# Probabilistic Forecasts for Hierarchical Time Series

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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 (see for example, Dunn et al. (1976), Gross & Sohl (1990), Athanasopoulos et al. (2009), Hyndman et al. (2011) and Wickramasuriya et al. (2019)). 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 allows us to derive further results for parametric as well as non-parametric distributional forecasts for hierarchical time series.

A shortcoming of the existing hierarchical forecasting 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, Ben Taieb et al. (2017) and Jeon et al. (2019) are the only papers to deal with probabilistic forecasts in hierarchical literature. In Ben Taieb et al. (2017), although they reconcile the means of predictive distributions, the overall distributions are constructed in a bottom-up fashion rather than using a reconciliation process. Jeon et al. (2019) proposed a novel method for probabilistic forecast reconciliation based on cross-validation which in particular applied

to the temporal hierarchies. In contrast to these studies, the main objective of our paper is to generalise both coherence and reconciliation from point to probabilistic forecasting.

Extending the geometric interpretation on point forecast reconciliation in cite first paper we provide new definitions of coherence and forecast reconciliation in the probabilistic setting. 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.

When parametric density assumptions are made we describe how the probabilistic forecast 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.

Further we propose a new method to generate coherent forecasts when the parametric distributional assumptions are not applicable. This method uses a non-parametric bootstrap based approach to generate future paths for all series in the hierarchy and then reconcile each sample path using projections. This will provide a possible sample from the reconciled predictive density of the hierarchy. An extensive simulation study was carried out to find the optimal reconciliation of bootstrap future paths with respect to a proper scoring rule. This has shown that the MinT method is at least as good as the optimal

method for reconciling future paths.

Finally we applied both parametric and non-parametric approaches to generate probabilistic forecasts for domestic tourism flow in Australia. The results shows that reconciliation improves forecast accuracy compared to incoherent forecasts in both parametric and non-parametric approaches and further, MinT reconciliation is performing best.

The remainder of the paper is structured as follows. In Section 2 notation and some preliminary work on point forecast reconciliation is discussed. Section 3 contains the definitions and interpretation of coherent probabilistic forecasts and reconciliation. In Section 4 we consider the evaluation of probabilistic hierarchical forecasts via scoring rules. Parametric forecast reconciliation and some theoretical results related to elliptical distributions are discussed in Section 5 while the non-parametric approach is introduced in Section 6. An empirical application on tourism forecasting is contained in Section 7. Finally Section 8 concludes with some discussion and thoughts on future research.

# 2 Notations and preliminaries

Following cite first paper we define our notations and some preliminary work on hierarchical time series and forecasting.

#### 2.1 Notations

Hierarchical time series are a collection of n time series which are formed by aggregating m number of linearly independent series. In conventional hierarchies the bottom level series are linearly independent and these will be aggregated to the upper level series. Let us denote with  $y_t$ , a n dimensional vector containing observations of all series in the hierarchy at time t. Further, let  $b_t \in \mathbb{R}^m$  contain the observations of only the bottom level series of

the hierarchy at time t. Due to the aggregation constraints of the hierarchy we can write,

$$y_t = Sb_t, \tag{1}$$

where S is an  $n \times m$  constant matrix for a given hierarchical structure.

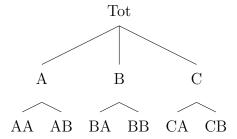


Figure 1: An example of a two level hierarchical structure.

To make explicit this notation, we refer to the hierarchy in Figure 1. This hierarchy consists of m=4 bottom level series with n=7 total number of series. Further,  $\boldsymbol{y}_t=[y_{Tot,t},y_{A,t},y_{B,t},y_{AA,t},y_{AB,t},y_{BA,t},y_{BB,t}]'$ ,  $\boldsymbol{b}_t=[y_{AA,t},y_{AB,t},y_{BA,t},y_{BB,t}]'$  and

$$m{S} = egin{pmatrix} 1 & 1 & 1 & 1 \ 1 & 1 & 0 & 0 \ 0 & 0 & 1 & 1 \ & m{I}_4 \end{pmatrix},$$

where  $I_4$  is the  $4 \times 4$  identity matrix.

The columns of S define the aggregation constraints of the hierarchy and they span a subspace  $\mathfrak{s} \subset \mathbb{R}^n$  which all  $y_t$  lie on. This subspace is referred to as the *coherent subspace*. Any point that lies in this subspace is referred to as a *coherent point*. In particular, all observations are coherent by construction. Further, any point forecast is said to be coherent if it lies in the coherent subspace.

It will sometimes be useful to think of pre-multiplication by S in equation (1) as a mapping from  $\mathbb{R}^m$  to  $\mathbb{R}^n$ , in which case we use the notation s(.). Although the codomain of s(.) is  $\mathbb{R}^n$ , its image is the coherent space  $\mathfrak{s}$  as depicted in Figure 2.

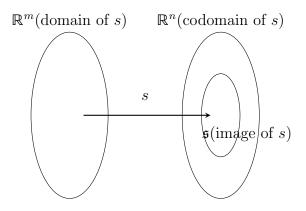


Figure 2: The domain, codomain and image of the mapping s.

### 2.2 Hierarchical point forecasts

Cite first paper provide insights to coherent point forecasts and forecast reconciliation in terms of geometric concepts. We briefly address these to facilitate extension into probabilistic framework discussed in Section 3.

Suppose we have a vector of point forecasts at time t + h derived by using information up to and including time t. Let these forecasts be stacked in a vector with the same order as  $\mathbf{y}_t$  and denoted by  $\hat{\mathbf{y}}_{t+h|t} \in \mathbb{R}^n$ . These are referred to as incoherent point forecasts as they do not satisfy the aggregation constraints. Assume a linear function that converts these incoherent forecasts into new bottom level forecasts. Let  $\mathbf{G}$  and  $\mathbf{d}$  be an  $m \times n$  matrix and  $m \times 1$  vector respectively, and let  $g : \mathbb{R}^n \to \mathbb{R}^m$  be the mapping  $g(\mathbf{y}) = \mathbf{G}\mathbf{y} + \mathbf{d}$ . A composition of g(.) and s(.) gives the reconciled point forecasts as,

$$\tilde{\boldsymbol{y}}_{t+h|t} = \boldsymbol{S}(\boldsymbol{G}\hat{\boldsymbol{y}}_{t+h|t} + \boldsymbol{d}). \tag{2}$$

Several choices of g(.) are currently extant in the literature, including the Bottom-up, OLS, WLS and MinT methods (see for example (Dunn et al. 1976), Hyndman et al. (2011) and Wickramasuriya et al. (2019)). These are special cases where  $s \circ g$  is a projection. These can be defined so that  $G = (R'_{\perp}S)^{-1}R'_{\perp}$  and d = 0, where,  $R_{\perp}$  is a  $n \times m$  orthogonal complement to an  $n \times (n - m)$  matrix R, where the columns of the latter span the null space of  $\mathfrak{s}$ . For example, a straightforward choice of R for the most simple three variable hierarchy where  $y_{1,t} = y_{2,t} + y_{3,t}$ , is the vector (1, -1, -1) which is orthogonal (in the Euclidean sense) to the columns of S. In this case, the matrix R can be interpreted as a 'restrictions' matrix since it has the property that R'y = 0 for coherent y. For this three variable hierarchy,  $R'_{\perp} = S$  and reconciliation corresponds to the OLS method. For the case where  $R'_{\perp} \neq S$ , for example WLS and MinT,  $R'_{\perp}$  is usually written in the form  $S'W^{-1}$ . These projections can be thought of as orthogonal projections after premultiplying by  $W^{-1/2}$ . More detailed explanation on this can be found in cite first paper. Table 1 summarises existing reconciliation methods.

The columns of S and R provide a basis for  $\mathbb{R}^n$ . Therefore any incoherent set of point forecasts  $\hat{y}_{t+h|t}$  can be expressed in terms of coordinates in the basis defined by S and R. Let  $\tilde{b}_{t+h|t}$  and  $\tilde{a}_{t+h|t}$  be the coordinates corresponding to S and R respectively, after a change of basis. The process of reconciliation involves setting the values of the reconciled bottom-level series to be  $\tilde{b}_{t+h|t}$ , and ignoring  $\tilde{a}_{t+h|t}$  to ensure coherence. From properties of linear algebra it follows that

$$\hat{m{y}}_{t+h|t} = (m{S} \; m{R}) egin{pmatrix} ilde{m{b}}_{t+h|t} \ ilde{m{a}}_{t+h|t} \end{pmatrix} = m{S} ilde{m{b}}_{t+h|t} + m{R} ilde{m{a}}_{t+h|t},$$

Table 1: Summary of reconciliation methods that are projections. Here,  $\hat{\boldsymbol{W}}^{sam}$  is the variance covariance matrix of one-step ahead forecast errors,  $\hat{\boldsymbol{W}}^{shr}$  is a shrinkage estimator more suited to large dimensions proposed by Schäfer & Strimmer (2005),  $\hat{\boldsymbol{W}}^{wls}$  is the diagonal matrix with diagonal elements  $w_{ii}$ , and  $\tau = \frac{\sum_{i \neq j} \hat{Var}(\hat{w}_{ij})}{\sum_{i \neq j} \hat{w}_{ij}^2}$ , where  $w_{ij}$  denotes the (i,j)th element of  $\hat{\boldsymbol{W}}^{sam}$ .

Method	W	$oldsymbol{R}'_{\perp}$
OLS	I	S'
MinT(Sample)	$\hat{W}^{sam}$	$m{S}'(\hat{m{W}}^{sam})^{-1}$
MinT(Shrink)	$\tau \operatorname{Diag}(\hat{\boldsymbol{W}}^{sam}) + (1-\tau)\hat{\boldsymbol{W}}^{sam}$	$oldsymbol{S'}(\hat{oldsymbol{W}}^{shr})^{-1}$
WLS	$ ext{Diag}(\hat{oldsymbol{W}}^{sam})$	$m{S}'(\hat{m{W}}^{wls})^{-1}$

while the reconciled point forecast is

$$ilde{m{y}}_{t+h|t} = m{S} ilde{m{b}}_{t+h|t}.$$

In order to find  $\tilde{\boldsymbol{b}}_{t+h|t}$  we require the inverse  $(\boldsymbol{S}|\boldsymbol{R})^{-1}$  which is given by

$$(\boldsymbol{S} \ \boldsymbol{R})^{-1} = \begin{pmatrix} (\boldsymbol{R}_{\perp}' \boldsymbol{S})^{-1} \boldsymbol{R}_{\perp}' \\ (\boldsymbol{S}_{\perp}' \boldsymbol{R})^{-1} \boldsymbol{S}_{\perp}' \end{pmatrix} ,$$
 (3)

where  $S_{\perp}$  is the orthogonal complements of S. Thus it follows that  $\tilde{\boldsymbol{b}}_{t+h|t} = (\boldsymbol{R}'_{\perp}\boldsymbol{S})^{-1}\boldsymbol{R}'_{\perp}\hat{\boldsymbol{y}}_{t+h|t}$  and  $\tilde{\boldsymbol{y}}_{t+h|t} = \boldsymbol{S}(\boldsymbol{R}'_{\perp}\boldsymbol{S})^{-1}\boldsymbol{R}'_{\perp}\hat{\boldsymbol{y}}_{t+h|t}$ . Here  $(\boldsymbol{R}'_{\perp}\boldsymbol{S})^{-1}\boldsymbol{R}'_{\perp}$  corresponds to  $\boldsymbol{G}$  as defined previously.

## 3 Hierarchical probabilistic forecasts

The geometric intuition in hierarchical point forecasts provides a solid basis for extending the idea into probabilistic framework. We start with providing definitions for coherent probabilistic forecasts and probabilistic forecast reconciliation.

### 3.1 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  $\sigma$ -algebra on  $\mathbb{R}^m$ . Let  $\check{\nu}$  be a probability measure on  $\mathfrak{s}$  with  $\sigma$ -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 3.1** (Coherent Probabilistic Forecasts). The measure  $\check{\nu}$  is coherent if it has the property

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

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

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 definition of probabilistic forecast reconciliation to which we now turn our attention.

#### 3.2 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 3.2.** The reconciled probability measure of  $\hat{\nu}$  with respect to the mapping g(.) is a probability measure  $\tilde{\nu}$  on  $\mathfrak{s}$  with  $\sigma$ -algebra  $\mathscr{F}_{\mathfrak{s}}$  such that

$$\tilde{\nu}(s(\mathcal{B})) = \nu(\mathcal{B}) = \hat{\nu}(g^{-1}(\mathcal{B})) \qquad \forall \mathcal{B} \in \mathscr{F}_{\mathbb{R}^m},$$
(4)

where  $g^{-1}(\mathcal{B}) := \{ \check{\boldsymbol{y}} \in \mathbb{R}^n : g(\check{\boldsymbol{y}}) \in \mathcal{B} \}$  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 3 schematically when  $s \circ g$  is a projection.

Following these definitions we can derive the probabilistic forecasts for parametric distributions which we will elaborate in Section 5. Now we turn our attention to the evaluation of hierarchical probabilistic forecasts.

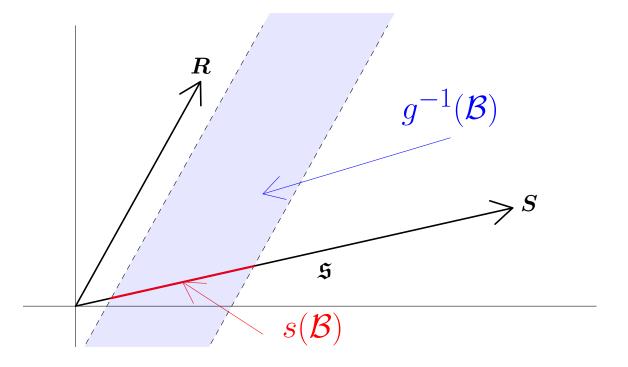


Figure 3: Summary of probabilistic forecast reconciliation. The probability that  $y_{t+h}$  lies in the red line segment under the reconciled probabilistic forecast is defined to be equal to the probability that  $y_{t+h}$  lies in the shaded blue area under the unreconciled probabilistic forecast. Note that since the smallest possible hierarchy involves three dimensions, this figure is only a schematic.

## 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  $\omega$  be a realization from Q. Then a scoring rule is a function  $S(P, \omega)$  that maps  $P, \omega$  to  $\mathbb{R}$ . It is a "proper" scoring rule if

$$E_{\mathbf{O}}[S(Q,\omega)] \le E_{\mathbf{O}}[S(P,\omega)],$$
 (5)

where  $E_Q[S(P,\omega)]$  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. 2019). 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 time series in the hierarchy. A summary can be taken of the expected scores across each margin, for example a mean or median. 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 continuous rank probability score generalises mean square error and is given by

$$CRPS(\breve{F}_i, y_i) = \int \left( \breve{F}_i(\breve{Y}_i) - \mathbb{1}(\breve{Y}_i < y_i) \right) d\breve{Y}_i \tag{6}$$

$$= E_{\check{Y}_{i}} |\check{Y}_{i} - y_{i}| - \frac{1}{2} E_{\check{Y}_{i}} |\check{Y}_{i} - \check{Y}_{i}^{*}|, \qquad (7)$$

where  $\check{F}_i$  is the cumulative distribution function of the  $i^{\text{th}}$  margin of the probabilistic forecast,  $\check{Y}_i$  and  $\check{Y}_i^*$  are independent copies of a random variable with distribution  $\check{F}_i$ , and

 $y_i$  is the outcome of the  $i^{th}$  margin. The expectations in the second line can be approximated by Monte Carlo when a sample from the predictive distribution is available.

An advantage of this approach is that it allows the forecaster to separately evaluate different levels and individual series of the hierarchy to determine 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. 2019) 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

$$\mathrm{ES}(\breve{\boldsymbol{Y}}_{T+h}, \boldsymbol{y}_{T+h}) = \mathrm{E}_{\breve{\boldsymbol{Y}}} ||\breve{\boldsymbol{Y}}_{T+h} - \boldsymbol{y}_{T+h}||^{\alpha} - \frac{1}{2} \mathrm{E}_{\breve{\boldsymbol{Y}}} ||\breve{\boldsymbol{Y}}_{T+h} - \breve{\boldsymbol{Y}}_{T+h}^{*}||^{\alpha}, \ \alpha \in (0, 2],$$
(8)

lends itself to easy computation when samples from the probabilistic forecast are available and given as,

$$ES(\breve{\boldsymbol{Y}}_{T+h}, \boldsymbol{y}_{T+h}) \approx \frac{1}{M} \sum_{i=1}^{M} ||\boldsymbol{S}\boldsymbol{G}\breve{\boldsymbol{y}}_{T+h,i} - \boldsymbol{y}_{T+h}|| - \frac{1}{2(M-1)} \sum_{i=1}^{M-1} ||\boldsymbol{S}\boldsymbol{G}(\breve{\boldsymbol{y}}_{T+h,i} - \breve{\boldsymbol{y}}_{T+h,i+1})||,$$
(9)

where,  $\check{y}_{T+h,i}$  is the  $i^{\text{th}}$  Monte-Carlo sample from the forecast distribution. 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  $\check{\boldsymbol{y}}$  is a random variable from probabilistic forecast  $\check{F}$ , the empirical variogram score is defined as

$$VS(\breve{F}, \boldsymbol{y}) = \sum_{i=1}^{n} \sum_{j=1}^{n} w_{ij} \left( |y_i - y_j|^p - E_{\breve{Y}_i, \breve{Y}_j} |\breve{Y}_i - \breve{Y}_j|^p \right)^2.$$
 (10)

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 3. 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,  $z_t = Uy_t$ , so that the first m elements of  $z_t$  denoted  $z_t^{(1)}$  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

$$LS\left(\hat{f}, \mathbf{z}_{t}^{(1)}\right) = -\log f_{1}(\mathbf{z}_{t}^{(1)}) - \log f_{2}(\mathbf{z}_{t}^{(1)})$$
(11)

$$= -\log f_1(\mathbf{z}_t^{(1)}) + \frac{n-m}{2}\log(2\pi\sigma^2)$$
 (12)

$$< -\log f_1(\boldsymbol{z}_t^{(1)}) = LS\left(f, \boldsymbol{z}_t^{(1)}\right).$$
 (13)

After taking expectations  $E[LS(f, f)] > E[LS(\hat{f}, f)]$ , violating the condition in Equation (5) 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 3.1. 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(b). The density for the full hierarchy is given by  $f(y) = f(Sb) = f(b)J^{-1}$ , where  $J = \prod_{j=1}^{m} \lambda_j$  is a pseudo-determinant of the non-square matrix S and  $\lambda_j$  are the non-zero singular values of 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 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 probabilistic forecasts are summarised in Table 2.

Table 2: Summary of properties of scoring rules in the context of reconciled probabilistic forecasts.

	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

## 5 Parametric reconciliation

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.  $\tilde{a}_{t+h|t}$  is discarded and  $\tilde{b}_{t+h|t}$  are kept as the bottom-level reconciled forecasts.
- 3. Reconciled forecasts for the entire hierarchy are recovered via  $\tilde{y}_{t+h|t} = S\tilde{b}_{t+h|t}$ .

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  $\hat{y}_{t+h|t}$ , 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 point forecast reconciliation where  $\hat{y}_{t+h|t} = S\tilde{b}_{t+h|t} + R\tilde{a}_{t+h|t}$ , we obtain

$$f(\hat{\mathbf{y}}_{t+h|t}) = f(\mathbf{S}\tilde{\mathbf{b}}_{t+h|t} + \mathbf{R}\tilde{\mathbf{a}}_{t+h|t})|(\mathbf{S}\ \mathbf{R})|$$
(14)

The expression  $\hat{\nu}(g^{-1}(\mathcal{B}))$  in Definition 3.2 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

$$\Pr(\hat{\boldsymbol{y}}_{t+h|t} \in g^{-1}(\mathcal{B})) = \int_{g^{-1}(\mathcal{B})} f(\hat{\boldsymbol{y}}_{t+h|t}) d\hat{\boldsymbol{y}}_{t+h|t}$$
(15)

$$= \int_{\mathcal{B}} \int f(\mathbf{S}\tilde{\mathbf{b}}_{t+h|t} + \mathbf{R}\tilde{\mathbf{a}}_{t+h|t}) |(\mathbf{S}\ \mathbf{R})| d\tilde{\mathbf{a}}_{t+h|t} d\tilde{\mathbf{b}}_{t+h|t}. \tag{16}$$

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 lies in the region  $\mathcal{B}$ . This corresponds to  $\nu(\mathcal{B})$  in Definition 3.2. To make a valid probability statement about the entire hierarchy we simply use the bottom-level probabilistic forecasts together with Definition 3.1.

### **Example: Gaussian Distributions**

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

$$f(\hat{\mathbf{y}}) = (2\pi)^{-n/2} |\hat{\mathbf{\Sigma}}|^{-1/2} \exp\left\{-\frac{1}{2} \left[ (\hat{\mathbf{y}} - \hat{\boldsymbol{\mu}})' \hat{\mathbf{\Sigma}}^{-1} (\hat{\mathbf{y}} - \hat{\boldsymbol{\mu}}) \right] \right\}.$$
 (17)

In an alternative basis,

$$f(\tilde{\boldsymbol{b}}, \tilde{\boldsymbol{a}}) = (2\pi)^{-\frac{n}{2}} \left| \hat{\boldsymbol{\Sigma}} \right|^{-\frac{1}{2}} \left| (\boldsymbol{S} \ \boldsymbol{R}) \right| \exp\{-\frac{1}{2}q\},$$
 (18)

where

$$q = (\mathbf{S}\tilde{\mathbf{b}} + \mathbf{R}\tilde{\mathbf{a}} - \hat{\boldsymbol{\mu}})'\hat{\boldsymbol{\Sigma}}^{-1}(\mathbf{S}\tilde{\mathbf{b}} + \mathbf{R}\tilde{\mathbf{a}} - \hat{\boldsymbol{\mu}}). \tag{19}$$

The quadratic form q can be rearranged as

$$q = \left( (\boldsymbol{S} \ \boldsymbol{R}) \begin{pmatrix} \tilde{\boldsymbol{b}} \\ \tilde{\boldsymbol{a}} \end{pmatrix} - \hat{\boldsymbol{\mu}} \right)' \hat{\boldsymbol{\Sigma}}^{-1} \left( (\boldsymbol{S} \ \boldsymbol{R}) \begin{pmatrix} \tilde{\boldsymbol{b}} \\ \tilde{\boldsymbol{a}} \end{pmatrix} - \hat{\boldsymbol{\mu}} \right),$$

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

Recall that

$$(oldsymbol{S} \ oldsymbol{R})^{-1} = egin{pmatrix} (oldsymbol{R}'_oldsymbol{oldsymbol{S}}' \ (oldsymbol{S}'_oldsymbol{L} oldsymbol{R})^{-1} oldsymbol{S}'_oldsymbol{oldsymbol{L}}' \end{pmatrix} := egin{pmatrix} oldsymbol{G} \ oldsymbol{H} \end{pmatrix} \ .$$

Then q can be rearranged further as

$$q = \left[egin{pmatrix} ilde{m{b}} & - igg( m{G} \ m{\mu} \end{pmatrix} \hat{m{\mu}}_{t+h} 
ight]' \left[igg( m{G} \ m{H} \end{pmatrix} m{\Sigma}_{t+h}^{\hat{}} igg( m{G} \ m{H} \end{pmatrix}' 
ight]^{-1} \left[igg( ilde{m{b}} \ m{a} \end{pmatrix} - igg( m{G} \ m{H} \end{pmatrix} \hat{m{\mu}}_{t+h} 
ight]$$
 $= egin{pmatrix} ilde{m{b}} - G\hat{m{\mu}} \ ilde{m{a}} - H\hat{m{\mu}} \end{pmatrix}' \left[igg( m{G} \ m{H} \end{pmatrix} m{\Sigma}_{t+h}^{\hat{}} igg( m{G} \ m{H} \end{pmatrix}' 
ight]^{-1} egin{pmatrix} ilde{m{b}} - G\hat{m{\mu}} \ ilde{m{a}} - H\hat{m{\mu}} \end{pmatrix}.$ 

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

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

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

$$f(\tilde{\boldsymbol{b}}) = (2\pi)^{-\frac{m}{2}} \left| \boldsymbol{G} \hat{\boldsymbol{\Sigma}} \boldsymbol{G}' \right|^{\frac{1}{2}} \exp \left\{ -\frac{1}{2} (\tilde{\boldsymbol{b}} - \boldsymbol{G} \hat{\boldsymbol{\mu}})' (\boldsymbol{G} \hat{\boldsymbol{\Sigma}} \boldsymbol{G}')^{-1} (\tilde{\boldsymbol{b}} - \boldsymbol{G} \hat{\boldsymbol{\mu}}) \right\}.$$
(20)

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

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

Theorem 5.1 (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  $g(\boldsymbol{y}) = \boldsymbol{G}_{opt}\boldsymbol{y} + \boldsymbol{d}_{opt}$  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  $SG_{opt}\hat{\Sigma}G'_{opt}S'$ , while the location matrix is given by  $SG_{opt}\hat{\mu} + d_{opt}$ . The reconciled

scale matrix is

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

For the choices of  $G_{opt}$  and  $d_{opt}$  given above, the reconciled location vector is

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

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 5.2** (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:

$$sp(\hat{\boldsymbol{\mu}} - \boldsymbol{\mu}) \subset sp(\boldsymbol{R})$$
 (21)

$$sp(\hat{\Sigma}^{1/2} - \Sigma^{1/2}) \subset sp(\mathbf{R})$$
 (22)

(23)

*Proof.* The reconciled location vector will be given by

$$egin{aligned} ilde{m{\mu}} &= m{S}(m{R}_{\perp}'m{S})^{-1}m{R}_{\perp}'\hat{m{\mu}} \ &= m{S}(m{R}_{\perp}'m{S})^{-1}m{R}_{\perp}'\left(\hat{m{\mu}} + m{\mu} - m{\mu}
ight) \ &= m{S}(m{R}_{\perp}'m{S})^{-1}m{R}_{\perp}'m{\mu} + m{S}(m{R}_{\perp}'m{S})^{-1}m{R}_{\perp}'\left(\hat{m{\mu}} - m{\mu}
ight). \end{aligned}$$

Since  $S(R'_{\perp}S)^{-1}R'_{\perp}$  is a projection onto  $\mathfrak{s}$  and  $\mu \in \mathfrak{s}$ , the first term simplifies to  $\mu$ . If  $\mu - \hat{\mu}$  lies in the span of R, then multiplication by  $R'_{\perp}$  reduces the second term to  $\mathbf{0}$ . By a similar argument it can be shown that  $\tilde{\Sigma}^{1/2} = \Sigma^{1/2}$ . 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  $\hat{\mu}$  were equi-probable in all directions, then a projection orthogonal to  $\mathfrak{s}$  would be a sensible choice for R since it would in some sense represent a 'median' direction for  $\mu - \hat{\mu}$ . However, the one-step-ahead in-sample errors are usually correlated suggesting that  $\hat{\mu}$  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 we demonstrate this in a simulation setting in the following subsection.

#### 5.2 Simulations

To compare different reconciliation methods in parametric densities we assume a Gaussian predictive distribution for the hierarchy. We choose the Gaussian case due to its analytical tractability which allows for evaluation using all scoring rules (including the log score).

#### 5.2.1 Data generating process (DGP)

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.

First  $\{w_{AA,t}, w_{AB,t}, w_{BA,t}, w_{BB,t}\}$  are generated from ARIMA(p,d,q) processes, where (p,q) and d take integers from  $\{1,2\}$  and  $\{0,1\}$  respectively with equal probability. The parameters for the AR and MA components are randomly and uniformly generated from [0.3, 0.5] and [0.3, 0.7] respectively. The errors driving the ARIMA processes were generated from Gaussian and non-Gaussian distributions separately. This will allow us to demonstrate impact of true DGP for the parametric reconciliation approach.

#### Gaussian errors:

Errors were generated from jointly normal distribution, and denoted by  $\{\varepsilon_{AA,t}, \varepsilon_{AB,t}, \varepsilon_{BA,t}, \varepsilon_{BB,t}\} \stackrel{iid}{\sim} \mathcal{N}(\mathbf{0}, \mathbf{\Sigma}) \ \forall t$ . Further we choose,

$$\Sigma = \begin{pmatrix} 5.0 & 3.1 & 0.6 & 0.4 \\ 3.1 & 4.0 & 0.9 & 1.4 \\ 0.6 & 0.9 & 2.0 & 1.8 \\ 0.4 & 1.4 & 1.8 & 3.0 \end{pmatrix} . \tag{24}$$

#### Non-Gaussian errors:

Non-Gaussian errors were generated from a Gumbel copula model with beta margins. Using a copula model helps to impose the dependency structure among the series. A two dimensional Gumbel copula is given by,

$$C_{\theta}(u_1, u_2) = exp\{-[(-ln(u_1))^{\theta} + (-ln(u_2))^{\theta}]^{1/\theta}\}.$$

We generate random variates  $\{u_{AA}, u_{AB}\}$  from  $C_{\theta=10}(.)$  and  $\{u_{BA}, u_{BB}\}$  from  $C_{\theta=8}(.)$  for series  $\{AA, AB\}$  and  $\{BA, BB\}$  respectively. Next we generate the errors,  $\{\varepsilon_{AA}, \varepsilon_{AB}, \varepsilon_{BA}, \varepsilon_{BB}\}$  as the quantiles from beta distributions with shape parameters  $\alpha = 1$  and  $\beta = 3$  correspond to  $\{u_{AA}, u_{AB}, u_{BA}, u_{BB}\}$ .

Although the copulas more beyond the concepts of linear dependence, we will apply a Gaussian assumption to the data to investigate model misspecification. To give some idea of the covariance matrix of  $\{\varepsilon_{AA}, \varepsilon_{AB}, \varepsilon_{BA}, \varepsilon_{BB}\}$ , the sample estimate is,

$$\Sigma = \begin{pmatrix} 0.0388 & 0.0385 & 0.0010 & 0.0010 \\ 0.0385 & 0.0390 & 0.0008 & 0.0008 \\ 0.0010 & 0.0008 & 0.0387 & 0.0377 \\ 0.0010 & 0.0008 & 0.0377 & 0.0381 \end{pmatrix}. \tag{25}$$

#### Signal-to-noise ratio:

In practice, hierarchical time series are likely to have much noisier series at lower levels of aggregation. Following the method proposed by Wickramasuriya et al. (2019), we replicate this feature in our simulations by generating the bottom-level series  $\{y_{AA,t}, y_{AB,t}, y_{BA,t}, y_{BB,t}\}$  as follows:

$$y_{AA,t} = w_{AA,t} + u_t - 0.5v_t,$$
  

$$y_{AB,t} = w_{AB,t} - u_t - 0.5v_t,$$
  

$$y_{BA,t} = w_{BA,t} + u_t + 0.5v_t,$$
  

$$y_{BB,t} = w_{BB,t} - u_t + 0.5v_t,$$

where  $u_t \sim \mathcal{N}(0, \sigma_u^2)$  and  $v_t \sim \mathcal{N}(0, \sigma_v^2)$ . The aggregate series in the middle-level are given by:

$$y_{A,t} = w_{AA,t} + w_{AB,t} - v_t,$$
  
 $y_{B,t} = w_{BA,t} + w_{BB,t} + v_t,$ 

and the total series is given by

$$y_{Tot,t} = w_{AA,t} + w_{AB,t} + w_{BA,t} + w_{BB,t}.$$

To ensure the disaggregate series are noisier than the aggregate series, we choose  $\sigma_u^2$  and  $\sigma_v^2$  such that

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

Similar inequalities hold when  $\varepsilon_{AA,t}$  is replaced by  $\varepsilon_{AB,t}$ ,  $\varepsilon_{BA,t}$  and  $\varepsilon_{BB,t}$  in the third term. Thus for the Gaussian DGP we choose  $\sigma_u^2 = 24$  and  $\sigma_u^2 = 18$  whereas for non-Gaussian DGP we choose  $\sigma_u^2 = 10$  and  $\sigma_v^2 = 7$ .

We generate 2500 observations for each series from this Gaussian and non-Gaussian DGP. We ignore the first 500 observations from each series to avoid the impact from initial values. Choosing a rolling window of T=500 observations, univariate ARIMA models were fitted for each series using the auto.arima() function in the forecast package (Hyndman 2019) in R (R Core Team 2018). Using the fitted models, h=3-steps ahead base (incoherent) Gaussian probabilistic forecasts were generated. We estimate the mean and the variance of this incoherent Gaussian density as the h-step ahead point forecasts  $\hat{y}_{t+h|t}$  and shrinkage estimator for variance covariance matrix of one-step ahead forecast errors  $\hat{W}^{\text{shr}}$  respectively. These were then reconciled using different projections summarised in Table 1. This process was replicated for 1000 times by rolling the window one step at a time.

To assess the predictive performance of different forecasting methods, we use scoring rules as discussed in Section 4. To facilitate comparisons, we report skill scores (Gneiting & Raftery 2007). For a given forecasting method, evaluated by a particular scoring rule, the skill score gives the percentage improvement of the preferred forecasting method relative to a reference method. A negative valued skill score indicates that a method is worse than the reference method, whereas any positive value indicates that the method is superior to the reference method.

Table 3 summarizes the forecasting performance of unreconciled, bottom-up, OLS, WLS and two MinT reconciliation methods using log score, energy score and variogram score. The top panel refers to the Gaussian DGP whereas the bottom panel refers to the non-Gaussian DGP. In all cases skill scores are calculated with the bottom-up method as reference. All log scores are evaluated on the basis of bottom-level series only, however these only differ from the log scores for the full hierarchy by a fixed constant. The cell for log score of unreconciled forecasts is left blank since the log score is not proper in this context. Overall, the MinT methods provide the best performance irrespective of the scoring rule, and all methods that reconcile using information at all levels of the forecast improve upon unreconciled forecasts. Bottom-up forecasts perform even worse than unreconciled forecasts in some cases. These results hold for both Gaussian as well as non-Gaussian DGP.

Tables 4 and 5 break down the forecasting performance of different reconciliation methods by considering univariate scores on each individual margin. Tables 4 summarises results for the top and middle-level, Table 4 does the same for bottom-level. Univariate log score and CRPS are considered, while skill scores are computed with the unreconciled forecast as a reference. When broken down in this fashion, irrespective of DGP, the methods based on MinT perform best for most series and always outperform bottom-up forecasts.

Table 3: Comparison of coherent forecasts in forecast horizons h=1, h=2 and h=3. All entries shows the percentage skill score with reference to the bottom-up method. Top panel shows the results from Gaussian DGP and bottom panel shows the results from non-Gaussian DGP. "ES" and "VS" columns give scores based on the joint forecast distribution of the whole hierarchy. "LS" column gives the log scores of the joint forecast distribution of the bottom-level.

		h=1			h=2		h=3							
Method	ES(%)	VS(%)	LS(%)	ES(%)	VS(%)	LS(%)	ES(%)	VS(%)	LS(%)					
	Gaussian DGP													
MinT(Shrink)	19.48	9.78	3.16	19.57	14.16	6.53	16.47	8.34						
MinT(Sample)	19.48	9.74	3.09	19.50	14.16	6.51	16.28	16.28 16.42						
WLS	18.08	7.21	0.64	17.68	10.97	2.31	14.99	14.99 13.17						
OLS	16.01	5.80	-0.79	15.38	8.43	0.05	13.03	10.26	0.82					
Bottom up	0.00	0.00	0.00	0.00	0.00 0.00		0.00	0.00	0.00					
Incoherent	11.65	-0.12		10.58	1.71		8.75	3.64						
			Non-	Gaussian	DGP									
MinT(Shrink)	15.04	0.69	4.52	16.98	1.34	4.55	18.00	0.66	4.01					
MinT(Sample)	15.02	0.59	4.40	16.94	04 1.02 4.30		17.88	0.64	3.42					
WLS	12.72	12.72 0.00		14.22	0.41	1.34	15.20	-0.42	0.89					
OLS	11.26	0.17	0.65	12.27	0.48	0.47	13.12	-0.24	0.10					
Bottom up	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00					
Incoherent	8.47	-2.79		8.94	-2.09		9.20	-3.62						

Table 4: Comparison of incoherent vs coherent forecasts based on the univariate forecast distribution of aggregate series. Each entry represents the percentage skill score with reference to the incoherent forecasts based on "CRPS" and "LS". These entries show the percentage increase in score for different forecasting methods relative to the incoherent forecasts for h=1, h=2 and h=3 forecast horizons. Results from Gaussian DGP are presented in the top panel whereas the results from non-Gaussian DGP are presented in the bottom panel

			h=1						h=	2		h=3							
	To	otal	A		В		Tot	Total		A			Total		A		В		
R.method	CRPS	LS	CRPS	LS	CRPS	LS	CRPS	LS	CRPS	LS	CRPS	LS	CRPS	LS	CRPS	LS	CRPS	LS	
	Gaussian DGP																		
MinT(Shrink)	-0.13	-0.01	9.37	3.12	5.42	1.67	0.34	-0.08	10.67	3.32	5.79	1.59	0.08	-0.17	8.13	1.58	4.17	1.04	
$\operatorname{MinT}(\operatorname{Sample})$	-0.08	-0.04	9.37	3.13	5.24	1.67	0.27	-0.10	10.76	3.39	5.67	1.62	0.04	-0.23	8.14	1.69	4.19	1.10	
WLS	-2.91	-1.24	8.78	2.86	5.49	1.73	-0.41	1.02	9.99	2.97	6.01	1.73	0.10	2.97	7.72	1.57	4.46	1.26	
OLS	-19.22	-6.86	6.28	2.06	4.86	1.58	-5.99	4.05	7.17	2.03	5.83	1.70	-2.13	13.11	5.30	0.97	4.41	1.30	
Bottom up	-140.27	-33.67	-13.75	-3.89	-11.10	-3.17	-60.07	2.72	-13.82	-3.86	-9.04	-2.37	-30.95	30.34	-13.57	-3.37	-8.47	-1.87	
Incoherent	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	
							Non	-Gaussia	an DGP										
MinT(Shrink)	-1.16	-0.26	0.92	0.27	11.90	4.91	-0.70	-1.16	0.71	0.29	16.53	6.83	-0.30	-1.35	0.60	0.25	19.53	8.28	
$\operatorname{MinT}(\operatorname{Sample})$	-1.16	-0.72	0.92	0.28	11.90	4.94	-0.70	-1.53	0.71	0.31	16.53	6.87	-0.30	-1.61	0.60	0.31	19.53	8.35	
WLS	0.01	0.35	-1.02	-0.52	9.95	4.07	-0.11	-0.15	-2.50	-1.09	13.87	5.55	-0.02	-0.40	-3.96	-1.60	16.14	6.78	
OLS	-96.77	-84.90	0.55	0.08	6.48	2.57	-44.06	-14.27	-0.18	-0.12	8.72	3.44	-22.75	19.51	-0.71	-0.32	10.48	4.27	
Bottom up	-541.40	-246.37	-4.60	-1.87	-8.99	-3.11	-273.80	-68.47	-4.20	-1.67	-8.78	-2.84	-159.47	10.59	-4.71	-1.77	-8.06	-2.27	
Incoherent	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	

Table 5: Comparison of incoherent vs coherent forecasts based univariate forecast distribution of bottom-level series. Each entry represents the skill score with reference to Incoherent forecasts based on "CRPS" and "LS"

	h=1									h=2								h=3								
	AA		Al	AB		BA		BB		AA		AB		BA		BB		AA		AB		BA		В		
R.method	CRPS	LS	CRPS	LS	CRPS	LS	CRPS	LS	CRPS	LS	CRPS	LS	CRPS	LS	CRPS	LS	CRPS	LS	CRPS	LS	CRPS	LS	CRPS	LS		
	Gaussian DGP																									
$\operatorname{MinT}(\operatorname{Shrink})$	3.91	1.30	12.04	3.82	10.07	3.12	1.47	0.47	3.80	1.28	19.37	6.55	13.61	4.44	-0.08	-0.14	2.54	0.83	19.58	6.92	13.94	4.83	-2.64	-0.96		
$\operatorname{MinT}(\operatorname{Sample})$	4.12	1.38	11.99	3.82	9.90	3.10	1.57	0.51	4.06	1.33	19.23	6.53	13.21	4.34	-0.24	-0.19	2.24	0.68	19.33	6.73	13.44	4.62	-3.44	-1.21		
WLS	1.10	0.42	10.37	3.21	9.12	2.78	-1.14	-0.26	-0.55	-0.09	15.52	5.05	12.17	3.91	-3.48	-1.25	-1.52	-0.46	15.75	5.32	12.63	4.34	-5.74	-2.04		
OLS	0.80	0.25	8.47	2.59	7.91	2.39	-1.52	-0.49	-1.23	-0.30	12.09	3.83	10.19	3.25	-4.42	-1.57	-2.04	-0.60	11.96	3.93	10.44	3.45	-6.72	-2.36		
Bottom up	0.01	0.00	0.04	0.00	0.15	0.00	-0.09	0.00	-0.01	0.00	0.17	-0.01	0.12	0.00	0.17	0.00	-0.23	0.00	-0.01	-0.02	0.01	-0.01	-0.13	0.00		
Base	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00		
										N	on-Gaus	sian DO	ЗP													
MinT(Shrink)	3.40	1.31	-0.11	-0.11	13.22	5.00	2.37	0.87	3.67	1.30	-0.11	-0.18	16.19	6.12	2.29	0.80	3.38	1.22	-1.21	-0.47	17.90	6.92	2.09	0.76		
$\operatorname{MinT}(\operatorname{Sample})$	3.40	1.29	-0.11	-0.13	13.22	4.99	2.37	0.91	3.67	1.25	-0.11	-0.24	16.19	6.01	2.29	0.76	3.38	1.16	-1.21	-0.58	17.90	6.71	2.09	0.64		
WLS	2.92	1.20	-1.90	-0.74	8.50	3.13	-0.96	-0.26	3.34	1.24	-2.51	-1.00	10.79	3.96	-1.27	-0.38	3.47	1.23	-3.11	-1.12	12.60	4.78	-1.21	-0.41		
OLS	2.70	1.07	-1.46	-0.55	6.19	2.25	-0.81	-0.21	2.95	1.15	-1.85	-0.73	7.61	2.74	-1.19	-0.32	3.22	1.18	-2.13	-0.76	8.85	3.25	-1.13	-0.35		
Bottom up	-0.10	0.00	-0.12	0.00	-0.02	0.00	-0.08	0.00	-0.17	0.00	0.09	0.00	0.03	-0.01	-0.10	0.00	-0.20	0.00	-0.03	0.00	-0.05	-0.01	-0.22	0.00		
Base	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00		

## 6 A novel non-parametric bootstrap approach

Often in practice we come across with hierarchical time series that has high level of disaggregation and/or contains more discrete data. For these time series, the parametric distributional assumptions are misleading. An alternative for such cases is to follow non-parametric approaches. Hence we propose a novel non-parametric bootstrap based approach for obtaining coherent probabilistic forecasts.

Our proposed method initially involves obtaining probabilistic forecasts without considering the aggregation constraints. These incoherent probabilistic forecasts are then reconcile to make them coherent. Let us first focus on the methodology for obtaining base forecasts.

## 6.1 Incoherent probabilistic forecasts

First we fit appropriate univariate models for each series in the hierarchy based on the training data  $\mathbf{y}_{1:T}$ . Then we compute 1-step-ahead training errors as  $e_{i,t} = y_{i,t} - \hat{y}_{i,t}$  for i = 1, ..., n and t = 1, ..., T where  $\hat{y}_{i,t} = E(y_{i,t}|y_{i,1:t-1})$ . These training errors will be stored in a matrix  $\mathbf{\Gamma}_{(T\times n)} = (\mathbf{e}_1, ..., \mathbf{e}_T)'$  where  $\mathbf{e}_t = (e_{1,t}, ..., e_{n,t})$  stored in the same order as  $\mathbf{y}_t$  for t = 1, ..., T. Next we block bootstrap a sample of size H from  $\mathbf{\Gamma}_{(T\times n)}$ . That is, we randomly select H consecutive rows from  $\mathbf{\Gamma}$  and store in a matrix  $\mathbf{\Gamma}_{(H\times n)}^b = (\mathbf{e}_1^b, ..., \mathbf{e}_H^b)'$  and repeat this for b = 1, ..., B.

Finally we generate the h-step-ahead future paths using the fitted univariate models conditioning on the past observations. We also incorporate the bootstrapped training errors as the error series for generating these future paths, and by doing so we implicitly model the contemporaneous correlation structure of the hierarchy. Further the use of consecutive (block) training errors will ensure that the serial correlation of the series is accounted for. To explain this process more explicitly consider the following example.

**Example:** Suppose we have fitted an ARMA(p,q) model for the  $i^{th}$  series of the hierarchy. i.e.

$$y_{i,t} = \alpha_1 y_{i,t-1} + \alpha_2 y_{i,t-2} + \dots + \alpha_p y_{i,t-p} + \beta_1 \epsilon_{i,t-1} + \beta_1 \epsilon_{i,t-2} + \dots + \beta_q \epsilon_{i,t-q} + \epsilon_{i,t},$$
  
$$y_{i,t} = (\alpha_1 + \alpha_2 L + \dots + \alpha_p L^{p-1}) y_{i,t-1} + (\beta_1 + \beta_1 L + \dots + \beta_q L^{q-1}) \epsilon_{i,t-1} + \epsilon_{i,t}.$$

where L is the well known lag/backshift operator. Then the h-step-ahead b<sup>th</sup> future path for the i<sup>th</sup> series is produced as,

$$\hat{y}_{i,t+h}^b = (\hat{\alpha}_1 + \hat{\alpha}_2 L + \dots + \hat{\alpha}_p L^{p-1}) y_{i,t+h-1} + (\hat{\beta}_1 + \hat{\beta}_1 L + \dots + \hat{\beta}_q L^{q-1}) \epsilon_{i,t+h-1} + e_{i,h}^b.$$

where,  $e_{i,h}^b$  is the  $(h \times i)^{\text{th}}$  element from  $\Gamma^b$ ,

$$y_{i,t+h-1} = \begin{cases} y_{i,1} : y_{i,T} & \text{for } t+h-1 \le T \\ \hat{y}_{i,T+1}^b : \hat{y}_{i,T+h-1}^b & \text{for } t+h-1 > T \end{cases}$$

and

$$\epsilon_{i,t+h-1} = \begin{cases} \epsilon_{i,1} : \epsilon_{i,T} & \text{for } t+h-1 \le T \\ e^b_{i,1} : e^b_{i,h-1} & \text{for } t+h-1 > T \end{cases}.$$

Once we obtain the h-step-ahead sample path for all n series in the hierarchy, we stack them in the same order as  $\hat{y}_{t+h}$ . Repeating the same process for b = 1, ..., B we will get a set of h-step-ahead bootstrapped future path of size B. We denote this as  $\hat{\Upsilon}_{T+h} = (\hat{y}_{T+h}^1, ..., \hat{y}_{T+h}^B)'$  where  $b^{\text{th}}$  row of  $\hat{\Upsilon}_{T+h}$  represent the h-step-ahead  $b^{\text{th}}$  sample paths for all series in the hierarchy.

We note that  $\hat{\mathbf{\Upsilon}}_{T+h}$  is a empirical sample from the incoherent probability distribution of the hierarchy. Since the aggregation constraints are not imposed while generating  $\hat{\mathbf{\Upsilon}}_{T+h}$ , it is very unlikely that they lie in the coherent subspace. Thus it requires reconciliation to which we now turn our attention.

## 6.2 Reconciliation of incoherent future paths

To reconcile the incoherent sample paths, we follow the definition of reconciliation. We project each sample path in  $\hat{\Upsilon}_{T+h}$  to the coherent subspace via the projection SG. i.e. for any G we can write,

$$\tilde{\mathbf{y}}_{T+h}^b = \mathbf{S}\mathbf{G}\hat{\mathbf{y}}_{T+h}^b,\tag{26}$$

consequently we have,

$$\tilde{\Upsilon}_{T+h} = SG\hat{\Upsilon}'_{T+h},\tag{27}$$

where, each row in  $\tilde{\mathbf{\Upsilon}}'_{T+h}$  represent a single reconciled sample path. Further  $\tilde{\mathbf{\Upsilon}}'_{T+h}$  form an empirical sample from the reconciled forecast distribution of the hierarchy. Any G matrix introduced in point forecast reconciliation (also given in Table 1) can be used for this sample path reconciliation. However, in the following subsection we discuss a method to find G that is optimal for probabilistic forecasts with respect to a proper scoring rule.

## 6.3 Optimal reconciliation of incoherent future paths

Let us now propose to find an optimal G for reconciling future paths by minimising a proper multivariate scoring rule. The respective objective function can be written as,

$$\underset{\boldsymbol{G}_{h}}{\operatorname{argmin}} \quad \mathbf{E}_{\boldsymbol{Q}}[S(\boldsymbol{S}\boldsymbol{G}_{h}\hat{\boldsymbol{\Upsilon}}'_{T+h}, \boldsymbol{y}_{T+h})], \tag{28}$$

where S is a proper scoring rule that follows equation (5). We use the subscript h on G to emphasis distinct G matrices for different forecast horizons. Recall that the energy score given in equation (8) is a proper scoring rule. Let  $\alpha = 1$  and following equation (9) we can write,

$$ES(\mathbf{S}\mathbf{G}_{h}\hat{\mathbf{\Upsilon}}'_{T+h}, \mathbf{y}_{T+h}) \approx \frac{1}{B} \sum_{b=1}^{B} ||\mathbf{S}\mathbf{G}_{h}\hat{\mathbf{y}}^{b}_{T+h,j} - \mathbf{y}_{T+h}|| - \frac{1}{2(B-1)} \sum_{b=1}^{B-1} ||\mathbf{S}\mathbf{G}_{h}(\hat{\mathbf{y}}^{b}_{T+h,j} - \hat{\mathbf{y}}^{b+1}_{T+h,j})||.$$
(29)

where B is the empirical sample size from the coherent forecast distribution. Now we can rewrite the objective function in (28) as,

$$\underset{\boldsymbol{G}}{\operatorname{argmin}} \frac{1}{N} \sum_{j=1}^{N} \left\{ \frac{1}{B} \sum_{b=1}^{B} || \boldsymbol{S} \boldsymbol{G}_{h} \boldsymbol{y}_{T+h,j}^{b} - \boldsymbol{y}_{T+h,j} || - \frac{1}{2(B-1)} \sum_{b=1}^{B-1} || \boldsymbol{S} \boldsymbol{G}_{h} (\boldsymbol{y}_{T+h,j}^{b} - \boldsymbol{y}_{T+h,j}^{b+1}) || \right\}$$
(30)

where, the expectation  $E_{\mathbf{Q}}$  over true forecast distribution  $\mathbf{Q}$  is approximated through the sample mean over  $\{\mathrm{ES}(\mathbf{S}\mathbf{G}_h\hat{\mathbf{\Upsilon}}'_{T+h,1}, \mathbf{y}_{T+h,1}), ..., \mathrm{ES}(\mathbf{S}\mathbf{G}_h\hat{\mathbf{\Upsilon}}'_{T+h,N}, \mathbf{y}_{T+h,N})\}$ . We can use numerical optimization methods to estimate the matrix  $\mathbf{G}_h$  that minimizes above objective function and thus obtain the optimally reconciled future paths.

### 6.3.1 Reparameterisation of G

We consider different reparameterisations when estimating the optimal  $G_h$  via the proposed optimisation process. Let,

$$G_h = (S'W_hS)^{-1}S'W_h. \tag{31}$$

This structure for  $G_h$  will ensure  $SG_h$  is a projection matrix and it projects each sample path onto  $\mathfrak{s}$ .

- **Method 1** Minimising the objective function in (30) over symmetric  $W_h$ . This solves an unconstrained optimisation problem
- **Method 2** Consider the Cholesky decomposition of  $W_h$ . i.e. let  $W_h = R'_h R_h$  where  $R_h$  is an upper triangular matrix. Thus minimising (30) over  $R_h$
- **Method 3** Similar to method 2, minimising (30) over cholesky decomposition of  $W_h$  but restricted for scaling. i.e.,  $W_h = R'_h R$  s.t  $i'W_h i = 1$  where i = (1, 0, ..., 0)'
- Method 4 Minimising (30) over  $G_h$  such that  $G_hS = I$ . This constraint is an alternative way to ensure that  $SG_h$  is a projection onto  $\mathfrak{s}$

## 6.4 Simulation study

We now compare different reconciliation methods with optimal reconciliation in a simulation setting. We use the same Gaussian and non-Gaussian DGP explained in Subsection 5.2.1 corresponding to the hierarchy in Figure 1.

#### 6.4.1 Simulation set up for optimal reconciliation

- 1. Generate time series with 2500 data points for each series in the hierarchy.
- 2. Consider a rolling window of 600 observations. We call this the "outer" rolling window.
  - i. Inside this outer rolling window consider an inner rolling window of T=500 observations.
  - ii. For this inner rolling window, fit univariate ARIMA models to each series in the hierarchy.
  - iii. Based on these fitted models, we generate B = 1000 of h = 3 step-ahead incoherent future paths incorporating bootstrap errors as described in Subsection 6.1. Thus we get  $\{\hat{\Upsilon}_{T+1,j=1}, \hat{\Upsilon}_{T+2,j=1}, \hat{\Upsilon}_{T+3,j=1}\}$ .
  - iv. Repeat step (iii) for j = 1, ..., N where N = 100 by rolling the inner window by one step ahead at a time.
  - v. Collect  $\{\hat{\mathbf{\Upsilon}}_{T+h,j=1},...,\hat{\mathbf{\Upsilon}}_{T+h,j=100}\}$  for h=1,...,3 into separate arrays of matrices.
  - vi. For each forecast horizon h, estimate the optimal  $G_h$  that will reconcile  $\{\hat{\mathbf{\Upsilon}}_{T+h,j=1},...,\hat{\mathbf{\Upsilon}}_{T+h,j=100}\}$  by minimising the average energy score as explained in Subsection 6.3. Also use different reparameterisation of  $G_h$  as explained in Subsection 6.3.1. Denote this as  $G_h^{Opt}$ .

- vii. Roll the inner rolling window another one step ahead and repeat step (ii) and (iii). Let these future paths denoted by  $\hat{\Upsilon}_{T+h}$  for h = 1, 2, 3.
- viii. Compute  $\tilde{\mathbf{\Upsilon}}_{T+h} = \mathbf{S}\mathbf{G}_h\hat{\mathbf{\Upsilon}}'_{T+h}$  for h = 1, 2, 3 using  $\mathbf{G}_h^{Opt}$  as well as using other  $\mathbf{G}$  matrices given in Table 1.
- 3. Repeat Step 2 for 1000 times by rolling the outer rolling window one step ahead at each time. Collect 1000 of these reconciled future paths,  $\tilde{\Upsilon}_{T+h}$ , from different reconciliation methods for h = 1, 2, 3 and evaluate the forecasting performances.

#### 6.4.2 Evaluation

Following the simulation process explained before, the reconciled non-parametric probabilistic forecasts were generated separately for Gaussian data and non-Gaussian data. To assess the predictive performance of these forecasts from different reconciliation methods, we use energy score and variogram scores as discussed in Section 4. Results are presented in Table 6.

We see that the scores for reconciled forecasts for different optimal methods are equivalent irrespective to the forecast horizon or the DGP. This implies that there is no difference in results due to different reparameterisations of G. Further, Mann-Whitney tests for location comparison support that the ES and VS for all reconciled forecasts are significantly lower than those of base/incoherent forecasts. This implies that all reconciliation methods produce coherent probabilistic forecasts with improved predictive ability compared to incoherent forecasts. In addition to that, the MinT(Shrink) and Optimal methods have similar prediction accuracy as there is no significant difference between the scores from these reconciliation methods. These results are consistent for both Gaussian and non-Gaussian data.

Table 6: Energy scores (ES) and variogram scores (VS) for probabilistic forecasts from different reconciliation methods are presented. Bottom row represent the scores for base forecasts which are not coherent. The smaller the scores, the better the forecasts are.

	Non-Gaussian DGP					Gaussian DGP						
Reconciliation	econciliation h=1		h=2		h=3		h=1		h=2		h=3	
method	ES	VS	ES	VS	ES	VS	ES	VS	ES	VS	ES	VS
Optimal(Method-1)	5.36	1.21	5.51	1.27	5.83	1.38	9.59	4.86	11.50	5.38	13.80	6.13
Optimal(Method-2)	5.37	1.21	5.53	1.27	5.83	1.37	9.58	4.85	11.50	5.37	13.80	6.14
Optimal(Method-3)	5.37	1.21	5.53	1.27	5.83	1.37	9.58	4.85	11.50	5.37	13.80	6.14
Optimal(Method-4)	5.38	1.21	5.54	1.27	5.83	1.38	9.58	4.85	11.50	5.37	13.80	6.14
MinT(Shrink)	5.33	1.19	5.50	1.26	5.77	1.34	9.43	4.78	11.40	5.33	13.70	6.09
WLS	5.43	1.23	5.60	1.30	5.89	1.40	9.64	4.93	11.70	5.60	14.10	6.39
OLS	5.51	1.23	5.70	1.30	5.98	1.40	9.91	4.93	12.10	5.60	14.50	6.39
Base	5.71	1.28	5.94	1.37	6.27	1.49	10.40	5.31	12.70	6.22	15.20	7.14

However, optimal reconciliation required a high computational cost for larger hierarchies. Further, it requires sufficient data points to learn the G matrix. Thus we claim to use the MinT G for reconciling bootstrapped future paths for two reasons. Firstly it is computationally efficient relative to the optimal method and secondly, it produces accurate probabilistic forecasts that are at least as good as the Optimal method with respect to the energy score.

# 7 Application: Forecasting Australian domestic tourism flow

In this section we illustrate how the probabilistic forecast reconciliation methods can be used in practice. We use an application to forecasting the domestic tourism flow in Australia. Previous related studies have shown that hierarchical forecasting methods will improve the forecast accuracy in point forecasts. For example see Athanasopoulos et al. (2009), Hyndman et al. (2011) and Wickramasuriya et al. (2019). However, this study is the first to apply the reconciliation methods for tourism forecasting in a probabilistic framework.

#### 7.1 Data

As a measure of domestic tourism flow, we consider the "overnight trips" to different destinations across the country. An Australian citizen going on a trip within the country, to a minimum of 40km away from the residence and spending at least one night is considered as an overnight trip. Data were collected through the National Visitor Survey (NVS) managed by Tourism Research Australia based on an annual sample of 120,000 Australian residents aged 15 years or more, through telephone interviews (Tourism Research Australia 2019).

The total number of overnight trips in Australia can naturally disaggregate through a geographical hierarchy. This hierarchy consists of 7 states <sup>1</sup> in the 1st level of disaggregation, 27 zones in the 2nd level of disaggregation and 76 regions in the bottom level and thus comprises 110 series altogether. More details about the individual series are provided

<sup>&</sup>lt;sup>1</sup>We have considered ACT as a part of New South Wales and Northern Territory as a state.

in Table 7. We consider monthly overnight trips for all series spanning the period from January 1998 to December 2018. This gives 152 observations per series.

### 7.2 Forecasting methodology

We apply the both parametric and non-parametric reconciliation approaches as discussed in previous sections. We use a rolling window of 100 observations as the training sample where the first training sample will span from Jan-1998 to Apr-2006. Based on this training set we fit univariate ARIMA and ETS models for each series in the hierarchy using automated functions  $\mathtt{auto.arima()}$  and  $\mathtt{ets()}$  from the forecast package in R software. Then we generate parametric and non-parametric probabilistic forecasts for half a year ahead, i.e for h=1,...,6. For parametric forecasts, we assume Gaussian densities and obtain the incoherent mean and variance forecasts. These are then reconciled using the methods described in Section 5. For non-parametric forecasts, we generate the bootstrapped future paths and then reconcile each sample path as described in Section 6. We note that the MinT(Sample) reconciliation was ignored in both approaches as the sample size of training data set is less than the dimension of the hierarchy. Finally we roll the training window one month ahead at a time and replicate the process until the end of the sample. This yields, 152 1-step ahead, 151 2-steps ahead through 147 6-step ahead sets of probabilistic forecasts left for evaluation.

#### 7.3 Evaluation, results and discussion

We evaluate the predictive accuracy using scoring rules. Energy score and Variogram score are used to assess the predictive accuracy of multivariate forecast distributions for the whole hierarchy as well as for the different disaggregation levels. CRPS is used to assess predictive

accuracy of the univariate forecast distributions of each series in the hierarchy. Average scores were calculated over the replications for each forecast horizons separately. Finally the skill scores were calculated for each reconciled predictive distribution with reference to the incoherent forecast distribution. Positive values in the skill score indicate improved forecast accuracy and negative values indicate weaker forecast accuracy relative to the incoherent forecast distribution.

Figure 4 shows the skill scores with respect to the multivariate predictive distribution of the whole hierarchy from different reconciliation methods. Figure 5 shows evaluation with respect to the multivariate forecast distributions of each level of the hierarchy. Top panel/s represent the results from Gaussian reconciled predictive distribution and bottom panel/s represent the results from non-parametric predictive densities. From both figures we see that almost all the reconciliation methods improve forecast accuracy irrespective of whether the parametric or non-parametric approaches is taken. Further, bottom-up approach performs worse than incoherent forecasts at all forecast horizons. This is due to the fact that bottom level series are more volatile and therefore challenging to forecast. Finally and most importantly, MinT(Shrink) outperforms all probabilistic forecast reconciliation methods for both parametric and non-parametric approaches.

Figure 6 shows the predictive accuracy of univariate forecast distributions for the Total overnight trips. We see that reconciliation with OLS and MinT(Shrink) methods provide improved univariate forecast distributions for the top level of the hierarchy for both approaches.

As a final note, we have presented results follows using ARIMA models only. The results are similar for ETS models as well and we present these in the appendix.

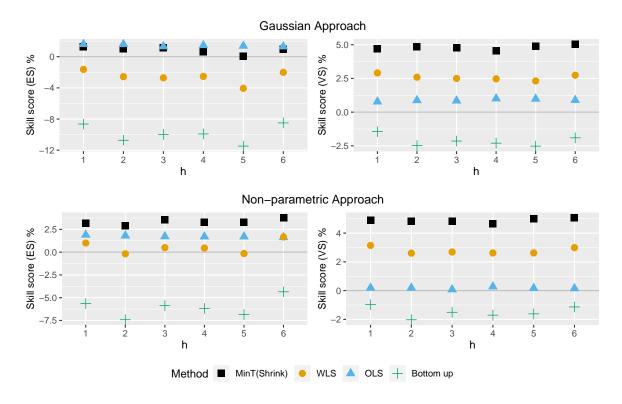


Figure 4: Skill scores with reference to incoherent forecasts for multivariate predictive distribution of the whole hierarchy from different reconciliation methods are presented. Top panel shows the results from Gaussian approach and the bottom panel shows the results from non-parametric approach. Left and right panels shows the skill scores based on energy score and variogram score respectively.

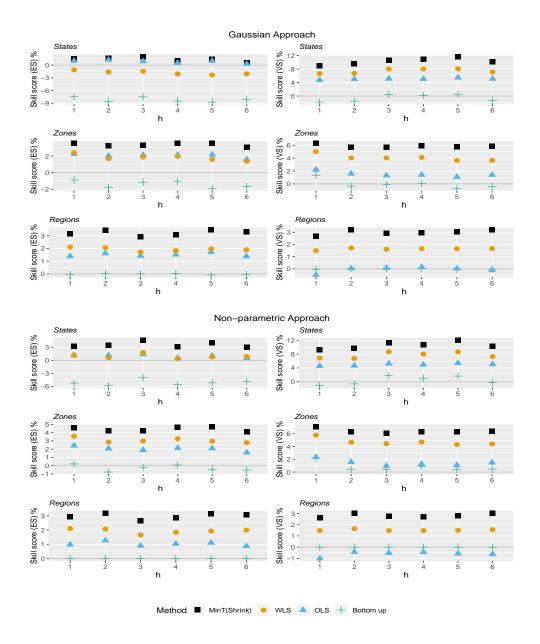


Figure 5: Skill score for multivariate probabilistic forecasts of different levels of the hierarchy are presented. Results from Gaussian approach are presented in the top three panels and results from the non-parametric approach are presented in the bottom three panels.

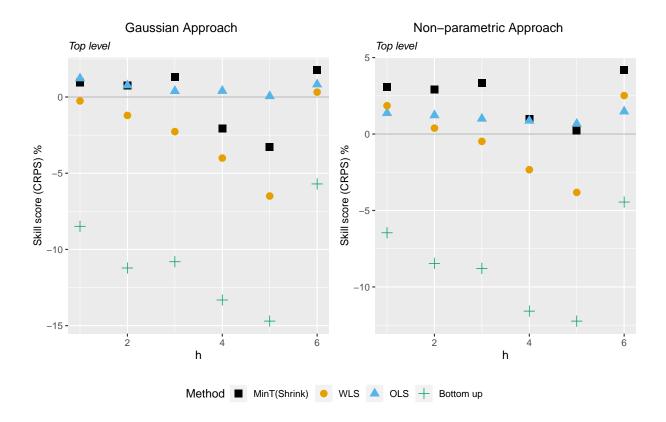


Figure 6: Skill score based on CRPS (with reference to the incoherent forecasts) for univariate probabilistic forecasts for the Total (top level) overnight trips are presented. Left panel shows the results from Gaussian approach and right panel shows the results from non-parametric approach.

## 8 Conclusions

Although the problem of hierarchical point forecasts is well studied in the literature, there is a lack of attention in the context of probabilistic forecasts. Thus we fill this gap in the literature by providing substantial theoretical background to the problem.

The geometric interpretation of point forecast reconciliation allowed us to extend these concepts to the probabilistic setting. We have also discussed strategies for evaluating probabilistic forecasts for hierarchical time series advocating the use of multivariate scoring rules on the full hierarchy, while establishing a key result regarding the impropriety of the log score with respect to incoherent forecasts.

We have shown that for elliptical distributions the true predictive density can be recovered by linear reconciliation and we have established conditions for when this is a projection. Although this projection cannot feasibly be obtained in practice, a projection similar to the MinT procedure provides a good approximation in applications. This is supported by the results of a simulation study as well as the empirical application.

We have further proposed a novel non-parametric approach for obtaining coherent probabilistic forecasts when the parametric densities are unavailable. Initially this method involves generating thousands of sample paths using bootstrapped forecast errors. Then each sample path will be reconciled via projections. Using an extensive simulation setting we have shown that MinT projection is at least as good as the optimal projection with respect to minimising Energy score. Further we have shown reconciled probabilistic forecasts via MinT has improved the forecast accuracy in the empirical application.

In many ways this paper sets up a substantial future research agenda. For example, having defined what amounts to an entire class of reconciliation methods for probabilistic forecasts it will be worthwhile investigating which specific projections are optimal. This

is likely to depend on the specific scoring rule employed as well as the properties of the base forecasts. Another avenue worth investigating is to consider whether it is possible to recover the true predictive distribution for non-elliptical distributions via a non-linear function g(.).

# 9 Appendix

# 9.1 Results from ETS base forecasts

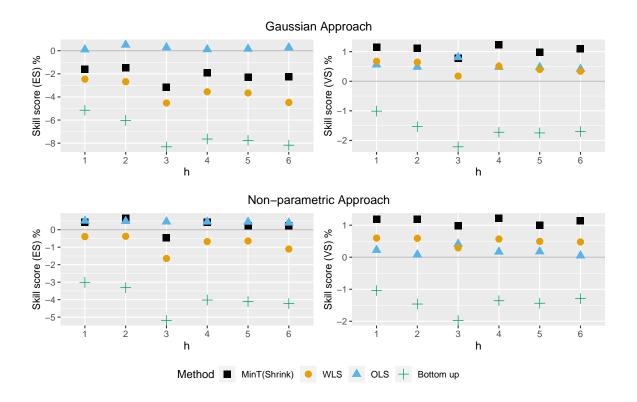


Figure 7: Skill scores with reference to ETS base forecasts for multivariate predictive distribution of the whole hierarchy from different reconciliation methods are presented. Top panel shows the results from Gaussian approach and the bottom panel shows the results from non-parametric approach. Left and right panels shows the skill scores based on energy score and variogram score respectively.

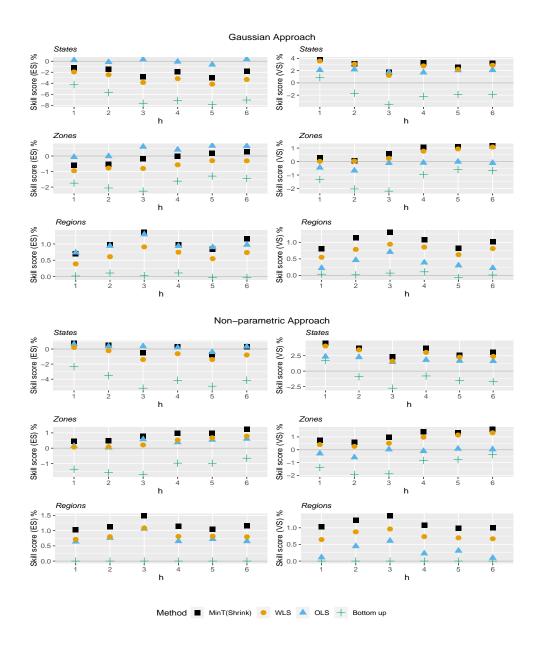


Figure 8: Skill score (with reference to ETS base forecasts) for multivariate probabilistic forecasts of different levels of the hierarchy are presented. Results from Gaussian approach are presented in the top three panels and results from the non-parametric approach are presented in the bottom three panels.

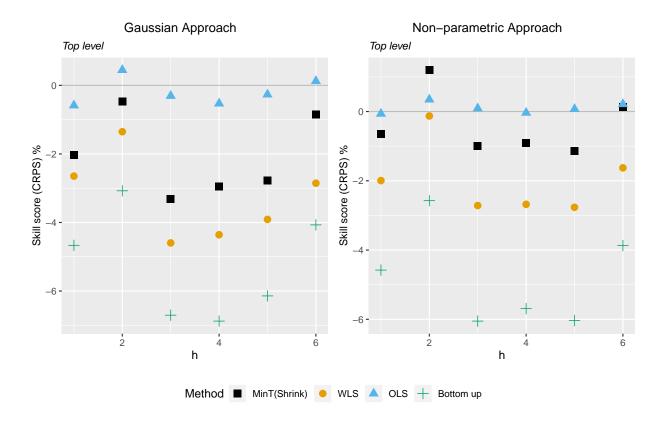


Figure 9: Skill score based on CRPS (with reference to the ETS base forecasts) for univariate probabilistic forecasts for the Total (top level) overnight trips are presented. Left panel shows the results from Gaussian approach and right panel shows the results from non-parametric approach.

9.2 Geographical hierarchy of Australia

Table 7: Geographical hierarchy of Australian tourism flow

	Level 0 - Total		$Regions\ cont.$			Regions cont.			
1	Tot	Australia	37	AAB	Central Coast	75	CBD	Mackay	
	Level 1 - States		38	ABA	Hunter	76	CBE	Capricorn	
2	A	NSW	39	ABB	North Coast NSW	77	CBF	Gladstone	
3	В	Victoria	40	ACA	South Coast	78	CCA	Whitsundays	
4	$\mathbf{C}$	Queensland	41	ADA	Snowy Mountains	79	CCB	Townsville	
5	D	South Australia	42	${\rm ADB}$	Capital Country	80	CCC	Tropical North Queensland	
6	$\mathbf{E}$	Western Australia	43	$\operatorname{ADC}$	The Murray	81	$\mathrm{CDA}$	Southern QLD country	
7	F	Tasmania	44	$\operatorname{ADD}$	Riverina	82	${\rm CDB}$	Outback QLD	
8_	G	Northern Territory	45	AEA	Central NSW	83	DAA	Adelaide	
	Level 2 - Zones		46	AEB	New England North West	84	DAB	Barossa	
9	AA	Metro NSW	47	AEC	Outback NSW	85	DAC	Adelaide Hills	
10	AB	North Coast NSW	48	$\operatorname{AED}$	Blue Mountains	86	DBA	Limestone Coast	
11	AC	South Coast NSW	49	AFA	Canberra	87	DBB	Fleurieu Peninsula	
12	AD	South NSW	50	${\rm BAA}$	Melbourne	88	$\operatorname{DBC}$	Kangaroo Island	
13	AE	North NSW	51	BAB	Peninsula	89	DCA	Murraylands	
14	AF	ACT	52	${\rm BAC}$	Geelong	90	DCB	Riverland	
15	BA	Metro VIC	53	$\operatorname{BBA}$	Western	91	DCC	Clare Valley	
16	BB	West Coast VIC	54	$\operatorname{BCA}$	Lakes	92	DCD	Flinders Range and Outback	
17	$_{\mathrm{BC}}$	East Coast VIC	55	$\operatorname{BCB}$	Grippsland	93	$\mathrm{DDA}$	Eyre Peninsula	
18	BD	North East VIC	56	$\operatorname{BCC}$	Phillip Island	94	DDB	Yorke Peninsula	
19	BE	North West VIC	57	$\operatorname{BDA}$	Central Murray	95	EAA	Australia's Coral Coast	
20	CA	Metro QLD	58	$\operatorname{BDB}$	Goulburn	96	EAB	Experience Perth	
21	$^{\mathrm{CB}}$	Central Coast QLD	59	$\operatorname{BDC}$	High Country	97	EAC	Australia's South West	
22	CC	North Coast QLD	60	$\operatorname{BDD}$	Melbourne East	98	EBA	Australia's North West	
23	$^{\mathrm{CD}}$	Inland QLD	61	$\operatorname{BDE}$	Upper Yarra	99	ECA	Australia's Golden Outback	
24	DA	Metro SA	62	$\operatorname{BDF}$	Murray East	100	FAA	Hobert and South	
25	DB	South Coast SA	63	$\operatorname{BEA}$	Wimmera+Mallee	101	FBA	East Coast	
26	DC	Inland SA	64	BEB	Western Grampians	102	$\operatorname{FBB}$	Launceston, Tamar & North	
27	DD	West Coast SA	65	$\operatorname{BEC}$	Bendigo Loddon	103	FCA	North West	
28	$\mathrm{E}\mathrm{A}$	West Coast WA	66	$\operatorname{BED}$	Macedon	104	FCB	West coast	
29	EB	North WA	67	BEE	Spa Country	105	GAA	Darwin	
30	EC	South WA	68	$\operatorname{BEF}$	Ballarat	106	$\operatorname{GAB}$	Litchfield Kakadu Arnhem	
31	FA	South TAS	69	$\operatorname{BEG}$	Central Highlands	107	GAC	Katherine Daly	
32	FB	North East TAS	70	CAA	Gold Coast	108	$\operatorname{GBA}$	Barkly	
33	FC	North West TAS	71	CAB	Brisbane	109	$_{\mathrm{GBB}}$	Lasseter	
34	GA	North Coast NT	72	CAC	Sunshine Coast	110	$_{\mathrm{GBC}}$	Alice Springs	
35	GB	Central NT	73	CBB	Bundaberg	111	GBD	MacDonnell	
	Lev	vel 2 - Regions	74	CBC	Fraser Coast				
36	AAA	Sydney							

# References

- Athanasopoulos, G., Ahmed, R. A. & Hyndman, R. J. (2009), 'Hierarchical forecasts for Australian domestic tourism', *International Journal of Forecasting* **25**(1), 146 166.
- Athanasopoulos, G., Hyndman, R. J., Kourentzes, N. & Petropoulos, F. (2017), 'Forecasting with temporal hierarchies', European Journal of Operational Research 262(1), 60–74.
- Ben Taieb, S., Huser, R., Hyndman, R. J. & Genton, M. G. (2017), 'Forecasting uncertainty in electricity smart meter data by boosting additive quantile regression', *IEEE Transactions on Smart Grid* **7**(5), 2448–2455.
- Dunn, D. M., Williams, W. H. & Dechaine, T. L. (1976), 'Aggregate Versus Subaggregate Models in Local Area Forecasting', *Journal of American Statistical Association* **71**(353), 68–71.
- Gneiting, T. & Katzfuss, M. (2014), 'Probabilistic Forecasting', Annual Review of Statistics and Its Application 1, 125–151.
- Gneiting, T. & Raftery, A. E. (2007), 'Strictly Proper Scoring Rules, Prediction, and Estimation', Journal of the American Statistical Association 102(477), 359–378.
- Gneiting, T., Stanberry, L. I., Grimit, E. P., Held, L. & Johnson, N. A. (2008), Assessing probabilistic forecasts of multivariate quantities, with an application to ensemble predictions of surface winds.
- Gross, C. W. & Sohl, J. E. (1990), 'Disaggregation methods to expedite product line forecasting', *Journal of Forecasting* **9**(3), 233–254.

- Hyndman, R. (2019), 'forecast: Forecasting Functions for Time Series and Linear Models, R package version 8.9', *URL: http://github.com/robjhyndman/forecast*.
- Hyndman, R. J., Ahmed, R. A., Athanasopoulos, G. & Shang, H. L. (2011), 'Optimal combination forecasts for hierarchical time series', *Computational Statistics and Data Analysis* **55**(9), 2579–2589.
- Jeon, J., Panagiotelis, A. & Petropoulos, F. (2019), 'Probabilistic forecast reconciliation with applications to wind power and electric load', European Journal of Operational Research 279(2), 364–379.
- Jordan, A., Krüger, F. & Lerch, S. (2017), 'Evaluating probabilistic forecasts with the R package scoringRules'.

**URL:** http://arxiv.org/abs/1709.04743

- Pinson, P. & Tastu, J. (2013), Discrimination ability of the Energy score, Technical report, Technical University of Denmark.
- R Core Team (2018), R: A Language and Environment for Statistical Computing, R Foundation for Statistical Computing, Vienna, Austria.

**URL:** https://www.R-project.org/

- Schäfer, J. & Strimmer, K. (2005), 'A Shrinkage Approach to Large-Scale Covariance Matrix Estimation and Implications for Functional Genomics', *Statistical Applications in Genetics and Molecular Biology* 4(1).
- Scheuerer, M. & Hamill, T. M. (2015), 'Variogram-Based Proper Scoring Rules for Probabilistic Forecasts of Multivariate Quantities', *Monthly Weather Review* **143**(4), 1321–1334.

- Székely, G. J. & Rizzo, M. L. (2013), 'Energy statistics: A class of statistics based on distances', *Journal of Statistical Planning and Inference* **143**(8), 1249–1272.
- Tourism Research Australia (2019), Tourism forecasts, Technical report, Tourism Research Australia, Canberra.
- Wickramasuriya, S. L., Athanasopoulos, G. & Hyndman, R. J. (2019), 'Optimal Forecast Reconciliation for Hierarchical and Grouped Time Series Through Trace Minimization', Journal of the American Statistical Association 114(526), 804–819.