Empirical Risk Minimization as Parameter Choice Rule for General Linear Regularization Methods

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1 joint work with Housen Li
Ill-posed linear models

Model: Recover unknown $f$ from $n$ indirect noisy samples

$$ Y = Tf + \sigma \xi $$
with $T \in \mathbb{R}^{n \times p}$, $\text{rank}(T) = p$, $\xi$ standard Gaussian.

Eigenvalues of $T^* T$: $\lambda_1 \geq \cdots \geq \lambda_p > 0$, assume

$$ \lambda_k \asymp k^{-a} \quad \text{with some } a > 1. $$

Normalized eigenvectors $e_1, \ldots, e_p$ \\[ \sim \] Equivalent sequence model:

$$ Y_k = \sqrt{\lambda_k} f_k + \sigma \xi_k, \quad k = 1, \ldots, p, $$

where $Y_k := \langle \lambda_k^{-1/2} Te_k, Y \rangle$, $f_k = \langle f, e_k \rangle$, $\xi_k := \langle \lambda_k^{-1/2} Te_k, \xi \rangle \overset{\text{i.i.d.}}{\sim} \mathcal{N}(0, 1)$. 
Linear regularization methods

Recall: least square estimator $\hat{f} := (T^* T)^{-1} T^* Y$.

Ill-posedness $\Rightarrow$ stable approximation $q_\alpha(\cdot)$ of $(\cdot)^{-1}$, that is,

$$\text{linear regularization methods: } \hat{f}_\alpha := q_\alpha(T^* T) T^* Y.$$

**Definition**

We call $q_\alpha : [0, \lambda_1] \to \mathbb{R}$ with $\alpha \in \mathcal{A} \subseteq \mathbb{R}_+$ an ordered filter if

(i) There exist $C'_q, C''_q > 0$ s.t. for every $\alpha \in \mathcal{A}$ and every $\lambda \in [0, \lambda_1]$

$$\alpha |q_\alpha(\lambda)| \leq C'_q$$

and

$$\lambda |q_\alpha(\lambda)| \leq C''_q.$$

(ii) $\alpha \mapsto (q_\alpha(\lambda_k))_{k=1}^p$ is strictly monotone and continuous.
Smoothness assumptions

We want to obtain minimax optimality over ellipsoids of the form

$$\mathcal{W} := \left\{ f \in \mathbb{R}^p : \sum_{k=1}^{p} w_k f_k^2 \leq 1 \right\} \quad \text{with } w_k \asymp k^b.$$ 

But therefore, $q_\alpha$ must be able to take advantage of this!

Shorthand notation: $s_\alpha(\lambda) := \lambda q_\alpha(\lambda)$. Qualification condition

$$\sup_{\alpha \in \mathcal{A}, \lambda \in [0, \lambda_1]} \alpha^{-\nu} \lambda^{\nu} |1 - s_\alpha(\lambda)| \leq C_\nu < \infty \quad \text{for all } 0 < \nu \leq \nu_0.$$ 

The largest possible $\nu_0$ is called the polynomial qualification index.
Examples

Table: Summary of some ordered filters

<table>
<thead>
<tr>
<th>Method</th>
<th>$q_\alpha(\lambda)$</th>
<th>$C'_q$</th>
<th>$C''_q$</th>
<th>$\nu_0$</th>
<th>Need SVD</th>
</tr>
</thead>
<tbody>
<tr>
<td>Spectral cut-off</td>
<td>$\frac{1}{\lambda} 1_{[\alpha, \infty)}(\lambda)$</td>
<td>1</td>
<td>1</td>
<td>$\infty$</td>
<td>Yes</td>
</tr>
<tr>
<td>Tikhonov</td>
<td>$\frac{1}{\lambda + \alpha}$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>No</td>
</tr>
<tr>
<td>$m$-iterated Tikhonov</td>
<td>$\frac{(\lambda + \alpha)^m - \alpha^m}{\lambda(\lambda + \alpha)^m}$</td>
<td>$m$</td>
<td>1</td>
<td>$m$</td>
<td>No</td>
</tr>
<tr>
<td>Landweber ($| T | \leq 1$)</td>
<td>$\sum_{j=0}^{\lfloor \alpha \rfloor - 1} (1 - \lambda)^j$</td>
<td>1</td>
<td>1</td>
<td>$\infty$</td>
<td>No</td>
</tr>
<tr>
<td>Showalter</td>
<td>$\frac{1 - \exp\left(-\frac{\lambda}{\alpha}\right)}{\lambda}$</td>
<td>1</td>
<td>1</td>
<td>$\infty$</td>
<td>No</td>
</tr>
</tbody>
</table>
A-priori parameter choice

Proposition (Bissantz et al. ‘07)

Let $\hat{f}_\alpha := q_\alpha(T^* T) T^* Y$ with a filter $q_\alpha$, and $\alpha = \alpha_{or} \asymp (\sigma^2)^{a/(a+b+1)}$.

- If the qualification index $v_0 \geq b/(2a)$, then

$$R(\alpha_{or}, \mathcal{W}) := \sup_{f \in \mathcal{W}} \mathbb{E} \left[ \| \hat{f}_{\alpha_{or}} - f \|^2 \right] \lesssim (\sigma^2)^{b/(a+b+1)}.$$

- If further $v_0 \geq b/(2a) + 1/2$, then

$$r(\alpha_{or}, \mathcal{W}) := \sup_{f \in \mathcal{W}} \mathbb{E} \left[ \| T \hat{f}_{\alpha_{or}} - Tf \|^2 \right] \lesssim (\sigma^2)^{a+b/(a+b+1)}.$$

Such rates are minimax optimal in order over $\mathcal{W}$. 
Empirical prediction risk minimization

The optimality on the last slide relies on the smoothness of $f$ (via $\alpha_{or}$). We consider the parameter choice rule $\hat{\alpha}$ given by

$$\hat{\alpha} := \text{argmin}_{\alpha \in A} \left[ \| T \hat{f}_\alpha - Y \|^2 + 2\sigma^2 \text{Trace} \left( s_\alpha \left( T^* T \right) \right) \right].$$

Intuition: minimize an unbiased estimator of the prediction risk

$$r(\alpha, f) := \mathbb{E} \left[ \| T (\hat{f}_\alpha - f) \|^2 \right] = \sum_{k=1}^{p} \lambda_k (1 - s_\alpha(\lambda_k))^2 f_k^2 + \sigma^2 \sum_{k=1}^{p} s_\alpha(\lambda_k)^2,$$

since

$$\mathbb{E} \left[ \| T \hat{f}_\alpha - Y \|^2 \right] = \sum_{k=1}^{p} \lambda_k (1 - s_\alpha(\lambda_k))^2 f_k^2 + \sigma^2 \sum_{k=1}^{p} s_\alpha(\lambda_k)^2 - 2\sigma^2 \sum_{k=1}^{p} s_\alpha(\lambda_k) + p\sigma^2.$$
Empirical prediction risk minimization (cont’)

The $\hat{\alpha}$ was first introduced in (Mallows ‘73), thus a.k.a. Mallows $C_L$.

Practice: it is popular & attractive.

Theory: $\hat{\alpha}$ is order optimal w.r.t. prediction risk $r(\alpha, f)$ (Kneip ‘94).

- **Unknown:** Is $\hat{\alpha}$ also optimal for the risk $R(\alpha, f) := \mathbb{E} \left[ \| \hat{f}_\alpha - f \|^2 \right]$?
  - It is way more informative than $r(\alpha, f)$ due to the ill-posedness.
  - Spectral cut-off: this has recently been shown in (Chernousova & Golubev ‘14.)

- **Our goal:** Extend it to general linear regularization methods.
  - Why? Spectral cut-off relies on full SVD, thus impractical.
Order inequality

Assumption

(i) As $\alpha \downarrow 0$, $s_\alpha(\alpha) \equiv \alpha q_\alpha(\alpha) \geq c_q > 0$.

(ii) For $\alpha \in \mathcal{A}$, the function $\lambda \mapsto s_\alpha(\lambda)$ is non-decreasing.

All mentioned regularization methods satisfy the assumption.

It requires proper parametrization. E.g. Tikhonov with re-parametrization $\alpha \mapsto \sqrt{\alpha}$, i.e. $q_\alpha(\lambda) = 1/(\sqrt{\alpha} + \lambda)$, still an ordered filter, but violates Ass. (i).

Theorem (Oracle inequality)

Let $r(\alpha_{\text{or}}, f) := \min_{\alpha \in \mathcal{A}} r(\alpha, f)$. Then for all $f \in \mathcal{W}$

$$
\mathbb{E} \left[ \| \hat{f}_\alpha - f \|_2^2 \right] \lesssim r(\alpha_{\text{or}}, f)^{\frac{b}{a+b}} + \sigma^{-2a} r(\alpha_{\text{or}}, f)^{1+a} + \sigma^{1-2a} r(\alpha_{\text{or}}, f)^{\frac{1+2a}{2}}. 
$$
Order optimality

\[ \mathbb{E} \left[ \| \hat{f}_\alpha - f \|^2 \right] \lesssim r(\alpha_{or}, f)^{\frac{b}{a+b}} + \sigma^{-2a} r(\alpha_{or}, f)^{1+a} + \sigma^{1-2a} r(\alpha_{or}, f)^{\frac{1+2a}{2}}. \]

Recall:

\[ r(\alpha_{or}, f) \lesssim \sigma^{\frac{2(a+b)}{a+b+1}} \quad \text{if} \quad v_0 \geq b/(2a) + 1/2 \]

Thus, if \( v_0 \geq b/(2a) + 1/2 \),

\[ \mathbb{E} \left[ \| \hat{f}_\alpha - f \|^2 \right] \lesssim \sigma^{\frac{2b}{a+b+1}}. \quad \text{(order optimal)} \]

\( v_0 \geq b/(2a) + 1/2 \) means we need higher qualification (early saturation)

- Same price for the deterministic discrepancy principle and GCV, which also rely on the residual \( \| T\hat{f}_\alpha - Y \| \).
- Better than Lepskiï ('90) principle, where one typically looses a log-factor.
Further results
Oracle inequality & optimality actually holds...

... in a more general setting \( Y = Tf + \sigma \xi \) where

- \( T \) is an injective and compact operator between Hilbert spaces,
- the Eigenvalues of \( T^*T \) decay in a general way,
- \( \xi \) is sub-Gaussian noise, and \( \sigma \) is unknown.

... under general smoothness assumptions:

- Source condition
  \[ f = \phi(T^*T)w \quad \text{for some } \omega \text{ with } \|w\| \leq C. \]

- Qualification condition
  \[ \sup_{\lambda \in [0, \lambda_1]} \sqrt{\lambda} \phi(\lambda) |1 - s_{\alpha}(\lambda)| \lesssim \sqrt{\alpha} \phi(\alpha). \]
Experiment setting

Forward operator \( T : \mathbf{L}^2([0, 1]) \to \mathbf{L}^2([0, 1]) \)

\[
(Tf)(x) = \int_0^1 k(x, y) f(y) \, dy, \quad \text{with } k(x, y) = \min\{x(1-y), y(1-x)\}.
\]

Obviously, \((Tf)'' = -f\), so the eigenvalues \(\lambda_k\) of \(T^*T\) satisfy \(\lambda_k \asymp k^{-4}\).

The unknown truth

\[
f(x) = \begin{cases} 
x & \text{if } 0 \leq x \leq \frac{1}{2}, \\
1 - x & \text{if } \frac{1}{2} \leq x \leq 1.
\end{cases}
\]

Then \(f_k = \frac{(-1)^k - 1}{4\pi^3 k^2}\) and the optimal rate is \(O\left(\sigma^{\frac{3}{4} - \varepsilon}\right)\) for any \(\varepsilon > 0\).
Numerical Simulations

Results

Figure: Average of $\| \hat{f} - f \|_2^2$ over $10^4$ repetitions.
Conclusion

**Theoretical explanations** for the well-known parameter choice rule via empirical prediction risk minimization

Open questions

- Nonlinear problems;
- Different noise models;
- Exponentially ill-posed problems.


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