Optimal Predictor Selection for High-dimensional Nonparametric Forecasting

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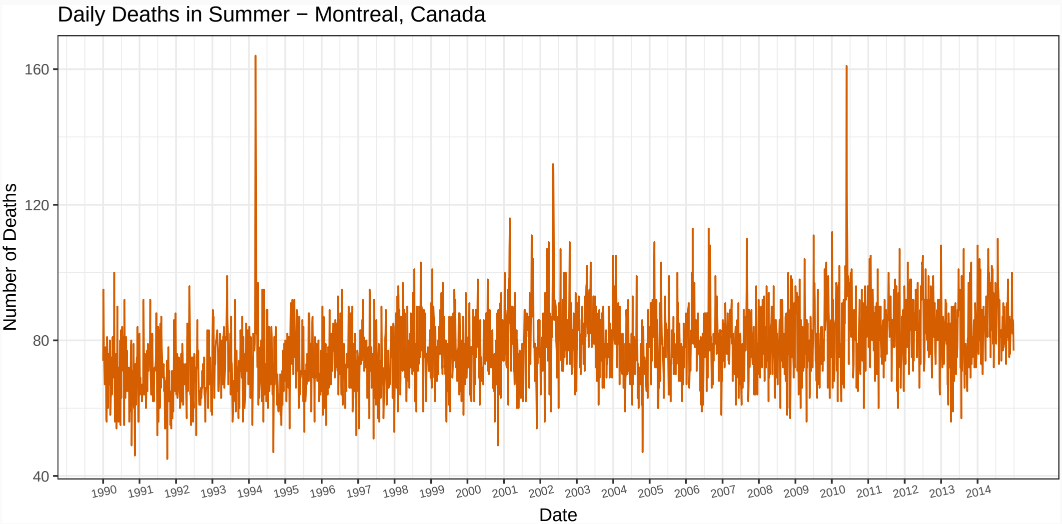
Heat Exposure Related Daily Mortality



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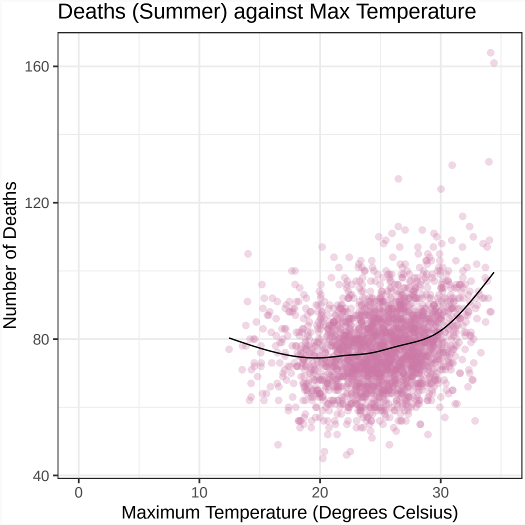

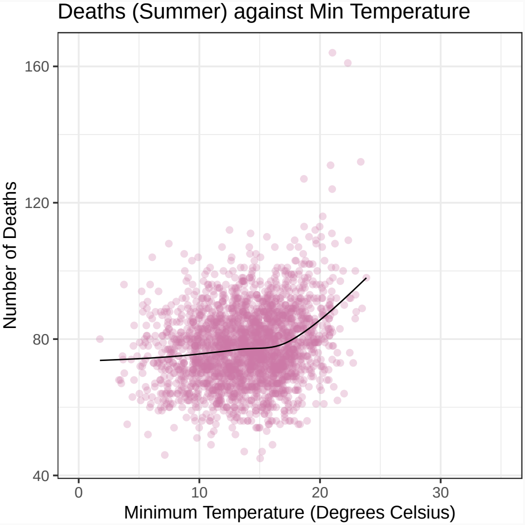

Background

- ***Nonlinear "Transfer Function" model***

$$y_t = f(\boldsymbol{x}_t, \boldsymbol{x}_{t-1}, \dots, \boldsymbol{x}_{t-k}, y_1, \dots, y_{t-l}) + \varepsilon_t$$

y_t – variable to forecast

$\boldsymbol{x}_t$ – a vector of predictors

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$$f(\boldsymbol{x}_t, \boldsymbol{x}_{t-1}, \dots, \boldsymbol{x}_{t-k}) = \sum_{a=0}^{k} f_a(\boldsymbol{x}_{t-a}) \leftarrow$$ **Nonparametric Additive Model**

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Issues:

1. Challenging to estimate in a high-dimensional setting
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Index Models:

- **Mitigate difficulty of estimating a nonparametric component for each predictor**
- **Improve flexibility**

$$y_i = g\left(\boldsymbol{\alpha}^T \boldsymbol{x}_i\right) + \varepsilon_i$$

Sparse Multiple Index (SMI) Model

Semi-parametric model

$$y_i = \beta_0 + \sum_{j=1}^{p} g_j(\boldsymbol{\alpha}_j^T \boldsymbol{x}_{ij}) + \sum_{k=1}^{d} f_k(w_{ik}) + \boldsymbol{\theta}^T \boldsymbol{u}_i + \varepsilon_i, \quad i = 1, \dots, n,$$

- y_i – univariate response
- $\boldsymbol{x}_{ij} \in \mathbb{R}^{\ell_j}$, $j = 1, \dots, p$ – p subsets of predictors entering indices
- $\boldsymbol{\alpha}_j$ – ℓ_j-dimensional vectors of index coefficients
- g_j, f_k – smooth nonlinear functions
- Additional predictors :
  - w_{ik} – nonlinear
  - $\boldsymbol{u}_i$ – linear

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Allow elements equal to zero in $\boldsymbol{\alpha}_j$ – ”Sparse”

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Both "p" and the predictor grouping among indices are unknown.

Overlapping of predictors among indices is not allowed.

Optimisation Problem

Let q be the *total number of predictors* entering indices.

$$\min_{\beta_0, p, \boldsymbol{\alpha}, \boldsymbol{g}, \boldsymbol{f}, \boldsymbol{\theta}} \quad \sum_{i=1}^{n} \left[y_i - \beta_0 - \sum_{j=1}^{p} g_j(\boldsymbol{\alpha}_j^T \boldsymbol{x}_i) - \sum_{k=1}^{d} f_k(w_{ik}) - \boldsymbol{\theta}^T \boldsymbol{u}_i \right]^2$$

$$+ \lambda_0 \sum_{j=1}^{p} \sum_{m=1}^{q} \mathbb{1}(\alpha_{jm} \neq 0) + \lambda_2 \sum_{j=1}^{p} \|\boldsymbol{\alpha}_j\|_2^2$$

$$\text{s.t.} \quad \sum_{j=1}^{p} \mathbb{1}(\alpha_{jm} \neq 0) \in \{0, 1\} \quad \forall m$$

- $\lambda_0 > 0$ – controls the number of selected predictors
- $\lambda_2 \geq 0$ – controls the strength of the additional shrinkage

MIQP Formulation

$$\min_{\beta_0, p, \boldsymbol{\alpha}, \boldsymbol{g}, \boldsymbol{f}, \boldsymbol{\theta}, \boldsymbol{z}} \quad \sum_{i=1}^{n} \left[y_i - \beta_0 - \sum_{j=1}^{p} g_j(\boldsymbol{\alpha}_j^T \boldsymbol{x}_i) - \sum_{k=1}^{d} f_k(w_{ik}) - \boldsymbol{\theta}^T \boldsymbol{u}_i \right]^2 + \lambda_0 \sum_{j=1}^{p} \sum_{m=1}^{q} z_{jm} + \lambda_2 \sum_{j=1}^{p} \sum_{m=1}^{q} \alpha_{jm}^2$$

$$\text{s.t.} \quad |\alpha_{jm}| \leq M z_{jm} \quad \forall j, \forall m,$$

$$\sum_{j=1}^{p} z_{jm} \leq 1 \quad \forall m,$$

$$z_{jm} \in \{0, 1\} \quad \leftarrow \quad z_{jm} = \mathbb{1}(\alpha_{jm} \neq 0)$$

- $M < \infty$: If $\boldsymbol{\alpha}^*$ is an optimal solution, then $\max\left(\{|\alpha_{jm}^*|\}_{j \in [p], m \in [q]}\right) \leq M$

Estimation Algorithm

Step 1 : Initialise index structure and index coefficients

Estimation Algorithm

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- **PPR:** Projection Pursuit Regression Based Initialisation
- **Additive:** Nonparametric Additive Model Based Initialisation
- **Linear:** Linear Regression Based Initialisation
- **Multiple:** Pick One From Multiple Initialisations

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Step 4 : Iterate steps 2 and 3 – until:

- convergence
- loss increases for 3 consecutive iterations OR
- max iterations

Estimation Algorithm

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Step 5 : Add a new index with dropped predictors, and repeat step 4

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Step 6 : Increase p by 1 in each iteration of step 5 – until:

- no.of indices reaches q
- loss increases after the increment model OR
- solution maintains same no.of indices as previous iteration, and abs(difference of index coefficients between two successive iterations) $<=$ tolerance

Forecasting Heat Exposure Related Daily Mortality

Variables

- **Response: Daily deaths in Summer** – 1990 to 2014 – Montreal, Canada
- **Index Variables:**
  - Death lags
  - Max temperature lags
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Data Split

- **Training Set:** 1990 to 2012
- **Validation Set:** 2013
- **Test Set:** 2014

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Results

Model	Predictors	Indices	Test Set 1		Test Set 2	
			MSE	MAE	MSE	MAE
SMI Model (5, 12) - PPR	61	7	**85.233**	**7.140**	**97.353**	**7.772**
SMI Model (1, 0) - Additive	61	59	96.398	7.481	112.199	8.156
SMI Model (6, 11) - Linear	61	2	100.231	7.719	120.542	8.598
Backward Elimination	40	—	136.204	9.319	140.867	9.385
Group-wise Additive Index Model	61	4	90.763	7.247	106.251	7.928
Projection Pursuit Regression	61	4	90.698	7.343	110.497	8.057

SMI Model (a, b) $\rightarrow$ $\boldsymbol{\lambda}_0 = a, \boldsymbol{\lambda}_2 = b$

- **Test Set 1:** Three months (June, July and August 2014)
- **Test Set 2:** One month (June 2014)

Summary

Key features:

- Automatic selection of number of indices and predictor grouping
- Automatic predictor selection
- A wide spectrum: from single index models to additive models

Limitations:

- Initialisation: we encourage trial-and-error
- Computational cost: increases with number of predictors and indices

Paper : github.com/nuwani-palihawadana/smimodel_paper

R Package - smimodel

- Open source implementation of **SMI Modelling Algorithm**
  - **model_smimodel()**
- Penalty parameter tuning with greedy search
  - **greedy_smimodel()**
- Functions to fit benchmark models
  - **model_backward()**
  - **model_gaim()**
  - **model_ppr() etc.**

github.com/nuwani-palihawadana/smimodel

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- **"Uncertainty"** of a forecast $\rightarrow$ **Prediction Interval (PI)**

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- Theoretical $100(1-\alpha)\%$ prediction interval:

$$\hat{y}_{t+h|t} \pm z_{\alpha/2} * \hat{\sigma}_h,$$

where

- y – time series $y_1, \dots, y_T$
- $\hat{y}_{t+h|t}$ – h steps ahead point forecast for y_{t+h}
- $z_{\alpha/2}$ – $\alpha/2$ quantile of standard normal distribution
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  - $\hat{\sigma}_h$ – an estimate of std. deviation of h-step forecast distribution
- Nonparametric Additive Models:
  - No distributional assumptions
  - Serially correlated errors $\rightarrow$ **Impossible to estimate theoretical PIs**

Methodology

Block Bootstrap

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- Resampling from empirical distribution of historical model residuals $\rightarrow$ Bootstrapping
- Randomly resample blocks from the historical model residuals, and join together $\rightarrow$ **Block Bootstrapping**
- Retains serial correlation in the data
- block length:
  - Long enough to capture autocorrelation patterns
  - Short enough to construct sufficient number of blocks

Methodology

Conformal Prediction (CP) – Vovk et al. (2005)

- A distribution-free approach
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Split Conformal Prediction (SCP)

- A holdout method for generating prediction intervals
  - **Training set** – forecasting model is trained
  - **Calibration set** – forecasting errors (*nonconformity scores*) are calculated
  - **Test set** – prediction intervals are obtained

Methodology

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Weighted Conformal Prediction (WCP) Methods

- Tibshirani et al. (2019):
  - Depends on **”covariate shift”** assumption
  - *Nonconformity scores* are weighted using ratio of likelihoods of training and test covariate distributions
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- Barber et al. (2023):
  - Weighting *quantiles* to avoid assumption of exchangeability
  - Weights are "fixed" rather than being data dependent

Methodology

- CP methods for **non-exchangeable data**:

Adaptive Conformal Prediction (ACP) – Gibbs & Candès (2021)

- Update nominal α based on achieved coverage
  - If achieved coverage is larger – increase α
  - If achieved coverage is smaller – decrease α

Methodology

- Prediction interval construction methods
  - Block Bootstrapping (BB)
  - Conformal Prediction (CP) methods: SCP, WSCP, ACP

- Applied using *online learning framework* proposed by *Wang and Hyndman (2024)*

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Data Recap

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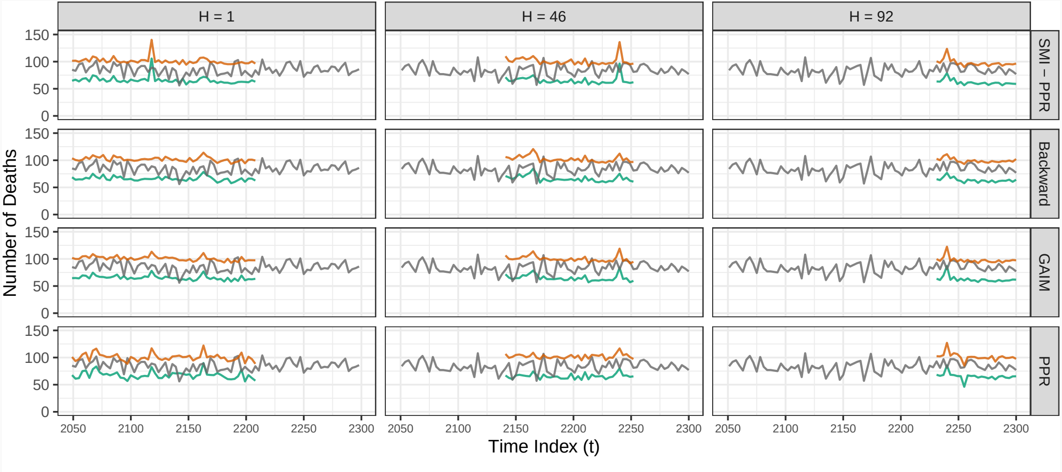
New Data Split

- **Training Set:** 1990 to 2007
- **Validation Set:** 2008
- **Test Set:** 2009 to 2014

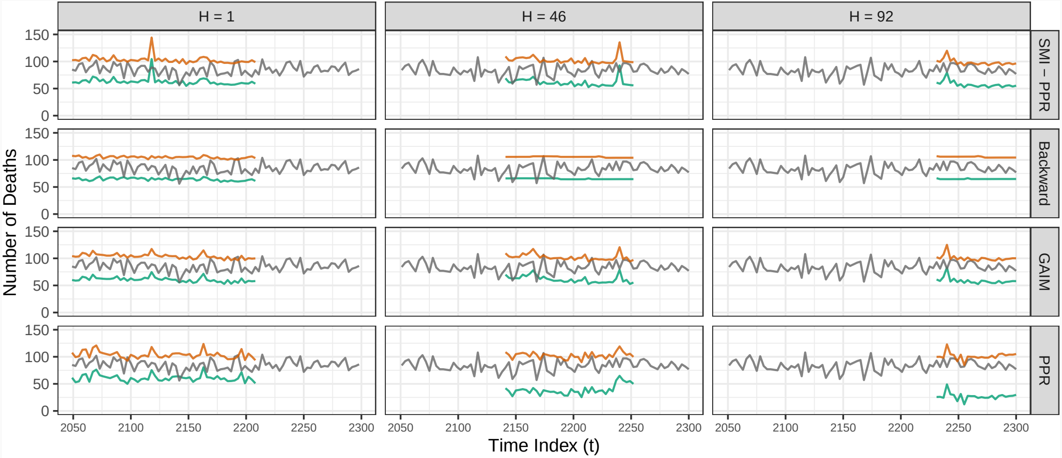
Results

Block Bootstrap 95% Prediction Intervals (block length = 59):

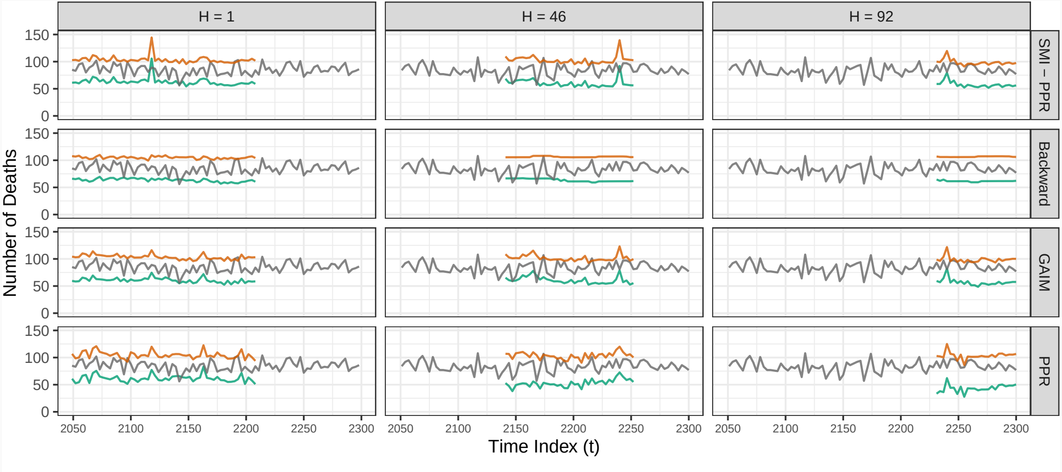


Results

Split Conformal Prediction 95% Prediction Intervals:

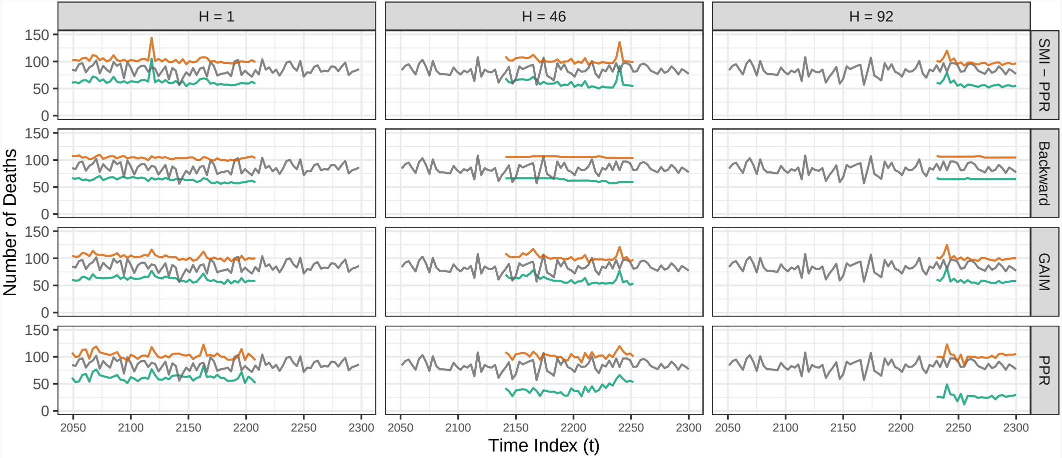


Weighted Split Conformal Prediction 95% Prediction Intervals:



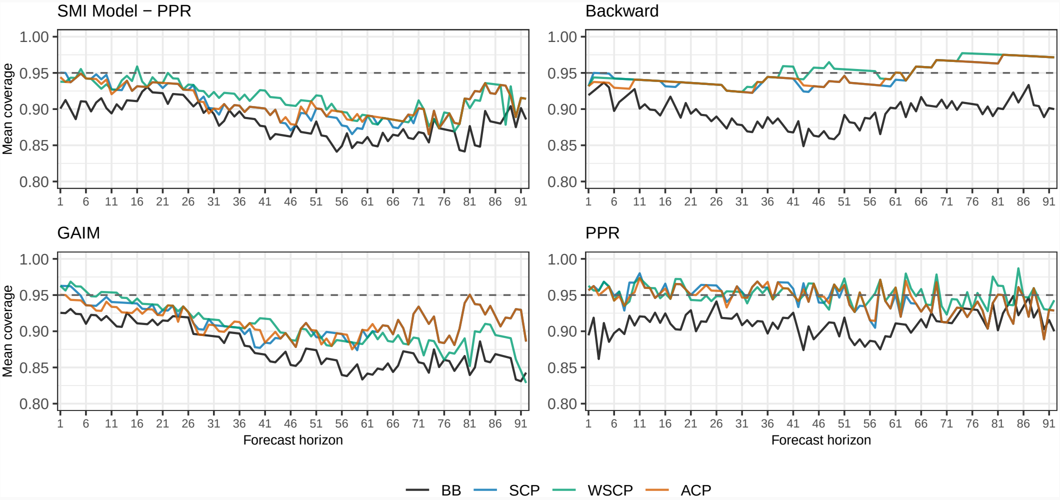
Results

Adaptive Conformal Prediction 95% Prediction Intervals:



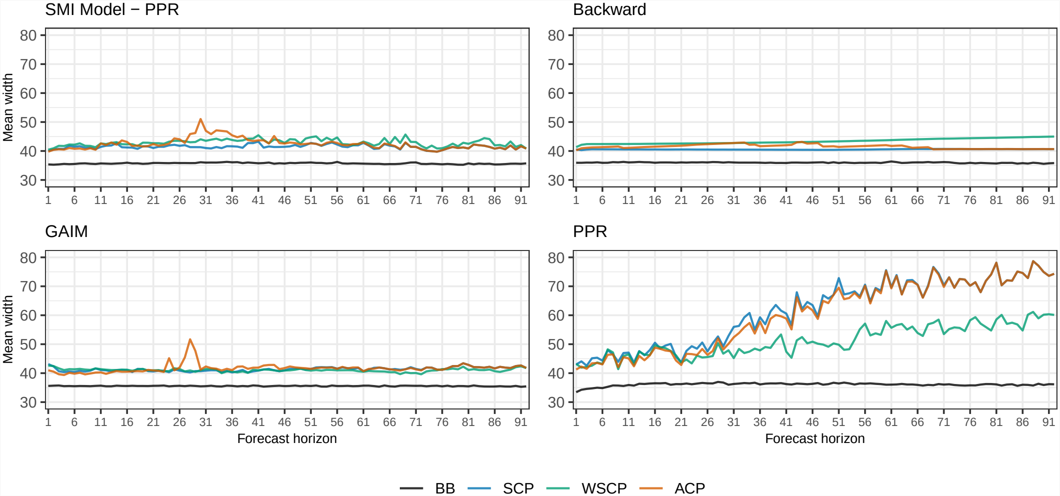
Results

Mean Coverage:



Results

Mean Width:



Summary

Summary of Results (work-in-progress):

- **Block Bootstrap** – Under-coverage; too narrow
- **Conformal Prediction** – Better achieves a target coverage, with acceptable sharpness

Limitations:

- Test set is not long enough for larger forecast horizons
- Hyper-parameter choices

Future Work

- We propose a novel methodology: **Conformal Block Bootstrap (CBB)**
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