NIXTLA

Time Series Research and Deployment

Hierarchical Forecasting in Python

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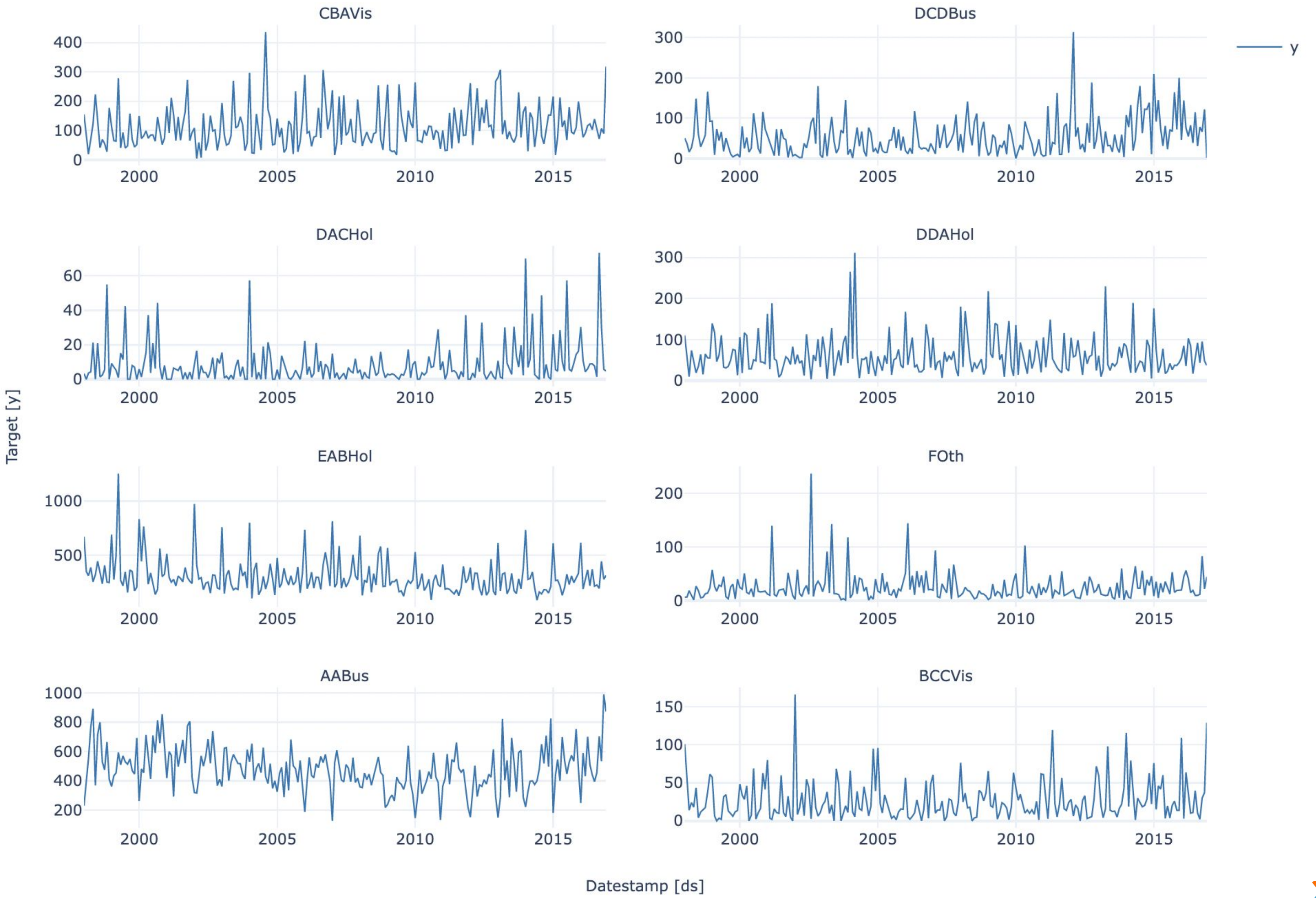
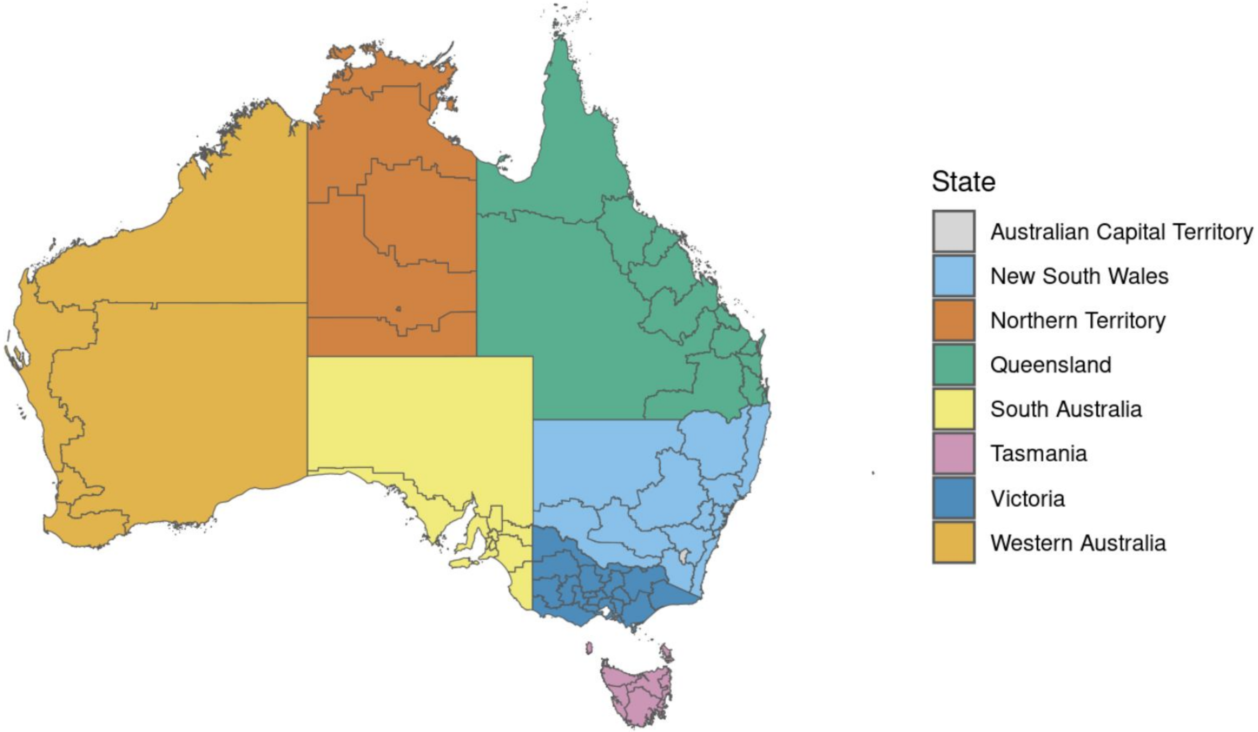
Setting: you are the minister of tourism in Australia

Question: how many tourists are going to visit Australia?


CBAVis
DCDBus
DACHol
DDAHol
EABHol
FOth
AABus
BCCVis
y
Target [y]
Datestamp [ds]

- How should we staff the airports?
- How will the economy grow?

Australia's has: 7 states, 27 zones and 76 regions.



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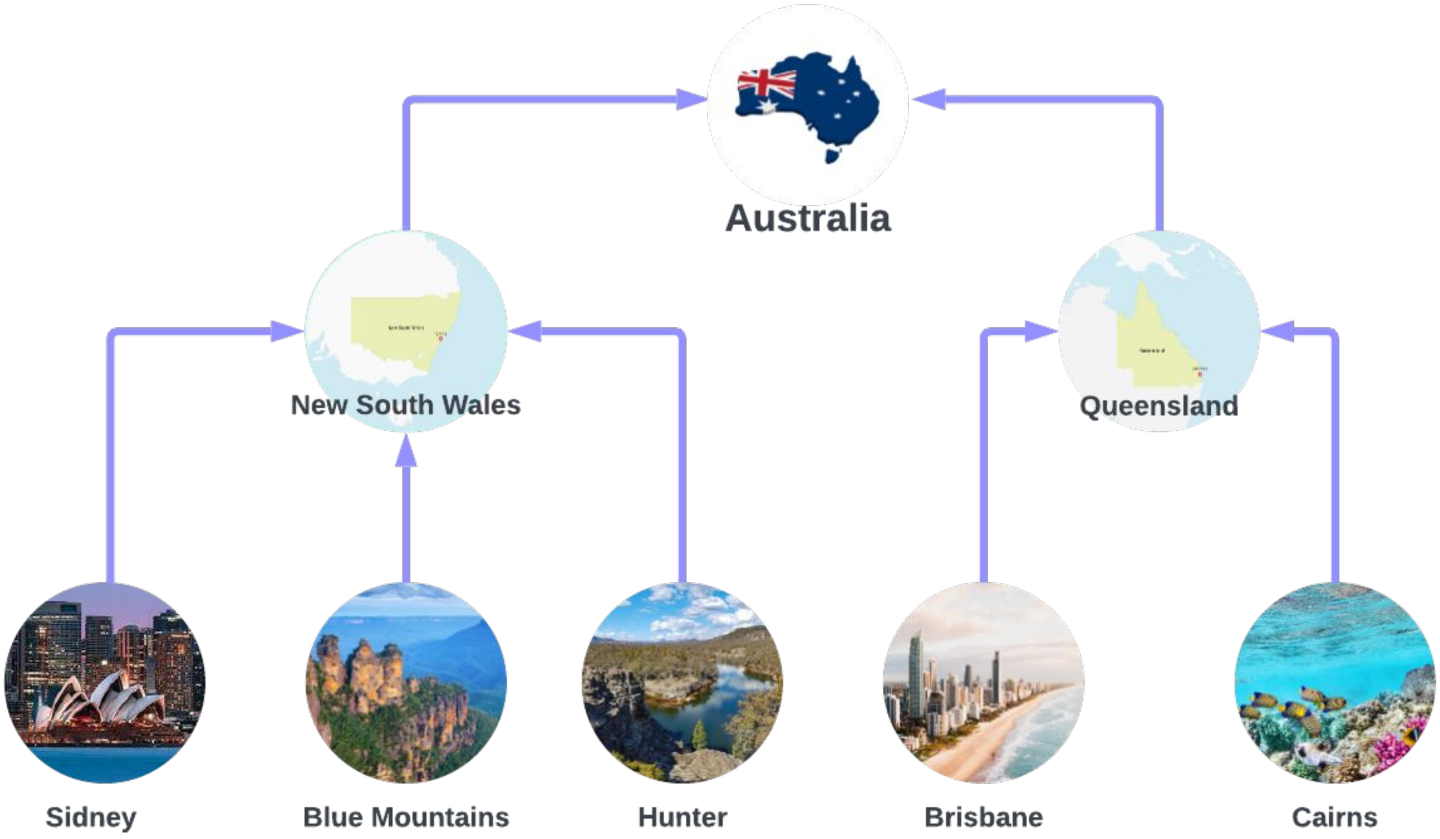
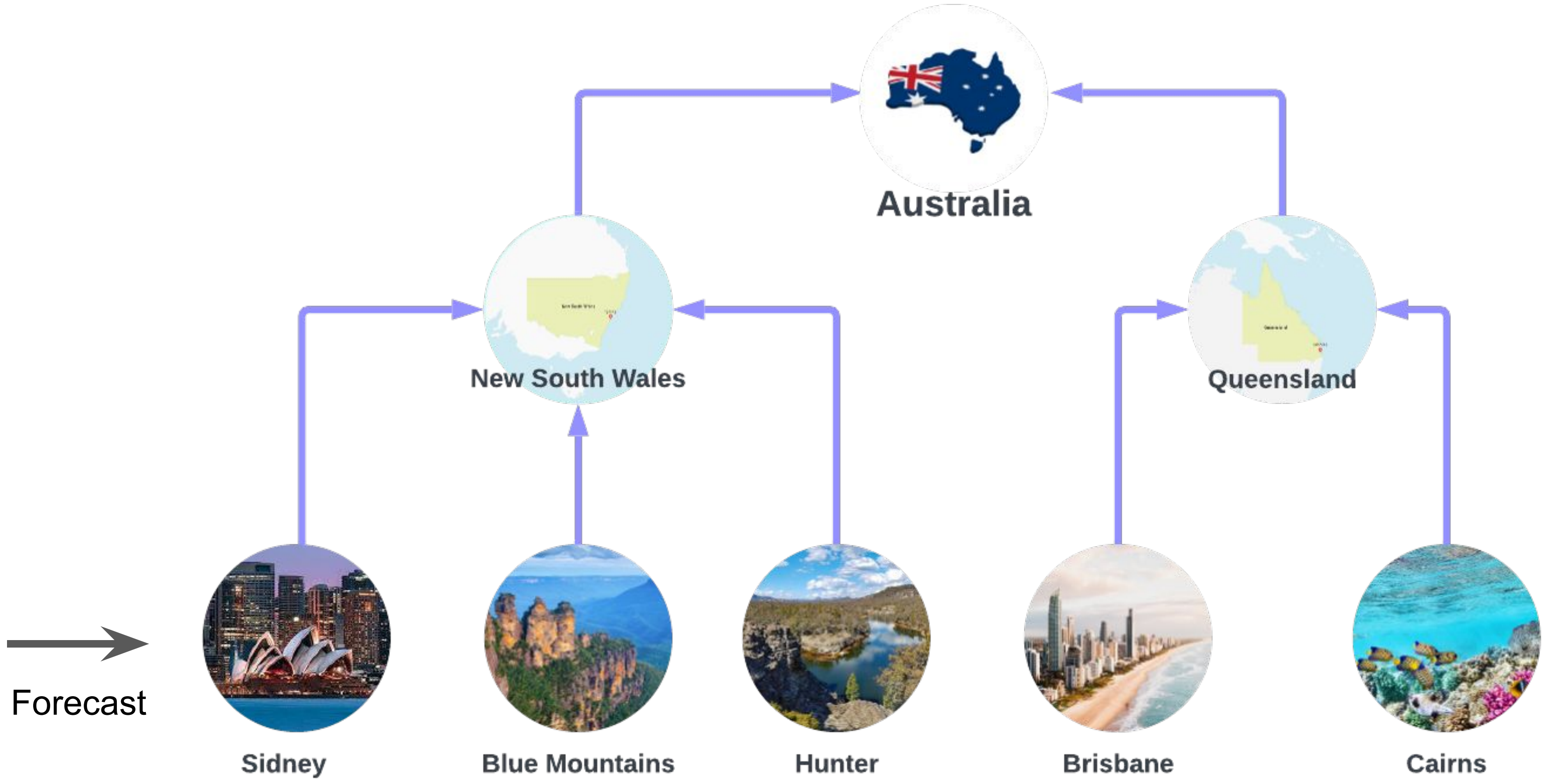
We need forecasts for the whole of Australia, for each of the states, territories, and regions.

Table A2: Australian Tourism flows.

Geographical Level	**Series per Level**	**Series per Level & Purpose**	**Total**
Australia	1	4	5
States	7	28	35
Zones	27	108	135
Regions	76	304	380
Total	111	444	555

Approach 1: Bottom UP


Australia
New South Wales
Queensland
Sidney
Blue Mountains
Hunter
Brisbane
Cairns



Australia
New South Wales
Queensland
Forecast
Sidney
Blue Mountains
Hunter
Brisbane
Cairns

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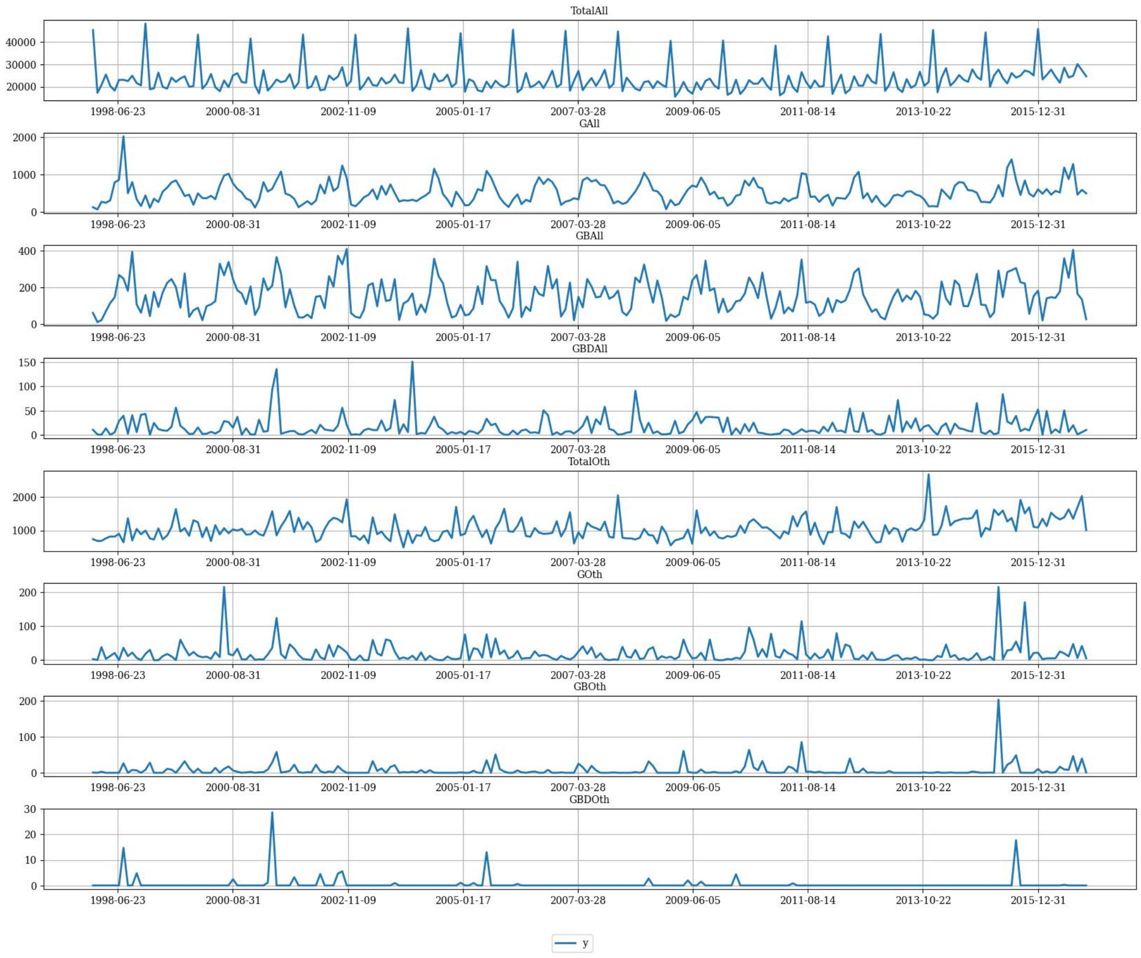

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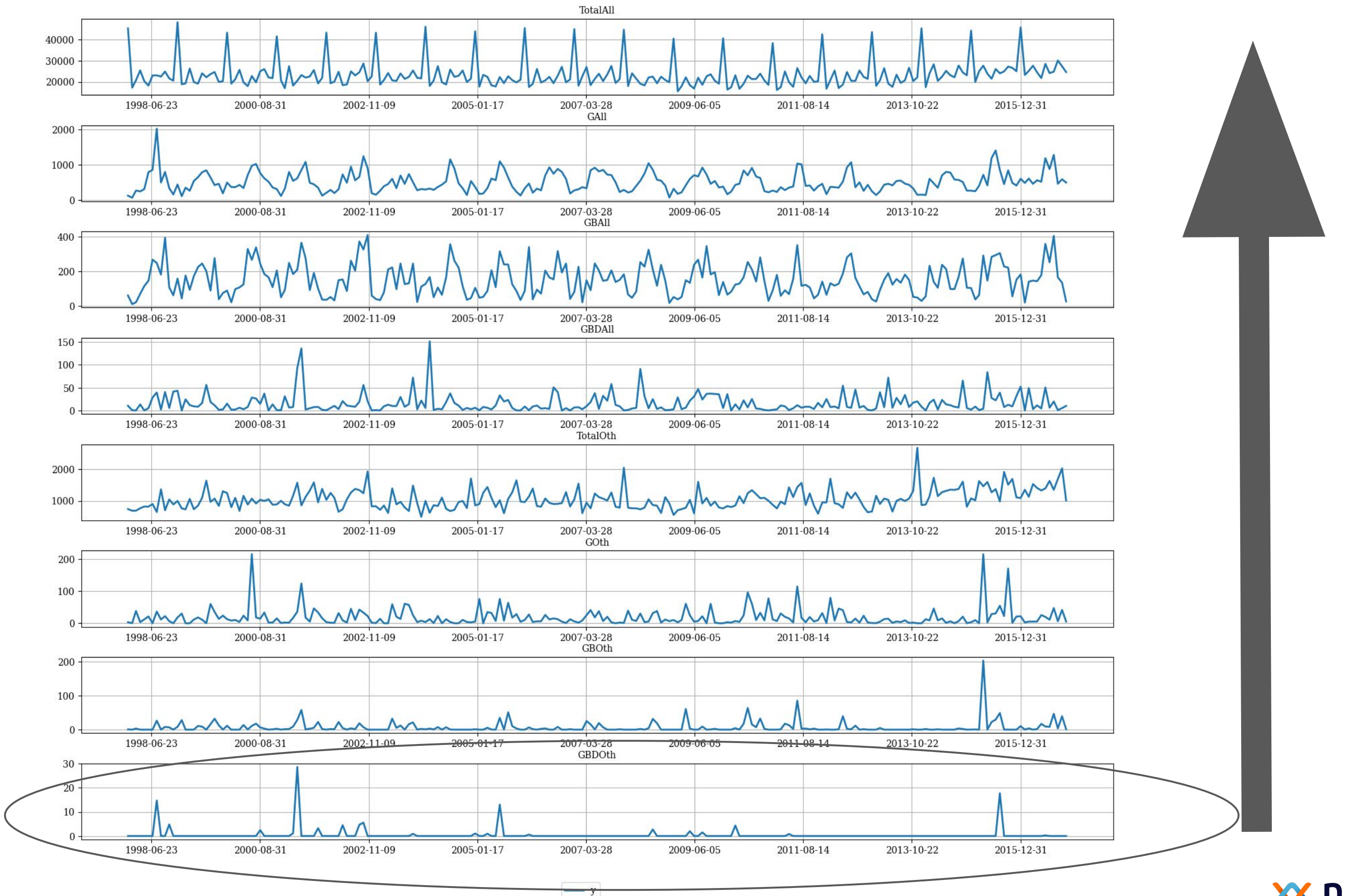
y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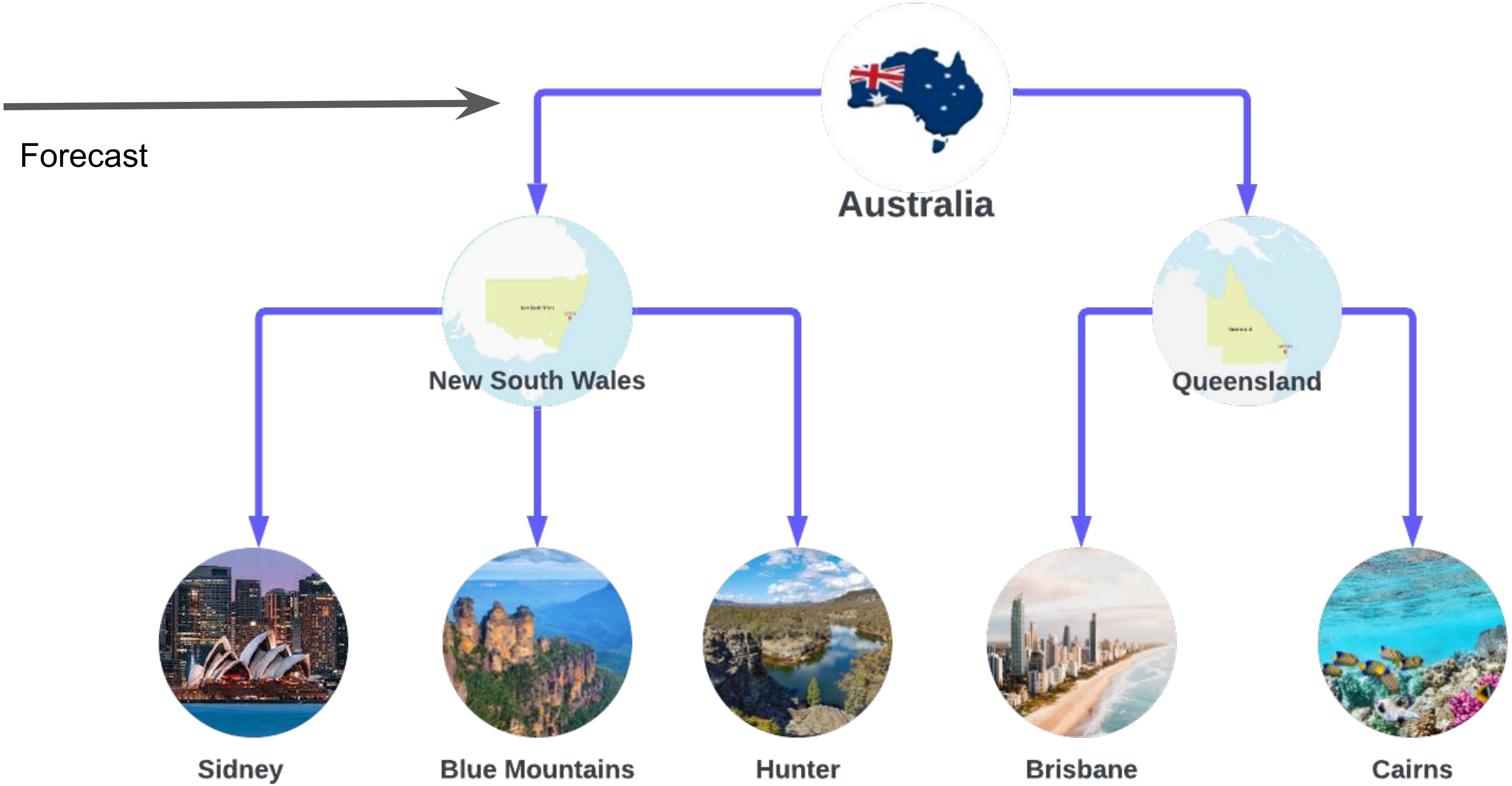
2013-10-22
2015-12-31
y

Approach 2: Top Down


Forecast
Australia
New South Wales
Queensland
Sidney
Blue Mountains
Hunter
Brisbane
Cairns

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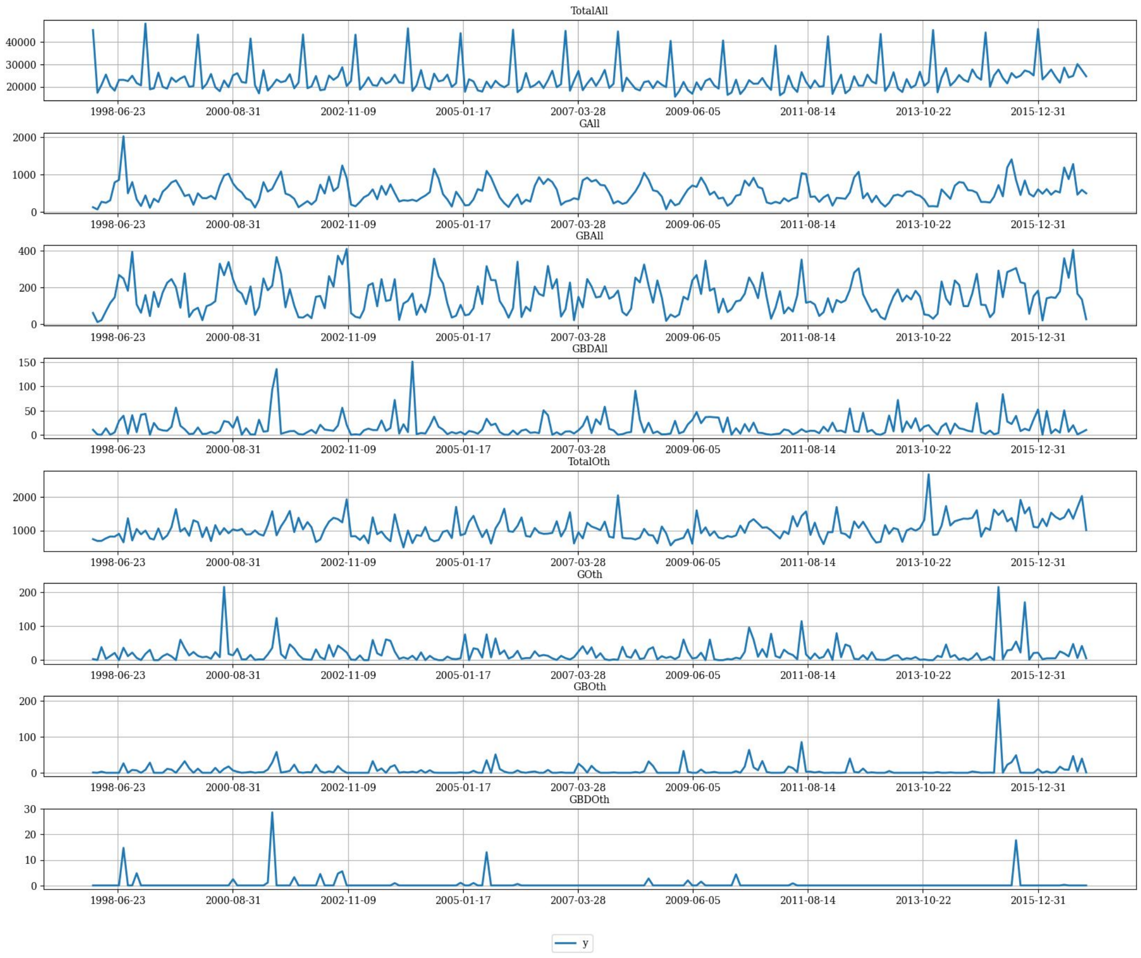

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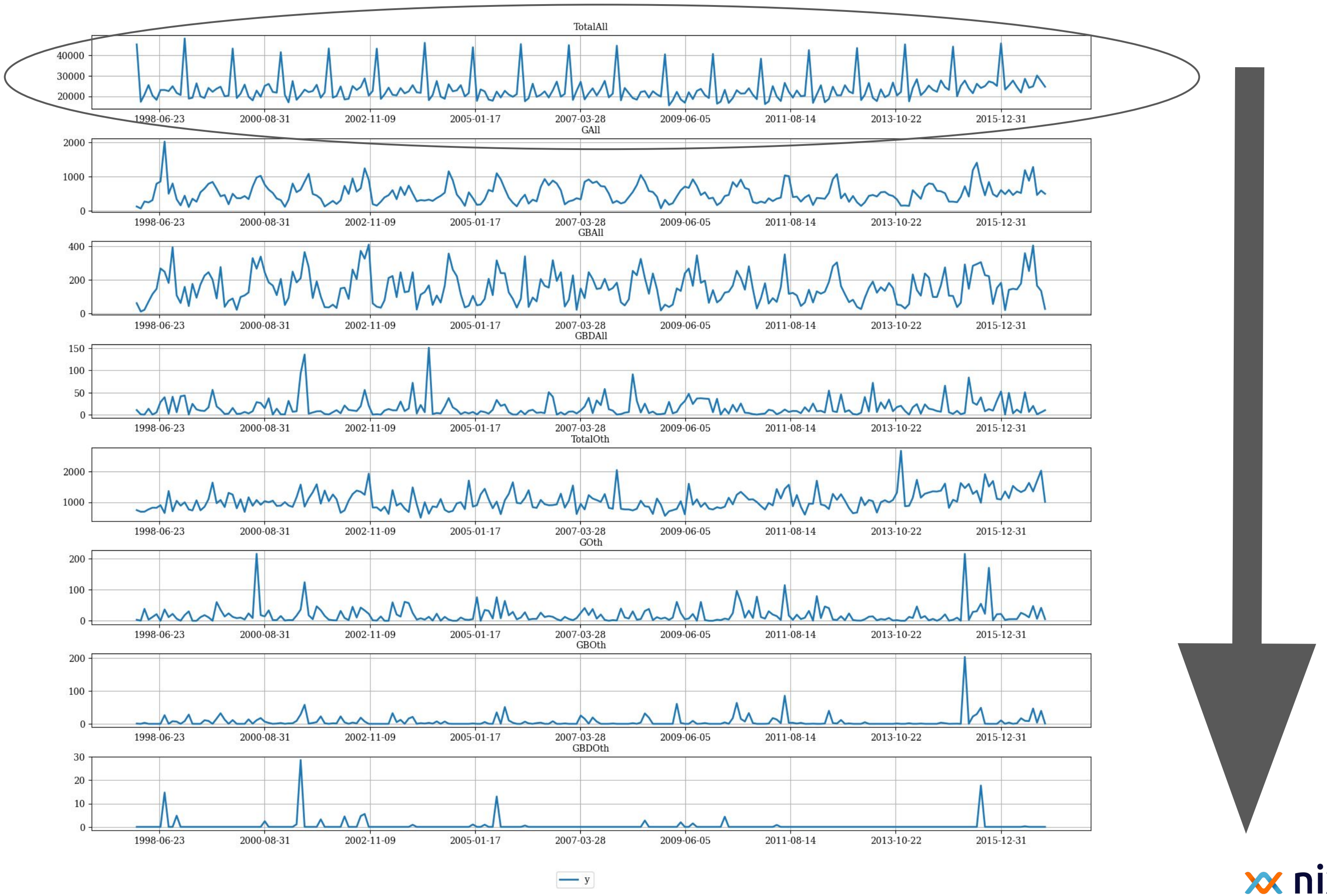
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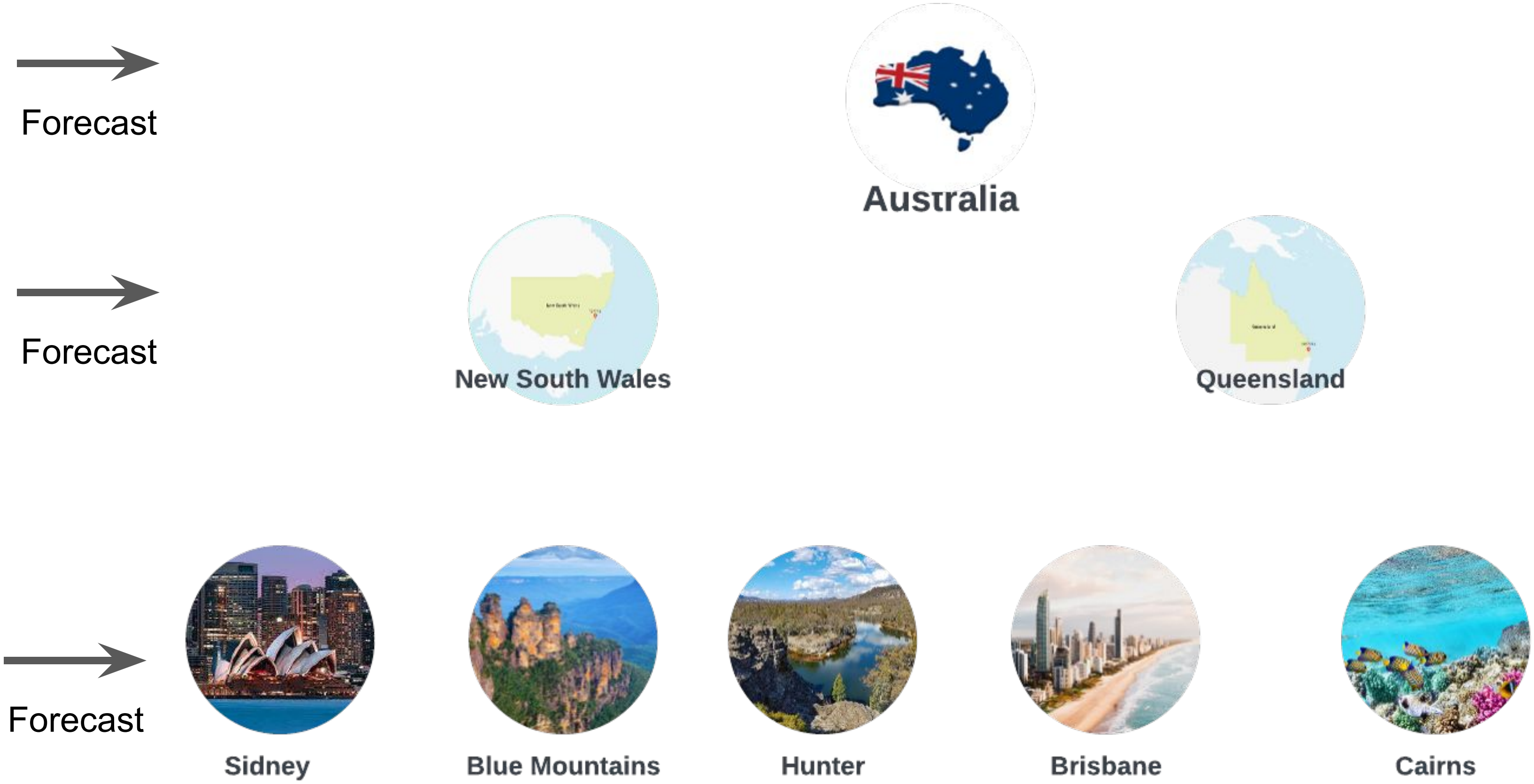
y

Approach 3: forecast all series!


Forecast
Australia
Forecast
New South Wales
Queensland
Forecast
Sidney
Blue Mountains
Hunter
Brisbane
Cairns

How to forecast hundreds or millions of series?

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Open Source Time Series Ecosystem

Stars 5k

⚡ StatsForecast

Lightning fast forecasting with statistical and econometric models.

Github

🤖 MLForecast

Scalable machine learning for time series forecasting.

Github

🧠 NeuralForecast

Scalable and user friendly neural forecasting algorithms for time series data.

Github

```
pip install mlforecast
```

```python
import lightgbm as lgb
from mlforecast import MLForecast
from window_ops.expanding import expanding_mean
from window_ops.rolling import rolling_mean

# Create an instance of MLForecast with specified models, frequency, differences, lags, and lag_transforms
mlf = MLForecast(
    models=[lgb.LGBMRegressor()],   # List of models to use, in this case, a LightGBM Regressor
    freq='MS',                      # Frequency of the time series data (monthly start)
    differences=[12],               # List of differences to apply, in this case, a seasonal difference of 12 periods
    lags=[1, 12],                   # List of lags to use as features, in this case, lags of 1 and 12 periods
    lag_transforms={                # Dictionary of lag transformations to apply on the selected lags
        1: [expanding_mean],        # Apply expanding mean transformation on the 1-period lag
        12: [(rolling_mean, 24)],   # Apply rolling mean transformation with a window size of 24 on the 12-period lag
    },
)
```

```python
# Fit the MLForecast model to the tourism dataset
mlf.fit(
    tourism_df,                          # Input dataset (Tourism)
    id_col='unique_id',                  # Column containing unique time series identifiers
    time_col='ds',                       # Column containing timestamps
    target_col='y'                       # Column containing the target variable to forecast
)

# Generate forecasts using the MLForecast model for 12 steps ahead
base_forecasts_df = mlf.predict(12)
```


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1997-05-19
2000-02-13
2002-11-09
2005-08-05
2008-05-01
2011-01-26
2013-10-22
2016-07-18
y
LGBMRegressor

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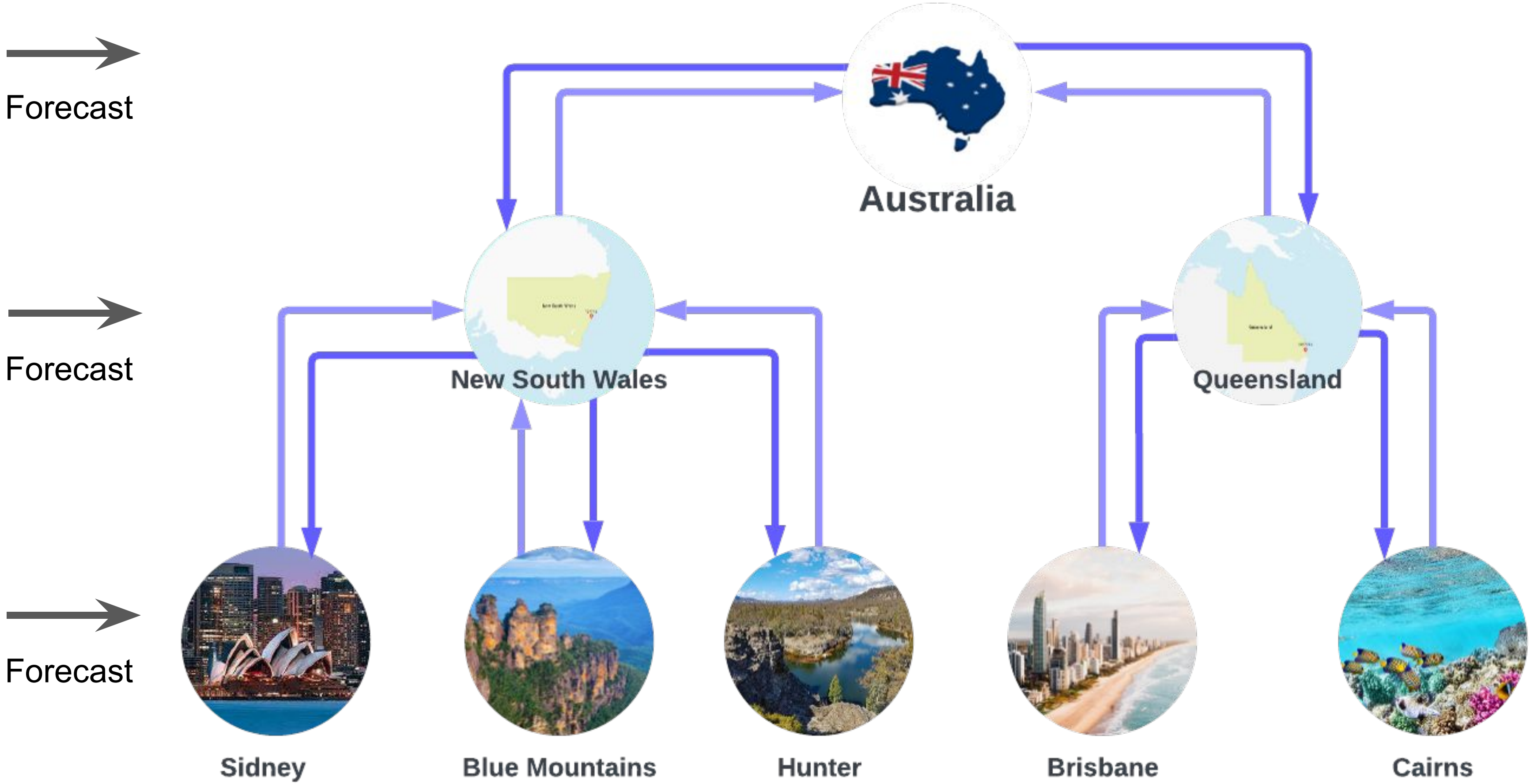
Why is the national forecast different from the sum of all the states!?

Problem: the forecast at different levels don’t add up.

What is the optimal solution?


Forecast
Forecast
Forecast
Australia
New South Wales
Queensland
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Brisbane
Cairns

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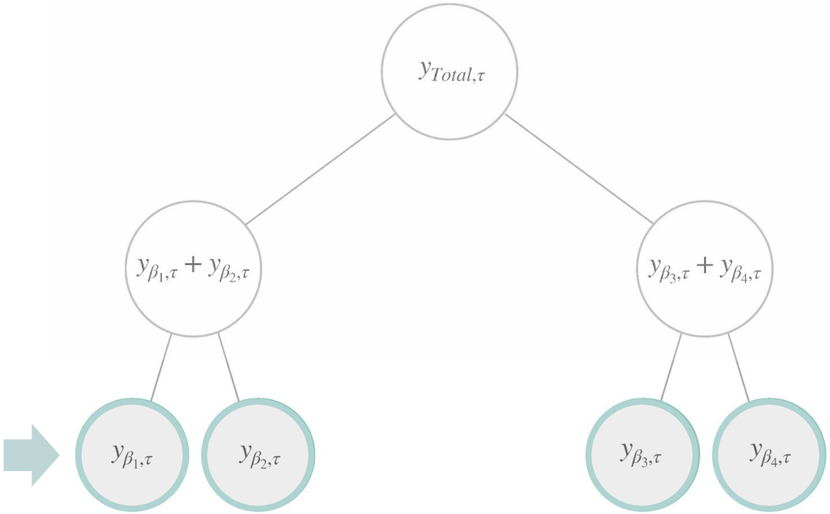
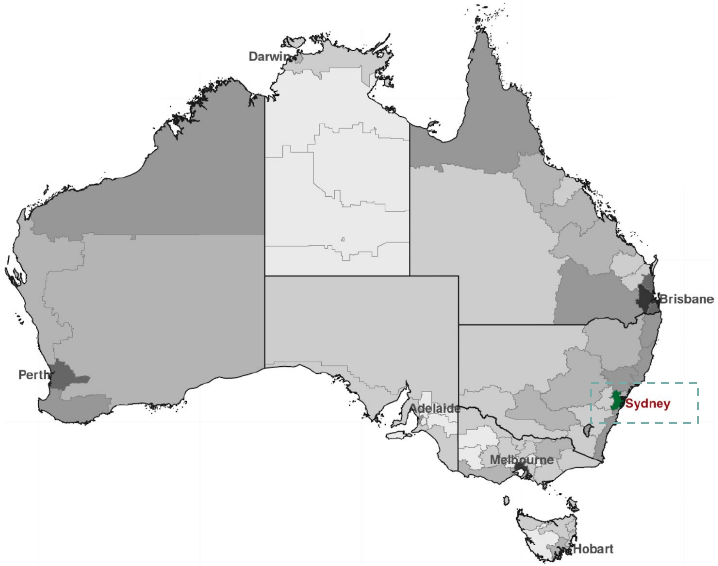
Hierarchical Reconciliation



$y_{Total,\tau}$
$y_{\beta_1,\tau} + y_{\beta_2,\tau}$
$y_{\beta_3,\tau} + y_{\beta_4,\tau}$
$y_{\beta_1,\tau}$
$y_{\beta_2,\tau}$
$y_{\beta_3,\tau}$
$y_{\beta_4,\tau}$



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Sydney
Adelaide
Melbourne
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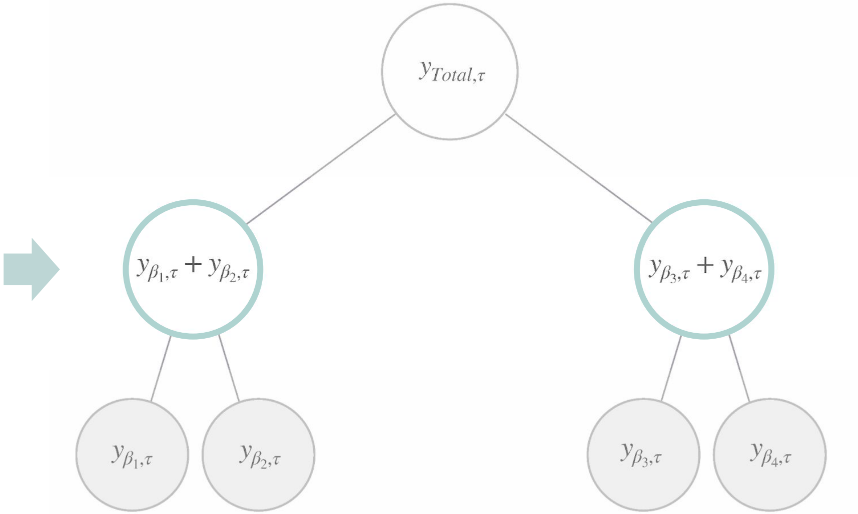
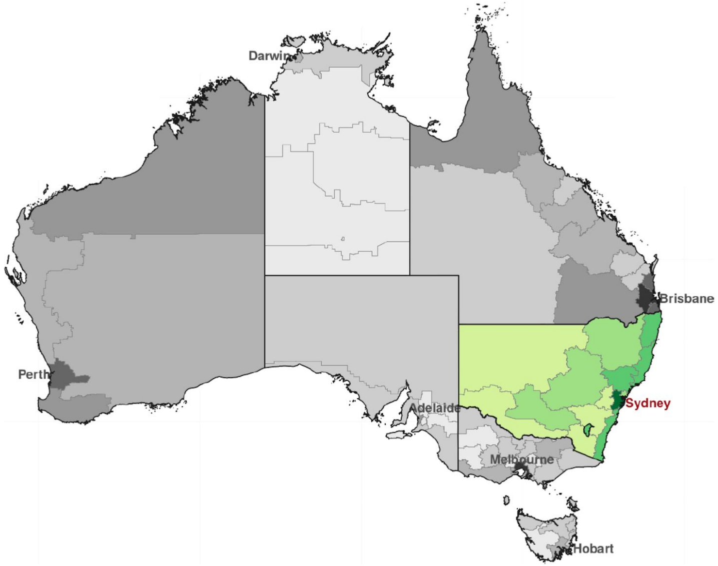

$y_{Total,\tau}$
$y_{\beta_1,\tau} + y_{\beta_2,\tau}$
$y_{\beta_3,\tau} + y_{\beta_4,\tau}$
$y_{\beta_1,\tau}$
$y_{\beta_2,\tau}$
$y_{\beta_3,\tau}$
$y_{\beta_4,\tau}$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Melbourne
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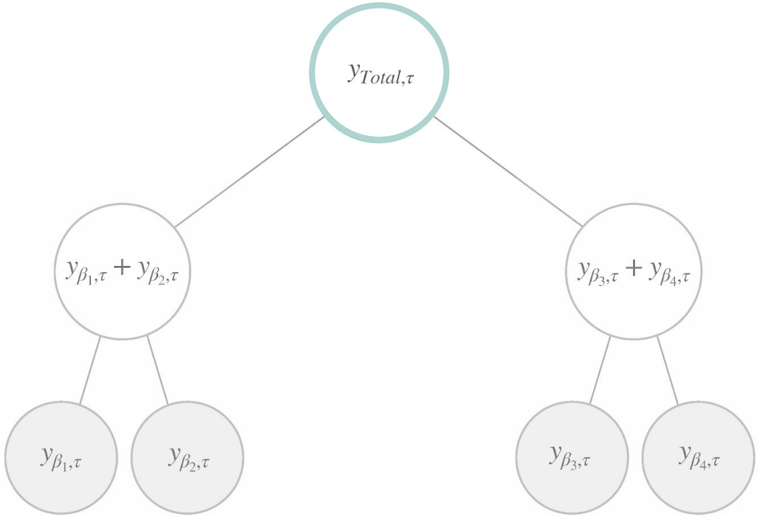
$y_{Total,\tau}$
$y_{\beta_1,\tau} + y_{\beta_2,\tau}$
$y_{\beta_3,\tau} + y_{\beta_4,\tau}$
$y_{\beta_1,\tau}$
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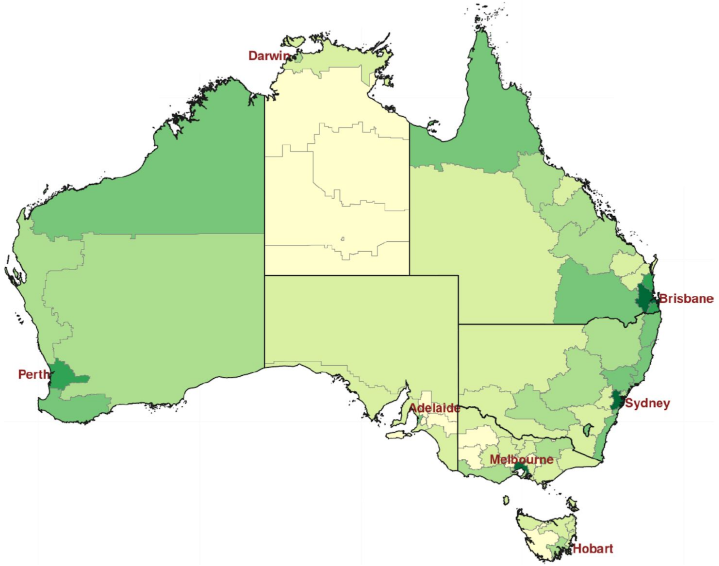
$y_{\beta_3,\tau}$
$y_{\beta_4,\tau}$


Darwin
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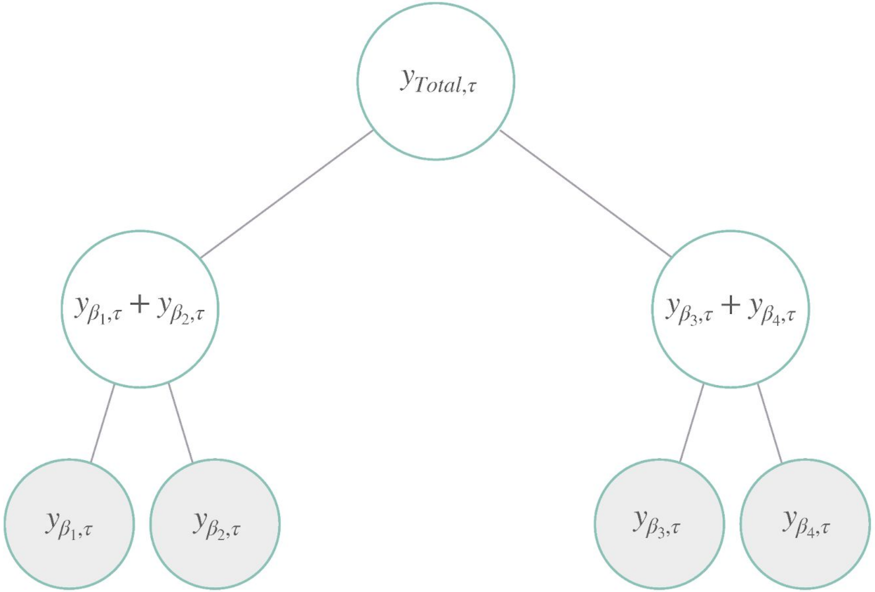
Notation



The example's hierarchical, aggregated and base series are:

$$y_{\text{Total},\tau} = y_{\beta_1,\tau} + y_{\beta_2,\tau} + y_{\beta_3,\tau} + y_{\beta_4,\tau}$$

$$\mathbf{y}_{[a],\tau} = \left[y_{\text{Total},\tau},\; y_{\beta_1,\tau} + y_{\beta_2,\tau},\; y_{\beta_3,\tau} + y_{\beta_4,\tau}\right]^{\intercal}$$

$$\mathbf{y}_{[b],\tau} = \left[y_{\beta_1,\tau},\; y_{\beta_2,\tau},\; y_{\beta_3,\tau},\; y_{\beta_4,\tau}\right]^{\intercal}$$

The summing matrix of the example can be written as:

$$\mathbf{H} = \begin{bmatrix} \mathbf{S}_{[a][b]} \\ \\ \mathbf{I}_{[b][b]} \end{bmatrix} = \left[\begin{array}{cccc} 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ \hline 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{array}\right]$$

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2 Step Reconciliation Strategies

Two-stage process, first a set of base forecasts $\hat{\mathbf{y}}_{[a,b],\tau} \in \mathbb{R}^{N_a+N_b}$ is created and

then adapted into coherent forecasts $\tilde{\mathbf{y}}_{[a,b],\tau}$

They can be expressed by:

$$\tilde{\mathbf{y}}_{[a,b],\tau} = \mathbf{H}\mathbf{P}\hat{\mathbf{y}}_{[a,b],\tau}$$

With the hierarchical constraints matrix and a projection matrix $\mathbf{P} \in \mathbb{R}^{N_b \times (N_a+N_b)}$

Gross, C. W., & Sohl, J. E. (1990). Disaggregation methods to expedite product line forecasting. Journal of Forecasting, 9, 233–254. Available at https://onlinelibrary.wiley.com/doi/abs/10.1002/for.3980090304.

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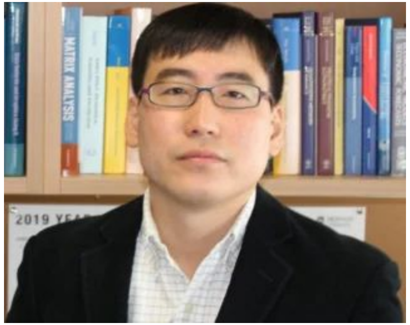
Statistical Approach: Minimize Variance

MONASH University



MinTrace

Wickramasuriya et al. (2019) show that the variance-covariance matrix of the h-step-ahead coherent forecast errors is given by

$$V_h = Var\left(\mathbf{y}_{T+h} - \tilde{\mathbf{y}}_h\right) = HPW_hP^TH^T$$

Where $W_h = Var\left(\mathbf{y}_{T+h} - \hat{\mathbf{y}}_h\right)$ is the variance-covariance matrix of the corresponding base forecast errors.

Wickramasuriya et al. (2019) show that the matrix P which minimizes the trace of V_h (the sum of all the error variances) such that $HPH = P$, is given by,

$$P = (H^TW_h^{-1}H)^{-1}H^TW_h^{-1}$$

Therefore, the optimally reconciled forecasts are given by,

$$\tilde{\mathbf{y}}_h = HG\hat{\mathbf{y}}_h = H(H^TW_h^{-1}H)^{-1}H^TW_h^{-1}\hat{\mathbf{y}}_h$$

To use this in practice, we need to estimate W_h, the forecast error variance of the h-step-ahead base forecasts. Usually, the matrix can be approximated (for example $W_h = k_hI$ recovers the ols method).

ERM

The Empirical Risk Minimization reconciliation strategy (Taieb et al., 2019) relaxes the unbiasedness assumptions from previous reconciliation methods like MinT and optimizes square errors between the reconciled predictions and the validation data to obtain an optimal reconciliation matrix P.

The exact solution for P follows the expression:

$$P^{*} = (H^{\intercal}H)^{-1}\,\mathbf{y}_{h}^{\intercal}\hat{\mathbf{y}}_{h}\,(\hat{\mathbf{y}}_{h}\hat{\mathbf{y}}_{h})^{-1}$$

The alternative Lasso regularized $\mathbf{P}$ solution is useful when the observations of validation data is limited or the exact solution has low numerical stability.

$$P^{*} = \text{argmin}_{P}||\mathbf{y}_{h} - HP\hat{\mathbf{y}}_{h}||_{2}^{2} + \lambda||P - P_{\text{BU}}||_{1}$$

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That sounds hard.

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Open Source Time Series Ecosystem

Stars 5k

⚡ StatsForecast

Lightning fast forecasting with statistical and econometric models.

Github

🤖 MLForecast

Scalable machine learning for time series forecasting.

Github

🧠 NeuralForecast

Scalable and user friendly neural forecasting algorithms for time series data.

Github

👑 Hierarchical Forecast

Probabilistic Hierarchical forecasting with statistical and econometric methods.

Github

🔧 TS features

Calculates various features from time series data. Python implementation of the R package *tsfeatures*.

Github

```
pip install hierarchicalforecast
```

```python
# Import aggregate function to construct hierarchies,
# summing matrix (H), and tags
from hierarchicalforecast.utils import aggregate

# Define different hierarchy levels
hierarchies = [['Country'], ['Country', 'State'], ['Country', 'State', 'Region']]

# Use aggregate function to create hierarchical time series dataframe, summing matrix (H), and tags
tourism_df, H_df, tags = aggregate(
    bottom_tourism_df,  # Input bottom-level time series
    spec=hierarchies    # Specify hierarchies to be created
)
```

```python
# Import HierarchicalReconciliation class
from hierarchicalforecast.core import HierarchicalReconciliation

# Instantiate the HierarchicalReconciliation object with a list of reconcilers
hrec = HierarchicalReconciliation(
    reconcilers=[
        MinTrace(method='ols', nonnegative=True),  # Minimum trace method using OLS with nonnegative constraints
        ERM(method='closed'),                     # Empirical Risk Minimization using the closed form solution
    ]
)
```

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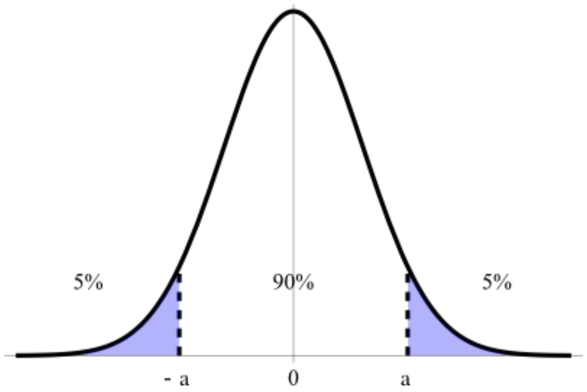
```python
# Reconcile the base forecasts using the HierarchicalReconciliation object
reconciled_fcsts_df = hrec.reconcile(
    base_forecasts_df,  # Base forecasts dataframe
    summing_matrix_df,  # Summing matrix dataframe
    tags,               # Hierarchy tags
    fitted_values_df    # Fitted values dataframe
)
```

What about uncertainty quantification?



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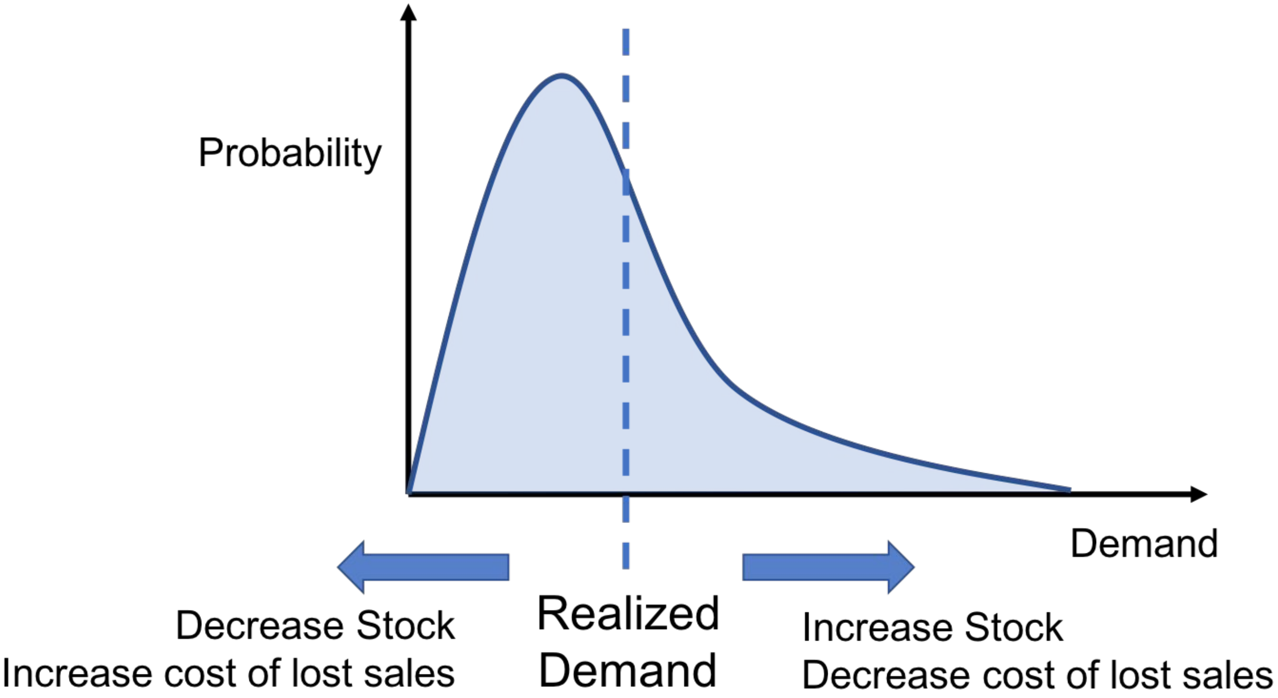
Not all errors are the same.



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Ok… that sounds hard.

```python
# Fit the model to the tourism_df dataset
mlf.fit(
    tourism_df,
    id_col='unique_id',                        # Unique identifier column
    time_col='ds',                             # Timestamp column
    target_col='y',                            # Target variable column
    prediction_intervals=PredictionIntervals( # Prediction intervals configuration
        n_windows=4,                           # Number of cross validation windows (conformal scores)
        window_size=12,                        # forecast horizon (1 year)
    )
)

# Generate predictions for the next 12 months and produce 80, and 90 prediction intervals
base_forecasts_df = mlf.predict(12, level=[80, 90])
```

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Confidence Intervals with Conformal Prediction

```python
# Fit the model to the tourism_df dataset
mlf.fit(
    tourism_df,
    id_col='unique_id',                          # Unique identifier column
    time_col='ds',                               # Timestamp column
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    time_col='ds',                          # Timestamp column
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# Generate predictions for the next 12 months and produce 80, and 90 prediction intervals
base_forecasts_df = mlf.predict(12, level=[80, 90])
```


GABAll
ECABus
BDHol
AFABus
CVis
BDABus
BDDHol
CBBVis
y
LGBMRegressor
LGBMRegressor_level_80
LGBMRegressor_level_90
Target [y]
Datestamp [ds]
2013
2014
2015
2016
2017

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```python
# Reconcile the base forecasts using the HierarchicalReconciliation object
reconciled_fcsts_df = hrec.reconcile(
    base_forecasts_df,  # Base forecasts dataframe
    summing_matrix_df,  # Summing matrix dataframe
    tags,               # Hierarchy tags
    fitted_values_df,   # Fitted values dataframe
    level=[80, 90],     # Prediction intervals
)
```

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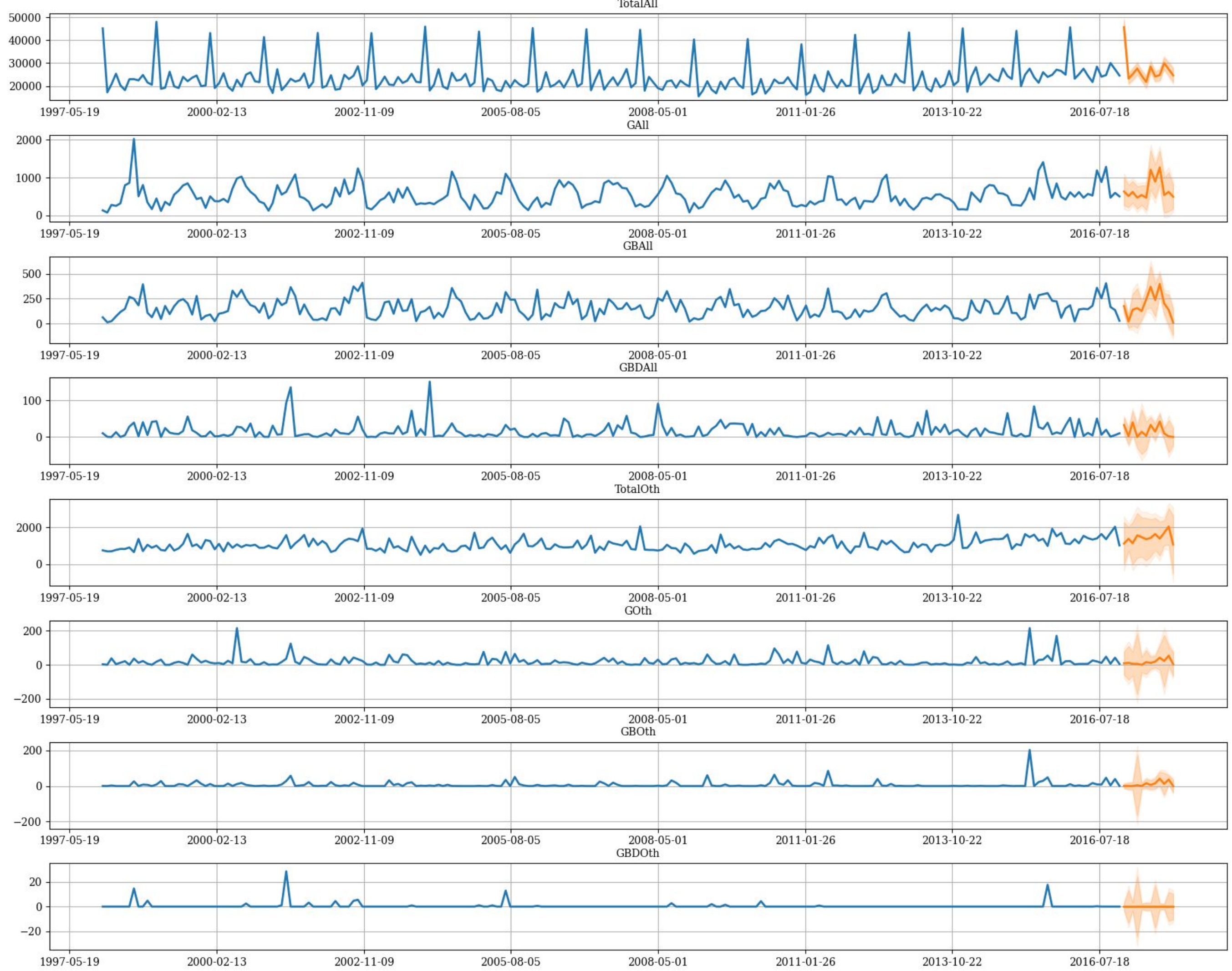
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1997-05-19
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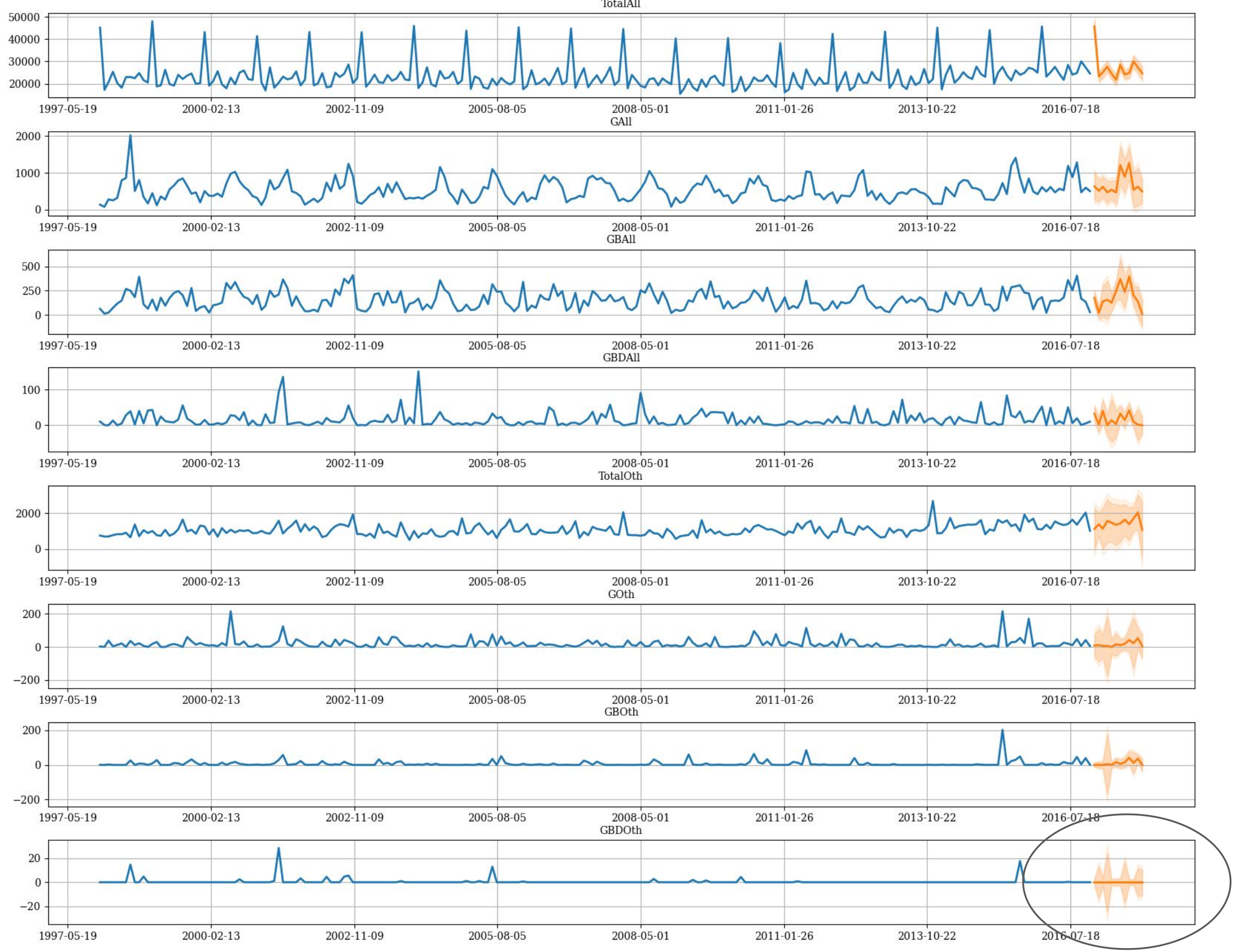
2011-01-26
2013-10-22
2016-07-18

Warning!
Scientists at work

Problems with classical approaches

Normality assumption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2011-01-26
2013-10-22
2016-07-18
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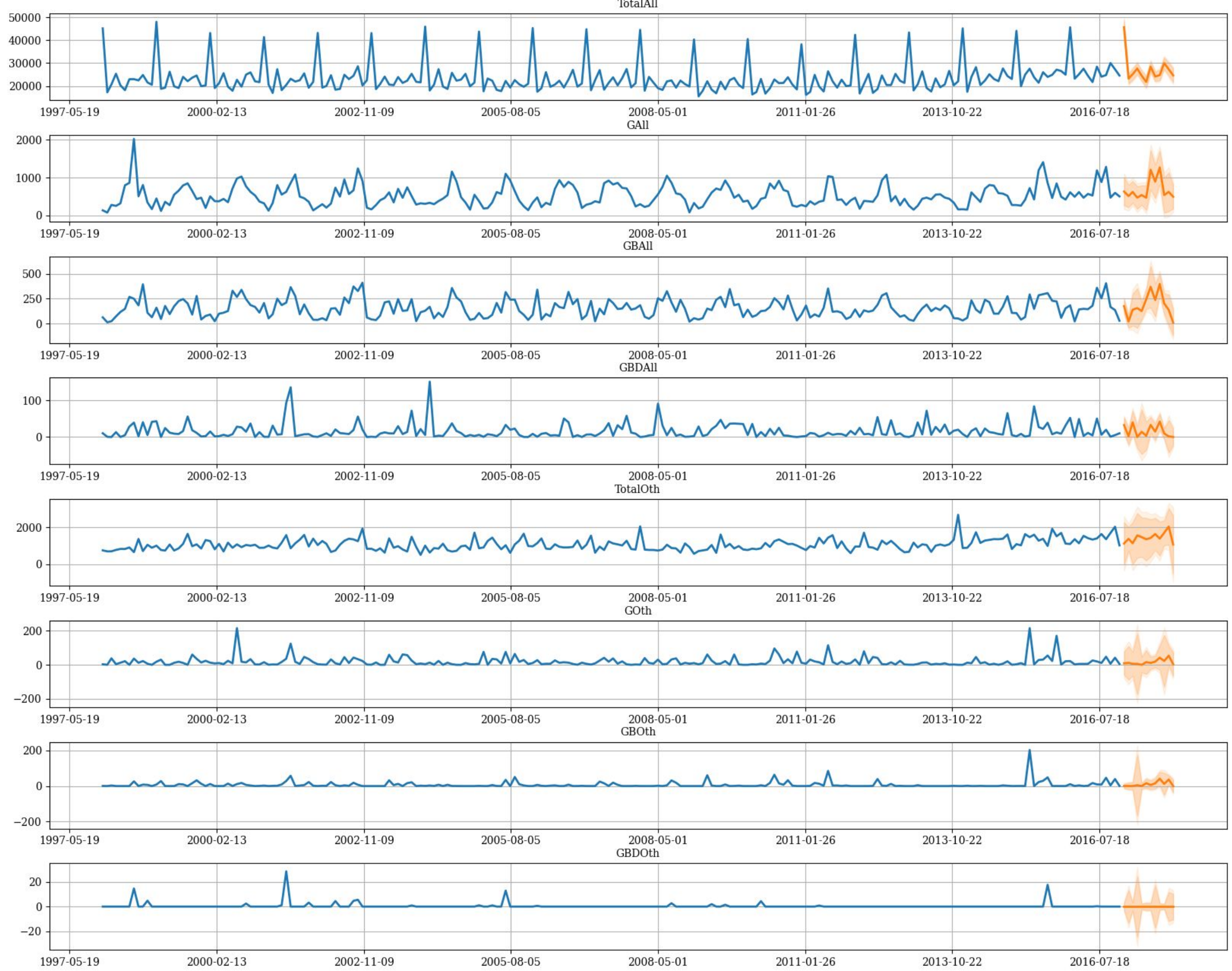
Univariate approach



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1997-05-19
2000-02-13
2002-11-09
2005-08-05
2008-05-01
2011-01-26
2013-10-22
2016-07-18

Complex pipeline (2 steps)

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Solution?

Hierarchical Mixture Networks (HINT)

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Flexible (mixture) and efficient (composite likelihood) multivariate probability.

Expands vast collection of neural forecasting methods in a single framework.

Mixtures Mesh

Probabilistic Coherent Distribution

A probabilistic hierarchical coherent distribution, is a multivariate forecasting system that satisfies that for a set of random variables (A, B, C) with $C = A + B$.

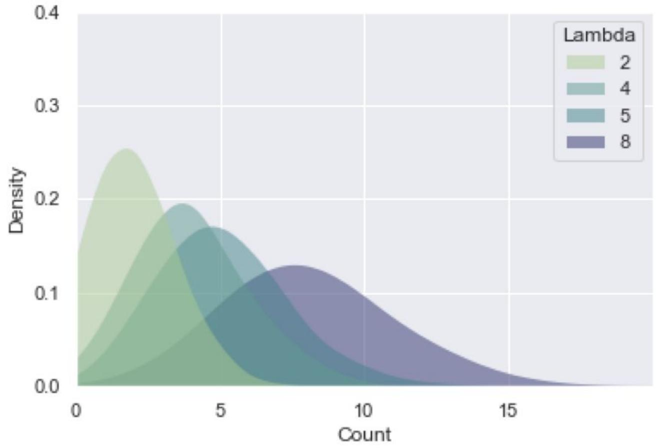
The marginal distributions satisfy:

$$\mathrm{P}(A) = \sum_{B} \mathrm{P}(A, B) \quad \text{and} \quad \mathrm{P}(B) = \sum_{A} \mathrm{P}(A, B)$$

$$\mathrm{P}(C) = \sum_{A,B} \mathrm{P}(A, B)\, \mathbb{1}(C = A + B)$$

Poisson Mixtures Mesh

The foundation of HINT models is the assumption that the joint distribution of a a time series $\mathbf{y}_{[b][t+1:t+H]}$ is described by a Mixture distribution with the **component matching assumption**, that achieves by construction probabilistic hierarchical coherence.



$$\mathbb{P}(\mathbf{y}_{[b][t+1:t+H]}) = \sum_{k=1}^{N_k} w_k \prod_{(\beta,\tau)\in[b][t+1:t+H]} \text{Poisson}(y_{\beta,\tau} \mid \lambda_{\beta,\tau})$$

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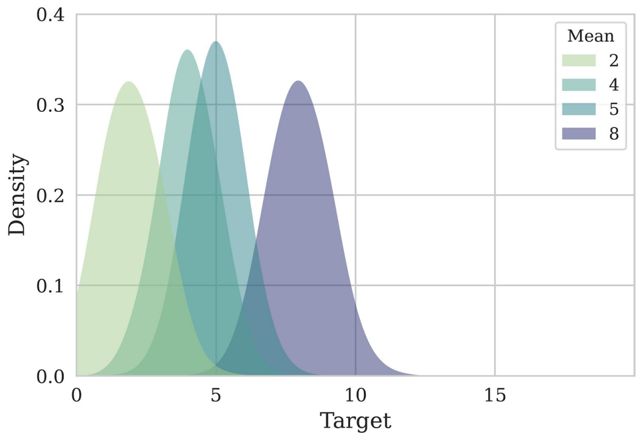
Gaussian Mixture Mesh

The foundation of HINT models is the assumption that the joint distribution of a a time series is described by a Mixture distribution with the **component matching assumption**, that achieves by construction probabilistic hierarchical coherence.



$$\mathbb{P}(\mathbf{y}_{[b][t+1:t+H]}) = \sum_{\kappa=1}^{K} w_{\kappa} \prod_{(\beta,\tau)\in[b][t+1:t+H]} \mathrm{Normal}(y_{\beta,\tau} \mid \mu_{\beta,\tau,\kappa},\ \sigma_{\beta,\tau,\kappa})$$

We reached the maximum number of allowed equations…

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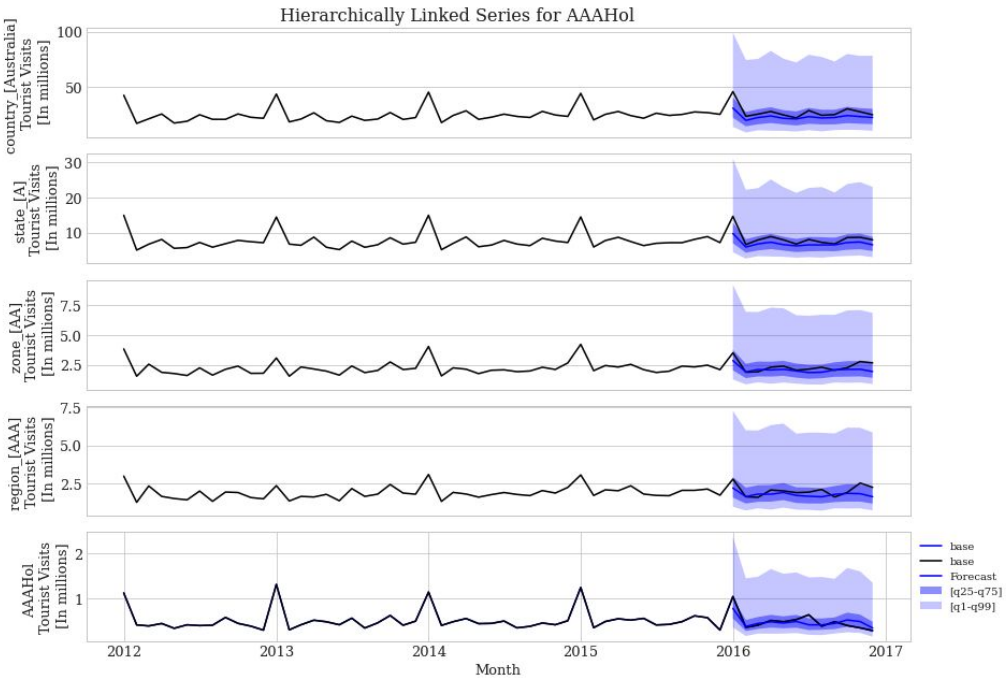
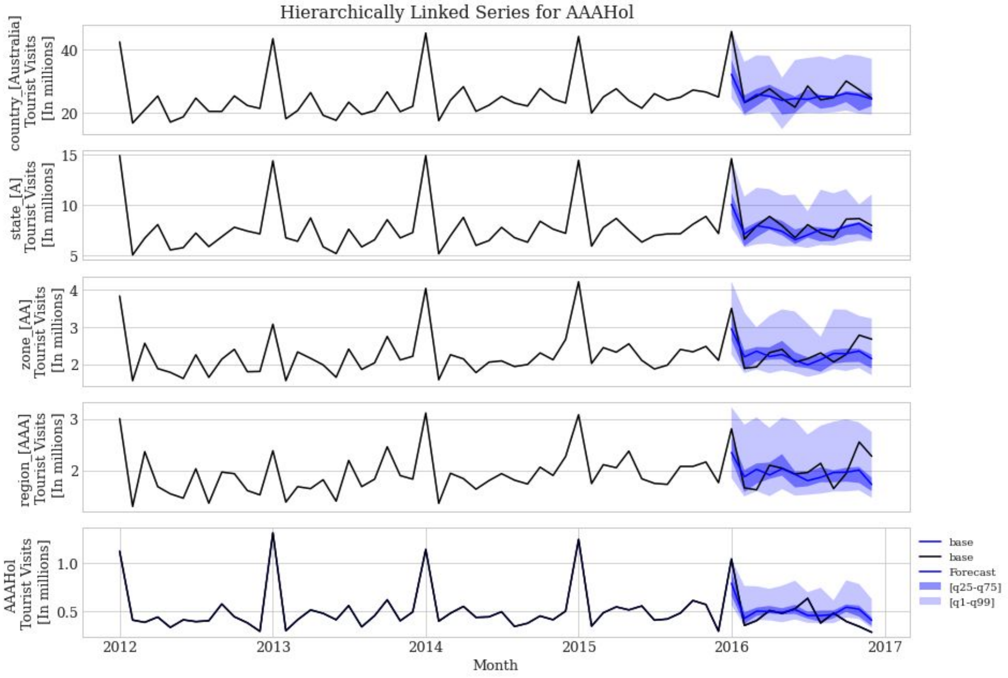
Naive Approach (Independence)



Informed approach (Correlation Groups)



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Why is this cool?

Now you can do hierarchical forecasting with your favorite deep learning model

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Ok… but this time it must be hard…

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Open Source Time Series Ecosystem

Stars 5k

⚡ StatsForecast

Lightning fast forecasting with statistical and econometric models.

Github

🤖 MLForecast

Scalable machine learning for time series forecasting.

Github

🧠 NeuralForecast

Scalable and user friendly neural forecasting algorithms for time series data.

Github

```
pip install neuralforecast
```

Let’s fit a hierarchical coherent LSTM with a PMM

```python
from neuralforecast import NeuralForecast
from neuralforecast.models import NHITS, LSTM, HINT
from neuralforecast.losses.pytorch import GMM, PMM

# Base models
# LSTM with Poisson Mixture
lstm = LSTM(h=12,
            loss=PMM(n_components=2, num_samples=100, quantiles=list(np.arange(100)/100)))

# Hierarchical Reconciliation using LSTM model
lstm_hint = HINT(h=12, model=lstm, H=H_df, group_level=1, reconciliation='bottom_up')

# Fit and Predict
fcst = NeuralForecast(
    models=[lstm_hint], # Define models
    freq='MS',                    # Monthly frequency
)
fcst.fit(df=tourism_df) # Fit neuralforecast
forecasts = fcst.predict() # Predict using trained model
```

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```

```python
from neuralforecast import NeuralForecast
from neuralforecast.models import NHITS, LSTM, HINT
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# Base models
# LSTM with Poisson Mixture
lstm = LSTM(h=12,
            loss=PMM(n_components=2, num_samples=100, quantiles=list(np.arange(100)/100)))

# Hierarchical Reconciliation using LSTM model
lstm_hint = HINT(h=12, model=lstm, H=H_df, group_level=1, reconciliation='bottom_up')

# Fit and Predict
fcst = NeuralForecast(
    models=[lstm_hint], # Define models
    freq='MS',                    # Monthly frequency
)
fcst.fit(df=tourism_df) # Fit neuralforecast
forecasts = fcst.predict() # Predict using trained model
```

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Let’s include a hierarchical coherent NHiTS with a GMM

```python
from neuralforecast import NeuralForecast
from neuralforecast.models import NHITS, LSTM, HINT
from neuralforecast.losses.pytorch import GMM, PMM

# Base models
# LSTM with Poisson Mixture
lstm = LSTM(h=12,
            loss=PMM(n_components=2, num_samples=100, quantiles=list(np.arange(100)/100)))

#  NHITS with Gaussian Mixture
nhits = NHITS(h=12,
              input_size=24,
              loss=GMM(n_components=2, num_samples=100, quantiles=list(np.arange(100)/100)))

# Hierarchical Reconciliation using LSTM model
lstm_hint = HINT(h=12, model=lstm, H=H_df, group_level=1, reconciliation='bottom_up')
# Hierarchical Reconciliation using NHITS model
nhits_hint = HINT(h=12, model=nhits, H=H_df, group_level=1, reconciliation='bottom_up')

# Fit and Predict
fcst = NeuralForecast(
    models=[lstm_hint, nhits_hint], # Define models
    freq='MS',                      # Monthly frequency
)
fcst.fit(df=tourism_df) # Fit neuralforecast
forecasts = fcst.predict() # Predict using trained model
```

```python
from neuralforecast import NeuralForecast
from neuralforecast.models import NHITS, LSTM, HINT
from neuralforecast.losses.pytorch import GMM, PMM

# Base models
# LSTM with Poisson Mixture
lstm = LSTM(h=12,
            loss=PMM(n_components=2, num_samples=100, quantiles=list(np.arange(100)/100)))

#  NHITS with Gaussian Mixture
nhits = NHITS(h=12,
              input_size=24,
              loss=GMM(n_components=2, num_samples=100, quantiles=list(np.arange(100)/100)))

# Hierarchical Reconciliation using LSTM model
lstm_hint = HINT(h=12, model=lstm, H=H_df, group_level=1, reconciliation='bottom_up')
# Hierarchical Reconciliation using NHITS model
nhits_hint = HINT(h=12, model=nhits, H=H_df, group_level=1, reconciliation='bottom_up')

# Fit and Predict
fcst = NeuralForecast(
    models=[lstm_hint, nhits_hint], # Define models
    freq='MS',                      # Monthly frequency
)
fcst.fit(df=tourism_df) # Fit neuralforecast
forecasts = fcst.predict() # Predict using trained model
```

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```python
from neuralforecast import NeuralForecast
from neuralforecast.models import NHITS, LSTM, HINT
from neuralforecast.losses.pytorch import GMM, PMM

# Base models
# LSTM with Poisson Mixture
lstm = LSTM(h=12,
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nhits = NHITS(h=12,
              input_size=24,
              loss=GMM(n_components=2, num_samples=100, quantiles=list(np.arange(100)/100)))

# Hierarchical Reconciliation using LSTM model
lstm_hint = HINT(h=12, model=lstm, H=H_df, group_level=1, reconciliation='bottom_up')
# Hierarchical Reconciliation using NHITS model
nhits_hint = HINT(h=12, model=nhits, H=H_df, group_level=1, reconciliation='bottom_up')

# Fit and Predict
fcst = NeuralForecast(
    models=[lstm_hint, nhits_hint], # Define models
    freq='MS',                      # Monthly frequency
)
fcst.fit(df=tourism_df) # Fit neuralforecast
forecasts = fcst.predict() # Predict using trained model
```

Wrap Up


FORECASTING ALL LEVELS
RECONCILING HIERACHIES
PROBABILISTIC RECONCILATION
HIERARCHICAL MIXTURE NETWORKS (HINT)
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Show some love

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👑 Hierarchical Forecast

Probabilistic Hierarchical forecasting with statistical and econometric methods.

Github

🧠 NeuralForecast

Scalable and user friendly neural forecasting algorithms for time series data.

Github

🤖 MLForecast

Scalable machine learning for time series forecasting.

Github

HierarchicalForecast: A Reference Framework for Hierarchical Forecasting in Python

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Forecasting: Principles and Practice (3rd ed)

Rob J Hyndman and George Athanasopoulos

Monash University, Australia

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