

## A Theorem Proofs

### A.1 Proof of Theorem 4.1 and Theorem 4.2

Consider the region  $\mathcal{I}$  given by the Cartesian product of intervals  $(l_1, u_1), (l_2, u_2), \dots, (l_m, u_m)$ . We derive the probability, under the reconciled measure, that the bottom-level series lie in  $\mathcal{I}$ , i.e.  $\Pr(\boldsymbol{\ell} > \mathbf{b} > \mathbf{u})$ , where  $\boldsymbol{\ell} = (\ell_1, \ell_2, \dots, \ell_m)$ ,  $\mathbf{u} = (u_1, u_2, \dots, u_m)$  and  $>$  denotes element-wise inequality between vectors. The pre-image of  $\mathcal{I}$  under  $g$  can similarly be denoted as all points  $\mathbf{y}$  satisfying  $\boldsymbol{\ell} > \mathbf{G}\mathbf{y} > \mathbf{u}$ . Using Definition 3.2,

$$\Pr(\boldsymbol{\ell} > \mathbf{b} > \mathbf{u}) = \int_{\boldsymbol{\ell} > \mathbf{G}\mathbf{y} > \mathbf{u}} \hat{f}(\mathbf{y}) d\mathbf{y},$$

where  $\hat{f}$  is the density of the base probabilistic forecast. Now consider a change of variables to an  $n$ -dimensional vector  $\mathbf{z}$  where  $\mathbf{y} = \mathbf{G}^* \mathbf{z}$ . Recall,  $\mathbf{G}^* = (\mathbf{G}^- \vdots \mathbf{G}_\perp)$ ,  $\mathbf{G}^-$  is a generalised inverse of  $\mathbf{G}$ , and  $\mathbf{G}_\perp$  is an orthogonal complement of  $\mathbf{G}$ . By the change of variables

$$\begin{aligned} \Pr(\boldsymbol{\ell} > \mathbf{b} > \mathbf{u}) &= \int_{\boldsymbol{\ell} > \mathbf{G}\mathbf{y} > \mathbf{u}} \hat{f}(\mathbf{y}) d\mathbf{y} \\ &= \int_{\boldsymbol{\ell} > \mathbf{G}\mathbf{G}^* \mathbf{z} > \mathbf{u}} \hat{f}(\mathbf{G}^* \mathbf{z}) |\mathbf{G}^*| d\mathbf{z} \\ &= \int_{\boldsymbol{\ell} > \mathbf{z}_1 > \mathbf{u}} \hat{f}(\mathbf{G}^* \mathbf{z}) |\mathbf{G}^*| d\mathbf{z}, \end{aligned}$$

where  $\mathbf{z}_1$  denotes the first  $m$  elements of  $\mathbf{z}$ . Letting  $\mathbf{a}$  denote the last  $n - m$  elements of  $\mathbf{z}$  the integral above can be written as

$$\Pr(\mathbf{b} \in \mathcal{I}) = \int \int_{\boldsymbol{\ell} > \mathbf{z}_1 > \mathbf{u}} \hat{f}(\mathbf{G}^- \mathbf{z}_1 + \mathbf{G}_\perp \mathbf{a}) |\mathbf{G}^*| d\mathbf{a} d\mathbf{z}_1$$

Replacing  $\mathbf{z}_1$  with  $\mathbf{b}$ , it can be seen that the term inside the outer integral is a density for the bottom-level series. Therefore

$$\tilde{f}_b(\mathbf{b}) = \int \hat{f}(\mathbf{G}^- \mathbf{b} + \mathbf{G}_\perp \mathbf{a}) |\mathbf{G}^*| d\mathbf{a}, \quad (6)$$

is the density of  $\mathbf{b}$ . To obtain the density of the full hierarchy we first augment the density in Equation (6) by  $n - m$  variables denoted  $\mathbf{u}$

$$f(\mathbf{b}, \mathbf{u}) = \tilde{f}_b(\mathbf{b}) \mathbb{1}\{\mathbf{u} = 0\}, \quad (7)$$

such that the density  $f(\mathbf{b}, \mathbf{u})$  is a density for  $n$ -dimensional vector that is degenerate across the dimensions corresponding to  $\mathbf{u}$ . Using the change of variables,

$$\mathbf{y} = (\mathbf{S} : \mathbf{S}_{\perp}^{-}) \begin{pmatrix} \mathbf{b} \\ \mathbf{u} \end{pmatrix},$$

where  $\mathbf{S}_{\perp}^{-}$  is a generalised inverse such that  $\mathbf{S}'_{\perp} \mathbf{S}_{\perp}^{-} = \mathbf{I}$  and noting the inverse of  $(\mathbf{S} : \mathbf{S}_{\perp})$  is

$$\mathbf{S}^* := \begin{pmatrix} \mathbf{S}^{-} \\ \mathbf{S}'_{\perp} \end{pmatrix},$$

it can be seen that  $\mathbf{b} = \mathbf{S}^{-} \mathbf{y}$  and  $\mathbf{u} = \mathbf{S}'_{\perp} \mathbf{y}$ . Applying this change of variables yields the density

$$\tilde{f}_{\mathbf{y}}(\mathbf{y}) = |\mathbf{S}^*| \tilde{f}_{\mathbf{b}}(\mathbf{S}^{-} \mathbf{y}) \mathbb{1}_{\{\mathbf{S}'_{\perp} \mathbf{y} = \mathbf{0}\}}.$$

Since  $\mathbf{S}'_{\perp}$  is the orthogonal complement of  $\mathbf{S}$  and since the columns of  $\mathbf{S}$  span the coherent subspace, the statement  $\mathbf{S}'_{\perp} \mathbf{y} = 0$  is equivalent to the statement  $\mathbf{y} \in \mathfrak{s}$ . As such, the reconciled density is given by

$$\tilde{f}_{\mathbf{y}}(\mathbf{y}) = |\mathbf{S}^*| \tilde{f}_{\mathbf{b}}(\mathbf{S}^{-} \mathbf{y}) \mathbb{1}_{\{\mathbf{y} \in \mathfrak{s}\}}.$$

## A.2 Proof of Theorem 4.4

Let  $\hat{\Sigma} = \Sigma + \mathbf{D} = \mathbf{S} \Omega \mathbf{S}' + \mathbf{D}$ . If reconciliation is via a projection onto  $\mathfrak{s}$ , then  $\mathbf{S} \mathbf{G} \mathbf{S} = \mathbf{S}$  and

$$\begin{aligned} \tilde{\Sigma} &= \mathbf{S} \mathbf{G} \hat{\Sigma} \mathbf{G}' \mathbf{S}' \\ &= \mathbf{S} \mathbf{G} \mathbf{S} \Omega \mathbf{S}' \mathbf{G}' \mathbf{S}' + \mathbf{S} \mathbf{G} \mathbf{D} \mathbf{G}' \mathbf{S}' \\ &= \mathbf{S} \Omega \mathbf{S}' + \mathbf{S} \mathbf{G} \mathbf{D} \mathbf{G}' \mathbf{S}' \\ &= \Sigma + \mathbf{S} \mathbf{G} \mathbf{D} \mathbf{G}' \mathbf{S}'. \end{aligned}$$

Therefore to recover the true predictive using a projection, some  $\mathbf{G}_{\text{opt}}$  must be found such that  $\mathbf{G}_{\text{opt}} \mathbf{D} = \mathbf{0}$ . Let the eigenvalue decomposition of  $\mathbf{D}$  be given by  $\mathbf{R} \mathbf{\Lambda} \mathbf{R}'$ , where  $\mathbf{R}$  is an  $n \times q$  matrix with  $q = \text{rank}(\mathbf{D})$  and  $\mathbf{\Lambda}$  is an  $q \times q$  diagonal matrix containing non-zero eigenvalues of  $\mathbf{D}$ . By the rank nullity theorem,  $\mathbf{R}$  will have an orthogonal complement  $\mathbf{R}_{\perp}$  of dimension  $n \times (n - q)$ . If  $q = n - m$  then the number of columns of  $\mathbf{R}_{\perp}$  is  $m$  and  $\mathbf{G}_{\text{opt}}$  can be formed as the  $m \times n$  matrix  $(\mathbf{R}'_{\perp} \mathbf{S})^{-1} \mathbf{R}'_{\perp}$ . If  $q < n - m$  the number of columns of  $\mathbf{R}_{\perp}$  is greater than  $m$ , and any  $m$  columns of  $\mathbf{R}_{\perp}$  can be used to form  $\mathbf{G}_{\text{opt}}$  in a similar fashion. However when  $q > n - m$ , the number of columns of  $\mathbf{R}_{\perp}$  is less than  $m$  and no such  $m \times n$  matrix  $\mathbf{G}_{\text{opt}}$  can be formed. Therefore the true predictive can only be recovered via a projection when  $\text{rank}(\mathbf{D}) \leq n - m$ .

With respect to the location, if  $\mathbf{S} \mathbf{G}$  is a projection, reconciled forecasts will be unbiased if the base forecasts are also unbiased. Biased base forecasts can be bias corrected before reconciliation as described by Panagiotelis et al. (2021) in the point forecasting setting.

### A.3 Proof of Theorem 5.1

The proof relies on the following change of variables,

$$\mathbf{y} = (\mathbf{S} \vdash \mathbf{S}_\perp) \begin{pmatrix} \mathbf{b} \\ \mathbf{u} \end{pmatrix}.$$

Also recall from the proof of Theorem 4.2 that  $\mathbf{S}^* = (\mathbf{S} \vdash \mathbf{S}_\perp)^{-1}$

Let the density of the true predictive  $f(\mathbf{y})$  after a change of variables, be given by  $|\mathbf{S}^*|^{-1} f_{\mathbf{b}}(\mathbf{b}) \mathbb{1}\{\mathbf{u} = \mathbf{0}\}$ . To prove that the log score is improper we construct an incoherent base density  $\hat{f}$  such that  $E_f[LS(\hat{f}, \mathbf{y})] < E_f[LS(f, \mathbf{y})]$ . This incoherent density is constructed, so that after the same change of variables it can be written as  $|\mathbf{S}^*|^{-1} \hat{f}_{\mathbf{b}}(\mathbf{b}) \hat{f}_{\mathbf{u}}(\mathbf{u})$ . We require  $\hat{f}_{\mathbf{u}}(\mathbf{0}) > 1$ , i.e.,  $\mathbf{u}$  is highly concentrated around  $\mathbf{0}$  but still non-degenerate. An example is an independent normal with mean 0 and variance less than  $(2\pi)^{-1}$ . Now, let  $\mathbf{y}^*$  be a realisation from  $f$ . Let the first  $m$  elements of  $\mathbf{S}^* \mathbf{y}^*$  be  $\mathbf{b}^*$ , and the remaining elements be  $\mathbf{u}^*$ . The log score for  $f$  is thus,

$$\begin{aligned} LS(f, \mathbf{y}^*) &= -\log f(\mathbf{y}^*) \\ &= -\log |\mathbf{S}^*| - \log f_{\mathbf{b}}(\mathbf{b}^*) - \log(\mathbb{1}\{\mathbf{u}^* = \mathbf{0}\}) \\ &= -\log |\mathbf{S}^*| - \log f_{\mathbf{b}}(\mathbf{b}^*), \end{aligned} \tag{8}$$

where the third term in Equation (8) is equal to zero since the fact that  $\mathbf{y}^* \in \mathfrak{s}$  implies that  $\mathbf{u}^* = \mathbf{0}$ . The log score for  $\hat{f}$  is

$$LS(\hat{f}, \mathbf{y}^*) = -\log |\mathbf{S}^*| - \log f_{\mathbf{b}}(\mathbf{b}^*) - \log f_{\mathbf{u}}(\mathbf{0}).$$

Since  $f_{\mathbf{u}}(\mathbf{0}) > 1$  by construction,  $-\log f_{\mathbf{u}}(\mathbf{0}) < 0$ , therefore

$$LS(\hat{f}, \mathbf{y}^*) < -\log |\mathbf{S}^*| - \log f_{\mathbf{b}}(\mathbf{b}^*) = LS(f, \mathbf{y}^*)$$

Since this holds for any possible realisation, it will also hold after taking expectations (by the monotonicity of expectations). Thus  $\hat{f}$  violates the condition for a proper scoring rule.

## B Reconciled Forecast for Gaussian Distribution

Suppose the incoherent base forecasts are Gaussian with mean  $\hat{\boldsymbol{\mu}}$ , covariance matrix  $\hat{\boldsymbol{\Sigma}}$  and density,

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

Then, using Theorem 4.1, the reconciled density for the bottom-level series is given by

$$\tilde{f}_{\mathbf{b}}(\mathbf{b}) = \int (2\pi)^{-\frac{n}{2}} |\hat{\Sigma}|^{-\frac{1}{2}} |\mathbf{G}^*| e^{-q/2} d\mathbf{a},$$

where

$$\begin{aligned} q &= \left[ \mathbf{G}^* \begin{pmatrix} \mathbf{b} \\ \mathbf{a} \end{pmatrix} - \hat{\mu} \right]' \hat{\Sigma}^{-1} \left[ \mathbf{G}^* \begin{pmatrix} \mathbf{b} \\ \mathbf{a} \end{pmatrix} - \hat{\mu} \right] \\ &= \left[ \begin{pmatrix} \mathbf{b} \\ \mathbf{a} \end{pmatrix} - \mathbf{G}^{*-1} \hat{\mu} \right]' \left[ \mathbf{G}^{*-1} \hat{\Sigma} (\mathbf{G}^{*-1})' \right]^{-1} \left[ \begin{pmatrix} \mathbf{b} \\ \mathbf{a} \end{pmatrix} - \mathbf{G}^{*-1} \hat{\mu} \right]. \end{aligned}$$

Noting that

$$\mathbf{G}^{*-1} = \begin{pmatrix} \mathbf{G} \\ \mathbf{G}_{\perp}^{-} \end{pmatrix},$$

where  $\mathbf{G}_{\perp}^{-}$  is an  $(n - m) \times n$  matrix such that  $\mathbf{G}_{\perp}^{-} \mathbf{G}_{\perp} = \mathbf{I}$ ,  $q$  can be rearranged as

$$\left[ \begin{pmatrix} \mathbf{b} \\ \mathbf{a} \end{pmatrix} - \begin{pmatrix} \mathbf{G} \\ \mathbf{G}_{\perp}^{-} \end{pmatrix} \hat{\mu} \right]' \left[ \begin{pmatrix} \mathbf{G} \\ \mathbf{G}_{\perp}^{-} \end{pmatrix} \hat{\Sigma} \begin{pmatrix} \mathbf{G} \\ \mathbf{G}_{\perp}^{-} \end{pmatrix}' \right]^{-1} \left[ \begin{pmatrix} \mathbf{b} \\ \mathbf{a} \end{pmatrix} - \begin{pmatrix} \mathbf{G} \\ \mathbf{G}_{\perp}^{-} \end{pmatrix} \hat{\mu} \right].$$

After the change of variables, the density can be recognised as a multivariate Gaussian in  $\mathbf{b}$  and  $\mathbf{a}$ . The mean and covariance matrix for the margins of the first  $m$  elements are  $\mathbf{G}\hat{\mu}$  and  $\mathbf{G}\hat{\Sigma}\mathbf{G}'$  respectively. Marginalising out  $\mathbf{a}$ , the reconciled forecast for the bottom-level is  $\tilde{\mathbf{b}} \sim \mathcal{N}(\mathbf{G}\hat{\mu}, \mathbf{G}\hat{\Sigma}\mathbf{G}')$ . Using standard results from matrix algebra of normals,  $\tilde{\mathbf{y}} \sim \mathcal{N}(\mathbf{S}\mathbf{G}\hat{\mu}, \mathbf{S}\mathbf{G}\hat{\Sigma}\mathbf{G}'\mathbf{S}')$ .

## C Comparison using only bottom-level series

If a probabilistic forecast is available for any  $m$  series, then a probabilistic forecast for the full hierarchy can be derived. Definition 3.1 provides an example using the bottom-level series. This suggests that it may be adequate to merely compare two coherent forecasts to one another using the bottom-level series only. This is true for the log score.

Consider a coherent probabilistic forecast with density  $\tilde{f}_{\mathbf{y}}$  for the full hierarchy and  $\tilde{f}_{\mathbf{b}}$  for the bottom-level series. By Theorem 4.2,  $\tilde{f}_{\mathbf{y}}(\mathbf{y}) = |\mathbf{S}^*| \tilde{f}_{\mathbf{b}}(\mathbf{S}^{-}\mathbf{y}) \mathbb{1}\{\mathbf{y} \in \mathfrak{s}\}$ . Any realisation  $\mathbf{y}^*$  will lie on the coherent subspace and can be written as  $\mathbf{S}\mathbf{b}^*$ . The expression for the log score is therefore

$$\begin{aligned} \text{LS}(\tilde{f}_{\mathbf{y}}, \mathbf{y}^*) &= -\log(|\mathbf{S}^*| \tilde{f}_{\mathbf{b}}(\mathbf{S}^{-}\mathbf{S}\mathbf{b}^*)) \\ &= -\log|\mathbf{S}^*| - \log \tilde{f}_{\mathbf{b}}(\mathbf{b}^*). \end{aligned}$$

For coherent densities, the log score for the full hierarchy differs from the log score for the bottom-level series only by  $-\log|\mathbf{S}^*|$ . This term is independent of the choice of  $\mathbf{G}$ .

Consequently, rankings of different reconciliation methods using the log score for the full hierarchy will not change if only the bottom-level series is used.

The same property does not hold for all scores. For example, the energy score is invariant under orthogonal transformations (Székely and Rizzo, 2013) but not under linear transformations in general. Therefore it is possible for one method to outperform another when energy score is calculated using the full hierarchy, but for these rankings to change if only bottom-level series are considered. We therefore recommend computing the energy score using the full hierarchy. The properties of multivariate scoring rules in the context of evaluating reconciled probabilistic forecasts are summarised in Table 2.

**Table 2:** *Properties of scoring rules for reconciled probabilistic forecasts.*

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

## D Data generating process

To ensure that bottom-level series are noisier than bottom-level series (a feature often observed empirically), noise is added to the bottom-level series in the following manner

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

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

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

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

where  $w_{AA,t}, w_{AB,t}, w_{BA,t}, w_{BB,t}$  are generated from ARIMA processes as described in Section 7.1 with innovations  $\varepsilon_{AA,t}, \varepsilon_{AB,t}, \varepsilon_{BA,t}, \varepsilon_{BB,t}$ .

For the Gaussian DGP,  $u_t \sim \mathcal{N}(0, \sigma_u^2)$  and  $v_t \sim \mathcal{N}(0, \sigma_v^2)$  and  $\{\varepsilon_{AA,t}, \varepsilon_{AB,t}, \varepsilon_{BA,t}, \varepsilon_{BB,t}\} \stackrel{iid}{\sim} \mathcal{N}(\mathbf{0}, \mathbf{\Sigma}) \forall t$ . We follow Wickramasuriya et al. (2019) and set

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

and  $\sigma_u^2 = 28$  and  $\sigma_v^2 = 22$ . This ensures that the following inequalities are satisfied,

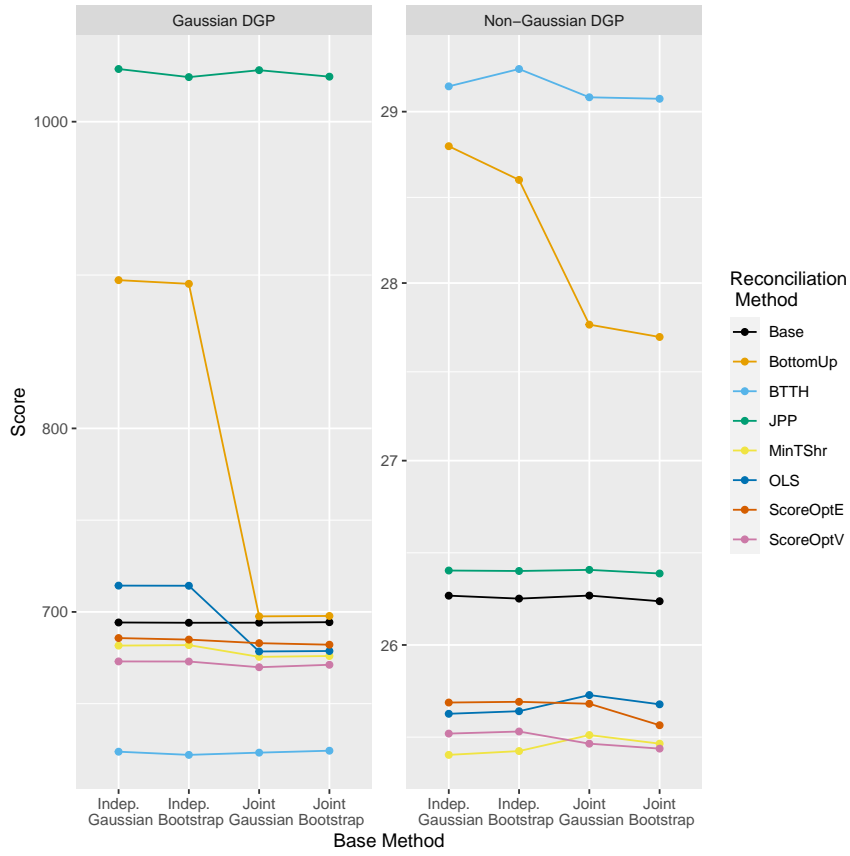
$$\begin{aligned}\text{Var}(\varepsilon_{AA,t} + \varepsilon_{AB,t} + \varepsilon_{BA,t} + \varepsilon_{BB,t}) &\leq \text{Var}(\varepsilon_{AA,t} + \varepsilon_{AB,t} - v_t) \leq \text{Var}(\varepsilon_{AA,t} + u_t - 0.5v_t), \\ \text{Var}(\varepsilon_{AA,t} + \varepsilon_{AB,t} + \varepsilon_{BA,t}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

For the non-Gaussian case, errors are generated from a Gumbel copula with Beta margins as described in Section 7.1. Rather than add Gaussian noise, we simulate  $u_t$  and  $v_t$  from skew t distributions using the `sn` package (Azzalini, 2020). The scale, skew and degrees of freedom parameters are chosen as 0.5, 1.5 and 4 and 0.9, 2 and 8 for  $u_t$  and  $v_t$  respectively. Monte Carlo simulations show that these values satisfy the inequalities described above.

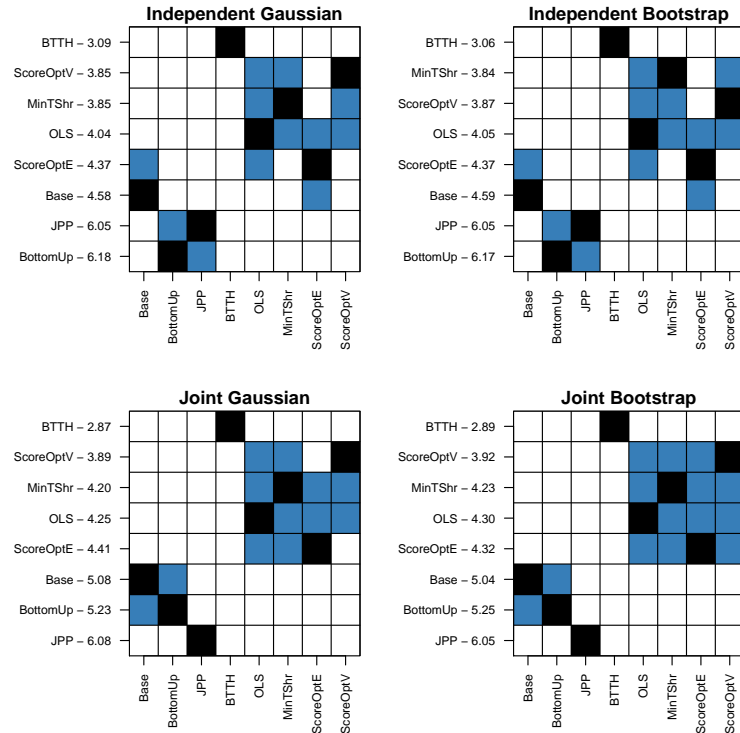
## E Results for Variogram Score for Simulation

Figure 10 shows the mean variogram score for different reconciliation methods and different methods of generating base forecasts. The results on the left panel are for a Gaussian DGP while the results on the right panel are for a non-Gaussian DGP. For this specific DGP, base model and score, BTTH significantly outperforms all other methods. However, this result was not observed when using BTTH for any other simulation scenario, including those discussed earlier in the paper as well as the results for the non-Gaussian DGP shown in the right panel. Excluding this result, score optimisation with respect to the variogram score is the best performing method with MinTShr and OLS also performing well. Score optimisation, OLS, MinTShr and BTTH all lead to significant improvements relative to base, bottom-up and JPP.

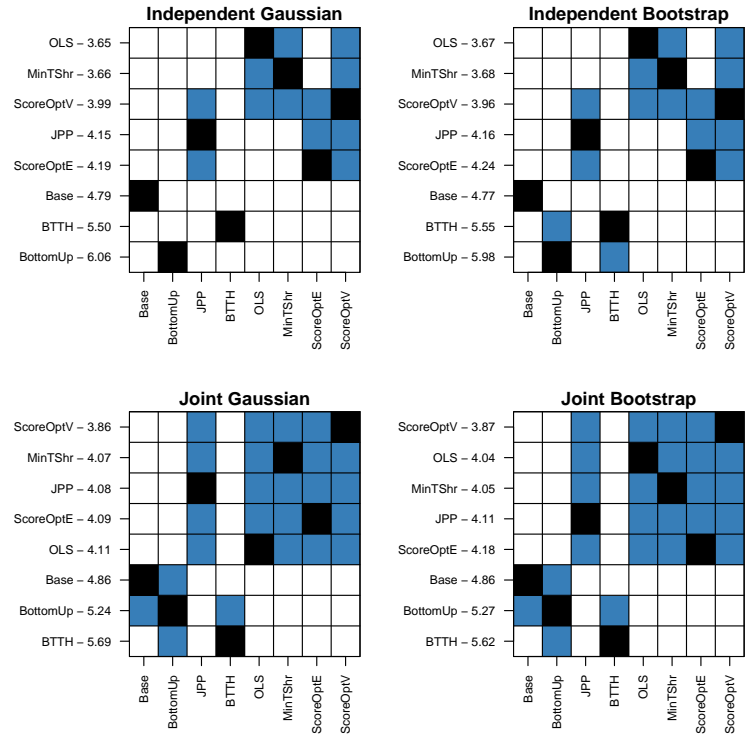
For the non-Gaussian DGP score optimisation with respect to the variogram score yields the best performance when base forecasts are dependent, while MinTShr yields the best performance when base forecasts are independent. In contrast to the Gaussian DGP, the JPP method leads to significant improvements over base forecasts, while the BTTH method leads to a significantly worse performance than base forecasts. The Nemenyi matrix is presented in Figure 12.



**Figure 10:** Mean variogram scores using different base forecast and reconciliation methods. Left panel is the Gaussian data, right panel is the non-Gaussian data.



**Figure 11:** Nemenyi matrix for Variogram score for Gaussian DGP.

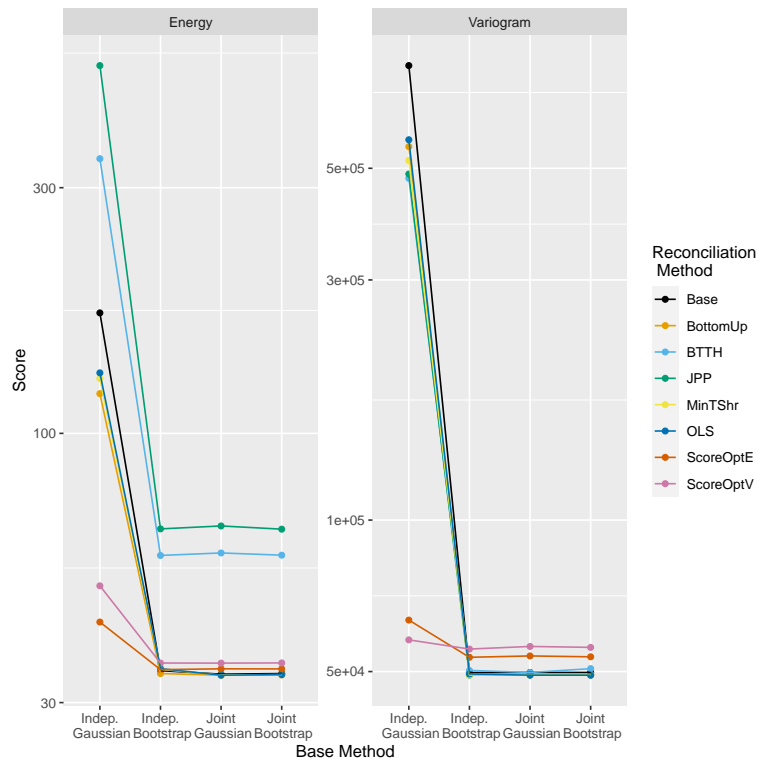


**Figure 12:** Nemenyi matrix for Variogram score with a non-Gaussian DGP.

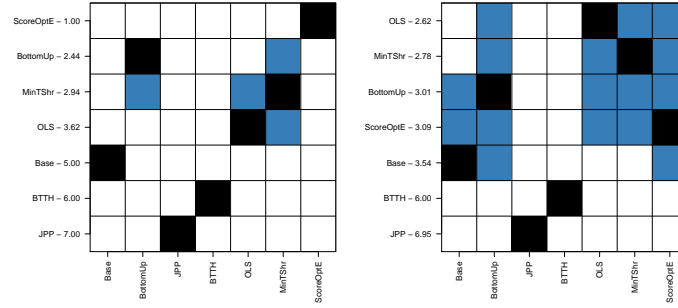


## F Results from Vector Autoregression

The results in this section were applied to the same data as Section 8, however base forecasts were obtained from a vector autoregressive model. Up to 7 lags (one week) were considered and regularisation was achieved via a lasso penalty on the VAR coefficients. Similar conclusions can be drawn from Figure 13 as for Figure 8, namely that the score optimisation method (and to a lesser extent MinT) lead to substantial improvements in base forecasts under the assumptions of Gaussianity and independence. For base forecasts that use either bootstrapping or assume dependence (or both), the improvements from applying forecast reconciliation are not as obvious. However, Figure 14 does show that there is a statistically significant improvement over base forecasts from using OLS reconciliation and the MinT method.



**Figure 13:** Mean Energy score for the electricity application using a VAR model under different base forecasting assumptions and different reconciliation methods.



**Figure 14:** Nemenyi matrices for Energy score for the electricity application with base forecasts from a VAR model. Left: base forecasts are (contemporaneously) independent and Gaussian. Right: base forecasts are obtained by jointly bootstrapping residuals.