

Joint estimation of the conditional mean and the conditional variance in high-dimensions

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I. Problem presentation

Heteroscedastic Regression

Observations : finite collection of pairs $\{(\mathbf{x}_t, y_t); t = 1, \dots, T\}$

- $\mathbf{x}_t \in \mathbb{R}^d$ multidimensional feature vector ;
- $y_t \in \mathbb{R}$ real valued label.

Prediction : for a new feature \mathbf{x}_{T+1} , predict y_{T+1} .

- Quadratic loss : $\ell[y_{T+1}, \mathbf{b}(\mathbf{x}_{T+1})] = (y_{T+1} - \mathbf{b}(\mathbf{x}_{T+1}))^2$.
- Bayes predictor : $\mathbf{b}^* = \arg \min_{\mathbf{b}} \mathbf{E}\{\ell[y_{T+1}, \mathbf{b}(\mathbf{x}_{T+1})]\}$

$$\mathbf{b}^*(\mathbf{x}) = \mathbf{E}[y_{T+1} | \mathbf{x}_{T+1} = \mathbf{x}].$$

- Given $\mathbf{x}_{T+1} = \mathbf{x}$, the average loss of the Bayes predictor :

$$s^{*2}(\mathbf{x}) = \mathbf{E}\{\ell[y_{T+1}, \mathbf{b}^*(\mathbf{x}_{T+1})] | \mathbf{x}_{T+1} = \mathbf{x}\} = \mathbf{Var}[y_{T+1} | \mathbf{x}_{T+1} = \mathbf{x}].$$

The goal is to estimate the functions \mathbf{b}^* and s^* .

Problem reformulation

Observations : finite collection $(\mathbf{x}_t, y_t) \in \mathbb{R}^d \times \mathbb{R}$ obeying

$$y_t = \mathbf{b}^*(\mathbf{x}_t) + \mathbf{s}^*(\mathbf{x}_t) \xi_t, \quad t \in \mathcal{T} = \{1, \dots, T\},$$

where $\mathbf{b}^* : \mathbb{R}^d \rightarrow \mathbb{R}$ and $\mathbf{s}^* : \mathbb{R}^d \rightarrow \mathbb{R}_+$ such that

Conditional mean : $\mathbf{E}[y_t | \mathbf{x}_t] = \mathbf{b}^*(\mathbf{x}_t)$.

Conditional variance : $\mathbf{Var}[y_t | \mathbf{x}_t] = \mathbf{s}^{*2}(\mathbf{x}_t)$.

Therefore, ξ_t 's are such that $\mathbf{E}[\xi_t | \mathbf{x}_t] = 0$ and $\mathbf{Var}[\xi_t | \mathbf{x}_t] = 1$. They are often assumed Gaussian $\mathcal{N}(0, 1)$ for simplicity.

Goal : to jointly estimate the functions \mathbf{b}^* and \mathbf{s}^* by a computationally tractable procedure with strong theoretical guarantees.

Sparsity Assumption

- In these settings, estimating \mathbf{b}^* and \mathbf{s}^* under no further assumption is an ill-posed problem.
- Sparsity scenario : \mathbf{b}^* and \mathbf{s}^* belong to some low dimensional spaces.

Example : Homoscedastic regression

$$\forall \mathbf{x}, \quad \mathbf{b}^*(\mathbf{x}) = \sum_{j=1}^p f_j(\mathbf{x})\beta_j^* = [f_1(\mathbf{x}), \dots, f_p(\mathbf{x})]\beta^*, \quad \text{and} \quad \mathbf{s}^*(\mathbf{x}) \equiv \sigma^*$$

↪ Dictionary $\{f_1, \dots, f_p\}$ of functions from \mathbb{R}^d to \mathbb{R}

↪ Unknown vector $(\beta^*, \sigma^*) \in \mathbb{R}^p \times \mathbb{R}$, sparse vector β^*

↪ Sparsity index : $p^* = |\beta^*|_0 := \sum_{j=1}^p \mathbb{1}(\beta_j^* \neq 0)$ with $p^* \ll p$

Some remarks

- Because of its nonparametric nature, this problem is hard even for small values of the dimension d .
- The literature on estimating \mathbf{s}^* is very scarce as compared to the literature on estimating \mathbf{b}^* .
- Estimators of \mathbf{s}^* may be used for constructing confidence intervals for the predictions.
- The case of time-inhomogeneous observations is included in the previous set-up. Indeed, if

$$\mathbf{b}_t^*(\mathbf{x}) = \mathbf{E}[y_t | \mathbf{x}_t = \mathbf{x}]$$

depends on “time” t , one can include the time as a feature $\bar{\mathbf{x}}_t = (\mathbf{x}_t, t)$ and set $\bar{\mathbf{b}}^*(\bar{\mathbf{x}}_t) = \mathbf{b}_t^*(\mathbf{x}_t)$.

II. Previous work

Homoscedastic regression

The model is

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta}^* + \sigma^* \boldsymbol{\xi}$$

Observations : $\mathbf{Y} = [y_1, \dots, y_T]^\top \in \mathbb{R}^T$

Noise : $\boldsymbol{\xi} = [\xi_1, \dots, \xi_T]^\top \in \mathbb{R}^T$

Design Matrix : $\mathbf{X} = x_{t,j}$ with $x_{t,j} = [f_j(\mathbf{x}_t)] \in \mathbb{R}$

Coefficients : $\boldsymbol{\beta}^* = [\beta_1^*, \dots, \beta_p^*]^\top \in \mathbb{R}^p$

Standard deviation : $\mathbf{s}^*(\mathbf{x}_t) \equiv \sigma^* \in \mathbb{R}_*^+$

Recall that the sparsity assumption postulates that $|\boldsymbol{\beta}^*|_0 = p^* \ll p$.

Most popular methods : Lasso and Dantzig selector

- ◀ The LASSO of Tibshirani (1996) is defined as

$$\hat{\beta}^{\text{Lasso}} = \arg \min_{\beta \in \mathbb{R}^p} \left(\frac{\|\mathbf{Y} - \mathbf{X}\beta\|_2^2}{2\sigma^{*2}} + \lambda \sum_{j=1}^p |\mathbf{x}_j|_2 |\beta_j| \right)$$

- ◀ The Dantzig selector of Candès and Tao (2007) is

$$\hat{\beta}^{\text{DS}} = \arg \min_{\beta \in \mathbb{R}^p} \left\{ \sum_{j=1}^p |\mathbf{x}_j|_2 |\beta_j| : \max_{j=1, \dots, p}, \frac{|\mathbf{x}_j^\top (\mathbf{Y} - \mathbf{X}\beta)|}{|\mathbf{x}_j|_2} \leq \lambda \right\}$$

For a tuning parameter satisfying $\lambda \propto 1/\sigma^*$, if \mathbf{X} is “nice”, sharp oracle inequalities are available, e.g., Bickel *et al.* (2009).

$$\mathbf{E} \left(\frac{1}{T} \|\mathbf{X}(\hat{\beta}^\bullet - \beta)\|_2^2 \right) \leq C \frac{p^* \log(p)}{T}.$$

To correctly tune the parameter λ , the knowledge of σ^* is necessary.

Joint estimation of β^* and σ^* (1/2)

- ◀ Scaled Lasso, [Städler et al. \(2010\)](#),

$$(\hat{\beta}^{\text{ScL}}, \hat{\sigma}^{\text{ScL}}) = \arg \min_{\beta, \sigma} \left(T \log(\sigma) + \frac{\|\mathbf{Y} - \mathbf{X}\beta\|_2^2}{2\sigma^2} + \frac{\lambda}{\sigma} \sum_{j=1}^p \|\mathbf{x}_j\|_2 |\beta_j| \right).$$

This can be recast in a convex problem (do $\rho := \frac{1}{\sigma}$ and $\phi := \frac{\beta}{\sigma}$):

$$\arg \min_{\phi, \rho} \left(-T \log(\rho) + \frac{\|\rho \mathbf{Y} - \mathbf{X}\phi\|_2^2}{2} + \lambda \sum_{j=1}^p \|\mathbf{x}_j\|_2 |\phi_j| \right).$$

- ◀ Scaled DS version proposed by [Dalalyan & Chen \(2012\)](#): sharp analysis and computational advantages.

Joint estimation of β^* and σ^* (2/2)

- ◀ Square-Root Lasso Antoniadis (2010), Belloni *et al.* (2011), Sun & Zhang (2012),

$$\hat{\beta}^{\text{SqR-Lasso}} = \arg \min_{\beta} \left(\|\mathbf{Y} - \mathbf{X}\beta\|_2 + \lambda \sum_{j=1}^p |\mathbf{X}_j|_2 |\beta_j| \right)$$

$$\hat{\sigma}^{\text{SqR-Lasso}} = T^{-1/2} \|\mathbf{Y} - \mathbf{X}\hat{\beta}^{\text{SqR-Lasso}}\|_2.$$

- ◀ Self Tuning Instrumental Variables (STIV) Gautier & Tsybakov (2011), $(\hat{\beta}^{\text{STIV}}, \hat{\sigma}^{\text{STIV}})$ minimizes

$$\sigma + \lambda \sum_{j=1}^p |\mathbf{X}_j|_2 |\beta_j|$$

subject to the constraints

$$\|\mathbf{Y} - \mathbf{X}\beta\|_2 \leq \sigma; \quad \forall j = 1, \dots, p, |\mathbf{X}_j^\top (\mathbf{Y} - \mathbf{X}\beta)| \leq \tilde{\lambda} |\mathbf{X}_j|_2.$$

If the two tuning parameters coincide $\lambda = \tilde{\lambda}$, STIV = SqR-Lasso.

Some remarks

- If the design matrix \mathbf{X} satisfies some “nice” conditions (RIP, RE,...), the theoretical guarantees for the methods presented in this part are almost as strong as for the Lasso and the DS with known σ^* .
- All the estimators presented in this part are computable by solving a simple convex program. This can be done efficiently even for large dimensions p .
- Extensions to the matrix estimation under the rank-sparsity available [Klopp \(2012\)](#).

III. Main results

Functional transformation

- Re-parametrize by the inverse of the conditional standard deviation s^*

$$r^*(\mathbf{x}) = \frac{1}{s^*(\mathbf{x})} \quad \text{and} \quad f^*(\mathbf{x}) = \frac{b^*(\mathbf{x})}{s^*(\mathbf{x})}.$$

- This leads to

$$r^*(\mathbf{x}_t) \cdot y_t = f^*(\mathbf{x}_t) + \xi_t, \quad t = 1, \dots, T,$$

where $r^* : \mathbb{R}^d \rightarrow \mathbb{R}$ is the inverse of conditional standard deviation (StD) and f^* is the conditional signal-to-noise ratio.

- We impose modeling assumptions on the pair (r^*, f^*) rather than on (s^*, b^*) .

Main assumptions on b^* and s^*

Group Sparsity Assumption

For p given functions f_1, \dots, f_p mapping \mathbb{R}^d into \mathbb{R} , there is a vector $\phi^* \in \mathbb{R}^p$ such that

$$f^*(\mathbf{x}) = \sum_{j=1}^p \phi_j^* f_j(\mathbf{x}).$$

Furthermore, for a given partition G_1, \dots, G_K of $\{1, \dots, p\}$, the vector ϕ^* is group-sparse that is

$$\text{Card}(\{k : |\phi_{G_k}^*|_2 \neq 0\}) \ll K.$$

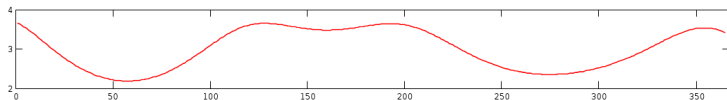
Low dimensional inverse StD assumption

For q given functions r_1, \dots, r_q mapping \mathbb{R}^d into \mathbb{R}_+ , there is a vector $\alpha^* \in \mathbb{R}^q$ such that

$$r^*(\mathbf{x}) = \sum_{\ell=1}^q \alpha_\ell^* r_\ell(\mathbf{x}), \quad \forall \mathbf{x} \in \mathbb{R}^d.$$

Motivations for these assumptions

- ▶ **Group sparsity assumption** is relevant in a sparse additive model, that is when
 - ↪ $\mathbf{f}^*(\mathbf{x}) = \psi_1(x_1) + \dots + \psi_d(x_d)$ s.t. $\psi_j \equiv \mathbf{0}$ for most j ,
 - ↪ projection on basis $\psi_j(x_j) \approx \sum_{\ell=1}^{K_j} \phi_{\ell,j}^* f_{\ell}(x_j)$,
 - ↪ group sparsity of $\phi = (\phi_{\ell,j})$.
- ▶ **Low dimensionality of the inverse StD** occurs, for instance when the noise is block-wise homoscedastic or periodic.



Estimation for heteroscedastic regression

Observations : $(\mathbf{x}_t, y_t)_{t=1, \dots, T}$ obeying

$$y_t = \mathbf{b}^*(\mathbf{x}_t) + \mathbf{s}^*(\mathbf{x}_t) \xi_t = \mathbf{r}^*(\mathbf{x}_t)^{-1} (\mathbf{f}^*(\mathbf{x}_t) + \xi_t).$$

Under our assumptions

$$\begin{aligned} \mathbf{f}^*(\mathbf{x}_t) &= \sum_{j=1}^p \phi_j^* \mathbf{f}_j(\mathbf{x}_t) = \mathbf{X}(t) \boldsymbol{\phi}^*, \\ \mathbf{r}^*(\mathbf{x}_t) &= \sum_{\ell=1}^q \alpha_\ell^* r_\ell(\mathbf{x}_t) = \mathbf{R}(t) \boldsymbol{\alpha}^*. \end{aligned}$$

Thus,

$$\begin{bmatrix} \mathbf{f}^*(\mathbf{x}_1) \\ \vdots \\ \mathbf{f}^*(\mathbf{x}_T) \end{bmatrix} = \mathbf{X} \boldsymbol{\phi}^* \quad \text{and} \quad \begin{bmatrix} \mathbf{r}^*(\mathbf{x}_1) \\ \vdots \\ \mathbf{r}^*(\mathbf{x}_T) \end{bmatrix} = \mathbf{R} \boldsymbol{\alpha}^*.$$

This leads to

$$\mathbf{D}_Y \mathbf{R} \boldsymbol{\alpha}^* = \mathbf{X} \boldsymbol{\phi}^* + \boldsymbol{\xi}, \quad \mathbf{D}_Y = \text{diag}(y_1, \dots, y_T).$$

Estimation for heteroscedastic regression

Scaled Heteroscedastic Lasso : $(\hat{\phi}^{\text{ScHeL}}, \hat{\alpha}^{\text{ScHeL}})$ solution to

$$\min_{(\phi, \alpha)} \left\{ \underbrace{-\sum_{t=1}^T \log(\mathbf{R}(t)\alpha) + \frac{1}{2} \|\mathbf{D}_Y \mathbf{R}\alpha - \mathbf{X}\phi\|_2^2}_{\text{Gaussian negative log-likelihood}} + \underbrace{\sum_{k=1}^K \lambda_k \|\mathbf{X}_{G_k} \phi_{G_k}\|_2}_{\text{sparsity promoting penalty}} \right\}.$$

- The optimization problem is convex.
- ... but the gradient of the objective is not Lipschitz.

Scaled Heteroscedastic Dantzig selector (ScHeDs) :

$(\hat{\phi}^{\text{ScHeDs}}, \hat{\alpha}^{\text{ScHeDs}})$ solution to

$$\min_{(\phi, \alpha) \in \mathbb{R}^{p+q}} \sum_{k=1}^K \lambda_k |\mathbf{X}_{G_k} \phi_{G_k}|_2 \quad \text{s.t.}$$

$$\left| \mathbf{\Pi}_{G_k} (\text{diag}(\mathbf{Y}) \mathbf{R} \alpha - \mathbf{X} \phi) \right|_2 \leq \lambda_k, \quad \forall k \in \{1, \dots, K\};$$

$$\sum_{t=1}^T \frac{\mathbf{R}_{t\ell}}{\mathbf{R}_{t,:} \alpha} \leq (y_t \mathbf{R}_{t,:} \alpha - \mathbf{X}_{t,:} \phi) y_t \mathbf{R}_{t\ell}, \quad \forall \ell \in \{1, \dots, q\};$$

Theorem : ScHeDs can be solved by an SOCP. Furthermore, the feasible set of this problem is not empty and contains, in particular, the ScHeL.

Comments on the procedure

- Degrees of freedom :
 - ↪ Many tuning parameters in the procedure
 - ↪ Theory : $\lambda_k = \lambda_0 \sqrt{r_k}$ with $\lambda_0 > 0$ and $r_k = \text{rank}(\mathbf{X}_{G_k})$
 - ↪ Most papers use $\lambda_k \propto \sqrt{|G_k|}$ ($k = 1, \dots, K$)
- One can include additional constraints of boundedness of the conditional mean or conditional standard deviation without breaking convexity.
- Bias Correction, practical improvement :
 - ↪ Classical two-steps methods :
 - our algorithm with $\lambda_k = \lambda_0 \sqrt{r_k}$ ($k = 1, \dots, K$)
 - Least squares on the selected variables ($\lambda = 0$)

Comments on the implementation

Several off-the-shelves toolboxes (for instance in Matlab) exist to deal with SOCP

- Sedumi **Sturm (1999)** : popular interior point methods
<http://sedumi.ie.lehigh.edu/>
↪ highly accurate solution for moderately large datasets, *e.g.* $p, T \leq 2000$
- Tfocs **Becker et al. (2011)** : first-order proximal method
<http://cvxr.com/tfocs/>
↪ less accurate (but do we need high accuracy in a noisy setting ?)
BUT can handle large scale datasets.

Finite sample risk bounds for the ScHeDs

Theorem

Consider the aforementioned heteroscedastic model with sub-Gaussian errors ξ . Let K^* (resp. p^*) be the number of relevant groups (resp. coordinates of ϕ^*). Let $\varepsilon \in (0, 1)$ be a tolerance level and set

$$\lambda_k = 4(\sqrt{\text{rank}(\mathbf{X}_{G_k})} + \sqrt{\log(K/\varepsilon)}).$$

Under some assumptions, with probability at least $1 - 2\varepsilon$,

$$\|\mathbf{X}(\hat{\phi} - \phi^*)\|_2 \leq D_{T,\varepsilon}^{3/2} \sqrt{q \log(2q/\varepsilon)} + D_{T,\varepsilon} \sqrt{p^* + K^* \log(K/\varepsilon)}.$$

$$\|\mathbf{R}(\hat{\alpha} - \alpha^*)\|_2 \leq D_{T,\varepsilon}^{3/2} \sqrt{q \log(2q/\varepsilon)} + D_{T,\varepsilon} \sqrt{p^* + K^* \log(K/\varepsilon)},$$

where $D_{T,\varepsilon} \propto (\max_t |f^*(\mathbf{x}_t)| + \log(2T/\varepsilon))$.

IV. Numerical experiments

Homoscedastic noise

Data : 500 repetitions :

- Design matrix : $\mathbf{X} \in \mathbb{R}^{T \times p}$ i.i.d. entries $\mathcal{N}(0, 1)$
- Noise vector : $\boldsymbol{\xi} \sim \mathcal{N}(\mathbf{0}_T, \mathbf{I}_{T \times T})$ independent of \mathbf{X} ; $\sigma_t \equiv \sigma^*$
- Regression vector : $\boldsymbol{\beta}^0 = [\mathbf{1}_{p^*}, \mathbf{0}_{p-p^*}]^\top$;
 \hookrightarrow permutation of the entries of $\boldsymbol{\beta}^0$ gives $\boldsymbol{\beta}^*$;
- Response vector : $\mathbf{Y} = \mathbf{X}\boldsymbol{\beta}^* + \sigma^*\boldsymbol{\xi}$.

Setting : 8 different settings varying (T, p, p^*, σ^*)

Challenger : Square-root Lasso

Tuning parameter : universal choice for both $\lambda = \sqrt{2 \log(p)}$ as good in most cases as Cross Validation, cf. Sun and Zhang (2012)

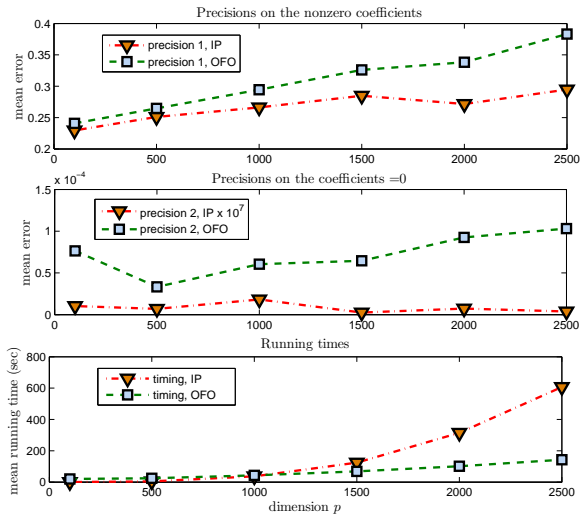


FIGURE: Comparing interior point (IP) vs. optimal first-order (OFO) method. Top & middle : MSE of $\hat{\beta}^{\text{ScHeDs}}$. Bottom : running times.

Experiment with bias correction for the two methods :

ScHeDs (T, ρ, i^*, σ^*)	$ \hat{\beta} - \beta^* _2$		$ \hat{\rho} - \rho^* $		$10 \hat{\sigma} - \sigma^* $	
	Ave	StD	Ave	StD	Ave	StD
(100, 100, 2, .5)	.06	.03	.00	.00	.29	.21
(100, 100, 5, .5)	.11	.08	.01	.12	.32	.37
(100, 100, 2, 1)	.13	.07	.03	.16	.57	.46
(100, 100, 5, 1)	.28	.23	.10	.33	.77	.68
(200, 100, 5, .5)	.08	.02	.00	.00	.23	.16
(200, 100, 5, 1)	.16	.05	.00	.01	.09	.29
(200, 500, 8, .5)	.09	.03	.00	.00	.22	.16
(200, 500, 8, 1)	.21	.11	.03	.17	.48	.43

SqR Lasso	$ \hat{\beta} - \beta^* _2$		$ \hat{\rho} - \rho^* $		$10 \hat{\sigma} - \sigma^* $	
	Ave	StD	Ave	StD	Ave	StD
(100, 100, 2, .5)	.08	.06	.19	.44	.32	.23
(100, 100, 5, .5)	.12	.04	.18	.42	.33	.24
(100, 100, 2, 1)	.16	.10	.19	.44	.59	.48
(100, 100, 5, 1)	.25	.16	.21	.43	.68	.47
(200, 100, 5, .5)	.09	.03	.21	.45	.24	.17
(200, 100, 5, 1)	.18	.07	.21	.48	.48	.32
(200, 500, 8, .5)	.10	.03	.14	.38	.23	.17
(200, 500, 8, .5)	.21	.07	.18	.40	.46	.34

Real data : temperature in Paris

Data : daily temperature in Paris from 2003 to 2008 ;

↪ National Climatic Data Center (NCDC).

- Response variable y_t : the difference of temperature between two successive days.
- Covariates $\mathbf{x}_t = (t, \mathbf{u}_t)$: 17 dimensional vector (16+1)
 - ↪ time t ;
 - ↪ increments of temperature over the past 7 days ;
 - ↪ maximal intraday variation of temperature over the past 7 days ;
 - ↪ wind speed of the day before.

Construction of \mathbf{R} : $T \times 11$ matrix with columns r_ℓ .

$$r_1(\mathbf{x}_t) = 1; \quad r_2(\mathbf{x}_t) = t; \quad r_3(\mathbf{x}_t) = 1/(t + 2 \times 365)^{\frac{1}{2}};$$

$$r_\ell(\mathbf{x}_t) = 1 + \cos(2\pi(\ell - 3)t/365); \quad \ell = 4, \dots, 7;$$

$$r_\ell(\mathbf{x}_t) = 1 + \cos(2\pi(\ell - 7)t/365); \quad \ell = 8, \dots, 11.$$

Construction of \mathbf{X} : $T \times 2176$ matrix with columns \mathbf{f}_j . \leftrightarrow

Time-varying second-order polynomial in \mathbf{u}_t :

$$\mathbf{f}_j(t) = \psi_\ell(t) \times \chi_{m,m'}(\mathbf{u}_t);$$

$$|\{\mathbf{f}_j\}| = 16 \times 16 \times 17/2 = 2176.$$

Construction of groups : 136 groups of 16 functions

$$\mathcal{G}_{m,m'} = \{\psi_\ell(t) \times \chi_{m,m'}(\mathbf{u}_t) : \ell = 1, \dots, 16\}.$$

Samples :

- ↪ Training set : temperatures from 2003 to 2007 (that is, 2172 values) ;
- ↪ Test set : temperatures from 2008 (that is, 366 values, leap year).

Conclusions of the study :

- Dimension reduction : from 2176 to 26 ;
- Sign estimation : 62% of right estimation ;
- Volatility estimation : the oscillation of the temperature during the period between May and July is significantly higher than in March, September and October ;

Summary

New procedures named ScHeL and ScHeDs :

- ◀ Suitable for fitting the heteroscedastic regression model.
- ◀ Simultaneous estimation of the mean and the variance functions.
- ◀ Takes into account group sparsity.
- ◀ Implemented using two different solvers :
 - ↪ primal-dual interior point method (highly accurate),
 - ↪ optimal first-order method (moderately accurate but with cheap iterations).
- ◀ Competitive with state-of-the art algorithms
 - ↪ applicable in a much more general framework.

Manuscript is available on arxiv, codes are available on request.



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