Regularization Parameter Tool

Theoretical Aspects

A Package for Comparing Regularization Parameter Rules and Solving Discrete Ill-Posed Problems by Tikhonov method

Uno Hämarik, Reimo Palm, Toomas Raus

The purpose of this package is to provide the user tools for comparing and analysis of different rules for choice of the regularization parameter if discrete illposed problems are solved by Tikhonov method. The user can choose the problem from the set of test problems or to use the own problem. The user can choose certain version from many possibilities to generate the noise and to give information about the noise level. If no information about the noise level is given, the regularization parameter may be chosen by one of heuristic rules, otherwise many rules for parameter choice are available depending information about the noise level.

Contents

1. Discrete ill-posed problem. Tikhonov method	3
2. Choice of the regularization parameter	3
2.1 Delta-rules	4
Discrepancy principle	4
Modified discrepancy principle (Raus-Gfrerer rule)	4
Monotone error rule	5
Monotone error rule with post-estimation	5
Adjusted monotone error rule	5
Rule R1(k) (transformed discrepancy principle)	5
Balancing principle	6
Rules R2 $(q = 2, l = 1/2, k = 1)$ and R2 $(q = 2, l = 1/2, k = 2)$	6
2.2. Heuristic rules	7
Quasi-optimality criterion	8
Hanke-Raus rule	8
L-curve and the Reginska's rule	8
Modified Reginska's rule	8
Hybrid rule	9
Brezinski –Rodriguez-Seatzu rule	10
Residual method.	10
Generalized maximum likelihood rule	11
Generalized cross-validation rule	11
Robust generalized cross-validation	11
Strong robust generalized cross-validation	11
Modified generalized cross-validation	11
2.3. Parameter choice rules which uses	12
the adjusting mechanism of the hybrid rule	12
Adjusting mechanism	12
Adjusted ME rule (MEa)	12
Choice of the regularization parameter in case of approximately known noise	
level	13
Choice of the regularization parameter in case of approximately known standar	:d
deviations	13
3. Noise generation	14
3.1. Noise in the right-hand side	14
Actual noise level	14
Standard deviation of the noise	15
3.2. Noise in the matrix	15
Actual noise level	15
Standard deviation of the noise	15
4. Output	15
4.1. The table of the results in the case of test problem if number of runs $K = 1$	16
4.2. The table of the results in the case of test problem if number of runs $K > 1$	17
4.3. The table of the results in case the of unknown solution	18
References	19

1. Discrete ill-posed problem. Tikhonov method

We consider the solving of the discrete linear ill-posed problem

Ь

$$A_0 u = f_0, \ A_0 \in \mathbb{R}^{n \times n},$$
 (1)

where the matrix A_0 is of ill-determined rank, i.e, the singular values of A_0 "cluster" at the origin. We assume that the equation (1) has unique solution u_* . The typical examples of discrete ill-posed problems are systems of linear equations arising from the discretization of ill-posed problems, such as Fredholm integral equations of the first kind with a square integrable kernel

$$\int_{a}^{b} K(t,s)u(s)ds = f(t), \quad c \le t \le d \; .$$

Instead exact right-hand side vector $f_0 \in \mathbb{R}^n$ typically only noisy right-hand side is available: $f = f_0 + \xi$, $\xi \in \mathbb{R}^n$. We consider also the case, where the matrix A_0 is given with errors: $A = A_0 + \zeta$, $\zeta \in \mathbb{R}^{n^*n}$.

To compute stable solution of such system with noisy data we use Tikhonov method $u_{\alpha} = (\alpha I + A^{T} A)^{-1} A^{T} f,$

where $\alpha > 0$ is the regularization parameter.

2. Choice of the regularization parameter

An important problem in applying the Tikhonov method is the proper choice of the regularization parameter α . If α is too small, the numerical implementation will be unstable and the approximation u_{α} will be useless; if α is too big, the approximation

 u_{α} will be too smooth.

The rules for the choice of the regularization parameter can be classified into three groups according to the information they require:

- a) a priori rules
- b) a posteriori rules which use the information about noise level (in the following we call they delta-rules)
- c) heuristic rules.

A priori rules use the noise level δ, η and for accurate results also smoothness information about the solution is needed. A posteriori rules use in parameter choice the quantities which arise in computations. These rules do not need information about the smoothness of the solution. A posteriori rules are divided into two groups, where rules of the first group use the noise level information and the rules of the second group (heuristic rules) do not need this. Heuristic rules have the advantage that they do not need require any information about the solution or noise levels of the initial data. In Regularization Parameter Tool we consider the delta-rules and the heuristic rules for the parameter choice.

In the following we consider the search of the proper regularization parameter on the sequence α_j , $\alpha_j = q\alpha_{j-1}$, $j = 1, 2, 3, ..., \alpha_j \le \alpha_M$, where α_0, α_M and q, 0 < q < 1 are given constants.

2.1 Delta-rules

To use the delta-rules for choosing regularization parameter, the upper bounds of the noise levels are needed:

$$||f - f_0|| \le \delta, ||A - A_0|| \le \eta.$$
 (2)

Here we use the Euclidean norms $||x|| = ||x||_2 = \sqrt{\sum_{i=1}^n x_i^2}$. If the inequalities (2) hold

and the parameter $\alpha = \alpha(\delta, \eta)$ is chosen by the delta-rules given below, then approximate solution converges to the exact solution u_* of the equation (1):

$$\|u_{\alpha(\delta,\eta)}-u_*\| \to 0 \quad (\delta \to 0, \eta \to 0).$$

Delta-rules can be divided into two groups: unstable and stable delta-rules. The discrepancy principle, the modified discrepancy principle and the monotone error rule (and its different versions) are unstable rules in the sense that if the actual error of the right-hand side is only slightly larger than $b\delta$ ($b \ge 1$ - constant which is used in rule), then the error of the approximate solution may be arbitrarily large, regardless of the value of the ratio of the actual and supposed noise level. For stable delta-rules (rule R1, balancing principle, rules R2) the convergence

$$\|u_{\alpha(\delta)} - u_*\| \to 0 \quad (\delta \to 0)$$

holds, if in the process $\delta \to 0$ the ratio of the actual and supposed error level is bounded: $||f - f_0||/\delta \le c$. Stable delta-rules can be used also in case if $f_i = f_{0,i} + \xi_i$, i = 1,2,...,n with $E\xi_i = 0$ and we know the upper bound of the variance σ^2 of the noise: $E||\xi_i||^2 \le \sigma^2$.

Discrepancy principle

Discrepancy principle [35,33,21] is one of the oldest rules for the parameter choice. Here the regularization parameter is found as the largest parameter $\alpha(\delta,\eta) = \alpha_j$, for which

$$\left\|Au_{\alpha} - f\right\| \le b\left(\delta + \eta \left\|u_{\alpha}\right\|\right), \ b \ge b_0 = 1$$

Note that in the case of noisy matrix the discrepancy principle was considered in [11,49], other delta-rules in [41].

Modified discrepancy principle (Raus-Gfrerer rule)

Modified discrepancy principle [36,8] is the delta-rule, which yields optimal convergence rates $||u_{\alpha(\delta,\eta)} - u_*|| = O((\delta + \eta)^{p/(p+1)})$ under assumption $u_* \in R((A_0^T A_0)^{p/2})$ for all $p \in [0,2]$. We take for the regularization parameter the largest parameter $\alpha(\delta, \eta) = \alpha_j$, for which

$$\left\| B_{\alpha} \left(A u_{\alpha} - f \right) \right\| \leq b \left(\delta + \eta \left\| u_{\alpha} \right\| \right), \quad b \geq b_0 = 1.$$

Here $B_{\alpha} = \sqrt{\alpha} (\alpha I + AA^T)^{-1/2}$ and the norm $||B_{\alpha}(Au_{\alpha} - f)||$ can be computed by the formula $||B_{\alpha}(Au_{\alpha} - f)|| = \langle Au_{2,\alpha} - f, Au_{\alpha} - f \rangle^{1/2}$, where $u_{2,\alpha}$ is the two-times iterated Tikhonov approximation $u_{2,\alpha} = (\alpha I + A^T A)^{-1} (\alpha u_{\alpha} + A^T f)$.

Monotone error rule

Monotone error (ME) rule was proposed in [46]. For the regularization parameter we choose the largest parameter $\alpha(\delta, \eta) = \alpha_i$, for which

$$\frac{\|B_{\alpha}(Au_{\alpha}-f)\|^{2}}{\|B_{\alpha}^{2}(Au_{\alpha}-f)\|} = \frac{(Au_{2,\alpha}-f,Au_{\alpha}-f)}{\|Au_{2,\alpha}-f\|} \le b(\delta+\eta\|u_{\alpha}\|), \ b\ge b_{0}=1.$$

Monotone error rule with post-estimation

In the ME rule with post-estimation [15] we take for the regularization parameter $\alpha(\delta,\eta) = \gamma \alpha_{ME}(\delta,\eta)$, $0 < \gamma < 1$, where $\alpha_{ME}(\delta,\eta)$ is chosen by the monotone error rule. The post-estimation is justified by the property $||u_{\alpha_{ME}} - u_*|| \le ||u_{\alpha} - u_*||$ for $\alpha > \alpha_{ME}$. We recommend to take $\gamma = 0.4$.

Adjusted monotone error rule

See Section 3.3

Rule R1(k) (transformed discrepancy principle)

Rule R1(k) [37,38] is the first stable parameter rule. Fix k > 0, $2k \in N$. Denote $D_{\alpha} = \alpha^{-1}AA^{T}B_{\alpha}^{2}$. Fix k > 0: $2k \in N$. For the regularization parameter we choose the largest parameter $\alpha(\delta, \eta) = \alpha_{j}$, for which

$$\left\| D_{\alpha_{j-1}}^{k} B_{\alpha_{j-1}} \left(A u_{\alpha_{j-1}} - f \right) \right\| > b \left(\delta + \eta \left\| u_{\alpha_{j-1}} \right\| \right),$$
$$\left\| D_{\alpha_{j}}^{k} B_{\alpha_{j}} \left(A u_{\alpha_{j}} - f \right) \right\| \le b \left(\delta + \eta \left\| u_{\alpha_{j}} \right\| \right).$$

It is recommended to choose the constant *b* near to the value $b_0 = \left(\frac{3}{2}\right)^{\frac{3}{2}} \frac{k^k}{(k+3/2)^{k+3/2}}.$

The norm $\left\| D_{\alpha}^{k} B_{\alpha} (Au_{\alpha} - f) \right\|$ can be computed by the formula

$$\left\|D_{\alpha}^{k}B_{\alpha}(Au_{\alpha}-f)\right\| = \begin{cases} \alpha^{-k} \left\|\left(A^{T}A\right)^{k-1/2}A^{T}\left(Au_{k+1/2,\alpha}-f\right)\right\|, & \text{if } k+1/2 \in N\\ \alpha^{-k}\left(\left(AA^{T}\right)^{k}\left(Au_{k+2,\alpha}-f\right),\left(AA^{T}\right)^{k}\left(Au_{k+1,\alpha}-f\right)\right)^{1/2}, & \text{if } k \in N \end{cases}$$

where $u_{k,\alpha}$ is the approximate solution in k-times iterated Tikhonov method

$$u_{m,\alpha} = (\alpha I + A^T A)^{-1} (\alpha u_{\alpha,m-1} + A^T f), m = 1,2,..,k.$$

The more detailed recommendations for numerical realization of many rules for choice of the regularization parameter are given in [40].

Balancing principle

This rule has a different form in different papers [2,28-32]. Here we consider the rule from [28-32]. For the regularization parameter we choose the largest parameter $\alpha(\delta,\eta) = \alpha_i$, for which

$$\frac{\sqrt{\alpha_j}\sqrt{q}\left\|u_{\alpha_j}-u_{\alpha_{j-1}}\right\|}{(1-q)} \leq b\delta \quad \text{and} \quad \frac{\sqrt{\alpha_{j-1}}\sqrt{q}\left\|u_{\alpha_{j-1}}-u_{\alpha_{j-2}}\right\|}{(1-q)} > b\delta.$$

It is recommended to choose the constant *b* near to the value $b_0 = \frac{3\sqrt{3}}{16}$. Note that the balancing principle can be considered as an discrete version of the rule R1 with k = 1/2 (see [13]).

<u>Rules R2</u> (q = 2, l = 1/2, k = 1) and **R2** (q = 2, l = 1/2, k = 2)

These rules are examples of the general family of rules [14]. The general rule is the following. Fix the parameters $3/2 \le q \le 2$, $l \ge 0$, $k \ge l/q$. We choose the regularization as the largest parameter $\alpha(\delta, \eta) = \alpha_j$, for which

$$d(\alpha,q,l,k) = \frac{\kappa(\alpha)^{\mu} \left\| D_{\alpha}^{k} B_{\alpha} (Au_{\alpha} - f) \right\|^{\frac{q}{q-1}}}{\left\| D_{\alpha}^{l} B_{\alpha}^{2q-2} (Au_{\alpha} - f) \right\|^{\frac{1}{q-1}}} \leq b\delta.$$

Here $\kappa(\alpha) := 1 + \alpha ||A||^{-2}$, $\mu = \frac{kq - l + sq/2}{q - 1}$, $s = \begin{cases} 0, & \text{if } k = l/q \\ 1, & \text{if } k > l/q \end{cases}$.

If k = l/q, then $b \ge b_0$, where

$$b_{0} = \left(\frac{3}{2}\right)^{\frac{3}{2}} \left(\frac{k^{k}}{\left(k+3/2\right)^{k+3/2}}\right) \left(\frac{k^{k}\left(l+3/2\right)^{l+3/2}}{\left(k+3/2\right)^{k+3/2}l^{l}}\right)^{1/(q-1)}$$

If k > l/q then it is recommended to choose the constant *b* near to the value b_0 . Note that the general rule includes as special case the monotone error rule (q = 2, l = k = 0), the modified discrepancy principle (q = 3/2, l = k = 0) and Rule R1 (q = 3/2, l = k).

For the Rule R2 (q = 2, l = 1/2, k = 1) the function $d(\alpha, q, l, k)$ has the form

$$d(\alpha,2,1/2,1) = \kappa(\alpha)^{5/2} \frac{\left\|D_{\alpha}B_{\alpha}(Au_{\alpha}-f)\right\|^{2}}{\left\|D_{\alpha}^{1/2}B_{\alpha}^{2}(Au_{\alpha}-f)\right\|}$$

and for the rule R2 (q = 2, l = 1/2, k = 2) the function $d(\alpha, q, l, k)$ has the form

$$d(\alpha,2,1/2,2) = \kappa(\alpha)^{9/2} \frac{\left\|D_{\alpha}^{2}B_{\alpha}(Au_{\alpha}-f)\right\|^{2}}{\left\|D_{\alpha}^{1/2}B_{\alpha}^{2}(Au_{\alpha}-f)\right\|}.$$

Note that the stable delta-rules can be used in case of known variance of the noise. Let, for example, we know the upper bound σ^2 of the variance of the noise in the right-hand side: $f_i = f_{0,i} + \xi_i$, $E \|\xi_i\|^2 \le \sigma^2$, i = 1, 2, ..., n, where ξ_i are independent normally distributed random variables with zero mean. Then for choosing the regularization parameter we can use some stable delta-rule (Rule R1, balancing principle or Rules R2 (q = 2, l = 1/2, k = 1), R2 (q = 2, l = 1/2, k = 2)) where instead of δ we use $\sigma \sqrt{n}$.

2.2. Heuristic rules

If the noise level is unknown, then, as shown by Bakushinskii [1], no rule for choosing the regularization parameter can guarantee the convergence of the regularized solution to the exact one as $\delta \rightarrow 0$.

In Regularization Parameter Tool we consider the heuristic parameter choice rules, which can be represented in the form

$$\alpha_h = \underset{\alpha_M \le \alpha \le \alpha_0}{\arg \min} \psi(\alpha) \quad . \tag{3}$$

For all heuristic rules considered below there is the possibility to use the following modifications of the general rule (3).

1. In [16] was mentioned that if the problem (1) has a unique solution, then the function $\psi(\alpha)$ of the Hanke-Raus rule converges to 0 as $\alpha \to 0$. The same holds for other functions $\psi(\alpha)$ considered below. Therefore, in [34] was proposed to find the minimizer of $\psi(\alpha)$ in the interval $[\lambda_{\min}, \alpha_0]$, where λ_{\min} is the minimal eigenvalue of the matrix $A^T A$. Taking into account that $\alpha \ge \alpha_M$, we get

$$\alpha_h = \arg\min_{\max\{\alpha_M, \lambda_{\min}\} \le \alpha \le \alpha_0} \psi(\alpha)$$

2. The minimizing function has usually the property $\lim_{\alpha \to \infty} \psi(\alpha) = 0$ and to use the heuristic rule in the form (3), we must carefully choose the proper α_0 ; otherwise there may be possibility that $\alpha_h = \alpha_0$ which is not good parameter choice usually. Therefore for all parameter choice rules considered below we consider the following general rule

$$\alpha_h = \arg\min_{\alpha_M \le \alpha \le \alpha_0} \kappa(\alpha)^{\mu} \psi(\alpha),$$

where $\kappa(\alpha) = 1 + \alpha / ||A^T A||$ and $\rho > 0$ is the value, for which

$$\lim_{\alpha \to \infty} \kappa(\alpha)^{\mu} \psi(\alpha) = c_1 ||f||, \ 0 < c_1 < \infty.$$
(4)

Quasi-optimality criterion

The quasi-optimality criterion [47,48,9] is one of the oldest parameter choice rules. In case of the continuous version of the quasi-optimality criterion the function $\psi(\alpha)$ has the form

$$\psi_{\varrho}(\alpha) = \alpha \left\| \frac{du_{\alpha}}{d\alpha} \right\| = \alpha^{-1/2} \left\| D_{\alpha}^{1/2} B_{\alpha} (Au_{\alpha} - f) \right\| = \alpha^{-1} \left\| A^{T} (Au_{2,\alpha} - f) \right\|.$$

We get the discrete version of the quasi-optimality criterion, if we use a difference quotient in place of the derivative: $\psi_{QD}(\alpha) = ||u_{\alpha} - u_{\alpha q}||$. The parameter μ in (4) is one.

Hanke-Raus rule

For the Hanke-Raus rule [16] the minimizing function is

$$\psi_{HR}(\alpha) = \alpha^{-1/2} \|B_{\alpha}(Au_{\alpha} - f)\| = \alpha^{-1/2} (Au_{2,\alpha} - f, Au_{\alpha} - f)^{1/2}$$

and the parameter $\mu = 1/2$.

L-curve and the Reginska's rule

The L-curve rule was proposed by Hansen [17,19,20], see also [25]. The name of this method is justified by the fact that log-log parametric plot of $(||Au_{\alpha} - f||, ||u_{\alpha}||)$ has for many problems a distinct L-shape and the "corner point" of the L-curve defines a good value of the regularization parameter. There are several variants to choose the "corner point" of the L-curve. In case of Reginska's rule [44] we choose the "corner point" as global minimizer of the function

$$\psi_R(\alpha) = \|Au_\alpha - f\|\|u_\alpha\|^{\tau},$$

where $\tau = 1$. In case of the generalized Reginska's rule $\tau \ge 1$. The parameter μ in (4) has the form $\mu = \tau$.

Modified Reginska's rule

Numerical experiments show that the Reginska's rule does not work well in case of smooth solution. Motivated by this, in [42] the modification of the Reginska's rule was proposed. The logic behind this rule is the following. For Tikhonov method we can present the minimizing function of the Reginska's rule in the form

$$\|Au_{\alpha}-f\|\|u_{\alpha}\|=\alpha^{-1/2}\|Au_{\alpha}-f\|\|\overline{D}_{\alpha}^{1/2}(Au_{\alpha}-f)\|,$$

where the operator $\overline{D}_{\alpha} = \alpha^{-1}AA^{T}$. We know that in Tikhonov method the corresponding delta-rules

 $||Au - f|| = b(\delta + \eta ||u_{\alpha}||), b \ge 1,$ $||\overline{D}_{\alpha}^{1/2}(Au_{\alpha} - f)|| = b(\delta + \eta ||u_{\alpha}||), b \ge b_0$ are orderoptimal delta-rules not for the full range of the smoothness index p: if $u_* \in R((A_0^T A_0)^{p/2})$ and the parameter $\alpha(\delta, \eta)$ is chosen by these delta-rules, then $\begin{aligned} \left\|u_{\alpha(\delta)} - u_*\right\| &\leq c(\delta + \eta)^{p/(p+1)}, \ 0 Thus, in the case of modified Reginska's rule the minimizing function has the form
<math display="block">w_{\alpha}(\alpha) = \alpha^{-1/2}\|B_{\alpha}(Au_{\alpha} - f)\| = b(\Delta + \eta\|u_{\alpha}\|), \ b \geq b_{0}. \end{aligned}$

$$\psi_{MR}(\alpha) = \alpha^{-1/2} \left\| B_{\alpha} (Au_{\alpha} - f) \right\| \left\| D_{\alpha}^{1/2} B_{\alpha} (Au_{\alpha} - f) \right\|$$

and the parameter $\mu = 1$ in (4). Note that $\psi_{MR}(\alpha) = \alpha^{1/2} \psi_Q(\alpha) \psi_{HR}(\alpha)$.

Hybrid rule

Theoretical [22-24] and experimental results show that for some problems Hanke-Raus rule fails less frequently than the quasi-optimality criterion or the (modified) Reginska's rule, but in most cases the average performance of the two last rules is much better. Main idea of the following algorithm is to use the functions of all three rules in one hybrid rule for getting the same stability as in HR-rule and the same accuracy as in the quasi-optimality criterion and in the (modified) Reginska's rule. The hybrid rule was proposed in [42]. Another variant of the hybrid rule was given in [43].

Denote

$$\begin{aligned} \overline{\alpha}_{M} &\coloneqq \min\{\alpha_{j} : \alpha_{j} = \alpha_{0}q^{j}, \alpha_{j} \ge \max\{\lambda_{\min}, \alpha_{M}\}\}, \\ \overline{\alpha}_{Q} &\coloneqq \underset{\overline{\alpha}_{M} \le \alpha_{j} \le \alpha_{0}}{\operatorname{smin}} \psi_{Q,\kappa}(\alpha_{j}), \quad \psi_{Q,\kappa}(\alpha) = \kappa(\alpha)\alpha^{-1/2} \left\| D_{\alpha}^{1/2} B_{\alpha}(Au_{\alpha} - f) \right\|, \\ \overline{\alpha}_{HR} &\coloneqq \underset{\overline{\alpha}_{M} \le \alpha_{j} \le \alpha_{0}}{\operatorname{smin}} \psi_{HR,\kappa}(\alpha_{j}), \quad \psi_{HR,\kappa}(\alpha) = \sqrt{\kappa(\alpha)}\alpha^{-1/2} \left\| B_{\alpha}(Au_{\alpha} - f) \right\|, \\ \overline{\alpha}_{MR} &\coloneqq \underset{\overline{\alpha}_{M} \le \alpha_{j} \le \alpha_{0}}{\operatorname{smin}} \psi_{MR,\kappa}(\alpha_{j}), \quad \psi_{MR,\kappa}(\alpha) = \kappa(\alpha)\alpha^{-1/2} \left\| B_{\alpha}(Au_{\alpha} - f) \right\| \left\| D_{\alpha}^{1/2} B_{\alpha}(Au_{\alpha} - f) \right\|, \\ \overline{\alpha}_{QMR} &\coloneqq \left\{ \overline{\alpha}_{QRR}, \quad \text{if } \overline{\alpha}_{MR} > \overline{\alpha}_{M}, \\ \overline{\alpha}_{Q}, \quad \text{if } \overline{\alpha}_{MR} = \overline{\alpha}_{M}. \end{aligned}$$

Form the set of parameters $\boldsymbol{\mathcal{A}}$:

$$\boldsymbol{\mathcal{A}} = \begin{cases} \{\overline{\alpha}_{HR}\}, & \text{if } \overline{\alpha}_{QMR} \ge \overline{\alpha}_{HR} \\ \{\overline{\alpha}_{HR}, \alpha_{Q}^{(1)}, ..., \alpha_{Q}^{(k)}, \overline{\alpha}_{QMR}\}, & \text{if } \overline{\alpha}_{HR} > \overline{\alpha}_{QMR} > \overline{\alpha}_{M} \\ \{\overline{\alpha}_{HR}, \alpha_{Q}^{(1)}, ..., \alpha_{Q}^{(k)}\}, & \text{if } \overline{\alpha}_{HR} > \overline{\alpha}_{QMR} \text{ and } \overline{\alpha}_{QMR} = \overline{\alpha}_{M} \end{cases}$$

Here $\alpha_Q^{(1)}, \alpha_Q^{(2)}, ..., \alpha_Q^{(k)}$ are the local minimum points of the quasi-optimality criterion function $\psi_{Q,\kappa}(\alpha)$ between parameters $\overline{\alpha}_{QMR}$ and $\overline{\alpha}_{HR}$:

$$\overline{\alpha}_{HR} > \alpha_Q^{(1)} > \alpha_Q^{(2)} > \dots > \alpha_Q^{(k)} > \overline{\alpha}_{QMR} \quad .$$

Let $\overline{\alpha}_{H} := \min\{\alpha \in \mathcal{A} : T(\alpha, \overline{\alpha}_{HR}) \le C_1\}$, where $T(\alpha_1, \alpha_2) = \frac{\|u_{\alpha_1} - u_{\alpha_2}\|}{\psi_{Q,\kappa}(\alpha_2)}$ and C_1 is

the fixed number from the interval [20,50]. In case $\lambda_{\min} < \alpha_M$ we take for the regularization parameter $\alpha_H = \overline{\alpha}_H$.

In case $\lambda_{\min} \ge \alpha_M$ we take for the regularization parameter

$$\alpha_{H} = \begin{cases} \alpha_{M}, & \text{if } T(\alpha_{M}, \overline{\alpha}_{H}) \leq C_{2} \\ \overline{\alpha}_{H}, & \text{if } T(\alpha_{M}, \overline{\alpha}_{H}) > C_{2} \end{cases},$$

where $C_2 \in [2,5]$. In Regularization Parameter Tool the constants C_1 and C_2 are $\|u_{\alpha} - u_{\alpha}\|$

fixed: $C_1 = 25$, $C_2 = 3$. Note that the function $T(\alpha_1, \alpha_2) = \frac{\|u_{\alpha_1} - u_{\alpha_2}\|}{\psi_Q(\alpha_2)}$ characterizes

the maximal possible error of the approximate solution u_{α_1} with respect to $||u_{\alpha_2} - u_*||$. Namely, the following error estimate holds

$$\|u_{\alpha_1}-u_*\|\leq (1+T(\alpha_1,\alpha_2))\Phi(\alpha_2),$$

where the function $\Phi(\alpha) = \|\alpha(\alpha I + A^T A)^{-1} u_*\| + \|(\alpha I + A^T A)^{-1} A^T (f - f_0)\|$ is an upper bound of the error of the approximate solution u_{α} :

$$||u_{\alpha} - u_{*}|| \leq ||\alpha(\alpha I + A^{T}A)^{-1}u_{*}|| + ||(\alpha I + A^{T}A)^{-1}A^{T}(f - f_{0})||.$$

Brezinski – Rodriguez-Seatzu rule

In [5,6] the heuristic rule was proposed, where the minimizing function has the form

$$\psi_{BRS}(\alpha) = \frac{\|Au_{\alpha} - f\|^{2}}{\|A^{T}(Au_{\alpha} - f)\|} = \alpha^{-1/2} \frac{\|Au_{\alpha} - f\|^{2}}{\|\overline{D}_{\alpha}^{1/2}(Au_{\alpha} - f)\|}$$

The parameter $\mu = 1/2$ in (4).

On presentation of the following rules we rely on the paper [3].

Residual method

The residual method was proposed in [4] for spectral cut-off regularization method. The minimizing function has the form

$$\psi_{RES}(\alpha) = \frac{\|Au_{\alpha} - f\|}{\left(trace(AK_{\alpha})^{T}(AK_{\alpha})\right)^{1/4}},$$

where $K_{\alpha} = (\alpha I + A^T A)^{-1} A^T$ and $trace(C) = \sum_{i=1}^{n} c_{ii}$ for the matrix $C = (c_{ij}) \in R^{nxn}$. For the residual method $\mu = 1/2$.

Generalized maximum likelihood rule

The generalized maximum likelihood rule was proposed by Wahba [52]. The minimizing function has the form

$$\psi_{GML}(\alpha) = \frac{\|Au_{\alpha} - f\|^{2}}{\left[\det^{+}(I - AK_{\alpha})\right]^{1/n_{1}}} = \alpha^{-1} \frac{\|Au_{\alpha} - f\|^{2}}{\left[\det^{+}(\alpha I + AA^{T})^{-1}\right]^{1/n_{1}}},$$

where $n_1 = rank(I - AK_{\alpha})$ and det⁺ is the product of the nonzero eigenvalues. The parameter $\mu = 1$.

Generalized cross-validation rule

Generalized cross-validation (GCV) rule was proposed in [10,51]. The minimizing function has the form

$$\psi_{GCV}(\alpha) = \frac{\|Au_{\alpha} - f\|^{2}}{\left(n^{-1}trace(I - AK_{\alpha})\right)^{2}} = \alpha^{-1}\frac{\|Au_{\alpha} - f\|^{2}}{\left(n^{-1}trace(\alpha I + AA^{T})^{-1}\right)^{2}}$$

and the parameter $\mu = 1$ in (4).

Robust generalized cross-validation

Robust GCV rule has been developed in [26,45]. The minimizing function has the form

$$\psi(\alpha) = \frac{\left\|Au_{\alpha} - f\right\|^{2}}{\left(n^{-1}trace(I - AK_{\alpha})\right)^{2}} \left(\gamma + (1 - \gamma)n^{-1}trace((AK_{\alpha})^{2})\right), 0 < \gamma < 1,$$

where $\gamma \in (0,1)$ is a robustness parameter. In [3] $\gamma = 0.1$ was used. The parameter $\mu = 1$.

Strong robust generalized cross-validation

Strong robust GCV rule was considered in [27]. The minimizing function has the form

$$\psi(\alpha) = \frac{\|Au_{\alpha} - f\|^2}{\left(n^{-1}trace(I - AK_{\alpha})\right)^2} \left(\gamma + (1 - \gamma)n^{-1}trace(K_{\alpha}^T K_{\alpha})\right)$$

where $\gamma \in (0,1)$ is a robustness parameter. In [3] $\gamma = 0.95$ was used. The parameter $\mu = 1$.

Modified generalized cross-validation

Modified GCV rule was considered in [7,50]. The minimizing function has the form

$$\psi(\alpha) = \frac{\left\|Au_{\alpha} - f\right\|^{2}}{\left(n^{-1}trace(I - cAK_{\alpha})\right)^{2}}$$

with parameter c > 1. In [3] c = 3 was used. The parameter $\mu = 1$.

2.3. Parameter choice rules which uses

the adjusting mechanism of the hybrid rule

We can consider the heuristic hybrid rule as a two-stage rule. In the first stage we choose the parameter using the Hanke-Raus rule. In the second stage we adjust the selected parameter using local minimizers of the quasi-optimality criterion and the global minimizer of the modified Reginska's rule. It turns out that such adjusting of previously chosen parameter is useful also in cases, if we have some information about the noise level of the data.

Adjusting mechanism

Let the parameter $\alpha(\delta,\eta)$ be chosen according to some delta-rule. Then adjusting mechanism of the parameter $\alpha(\delta,\eta)$ is the following.

Form the set of parameters $\boldsymbol{\mathcal{A}}$:

$$\boldsymbol{\mathcal{A}} = \begin{cases} \{\alpha(\delta,\eta)\}, & \text{if } \overline{\alpha}_{QMR} \ge \alpha(\delta,\eta) \\ \{\alpha(\delta,\eta), \alpha_Q^{(1)}, ..., \alpha_Q^{(k)}, \overline{\alpha}_{QMR}\}, & \text{if } \alpha(\delta,\eta) > \overline{\alpha}_{QMR} > \overline{\alpha}_M \\ \{\alpha(\delta,\eta), \alpha_Q^{(1)}, ..., \alpha_Q^{(k)}\}, & \text{if } \alpha(\delta,\eta) > \overline{\alpha}_{QMR} \text{ and } \overline{\alpha}_{QMR} = \overline{\alpha}_M \end{cases}$$

Here $\alpha_Q^{(1)}, \alpha_Q^{(2)}, ..., \alpha_Q^{(k)}$ are the local minimum points of the quasi-optimality criterion function $\psi_{Q,\kappa}(\alpha)$ between parameters $\overline{\alpha}_{QMR}$ and $\alpha(\delta, \eta)$:

$$\alpha(\delta,\eta) > \alpha_Q^{(1)} > \alpha_Q^{(2)} > \dots > \alpha_Q^{(k)} > \overline{\alpha}_{QMR}$$

Let $\overline{\alpha}_{adj} := \min\{\alpha \in \mathcal{A} : T(\alpha, \alpha(\delta, \eta)) \le C_1\}$. In case $\lambda_{\min} < \alpha_M$ we take for the regularization parameter $\alpha_{adj}(\delta, \eta) = \overline{\alpha}_{adj}(\delta, \eta)$. In case $\lambda_{\min} \ge \alpha_M$ we take for the regularization parameter

$$\alpha_{adj}(\delta,\eta) = \begin{cases} \alpha_{_M}, & \text{if } T(\alpha_{_M},\overline{\alpha}_{_{adj}}(\delta,\eta)) \leq C_2 \\ \overline{\alpha}_{_{adj}}(\delta,\eta), & \text{if } T(\alpha_{_M},\overline{\alpha}_{_{adj}}(\delta,\eta)) > C_2 \end{cases}$$

Adjusted ME rule (MEa)

In case of this rule we choose at first the parameter $\alpha(\delta,\eta)$ using monotone error rule and adjust this parameter using adjusting mechanism. In Regularization Parameter Tool the constants C_1 and C_2 of the adjusting mechanism are fixed: $C_1 = 3$, $C_2 = 3$. Numerical results show that this rule works better than other delta-rules if noise ξ in the right-hand side has the positive correlation or the Poisson distribution.

<u>Choice of the regularization parameter in case of approximately known noise</u> <u>level</u>

The delta-rules works well in practice, if we have fairly accurate estimate of the noise level of the data. In case of overestimating of the noise level the heuristic parameter choice rules works often better than delta-rules. On the other hand, heuristic rules may fail for some problems. Motivated by this, we present (see [42]) the rule for the case if the noise level is known approximately.

In the following we assume that we know some upper bounds δ_0, η_0 of the noise level: $||A - A_0|| \le \eta_0, ||f_0 - f|| \le \delta_0$, but probably the norms of noise are larger than δ_1, η_1 : $\delta_1 \le \delta_0, \eta_1 \le \eta_0$. Then for the regularization parameter we choose the parameter

$$\alpha(\delta_0, \eta_0, \delta_1, \eta_1) = \max\{\alpha_{MEe}(\delta_1, \eta_1), \min\{\alpha_{MEe}(\delta_0, \eta_0), \alpha_{adj}(\delta_0, \eta_0)\}\}.$$
(5)

Here the parameters $\alpha_{MEe}(\delta_0, \eta_0)$ and $\alpha_{MEe}(\delta_1, \eta_1)$ are the parameters which are chosen by post-estimated monotone error rule. If for $\alpha \ge \alpha_M$

$$\frac{\left\|B_{\alpha}(Au_{\alpha}-f)\right\|^{2}}{\left\|B_{\alpha}^{2}(Au_{\alpha}-f)\right\|} > \delta_{1}+\eta_{1}\left\|u_{\alpha}\right\|,$$

then we take $\alpha_{MEe}(\delta_1, \eta_1) = \alpha_M$. The parameter $\alpha_{adj}(\delta_0, \eta_0)$ in (5) is the adjusted parameter of the parameter $\alpha(\delta_0, \eta_0) = \min\{\overline{\alpha}_{HR}, \alpha_{ME}(\delta_0, \eta_0)\}$. In adjustment we use

the constant $C_1 = \min\left\{25, 3\left(\frac{\Delta_0}{\Delta_1}\right)^2\right\}$, where $\Delta_j = \delta_j + \eta_j \|f\| \|A\|^{-1}$, j = 0,1 and the

constant $C_2 = 3$.

If $||f - f_0|| \le \delta_0$, $||A - A_0|| \le \eta_0$, then this rule guarantees the convergence of the approximate solution, if $\delta_0, \eta_0 \to 0$ and $\delta_0/\delta_1 \le const$, $\eta_0/\eta_1 \le const$ in the process $\delta_0, \eta_0 \to 0$. Numerical examples show that if $\delta_0/\delta_1 \le C$, $\eta_0/\eta_1 \le C$, where constant *C* is not very large (for example, C = 100), then this rule gives on average better results than the monotone error rule

$$\frac{\|B_{\alpha}(Au_{\alpha} - f)\|^{2}}{\|B_{\alpha}^{2}(Au_{\alpha} - f)\|} = b(\|f - f_{0}\| + \|A - A_{0}\|\|u_{\alpha}\|)$$

in case of exactly known noise levels if $\delta_1 \leq \|f - f_0\| \leq \delta_0, \eta_1 \leq \|A - A_0\| \leq \eta_0$.

<u>Choice of the regularization parameter in case of approximately known standard</u> <u>deviations</u>

In the following we assume that we know some upper bounds $\sigma_0, \sigma_{\eta,0}$ of the standard deviations of the right-hand side and matrix noise $: f_i = f_{0,i} + \xi_i$, $E \|\xi_i\|^2 \le \sigma_0^2$, i = 1, 2, ..., n and $a_{ij} = a_{ij}^0 + \xi_{ij}$, $E \|\xi_{ij}\|^2 \le \sigma_{\eta,0}^2$, i, j = 1, 2, ..., n. Here $A = (a_{ij}), A_0 = (a_{ij}^0)$. We know also that probably these standard deviations are larger

than $\sigma_1, \sigma_{\eta,1}$: $\sigma_1 \leq \sigma_0, \sigma_{\eta,1} \leq \sigma_{\eta,0}$. Then for the regularization parameter we choose the parameter

$$\alpha(\sigma_0, \sigma_{\eta,0}, \sigma_1, \sigma_{\eta,1}) = \max\{\alpha_{ME}(\sqrt{n}\sigma_1/3, 2\sigma_{\eta,1}\sqrt{n}/3), \alpha_{adj}(\sigma_0, \sigma_{\eta,1})\}.$$

Here the parameter $\alpha_{ME}(\sqrt{n\sigma_1/3}, 2\sigma_{\eta,1}\sqrt{n/3})$ is the parameter which is chosen by the monotone error rule, chosen as largest α for which

$$\frac{\left\|B_{\alpha}\left(Au_{\alpha}-f\right)\right\|^{2}}{\left\|B_{\alpha}^{2}\left(Au_{\alpha}-f\right)\right\|} \leq \left(\sigma_{1}\sqrt{n}+2\sigma_{\eta,1}\sqrt{n}\left\|u_{\alpha}\right\|\right)/3.$$

If there is no $\alpha \le \alpha_M$ for which this inequality holds, then we take $\alpha_{ME}(\sigma_1\sqrt{n}/3, 2\sigma_{\eta,1}\sqrt{n}/3) = 0$. The parameter $\alpha_{adj}(\sigma_0, \sigma_{\eta,0})$ is the adjusted parameter of the parameter $\alpha(\sigma_0, \sigma_{\eta,0}) = \min\{\overline{\alpha}_{HR}, \alpha_{R2}(3\sqrt{n}\sigma_0, 6\sigma_{\eta,0}\sqrt{n})\}$. Here the parameter $\alpha_{R2}(3\sqrt{n}\sigma_0, 6\sigma_{\eta,0}\sqrt{n})$ is chosen by the rule R2 (q = 2, l = 1/2, k = 1):

$$\kappa(\alpha)^{5/2} \frac{\left\|D_{\alpha}B_{\alpha}(Au_{\alpha}-f)\right\|^{2}}{\left\|D_{\alpha}^{1/2}B_{\alpha}^{2}(Au_{\alpha}-f)\right\|} \leq 3\left(\sigma_{0}\sqrt{n}+2\sigma_{\eta,0}\sqrt{n}\left\|u_{\alpha}\right\|\right).$$

In adjustment we use the constants $C_1 = 25$ and $C_2 = 3$.

3. Noise generation

3.1. Noise in the right-hand side

To generate noise of the right-hand side one can set up actual noise level or standard deviation of the noise. In both cases there is possibility to set up absolute or relative value of the corresponding quantity.

Actual noise level

The noisy right-hand side is computed in the case of absolute noise level δ_{abs} by the formula $f = f_0 + \delta_{abs} \|\xi\|^{-1} \xi$ and in the case of relative noise level δ_{rel} by the formula $f = f_0 + \delta_{rel} \|f_0\| \|\xi\|^{-1} \xi$. Here the components ξ_i of the vector $\xi \in \mathbb{R}^n$ are random variables with chosen distribution.

The components ξ_i are computed by the formulas

$$\xi_1 = (1 - \rho^2)^{-1/2} \varepsilon_1, \ \xi_i = \rho \xi_{i-1} + \varepsilon_i, \ i = 2, 3, ..., n$$

where $\rho \in (-1,1)$ is the correlation coefficient and ε_i are independent random variables with standard normal distribution, with uniform distribution U[-1,1] or with Poisson distribution with parameter λ .

In the case of **normal distribution with outlier** the components ξ_i are computed by the formulas

$$\xi_i = \begin{cases} \varepsilon_i, & i = 1, 2, 3, \dots, n, \ i \neq n_0 \\ \varepsilon_i + d_{\pm} \sqrt{n}, & i = n_0 \end{cases}$$

where ε_i are independent random variables with standard normal distribution. The numbers $d_{\pm} \in \{-1,1\}$ and $n_0 \in N : 1 \leq n_0 \leq n$ are chosen randomly. In case of such distribution approximately half of the noise of the right-hand side is distributed randomly and the remaining noise is placed in a single component.

Standard deviation of the noise

The noisy right-hand side is computed in the case of absolute standard deviation σ_{abs} by the formula $f = f_0 + \sigma_{abs} \xi$ and in the case of relative standard deviation σ_{rel} by the formula $f = f_0 + \sigma_{rel} ||f_0|| \xi$. The components ξ_i of the vector $\xi \in \mathbb{R}^n$ are computed by the formulas

$$\xi_1 = (1 - \rho^2)^{-1/2} \varepsilon_1, \ \xi_i = \rho \xi_{i-1} + \varepsilon_i, \ i = 2, 3, ..., n,$$

where $\rho \in (-1,1)$ is the correlation coefficient and ε_i are independent normally distributed random variables with zero mean and with the variance $1 - \rho^2$ in the case of normal distribution or independent random variables with uniform distribution $U\left[-\sqrt{3(1-\rho^2)}, \sqrt{3(1-\rho^2)}\right]$ in the case of uniform distribution.

3.2. Noise in the matrix

To generate noisy matrix one can set up actual noise level or standard deviation of the noise. In both cases there is possibility to set up absolute or relative value of the corresponding quantity.

Actual noise level

The noisy matrix $A = (a_{ij})$ is computed by the formula $a_{ij} = a_{ij}^0 + c\xi_{ij}$, where $A_0 = (a_{ij}^0)$ and the components ξ_{ij} are independent random variables with standard normal distribution or with uniform distribution. The constant *c* is chosen so that in the case of absolute noise level $||A - A_0|| = \eta$ and in the case of relative noise level $||A - A_0|| = \eta$

Standard deviation of the noise

The noisy matrix $A = (a_{ij})$ is computed by the formula $a_{ij} = a_{ij}^0 + \sigma_\eta \xi_{ij}$, where $A_0 = (a_{ij}^0)$ and the components ξ_{ij} are independent random variables with standard normal distribution or with uniform distribution $U\left[-\sqrt{3},\sqrt{3}\right]$.

4. Output

The Regularization Parameter Tool gives for the output the table of results and for each run the graphs of the approximate solutions and the graph of functions use in rules. If the exact solution is known, then the graph of the exact solution and the graph of approximate solution with the optimal parameter are presented. The table of results depends on the number of runs (one run or more) and on that is the exact solution of the problem known or not.

4.1. The table of the results in the case of test problem if number of runs K = 1.

	Rule 1	Rule 2	Rule 3	Rule 4	Rule 5	Optimal
Parameter	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX
Error	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX
Relative error	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX
Error ratio	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX	
Quasi ratio	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX	
\overline{T} 1(α)	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX	
$\overline{T}2(\alpha)$	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX	
Link to solution	Link	Link	Link	Link	Link	Link

In the case of single run the table of results is the following

In the case of single run the regularization parameter, the error of the approximate solution $||u_{\alpha(R)} - u_*||$, relative error of the approximate solution $||u_{\alpha(R)} - u_*||/||u_*||$, the error ratio $E(\alpha(R))$ and the quasi-error ratio $Q(\alpha(R))$ are presented for each chosen rule. For each problem we define the optimal regularization parameter by $\alpha_{opt} = \underset{\alpha_M \leq \alpha_j \leq \alpha_0}{\min} ||u_{\alpha_j} - u_*||$, where u_* is the solution of the equation $A_0 u = f_0$. Then the accuracy of the chosen regularization parameter $\alpha(R)$ by rule R is characterized by the error ratio

$$E(\alpha(R)) = \frac{\left\|u_{\alpha(R)} - u_*\right\|}{\left\|u_{\alpha_{opt}} - u_*\right\|} \ge 1.$$

and by the quasi-error ratio

$$Q(\alpha(R)) = \frac{\left\| u_{\alpha(R)} - u_* \right\|}{\min_{\alpha_j, \alpha_M \le \alpha_j \le \alpha_0} \Psi(\alpha_j)},$$

where the function $\Psi(\alpha) = \left\| \alpha \left(\alpha I + A^T A \right)^{-1} u_* \right\| + 2^{-1} \alpha^{-1/2} \left(\left\| f - f_0 \right\| + \left\| A - A_0 \right\| \| u_* \| \right) \right)$ is an upper bound of error of the approximate solution:

$$||u_{\alpha} - u_{*}|| \leq ||\alpha(\alpha I + A^{T}A)^{-1}u_{*}|| + 2^{-1}\alpha^{-1/2}(||f - f_{0}|| + ||A - A_{0}||||u_{*}||).$$

The quantities

$$\overline{T_1}(\alpha(R)) = \max_{\alpha_H \le \alpha \le \alpha_0} \frac{\|u_{\alpha(R)} - u_{\alpha}\|}{\psi_{HR}(\alpha)}, \ \overline{T_2}(\alpha(R)) = \max_{\max(\alpha_M, \lambda_{\min}) \le \alpha \le \alpha_H} \frac{\|u_{\alpha(R)} - u_{\alpha}\|}{\psi_{HR}(\alpha)}$$
 characterize a posteriori error estimate for the approximate solution:

posteriori error estimate for the approximate solution:

$$\left\|u_{\alpha(R)}-u_*\right\|\leq \left(1+\max(\overline{T_1}(\alpha(R)),\overline{T_2}(\alpha(R)))\right)\min_{\alpha_{M}\leq\alpha\leq\alpha_0}\Psi(\alpha).$$

The quantity $\overline{T_1}(\alpha(R))$ will be large (for example $\overline{T_1}(\alpha(R)) \ge 30$), if the parameter choice fails and the rule chooses too small parameter.

In the column 'Optimal' the optimal parameter and corresponding absolute and relative error of the approximate solution are presented. At the end of the table the links to the files of the approximate solution vectors are presented.

Nr		Rule 1	Rule 2	Rule 3	Rule 4	Rule 5	Optimal
1	Parameter	xxx.xx	XXX.XX	xxx.xx	XXX.XX	xxx.xx	xxx.xx
	Parameter	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX
Κ	Parameter	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX
1	Error ratio	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX	xxx.xx*
	Error ratio	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX	xxx.xx*
Κ	Error ratio	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX	xxx.xx*
Avera	ige error	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX
Avg	rel error	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX
Avg	error ratio	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX	
Medi	an error ratio	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX	
Max	error ratio	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX	
Avg	quasi ratio	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX	
Max	quasi ratio	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX	
1	Link to solution	Link	<u>Link</u>	<u>Link</u>	Link	<u>Link</u>	<u>Link</u>
	Link to solution	Link	Link	<u>Link</u>	Link	<u>Link</u>	<u>Link</u>
K	Link to solution	Link	Link	Link	Link	Link	Link

In the case of multiple runs the table of results is the following

For each run and for each selected rule the chosen regularization parameter and the error ratio $E(\alpha(R))$ are presented. In the column 'Optimal' the optimal parameter and corresponding absolute error of approximate solution are presented.

For all runs the following aggregates are presented:

- 1) Average error of the approximate solution $K^{-1} \sum_{i=1}^{K} \left\| u_{\alpha^{i}(R)} u_{*} \right\|$, where $\alpha^{i}(R)$ is the regularization parameter chosen by rule *R* for run *i*;
- 2) Average relative error of the approximate solution $K^{-1}\sum_{i=1}^{K} \left(\left\| u_{\alpha^{i}(R)} u_{*} \right\| / \left\| u_{*} \right\| \right);$
- 3) Average error ratio $E_{avg} = K^{-1} \sum_{i=1}^{K} E(\alpha^{i}(R))$
- 4) Median error ratio E_{med}

- 5) Maximal error ratio $E_{\max} = \max_{1 \le i \le K} E(\alpha^i(R))$
- 6) Average quasi-error ratio $Q_{avg} = K^{-1} \sum_{i=1}^{K} Q(\alpha^{i}(R))$ 7) Maximal quasi-error ratio $Q_{max} = K^{-1} \sum_{i=1}^{K} Q(\alpha^{i}(R)).$

4.3. The table of the results in case the of unknown solution

In the case of unknown solution the table of results has the following form:

	Rule 1	Rule 2	Rule 3	Rule 4	Rule 5
Parameter	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX
$\overline{T}1(\alpha_{_H})$	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX
$\overline{T}2(\alpha_{_H})$	XXX.XX	XXX.XX	XXX.XX	XXX.XX	XXX.XX
Link to solution	Link	Link	Link	Link	Link

For each selected rule the chosen regularization parameter, the quantities $\overline{T_1}(\alpha(R))$, $\overline{T_2}(\alpha(R))$ and the link to the file of the approximate solution vector are presented.

References

[1] A.B. Bakushinskii, Remarks on choosing a regularization parameter using the quasi-optimality and ratio criterion, Comput. Math. Math. Phys. 24 (4) (1984) 181–182.

[2] F. Bauer, T. Hohage, A Lepskij-type stopping rule for regularized Newton methods, Inverse Problems 21 (6) (2005) 1975–1991.

[3] F. Bauer, M.A. Lukas, Comparing parameter choice methods for regularization of ill-posed problems, Math. Comput. Simul. 81 (2011) 1795–1841.

[4] F. Bauer, P. Mathé, Parameter choice methods using minimization schemes, J. Complexity (2010), doi:10.1016/j.jco.2010.10.001.

[5] C. Brezinski, G. Rodriguez, S. Seatzu, Error estimates for linear systems with applications to regularization, Numer. Algorithms 49 (2008) 85–104.

[6] C. Brezinski, G. Rodriguez, S. Seatzu, Error estimates for the regularization of least squares problems, Numer. Algorithms 51 (2009) 61–76.

[7] D.J. Cummins, T.G. Filloon, D. Nychka, Confidence intervals for nonparametric curve estimates: toward more uniform pointwise coverage, J. Am. Stat. Assoc. 96 (2001) 233–246.

[8] H. Gfrerer, An a posteriori parameter choice for ordinary and iterated Tikhonov regularization of ill-posed problems leading to optimal convergence rates, Math. Comput. 49 (1987) 507–522.

[9] V. Glasko, Y. Kriksin, On the quasioptimality principle for linear ill-posed problems in Hilbert space. Zh. Vychisl. Mat. Mat. Fiz. 24(11), 1603–1613 (1984) In Russian.

[10] G.H. Golub, M. Heath, G. Wahba, Generalized cross-validation as a method for choosing a good ridge parameter, Technometrics 21 (1979), 215–223.

[11]. A.V. Goncharski, A.S. Leonov, A.G.Yagola, A generalized discrepancy principle. USSR Comput. Math. Math. Phys. 13(2), (1973) 25–37.

[12] U. Hämarik, T. Raus, On the choice of the regularization parameter in ill-posed problems with approximately given noise level of data, J.Inverse Ill-Posed Probl. 14 (2006) 251–266.

[13] U. Hämarik, T. Raus, About the balancing principle for choice of the regularization parameter, Numerical Functional Analysis and Optimization, 30(9 & 10), (2009) 951 - 970.

[14] U. Hämarik, R. Palm, T. Raus, A family of rules for parameter choice in Tikhonov regularization of ill-posed problems with inexact noise level, Journal of Computational and Applied Mathematics, 236(8), (2012), 2146 - 2157.

[15] U. Hämarik, R. Palm, T. Raus, On minimization strategies for choice of the regularization parameter in ill-posed problems. Numerical Functional Analysis and Optimization, 30(9&10), (2009), 924 - 950.

[16] M. Hanke, T. Raus, A general heuristic for choosing the regularization parameter in ill-posed problems, SIAM J. Sci. Comput. 17 (1996), 956–972.

[17] P.C. Hansen, Analysis of discrete ill-posed problems by means of the L-curve, SIAM Rev. 34 (1992) 561–580.

[18] P.C. Hansen, Regularization tools: a Matlab package for analysis and solution of discrete ill-posed problems, Numer. Algorithms 6(1)(1994) 1–35.

[19] P.C. Hansen, Rank-Deficient and Discrete Ill-Posed Problems, SIAM, Philadelphia, 1998.

[20] P.C. Hansen, D.P. O'Leary, The use of the L-curve in the regularization of discrete ill-posed problems, SIAM J. Sci. Comput. 14 (1993), 1487–1503.

[21] V.K. Ivanov, The approximate solution of operator equations of the first kind, Zh. Vychisl. Mat. i Mat. Fig. 6: 6 (1966), pp. 1089-1094. (In Russian).

[22] S. Kindermann, A. Neubauer, On the convergence of the quasioptimality criterion for (iterated) Tikhonov regularization, Inverse Probl. Imaging 2(2), (2008), 291–299.

[23] S. Kindermann, Convergence Analysis for minimization based noise level-free parameter choice rules for linear ill-posed problems, ETNA, Vol. 38, (2011), pp. 233-257.

[24] S. Kindermann, Discretization independent convergence rates for noise level-free parameter choice rules in the regularization of ill-conditioned problems, ETNA, 40 (2013), pp 58-81.

[25] C.L. Lawson, R.J. Hanson, Solving least squares problems, SIAM (1974).

[26] M.A. Lukas, Robust generalized cross-validation for choosing the regularization parameter, Inverse Probl. 22 (2006) 1883–1902.

[27] M.A. Lukas, Strong robust generalized cross-validation for choosing the regularization parameter, Inverse Probl. 24 (2008) 034006, 16.

[28] P. Mathé, The Lepskii principle revisited, Inverse Problems 22 (3) (2006) L11–L15.

[29] P. Mathé and S.V. Pereverzev, Discretization strategy for linear ill-posed problems in variable Hilbert scales, *Inverse Probl.* 19 (2003), 1263–1277.

[30] P. Mathé and S.V. Pereverzev, Geometry of linear ill-posed problems in variable Hilbert scales, *Inverse Probl.* 19 (2003), 789–803.

[31] P. Mathé and S.V. Pereverzev, Regularization of some linear ill-posed problems with discretized random noisy data, *Math. Comp.* 75 (2006), 1913–1929.

[32] P. Mathé and S.V. Pereverzev, The discretized discrepancy principle under general source conditions, *J. Complexity* 22 (2006), 371–381.

[33] V.A. Morozov, On the solution of functional equations by the method of regularization, Soviet Math. Dokl. 7 (1966) 414–417.

[34] A. Neubauer, The convergence of a new heuristic parameter selection criterion for general regularization methods, Inverse Probl. 24, 055005 (2008), ...

[35] D. Phillips, A technique for the numerical solution of certain integral equations of the first kind, J. Assoc. Comput. Mach. 9 (1962) 84–97.

[36] T. Raus, The principle of the residual in the solution of ill-posed problems with nonselfadjoint operator, Tartu Riikl. Ül. Toimetised 715 (1985), 12–20.

[37] T. Raus, About regularization parameter choice in case of approximately given error bounds of data, , Tartu Riikl. Ül. Toimetised 937 (1992), 77-89.

[38] T. Raus, U. Hämarik, On the quasioptimal regularization parameter choices for solving ill-posed problems, Journal of Inverse and Ill-Posed Problems, 15(4) (2007), 419 - 439.

[39] T. Raus, U. Hämarik, New Rule for Choice of the Regularization Parameter in (Iterated) Tikhonov Method, Mathematical Modelling and Analysis, 14(2) (2009), 187 - 198.

[40] T.Raus, U.Hämarik, On numerical realization of quasioptimal parameter choices in (iterated) Tikhonov and Lavrentiev regularization, Mathematical Modelling and Analysis, 14(1) (2009), 99 - 108.

[41] T. Raus, U. Hämarik, On the quasi-optimal rules for the choice of the regularization parameter in case of a noisy operator. Advances in Computational Mathematics, 36(2) (2012), 221 - 233.

[42] T.Raus, A new heuristic hybrid rule for choice of the regularization parameter in Tikhonov method, (to appear).

[43] T. Raus, Heuristic hybrid rule for choosing regularization parameter. In: Abstracts of the 7th International Conference "Inverse Problems: Modeling and Simulation": 7th International Conference "Inverse Problems: Modeling and Simulation"; Fethiye, Turkey; May 26-30, 2014. Izmir : Izmir University, 2014,

[44] T. Reginska, A regularization parameter in discrete ill-posed problems, SIAM J. Sci. Comput. 17 (1996) 740–749.

[45] T. Robinson, R. Moyeed, Making robust the cross-validatory choice of smoothing parameter in spline smoothing regression, Commun. Stat., Theory Methods 18 (1989) 523–539.

[46] U. Tautenhahn, U. Hämarik, The use of monotonicity for choosing the regularization parameter in ill-posed problems, Inverse Probl. 15 (1999) 1487–1505.

[47] A. Tikhonov, V. Arsenin, Solutions of Ill-posed Problems, Wiley, New York, 1977.

[48] A. Tikhonov, V. Glasko, Use of the regularization method in non-linear problems, U.S.S.R. Comput. Math. Math. Phys. 5 (1965) 93–107.

[49]. G. Vainikko, A. Veretennikov, Iteration Procedures in Ill-Posed Problems, Nauka, Moscow (1986) (in Russian).

[50] R. Vio, P. Ma, W. Zhong, J. Nagy, L. Tenorio, W. Wamsteker, Estimation of regularization parameters in multiple-image deblurring, Astron. Astrophys. 423 (2004) 1179–1186.

[51] G. Wahba, Practical approximate solutions to linear operator equations when the data are noisy, SIAM J. Numer. Anal. 14 (1977) 651–667.

[52] G. Wahba, A comparison of GCV and GML for choosing the smoothing parameter in the generalized spline smoothing problem, Ann. Stat.13 (1985) 1378–1402.