Discrepancy based model selection in statistical inverse problems

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based on joint work with G. Blanchard, Q. Jin and S. Lu, 2012-2014.

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Outline

Problem formulation

We will prototypically discuss *linear inverse problems* in Hilbert space, given as

$$y^\sigma = Tx + \sigma\xi,$$

where

- $T: X \to Y$ is a *(compact) linear operator* between (real) Hilbert spaces X and Y,
- x is the (unknown) *solution*,
- ξ represents *Gaussian white noise*, i.e., it is a (weak) Gaussian element, with
  - weak second moments $\mathbb{E}\langle\xi, y\rangle^2 < \infty$, and
  - identity covariance $\mathbb{E}\langle\xi, y_1\rangle\langle\xi, y_2\rangle = \langle y_1, y_2\rangle$.
- σ is the *(known) noise level*, and
- y^σ are the given *observations*.

Remark

Further restrictions will be imposed below.

Challenges

Within the present context we face two major problems

- The observations y^σ do not belong to the space Y;
- The solution operator T^{-1} is not boundedly invertible.

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Therefore we will discuss

- how to precondition the equation in order to have data right, and
- how to *regularize* the problem in order to obtain a stable reconstruction of the solution.

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- how to *regularize* the problem in order to obtain a stable reconstruction of the solution.

Literature:

- G. Blanchard, M., *Discrepancy principle for statistical inverse problems with application to conjugate gradient regularization*, *Inverse Problems*, 28(11):pp. 115011, 2012.
- Q. Jin, M., *Oracle inequality for a statistical Raus–Gfrerer–type rule*, *SIAM/ASA J. on UQ*, 1(1):386–407, 2013.
- S. Lu, M., *Discrepancy based model selection in statistical inverse problems*, *J. Complexity*, 30(3):290–308, 2014.

Preconditioning

Preconditioning is achieved by *smoothing* the equation, i.e., by applying some $S\colon Y \to X$ such that $T\xi \in X$ (a.s.).

Theorem (Sazonov, 1958)

$S\xi$ is an element in X if and only if the operator S has square summable singular numbers.

Definition (Hilbert–Schmidt operator)

A bounded operator $S\colon Y \to X$ in Hilbert space is called Hilbert–Schmidt operator if $\mathrm{tr}[S^*S] = \sum_{s_j>0} s_j^2 < \infty$.

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This can be used in two situations

smoothing $S := T^*$ provided that T is Hilbert–Schmidt, or

discretization $S := P_n T^*\colon Y \to X$ with P_n being finite, otherwise.

Regularization

In the following we do not consider *discretization*, instead we assume that *T is Hilbert–Schmidt*, and we consider new data

$$z^\sigma = T^* y^\sigma = T^* T x + \sigma T^* \xi = T^* T x + \sigma \zeta$$

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Now, the data $z^\sigma \in X$ are o.k., but, still the solution operator $T^* T$ is not boundedly invertible. We confine our discussion to *Tikhonov regularization*: We determine a *parametric family*

$$x_{\alpha,\sigma} := (T^* T + \alpha I)^{-1} T^* y^\sigma = (T^* T + \alpha I)^{-1} z^\sigma, \quad \alpha > 0.$$

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Problem

How to choose α?

Bias-variance decomposition

The estimators are *linear functions of the data z^σ*. In this case we have a natural error decomposition.

Theorem

Let $z^\sigma \to \hat{x}(z^\sigma)$ be any linear (Hilbert–Schmidt) estimator. Then

$$\mathbb{E}\|x - \hat{x}(z^\sigma)\|^2 = \|x - \hat{x}(Tx)\|^2 + \sigma^2 \mathbb{E}\|\hat{x}(\xi)\|^2$$

- The quantity $\|x - \hat{x}(Tx)\|$ is called *bias* (regularization error).
- The quantity $\sigma^2 \mathbb{E}\|\hat{x}(\xi)\|^2 = \sigma^2 \operatorname{tr}[(\hat{x})^* \hat{x}]$ is the variance.

We shall ignore the bias, here. There are sharp bounds under natural smoothness conditions.

Controlling the variance: The effective dimension

We need to control the trace $\mathrm{tr}[(\hat{x})^*\hat{x}]$. The following function is important.

Definition (effective dimension)

Let T be a Hilbert Schmidt operator. The function

$$\mathcal{N}(t) := \mathrm{tr}[(tI + T^*T)^{-1} T^*T], \quad t > 0,$$

is called effective dimension.

Lemma

Let T be a Hilbert–Schmidt operator with infinite range. For Tikhonov regularization $x_{\alpha,\sigma} = (T^*T + \alpha)^{-1} z^\sigma$ we have that

$$\mathrm{tr}[(\hat{x})^*\hat{x}] \le \frac{\mathcal{N}(\alpha)}{\alpha}, \quad \alpha > 0.$$

Goal

Find a discrepancy which takes $\mathcal{N}$ into account!

Previous approaches

- Observation:

$$\mathbb{E}\|(\lambda I + T^* T)^{-1/2} T^* \xi\|^2 = \mathcal{N}(\lambda)$$

Thus, as in [1] we might consider the *weighted discrepancy*

$$\|(\lambda I + T^* T)^{-1/2} (T^* T x_{\alpha,\sigma} - z^\sigma)\|^2 \leq \tau\sigma\sqrt{\mathcal{N}(\lambda)}$$

- Observation: The best *a priori choice of λ* coincides with the best *a priori choice of α*!

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$$\|\,(\lambda I + T^*T)^{-1/2}\,(T^*Tx_{\alpha,\sigma} - z^\sigma)\|^2 \leq \tau\sigma\sqrt{\mathcal{N}(\lambda)}$$

- Observation: The best *a priori choice of* λ coincides with the best *a priori choice of* α!
- Thus, as in [6] we let $\lambda = \alpha$ in above formula and we consider

$$\|\,(\alpha I + T^*T)^{-1/2}\,(T^*Tx_{\alpha,\sigma} - z^\sigma)\|^2 \leq \tau\sigma\sqrt{\mathcal{N}(\alpha)}!$$

Varying discrepancy principle

We choose α from a grid

$$\Delta := \{\alpha_0 > \alpha_1 := q\alpha_0 > \cdots > \alpha_n := q^n\alpha_0 > \cdots > 0\},$$

for a pre-specified value $0 < q < 1$.

Definition (varying discrepancy principle, cf. Lu/M. [6], 2014)

Given positive constants $\tau > 1$, $\eta > 0$ and $\kappa > 0$ the parameter α_{VDP} *is chosen as the largest $\alpha \in \Delta$ for which either*

$$\| (\alpha I + T^*T)^{-1/2} (z^\sigma - T^*Tx_{\alpha,\sigma}) \| \leq \tau(1+\kappa)\sigma\sqrt{\mathcal{N}(\alpha)} \quad \textit{(regular stop), or}$$

$$\sqrt{q\alpha} \leq \eta(1+\kappa)\sigma\sqrt{\mathcal{N}(\alpha)} \quad \textit{(emergency stop)}.$$

Remark

This parameter choice works, however it suffers from early saturation*!*
The emergency stop prevents outliers*!*

Oracle inequalities

There are many variants for formulating *oracle-type inequalities*. Here we shall focus on one based on the error decomposition from before.

Definition (generic oracle inequality, quasi-optimality)

Let $x_{\alpha,\sigma}$ be any regularization scheme, and let α_* be chosen according to some parameter choice. *This choice allows for an oracle inequality, if*

$$\left(\mathbb{E}\|x - x_{\alpha_*,\sigma}(z^\sigma)\|^2\right) \leq \inf_{0<\alpha<\infty}\left\{\|x - x_{\alpha,\sigma}(Tx)\| + \sigma\sqrt{\frac{\mathcal{N}(\alpha}{\alpha}}\right\}$$

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Remark

If the regularization has certain qualification, then we obtain the best possible error bound for this regularization. So, necessarily *the parameter choice* cannot have early saturation*!*

The varying discrepancy principle does not allow for an oracle inequality.

Statistical Raus–Gfrerer rule

Definition (statistical RG-rule, cf. Jin/M. [4], 2013)

Given $\tau > 1 > \eta > 0$, *and* $\kappa \geq 0$.
Let $\alpha_{RG} \in \Delta$ be the largest parameter *for which either*

$$\text{(reg. stop): } \left\| \left(\alpha I + T^* T\right)^{-1} \left(T^* T x_{\alpha,\sigma} - z^\sigma\right)\right\| \leq \tau(1+\kappa)\sigma\sqrt{\mathcal{N}(\alpha)},$$

or

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Remark

This approach goes back to Raus/Gfrerer [8, 3], 1984/87.
It resolves the early saturation of the discrepancy principle.

Outline

Main result for the statistical RG-rule

Theorem (Jin/M. [4], 2013)

If $\alpha_{RG} \leq \alpha_0$ is chosen according to statistical RG-rule *with* $\kappa = \sqrt{8(1 + |\log(1/\sigma)|)/\mathcal{N}(\alpha_0)}$, *then*

$$\left(\mathbb{E}\|x - x^{\delta}_{\alpha_{\alpha_{RG}}}\|^2\right)^{1/2} \leq C \inf_{0<\alpha\leq\alpha_0} \left\{ \|x - x_\alpha\| + \sigma\sqrt{|\log 1/\sigma|}\sqrt{\frac{\mathcal{N}(\alpha}{\alpha}} \right\},$$

provided that Assumption 2 *holds.*

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provided that Assumption 2 *holds.*

Remark

Under smoothness in terms of general source conditions *this gives the optimal order of reconstruction* up to the log-factor $\sqrt{|\log 1/\sigma|}$*!*

General proof strategy

We consider the set
$Z_{\kappa,\alpha} = \left\{ \zeta : \left\| (\alpha I + T^* T)^{-1/2} \zeta \right\| \leq (1+\kappa)\sqrt{\alpha \mathcal{N}(\alpha)} \right\}$. Then

$$\left(\mathbb{E} \| x - x_{\alpha,\sigma} \|^2 \right)^{1/2} \leq \sup_{\zeta \in Z_{\kappa,\alpha}} \| x - x_{\alpha,\sigma}(\zeta) \| + \left(\mathbb{E} \| x - x_{\alpha,\sigma} \|^4 \right)^{1/4} \mathbb{P}\left[Z^C_{\kappa,\alpha} \right]^{1/4}.$$

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The set $Z_{\kappa,\alpha}$ *of noise realizations is designed* such that

- The 4th moment is bounded (*emergency stop*),
- the set $Z_{\kappa,\alpha}$ has (exponentially) small probability (*concentration*),
- we can control the parameter choice on $\zeta \in Z_{\kappa,\alpha}$ (*crucial part!*).

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Goal

Analyze ill-posed problem under general noise assumption*!*
Such analysis was initiated by P. Eggermont et al. *[2], 2009!*

Outline

General noise

Assumption

There is a function $\alpha \to \delta(\alpha) > 0$ *that is* non-decreasing, *while* $\alpha \to \delta(\alpha)/\sqrt{\alpha}$ is non-increasing *such that the noise* ζ *obeys*

$$\delta \| (\alpha I + T^* T)^{-1/2} \zeta \| \leq \delta(\alpha), \qquad \hat{\alpha} \leq \alpha \in \Delta_q,$$

where $\hat{\alpha} \in \Delta_q$ *is the largest parameter such that* $\hat{\alpha} \leq \eta \delta(\hat{\alpha})$ *with* $\eta > 0$ *being a given small number.*

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Remark

There are interesting special cases.

- *If* $\| (T^* T)^{-1/2} \zeta \| = \|\xi\| \leq 1$ *then* usual noise *assumption* $\delta(\alpha) = \delta$,
- *if* $\|\zeta\| = \| T^* \xi \| \leq 1$ *then* large noise $\delta(\alpha) = \delta/\sqrt{\alpha}$*!*

$\alpha > \alpha_{RG}$:

Lemma

Under the noise assumption 1 we have the following natural error decomposition

$$\|x - x_{\alpha,\sigma}\| \leq \|x - x_\alpha\| + c_* \frac{\delta(\alpha)}{\alpha}.$$

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Lemma

If $\alpha > \alpha_{RG}$ *then*

$$\frac{\delta(\alpha)}{\alpha} \leq \frac{1}{\tau - 1}\|x_\alpha - x\|.$$

Thus the bias dominates the noise term*!*

Therefore we need to consider the case $\alpha \leq \alpha_{RG}$!

Bounding the bias: *Qinian's inequality*

Lemma (Q. Jin, 2009/10)

For $0 < \alpha \leq \beta$ *we have*

$$\|x_\beta - x_\alpha\| \leq (1+\gamma_*)\sqrt{\frac{\beta}{\alpha}}\|T^{1/2}(\beta + T)^{-1/2}(x - x_\beta)\|.$$

Remark

This allows to establish an oracle inequality for the RG-rule under classical noise assumptions, Q. Jin, *unpublished.*

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This allows to establish an oracle inequality for the RG-rule under classical noise assumptions, Q. Jin, *unpublished.*

In our setup we need to *lift* the norm on the right as

$$\| T^{1/2} (\beta + T)^{-1/2} (x - x_\beta)\| \leq C\| (\beta + T)^{-1} T(x - x_\beta)\|.$$

The latter bound *can be controlled by the RG-rule*!

Lifting: The Kindermann–Neubauer condition

Assumption (Ass. 2, Kindermann/Neubauer [5], 2008)

There exist $c_1 > 1$, $0 < c_2 < 1$ and $0 < t_0 < \|T^*T\|$ such that

$$\int_0^{\alpha} d\|E_t x\|^2 \leq c_1^2 \int_{c_2\alpha}^{\infty} r_\alpha^2(t)\, d\|E_t x\|^2$$

for all $0 < \alpha \leq t_0$.

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for all $0 < \alpha \leq t_0$.

Lemma

Under Assumption 2 *there is a constant C such that*

$$\| T^{1/2} (\beta + T)^{-1/2} (x - x_\beta)\| \leq C \| (\beta + T)^{-1} T(x - x_\beta)\|.$$

Consequently, we have that

$$\|x_\beta - x_\alpha\| \leq C\sqrt{\frac{\beta}{\alpha}} \| (\beta + T)^{-1} T(x - x_\beta)\|.$$

Deterministic oracle inequality

Theorem (Jin/M., 2013, [4])

For the general noise model, *and* under Assumption 2 *there is a constant such that the following holds.*
If α_{RG} is the parameter chosen according to the RG-rule *then*

$$\|x - x^{\delta}_{\alpha_{RG}}\| \leq C \inf_{0<\alpha\leq\alpha_0} \left\{ \|x - x_\alpha\| + \frac{\delta(\alpha)}{\alpha} \right\}.$$

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Goal

When does the Kindermann–Neubauer Assumption 2 hold?

The Kindermann–Neubauer Assumption

We did not talk about *smoothness* so far.
In order to understand the validity of the KN-assumption we introduce source sets.

Definition (source set)

For a non-decreasing continuous function $\psi\colon (0,\infty) \to \mathbb{R}^+,\ \psi(0+) = 0$ *we measure smoothness of an element* $x \in X$ *by assuming that*

$$x \in H_\psi := \{x, \quad x = \psi(T^* T)v,\ \|v\| \leq 1\} \subset X_\psi.$$

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Theorem (Lu/M., 2014)

The set of $x \in X$ *for which Assumption 2 holds true is* everywhere dense *in* every source set H_ψ *(in* X_ψ*).*

Outline

Summary

- We discussed *linear statistical ill-posed problems* in Hilbert space $y^\sigma = Tx + \delta\xi$ under *Gaussian white noise*.
- We indicated the optimal order of reconstruction.
- The error can be expressed in terms of the *effective dimension* $\mathcal{N}$.

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- The error can be expressed in terms of the *effective dimension* $\mathcal{N}$.
- We discussed the *statistical RG-rule*.
- We highlighted the importance of the *Kindermann–Neubauer type assumptions*.
- Under this assumption an *oracle-type bound* for the reconstruction error can be proven both
  - for *general noise assumptions*, and
  - for regularization under *Gaussian white noise*.

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Thank you for the attention!

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