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On modelling planning under uncertainty in manufacturing*

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Abstract

We present a modelling framework for two-stage and multi-stage mixed 0−1 problems under uncertainty for strategic Supply Chain Management, tactical production planning and operations assignment and scheduling. A scenario tree based scheme is used to represent the uncertainty. We present the Deterministic Equivalent Model of the stochastic mixed 0−1 programs with complete recourse that we study. The constraints are modelled by compact and splitting variable representations via scenarios.

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1 Introduction

1.1 Motivation and organization of the work

Very frequently, mainly in problems with a given time horizon to exploit, some coefficients in the objective function and the right-hand-side (*rhs*) vector and, to a lesser

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extent, the constraint matrix are not known with certainty when decisions are to be made, but certain information is available. The paper deals with important manufacturing problems. With this objective we follow the classic taxonomy of planning/scheduling problems in strategic, tactical and operational problems proposed by [11]. The models of most of the problems require 0−1 variables and, so, we will use a modelling methodology based on Stochastic Integer Programming (*SIP*). It has a broad field of application, mainly, in production planning and logistics of transportation and distribution, see [2–4, 6, 7, 38, 41, 52, 56, 57, 61, 73, 82], among others. See in [54] a good survey of coordination mechanisms of supply chain systems.

Many of the *SIP* approaches represent the uncertainty by a set of scenarios. The problem is formulated by the so-called Deterministic Equivalent Model (*DEM*), and use Benders decomposition [10, 17, 20, 23, 36, 53, 73], Lagrangian decomposition [22, 42, 45, 51, 72, 75–77, 84], disjunctive decomposition [63, 79], stochastic branch-and-cut [78], Benders decomposition based branch-and-bound [80], branch-and-fix coordination [3, 5, 7, 37] and stochastic dynamic programming [26], among others. See also [74].

Most of the approaches deal with the optimization of the objective function expected value alone. However, there are some approaches that additionally deal with mean-risk measures, by considering semi-deviations [66], excess probabilities [76] and conditional value-at-risk [70, 77] as risk measure-based functions to optimize. See also [1, 7, 57, 74, 86, 89], among others.

The remainder of the paper is organized as follows. Sections 1.2 and 1.3 present the objective functions min expected value and min mean-risk to optimize. Subsections 1.4 and 1.5 introduce the stochastic modelling paradigm to use in the rest of the work. Section 2 presents the problem and modelling approach for strategic Supply Chain Management determining the production topology and product selection via a two-stage complete recourse mixed 0−1 *DEM*. Section 3 presents the strategic Multiperiod Single Sourcing Problem (MPSSP) and its modelling as a two stage complete recourse mixed 0−1 problem. Section 4 presents the tactical single level Production Planning and Raw Material Supplying problem as a multi-stage mixed 0−1 problem. Section 5 deals with the difficult tactical multilevel Supply Chain Management problem as a multi-stage complete recourse continuous problem. Section 6 presents the difficult operational Stochastic Sequencing and Scheduling (S3) problem for assigning the operations to a time schedule with limited resources as a multi-stage complete recourse pure 0−1 problem. Finally, Section 7 concludes.

1.2 Objective function expected value

Consider the following deterministic model

$$\begin{aligned} &\min\ cx + ay \\ &\text{subject to (s.t.) } Ax + By = b \\ &x \in \{0,1\}^n, y \geq 0, \end{aligned} \tag{1}$$

where c and a are the n- and n_c-row vectors of the objective function coefficients, respectively, b is the column right-and-side *rhs* m-vector, A and B are the $m \times n$ and $m \times n_c$ constraint matrices, respectively, x and y are the n– and n_c–vectors of the 0−1 and continuous variables to optimize over a set of stages $\mathcal{T}$, respectively, and m, n and nc are the number of constraints, and the 0−1 variables and continuous variables, respectively. The model must be extended in order to deal properly with the uncertainty in the values of some parameters. Thus, an approach to model the uncertainty in the problem data is needed.

Definition 1 *A* stage *of a given time horizon is a set of time periods where the realization of the uncertain parameters takes place.*

Definition 2 *A* scenario *is one realization of the uncertain parameters along the stages of the given time horizon.*

Definition 3 *A* scenario group *for a given stage is the set of scenarios with the same realization of the uncertain parameters up to the stage.*

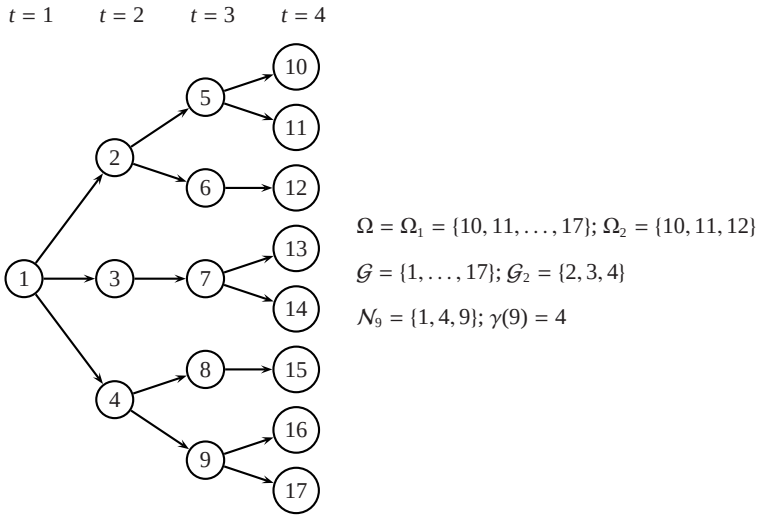


Figure 1: *Scenario tree*

Many approaches at present for stochastic programming and, certainly, *SIP* are scenario-based approaches to deal with the uncertainty. To illustrate this concept, see [4], consider Figure 1: each node in the figure represents a point in time where a decision can be made. Once a decision has been made, some contingencies can occur (e.g., in this example the number of contingencies is three for time period $t = 2$), and information related to these contingencies is available at the beginning of the stage (here, time period). This information structure is visualized as a tree, where each root-to-leaf path represents one specific scenario and corresponds to one realization of the whole set of the uncertain parameters. Each node in the tree can be associated with a scenario group, such that two scenarios belong to the same group in a given stage, provided that they have the same realizations of the uncertain parameters up to the stage. Accordingly with the *non-anticipativity* principle, see [20, 71], both scenarios should have the same value for the related variables with the time index up to the given stage.

Let the following notation related to the scenario tree:

$\mathcal{T}$, set of stages along the time horizon. $\mathcal{T}^- \equiv \mathcal{T} - \{|\mathcal{T}|\}$.

Ω, set of scenarios.

$\mathcal{G}$, set of scenario groups, so that we have a directed graph where $\mathcal{G}$ is the set of nodes.

$\mathcal{G}_t$, set of scenario groups in stage t, for $t \in \mathcal{T}$ ($\mathcal{G}_t \subseteq \mathcal{G}$).

Ω_g, set of scenarios in group g, for $g \in \mathcal{G}$ ($\Omega_g \subseteq \Omega$).

$\gamma(g)$, immediate ancestor node of node g, for $g \in \mathcal{G}$.

$\mathcal{N}_g$, set of scenario groups $\{k\}$ such that $\Omega_g \subseteq \Omega^k$, for $g \in \mathcal{G}$ ($\mathcal{N}^g \subset \mathcal{G}$). That is, set of ancestor scenario groups to scenario group g, including itself.

$\mathcal{N}^g$, set of successor nodes to node g. That is, set of successor scenario groups to scenario group g, including itself.

w_g, weight factor representing the likelihood that is associated with scenario group g, for $g \in \mathcal{G}$. Note: $w_g = \sum_{\omega \in \Omega_g} w^\omega$, where w^ω gives the likelihood that the modeller associates with scenario ω, for $\omega \in \Omega$, and $\sum_{\omega \in \Omega} w^\omega = 1$ and $\sum_{g \in \mathcal{G}_t} w_g = 1 \; \forall t \in \mathcal{T}$.

Let ω' be a given scenario in Ω_g for $g \in \mathcal{G}$.

Different types of models can be presented depending upon the type of recourse to consider, namely, simple, partial and complete recourse. Let us consider the minimization of the objective function expected value with complete recourse. In this

case, the stochastic version of program (1) has the following *DEM*,

$$\begin{aligned} \min\ & Q_E = \sum_{\omega\in\Omega} w^{\omega}(c^{\omega}x^{\omega} + a^{\omega}y^{\omega}) \\ \text{s.t. } & Ax^{\omega} + By^{\omega} = b^{\omega} && \forall \omega \in \Omega \\ & (x, y) \in \mathcal{N} \\ & x^{\omega} \in \{0,1\}^{n}, y^{\omega} \geq 0 && \forall \omega \in \Omega, \end{aligned} \tag{2}$$

where c^{ω} and a^{ω} are the row vectors of the objective function coefficients, x^{ω} and y^{ω} are the vectors of the related variables and b^{ω} is the *rhs* vector for scenario ω, and $\mathcal{N}$ is the so-called feasible space to satisfy the *non-anticipativity* constraints for the x– and y–variables, such that

$$v \in \mathcal{N} = \{v_t^{\omega} | v_t^{\omega} = v_t^{\omega'} \quad \forall \omega \in \Omega_g, g \in \mathcal{G}_t, t \in \mathcal{T}^{-}\}, \tag{3}$$

where $v = (x, y)$ and v_t^{ω} is such that $v^{\omega} = (v_t^{\omega},\ \forall t \in \mathcal{T})$.

Two approaches can be used to represent the constraints (3), namely, *splitting variable* and *compact* representations. The first approach has two types of formulations. One is so-called *node*-related (or scenario group related) representation. It requires to produce siblings of the variables that have nonzero elements in the constraints that belong to different stages. Another, so-called *scenario*-related representation, requires siblings of all variables in the model. In both cases, the *non-anticipativity* constraints must be explicitly added, but the second type preserves the model's structure in a more amenable way for the approach considered in this work; its model is as follows,

$$\begin{aligned} \min\ & Q_E = \sum_{\omega\in\Omega} w^{\omega}(c^{\omega}x^{\omega} + a^{\omega}y^{\omega}) \\ \text{s.t. } & Ax^{\omega} + By^{\omega} = b^{\omega} && \forall \omega \in \Omega \\ & v_t^{\omega} - v_t^{\omega'} = 0 && \forall \omega \in \Omega_g, g \in \mathcal{G}_t, t \in \mathcal{T}^{-} \\ & x^{\omega} \in \{0,1\}^{n}, y^{\omega} \geq 0 && \forall \omega \in \Omega. \end{aligned} \tag{4}$$

The *compact* representation requires to model the relationships of the variables in more detail. For illustrative purposes, assume that the variables vector v_t^{ω} has nonzero coefficients in the constraints related to the stages t and $t+1$, such that the deterministic model can be written as follows,

$$\begin{aligned} \min\ & cx + ay \\ \text{s.t. } & A_t^{-}x_{t-1} + A_t x_t + B_t^{-}y_{t-1} + B_t y_t = b_t && \forall t \in \mathcal{T} \\ & x_t \in \{0,1\}^{n'}, y_t \geq 0 && \forall t \in \mathcal{T}, \end{aligned} \tag{5}$$

where x_t and y_t are the vectors of the variables for stage t such that $x = (x_t \ \forall \in \mathcal{T})$ and $y = (y_t \ \forall \in \mathcal{T})$, n' gives the dimension of the vectors x_t, and A_t^-, A_t, B_t^- and B_t are the related constraint matrices. By slightly abusing the notation, the stochastic version of the model can be expressed

$$\begin{aligned} \min\ & Q_E = \sum_{g \in \mathcal{G}} w_g (c_g x_g + a_g y_g) \\ \text{s.t. } & A_t^- x_{\gamma(g)} + A_t x_g + B_t^- y_{\gamma(g)} + B_t y_g = b_g \quad \forall g \in \mathcal{G}_t, t \in \mathcal{T} \\ & x_g \in \{0,1\}^{n'}, y_g \geq 0 \qquad\qquad \forall g \in \mathcal{G}, \end{aligned} \tag{6}$$

where c_g and a_g are the row vectors of the objective function coefficients, b_g is the *rhs* vector, and x_g and y_g are the vectors of the variables for scenario group g, such that $c_g = c_t^\omega$, $a_g = a_t^\omega$ and $b_g = b_t^\omega$ where, in general, $d^\omega = (d_t^\omega \ \forall t \in \mathcal{T})$, for $\omega \in \Omega_g, g \in \mathcal{G}_t, t \in \mathcal{T}$.

1.3 Mean-risk objective function

The models that we have considered in the previous section aim to minimize the objective function expected value. However, there are some other approaches that additionally deal with the risk measures by also considering, e.g., semi-deviations [66], *excess probabilities* [76] and conditional value-at-risk [77] as we mentioned above. Those approaches are more amenable than the classical mean-variance schemes, mainly in the presence of 0−1 variables.

Let ϕ denote a prescribed threshold for the *excess probability*, say, Q_P, such that

$$Q_P = P(\omega \in \Omega : c^\omega x^\omega + a^\omega y^\omega > \phi). \tag{7}$$

So, alternatively to min Q_E (2), the mean-risk function to minimize is as follows,

$$Q_E + \eta Q_P, \tag{8}$$

where η is a positive weighting parameter.

A more amenable expression of (8) for computational purposes, at least, can be

$$\begin{aligned} \min\ & \sum_{\omega \in \Omega} w^\omega (c^\omega x^\omega + a^\omega y^\omega + \eta \nu^\omega) \\ \text{s.t. } & c^\omega x^\omega + a^\omega y^\omega \leq \phi + M\nu^\omega \qquad \forall \omega \in \Omega \\ & \nu^\omega \in \{0,1\} \qquad\qquad\qquad\quad \forall \omega \in \Omega, \end{aligned} \tag{9}$$

where ν^ω is a 0−1 variable, such that its value is 1 if the objective function value for scenario ω is greater than threshold ϕ and, otherwise, is 0, and M is a parameter,

preferably, the smallest one which does not eliminate any feasible solution of the stochastic program under any scenario.

1.4 Branch-and-Bound bounding

The instances of the mixed 0−1 *DEM* (4) can have such large dimensions that the plain using of a state-of the-art optimization engine can make it unaffordable. Benders Decomposition schemes can be used as we mentioned above. Alternatively, we can execute a *Branch-and-Bound* (*BB*) scheme for optimizing the *DEM*, such that a Lagrangean *Decomposition* approach can be used at each *BB* node by dualizing the *nonanticipativity* constraints

$$v_t^{\omega} - v_t^{\omega'} = 0 \quad \forall \omega \in \Omega_g, g \in \mathcal{G}_t, t \in \mathcal{T}^-, \tag{10}$$

see references above. In any case, heuristic Lagrangeans should be used.

The Lagrangean model is as follows,

$$\begin{aligned} \min & \sum_{\omega \in \Omega} w^{\omega}(c^{\omega}x^{\omega} + a^{\omega}y^{\omega} + \beta v^{\omega}) + \sum_{t \in \mathcal{T}^-, g \in \mathcal{G}_t, \omega \in \Omega_g} \mu_t^{\omega}(v_t^{\omega} - v_t^{\omega'}) \\ \text{s.t. } & c^{\omega}x^{\omega} + a^{\omega}y^{\omega} \leq \phi + Mv^{\omega} && \forall \omega \in \Omega \\ & Ax^{\omega} + By^{\omega} = b^{\omega} && \forall \omega \in \Omega \\ & 0 \leq x^{\omega} \leq 1, 0 \leq v^{\omega} \leq 1, y^{\omega} \geq 0 && \forall \omega \in \Omega, \end{aligned} \tag{11}$$

where $\mu_t^{\omega}, \ \forall \omega \in \Omega_g, g \in \mathcal{G}_t, t \in \mathcal{T}^-$ denotes the row vector of the Lagrange multipliers associated with the *non-anticipativity* constraints (10). Notice that the number of Lagrange multipliers depends on the number of variables in the *v*–vector and the number of scenarios in each group.

1.5 Scenario clusters and Twin Node Families

Alternatively to a *Branch-and-Bound* framework, we consider a variant of the *Branch-and-Fix Coordination (BFC)* approach, such that it treats in a coordinate way the $|\Omega|$ independent models (12) that result from the relaxation of the constraints (10).

$$\begin{aligned} \min & \ c^{\omega}x^{\omega} + a^{\omega}y^{\omega} + \beta v^{\omega} \\ \text{s.t. } & c^{\omega}x^{\omega} + a^{\omega}y^{\omega} \leq \phi + Mv^{\omega} \\ & Ax^{\omega} + By^{\omega} = b^{\omega} \\ & x^{\omega} \in \{0,1\}^n, v^{\omega} \in \{0,1\}, y^{\omega} \geq 0. \end{aligned} \tag{12}$$

Moreover, Lagrangeans can be used on the top. *BFC* is specially designed to coordinate the selection of the branching variable and branching node for each scenario-related *Branch-and-Fix (BF)* tree, such that the relaxed constraints (10) are satisfied when fixing the appropriate variables to either one or zero. The approach also coordinates and reinforces the scenario-related *BF* node pruning, the variable fixing and the objective function bounding of the subproblems attached to the nodes.

The presentation of the scheme below is an extension of the scheme presented in [5]. See [3,4,6,8] for applications to the two-stage mixed 0−1 problem, where the first stage is only included by 0−1 variables, [37] for an application to the two-stage mixed 0−1 problem where the first stage is included by 0−1 variables and continuous variables and [7] for an application to the multistage pure 0−1 problem.

For the presentation of the *BFC* approach, let $\mathbb{R}^{\omega}$ denote the *BF* tree associated with scenario ω, $\mathcal{A}^{\omega}$ be the set of active nodes in $\mathbb{R}^{\omega}$ for $\omega \in \Omega$, $\mathcal{I}$ the set of indices of the variables in any vector x_t^{ω}, and $(x_t^{\omega})_i$ the i-th variable in x_t^{ω}, for $t \in \mathcal{T}, \omega \in \Omega, i \in \mathcal{I}$.

Definition 4 *Two variables, say,* $(x_t^{\omega})_i$ *and* $(x_t^{\omega'})_i$ *are said to be* common *variables for the scenarios* ω *and* ω'*, if* $\omega, \omega' \in \Omega_g$, $g \in \mathcal{G}_t$, *for* $\omega \neq \omega', t \in \mathcal{T}^-, i \in \mathcal{I}$. *Notice that two* common *variables have nonzero elements in the* non-anticipativity *constraint related to a given scenario group.*

Definition 5 *Any two nodes, say,* $a \in \mathcal{A}^{\omega}$ *and* $a' \in \mathcal{A}^{\omega'}$ *are said to be* twin nodes *with respect to a given scenario group if the paths from their root nodes to each of them in their own* BF *trees* $\mathbb{R}^{\omega}$ *and* $\mathbb{R}^{\omega'}$*, respectively, either having not yet branched on/fixed their* common *variables, if any, or having the same* 0−1 *value for their branched on/fixed their* common *variables* $(x_t^{\omega})_i$ *and* $(x_t^{\omega'})_i$, *for* $\omega, \omega' \in \Omega_g, g \in \mathcal{G}_t, t \in \mathcal{T}^-, i \in \mathcal{I}$.

Definition 6 *A* Twin Node Family (TNF)*, say,* $\mathcal{J}_f$ *is a set of nodes such that any node is a* twin *node to all the other node members in the family, for* $f \in \mathcal{F}$*, where* $\mathcal{F}$ *is the set of the families. Note: For practical reasons, all* BF *nodes belong to one* TNF*, at least, even if its cardinality is one.*

Definition 7 *A* candidate TNF *is a* TNF *whose members have not yet branched on/fixed all their* common *variables.*

Definition 8 *A* TNF integer set *is a set of* TNFs *where all x– and v–variables take integer values, there is one node per each* BF *tree and the* nonanticipativity *constraints* $(x_t^{\omega})_i - (x_t^{\omega'})_i = 0$ *are satisfied,* $\forall \omega, \omega' \in \Omega_g$, $g \in \mathcal{G}_t, t \in \mathcal{T}^-, i \in \mathcal{I}$. *Note: The cardinality of each* TNF *is one in any integer set.*

Let us consider the scenario tree and the *BF* trees shown in Figure 2, where x_h^{ω} denotes a given variable subscripted h under scenario ω and x_h gives the generic notation for the variable. For illustrative purposes, let the branching ordering be $x_1, x_2, \ldots, x_6$. We can see that the first *candidate TNF* is J_1, since the variables from stage 1 are *common*

variables to all nodes. Additionally, J_2 is a family that has already been branched on the same value of the *common* variable x_1. It is also a *candidate TNF* since the *common* variable x_2 has not been branched on (and, suppose that it has not been fixed either). Similarly, J_3 is another *candidate TNF*. However, J_4 is not a *candidate TNF* since all the *common* variables for their node members have been already branched on. The family J_4 is split into the families J_5 and J_6 to branch independently on the variables x_3 and x_4, since the nodes 10 and 11 are *twin* nodes for these variables, while node 12 is not. Finally, note that J_7 and J_8 are also *candidate TNFs*, since the variable x_4 is not yet branched and, on the other hand, it is a *common* variable for the node members of those families.

It is clear that the relaxation of the *non-anticipativity* constraints (10) is not required for all pairs of scenarios in order to gain computational efficiency. The number of scenarios to consider in a given model basically depends on the dimensions of the scenario related model (12).

Definition 9 *A* scenario cluster *is a set of scenarios whose* non-anticipativity *constraints are explicitly considered in the model.*

The criterion for scenario clustering in the sets, say, $\Omega^1, \ldots, \Omega^q$, where q is the number of *scenario clusters*, is instance dependent. However, we favour the approach that shows higher scenario clustering for greater number of scenario groups in common. In any case, notice that $\Omega^p \bigcap \Omega^{p'} = \emptyset$, $p, p' = 1, \ldots, q : p \neq p'$ and $\Omega = \cup_{p=1}^{q} \Omega^p$.

The model to consider for scenario *cluster* $p = 1, \ldots, q$ can be expressed by the *compact* representation (13), where ω for $d \in G_{|\mathcal{T}|}$ is the unique scenario such that $\omega \in \Omega_d$ and, on the other hand, $\mathcal{G}^p = \{g \in \mathcal{G} : \Omega_g \bigcap \Omega^p \neq \emptyset\}$.

$$
\begin{aligned}
\min \; & \sum_{d \in \mathcal{G}_{|\mathcal{T}|} \bigcap \mathcal{G}^p} w^\omega \sum_{g \in \mathcal{N}_d} (c_g x_g + a_g y_g) + \beta \sum_{\omega \in \Omega^p} w^\omega \nu^\omega & & \\
\text{s.t.} \; & \sum_{g \in \mathcal{N}_d} (c_g x_g + a_g y_g) \leq \phi + M \nu^\omega & & \forall d \in \mathcal{G}_{|\mathcal{T}|} \bigcap \mathcal{G}^p \\
& A_t^- x_{\gamma(g)} + A_t x_g + B_t^- y_{\gamma(g)} + B_t y_g = b_g & & \forall g \in \mathcal{G}_t \bigcap \mathcal{G}^p, t \in \mathcal{T} \\
& x_g \in \{0,1\}^{n'}, y_g \geq 0, & & \forall g \in \mathcal{G}^p \\
& \nu^\omega \in \{0,1\} & & \forall \omega \in \Omega^p.
\end{aligned}
\tag{13}
$$

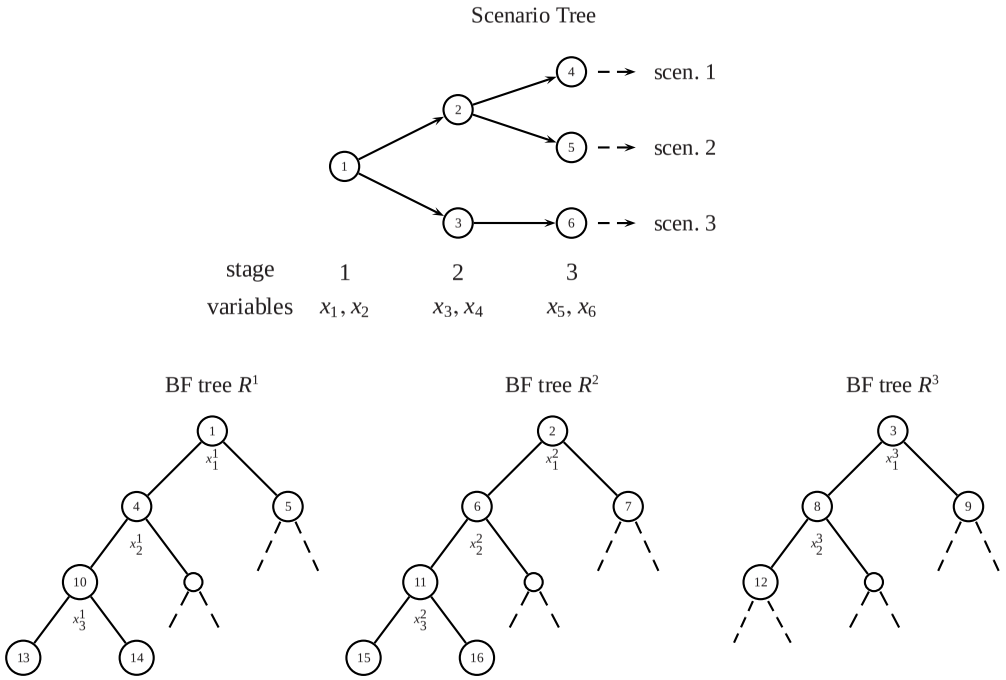
Remind that $\mathcal{N}_d$ gives the set of nodes in the ancestor path from leaf-node d to root node 1. Note: $n' \equiv |I|$.

The *scenario cluster* models (13) are linked by the *non-anticipativity* constraints:

$$x_{g^p} - x_{g^{p'}} = 0 \tag{14}$$

$$y_{g^p} - y_{g^{p'}} = 0, \tag{15}$$

for $p, p' = 1, \ldots, q : p \neq p'$, where $g^p \in \mathcal{G}^p, g^{p'} \in \mathcal{G}^{p'}$ and $g^p = g^{p'}$.



Branching variables ordering: $x_1, x_2, x_3, x_4, x_5, x_6$

Some Twin Node Families (*TNFs*)

$\mathcal{J}_1 = \{1, 2, 3\}$, $\mathcal{J}_2 = \{4, 6, 8\}$, $\mathcal{J}_3 = \{5, 7, 9\}$, $\mathcal{J}_4 = \{10, 11, 12\}^*$,

$\mathcal{J}_5 = \{10, 11\}$, $\mathcal{J}_6 = \{12\}$, $\mathcal{J}_7 = \{13, 15\}$, $\mathcal{J}_8 = \{14, 16\}$

$*$ A non candidate *TNF*

Figure 2: *Branch and Fix Coordination scheme*

2 Strategic Supply Chain Management

2.1 Introduction

Supply Chain Management *SCM* is concerned with determining supply, production and stock levels in raw materials, subassemblies at different levels of the given *Bills of Material (BoM)*, end products and information exchange through (possibly) a set of factories, depots and dealer centres of a given production and service network to meet fluctuating demand requirements, see [38, 43, 61], among others. Four key aspects of the problem are identified, namely, *supply chain topology, time, uncertainty* and *cost*. The uncertainty aspect of the problem is due to the stochasticity inherent in some parameters for dynamic (multiperiod) planning problems; in our case, the main uncertain parameters are product demand and net profit, raw material supply cost and production cost. See [3, 5, 6].

The tactical supply chain planning problem consists of deciding on the best utilization of the available resources included by vendors, factories, depots and dealer centers along the time horizon, such that given targets are met at a minimum cost. It assumes that the supply chain topology is given, see Section 5. The subject of this section is the strategic planning for supply chains and, so, the problem consists of deciding on the production topology, plant sizing, product selection, product allocation among plants and vendor selection for raw materials. The objective is the maximization (in constant terms) of the expected benefit given by the product net profit over the time horizon minus the investment depreciation and operation costs.

There is an extensive literature on dynamic production/scheduling planning. See hierarchical approaches in [21]; single level based systems in [49]; multi-level based systems in [32]; systems for line balancing in [69]; and systems with lot sizing, inventory holding and setup considerations in [28, 81, 91, 94], among others. See in [25, 81] models for global optimization of multi-level supply chains. These references present models and algorithmic schemes for deterministic environments. So, the uncertainty inherent to most of the important parameters is not dealt with.

This section presents a two stage complete recourse mixed $0-1$ model that considers the uncertainty in the parameters. See other approaches in [2, 13, 24, 29, 35, 61, 62, 85, 90, 95], among others.

2.2 Problem Statement

A *time horizon* is a set of (consecutive and integer) time periods of non necessarily equal length where the operations planning will be considered. A *product* is any item whose production volume, location and scheduling is decided by the Supply Chain Management (*SCM*). An *end product* is the final output of the supply chain network. A

subassembly is a product that is assembled by the supply chain and, together with other items, is used to produce other products. By the term *product* we will refer to both end products and subassemblies. Their own *BoM* is a concern of the *SCM*. Multiple external demand sources for a product (either an end product or a subassembly) are also allowed. We will name *raw material* any storable item that is required in the products' *BoM*, but whose own *BoM* is not a concern of the *SCM*, i.e., the supply is only from outside sources. Let us use the term *component* to describe any storable item that is required for the production. We may observe that a subassembly is a component in a given *BoM* of some other product. So, subassemblies and raw materials are *components*. The *stock* of an item (either a product or a raw material) is its available volume at the end of a given time period. Let us assume that the cycle time (i.e., lead time) of any unit product is smaller than the length of the given periods in the time horizon.

We may notice that the *BoM* of a product is the structuring of the set of components that are required for its manufacturing/assembly, see Figure 3. The *BoM* can be described as a set of tiers, i.e., a set of levels in the supply chain. A so-called *first tier* component in a *BoM* of a given product is a component that is directly required for its manufacturing/assembly.

Let us term *vendor* any external source for the supplying of raw materials. A warehouse within the supply chain can be associated to any item. A *plant* is a capacitated physical location where the products are processed. The plants may have different capacity production levels. The term *plant investment for level k* will be used for the amount of a given currency that is needed for expanding a plant from, say, level $k-1$ to level k. We may observe that the expansion to level $k=1$ means that a plant will be open.

Note that single-level production requires that the components of a given *BoM* are assembled sequentially along the cycle time of the product, see Section 4. On the contrary, multilevel production, as it is in supply chain environments, allows the subsets of components to be assembled independently and then, the production resources can be better utilized.

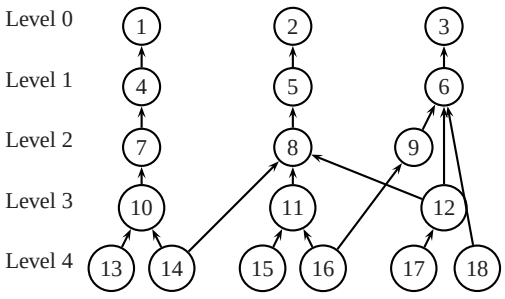


Figure 3: *Bill of Material*

Some parameters are deterministic by nature or the optimal solution may not be very sensitive to their variability. However, the product net profit and demand, as well as the raw material cost (and, with less intensity, the production cost) are uncertain parameters, mainly for long time horizons, as is usually the case for strategic planning. The available information for the uncertain parameters is structured in a set of scenarios.

The goal of the strategic *SCM* problem that is addressed in this work, consists of determining the production topology, plant sizing, product selection, product allocation among plants and vendor selection for raw material. The objective is the maximization (in constant terms) of the expected benefit given by the product net profit minus the operation costs and the plant investment depreciation cost over the time horizon, by considering the set of given scenarios for the uncertain parameters.

Two stages are considered in the problem. The first stage is devoted to the *strategic* decisions involving plant sizing, product allocation to plants and raw materials vendor selection. The second stage is devoted to the *tactical* decisions involving the raw material volume to be supplied from vendors, product volume to be processed in plants, stock volume of product/raw material to be stored in plants/warehouses, component volume to be transported from origin plants/warehouses to destination plants and product volume to be shipped from plants to market sources at each time period along the time horizon, given the supply chain topology decided on at the first stage. Obviously, the strategic decisions, besides satisfying their related first stage constraints, will take into consideration the product net profit and operation cost related to the tactical environment besides the investment depreciation cost.

We use the following notation.

***Sets**:*

$\mathcal{I}$, set of plants.
$\mathcal{J}$, set of products (end products and subassemblies).
$\mathbb{C}$, set of components (raw materials and subassemblies).
$\mathcal{L}$, set of subassemblies ($\mathcal{L} = \mathcal{J} \bigcap \mathbb{C}$).
$\mathbb{R}$, set of raw materials.
$\mathcal{E}$, set of items (raw materials and products).
$\mathcal{V}$, set of vendors (or zones) for the supply of raw materials.
$\mathbb{C}_j$, set of first tier components required by product j, $\forall j \in \mathcal{J}$.
$\mathcal{I}_j$, set of plants that are available to process product j, $\forall j \in \mathcal{J}$, ($\mathcal{I}_j \subseteq \mathcal{I}$), and set of candidate vendors (or zones) for raw material j, $\forall j \in \mathbb{R}$, ($\mathcal{I}_j \subseteq \mathcal{V}$).
$\mathcal{T}_i$, set of time periods where a capacity expansion for plant i is allowed, $\forall i \in \mathcal{I}$($\mathcal{T}_i \subseteq \mathcal{T}$), besides time period $t = 0$ (i.e., first stage).
$\mathcal{K}_i$, set of capacity expansion levels for plant i, $\forall i \in \mathcal{I}$.
$\mathcal{M}_j$, set of market sources for product j, $\forall j \in \mathcal{J}$.

Deterministic parameters:

$\widetilde{N}$, maximum number of plants that can be open.
$\widehat{N}$, maximum number of end products that can be processed.
$\underline{N}_j, \overline{N}_j$, minimum and maximum number of plants where product j can be processed, respectively, if any, $\forall j \in \mathcal{J}$, and minimum and maximum number of vendors for raw material j, respectively, if any, $\forall j \in \mathbb{R}$.
$\overline{N}^i$, maximum number of products to be processed in plant i at any time period, $\forall i \in \mathcal{I}$, and maximum number of raw materials to be supplied by vendor (or zone) i, $\forall i \in \mathcal{V}$.
P_t, available budget for plant capacity building/expansion at time period t, for $t \in \{0\} \cup \mathcal{T}$. Note: By convention, plant building (i.e., capacity expansion level $k = 1$) can only occur at time period $t = 0$.
$\underline{X}^i_j, \overline{X}^i_j$, minimum and maximum volume of raw material j that can be supplied from vendor i at any time period, respectively, if any, $\forall i \in \mathcal{I}_j$, $j \in \mathbb{R}$, and minimum and maximum volume of product j that can be processed in plant i at any time period, respectively, if any, $\forall i \in \mathcal{I}_j$, $j \in \mathcal{J}$.
$\underline{S}^i_{jt}, \overline{S}^i_j$ minimum and maximum volume of raw material j that can be in stock from vendor (or zone) i at the end of time period t and at any time period, respectively, if any, $\forall i \in \mathcal{I}_j$, $j \in \mathbb{R}, t \in \mathcal{T}$ and minimum and maximum volume of product j that can be in stock in plant i at the end of time period t and at any time period, respectively, if any, $\forall i \in \mathcal{I}_j$, $j \in \mathcal{J}, t \in \mathcal{T}$.
o^i_j, unit capacity usage of plant i by product j, $\forall i \in \mathcal{I}_j$, $j \in \mathcal{J}$.
$\underline{p}_i$, minimum capacity usage of plant i at any time period, if any.
p^k_i, production capacity increment from level $k-1$ to level k in plant i, $\forall k \in \mathcal{K}_i, i \in \mathcal{I}$.
N_{gj}, volume of component g required by one unit of product j in its *BoM*, $\forall g \in \mathbb{C}_j$, $j \in \mathcal{J}$.
D^m_{jt}, demand of product j from market source m at time period t, $\forall m \in \mathcal{M}_j$, $j \in \mathcal{J}, t \in \mathcal{T}$.

Cost parameters:

a^k_{it} : budget required for the capacity expansion from level $k-1$ to level k in plant i at time period t, $\forall k \in \mathcal{K}_i, t \in \{0\} \cup \mathcal{T}_i, i \in \mathcal{I}$.
q^k_{it} : depreciation cost (along the time horizon) of the investment a^k_{it} related to the kth capacity expansion level in plant i at time period t, $\forall k \in \mathcal{K}_i, t \in \{0\} \cup \mathcal{T}_i, i \in \mathcal{I}$.
p^{im}_{jt} : net unit profit of selling product j from plant i to market source m at time period t, including product price, local taxes, transport cost and others, $\forall i \in \mathcal{I}_j, m \in \mathcal{M}_j$, $j \in \mathcal{J}, t \in \mathcal{T}$.
c^i_{jt} : processing unit cost of product j in plant i at time period t, $\forall i \in \mathcal{I}_j$, $j \in \mathcal{J}, t \in \mathcal{T}$, and supplying unit cost of raw material j from vendor i at time period t, $\forall i \in \mathcal{I}_j$, $j \in \mathbb{R}, t \in \mathcal{T}$.

h^i_{jt} : holding unit cost of product/raw material j in plant/warehouse i at time period t, $\forall i \in \mathcal{I}_j, j \in \mathcal{E}, t \in \mathcal{T}$.

b^{fi}_g : transport unit cost of component g from plant/ warehouse f to plant i at any time period, $\forall f \in \mathcal{I}_g, g \in \mathbb{C}_j, i \in \mathcal{I}_j, j \in \mathcal{J}$.

The goal consists of determining the production topology (i.e., location of plants to open), plant sizing, end product selection, product allocation among plants and vendor selection for raw materials to maximize the total expected net revenue.

2.3 Scenario-based modelling

This section is devoted to the scenario version of the strategic supply chain management model and, so, the goal is to obtain the optimal solution for a problem where all parameters are known. The so-called *step variables* are considered. The basic idea for this type of representation of the variables is taken from [18] for scheduling air traffic in a network of airports.

Strategic variables:

α_j, 0−1 variable such that its value is 1 if product/raw material j is selected for processing/supplying, and 0 otherwise, $\forall j \in \mathcal{E}$.

β^i_j, 0−1 variable such that its value is 1 if product/raw material j is processed in plant i/supplied by vendor i, and 0 otherwise, $\forall i \in \mathcal{I}_j, j \in \mathcal{E}$.

γ^k_{it}, 0−1 variable such that its value is 1 if plant i has capacity level k *at least* at period t, and 0 otherwise, $\forall k \in \mathcal{K}_i, i \in \mathcal{I}, t \in \{0\} \cup \mathcal{T}$. Notice that the capacity level k can be reached either at period t or earlier, for $\gamma^k_{it} = 1$.

Tactical variables:

x^i_{jt}, volume of product j to be processed in plant i at time period t, $\forall i \in \mathcal{I}_j, j \in \mathcal{J}, t \in \mathcal{T}$, and volume of raw material j to be supplied from vendor i at time period t, $\forall i \in \mathcal{I}_j, j \in \mathbb{R}, t \in \mathcal{T}$.

s^i_{jt}, stock volume of product/raw material j in plant/warehouse i at (the end of) time period t, $\forall i \in \mathcal{I}_j, j \in \mathcal{E}, t \in \mathcal{T}$.

e^{fji}_{gt}, volume of component g to be transported from plant/warehouse (origin) f to plant (destination) i at time period t for processing product j, $\forall f \in \mathcal{I}_g, g \in \mathbb{C}_j$, $i \in \mathcal{I}_j, j \in \mathcal{J}, t \in \mathcal{T}$.

y^{im}_{jt}, volume of product j to be shipped from plant i to market source m at time period t, $\forall i \in \mathcal{I}_j, m \in \mathcal{M}_j, j \in \mathcal{J}, t \in \mathcal{T}$.

Objective

Maximize the total net revenue, given by $z_2 - z_1$, see below.

Stage 1 (Strategic) Submodel

$$z_1 = \sum_{i\in\mathcal{I}} \sum_{k\in\mathcal{K}_i} q_{i0}^k \gamma_{i0}^k \tag{16}$$

subject to

$$\sum_{i\in\mathcal{I}} \gamma_{i0}^1 \leq \widetilde{N} \tag{17}$$

$$\gamma_{i0}^{k-1} \geq \gamma_{i0}^k \quad \forall k \in \mathcal{K}_i \setminus \{1\},\ i \in \mathcal{I} \tag{18}$$

$$\sum_{i\in\mathcal{I}} \sum_{k\in\mathcal{K}_i} a_{i0}^k \gamma_{i0}^k \leq P_0 \tag{19}$$

$$\sum_{j\in\mathcal{J}\setminus\mathcal{L}} \alpha_j \leq \widehat{N} \tag{20}$$

$$\alpha_j \leq \alpha_g \quad \forall g \in \mathbb{C}_j,\ j \in \mathcal{J} \tag{21}$$

$$\underline{N}_j \alpha_j \leq \sum_{i\in\mathcal{I}_j} \beta_j^i \leq \overline{N}_j \alpha_j \quad \forall j \in \mathcal{E} \tag{22}$$

$$\beta_j^i \leq \gamma_{i0}^1 \quad \forall i \in \mathcal{I}_j,\ j \in \mathcal{J} \tag{23}$$

$$\sum_{j\in\mathcal{J}/i\in\mathcal{I}_j} \beta_j^i \leq \overline{N}^i \gamma_{i0}^1 \quad \forall i \in \mathcal{I} \tag{24}$$

$$\sum_{j\in\mathbb{R}/i\in\mathcal{I}_j} \beta_j^i \leq \overline{N}^i \quad \forall i \in \mathcal{V} \tag{25}$$

$$\alpha_j \in \{0,1\} \quad \forall j \in \mathcal{E} \tag{26}$$

$$\beta_j^i \in \{0,1\} \quad \forall i \in \mathcal{I}_j,\ j \in \mathcal{E} \tag{27}$$

$$\gamma_{i0}^k \in \{0,1\} \quad \forall k \in \mathcal{K}_i, i \in \mathcal{I} \tag{28}$$

Constraints (17) ensure that the number of plants in the supply chain will not exceed the allowed maximum. Constraints (18) ensure that the γ–variables are well defined. Constraints (19) take into account the investment budget. Constraints (20) restrict the number of end products for processing. Constraints (21) determine the production/supplying of the first tier components of any product selected. By considering the *BoM* requirements in the operation submodel, see below specifically constraints (39), it is easy to see the redundancy of (21). However, this type of

cuts reduces the linear programming (*LP*) solution space and, then, helps to tighten the model. Constraints (22) conditionally lower and upper limit the number of plants/vendors for each product/raw material. Constraints (23) restrict the processing of products to those plants that are in operation. Constraints (24) and (25) ensure that the number of products/raw materials for processing in plant/supplying from vendor i will not exceed the allowed maximum.

We can observe that the *rhs* of (24) has been reinforced by multiplying it by γ^1_{io}. On the other hand, enlarging the model by appending the variable upper bound $\beta^i_j \leq \alpha_j$, $i \in \mathcal{I}_j$, $j \in \mathcal{E}$ results in a 0−1 *LP* equivalent stronger model as well. However, given the potentially high number of β-variables, the appending should only be performed for violated cuts by the current *LP* solution.

Stage 2 (Operation) Submodel

Stage 2 submodel. Time period indexed profit function to maximize

$$z_2 = \sum_{t\in\mathcal{T}}\sum_{j\in\mathcal{J}}\sum_{i\in\mathcal{I}_j}\sum_{m\in\mathcal{M}_j} p^{im}_{jt} y^{im}_{jt} - \sum_{t\in\mathcal{T}}\sum_{j\in\mathcal{E}}\sum_{i\in\mathcal{I}_j}(c^i_{jt}x^i_{jt} + h^i_{jt}s^i_{jt}) - \\ - \sum_{t\in\mathcal{T}}\sum_{j\in\mathcal{J}}\sum_{g\in\mathbb{C}_j}\sum_{f\in\mathcal{I}_g}\sum_{i\in\mathcal{I}_j} b^{fi}_g e^{fji}_{gt} - \sum_{i\in\mathcal{I}}\sum_{k\in\mathcal{K}_i\setminus\{1\}}\sum_{t\in\mathcal{T}_i} q^k_{it}(\gamma^k_{it} - \gamma^k_{i,t-1}) \quad (29)$$

Stage 2 submodel. Time period indexed capacity expansion constraints

$$\gamma^1_{i,t-1} = \gamma^1_{it} \quad \forall i \in \mathcal{I}, t \in \mathcal{T} \quad (30)$$

$$\gamma^k_{i,t-1} = \gamma^k_{it} \quad \forall k \in \mathcal{K}_i \setminus \{1\}, t \in \mathcal{T} \setminus \mathcal{T}_i, i \in \mathcal{I} \quad (31)$$

$$\gamma^k_{i,t-1} \leq \gamma^k_{it} \quad \forall k \in \mathcal{K}_i \setminus \{1\}, t \in \mathcal{T}_i, i \in \mathcal{I} \quad (32)$$

$$\gamma^{k-1}_{it} \geq \gamma^k_{it} \quad \forall k \in \mathcal{K}_i \setminus \{1\}, i \in \mathcal{I}, t \in \mathcal{T} \quad (33)$$

$$\sum_{i\in\mathcal{I}}\sum_{k\in\mathcal{K}_i\setminus\{1\}} a^k_{it}(\gamma^k_{it} - \gamma^k_{i,t-1}) \leq P_t \quad \forall t \in \mathcal{T} \quad (34)$$

$$\underline{p}_i \gamma^1_{i0} \leq \sum_{j\in\mathcal{J}/i\in\mathcal{I}_j} o^i_j x^i_{jt} \leq \sum_{k\in\mathcal{K}_i} p^k_i \gamma^k_{it} \quad \forall i \in \mathcal{I}, t \in \mathcal{T} \quad (35)$$

Stage 2 submodel. Time period indexed operation constraints

$$s^i_{j,t-1} + x^i_{jt} = \rho^i_{jt} + \sigma^i_{jt} + s^i_{jt} \quad \forall i \in \mathcal{I}_j, j \in \mathcal{E}, t \in \mathcal{T} \quad (36)$$

$$\underline{X}^i_j \beta^i_j \leq x^i_{jt} \leq \overline{X}^i_j \beta^i_j \quad \forall i \in \mathcal{I}_j, j \in \mathcal{E}, t \in \mathcal{T} \quad (37)$$

$$\underline{S}^i_{jt}\beta^i_j \leq s^i_{jt} \leq \overline{S}^i_j\beta^i_j \quad \forall i \in \mathcal{I}_j,\, j \in \mathcal{E}, t \in \mathcal{T} \tag{38}$$

$$\sum_{f \in \mathcal{I}_g} e^{fji}_{gt} = N_{gj} x^i_{jt} \quad \forall g \in \mathbb{C}_j,\, i \in \mathcal{I}_j,\, j \in \mathcal{J}, t \in \mathcal{T} \tag{39}$$

$$\sum_{i \in \mathcal{I}_j} y^{im}_{jt} \leq D^m_{jt} \quad \forall m \in \mathcal{M}_j,\, j \in \mathcal{J}, t \in \mathcal{T} \tag{40}$$

$$y^{im}_{jt} \geq 0 \quad \forall i \in \mathcal{I}_j, m \in \mathcal{M}_j,\, j \in \mathcal{J}, t \in \mathcal{T} \tag{41}$$

$$e^{fji}_{gt} \geq 0 \quad \forall f \in \mathcal{I}_g, g \in \mathbb{C}_j, i \in \mathcal{I}_j,\, j \in \mathcal{J}, t \in \mathcal{T} \tag{42}$$

where

$$\rho^i_{jt} \equiv \begin{cases} \displaystyle\sum_{\ell \in \mathcal{J}\,/\, j \in \mathbb{C}_\ell} \sum_{f \in \mathcal{I}_\ell} e^{i\ell f}_{jt}, & \text{for } j \in \mathbb{C} \\ 0, & \text{for } j \in \mathcal{J} \setminus \mathcal{L} \end{cases}$$

and

$$\sigma^i_{jt} \equiv \begin{cases} \displaystyle\sum_{m \in \mathcal{M}_j} y^{im}_{jt}, & \text{for } j \in \mathcal{J} \\ 0, & \text{for } j \in \mathbb{R} \end{cases}$$

The constraints have been divided into two blocks, namely, capacity expansion related constraints (30)-(35) and operation related constraints (36)-(42). Constraints (30) ensure that the plants are only open at time period $t = 0$. Constraints (31) ensure that the capacity expansion of the plants will only occur at permitted time periods. Constraints (32) and (33) assure that the γ-variables are well defined. Constraints (34) take into account the capacity expansion budget. Constraints (35) limit the production from each plant to a conditional minimum, as well as to the maximum capacity given by the expansion plan. Constraints (36) are the stock balance equations for products and raw materials. Constraints (37) and (38) define the semi-continuous character of the production and stock variables. These constraints imply the non-negativity of the variables x^i_{jt} and s^i_{jt}, $\forall i \in \mathcal{I}_j,\, j \in \mathcal{E}, t \in \mathcal{T}$. Constraints (39) define the *BoM* requirements for the products. Constraints (40) ensure that the product shipment to the market sources will not exceed the related demand.

The objective of the strategic *SCM* is to maximize the expected benefit over the scenarios, given the uncertainty in the production/supplying cost c^i_{jt}, product demand D^m_{jt} and net profit p^{im}_{jt}. So, the uncertain parameters and all the variables have the superindex ω in the splitting variable representation for $\omega \in \Omega$, such that the following non-anticipativity constraints are satisfied,

$$\alpha_j^{\omega} - \alpha_j^{\omega'} = 0 \tag{43}$$

$$\beta_j^{i\omega} - \beta_j^{i\omega'} = 0 \tag{44}$$

$$\gamma_{i0}^{k\omega} - \gamma_{i0}^{k\omega'} = 0. \tag{45}$$

Let an instance with $|\mathcal{I}| = 6$ plants, $|\mathcal{K}_i| = 3$ capacity levels each, $|\mathcal{J}| = 12$ products, where $|\mathcal{L}| = 8$ are subassemblies, $|\mathbb{R}| = 12$ raw materials, $|\mathcal{V}| = 24$ vendors, $|\mathcal{M}_j| = 2$ markets for each of the products, $|\mathcal{T}| = 10$ time periods and $|\Omega| = 23$ scenarios. The dimensions of *DEM*, compact representation are 69871 constraints, 56785 continuous variables and 895 0−1 variables.

Given the large dimensions of the real-life instances, the plain use of state-of-the-art optimization engines cannot provide the solution in affordable computing time. So, we propose to use the Branch-and-Fix Coordination approach given in [3, 5].

3 Multi-Period Single Sourcing problem

3.1 Introduction

In this section we deal with a modelling of a two-stage stochastic mixed 0−1 problem where the continuous variables only appear in the second stage, the so-called Multi Period Single Sourcing Problem (*MPSSP*) under uncertainty, where the objective function is included by the mean function and the weighted excess probability functional. Given a time horizon, a set of retailers and a set of facilities (e.g., production plants), the *MPSSP* is concerned with assigning each retailer to a unique facility at the beginning of the time horizon. The aim is to minimize the composite function of the expected assignment, inventory holding and backlogging costs and the weighted function of the probability of the excess cost with respect to a given target subject to the satisfaction of retailers' demands and the production capacity constraints at the facilities. The assignment cost includes the production and distribution costs. The problem can be viewed as an assignment problem where the goodness of the retailers' assignment can be measured against its performance along the time horizon. There are substantial differences between the procedures for solving the expected objective function minimization and the mean-risk functional minimization. See [9].

3.2 Problem statement

Consider a production/distribution network of a single product including a set of *facilities* and a set of *retailers*. Each facility can be interpreted as a production plant

with an associated warehouse. Each retailer needs to be served by (assigned to) a unique facility. The product demand and all costs along a given time horizon are unknown, but it is assumed that the uncertainty can be represented by a set of scenarios. Each production plant has a finite, known production capacity. We assume that each warehouse has sufficient capacity to be able to store the cumulative excess production of its corresponding production plant, even if this production plant produces to complete capacity in each time period. We assume that the product can only be stored at the facilities. Backlogging is also allowed at the facilities. The aim is to allocate the retailers to the facilities so that the objective function value is minimized.

Sets:

$\mathcal{I}$, set of facilities.

$\mathcal{J}$, set of retailers.

Deterministic parameter:

b_{it}, production capacity of facility i at time period t, for $i \in \mathcal{I}, t \in \mathcal{T}$.

Uncertain parameters:

D_{jt}^{ω}, product's demand from retailer j at time period t under scenario ω, for $j \in \mathcal{J}$, $t \in \mathcal{T}$, $\omega \in \Omega$.

c_{ij}^{ω}, assignment cost of retailer j to facility i under scenario ω, consisting of the total production and distribution costs, for $i \in \mathcal{I}$, $j \in \mathcal{J}$, $\omega \in \Omega$.

$h_{it}^{+\omega}$, unit inventory holding cost in facility i at time period t under scenario ω, for $i \in \mathcal{I}$, $t \in \mathcal{T}$, $\omega \in \Omega$.

$h_{it}^{-\omega}$, unit backlogging cost in facility i at time period t under scenario ω, for $i \in \mathcal{I}, t \in \mathcal{T}$, $\omega \in \Omega$.

Strategic variables:

x_{ij}, 0−1 variable such that its value is 1 if retailer j is assigned to facility i and 0 otherwise, for $\forall i \in \mathcal{I}, j \in \mathcal{J}$

Tactical variables:

$s_{it}^{+\omega}, s_{it}^{-\omega}$, product's inventory and backlogging in facility i at (the end of) time period t under scenario ω, respectively, for $i \in \mathcal{I}, t \in \mathcal{T}, \omega \in \Omega$.

3.3 Mixed 0−1 DEM. *Expected cost function minimization*

The following is a *compact* representation of the mixed 0−1 *DEM* for the two-stage stochastic *MPSSP* with complete recourse to minimize the expected cost.

$$\min Q_E = \sum_{\omega\in\Omega} w^{\omega}\Big(\sum_{i\in\mathcal{I}} \sum_{j\in\mathcal{J}} c_{ij}^{\omega} x_{ij} + \sum_{i\in\mathcal{I}} \sum_{t\in\mathcal{T}} (h_{it}^{+\omega} s_{it}^{+\omega} + h_{it}^{-\omega} s_{it}^{-\omega})\Big) \tag{46}$$

subject to

$$\sum_{i\in\mathcal{I}} x_{ij} = 1 \quad \forall j \in \mathcal{J} \tag{47}$$

$$\sum_{j\in\mathcal{J}} D_{jt}^{\omega} x_{ij} + s_{it}^{+\omega} + s_{i,t-1}^{-\omega} \leq b_{it} + s_{i,t-1}^{+\omega} + s_{it}^{-\omega} \quad \forall i \in \mathcal{I}, t \in \mathcal{T}, \omega \in \Omega \tag{48}$$

$$s_{i0}^{+\omega} = s_{i0}^{-\omega} = 0 \quad \forall i \in \mathcal{I}, \omega \in \Omega \tag{49}$$

$$x_{ij} \in \{0,1\} \quad \forall i \in \mathcal{I}, j \in \mathcal{J} \tag{50}$$

$$s_{it}^{+\omega}, s_{it}^{-\omega} \geq 0 \quad \forall i \in \mathcal{I}, t \in \mathcal{T}, \omega \in \Omega. \tag{51}$$

The objective function (46) consists of the expected assignment, inventory holding and backlogging costs along the time horizon over the scenarios. Constraints (47), together with constraints (50), ensure that each retailer is assigned to exactly one facility. Constraints (48) ensure that the production capacity of the facilities is not violated. Notice that the model (46)–(51) is always feasible.

We propose in [8] an equivalent formulation of the *compact* representation (46)–(51) based on *splitting* the assignment variables. In particular, we replace each variable x_{ij} by x_{ij}^{ω} $\forall w \in \Omega$ and append to the model the so-called *non-anticipativity* constraints (52) to ensure that the assignments are not subordinated to any of the scenarios.

$$x_{ij}^{\omega} - x_{ij}^{\omega+1} = 0 \qquad \forall i \in \mathcal{I}, j \in \mathcal{J}, \omega \in \Omega - \{|\Omega|\}. \tag{52}$$

Let an instance with $|\mathcal{I}| = 10$ facilities, $|\mathcal{J}| = 150$ retailers, $|\mathcal{T}| = 6$ time periods and $|\Omega| = 400$ scenarios. The dimensions of *DEM*, compact representation are 24150 constraints, 48000 continuous variables and 1500 0−1 variables. See in [8] the specialization of the Branch-and-Fix Coordination approach used for minimizing the expected cost as well as the computational experience. The proposed approach outperform a state-of-the-art optimization engine as well as the approach based on the average scenario.

3.4 Mixed 0−1 DEM*. Mean-risk function minimization*

The above model aims to minimize the objective function expected value. However, one of the approaches that in addition deals with the risk measure considers the *excess probability* functional [76] as we mentioned above.

Recall that ϕ denotes a prescribed threshold for the *excess probability*, say, Q_P, such that

$$Q_P = P(\omega \in \Omega : c^\omega x^\omega + h^\omega s^\omega > \phi). \tag{53}$$

where c^ω and h^ω are the row vectors of the objective function coefficients for the x and s variables, respectively, So, alternatively to min Q_E (46), we propose to minimize the mean-risk function

$$Q_E + \eta Q_P. \tag{54}$$

A more amenable expression of (54) for computational purposes at least, can be

$$\begin{aligned} &\min\ Q_E + \ \eta \sum_{\omega\in\Omega} w^\omega v^\omega \\ &\text{s.t.} \sum_{i\in\mathcal{I}} \sum_{j\in\mathcal{J}} c_{ij}^\omega x_{ij} + \sum_{i\in\mathcal{I}} \sum_{t\in\mathcal{T}} (h_{it}^{+\omega} s_{it}^{+\omega} + h_{it}^{-\omega} s_{it}^{-\omega}) \le \phi + M v^\omega \quad \forall \omega \in \Omega \\ &\quad v^\omega \in \{0,1\} \qquad\qquad \forall \omega \in \Omega, \end{aligned} \tag{55}$$

where η, v^ω and M as above, see Section 1.3.

Let the synthesized model of the *splitting variable* representation of the mixed 0−1 *DEM* min (55) subject to (47)–(51) be expressed

$$\begin{aligned} Z_{IP} = \min &\sum_{\omega\in\Omega} w^\omega \left(c^\omega x^\omega + h^\omega s^\omega + \eta v^\omega \right) \\ \text{s.t. } & c^\omega x^\omega + h^\omega s^\omega \le \phi + M v^\omega && \forall \omega \in \Omega \\ & \sum_{i\in\mathcal{I}} x_{ij}^\omega = 1 && \forall j \in \mathcal{J}, \omega \in \Omega \\ & D^\omega x^\omega + B s^\omega = b && \forall \omega \in \Omega \\ & x_{ij}^\omega - x_{ij}^{\omega+1} = 0 && \forall i \in \mathcal{I}, j \in \mathcal{J}, \omega \in \Omega - \{|\Omega|\} \\ & s_0^\omega = 0^{2m} && \forall \omega \in \Omega \\ & x^\omega \in \{0,1\}^{mn} && \forall \omega \in \Omega \\ & s^\omega \ge 0^r && \forall \omega \in \Omega \\ & v^\omega \in \{0,1\} && \forall \omega \in \Omega, \end{aligned} \tag{56}$$

where c^ω and h^ω are as above, D^ω is the time indexed constraint matrix for the product's demand from the retailers, B is the time indexed constraint matrix $(+1, -1, 0)$ for the product's inventory and backlogging, b is the *rhs* vector, $x^\omega = (x_{ij}^\omega)_{i\in\mathcal{I}, j\in\mathcal{J}}$ gives the $m \times n$-vector of the 0−1 variables, S^ω gives the r-vector for the continuous variables, where $m = |\mathcal{I}|$, $n = |\mathcal{J}|$ and $r = 2m|\mathcal{T}|$, for $\omega \in \Omega$, M and v are as above and S_0^ω gives the vector for the continuous variables when $t = 0$.

Consider an example with $|\mathcal{I}| = 10$ facilities, $|\mathcal{J}| = 100$ retailers, $|\mathcal{T}| = 6$ time periods and $|\Omega| = 100$ scenarios. The dimensions of *DEM*, compact representation are 6200 constraints, 12000 continuous variables and 1100 0−1 variables. Due to the type of objective function in model (56), the computational experience with plain use of a general state-of-art optimization engine does not give good results, nor the plain use of the Branch-and-Fix Coordination approach [5]. Moreover, the implementation of the heuristic algorithm so-called the Fix-and-Relax Coordination introduced in [9] provides better results in an affordable computing time.

4 Single level Production Planning and Raw Material Supplying under Uncertainty

4.1 Problem statement

The planning of the production capacity utilization and the supplying of raw material is one of the most important managerial tactical responsibilities in manufacturing. In particular, the problem consists of deciding how much production and raw material supply, and how much product demand loss and backlogging can be expected at each period along a time horizon. The production capacity constraints, the product stock limitations, some logistic constraints related to the production lot sizing and the product demand requirements should be satisfied at a minimum cost.

There is a vast amount of literature on the deterministic version of the problem. See the seminal paper of [91] for considering only continuous variables. See [16, 28, 60, 69, 81, 83, 94], among others, for considering lot sizing limitations and other logical constraints (and, then, considering 0−1 variables). But there are not too many papers on the stochastic version of the problem.

However, very frequently the production decisions must be made in the presence of uncertainty in several important parameters, such as raw material and production cost, product demand and resource availability along a multi-stage time horizon.

We present below a mixed 0−1 model for production planning and raw material supplying, where the uncertainty is treated via a scenario tree based scheme, such that the occurrence of the events is represented by a multi-stage scenario tree. In particular, the 0−1 variables as well as the continuous variables appear at any stage along the time horizon.

The unit cost of the raw material supplying is not constant but it is decreasing while the supplying volume is increasing. This nonlinear separable function can be modelled via a function with linear segments.

4.2 Complete recourse mixed 0–1 DEM

The following is the notation for the sets and parameters used in the tactical production planning model.

Sets:

$\mathcal{I}$, set of raw materials.
$\mathcal{I}_j$, set of raw materials required by product j, for $j \in \mathcal{J}$.
$\mathcal{J}$, set of products.
$\mathbb{R}$, set of resources.

Deterministic parameters:

$\widehat{N}$, maximum number of products to be produced in a single time period.
$\underline{X}_{jt}, \overline{X}_j$, minimum and maximum volume of product j that can be produced at time period t, respectively, if any, for $j \in \mathcal{J}$, $t \in \mathcal{T}$.
$\overline{S}_j$, maximum volume of raw material or product j that can be in stock at any time period, for $j \in \mathcal{I} \bigcup \mathcal{J}$.
σ_j, fraction of the accumulated non-served demand that is lost.
o_{rj}, unit capacity consumption of resource r by product j, for $r \in \mathcal{R}$, $j \in \mathcal{J}$.
N_{ij}, volume of raw material i required by one unit of product j, for $i \in \mathcal{I}_j$, $j \in \mathcal{J}$.
h_j, unit holding cost of raw material or product j at any time period, for $j \in \mathcal{I} \bigcup \mathcal{J}$.
a_j, unit demand backlog penalty for product j, for $j \in \mathcal{J}$.
ρ_j, unit lost demand penalty for product j, for $j \in \mathcal{J}$.
f_j, fixed cost to be incurred for producing product j at any time period, for $j \in \mathcal{J}$.
d_i, delay time since the ordering of raw material i until its availability for processing, for $i \in \mathcal{I}$.

Uncertain parameters under scenario group $g \in \mathcal{G}$***:***

O_r^g, available capacity of resource r at time period $t(g)$, for $r \in \mathcal{R}$.
D_j^g, demand of product j at time period $t(g)$, for $j \in \mathcal{J}$.
c_j^g, unit supplying cost of raw material j, for $j \in \mathcal{I}$, and unit processing cost of product j at time period $t(g)$, for $j \in \mathcal{J}$.
$(\overline{c}_{ip}^g, a_{ip})$, pair of points (ordinate supplying cost, abscissa supplying volume) to define the supplying cost function of raw material i at time period $t(g)$, where $p = 1, \ldots, q$ is a given pair and q is the number of pairs.

Variables under scenario group $g \in \mathcal{G}$***:***

δ_j^g, 0−1 variable such that its value is 1 if product j is produced under scenario group g, and 0 otherwise, for $j \in \mathcal{J}$.

x_j^g, ordering volume of raw material j at (the end of) time period $t(g)$, for $j \in \mathcal{I}$, and production volume of product j at time period $t(g)$, for $j \in \mathcal{J}$.

s_j^g, stock volume of raw material j, for $j \in \mathcal{I}$ and product j, for $j \in \mathcal{J}$ at (the end of) time period $t(g)$.

z_j^g, served demand of product j at time period $t(g)$, for $j \in \mathcal{J}$.

y_j^g, lost demand of product j from time period $t(g)$, for $j \in \mathcal{J}$.

b_j^g, demand backlog of product j from time period $t(g)$, for $j \in \mathcal{J}$.

Raw material supplying cost function:

Alternative 1

The cost function is modelled by using the special ordered sets of type 2, or *S2* sets. These are sets of ordered continuous nonnegative variables, say, λ_{ip}^g for each pair $p = 1, \ldots, q$ of which no more than two members may be nonzero with the further condition that if there are many as two they must be adjacent, for $g \in \mathcal{G}, i \in \mathcal{I}$, see [14, 15]. The formulation is as follows,

$$\begin{aligned} c_i^g x_i^g &\equiv \sum_{p=1,\ldots,q} \overline{c}_{ip}^g \lambda_{ip}^g \quad \forall g \in \mathcal{G}, i \in \mathcal{I} \\ x_i^g &\equiv \sum_{p=1,\ldots,q} a_{ip} \lambda_{ip}^g \quad \forall g \in \mathcal{G}, i \in \mathcal{I} \\ \sum_{p=1,\ldots,q} \lambda_{ip}^g &= 1 \quad \forall g \in \mathcal{G}, i \in \mathcal{I} \end{aligned} \tag{57}$$

Alternative 2

The cost function is modelled by using the 0−1 variables, say, λ_{ip}^g for each pair $p = 1, \ldots, q$ and the continuous variables x_{ip}^g, for $g \in \mathcal{G}, i \in \mathcal{I}$. The formulation is as follows,

$$\begin{aligned} c_i^g x_i^g \equiv \sum_{p=1,\ldots,q} \left((\overline{c}_{ip}^g - \overline{c}_{i,p-1}^g)/(a_{ip}^g - a_{i,p-1}^g) \right) x_{ip}^g \quad & \forall g \in \mathcal{G}, i \in \mathcal{I} \\ \text{where } \overline{c}_{i0}^g = 0 \text{ and } a_{i0}^g = 0 & \\ x_i^g \equiv \sum_{p=1,\ldots,q} x_{ip}^g \quad & \forall g \in \mathcal{G}, i \in \mathcal{I} \\ a_{i1}^g \lambda_{i2}^g \le x_{i1}^g \le a_{i1}^g & \\ (a_{i2}^g - a_{i1}^g) \lambda_{i3}^g \le x_{i2}^g \le (a_{i2}^g - a_{i1}^g) \lambda_{i2}^g & \\ \ldots & \\ 0 \le x_{iq}^g \le (a_{iq}^g - a_{i,q-1}^g) \lambda_{iq}^g & \end{aligned} \tag{58}$$

The following is a *compact* representation of the *DEM* for the *multi-stage* stochastic problem with *complete recourse*.

Objective

Determine the production, supplying and stock management policy to minimize the expected production, supply and stock cost, the demand backlog penalty and the lost demand penalty plus the production fixed cost over the scenarios along the time horizon, subject to the constraints (60)- (69). Note: $c_j^g x_j^g$ and x_j^g below can be represented by either (57) or (58).

$$\min \sum_{g\in\mathcal{G}} w_g\Big(\sum_{j\in\mathcal{I}\bigcup\mathcal{J}} [c_j^g x_j^g + h_j s_j^g] + \sum_{j\in\mathcal{J}} [a_j b_j^g + \rho_j y_j^g + f_j \delta_j^g]\Big) \tag{59}$$

Constraints

$$s_i^{\gamma(g)} + x_i^{\pi(g)} = \sum_{j\in\mathcal{J}:i\in\mathcal{I}_j} N_{ij} x_j^g + s_i^g \quad \forall i \in \mathcal{I}, g \in \mathcal{G} \tag{60}$$

$$\sum_{j\in\mathcal{J}} o_{rj} x_j^g \le O_r^g \quad \forall r \in \mathcal{R}, g \in \mathcal{G} \tag{61}$$

$$\underline{X}_{j,t(g)} \delta_j^g \le x_j^g \le \overline{X}_j \delta_j^g \quad \forall j \in \mathcal{J}, g \in \mathcal{G} \tag{62}$$

$$\sum_{j\in\mathcal{J}} \delta_j^g \le \widehat{N} \quad \forall g \in \mathcal{G} \tag{63}$$

$$s_j^{\gamma(g)} + x_j^g = z_j^g + s_j^g \quad \forall j \in \mathcal{J}, g \in \mathcal{G} \tag{64}$$

$$b_j^{\gamma(g)} + D_j^g = z_j^g + b_j^g + y_j^g \quad \forall j \in \mathcal{J}, g \in \mathcal{G} \tag{65}$$

$$y_j^g \equiv \sigma_j (b_j^{\gamma(g)} + D_j^g - z_j^g) \ge 0 \quad \forall j \in \mathcal{J}, g \in \mathcal{G} \tag{66}$$

$$0 \le s_j^g \le \overline{S}_j \quad \forall j \in \mathcal{I}\bigcup\mathcal{J}, g \in \mathcal{G} \tag{67}$$

$$z_j^g, b_j^g \ge 0 \quad \forall j \in \mathcal{J}, g \in \mathcal{G} \tag{68}$$

$$\delta_j^g \in \{0,1\} \quad \forall j \in \mathcal{J}, g \in \mathcal{G} \tag{69}$$

where $\pi(g)$ for a given i is the scenario group whose time period $t(\pi(g))$ is the ordering time period of raw material i, so that $t(\pi(g)) + d_i + 1 = t(g)$ and $\pi(g) = G_{t(\pi(g))} \bigcap \mathcal{N}_g$.

Constraints (60) define the balance equations of the (internal) demand of the raw materials. The knapsack constraints (61) ensure that the consumption of the resources does not exceed the availability. Constraints (62) define the semi-continuous character of the production volume. The cover induced constraints (63) do not allow to produce more products in a single time period than the maximum allowed. Constraints (64) define the production and served product demand. Constraints (65) define the product demand balance equations, such that the demand deficit is either backlogged or lost. Constraints (66) define the nonnegative product lost demand. Constraints (67) give the upper bounds of the raw materials and product stock.

The instances of the mixed 0−1 *DEM* (59)-(69) can have such large dimensions that the using of state-of the-art optimization engines can make it unaffordable. Benders, Lagrangian and Branch-and-Fix Coordination decomposition schemes can be used, although the instances dimensions should be medium-sized.

It is well known that the deterministic version of model (59)-(69) is weaker than the version of the model where the *x*–variables de-aggregate the production to satisfy the demand at different time periods and, then, the *s*–variables are only implicit in the model, see [94]. However, the stochastic version of the above model gives better results than the other model. Its optimization can be performed by using a stochastic dynamic programming approach (*SDP*), see [26].

Consider an example with $|\mathcal{J}| = 50$ products, $|\mathbb{R}| = 10$ resources, $|\mathcal{T}| = 13$ time periods, $|\mathcal{G}| = 855$ scenario groups and $|\Omega| = 432$ scenarios. The dimensions of *DEM*, compact representation are 158805 constraints, 106650 continuous variables and 42750 0−1 variables. CPLEX, a state-of-the-art optimization engine, obtains a solution in a time limit, 8 hours, that is 0.8 per cent better than the solution obtained by using a *SDP* approach, but this one requires only 22.35 seconds. An instance with $|\mathcal{J}| = 100$ products, $|\mathbb{R}| = 50$ resources, $|\mathcal{T}| = 16$ time periods, $|\mathcal{G}| = 11684$ scenario groups and $|\Omega| = 7776$ scenarios cannot be solved by CPLEX (it does not produce any solution) in the time limit, but a solution is provided by the *SDP* approach in 75 minutes. The *DEM* dimensions are 4258204 constraints, 2727600 continuous variables and 1168400 0−1 variables.

5 Tactical multilevel Supply Chain Management (*SCM*)

5.1 Problem statement

A company with multiple suppliers at different production levels and multiple markets may seek to allocate demand quantities to different plants over a given time horizon. Its objective can be to determine the production, supplying and stock policy that best utilize the available resources in the whole supply chain system.

Let the problem elements be those presented in Section 2.2. Additionally, let the *cycle time* of a product be the set of consecutive and integer time periods that are required for its completion from its release in the assembly line until its availability for use. A *production period* is a time period in the cycle time of the product. Multiple market sources for end-products are allowed. A *LP* modelling approach is presented in [32] for the deterministic case. See also [25, 81], among others.

The uncertain parameters at the time of the planning are the product demand and the lost demand fraction, the resource availability, the unit production cost and the raw material supply cost. A two-stage stochastic *LP* model is introduced in [35]. It also

includes some other features, such as different modes for component procurement, say, standard and expediting modes, effective period segments where the components are required in the *BoM* (a very interesting structure for modelling engineering changes), alternate components of the so-called prime components, raw material and product groups, etc. See also [6].

One of the important decisions to be made in tactical supply chain management consists of determining the *ordering time period* for raw material supplying and product manufacturing/assembling along the time horizon. There is usually a time interval between ordering and delivering the components in the supply chain. In the case that the interval is not subject to specific constraints, a deterministic model can consider that the ordering time is the same as the delivering time. However, in the stochastic setting the related time interval is important, since the production and market environments can vary along the interval as we can also see in Section 4.

In this section we present a *LP DEM* for the multi-stage stochastic problem with significant time interval between the component ordering and delivering times.

5.2 LP DEM

The following is additional notation for the sets and parameters used in the tactical multilevel supply chain model.

Sets:

$\mathcal{J}$, set of products.
$\mathcal{JE}$, set of end products.
$\mathcal{JS}$, set of subassemblies. Note: $\mathcal{J} = \mathcal{JE} \bigcup \mathcal{JS}$.
$\mathcal{DS}_j$, set of market sources for end product j, for $j \in \mathcal{JE}$. Note: It is assumed that no subassembly has external demand, but the assumption can easily be removed.
$\mathcal{I}$, set of components.
$\mathcal{IR}$, set of raw materials. Note: $\mathcal{I} = \mathcal{JS} \bigcup \mathcal{IR}$.
$\mathcal{I}_j$, set of first tier components for product j, for $j \in \mathcal{J}$.
$\mathcal{R}$, set of resources.
$\mathcal{DS} = \bigcup_{j \in \mathcal{J}} \mathcal{DS}_j$.

Deterministic parameters market:

$\overline{B}_{dt}$, maximum backlog from market source d that is allowed at time period t, for $d \in \mathcal{DS}, t \in \mathcal{T}$.
τ_d, delivery lag time, i.e., number of time periods after its completion to deliver the related product to market source d, for $d \in \mathcal{DS}$. Note: It is assumed that the

delivery time is the same for all plants where the product is produced, but the assumption can easily be removed.

ρ_{dt}, σ_{dt}, unit lost demand penalty and backlog penalty for market source d at time period t, respectively, for $d \in \mathcal{DS}, t \in \mathcal{T}$.

Bill of Material (*BoM*):

c_j, cycle time of product j, for $j \in \mathcal{J}$.

p_{ij}, production time period in the cycle time of product j, where first tier component i is needed, for $i \in \mathcal{I}_j$, $j \in \mathcal{J}$.

N_{ij}, volume of first tier component i that is needed per unit of product j, for $i \in \mathcal{I}_j$, $j \in \mathcal{J}$.

τ_{ij}, number of time periods required to deliver component i from its depot to the plant where product j is manufactured/assembled, for $i \in \mathcal{I}_j$, $j \in \mathcal{J}$. Note: It is assumed that the delivery time is the same for all sites where the components and products are produced, but the assumption can easily be removed.

Component availability:

$\overline{X}_{it}$, maximum volume of raw material i that can be ordered at time period t, for $i \in \mathcal{IR}, t \in \mathcal{T}$.

τ^i, number of time periods required to supply raw material i to its depot, for $i \in \mathcal{IR}$.

Production and stock restrictions:

$\overline{Z}_{jt}$, maximum volume to release that is allowed for product j at time period t, for $j \in \mathcal{J}, t \in \mathcal{T}$.

$\underline{S}_{jt}, \overline{S}_j$, minimum and maximum volume of item j that can be in stock at (the end of) time period t, respectively, for $j \in \mathcal{J} \bigcup \mathcal{IR}, t \in \mathcal{T}$.

o_{rj}, unit capacity consumption of resource r by product j, for $r \in \mathcal{R}, j \in \mathcal{J}$. It is assumed that the resource is required at the time the product is released. Again this restriction can easily be removed, see Section 6.

Cost coefficients:

h_j, unit holding cost of item j at any time period, for $j \in \mathcal{J} \bigcup \mathcal{IR}$.

Uncertain parameters under scenario group $g \in \mathcal{G}$***:***

D_d^g, demand from market source d at time period $t(g)$, for $d \in \mathcal{DS}$.

f_d^g, lost fraction of nonserved accumulated demand from market source d, for $d \in \mathcal{DS}$.

O_r^g, available capacity of resource r, for $r \in \mathcal{R}$.
pc_j^g, unit production cost for product j, for $j \in \mathcal{J}$.
sc_i^g, unit supply cost for raw material i, for $i \in \mathcal{I}R$.

Variables under scenario group $g \in \mathcal{G}$***:***

z_j^g, volume of product j that is released in the production line at (the beginning of) time period $t(g)$, for $j \in \mathcal{J}$.
x_i^g, volume of raw material i that is *ordered* at (the end of) time $t(g)$, for $i \in \mathcal{I}R$.
y_d^g, volume of served demand from market source d that is being shipped at (the end of) time period $t(g)$, for $d \in \mathcal{D}S$.
s_j^g, stock volume of item j at (the end of) time period $t(g)$, for $j \in \mathcal{J} \bigcup \mathcal{I}R$.
b_d^g, backlog volume from market source d at (the end of) time period $t(g)$, for $d \in \mathcal{D}S$.
ℓ_d^g, lost demand from market source d at time period $t(g)$, for $d \in \mathcal{D}S$.

The following is a *compact* representation of the *DEM* for the *multi-stage* stochastic problem.

Objective

Determine the master production planning to minimize the expected production, supply and stock cost plus the expected penalty due to demand loss and backlogging over the scenarios along the time horizon, subject to the constraints (71)-(79).

$$\min \sum_{g \in \mathcal{G}} w_g \Big[\sum_{j \in \mathcal{J}} pc_j^g z_j^g + \sum_{i \in \mathcal{I}R} sc_i^g x_i^g + \sum_{j \in \mathcal{J} \bigcup \mathcal{I}R} h_j s_j^g + \sum_{d \in \mathcal{D}S} (\rho_{d,t(g)} \ell_d^g + \sigma_{d,t(g)} b_d^g) \Big] \tag{70}$$

Constraints

$$s_j^{\gamma(g)} + z_j^n = \sum_{d \in \mathcal{D}S_j} y_d^g + s_j^g \quad \forall j \in \mathcal{J}E, g \in \mathcal{G} \tag{71}$$

$$\text{where } n \in \mathcal{N}_g : t(n) = t(g) - c_j + 1$$

$$s_i^{\gamma(g)} + q_i^n = \sum_{j \in \mathcal{J} : i \in \mathcal{I}_j} N_{ij} z_j^h + s_i^g \quad \forall i \in \mathcal{I}, g \in \mathcal{G} \tag{72}$$

$$\text{where } q_i^n \equiv \begin{cases} z_i^n, & \text{for } i \in \mathcal{J}S \text{ where } n \in \mathcal{N}_g : t(n) = t(g) - c_i + 1 \\ x_i^n, & \text{for } i \in \mathcal{I}R \text{ where } n \in \mathcal{N}_g : t(n) = t(g) - \tau^i + 1 \end{cases}$$

$$h \in \mathcal{N}_g : t(h) = t(g) - c_j + p_{ij} + 1$$

$$b_d^{\gamma(g)} + D_d^g = y_d^e + \ell_d^g + b_d^g \quad \forall d \in \mathcal{D}S, g \in \mathcal{G} \tag{73}$$

$$\ell_d^g \equiv f_d^g(b_d^{\gamma(g)} + D_d^g - y_d^e) \geq 0 \tag{74}$$

$$\sum_{j\in\mathcal{J}} o_{rj} z_j^g \leq O_r^g \quad \forall r \in \mathcal{R}, g \in \mathcal{G} \tag{75}$$

$$0 \leq z_j^g \leq \overline{Z}_{j,t(g)} \quad \forall j \in \mathcal{J}, g \in \mathcal{G}, \tag{76}$$

$$\underline{S}_{j,t(g)} \leq s_j^g \leq \overline{S}_j \quad \forall j \in \mathcal{J} \cup \mathcal{IR}, g \in \mathcal{G} \tag{77}$$

$$0 \leq x_i^g \leq \overline{X}_{i,t(g)} \quad \forall i \in \mathcal{IR}, g \in \mathcal{G} \tag{78}$$

$$0 \leq b_d^g \leq \overline{B}_d^g \quad \forall d \in \mathcal{DS}, g \in \mathcal{G} \tag{79}$$

where $e \in \mathcal{N}_g : t(e) = t(g) - \tau_d$. Notice that y_d^e gives the served demand that is shipped at time period $t(e)$ (under scenario group e) to satisfy the product demand from market source d at time period $t(g)$ under any scenario in group $G_{t(g)} \bigcap \mathcal{N}^g$.

Constraints (71) and (72) are the stock balance equations for the end products and the components, respectively. Constraints (72) define the *BoM* requirements. Notice that $t(h)$ gives the time period for the release of product, say, j under scenario group h such that h belongs to the ancestor path $\mathcal{N}_g$. Constraints (73) and (74) define the balance equations of the product demand. Constraints (75) ensure that the consumption of the resources (to be used at the release time of the products) does not exceed its availability. Finally, the system (76)-(79) restricts the variables.

The *compact* representation (70)-(79) can be transformed in a *splitting variable* representation, such that the variable, say, x_i^g is replaced with its sibling, say, x_{it}^{ω} for $t = t(g)$, $\omega \in \Omega_g$, etc. Additionally, the non-anticipativity constraints (80)-(84) are appended to the model, for $\omega, \omega' \in \Omega_g : \omega \neq \omega', g \in \mathcal{G}_t, t \in \mathcal{T}$.

$$x_{it}^{\omega} - x_{it}^{\omega'} = 0 \quad \forall i \in \mathcal{IR} \tag{80}$$

$$z_{jt}^{\omega} - z_{jt}^{\omega'} = 0 \quad \forall j \in \mathcal{J} \tag{81}$$

$$s_{jt}^{\omega} - s_{jt}^{\omega'} = 0 \quad \forall j \in \mathcal{J} \cup \mathcal{IR} \tag{82}$$

$$y_{dt}^{\omega} - y_{dt}^{\omega'} = 0 \quad \forall d \in \mathcal{DS} \tag{83}$$

$$b_{dt}^{\omega} - b_{dt}^{\omega'} = 0 \quad \forall d \in \mathcal{DS}. \tag{84}$$

The instances of the *compact* representation (70)-(79) can have such big dimensions that decomposition approaches are needed. For illustrative purposes let the dimensions of a real-life instance from the automation sector: $|\mathcal{T}| = 13$ time periods, $|\mathcal{JE}| = 23$ end products, $|\mathcal{JS}| = 104$ subassemblies, $|\mathcal{IR}| = 5821$ raw components and $|\mathcal{DS}| = 525$ market sources. The related dimensions of the compact *DEM* for the two-stage stochastic version with two periods in the first stage, 11 periods in the second stage and $|\Omega| = 100$ scenarios are 2893683 constraints, 6014547 variables and 83304251 nonzero constraint elements.

See in [33] the Lagrangean based approach that we propose for solving multi-stage Stochastic Linear Programming problems.

6 Stochastic Sequencing and Scheduling problem

6.1 Introduction

Sequencing and Scheduling Problems (*SSPs*) arise in many practical circumstances when planning the utilization of a production/manufacturing system. Many problems are basically optimization problems having the following form: given a set of operations to be executed along a time horizon, find a schedule to minimize the value of a given objective function subject to various constraints. Typical elements are: limited availability of the resources, multiperiod operations, subsets of jobs with exclusivity constraints, precedence relationships in the execution of the operations, etc. See [6, 7].

This type of problems can be formulated as $0-1$ models and fall into the category of $\mathcal{NP}-hard$ problems. Traditional branch-and-bound methods have proved to be very inefficient to solve them. Instead, heuristic and meta-heuristic approaches have been found to obtain satisfactory solutions for special classes of this type of problems, such as problems with single period operations and special objective functions (e.g., *makespan* minimization). See [12, 44] for a survey and research potentials in project scheduling under uncertainty, among others.

On the other hand, there is a vast amount of literature on the polyhedral analysis of the problem and, then, on tightening $0-1$ models and facet defining inequalities identification for the deterministic version of the problem, see [93, 94], among others.

Application cases of the *SSP* considered in this paper can be found in investment planning, see [39], and production units maintenance planning, see [30], besides the proper application in production/manufacturing, see [31, 93, 94], among others. All of these works only consider the deterministic version of the problem. However, very frequently the resource availability as well as the resource consumption by the operations execution and, as a consequence, their execution cost are uncertain parameters.

6.2 Problem statement

Consider a set of *jobs*, each of them comprises a set of *operations* to be executed along the given time horizon. Each operation has a *time window* for its execution. The operations must be executed during a given number of consecutive so-called *production time periods* without preemption. Some jobs are alternative in the sense that one and only one of these jobs can be executed. Let us call a *class* to a set of alternative jobs. If a job is executed then the operations of the other jobs that belong to the same class cannot be executed (i.e., they cannot be assigned).

It is assumed that some operations have assigned a dedicated machine (or working station) for their execution. Let us say that the operations with the same dedicated

machine belong to the same *type*, such that the simultaneous execution of these operations is not allowed. A *setup* in a dedicated machine can be required between the consecutive execution of two operations. It is allowed that one operation can belong to more than one type.

There are *precedence* relationships in the execution of the operations. They can be expressed by a directed acyclic graph, where the nodes are associated with the operations and the arcs refer to the existence of a direct precedence between the execution of the operations represented by the from-node and the to-node of the arcs. The precedences have the transitivity property. Two types of precedences are considered, such that a minimum number (type 1) and a maximum number (type 2) of time periods are required between the starting of the executions.

A set of *resources* with uncertain availability along the time horizon is considered. The operations' execution can require resource consumption in each of its production periods. The resource amount to be utilized depends on several factors and it is also an uncertain parameter. Although the resource availability is uncertain at the *planning time* period, it is assumed to be known at the (beginning of the) period where the resource is required. However, the resource consumption by the operations execution is only known at the *consumption time*, what means that the occurrence of the resource consumption scenario at a given time period is not known in advance.

The goal consists of determining the time period at which each operation will start its execution (i.e., assignment), if any, such that a set of constraints is satisfied along the scenario tree. The objective function to minimize consists of the expected execution cost of the operations over the scenarios.

6.3 Pure 0–1 DEM

The following is additional notation for the sets and parameters to be used in the section.

Sets:

$\mathbb{R}$, set of resources.
$\mathcal{I}$, set of operations.
$\mathcal{J}$, set of jobs.
$\mathbb{C}$, set of classes of jobs.
$\mathcal{T}_i$, set of feasible time periods to start the execution of operation i, for $i \in \mathcal{I}$ ($\mathcal{T}_i \subseteq \mathcal{T}$).
$\mathcal{I}_j$, set of operations included in job j, for $j \in \mathcal{J}$ ($\mathcal{I}_j \subseteq \mathcal{I}$).
$\mathcal{J}_c$, set of jobs that belong to class c, for $c \in \mathbb{C}$ ($\mathcal{J}_c \subseteq \mathcal{J}$).
$\mathcal{M}$, set of types of operations.
$\mathcal{I}^m$, set of operations that belong to type m, for $m \in \mathcal{M}$ ($\mathcal{I}^m \subseteq \mathcal{I}$).

$\mathcal{A}^1$ (resp., $\mathcal{A}^2$), set of ordered pairs of operations with precedence relationship type 1 (resp., type 2).

Deterministic parameters:

e_i, ℓ_i**,** earliest and latest time periods for starting the execution of operation i, respectively, for $i \in \mathcal{I}$. Note: $e_i, \ell_i \in \mathcal{T}_i$ and $\mathcal{T}_i \subseteq \{e_i, e_{i+1}, \ldots, \ell_i\}$.

d_i**,** number of the so-called production time periods that are required for the execution of operation i, for $i \in \mathcal{I}$. Note: $t \in \mathcal{T}_i$ implies that $1 \leq t \leq |\mathcal{T}| - d_i + 1$.

d^m**,** setup time between the ending and the starting of the execution of two operations that belong to type m, for $m \in \mathcal{M}$.

p^1_{ab} and p^2_{ab}**,** minimum and maximum number of time periods (so-called time lag) between the starting of the execution of the operations a and b, for $(a, b) \in \mathcal{A}^1$ and $(a, b) \in \mathcal{A}^2$, respectively.

Uncertain parameters under scenario group $g \in \mathcal{G}$***:***

o^g_{rih}, amount of resource r that is required by the execution of operation i during its hth production time period under scenario group g, for $r \in \mathbb{R}$, $h = 1, 2, \ldots, d_i, i \in \mathcal{I}$.

O^g_r, available capacity of resource r at time period $t(g)$, for $r \in \mathbb{R}$.

c^g_i, execution cost of operation i at time period $t(g)$, for $i \in \mathcal{I}$.

Among the different alternatives to model the problem, we use the *step variable* based formulation given in [18].

Strategic variables:

y_j, 0−1 variable such that its value is 1 if job j is selected for execution, and 0 otherwise, $\forall j \in \mathcal{J}$.

Sequencing and scheduling variables:

z^g_i, 0−1 variable such that its value is 1 if operation i starts its execution **by** time period $t(g)$ under scenario group g, and 0 otherwise, $\forall g \in \mathcal{G}_t, t \in \mathcal{T} : e_i \leq t, i \in \mathcal{I}$.

The execution time interval for operation i is $t(g), t(g) + 1, \ldots, t(g) + d_i - 1$ for $z^g_i = 1$ and $z^{\gamma(g)}_i = 0$.

The following is a *compact* representation of the *DEM* for the *multi-stage* stochastic problem with *complete recourse*.

Objective

Determine the execution sequencing and scheduling of the operations in order to minimize the expected cost of the operations' execution over the scenarios along a time horizon, subject to the constraints (86)– (96). It can be expressed

$$\min \sum_{i\in\mathcal{I}} \sum_{t\in\mathcal{T}_i} \sum_{g\in\mathcal{G}_t} w_g c_i^g (z_i^g - z_i^{\gamma(g)}). \tag{85}$$

Constraints

$$\sum_{j\in\mathcal{J}_c} y_j = 1 \quad \forall c \in \mathbb{C} \tag{86}$$

$$z_i^g = y_j \quad \forall g \in \mathcal{G}_{\ell_i}, i \in \mathcal{I}_j, j \in \mathcal{J} \tag{87}$$

$$z_i^{\gamma(g)} \le z_i^g \quad \forall g \in \mathcal{G}_t, t \in \mathcal{T}_i \setminus \{e_i\} \tag{88}$$

$$z_i^{\gamma(g)} = z_i^g \quad \forall g \in \mathcal{G}_t, t \in \mathcal{T} \setminus T_i : e_i < t < \ell_i, i \in \mathcal{I} \tag{89}$$

$$z_i^{g'} = z_i^g \quad \forall g' \in \mathcal{N}^g \setminus \{g\}, g \in \mathcal{G}_{\ell_i}, i \in \mathcal{I} \tag{90}$$

$$\sum_{i\in\mathcal{I}^m} \rho_{it}(z_i^g - \mu_{it} z_i^{g'}) \le 1 \quad \forall m \in \mathcal{M}, g \in \mathcal{G}_t, t \in \mathcal{T} \tag{91}$$

where $\rho_{it} \equiv \begin{cases} 1, & e_i \le t < \ell_i + d_i + d^m \\ 0, & \text{otherwise} \end{cases}$

$\mu_{it} \equiv \begin{cases} 1, & e_i + d_i + d^m \le t \\ 0, & \text{otherwise} \end{cases}$

$g' = \mathcal{N}_g \cap \mathcal{G}_{t-d_i-d^m}$

$$z_a^{g'} \ge z_b^g \quad \forall g \in \mathcal{G}_t, t \in \mathcal{T}_b : t < \ell_a + p_{ab}^1, (a,b) \in \mathcal{A}^1 \tag{92}$$

where $g' = \mathcal{N}_g \cap \mathcal{G}_{t-p_{ab}^1}$

$$z_a^g \le z_b^{g'} \quad \forall g' \in \mathcal{N}^g \cap \mathcal{G}_{t+p_{ab}^2}, g \in \mathcal{G}_t, t \in \mathcal{T}_a : t < \ell_b - p_{ab}^2, (a,b) \in \mathcal{A}^2 \tag{93}$$

$$\sum_{i\in\mathcal{I}} \sum_{k\in F_i} o_{rih}^g (z_i^k - \alpha_{it} z_i^{\gamma(k)}) \le O_r^g \quad \forall r \in \mathbb{R}, g \in \mathcal{G}_t, t \in \mathcal{T} \tag{94}$$

where $F_i \equiv \{k \in \mathcal{N}_g : t(k) \in \mathcal{T}_i, t - d_i < t(k)\}$

$\alpha_{it} = \begin{cases} 1, & e_i < t \\ 0, & \text{otherwise} \end{cases}$

$h = t - t(k) + 1$

$$z_i^g \in \{0,1\} \quad \forall g \in \mathcal{G}_t, t \in \mathcal{T} : e_i \leq t, i \in \mathcal{I} \tag{95}$$

$$y_j \in \{0,1\} \quad \forall j \in \mathcal{J}. \tag{96}$$

Constraints (86) force the assignment (i.e., the execution) of one and only one job for each class.

Constraints (87) force the execution of all operations that are required by the selected jobs under any scenario, and prevent the execution of the operations that are required by the jobs that have not been selected. Notice that it is enough that $g \in \mathcal{G}_{\ell_i}$ in the domain of the constraints.

Constraints (88) ensure that the value 0 for the variable z_i^g is propagated through the ancestor path from node g down to node k for $t(k) = e_i$ in the scenario tree, for $t(g) \in \mathcal{T}_i \setminus \{e_i\}$. The constraints also ensure that the value 1 for the variable $z^{\gamma(g)}$ is propagated through the subtree with root node $\gamma(g)$ in the scenario tree.

Constraints (89) avoid the operations starting their execution in non-feasible time periods, independently of the scenario being considered. Note: From a computational point of view, the constraints (89) are not included in the model and the variable z_i^g, $g \in \mathcal{G}_t, t \in \mathcal{T} \setminus T_i : e_i \leq t < \ell_i$ is replaced with the variable z_i^g, $g \in \mathcal{G}_\tau, \tau \in \mathcal{T}_i$ in any other constraint, where $\tau = \max t' \in \mathcal{T}_i : t' < t$.

Constraints (90) formally state the propagation of the z-value to the scenario groups in the subtrees whose root nodes are the latest start of the operations' execution. Note: From a computational point of view, the constraints (90) are not included in the model and the variable $z_i^{g'}$, $g' \in \mathcal{N}^g \setminus \{g\}$ is replaced with the variable z_i^g, $g \in \mathcal{G}_{\ell_i}$ in any other constraint. Let us name *configuration* system to the constraint system (86)–(90) and (95)-(96).

Constraints (91), jointly with the *configuration* system, prevent the assignment of more than one operation of a given type at the same time period. Notice that the difference $z_i^g - z_i^{g'}$ equals 1 (and, so, the assignment of operation i prevents the assignment of any other operation of the same type at time period $t(g)$) if operation i starts its execution in the time interval given by the periods $t(g) - d_i - d^m + 1$ and $t(g)$.

Constraints (92) and (93) ensure that the precedence relationships types 1 and 2 are not violated, respectively. By constraints (92), if operation b starts at time period $t(g)$, then operation a must start p_{ab}^1 periods earlier, at least, under the given ancestor scenario group from $\mathcal{G}_{t(g)-p_{ab}^1}$, for $(a,b) \in \mathcal{A}^1$. By constraints (93), if operation a starts at time period $t(g)$, then operation b must start p_{ab}^2 periods later, at most, under any successor scenario group from $\mathcal{G}_{t(g)+p_{ab}^2}$, for $(a,b) \in \mathcal{A}^2$.

Constraints (94), jointly with the *configuration* system, ensure that the consumption of the resources does not exceed their availability.

The *compact* representation (85)–(96) can also be transformed into a *splitting variable* representation by replacing the y– and z–variables with their respective siblings, where y_j is replaced with y_j^ω $\forall \omega \in \Omega$ and z_i^g is replaced with z_{it}^ω $\forall \omega \in \Omega^g$, for $t = t(g)$,

so that there is a submodel for each scenario $\omega \in \Omega$. The non-anticipativity constraints (97)-(98) are appended to the new model.

$$y_j^{\omega} - y_j^{\omega'} = 0 \quad \forall \omega, \omega' \in \Omega : \omega \neq \omega', j \in \mathcal{J} \tag{97}$$

$$z_{it}^{\omega} - z_{it}^{\omega'} = 0 \quad \forall \omega, \omega' \in \Omega^g : \omega \neq \omega', g \in \mathcal{G}_t, t \in \mathcal{T} : e_i \leq t, i \in \mathcal{I}. \tag{98}$$

Consider an example with $|\mathbb{C}| = 20$ classes, $|\mathcal{J}| = 31$ jobs, $|I| = 399$ operations, $|\mathcal{T}| = 7$ time periods, $|\Omega| = 128$ and $|\mathcal{G}| = 255$ scenario groups. The dimensions of *DEM*, compact representation are 208170 constraints and 185015 0−1 variables.

From a practical point of view, due to the large-scale of the problem and its combinatorial nature, it cannot be solved up to optimality in affordable computing time but for moderated size instances, mainly in the number of scenarios. So, efficient heuristic approaches should be used. We consider in [7] an heuristic based on a mixture of a Fix-and-Relax approach, see [28, 39], for providing good solutions to the scenario–related sequencing and scheduling problem, and a Branch-and-Fix Coordination scheme, see [3, 5], for coordinating the branching phase in the scenario cluster–related Branch-and-Fix trees, so that the constraints (97)–(98) are satisfied. The results reported in [7] for large-scale instances are very encouraging, outperforming a state-of-the-art optimization engine.

7 Conclusions

We have presented some modelling schemes in supply chain management and production planning under uncertainty by using a sample set of problems. The uncertainty is represented by a scenario tree. All the problems lie within the complete recourse environment. In any case, the presence of 0−1 variables is very frequent, mainly, for modelling the either-or decisions and the operations assignment, sequencing and scheduling. Two approaches can be used depending basically upon the amount of information that is available on the uncertain parameters, namely, two-stage Stochastic Integer Programming (*SIP*) (where the continuous variables only appear in the second stage) and multi-stage *SIP* (where the continuous variables and the 0−1 variables appear at any stage). There are good exact solutions for the two-stage and good heuristic approaches for the multi-stage, but there are very few exact algorithms for large-scale multi-stage problems. In any case, the *SIP* discipline has been proved to be essential for modelling and solving real-life Supply Chain and production planning and assignment problems.

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Discussion of “On Modelling Planning under Uncertainty in Manufacturing” by A. Alonso-Ayuso, L.F. Escudero and M.T. Ortuño

Monique Guignard

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This paper shows how to approach uncertainty in various aspects of manufacturing, both at a strategic and at a tactical level. It considers a number of specific problems, from strategic to tactical multilevel supply chain management, with in between single sourcing, production planning, raw material supplying, and sequencing and scheduling. All involve a number of critical decisions that must often be made in a very uncertain environment. After presenting a broad picture of possible ways to represent uncertainty via scenarios and scenario trees, and two possible objectives, namely minimizing expected costs or maximizing expected benefits, and minimizing a mean-risk function, the authors turn to specific problems. These are often complicated by the fact that in addition to uncertainly, they contain 0-1 variables, which would make them difficult to solve even in a deterministic environment. For each problem, the authors carefully define the data/decision variables and present models for complete recourse for 2-stage or multi-stage Stochastic Integer Programming. In most instances, then, they refer the readers to their numerous contributions to the field, or to some other papers in the literature, for more detailed solution approaches, such as Benders, Lagrangean or Branch-and-Fix coordination decomposition, or Fix-and-Relax schemes.

This paper is thus a very nice introduction to modelling for several important problems in manufacturing under uncertain conditions, and the reader is directed to a number of important papers on the topic, making it at the same time a valuable survey paper.

I have three questions for the authors.

1. Much of the optimization is related to choosing a set of scenarios. While scenario generation schemes may present themselves naturally in problems related to, say, interest rates, for the problems considered here, it is not clear how to generate them. Yet, the results obtained will probably critically depend upon this initial decision. Could the authors discuss how they would suggest generating scenarios, including their number, and how they think this choice will affect the solutions to their models? Are more scenarios better? In general, what characterizes a ”better set” of scenarios?
2. In this as well as in some other papers on stochastic optimization, one finds statements to the effect that a certain approach “outperforms” other approaches,

or that a particular model "gives better results" than another model. Could the authors expand on this concept?

3. What other alternative approaches are there? In particular, what role do/can approximation algorithms play for solving such problems?

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Gautam Mitra

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CARISMA: The Centre for the Analysis of Risk and Optimisation Modelling Applications.

This paper contains a splendid review of the supply chain planning under uncertainty.

A family of planning models is introduced taking into consideration the taxonomy of planning problems introduced by Anthony and covering Strategic, Tactical and Operational decision making.

The models are carefully constructed and clearly set out. The models provide considerable details encompassing bill of materials, supply chain topology, vendor contributions and cost uncertainties in the supply side and depots, and demand uncertainties in the demand side.

At the modelling level the authors consider both the expected value and the mean-risk as objective functions of their models. The consideration of the risk objective is quite insightful. It is our opinion that in future supply chain management models will take into consideration the risk exposure of the raw material supply, their volatile prices and risk of disruption in the network. Indeed a special issue (January 2008) of the *Journal of the Operational Research Society* (GB) has been edited by us and devoted to this topic: Risk Based Methods for Supply Chain Planning and Management.

The authors quite justifiably highlight the importance of computational algorithms in general and stochastic integer programming in particular.

In our paper (Chandra, Lucas and Mitra, 2008) we consider a strategic supply chain planning problem formulated as a two-stage Stochastic Integer Programming (SIP) model. The large-scale SIP problem is solved through Benders' decomposition, and we approximate the probability distribution of the random varibles using the Generalised Lambda distribution and through simulations, calculate the performance statistics and the risk measures for the two models, namely the expected-value of the here-and-now.

In conclusion, the authors Alonso-Ayuso, Escudero and Ortuno have made a substantial contribution and provided insights into supply chain modelling under uncertainty and risk which is going to be the central theme of the future developments in this domain.

Reference

Poojari, C.A., Lucas, C. and Mitra, G. (2008). Robust solutions and risk measures for a supply chain planning problem under uncertainty. *Journal of the Operational Research Society*, 59, 2-12.

Francisco J. Prieto

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1 Introduction

This paper presents and discusses several formulation approaches to relevant production planning problems, with a particular emphasis on the treatment of uncertainty and risk within the corresponding frameworks.

These are relevant and timely contributions, presented in a careful and detailed manner. While, as illustrated in the references for the paper, a significant amount of work has been carried out on the modelling of production and logistics problems for the deterministic case, a more limited effort has been devoted to the treatment of the uncertainty in these problems. In many practical applications within this context, issues related to the robustness of the solutions are very relevant; in a production world of small inventories and tight schedules, unforeseen disruptions can have a large impact on final results for any company. In this production context, robustness is possibly much more relevant than financial risk as a criterion to be modelled.

Many improvements have taken place in recent years both regarding solvers for mixed integer programs and in approximation and decomposition algorithms, including several contributions from the authors ([6] or [10], for example). These improvements have brought the corresponding problems much closer to gaining widespread consideration within normal production planning processes. Perhaps in the near future it will be possible to see tools based on these models, and the corresponding solution techniques, incorporated as part of the most common decision support systems for production planning and business software in general. By giving a complete, clear and coherent presentation of these problems, this paper provides a significant contribution to this end.

2 Some comments

The model descriptions and comments presented by the authors unavoidably give rise to many related and interesting issues. While they do not directly affect the contents of the paper, they may help to provide additional insights on these models and their practical application.

- One important issue that might merit some additional discussion is that of two-stage vs. multi-stage formulations for the uncertainty. This modelling decision has implications on several aspects: the choice of a solution procedure, as any decomposition approach would depend significantly on the structure of the resulting problem; the uncertainty representation through the scenario trees: while its dependence structure would be in principle richer in the multi-stage setting, it would also require additional computational effort to generate and to handle; and the quality of the solution, as a better adapted set of values of the variables would potentially provide a more realistic solution.
  In the paper, the two-stage approach is preferred in most cases, except for the Production Planning and Raw Material Supplying problem and the Stochastic Sequencing and Scheduling problem. Nevertheless, in both these cases the temporal structure of the decisions is similar to that of the other problems, including both decisions taken now (without considering any future information) and future decisions adapted to the uncertainty, that can be reevaluated and optimized again later on.
  It is not clear that there is any significant advantage gained by not treating these problems also as two-stage ones. This approach would not seem to compromise much of the quality of the solutions, and might simplify (and homogenize) the modelling, while presenting computational advantages.

- In most approaches to uncertainty planning in the literature, the uncertain values are associated to highly variable parameters, such as prices/costs or demand. This seems reasonable for everyday situations where the variability in the optimal decisions is mostly associated to these values, but in the production setting considered in the paper it could be argued that it would be as important to take into account the variability associated to unforeseen changes in capacity availability.
  For example, in model (10)–(22) both P_t and $\bar{N}^i$ could be treated as stochastic parameters, and similarly for $\bar{X}^i_j$ in (23)–(36).
  This consideration raises an interesting issue: the treatment of low-probability situations within a scenario framework, such as those indicated above, as their treatment may have a significant impact on the quality of the solution. Using a MonteCarlo simulation analogy, there may be a problem with the variance of the estimates, as in principle only a few of these situations would be considered within the usual scenario generation approaches. Variance reduction techniques, such as importance sampling, could be helpful to improve the quality of the solutions in these cases.
  Additionally, scenario-tree reduction techniques based on moment-approximation may give results that are not particularly precise, as they are fitting a distribution for the input variables not knowing in advance which parts of that distribution are more relevant for the precise characterization of the distribution for the output variables.

Other approaches, such as dynamic scenario generation strategies, may be able to adapt to these situations and provide better answers in these settings (low-probability but significant events). Of course, they would also have an impact on problem formulation and solution techniques, as the structure of the problem could be modified from iteration to iteration, and they may present significant difficulties in multi-stage settings.

- Another question raised by the models in the paper is related to its prevalent use of an objective function based on a profit or cost criterion, possibly augmented with the inclusion of measures for excess probabilities associated with them.
  In manufacturing problems it is quite often the case that the goal is obtaining production/distribution schedules that are robust, that is, do not require much modification in the presence of perturbations. Also, in the uncertainty setting contemplated in the paper, other criteria related to quality become also relevant for the objective function. This raises the issue of the use of different objective functions/risk measures in this context.
  For example, and regarding the objective functions considered in several of the models, such as for example that of Section 2, it might be reasonable to include in them explicit measures of the delay in the satisfaction of the demand. In that particular case, a possible modification of the model might introduce variables covering separately the demand whose satisfaction has been delayed k periods at time t, and updating them through an expanded conservation law similar to (30).
  In the case of the model in Section 6 it might be of interest to relax its formulation to allow for delays (that would otherwise be associated with infeasible solutions in the formulation presented in the paper), and to account for the number of periods that the execution extended beyond the latest time period allowed to complete it. This would require an extensive and complex modification of the model.
  Note that under uncertainty infeasibility becomes a more likely end result for formulations that are not sufficiently flexible to accommodate extreme outcomes in the values of the variables.
  The definition of robust solutions is also very relevant in this context. The objective function could include measures for the changes in solutions for different scenarios, and look for those that require smaller modifications between scenarios. For example, this could be done by considering the deterministic solutions for each scenario as references. Of course, a question open to debate would be the choice of an appropriate metric to compare these changes.

- On a more specific topic, and regarding the models used in Sections 2 and 4 (Strategic Supply Chain Management and Single Level Production Planning), their treatment in an uncertain setting would suggest the possibility of giving explicit consideration within the model to futures and other instruments, to hedge some purchasing decisions against price (and availability) changes. In practice, this

would make particular sense at least regarding those raw materials that are traded in open markets (gas, fuel or electricity, for example).

The additional terms required would not need to complicate the model significantly. It might be enough to introduce a portfolio of contracts with predefined time availabilities and costs, and zero-one variables related to the purchasing of the contracts and/or their usage within the model. That is, there would be additional suppliers with availabilities linked to stage-one decisions and having deterministic parameters in the model.

Andres Weintraub

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The issue of incorporating uncertainty explicitly is becoming increasingly central in modelling, driven largely by research sophistication, but also due to needs for more robust planning.

There are several ways in which to incorporate uncertainty, and also to evaluate the need to actually do it explicitly.

In this excellent paper by Alonso-Ayuso, Escudero and Ortuno,the authors present a summary, an integration of their important work in this field, in relation to modelling problems in manufacturing.

Here they consider several levels of planning, going from strategic to tactical to operational decisions. Uncertainty is considered, depending on the level of decision in parameters dealing with demand, production costs, costs for raw materials, resource availability. Their approach to uncertainty is to consider tree scenarios, assigning probabilities to the scenarios, and finding deterministic equivalents with complete recourse. Given that the models they present deal with discrete decisions, all models have a MIP structure, and the approaches proposed are based on the non-anticipativity constraints to force same decisions for same scenarios up to any point in time. This can be represented by splitting variable or a compact representation, which allows to solve the problems in a decomposed form. I see here several main contributions. First, the form of representing uncertainty. While in theory probability distribution functions can be defined to represent uncertainty, in practice in most cases it is very difficult to determine such functions with accuracy. But planners can feel more comfortable thinking of scenarios, and assign probabilities to them. In some cases, there is a reasonably rigorous basis for establishing probabilities for scenarios. In other cases, the scenarios defined, and the probabilities are more like guesses. One open problem here could be analyzing the robustness of the decisions to variability in the probabilities of the scenarios.

Considering the scenario approach, expressed in equation (2), there is ample experience to show that for large scale problems, which are usually the real ones, it is computationally infeasible to solve the problem as stated. Here comes the main contribution of the authors in their different works. They propose a successful way to decompose the problems, based on the non-anticipativity constraints. Perhaps here the

authors should help the reader by expanding Section 1.2, to clearly show how the two approaches work, the solution process, in particular for the compact representation. A small example might be of help here.

It should be noted that the approaches proposed require a limited number of scenarios to be computationally tractable. While this condition on the number of scenarios in some cases can be a significant limitation, it can be considered to fall in line with the difficulties of planners of thinking of too many scenarios.

The authors present several specific models for manufacturing. The models are not simple, can be considered similar to real, simplified cases, and uncertainty is incorporated into them where logic would indicate.

Here we need to view two aspects I think. One is the way uncertainty is approached. The second are the models themselves. While these models need to be represented as they are, in some cases they are not easy to read. Maybe the relative complexity of the model formulation can overshadow the main result, which is the consideration of uncertainty.

As for uncertainty, I believe the authors could present their results in a stronger way, by explaining more explicitly why they used a given approach for each problem. For example, in Section 2, why propose to use Branch and Fix Coordination, what are the results obtained? What is gained by the proposed approach as compared to more traditional approaches, including not considering uncertainty in an explicit form. So, in this case, there are two issues to consider, one is in relation to the improvement in robustness of the solutions when uncertainty is considered explicitly, and what is the cost due to this insurance. Note that these approaches by requiring to satisfy feasibility under all scenarios, have a component of being conservative. The second issue is related to the comparison of the proposed approaches with other alternatives.

In Section 3.4, the Fix and Relax Coordination approach is presented. Again the paper I think would gain by explaining the method, why it was proposed and a short discussion of the results obtained through the use of this approach. The same comment applies to the approaches mentioned as solution methods in the other sections, and other problems presented.

Basically the objective function is expressed in terms of expected value, and in some cases as excess probabilities. The latter adds another component to variability, trying to avoid solutions where the objective under certain scenarios are above a certain threshold value (this is used in Section 3.4, for example.). I believe a discussion is needed on why consider excess probability, why in specific problems, and what is gained by this consideration in Section 3.4 compared to Section 3.3.

I think the conclusion could be enriched by commenting in a general way on what are the conclusions of their work. How can they can link the different problems and models conceptually.

These comments should be considered as a way to enrich the presentation of this work of very high quality, which opens a novel way to look at uncertainty and how to deal with it. It should be noted that the approaches presented in this paper are useful in other problem settings also.

Rejoinder

First of all we would like to thank all the discussants for their comments and suggestions that we appreciate.

To the remarks from prof. Monique Guignard

On Question #1. The discussant addresses one of the most important issues in stochastic programming, namely, the generation of a set of enough representative scenarios and their probabilities. She offers a very comprehensive set of references that deal with the issue. We are not specialists on the matter and little more we can add, except to remark that there are approaches, see [26] as one example, that allow to generate thousands of scenarios to provide approximate solutions where state-of-the art optimization engines cannot provide any.

On Question #2. Effectively, in most of the papers dealing with the computational aspects of algorithmic proposals, one finds statements related to one approach "outperforms" another. In deterministic environments it is an easy task, the approach with a better objective function value is "better" than the other one. In stochastic environments it is not so easy. One approach can be better than the other one for one scenario but worse and much worse for another one. Most of the approaches in stochastic programming deal with two-stage problems. For these approaches the methodology for deciding what approach outperforms some other is simple. Here, the result of the stochastic approach, say RP, that provides a solution for the first and the second variables, can be compared with the average scenario solution. The value of the first variables obtained by the average scenario approach is simulated for each scenario to consider, and the expected result of using the average solution, say EEV [20] is obtained. And, then, the values RP and EEV can be compared.

A more difficult question is related to the value of the stochastic solution in multistage problems, and to what extend a solution "outperforms" another. An approach to the problem can be seen in Escudero et al. (2007), see below, where the definition of the bounds for the optimal value of the objective function is generalized to multistage stochastic problems. The definition of the parameters EVPI=RP-WS and VSS=EEV-RP for the two stage problems [20], where WS is the expected value of the scenarios treated in an independent form, is extended to the multistage stochastic problem. It is proved in Escudero et al. (2007) a similar chain of inequalities as for two-stage environments, with the lower and upper bounds depending substantially on the structure of the problem.

On Question #3. Approximation algorithms are one of the future directions of research in stochastic programming, mainly for solving combinatorial problems of realistic size. The Fix-and-Relax Coordination (FRC) approach introduced in [7] and mentioned in Section 6 of the paper while dealing with the Stochastic Sequencing and Scheduling problem is a good example of approximation algorithms. Note how difficult it is to solve most of the combinatorial optimization problems, NP and, on the other hand, some of their parameters refer to a time horizon and, then, probably, are also uncertain.

To the remarks from prof. Gautam Mitra

We completely agree with the remarks of the discussant about the objective function. The expected value to optimize should be replaced most of the times by risk exposure measures, such as the mean-risk objective function. We agree to consider the risk exposure of the raw material supply disruption and prices volatility. Besides the excess probability measure [76], we suggest in the paper some other risk measures to use such as semi-deviations [66] and conditional value-at-risk [77]. Unfortunately, this type of measures requires extra 0-1 variables that sometimes can make impractical some of the current algorithms. However, it is important to continue working in that direction.

To the remarks from prof. Francisco J. Prieto

On comment #1. We agree that one of the important issues in today stochastic programming is the discussion about the two-stage setting versus the multi-stage setting. Most of the algorithmic approaches are related to the two-stage setting. It is partly due to the difficulty on tackling algorithms for problem solving in the multi-stage setting, partly due to the difficulty on estimating representative scenario trees. In our approach we preferred in all cases, but two, two-stage environments due to the real-life type of problems that we were studying where the scenario estimation is a hard problem. However, it is our opinion that it is more accurate to represent the uncertainty by multi-stage scenario trees. An exercise to be done is a computational comparison between two-stage and multi-stage settings for the same problem. In this way we could assess if two-stage approaches do “not compromise much of the quality of the solutions”; certainly, they present problem solving advantages.

On comment #2. The discussant’s observation is well taken. We agree that some of the uncertainties on today production planning setting are the unforeseen changes in capacity availability. In this regard, the parameters available “budget for plant generation / expansion”, “maximum number of products to be processed in the plants” and “maximum number of raw materials to be supplied by the vendors” as well as “maximum volume of raw materials” and “maximum volume of products to be processed by the plants” in Section 2 of the paper: Strategic Supply Chain Management

should have been considered as stochastic parameters. Moreover, we consider the available capacity of the resources as an uncertain parameter in the models presented in Sections 4, 5 and 6.

We agree with the discussant that special care has to be taken for considering low-probability extreme scenarios to occur. Certain types of scenario generation approaches consider them as outliers and, then, not worthy of consideration. We agree that importance sampling type of approaches, see Dantzig and Thapa (2003), helps to consider them. One of the future directions of research in stochastic programming is the dynamic scenario generation strategies in multi-stage settings. We agree with the discussant about the difficulty that the modification of the structure of the problem from iteration to iteration, has in multi-stage settings.

On comment #3. We agree that in manufacturing planning one of the considerations in the objective function should be a measure to reduce the impact of the delay on the satisfaction of the product demand and the tardiness (i.e., the delay on the project finishing) in sequencing and scheduling problems. The price to be paid is a possible increase in the number of 0-1 variables to consider, but it is worthy to try it.

Another relevant issue pointed out by the discussant, although beyond the scope of our paper, is the robustness of the solution. And, in particular, the treatment of measures to favour solutions that require small modifications between scenarios. It is another future direction of research.

On comment #4. Another very important issue is the relevance of futures and other financial instruments to hedge the solutions against the uncertainty in the parameters, mainly regarding the price volatility and delivery disruptions of the raw materials traded in open markets as it is pointed out by the discussant. Again, the possible price to be paid could be the increase in the number of 0-1 variables to consider. Precisely, we are currently working on a stochastic model for structuring bilateral trading (selling and purchasing) energy contract portfolios in competitive markets, where financial futures are implicitly considered.

To the remarks from prof. Andres Weintraub

We completely agree with the remarks of the discussant about the need to incorporate uncertainty in the models, in particular, for the strategic and tactical supply chain management, and sequencing and scheduling. We also prefer to represent the uncertainty by “thinking of scenarios and assigning probabilities to them”. We also agree on future research directions for analyzing the robustness of the decisions to the variability of the scenario weights.

According to the suggestions from the discussant we expanded Section 1 to explain our approach for using the non-anticipativity principle to handle the uncertainty in problems with 0-1variables.

After presenting each stochastic model we have added, based on his suggestion, some comments on the dimensions of the models and the performance of our approach Branch-and-Fix Coordination (BFC) [5]. Sometimes, in particular for the Stochastic Sequencing and Scheduling problem, an exact solution cannot be obtained for a practical solving of real-life problems. In this case, we proposed the heuristic FRC [7], which based on BFC, produces quasi-optimal solutions clearly without guaranteeing the optimality.

We give the appropriate references where the specialization of BFC and FRC are presented for each of the models discussed in the paper. The computational comparisons are performed against the plain using of state-of-the-art optimization engines and the scenario average approach (i.e., the using of the deterministic solution offered by the average of the different scenarios to consider).

The discussion on the reason for using the excess probabilities concept as a risk measure instead of using the expected value alone may require more space than allowed but, agreeing with the discussant, it reduces the risk (i.e., probability) of occurring scenarios whose objective function is greater (for a minimization) than a given non-desired threshold.

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Poverty measures and poverty orderings*

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Abstract

We examine the conditions under which unanimous poverty rankings of income distributions can be obtained for a general class of poverty indices. The "per-capita income gap" and the Shorrocks and Thon poverty measures are particular members of this class. The conditions of dominance are stated in terms of comparisons of the corresponding TIP curves and areas.

MSC: 91B82; 60E15

Keywords: Poverty measure; poverty ordering; TIP curve

1 Introduction

Following the publication of Sen's (1976) influential work on poverty measurement, much has been written on this topic and related issues. Because an important reason for measuring poverty is to make poverty comparisons, part of the literature on poverty measurement has developed by focusing on partial poverty orderings.

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Given the poverty line (that is, the income level below which one is considered poor), the simplest way of comparing two income distributions in terms of poverty is by comparing some associated poverty measure. However, the choice of a single measure can be arbitrary and, hence, so can the conclusions based on this measure. In addition, different measures may produce contradictory conclusions. As pointed out by various authors (see, for example, Atkinson (1970, 1987) and Foster (1984)), this arbitrariness can be reduced by using a class of poverty measures rather than a single measure. This approach yields partial orders, by making judgements only if all members of a wide class of measures lead to the same conclusion.

Several authors, including Atkinson (1970, 1987), Foster and Shorrocks (1988a, 1988b), Spencer and Fisher (1992), Howes (1993), Jenkins and Lambert (1993, 1997, 1998) and Zheng (1999) have examined the conditions under which unanimous poverty orderings of income random variables are implied by large classes of indices. A comprehensive review of this topic is given by Zheng (2000). If C denotes a class of poverty measures and $I(X,z) \in C$ indicates the degree of poverty associated with the income random variable, X, when the poverty line is at an income level $z > 0$, the results are usually of the form

$$I(X,z) \leq I(Y,z) \text{ for all } I \in C, \text{ for all } z \in \Theta \subseteq \mathbf{R}^+ \tag{1}$$

if and only if

$$X \prec_P Y$$

where $\prec_P$ denotes the ordering that is induced by some comparison principle, P. Because (1) yields a multitude of inequalities, the potential applications of these characterizations are obvious, particularly when $X \prec_P Y$ is easy to verify.

In this work, we consider a comparison principle P based on comparing TIP (Three I's of Poverty) curves and areas. The TIP curve is a graphical device (also called the cumulative poverty gap (CPG) curve or the poverty profile curve) due to Jenkins and Lambert (1997) (see also Spencer and Fisher (1992) and Shorrocks (1995)). In order to introduce this curve, let X be a non-negative income random variable with a distribution function, F, and let F^{-1} be the right continuous quantile function of F, which is defined by

$$F^{-1}(t) = \sup\{x : F(x) \leq t\}, \quad t \in [0,1].$$

Suppose that a poverty line is established at an income level $z > 0$. The proportion of poor people is denoted by r_z^X; that is,

$$r_z^X = \sup\{F(x) : x < z\}.$$

Let $X_z^* = \min\{X, z\}$ be the random variable, X, censored at z, with a distribution function, F_z. Its corresponding quantile function is F_z^{-1}, where

$$F_z^{-1}(t) = \begin{cases} F^{-1}(t) & \text{if} \quad t < r_z^X \\ z & \text{if} \quad t \geq r_z^X \end{cases},$$

for all $t \in [0, 1]$. The relative poverty gap associated with income $F^{-1}(t)$ is defined as

$$\frac{z - F_z^{-1}(t)}{z}$$

and the corresponding TIP curve (see Spencer and Fisher (1992), Shorrocks (1995) and Jenkins and Lambert (1998a)) is given by

$$G_X(p, z) = \int_0^p \left(z - F_z^{-1}(t)\right) dt, \quad p \in [0, 1].$$

The curve $G_X(p, z)$ is increasing and concave and begins at the origin and rises continuously over the interval $[0, r_z^X]$. At $p = r_z^X$ the curve becomes horizontal at a height equal to the mean poverty gap. As Jenkins and Lambert (1997) have pointed out, this curve summarizes three aspects of poverty: incidence, given by r_z^X; intensity, given by the height of the curve at $p = 1$; and inequality, represented by the degree of concavity of the non-horizontal section of the curve. Applications of this curve to the study of the evolution of poverty in Spain during the 1980s can be found in Del Río y Ruiz-Castillo (2001a, 2001b).

As shown by Jenkins and Lambert (1998a, 1998b), orderings of distributions by non-intersecting TIP curves correspond to unanimous orderings according to the class Γ of generalized poverty gap (GPG) poverty indices, which are increasing Schur-convex functions of absolute poverty gaps. Members of Γ satisfy the Focus, Monotonicity, Transfer, Symmetry and Replication invariance axioms (as defined, for example, by Foster 1984). However, it is well-known that TIP curves often intersect, so that clear rankings of income distributions would not be possible by simple TIP curve comparisons. Although, as shown by Jenkins and Lambert (1998a), unambiguous results are still possible when TIP curves cross once, little has been known about the exact ordering conditions when TIP curves present multiple crossings.

In this paper, we suggest a poverty comparison principle based on comparing TIP areas, which can be used when curves intersect more than once. The normative significance of using this comparison principle is analyzed in terms of a class of poverty indices, C, that are linear in incomes and given by the following functional forms:

$$I_X(\Phi, z) = \int_0^1 \left(\frac{z - F_z^{-1}(t)}{z}\right) d\Phi(t), \tag{2}$$

where the relative poverty gaps are weighted using a continuous probability distribution, Φ, with support $supp(\Phi) \subseteq [0,1]$ (the integral is interpreted in the Riemann–Stieltjes sense). The class, C, considered recently by Davidson and Duclos (2000), Duclos and Grégoire (2002) and Duclos and Araar (2006), is analogous to the class of linear inequality measures proposed by Mehran (1976) and contains some poverty measures that are well known from the literature. It includes the so-called "per-capita income gap" proposed by Foster et al. (1984) and is obtained when $\Phi(t)$ is the uniform distribution on $(0,1)$. The Thon (1979) and Shorrocks (1995) poverty indices are members of C, given that $\Phi(t) = 1-(1-t)^2$, and the general class of poverty indices proposed by Thon (1983) is also obtained from (2) by choosing

$$\Phi(t) = \frac{c^2}{4(c-1)} - \frac{1}{c-1}\left(\frac{c}{2} - t\right)^2, \; c > 2.$$

Hagenaars (1987) and Shorrocks (1998) also evaluate indices of the form (2) at the income distribution of a finite population.

The desirability of a poverty measure is evaluated by the axioms it satisfies. In this sense, it can be easily proven that each member $I_X(\Phi, z) \in C$ satisfies the following reasonable axioms: monotonicity ($I_X(\Phi, z)$ increases if a poor person's income decreases), scale invariance ($I_X(\Phi, z)$ is not affected if we multiply income and poverty line by a common factor $a > 0$), focus ($I_X(\Phi, z)$ is not affected by changes in nonpoor incomes) and symmetry ($I_X(\Phi, z)$ is not affected if two people switch their incomes). All these axioms are well-known in the literature and have been discussed thoroughly (see, for example, Foster (1984) and Zheng (2000)). In addition, as proved by Mehran (1976) in the context of income inequality, members of the class C_1 given by

$$C_1 = \{I(\Phi, z) \in C \text{ such that } \Phi \text{ is concave}\}$$

satisfy the Pigou-Dalton Principle of Transfers (any mean-preserving transfer from a poor person to a poorer person that leaves unchanged their relative rank in the distribution, must decrease poverty) and members of C_2, given by

$$C_2 = \{I(\Phi, z) \in C_1 \text{ such that } \phi \text{ is convex, where } \Phi'(t) = \phi(t) \text{ a.e.}\}.$$

satisfy the stronger Diminishing Transfer Principle, which requires that a small transfer from a poor person to a poorer person, with a given proportion of the population in between them, decreases poverty and the decrease is larger the poorer the recipient. In other words, the relative ethical weight assigned to the effect of income changes occurring at the bottom of the distribution is higher in C_2 than in C_1.

We prove in this paper that non-intersecting TIP curves principle is equivalent to unambiguous poverty ranking by all measures in C_1 (this result is well-known and it appears, for instance, in Duclos and Araar (2006)). In order to obtain unambiguous

poverty ranking by all measures in C_2, we use a weaker comparison principle based on comparing TIP areas. This weaker principle is, therefore, more sensitive to the distribution of income among the poorest.

The plan of the paper is as follows. In Section 2, we show that two income random variables can be unanimously ranked by all poverty indices in C with Φ concave if and only if their TIP curves do not intersect. In this section, we also provide a condition for stochastic equality of the censored random variables, X_z^* and Y_z^*, under the hypothesis of non-intersecting TIP curves. More precisely, we prove that, if the TIP curves do not intersect and if $I_X(\Phi, z) = I_Y(\Phi, z)$ for some strictly concave distribution function Φ, then X_z^* and Y_z^* are stochastically equal. Section 2 includes examples. In Section 3, we show that, when the TIP curves intersect, unambiguous rankings are still possible. In this case, the ordering condition is based on comparisons of the respective TIP areas. Section 4 contains concluding remarks.

2 Characterization in terms of TIP curves

Denote

$$C_1 = \{I(\Phi, z) \in C \text{ such that } \Phi \text{ is concave}\}.$$

The following result connects the unambiguous poverty ordering of two income random variables based on the class C_1 of poverty indices with the non-intersection of the corresponding TIP curves.

Theorem 1 *Let X and Y be two non-negative income random variables and let $z > 0$ be a fixed poverty line. Then,*

$$G_X(p, z) \leq G_Y(p, z) \text{ for all } p \in [0, 1] \tag{3}$$

if and only if

$$I_X(\Phi, z) \leq I_Y(\Phi, z), \text{ for all } I(\Phi, z) \in C_1. \tag{4}$$

Proof ($\Longrightarrow$) Let F and G be the distribution functions of X and Y, respectively, and let F^{-1} and G^{-1} be the corresponding quantile functions. Note that (2) can be written as

$$I_X(\Phi, z) = \int_0^{r_z^X} \left(\frac{z - F^{-1}(t)}{z}\right) d\Phi(t). \tag{5}$$

Integration by parts in (5) for Riemann–Stieltjes integrals, given that $\Phi(0) = 0$, yields

$$I_X(\Phi, z) = \frac{1}{z} \int_0^{r_z^X} \Phi(t)\, dF^{-1}(t) \tag{6}$$

and, analogously,

$$I_Y(\Phi, z) = \frac{1}{z} \int_0^{r_z^Y} \Phi(t)\, dG^{-1}(t). \tag{7}$$

On the other hand, condition (3) is equivalent to the condition

$$\int_0^p \frac{F_z^{-1}(t)}{z}\, dt \geq \int_0^p \frac{G_z^{-1}(t)}{z}\, dt, \text{ for all } p \in [0,1]. \tag{8}$$

Since the functions, $F_z^{-1}(t)/z$ and $G_z^{-1}(t)/z$, can be considered analogous to two distribution functions defined on $\left[0, r_z^X\right]$ and $\left[0, r_z^Y\right]$, respectively, it follows from Theorem 1.4.1 of Stoyan (1983) that (8) holds if and only if

$$\int_0^{r_z^X} \Phi(t)\, d\left[\frac{F_z^{-1}(t)}{z}\right] \leq \int_0^{r_z^Y} \Phi(t)\, d\left[\frac{G_z^{-1}(t)}{z}\right]$$

for all non-decreasing and concave functions, Φ, or, equivalently, if and only if

$$\frac{1}{z} \int_0^{r_z^X} \Phi(t)\, dF^{-1}(t) \leq \frac{1}{z} \int_0^{r_z^Y} \Phi(t)\, dG^{-1}(t) \tag{9}$$

for all non-decreasing and concave functions, Φ. Combining (9), (6) and (7) implies (4). ($\Longleftarrow$) For $p = 0$, (3) is obvious because $G_X(0, z) = G_Y(0, z) = 0$. Now, for each $p \in (0, 1]$, the distribution function defined by

$$\Phi_p(t) = \begin{cases} t/p & \text{if} \quad 0 \leq t < p \\ 1 & \text{if} \quad t \geq p \end{cases}$$

is concave. Hence,

$$I_X(\Phi_p, z) \leq I_Y(\Phi_p, z), \text{ for all } p \in (0, 1]. \tag{10}$$

Since $I_X(\Phi_p, z) = (pz)^{-1} G_X(p, z)$ and $I_Y(\Phi_p, z) = (pz)^{-1} G_Y(p, z)$, (3) follows directly from (10). □

Example 2 The Pareto income distribution has become one of the most popular and widely used models for empirical income data. Thus, it would be interesting to compare the TIP curves of such distributions in terms of their parameters. In this way, we can

obtain their unanimous poverty rankings based on the class C_1. The corresponding distribution function of a Pareto random variable with parameters ε and α is

$$F(x) = 1 - \left(\frac{\varepsilon}{x}\right)^{\alpha}, \quad x \geq \varepsilon, \quad \alpha > 0, \quad \varepsilon > 0.$$

From straightforward computation, the corresponding TIP curve is

$$G(p,z) = \begin{cases} zp + \dfrac{\varepsilon\alpha}{(\alpha-1)}\left((1-p)^{\frac{\alpha-1}{\alpha}} - 1\right), & \text{if } 0 \leq p < 1 - \left(\dfrac{\varepsilon}{z}\right)^{\alpha} \\ z + \dfrac{z}{\alpha-1}\left(\dfrac{\varepsilon}{z}\right)^{\alpha} - \dfrac{\varepsilon\alpha}{(\alpha-1)}, & \text{if } 1 - \left(\dfrac{\varepsilon}{z}\right)^{\alpha} \leq p \leq 1. \end{cases} \tag{11}$$

Let $X_i (i = 1, 2)$ be two Pareto variables with parameters $(\varepsilon_i, \alpha_i)$. Let $z > 0$ be a fixed poverty line. If $\alpha_1 = \alpha_2 > 1$ and $\varepsilon_1 \leq \varepsilon_2$, it can be easily verified that $G_{X_2}(t; z) \leq G_{X_1}(t; z)$ for $0 \leq t \leq 1$. Using Theorem 1, we have $I_{X_2}(\Phi, z) \leq I_{X_1}(\Phi, z)$, for all $I(\Phi, z) \in C_1$. Note that the distribution with a lower minimum income implies higher poverty according to all members of C_1. If we fixed $\varepsilon_1 = \varepsilon_2 > 0$ and $\alpha_1 \geq \alpha_2 > 1$, we reach the same conclusion. Since $E[X_i] = \alpha_i\varepsilon_i/(\alpha_i - 1)$, the distribution with the lower average value implies higher poverty according to all members of C_1.

If X and Y are income random variables such that $G_X(p, z) \leq G_Y(p, z)$ for all $p \in [0, 1]$, it is interesting and natural to ask what simple sufficient condition would imply the stochastic equivalence of their corresponding censored random variables, X_z^* and Y_z^*. In the existing literature, conditions implying equality in the distributions of random variables under various stochastic orderings can be found in Baccelli and Makowski (1989), Bhattacharjee and Sethuraman (1990), Scarsini and Shaked (1990), Bhattacharjee (1991), Jun (1994), Li and Zhu (1994), Cai and Wu (1997), Denuit et al. (2000) and Bhattacharjee and Bhattacharya (2000). In this tradition, we obtain the following theorem.

Theorem 3 *Let X and Y be two non-negative income random variables and let $z > 0$ be a fixed poverty line. If*

$$G_X(p, z) \leq G_Y(p, z) \text{ for all } p \in [0, 1] \tag{12}$$

and if

$$I_X(\Phi, z) = I_Y(\Phi, z) \tag{13}$$

for some strictly concave distribution function, Φ, then the censored random variables, X_z^* and Y_z^*, have the same distribution.

Proof. Suppose that Φ is a strictly concave distribution function. Then, there exists a strictly decreasing, non-negative and integrable function, φ, such that

$$\Phi(t) = \int_0^t \varphi(u)\, du,\ t \in [0,1)$$

(see Zygmund, 1959). Using the properties of the Riemann–Stieltjes integral, we have

$$z \cdot I_X(\Phi, z) = \int_0^1 \left(z - F_z^{-1}(t)\right) d\Phi(t) = \int_0^1 \varphi(t)\, dG_X(t,z). \tag{14}$$

Partial integration of (14) and $G_X(0,z) = 0$ reveals that

$$z \cdot I_X(\Phi, z) = \varphi(1) G_X(1,z) - \int_0^1 G_X(t,z)\, d\varphi(t). \tag{15}$$

Analogously, it can be shown that

$$z \cdot I_Y(\Phi, z) = \varphi(1) G_Y(1,z) - \int_0^1 G_Y(t,z)\, d\varphi(t). \tag{16}$$

Combining (13), (15) and (16) yields

$$\varphi(1)\left[G_Y(1,z) - G_X(1,z)\right] - \int_0^1 \left[G_Y(t,z) - G_X(t,z)\right] d\varphi(t) = 0. \tag{17}$$

Since $G_X(p,z) \le G_Y(p,z)$ for all $p \in [0,1]$, $\varphi(1) \ge 0$ and

$$d\varphi(t) < 0, \tag{18}$$

from (17), it follows that

$$\int_0^1 \left[G_Y(t,z) - G_X(t,z)\right] d\varphi(t) = 0. \tag{19}$$

Given(12), the continuity of the TIP curves and (18), from (19), we obtain

$$G_Y(t,z) = G_X(t,z) \text{ for all } t \in [0,1]. \tag{20}$$

Taking the derivative completes the proof. □

Example 4 Let X and Y be two non-negative income random variables and let $z > 0$ be a fixed poverty line. If $G_X(p,z) \le G_Y(p,z)$ for all $p \in [0,1]$ and if $T(X,z) = T(Y,z)$ (where $T(\cdot,z)$ denotes Thon's poverty index), then X_z^* and Y_z^* have the same distribution. In particular, $I_X(\Phi,z) = I_Y(\Phi,z)$ for all $I(\Phi,z) \in C$.

3 Characterization in terms of TIP areas

We have shown in Theorem 1 that non-intersecting TIP curves are equivalent to a unanimous poverty ordering by all indices in C_1. However, in practical applications, TIP curves often intersect. In this case, we can still order the distributions by a subclass of C_1. Taking into account that, for a concave Φ, its derivative, Φ', exists (except possibly at a countable number of points), we consider the class, C_2, in which functionals are of the form of (2), where Φ is concave and differentiable almost everywhere (a.e.) with a convex derivative; that is,

$$C_2 = \{I(\Phi, z) \in C_1 \text{ such that } \phi \text{ is convex, where } \Phi'(t) = \phi(t) \text{ a.e.}\}.$$

Theorem 5 *Let X and Y be two non-negative income random variables and let $z > 0$ be a fixed poverty line. Then,*

$$\int_0^p G_X(t,z)\,dt \le \int_0^p G_Y(t,z)\,dt, \text{ for all } p \in [0,1] \text{ and } G_X(1,z) \le G_Y(1,z) \tag{21}$$

if and only if

$$I_X(\Phi, z) \le I_Y(\Phi, z), \quad \text{for all} \quad I(\Phi, z) \in C_2. \tag{22}$$

Proof. ($\Rightarrow$) Let $I(\Phi, z) \in C_2$. Suppose that $\Phi' = \phi$ a.e. for some non-increasing convex and non-negative function, ϕ. Then, there exists a non-increasing non-negative function, φ, such that

$$\phi(t) - \phi(1) = \int_t^1 \varphi(p)\,dp, \quad p \in (0,1].$$

Using integration by parts, it follows, for $p \in (0,1]$ that

$$\phi(t) = \phi(1) + (1-t)\varphi(1) - \int_0^1 (p-t)^+\,d\varphi(p). \tag{23}$$

Because of the properties of the Riemann–Stieltjes integral, we can write

$$z \cdot I_X(\Phi, z) = \int_0^1 \left(z - F^{-1}(t)\right) d\Phi(t) = \int_0^1 \phi(t)\,dG_X(t,z),$$

and using (23), we obtain

$$z \cdot I_X(\Phi, z) = \int_0^1 \left[\phi(1) + (1-t)\varphi(1) - \int_0^1 (p-t)^+\,d\varphi(p)\right] dG_X(t,z). \tag{24}$$

The additivity properties of integrals, Fubini's Theorem and $G_X(0,z) = 0$ imply that (24) can be rewritten as follows:

$$\phi(1)G_X(1,z) + \varphi(1)\int_0^1 (1-t)\,dG_X(t,z) - \int_0^1\int_0^p (p-t)\,dG_X(t,z)\,d\varphi(p). \qquad (25)$$

Using integration by parts, for each p, we obtain

$$\int_0^p (p-t)\,dG_X(t,z) = \int_0^p G_X(t,z)\,dt,$$

which, when combined with (25), implies

$$z\cdot I_X(\Phi,z) = \phi(1)G_X(1,z) + \varphi(1)\int_0^1 G_X(t,z)\,dt - \int_0^1\int_0^p G_X(t,z)\,dt\,d\varphi(p).$$

We complete the proof by noting that $\phi(1) \geq 0$, $\varphi(1) \geq 0$, $d\varphi(p) \leq 0$ and (21).

($\Leftarrow$) The condition given in (22) implies $G_X(1,z) \leq G_Y(1,z)$ when $\Phi(t)$ is a uniform distribution on $(0,1)$.

For $p = 0$, it is obvious that the first condition in (21) is satisfied. Now, for each $p \in (0,1]$, the following distribution function in $[0,1]$ is concave and has a convex derivative:

$$\Phi_p(t) = \begin{cases} (2pt - t^2)/p^2 & \text{if} \quad 0 \leq t < p \\ 1 & \text{if} \quad t \geq p \end{cases}.$$

Hence, it follows that

$$I_X(\Phi_p, z) \leq I_Y(\Phi_p, z), \text{ for all } p \in (0,1].$$

Integration by parts leads to

$$I_X(\Phi_p, z) = \frac{2}{zp^2}\int_0^p G_X(t;z)\,dt,$$

and the proof is complete. □

4 Concluding remarks

In this paper, we have characterized the comparisons of TIP curves in terms of a class C_1 of linear poverty measures. When TIP curves intersect (possibly more than once) we have shown that unambiguous poverty orderings are still possible, by focusing on

a more restricted class $C_2 \subset C_1$. The criterion, then, is to compare the underlying TIP areas. Because of the axioms that the members of this class must fulfill, it must be the case that, in order to use this criteria, decision-makers should be ready to assume a larger sensitivity of poverty measures to the distribution of income among the poorest.

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Bayesian joint modelling of the mean and covariance structures for normal longitudinal data

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Abstract

We consider the joint modelling of the mean and covariance structures for the general antedependence model, estimating their parameters and the innovation variances in a longitudinal data context. We propose a new and computationally efficient classic estimation method based on the Fisher scoring algorithm to obtain the maximum likelihood estimates of the parameters. In addition, we also propose a new and innovative Bayesian methodology based on the Gibbs sampling, properly adapted for longitudinal data analysis, a methodology that considers linear mean structures and unrestricted covariance structures for normal longitudinal data. We illustrate the proposed methodology and study its strengths and weaknesses by analyzing two examples, the race and the cattle data sets.

MSC: 62F15; 62J05; 62F10; 62P10

Keywords: Antedependence models; Bayes estimation; Fisher scoring; Gibbs sampling

1 Introduction

Continuous longitudinal data consist of repeated measurements on the same subject over time. These measurements are typically correlated and there have been several proposals in the literature to handle stationary or nonstationary correlations and variances, as well as balanced or unbalanced longitudinal data (see, e.g., Laird and Ware, 1982; Diggle *et al.*, 1994 or Zimmerman and Núñez-Antón, 2001).

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In the context of the parametric multivariate regression model for longitudinal data and under normality, the response variable for each of the m experimental units under study, each having n observations over time, is denoted by $\mathbf{Y}_i = (Y_{i1}, \ldots, Y_{in})'$, $i = 1, \ldots, m$. In this way, the $nm \times 1$ response vector $\mathbf{Y} = (\mathbf{Y}_1, \ldots, \mathbf{Y}_m)'$ contains the responses for all subjects under study, and it is assumed that the $\mathbf{Y}_i$'s are independently normally distributed as $N(\boldsymbol{\mu}, \Sigma_i = \sigma^2 \mathbf{I}_n)$, with $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_n)' = \mathbf{X}\boldsymbol{\beta}$ and $\mathbf{I}_n$ being the identity matrix of order n. Here, X is the $n \times p$ design matrix containing the set of explanatory variables, and $\boldsymbol{\beta}$ is the set of mean parameters, so that $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_p)'$. This model can be formally written as

$$\mathbf{Y}_i = \boldsymbol{\mu} + \boldsymbol{\epsilon}_i, \text{ with } \boldsymbol{\epsilon}_i \sim N(\mathbf{0}, \Sigma_i = \sigma^2 \mathbf{I}_n), \tag{1}$$

As is well known, this model assumes that the errors are independently and normally distributed with mean zero and unknown constant variance σ^2. Under the model above, we have that $E(\mathbf{Y}) = \boldsymbol{\mu}^* = (\boldsymbol{\mu}, \ldots, \boldsymbol{\mu})'$ and that $\Sigma_{\mathbf{Y}}$ is a block-diagonal matrix with diagonal matrix elements given by $\Sigma_i = \sigma^2 \mathbf{I}_n$, $i = 1, \ldots, m$.

If ϵ_{ij} and ϵ_{ik}, $j \neq k$, $i = 1, \ldots, m$, are not independent, then $Var(\boldsymbol{\epsilon}_i) = \Sigma_i$ is no longer a diagonal matrix and it would be necessary to model and estimate the off-diagonal elements of the covariance matrix. This modelling approach usually requires to impose some constraints on the elements of Σ_i to guarantee its positive definiteness. For example, in stationary Gaussian processes, such as the ones used in Geostatistics, the covariance between two observations is explicitly determined by their correlation function. More specifically, it is modelled as a function of the (Euclidean) distance between these two observations. Moreover, and given that some of the properties of this function are imposed by its spatial structure, only correlation functions belonging to the families where these requirements hold can be considered (see, e.g., Diggle and Verbyla, 1998, or Stein, 1999).

Longitudinal data typically consist of several measurements taken over time in each of the experimental units in the sample. It falls into the framework of correlated observations on the same subject and/or experimental unit, and it requires the specification and estimation of both the mean and the covariance structures. Most of the parametric approaches have concentrated on normal linear models (see, e.g., Pourahmadi, 1999 and 2000, or Zimmerman and Núñez-Antón, 2001). A central idea to be able to efficiently estimate the covariance matrix was first introduced by Macchiavelli and Arnold (1994) and Macchiavelli and Moser (1997) and it was based on its Cholesky decomposition. This approach has been used for several joint modelling proposals for the mean and covariance structures in the context of longitudinal data (see, e.g., Pourahmadi, 1999 and 2000, Pan and MacKenzie, 2003, 2006 and 2007 or Pan and Ye, 2006). Zimmerman and Núñez-Antón (1997) and Zimmerman, Núñez-Antón and El Barmi (1998) also proposed a joint modelling of the mean and covariance structures, and Núñez-Antón and Zimmerman (2000) addressed the possibility of having random coefficients and other alternative nonstationary models in a joint modelling proposal for

the mean and covariance structures in the context of longitudinal data. In addition, there have been only a few proposals within the Bayesian framework (see, e.g., Cepeda, 2001, Cepeda and Gamerman, 2000 and 2004, Daniels and Pourahmadi, 2002, or Pourahmadi and Daniels, 2002) and all of them proposed specific and restricted parametric structures for the mean, the innovation variances and the autoregressive parameters in the model. Cepeda and Gamerman (2000) proposed a Bayesian methodology for modeling mean and variance heterogeneity, using normal prior distributions for both the mean and variance parameters in the regression model. Cepeda (2001), also using normal prior distributions, extended this methodology to allow for a joint modelling of the mean and covariance structures. These latter results are included in Cepeda and Gamerman (2004). Independently, Daniels and Pourahmadi (2002) and Pourahmadi and Daniels (2002), also proposed the use of normal prior distributions for both the mean and covariance parameters, but they did not include any explicit algorithm to fit the joint mean and covariance model and use a data set (Pourahmadi and Daniels, 2002) and simulations (Daniels and Pourahmadi, 2002) to illustrate their proposals. Moreover, their proposals focused on modelling the covariance structure and did not include simulations or applications where there was a joint modelling approach proposal for the mean and covariance structure. In this paper, we consider the general antedependence model (Gabriel, 1962, Macchiavelli and Arnold, 1994, or Zimmerman and Núñez-Antón, 1997), and propose a joint modelling approach for the mean and covariance structures, estimating the mean and autoregressive parameters, and the innovation variances in the longitudinal data context. This general model does not impose any specific or restricted parametric structure on the innovation variances and autoregressive parameters, as was the case in previous proposal. We initially consider a new and computationally efficient classical estimation algorithm based on the Fisher scoring algorithm to obtain the estimators of the parameters. This proposal is very convenient and appealing in many cases, especially in the ones where the number of observational units in the study is large, such as in the examples used here to illustrate our proposals (i.e., the race data and the cattle data). In these cases there is a better agreement between sample regressograms and fitted autoregressive parameters and innovation variances, resulting in a better estimation of the parameters in the mean structure. In addition, we also propose a new and innovative Bayesian methodology based on the Gibbs Sampling (Geman and Geman, 1984), properly adapted for longitudinal data analysis, a methodology that considers linear mean structures and unrestricted covariance structures for normal longitudinal data. This methodology allows the researcher to be able to incorporate relevant prior information in the data analysis, as well as to obtain the parameter estimates when the number of observational units in the study is small. In this specific case, we can also estimate credibility intervals for the parameters of interest in the model.

We illustrate the proposed methodology and study its relative strengths and weaknesses when compared to other proposed methods by analyzing two examples,

the race and the cattle data sets. Moreover and for the cases where no prior information is available to be implemented in our Bayesian methodology proposal, we also include the methodology for the possibility of using noninformative priors. The comparison of the results obtained with the classic methodology proposal and with the noninformative priors Bayesian proposal allows us to be able to evaluate their efficiency. As will be seen in the examples presented here, the estimates obtained under these two alternative proposals are very similar.

The paper is organized as follows. Section 2 introduces the general model used in the context of longitudinal data analysis. In Section 3 we introduce the proposed classic methodology for this type of data. Section 4 includes the proposed Bayesian methodology, which is finally applied to the race and cattle data sets in Section 5. Section 6 includes some general conclusions.

2 The General Model

As we have already indicated, one of the main issues in the modelling approach we propose requires $Var(\boldsymbol{\epsilon}_i) = \Sigma_i$, $i = 1, \ldots, m$, to be nonnegative definite so that its inverse can be efficiently calculated and, in addition, it should also be allowed to have a general form so that it is not too restrictive. Pourahmadi (1999) proposed a general approach where all of these conditions hold. Note that, since observations on different subjects are assumed to be independent and, thus, only within-subject covariance structures need to be considered, we suppress the subscript i (identifying the subjects) when describing these structures. More specifically and following the general model settings presented in Cepeda and Gamerman (2004), let us consider the general antedependence model (Gabriel, 1962 or Zimmerman and Núñez-Antón, 1997), where for a given individual having n observations we have that:

$$Y_{ij} - \mu_j = \sum_{k=1}^{j-1} \phi_{jk}(Y_{ik} - \mu_k) + \nu_j, \qquad \nu_j \sim N(0, \sigma_j^2), \qquad (2)$$
$$i = 1, \ldots, m, \qquad j = 1, \ldots, n,$$

and that $E(Y_{ij}) = \mu_j$, where μ_j is assumed to be a linear function of the vector of parameters $\boldsymbol{\beta}$. In addition, the ν_j's are assumed to be mutually independent and, by convention, we set all empty sums to zero, that is $\sum_{k=1}^{0} z_k = 0$. In this way, (2) can be rewritten in matrix form as

$$\boldsymbol{\nu} = \mathbf{T}(\mathbf{Y}_i - \boldsymbol{\mu}), \boldsymbol{\nu} \sim N(\mathbf{0}, \mathbf{D}), \text{ and } \mathbf{D} = diag(\sigma_1^2, \ldots, \sigma_n^2), \qquad (3)$$

where $\boldsymbol{\nu} = (\nu_1, \ldots, \nu_n)'$, $\boldsymbol{\mu} = (\mu_1, \ldots, \mu_n)'$, $\mathbf{T} = \{t_{ij}\}_{i=1,\ldots,n}^{j=1,\ldots,n}$, with

$$t_{ij} = \begin{cases} 1 & \text{if } j = i \\ -\phi_{ij} & \text{if } j < i \\ 0 & \text{otherwise} \end{cases}$$

and

$$Var(\boldsymbol{\nu}) = \mathbf{D} = \mathbf{T}\, Var(\mathbf{Y}_i - \boldsymbol{\mu})\, \mathbf{T}' = \mathbf{T}\Sigma_i\mathbf{T}' = \mathbf{T}\Sigma\mathbf{T}' \tag{4}$$

As a direct result of equations (3) and (4), Σ can be indirectly calculated by computing $\mathbf{D}$ and $\mathbf{T}$. In addition, we should point out that the triangular decomposition in equation (4) is unique. Moreover, given that Σ is a symmetric matrix if and only if there exists a unique lower triangular matrix $\mathbf{T}$, with ones in the diagonal, and a unique diagonal matrix $\mathbf{D}$ with positive diagonal entries such that $\mathbf{T}\Sigma\mathbf{T}' = \mathbf{D}$, we also have that Σ is positive definite (Pourahmadi, 1999). Therefore, from (3), we have that

$$\tilde{\mathbf{Y}}_i = (\mathbf{I}_n - \mathbf{T})\tilde{\mathbf{Y}}_i + \boldsymbol{\nu} = \Phi\tilde{\mathbf{Y}}_i + \boldsymbol{\nu},\ i = 1, \ldots, m, \tag{5}$$

where $\tilde{\mathbf{Y}}_i = (\mathbf{Y}_i - \boldsymbol{\mu})$, and the k-th row of the $n \times n$ matrix $\Phi = (\mathbf{I}_n - \mathbf{T})$ contains $[n - (k-1)]$ zeroes and the $(k-1)$ components of the autoregressive parameter vector $\boldsymbol{\phi}_k = (\phi_{k1}, \ldots, \phi_{k,k-1})'$, $k = 2, \ldots, n$.

3 Classic Methodology

Under the assumption that $\mathbf{Y}_i = (Y_{i1}, \ldots, Y_{in})' \sim$ *i.i.d.* $N(\boldsymbol{\mu}, \Sigma)$, $i = 1, \ldots, m$, where $\boldsymbol{\mu}$ is assumed to depend linearly on $\boldsymbol{\beta}$ (i.e., $\boldsymbol{\mu} = \mathbf{X}\boldsymbol{\beta}$, $\mathbf{X}$ being the $n \times p$ design matrix), and $\Sigma^{-1} = \mathbf{T}'\mathbf{D}^{-1}\mathbf{T}$, the likelihood function is given by

$$L(\boldsymbol{\beta}, \Phi, \mathbf{D}|\mathbf{Y}) \propto |\mathbf{D}|^{-m/2} \exp\left\{-\frac{1}{2}(\mathbf{Y} - \boldsymbol{\mu}^*)'\Sigma_{\mathbf{Y}}^{-1}(\mathbf{Y} - \boldsymbol{\mu}^*)\right\},$$

where $\mathbf{Y} = (\mathbf{Y}_1, \ldots, \mathbf{Y}_m)' \sim N(\boldsymbol{\mu}^*, \Sigma_{\mathbf{Y}})$ and $|\Sigma| = |\mathbf{T}'|\,|\mathbf{D}|\,|\mathbf{T}| = |\mathbf{D}|$. Note that in the equation above, $\boldsymbol{\mu}^* = (E(\mathbf{Y}_1), \ldots, E(\mathbf{Y}_m))' = (\boldsymbol{\mu}, \ldots, \boldsymbol{\mu})'$ and $\Sigma_{\mathbf{Y}}$ is a block diagonal matrix with diagonal matrix elements given by Σ, so that $\Sigma_{\mathbf{Y}}^{-1}$ is a block diagonal matrix with diagonal matrix elements given by $\Sigma^{-1} = \mathbf{T}'\mathbf{D}^{-1}\mathbf{T}$.

Therefore, the log-likelihood function can be written as $\ell(\boldsymbol{\beta}, \Phi, \mathbf{D}|\mathbf{Y}) = \log L(\boldsymbol{\beta}, \Phi, \mathbf{D}|\mathbf{Y}) \propto -m \log|\mathbf{D}| - (\mathbf{Y} - \boldsymbol{\mu}^*)'\Sigma_{\mathbf{Y}}^{-1}(\mathbf{Y} - \boldsymbol{\mu}^*)$, so that the components of the corresponding score function are given by

$$\begin{aligned}\frac{\partial \ell}{\partial \boldsymbol{\beta}} &= -\mathbf{X}^{*\prime}\Sigma_{\mathbf{Y}}^{-1}(\mathbf{Y}-\mathbf{X}^{*}\boldsymbol{\beta}) \\ \frac{\partial \ell}{\partial \phi_{ij}} &= -\frac{1}{2}(\mathbf{Y}-\mathbf{X}^{*}\boldsymbol{\beta})'\left(\frac{\partial \Sigma_{\mathbf{Y}}^{-1}}{\partial \phi_{ij}}\right)(\mathbf{Y}-\mathbf{X}^{*}\boldsymbol{\beta}) \\ & \quad (i=1,\ldots,n,\ j=1,\ldots,i-1),\end{aligned}$$

where $\mathbf{X}^{*} = (X',\ldots,X')'$ is the $nm \times p$ design matrix. Thus, we have that

$$\begin{aligned}I_{\boldsymbol{\beta},\phi} &= E\left(\frac{\partial^2 \ell}{\partial \boldsymbol{\beta}\partial\phi}\right) = 0 \\ I_{\boldsymbol{\beta},\sigma^2} &= E\left(\frac{\partial^2 \ell}{\partial \boldsymbol{\beta}\partial\sigma^2}\right) = 0\end{aligned}$$

Now, given that the log-likelihood function can be written as $\ell = \log L \propto -m\log|\mathbf{D}| - \frac{1}{\sigma_1^2}\mathbf{Y}_1^{*\prime}\mathbf{Y}_1^{*} - \cdots - \frac{1}{\sigma_n^2}(\mathbf{Y}_n^{*}-\tilde{\boldsymbol{\mu}}_n)(\mathbf{Y}_n^{*}-\tilde{\boldsymbol{\mu}}_n)$, where $\mathbf{Y}_1^{*}$ is the m-dimensional vector with i-th component given by $(Y_{i1}-\mu_1)$, $\mathbf{Y}_k^{*}$ $(k=2,\ldots,n)$ is the m-dimensional vector with i-th component given by $(Y_{ik}-\mu_k)$, and $\tilde{\boldsymbol{\mu}}_k$, $k=2,\ldots,n$, is the m-dimensional vector with i-th component given by $\phi_{k1}(Y_{i1}-\mu_1)+\cdots+\phi_{k,k-1}(Y_{i,k-1}-\mu_{k-1})$, we can write

$$\begin{aligned}\frac{\partial \ell}{\partial \mu_1} &= \frac{1}{\sigma_1^2}\sum_{i=1}^{m}(Y_{i1}-\mu_1) \\ \frac{\partial \ell}{\partial \sigma_1^2} &= -\frac{m}{2\sigma_1^2}+\frac{1}{2\sigma_1^4}\mathbf{Y}_1^{*\prime}\mathbf{Y}_1^{*}\end{aligned}$$

Therefore, the maximum likelihood estimators of μ_1 and σ_1^2 are given by $\hat{\mu}_1 = \frac{1}{m}\sum_{i=1}^{m} Y_{i1}$ and $\hat{\sigma}_1^2 = \frac{1}{m}\mathbf{Y}_1^{*\prime}\mathbf{Y}_1^{*}$. Now, for $\boldsymbol{\phi}_k = (\phi_{k1},\ldots,\phi_{k,k-1})$ and σ_k^2, $k=2,\ldots,n$, and if we let $\tilde{\mathbf{X}}_k$ be an $m\times(k-1)$ matrix with columns given by $\mathbf{Y}_1^{*},\ldots,\mathbf{Y}_{k-1}^{*}$, we have that

$$\begin{aligned}\frac{\partial \ell}{\partial \boldsymbol{\phi}_k} &= \frac{1}{\sigma_1^2}\tilde{\mathbf{X}}_k'(\mathbf{Y}_k^{*}-\tilde{\mathbf{X}}_k\boldsymbol{\phi}_k) \\ \frac{\partial \ell}{\partial \sigma_k^2} &= -\frac{m}{2\sigma_k^2}+\frac{1}{2\sigma_k^4}(\mathbf{Y}_k^{*}-\tilde{\boldsymbol{\mu}}_k)'(\mathbf{Y}_k^{*}-\tilde{\boldsymbol{\mu}}_k)\end{aligned}$$

Thus, the maximum likelihood estimators of $\boldsymbol{\phi}_k$ and σ_k^2 $(k=2,\ldots,n)$ are given by

$$\begin{aligned}\hat{\boldsymbol{\phi}}_k &= (\tilde{\mathbf{X}}_k'\tilde{\mathbf{X}}_k)^{-1}(\tilde{\mathbf{X}}_k'\mathbf{Y}_k^{*}) \\ \hat{\sigma}_k^2 &= \frac{1}{m}(\mathbf{Y}_k^{*}-\tilde{\boldsymbol{\mu}}_k)'(\mathbf{Y}_k^{*}-\tilde{\boldsymbol{\mu}}_k)\end{aligned} \tag{6}$$

The steps of the algorithm used to obtain the maximum likelihood estimators of both the mean and variance parameters follow:

1. Set some arbitrary initial values for $\boldsymbol{\phi}_k$ and positive initial values for σ_k^2, $k = 1, \ldots, n$.
2. Compute Σ and update $\boldsymbol{\beta}$ by using $\dfrac{\partial \ell(\boldsymbol{\beta}, \Phi, \mathbf{D}|\mathbf{Y})}{\partial \boldsymbol{\beta}} = 0$.
3. Update $\boldsymbol{\phi}_k$ and σ_k^2, by solving the equations $\dfrac{\partial \ell(\boldsymbol{\beta}, \Phi, \mathbf{D}|\mathbf{Y})}{\partial \boldsymbol{\phi}_k} = 0$ and $\dfrac{\partial \ell(\boldsymbol{\beta}, \Phi, \mathbf{D}|\mathbf{Y})}{\partial \sigma_k^2} = 0$, $k = 1, \ldots, n$.
4. Repeat steps 2 and 3 until convergence.

4 Bayesian Methodology

As in the classic approach, we also assume that $\mathbf{Y}_i = (Y_{i1}, \ldots, Y_{in})'$ *i.i.d.* $\sim N(\boldsymbol{\mu}, \Sigma)$, $i = 1, \ldots, m$, where $\boldsymbol{\mu}$ is assumed to depend linearly on $\boldsymbol{\beta}$, and $\Sigma^{-1} = \mathbf{T}' \mathbf{D}^{-1} \mathbf{T}$. Therefore, the likelihood function is given by

$$L(\boldsymbol{\beta}, \Phi, \mathbf{D}|\mathbf{Y}) \propto |\mathbf{D}|^{-m/2} \exp\left\{-\frac{1}{2}(\mathbf{Y} - \boldsymbol{\mu}^*)' \Sigma_{\mathbf{Y}}^{-1} (\mathbf{Y} - \boldsymbol{\mu}^*)\right\},$$

where $\mathbf{Y} = (\mathbf{Y}_1, \ldots, \mathbf{Y}_m)'$, $|\Sigma| = |\mathbf{T}'|\,|\mathbf{D}|\,|\mathbf{T}| = |\mathbf{D}|$ and $\Phi = (\mathbf{I}_n - \mathbf{T})$.

If we now let $\boldsymbol{\theta} = (\boldsymbol{\beta}, \Phi, \mathbf{D})'$, under the Bayesian approach and in order to obtain the posterior distribution for the parameters, we need to assume a prior distribution $P(\boldsymbol{\theta})$ for $\boldsymbol{\theta}$. Without loss of generality and for simplicity, we assume independent prior distributions such that $\boldsymbol{\beta} \sim N(\mathbf{b}_0, \mathbf{B})$, $\boldsymbol{\phi}_k \sim N(\mathbf{l}_{0k}, \Sigma_{\boldsymbol{\phi}_k})$, $\psi_1 = 1/\sigma_1^2 \sim G(\alpha_1, \lambda_1)$ and $\psi_k = 1/\sigma_k^2 \sim G(\alpha_k, \lambda_k)$ $(k = 2, \ldots, n)$, where $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_n)'$, $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_n)'$, $\Psi = (\psi_1, \ldots, \psi_n)'$, and $G(r, s)$, represents the gamma distribution with parameters $r > 0$ and $s > 0$. As usual, another possibility for the prior distribution for $\boldsymbol{\theta}$ could be to assume a noninformative prior distribution such as, for example, assume Jeffreys prior distributions.

From Bayes' theorem, the posterior conditional distribution for $\boldsymbol{\beta}$, $\pi_{\boldsymbol{\beta}} = \pi(\boldsymbol{\beta}|\Phi, \Psi, \mathbf{Y})$, is given by

$$\begin{aligned} \pi(\boldsymbol{\beta}|\Phi, \Psi, \mathbf{Y}) &\propto \exp\left\{-\frac{1}{2}(\mathbf{Y} - \mathbf{X}^*\boldsymbol{\beta})' \Sigma_{\mathbf{Y}}^{-1} (\mathbf{Y} - \mathbf{X}^*\boldsymbol{\beta}) - \frac{1}{2}(\boldsymbol{\beta} - \mathbf{b}_0)' \mathbf{B}^{-1} (\boldsymbol{\beta} - \mathbf{b}_0)\right\} \\ &\propto \exp\left\{-\frac{1}{2}(\boldsymbol{\beta} - \mathbf{b}^*)' \mathbf{B}^{*-1} (\boldsymbol{\beta} - \mathbf{b}^*)\right\}, \end{aligned} \tag{7}$$

where $\mathbf{b}^* = \mathbf{B}^*(\mathbf{B}^{-1}\mathbf{b}_0 + \mathbf{X}^{*\prime}\Sigma_{\mathbf{Y}}^{-1}\mathbf{Y})$ and $\mathbf{B}^* = (\mathbf{B}^{-1} + \mathbf{X}^{*\prime}\Sigma_{\mathbf{Y}}^{-1}\mathbf{X}^*)^{-1}$. Therefore, we have that $\pi_{\boldsymbol{\beta}} = \pi(\boldsymbol{\beta}|\Phi, \Psi, \mathbf{Y}) \sim N(\mathbf{b}^*, \mathbf{B}^*)$ and, thus, it would be possible to sample $\boldsymbol{\beta}$ directly from $\pi_{\boldsymbol{\beta}}$. That is, values of $\boldsymbol{\beta}$ can be proposed directly from $\pi_{\boldsymbol{\beta}}$ and accepted with probability one. This is the basic description and motivation for the Gibbs sampler (Geman and Geman, 1984).

Now, given that $\Sigma^{-1} = \mathbf{T}'\mathbf{D}^{-1}\mathbf{T}$, we have that, for $i = 1, \ldots, m$,

$$\tilde{\mathbf{Y}}_i'\mathbf{T}'\mathbf{D}^{-1}\mathbf{T}\tilde{\mathbf{Y}}_i \quad = \quad [(\mathbf{I}_n - \Phi)\tilde{\mathbf{Y}}_i]'\mathbf{D}^{-1}[(\mathbf{I}_n - \Phi)\tilde{\mathbf{Y}}_i]$$

Therefore, by taking into account the independence between individuals and using the equation above, the quadratic form appearing in the log-likelihood function, $Q(\mathbf{Y}) = (\mathbf{Y} - \boldsymbol{\mu}^*)'\Sigma_{\mathbf{Y}}^{-1}(\mathbf{Y} - \boldsymbol{\mu}^*)$, can be rewritten as

$$Q(\mathbf{Y}) \quad = \quad \frac{1}{\sigma_1^2}\mathbf{Y}_1^{*\prime}\mathbf{Y}_1^* + \cdots + \frac{1}{\sigma_n^2}(\mathbf{Y}_n^* - \tilde{\boldsymbol{\mu}}_n)'(\mathbf{Y}_n^* - \tilde{\boldsymbol{\mu}}_n),$$

where $\tilde{\boldsymbol{\mu}}_k$, $k = 2, \ldots, n$ is the m-dimensional vector with i-th component given by $\phi_{k1}(Y_{i1} - \mu_1) + \cdots + \phi_{k,k-1}(Y_{i,k-1} - \mu_{k-1})$, $\mathbf{Y}_1^* = (Y_{11} - \mu_1, Y_{21} - \mu_1, \ldots, Y_{m1} - \mu_1)'$ is the vector of centered observations for all m individuals at the first time point; $\mathbf{Y}_2^* = (Y_{12} - \mu_2, Y_{22} - \mu_2, \ldots, Y_{m2} - \mu_2)'$, is the vector of centered observations for all m individuals at the second time point; and $\mathbf{Y}_n^* = (Y_{1n} - \mu_n, Y_{2n} - \mu_n, \ldots, Y_{mn} - \mu_n)'$ is the vector of centered observations for all m individuals at the n-th time point.

In this way, the maximum likelihood function can be written as:

$$L(\boldsymbol{\beta}, \Phi, \mathbf{D}) \propto |\mathbf{D}|^{-m/2} \exp\left\{-\frac{1}{2\sigma_1^2}\mathbf{Y}_1^{*\prime}\mathbf{Y}_1^* - \cdots - \frac{1}{2\sigma_n^2}(\mathbf{Y}_n^* - \tilde{\boldsymbol{\mu}}_n)'(\mathbf{Y}_n^* - \tilde{\boldsymbol{\mu}}_n)\right\} \tag{8}$$

Thus, if we assume independent normal prior for the $\boldsymbol{\phi}_k$'s, we can obtain, from the application of Bayes' theorem, that the posterior full conditional distribution for $\boldsymbol{\phi}_k$ is given by

$$\pi(\boldsymbol{\phi}_k|\boldsymbol{\beta}, \mathbf{D}, \Phi_{-k}) \propto \sigma_k^{-1} \exp\Big\{ - \frac{1}{2\sigma_k^2}(\mathbf{Y}_k^* - \tilde{\boldsymbol{\mu}}_k)'(\mathbf{Y}_k^* - \tilde{\boldsymbol{\mu}}_k) - \frac{1}{2}(\boldsymbol{\phi}_k - \mathbf{l}_{0k})'\Sigma_{\boldsymbol{\phi}_k}^{-1}(\boldsymbol{\phi}_k - \mathbf{l}_{0k})\Big\}, \tag{9}$$

where Φ_{-k} represent the parameters in Φ excluding the corresponding ones for $\boldsymbol{\phi}_k$. Therefore, the conditional posterior distribution is given by

$$\tilde{\pi}(\boldsymbol{\phi}_k|\boldsymbol{\alpha}, \boldsymbol{\lambda}) \quad \propto \quad \exp\left\{-\frac{1}{2}(\boldsymbol{\phi}_k - \mathbf{l}_k^*)'\Sigma_k^{*-1}(\boldsymbol{\phi}_k - \mathbf{l}_k^*)\right\},$$

where $\mathbf{l}_k^* = \Sigma_k^*\left(\Sigma_{\boldsymbol{\phi}_k}\mathbf{l}_{0k} + \frac{1}{\sigma_k^2}\tilde{\mathbf{X}}_k'\tilde{\mathbf{Y}}_k\right)$ and $\Sigma_k^* = \left(\Sigma_{\boldsymbol{\phi}_k}^{-1} + \frac{1}{\sigma_k^2}\tilde{\mathbf{X}}_k'\tilde{\mathbf{X}}_k\right)^{-1}$. From the above, we have that

$$\pi_{\boldsymbol{\phi}_k} = \pi(\boldsymbol{\phi}_k|\boldsymbol{\beta}, \mathbf{D}, \Phi_{-k}, \mathbf{Y}) \sim N(\mathbf{l}_k^*, \Sigma_k^*) \tag{10}$$

So it is possible to sample $\boldsymbol{\phi}_k$ directly from $\pi_{\boldsymbol{\phi}_k}$. Values of $\boldsymbol{\phi}_k$ can be proposed directly from $\pi_{\boldsymbol{\phi}_k}$ and accepted with probability 1. This is the basic description and motivation for the Gibbs sampler (Geman and Geman, 1984).

Finally, to be able to sample σ_k^2, $k = 1, 2, 3, \ldots, n$, as we have already seen before, we propose the use of gamma priors for the ψ_k's and, thus, from the straight application

of Bayes' theorem, we obtain gamma posterior distributions for the ψ_k's, so that the sampling procedure can be easily handled by using the Gibbs sampler.

More concretely, let $\tilde{\mathbf{Y}}_k^* = (\mathbf{Y}_k^* - \tilde{\boldsymbol{\mu}}_k)$ be a random sample of size m from a $N(\mathbf{0}, \sigma_k^2)$ distribution ($k = 1, \ldots, n$), with $\psi_k = 1/\sigma_k^2$. That is, $\tilde{\mathbf{Y}}_k^*$ represents a sample of m individuals at time t_k, $k = 1, \ldots, n$. Now, given that the gamma family is closed under sampling, we can assume a gamma prior distribution so that $\psi_k \sim G(\alpha_k = n_{0k}/2, n_0\sigma_{0k}^2)$, where n_{0k} is a natural number and $\sigma_{0k}^2 > 0$. Therefore, the posterior distribution of ψ_k can be directly obtained by using Bayes' theorem, so that

$$\pi(\psi_k|\boldsymbol{\beta}, \mathbf{D}, \tilde{\mathbf{Y}}_k^*) \propto \psi_k^{[(n_{0k}+m)/2]-1} \exp\{-(n_{0k}\sigma_{0k}^2 + ms_{0k}^2)\psi_k/2\} \tag{11}$$

This expression corresponds to the kernel of the gamma distribution. Thus, we have that

$$\pi(\psi_k|\boldsymbol{\beta}^{(c)}, \boldsymbol{\phi}^{(c)}) = G\Big(\frac{n_{0k}+m}{2}, \frac{n_{0k}\sigma_{0k}^2 + ms_{0k}^2}{2}\Big),$$

where $s_{0k}^2 = \frac{1}{m}\Sigma_{i=1}^m \tilde{\mathbf{Y}}_k^{*\prime}\tilde{\mathbf{Y}}_k^*$, $k = 1, \ldots, n$.

If we decide to assume constant or noninformative priors, the sampling procedure for each of the parameters involved in the estimation process is described below.

Given $\mathbf{D}$, Φ and a constant prior distribution for $\boldsymbol{\beta}$, we can sample $\boldsymbol{\beta}$ from

$$\pi(\boldsymbol{\beta}|\Phi, \Psi, \mathbf{Y}) \quad \propto \quad \left\{-\frac{1}{2}(\boldsymbol{\beta} - \mathbf{b}^*)'\mathbf{B}^{*-1}(\boldsymbol{\beta} - \mathbf{b}^*)\right\}, \tag{12}$$

where $\mathbf{b}^* = \mathbf{B}^*(\mathbf{X}^{*\prime}\Sigma_{\mathbf{Y}}^{-1}\mathbf{Y})$ and $\mathbf{B}^* = (\mathbf{X}^{*\prime}\Sigma_{\mathbf{Y}}^{-1}\mathbf{X}^*)^{-1}$.

Given $\boldsymbol{\beta}$, $\mathbf{D}$ and a constant prior distribution for the $\boldsymbol{\phi}_k$'s, and letting Φ_{-k} represent the parameters in Φ excluding the corresponding ones for $\boldsymbol{\phi}_k$, we can sample the $\boldsymbol{\phi}_k$'s ($k = 1, 2, \ldots, n$) from (9) by following the procedure below:

1. Sample $\boldsymbol{\phi}_1$ from $\pi(\boldsymbol{\phi}_1|\boldsymbol{\beta}, \mathbf{D}, \Phi_{-1}) \propto \sigma_1^{-1} \exp\left\{-\frac{1}{2\sigma_1^2}\mathbf{Y}_1^{*\prime}\mathbf{Y}_1^*\right)\right\}$.
2. Sample $\boldsymbol{\phi}_2$ from $\pi(\boldsymbol{\phi}_2|\boldsymbol{\beta}, \mathbf{D}, \Phi_{-2}) \propto \sigma_2^{-1} \exp\left\{-\frac{1}{2\sigma_2^2}(\mathbf{Y}_2^* - \tilde{\boldsymbol{\mu}}_2)'(\mathbf{Y}_2^* - \tilde{\boldsymbol{\mu}}_2)\right\}$.
3. And so on, up to sample $\boldsymbol{\phi}_n$ from

$$\pi(\boldsymbol{\phi}_n|\boldsymbol{\beta}, \mathbf{D}, \Phi_{-n}) \propto \sigma_n^{-1} \exp\left\{-\frac{1}{2\sigma_n^2}(\mathbf{Y}_n^* - \tilde{\boldsymbol{\mu}}_n)'(\mathbf{Y}_n^* - \tilde{\boldsymbol{\mu}}_n)\right\}.$$

Finally, given $\mathbf{D}, \boldsymbol{\beta}$ and a constant prior for the ψ_k's, we can sample the ψ_k's from

$$\pi(\psi_k|\boldsymbol{\beta}^{(c)}, \boldsymbol{\phi}^{(c)}) = G\Big(\frac{m}{2}, \frac{ms_{0k}^2}{2}\Big),$$

where s_{0k}^2 is defined as before.

5 Examples

In order to illustrate and motivate the methods proposed in this paper, we present the analysis of two data sets, referred to here as the race data and the cattle data. Previous approaches for analyzing these data sets have been reported elsewhere (Zimmerman and Núñez-Antón, 1997; Zimmerman *et al.*, 1998; Pourahmadi, 1999, 2000 and 2002; Zimmerman, 2000; Núñez-Antón and Zimmerman, 2000; Wu and Pourahmadi, 2003; Pan and MacKenzie, 2003, 2006 and 2007).

The race data consist of the "split" times for each of $m = 80$ competitors in each 10-km section of a 100-km race held in 1984 in the United Kingdom. The data include, in addition to the split times, the ages of all but four of the competitors. Measurement times are evenly spaced and common to all subjects in the study and no observations were missing. A previous analysis (Zimmerman *et al.*, 1998) showed the age variable to be non-significant, so we will ignore it here. Our analysis centres on the study of how competitor performance on each 10-km section is related to the section number ($t = 1, 2, \ldots, 10$) (i.e., $n = 10$), as well as on the adequate modelling of the variances and the correlations between successive measurements being made on any given subject.

The cattle data (Kenward, 1987) come from a designed experiment in which cattle receiving two treatments, say A and B, for intestinal parasites were weighed $n = 11$ times over a 133-day period. Thirty animals received treatment A and thirty received treatment B (i.e., $m = 60$). The first 10 measurements on each animal were made at two-week intervals and the final measurement was made after a one-week interval. Measurement times were common across animals and rescaled to $t = 1, \ldots, 9, 10, 10.5$, and no observations were missing. We wish to study how cattle growth is affected by the different treatments and, in addition, we concentrate on how the mean changes with time, as well as on the adequate modelling of the variances and the correlations between successive measurements being made on any given experimental unit.

5.1 Analysis of the Race Data

Figure 1 shows the profile plot for the race data. The profile plot indicates that the mean split time tends to increase over the first 80 km of the race but then levels off (perhaps reflecting the "kick" that well-conditioned runners generally show near the end of a race). Figure 1 also shows that variances tend to increase over the course of the race, and that the behaviour of many runners in the later sections of the race is more erratic, in the sense that consecutive same-runner split times fluctuate more. The increase of the mean does not seem to be linear with time and, thus, a quadratic or cubic model in time may be more appropriate to model the overall mean growth in this data set. Based on this and, as in Zimmerman *et al.* (1998), we use a cubic in time model for the overall mean weight. That is, the overall mean weight, as a function of the section number t,

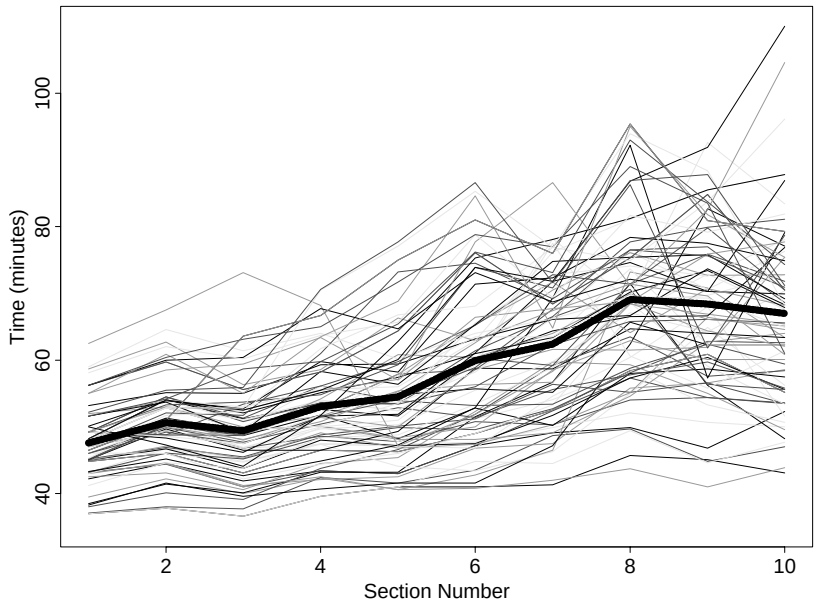

Figure 1: *Profile plot for the race data. The thicker line indicates the mean profile for all individuals in the study.*

will be given by:

$$\mu_j = \beta_0 + \beta_1 t_j + \beta_2 t_j^2 + \beta_3 t_j^3, \quad j = 1, \ldots, 10,$$

where

$$\boldsymbol{\mu} = (\mu_1, \mu_2, \ldots, \mu_{10})' = (\mu_{\{t_1=1\}}, \ldots, \mu_{\{t_{10}=10\}})'$$

and $\boldsymbol{\beta} = (\beta_0, \beta_1, \beta_2, \beta_3)'$.

We also need to estimate the variance-covariance matriz Σ. In order to do so, and as a direct result from equations (3) and (4), both the elements of the diagonal matrix **D** and the ϕ_{ij}'s in the lower triangular matrix **T** need to be estimated. In order to have a not too restrictive and a more general procedure, we consider noninformative prior distributions in all mean and covariance parameters. As it is well known and as we will see later on in this section, with the use of noninformative prior information, the parameter estimates (both for the mean and variance-covariance matrix) obtained with the proposed Bayesian methodology are very similar to the ones obtained with the proposed classic methodology.

The estimates for the mean parameters obtained with the proposed Bayesian methodology, together with their standard deviations in parenthesis, are

$$\boldsymbol{\beta} = (46.320(0.711), 1.267(0.483), 0.556(0.167), -0.047(0.014))',$$

Table 1: *Estimated means, variances and correlations for the race data set with the Bayesian methodology. In the table, Section refers to the section number.*

Section	1	2	3	4	5	6	7	8	9	10
Correlations										
	1.0									
	.94	1.0								
	.75	.72	1.0							
	.72	.70	.92	1.0						
	.49	.44	.76	.87	1.0					
	.57	.54	.72	.84	.91	1.0				
	.47	.43	.60	.69	.75	.84	1.0			
	.49	.53	.54	.64	.66	.80	.72	1.0		
	.53	.50	.55	.65	.69	.76	.68	.75	1.0	
	.37	.35	.47	.51	.54	.65	.72	.62	.77	1.0
Means	48.1	50.7	53.9	57.3	60.7	63.8	66.3	68.0	68.5	67.6
Variances	27.0	39.7	48.5	56.2	94.9	142.1	105.6	154.7	144.2	165.6

and the ones obtained with the proposed classic approach are

$$\boldsymbol{\beta} = (46.247, 1.258, 0.564, -0.048)'.$$

Given that, as expected, the estimates obtained with the proposed classic methodology are very similar to the ones obtained with the Bayesian methodology, we do not include their estimated standard deviations. Note that all coefficients in the linear model are different from zero at a 95% credibility level and that the signs of the coefficients are consistent with the behaviour seen in Figure 1. In addition, our estimates are also similar to the ones obtained by Zimmerman *et al.* (1998) with the difference that our variance-covariance structure is more general than theirs because they have assumed a structured antedependent model of order one and we have a general unstructured antedependent model. As a way of comparing the estimated mean time as a function of the section number, as in Figure 1, Table 1 shows these estimated values using the estimates obtained from the Bayesian approach. As can be seen, this behaviour is consistent with the one observed in Figure 1.

The estimated innovation variances obtained with the proposed Bayesian methodology under noninformative priors with their corresponding estimated standard deviations in parenthesis, as well as those obtained with the proposed classic methodology are

Table 2: *Estimated autoregressive parameters obtained with the proposed Bayesian methodology for the race data set. Estimated standard deviations, in parenthesis, are also included. As in the* **T** *matrix (see Section 2), there are ones on the main diagonal.*

1									
1.137	1								
(0.028)									
0.773	0.215	1							
(0.216)	(0.158)								
−0.010	0.105	0.924	1						
(0.076)	(0.091)	(0.043)							
0.293	−0.701	−0.179	1.554	1					
(0.079)	(0.067)	(0.043)	(0.038)						
−0.053	0.517	−0.370	0.100	1.117	1				
(0.103)	(0.100)	(0.084)	(0.063)	(0.028)					
0.200	−0.308	0,221	−0.078	−0.199	0.858	1			
(0.102)	(0.144)	(0.086)	(0.060)	(0.055)	(0.033)				
−0.897	1.028	−0.150	−0.093	−0.197	0.849	0.240	1		
(0.159)	(0.138)	(0.117)	(0.073)	(0.067)	(0.055)	(0.031)			
0.749	−0.261	−0.211	−0.058	0.298	0.156	0.092	0.397	1	
(0.091)	(0.155)	(0.110)	(0.066)	(0.061)	(0.039)	(0.028)	(0.029)		
−0.610	0.073	0.612	−0.283	−0.608	0.308	0.576	−0.118	0.726	1
(0.143)	(0.193)	(0.145)	(0.082)	(0.072)	(0.050)	(0.031)	(0.037)	(0.022)	

$$\begin{pmatrix} \hat{\sigma}_1^2 \\ \hat{\sigma}_2^2 \\ \hat{\sigma}_3^2 \\ \hat{\sigma}_4^2 \\ \hat{\sigma}_5^2 \\ \hat{\sigma}_6^2 \\ \hat{\sigma}_7^2 \\ \hat{\sigma}_8^2 \\ \hat{\sigma}_9^2 \\ \hat{\sigma}_{10}^2 \end{pmatrix}_{\text{Bayes}} = \begin{pmatrix} 27.653(4.489) \\ 4.811(1.162) \\ 21.818(4.736) \\ 9.085(1.493) \\ 16.496(2.812) \\ 19.616(3.319) \\ 31.837(5.182) \\ 47.552(7.980) \\ 50.997(8.399) \\ 49.414(8.123) \end{pmatrix}, \quad \begin{pmatrix} \hat{\sigma}_1^2 \\ \hat{\sigma}_2^2 \\ \hat{\sigma}_3^2 \\ \hat{\sigma}_4^2 \\ \hat{\sigma}_5^2 \\ \hat{\sigma}_6^2 \\ \hat{\sigma}_7^2 \\ \hat{\sigma}_8^2 \\ \hat{\sigma}_9^2 \\ \hat{\sigma}_{10}^2 \end{pmatrix}_{\text{Classic}} = \begin{pmatrix} 27.980 \\ 4.544 \\ 21.167 \\ 8.803 \\ 16.463 \\ 19.009 \\ 30.946 \\ 46.477 \\ 49.537 \\ 47.683 \end{pmatrix}$$

The estimated values of all innovation variances are somehow consistent with the increasing behaviour of variances seen in Table 1 and Figure 1. However, we must be cautious about this issue because these are not the response variances. We will come back to this matter when reporting the estimated variances and correlations for the race data (see Table 1). Table 2 shows the estimated autoregressive parameters obtained with the Bayesian approach. Moreover, the standard deviations obtained with the proposed

Bayesian approach show that some of the autoregressive parameters are not different from zero at a 95% credibility level. For brevity and because estimates obtained for the autoregressive parameters with the classic approach are similar to those obtained with the Bayesian approach, we do not include them. However, as estimates obtained with the use of the two proposed approaches are quite similar, we can see that some of the autoregressive parameters are not statistically significant at the same level. Finally, Table 1 shows the estimated variances and correlations for the race data obtained with the Bayesian approach. The behaviour of these estimated values is consistent with the one observed in the corresponding sample variances and correlations (not included here for brevity).

5.2 Analysis of the Cattle Data

For brevity, and as in Zimmerman and Núñez-Antón (1997), we report here the results for group A only. Figure 2 shows the profile plot for cattle in group A of the cattle data. The profile plot indicates that the means and variances of the responses are increasing over the course of the experiment, with the more rapid growth occurring in the first few weeks of the study. The increase of the mean does not seem to be linear with time and, thus, a quadratic or cubic model in time may be more appropriate to model the overall mean growth in this cattle group. Based on the analysis above and, as in Pourahmadi

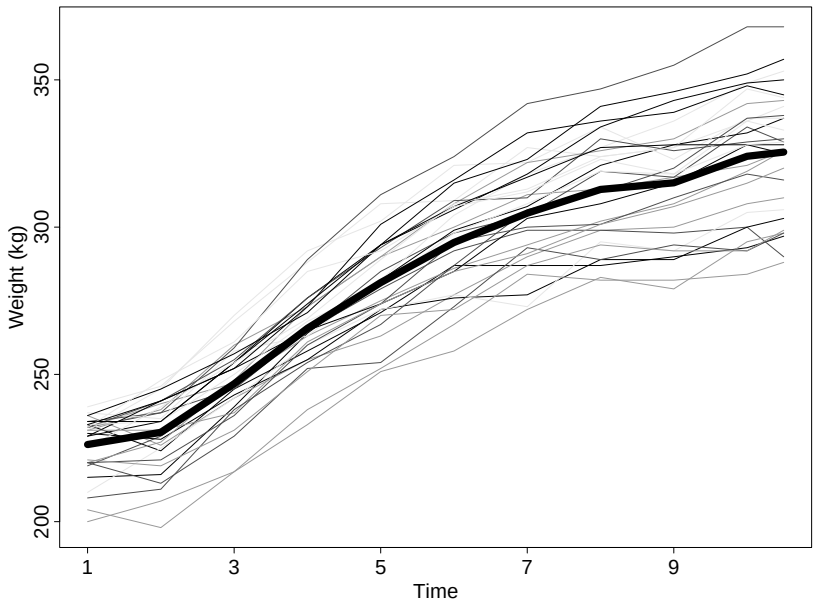

Figure 2: *Profile plot for the cattle data, treatment A. The thicker line indicates the mean profile for all individuals in this group.*

(1999) or Cepeda (2001), we use a cubic in time model for the overall mean weight. That is, the overall mean weight, as a function of the section number t, will be given by:

$$\mu_j = \beta_0 + \beta_1 t_j + \beta_2 t_j^2 + \beta_3 t_j^3, \quad j = 1, \ldots, 11,$$

where

$$\boldsymbol{\mu} = (\mu_1, \mu_2, \ldots, \mu_{11})' = (\mu_{\{t_1=1\}}, \ldots, \mu_{\{t_{10}=10\}}, \mu_{\{t_{11}=10.5\}})'$$

and $\boldsymbol{\beta} = (\beta_0, \beta_1, \beta_2, \beta_3)'$. As in the analysis of the race data, we estimate the variance-covariance matriz $\boldsymbol{\Sigma}$ from equations (3) and (4), by estimating the elements of the diagonal matrix $\mathbf{D}$ and the ϕ_{ij}'s in the lower triangular matrix $\mathbf{T}$. In this case, we also consider noninformative prior distributions in all mean and covariance parameters. Given the similarity of the estimates obtained from the Bayesian and classic approaches when considering this type of priors, we only report the ones from the Bayesian methodology. The estimates for the mean parameters obtained with the proposed Bayesian methodology, together with their standard deviations in parenthesis, are

$$\boldsymbol{\beta} = (227.575(3.041), 10.003(2.565), 1.154(0.541), -0.117(0.034))'.$$

Note that all coefficients in the linear model are different from zero at a 95% credibility level, and that the signs of the coefficients are consistent with the behaviour seen in Figure 2. In addition, our estimates are also similar to the ones obtained by previous authors that have analyzed this data, with the difference that our variance-

Table 3: *Estimated means, variances and correlations for the group A cattle data set with the Bayesian methodology.*

Time	1	2	3	4	5	6	7	8	9	10	10.5
Correlations											
	1.0										
	.74	1.0									
	.74	.89	1.0								
	.62	.68	.87	1.0							
	.58	.59	.79	.94	1.0						
	.53	.53	.75	.91	.95	1.0					
	.49	.50	.70	.83	.87	.93	1.0				
	.51	.58	.75	.83	.88	.92	.93	1.0			
	.51	.62	.73	.73	.76	.82	.89	.83	1.0		
	.46	.52	.68	.73	.78	.85	.88	.94	.94	1.0	
	.44	.44	.63	.70	.75	.81	.86	.92	.92	.98	1.0
Means	238.62	251.3	264.8	278.6	291.8	303.9	314.0	321.6	325.8	326.0	324.4
Variances	109.5	228.4	194.6	202.5	269.7	317.5	335.1	372.2	452.3	510.5	454.8

covariance structure is more general than theirs. As a way of comparing the estimated cattle weight as a function of time, as in Figure 2, Table 3 shows these estimated values using the estimates obtained from the Bayesian approach. As can be seen, this behaviour is consistent with the behaviour observed in Figure 2.

The estimated innovation variances obtained with the proposed Bayesian methodology under noninformative priors with their corresponding estimated standard deviations in parenthesis are

$$\begin{pmatrix} \hat{\sigma}_1^2 \\ \hat{\sigma}_2^2 \\ \hat{\sigma}_3^2 \\ \hat{\sigma}_4^2 \\ \hat{\sigma}_5^2 \\ \hat{\sigma}_6^2 \\ \hat{\sigma}_7^2 \\ \hat{\sigma}_8^2 \\ \hat{\sigma}_9^2 \\ \hat{\sigma}_{10}^2 \\ \hat{\sigma}_{11}^2 \end{pmatrix}_{\text{Bayes}} = \begin{pmatrix} 109.524(30.490) \\ 102.496(42.180) \\ 38.595(15.072) \\ 42.015(13.012) \\ 29.769(8.330) \\ 29.811(8.357) \\ 45.612(12.784) \\ 32.955(9.345) \\ 23.515(6.791) \\ 37.974(11.438) \\ 10.805(3.024) \end{pmatrix}$$

The estimated values of all innovation variances are somehow consistent with the increasing behaviour of variances seen in Table 3 and Figure 2. However, we must be cautious about this issue because these are not the response variances. We will come back to this matter when reporting the estimated variances and correlations for the group A cattle data (see Table 3). If we wish to compare these results with those reported in Pourahmadi (1999) or Cepeda (2001), we could estimate the log-innovation variances. We have done so and estimates are very similar to theirs. Thus, this can be used as a way to indicate that log-innovation variances could be modelled as cubic polynomials (see Pourahmadi, 1999 or Cepeda, 2001). We do not consider it necessary to include these estimated values here.

Table 4 shows the estimated autoregressive parameters with the Bayesian approach. The standard deviations obtained with the proposed Bayesian approach show that the autoregressive parameters are different from zero at a 95% credibility level and they are all consistent with the results presented in Pourahmadi (1999). Finally, Table 3 shows the estimated variances and correlations for the group A cattle data obtained with the Bayesian approach. The behaviour of these estimated values is consistent with the one observed in the corresponding sample variances and correlations (not included here for brevity).

Table 4: *Estimated autoregressive parameters obtained with the proposed Bayesian methodology for the group A cattle data set. Estimated standard deviations, in parenthesis, are also included. As in the* **T** *matrix (see Section 2), there are ones on the main diagonal.*

1										
1.072	1									
(0.172)										
0.236	0.698	1								
(0.110)	(0.097)									
0.062	−0.416	1.251	1							
(0.118)	(0.150)	(0.181)								
0.104	−0.133	−0.015	1.146	1						
(0.050)	(0.071)	(0.059)	(0.068)							
−0.014	−0.200	0.166	0.295	0.789	1					
(0.059)	(0.087)	(0.060)	(0.075)	(0.039)						
−0.027	0.017	0.116	−0.278	0.050	1.044	1				
(0.085)	(0.092)	(0.069)	(0.099)	(0.056)	(0.069)					
−0.182	0.261	0.100	−0.386	0.150	0.538	0.516	1			
(0.069)	(0.110)	(0.059)	(0.087)	(0.060)	(0.053)	(0.063)				
−0.011	0.208	0.166	−0.362	−0.216	−0.204	0.416	1.053	1		
(0.077)	(0.058)	(0.072)	(0.062)	(0.055)	(0.067)	(0.037)	(0.067)			
0.052	−0.306	0.226	−0.147	0.007	0.112	−0.122	0.562	0.617	1	
(0.099)	(0.103)	(0.077)	(0.072)	(0.058)	(0.065)	(0.042)	(0.083)	(0.072)		
0.192	−0.330	−0.011	0.269	0.047	−0.292	−0.050	−0.015	0.213	0.907	1
(0.042)	(0.051)	(0.077)	(0.058)	(0.048)	(0.052)	(0.037)	(0.057)	(0.073)	(0.048)	

6 Conclusions

We have proposed a joint modelling approach for the mean and covariance structures in the context of normal longitudinal data. In the proposals presented here, the mean is modelled in a linear form and the covariance structure is left unrestricted in the sense that no specific parametric model is imposed on it, except for the fact that its modelling makes use of the general antedependence model specification, which has shown to be most useful in practice for nonstationary situations such as the ones present in the data sets analyzed here (see, e.g., Kenward, 1987, Pourahmadi, 1999 and 2000, Núñez-Antón and Zimmerman, 2000 or Zimmerman and Núñez-Antón, 2001). The proposals include both a classic and a Bayesian approach, allowing for the possibility of having noninformative priors for the latter. The behaviour of the proposed methodology is evaluated by analyzing two data sets and it has proved to be consistent and reasonable when compared to previous and less general proposals.

Extensions allowing for nonlinear mean structures are being considered at the moment but are beyond the scope of this paper.

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Book review

PATTERN RECOGNITION AND MACHINE LEARNING

Cristopher M. Bishop

Information Science and Statistics

Springer 2006, 738 pages

As the author writes in the preface of the book, pattern recognition has its origin in engineering, whereas machine learning grew out of computer science. However, these activities can be viewed as two facets of the same field, and they have undergone substantial development over the past years.

Bayesian methods are widely used, while graphical models have emerged as a general framework for describing and applying probabilistic models. Similarly new models based on kernels have had significant impact on both algorithms and applications.

This textbook reflects these recent developments while providing a comprehensive introduction to the fields of pattern recognition and machine learning. It is aimed at advanced undergraduate or first year PhD students, as well as researchers and practitioners. It can be consider as an introductory course to the subject.

The first four chapters are devoted to the concepts of Probability and Statistics that are needed for reading the rest of the book, so we can imagine that the speed is high in order to get from zero to infinity. I believe that it is better to study the book after a previous course on Probability and Statistics. On the other hand, a basic knowledge of linear algebra and multivariate calculus is assumed.

The other chapters give to a classic probabilist or statistician a point of view on some applications that are very interesting but far from his usual world. In all the text the mathematical aspects are at the second level in relation with the ideas and intuitions that the author wants to communicate.

The book is supported by a great deal of additional material, including lecture slides as well as the complete set of figures used in it, and the reader is encouraged to visit the book web site for the latest information. So it can be very useful for a course or a talk about the subject.

The exercises that appear at the end of the chapters form an important component of the book. They reinforce or generalize concepts explained in the text, and are graded according to difficulty. The solutions to the exercises considered by the author to amplify key points or fill in important details can be found also as a PDF file in the web book site.

This book focuses on concepts and principles and not on the use of key algorithms for appropriate data sets. The author announces a companion volume in 2008, which will deal with practical aspects of pattern recognition and machine learning. It will be accompanied by Matlab software, implementing most of the algorithms discussed in this text. This second part is necessary to complete the gap of the present volume.

Though this book has to be considered a first contact with these interesting fields, the list of references is wide enough to satisfy our curiosity.

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A recursion formula for expected negative and positive powers of the central Wishart distribution

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Abstract

We use Haff's fundamental identity to express the expectation of S^p in lower-order terms, where S follows the central Wishart distribution.

MSC: primary 62H10, secondary 15A69

Keywords: Haff's Fundamental Identity, matrix differentiation, central Wishart distribution.

1 The recursion formula

Let $S \sim W_m(\Omega, n)$ the Wishart distribution with scale matrix $\Omega > 0$ and n degrees of freedom. We use Haff's Fundamental Identity (FI):

$$\mathcal{E}\, F_1 \Omega^{-1} F_2 = 2\, \mathcal{E} F_1\, \nabla\, F_2 + 2\, (\mathcal{E}\, F_2'\, \nabla\, F_1')' + (n - m - 1)\, \mathcal{E}\, F_1\, S^{-1}\, F_2,$$

with $F_1 = F_1(S)$ a differentiable matrix function of S and $n > m + 1$. Further ∇ is a matrix of differential operators with typical element

$$d_{ij} = \frac{1}{2}\,(1 + \delta_{ij})\,\frac{\partial}{\partial\, s_{ij}} \quad (i, j = 1, \ldots, m),$$

where δ_{ij} is a Kronecker delta: $\delta_{ii} = 1$ and $\delta_{ij} = 0$ $(i \neq j)$.

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All matrices are square of dimension m. A very useful property is: when $dF = P'(dS)Q$ then $2\nabla F = PQ + (\operatorname{tr} P)Q$, where dF is the differential of F. For these properties see, e.g. Neudecker (2001). Further $\mathcal{E}$ is the expectation operator.

We choose $F_1 = I_m$ and $F_2 = S^p$. By Haff's FI we get:

$$\mathcal{E}\,\Omega^{-1} S^p = 2\,\mathcal{E}\,\nabla S^p + (n - m - 1)\,\mathcal{E}\,S^{p-1},$$

because $\nabla I = 0$. For definition and computation of $\nabla(\cdot)$ see also Neudecker (2000).

Clearly

$$d S^p = \sum_{k=0}^{p-1} S^k (dS) S^{p-k-1}$$

where $S^0 = I_m$.

Hence

$$2\nabla S^p = (m + p) S^{p-1} + \sum_{k=1}^{p-1} \left(\operatorname{tr} S^k\right) S^{p-k-1}.$$

Then

$$\mathcal{E}\,\Omega^{-1} S^p = (n + p - 1)\,\mathcal{E}\,S^{p-1} + \mathcal{E} \sum_{k=1}^{p-1} \left(\operatorname{tr} S^k\right) S^{p-k-1}$$

or equivalently

$$\mathcal{E}\,S^p = (n + p - 1)\Omega\,\mathcal{E}\,S^{p-1} + \Omega\,\mathcal{E} \sum_{k=1}^{p-1} \left(\operatorname{tr} S^k\right) S^{p-k-1}.$$

2 Discussion (positive powers)

The second recursion formula is not really suited for finding $\mathcal{E}\,S^p$, because this requires knowledge of $\mathcal{E}\,(\operatorname{tr} S^k)\,S^{p-k-1}$ for $1 \le k \le p - 1$. This expression has to be found by other methods. See Neudecker (2001). The formula is, however, suited for establishing Loewner orderings. Relevant is that $\Omega\,\mathcal{E}\,S^p = \mathcal{E}\,S^p\,\Omega > 0$ (positive definite). This indirectly follows from the first recursion formula, which yields the identity $\Omega^{-1}\,\mathcal{E}\,S^p = \mathcal{E}\,S^p\,\Omega^{-1}$ and further the positive definiteness of the two expressions. Pre- and postmultiplication of the identity by matrix Ω yields: $\Omega\,\mathcal{E}\,S^p = \mathcal{E}\,S^p\,\Omega$. As Ω and $\mathcal{E}\,S^p$ are two conmuting positive definite matrices, they are simultaneously diagonizable by an orthogonal similarity transformation. Hence $T'\,\Omega\,T = \Lambda$ and $T'\,\mathcal{E}\,S^p\,T = M$, say,

and consequently $\Omega \mathcal{E} S^p = T \Lambda T' T M T' = T \Lambda M T' > 0$ (positive definite), as both Λ and M are diagonal positive definite. See e.g. Hadley (1972, ex. 7-14).

We further conclude that $\Omega^{-1} \mathcal{E} S^p > (n+p-1)\mathcal{E} S^{p-1}$ or equivalently $(\mathcal{E} S)^{-1} \mathcal{E} S^p > n^{-1}(n+p-1)\mathcal{E} S^{p-1}$ as $\mathcal{E} S = n\Omega$ $(p \geq 2)$. The first inequality follows from the second recursion formula. Repeated substitution finally yields the inequations

$$\mathcal{E} S^p > (\mathcal{E} S)^p$$

3 The recursion formula (negative powers)

With $F_1 = I_m$ and $F_2 = S^{-p}$, by Haff's FI we get

$$\Omega^{-1} \mathcal{E} S^{-p} = 2 \mathcal{E} \nabla S^{-p} + (n-m-1) \mathcal{E} S^{-(p+1)} \tag{1}$$

For $p = 1, 2, \ldots, n-m-2$, we clearly have

$$dS^{-p} = -\sum_{k=1}^{p} S^{-k} (dS) S^{k-(p+1)}$$

Hence

$$\begin{aligned} \nabla S^{-p} &= \tfrac{1}{2} \sum_{k=1}^{p} S^{-(p+1)} - \frac{1}{2} \sum_{k=1}^{p} \left(\operatorname{tr} S^{-k} \right) S^{k-(p+1)} \\ &= -\tfrac{1}{2} p S^{-(p+1)} - \tfrac{1}{2} \sum_{k=1}^{p} \left(\operatorname{tr} S^{-k} \right) S^{k-(p+1)} \end{aligned}$$

Insertion in (1) leads to the recursion formula

$$\Omega^{-1} \mathcal{E} S^{-p} = (n-m-p-1) \mathcal{E} S^{-(p+1)} - \sum_{k=1}^{p} \mathcal{E} \left(\operatorname{tr} S^{-k} \right) S^{k-(p+1)} \tag{2}$$

or equivalently

$$\mathcal{E} S^{-p} = (n-m-p-1) \Omega \mathcal{E} S^{-(p+1)} - \Omega \sum_{k=1}^{p} \mathcal{E} \left(\operatorname{tr} S^{-k} \right) S^{k-(p+1)} \tag{3}$$

4 Discussion and application (negative powers)

Because of the symetry of the RHS of (2) we have

$$\Omega^{-1}\,\mathcal{E}\,S^{-p} = (\mathcal{E}\,S^{-p})\,\Omega^{-1}. \tag{4}$$

We shall prove that $\Omega^{-1}\,\mathcal{E}\,S^{-p} > 0$ (positive definite).

Proof. From the commutativity property (4) we conclude that $\mathcal{E}\,S^{-p} = T\,\Lambda_p\,T'$ say and $\Omega^{-1} = T\,M\,T'$ where T is orthogonal and M and Λ_p are diagonal positive definite. Hence

$$\Omega^{-\frac{1}{2}} = T\,M^{\frac{1}{2}}\,T'$$

and

$$\begin{aligned}\Omega^{-\frac{1}{2}}\,(\mathcal{E}\,S^{-p})\,\Omega^{-\frac{1}{2}} &= T\,M^{\frac{1}{2}}\,T'\,\Lambda_p\,T'\,T\,M^{\frac{1}{2}}\,T' \\ &= T\,M^{\frac{1}{2}}\,\Lambda_p\,M^{\frac{1}{2}}\,T' = T\,M\,\Lambda_p\,T' = T\,M\,T'\,T\,\Lambda_p\,T' \\ &= \Omega^{-1}\,\mathcal{E}\,S^{-p}\end{aligned}$$

Hence

$$\Omega^{-1}\,\mathcal{E}\,S^{-p} > 0 \quad \text{as} \quad \Omega^{-1}\,(\mathcal{E}\,S^{-p})\,\Omega^{-\frac{1}{2}} > 0 \quad \square$$

Because $\mathcal{E}\,S^{-(p+1)} > 0$ and $\sum_{k=1}^{p} \mathcal{E}\left(\operatorname{tr} S^{-k}\right) S^{k-(p+1)} > 0$ we conclude from (2) that

$$\Omega^{-1}\,\mathcal{E}\,S^{-p} < (n-m-p-1)\mathcal{E}\,S^{-(p+1)} \tag{5}$$

when $p < n-m-1$. Or equivalently

$$\left(\mathcal{E}\,S^{-1}\right)\mathcal{E}\,S^{-p} < (n-m-1)^{-1}(n-m-p-1)\mathcal{E}\,S^{-(p+1)} < \mathcal{E}\,S^{-(p+1)} \tag{6}$$

as

$$\mathcal{E}\,S^{-1} = (n-m-1)^{-1}\,\Omega^{-1}$$

and $(n-m-1)^{-1}(n-m-p-1) < 1$.

The inequality (6) ultimately leads by successive substitution to the inequality

$$\mathcal{E}\,S^{-p} > \left(\mathcal{E}\,S^{-1}\right)^{p} \quad (p \geq 2) \tag{7}$$

As $\mathcal{E}\,S^{-1} = n(n-m-1)^{-1}\,(\mathcal{E}\,S)^{-1} > (\mathcal{E}\,S)^{-1}$, we can get the inequality

$$\mathcal{E}\,S^{-p} > \left(\mathcal{E}\,S^{-1}\right)^{p} > (\mathcal{E}\,S)^{-p} \tag{8}$$

It is known that

$$\mathcal{E}\,S^{p} > (\mathcal{E}\,S)^{p} \qquad p \geq 2 \tag{9}$$

See the end of section 2.

Combining (8) and (9) we finally have the inequality

$$\mathcal{E}\,S^{-p} > \left(\mathcal{E}\,S^{-1}\right)^{p} > (\mathcal{E}\,S)^{-p} > (\mathcal{E}\,S^{p})^{-1} \tag{10}$$

5 References

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Book review

PATTERN RECOGNITION AND MACHINE LEARNING

Cristopher M. Bishop

Information Science and Statistics

Springer 2006, 738 pages

As the author writes in the preface of the book, pattern recognition has its origin in engineering, whereas machine learning grew out of computer science. However, these activities can be viewed as two facets of the same field, and they have undergone substantial development over the past years.

Bayesian methods are widely used, while graphical models have emerged as a general framework for describing and applying probabilistic models. Similarly new models based on kernels have had significant impact on both algorithms and applications.

This textbook reflects these recent developments while providing a comprehensive introduction to the fields of pattern recognition and machine learning. It is aimed at advanced undergraduate or first year PhD students, as well as researchers and practitioners. It can be consider as an introductory course to the subject.

The first four chapters are devoted to the concepts of Probability and Statistics that are needed for reading the rest of the book, so we can imagine that the speed is high in order to get from zero to infinity. I believe that it is better to study the book after a previous course on Probability and Statistics. On the other hand, a basic knowledge of linear algebra and multivariate calculus is assumed.

The other chapters give to a classic probabilist or statistician a point of view on some applications that are very interesting but far from his usual world. In all the text the mathematical aspects are at the second level in relation with the ideas and intuitions that the author wants to communicate.

The book is supported by a great deal of additional material, including lecture slides as well as the complete set of figures used in it, and the reader is encouraged to visit the book web site for the latest information. So it can be very useful for a course or a talk about the subject.

The exercises that appear at the end of the chapters form an important component of the book. They reinforce or generalize concepts explained in the text, and are graded according to difficulty. The solutions to the exercises considered by the author to amplify key points or fill in important details can be found also as a PDF file in the web book site.

This book focuses on concepts and principles and not on the use of key algorithms for appropriate data sets. The author announces a companion volume in 2008, which will deal with practical aspects of pattern recognition and machine learning. It will be accompanied by Matlab software, implementing most of the algorithms discussed in this text. This second part is necessary to complete the gap of the present volume.

Though this book has to be considered a first contact with these interesting fields, the list of references is wide enough to satisfy our curiosity.

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