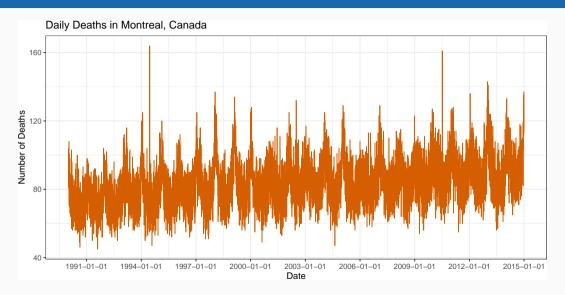
Sparse Multiple Index (SMI)
Models for High-dimensional
Nonparametric Forecasting

Nuwani Palihawadana

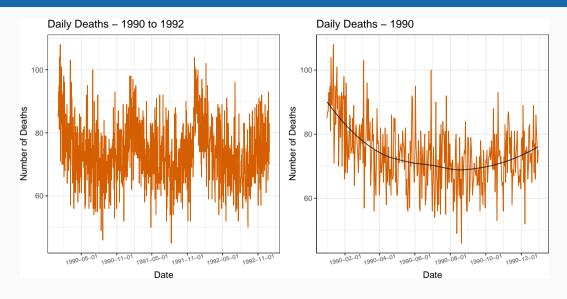
Joint work with: Rob Hyndman, Xiaoqian Wang

1 July 2024

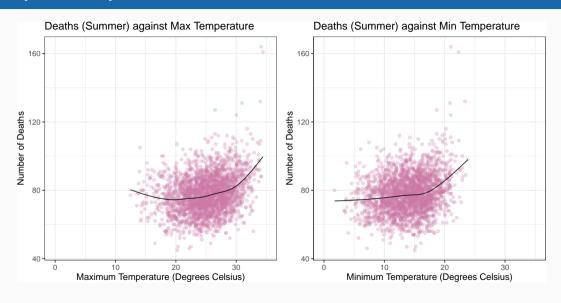
# **Daily Mortality Data**



# **Daily Mortality Data**



## **Daily Mortality Data**



#### ■ Nonlinear "Transfer Function" model

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

 $y_t$  – variable to forecast

 $oldsymbol{x}_t$  – a vector of predictors

 $\varepsilon_t$  – random error

#### ■ Nonlinear "Transfer Function" model

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

 $y_t$  – variable to forecast

 $oldsymbol{x}_t$  – a vector of predictors

 $\varepsilon_t$  – random error

■ Impossible to estimate f for large p – curse of dimensionality

#### Nonlinear "Transfer Function" model

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

 $y_t$  – variable to forecast

 $oldsymbol{x}_t$  – a vector of predictors

 $\varepsilon_t$  – random error

- Impossible to estimate f for large p curse of dimensionality
- Reasonable to impose additivity constraints

$$f(\boldsymbol{x}_t, \boldsymbol{x}_{t-1}, \dots, \boldsymbol{x}_{t-p}) = \sum_{i=0}^p f_i(\boldsymbol{x}_{t-i})$$

#### Nonlinear "Transfer Function" model

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

 $y_t$  – variable to forecast

 $oldsymbol{x}_t$  – a vector of predictors

 $\varepsilon_t$  – random error

- Impossible to estimate f for large p curse of dimensionality
- Reasonable to impose additivity constraints

$$f(m{x}_t, m{x}_{t-1}, \dots, m{x}_{t-p}) = \sum_{i=0}^p f_i(m{x}_{t-i}) \leftarrow extsf{Nonparametric Additive Model}$$

ľ

- **A** Issues:
- Challenging to estimate in a high-dimensional setting
- Subjectivity in predictor selection, and predictor grouping to model interactions

#### Issues:

- Challenging to estimate in a high-dimensional setting
- Subjectivity in predictor selection, and predictor grouping to model interactions

#### i Index Models:

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

#### **SMI Model**

#### Semi-parametric model

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

- $y_i$  univariate response
- $m{x}_{ij} \in \mathbb{R}^{\ell_j}$ ,  $j=1,\ldots,p$  p subsets of predictors entering indices
- $lacktriangleq oldsymbol{lpha}_i$   $\ell_i$ -dimensional vectors of index coefficients
- $\blacksquare g_i, f_k$  smooth nonlinear functions
- Additional predictors :
  - $ightharpoonup w_{ik}$  nonlinear
  - $lackbox{m{u}}_i$  linear

#### **SMI Model**

#### Semi-parametric model

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

- $\blacksquare$   $y_i$  univariate response
- $m{x}_{ij} \in \mathbb{R}^{\ell_j}$ ,  $j=1,\ldots,p$  p subsets of predictors entering indices
- $lacktriangleq oldsymbol{lpha}_j$   $\ell_j$ -dimensional vectors of index coefficients
- $\blacksquare g_i, f_k$  smooth nonlinear functions
- Additional predictors :
  - $ightharpoonup w_{ik}$  nonlinear
  - $ightharpoonup u_i$  linear

Allow elements equal to zero in  $\alpha_i$  – "Sparse"

#### **SMI Model**

#### Semi-parametric model

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

- $\blacksquare$   $y_i$  univariate response
- $m{x}_{ij} \in \mathbb{R}^{\ell_j}$ ,  $j=1,\ldots,p$  p subsets of predictors entering indices
- $lacktriangleq oldsymbol{lpha}_j$   $\ell_j$ -dimensional vectors of index coefficients
- lacksquare  $g_j, f_k$  smooth nonlinear functions
- Additional predictors :
  - $ightharpoonup w_{ik}$  nonlinear
  - $lackbox{m u}_i$  linear

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.

$$\begin{split} \min_{\beta_0, p, \boldsymbol{\alpha}, \boldsymbol{g}, \boldsymbol{f}, \boldsymbol{\theta}} \quad & \sum_{i=1}^n \left[ y_i - \beta_0 - \sum_{j=1}^p g_j(\boldsymbol{\alpha}_j^T \boldsymbol{x}_i) - \sum_{k=1}^d f_k(w_{ik}) - \boldsymbol{\theta}^T \boldsymbol{u}_i \right]^2 \\ & \quad + \lambda_0 \sum_{j=1}^p \sum_{m=1}^q \mathbb{1}(\alpha_{jm} \neq 0) + \lambda_2 \sum_{j=1}^p \|\boldsymbol{\alpha}_j\|_2^2 \\ \text{s.t.} \quad & \sum_{j=1}^p \mathbb{1}(\alpha_{jm} \neq 0) \in \{0, 1\} \quad \forall m \end{split}$$

## **Optimisation Problem**

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

$$\begin{split} \min_{\beta_0, p, \boldsymbol{\alpha}, \boldsymbol{g}, \boldsymbol{f}, \boldsymbol{\theta}} \quad & \sum_{i=1}^n \left[ y_i - \beta_0 - \sum_{j=1}^p g_j(\boldsymbol{\alpha}_j^T \boldsymbol{x}_i) - \sum_{k=1}^d f_k(w_{ik}) - \boldsymbol{\theta}^T \boldsymbol{u}_i \right]^2 \\ & \quad + \lambda_0 \sum_{j=1}^p \sum_{m=1}^q \mathbb{1}(\alpha_{jm} \neq 0) + \lambda_2 \sum_{j=1}^p \|\boldsymbol{\alpha}_j\|_2^2 \end{split}$$
 s.t. 
$$\sum_{j=1}^p \mathbb{1}(\alpha_{jm} \neq 0) \in \{0, 1\} \quad \forall m \end{split}$$

lacksquare  $\lambda_0>0$  – controls the number of selected predictors

## **Optimisation Problem**

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

$$\begin{split} \min_{\beta_0,p,\boldsymbol{\alpha},\boldsymbol{g},\boldsymbol{f},\boldsymbol{\theta}} \quad & \sum_{i=1}^n \left[ y_i - \beta_0 - \sum_{j=1}^p g_j(\boldsymbol{\alpha}_j^T\boldsymbol{x}_i) - \sum_{k=1}^d f_k(w_{ik}) - \boldsymbol{\theta}^T\boldsymbol{u}_i \right]^2 \\ & \quad + \lambda_0 \sum_{j=1}^p \sum_{m=1}^q \mathbb{1}(\alpha_{jm} \neq 0) + \lambda_2 \sum_{j=1}^p \|\boldsymbol{\alpha}_j\|_2^2 \end{split}$$
 s.t. 
$$\sum_{j=1}^p \mathbb{1}(\alpha_{jm} \neq 0) \in \{0,1\} \quad \forall m \end{split}$$

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

### **MIQP Formulation**

$$\begin{split} \min_{\beta_0,p,\boldsymbol{\alpha},\boldsymbol{g},\boldsymbol{f},\boldsymbol{\theta},\boldsymbol{z}} \quad & \sum_{i=1}^n \left[ y_i - \beta_0 - \sum_{j=1}^p g_j(\boldsymbol{\alpha}_j^T\boldsymbol{x}_i) - \sum_{k=1}^d f_k(w_{ik}) - \boldsymbol{\theta}^T\boldsymbol{u}_i \right]^2 \\ & \quad + \lambda_0 \sum_{j=1}^p \sum_{m=1}^q z_{jm} + \lambda_2 \sum_{j=1}^p \sum_{m=1}^q \alpha_{jm}^2 \\ \text{s.t.} \quad & |\alpha_{jm}| \leq M z_{jm} \quad \forall j, \forall m, \\ & \quad \sum_{j=1}^p z_{jm} \leq 1 \quad \forall m, \\ & \quad z_{jm} \in \{0,1\} \end{split}$$

### **MIQP Formulation**

$$\begin{split} \min_{\beta_0,p,\boldsymbol{\alpha},\boldsymbol{g},\boldsymbol{f},\boldsymbol{\theta},\boldsymbol{z}} \quad & \sum_{i=1}^n \left[ y_i - \beta_0 - \sum_{j=1}^p g_j(\boldsymbol{\alpha}_j^T\boldsymbol{x}_i) - \sum_{k=1}^d f_k(w_{ik}) - \boldsymbol{\theta}^T\boldsymbol{u}_i \right]^2 \\ & \quad + \lambda_0 \sum_{j=1}^p \sum_{m=1}^q z_{jm} + \lambda_2 \sum_{j=1}^p \sum_{m=1}^q \alpha_{jm}^2 \\ \text{s.t.} \quad & |\alpha_{jm}| \leq M z_{jm} \quad \forall j, \forall m, \\ & \quad \sum_{j=1}^p z_{jm} \leq 1 \quad \forall m, \\ & \quad z_{jm} \in \{0,1\} \quad \leftarrow \quad z_{jm} = \mathbb{1}(\alpha_{jm} \neq 0) \end{split}$$

### **MIQP Formulation**

$$\begin{split} \min_{\beta_0,p,\boldsymbol{\alpha},\boldsymbol{g},\boldsymbol{f},\boldsymbol{\theta},\boldsymbol{z}} \quad & \sum_{i=1}^n \left[ y_i - \beta_0 - \sum_{j=1}^p g_j(\boldsymbol{\alpha}_j^T\boldsymbol{x}_i) - \sum_{k=1}^d f_k(w_{ik}) - \boldsymbol{\theta}^T\boldsymbol{u}_i \right]^2 \\ & \quad + \lambda_0 \sum_{j=1}^p \sum_{m=1}^q z_{jm} + \lambda_2 \sum_{j=1}^p \sum_{m=1}^q \alpha_{jm}^2 \\ \text{s.t.} \quad & |\alpha_{jm}| \leq M z_{jm} \quad \forall j, \forall m, \\ & \quad \sum_{j=1}^p z_{jm} \leq 1 \quad \forall m, \\ & \quad z_{jm} \in \{0,1\} \quad \leftarrow \quad \boldsymbol{z}_{jm} = \mathbb{1}(\alpha_{jm} \neq 0) \end{split}$$

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

**Step 1:** Initialise index structure and index coefficients

**Step 1:** Initialise index structure and index coefficients

**Step 2:** Estimate nonlinear functions

**Step 1:** Initialise index structure and index coefficients

**Step 2:** Estimate nonlinear functions

**Step 3:** Update index coefficients

**Step 1:** Initialise index structure and index coefficients

Step 2: Estimate nonlinear functions

Step 3: Update index coefficients

**Step 4:** Iterate steps 2 and 3 – until:

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

Step 1: Initialise index structure and index coefficients

**Step 2:** Estimate nonlinear functions

**Step 3:** Update index coefficients

**Step 4:** Iterate steps 2 and 3 – until:

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

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

**Step 1:** Initialise index structure and index coefficients

Step 2: Estimate nonlinear functions

Step 3: Update index coefficients

Step 4: Iterate steps 2 and 3 – until:

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

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

**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</li>

# **Forecasting Heat Exposure Related Mortality**

#### **Variables**

- Response: Daily deaths in Summer
  - 1990 to 2014 Montreal, Canada
- Index Variables:
  - Death lags
  - Max temperature lags
  - Min temperature lags
  - Vapor pressure lags
- Nonlinear: DOS (day of the season), Year

# **Forecasting Heat Exposure Related Mortality**

#### **Variables**

- Response: Daily deaths in Summer
  - 1990 to 2014 Montreal, Canada
- Index Variables:
  - Death lags
  - Max temperature lags
  - Min temperature lags
  - Vapor pressure lags
- Nonlinear: DOS (day of the season), Year

#### **Data Split**

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

# **Forecasting Heat Exposure Related Mortality**

#### **Variables**

- Response: Daily deaths in Summer
- 1990 to 2014 Montreal, Canada
- Index Variables:
  - Death lags
  - Max temperature lags
  - Min temperature lags
  - Vapor pressure lags
- Nonlinear: DOS (day of the season), Year

### **Data Split**

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

$$\mathbf{Deaths} = \beta_0 + \sum_{i=1}^r g_j(\boldsymbol{X}\boldsymbol{\alpha}_j) + f_1(\mathbf{DOS}) + f_2(\mathbf{Year}) + \varepsilon,$$

#### Results

			Test Set 1		Test Set 2	
Model	Predictors	Indices	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) 
$$ightarrow oldsymbol{\lambda}_0 = oldsymbol{a}, oldsymbol{\lambda}_2 = oldsymbol{b}$$

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

#### **Conclusion**

#### i Key features:

- Automatic selection of number of indices and predictor grouping
- Automatic predictor selection
- A wide spectrum: from single index models to additive models
- Flexibility to include separate nonlinear and linear predictors

### **Conclusion**

#### i Key features:

- Automatic selection of number of indices and predictor grouping
- Automatic predictor selection
- A wide spectrum: from single index models to additive models
- Flexibility to include separate nonlinear and linear predictors

### ▲ Things to improve:

- Initialisation: we encourage trial-and-error
- Applicability: more applications are needed
- Computational time: increases with number of predictors and indices



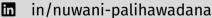
R package:

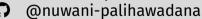
github.com/nuwani-palihawadana/smimodel

Paper:

github.com/nuwani-palihawadana/smimodel\_paper

#### Find me:





nuwani.kodikarapalihawadana@monash.edu