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Saddle Point Model Selection in Inverse Problems

Outline

1 Motivation

- Penalized model selection
- Saddle point model selection

2 SURE in linear inverse problem

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- A bound for the excess loss
- Projection estimates
- One-sided concentration: $\mathcal{N} > \mathcal{N}^*$
- One-sided concentration: $\mathcal{N} < \mathcal{N}^*$
- Spectral cut-off estimation
- Unordered case

3 Saddle point model selection

- Penalty calibration
- Oracle bound for a SP selector
- Special cases

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- ▶ Observed a vector $\mathbf{Y} = (Y_1, \dots, Y_n) \in \mathbb{R}^n$.
- ▶ Model

$$Y_i = s_i + \sigma_i \varepsilon_i$$

where ε_i are iid standard normal and σ_i are given numbers.

- ▶ Direct problem: $\sigma_i \equiv \sigma$.
- ▶ Inverse problem: $\sigma_i \nearrow \infty$.
- ▶ Target: $\mathbf{s} = (s_i)$.

Linear estimates

Linear estimates \tilde{s} of s defined by a vector \mathcal{X}

$$\tilde{s} = \tilde{s}(\mathcal{X}).$$

The **estimation loss** and **risk** are given by

$$\rho(\mathcal{X}) = \sum_i [\tilde{s}_i(\mathcal{X}) - s_i]^2,$$

$$\mathcal{R}(\mathcal{X}) = \mathbb{E} \sum_i [\tilde{s}_i(\mathcal{X}) - s_i]^2.$$

Oracle choice of an estimate:

$$\mathcal{X}^* \stackrel{\text{def}}{=} \underset{\mathcal{X}}{\operatorname{argmin}} \mathcal{R}(\mathcal{X}).$$

Some previous works

- ▶ Unbiased Risk Estimation (SURE): C_p -Mallows (73), Akaike (74), Donoho and Johnstone (1995).
- ▶ Blockwise SURE: Pinsker (1984), Tsybakov (2001),
- ▶ Adaptive estimation for inverse problems: Cavalier and Tsybakov (2002), Goldenshluger (1999), Cavalier, Golubev, Lepski, Tsybakov (2003).
- ▶ Penalized Gaussian Model Selection (PMS): Birgé and Massart (2001, 2007), Baraud, Huet and Laurent (2003).
- ▶ Pairwise comparison, (Test) T-estimation: Lepski (1990), Goldenshluger and Lepski (2009), Birgé (2006), Baraud et al. (2009).
- ▶ Sparse Methods: thresholding, LASSO, regularized LASSO etc.: Donoho and Johnstone (1995), Tibshirani (1995), Candes Tao (2007), van de Geer (2007), Bickel, Ritov, Tsybakov (2009) ...

Unbiased risk estimate

The unbiased risk estimate is given by

$$\ell(\boldsymbol{\varkappa}) = \sum_i \{ [\tilde{s}_i(\boldsymbol{\varkappa}) - Y_i]^2 - \mathbb{E} [\tilde{s}_i(\boldsymbol{\varkappa}) - Y_i]^2 + \mathbb{E} [\tilde{s}_i(\boldsymbol{\varkappa}) - s_i]^2 \},$$

where

$$\mathbb{E} [\tilde{s}_i(\boldsymbol{\varkappa}) - Y_i]^2 - \mathbb{E} [\tilde{s}_i(\boldsymbol{\varkappa}) - s_i]^2$$

does not depend on \boldsymbol{s} because $\tilde{\boldsymbol{s}}(\boldsymbol{\varkappa})$ is linear. Obviously,

$$\mathbb{E} \ell(\boldsymbol{\varkappa}) = \mathbb{E} \sum_i [\tilde{s}_i(\boldsymbol{\varkappa}) - s_i]^2 = \mathcal{R}(\boldsymbol{\varkappa}).$$

SURE/AIC method

The minimization of SURE: define $\tilde{\varkappa}$ by minimizing the empirical counterpart $\ell(\varkappa)$ of $\mathcal{R}(\varkappa)$:

$$\tilde{\varkappa} = \operatorname{argmin}_{\varkappa} \ell(\varkappa).$$

Aim: to mimic the oracle choice:

$$\varkappa^* \stackrel{\text{def}}{=} \operatorname{argmin}_{\varkappa} \mathcal{R}(\varkappa).$$

Problem: poor performance for inverse problems, especially for severely ill-posed.

Ultimate Goal: establish a concentration property (oracle bound) regardless particular features of the risk function and degree of ill-posedness.

Penalized model selection (PMS) approach:

$$\hat{\mathcal{X}} = \underset{\mathcal{X}}{\operatorname{argmin}} \{ \ell(\mathcal{X}) + 2 \operatorname{pen}(\mathcal{X}) \},$$

where $z(\mathcal{X})$ mimics the complexity related to the choice of the estimate $\tilde{\mathcal{S}}(\mathcal{X})$. Can be rewritten in the form

$$\ell(\hat{\mathcal{X}}) + 2 \operatorname{pen}(\hat{\mathcal{X}}) \leq \ell(\mathcal{X}) + 2 \operatorname{pen}(\mathcal{X})$$

for all \mathcal{X} , or equivalently,

$$\ell(\hat{\mathcal{X}}, \mathcal{X}) \leq 2 \operatorname{pen}(\hat{\mathcal{X}}) - 2 \operatorname{pen}(\mathcal{X}).$$

Limitations of PMS. Alternative approaches

Major problem: $2[\text{pen}(\mathcal{M}') - \text{pen}(\mathcal{M})]$ is a poor critical value for $\ell(\mathcal{M}', \mathcal{M})$.

Alternative idea (to PMS) is to consider a bivariate function
 $\ell(\mathcal{M}', \mathcal{M}) = \ell(\mathcal{M}') - \ell(\mathcal{M})$.

Related proposals:

- ▶ Lepski (1990): ordered model selection via pairwise comparison of different estimates. Extensions to inverse problems due to Mathe and Pereversev among others.
- ▶ Goldenshluger and Lepski (2009): extension to unordered case.
- ▶ Birgé (2006): T-estimation (ideas already in Le Cam 1973, Birgé 1983).
- ▶ Dümbgen and Rohde (2009): for model selection via multiple testing; worst case calibration.

Risk minimization vs saddle point

Consider the risk difference as **functions of two arguments** \varkappa, \varkappa' :

$$\mathcal{R}(\varkappa, \varkappa') \stackrel{\text{def}}{=} \mathcal{R}(\varkappa) - \mathcal{R}(\varkappa').$$

The definition of \varkappa^* as the minimizer of the risk function $\mathcal{R}(\varkappa)$ can be rewritten in the form:

$$\varkappa^* = \underset{\varkappa}{\operatorname{argmin}} \mathcal{R}(\varkappa, \varkappa^*) = \underset{\varkappa}{\operatorname{argmax}} \mathcal{R}(\varkappa^*, \varkappa).$$

In other words, $(\varkappa^*, \varkappa^*)$ is a **saddle point** of the function $\mathcal{R}(\varkappa, \varkappa')$:

$$\varkappa^* = \underset{\varkappa}{\operatorname{argmin}} \max_{\varkappa'} \mathcal{R}(\varkappa, \varkappa') = \underset{\varkappa}{\operatorname{argmax}} \min_{\varkappa'} \mathcal{R}(\varkappa, \varkappa')$$

Model selection as a SP-problem

Basic observation: the minimizer of SURE $\ell(\mathcal{X})$ is a saddle point of $\ell(\mathcal{X}, \mathcal{X}') = \ell(\mathcal{X}) - \ell(\mathcal{X}')$.

SP-Approach: consider a penalized **bivariate** function

$$\ell(\mathcal{X}, \mathcal{X}') + 2 \text{PEN}(\mathcal{X}, \mathcal{X}') = \ell(\mathcal{X}) - \ell(\mathcal{X}') + 2 \text{PEN}(\mathcal{X}, \mathcal{X}')$$

and define the **penalized choice** of $\hat{\mathcal{X}}$ via the **smallest saddle point**:

$$\hat{\mathcal{X}} \stackrel{\text{def}}{=} \underset{\mathcal{X}}{\text{argmin}} \max_{\mathcal{X}'} \{ \ell(\mathcal{X}, \mathcal{X}') - 2 \text{PEN}(\mathcal{X}, \mathcal{X}') \}.$$

In other words, the value $\hat{\mathcal{X}}$ is a SP if it holds for any \mathcal{X}° :

$$\max_{\mathcal{X}} \{ \ell(\hat{\mathcal{X}}, \mathcal{X}) - 2 \text{PEN}(\hat{\mathcal{X}}, \mathcal{X}) \} \leq \max_{\mathcal{X}} \{ \ell(\mathcal{X}^\circ, \mathcal{X}) - 2 \text{PEN}(\mathcal{X}^\circ, \mathcal{X}) \}.$$

Implication of the SP choice

The value $\hat{\varkappa}$ is a SP if it holds for any \varkappa° :

$$\max_{\varkappa} \{ \ell(\hat{\varkappa}, \varkappa) - 2 \text{PEN}(\hat{\varkappa}, \varkappa) \} \leq \max_{\varkappa} \{ \ell(\varkappa^\circ, \varkappa) - 2 \text{PEN}(\varkappa^\circ, \varkappa) \}.$$

In particular, this inequality can be applied with $\varkappa = \varkappa^*$ yielding

$$\ell(\hat{\varkappa}, \varkappa^*) - 2 \text{PEN}(\hat{\varkappa}, \varkappa^*) \leq \max_{\varkappa} \{ \ell(\varkappa^*, \varkappa) - 2 \text{PEN}(\varkappa^*, \varkappa) \}. \quad (1)$$

If the penalty $\text{PEN}(\varkappa, \varkappa')$ ensures (with high proba) that

$$\max_{\varkappa} \{ \ell(\varkappa^*, \varkappa) - 2 \text{PEN}(\varkappa^*, \varkappa) \} \leq \xi^*$$

Then (1) implies

$$\boxed{\ell(\hat{\varkappa}, \varkappa^*) - 2 \text{PEN}(\hat{\varkappa}, \varkappa^*) \leq \xi^*}.$$

Relation to multiple testing idea

“ $\hat{\mathcal{N}}$ is a SP” can be rewritten as

$$\ell(\hat{\mathcal{N}}) - \ell(\mathcal{N}) \leq t(\hat{\mathcal{N}}, \mathcal{N})$$

for all $\mathcal{N} > \hat{\mathcal{N}}$, where

$$t(\hat{\mathcal{N}}, \mathcal{N}) = 2 \text{PEN}(\mathcal{N}, \hat{\mathcal{N}}).$$

Interpretation: $T(\mathcal{N}, \mathcal{N}') = \ell(\mathcal{N}) - \ell(\mathcal{N}')$, a **test statistic** for testing \mathcal{N} against \mathcal{N}' and $t(\mathcal{N}, \mathcal{N}')$ is the critical value of the test.

$\hat{\mathcal{N}}$ accepted if $\hat{\mathcal{N}}$ is not rejected against any $\mathcal{N} > \hat{\mathcal{N}}$.

Key words for the next:

- ▷ Cross-concentration bounds for excess loss
- ▷ One-sided concentration
- ▷ Oracle bound for saddle point model selection

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SURE: Problem formulation

“Oracle”:

$$\mathcal{X}^* \stackrel{\text{def}}{=} \underset{\mathcal{X}}{\operatorname{argmin}} \mathcal{R}(\mathcal{X})$$

Define

$$L_1(\mathcal{X}, \mathcal{X}^*) \stackrel{\text{def}}{=} \frac{1}{2} \{ \ell(\mathcal{X}^*) - \ell(\mathcal{X}) \}.$$

Then

$$\tilde{\mathcal{X}} = \underset{\mathcal{X}}{\operatorname{argmin}} \ell(\mathcal{X}) = \underset{\mathcal{X}}{\operatorname{argmax}} L_1(\mathcal{X}, \mathcal{X}^*).$$

Problem: to bound **excess loss**

$$L_0(\tilde{\mathcal{X}}, \mathcal{X}^*) \stackrel{\text{def}}{=} \frac{1}{2} \{ \rho(\tilde{\mathcal{X}}) - \rho(\mathcal{X}^*) \}.$$

Rate function

For $L_1(\boldsymbol{x}, \boldsymbol{x}^*) \stackrel{\text{def}}{=} \frac{1}{2} \{ \ell(\boldsymbol{x}^*) - \ell(\boldsymbol{x}) \}$ and a fixed $\mu_1 > 0$, define

$$\mathcal{M}_1(\mu_1, \boldsymbol{x}, \boldsymbol{x}^*) \stackrel{\text{def}}{=} -\log \mathbb{E} \exp\{\mu_1 L_1(\boldsymbol{x}, \boldsymbol{x}^*)\}$$

implying

$$\mathbb{E} \exp\{\mu_1 L_1(\boldsymbol{x}, \boldsymbol{x}^*) + \mathcal{M}_1(\mu_1, \boldsymbol{x}, \boldsymbol{x}^*)\} = 1.$$

Define the **rate function**

$$\mathcal{M}_1(\boldsymbol{x}, \boldsymbol{x}^*) = \mathcal{M}_1(\mu_1(\boldsymbol{x}, \boldsymbol{x}^*), \boldsymbol{x}, \boldsymbol{x}^*),$$

where $\mu_1(\boldsymbol{x}, \boldsymbol{x}^*)$ (nearly) maximizes $\mathcal{M}_1(\mu_1, \boldsymbol{x}, \boldsymbol{x}^*)$ w.r.t. μ_1 .

Concentration of the empirical risk $\ell(\mathcal{x}, \mathcal{x}^*)$

Theorem

Let \mathcal{K} be a *discrete set* and let $z(\mathcal{x}, \mathcal{x}^*)$ satisfy

$$\sum_{\mathcal{x} \in \mathcal{K}} \exp\{-z(\mathcal{x}, \mathcal{x}^*)\} = \Omega^* < \infty.$$

Then

$$\mathcal{C}_1(\mathcal{x}, \mathcal{x}^*) \stackrel{\text{def}}{=} \mathcal{M}_1(\mathcal{x}, \mathcal{x}^*) - z(\mathcal{x}, \mathcal{x}^*)$$

is a *concentration function* for $L_1(\mathcal{x}, \mathcal{x}^*)$ in the sense that

$$\mathbb{E} \sup_{\mathcal{x} \in \mathcal{K}} \exp\{\mu_1(\mathcal{x}, \mathcal{x}^*)L_1(\mathcal{x}, \mathcal{x}^*) + \mathcal{C}_1(\mathcal{x}, \mathcal{x}^*)\} \leq \Omega^*.$$

Concentration sets

Concentration bound: for $\mathcal{C}_1(\mathcal{X}, \mathcal{X}^*) = \mathcal{M}_1(\mathcal{X}, \mathcal{X}^*) - z(\mathcal{X}, \mathcal{X}^*)$

$$\mathbb{E} \sup_{\mathcal{X} \in \mathcal{K}} \exp\{\mu_1(\mathcal{X}, \mathcal{X}^*)L_1(\mathcal{X}, \mathcal{X}^*) + \mathcal{C}_1(\mathcal{X}, \mathcal{X}^*)\} \leq \Omega^*,$$

Concentration set: $\mathcal{A}_1(\mathfrak{z}) \stackrel{\text{def}}{=} \{\mathcal{X} : \mathcal{C}_1(\mathcal{X}, \mathcal{X}^*) \leq \mathfrak{z}\}$. By $L_1(\tilde{\mathcal{X}}, \mathcal{X}^*) \geq 0$:

$$\mathbb{P}(\tilde{\mathcal{X}} \notin \mathcal{A}_1(\mathfrak{z})) = \mathbb{P}(\mathcal{C}_1(\mathcal{X}, \mathcal{X}^*) > \mathfrak{z}) \leq \Omega^* e^{-\mathfrak{z}}.$$

Concentration of emp. risk: with $\mathfrak{b}_1(\mathfrak{z}) \stackrel{\text{def}}{=} \min_{\mathcal{X} \in \mathcal{K}} \{\mathfrak{z}\mu_1(\mathcal{X}, \mathcal{X}^*) + \mathcal{C}_1(\mathcal{X}, \mathcal{X}^*)\}$

$$\mathbb{P}(L_1(\tilde{\mathcal{X}}, \mathcal{X}^*) > \mathfrak{z}) \leq \Omega^* \exp\{-\mathfrak{b}_1(\mathfrak{z})\}.$$

Concentration of the loss

Consider

$$L_0(\varkappa, \varkappa^*) \stackrel{\text{def}}{=} \{\rho(\varkappa) - \rho(\varkappa^*)\}/2$$

$$\mathcal{M}_0(\mu_0, \varkappa, \varkappa^*) \stackrel{\text{def}}{=} -\log \mathbb{E} \exp\{\mu_0 L_0(\varkappa, \varkappa^*)\}.$$

Assume $\mu_0(\varkappa, \varkappa^*)$ is fixed for $\varkappa \in \mathcal{K}$ defining

$$\mathcal{M}_0(\varkappa, \varkappa^*) \stackrel{\text{def}}{=} \mathcal{M}_0(\mu_0(\varkappa, \varkappa^*), \varkappa, \varkappa^*) \geq 0.$$

For $\mathcal{C}_0(\varkappa, \varkappa^*) = \mathcal{M}_0(\varkappa, \varkappa^*) - z(\varkappa, \varkappa^*)$, it holds:

$$\mathbb{E} \sup_{\varkappa \in \mathcal{K}} \exp\{\mu_0(\varkappa, \varkappa^*) L_0(\varkappa, \varkappa^*) + \mathcal{C}_0(\varkappa, \varkappa^*)\} \leq \Omega^*.$$

Yields **concentration sets** and **concentration bound**.

Cross Concentration

Now consider

$$L_0(\boldsymbol{x}, \boldsymbol{x}^*) \stackrel{\text{def}}{=} \{\rho(\boldsymbol{x}) - \rho(\boldsymbol{x}^*)\}/2.$$

Aim: a bound for $L_0(\tilde{\boldsymbol{x}}, \boldsymbol{x}^*)$ with

$$\tilde{\boldsymbol{x}} = \underset{\boldsymbol{x}}{\operatorname{argmin}} \ell(\boldsymbol{x}) = \underset{\boldsymbol{x}}{\operatorname{argmax}} L_1(\boldsymbol{x}, \boldsymbol{x}^*).$$

Idea: consider **linear combinations**

$$\mathcal{L}(\boldsymbol{x}, \boldsymbol{x}^*) \stackrel{\text{def}}{=} \mu_1(\boldsymbol{x}, \boldsymbol{x}^*)L_1(\boldsymbol{x}, \boldsymbol{x}^*) + \mu_0(\boldsymbol{x}, \boldsymbol{x}^*)L_0(\boldsymbol{x}, \boldsymbol{x}^*).$$

Define the rate function

$$\mathcal{M}(\boldsymbol{x}, \boldsymbol{x}^*) \stackrel{\text{def}}{=} -\log \mathbb{E} \exp\{\mathcal{L}(\boldsymbol{x}, \boldsymbol{x}^*)\}.$$

Concentration bound

Theorem

Let

$$\sum_{\mathcal{K}} \exp\{-z(\mathcal{u}, \mathcal{u}^*)\} = \Omega^* < \infty.$$

Then

$$\mathcal{C}(\mathcal{u}, \mathcal{u}^*) \stackrel{\text{def}}{=} \mathcal{M}(\mathcal{u}, \mathcal{u}^*) - z(\mathcal{u}, \mathcal{u}^*)$$

is a *concentration function* for $\mathcal{L}(\mathcal{u}, \mathcal{u}^*)$ in the sense that

$$\mathbb{E} \sup_{\mathcal{u} \in \mathcal{K}} \exp\{\mathcal{L}(\mathcal{u}, \mathcal{u}^*) + \mathcal{C}(\mathcal{u}, \mathcal{u}^*)\} \leq \Omega^*.$$

Concentration of the excess loss

Corollary

Let

$$\mathbb{E} \sup_{\mathcal{K}} \exp \left\{ \mathcal{L}(\mathcal{K}, \mathcal{K}^*) + \mathcal{C}(\mathcal{K}, \mathcal{K}^*) \right\} \leq \mathfrak{Q}^*.$$

Define for $\mathfrak{z} \geq 0$

$$\mathfrak{b}(\mathfrak{z}) \stackrel{\text{def}}{=} \inf_{\mathcal{K} \in \mathcal{K}} \left\{ \mathfrak{z} \mu_0(\mathcal{K}, \mathcal{K}^*) + \mathcal{C}(\mathcal{K}, \mathcal{K}^*) \right\}.$$

Then for any $\mathfrak{z} \geq 0$, it holds for $L_0(\tilde{\mathcal{K}}, \mathcal{K}^*) = \{\rho(\tilde{\mathcal{K}}) - \rho(\mathcal{K}^*)\}/2$

$$\mathbb{P} \left\{ L_0(\tilde{\mathcal{K}}, \mathcal{K}^*) > \mathfrak{z} \right\} = \mathbb{P} \left\{ \rho(\tilde{\mathcal{K}}) - \rho(\mathcal{K}^*) > 2\mathfrak{z} \right\} \leq \mathfrak{Q}^* e^{-\mathfrak{b}(\mathfrak{z})}.$$

Proof

From definition, $L_1(\tilde{\mathcal{X}}, \mathcal{X}^*) \geq 0$ and

$$\mathfrak{b}(\mathfrak{z}) \leq \{\mathfrak{z} \mu_0(\tilde{\mathcal{X}}, \mathcal{X}^*) + \mathcal{C}(\tilde{\mathcal{X}}, \mathcal{X}^*)\}.$$

Therefore

$$\begin{aligned} & \mathbb{P}\{L_0(\tilde{\mathcal{X}}, \mathcal{X}^*) > \mathfrak{z}\} \\ & \leq \mathbb{P}\{\mu_0(\tilde{\mathcal{X}}, \mathcal{X}^*)L_0(\tilde{\mathcal{X}}, \mathcal{X}^*) + \mu_1(\tilde{\mathcal{X}}, \mathcal{X}^*)L_1(\tilde{\mathcal{X}}, \mathcal{X}^*) > \mu_0(\tilde{\mathcal{X}}, \mathcal{X}^*)\mathfrak{z}\} \\ & \leq \mathbb{P}\{\mathcal{L}(\tilde{\mathcal{X}}, \mathcal{X}^*) + \mathcal{C}(\tilde{\mathcal{X}}, \mathcal{X}^*) > \mu_0(\tilde{\mathcal{X}}, \mathcal{X}^*)\mathfrak{z} + \mathcal{C}(\tilde{\mathcal{X}}, \mathcal{X}^*)\} \\ & \leq \mathbb{P}\{\mathcal{L}(\tilde{\mathcal{X}}, \mathcal{X}^*) + \mathcal{C}(\tilde{\mathcal{X}}, \mathcal{X}^*) > \mathfrak{b}(\mathfrak{z})\} \\ & \leq e^{-\mathfrak{b}(\mathfrak{z})} \mathbb{E} \exp\{\mathcal{L}(\tilde{\mathcal{X}}, \mathcal{X}^*) + \mathcal{C}(\tilde{\mathcal{X}}, \mathcal{X}^*)\}. \end{aligned}$$

Projection estimates

Consider $\tilde{s}_i(\boldsymbol{\varkappa}) = \varkappa_i Y_i$, where $\boldsymbol{\varkappa} = (\varkappa_i)$, with $\varkappa_i \in \{0, 1\}$. Then

$$\rho(\boldsymbol{\varkappa}) = \sum_i (\varkappa_i Y_i - s_i)^2 = \sum_{i: \varkappa_i=0} s_i^2 + \sum_{i: \varkappa_i=1} (Y_i - s_i)^2,$$

$$\mathcal{R}(\boldsymbol{\varkappa}) = \mathbb{E} \sum_i (\varkappa_i Y_i - s_i)^2 = \sum_{i: \varkappa_i=0} s_i^2 + \sum_{i: \varkappa_i=1} \sigma_i^2$$

$$\mathcal{R}(\boldsymbol{\varkappa}, \boldsymbol{\varkappa}^*) \stackrel{\text{def}}{=} \mathcal{R}(\boldsymbol{\varkappa}) - \mathcal{R}(\boldsymbol{\varkappa}^*) = - \sum_i \delta_i (s_i^2 - \sigma_i^2) \geq 0,$$

where $\delta_i = \varkappa_i - \varkappa_i^* \in \{1, 0, -1\}$.

One-sided concentration: $\mathcal{K} > \mathcal{K}^*$

Let $\mathcal{K}^* = \operatorname{argmin}_{\mathcal{K}} \mathcal{R}(\mathcal{K}) = \operatorname{argmin}_{\mathcal{K}} \mathcal{R}(\mathcal{K}, \mathcal{K}^*)$.

Let $\mathcal{K} \geq \mathcal{K}'$ mean partial ordering. Consider

$$\mathcal{K}^+(\mathcal{K}^*) = \{\mathcal{K} \in \mathcal{K} : \mathcal{K} > \mathcal{K}^*\}.$$

Requirement to the procedure: restricted to $\mathcal{K}^+(\mathcal{K}^*)$, the selected model should be nearly oracle. Equivalently: the event

$$\{L_1(\mathcal{K}, \mathcal{K}^*) < 0\} = \{\ell(\mathcal{K}) - \ell(\mathcal{K}^*) < 0\}, \quad \mathcal{K} > \mathcal{K}^*$$

only possible for $\mathcal{K} \approx \mathcal{K}^*$. Expected if

$$\mathbb{E}L_1(\mathcal{K}, \mathcal{K}^*) = \mathcal{R}(\mathcal{K}, \mathcal{K}^*) \gg \operatorname{Var}^{1/2}(L_1(\mathcal{K}, \mathcal{K}^*)).$$

$\mathcal{N} > \mathcal{N}^*$: loss and risk

We write $\mathcal{N} \geq \mathcal{N}^*$ if $\mathcal{N}_i \geq \mathcal{N}_i^*$ for all i . For projection estimates, this means $\mathcal{J}_{\mathcal{N}^*} \subset \mathcal{J}_{\mathcal{N}}$, where $\mathcal{J}_{\mathcal{N}} = \{i : \mathcal{N}_i = 1\}$.

Define

$$V^2(\mathcal{N}, \mathcal{N}^*) \stackrel{\text{def}}{=} \sum_{\mathcal{J}_{\mathcal{N}} \setminus \mathcal{J}_{\mathcal{N}^*}} \sigma_i^2, \quad B(\mathcal{N}, \mathcal{N}^*) \stackrel{\text{def}}{=} \sum_{\mathcal{J}_{\mathcal{N}} \setminus \mathcal{J}_{\mathcal{N}^*}} s_i^2.$$

It holds

$$\mathcal{R}(\mathcal{N}, \mathcal{N}^*) = \sum_{\mathcal{J}_{\mathcal{N}} \setminus \mathcal{J}_{\mathcal{N}^*}} (-s_i^2 + \sigma_i^2) = V^2(\mathcal{N}, \mathcal{N}^*) - B(\mathcal{N}, \mathcal{N}^*).$$

The definition of \mathcal{N}^* implies $B(\mathcal{N}, \mathcal{N}^*) \leq V^2(\mathcal{N}, \mathcal{N}^*)$ and $\mathcal{R}(\mathcal{N}, \mathcal{N}^*) \leq V^2(\mathcal{N}, \mathcal{N}^*)$.

$\varkappa > \varkappa^*$: rate function

Fix μ_0, μ_1 and $\mathcal{L}(\varkappa, \varkappa^*) = \mu_0 L_0(\varkappa, \varkappa^*) + \mu_1 L_1(\varkappa, \varkappa^*)$:

If $\mu_1 + \mu_0 < \sigma^{-2}(\varkappa, \varkappa^*)$ with $\sigma(\varkappa, \varkappa^*) = \max_{i \in \mathcal{J}_\varkappa} \sigma_i$, then

$$\mathbb{E}\mathcal{L}(\mu_0, \mu_1, \varkappa, \varkappa^*) = \frac{\mu_1 - \mu_0}{2} \mathcal{R}(\varkappa, \varkappa^*),$$

$$\text{Var}(\mathcal{L}(\mu_0, \mu_1, \varkappa, \varkappa^*)) \asymp (\mu_0 + \mu_1)^2 \sigma^2(\varkappa, \varkappa^*) V^2(\varkappa, \varkappa^*),$$

and

$$\mathcal{M}(\mu_0, \mu_1, \varkappa, \varkappa^*) \geq \frac{\mu_1 - \mu_0}{2} \mathcal{R}(\varkappa, \varkappa^*) - C(\mu_0 + \mu_1)^2 \sigma^2(\varkappa, \varkappa^*) V^2(\varkappa, \varkappa^*).$$

$\varkappa > \varkappa^*$: correction for multiplicity

Let

$$\sum_{\varkappa > \varkappa^*} \exp\{-z(\varkappa, \varkappa^*)\} \leq \Omega^+.$$

Define

$$\mu(\varkappa, \varkappa^*) \stackrel{\text{def}}{=} \frac{\sqrt{z(\varkappa, \varkappa^*)}}{\sigma(\varkappa, \varkappa^*)V(\varkappa, \varkappa^*)} \quad \varkappa > \varkappa^*,$$

and for some $\alpha_0 \leq \alpha_1$, set

$$\mu_0(\varkappa, \varkappa^*) = \alpha_0 \mu(\varkappa, \varkappa^*) \quad \mu_1(\varkappa, \varkappa^*) = \alpha_1 \mu(\varkappa, \varkappa^*)$$

Denote

$$\mathcal{M}(\varkappa, \varkappa^*; \alpha_0, \alpha_1) \stackrel{\text{def}}{=} \mathcal{M}(\alpha_0 \mu(\varkappa, \varkappa^*), \alpha_1 \mu(\varkappa, \varkappa^*), \varkappa, \varkappa^*).$$

$\varkappa > \varkappa^*$: One-sided concentration

Theorem

Let $\sum_{\varkappa > \varkappa^*} \exp\{-z(\varkappa, \varkappa^*)\} \leq \Omega^+$. Let $\alpha_1 > \alpha_0$ be s.t.

$$(\alpha_0 + \alpha_1)\mu(\varkappa, \varkappa^*)\sigma^2(\varkappa, \varkappa^*) = \frac{(\alpha_0 + \alpha_1)\sigma(\varkappa, \varkappa^*)\sqrt{z(\varkappa, \varkappa^*)}}{V(\varkappa, \varkappa^*)} \leq c < 1,$$

Then

$$\mathbb{P}\left(\rho(\tilde{\varkappa}) - \rho(\varkappa^*) \geq 2\mathfrak{z}, \tilde{\varkappa} > \varkappa^*\right) \leq \Omega^+ \exp\{-\mathfrak{b}^+(\mathfrak{z}; \alpha_0, \alpha_1)\}$$

with

$$\mathfrak{b}^+(\mathfrak{z}; \alpha_0, \alpha_1) \stackrel{\text{def}}{=} \min_{\varkappa > \varkappa^*} \{\mathfrak{z} \alpha_0 \mu(\varkappa, \varkappa^*) + \mathcal{M}(\varkappa, \varkappa^*; \alpha_0, \alpha_1) - z(\varkappa, \varkappa^*)\}.$$

$\varkappa > \varkappa^*$: Conditions on the risk function

Theorem

If for every $\varkappa > \varkappa^*$

$$\mathcal{R}(\varkappa, \varkappa^*) \geq \mathfrak{t} \sigma(\varkappa, \varkappa^*) V(\varkappa, \varkappa^*) \sqrt{z(\varkappa, \varkappa^*)},$$

where the constant \mathfrak{t} is sufficiently large to ensure that

$$\delta \stackrel{\text{def}}{=} \frac{1}{2} \left[\mathfrak{t}(\alpha_1 - \alpha_0) - q^+(c)(\alpha_1 + \alpha_0)^2 - (1 - c)^{-1} \alpha_1^2 \right] - 1 > 0,$$

then

$$\mathfrak{b}^+(\mathfrak{z}; \alpha_0, \alpha_1) \geq \min_{\varkappa > \varkappa^*} \left\{ \frac{\mathfrak{z} \alpha_0 \sqrt{z(\varkappa, \varkappa^*)}}{\sigma(\varkappa, \varkappa^*) V(\varkappa, \varkappa^*)} + \delta z(\varkappa, \varkappa^*) \right\}.$$

Discussion

SURE/AIC **works** if $\mathcal{R}(\kappa, \kappa^*)$ grows sufficiently fast, so that

$$\mathcal{R}(\kappa, \kappa^*) \geq t \sigma(\kappa, \kappa^*) V(\kappa, \kappa^*) \sqrt{z(\kappa, \kappa^*)}.$$

SURE/AIC **does not work** if

- ▷ $\mathcal{R}(\kappa)$ is flat and thus $\mathcal{R}(\kappa, \kappa^*)$ is small.
- ▷ $\sigma_{\kappa}^2 \asymp V^2(\kappa, \kappa^*)$ i.e. for severely ill-posed cases.

Interpretation: Risk is significant relative to the variation of the empirical risk: $\text{Var}(L_1(\kappa, \kappa^*)) \asymp \sigma^2(\kappa, \kappa^*) V^2(\kappa, \kappa^*)$.

$\varkappa < \varkappa^*$: loss and risk

$\varkappa < \varkappa^*$ means $\mathcal{J}_\varkappa \subset \mathcal{J}_{\varkappa^*}$.

The excess risk $\mathcal{R}(\varkappa, \varkappa^*)$ can be represented as

$$\mathcal{R}(\varkappa, \varkappa^*) = -B(\varkappa, \varkappa^*) - V^2(\varkappa, \varkappa^*)$$

where $V^2(\varkappa, \varkappa^*) = V^2(\varkappa^*, \varkappa) = V^2(\varkappa^*) - V^2(\varkappa)$ and $B(\varkappa, \varkappa^*) = B(\varkappa^*) - B(\varkappa)$.

The definition of \varkappa^* implies that $-B(\varkappa, \varkappa^*) > V^2(\varkappa, \varkappa^*)$.

$\kappa < \kappa^*$: rate functions

With $\mathcal{I}(\kappa^*, \kappa) = \mathcal{I}(\kappa^*) \setminus \mathcal{I}(\kappa)$, it holds

$$\mathcal{M}_0(\mu_0, \kappa, \kappa^*) = -\frac{\mu_0}{2} \mathcal{R}(\kappa, \kappa^*) - \frac{1}{2} \sum_{\mathcal{I}(\kappa^*, \kappa)} Q(-\mu_1 \sigma_i^2),$$

$$\mathcal{M}_1(\mu_1, \kappa, \kappa^*) = \frac{\mu_1}{2} \mathcal{R}(\kappa, \kappa^*) - \frac{1}{2} \sum_{\mathcal{I}(\kappa^*, \kappa)} \left\{ Q(-\mu_1 \sigma_i^2) + \frac{\mu_1^2 s_i^2 \sigma_i^2}{1 + \mu_1 \sigma_i^2} \right\}$$

$$\begin{aligned} \mathcal{M}(\mu_0, \mu_1, \kappa, \kappa^*) &= \frac{\mu_1 - \mu_0}{2} \mathcal{R}(\kappa, \kappa^*) \\ &\quad - \frac{1}{2} \sum_{\mathcal{I}(\kappa^*, \kappa)} \left\{ Q(-(\mu_1 + \mu_0) \sigma_i^2) + \frac{\mu_1^2 s_i^2 \sigma_i^2}{1 + (\mu_1 + \mu_0) \sigma_i^2} \right\}. \end{aligned}$$

$\varkappa < \varkappa^*$

Define $z^*(\varkappa^*) = \max_{\varkappa < \varkappa^*} z(\varkappa, \varkappa^*)$ and set for $\varkappa < \varkappa^*$

$$\mu(\varkappa, \varkappa^*) \equiv \mu^-(\varkappa^*) \stackrel{\text{def}}{=} \frac{\sqrt{z^*(\varkappa^*)}}{\sigma(\varkappa^*)V(\varkappa^*)}$$

with $\sigma(\varkappa^*) \stackrel{\text{def}}{=} \max_{I(\varkappa^*)} \sigma_i$. Also

$$\mu_0(\varkappa, \varkappa^*) = \alpha_0 \mu(\varkappa, \varkappa^*) \quad \mu_1(\varkappa, \varkappa^*) = \alpha_1 \mu(\varkappa, \varkappa^*)$$

for some $\alpha_0 \leq \alpha_1$. Write

$$\mathcal{M}(\varkappa, \varkappa^*; \alpha_0, \alpha_1) \stackrel{\text{def}}{=} \mathcal{M}(\alpha_0 \mu(\varkappa, \varkappa^*), \alpha_1 \mu(\varkappa, \varkappa^*), \varkappa, \varkappa^*).$$

Theorem ($\varkappa < \varkappa^*$: One-sided concentration)

Let $\sum_{\varkappa < \varkappa^*} \exp\{-z(\varkappa, \varkappa^*)\} \leq \Omega^-$, $z^*(\varkappa^*) = \max_{\varkappa < \varkappa^*} z(\varkappa, \varkappa^*)$, and $(\alpha_0 + \alpha_1)\sqrt{z^*(\varkappa^*)}\sigma(\varkappa^*)/V(\varkappa^*) \leq c < 1$. Define

$$\mathfrak{b}^-(\mathfrak{z}; \alpha_0, \alpha_1) \stackrel{\text{def}}{=} \min_{\varkappa < \varkappa^*} \{\mathfrak{z} \mu_0(\varkappa, \varkappa^*) + \mathcal{M}(\varkappa, \varkappa^*; \alpha_0, \alpha_1) - z(\varkappa, \varkappa^*)\}.$$

Then for any $u > 0$

$$\begin{aligned} \mathbb{P}\left(\frac{1}{\sigma(\varkappa^*)V(\varkappa^*)\sqrt{z^*(\varkappa^*)}}[\rho(\tilde{\varkappa}) - \rho(\varkappa^*)] \geq 2u, \tilde{\varkappa} < \varkappa^*\right) \\ \leq \Omega^- \exp\{\mathfrak{b}^-(\mathfrak{z}; \alpha_0, \alpha_1)\} \\ \leq \Omega^- \exp\left\{-[u\alpha_0 - g^-(c)(\alpha_0 + \alpha_1)^2/2 - 1]z^*(\varkappa^*)\right\}. \end{aligned}$$

Spectral cut-off procedure

\varkappa is an integer and $\mathcal{I}_\varkappa = \{1, \dots, \varkappa\}$, that is,

$$\tilde{s}_i(\varkappa) = \begin{cases} Y_i & i \leq \varkappa, \\ 0 & \text{otherwise.} \end{cases}$$

For a specific \varkappa , the corresponding loss and risk read as

$$\rho(\varkappa) = \sum_{i \leq \varkappa} (Y_i - s_i)^2 + \sum_{i > \varkappa} s_i^2 \quad \mathcal{R}(\varkappa) = \sum_{i \leq \varkappa} \sigma_i^2 + \sum_{i > \varkappa} s_i^2.$$

For the empirical risk holds

$$\ell(\varkappa) = \sum_{i \leq \varkappa} \sigma_i^2 + \sum_{i > \varkappa} (Y_i^2 - \sigma_i^2), \quad \mathbb{E}\ell(\varkappa) = \mathcal{R}(\varkappa).$$

Optimal choice: $\varkappa^* = \operatorname{argmin}_{\varkappa \in \mathcal{K}} \mathcal{R}(\varkappa) = \operatorname{argmin}_{\varkappa \in \mathcal{K}} \left\{ \sum_{i < \varkappa} \sigma_i^2 + \sum_{i > \varkappa} s_i^2 \right\}$

Oracle two-sided bound

Let $z_0(k)$ satisfy

$$\sum_{k=1}^{\infty} \exp\{-z_0(k)\} = \Omega.$$

An example: $z_0(k) = (1 + \delta) \log(k)$ for $\delta > 0$. Define

$$z(\mathcal{K}, \mathcal{K}^*) = z_0(k(\mathcal{K}, \mathcal{K}^*)), \quad k(\mathcal{K}, \mathcal{K}^*) = \#\{\mathcal{K}(\mathcal{K}, \mathcal{K}^*)\}. \quad (2)$$

Theorem

Let the set \mathcal{K} be ordered and let $z(\mathcal{K}, \mathcal{K}^*)$ be defined by (2). Then

$$\mathbb{P}\left(\rho(\tilde{\mathcal{K}}) - \rho(\mathcal{K}^*) \geq 2\delta\right) \leq \Omega e^{-b^+(\delta)} + \Omega e^{-b^-(\delta)}$$

Problem of choosing a subset

\mathcal{K} , a set of subsets in \mathcal{I} .

$\mathcal{x} < \mathcal{x}'$ means $\mathcal{I}_{\mathcal{x}} \subset \mathcal{I}_{\mathcal{x}'}$.

Let $\mathcal{x}^* = \operatorname{argmin}_{\mathcal{I}} \mathcal{R}(\mathcal{x})$ be the oracle choice.

Idea of the study: reduce the general oracle bound to the cases with $\mathcal{x} < \mathcal{x}^*$ and $\mathcal{x} > \mathcal{x}^*$.

Approach: given $\mathcal{x}, \mathcal{x}^*$ consider ordered pairs $(\mathcal{x} \vee \mathcal{x}^*, \mathcal{x}^*)$ and $(\mathcal{x}^*, \mathcal{x} \wedge \mathcal{x}^*)$:

$$\mathcal{x} \triangle \mathcal{x}^* = \mathcal{I}(\mathcal{x} \vee \mathcal{x}^*, \mathcal{x}^*) \cup \mathcal{I}(\mathcal{x}^*, \mathcal{x} \wedge \mathcal{x}^*)$$

Construction of $z(\varkappa, \varkappa^*)$

Suppose that two functions $z^+(\varkappa, \varkappa^*)$ for $\varkappa > \varkappa^*$ and $z^-(\varkappa, \varkappa^*)$ for $\varkappa < \varkappa^*$ be fixed in a way that

$$\sum_{\varkappa > \varkappa^*} \exp\{-z^+(\varkappa, \varkappa^*)\} \leq \Omega^+, \quad \sum_{\varkappa < \varkappa^*} \exp\{-z^-(\varkappa, \varkappa^*)\} \leq \Omega^-$$

for some fixed constants Ω^\pm . Define for any $\varkappa \in \mathcal{K}$

$$z(\varkappa, \varkappa^*) \stackrel{\text{def}}{=} z^+(\varkappa \vee \varkappa^*, \varkappa^*) + z^-(\varkappa \wedge \varkappa^*, \varkappa^*).$$

Obviously

$$\sum_{\varkappa} \exp\{-z(\varkappa, \varkappa^*)\} \leq \Omega^+ \Omega^-.$$

Theorem (Oracle bound)

Let α be s.t. $2\alpha\sqrt{z(\varkappa, \varkappa^*)}\sigma(\varkappa, \varkappa^*)/V(\varkappa, \varkappa^*) \leq c < 1$ for $\varkappa < \varkappa^*$.
Then for any $u > 0$ and $\mathfrak{z} = u\sigma(\varkappa^*)V(\varkappa^*)\sqrt{z^*(\varkappa^*)}$:

$$\begin{aligned} \mathbb{P}\left(\frac{1}{\sigma(\varkappa^*)V(\varkappa^*)\sqrt{z^*(\varkappa^*)}}[\rho(\tilde{\varkappa}) - \rho(\varkappa^*)] \geq 2u, \tilde{\varkappa} < \varkappa^*\right) \\ \leq \Omega^- \exp\{-\mathfrak{b}^-(\mathfrak{z}; \alpha, \alpha)\} \\ \leq \Omega^- \exp\left\{-[u\alpha - 2g^-(c)\alpha^2 - 1]z^*(\varkappa^*)\right\}. \end{aligned}$$

Let $(\alpha_0 + \alpha_1)\sqrt{z(\varkappa, \varkappa^*)}\sigma(\varkappa, \varkappa^*)/V(\varkappa, \varkappa^*) < 1$ for $\varkappa > \varkappa^*$. Then

$$\begin{aligned} \mathbb{P}\left(\rho(\tilde{\varkappa}) - \rho(\varkappa^*) \geq 2\mathfrak{z}^- + 2\mathfrak{z}^+, \tilde{\varkappa} \vee \varkappa^* > \varkappa^*\right) \\ \leq \Omega^+ \Omega^- \exp\{-\mathfrak{b}^+(\mathfrak{z}^+; \alpha_0, \alpha_1) - \mathfrak{b}^-(\mathfrak{z}^-; \alpha_0, \alpha_1)\} \end{aligned}$$

Define $\mu(\varkappa, \varkappa^*) = \sqrt{z(\varkappa, \varkappa^*)} \sigma(\varkappa, \varkappa^*) / V(\varkappa, \varkappa^*)$, $\varkappa > \varkappa^*$.

Theorem (cont)

Let the risk excess $\mathcal{R}(\varkappa, \varkappa^*)$ fulfill

$$\mu(\varkappa, \varkappa^*) \mathcal{R}(\varkappa, \varkappa^*) \geq \mathfrak{t} z(\varkappa, \varkappa^*), \quad \varkappa > \varkappa^*$$

where the constant \mathfrak{t} is sufficiently large to ensure

$$\delta \stackrel{\text{def}}{=} \frac{1}{2} [\mathfrak{t}(\alpha_1 - \alpha_0) - q^+(c)(\alpha_1 + \alpha_0)^2 - (1 - c)^{-1} \alpha_1^2] - 1 > 0.$$

Then

$$\mathfrak{b}^+(\mathfrak{z}; \alpha_0, \alpha_1) \geq \min_{\varkappa > \varkappa^*} \{ \mathfrak{z} \alpha_0 \mu(\varkappa, \varkappa^*) + \delta z(\varkappa, \varkappa^*) \}.$$

Outline

1 Motivation

- Penalized model selection
- Saddle point model selection

2 SURE in linear inverse problem

- Cross-concentration
- A bound for the excess loss
- Projection estimates
- One-sided concentration: $\mathcal{R} > \mathcal{R}^*$
- One-sided concentration: $\mathcal{R} < \mathcal{R}^*$
- Spectral cut-off estimation
- Unordered case

3 Saddle point model selection

- Penalty calibration
- Oracle bound for a SP selector
- Special cases

SPM: discussion

New procedure should overcome the main drawbacks of the SURE/AIC approach.

Ultimate Goal:

- ▶ establish a concentration property (oracle bound) regardless degree of ill-posedness and risk flatness.
- ▶ suggest a unified principle for choosing a penalty function.

Risk minimization vs saddle point

Consider the risk difference as **functions of two arguments** $\mathcal{N}, \mathcal{N}'$:

$$\mathcal{R}(\mathcal{N}, \mathcal{N}') \stackrel{\text{def}}{=} \mathcal{R}(\mathcal{N}) - \mathcal{R}(\mathcal{N}').$$

The definition of \mathcal{N}^* as the minimizer of the risk function $\mathcal{R}(\mathcal{N})$ can be rewritten in the form:

$$\mathcal{N}^* = \underset{\mathcal{N}}{\operatorname{argmin}} \mathcal{R}(\mathcal{N}, \mathcal{N}^*) = \underset{\mathcal{N}}{\operatorname{argmax}} \mathcal{R}(\mathcal{N}^*, \mathcal{N}).$$

In other words, $(\mathcal{N}^*, \mathcal{N}^*)$ is a **saddle point** of the function $\mathcal{R}(\mathcal{N}, \mathcal{N}')$:

$$0 \equiv \mathcal{R}(\mathcal{N}^*, \mathcal{N}^*) \geq \mathcal{R}(\mathcal{N}^*, \mathcal{N}), \quad 0 \equiv \mathcal{R}(\mathcal{N}^*, \mathcal{N}^*) \leq \mathcal{R}(\mathcal{N}, \mathcal{N}^*), \quad \forall \mathcal{N}.$$

Model selection as a SP-problem

Basic observation: the minimizer of SURE $\ell(\mathcal{X})$ is a saddle point of $\ell(\mathcal{X}, \mathcal{X}') = \ell(\mathcal{X}) - \ell(\mathcal{X}')$.

SP-Approach: consider a penalized **bivariate** function

$$\ell(\mathcal{X}, \mathcal{X}') + 2 \text{PEN}(\mathcal{X}, \mathcal{X}') = \ell(\mathcal{X}) - \ell(\mathcal{X}') + 2 \text{PEN}(\mathcal{X}, \mathcal{X}')$$

and define the **penalized choice** of $\hat{\mathcal{X}}$ via the **smallest saddle point**:

$$\hat{\mathcal{X}} \stackrel{\text{def}}{=} \underset{\mathcal{X}}{\text{argmin}} \max_{\mathcal{X}'} \{ \ell(\mathcal{X}, \mathcal{X}') - 2 \text{PEN}(\mathcal{X}, \mathcal{X}') \}.$$

In other words, the value $\hat{\mathcal{X}}$ is a SP if it holds for any \mathcal{X}° :

$$\max_{\mathcal{X}} \{ \ell(\hat{\mathcal{X}}, \mathcal{X}) - 2 \text{PEN}(\hat{\mathcal{X}}, \mathcal{X}) \} \leq \max_{\mathcal{X}} \{ \ell(\mathcal{X}^\circ, \mathcal{X}) - 2 \text{PEN}(\mathcal{X}^\circ, \mathcal{X}) \}.$$

The choice of a bivariate penalty function $\text{PEN}(\mathcal{X}, \mathcal{X}')$

Main requirements:

concentration property on each set $\mathcal{X} \geq \mathcal{X}^$.*

Is granted if a uniform exponential bound can be established for the linear combination

$$\mathcal{L}(\mathcal{X}, \mathcal{X}^*) = \mu_1(\mathcal{X}, \mathcal{X}^*)L_1(\mathcal{X}, \mathcal{X}^*) + \mu_0(\mathcal{X}, \mathcal{X}^*)L_0(\mathcal{X}, \mathcal{X}^*)$$

e.g. in the form

$$\mathbb{E} \sup_{\mathcal{X} > \mathcal{X}^*} \exp\{\mathcal{L}(\mathcal{X}, \mathcal{X}^*) - \text{PEN}(\mathcal{X}, \mathcal{X}^*)\} \leq \Omega^* .$$

Construction of Penalty: ordered case

Suppose that for every $\varkappa^* \in \mathcal{K}$

$$\sum_{\mathcal{K}} \exp\{-z(\varkappa, \varkappa^*)\} \leq \Omega^* < \infty, \quad \forall \varkappa^* \in \mathcal{K}.$$

Define a penalty function for $\varkappa > \varkappa'$:

$$\text{PEN}(\varkappa, \varkappa') \stackrel{\text{def}}{=} \tau \sqrt{z(\varkappa, \varkappa')} \sigma(\varkappa, \varkappa') V(\varkappa, \varkappa') \quad \varkappa > \varkappa',$$

Construction of Penalty: unordered case

For any $\mathcal{X}, \mathcal{X}'$, the value $\text{PEN}(\mathcal{X}, \mathcal{X}')$ is defined as:

$$\text{PEN}(\mathcal{X}, \mathcal{X}') \stackrel{\text{def}}{=} \text{PEN}(\mathcal{X} \vee \mathcal{X}', \mathcal{X}')$$

Interpretation: $\text{PEN}(\mathcal{X}, \mathcal{X}')$ reflects increased complexity of \mathcal{X} relative to \mathcal{X}' .

► $\text{PEN}(\mathcal{X} \vee \mathcal{X}', \mathcal{X}')$ accounts for the **increase of complexity** by adding new components $\mathcal{X} \setminus \mathcal{X}'$ to \mathcal{X}' .

Define

$$\mu(\mathcal{X}, \mathcal{X}') = \frac{\sqrt{z(\mathcal{X}, \mathcal{X}')}}{\sigma(\mathcal{X}, \mathcal{X}')V(\mathcal{X}, \mathcal{X}')},$$

$$\mu_0(\mathcal{X}, \mathcal{X}^*) = \alpha_0 \mu(\mathcal{X}, \mathcal{X}^*),$$

$$\mu_1(\mathcal{X}, \mathcal{X}^*) = \alpha_1 \mu(\mathcal{X}, \mathcal{X}^*),$$

where $\alpha_0 \leq \alpha_1$ are some constants. Set

$$\mathcal{L}(\mathcal{X}, \mathcal{X}^*; \alpha_0, \alpha_1) = \mu_1(\mathcal{X}, \mathcal{X}^*)L_1(\mathcal{X}, \mathcal{X}^*) + \mu_0(\mathcal{X}, \mathcal{X}^*)L_0(\mathcal{X}, \mathcal{X}^*)$$

$$\mathcal{M}(\mathcal{X}, \mathcal{X}^*; \alpha_0, \alpha_1) = -\log \mathbb{E} \exp\{\mathcal{L}(\mathcal{X}, \mathcal{X}^*; \alpha_0, \alpha_1)\}$$

Theorem (Oracle concentration bound)

Let $(\alpha_0 + \alpha_1)\mu(\boldsymbol{\kappa}, \boldsymbol{\kappa}^*)\sigma^2(\boldsymbol{\kappa}, \boldsymbol{\kappa}^*) \leq c < 1$. Then it holds

$$\begin{aligned} \mathbb{P}\left(\rho(\tilde{\boldsymbol{\kappa}}) - \rho(\boldsymbol{\kappa}^*) \geq 2\boldsymbol{z}^- + 2\boldsymbol{z}^+ + 2\boldsymbol{z}_1\right) \\ \leq \Omega^- \exp\{-\mathbf{b}^-(\boldsymbol{z}^-; \alpha_0, \alpha_1)\} \\ + \Omega^+ \Omega^- \exp\{-\mathbf{b}^+(\boldsymbol{z}^+; \alpha_0, \alpha_1) - \mathbf{b}^-(\boldsymbol{z}^-; \alpha_0, \alpha_1)\} \\ + \Omega^+ \Omega^- \exp\{-\mathbf{b}_1(\boldsymbol{z}_1; \alpha_1)\}. \end{aligned}$$

Theorem (Oracle concentration bound. cont)

Let also the constant τ in the definition

$$\text{PEN}(\varkappa, \varkappa^*) = \tau \sqrt{z(\varkappa, \varkappa')} \sigma(\varkappa, \varkappa') V(\varkappa, \varkappa'), \quad \varkappa > \varkappa',$$

fulfill

$$\delta \stackrel{\text{def}}{=} \frac{1}{2} [\tau \alpha_1 - q^+(c)(\alpha_1 + \alpha_0)^2 - (1 - c)^{-1} \alpha_1^2] - 1 > 0.$$

Then

$$\mathfrak{b}_1(\mathfrak{z}; \alpha_1) \geq \mathfrak{b}^+(\mathfrak{z}; \alpha_0, \alpha_1) \geq \min_{\varkappa > \varkappa^*} \{ \mathfrak{z} \alpha_0 \mu(\varkappa, \varkappa^*) + \delta z(\varkappa, \varkappa^*) \}.$$

Ordered model choice: $\mathcal{K} = \{1, 2, \dots, K\}$

Homogeneous noise: $\sigma_i = \sigma$, $V^2(\mathcal{K}, \mathcal{K}^*) = \sigma^2 |\mathcal{K} - \mathcal{K}^*|$. The choice

$$\text{PEN}(\mathcal{K}, \mathcal{K}') = C \sqrt{\log(|\mathcal{K} - \mathcal{K}'|)} \quad \mathcal{K} > \mathcal{K}'$$

yields the bound for excess loss of order $\sigma(\mathcal{K}^*)V(\mathcal{K}^*)\sqrt{\log n}$.

Inverse problem: σ_i grows with i . Then $\sigma(\mathcal{K}, \mathcal{K}^*) = \max_{i \in \mathcal{K} \setminus \mathcal{K}^*} \sigma_i$ and

$$\text{PEN}(\mathcal{K}, \mathcal{K}^*) = C \sqrt{\sigma(\mathcal{K}, \mathcal{K}')V(\mathcal{K}, \mathcal{K}') \log(|\mathcal{K} - \mathcal{K}'|)} \quad \mathcal{K} > \mathcal{K}'$$

still yields the oracle bound for $\sigma(\mathcal{K}, \mathcal{K}') \ll V(\mathcal{K}, \mathcal{K}')$.

Severely ill-posed case: $\sigma(\mathcal{K}, \mathcal{K}^*) \asymp V(\mathcal{K}, \mathcal{K}^*)$.

Then $L_0(\tilde{\mathcal{K}}, \mathcal{K}^*) \asymp \sqrt{\sigma(\mathcal{K}^*)V(\mathcal{K}^*) \log(n)} \gg \mathcal{R}(\mathcal{K}^*) \asymp V^2(\mathcal{K}^*)$.

Subset selection

\mathcal{K} = "set of all subsets" + "homogeneous noise" $\sigma_i \equiv \sigma$.

The choice

$$\text{PEN}(\mathcal{K}, \mathcal{K}') = C\sigma\sqrt{(|\mathcal{K}| - |\mathcal{K}'|)\log(n - |\mathcal{K}'|)} \quad \mathcal{K} > \mathcal{K}'$$

yields the oracle bound.

The excess loss bound is of order $|\mathcal{K}^*|\sqrt{\log(n - |\mathcal{K}^*|)}$, much larger than the oracle risk $\mathcal{R}(\mathcal{K}^*) \asymp |\mathcal{K}^*|$.

Outlooks

- ▶ New SP-approach is only relevant for practical use, if an efficient implementation is available. A choice of a SP can be reduced to a semi-definite programming provided that the objective function is convex-concave. This seems to be possible to achieve for typical examples.
- ▶ Extensions to linear models, non-Gaussian/correlated errors, etc. are called for.
- ▶ Numerical examples still missing.