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Rob J Hyndman, Alan Lee, and Earo Wang

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Rob J Hyndman
Department of Econometrics and Business Statistics,
Monash University, VIC 3800
Australia.
Email: rob.hyndman@monash.edu

Alan J Lee
Department of Statistics,
University of Auckland,
New Zealand
Email: lee@stat.auckland.ac.nz

Earo Wang
Department of Econometrics and Business Statistics,
Monash University, VIC 3800
Australia.
Email: yiru.wang@monash.edu

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Abstract

We describe some fast algorithms for reconciling large collections of time series forecasts with aggregation constraints. The constraints arise due to the need for forecasts of collections of time series with hierarchical or grouped structures to add up in the same manner as the observed time series. We show that the least squares approach to reconciling hierarchical forecasts can be extended to more general non-hierarchical groups of time series, and that the computations can be handled efficiently by exploiting the structure of the associated design matrix. Our algorithms will reconcile hierarchical forecasts with hierarchies of unlimited size, making forecast reconciliation feasible in business applications involving very large numbers of time series.

Keywords: combining forecasts; grouped time series; hierarchical time series; reconciling forecasts; weighted least squares.

1 Introduction

Time series can often be naturally disaggregated in a hierarchical or grouped structure. For example, a manufacturing company can disaggregate total demand for their products by country of sale, retail outlet, product type, package size, and so on. As a result, there can be tens of thousands of individual time series to forecast at the most disaggregated level, plus additional series to forecast at higher levels of aggregation.

The most disaggregated series often have a high degree of volatility (and are therefore hard to forecast), while the most aggregated time series is usually smooth and less noisy (and is therefore easier to forecast). Consequently, forecasting only the most disaggregated series and summing the results tends to give poor results at the higher levels of aggregation. On the other hand, if all the series at all levels of aggregation are forecast independently, the forecasts will not add up consistently between levels of aggregation. Therefore, it is necessary to reconcile the forecasts to ensure that the forecasts of the disaggregated series add up to the forecasts of the aggregated series (Fliedner, 2001).

In some cases, the disaggregation can be expressed in a hierarchical structure. For example, time series of sales may be disaggregated geographically by country, state and region, where each level of disaggregation sits within one node at the higher level (a region is within a state which is within a country).

In other cases, the disaggregation may not be uniquely hierarchical. For example, time series of sales may involve a geographical grouping (by country) and a product grouping (by type of product sold). Each of these grouping variables leads to a unique hierarchy, but if we wish to use both grouping variables, the order in which the disaggregation occurs is not unique. We may disaggregate by geography first, then by product type, or we may disaggregate by product type, then by geography. Both types of disaggregation may be useful, so choosing only one of these hierarchies is not appropriate. We call this a grouped time series. In general, there can be many different grouping variables, some of which may be hierarchical.

Hyndman et al. (CSDA 2011) proposed a method for optimally reconciling forecasts of all series in a hierarchy to ensure they add up. We show that this result is easily extended to cover more general (non-hierarchical) groups of time series.

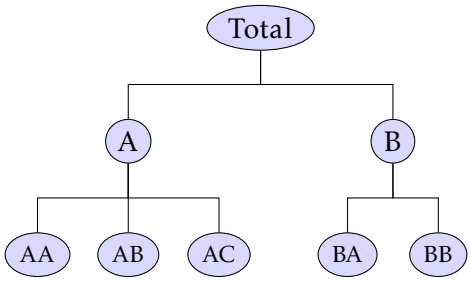
The optimal reconciliation method involves fitting a linear regression model where the design matrix has one column for each of the series at the most disaggregated level. Consequently, for problems involving tens of thousands (or even millions) of series, the model is impossible to estimate using standard regression algorithms such as the QR decomposition.

In this paper, we propose a solution to this problem, exploiting the unique structure of the linear model to efficiently estimate the coefficients, even when there are millions of time series at the most disaggregated level. Our solution involves two important cases: (1) where there can be any number of groups that are strictly hierarchical; and (2) where there are two groups that may not be hierarchical.

Our solution makes forecast reconciliation on very large collections of grouped and hierarchical time series feasible in practice. The algorithm has applications in any situation where large numbers of related time series need to be forecast, particularly in forecasting demand in product hierarchies, or geographical hierarchies.

For smaller hierarchies, where the computation is tractable without our new algorithm, good results have been obtained in forecasting tourism demand in Australia (Athanasopoulos, Ahmed, and Hyndman, 2009) and inflation in Mexico (Capistrán, Constandse, and Ramos-Francia, 2010).

Figure 1: *A simple hierarchy of time series containing five bottom-level series.*



2 Optimal reconciliation of hierarchical and grouped time series

2.1 Hierarchical time series

To introduce the notation and key ideas, we will use a very small and simple hierarchy, shown in Figure 1, with five series at the most disaggregated level. The "Total" node is the most aggregate level of the data, with the tth observation denoted by y_t. It is disaggregated into series A and B, which are each further disaggregated into the five bottom-level series. The tth observation at node X is denoted by $y_{X,t}$.

For any time t, the observations of the bottom level series will aggregate to the observations of the series above. To represent this in matrix notation, we introduce the $n \times n_K$ "summing" matrix $\boldsymbol{S}$. For the hierarchy in Figure 1 we can write

$$\begin{bmatrix} y_t \\ y_{\mathrm{A},t} \\ y_{\mathrm{B},t} \\ y_{\mathrm{AA},t} \\ y_{\mathrm{AB},t} \\ y_{\mathrm{AC},t} \\ y_{\mathrm{BA},t} \\ y_{\mathrm{BB},t} \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} y_{\mathrm{AA},t} \\ y_{\mathrm{AB},t} \\ y_{\mathrm{AC},t} \\ y_{\mathrm{BA},t} \\ y_{\mathrm{BB},t} \end{bmatrix}$$

or in more compact notation $\boldsymbol{y}_t = \boldsymbol{S}\boldsymbol{b}_t$, where $\boldsymbol{y}_t$ is a vector of all the observations in the hierarchy at time t, $\boldsymbol{S}$ is the summing matrix as defined above, and $\boldsymbol{b}_t$ is a vector of all the observations in the bottom level of the hierarchy at time t.

We are interested in generating forecasts for each series in the hierarchy. Let $\hat{y}_{X,h}$ be an h-step-ahead forecast for the series at node X and let $\hat{y}_h$ be an h-step-ahead forecast generated for the "Total" series, computed using the data to time T. These forecasts are computed independently

for each series, using only the history of the series and not taking account of any relationships with other series in the hierarchy. We refer to these as "base forecasts". The sum of the base forecasts at lower levels are unlikely to be equal to the base forecast of their parent nodes.

We wish to adjust these base forecasts so that they are consistent with the structure of the hierarchy, with adjusted forecasts aggregating to be equal to the adjusted forecast of their parent node. We refer to the adjusted forecasts as "reconciled forecasts".

Hyndman et al. (2011) proposed the linear model

$$\hat{\boldsymbol{y}}_h = \boldsymbol{S}\boldsymbol{\beta}_h + \boldsymbol{\varepsilon}_h \tag{1}$$

where $\hat{\boldsymbol{y}}_h$ is the vector of the h-step-ahead base forecasts for the whole hierarchy, $\boldsymbol{\beta}_h = \mathrm{E}(\boldsymbol{b}_{T+h} \mid \boldsymbol{y}_1, \ldots, \boldsymbol{y}_T)$ is the unknown conditional mean of the future values of the bottom level series, and $\boldsymbol{\varepsilon}_h$ represents the "aggregation error" (the difference between the base forecasts and their expected values if they were reconciled). We assume that $\boldsymbol{\varepsilon}_h$ has zero mean and covariance matrix $\boldsymbol{\Sigma}_h$. Then the optimally reconciled forecasts are given by the generalized least squares (GLS) solution

$$\tilde{\boldsymbol{y}}_h = \boldsymbol{S}\hat{\boldsymbol{\beta}}_h = \boldsymbol{S}(\boldsymbol{S}'\boldsymbol{\Sigma}_h^{\dagger}\boldsymbol{S})^{-1}\boldsymbol{S}'\boldsymbol{\Sigma}_h^{\dagger}\hat{\boldsymbol{y}}_h, \tag{2}$$

where $\boldsymbol{\Sigma}_h^{\dagger}$ is a generalized inverse of $\boldsymbol{\Sigma}_h$. This approach combines the independent base forecasts and generates a set of reconciled forecasts that are as close as possible (in an L_2 sense) to the original forecasts but also aggregate consistently with the hierarchical structure. A similar idea has been used for imposing aggregation constraints on time series produced by national statistical agencies (Quenneville and Fortier, 2012).

Unfortunately, $\boldsymbol{\Sigma}_h$ is not known and very difficult (or impossible) to estimate for large hierarchies. Instead, we could use the weighted least squares (WLS) solution given by

$$\tilde{\boldsymbol{y}}_h = \boldsymbol{S}(\boldsymbol{S}'\boldsymbol{\Lambda}_h\boldsymbol{S})^{-1}\boldsymbol{S}'\boldsymbol{\Lambda}_h\hat{\boldsymbol{y}}_h, \tag{3}$$

where $\boldsymbol{\Lambda}_h$ is a diagonal matrix with elements equal to the inverse of the variances of $\boldsymbol{\varepsilon}_h$. But even in this case, estimates of $\boldsymbol{\Lambda}_h$ are not readily available.

An alternative approach is to use ordinary least squares (OLS) instead of GLS or WLS. Then the set of reconciled forecasts is given by

$$\tilde{\boldsymbol{y}}_h = \boldsymbol{S}(\boldsymbol{S}'\boldsymbol{S})^{-1}\boldsymbol{S}'\hat{\boldsymbol{y}}_h. \tag{4}$$

Hyndman et al. (2011) noted that the GLS estimates (2) are identical to the OLS estimates (4) when the aggregation errors approximately satisfy the same aggregation structure as the original data, (i.e., $\varepsilon_h \approx \boldsymbol{S}\varepsilon_{b,h}$ where $\varepsilon_{b,h}$ contains the aggregation errors in the bottom level). Even if the aggregation errors do not satisfy this assumption, the OLS solution will still be a consistent way of reconciling the base forecasts.

We may also regard the OLS and WLS solutions in approximation terms: the solution gives the adjusted base forecasts with the property that the whole set of adjusted reconciled forecasts $\tilde{\boldsymbol{y}}_h$ best approximates the unadjusted base forecasts in the least squares or weighted least squares sense. In this interpretation, the weights could be used to control how much the adjusted forecasts are allowed to differ from the unadjusted ones. Series with more accurate forecasts might well have a larger weight.

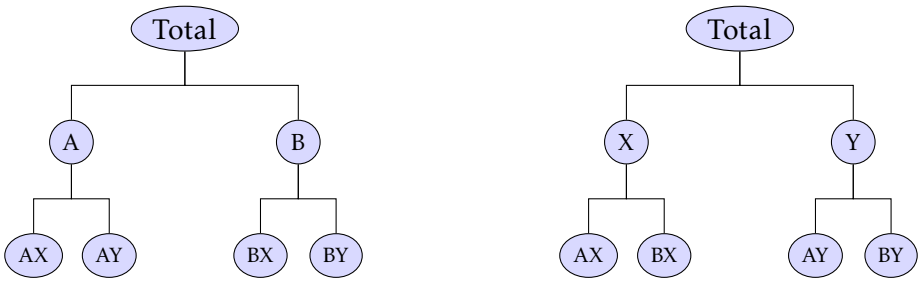
Consequently, in practice, we either use OLS, or we use WLS where the elements of Λ_h are set to the inverse of the variances of the base forecasts, $\text{var}(\boldsymbol{y}_{T+1} - \hat{\boldsymbol{y}}_1)$, which are readily available as the residual variances for each of the base forecasting models.

However, even with these simpler solutions (3) or (4), the problem of inverting the potentially large matrix $\boldsymbol{S}'\boldsymbol{S}$ remains.

Grouped time series

It is not difficult to see that the same linear model (1) will be satisfied in situations with more general groups of time series. Consider the example shown in Figure 2. These data can form two alternative hierarchies depending on which variable is first used to disaggregate the data. Another way to think of these data is in a two way table as shown in Table 1.

Figure 2: *A simple example of grouped time series with four bottom-level series. The series can be split into groups A and B first, then into groups X and Y (shown on the left), or they can be split first into groups X and Y, and then into groups A and B (shown on the right).*



			Sum
	AX	BX	X
	AY	BY	Y
Sum	A	B	Total

Table 1: *Two-way table representation of the groups of time series shown in Figure 2.*

Then if forecasts of all bottom level series, and of each grouping aggregate, are obtained, then the same simple linear model (1) can be used to represent them where

$$\boldsymbol{y}_t = \begin{pmatrix} y_t \\ y_{A,t} \\ y_{B,t} \\ y_{X,t} \\ y_{Y,t} \\ y_{AY,t} \\ y_{AX,t} \\ y_{BX,t} \\ y_{BY,t} \end{pmatrix}, \qquad \boldsymbol{S} = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \qquad \text{and} \qquad \boldsymbol{b}_t = \begin{pmatrix} y_{AX,t} \\ y_{AY,t} \\ y_{BX,t} \\ y_{BY,t} \end{pmatrix}.$$

More complicated grouping structures can be represented similarly. Each grouping aggregate of interest is included in vector $\boldsymbol{y}_t$, and the corresponding row in $\boldsymbol{S}$ defines how the bottom-level series are grouped for that aggregation. Then the same GLS, WLS, or OLS solutions can be used to reconcile the base forecasts.

We now proceed to consider fast algorithms for computing the WLS solution given by (3) when the time series are either strictly hierarchical, or there are two non-hierarchical grouping variables. The OLS solution (4) can be considered as a special case of the WLS results.

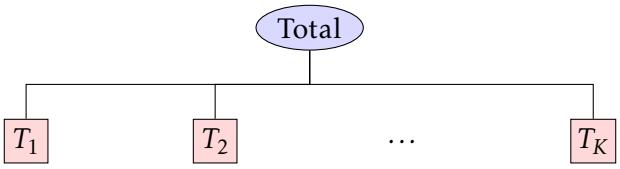
3 Fast computation to reconcile hierarchical time series

Every hierarchical time series can be represented recursively as a tree of trees. Consider the hierarchy depicted in Figure 3, consisting of a root node (labelled Total) and several appended sub-trees, denoted by $T_1, T_2, \ldots, T_K$.

Each of the sub-trees are themselves hierarchies of time series. Suppose that the trees $T_1, T_2, \ldots, T_K$ contain $n_1, n_2, \ldots, n_K$ terminal nodes respectively.

Let $\boldsymbol{y}_{k,t}$ be the vector of time series associated with the tree T_k, and let $\boldsymbol{S}_1, \boldsymbol{S}_2, \ldots, \boldsymbol{S}_K$ be the summing matrices corresponding to the subtrees $T_1, T_2, \ldots, T_K$. Then the summing matrix

Figure 3: *A recursive hierarchical tree diagram.*



corresponding to the whole tree T is

$$\boldsymbol{S} = \begin{bmatrix} \mathbf{1}'_{n_1} & \mathbf{1}'_{n_2} & \cdots & \mathbf{1}'_{n_K} \\ \boldsymbol{S}_1 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \boldsymbol{S}_2 & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \boldsymbol{S}_K \end{bmatrix} \tag{5}$$

where $\mathbf{1}_n$ is an n-vector of ones.

We want to produce the adjusted forecasts given by (3). Direct computation by standard least squares methods may be difficult if the matrix $\boldsymbol{S}$ is too large. Instead, we consider a recursive method for computing the adjusted forecasts which can handle quite large tree structures, particularly if the number of forecasts being aggregated at the lowest level is large compared to those being aggregated at higher levels. The method can also handle different forecast weights, and allows efficient computation of the matrix $(\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S})^{-1}$ by exploiting the structure of $\boldsymbol{S}$.

Write

$$\boldsymbol{\Lambda} = \begin{bmatrix} \lambda_0 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Lambda}_1 & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \boldsymbol{\Lambda}_K \end{bmatrix}$$

where λ_0 is the weight associated with the root node, and $\boldsymbol{\Lambda}_1, \ldots, \boldsymbol{\Lambda}_K$ are the diagonal weight matrices associated with the nodes in $T_1, \ldots, T_K$. Then

$$\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S} = \lambda_0 \boldsymbol{J}_n + \begin{bmatrix} \boldsymbol{S}'_1\boldsymbol{\Lambda}_1\boldsymbol{S}_1 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \boldsymbol{S}'_2\boldsymbol{\Lambda}_2\boldsymbol{S}_2 & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \boldsymbol{S}'_k\boldsymbol{\Lambda}_K\boldsymbol{S}_K \end{bmatrix}, \tag{6}$$

where $\boldsymbol{J}_n$ is an $n \times n$ matrix of ones, and $n = \sum_k n_k$. Using the rank-one update formula (see, e.g., Seber and Lee, 2003, p.467) we can express the inverse of $\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S}$ as

$$(\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S})^{-1} = \begin{bmatrix} (\boldsymbol{S}_1'\boldsymbol{\Lambda}_1\boldsymbol{S}_1)^{-1} & \boldsymbol{0} & \cdots & \boldsymbol{0} \\ \boldsymbol{0} & (\boldsymbol{S}_2'\boldsymbol{\Lambda}_2\boldsymbol{S}_2)^{-1} & \cdots & \boldsymbol{0} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{0} & \boldsymbol{0} & \cdots & (\boldsymbol{S}_k'\boldsymbol{\Lambda}_K\boldsymbol{S}_K)^{-1} \end{bmatrix} - c\boldsymbol{S}_0, \tag{7}$$

where the $n \times n$ matrix $\boldsymbol{S}_0$ can be partitioned into K^2 blocks, and the j,k block (of dimension $n_j \times n_k$) is $(\boldsymbol{S}_j'\boldsymbol{\Lambda}_j\boldsymbol{S}_j)^{-1}\boldsymbol{J}_{n_j,n_k}(\boldsymbol{S}_k'\boldsymbol{\Lambda}_k\boldsymbol{S}_k)^{-1}$, where $\boldsymbol{J}_{n_j,n_k}$ is a $n_j \times n_k$ matrix of ones. The constant c is given by

$$c^{-1} = \lambda_0^{-1} + \sum_j \boldsymbol{1}_{n_j}'(\boldsymbol{S}_j'\boldsymbol{\Lambda}_j\boldsymbol{S}_j)^{-1}\boldsymbol{1}_{n_j}.$$

3.1 Recursive calculation of the inverse

We can establish the form of $(\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S})^{-1}$ more precisely by an inductive argument: consider a simple tree consisting of a root node and n terminal nodes, as depicted in Figure 4. In this case, the matrix $\boldsymbol{S}$ is of the form

$$\boldsymbol{S} = \begin{bmatrix} \boldsymbol{1}_n' \\ \boldsymbol{I}_n \end{bmatrix} \tag{8}$$

where $\boldsymbol{I}_n$ is an $n \times n$ identity matrix. Then

$$\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S} = \text{diag}(\boldsymbol{\lambda}) + \lambda_0\boldsymbol{J}_n \tag{9}$$

where the elements of $\boldsymbol{\lambda}$ are the weights of the terminal nodes, and

$$(\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S})^{-1} = \text{diag}(\boldsymbol{d}) - c\boldsymbol{d}\boldsymbol{d}' \tag{10}$$

where $\boldsymbol{d}$ is the vector whose elements are the reciprocals of those of $\boldsymbol{\lambda}$, $d_0 = \lambda_0^{-1}$ and $c^{-1} = d_0 + \boldsymbol{d}'\boldsymbol{1}_n$.

Figure 4: *A simple tree with two levels.*

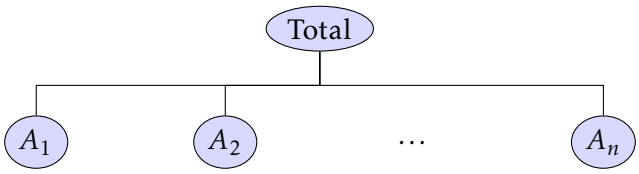
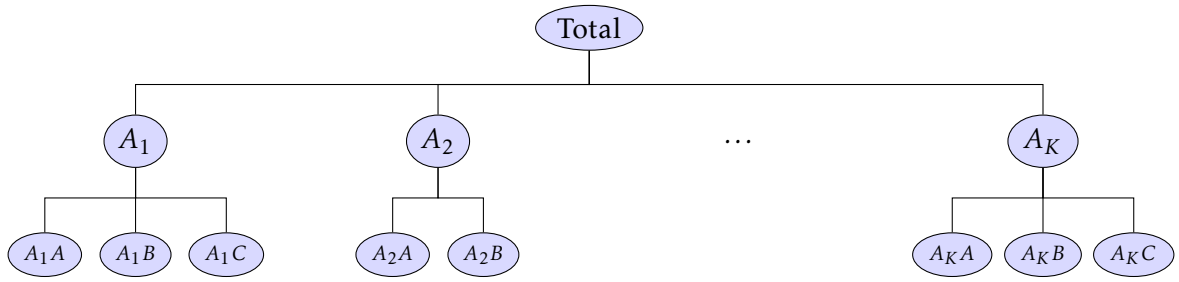


Figure 5: *A tree with three levels.*



Now consider the situation in Figure 5, with a tree having three levels, where the K subtrees $T_1, T_2, \ldots, T_K$ of Figure 3 have the simple form depicted in Figure 4. Let $\boldsymbol{d}_j$ be the vector of reciprocal weights for the terminal nodes of the subtrees T_j, d_{j0} the reciprocal weight of the root node of T_j, d_0 the reciprocal weight of the root node of the whole tree and $c_j = d_{j0} + \boldsymbol{d}_j'\mathbf{1}_{n_j}$. Then

$$(\boldsymbol{S}_j'\boldsymbol{\Lambda}_j\boldsymbol{S}_j)^{-1}\boldsymbol{J}_{n_j,n_k}(\boldsymbol{S}_k'\boldsymbol{\Lambda}_k\boldsymbol{S}_k)^{-1} = (1-c_j\boldsymbol{d}_j'\mathbf{1}_{n_j})(1-c_k\boldsymbol{d}_k'\mathbf{1}_{n_k})\boldsymbol{d}_j\boldsymbol{d}_k'$$

and

$$\sum_j \mathbf{1}_{n_j}'(\boldsymbol{S}_j'\boldsymbol{\Lambda}_j\boldsymbol{S}_j)^{-1}\mathbf{1}_{n_j} = \sum_j \boldsymbol{d}_j'\mathbf{1}_{n_j} - c_j(\boldsymbol{d}_j'\mathbf{1}_{n_j})^2.$$

Thus, by (7), the (j,j) block of $(\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S})^{-1}$ is

$$(\boldsymbol{S}_j'\boldsymbol{\Lambda}_j\boldsymbol{S}_j)^{-1} - c(\boldsymbol{S}_j'\boldsymbol{\Lambda}_j\boldsymbol{S}_j)^{-1}\boldsymbol{J}_{n_j,n_j}(\boldsymbol{S}_j'\boldsymbol{\Lambda}_j\boldsymbol{S}_j)^{-1} = \operatorname{diag}(\boldsymbol{d}_j) - \left\{c_j + c(1-c_j\boldsymbol{d}_j'\mathbf{1}_{n_j})^2\right\}\boldsymbol{d}_j\boldsymbol{d}_j', \tag{11}$$

where $c^{-1} = d_0 + \sum_j \boldsymbol{d}_k'\mathbf{1}_{n_j} - c_j(\boldsymbol{d}_j'\mathbf{1}_{n_j})^2$. For $j \neq k$, the (j,k) block is $-c(1-c_j\boldsymbol{d}_j'\mathbf{1}_{n_j})(1-c_k\boldsymbol{d}_k'\mathbf{1}_{n_k})\boldsymbol{d}_j\boldsymbol{d}_k'$. We can write this more compactly by defining

$$\tilde{\boldsymbol{D}} = \begin{bmatrix} \boldsymbol{d}_1 & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \boldsymbol{d}_2 & \cdots & \mathbf{0} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \boldsymbol{d}_K \end{bmatrix}. \tag{12}$$

Then we can write $(\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S})^{-1} = \boldsymbol{D} - \tilde{\boldsymbol{D}}\boldsymbol{C}\tilde{\boldsymbol{D}}'$ where the symmetric matrix $\boldsymbol{C}$ has elements

$$c_{jk} = \begin{cases} c_j + c(1-c_j\boldsymbol{d}_j'\mathbf{1}_{n_j})(1-c_k\boldsymbol{d}_k'\mathbf{1}_{n_k}) & j = k, \\ c(1-c_j\boldsymbol{d}_j'\mathbf{1}_{n_j})(1-c_k\boldsymbol{d}_k'\mathbf{1}_{n_k}) & j \neq k; \end{cases}$$

and

$$\boldsymbol{D} = \begin{bmatrix} \text{diag}(\boldsymbol{d}_1) & \boldsymbol{0} & \cdots & \boldsymbol{0} \\ \boldsymbol{0} & \text{diag}(\boldsymbol{d}_2) & \cdots & \boldsymbol{0} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{0} & \boldsymbol{0} & \cdots & \text{diag}(\boldsymbol{d}_K) \end{bmatrix}. \tag{13}$$

This pattern for the inverse also applies at higher levels in the hierarchy. Assume that for $j = 1,\dots,K$, the matrix $(\boldsymbol{S}_j'\boldsymbol{\Lambda}_j\boldsymbol{S}_j)^{-1}$ has the form

$$(\boldsymbol{S}_j'\boldsymbol{\Lambda}_j\boldsymbol{S}_j)^{-1} = \boldsymbol{D}_j - \tilde{\boldsymbol{D}}_j\boldsymbol{C}_j\tilde{\boldsymbol{D}}_j' \tag{14}$$

where $\tilde{\boldsymbol{D}}_j$ and $\boldsymbol{D}_j$ have the form (12) and (13) for vectors $\boldsymbol{d}_{j1},\dots,\boldsymbol{d}_{jm_j}$. Substituting these in equation (7) we get

$$(\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S})^{-1} = \boldsymbol{D} - \tilde{\boldsymbol{D}}\boldsymbol{C}\tilde{\boldsymbol{D}}' \tag{15}$$

where $\boldsymbol{C}$ is symmetric with its j,k block equal to

$$\boldsymbol{C}_{jk} = \begin{cases} \boldsymbol{C}_j + c(\boldsymbol{1}_{m_j} - \boldsymbol{C}_j\tilde{\boldsymbol{D}}_j'\boldsymbol{1}_{n_j})(\boldsymbol{1}_{m_k} - \boldsymbol{C}_k\tilde{\boldsymbol{D}}_k'\boldsymbol{1}_{n_k})', & j = k, \\ c(\boldsymbol{1}_{m_j} - \boldsymbol{C}_j\tilde{\boldsymbol{D}}_j'\boldsymbol{1}_{n_j})(\boldsymbol{1}_{m_k} - \boldsymbol{C}_k\tilde{\boldsymbol{D}}_k'\boldsymbol{1}_{n_k})', & j \neq k, \end{cases} \tag{16}$$

$$c^{-1} = d_0 + \text{trace}\,\boldsymbol{D} - \sum_j \boldsymbol{1}_{n_j}'\tilde{\boldsymbol{D}}_j\boldsymbol{C}_j\tilde{\boldsymbol{D}}_j'\boldsymbol{1}_{n_j}, \tag{17}$$

and

$$\tilde{\boldsymbol{D}} = \begin{bmatrix} \tilde{\boldsymbol{D}}_1 & \boldsymbol{0} & \cdots & \boldsymbol{0} \\ \boldsymbol{0} & \tilde{\boldsymbol{D}}_2 & \cdots & \boldsymbol{0} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{0} & \boldsymbol{0} & \cdots & \tilde{\boldsymbol{D}}_K \end{bmatrix}, \qquad \boldsymbol{D} = \begin{bmatrix} \boldsymbol{D}_1 & \boldsymbol{0} & \cdots & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{D}_2 & \cdots & \boldsymbol{0} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{0} & \boldsymbol{0} & \cdots & \boldsymbol{D}_K \end{bmatrix}. \tag{18}$$

Using these recursions, we can calculate the matrix $\boldsymbol{C}$ of for each subtree in the tree. If the tree has L levels, labeled $1,2,\dots,L$, we start with the set of "terminal" subtrees whose root nodes are the nodes at level $L-1$. We calculate the $\boldsymbol{C}$-matrix (which consists of a single element) for each subtree, using equation (10), so that the matrix corresponding to a node at level $L-1$ has the single element $d_0 + \boldsymbol{d}'\boldsymbol{1}_{n_j}$. Using these $\boldsymbol{C}$-matrices, we can use (16) and (17) to calculate the $\boldsymbol{C}$-matrices for all subtrees whose root nodes are the nodes at the next level $L-2$. Proceeding in this way, we eventually arrive at the single $\boldsymbol{C}$-matrix which represents the inverse for the whole tree. The dimension of the final $\boldsymbol{C}$ is equal to the number of nodes at the second-to-bottom level of the tree. Thus, if the number of terminal nodes at level L is considerably greater than the

number of nodes at level $L-1$, the dimensions of this matrix will be considerably less than that of $\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S}$.

Note that if $\boldsymbol{d}_1,\ldots,\boldsymbol{d}_N$ are the vectors of inverse weights of the N terminal trees, the elements of these vectors are the diagonal elements of the matrix $\boldsymbol{D}$ in (13), and the matrix $\tilde{\boldsymbol{D}}$ is

$$\tilde{\boldsymbol{D}} = \begin{bmatrix} \boldsymbol{d}_1 & \boldsymbol{0} & \cdots & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{d}_2 & \cdots & \boldsymbol{0} \\ \vdots & \vdots & \ddots & \vdots \\ \boldsymbol{0} & \boldsymbol{0} & \cdots & \boldsymbol{d}_N \end{bmatrix}.$$

3.2 Calculation of the adjusted forecasts

The elements of the vector $\boldsymbol{S}'\boldsymbol{\Lambda}\hat{\boldsymbol{y}}$, where $\hat{\boldsymbol{y}}$ is the vector of unadjusted forecasts, can also be calculated recursively. If $\hat{\boldsymbol{y}}_1,\hat{\boldsymbol{y}}_2,\ldots,\hat{\boldsymbol{y}}_K$ are the forecasts corresponding to the subtrees $T_1,T_2,\ldots,T_K$ and $\hat{y}_0$ is the forecast of the aggregate, then

$$\boldsymbol{S}'\boldsymbol{\Lambda}\hat{\boldsymbol{y}} = \begin{bmatrix} \boldsymbol{1}_{n_1} & \boldsymbol{S}_1' & \cdots & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{1}_{n_2} & \boldsymbol{0} & \cdots & \boldsymbol{0} & \boldsymbol{0} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \boldsymbol{1}_{n_k} & \boldsymbol{0} & \cdots & \boldsymbol{0} & \boldsymbol{S}_K' \end{bmatrix} \begin{bmatrix} \lambda_0\hat{y}_0 \\ \boldsymbol{\Lambda}_1\hat{\boldsymbol{y}}_1 \\ \boldsymbol{\Lambda}_2\hat{\boldsymbol{y}}_2 \\ \vdots \\ \boldsymbol{\Lambda}_K\hat{\boldsymbol{y}}_K \end{bmatrix} = \hat{y}_0\lambda_0\boldsymbol{1}_n + \begin{bmatrix} \boldsymbol{S}_1'\boldsymbol{\Lambda}_1\hat{\boldsymbol{y}}_1 \\ \boldsymbol{S}_2'\boldsymbol{\Lambda}_2\hat{\boldsymbol{y}}_2 \\ \vdots \\ \boldsymbol{S}_K'\boldsymbol{\Lambda}_K\hat{\boldsymbol{y}}_K \end{bmatrix}. \tag{19}$$

The recursion is started off at level $L-1$ using the equation

$$\boldsymbol{S}'\boldsymbol{\Lambda}\hat{\boldsymbol{y}} = \begin{bmatrix} \lambda_0\hat{y}_0 + \lambda_1\hat{\boldsymbol{y}}_1 \\ \vdots \\ \lambda_0\hat{y}_0 + \lambda_n\hat{\boldsymbol{y}}_n \end{bmatrix} \tag{20}$$

where $\hat{\boldsymbol{y}}_1,\ldots,\hat{\boldsymbol{y}}_n$ are the forecasts corresponding to the terminal nodes and $\hat{y}_0$ is the forecast of the aggregate.

Partition $\boldsymbol{S}'\boldsymbol{\Lambda}\hat{\boldsymbol{y}}$ into subvectors $\boldsymbol{s}_1,\ldots,\boldsymbol{s}_N$ corresponding to the N terminal subtrees and let $t_j = \boldsymbol{d}_j'\boldsymbol{s}_j$. Put $\boldsymbol{t} = (t_1,\ldots,t_N)'$. Then the vector of "bottom level" adjusted forecasts is

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S})^{-1}\boldsymbol{S}'\boldsymbol{\Lambda}\hat{\boldsymbol{y}} = \begin{bmatrix} \boldsymbol{d}_1\cdot\boldsymbol{s}_1 \\ \vdots \\ \boldsymbol{d}_N\cdot\boldsymbol{s}_N \end{bmatrix} - \begin{bmatrix} (\boldsymbol{C}\boldsymbol{t})_1\boldsymbol{d}_1 \\ \vdots \\ (\boldsymbol{C}\boldsymbol{t})_N\boldsymbol{d}_N \end{bmatrix}, \tag{21}$$

where $\cdot$ denotes an elementwise product.

Finally, the whole vector of adjusted forecasts can be calculated from the recursion

$$S\hat{\beta} = \begin{bmatrix} \mathbf{1}'_{n_1} & \mathbf{1}'_{n_2} & \cdots & \mathbf{1}'_{n_{K-1}} & \mathbf{1}'_{n_K} \\ S_1 & \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} & S_K \end{bmatrix} \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \\ \vdots \\ \hat{\beta}_K \end{bmatrix} = \begin{bmatrix} \hat{\beta}'_1\mathbf{1}_{n_1} + \cdots + \hat{\beta}'_K\mathbf{1}_{n_K} \\ S_1\hat{\beta}_1 \\ \vdots \\ S_K\hat{\beta}_K \end{bmatrix}, \tag{22}$$

where $\hat{\beta}_1, \ldots, \hat{\beta}_K$ are the vectors of "bottom level" adjusted forecasts for the subtrees $T_1, \ldots, T_K$.

When the weights are all unity (as for OLS), the formulas above simplify considerably. In this case at each stage the matrix $(S'_jS_j)^{-1}$ is of the form $(S'_jS_j)^{-1} = \boldsymbol{I}_{n_j} - \boldsymbol{R}$ where the matrix $\boldsymbol{R}$ consists of blocks of equal elements, whose common value is given by the corresponding element of the $\boldsymbol{C}$-matrix.

3.3 The algorithm

We may summarize the algorithm described above as follows:

Step 1: Calculate the (1×1) $\boldsymbol{C}$-matrices corresponding to level $L-1$ of the tree, using equation (7), and for each forecast horizon h, the list of vectors $S'_k\boldsymbol{\Lambda}_k\hat{\boldsymbol{y}}_{kh}$, using equation (20).

Step 2: For each level from $L-2$ to level 1, and each node in that level, calculate the updated $\boldsymbol{C}$-matrices and the updated vectors $S'\boldsymbol{\Lambda}\hat{\boldsymbol{y}}_h$, using equations (16), (17) and (19).

Step 3: Using the final $\boldsymbol{C}$-matrix and the final vector $\boldsymbol{s} = S'\boldsymbol{\Lambda}\hat{\boldsymbol{y}}_h$ corresponding to the whole tree, calculate the adjusted forecasts using equation (21) and (22).

4 A fast algorithm for grouped time series

In this section, we consider the case where the time series have a tabular rather than a hierarchical structure. We have a set of time series $\{y_{i,j,t}\}$, arranged in an $m \times n$ array, as in Table 1:

$$\begin{bmatrix} y_{1,1,t} & \cdots & y_{1,n,t} \\ \vdots & \cdots & \vdots \\ y_{m,1,t} & \cdots & y_{m,n,t} \end{bmatrix}. \tag{23}$$

For example, we might have separate time series for each gender and for each region of a country. As well as the series above, we will be interested in the aggregated series $y_{i,+,t}$, $y_{+,j,t}$ and $y_{+,+,t}$ of the row, column and grand totals.

Suppose we have h-step-ahead forecasts $\hat{y}_{ij}$ of the series $y_{i,j,t}$, and also separate forecasts of the series $y_{i,+,t}$, $y_{+,j,t}$, and $y_{+,+,t}$, which we denote by $\hat{y}_{i0}$, $\hat{y}_{0j}$ and $\hat{y}_{00}$ respectively.

Let $\boldsymbol{S}$ be the $(m+1)(n+1) \times mn$ summing matrix for this situation, satisfying

$$\boldsymbol{S}\begin{bmatrix} y_{1,1,t} \\ y_{1,2,t} \\ \vdots \\ y_{m,n,t} \end{bmatrix} = \begin{bmatrix} y_{+,+,t} \\ y_{+,1,t} \\ \vdots \\ y_{+,n,t} \\ y_{1,+,t} \\ \vdots \\ y_{m,+,t} \\ y_{1,1,t} \\ y_{1,2,t} \\ \vdots \\ y_{m,n,t} \end{bmatrix} \tag{24}$$

(Here and subsequently, when stringing the elements of a matrix out into a vector, we do this in the order first row, second row and so on). Let $\hat{\boldsymbol{y}}$ be the vector of $(m+1)(n+1)$ forecasts, arranged in the same order as the right side of (24). Ignoring the weights $\boldsymbol{\Lambda}$ for now, the adjusted unaggregated[1] forecasts are

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{S}'\boldsymbol{S})^{-1}\boldsymbol{S}'\hat{\boldsymbol{y}}. \tag{25}$$

and the aggregated adjusted forecasts are obtained by aggregating up the adjusted unaggregated forecasts, or, in matrix terms by $\boldsymbol{S}\hat{\boldsymbol{\beta}}$.

[1] By "unaggregated" forecasts we mean the forecasts of the unaggregated series $y_{ij,t}$ in (23).

4.1 Solving the normal equations

Using the ordering in (24), the matrix $\boldsymbol{S}$ can be written

$$\boldsymbol{S} = \begin{bmatrix} \mathbf{1}'_m \otimes \mathbf{1}'_n \\ \mathbf{1}'_m \otimes \boldsymbol{I}_n \\ \boldsymbol{I}_m \otimes \mathbf{1}'_n \\ \boldsymbol{I}_m \otimes \boldsymbol{I}_n \end{bmatrix}$$

where $\boldsymbol{I}_n$ is an $n \times n$ identity matrix and $\mathbf{1}_n$ an n-vector of ones. Using the properties of Kronecker products, we obtain

$$\begin{aligned}
\boldsymbol{S}'\boldsymbol{S} &= [\mathbf{1}_m \otimes \mathbf{1}_n \mid \mathbf{1}_m \otimes \boldsymbol{I}_n \mid \boldsymbol{I}_m \otimes \mathbf{1}_n \mid \boldsymbol{I}_m \otimes \boldsymbol{I}_n] \times \begin{bmatrix} \mathbf{1}'_m \otimes \mathbf{1}'_n \\ \mathbf{1}'_m \otimes \boldsymbol{I}_n \\ \boldsymbol{I}_m \otimes \mathbf{1}'_n \\ \boldsymbol{I}_m \otimes \boldsymbol{I}_n \end{bmatrix} \\
&= (\mathbf{1}_m \otimes \mathbf{1}_n)(\mathbf{1}'_m \otimes \mathbf{1}'_n) + (\mathbf{1}_m \otimes \boldsymbol{I}_n)(\mathbf{1}'_m \otimes \boldsymbol{I}_n) + (\boldsymbol{I}_m \otimes \mathbf{1}_n)(\boldsymbol{I}_m \otimes \mathbf{1}'_n) + (\boldsymbol{I}_m \otimes \boldsymbol{I}_n)(\boldsymbol{I}_m \otimes \boldsymbol{I}_n) \\
&= \boldsymbol{J}_m \otimes \boldsymbol{J}_n + \boldsymbol{J}_m \otimes \boldsymbol{I}_n + \boldsymbol{I}_m \otimes \boldsymbol{J}_n + \boldsymbol{I}_m \otimes \boldsymbol{I}_n \\
&= (\boldsymbol{I}_m + \boldsymbol{J}_m) \otimes (\boldsymbol{I}_n + \boldsymbol{J}_n),
\end{aligned}$$

and so

$$\begin{aligned}
(\boldsymbol{S}'\boldsymbol{S})^{-1} &= [(\boldsymbol{I}_m + \boldsymbol{J}_m) \otimes (\boldsymbol{I}_n + \boldsymbol{J}_n)]^{-1} \\
&= (\boldsymbol{I}_m + \boldsymbol{J}_m)^{-1} \otimes (\boldsymbol{I}_n + \boldsymbol{J}_n)^{-1} \\
&= (\boldsymbol{I}_m - \boldsymbol{J}_m/(m+1)) \otimes (\boldsymbol{I}_n - \boldsymbol{J}_n/(n+1)).
\end{aligned}$$

Finally, the solution of the normal equations is

$$\begin{aligned}
(\boldsymbol{S}'\boldsymbol{S})^{-1}\boldsymbol{S}'\hat{\boldsymbol{y}} = \frac{1}{(m+1)(n+1)} \Big\{ & \boldsymbol{J}_{mn}\hat{y}_{00} + \Big[(n+1)(\mathbf{1}_m \otimes \boldsymbol{I}_n) - \boldsymbol{J}_{mn,n}\Big]\hat{\boldsymbol{y}}_C \\
& + \Big[(m+1)(\boldsymbol{I}_m \otimes \mathbf{1}_n) - \boldsymbol{J}_{mn,m}\Big]\hat{\boldsymbol{y}}_R \\
& + \Big[(m+1)(n+1)\boldsymbol{I}_m - (m+1)(\boldsymbol{I}_m \otimes \boldsymbol{J}_n) - (n+1)(\boldsymbol{J}_m \otimes \boldsymbol{I}_n) - \boldsymbol{J}_{mn}\Big]\hat{\boldsymbol{y}}_B \Big\}
\end{aligned}$$

where $\hat{y}_{00}$ is the forecast of the grand total, and $\hat{\boldsymbol{y}}_C$, $\hat{\boldsymbol{y}}_R$ and $\hat{\boldsymbol{y}}_B$ are the vectors of column, row and unaggregated forecasts respectively, and $\boldsymbol{J}_{mn,n}$ is a $mn \times n$ matrix of ones. Writing this vector as an $m \times n$ matrix, the adjusted forecast for row i, column j is

$$\Big\{\hat{y}_{00} - \hat{y}_{0+} - \hat{y}_{+0} + \hat{y}_{++} + (m+1)\hat{y}_{i0} + (n+1)\hat{y}_{0j} \\ +(m+1)(n+1)\hat{y}_{ij} - (m+1)\hat{y}_{i+} - (n+1)\hat{y}_{+j}\Big\}\Big/(m+1)(n+1),$$

where + denotes summation of the unadjusted forecasts over $1, 2, \ldots, m$ or $1, 2, \ldots, n$.

4.2 Incorporating weights

Suppose now for each forecast we have a weight, and we calculate the adjusted unaggregated forecasts by

$$\hat{\boldsymbol{\beta}} = (\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S})^{-1}\boldsymbol{S}'\boldsymbol{\Lambda}\hat{\boldsymbol{y}} \tag{26}$$

instead of (25), where $\boldsymbol{\Lambda}$ is the diagonal matrix of weights. Direct computation of (26) may be difficult if m and/or n are large, since it involves dealing with a matrix of dimension $mn \times mn$. However, we can exploit the special structure of $\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S}$ to develop a more efficient computational scheme that does not involve forming such large matrices.

Let $\lambda_{ij}, i = 0, 1, \ldots, m; j = 0, 1, \ldots, n$ denote then weights corresponding to the forecast $\hat{y}_{ij}$, so that for example λ_{00} is the weight associated with the grand total forecast $\hat{y}_{00}$.

Also, denote by $\boldsymbol{\Lambda}_R$, $\boldsymbol{\Lambda}_C$ and $\boldsymbol{\Lambda}_U$ the diagonal matrices whose diagonal elements are the row weights $\lambda_{10}, \ldots, \lambda_{m0}$, the column weights $\lambda_{01}, \ldots, \lambda_{0n}$ and the "unaggregated" weights $\lambda_{11}, \lambda_{12}, \ldots, \lambda_{mn}$.

We can write $\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S}$ as

$$\begin{aligned}\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S} &= \lambda_{00}(\mathbf{1}_m \otimes \mathbf{1}_n)(\mathbf{1}'_m \otimes \mathbf{1}'_n) + (\boldsymbol{I}_m \otimes \mathbf{1}_n)\boldsymbol{\Lambda}_R(\boldsymbol{I}_m \otimes \mathbf{1}'_n) + (\mathbf{1}_m \otimes \boldsymbol{I}_n)\boldsymbol{\Lambda}_C(\mathbf{1}'_m \otimes \boldsymbol{I}_n) + \boldsymbol{\Lambda}_U \\ &= \lambda_{00}\boldsymbol{J}_{mn} + (\boldsymbol{\Lambda}_R \otimes \boldsymbol{J}_n) + (\boldsymbol{J}_m \otimes \boldsymbol{\Lambda}_C) + \boldsymbol{\Lambda}_U.\end{aligned}$$

The first three matrices in the above sum have ranks 1, m and n and the last has a simple, easily computed inverse as it is diagonal. This suggests we might be able to compute $(\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S})^{-1}$ efficiently by successive applications of the Sherman-Morrison-Woodbury (SMW) updating formula (see e.g. Seber and Lee (2003), p 467), and this turns out to be the case. We now turn to the details.

First, note that we can write

$$(\boldsymbol{J}_m \otimes \boldsymbol{\Lambda}_C) = (\mathbf{1}_m \otimes \boldsymbol{\Lambda}_C^{1/2})(\mathbf{1}'_m \otimes \boldsymbol{\Lambda}_C^{1/2}) = \boldsymbol{B}'_C\boldsymbol{B}_C$$

say. Thus if $\boldsymbol{A}_1 = ((\boldsymbol{J}_m \otimes \boldsymbol{\Lambda}_C) + \boldsymbol{\Lambda}_U)^{-1}$, by the SMW formula we have

$$\boldsymbol{A}_1 = \boldsymbol{\Lambda}_U^{-1} - \boldsymbol{\Lambda}_U^{-1}\boldsymbol{B}_C'(\boldsymbol{I}_n + \boldsymbol{B}_C\boldsymbol{\Lambda}_U^{-1}\boldsymbol{B}_C')^{-1}\boldsymbol{B}_C\boldsymbol{\Lambda}_U^{-1}.$$

Now write

$$\boldsymbol{\Lambda}_U = \begin{bmatrix} \boldsymbol{\Lambda}_1 & \boldsymbol{0} & \cdots & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{\Lambda}_2 & \cdots & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \vdots & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{0} & \cdots & \boldsymbol{\Lambda}_m \end{bmatrix}$$

so that the diagonal elements of $\boldsymbol{\Lambda}_i$ are λ_{ik}, $k = 1, 2, \ldots, n$. Then $\boldsymbol{B}_C\boldsymbol{\Lambda}_U^{-1}\boldsymbol{B}_C' = \boldsymbol{\Lambda}_C^{1/2}\sum_i \boldsymbol{\Lambda}_i^{-1}\boldsymbol{\Lambda}_C^{1/2}$ which is diagonal, so that $(\boldsymbol{I}_n + \boldsymbol{B}_C\boldsymbol{\Lambda}_U^{-1}\boldsymbol{B}_C')^{-1}$ is also a diagonal matrix with jth diagonal element $1/(1 + \lambda_{0j}\sum_i \lambda_{ij}^{-1})$. Finally,

$$\boldsymbol{B}_C'(\boldsymbol{I}_n + \boldsymbol{B}_C\boldsymbol{\Lambda}_U^{-1}\boldsymbol{B}_C')^{-1}\boldsymbol{B}_C = \boldsymbol{J}_m \otimes \boldsymbol{D}$$

where $\boldsymbol{D}$ is a diagonal matrix with elements $d_j = \lambda_{0j}/(1 + \lambda_{0j}\sum_i \lambda_{ij}^{-1})$. Thus, we have

$$\boldsymbol{A}_1 = \boldsymbol{\Lambda}_U^{-1} - \boldsymbol{\Lambda}_U^{-1}(\boldsymbol{J}_m \otimes \boldsymbol{D})\boldsymbol{\Lambda}_U^{-1}. \tag{27}$$

Now consider

$$\boldsymbol{A}_2 = (\boldsymbol{A}_1^{-1} + (\boldsymbol{\Lambda}_R \otimes \boldsymbol{J}_n))^{-1} = (\boldsymbol{A}_1^{-1} + \boldsymbol{B}_R'\boldsymbol{B}_R)^{-1}$$

where $\boldsymbol{B}_R = (\boldsymbol{\Lambda}_R^{1/2} \otimes \boldsymbol{1}_n')$. Again by SMW, we have

$$\boldsymbol{A}_2 = \boldsymbol{A}_1 - \boldsymbol{A}_1\boldsymbol{B}_R'(\boldsymbol{I}_m + \boldsymbol{B}_R\boldsymbol{A}_1\boldsymbol{B}_R')^{-1}\boldsymbol{B}_R\boldsymbol{A}_1. \tag{28}$$

The $m \times m$ matrix $\boldsymbol{M} = \boldsymbol{I}_m + \boldsymbol{B}_R\boldsymbol{A}_1\boldsymbol{B}_R'$ has i, j element

$$\begin{cases} 1 + \lambda_{i0}\sum_k \lambda_{ik}^{-1} - \lambda_{i0}\sum_k \lambda_{ik}^{-2}d_k, & i = j, \\ -\lambda_{i0}^{1/2}\lambda_{j0}^{1/2}\sum_k \lambda_{ik}^{-1}\lambda_{jk}^{-1}d_k, & i \neq j. \end{cases} \tag{29}$$

We can also get an explicit formula for the elements of the matrix $\boldsymbol{E} = \boldsymbol{A}_1\boldsymbol{B}_R'$. We can write

$$\boldsymbol{E} = \begin{bmatrix} e_{11} & \cdots & e_{1m} \\ \vdots & \ldots & \vdots \\ e_{m1} & \cdots & e_{mm} \end{bmatrix}$$

where the n-vectors e_{ij} have kth element

$$(e_{ij})_k = \begin{cases} \lambda_{i0}^{1/2}\lambda_{ik}^{-1} - \lambda_{i0}^{1/2}\lambda_{ik}^{-2}d_k, & i = j, \\ -\lambda_{j0}^{1/2}\lambda_{ik}^{-1}\lambda_{jk}^{-1}d_k, & i \neq j. \end{cases} \tag{30}$$

Thus,

$$\boldsymbol{A}_2 = \boldsymbol{A}_1 - \boldsymbol{E}\boldsymbol{M}^{-1}\boldsymbol{E}'. \tag{31}$$

Finally, set $\boldsymbol{A}_3 = (\boldsymbol{A}_2^{-1} + \lambda_{00}\boldsymbol{J}_{mn})^{-1} = (\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S})^{-1}$. This is just a rank one update, so

$$\boldsymbol{A}_3 = \boldsymbol{A}_2 - \frac{\boldsymbol{A}_2\mathbf{1}_{mn}\mathbf{1}_{mn}'\boldsymbol{A}_2}{1/\lambda_{00} + \mathbf{1}_{mn}'\boldsymbol{A}_2\mathbf{1}_{mn}}. \tag{32}$$

4.3 Computation of the adjusted forecasts

To compute the adjusted unaggregated forecasts efficiently when m and/or n are large, we must compute $(\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S})^{-1}\boldsymbol{S}'\boldsymbol{\Lambda}\hat{\boldsymbol{y}}$ without explicitly forming $\boldsymbol{S}$ or $(\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S})$. The formulae in the previous section suggest the following procedure:

1. Suppose we arrange $\boldsymbol{Z} = \boldsymbol{S}'\boldsymbol{\Lambda}\hat{\boldsymbol{y}}$ as a $m \times n$ matrix. Then the i, j element is

$$z_{ij} = \lambda_{00}\hat{y}_{00} + \lambda_{i0}\hat{y}_{i0} + \lambda_{0j}\hat{y}_{0j} + \lambda_{ij}\hat{y}_{ij}. \tag{33}$$

2. To compute $(\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S})^{-1}\boldsymbol{S}'\boldsymbol{\Lambda}\hat{\boldsymbol{y}} = \boldsymbol{A}_3\boldsymbol{Z}$, (regarding $\boldsymbol{Z}$ as a vector) we use the formulae of the last section.

   2.1. From (32) we have

$$\boldsymbol{A}_3\boldsymbol{Z} = \boldsymbol{A}_2\boldsymbol{Z} - \frac{(\mathbf{1}_{mn}'\boldsymbol{A}_2\boldsymbol{Z})\boldsymbol{A}_2\mathbf{1}_{mn}}{1/\lambda_{00} + \mathbf{1}_{mn}'\boldsymbol{A}_2\mathbf{1}_{mn}}. \tag{34}$$

   which involves the computation of $\boldsymbol{A}_2\boldsymbol{Z}$ and $\boldsymbol{A}_2\mathbf{1}_{mn}$.

   2.2 These are computed using

$$\boldsymbol{A}_2\boldsymbol{Z} = \boldsymbol{A}_1\boldsymbol{Z} - \boldsymbol{E}\boldsymbol{M}^{-1}\boldsymbol{E}'\boldsymbol{Z} \tag{35}$$

   and

$$\boldsymbol{A}_2\mathbf{1}_{mn} = \boldsymbol{A}_1\mathbf{1}_{mn} - \boldsymbol{E}\boldsymbol{M}^{-1}\boldsymbol{E}'\mathbf{1}_{mn} \tag{36}$$

   which involves computation of $\boldsymbol{A}_1\boldsymbol{Z}$, $\boldsymbol{A}_1\mathbf{1}_{mn}$, $\boldsymbol{E}'\boldsymbol{Z}$, $\boldsymbol{E}'\mathbf{1}_{mn}$ and $\boldsymbol{E}\boldsymbol{v}$ where the m-vector $\boldsymbol{v}$ is either $\boldsymbol{M}^{-1}\boldsymbol{E}'\boldsymbol{Z}$ or $\boldsymbol{M}^{-1}\boldsymbol{E}'\mathbf{1}_{mn}$.

2.3 Computation of the m-vector $\boldsymbol{E}'\boldsymbol{Z}$ can be done efficiently using the equations

$$(\boldsymbol{E}'\boldsymbol{Z})_i = \lambda_{i0}^{1/2} \sum_j \lambda_{ij}^{-1} z_{ij} - \lambda_{i0}^{1/2} \sum_j \sum_k \lambda_{ij}^{-1} \lambda_{kj}^{-1} d_j z_{kj} \tag{37}$$

with a similar equation for $\boldsymbol{E}'\mathbf{1}_{mn}$. If we arrange the mn-vector $\boldsymbol{E}\boldsymbol{v}$ as a matrix, its i,j element is

$$(\boldsymbol{E}\boldsymbol{v})_{ij} = \lambda_{i0}^{1/2} \lambda_{ij}^{-1} v_i - \lambda_{ij}^{-1} d_j \sum_k \lambda_{k0}^{1/2} \lambda_{kj}^{-1} v_k. \tag{38}$$

2.4 From (27), and arranging $\boldsymbol{A}_1\boldsymbol{Z}$ as a matrix, we have

$$(\boldsymbol{A}_1\boldsymbol{Z})_{ij} = \lambda_{ij}^{-1} z_{ij} - \lambda_{ij}^{-1} d_j z_{ij} \sum_k \lambda_{kj}^{-1}, \tag{39}$$

with a similar equation for $\boldsymbol{A}_1\mathbf{1}_{mn}$.

To summarize, the algorithm for the computation of $(\boldsymbol{S}'\boldsymbol{\Lambda}\boldsymbol{S})^{-1}\boldsymbol{S}'\boldsymbol{\Lambda}\hat{\boldsymbol{y}}$ proceeds as follows:

1. Calculate $\boldsymbol{Z} = \boldsymbol{S}'\boldsymbol{\Lambda}\hat{\boldsymbol{y}}$ using (33).
2. Calculate $\boldsymbol{A}_1\boldsymbol{Z}$ and $\boldsymbol{A}_1\mathbf{1}_{mn}$ using (39).
3. Calulate $\boldsymbol{E}'\boldsymbol{Z}$ and $\boldsymbol{E}'\mathbf{1}_{mn}$ using (37).
4. Calculate $\boldsymbol{M}^{-1}\boldsymbol{E}'\boldsymbol{Z}$ and $\boldsymbol{M}^{-1}\boldsymbol{E}'\mathbf{1}_{mn}$ using (29) and solving the linear system. Calculate $\boldsymbol{E}\boldsymbol{M}^{-1}\boldsymbol{E}'\boldsymbol{Z}$ and $\boldsymbol{E}\boldsymbol{M}^{-1}\boldsymbol{E}'\mathbf{1}_{mn}$ using (38).
5. Calculate $\boldsymbol{A}_2\boldsymbol{Z}$ and $\boldsymbol{A}_2\mathbf{1}_{mn}$ using (35) and (36).
6. Calculate $\boldsymbol{A}_3\boldsymbol{Z}$ using (34).

The major computational task is the calculation of $\boldsymbol{M}^{-1}\boldsymbol{E}\boldsymbol{Z}$ but as $\boldsymbol{M}$ is only an $m \times m$ matrix this should present no difficulty. Without loss of generality we can assume that $m \leq n$ (otherwise interchange rows and columns).

5 Application to forecasting the Australian labour market

We now demonstrate the algorithm described in Section 3.

The Australian and New Zealand Standard Classification of Occupations (ANZSCO) provides a detailed hierarchical classification of occupations (ABS, 2013). Occupations are organized into progressively larger groups based on the similarities of skill specialities and levels. ANZSCO

(version 1.2) lists 1023 occupations, grouped into 359 unit groups. These, in turn, form 97 minor groups, which make up 43 sub-major groups, which combine to give 8 major groups of occupations. For example, a statistician has ANZSCO code 224113, meaning it sits within the hierarchy as follows.

2 Professionals
  22 Business, Human Resource and Marketing Professionals
    224 Information and Organisation Professionals
      2241 Actuaries, Mathematicians and Statisticians
        224113 Statistician

Each of the first four digits represents the group at that level, the last two digits denote the occupation group at the bottom level of the hierarchy.

Detailed data on the occupation groups are only recorded for censuses, held every five years. However, the Australian Labour Force Survey provides data down to the level of unit groups for each quarter, based on a multi-stage area sample of approximately 26,000 private dwellings (ABS, 2014). Quarterly data on the numbers of people employed in each unit group were obtained from the Australian Bureau of Statistics for the period 1986:Q3 – 2013:Q2.

So the hierarchy consists of 359 unit groups, 97 minor groups, 43 sub-major groups, 8 major groups, and the total, giving 508 time series, each of length 108 observations. Compared to typical examples arising in manufacturing and sales, this is a very small hierarchy, but is sufficient to demonstrate our approach. Figure 6 shows some of the time series. The top panel shows the total number of people in the labour force aggregated across all occupations. The panel marked "Level 1" shows the total number of people in each of the 8 major groups. The remaining panels show only one time series per major group; specifically, the largest sub-group at each level from each of the major groups.

We fitted ARIMA models using the automatic algorithm of Hyndman and Khandakar (2008), as implemented in Hyndman (2014), to all series in the hierarchy. Thus, a separate ARIMA model was independently estimated for each of the 508 time series, and forecasts were obtained. These were then combined using the weighted least squares reconciliation approach defined in (3), where the weights were specified as the inverse of the one-step residual variances for each of the series. Figure 7 shows some examples of the original ARIMA (base) forecasts, along with the adjusted forecasts after reconciliation. The examples shown are those with the largest changes in the one-step forecast at each level.

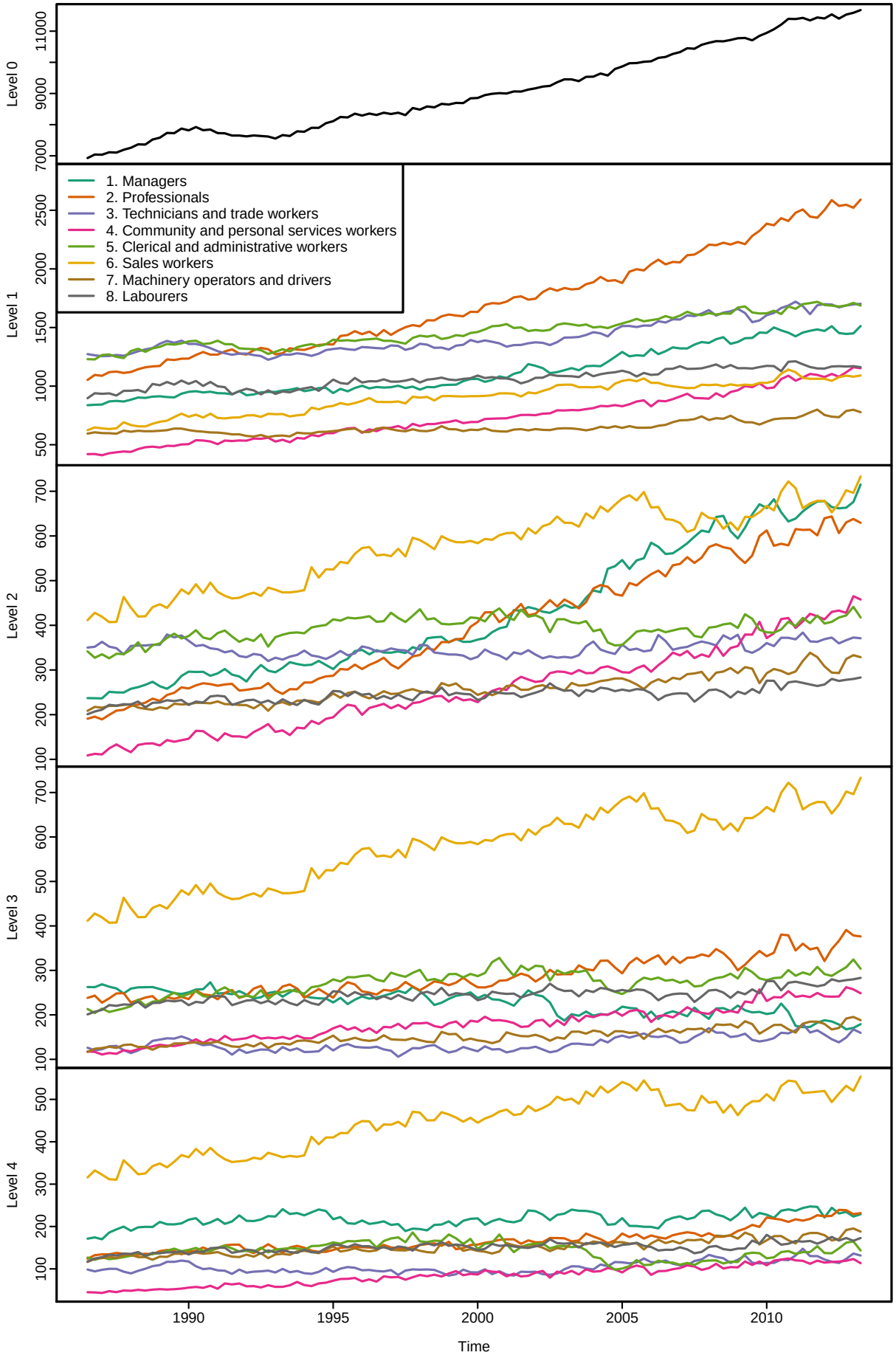


Figure 6: *Some of the 508 time series in the Australian labour force hierarchy. Top: total number of people aggregated across all occupations; Level 1 shows the total number of people in each of the 8 major occupation groups; the remaining panels show the largest sub-group at each level from each of the major groups.*

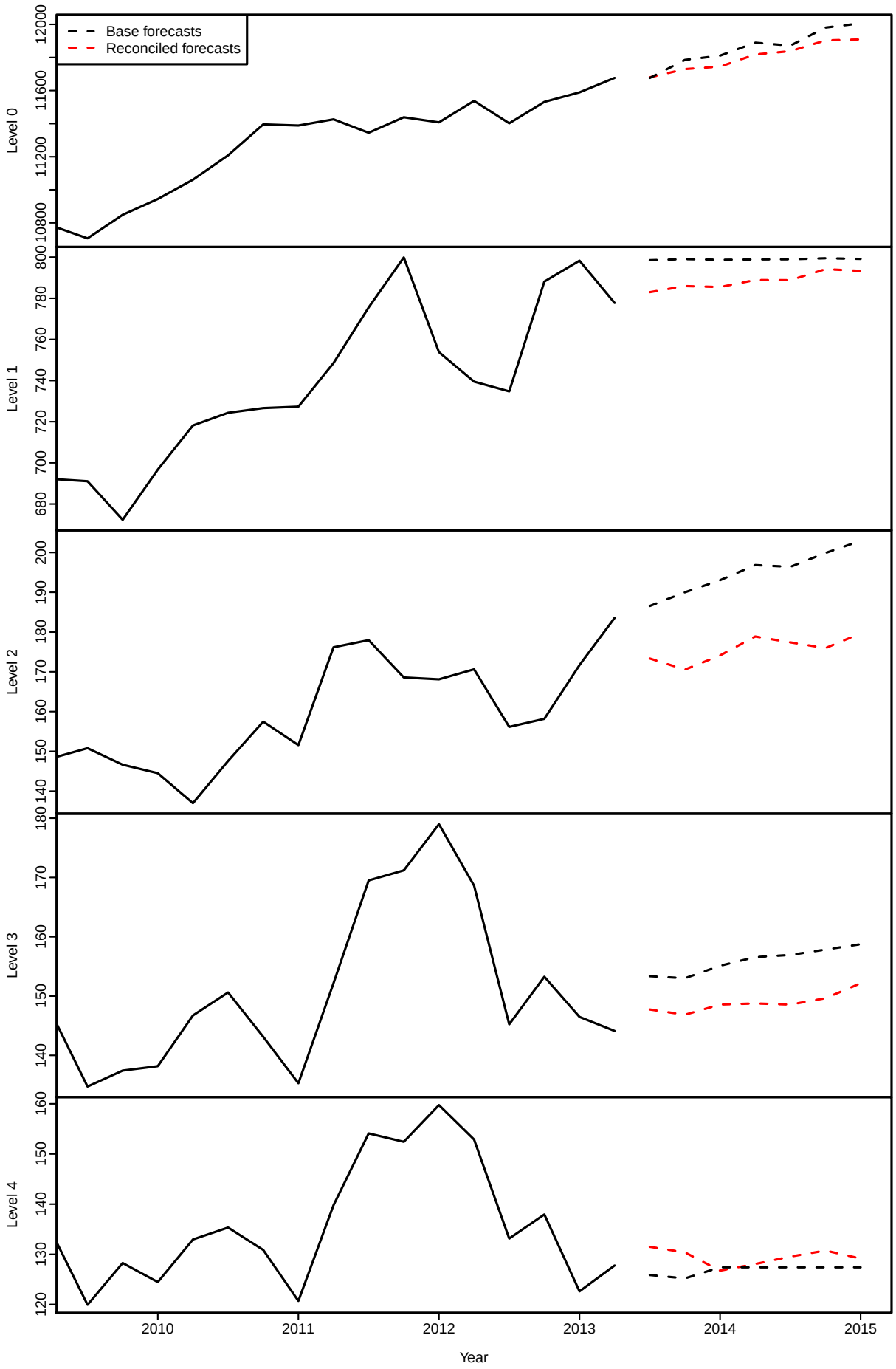


Figure 7: *Some examples of the base forecasts and the reconciled forecasts. The series plotted are those with the largest changes in the one-step forecast at each level.*

To compare the accuracy of our approach with alternative strategies for hierarchical forecasting, we computed forecasts based on a rolling forecast origin for the Australian labour market data. Beginning with a training set of 24 observations, we forecast eight steps ahead, and computed forecast errors using the first eight observations of the withheld data. Then the training set was increased by one observation and new forecast errors were obtained. The training set continued to increase in size, one observation at a time, until it comprised all but the last observation. In this way, we computed many forecast errors for horizons 1–8, and averaged their squares to obtain out-of-sample mean squared errors for each horizon.

We repeated this exercise for bottom-up forecasts, top-down forecasts with the proportions of disaggregation specified by the "forecast proportions" approach of Athanasopoulos, Ahmed, and Hyndman (2009), OLS reconciled forecasts and WLS reconciled forecasts. The resulting root MSE values are given in Table 2. The results show that on average the WLS reconciliation approach outperforms the other approaches at all levels except the very top level where the OLS method does slightly better.

Table 2: *Out-of-sample forecasting performance: Australian labour data*

	Forecast horizon (h)								
RMSE	1	2	3	4	5	6	7	8	Average
				Top level					
Bottom-up	74.71	102.02	121.70	131.17	147.08	157.12	169.60	178.93	135.29
Top-down FP	53.11	79.22	103.52	122.03	142.33	155.86	166.27	173.92	124.53
OLS	52.20	77.77	101.50	119.03	138.27	150.75	160.04	166.38	120.74
WLS	61.77	86.32	107.26	119.33	137.01	146.88	156.71	162.38	122.21
				Level 1					
Bottom-up	21.59	27.33	30.81	32.94	35.45	37.10	39.00	40.51	33.09
Top-down FP	22.42	29.24	33.72	36.76	40.19	42.82	45.24	47.80	37.27
OLS	21.89	28.55	32.74	35.58	38.82	41.24	43.34	45.49	35.96
WLS	20.58	26.19	29.71	31.84	34.36	35.89	37.53	38.86	31.87
				Level 2					
Bottom-up	8.78	10.72	11.79	12.42	13.13	13.61	14.14	14.65	12.40
Top-down FP	9.41	11.74	12.89	13.61	14.58	15.31	15.97	16.62	13.77
OLS	9.02	11.19	12.34	13.04	13.92	14.56	15.17	15.77	13.13
WLS	8.58	10.48	11.54	12.15	12.88	13.36	13.87	14.36	12.15
				Level 3					
Bottom-up	5.44	6.57	7.17	7.53	7.94	8.27	8.60	8.89	7.55
Top-down FP	5.71	7.00	7.64	8.04	8.56	8.98	9.34	9.69	8.12
OLS	5.55	6.78	7.42	7.81	8.29	8.68	9.04	9.37	7.87
WLS	5.35	6.46	7.06	7.42	7.84	8.17	8.48	8.76	7.44
				Bottom Level					
Bottom-up	2.35	2.79	3.02	3.15	3.29	3.42	3.54	3.65	3.15
Top-down FP	2.41	2.88	3.11	3.25	3.43	3.57	3.70	3.83	3.27
OLS	2.40	2.86	3.10	3.24	3.41	3.55	3.68	3.80	3.25
WLS	2.34	2.77	2.99	3.12	3.27	3.40	3.52	3.63	3.13

6 Discussion and conclusions

Our fast computational algorithms provide a way of handling enormous collections of time series in two special but important cases: when the time series are arranged in a hierarchy, and when the time series have a two-way grouping structure. In practice, more than two grouping variables are often available, and hierarchical data often have grouping variables available as well.

For example, with the Australian labour market data considered in Section 5, we also have the data disaggregated further by state, and by age group. As these two variables are not hierarchical, we did not include them in our forecast reconciliations. However, it would be better to allow all possible disaggregations and aggregate groupings of the available data in order to utilize all the available information. In this case, that would require a summing matrix that results from the cross-product of both grouping variables with the occupational hierarchy. While the reconciliation would follow the same equation (3), the computation of the resulting matrices is not possible using either of the fast algorithms described in Sections 3 and 4. For these more general problems, we have to resort to sparse matrix algebra which is much slower. An important future research need is to extend our results to fast computation of the reconciled forecasts for more general grouping structures.

A further research need is the estimation of the covariance matrix Σ_h so that the more general GLS solution (2) can be used. This is difficult because of the sheer size of the matrix, and standard estimators give very poor results. Even if Σ_h could be accurately estimated, computation of the reconciled forecasts would remain an issue as our fast algorithms do not apply in that case.

Our algorithms are implemented in the **hts** package for R (Hyndman, Lee, and Wang, 2014). Very general hierarchical and grouping structures are possible. When the time series are strictly hierarchical, the algorithm described in Section 3 is used. When the time series are grouped in a two-way structure, the algorithm described in Section 4 is used. In all other cases, the reconciliation is handled using sparse matrix algebra. The package provides facilities for creation of the $\boldsymbol{S}$ matrix and estimation of $\boldsymbol{\Lambda}$ from one-step forecast error variances, without requiring user input. The base forecasts are generated automatically using one of the algorithms described in Hyndman and Khandakar (2008).

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