Simultaneously Reconciled Quantile Forecasting of Hierarchically Related Time Series

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Abstract

Many real-life applications involve simultaneously forecasting multiple time series that are hierarchically related via aggregation or disaggregation operations. For instance, commercial organizations often want to forecast inventories simultaneously at store, city, and state levels for resource planning purposes. In such applications, it is important that the forecasts, in addition to being reasonably accurate, are also consistent w.r.t one another. Although forecasting such hierarchical time series has been pursued by economists and data scientists, the current state-of-the-art models use strong assumptions, e.g., all forecasts being unbiased estimates, noise distribution being Gaussian. Besides, state-of-the-art models have not harnessed the power of modern nonlinear models, especially ones based on deep learning. In this paper, we propose using a flexible nonlinear model that optimizes quantile regression loss coupled with suitable regularization terms to maintain the consistency of forecasts across hierarchies. The theoretical framework introduced herein can be applied to any forecasting model with an underlying differentiable loss function. A proof of optimality of our proposed method is also provided. Simulation studies over a range of datasets highlight the efficacy of our approach.

1 Introduction

Hierarchical time series refers to a set of time series organized in a logical hierarchy with the parent-children relations, governed by a set of aggregation and disaggregation operations (Hyndman et al., 2011; Taieb et al., 2017). These aggregations and disaggregations can occur across multiple time series or over the same time series across multiple time granularities. An example of the first kind can be forecasting demand at county, city, state, and country levels (Hyndman et al., 2011). An example of the second kind of hierarchy is forecasting demand at different time granularities like daily, weekly, and monthly (Athanasopoulos et al., 2017). The need to forecast multiple time series that are hierarchically related arise in many applications, from financial forecasting (sas) to demand forecasting (Hyndman et al., 2016; Zhao et al., 2016) and psephology (Lauderdale et al., 2019). The recently announced M5 competition[1] from the International Institute of Forecasters also involves hierarchical forecasting on Walmart data with a $100K prize. A novel challenge in such forecasting problems is to produce accurate forecasts while maintaining the consistency of the forecasts across multiple hierarchies.

Related Works Existing hierarchical forecasting methods predominantly employ linear auto-regressive (AR) models that are initially trained while ignoring the hierarchy. The output forecasts produced by these AR models are reconciled afterward for consistency. As shown in Figure 1(c), such reconciliation is achieved by defining a mapping matrix, often denoted by S, which encapsulates the mutual relationships among the time series (Hyndman et al., 2011). The reconciliation step involves inversion and multiplication of the S matrix that leads to the computational complexity of $\mathcal{O}(n^3 h)$, where n is the number of nodes, and h represents how many levels of hierarchy the set of time series are organized into. Thus, reconciling hundreds of thousands of time series at a time required for specific industrial applications becomes difficult. Improved versions of the reconciliation were proposed by employing trace minimization (Wickramasuriya et al., 2015) and sparse matrix computation (Hyndman et al., 2016). These

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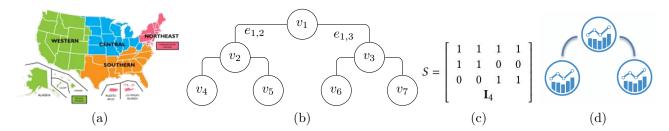[1]https://mofc.unic.ac.cy/m5-competition/

Figure 1: (a) Example of hierarchically related time series: state population growth forecast, the data is aggregated by geographical locations; (b) corresponding graph structure as nodes and vertices; (c) corresponding matrix representation with four bottom level time series and three aggregated levels; (d) time series forecast at each node.

algorithms assume that the individual base estimators are unbiased, which is unrealistic in many real-life applications. The unbiasedness assumption was relaxed in (Taieb et al., 2017) while introducing other assumptions like ergodicity with exponentially decaying mixing coefficient. Moreover, all these existing methods try to impose any reconciliation constraints among the time series as a post inference step, which possesses two challenges: 1. ignoring the relationships across time series during training can potentially lead to suboptimal solutions, 2. additional computational complexity in the inference step, owing to the inversion of S matrix, which makes it challenging to use the technique when a significant amount of time series are encountered in an industrial forecasting pipeline.

A critical development in time series forecasting has been the application of Deep Neural Networks (DNN) (e.g., Chung et al., 2014; Lai et al., 2018; Mukherjee et al., 2018; Oreshkin et al., 2019; Salinas et al., 2019; Sen et al., 2019; Zhu and Laptev, 2017) which have shown to outperform statistical auto-regressive or other statistical models in several situations. However, no existing method incorporates the hierarchical structure of the set of time series into the DNN learning step. Instead, one hopes that the DNN will learn the relationships from the data. Graph neural networks (GNN) (e.g., Franceschi et al., 2019; Lachapelle et al., 2019; Wu et al., 2020; Yu et al., 2017, 2019; Zhang et al., 2020; Zheng et al., 2018) have also been used to learn inherent relations among multiple time series; however, they need a pre-defined graph model that can adequately capture the relationships among the time series. Characterizing uncertainty of the DNN forecast is another critical aspect, which becomes even more complicated when additive noise does not follow a Gaussian distribution (e.g., Blundell et al., 2015; Iwata and Ghahramani, 2017; Kuleshov et al., 2018; Lakshminarayanan et al., 2017; Sun et al., 2019). If the observation noise model is misspecified, then the performance would be poor however complex neural network architecture one uses. Other works like Salinas et al. (2019) use multiple observation noise models (Gaussian, Negative Binomial) and

loss functions. It is left to human experts' discretion to select the appropriate loss based on the time series's nature. This approach cannot be generalized and involves human intervention; it is especially not feasible for an industrial forecasting pipeline where predictions are to be generated for a vast number of time series, which can have a widely varying nature of observation noise. Besides, Bayesian approaches also face problems as the prior distribution and loss function assumptions will not be met across all of the time series. One approach that does not need to specify a parametric form of distribution is through quantile regression. Prior works include combining sequence to sequence models with quantile loss to generate multi-step probabilistic forecasts (Wen et al., 2017) and modeling conditional quantile functions using regression splines (Gasthaus et al., 2019). These works are incapable of handling hierarchical structures within time series.

Key aspects of multiple, related time series forecasting addressed by our proposed model include:

1. introduction of a regularized loss function that captures the mutual relationships among each group of time series from adjacent aggregation levels,

2. generation of probabilistic forecasts using quantile regression and simultaneously reconciling each quantile during model training,

3. clear demonstration of superior model capabilities, especially on real e-commerce datasets with sparsity and skewed noise distributions.

Background: Hierarchical Time Series Forecast
Denote $b_t \in \mathbb{R}^m$, $a_t \in \mathbb{R}^k$ as the observations at time t for the m and k series at the bottom and aggregation level(s), respectively. Then $y_t = Sb_t \in \mathbb{R}^n$ contains observations at time t for all levels. Similarly, let $\hat{b}_T(h)$ be the $h-$step ahead forecast on the bottom-level at time T, we can obtain forecasts in higher aggregation levels by computing $\hat{y}_T(h) = S\hat{b}_T(h)$. This simple method is called bottom-up (BU), which guarantees

reconciled forecasts. However, the error from bottom-level forecasts will accumulate to higher levels, leading to poor results. BU also cannot leverage any training data that is available at the more granular levels. A more straightforward approach called base forecast is to perform forecasting for each time series independently without considering the structure at all, i.e., compute $\hat{y}_T(h) = \begin{bmatrix} \hat{a}_T(h)^\top & \hat{b}_T(h)^\top \end{bmatrix}^\top$, but this will apparently lead to irreconciled forecasts. Therefore, imposing constraints to revise the base forecasts is a natural choice to accommodate the hierarchical relationships. More specifically, the goal is to obtain some appropriately selected matrix $P \in \mathbb{R}^{m \times n}$ to combine the base forecasts linearly: $\tilde{y}_T(h) = SP\hat{y}_T(h)$, where $\tilde{y}_T(h)$ is the reconciled forecasts which are now coherent by construction. The role of P is to map the base forecasts into the forecasts at the most disaggregated level and sum them up by S to get the reconciled forecasts. The previously mentioned approach (Ben Taieb and Koo, 2019; Hyndman et al., 2011, 2016; Wickramasuriya et al., 2015) involves computing the optimal P under different situations. A more detailed introduction can be found in Appendix A.

2 Simultaneous Hierarchically Reconciled Quantile Forecasting

We propose a new method for hierarchical time-series forecasts. Our approach fundamentally differs from others in that we move the reconciliation into the training stage by enabling the model to simultaneously learn the time series data from adjacent aggregation levels, while also integrating quantile regression to provide coherent forecasts for uncertainty bounds. We call our method Simultaneous HierArchically Reconciled Quantile Regression (SHARQ) to highlight these properties.

2.1 Problem Formulation

Graph Structure Figure 1(b) shows a hierarchical graph structure where each node represents a time series, which is to be predicted over a horizon. The graph structure is represented by $\{V, E\}$, where $V := \{v_1, v_2, \ldots, v_n\}$ are the vertices of the graph and $E := \{e_{i_1,j_1}, e_{i_2,j_2}, \ldots, e_{i_p,j_p}\}$ are the set of edges. Also, $e_{i,j} \in \{-1, 1\}$ is a signed edge where i is the parent vertex and j is the child. An example of the negative-signed edge can be forecasting surplus production, which is the difference between production and demand. The time series for vertex i at time t is represented as $x_{v_i}(t)$. For sake of simplicity, we assume the value of a time series at a parent level will be the (signed) sum of the children vertices. This constraint relationship can be represented as $x_{v_i}(t) = \sum_{e_{i,k} \in E} e_{i,k}\, x_{v_k}(t)$. We

can later extend these to set of non-linear constraints: $x_{v_i}(t) = H_{v_i}\left(\sum_{e_{i,k} \in E} e_{i,k}\, x_{v_k}(t)\right)$, where $H_{v_i} \in \mathbb{C}^1$. But linear hierarchical aggregation has already covered most real-world applications. The graph has hierarchies $L := \{l_1, l_2, \ldots, l_i, \ldots, l_q\}$, where l_i is the set of all vertices belonging to the ith level of hierarchy. Note that the graph representation using $\{V, E\}$ is equivalent to the S matrix in defining a hierarchical structure.

Data Fit Loss Function We now formulate the learning problem for each node. Let $\{x_{v_i}(t) \mid t = 0, \ldots, T\}$ be the training data for vertex v_i, w be the window of the auto-regressive features, and h be horizon of forecast. Based on the window, we can create a sample of training data in the time stamp m as:

$$\{(X_m^i, Y_m^i) \mid X_m^i = [F\left(x_{v_i}(m), \ldots, x_{v_i}(m - w + 1)\right)],$$
$$Y_m^i = [x_{v_i}(m + 1), \ldots, x_{v_i}(m + h)]\},$$

where $F \colon \mathbb{R}^{w+1} \to \mathbb{R}^{n_f}$ is the featurization function, which will generate a set of features; n_f is the size of feature space, h is the horizon of the forecast. It can be noted that $n_f \geq \omega$. In this fashion, we transform the forecasting problem to a regression one, where n_f and h capture the size of the feature space and the response. For instance, we can create a set of features for an ARIMA(p, d, q) model based on the standard parameterization, where auto-regressive window size $w = p$ and the other features corresponding to the d, q parameters will form the rest of the features.

We represent a forecasting model that learns the mean as a point estimate. Denote function $g_i : \mathbb{R}^{n_f} \times \mathbb{R}^{n_\theta} \to \mathbb{R}^d$, where n_θ represents the number of model parameters which are represented as $\theta_i \in \mathbb{R}^{n_\theta}$. The estimate from the model for X_m^i will be $\hat{Y}_m^i := g_i(X_m^i, \theta_i)$. We can define a loss function for the mth sample at the ith vertex as $\mathcal{L}(\hat{Y}_m^i, Y_m^i) = \mathcal{L}(g_i(X_m^i, \theta_i), Y_m^i)$. We would assume the noise in training samples are of `i.i.d.` nature. As a consequence, the loss for the entire training data will be sum for each sample, i.e., $\sum_m \mathcal{L}(g_i(X_m^i, \theta_i), Y_m^i)$. Noted that this formulation will work for neural networks or ARIMA but not for Gaussian Processes, where we need to model the covariance of the uncertainties across the samples.

Reconciled Point Forecast We then describe how to incorporate reconciliation constraints into the loss functions for the vertices. The constraints at different levels of hierarchy will have different weights, which we denote as a function $w_c : L \to \mathbb{R}$. We define another function that maps any vertex to the hierarchy level, $LM : V \to L$. For any vertex v_i, the corresponding weight for the constraint is given by $\lambda_{v_i} := w_c \circ LM(v_i)$.

The constrained loss for vertex v_i will be

$$\mathcal{L}_c(g_i(X_m^i, \theta_i), Y_m^i, g_k(X_m^k, \theta_k)) := \mathcal{L}(g_i(X_m^i, \theta_i), Y_m^i)$$
$$+ \lambda_i \parallel g_i(X_m^i, \theta_i) - \sum_{e_{i,k} \in E} \left(e_{i,k} \ g_k(X_m^k, \theta_k) \right) \parallel^2 . \quad (1)$$

Note that the data fit loss and the reconciliation, as described thus far, are catered to the point estimate of the mean forecasts.

2.2 Reconciling Probabilistic Forecast using Quantiles

Generating probabilistic forecasts over a range of time is significant for wide-ranging applications. Real-world time series data is usually sparse and not uniformly sampled. It is unreasonable to assume that the uncertainty or error distribution at every future point of time as Gaussians. A standard approach to solve this problem is using quantile loss, which allows one to model the error distribution in a non-parametric fashion. The estimator will aim at minimizing a loss directly represented in terms of the quantiles. Simultaneously, quantile can be used to construct confidence intervals by fitting multiple quantile regressors to obtain estimates of upper and lower bounds for prediction intervals. The quantile loss $\rho_\tau(y)$ is defined as $\rho_\tau(y, \ Q_\tau) = (y - Q_\tau).(\tau - \mathbb{I}_{(y<Q_\tau)})$, where Q_τ is the τth quantile output by an estimator. We will adopt quantiles in our framework, and pre-specified quantile ranges will represent the forecasting distribution. For simplicity, we denote $Q_i^\tau = Q_i^\tau(X_m^i, \theta_i)$ as the τth quantile estimator for node i. Eq.(23) demonstrates a quantile version of the probabilistic estimator; it aims to produce multiple forecasts at different quantiles while maintaining a coherent median forecast which will be used to reconcile other quantiles:

$$\mathcal{L}_c(Q_i, Y_m^i, Q_k) :=$$
$$\sum_{\tau=\tau_0}^{\tau_q} \rho_\tau(Q_i^\tau, Y_m^i) + \lambda_i \parallel Q_i^{50} - \sum_{e_{i,k} \in E} e_{i,k} Q_i^{50} \parallel^2, \quad (2)$$

where $[\tau_0, \ldots, \tau_q]$ are a set of quantile levels, and $Q_i = [Q_i^{\tau_0}, \ldots, Q_i^{\tau_q}]$. To further guarantee that estimation at each quantile is coherent across the hierarchy, the straightforward solution is to add consistency regularization for each quantile like Eq.(23). However, too many regularization terms would not only increase the number of hyper-parameters, but also complicate the loss function, where the result may even be worse as it is hard to find a solution to balance each objective. Moreover, a quantile estimator does not hold the additive property. As an example, assume $X_1 \sim N(\mu_1, \sigma_1^2)$, $X_2 \sim N(\mu_2, \sigma_2^2)$ are independent random variables, and define $Y = X_1 + X_2$. Then $Q_Y^\tau = Q_{X_1}^\tau + Q_{X_2}^\tau$ is true

Algorithm 1 SHARQ

Input: Training data $\mathcal{I}_1 = \{X_i, Y_i\}_{i=1}^{T_1}$, testing data $\mathcal{I}_2 = \{X_i, Y_i\}_{i=1}^{T_2}$.
Process:
train each leaf node (e.g., v_4 to v_7 in Figure 1(b)) independently without regularization
for each vertex v at upper level l (e.g., $l = 2$ for v_3, v_2, then $l = 1$ for v_1) **do**
    train vertex v at level l using Eq.(23)
end for
Reconciled Median Forecast $\mathbf{MF} \leftarrow \mathbf{Models}(\mathcal{I}_2)$
for each vertex v at upper level l **do**
    train vertex v at level l using Eq.(3) and $\mathbf{MF}$
end for
Output: Reconciled forecasts at pre-specified quantiles.

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only if $X_1 = C \times X_2$, where C is arbitrary constant. This requirement cannot be satisfied. But for any τ, we have $(Q_Y^\tau - \mu_Y)^2 = (Q_{X_1}^\tau - \mu_{X_1})^2 + (Q_{X_2}^\tau - \mu_{X_2})^2$, the proof of above properties can be found in Appendix B. Given these properties, we can formulate a new objective to make an arbitrary quantile consistent:

$$\mathcal{L}_q(Q_i, Y_m^i, Q_k) := \quad (3)$$
$$\left[f \left(Q_i^\tau - Q_i^{50} \right) - \sum_{e_{i,k} \in E} e_{i,k} \ f \left(Q_k^\tau - Q_k^{50} \right) + \mathrm{Var}(\epsilon) \right]^2,$$

where ϵ is the mean forecast's inconsistency error, which is mostly a much smaller term for a non-sparse dataset, and f is the distance metric. Eq.(3) is zero when f is a squared function and the given data satisfies `i.i.d.` Gaussian assumption. Therefore, optimizing Eq.(3) "forces" this additive property in non-Gaussian cases and is equivalent to reconcile the quantile estimators, which can also be interpreted as reconciliation over the variance across adjacent aggregation levels. Empirically, this approach calibrates multiple quantile predictions to be coherent and mitigates the quantile crossing issue (Liu and Wu, 2009).

2.3 SHARQ Algorithm

Our formulation can be combined with a bottom-up training approach to reconciling forecasts for each quantile simultaneously. Since the time series at the leaf (disaggregated) level are independent of higher aggregation levels, we can use the lower-level forecasting results to progressively reconcile the forecasting models at higher levels without revisiting previous reconciliations, till the root is reached. In contrast, if top-down training is applied, one needs to reconcile both higher (previously visited) and lower-level data at an intermediate vertex, since other time series at that intermediate level may have changed. Algorithm 1 describes our procedure. We now address the remaining aspects.

Beyond Gaussian Noise Assumption. Noise distributions for many real-world datasets (e.g., e-commerce data) are heavily skewed, so a Gaussian model may not be appropriate. For multi-level time series, data at the most disaggregated (lowest) level is more likely to be sparse, which makes the quantile reconciliation in Eq.(3) less accurate. In such situations, one can substitute median with the mean estimator as in Eq.(1) for training lower-level time series. One can also mix-and-match between mean and median estimators at higher aggregation levels depending on the data characteristics. Finding a suitable function f for quantile reconciliation as in Eq.(3) is an alternative way to tackle non-symmetric errors (Li and Zhu, 2008).

Efficient Training and Inference SHARQ is time and memory efficient, scaling well in both aspects with large datasets. One can simultaneously train multiple time series and keep a running sum for reconciliation. Since coherent probabilistic forecasts are enforced during training, no extra post-processing time is needed (see Appendix E for details). Besides, SHARQ does not force one to use deep forecasting models or to use the same type of model at each node; in fact, any model where gradient-based optimization can be used is allowable, and one can also mix-and-match. For cases where the time series at a given level are structurally very similar (Zhu and Laptev, 2017), they can be grouped (e.g., by clustering), and a single model can be learned for the entire group.

3 Statistical Analysis of SHARQ

In this section, we theoretically demonstrate the advantages of SHARQ. We begin by showing the optimality of our formulation (1) in contrast to post-inference based methods, which solves the matrix P for $\tilde{y}_T(h) = SP\hat{y}_T(h)$. We emphasize our advantage in balancing coherency requirements and forecasting accuracy. We then present some desirable statistical properties of SHARQ.

THEOREM 1. *(Global Optimum) For $L_c \in C^1$, for an arbitrary parameterized smooth regressor model asymptotically,*

$$\mathcal{L}_c(g_i(X_m^i, \theta_i^\star), Y_m^i, g_k(X_m^k, \theta_k^\star))$$
$$\leq \mathcal{L}_c(g_i(X_m^i, \theta_i^{recon}), Y_m^i, g_k(X_m^k, \theta_k^{recon})) \quad (4)$$

where $\theta^\star$, θ^{recon} are the parameters for SHARQ, and post inference reconciled solution, respectively.

PROOF. By definition, SHARQ directly minimize Eq.(1),

$$\theta^\star = \arg\min_\theta \mathcal{L}_c(g_i(X_m^i, \theta_i), Y_m^i, g_k(X_m^k, \theta_k)), \quad (5)$$

where $\theta = \{\theta_i, \theta_k\}$. □

Since Ben Taieb and Koo (2019); Hyndman et al. (2011, 2016); Wickramasuriya et al. (2015) are performing the reconciliation as a post-processing step, those solutions are bound to be sub-optimal in comparison with $\theta^\star$.

PROPOSITION 2. *(Hard Constraint) For post-inference based methods, $P\hat{y}_T(h)$ is the bottom level reconciled forecast. In other words, it requires that*

$$g_i(X_m^i, \theta_i^\star) = \sum_{e_{i,k} \in E} g_k(X_m^k, \theta_k^{recon}). \quad (6)$$

Had we only considered the point forecast reconciliation, i.e. $\mathbb{E}[g_i(X_m^i, \theta_i^\star)] = \sum_{e_{i,k} \in E} \mathbb{E}[g_k(X_m^k, \theta_k^{recon})]$, the post inference processing still might have worked. However, due to the probabilistic nature of the variables $g_i(X_m^i, \theta_i^\star) = \mathbb{E}[g_i(X_m^i, \theta_i^\star)] + \varepsilon_i$, where ε_i is the observation noise, reconciling the mean won't suffice.

Remark To satisfy Eq.(6), it is required that $\varepsilon_i = \sum_{e_{i,k} \in E} \varepsilon_k$, which is not a realistic property to be satisfied in real-life problems. Intuitively, when a reconciliation matrix P is applied, the original, unbiased base forecasts with variation are "forced" to be summed up. However, our method does not impose this hard constraint, leading to different properties.

PROPOSITION 3. *(Unbiasedness Property) Consider a hierarchical structure with n nodes where the first κ nodes belong to aggregation levels, assume that the bottom level forecasting is unbiased:*

$$\mathbb{E}[g_k(X_m^k, \theta_k)] = Y_m^k, \quad k = \kappa + 1, ..., n \quad (7)$$

and the bottom level forecasting models are well optimized:

$$\text{Var}\left(\|g_k(X_m^k, \theta_k) - Y_m^k\|\right) = \epsilon, \quad \epsilon = \mathcal{O}(\frac{1}{m}). \quad (8)$$

Then we have that

$$\mathbb{E}[g_i(X_m^i, \theta_i)] = \mathbb{E}[\sum_{e_{i,k} \in E} g_k(X_m^k, \theta_k)]$$
$$= \sum_{e_{i,k} \in E} \mathbb{E}[g_k(X_m^k, \theta_k)]$$
$$= Y_m^i, \quad i = 1, ..., \kappa$$

Therefore, we claim that given the unbiased base forecast at the most disaggregated level, as well as well-specified models, our method can provide unbiased estimation at all aggregation levels.

PROPOSITION 4. *(Variance Reduction) Assume we are minimizing a quadratic loss function using our*

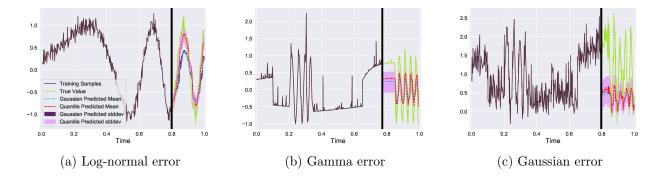(a) Log-normal error   (b) Gamma error   (c) Gaussian error

Figure 2: Forecasting results of simulated sequential data under different error distributions. The original function of (a) is sinusoidal with varying frequency; (b) and (c) are discontinuous step functions. Note that our baseline forecasts in (b) and (c) are overconfident (Lakshminarayanan et al., 2017; Li and Hoiem, 2020) and their prediction intervals are too small to be shown.

Error distribution		Log-normal	Gamma	Gaussian
MAPE	Quantile	**32.72**	**62.20**	**70.29**
	Baseline	49.88	73.69	73.36
LR	Quantile	**0.2218**	**0.5649**	**0.8634**
	Baseline	0.5661	0.7489	1.025

Table 1: Left: Quantitative results for simulation experiments. We use Mean Absolute Percentage Error (MAPE) (Makridakis and Hibon, 2000) to measure forecasting accuracy and Likelihood Ratio (LR) to evaluate uncertainty intervals. Right: A schematic of the multi-quantile forecaster used for simulation.

formulation, where

$$L_c(g_i(X_m^i, \theta_i), Y_m^i, g_k(X_m^k, \theta_k)) = \|g_i(X_m^i, \theta_i) - Y_m^i\|^2$$
$$+ \lambda_i \| g_i(X_m^i, \theta_i) - \sum_{e_{i,k} \in E} \left(e_{i,k} \ g_k(X_m^k, \theta_k) \right) \|^2 .$$

By solving the quadratic objective, we get

$$g_i(X_m^i, \theta_i) = \frac{Y_m^i + \lambda_i \sum_{e_{i,k} \in E} e_{i,k} \ g_k(X_m^k, \theta_k)}{\lambda_i + 1}. \quad (9)$$

Note that if we fit linear models that generalize in the bottom level, we have $\mathrm{Var}(\sum_{e_{i,k} \in E} e_{i,k} \ g_k(X_m^k, \theta_k)) = \mathcal{O}(\frac{1}{m})$ *(for other models, the variance should be at least in a smaller scale than* $\mathcal{O}(1)$, *which is the variance of observed samples). Therefore, by alternating* λ_i:

- $\mathrm{Var}(g_i(X_m^i, \theta_i)) = \mathrm{Var}(Y_m^i) = \mathcal{O}(1), \text{when } \lambda_i \to 0.$

- $\mathrm{Var}(g_i(X_m^i, \theta_i)) = \mathrm{Var}(\sum_{e_{i,k} \in E} e_{i,k} \ g_k(X_m^k, \theta_k))$
$$= \mathcal{O}(\frac{1}{m}), \text{when } \lambda_i \to \infty. \quad (10)$$

This tells us that by alternating the coefficient λ_i, the amount of estimator variance at higher aggregation

levels can be controlled. If lower-level models are accurate, then we can improve the higher-level models by this method. Instead of adding a hard coherency requirement like the post-inference methods, SHARQ provides more flexibility for controlling the variations.

4 Experimental Results

In this section, we validate the performance of SHARQ on multiple hierarchical time series datasets with different properties and use cases. The experiments are conducted on both simulated and real-world data. Results demonstrate that SHARQ can generate coherent and accurate forecasts and well-capture the prediction uncertainty at any specified level.

4.1 Simulation Experiments

We first demonstrate that quantile loss can handle various kinds of error distributions and thus provide more stable and accurate uncertainty estimation than methods under Gaussian error assumption. We trained vanilla RNN models on three different sequential data with distinct error distributions. We implemented a model that has multiple quantile estimators with shared

Table 2: Performance measured by MAPE (Makridakis and Hibon, 2000) on Australian Labour (755 time series), and M5 competition (42840 time series), lower values are better. Level 1 is the top aggregation level, and 4 is the bottom level.

Algorithm	RNN				Autoregressive				LST-Skip				N-Beats			
Reconciliation	Level				Level				Level				Level			
	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4
BU	15.23	15.88	19.41	**17.96**	19.29	20.14	21.09	22.13	16.13	17.59	16.88	**17.17**	14.23	14.75	15.67	**15.84**
Base	12.89	14.26	16.96	**17.96**	17.59	19.86	20.98	22.13	14.99	12.31	**15.12**	**17.17**	12.18	13.32	**14.32**	**15.84**
MinT-sam	14.98	15.94	17.79	19.23	18.82	19.98	21.59	22.26	15.12	14.41	16.42	18.62	13.11	14.63	14.86	15.96
MinT-shr	14.46	15.43	16.94	18.75	18.54	19.98	21.22	22.01	15.06	13.89	16.31	17.56	12.76	14.41	14.77	15.87
MinT-ols	15.01	15.96	18.75	19.21	19.14	20.02	21.74	22.34	15.12	14.41	16.41	18.74	13.29	14.49	14.85	16.83
ERM	14.73	16.62	19.51	20.13	17.89	20.11	20.33	**21.93**	16.61	16.84	18.75	19.21	14.52	15.26	17.02	17.29
SHARQ	**12.55**	**13.21**	**16.01**	**17.96**	17.65	**19.72**	**20.01**	22.13	**11.97**	**12.24**	15.64	**17.17**	**11.86**	**12.35**	14.53	**15.84**
BU	11.42	12.04	12.32	**11.72**	12.77	14.59	16.11	**16.56**	10.11	12.69	10.78	**10.94**	11.01	11.05	12.43	**11.34**
Base	10.63	10.15	11.23	**11.72**	11.64	13.91	15.67	**16.56**	8.96	11.38	10.59	**10.94**	9.64	9.88	11.11	**11.34**
MinT-sam	11.25	11.67	11.87	12.99	12.34	14.09	15.97	17.54	9.64	12.31	11.02	11.01	9.97	10.82	11.89	12.77
MinT-shr	10.76	11.03	11.49	12.81	11.92	13.85	15.76	17.33	9.19	11.97	10.71	10.99	9.78	10.69	11.56	12.63
MinT-ols	11.75	11.56	12.06	13.05	12.32	14.21	15.97	17.56	9.63	12.54	10.98	11.02	10.41	11.01	12.02	12.71
ERM	11.86	12.01	12.42	13.54	12.61	14.02	**15.41**	17.14	10.35	13.01	13.15	13.56	10.44	11.22	13.42	13.96
SHARQ	**9.87**	**9.68**	**10.41**	**11.72**	**11.23**	**13.84**	15.69	**16.56**	**8.68**	**9.49**	**10.23**	**10.94**	**9.67**	**9.76**	**10.75**	**11.34**

features, which enables more efficient training. The bagging method (Oliveira and Torgo, 2014) is used as a baseline where we utilize model ensembles to produce confidence intervals. Figure 2 shows the advantage of quantile estimators on simulated sequential data, and Table 1 compares forecasting results as well as demonstrates our model structure. Although it is difficult to capture the trend of discontinuous functions in Figure 2 (b) and (c), the quantile estimators are accurate and stable under both skewed and symmetric error distributions, where it also outperforms the baseline for all types of error distributions.

4.2 Hierarchical Time Series

We validate the performance of SHARQ on multiple real-world hierarchical time-series datasets, which include Australian Labour, FTSE (Doherty et al., 2005), M5 competition, and Wikipedia webpage views dataset (see Appendix D for details). This type of data usually contains categorical features (e.g., locations, genders) that can be used to aggregate across time series to construct hierarchical structures. We compare our method with state-of-the-art reconciliation algorithms MinT (Wickramasuriya et al., 2019) and ERM (Ben Taieb and Koo, 2019), along with other baselines, including bottom-up (BU) and base forecast. To have a fair comparison, we first pre-process each dataset using information from categorical features. The bottom-up training procedure in Algorithm 1 is then used for each method except for BU. Specifically, the model training settings of the base forecast, MinT and ERM are by default the same as SHARQ, except that they do not have mean and quantile reconciliation. As for MinT and ERM, extra reconciliations are performed after model training. In this case, the algorithm has access

to the hierarchical information about the dataset. We also incorporate different time series forecasting algorithms into our framework, which ranges from linear auto-regressive model and RNN-GRU (Chung et al., 2014) to advanced models such as LSTNet (Lai et al., 2018) and N-Beats (Oreshkin et al., 2019). Although these models are not originally designed for hierarchical time series problems, we show that the performance on this task can be improved under our framework.

Table 2 and 3 shows forecasting results across all reconciliation methods and models on Australian Labour (upper) and M5 (lower) dataset, the results are averaged across 3 runs. Specifically, MAPE (Makridakis and Hibon, 2000) measures accuracy for point forecast by Eq.(1), and *Continuous Ranked Probability Score* (CRPS) (Matheson and Winkler, 1976) measures the holistic accuracy of a probabilistic forecast, using multiple quantiles. Overall, SHARQ outperforms other reconciliation baselines, resulting in much lower MAPE and CRPS over all four models, particularly at the higher aggregation levels. Specifically, although the bottom-up training of SHARQ leads to the same bottom level performance as BU and Base method, the error accumulation and inconsistency across the hierarchy leads to higher error in other aggregation levels. More importantly, the better performance of SHARQ over Base and BU in multiple datasets validates the necessity of hierarchical construction in DNN training. Besides, comparing the autoregressive model results with others, SHARQ tends to perform better when the forecasting model is less parsimonious for the dataset. Figure 3 presents multi-step forecasting results, which possess the advantage of coherent estimation at multiple quantile levels.

(a) Labour (SHARQ)   (b) FTSE (SHARQ)   (c) M5 (SHARQ)   (d) Wiki (SHARQ)

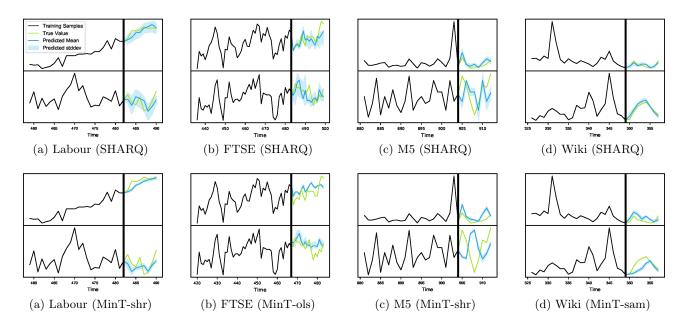(a) Labour (MinT-shr)   (b) FTSE (MinT-ols)   (c) M5 (MinT-shr)   (d) Wiki (MinT-sam)

Figure 3: Top and bottom level forecasts on four datasets using the LSTNet skip connection model. For each dataset, we plot the results of SHARQ and the second-best reconciliation method. P5 and P95 forecasts are the lower and upper boundaries of the forecast band. We use mean as the point estimator (also complement of P50) for all bottom-level data and other aggregation levels of Australian Labour and FTSE data.

Algorithm	RNN				Autoregressive				LST-Skip				N-Beats			
Reconciliation	Level				Level				Level				Level			
	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4
BU	0.244	0.221	0.186	**0.149**	0.401	0.367	0.303	0.231	0.241	0.222	0.193	**0.142**	0.232	0.211	0.196	0.154
Base	0.119	0.135	0.143	**0.149**	0.174	0.203	0.221	0.231	0.124	0.139	0.142	**0.142**	0.122	0.141	0.141	0.154
MinT-sam	0.106	0.135	0.139	0.152	0.167	0.191	0.214	0.227	0.106	0.125	0.133	0.156	0.106	0.119	0.141	**0.153**
MinT-shr	0.103	0.129	0.137	0.158	0.162	0.189	0.206	0.232	0.101	0.113	0.132	0.153	0.103	**0.114**	0.137	0.155
MinT-ols	0.109	0.133	0.142	0.159	0.167	0.194	0.215	0.233	0.109	0.124	0.133	0.154	0.111	0.123	0.142	0.155
ERM	0.126	0.147	0.152	0.156	0.164	**0.178**	**0.192**	**0.201**	0.132	0.145	0.149	0.162	0.121	0.138	0.143	0.158
SHARQ	**0.097**	**0.124**	**0.133**	0.149	**0.157**	0.187	0.199	0.231	**0.089**	**0.096**	**0.126**	**0.142**	**0.092**	0.115	**0.136**	0.154
BU	0.247	0.231	0.226	**0.208**	0.397	0.375	0.316	0.297	0.219	0.211	0.194	**0.164**	0.199	0.171	0.152	**0.135**
Base	0.162	0.167	0.193	**0.208**	0.231	0.257	0.265	0.297	0.146	0.152	0.175	**0.164**	0.079	0.128	0.136	**0.135**
MinT-sam	0.147	0.158	0.154	0.211	0.257	0.262	0.271	0.279	0.112	0.141	0.175	0.189	0.091	0.124	0.142	0.149
MinT-shr	0.134	0.142	0.146	0.213	0.256	0.248	0.268	0.288	0.096	0.137	0.134	0.171	0.083	0.112	0.147	0.166
MinT-ols	0.143	0.161	0.154	0.215	0.259	0.261	0.272	0.283	0.109	0.154	0.156	0.191	0.086	0.117	0.139	0.162
ERM	0.152	0.154	0.188	0.226	0.213	0.229	**0.241**	**0.267**	0.124	0.166	0.168	0.194	0.098	0.129	0.151	0.172
SHARQ	**0.071**	**0.063**	**0.114**	**0.208**	**0.189**	**0.225**	0.279	0.297	**0.069**	**0.074**	**0.108**	**0.164**	**0.067**	**0.069**	**0.096**	**0.135**

Table 3: Performance measured by CRPS (Matheson and Winkler, 1976) on Australian Labour (755 time series), and M5 competition (42840 time series), lower values are better. Level 1 is the top aggregation level, and 4 is the bottom aggregation level.

We pre-define the hyper-parameter λ_i for vertex v_i from Eq.(1) level-wise, where we use the same λs for all time series at the same level, and gradually decrease this value at higher aggregation levels. This is because time series at the same level possess similar magnitudes. With more vertices at lower levels, the chances of having consistency issues are higher, and error can accumulate to higher levels.

We then evaluate the effect of regularization strength on forecasting coherency across the hierarchical structure; we summarize the result in Figure 4.2, where the coherency loss drops dramatically after incorporating the hierarchical regularization at each level. Note that we mainly compare SHARQ with the Base method (SHARQ without regularization), as other reconciliation approaches generate absolute coherent results at the cost of sacrificing forecasting accuracy. More detailed evaluations can be found in Appendix E.
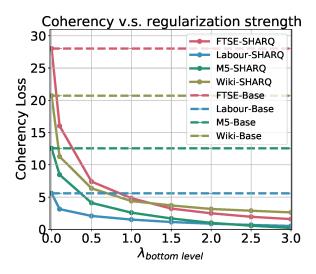
Figure 4: Coherency loss of SHARQ compared with the Base method on four datasets. Results are averaged across all the forecasting models.

4.3 Comparison with Baseline Methods

Learning inter-level relationships through regularization helps SHARQ generalize better while mitigating coherency issues. It also provides a learnable trade-off between coherency and accuracy. From a computational perspective, MinT and ERM require one to compute matrix inversion explicitly. Note that the ERM method could compute the weight matrix on a validation set, but additional matrix computations are required during inference. Crucially, they depend on the Gaussian and unbiasedness assumptions, as stated in Ben Taieb and Koo (2019); Hyndman et al. (2011); Wickramasuriya et al. (2015) and their performance degrades noticeably when faced with actual data that do not match these assumptions well.

5 Conclusion

This paper has proposed a distributed optimization framework to generate probabilistic forecasts for a set of time series subject to hierarchical constraints. In our approach, the forecasting model is trained in a bottom-up fashion. At any stage, the model training involves simultaneously updating model parameters at two adjacent levels while maintaining the coherency constraints. This enables manageable information exchange at different levels of data aggregation. Our framework can incorporate any forecasting model and the non-parametric quantile loss function to generate accurate and coherent forecasts with pre-specified confidence levels. We have analytically demonstrated

that by training the model with our modified objective function, the variance of time series data at higher aggregation levels can be reduced. We also compared our method empirically with the state-of-the-art hierarchical forecasting methods with cutting-edge base forecasters. The results show that our method produces relatively robust with accurate and coherent forecasts. Our proposed method reduces the inference complexity compared to the state-of-the-art algorithms, which perform a computationally expensive matrix inversion operation during the inference to achieve the reconciliation.

As for future work, we plan to extend our method to multi-variate time series to be forecast at different time granularities while obeying hierarchical relationships. Besides, we also plan to investigate incorporating exogenous variables and related metadata.

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Appendix

A Further Discussion on Related Works

As we mentioned in Section (1), state-of-the-art hierarchical forecasting algorithms (Ben Taieb and Koo, 2019; Hyndman et al., 2011, 2016; Wickramasuriya et al., 2015) involves computing the optimal P matrix to combine the base forecasts under different situations linearly. We now summarize these methods as follows.

A.1 Generalized Least Squares (GLS) Reconciliation

Denote $b_t \in \mathbb{R}^m$, $a_t \in \mathbb{R}^k$ as the observations at time t for the m and k series at the bottom and aggregation level(s), respectively. $S \in \{0,1\}^{n \times m}$ is the summing matrix. Each entry S_{ij} equals to 1 if the ith aggregate series contains the jth bottom-level series, where $i = 1, ..., k$ and $j = 1, ..., m$. Denote $\mathcal{I}_T = \{y_1, y_2, ..., y_T\}$ as the time series data observed up to time T; $\hat{b}_T(h)$ and $\hat{y}_T(h)$ as the $h-$step ahead forecast on the bottom-level and all levels based on $\mathcal{I}_T$.

Let $\hat{e}_T(h) = y_{T+h} - \hat{y}_T(h)$ be the $h-$step ahead conditional base forecast errors and $\beta_T(h) = E[\hat{b}_T(h) \mid \mathcal{I}_T]$ be the bottom-level mean forecasts. We then have $E[\hat{y}_T(h) \mid \mathcal{I}_T] = S\beta_T(h)$. Assume that $E[\hat{e}_T(h) \mid \mathcal{I}_T] = 0$, then a set of reconciled forecasts will be unbiased iff $SPS = S$, i.e., **Assumption A1:**

$$\mathbb{E}[\tilde{y}_T(h)|\mathcal{I}_T] = \mathbb{E}[\hat{y}_T(h)|\mathcal{I}_T] = S\beta_T(h) \qquad (11)$$

The optimal combination approach proposed by Hyndman et al. (2011), is based on solving the above regression problem using the generalized least square method:

$$\hat{y}_T(h) = S\beta_T(h) + \varepsilon_h, \qquad (12)$$

where ε_h is the independent coherency error with zero mean and $\text{Var}(\varepsilon_h) = \Sigma_h$. The GLS estimator of $\beta_T(h)$ is given by

$$\hat{\beta}_T(h) = (S'\Sigma_h'S)^{-1}S'\Sigma_h'\hat{y}_T(h), \qquad (13)$$

which is an unbiased, minimum variance estimator. The optimal P is $(S'\Sigma_h'S)^{-1}S'\Sigma_h'$. The reconciled mean and variance can therefore be obtained accordingly.

A.2 Trace Minimization (MinT) Reconciliation

Defining the reconciliation error as $\tilde{e}_T(h) = y_{T+h} - \tilde{y}_T(h)$, the original problem can also be formulated as

$$\min_{P \in \mathcal{P}} \mathbb{E}[\|\tilde{e}_T(h)\|_2^2 \mid \mathcal{I}_T]$$

$$\text{subject to } \mathbb{E}[\tilde{y}_T(h) \mid \mathcal{I}_T] = \mathbb{E}[\tilde{y}_T(h) \mid \mathcal{I}_T] \qquad (14)$$

If the assumption **A1** still holds, then minimizing Eq.(14) reduces to

$$\min_{P \in \mathcal{P}} \text{Tr}(\text{Var}[\tilde{e}_T(h) \mid \mathcal{I}_T]) \quad \text{subject to } \mathbf{A1}, \quad (15)$$

where $\text{Tr}(.)$ denotes the trace of a matrix. In Wickramasuriya et al. (2019), the proposed optimal solution of P obtained by solving this problem is given by

$$P = (S'W_h^{-1}S)^{-1}S'W_h^{-1}, \quad (16)$$

where $W_h = \mathbb{E}[\hat{e}_T(h)\hat{e}_T'(h) \mid \mathcal{I}_T]$ is the variance-covariance matrix of the $h-$step-ahead base forecast errors, which is different from the coherence errors Σ_h in GLS reconciliation method given in Eq.(13). There are various covariance estimators for W_h considered in Wickramasuriya et al. (2019), the most effective one is the shrinkage estimator with diagonal target, and can be computed by

$$\hat{W}_h = (1 - \alpha)\hat{W}_s + \alpha\hat{W}_d, \quad \hat{W}_s = \frac{1}{T}\sum_{t=1}^{T} \hat{e}_t(1)\hat{e}_t(1)', \quad (17)$$

where $\hat{W}_d = \text{diag}(\hat{W}_s)$ and $\alpha \in (0, 1]$.

A.3 Empirical Risk Minimization (ERM) Reconciliation

Most recently, Ben Taieb and Koo (2019) proposed a new method to relax the unbiasedness assumption **A1**. Specifically, the objective function in (14) can be decomposed as

$$\mathbb{E}[\|y_{T+h} - \tilde{y}_T(h)\|_2^2 \mid \mathcal{I}_T] \quad (18)$$
$$= \|SP(\mathbb{E}[\hat{y}_T(h)|\mathcal{I}_T] - \mathbb{E}[y_{T+h}|\mathcal{I}_T])$$
$$+ (S - SPS)\mathbb{E}[b_{T+h}|\mathcal{I}_T]\|_2^2 \quad (19)$$
$$+ \text{Tr}(\text{Var}[y_{T+h} - \tilde{y}_T(h)|\mathcal{I}_T], \quad (20)$$

where (19) and (20) are the bias and variance terms of the revised forecasts $\tilde{y}_T(h)$. The assumption **A1** in MinT method renders (19) to 0. Obviously, directly minimize the objective in (18) provides a more general form of reconciliation represented by following empirical risk minimization (ERM) problem:

$$\min_{P \in \mathcal{P}} \frac{1}{(T - T_1 - h + 1)n} \sum_{t=T_1}^{T-h} \|y_{t+h} - SP\hat{y}_t(h)\|_2^2, \quad (21)$$

where $T_1 < T$ is the number of observations used for model fitting. Empirically, this method demonstrates better performance than MinT according to Ben Taieb and Koo (2019), particularly when the forecasting models are mis-specified.

B Non-Additive Property of Quantile Loss

Here we prove the non-additive property of quantile loss as mentioned in Section (2.2).

THEOREM 5. *(Non-additive Property) Assume two independent random variables $X_1 \sim N(\mu_1, \sigma_1^2)$ and $X_2 \sim N(\mu_2, \sigma_2^2)$, and define $Y = X_1 + X_2$. Then $Q_Y(\tau) \neq Q_{X_1}(\tau) + Q_{X_2}(\tau)$.*

PROOF. The τth quantile of X_1 is given by:

$$Q_{X_1}(\tau) = F_{X_1}^{-1}(\tau) = inf\{x : F_{X_1}(x) \geq \tau\}, \quad (22)$$

where $F_{X_1}(x)$ is $\frac{1}{2}\left[1 + erf\left(\frac{x-\mu_1}{\sigma_1\sqrt{2}}\right)\right]$, and $erf(x) = \frac{1}{\sqrt{\pi}}\int_{-x}^{x} e^{-t^2}dt$. Therefore, we can further get:

$$Q_{X_1}(\tau) = \mu_1 + \sigma_1\Phi^{-1}(\tau) = \mu_1 + \sigma_1\sqrt{2}\ erf^{-1}(2\tau - 1)$$
$$Q_{X_2}(\tau) = \mu_2 + \sigma_2\Phi^{-1}(\tau) = \mu_2 + \sigma_2\sqrt{2}\ erf^{-1}(2\tau - 1)$$

According to the additive property of Gaussian distribution, we have $Y \sim N(\mu_1 + \mu_2, \sigma_1^2 + \sigma_2^2)$, and

$$Q_Y(\tau) = \mu_1 + \mu_2 + \sqrt{\sigma_1^2 + \sigma_2^2}\ \Phi^{-1}(\tau)$$
$$= \mu_1 + \mu_2 + \sqrt{\sigma_1^2 + \sigma_2^2}\ \sqrt{2}\ erf^{-1}(2\tau - 1). \quad (23)$$

Therefore, even if we have `i.i.d.` normal distribution with $Y = X_1 + X_2$, it still doesn't imply $Q_Y(\tau) = Q_{X_1}(\tau) + Q_{X_2}(\tau)$. The only case that the addition property hold true in any quantile is when $X_1 = C \times X_2$, where C is arbitrary constant. Obviously, this is not applicable. $\square$

In fact, under Gaussian assumption, we have the following additive property holds for any τ:

$$(Q_Y^\tau - \mu_Y)^2 = (Q_{X_1}^\tau - \mu_{X_1})^2 + (Q_{X_2}^\tau - \mu_{X_2})^2. \quad (24)$$

Since by Eq.(23), the left hand side of Eq.(24) is $2(\sigma_1^2 + \sigma_2^2)\left[erf^{-1}(2\tau - 1)\right]^2$, and the right hand side of Eq.(24) is $2\sigma_1^2\left[erf^{-1}(2\tau - 1)\right]^2 + 2\sigma_2^2\left[erf^{-1}(2\tau - 1)\right]^2$. Therefore, the additive property holds for any τ assume the RVs follow Gaussian distribution.

Table 4: Details of four hierarchical time-series datasets. Note that hierarchical levels mean the number of aggregation levels from bottom to top in the hierarchical structure used in the experiments.

Dataset	Total number of time series	Total length of time series	Hierarchical Levels
FTSE	73	2512	4
M5	42840	1969	4
Wiki	145000	550	5
Labour	755	500	4

(a) FTSE   (b) M5   (c) Labour   (d) Wikipedia
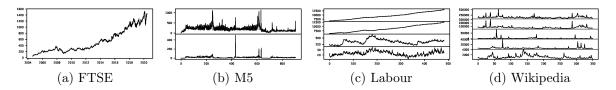
Figure 5: Visualization of hierarchical time series data. (a) Bottom level time series of FTSE (the open stock price of Google); (b) bottom and top level of unit sales record; (c) Australian Labour Force data at all aggregation levels; (d) Wikipedia page views data at all aggregation levels.

C KKT Conditions

An alternative way of solving the optimization problem defined in Section (2.1) Eq.(1) is to obtain the KKT conditions (Boyd and Vandenberghe, 2004). For notational simplicity, we express the constrained loss for i^{th} vertex and m^{th} data point as $L_c(i, m)$. As the optimization problem is unconstrained, the KKT conditions will lead to:

$$\frac{\partial}{\partial[\theta_i, \Theta_i]} L_c(i, m) = [\ \frac{\partial}{\partial \theta_i} L_c(i, m)\ ,\ \frac{\partial}{\partial \Theta_i} L_c(i, m)\ ] = 0,$$

which will further imply that

$$\lambda_i \left[\frac{\partial}{\partial g_i} L(g_i(X_m^i, \theta_i),\ Y_m^i) \right]^{\top}$$

$$\left[g_i(X_m^i, \theta_i) - \sum_{e_{i,k} \in E} e_{i,k} \cdot g_k(X_m^k, \theta_k) \right]$$

$$+ \frac{\partial}{\partial g_i} L(g_i(X_m^i, \theta_i),\ Y_m^i) \cdot \frac{\partial g_i}{\partial \theta_i} = 0,$$

and

$$\left(e_{i,j} \cdot g_j(X_m^j, \theta_j)\right)^T$$

$$\left(g_i(X_m^i, \theta_i) - \sum_{e_{i,k} \in E} e_{i,k} g_k(X_m^k, \theta_k) \right) = 0,\ \forall j | e_{i,j} \in E.$$

However, we found that SHARQ performs better and more efficiently than the KKT approach during our empirical evaluation. Solving the KKT conditions requires matrix inversion in most situations. Besides, SHARQ is more flexible in incorporating various forecasting models and performs probabilistic forecasts.

D Dataset Details

We first describe the details (dataset generation, processing, etc.) of each dataset used in the experiment. A summary of each dataset is shown in Table 4. Visualizations for some raw time series can be found in Figure 5.

D.1 FTSE Stock Market Data

The FTSE Global Classification System is a universally accepted classification scheme based on a market's division into Economic Groups, Industrial Sectors, and Industrial Sub-sectors. This system has been used to classify company data for over 30,000 companies from 59 countries. The FTSE 100 (Doherty et al., 2005) is the top 100 capitalized blue-chip companies in the UK and is recognized as the measure of UK stock market performance (Russell, 2017). Base on the FTSE classification system, we formulate a 4-level hierarchical structure (Economic Groups, Industrial Sectors, Industrial Sub-sectors, and companies) of 73 companies in Doherty et al. (2005). Our task is to model the stock market time series for each company. The stock market data of each company is available from the Yahoo Finance package[1]. Since the stock market time series starting time of each company is not the same, we use a common time window ranging from January 4, 2010, to May 1, 2020.
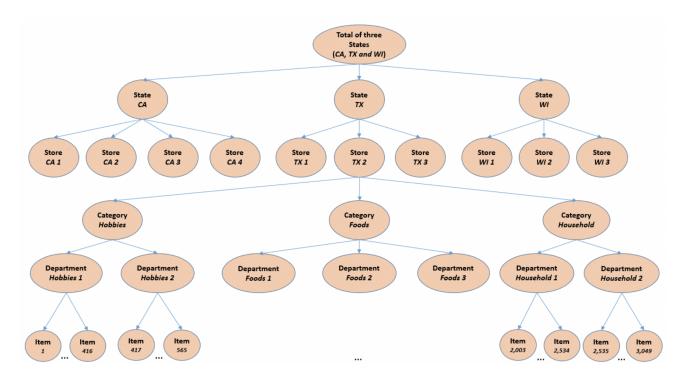
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[1]https://pypi.org/project/yfinance/

Figure 6: Hierarchical structure of the M5 dataset.

D.2 M5 Competition Data

The M5 dataset[2] involves the unit sales of various products ranging from January 2011 to June 2016 in Walmart. It involves the unit sales of 3,049 products, classified into 3 product categories (Hobbies, Foods, and Household) and 7 product departments, where the categories mentioned above are disaggregated. The products are sold across ten stores in three states (CA, TX, and WI). An overview of how the M5 series are organized is shown in Figure 6. Here, we formulate a 4-level hierarchy, starting from the bottom-level individual item to unit sales of all products aggregated for each store.

D.3 Wikipedia Webpage Views

This dataset[3] contains the number of daily views of 145k various Wikipedia articles ranging from July 2015 to Dec. 2016. We follow the data processing approach used in Ben Taieb and Koo (2019) to sample 150 bottom-level series from the 145k series and aggregate to obtain the upper-level series. The aggregation features include the type of agent, type of access, and

country codes. We then obtain a 5-level hierarchical structure with 150 bottom series.

D.4 Australian Labour Force

This dataset[4] contains monthly employment information ranging from Feb. 1978 to Aug. 2019 with 500 records for each series. The original dataset provides a detailed hierarchical classification of labor force data, while we choose three aggregation features to formulate a 4-level symmetric structure. Specifically, the 32 bottom level series are hierarchically aggregated using labor force location, gender, and employment status.

E Additional Experiments

In this section, we demonstrate our additional experiment results, including the full results on FTSE and Wiki as well as additional simulation experiments under unbiasedness and Gaussian assumptions. Reconciliation error is also measured for each method. We start by discussing our evaluation metrics.

E.1 Evaluation Metrics

We denote $\hat{Y}_T(h)$ and $Y_T(h)$ as the $h-$step ahead forecast at time T and its ground truth, respectively. To

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Table 5: MAPE$^\downarrow$ for small and large simulation dataset. The likelihood ratios are given in parentheses.

MAPE	Simulation Small			Simulation Large			
	Top level	Level 1	Level 2	Top level	Level 1	Level 2	Level 3
Base	1.29 (.69)	1.50 (.77)	2.41 (.91)	2.08 (.43)	2.20 (.61)	1.41 (.75)	0.72 (.85)
BU	2.14 (.73)	1.76 (.79)	2.41 (.91)	4.19 (.46)	3.48 (.64)	1.48 (.76)	0.72 (.85)
MinT-sam	0.54 (.66)	1.48 (.77)	2.24 (.89)	1.48 (.42)	2.55 (.65)	1.38 (.74)	0.63 (.83)
MinT-shr	0.45 (.65)	1.47 (.77)	**2.23** (.89)	**1.28** (.39)	2.31 (.63)	**1.35** (.74)	**0.59** (.81)
MinT-ols	**0.20** (.64)	1.72 (.78)	2.41 (.91)	1.69 (.41)	2.15 (.60)	1.41 (.75)	0.71 (.85)
ERM	1.23 (.69)	1.73 (.78)	2.55 (.93)	2.78 (.44)	2.86 (.69)	1.50 (.76)	0.75 (.86)
SHARQ	1.54 (.41)	**1.42** (.45)	2.41 (.73)	2.16 (.23)	**2.13** (.49)	1.44 (.67)	0.72 (.82)

Table 6: MAPE$^\downarrow$ on FTSE dataset. Level 1 is the top aggregation level; 4 is the bottom aggregation level.

Algorithm	RNN				Autoregressive				LST-Skip				N-Beats			
Reconciliation	Level				Level				Level				Level			
	1	2	3	4	1	2	3	4	1	2	3	4	1	2	3	4
BU	6.11	8.48	9.41	9.54	10.01	12.15	11.77	12.43	7.48	8.96	9.29	9.49	6.63	8.04	8.23	8.41
Base	4.82	6.27	8.55	9.54	**8.65**	10.46	10.88	12.43	6.02	7.79	8.76	9.49	5.86	**7.56**	**8.01**	8.41
MinT-sam	4.68	8.53	8.77	10.13	9.72	11.25	11.57	12.26	6.47	8.24	8.93	10.62	5.94	7.89	8.35	8.86
MinT-shr	**4.43**	8.46	8.59	9.75	9.23	10.91	11.02	**12.13**	6.12	8.11	8.81	10.57	5.67	7.74	8.22	**8.54**
MinT-ols	4.71	8.92	8.74	10.31	9.96	11.01	11.25	12.32	6.31	8.56	8.74	10.88	5.87	8.12	8.41	9.84
ERM	5.74	9.52	9.54	12.41	9.92	10.61	12.03	13.23	8.12	9.38	9.76	13.01	6.19	8.89	9.26	10.22
SHARQ	4.51	**8.28**	**8.08**	**9.54**	9.13	**9.35**	**10.61**	12.43	**5.01**	**7.14**	**8.52**	**9.49**	**5.44**	7.83	7.93	8.41

Table 7: MAPE$^\downarrow$ on Wiki dataset. Level 1 is the top aggregation level; 5 is the bottom aggregation level.

Algorithm	RNN					Autoregressive					LST-Skip					N-Beats				
Reconciliation	Level					Level					Level					Level				
	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5	1	2	3	4	5
BU	11.71	12.36	14.47	16.45	16.74	15.67	15.99	16.67	18.99	20.32	11.44	11.88	13.31	14.76	15.77	11.92	12.57	14.45	15.22	16.21
Base	11.12	11.52	14.06	16.11	16.74	**15.04**	15.23	16.02	17.83	20.32	11.21	11.24	12.88	14.35	15.77	11.84	12.02	14.17	15.16	16.21
MinT-sam	11.65	12.02	14.19	16.23	17.66	15.22	15.65	16.33	18.12	19.87	11.38	11.46	13.13	14.57	16.22	11.96	12.26	14.29	15.25	16.45
MinT-shr	11.32	11.86	13.87	**16.07**	17.54	15.17	15.12	15.98	17.69	**19.54**	11.24	11.15	12.91	**14.32**	16.14	11.75	12.19	14.03	15.02	16.39
MinT-ols	11.48	12.11	14.52	16.34	17.59	15.37	15.74	16.23	18.01	20.21	11.42	11.52	13.05	14.78	16.59	11.88	12.39	14.21	15.16	16.45
ERM	12.08	13.62	15.96	18.11	18.97	15.29	15.85	16.12	**17.58**	21.56	12.08	12.85	14.56	15.96	17.42	12.14	12.83	15.49	16.17	17.41
SHARQ	**10.84**	**11.07**	**13.54**	16.08	**16.74**	15.07	**15.05**	**15.87**	17.79	20.32	**11.07**	**11.09**	**12.65**	14.41	**15.77**	**11.64**	**11.67**	**13.81**	**15.02**	**16.21**

construct confidence intervals, we use the $95^{th}, 50^{th}$, and 5th quantiles as upper, median and lower forecasts.

E.1.1 Mean Absolute Percentage Error (MAPE)

The MAPE is commonly used to evaluate forecasting performance. It is defined by

$$\text{MAPE} = \frac{100}{H} \sum_{h=1}^{H} \frac{|Y_T(h) - \hat{Y}_T(h)|}{|Y_T(h)|}. \qquad (25)$$

E.1.2 Likelihood Ratio

We compute the likelihood ratio between the quantile prediction intervals versus the trivial predictors, which gives the specified quantile of training samples as forecasts. Specifically, define N ($N = 3$ in our case) as the number of quantile predictors. Then the likelihood

ratio at $h-$step forecast is:

$$\alpha = \frac{\sum_{i=1}^{N} \rho_{\tau_i}(Y_T(h) - Q_{Y_T(h)}(\tau_i))}{\sum_{i=1}^{N} \rho_{\tau_i}(Y_T(h) - Q_{\mathcal{I}_T}(\tau_i))}. \qquad (26)$$

Ideally, we should have $\alpha < 1$ if our estimator performs better than the trivial estimator.

E.1.3 Continuous Ranked Probability Score (CRPS)

CRPS measures the compatibility of a cumulative distribution function F with an observation x as:

$$\text{CRPS}(F, x) = \int_{\mathbb{R}} (F(z) - \mathbb{I}\{x \leq z\})^2 \, dz \qquad (27)$$

where $\mathbb{I}\{x \leq z\}$ is the indicator function which is one if $x \leq z$ and zero otherwise. Therefore, CRPS attains its minimum when the predictive distribution F and

Table 8: Average forecasting coherency on each dataset across 4 forecasting models. Bottom-level $\lambda = 3.0$, higher-level λs are decreased gradually.

Reconciliation	Dataset			
	FTSE	Labour	M5	Wiki
Base	28.01	5.59	12.56	20.71
BU	0	0	0	0
MINTsam	4.21E-15	4.60E-12	0	5.46E-10
MINTshr	2.50E-15	4.19E-12	0	6.40E-11
MINTols	6.22E-15	6.10E-12	0	1.08E-10
ERM	6.48E-12	2.27E-08	5.86E-12	2.40E-07
SHARQ	1.59	0.53	0.22	2.63

Table 9: Training and inference time (in second) comparison for each data set.

Time (s)	FTSE		Labour		M5		Wikipedia	
	training	inference	training	inference	training	inference	training	inference
Base	115.96	0.01	68.35	0.00	181.58	0.00	205.47	0.01
BU	65.83	0.03	57.06	0.00	105.45	0.00	142.53	0.01
MinT-sam	106.55	1,784.77	72.24	430.42	172.11	1,461.81	208.26	1,106.70
MinT-shr	104.35	1,148.49	60.83	317.02	175.83	1,039.53	198.16	788.31
MinT-ols	103.23	1,129.45	64.14	310.13	163.24	977.88	196.88	702.02
ERM	547.66	0.05	497.88	0.01	551.60	0.01	1,299.30	0.04
SHARQ	121.84	0.01	99.96	0.00	201.40	0.00	241.97	0.01

the data are equal. We used this library[5] to compute CRPS.

E.1.4 Reconciliation Error

We compute the reconciliation error of forecasts generated by each method on each dataset to measure the forecasting coherency. More specifically, assume a total of m vertices in the hierarchy at time T, the reconciliation error for the mean forecast is defined as

$$\frac{1}{H} \sum_{h=1}^{H} \sum_{i=1}^{m} \|\hat{Y}_T^i(h) - \sum_{e_{i,k} \in E} \hat{Y}_T^k(h)\|_1. \qquad (28)$$

E.2 Simulation under Unbiased Assumption

We follow the data simulation mechanism developed in Wickramasuriya et al. (2019); Ben Taieb and Koo (2019), which satisfies the ideal unbiased base forecast and Gaussian error assumptions. The bottom level series were first generated through an ARIMA(p, d, q) process, where the coefficients are uniformly sampled from a predefined parameter space. The contemporaneous error covariance matrix is designed to introduce a positive error correlation among sibling series, while moderately positive correlation among others. We simulate a small and a large hierarchy with 4 and 160 bottom series, respectively. The bottom series are then aggregated to obtain the whole hierarchical time series in groups of two and four. For each series in the

hierarchy, we generate 500 observations, and the final $h = 8, 16$ observations are used for evaluation for both the large and small hierarchies. We run the above simulation 100 times and report the average results. Table 5 shows the average MAPE by fitting an ARIMA model followed by reconciliation on two simulation datasets. We can see that the MinT methods generally perform the best, particularly for MinT methods with shrinkage estimators. This confirms the statements from Ben Taieb and Koo (2019); Hyndman et al. (2011) that under ideal unbiasedness assumption if the forecasting models are well specified, the MinT methods will provide the optimal solution. Simultaneously, the results of SHARQ are also satisfactory. In fact, it outperforms MinT methods at some levels.

E.3 Additional Results

Table 6 and 7 show the MAPE results of FTSE and Wiki dataset. Moreover, table 11 is the average likelihood ratio of each reconciliation method across four algorithms. The reported results are average across three random runs. We can see that SHARQ performs better overall in providing accurate probabilistic forecasts. Table 9 compares the average training and inference time across all forecasting models. Overall, the training time of SHARQ and base forecast are roughly the same, but the inference time of SHARQ is ignorable relative to MinT, and ERM approaches. Since both these methods require matrix inversion to compute the weight matrix. Even if ERM could calculate the weight

[5]https://github.com/TheClimateCorporation/properscoring

Table 10: Common Hyper-parameters for all experiments.

	Train/Valid/Test	Epoch	Learning Rate	Batch Size	Window Size	Horizon
Quantile Simulation	0.6/0.2/0.2	300	1.00E-03	64	128	1
Unbiased Simulation	0.6/0.2/0.2	100	1.00E-03	128	10	1-8
Real-world Data	0.6/0.2/0.2	1000	0.1	128	168	1-8

Table 11: Average likelihood ratio across forecasting horizons and models.

Likelihood Ratio	Labour	M5	FTSE	Wiki
BU	0.36	0.48	0.50	0.66
Base	0.36	0.48	0.51	0.66
MinT-sam	0.36	0.47	0.50	0.66
MinT-shr	0.35	0.49	0.51	0.68
MinT-ols	0.34	0.48	0.51	0.66
ERM	0.35	0.48	0.51	0.67
SHARQ	**0.07**	**0.25**	**0.32**	**0.65**

matrix on a separate validation set before inference, additional matrix computations are required to obtain the results.

E.4 Forecasting Coherency

Table 8 compares the forecasting coherency of each reconciliation method. We use the metric defined in (28) to compute the forecasting reconciliation error generated by previous experiments. As expected, the MinT and ERM approach give almost perfect coherent forecasts, as these methods can directly compute the close form of weight matrix P to optimally combine the original forecasts. Even though MinT and ERM can give perfectly coherent forecasts, the accuracy can sometimes be worse than the base method, which coincides with Proposition 2 (Hard Constraint). Although SHARQ could not give the most coherent results, there is still a significant improvement compared to incoherent base forecasts. Note that this can be further improved by increasing the penalty of the regularization term.

F Hyper-parameter Configurations

We present hyper-parameters for all the experiments mentioned above. Table 10 lists the common hyper-parameters used on each experiment. Model-specific hyper-parameters are as follows.

Quantile Simulation Experiment We simulate 500 samples for both step function and sinusoidal func-

tion; the data is trained on a vanilla RNN model with hidden dimension 5, layer dimension 2, and *tanh* nonlinearity. We used 10 ensembles of estimators for bagging, and each model is trained using random 64 samples.

LSTNet The number of CNN hidden units: 100; the number of RNN hidden units: 100; kernel size of the CNN layers: 6; window size of the highway component: 24; gradient clipping: 10; dropout: 0.2; skip connection: 24. Note that to enable LSTNet to produce multi-quantile forecast, we add the final layer of each quantile estimator after the fully connected layer of the original model. The same linear bypass then adds the obtained quantile estimators to produce the final results.

N-Beats We use the same parameter settings as shown in the public GitHub repository[6].

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[6]https://github.com/philipperemy/n-beats