JSS30, Summer School, COM5: Machine learning in inverse and ill-posed problems

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Methods of regularization of inverse problems: Morozov's discrepancy, balancing principle
Computer Session 2

Used literature

In this lecture is used material from the following books:

[BaK] A.B. Bakushinsky and M.Yu. Kokurin, *Iterative Methods for Approximate Solution of Inverse Problems*, Springer, New York, 2004.

[BeK] L. Beilina, M. Klibanov, *Approximate global convergence and adaptivity for coefficient inverse problems*, Springer, 2012.

[BKK] L. Beilina, E. Karchevskii, M. Karchevskii, *Numerical Linear Algebra: Theory and Applications*, Springer, 2017.

[IJ] K. Ito, B. Jin, *Inverse Problems: Tikhonov theory and algorithms*, Series on Applied Mathematics, V.22, World Scientific, 2015.

[TGSY] Tikhonov, A.N., Goncharsky, A., Stepanov, V.V., Yagola, A.G., *Numerical Methods for the Solution of Ill-Posed Problems*, ISBN 978-94-015-8480-7, 1995.

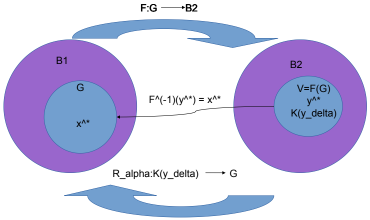
To solve ill-posed problems, regularization methods should be used. In this section we present main ideas of the regularization.

Definition Let B_1 and B_2 be two Banach spaces and $G \subset B_1$ be a set. Let the operator $F : G \to B_2$ be one-to-one. Consider the equation

$$F(x) = y. \tag{1}$$

Let y^* be the ideal noiseless right hand side of equation (2) and x^* be the ideal noiseless solution corresponding to y^*, $F(x^*) = y^*$. For every $\delta \in (0, \delta_0)$, $\delta_0 \in (0,1)$ denote

$$K_\delta(y^*) = \left\{ z \in B_2 : \|z - y^*\|_{B_2} \leq \delta \right\}.$$



Let $\alpha > 0$ be a parameter and $R_\alpha : K_{\delta_0}(y^*) \to G$ be a continuous operator depending on the parameter α. The operator R_α is called the *regularization operator* for

$$F(x) = y \tag{2}$$

if there exists a function $\alpha(\delta)$ defined for $\delta \in (0, \delta_0)$ such that

$$\lim_{\delta \to 0} \left\| R_{\alpha(\delta)}(y_\delta) - x^* \right\|_{B_1} = 0.$$

Regularization

The parameter α is called the regularization parameter. The procedure of constructing the approximate solution $x_{\alpha(\delta)} = R_{\alpha(\delta)}(y_\delta)$ is called the *regularization procedure*, or simply *regularization*.

There might be several regularization procedures for the same problem. In the case of CIPs, usually $\alpha(\delta)$ is a vector of regularization parameters, such as, e.g. the number of iterations, the truncation value of the parameter of the Laplace transform, the number of finite elements, etc..

The Tikhonov Regularization Functional

Let B_1 and B_2 be two Banach spaces. Let Q be another space, $Q \subset B_1$ as a set and $\overline{Q} = B_1$. In addition, we assume that Q is compactly embedded in B_1. Let $G \subset B_1$ be the closure of an open set. Consider a continuous one-to-one operator $F : G \to B_2$. Our goal is to solve

$$F(x) = y, \quad x \in G. \tag{3}$$

Let y^* be the ideal noiseless right hand side corresponding to the ideal exact solution x^*,

$$F(x^*) = y^*, \quad \|y - y^*\|_{B_2} < \delta. \tag{4}$$

To find an approximate solution of equation (3), we minimize the Tikhonov regularization functional $J_\alpha(x)$,

$$J_\alpha(x) = \frac{1}{2}\left\|F(x) - y\right\|_{B_2}^2 + \frac{\alpha}{2}\psi(x) = \varphi(x) + \frac{\alpha}{2}\psi(x), \tag{5}$$

$$J_\alpha : G \to \mathbb{R},$$

where $\alpha = \alpha(\delta) > 0$ is a small regularization parameter.

Different regularization terms

- The regularization term $\frac{\alpha}{2}\psi(x)$ encodes a priori available information about the unknown solution such that sparcity, smoothness, monotonicity
- Regularization term can be chosen as follows:
  - $\frac{\alpha}{2}||x||^p_{L^p}, \quad 1 \leq p \leq 2$
  - $\frac{\alpha}{2}||x||_{TV}$, TV means total variation, $||x||_{TV} = \int_G ||\nabla x||_2 dx$
  - $\frac{\alpha}{2}||x||_{BV}$, BV means bounded variation, a real-valued function whose TV is bounded (finite).
  - $\frac{\alpha}{2}||x||_{H^1}$
  - $\frac{\alpha}{2}(||x||_{L^1} + ||x||^2_{L^2})$

The Tikhonov Regularization Functional

We will consider the Tikhonov regularization functional $J_\alpha(x)$ in the form

$$J_\alpha(x) = \frac{1}{2}\left\|F(x) - y\right\|_{B_2}^2 + \frac{\alpha}{2}\|x - x_0\|_Q^2, \quad x_0 \in G \tag{6}$$

- Usually x_0 is a good first approximation for the exact solution x^*, it is sometimes called the *first guess* or the *first approximation*.
- The term $\alpha\|x - x_0\|_Q^2$ is called the *Tikhonov regularization term* or simply the *regularization term*.
- Consider a sequence $\{\delta_k\}_{k=1}^{\infty}$ such that $\delta_k > 0, \lim_{k\to\infty}\delta_k = 0$. Our goal is to construct sequences $\{\alpha(\delta_k)\}, \left\{x_{\alpha(\delta_k)}\right\}$ in a stable way such that

$$\lim_{k\to\infty}\left\|x_{\alpha(\delta_k)} - x^*\right\|_{B_1} = 0.$$

The Tikhonov Regularization Functional

Using (4) and (6), we obtain

$$J_\alpha(x^*) = \frac{1}{2}\left\|F(x^*) - y\right\|_{B_2}^2 + \frac{\alpha}{2}\|x^* - x_0\|_Q^2 \quad (7)$$

$$\leq \frac{\delta^2}{2} + \frac{\alpha}{2}\|x^* - x_0\|_Q^2 . \quad (8)$$

Let

$$m_{\alpha(\delta_k)} = \inf_G J_{\alpha(\delta_k)}(x) .$$

By (8)

$$m_{\alpha(\delta_k)} \leq \frac{\delta_k^2}{2} + \frac{\alpha(\delta_k)}{2}\|x^* - x_0\|_Q^2 .$$

Hence, there exists a point $x_{\alpha(\delta_k)} \in G$ such that

$$m_{\alpha(\delta_k)} \leq J_{\alpha(\delta_k)}\left(x_{\alpha(\delta_k)}\right) \leq \frac{\delta_k^2}{2} + \frac{\alpha(\delta_k)}{2}\|x^* - x_0\|_Q^2 . \quad (9)$$

The Tikhonov Regularization Functional

Hence, by (6) and (9)

$$\frac{1}{2}\left\|F(x_{\alpha(\delta_k)}) - y\right\|_{B_2}^2 + \frac{\alpha(\delta_k)}{2}\left\|x_{\alpha(\delta_k)} - x_0\right\|_Q^2 = J_\alpha\left(x_{\alpha(\delta_k)}\right) \qquad (10)$$

and thus,

$$\frac{1}{\alpha(\delta_k)}\left\|F(x_{\alpha(\delta_k)}) - y\right\|_{B_2}^2 + \left\|x_{\alpha(\delta_k)} - x_0\right\|_Q^2 = \frac{2}{\alpha(\delta_k)}J_\alpha\left(x_{\alpha(\delta_k)}\right),$$

or

$$\frac{1}{\alpha(\delta_k)}\left\|F(x_{\alpha(\delta_k)}) - y\right\|_{B_2}^2 \leq \frac{2}{\alpha(\delta_k)}J_\alpha\left(x_{\alpha(\delta_k)}\right)$$

and

$$\left\|x_{\alpha(\delta_k)} - x_0\right\|_Q^2 \leq \frac{2}{\alpha(\delta_k)}J_\alpha\left(x_{\alpha(\delta_k)}\right) \leq \frac{2}{\alpha(\delta_k)}\cdot\left[\frac{\delta_k^2}{2} + \frac{\alpha(\delta_k)}{2}\|x^* - x_0\|_Q^2\right]. \qquad (11)$$

The Tikhonov Regularization Functional

From (11) follows that

$$\left\|x_{\alpha(\delta_k)} - x_0\right\|_Q^2 \leq \frac{\delta_k^2}{\alpha(\delta_k)} + \|x^* - x_0\|_Q^2 . \quad (12)$$

Suppose that

$$\lim_{k\to\infty} \alpha(\delta_k) = 0 \text{ and } \lim_{k\to\infty} \frac{\delta_k^2}{\alpha(\delta_k)} = 0. \quad (13)$$

Then (12) implies that the sequence $\left\{x_{\alpha(\delta_k)}\right\} \subset G \subseteq Q$ is bounded in the norm of the space Q. Since Q is compactly embedded in B_1, then there exists a subsequence of the sequence $\left\{x_{\alpha(\delta_k)}\right\}$ which converges in the norm of the space B_1.

The Tikhonov Regularization Functional

We assume that the sequence $\left\{x_{\alpha(\delta_k)}\right\}$ itself converges to a point $\overline{x} \in B_1$,

$$\lim_{k\to\infty} \left\|x_{\alpha(\delta_k)} - \overline{x}\right\|_{B_1} = 0.$$

Then (9) and (13) imply that

$$\lim_{k\to\infty} J_{\alpha(\delta_k)}\left(x_{\alpha(\delta_k)}\right) = 0. \tag{14}$$

On the other hand, by the definition of Tikhonov's functional,

$$\lim_{k\to\infty} J_{\alpha(\delta_k)}\left(x_{\alpha(\delta_k)}\right) = \frac{1}{2}\lim_{k\to\infty}\left[\left\|F\left(x_{\alpha(\delta_k)}\right) - y\right\|_{B_2}^2 + \alpha\left(\delta_k\right)\left\|x_{\alpha(\delta_k)} - x_0\right\|_Q^2\right]$$

$$= \frac{1}{2}\lim_{k\to\infty}[\|F\left(x_{\alpha(\delta_k)}\right) - y^* + y^* - y\|_{B_2}^2 + \alpha\left(\delta_k\right)\left\|x_{\alpha(\delta_k)} - x_0\right\|_Q^2]$$

$$= \frac{1}{2}\left\|F\left(\overline{x}\right) - y^*\right\|_{B_2}^2.$$

Hence, by (14) and the above equation $\left\|F\left(\overline{x}\right) - y^*\right\|_{B_2} = 0$, which means that $F\left(\overline{x}\right) = y^*$. Since the operator F is one-to-one, then $\overline{x} = x^*$. Thus, we have constructed the sequence of regularization parameters $\{\alpha\left(\delta_k\right)\}_{k=1}^{\infty}$ and the sequence $\left\{x_{\alpha(\delta_k)}\right\}_{k=1}^{\infty}$: $\lim_{k\to\infty}\left\|x_{\alpha(\delta_k)} - x^*\right\|_{B_1} = 0$.

The Tikhonov Regularization Functional

- To ensure (13)

$$\lim_{k\to\infty} \alpha(\delta_k) = 0 \text{ and } \lim_{k\to\infty} \frac{\delta_k^2}{\alpha(\delta_k)} = 0. \quad (15)$$

  one can choose, for example $\alpha(\delta_k) = C\delta_k^{\mu}, \mu \in (0, 2)$.

- It is reasonable to call $\left\{x_{\alpha(\delta_k)}\right\}_{k=1}^{\infty}$ *regularizing sequence*.
- The sequence $\left\{x_{\alpha(\delta_k)}\right\}_{k=1}^{\infty}$ is called *minimizing sequence*.
- There are two inconveniences in the above construction:
  - First, it is unclear how to find the minimizing sequence computationally.
  - Second, the problem of multiple local minima and ravines of the functional (6) presents a significant complicating factor in the goal of the construction of such a sequence.

Regularized Solution

- The considered process of the construction of the regularized sequence does not guarantee that the functional $J_\alpha(x)$ indeed achieves it minimal value.
- Suppose now that the functional $J_\alpha(x)$ does achieve its minimal value, $J_\alpha(x_\alpha) = \min_G J_\alpha(x), \alpha = \alpha(\delta)$. Then $x_{\alpha(\delta)}$ is called a *regularized solution* of equation (3) for this specific value $\alpha = \alpha(\delta)$ of the regularization parameter.
- Let $\delta_0 > 0$ be a sufficiently small number. Suppose that for each $\delta \in (0, \delta_0)$ there exists an $x_{\alpha(\delta)}$ such that $J_{\alpha(\delta)}\left(x_{\alpha(\delta)}\right) = \min_G J_{\alpha(\delta)}(x)$.
- Even though one might have several points $x_{\alpha(\delta)}$, we select a single one of them for each $\alpha = \alpha(\delta)$.

Regularized Solution

- It follows from the construction of the minimizing sequence that all points $x_{\alpha(\delta)}$ are close to the exact solution x^*, as long as δ is sufficiently small.
- It makes sense now to relax a little bit the definition of the regularization operator

$$\lim_{\delta \to 0} \left\| R_{\alpha(\delta)} \left(y_\delta \right) - x^* \right\|_{B_1} = 0.$$

- Thus, instead of the existence of a function $\alpha\left(\delta\right)$, we now require the existence of a sequence $\{\delta_k\}_{k=1}^{\infty} \subset (0, 1)$ such that

$$\lim_{k \to \infty} \delta_k = 0 \text{ and } \lim_{k \to \infty} \left\| R_{\alpha(\delta_k)} \left(y_{\delta_k} \right) - x^* \right\|_{B_1} = 0.$$

Regularized Solution

- For every $\delta \in (0, \delta_0)$ and y_δ such that $\|y_\delta - y^*\|_{B_2} \leq \delta$ we define the operator $R_{\alpha(\delta)}(y) = x_{\alpha(\delta)}$, where $x_{\alpha(\delta)}$ is a regularized solution. Then it follows from the construction of the regularized sequence that $R_{\alpha(\delta)}(y)$ is a regularization operator.
- Consider now the case when the space B_1 is a finite dimensional space. Since all norms in finite dimensional spaces are equivalent, we can set $Q = B_1 = \mathbb{R}^n$. We denote the standard euclidean norm in $\mathbb{R}^n$ as $\|\cdot\|$. Hence, we assume now that $G \subset \mathbb{R}^n$ is the closure of an open bounded domain and G is a compact set.
- Let $x^* \in G$ and $\alpha = \alpha(\delta)$. We have

$$J_{\alpha(\delta)}(x) = \frac{1}{2}\left\|F(x) - y\right\|_{B_2}^2 + \frac{\alpha(\delta)}{2}\|x - x_0\|^2,$$

$$J_{\alpha(\delta)} : G \to \mathbb{R},\ x_0 \in G.$$

- By the Weierstrass' theorem the functional $J_{\alpha(\delta)}(x)$ achieves its minimal value on the set G. Let $x_{\alpha(\delta)}$ be a minimizer of the functional $J_{\alpha(\delta)}(x)$ on G (there might be several minimizers).

$$J_{\alpha(\delta)}\left(x_{\alpha(\delta)}\right) \le J_{\alpha(\delta)}(x^*) = \frac{1}{2}\left\|F(x^*) - y\right\|_{B_2}^2 + \frac{\alpha}{2}\|x^* - x_0\|^2$$
$$\le \frac{\delta^2}{2} + \frac{\alpha(\delta)}{2}\|x^* - x_0\|^2.$$

Hence, using

$$\left\|x_{\alpha(\delta_k)} - x_0\right\|_Q^2 \le \frac{2}{\alpha(\delta_k)} J_\alpha\left(x_{\alpha(\delta_k)}\right) \le \frac{2}{\alpha(\delta_k)}\left(\frac{\delta_k^2}{2} + \frac{\alpha(\delta_k)}{2}\|x^* - x_0\|^2\right). \tag{16}$$

for $\left\|x_{\alpha(\delta)} - x_0\right\|_Q^2$ we get

$$\left\|x_{\alpha(\delta)} - x_0\right\| \le \sqrt{\frac{\delta^2}{\alpha} + \|x^* - x_0\|^2} \le \frac{\delta}{\sqrt{\alpha}} + \|x^* - x_0\|. \tag{17}$$

We obtain from (17)

$$\left\|x_{\alpha(\delta)} - x^*\right\| = \left\|x_{\alpha(\delta)} - x_0 + x_0 - x^*\right\| \leq \|x_{\alpha(\delta)} - x_0\| + \|x_0 - x^*\| \leq \frac{\delta}{\sqrt{\alpha}} + 2\|x^* - x_0\|. \tag{18}$$

An important conclusion from (18) is that for a given pair $(\delta, \alpha(\delta))$ the accuracy of the regularized solution is determined by the accuracy of the first guess x_0.

The Accuracy of the Regularized Solution

Consider again the equation

$$F(x) = y,\ x \in G. \tag{19}$$

Let y^* be the ideal noiseless data corresponding to the ideal solution x^*,

$$F(x^*) = y^*, \quad \|y - y^*\|_{B_2} \le \delta. \tag{20}$$

To find an approximate solution of equation (19), we minimize

$$J_\alpha(x) = \frac{1}{2}\left\|F(x) - y\right\|_{B_2}^2 + \frac{\alpha}{2}\|x - x_0\|_Q^2, \tag{21}$$

- One can not a better accuracy of the solution than δ, Thus, it is usually acceptable that all other parameters are much larger than δ.
- For example, let the number $\mu \in (0,1)$. Since $\lim_{\delta\to 0}\left(\delta^{2\mu}/\delta^2\right) = \infty$, then there exists a sufficiently small number $\delta_0(\mu) \in (0,1)$ such that $\delta^{2\mu} > \delta^2, \forall\delta \in (0, \delta_0(\mu))$.
- Hence, we we can choose

$$\alpha(\delta) = \delta^{2\mu}, \mu \in (0,1). \tag{22}$$

The Accuracy of the Regularized Solution

- We introduce the dependence

$$\alpha(\delta) = \delta^{2\mu}, \mu \in (0,1). \tag{23}$$

for the sake of definiteness only. In fact other dependencies $\alpha(\delta)$ are also possible.

- Let $m_{\alpha(\delta)} = \inf_G J_{\alpha(\delta)}(x)$. Then

$$m_{\alpha(\delta)} \leq J_{\alpha(\delta)}(x^*). \tag{24}$$

- We cannot prove the existence of a minimizer of the functional J_α when $\dim B_1 = \infty$.
- Thus, we work now with the minimizing sequence. It follows from (21) and (24) that there exists a sequence $\{x_n\}_{n=1}^{\infty} \subset G$ such that

$$m_{\alpha(\delta)} \leq J_{\alpha(\delta)}(x_n) \leq \frac{\delta^2}{2} + \frac{\alpha}{2}\|x^* - x_0\|_Q^2 \text{ and } \lim_{n\to\infty} J_{\alpha(\delta)}(x_n) = m(\delta). \tag{25}$$

The Accuracy of the Regularized Solution

- By
$$\left\|x_{\alpha(\delta_k)} - x_0\right\|_Q^2 \leq \frac{\delta_k^2}{\alpha\left(\delta_k\right)} + \|x^* - x_0\|_Q^2 . \tag{26}$$
and (25)
$$\|x_n\|_Q \leq \left(\frac{\delta^2}{\alpha} + \|x^* - x_0\|_Q^2\right)^{1/2} + \|x_0\|_Q . \tag{27}$$
- Thus, it follows from (23) and (27) that $\{x_n\}_{n=1}^{\infty} \subset K\left(\delta, x_0\right)$, where $K\left(\delta, x_0\right) \subset Q$ is a precompact set in B_1 defined as
$$K\left(\delta, x_0\right) = \left\{x \in Q : \|x\|_Q \leq \sqrt{\delta^{2(1-\mu)} + \|x^* - x_0\|_Q^2} + \|x_0\|_Q\right\}. \tag{28}$$
- Note that the sequence $\{x_n\}_{n=1}^{\infty}$ depends on δ.
- Let $\overline{K}\left(\delta, x_0\right)$ be the closure of the set $K\left(\delta, x_0\right)$ in the norm of the space B_1. Hence, $\overline{K}\left(\delta, x_0\right)$ is a closed compact set in B_1.

Rules for choice of the regularization parameter

Rules for choosing α in the Tikhonov functional

$$J_\alpha(x) = \frac{1}{2}\|F(x) - y\|_{B_2}^2 + \frac{\alpha}{2}\psi(x) = \varphi(x) + \frac{\alpha}{2}\psi(x). \qquad (29)$$

A-priori rules. Let $\eta = (\delta, h)$, $\|F - F_h\| \leq h$, $\|y - y^*\| \leq \delta$.

- $\alpha(\eta) \to 0$ as $\eta \to 0$ [BaK, BeK, IJ, TGSY]
- $\frac{\delta^2}{\alpha(\delta)} \to 0$. Example: $\alpha(\delta) = C\delta^\mu, \mu \in (0,2), C = const. > 0$. [BaK, BeK]
- $\frac{(\delta+h)^2}{\eta} \to 0$ as $\eta \to 0$. [BaK, TGSY]

A-posteriori rules:

- Morozov's discrepancy principle [IJ, TGSY]
- Balancing principle [IJ]
- Quasi-optimality [IJ]
- L-curve, S-curve [IJ]

How to estimate noise in data?

- Test first algorithm for solution of the inverse problem on simulated data which have the same set-up as the set-up for generation of your experimental data. Simulated data can be obtained by reconstructing of already known object with known properties (dielectric permittivity, conductivity and so on).
- Solve the inverse problem to obtain $x_{\alpha(\delta)}$ and compute discrepancy, then the noise will be approximately

$$||F(x_{\alpha(\delta)}) - y|| \approx \delta, \tag{30}$$

- We can say that the simulated data (for the known object to be reconstructed) is approximately exact data y^*, then noisy data y_δ can be obtained as

$$y_\delta = y(1 + \delta\alpha), \tag{31}$$

where y is simulated "exact" data, $\alpha \in (-1, 1)$ is randomly distributed number and $\delta \in [0, 1]$ is the noise level. For example, if noise in data is 5%, then $\delta = 0.05$.

Different models for generation of noise in data

- You can use several Matlab's functions to test adding of the noise. Below is an example of the Matlab code which shows how to add noise for solution of Poisson's equation (example of section 8.4.4 of the book [BKK]) (the Figure 26 illustrates different type of noise):

```
r = randi([-1 1],size(u),1)
for j=1:n
  for i=1:n
    udelta(n*(i-1)+j) = u(n*(i-1)+j)*(1 + 0.1*r(n*(i-1)+j));
  end
end
```

- Another models for generation of noisy data are also possible. For example, normally distributed Gaussian noisy data is obtained using normally distributed Gaussian noise

$$N(y|\mu, \sigma^2) = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{-(y-\mu)^2}{2\sigma^2}}.$$

Here, μ is mean, σ^2 is variance, σ is standard deviation.

Here is an example how to add Gaussian noise $N(y|\mu, \sigma^2)$ with mean $\mu = 0$ and variance $\sigma^2 = 0.01$ to matrix A in MATLAB:

```
Anoise = A + 0.01*randn(size(A)) + 0;
```

Different models for generation of noise in data

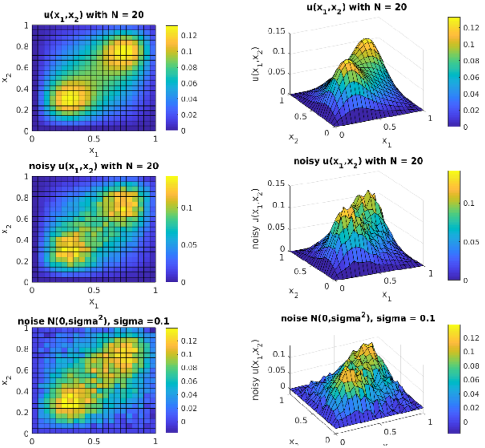


Figure 1: Top figures: Solution of Poisson's equation (example of section 8.4.4 of the book [BKK]). Middle figures: Noisy solution obtained via (31) with $\sigma = 0.1$. Bottom figures: noisy solution obtained via adding normally distributed Gaussian noise $N(y|0, 0.01), \sigma = 0.1$.

Morozov's discrepancy principle

- If the estimate of the noise level σ is available then the discrepancy principle is most popular.
- The principle determines the reg.parameter $\alpha = \alpha(\delta)$ such that

$$\|F(x_{\alpha(\delta)}) - y\| = c_m \delta, \tag{32}$$

  where $c_m \geq 1$ is a constant.
- Relaxed version of a discrepancy principle is:

$$c_{m,1}\delta \leq \|F(x_{\alpha(\delta)}) - y\| \leq c_{m,2}\delta, \tag{33}$$

  for some constants $1 \leq c_{m,1} \leq c_{m,2}$
- The main feature of the principle is that the computed solution $x_{\alpha(\delta)}$ can't be more accurate than the residual $\|F(x_{\alpha(\delta)}) - y\|$.
- Main methods for solution of (32) are the model function approach and a quasi-Newton method.

Morozov V.A., On the solution of functional equations by the method of regularization, Soviet Math.Dokl., 7, pp.414-417, 1966

Morozov's discrepancy principle

For the Tikhonov functional $J_\alpha(x)$ defined as

$$J_\alpha(x) = \frac{1}{2}\|F(x) - y\|^2_{B_2} + \alpha\psi(x) = \varphi(x) + \alpha\psi(x), \quad (34)$$

the value function $F(\alpha) : \mathbb{R}^+ \to \mathbb{R}$ is defined accordingly to [TA] as

$$F(\alpha) = \inf_x J_\alpha(x) \quad (35)$$

If there exists $F'(\alpha)$ at $\alpha > 0$ then from (34) and (35) follows that

$$F(\alpha) = \inf_x J_\alpha(x) = \underbrace{\varphi'(x)}_{\bar{\varphi}(\alpha)} + \alpha \underbrace{\psi'(x)}_{\bar{\psi}(\alpha)}. \quad (36)$$

Since $F'_\alpha(\alpha) = \psi'(x) = \bar{\psi}(\alpha)$ then from (36) folows

$$\bar{\psi}(\alpha) = F'(\alpha), \;\; \bar{\varphi}(\alpha) = F(\alpha) - \alpha F'(\alpha) \quad (37)$$

[TA] A.N.Tikhonov, V. Y. Arsenin, Solutions of ill-posed problems, John Wiley Sons, New-York, 1977.

Morozov's discrepancy principle: the model function approach

The main idea is to compute discrepancy $\bar{\varphi}(\alpha)$ using the value function $F(\alpha)$ and then approximate $F(\alpha)$ using rational functions like Padé approximations which are called model functions.
We note that

$$\varphi(x) = \frac{1}{2}\left\|F(x) - y\right\|^2 ; \bar{\varphi}(\alpha) = \varphi'(x_{\alpha(\delta)}) = \left\|F(x_{\alpha(\delta)}) - y\right\| F'(x_{\alpha(\delta)}). \quad (38)$$

If $\bar{\psi}(\alpha) \in C(\alpha)$ then the discrepancy equation

$$\|F(x_{\alpha(\delta)}) - y\| = c_m \delta \quad (39)$$

can be used in (38) to obtain $\bar{\varphi}(\alpha) = \frac{\delta^2}{2}$. Combining this with (37) we get

$$\bar{\varphi}(\alpha) = F(\alpha) - \alpha F'(\alpha) = \frac{\delta^2}{2}. \quad (40)$$

Our goal is to solve (40) for α. The value function is very nonlinear, the model function is used to approximate the value function.

Morozov's discrepancy principle: the model function approach

For example, one can use the following model function:

$$F(\alpha) \approx m(\alpha) = b + \frac{c}{t + \alpha}, \tag{41}$$

where b, c, t are constants to be determined.
Usually, b is determined using asymptotics of $m(0^+)$ or $m(+\infty)$, for example, as

$$b = \lim_{\alpha \to \infty} F(\alpha). \tag{42}$$

Then the formula (41) can be written in the iterative form as

$$F_k(\alpha) \approx m_k(\alpha) = b + \frac{c_k}{t_k + \alpha_k}, \tag{43}$$

The next step is to enforce the Hermite interpolation conditions at α_k such that

$$m_k(\alpha_k) = F(\alpha_k), \quad m_k'(\alpha_k) = F'(\alpha_k) \tag{44}$$

Morozov's discrepancy principle: the model function approach

The next step is to enforce the Hermite interpolation conditions at α_k such that

$$m_k(\alpha_k) = F(\alpha_k), \;\; m'_k(\alpha_k) = F'(\alpha_k), \tag{45}$$

what gives

$$\begin{aligned} m_k(\alpha_k) &= b + \frac{c_k}{t_k + \alpha_k} = F(\alpha_k) \rightarrow c_k = (F(\alpha_k) - b)(t_k + \alpha_k), \\ m'_k(\alpha_k) &= \frac{-c_k}{(t_k + \alpha_k)^2} = F'(\alpha_k) \rightarrow F'(\alpha_k) = \frac{-(F(\alpha_k) - b)(t_k + \alpha_k)}{(t_k + \alpha_k)^2} \end{aligned} \tag{46}$$

Morozov's discrepancy principle: the model function approach

From the first equation of (46) we get

$$c_k = (F(\alpha_k) - b)(t_k + \alpha_k), \tag{47}$$

and from the second equation of (46) we have

$$t_k + \alpha_k = \frac{-(F(\alpha_k) - b)}{F'(\alpha_k)} \tag{48}$$

Recall that

$$\bar{\psi}(\alpha_k) = F'(\alpha_k), \;\; \bar{\varphi}(\alpha_k) = F(\alpha_k) - \alpha_k F'(\alpha_k) \tag{49}$$

Substituting (48) into (47) we obtain

$$c_k = \frac{-(F(\alpha_k) - b)^2}{F'(\alpha_k)} = \frac{-(F(\alpha_k) - b)^2}{\bar{\psi}(\alpha_k)} \tag{50}$$

Morozov's discrepancy principle: the model function approach

From the second equation of (46) we get

$$F'(\alpha_k) = \frac{b - F(\alpha_k)}{t_k + \alpha_k} \to t_k = \frac{b - F(\alpha_k)}{F'(\alpha_k)} - \alpha_k. \qquad (51)$$

Then

$$t_k = \frac{(b - F(\alpha_k))}{\bar{\psi}(\alpha_k)} - \alpha_k. \qquad (52)$$

The sign of t_k is positive only if

$$b - F(\alpha_k) - \bar{\psi}(\alpha_k)\alpha_k > 0 \qquad (53)$$

which holds only for the same reg.parameter α_k. If $t_k > 0$ then the model function $m_k(\alpha)$ preserves the monotonicity, concavity and the asymptotic behaviour of $F(\alpha)$.

Morozov's discrepancy principle: the model function approach

The the discrepancy equation

$$F(\alpha) - \alpha F'(\alpha) = \frac{\delta^2}{2} \tag{54}$$

can be approximated as

$$m_k(\alpha) - \alpha m_k'(\alpha) = \frac{\delta^2}{2} \tag{55}$$

The equation (55) is nonlinear and can be solved vis Newton's method noting that

$$g(\alpha) = m_k(\alpha) - \alpha m_k'(\alpha) - \frac{\delta^2}{2} = 0. \tag{56}$$

Morozov's discrepancy principle: the model function approach

Then the Newton's method to solve $g(\alpha) = 0$ is:

$$\alpha_{k+1} = \alpha_k - \frac{g(\alpha_k)}{g'(\alpha_k)}, \tag{57}$$

where

$$g(\alpha_k) = m_k(\alpha_k) - \alpha_k m_k'(\alpha_k) - \frac{\delta^2}{2}$$

and

$$\begin{aligned} g'(\alpha_k) &= (m_k(\alpha) - \alpha m_k'(\alpha) - \frac{\delta^2}{2})'_\alpha(\alpha_k) \\ &= (m_k'(\alpha) - [m_k'(\alpha) + \alpha m_k''(\alpha)])(\alpha_k) \\ &= (-\alpha m_k''(\alpha))(\alpha_k) = -\alpha_k m_k''(\alpha_k). \end{aligned} \tag{58}$$

The model function approach

$$
\begin{aligned}
m_k(\alpha) &= b + \frac{c_k}{t_k + \alpha}, \\
m'_k(\alpha) &= \frac{-c_k}{(t_k + \alpha)^2}, \\
m''_k(\alpha) &= \frac{2c_k(t_k + \alpha)}{(t_k + \alpha)^4} = \frac{2c_k}{(t_k + \alpha)^3}.
\end{aligned} \tag{59}
$$

Then we can use following formulas

$$
\begin{aligned}
g(\alpha_k) &= m_k(\alpha_k) - \alpha_k m'_k(\alpha_k) - \frac{\delta^2}{2} = b + \frac{c_k}{t_k + \alpha_k} + \alpha_k \frac{c_k}{(t_k + \alpha_k)^2} - \frac{\delta^2}{2}, \\
g'(\alpha_k) &= \left(m_k(\alpha_k) - \alpha_k m'_k(\alpha_k) - \frac{\delta^2}{2} \right)'_{\alpha} (\alpha_k) = -\alpha_k m''_k(\alpha_k) = -\frac{2c_k \alpha_k}{(t_k + \alpha_k)^3}
\end{aligned} \tag{60}
$$

in the Newton's method (57) to get update of the coefficients α_k until convergence in α_k is achieved.

Algorithm: Morozov's discrepancy principle, the model function approach

1. Start with the initial approximations α_0 (take large value because of (42)) and compute the sequence of α_k in the following steps.
2. Compute the value function $F(\alpha_k) = \inf_x J_{\alpha_k}(x)$, b as in (42), c_k and t_k as in (50), (52), correspondingly.
3. Update the reg. parameter $\alpha := \alpha_{k+1}$ via Newton's method

$$\alpha_{k+1} = \alpha_k - \frac{g(\alpha_k)}{g'(\alpha_k)},$$

   where $g(\alpha_k), g'(\alpha_k)$ are computed as in (60), respectively.
4. For the tolerance $0 < \theta < 1$ chosen by the user, stop computing reg.parameters α_k if computed α_k are stabilized, or $|\alpha_k - \alpha_{k-1}| \leq \theta$. Otherwise, set $k := k + 1$ and go to Step 2.

The model function approach: study of convergence

We will show the the above algorithm is locally convergent. Let us define

$$G_k(\alpha) = m_k(\alpha) - \alpha m_k'(\alpha). \tag{61}$$

and assume $G_k(\alpha_k) > \delta^2/2, G_k(\alpha) \leq G_k(\alpha_k) \ \ \forall \alpha \in [0, \alpha_k]$. Using Taylor's expansion of $G_k(\alpha)$ we get approximation of it, $\bar{G}_k(\alpha) \approx G_k(\alpha)$, as

$$\bar{G}_k(\alpha) = G_k(\alpha) + G_k'(\alpha)(\alpha - \alpha_k) = G_k(\alpha) + \bar{\alpha}_k(G_k(\alpha) - G_k(\alpha_k)). \tag{62}$$

Since $F(\alpha) - \alpha F'(\alpha) = \frac{\delta^2}{2}$ then

$$\bar{G}_k(\alpha) \approx G_k(\alpha) = m_k(\alpha) - \alpha m_k'(\alpha) = \frac{\delta^2}{2}. \tag{63}$$

Assuming $\bar{G}_k(0) < \frac{\delta^2}{2}$, equation (63) has a unique solution. For example, one can choose $\bar{G}_k(0) = \gamma\delta^2 \ \ \forall \gamma \in [0, 0.5]$, then from (62)

$$\bar{\alpha}_k = \frac{\gamma\delta^2 - G_k(0)}{G_k(0) - G_k(\alpha_k)}$$

The model function approach: study of convergence

Theorem [K. Ito, B. Jin]
Let $\bar{\varphi}(\alpha)$ and $\bar{\psi}(\alpha)$ be continuous functions in α, then the solution α^* of the discrepancy equation

$$||F(x_{\alpha(\delta)}) - y|| = c_m \delta, \tag{64}$$

is unique with α_0 satisfying $G(\alpha_0) > \frac{\delta^2}{2}$. The sequence $\{\alpha_k\}$ generated by the Algorithm is well-defined, it is finite and terminates at α_k satisfying $G(\alpha_k) \leq \frac{\delta^2}{2}$, or it is infinite and converges to the solution α^* strictly monotonically decreasingly.
Proof. It is suffices to show that if $\bar{G}_k(\alpha_k) \leq \frac{\delta^2}{2}$ is never reached then α_k converges to α^*. Let us assume $\bar{G}_k(\alpha_k) > \frac{\delta^2}{2}$, then by monotonicity of $\bar{G}_k(\alpha_k)$ we get $\alpha_{k+1} < \alpha_k$. Since

$$\bar{G}_k(\alpha_k) = G_k(\alpha_k) = G(\alpha_k), \;\; \bar{G}_k(\alpha_k) > \frac{\delta^2}{2} \tag{65}$$

means that $\alpha_k > \alpha^*$. Thus, the sequence $\{\alpha_k\}$ converges to some $\bar{\alpha} > \alpha^*$ by the monotonne convergence theorem. Let is show that $\bar{\alpha} = \alpha^*$.

Now take limit in α_k, sequences $\{c_k\}, \{t_k\}$ are also converging. Then

$$G(\bar{\alpha}) = \lim_{k\to\infty} G(\alpha_{k+1}) = \lim_{k\to\infty} G_{k+1}(\alpha_{k+1}) = \lim_{k\to\infty} G_k(\alpha_{k+1}). \tag{66}$$

Here we have used the Lemma 3.10 in [K. Ito, B. Jin] that if the sequence α_k is converging to $\bar{\alpha}$, then

$$\lim_{k\to\infty} G_{k+1}(\alpha_{k+1}) = \lim_{k\to\infty} G_k(\alpha_{k+1}). \tag{67}$$

Then from the equation

$$\bar{G}_k(\alpha_{k+1}) = G_k(\alpha_{k+1}) + \bar{\alpha}_k(G_k(\alpha_{k+1}) - G_k(\alpha_k)) = \frac{\delta^2}{2}. \tag{68}$$

and (66), by the definition of $G_k(\alpha)$ and $\bar{\alpha}_k$ and the convergence of α_k we see that

$$\lim_{k\to\infty}(G_{k+1}(\alpha_{k+1}) - G_k(\alpha_k)) = 0. \tag{69}$$

Thus, $\bar{\alpha}_k$ are convergent, taking $\lim_{k\to\infty}$ in (68) $G(\bar{\alpha}) = \frac{\delta^2}{2}$. By the uniqueness assumption of the solution of the discrepancy equation $\bar{\alpha} = \alpha^*$. $\square$

Balancing principle

For the Tikhonov functional $J_\alpha(x)$ defined as

$$J_\alpha(x) = \frac{1}{2}\left\|F(x) - y\right\|^2_{B_2} + \alpha\psi(x) = \varphi(x) + \alpha\psi(x), \quad (70)$$

$$\bar{\psi}(\alpha) = F'(\alpha), \;\; \bar{\varphi}(\alpha) = F(\alpha) - \alpha F'(\alpha)$$

balancing principle (or Lepskii, see [LLP, M]) finds $\alpha > 0$ such that following expression is fullfilled

$$\bar{\varphi}(\alpha) = \gamma\alpha\bar{\psi}(\alpha) \quad (71)$$

where $\gamma = a_0/a_1$ is determined by the statistical a priori knowledge from shape parameters in Gamma distributions. When $\gamma = 1$ the method is called zero crossing method, see [JG].

[JG] P. R. Johnston, R.M. Gulrajani, A new method for regularization parameter determination in the inverse problem of electrocardiography, IEEE Transactions Biomed.Eng. 44, 1, pp. 19-39, 1997.
[LLP] R. D. Lazarov, S. Lu and S. V. Pereverzev, On the balancing principle for some problems of numerical analysis, Numer. Math.,106, 4, pp. 659-689.

[M] P. Mathé, The Lepskii principle revised, Inverse Problems, 22, 3, pp. L11-L15, 2006.

Balancing principle

Let us show that the balancing rule

$$\bar{\varphi}(\alpha) = \gamma\alpha\bar{\psi}(\alpha) \tag{72}$$

finds optimal $\alpha > 0$ minimizing the function

$$\Phi_\gamma(\alpha) = \frac{F^{1+\gamma}(\alpha)}{\alpha}$$

From

$$\bar{\psi}(\alpha) = F'(\alpha), \;\; \bar{\varphi}(\alpha) = F(\alpha) - \alpha F'(\alpha) \tag{73}$$

follows that

$$0 = \bar{\varphi}(\alpha) - \gamma\alpha\bar{\psi}(\alpha) = F(\alpha) - \alpha F'(\alpha) - \gamma\alpha F'(\alpha) = F(\alpha) - \alpha F'(\alpha)(1+\gamma)$$

or

$$F(\alpha) = \alpha F'(\alpha)(1+\gamma). \tag{74}$$

Balancing principle

The equation

$$F(\alpha) = \alpha F'(\alpha)(1+\gamma).$$

can be written as

$$\frac{1}{\alpha} = \frac{F'(\alpha)}{F(\alpha)}(1+\gamma) = \frac{dF/d\alpha}{F(\alpha)}(1+\gamma)$$

or

$$\frac{d\alpha}{\alpha} = \frac{dF}{F(\alpha)}(1+\gamma).$$

Integrating both sides of the above equation we get

$$\ln \alpha + C_1 = (1+\gamma) \ln F(\alpha) + C_2$$

or taking $C_1 = C_2$ we get

$$\alpha = \exp^{(1+\gamma)\ln F(\alpha)} = F(\alpha)^{1+\gamma}$$

which can be rewritten as the function to be minimized in the balancing principle

$$\Phi_\gamma(\alpha) = \frac{F^{1+\gamma}(\alpha)}{\alpha} = 1.$$

Balancing principle

We can check that the minimum of $\Phi_\gamma(\alpha)$ is achieved at

$$0 = (\Phi_\gamma(\alpha))'_\alpha = \frac{(1+\gamma)F'(\alpha)F^\gamma(\alpha)\alpha - F^{1+\gamma}(\alpha)}{\alpha^2}$$

From the above equation we get

$$(1+\gamma)F'(\alpha)F^\gamma(\alpha)\alpha = F^{1+\gamma}(\alpha) \rightarrow (1+\gamma)F'(\alpha)\alpha = F(\alpha)$$

This equation is the same as the equation (74) which gives the balancing principle

$$\bar{\varphi}(\alpha) = \gamma\alpha\bar{\psi}(\alpha) \tag{75}$$

Thus, the balancing principle computes optimal value of α where $(\Phi_\gamma(\alpha))'_\alpha = 0$.

Balancing principle: fixed point algorithm

For the Tikhonov functional $J_\alpha(x)$ defined as

$$J_\alpha(x) = \frac{1}{2}\left\|F(x) - y\right\|_{B_2}^2 + \alpha\psi(x) = \varphi(x) + \alpha\psi(x), \qquad (76)$$

the following fixed point algorithm for computing α is proposed.

1. Start with the initial approximations $\alpha_0 = \delta^\mu, \mu \in (0,2)$ and compute the sequence of α_k in the following steps.
2. Compute the value function $F(\alpha_k) = \inf_x J_{\alpha_k}(x)$ and get x_{α_k}.
3. Update the reg. parameter $\alpha := \alpha_{k+1}$ as

$$\alpha_{k+1} = \frac{1}{\gamma}\frac{\bar{\varphi}(x_{\alpha_k})}{\bar{\psi}(x_{\alpha_k})}$$

4. For the tolerance $0 < \theta < 1$ chosen by the user, stop computing reg.parameters α_k if computed α_k are stabilized, or $|\alpha_k - \alpha_{k-1}| \leq \theta$. Otherwise, set $k := k + 1$ and go to Step 2.