Probabilistic Forecasts for Hierarchical Time Series

Puwasala Gamakumara*
Department of Econometrics and Business Statistics,
Monash University,
VIC 3800, Australia.
Email: Puwasala.Gamakumara@monash.edu
and
Anastasios Panagiotelis
Department of Econometrics and Business Statistics,
Monash University,
VIC 3800, Australia.
Email: Anastasios.Panagiotelis@monash.edu
and
George Athanasopoulos
Department of Econometrics and Business Statistics,
Monash University,
VIC 3800, Australia.
Email: george.athanasopoulos@monash.edu
and
Rob J Hyndman
Department of Econometrics and Business Statistics,
Monash University,
VIC 3800, Australia.
Email: rob.hyndman@monash.edu

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Abstract

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1 Introduction

Large collections of time series often follow some aggregation structure. For example, the tourism flow of a country can be disaggregated along a geographic hierarchy of states, zones, and cities. These are ordinarily referred to as hierarchical time series. To ensure aligned decision making, it is important that forecasts at the most disaggregated level add up to forecasts at more aggregated levels. This property is called "coherence". On the other hand "reconciliation" is a process whereby incoherent forecasts are made coherent. Both of these concepts have been developed extensively for point forecasting. Generalising both of these concepts, particularly the latter, to probabilistic forecasting is a gap that we seek to address in this work. We do so by extending the geometric interpretation to coherence and reconciliation in the point forecasting case outlined in (cite the first paper) to the probabilistic framework. This is allowing us to derive further results for parametric as well as non-parametric distributional forecasts for hierarchical time series.

Traditional approaches to ensure coherent point forecasts produce first-stage forecasts at a single level of the hierarchy. To describe these we use the small hierarchy in Figure 1 where the variable labelled Tot is the sum of the series A and series B, the series A is the sum of series AA and series AB and the series B is the sum of the series BA and BB. In the bottom-up approach (Dunn et al. 1976), forecasts are produced at the most disaggregated level (series AA, AB, BA and BB) and then summed to recover forecasts for all higher-level series. Alternatively, in the top-down approach (Gross & Sohl 1990), a top-level forecast is first produced (series Tot) and bottom-level forecasts are recovered by disaggregating the forecast using either historical or forecasted proportions. A middle-out approach is a hybrid between these two, that for the hierarchy in Figure 1 would produce first stage forecasts for series A and B.

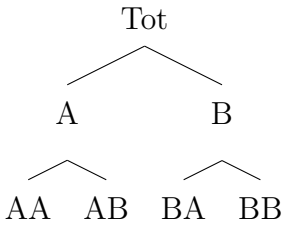

Figure 1: An example of a two level hierarchical structure.

In recent years, reconciliation methods introduced by Hyndman et al. (2011) have become increasingly popular. For these methods, first stage forecasts are independently produced for all series rather than series at a single level. Since these so-called 'base' forecasts are rarely coherent in practice, they are subsequently adjusted or 'reconciled' to ensure coherence. Note that we use coherence and reconciliation as distinct terms, in contrast to their at times ambiguous usage in the past. To date, reconciliation has typically been formulated as a regression problem with alternative reconciliation methods resembling different least squares estimators. These include Ordinary Least Squares OLS (Hyndman et al. 2011), Weighted Least Squares WLS (Athanasopoulos et al. 2017), and a Generalised Least Squares (GLS) estimator (Wickramasuriya et al. 2018) named MinT since it minimises the trace of the squared error matrix. These methods have been shown to outperform traditional alternatives across a range of simulated and real-world datasets (Athanasopoulos et al. 2009, van Erven & Cugliari 2014, Wickramasuriya et al. 2018) since they use information at all levels of the hierarchy and, in some sense, hedge against the risk of model misspecification at a single level.

A shortcoming of the existing literature is a focus on point forecasting despite an increased understanding over the past decade of the importance of providing a full predictive distribution for forecast uncertainty (see Gneiting & Katzfuss 2014, and references therein).

Indeed to the best of our knowledge, the (as yet unpublished) work of (Ben Taieb et al. 2017) is the only paper to deal with coherent probabilistic forecasts, and although they reconcile the means of the predictive distributions, the overall distributions are constructed in a bottom-up fashion rather than use a reconciliation process. In contrast, the main objective of our paper is to generalise both coherence and reconciliation from point to probabilistic forecasting.

To facilitate the extension of point forecast reconciliation to probabilistic forecasting, we first provide a geometric interpretation of existing point reconciliation methods, framing them in terms of projections. In addition to being highly intuitive, this allows us to establish a number of theoretical results. We prove two new theorems about point forecast reconciliation, the first showing that reconciliation via projections preserves the unbiasedness of base forecasts, while the second shows that reconciled forecasts dominate unreconciled forecasts via the distance reducing property of projections. We provide definitions of coherence and forecast reconciliation in the probabilistic setting, and describe how these definitions lead to a reconciliation procedure that merely involves a change of basis and marginalisation. We show that probabilistic reconciliation via linear transformations can recover the true predictive distribution as long as the latter is in the elliptical class. We provide conditions for which this linear transformation is a projection, and although this projection cannot be feasibly estimated in practice, we provide a heuristic argument in favour of MinT reconciliation.

We also cover the topic of forecast evaluation of probabilistic forecasts via scoring rules. In particular, we prove that for a coherent data generating process, the log score is not proper with respect to incoherent forecasts. Therefore we recommend the use of the energy score or variogram score for comparing reconciled to unreconciled forecasts. Two or more reconciled forecasts can be compared using log score, energy score or variogram score,

although we show that comparisons should be made on the full hierarchy for the latter two scores.

The remainder of the paper is structured as follows. In Section 2 coherence is defined geometrically for both point and probabilistic forecasts. Section 3 contains definitions of point and probabilistic forecast reconciliation as well as our main theoretical results. In Section 4 we consider the evaluation of probabilistic hierarchical forecasts via scoring rules, while a simulation study comparing unreconciled probabilistic forecasts and different kinds of reconciled probabilistic forecasts is provided in Section **??**. Section 7 concludes with some discussion and thoughts on future research.

2 Coherent forecasts

2.1 Notation and preliminaries

A *hierarchical time series* is a collection of n variables indexed by time, where some variables are aggregates of other variables. We let $\boldsymbol{y}_t \in \mathbb{R}^n$ be a vector comprising observations of all variables in the hierarchy at time t. The *bottom-level series* are defined as those m variables that cannot be formed as aggregates of other variables; we let $\boldsymbol{b}_t \in \mathbb{R}^m$ be a vector comprised of observations of all bottom-level series at time t. The hierarchical structure of the data implies that

$$\boldsymbol{y}_t = \boldsymbol{S}\boldsymbol{b}_t, \tag{1}$$

where $\boldsymbol{S}$ is an $n \times m$ constant matrix that encodes the aggregation constraints, holds for all t.

To clarify these concepts consider the example of the hierarchy in Figure 1. For this hierarchy, $n = 7$, $\boldsymbol{y}_t = [y_{Tot,t}, y_{A,t}, y_{B,t}, y_{C,t}, y_{AA,t}, y_{AB,t}, y_{BA,t}, y_{BB,t}]'$, $m = 4$, $\boldsymbol{b}_t =$

$[y_{AA,t}, y_{AB,t}, y_{BA,t}, y_{BB,t}]'$ and

$$\boldsymbol{S} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ & \boldsymbol{I}_4 & & \end{pmatrix},$$

where $\boldsymbol{I}_4$ is the 4×4 identity matrix.

While most applications of hierarchical time series to date have involved data that respect an aggregation structure, in principle the matrix $\boldsymbol{S}$ can encode any linear constraints including weighted sums or even cases where some variables in the hierarchy are formed by taking the difference of two other variables.

2.2 Coherent probabilistic forecasts

Let $(\mathbb{R}^m, \mathscr{F}_{\mathbb{R}^m}, \nu)$ be a probability triple, where $\mathscr{F}_{\mathbb{R}^m}$ is the usual Borel σ-algebra on $\mathbb{R}^m$. Let $\breve{\nu}$ be a probability measure on $\mathfrak{s}$ with σ-algebra $\mathscr{F}_{\mathfrak{s}}$. Here $\mathscr{F}_{\mathfrak{s}}$ is a collection of sets $s(\mathcal{B})$, where $s(\mathcal{B})$ denotes the image of the set $\mathcal{B} \in \mathscr{F}_{\mathbb{R}^m}$ under the mapping $s(.)$.

Definition 2.1 (Coherent Probabilistic Forecasts)**.** The measure $\breve{\nu}$ is coherent if it has the property

$$\breve{\nu}(s(\mathcal{B})) = \nu(\mathcal{B}) \quad \forall \mathcal{B} \in \mathscr{F}_{\mathbb{R}^m},$$

A probabilistic forecast for time $t+h$ is coherent if uncertainty in $\breve{\boldsymbol{y}}_{t+h}$ conditional on all information up to time t is characterised by the probability triple $(\mathfrak{s}, \mathscr{F}_{\mathfrak{s}}, \breve{\nu})$.

Add a sentence about taking bottom level series as basis series.

To the best of our knowledge, the only other definition of coherent probabilistic forecasts is given by Ben Taieb et al. (2017) who define coherent probabilistic forecasts in terms of convolutions. According to their definition, probabilistic forecasts are coherent when

a convolution of forecast distributions of disaggregate series is identical to the forecast distribution of the corresponding aggregate series. Their definition is consistent with our definition; our reason for providing a different definition is that the geometric understanding of coherence will facilitate our definitions of point and probabilistic forecast reconciliation to which we now turn our attention.

3 Forecast reconciliation

We extend this idea to the novel concept of probabilistic reconciliation.

3.1 Probabilistic forecast reconciliation

We now extend the methodology of point forecast reconciliation to probabilistic forecasts. Let $(\mathbb{R}^n, \mathscr{F}_{\mathbb{R}^n}, \hat{\nu})$ be a probability triple that is not coherent and which characterises forecast uncertainty for all variables in the hierarchy at time $t+h$ conditional on all information up to time t. This is obtained from the first stage of the forecasting process; e.g., by modelling and forecasting each series individually. Let $g : \mathbb{R}^n \to \mathbb{R}^m$ be a linear function, and let $(\mathbb{R}^m, \mathscr{F}_{\mathbb{R}^m}, \nu)$ be a probability triple defined on $\mathbb{R}^m$.

Definition 3.1. The reconciled probability measure of $\hat{\nu}$ with respect to the mapping $g(.)$ is a probability measure $\tilde{\nu}$ on $\mathfrak{s}$ with σ-algebra $\mathscr{F}_{\mathfrak{s}}$ such that

$$\tilde{\nu}(s(\mathcal{B})) = \nu(\mathcal{B}) = \hat{\nu}(g^{-1}(\mathcal{B})) \qquad \forall \mathcal{B} \in \mathscr{F}_{\mathbb{R}^m}\,, \tag{2}$$

where $g^{-1}(\mathcal{B}) := \{\breve{\boldsymbol{y}} \in \mathbb{R}^n : g(\breve{\boldsymbol{y}}) \in \mathcal{B}\}$ is the pre-image of $\mathcal{B}$, that is the set of all points in $\mathbb{R}^n$ that $g(.)$ maps to a point in $\mathcal{B}$.

This definition extends the notion of forecast reconciliation to the probabilistic setting. Under point reconciliation methods, the reconciled point forecast is equal to the

unreconciled point forecast after the latter is passed through two linear functions. Similarly, probabilistic forecast reconciliation assigns the same probability to two sets where the points in one set are obtained by passing all points in the other set through two linear functions. This is depicted in Figure 2 schematically when $s \circ g$ is a projection.

Recall that when $s \circ g$ is a projection, the case of point forecast reconciliation can be broken down into three steps.

1. $\hat{\boldsymbol{y}}_{t+h|t}$ is transformed into coordinates $\tilde{\boldsymbol{b}}_{t+h|t}$ and $\tilde{\boldsymbol{a}}_{t+h|t}$ via a change of basis.
2. $\tilde{\boldsymbol{a}}_{t+h|t}$ is discarded and $\tilde{\boldsymbol{b}}_{t+h|t}$ are kept as the bottom-level reconciled forecasts.
3. Reconciled forecasts for the entire hierarchy are recovered via $\tilde{\boldsymbol{y}}_{t+h|t} = \boldsymbol{S}\tilde{\boldsymbol{b}}_{t+h|t}$.

We now outline the analogous steps for probabilistic forecasts when predictive densities are available.

While $\hat{\nu}$ is a probability measure for an n-vector $\hat{\boldsymbol{y}}_{t+h|t}$, probability statements in terms of a different coordinate system can be made via an appropriate change of basis. Letting $f(.)$ be generic notation for a probability density function, and following the notation from our definition of point forecast reconciliation where $\hat{\boldsymbol{y}}_{t+h|t} = \boldsymbol{S}\tilde{\boldsymbol{b}}_{t+h|t} + \boldsymbol{R}\tilde{\boldsymbol{a}}_{t+h|t}$, we obtain

$$f(\hat{\boldsymbol{y}}_{t+h|t}) = f(\boldsymbol{S}\tilde{\boldsymbol{b}}_{t+h|t} + \boldsymbol{R}\tilde{\boldsymbol{a}}_{t+h|t})|(\boldsymbol{S}\ \boldsymbol{R})| \tag{3}$$

The expression $\hat{\nu}(g^{-1}(\mathcal{B}))$ in Definition 3.1 is equivalent to the probability statement $\Pr(\hat{\boldsymbol{y}}_{t+h|t} \in g^{-1}(\mathcal{B}))$. After the change of basis, this is equivalent to $\Pr(\tilde{\boldsymbol{b}} \in \mathcal{B})$, which implies

$$\Pr(\hat{\boldsymbol{y}}_{t+h|t} \in g^{-1}(\mathcal{B})) = \int_{g^{-1}(\mathcal{B})} f(\hat{\boldsymbol{y}}_{t+h|t}) d\hat{\boldsymbol{y}}_{t+h|t} \tag{4}$$

$$= \int_{\mathcal{B}} \int f(\boldsymbol{S}\tilde{\boldsymbol{b}}_{t+h|t} + \boldsymbol{R}\tilde{\boldsymbol{a}}_{t+h|t})|(\boldsymbol{S}\ \boldsymbol{R})| d\tilde{\boldsymbol{a}}_{t+h|t} d\tilde{\boldsymbol{b}}_{t+h|t}. \tag{5}$$

After integrating out over $\tilde{\boldsymbol{a}}_{t+h|t}$, a step analogous to setting $\tilde{\boldsymbol{a}}_{t+h|t} = 0$ for point forecasting, we obtain an expression that gives the probability that the reconciled bottom-level series

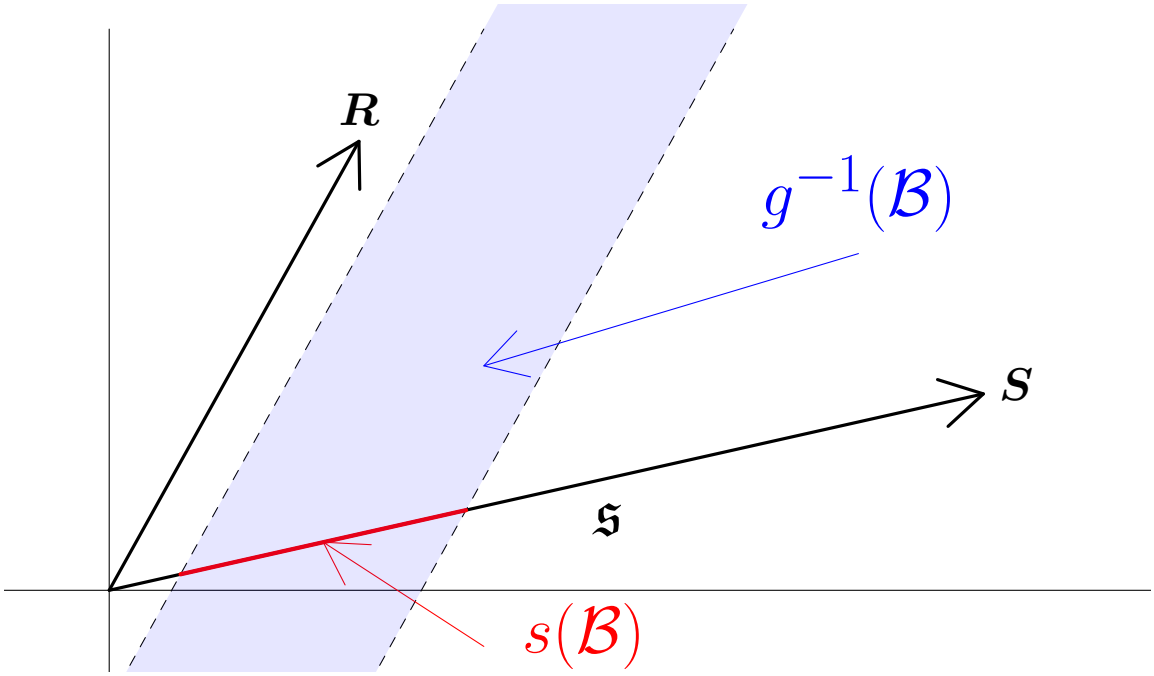

Figure 2: Summary of probabilistic forecast reconciliation. The probability that $\boldsymbol{y}_{t+h}$ lies in the red line segment under the reconciled probabilistic forecast is defined to be equal to the probability that $\boldsymbol{y}_{t+h}$ lies in the shaded blue area under the unreconciled probabilistic forecast. Note that since the smallest hierarchy involves three dimensions, this figure is only a schematic.

lies in the region $\mathcal{B}$. This corresponds to $\nu(\mathcal{B})$ in Definition 3.1. To make a valid probability statement about the entire hierarchy we simply use the bottom-level probabilistic forecasts together with Definition 2.1.

Example: Gaussian Distributions

Suppose an unreconciled probabilistic forecast is Gaussian with mean $\hat{\boldsymbol{\mu}}$ and variance-covariance matrix $\hat{\boldsymbol{\Sigma}}$. The subscripts $t+h|t$ are suppressed for brevity. Let the unreconciled density be given by

$$f(\hat{\boldsymbol{y}}) = (2\pi)^{-n/2}|\hat{\boldsymbol{\Sigma}}|^{-1/2}\exp\left\{-\frac{1}{2}\left[(\hat{\boldsymbol{y}}-\hat{\boldsymbol{\mu}})'\hat{\boldsymbol{\Sigma}}^{-1}(\hat{\boldsymbol{y}}-\hat{\boldsymbol{\mu}})\right]\right\}. \tag{6}$$

In an alternative basis,

$$f(\tilde{\boldsymbol{b}},\tilde{\boldsymbol{a}}) = (2\pi)^{-\frac{n}{2}}\left|\hat{\boldsymbol{\Sigma}}\right|^{-\frac{1}{2}}\left|(\boldsymbol{S}\ \boldsymbol{R})\right|\exp\{-\frac{1}{2}q\}, \tag{7}$$

where

$$q = (\boldsymbol{S}\tilde{\boldsymbol{b}}+\boldsymbol{R}\tilde{\boldsymbol{a}}-\hat{\boldsymbol{\mu}})'\hat{\boldsymbol{\Sigma}}^{-1}(\boldsymbol{S}\tilde{\boldsymbol{b}}+\boldsymbol{R}\tilde{\boldsymbol{a}}-\hat{\boldsymbol{\mu}}). \tag{8}$$

The quadratic form q can be rearranged as

$$\begin{aligned} q &= \left((\boldsymbol{S}\ \boldsymbol{R})\begin{pmatrix}\tilde{\boldsymbol{b}}\\ \tilde{\boldsymbol{a}}\end{pmatrix}-\hat{\boldsymbol{\mu}}\right)'\hat{\boldsymbol{\Sigma}}^{-1}\left((\boldsymbol{S}\ \boldsymbol{R})\begin{pmatrix}\tilde{\boldsymbol{b}}\\ \tilde{\boldsymbol{a}}\end{pmatrix}-\hat{\boldsymbol{\mu}}\right), \\ &= \left(\begin{pmatrix}\tilde{\boldsymbol{b}}\\ \tilde{\boldsymbol{a}}\end{pmatrix}-(\boldsymbol{S}\ \boldsymbol{R})^{-1}\hat{\boldsymbol{\mu}}_{t+h}\right)'\left[(\boldsymbol{SR})^{-1}\hat{\boldsymbol{\Sigma}_{t+h}}\left((\boldsymbol{S}\ \boldsymbol{R})^{-1}\right)'\right]^{-1}\left(\begin{pmatrix}\tilde{\boldsymbol{b}}\\ \tilde{\boldsymbol{a}}\end{pmatrix}-(\boldsymbol{S}\ \boldsymbol{R})^{-1}\hat{\boldsymbol{\mu}}_{t+h}\right). \end{aligned}$$

Recall that

$$(\boldsymbol{S}\ \boldsymbol{R})^{-1} = \begin{pmatrix}(\boldsymbol{R}_\perp'\boldsymbol{S})^{-1}\boldsymbol{R}_\perp'\\ (\boldsymbol{S}_\perp'\boldsymbol{R})^{-1}\boldsymbol{S}_\perp'\end{pmatrix} := \begin{pmatrix}\boldsymbol{G}\\ \boldsymbol{H}\end{pmatrix}.$$

Then q can be rearranged further as

$$q = \left[\begin{pmatrix}\tilde{\boldsymbol{b}}\\ \tilde{\boldsymbol{a}}\end{pmatrix} - \begin{pmatrix}\boldsymbol{G}\\ \boldsymbol{H}\end{pmatrix}\hat{\boldsymbol{\mu}}_{t+h}\right]' \left[\begin{pmatrix}\boldsymbol{G}\\ \boldsymbol{H}\end{pmatrix}\hat{\boldsymbol{\Sigma}}_{t+h}\begin{pmatrix}\boldsymbol{G}\\ \boldsymbol{H}\end{pmatrix}'\right]^{-1}\left[\begin{pmatrix}\tilde{\boldsymbol{b}}\\ \tilde{\boldsymbol{a}}\end{pmatrix} - \begin{pmatrix}\boldsymbol{G}\\ \boldsymbol{H}\end{pmatrix}\hat{\boldsymbol{\mu}}_{t+h}\right]$$

$$= \begin{pmatrix}\tilde{\boldsymbol{b}} - \boldsymbol{G}\hat{\boldsymbol{\mu}}\\ \tilde{\boldsymbol{a}} - \boldsymbol{H}\hat{\boldsymbol{\mu}}\end{pmatrix}' \left[\begin{pmatrix}\boldsymbol{G}\\ \boldsymbol{H}\end{pmatrix}\hat{\boldsymbol{\Sigma}}_{t+h}\begin{pmatrix}\boldsymbol{G}\\ \boldsymbol{H}\end{pmatrix}'\right]^{-1}\begin{pmatrix}\tilde{\boldsymbol{b}} - \boldsymbol{G}\hat{\boldsymbol{\mu}}\\ \tilde{\boldsymbol{a}} - \boldsymbol{H}\hat{\boldsymbol{\mu}}\end{pmatrix}.$$

Similar manipulations on the determinant of the covariance matrix lead to the following expression for the density:

$$f(\tilde{\boldsymbol{b}}, \tilde{\boldsymbol{a}}) = (2\pi)^{-\frac{n}{2}}\left|\begin{pmatrix}\boldsymbol{G}\hat{\boldsymbol{\Sigma}}\boldsymbol{G}' & \boldsymbol{G}\hat{\boldsymbol{\Sigma}}\boldsymbol{H}'\\ \boldsymbol{H}\hat{\boldsymbol{\Sigma}}\boldsymbol{G}' & \boldsymbol{H}\hat{\boldsymbol{\Sigma}}\boldsymbol{H}'\end{pmatrix}\right|^{-\frac{1}{2}} \exp\left\{-\frac{1}{2}\begin{pmatrix}\tilde{\boldsymbol{b}} - \boldsymbol{G}\hat{\boldsymbol{\mu}}\\ \tilde{\boldsymbol{a}} - \boldsymbol{H}\hat{\boldsymbol{\mu}}\end{pmatrix}'\right.$$
$$\left.\begin{pmatrix}\boldsymbol{G}\hat{\boldsymbol{\Sigma}}\boldsymbol{G}' & \boldsymbol{G}\hat{\boldsymbol{\Sigma}}\boldsymbol{H}'\\ \boldsymbol{H}\hat{\boldsymbol{\Sigma}}\boldsymbol{G}' & \boldsymbol{H}\hat{\boldsymbol{\Sigma}}\boldsymbol{H}'\end{pmatrix}^{-1}\begin{pmatrix}\tilde{\boldsymbol{b}} - \boldsymbol{G}\hat{\boldsymbol{\mu}}\\ \tilde{\boldsymbol{a}} - \boldsymbol{H}\hat{\boldsymbol{\mu}}\end{pmatrix}\right\}.$$

Marginalising out $\tilde{\boldsymbol{a}}$ leads to the following bottom-level reconciled forecasts:

$$f(\tilde{\boldsymbol{b}}) = (2\pi)^{-\frac{m}{2}}\left|\boldsymbol{G}\hat{\boldsymbol{\Sigma}}\boldsymbol{G}'\right|^{\frac{1}{2}} \exp\Big\{-\frac{1}{2}(\tilde{\boldsymbol{b}} - \boldsymbol{G}\hat{\boldsymbol{\mu}})'(\boldsymbol{G}\hat{\boldsymbol{\Sigma}}\boldsymbol{G}')^{-1}(\tilde{\boldsymbol{b}} - \boldsymbol{G}\hat{\boldsymbol{\mu}})\Big\}. \tag{9}$$

This implies that the reconciled probabilistic forecast for the bottom-level series is $\tilde{\boldsymbol{b}} \sim \mathcal{N}(\boldsymbol{G}\hat{\boldsymbol{\mu}}, \boldsymbol{G}\hat{\boldsymbol{\Sigma}}\boldsymbol{G}')$. The reconciled probabilistic forecasts for the whole hierarchy follow a degenerate Gaussian distribution with mean $\boldsymbol{SG}\hat{\boldsymbol{\mu}}$ and rank deficient covariance matrix $\boldsymbol{SG}\hat{\boldsymbol{\Sigma}}\boldsymbol{G}'\boldsymbol{S}'$.

3.2 Elliptical distributions

We now show that the true predictive distribution can be recovered for elliptical distributions by linear reconciliation via pre-multiplication and translation respectively by a matrix

we denote $\boldsymbol{G}_{opt}$ and vector we denote $\boldsymbol{d}_{opt}$. Here, for any square matrix $\boldsymbol{C}$, $\boldsymbol{C}^{1/2}$ and $\boldsymbol{C}^{-1/2}$ are defined to satisfy $\boldsymbol{C}^{1/2}(\boldsymbol{C}^{1/2})' = \boldsymbol{C}$ and $\boldsymbol{C}^{-1/2}(\boldsymbol{C}^{-1/2})' = \boldsymbol{C}^{-1}$, for example $\boldsymbol{C}^{1/2}$ may be obtained via the Cholesky or eigenvalue decompositions.

Theorem 3.1 (Reconciliation for Elliptical Distributions)**.** *Let an unreconciled probabilistic forecast come from the elliptical class with location parameter $\hat{\boldsymbol{\mu}}$ and scale matrix $\hat{\boldsymbol{\Sigma}}$. Let the true predictive distribution of $\boldsymbol{y}$ also belong to the elliptical class with location parameter $\boldsymbol{\mu}$ and scale matrix $\boldsymbol{\Sigma}$. Then the linear reconciliation mapping $g(\breve{\boldsymbol{y}}) = \boldsymbol{G}_{opt}\breve{\boldsymbol{y}} + \boldsymbol{d}_{opt}$ with $\boldsymbol{G}_{opt} = \boldsymbol{a}\hat{\boldsymbol{\Sigma}}^{-1/2}$ and $\boldsymbol{d}_{opt} = \boldsymbol{\mu} - \boldsymbol{S}\boldsymbol{G}_{opt}\hat{\boldsymbol{\mu}}$ recovers the true predictive density where $\boldsymbol{a}$ is any $m \times n$ matrix such that $\boldsymbol{a}\boldsymbol{a}' = \boldsymbol{\Omega}$ and $\boldsymbol{\Omega}$ is a sub-matrix of $\boldsymbol{\Sigma}$ corresponding to the bottom-level series.*

Proof. Since elliptical distributions are closed under affine transformations, and are closed under marginalisation, reconciliation of an elliptical distribution yields an elliptical distribution (although the unreconciled and reconciled distributions may be different members of the class of elliptical distributions). The scale matrix of the reconciled forecast is given by $\boldsymbol{S}\boldsymbol{G}_{opt}\hat{\boldsymbol{\Sigma}}\boldsymbol{G}'_{opt}\boldsymbol{S}'$, while the location matrix is given by $\boldsymbol{S}\boldsymbol{G}_{opt}\hat{\boldsymbol{\mu}} + \boldsymbol{d}_{opt}$. The reconciled scale matrix is

$$\tilde{\boldsymbol{\Sigma}}_{opt} = \boldsymbol{S}\boldsymbol{a}\hat{\boldsymbol{\Sigma}}^{-1/2}\hat{\boldsymbol{\Sigma}}\left(\hat{\boldsymbol{\Sigma}}^{-1/2}\right)'\boldsymbol{a}'\boldsymbol{S}' = \boldsymbol{S}\boldsymbol{\Omega}\boldsymbol{S}' = \boldsymbol{\Sigma}.$$

For the choices of $\boldsymbol{G}_{opt}$ and $\boldsymbol{d}_{opt}$ given above, the reconciled location vector is

$$\tilde{\boldsymbol{\mu}}_{opt} = \boldsymbol{S}\boldsymbol{G}_{opt}\hat{\boldsymbol{\mu}} + \boldsymbol{\mu} - \boldsymbol{S}\boldsymbol{G}_{opt}\hat{\boldsymbol{\mu}} = \boldsymbol{\mu}.$$

□

A number of insights can be drawn from this theorem. First, although a linear function $g(.)$ can be used to recover the true predictive in the elliptical case, the same does not hold

in general. Second, $g(.)$ is not, in general, a projection matrix. The conditions for which a the true predictive density can be recovered by a projection are given below.

Theorem 3.2 (True predictive via projection)**.** *Assume that the true predictive distribution is elliptical with location $\boldsymbol{\mu}$ and scale $\boldsymbol{\Sigma}$. Consider reconciliation via a projection $g(\boldsymbol{y}) = (\boldsymbol{R}_\perp' \boldsymbol{S})^{-1} \boldsymbol{R}_\perp' \boldsymbol{y}$. The true predictive distribution can be recovered via reconciliation of an elliptical distribution with location $\hat{\boldsymbol{\mu}}$ and scale $\hat{\boldsymbol{\Sigma}}$ when the following conditions hold:*

$$sp(\hat{\boldsymbol{\mu}} - \boldsymbol{\mu}) \subset sp(\boldsymbol{R}) \tag{10}$$

$$sp(\hat{\boldsymbol{\Sigma}}^{1/2} - \boldsymbol{\Sigma}^{1/2}) \subset sp(\boldsymbol{R}) \tag{11}$$

$$\tag{12}$$

Proof. The reconciled location vector will be given by

$$\begin{aligned}
\tilde{\boldsymbol{\mu}} &= \boldsymbol{S}(\boldsymbol{R}_\perp' \boldsymbol{S})^{-1} \boldsymbol{R}_\perp' \hat{\boldsymbol{\mu}} \\
&= \boldsymbol{S}(\boldsymbol{R}_\perp' \boldsymbol{S})^{-1} \boldsymbol{R}_\perp' \left(\hat{\boldsymbol{\mu}} + \boldsymbol{\mu} - \boldsymbol{\mu}\right) \\
&= \boldsymbol{S}(\boldsymbol{R}_\perp' \boldsymbol{S})^{-1} \boldsymbol{R}_\perp' \boldsymbol{\mu} + \boldsymbol{S}(\boldsymbol{R}_\perp' \boldsymbol{S})^{-1} \boldsymbol{R}_\perp' \left(\hat{\boldsymbol{\mu}} - \boldsymbol{\mu}\right).
\end{aligned}$$

Since $\boldsymbol{S}(\boldsymbol{R}_\perp' \boldsymbol{S})^{-1} \boldsymbol{R}_\perp'$ is a projection onto $\mathfrak{s}$ and $\boldsymbol{\mu} \in \mathfrak{s}$, the first term simplifies to $\boldsymbol{\mu}$. If $\boldsymbol{\mu} - \hat{\boldsymbol{\mu}}$ lies in the span of $\boldsymbol{R}$, then multiplication by $\boldsymbol{R}_\perp'$ reduces the second term to $\mathbf{0}$. By a similar argument it can be shown that $\tilde{\boldsymbol{\Sigma}}^{1/2} = \boldsymbol{\Sigma}^{1/2}$. The closure property of elliptical distributions under affine transformations ensures that the full true predictive distribution can be recovered. □

Although these conditions will rarely hold in practice and only apply to a limited class of distributions, they do provide some insight into selecting a projection for reconciliation. If the value of $\hat{\boldsymbol{\mu}}$ were equi-probable in all directions, then a projection orthogonal to $\mathfrak{s}$ would be a sensible choice for $\boldsymbol{R}$ since it would in some sense represent a 'median' direction for

$\boldsymbol{\mu} - \hat{\boldsymbol{\mu}}$. However, the one-step-ahead in-sample errors are usually correlated suggesting that $\hat{\boldsymbol{\mu}}$ is more likely to fall in some directions than others. Therefore an orthogonal projection after transformation by the inverse of the one-step-ahead in-sample error covariance matrix may be more intuitively appealing. This is exactly what the MinT projection provides, and as simulations will show in Section **??**, this projection leads to the best empirical results.

4 Evaluation of hierarchical probabilistic forecasts

The necessary final step in hierarchical forecasting is to make sure that our forecast distributions are accurate. In general, forecasters prefer to maximize the sharpness of the forecast distribution subject to calibration (Gneiting & Katzfuss 2014). Therefore the probabilistic forecasts should be evaluated with respect to these two properties.

Calibration refers to the statistical compatibility between probabilistic forecasts and realizations. In other words, random draws from a perfectly calibrated forecast distribution should be equivalent in distribution to the realizations. On the other hand, sharpness refers to the spread or the concentration of the predictive distributions and it is a property of the forecasts only. The more concentrated the forecast distributions, the sharper the forecasts (Gneiting et al. 2008). However, independently assessing the calibration and sharpness will not help to properly evaluate the probabilistic forecasts. Therefore we need to assess these properties simultaneously using scoring rules.

Scoring rules are summary measures obtained based on the relationship between the forecast distributions and the realizations. In some studies, researchers take the scoring rules to be positively oriented, in which case the scores should be maximized (Gneiting & Raftery 2007). However, scoring rules have also been defined to be negatively oriented, and then the scores should be minimized (Gneiting & Katzfuss 2014). We follow the latter

convention here.

Let P be a forecast distribution and let Q be the true data generating process respectively. Furthermore let ω be a realization from Q. Then a scoring rule is a function $S(P, \omega)$ that maps P, ω to $\mathbb{R}$. It is a "proper" scoring rule if

$$\mathrm{E}_{\boldsymbol{Q}}[S(Q, \omega)] \leq \mathrm{E}_{\boldsymbol{Q}}[S(P, \omega)], \tag{13}$$

where $\mathrm{E}_Q[S(P, \omega)]$ is the expected score under the true distribution Q (Gneiting et al. 2008, Gneiting & Katzfuss 2014). When this inequality is strict, the scoring rule is said to be strictly proper.

In the context of probabilistic forecast reconciliation there could be two motivations for using scoring rules. The first is to compare unreconciled densities to reconciled densities. Reconciliation itself is a valuable goal since it can be important in aligning decision making across, for example, different units of an enterprise. In the point forecasting literature, forecast reconciliation has also been shown to improve forecast performance (Athanasopoulos et al. 2017, Wickramasuriya et al. 2018). It will be worthwhile to see whether the same holds in the probabilistic forecasting case. The second motivation for using scoring rules is to compare two or more sets of reconciled probabilistic forecasts to one another. The objective here is to evaluate which reconciliation mapping $g(.)$ works best in practice.

4.1 Univariate scoring rules

One way to evaluate hierarchical probabilistic forecasts is via the application of univariate scoring rules to each variable in the hierarchy. A summary can be taken of the expected scores across each margin, for example a mean or median. In the simulations of Section **??**, we consider two such scoring rules. The log score is given by the log density, in this case for each margin of the probabilistic forecast. The cumulative rank probability score generalises

mean square error and is given by

$$\text{CRPS}(\breve{F}_i, y_i) = \int \left(\breve{F}_i(\breve{Y}_i) - \mathbb{1}(\breve{Y}_i < y_i) \right) d\breve{Y}_i \tag{14}$$

$$= \text{E}_{\breve{Y}_i} |\breve{Y}_i - y_i| - \frac{1}{2} \text{E}_{\breve{Y}_i} |\breve{Y}_i - \breve{Y}_i^*| \,, \tag{15}$$

where $\breve{F}_i$ is the cumulative distribution function of the ith margin of the probabilistic forecast, $\breve{Y}_i$ and $\breve{Y}_i^*$ are independent copies of a random variable with distribution $\breve{F}_i$, and y_i is the outcome of the ith margin. The expectations in the second line can be approximated by Monte Carlo when a sample from the predictive distribution is available.

An advantage to this approach is that it allows the forecaster to evaluate the levels and individual series of the hierarchy where the gains from reconciliation are greatest. For this reason this approach has been used in the limited literature on probabilistic forecasting for hierarchies (Ben Taieb et al. 2017, Jeon et al. 2018) to date. A major shortcoming of this approach however, is that evaluating univariate scores on the margins does not account for the dependence in the hierarchy.

4.2 Multivariate scoring rules

While a number of alternative proper scoring rules are available for univariate forecasts, the multivariate case is somewhat more limited. Here we focus on three scoring rules: the log score (LS), the energy score (ES) and the variogram score (VS).

The log score can be approximated using a sample of values from the probabilistic forecast density (Jordan et al. 2017); however it is more commonly used when a parametric form for the density is available for the probabilistic forecast.

The energy score on the other hand can be defined in terms of the characteristic function

of the probabilistic forecast, but the following representation in terms of expectations

$$\mathrm{ES}(\breve{\boldsymbol{Y}}_{T+h}, \boldsymbol{y}_{T+h}) = \mathrm{E}_{\breve{\boldsymbol{Y}}}||\breve{\boldsymbol{Y}}_{T+h} - \boldsymbol{y}_{T+h}||^{\alpha} - \frac{1}{2}\mathrm{E}_{\breve{\boldsymbol{Y}}}||\breve{\boldsymbol{Y}}_{T+h} - \breve{\boldsymbol{Y}}^{*}_{T+h}||^{\alpha},\ \alpha \in (0, 2]\,, \tag{16}$$

lends itself to easy computation when samples from the probabilistic forecast are available. An interesting limiting case is where $\alpha = 2$, where it can be easily shown that energy score simplifies to mean squared error around the mean of the predictive distribution. In this limiting case, the energy score is proper but not strictly proper. Pinson & Tastu (2013) also argue that the energy score has low discriminative ability for incorrectly specified covariances, even though it discriminates the misspecified means well.

In contrast, Scheuerer & Hamill (2015) have shown that the variogram score has a higher discrimination ability for misspecified means, variances and correlation structures than the energy score. When $\breve{\boldsymbol{y}}$ is a random variable from probabilistic forecast $\breve{F}$, the empirical variogram score is defined as

$$\mathrm{VS}(\breve{F}, \boldsymbol{y}) = \sum_{i=1}^{n}\sum_{j=1}^{n} w_{ij}\left(|y_i - y_j|^{p} - E_{\breve{Y}_i,\breve{Y}_j}|\breve{Y}_i - \breve{Y}_j|^{p}\right)^{2}. \tag{17}$$

Scheuerer & Hamill (2015) recommend using $p = 0.5$.

4.2.1 Comparing unreconciled forecasts to reconciled forecasts

For both reconciled and unreconciled densities it is possible to obtain a density from the probability measures defined in Section 2. Therefore it may seem sensible to compare unreconciled densities to reconciled densities on the basis of log score. However, the following theorem shows that using the log score may fail in the case of multivariate distributions with a degeneracy.

Theorem 4.1 (Impropriety of log score)**.** *When the true data generating process is coherent, then the log score is improper with respect to the class of incoherent measures.*

Proof. Consider a rotated version of hierarchical time series, $\boldsymbol{z}_t = \boldsymbol{U}\boldsymbol{y}_t$, so that the first m elements of $\boldsymbol{z}_t$ denoted $\boldsymbol{z}_t^{(1)}$ are unconstrained, while the remaining $n-m$ elements denoted $\boldsymbol{z}_t^{(2)}$ equal 0 when the aggregation constraints hold. An example of the $n \times n$ $\boldsymbol{U}$ is the matrix of left singular vectors of $\boldsymbol{S}$.

Consider the case where the true predictive density is $f_1(\boldsymbol{z}_t^{(1)})\mathbb{1}\left(\boldsymbol{z}_t^{(2)} = \boldsymbol{0}\right)$, and we evaluate an incoherent density given by $f_1(\boldsymbol{z}_t^{(1)})f_2(\boldsymbol{z}_t^{(2)})$, where f_2 is highly concentrated around 0 but still non-degenerate. For example, f_2 may be Gaussian with variance $\sigma^2\boldsymbol{I}$ with $\sigma^2 < (2\pi)^{-1}$. The log score under the true data generating process is

$$LS\left(f, \boldsymbol{z}_t^{(1)}\right) = -\log f_1\left(\boldsymbol{z}_t^{(1)}\right),$$

while that of the unreconciled density is

$$\begin{aligned} LS\left(\hat{f}, \boldsymbol{z}_t^{(1)}\right) &= -\log f_1(\boldsymbol{z}_t^{(1)}) - f_2(\boldsymbol{z}_t^{(1)}) && (18)\\ &= -\log f_1(\boldsymbol{z}_t^{(1)}) + \frac{n-m}{2}\log(2\pi\sigma^2) && (19)\\ &< -\log f_1(\boldsymbol{z}_t^{(1)}) = LS\left(f, \boldsymbol{z}_t^{(1)}\right). && (20) \end{aligned}$$

After taking expectations $E\left[LS(f,f)\right] > E\left[LS(\hat{f},f)\right]$, violating the condition in Equation (**??**) for a proper scoring rule. □

A similar issue also arises when discrete random variables are modelled as if they were continuous, an issue discussed in Section 4.1 of Gneiting & Raftery (2007). This implies that the log score should be avoided when comparing reconciled and unreconciled probabilistic forecasts.

4.2.2 Comparing reconciled forecasts to one another

Coherent probabilistic forecasts can be completely characterised in terms of basis series; if a probabilistic forecast is available for the basis series, then a probabilistic forecast can be

recovered for the entire hierarchy via Definition 2.1. This may suggest that it is adequate to merely compare two coherent forecasts to one another using the basis series only. We now show how this depends on the specific scoring rule used.

For the log score, suppose the coherent probabilistic forecast has density $f(\boldsymbol{b})$. The density for the full hierarchy is given by $f(\boldsymbol{y}) = f(\boldsymbol{S}\boldsymbol{b}) = f(\boldsymbol{b})J^{-1}$, where $J = \prod_{j=1}^{m} \lambda_j$ is a pseudo-determinant of the non-square matrix $\boldsymbol{S}$ and λ_j are the non-zero singular values of $\boldsymbol{S}$. Therefore for any coherent density, the log score of the full hierarchy differs from the log score for the bottom-level series by the term $log(J)$. This term depends only on the structure of the hierarchy and is fixed across different reconciliation methods. Therefore if one method achieves a lower expected log score compared to an alternative method using the bottom-level series only, the same ordering is preserved when an assessment is made on the basis of the full hierarchy.

The same property does not hold for all scores in general. For example, the energy score can be expressed in terms of expectations of norms. In general, since norms are invariant under orthogonal rotations, the energy score is also invariant under orthogonal transformations (Székely & Rizzo 2013, Gneiting & Raftery 2007). In the context of two coherent forecasts, the same is true of a semi-orthogonal transformation from a lower dimensional basis series to the full hierarchy. However, when $\boldsymbol{S}$ is the usual summing matrix, it is not semi-orthogonal. Therefore the energy score computed on the bottom-level series will differ from the energy score computed using the full hierarchy and the ordering of different reconciliation methods may change depending on the basis series used. In this case we recommend computing the energy score using the full hierarchy. Although the discussion here is related to energy score, the same logic holds for other multivariate scores, for example the variogram score.

The properties of multivariate scoring rules in the context of evaluating reconciled

	Coherent v Incoherent	Coherent v Coherent
Log Score	Not proper	Ordering preserved if compared using bottom-level only
Energy/	Proper	Full hierarchy should be used
Variogram Score	Proper	Full hierarchy should be used

Table 1: Summary of properties of scoring rules in the context of reconciled probabilistic forecasts.

probabilistic forecasts are summarised in Table 1.

5 A novel non-parametric bootstrap approach

5.1 Incoherent probabilistic forecasts

Our proposed method initially involves obtaining probabilistic forecasts without considering the aggregation constraints. That is we first get the incoherent probabilistic forecasts. Then we reconcile these to obtain the coherent probabilistic forecasts of the hierarchy.

Suppose we fit univariate models for each series in the hierarchy. Based on the fitted models, we obtain the sample paths at time $t+h$ as,

$$\boldsymbol{y}^{b}_{t+h} = E(\boldsymbol{y}_{t+h}|\boldsymbol{\mathcal{I}}_{t+h}) + \boldsymbol{e}^{b}_{t+h}, \tag{21}$$

where $E(\boldsymbol{y}_{t+h}|\boldsymbol{\mathcal{I}}_{t+h})$ is the conditional mean of the forecast distribution of the hierarchy at time $t+h$. $\boldsymbol{e}^{b}_{t+h}$ denotes the in-sample bootstrapped errors and these captures the contemporaneous correlation structure of the hierarchy.

Let $\hat{\boldsymbol{y}}_k \in \mathbb{R}^n$ is a vector comprising the fitted values of each series in the hierarchy at time k. Further let $\boldsymbol{\Gamma}_{(t\times n)} = (\boldsymbol{e}_1, \boldsymbol{e}_2, ..., \boldsymbol{e}_t)'$ denote the in-sample residual matrix where

$\boldsymbol{e}_k = \boldsymbol{y}_k - \hat{\boldsymbol{y}}_k$ for $k = 1, \cdots, t$. $\hat{\boldsymbol{e}}_k \in \mathbb{R}^n$ consists of residuals in each node at time k and stacked in the same order as $\boldsymbol{y}_k$. We block bootstrap a sample of size h from $\boldsymbol{\Gamma}$ which we denoted by $\boldsymbol{e}^b_{t+h}$. These bootstrapped errors will be incorporated as the error series for simulating future paths in (21). Taking blocked bootstrapped in-sample errors in generating future paths will implicitly model the dependency structure of the hierarchy.

Notice that $\boldsymbol{y}^b_{t+h} \in \mathbb{R}^n$ does not lie in the coherent subspace. Thus we call $\boldsymbol{y}^b_{t+h}$ as incoherent sample paths. Thousands of these sample paths will form an empirical sample from the incoherent forecast distribution of the hierarchy.

5.2 Reconciliation of incoherent future paths

It is expected that the probabilistic forecasts should be coherent in order to reflect the properties of real data. Thus we reconcile the incoherent future paths obtained in previous section to get coherent probabilistic forecasts.

Following the definition for reconciliation, we project each sample path to the coherent subspace $\mathfrak{s}$ via the projection $\boldsymbol{SG}$. Thus we have,

$$\tilde{\boldsymbol{y}}^b_{t+h} = \boldsymbol{SG}\boldsymbol{y}^b_{t+h}, \tag{22}$$

These reconciled future paths will form an empirical sample from the coherent forecast distribution that lies in the coherent subspace.

5.3 Optimal reconciliation of incoherent future paths

We propose to find the optimal $\boldsymbol{G}$ for reconciling future paths by minimising a proper multivariate scoring rule. The respective objective function can be written as,

$$\underset{\boldsymbol{G}}{\operatorname{argmin}} \quad \mathrm{E}_Q[S(\boldsymbol{SG}\boldsymbol{y}^b_{t+h}, \boldsymbol{y}_{t+h})]. \tag{23}$$

where S is a proper scoring rule that follows (13). Recall that the energy score given in (16) is a proper scoring rule and it can be approximated using Monte-Carlo sample paths as follows,

$$\text{ES}(\breve{\boldsymbol{Y}}_{T+h}, \boldsymbol{y}_{T+h}) \approx \frac{1}{B}\sum_{i=1}^{B} ||\boldsymbol{S}\boldsymbol{G}\boldsymbol{y}^{b}_{T+h,i,j} - \boldsymbol{y}_{T+h}|| - \frac{1}{2(B-1)}\sum_{i=1}^{B-1} ||\boldsymbol{S}\boldsymbol{G}(\boldsymbol{y}^{b}_{T+h,i,j} - \boldsymbol{y}^{b}_{T+h,i+1,j})||. \tag{24}$$

where B is the empirical sample size from the coherent forecast distribution. Now we can rewrite the objective function in (23) as,

$$\underset{\boldsymbol{G}}{\text{argmin}} \frac{1}{N}\sum_{j=1}^{N}\left\{\frac{1}{B}\sum_{i=1}^{B} ||\boldsymbol{S}\boldsymbol{G}\boldsymbol{y}^{b}_{T+h,i,j} - \boldsymbol{y}_{T+h}|| - \frac{1}{2(B-1)}\sum_{i=1}^{B-1} ||\boldsymbol{S}\boldsymbol{G}(\boldsymbol{y}^{b}_{T+h,i,j} - \boldsymbol{y}^{b}_{T+h,i+1,j})||\right\} \tag{25}$$

We can use numerical optimization methods to find the matrix $\boldsymbol{G}$ that minimizes above objective function and thus obtain the reconciled future paths.

5.4 Simulation study

We now turn our attention to comparing different reconciliation methods with optimal reconciliation in a simulation study.

For the data generating process, we consider the hierarchy given in Figure 1, comprising two aggregation levels with four bottom-level series. Each bottom-level series will be generated first, and then summed to obtain the data for the upper-level series. In practice, hierarchical time series tend to contain much noisier series at lower levels of aggregation. In order to replicate this feature in our simulations, we follow the data generating process proposed by Wickramasuriya et al. (2018).

Explain the data generating process - Dependence structure is imposed with copula.

To ensure the disaggregate series are noisier than the aggregate series, we choose $\mathbf{\Sigma}, \sigma_u^2$ and σ_v^2 such that

$$\text{Var}(\varepsilon_{AA,t} + \varepsilon_{AB,t} + \varepsilon_{BA,t} + \varepsilon_{BB,t}) \leq \text{Var}(\varepsilon_{AA,t} + \varepsilon_{AB,t} - v_t) \leq \text{Var}(\varepsilon_{AA,t} + u_t - 0.5v_t)\,,$$

and similar inequalities hold when $\varepsilon_{AA,t}$ is replaced by $\varepsilon_{AB,t}$, $\varepsilon_{BA,t}$ and $\varepsilon_{BB,t}$ in the third term. The values of $\mathbf{\Sigma}$, σ_u^2 and σ_v^2 that we use and which satisfy these constraints are $\sigma_u^2 = 10$, $\sigma_v^2 = 7$ and

$$\mathbf{\Sigma} = \begin{pmatrix} 5.0 & 3.1 & 0.6 & 0.4 \\ 3.1 & 4.0 & 0.9 & 1.4 \\ 0.6 & 0.9 & 2.0 & 1.8 \\ 0.4 & 1.4 & 1.8 & 3.0 \end{pmatrix}.$$

- Explain how the simulation is set up including the optimal reconciliation
- Evaluation process - Used skill scores
- Discussion of results

6 Forecasting Australian domestic tourism flow

7 Conclusions

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