Discrete ill–posed problems

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Introduction to ill–posed problems

We speak of a discrete ill–posed problem (DIP) when the solution is sensitive to perturbations of the data

Example:

$$A = \begin{pmatrix} 0.15 & 0.1 \\ 0.16 & 0.1 \\ 2.02 & 1.3 \end{pmatrix}, \quad c + \Delta c = A \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \begin{pmatrix} 0.01 \\ -0.032 \\ 0.01 \end{pmatrix}$$

The solution of the perturbed least squares problem (rounded to 4 decimals) using the QR factorization of A is

$$x_{QR} = \begin{pmatrix} -2.9977 \\ 7.2179 \end{pmatrix}$$

Why is it so?

The SVD of A is

$$U = \begin{pmatrix} -0.0746 & 0.7588 & -0.6470 \\ -0.0781 & -0.6513 & -0.7548 \\ -0.9942 & -0.0058 & 0.1078 \end{pmatrix}, \quad \Sigma = \begin{pmatrix} 2.4163 & 0 \\ 0 & 0.0038 \\ 0 & 0 \end{pmatrix}$$

$$V = \begin{pmatrix} -0.8409 & -0.5412 \\ -0.5412 & 0.8409 \end{pmatrix}$$

The component $(u^2)^T \Delta c / \sigma_2$ (u^2 being the second column of U) corresponding to the smallest nonzero singular value is large being 6.2161

This gives the large change in the solution

$$Ax \approx c = \bar{c} - e$$

where A is a matrix of dimension $m \times n, m \geq n$ and the right hand side $\bar{c}$ is contaminated by a (generally) unknown noise vector e

- The standard solution of the least squares problem $\min \|c - Ax\|$ (even using backward stable methods like QR) may give a vector x severely contaminated by noise
- This may seems hopeless
- The solution is to modify the problem by regularization
- We have to find a balance between obtaining a problem that we can solve reliably and obtaining a solution which is not too far from the solution without noise

Tikhonov regularization

Replace the LS problem by

$$\min_x \{\|c - Ax\|^2 + \mu \|x\|^2\}$$

where $\mu \geq 0$ is a regularization parameter to be chosen
For some problems (particularly in image restoration) it is better to consider

$$\min_x \{\|c - Ax\|^2 + \mu \|Lx\|^2\}$$

where L is typically the discretization of a derivative operator of first or second order
The solution x_μ of the problem solves the linear system

$$(A^T A + \mu I)x = A^T c$$

The main problem is to choose μ

- If μ is too small the solution is contaminated by the noise in the right hand side
- if μ is too large the solution is a poor approximation of the original problem
- Many methods have been devised for choosing μ
- Most of these methods lead to the evaluation of bilinear forms with different matrices

Some methods for choosing μ

- Morozov's discrepancy principle
  Ask for the norm of the residual to be equal to the norm of the noise vector

$$\|c - A(A^T A + \mu I)^{-1} A^T c\| = \|e\|$$

- The Gfrerer/Raus method

$$\mu^3 c^T (AA^T + \mu I)^{-3} c = \|e\|^2$$

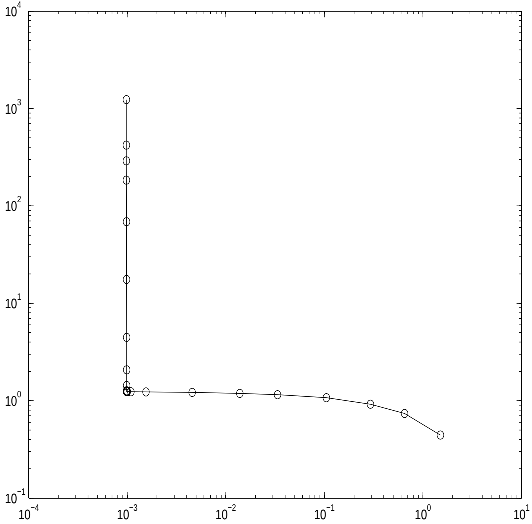
- The quasi–optimality criterion

$$\min[\mu^2 c^T A(A^T A + \mu I)^{-4} A^T c]$$

The L–curve criterion

- plot the curve $(\|x_\mu\|, \|b - Ax_\mu\|)$ obtained by varying the value of $\mu \in [0, \infty)$ in log–log scale
- In most cases this curve is shaped as an “L”
- Lawson and Hanson proposed to choose the value μ_L corresponding to the “corner” of the L–curve (the point of maximal curvature (see also Hansen; Hansen and O’Leary)
- This is done to have a balance between μ being too small and the solution contaminated by the noise, and μ being too large giving a poor approximation of the solution. The “vertex” of the L–curve gives an average value between these two extremes

An example of L–curve



The L-curve for the `Baart` problem, $m = n = 100$, *noise* $= 10^{-3}$

How to locate the corner of the L–curve?

see Hansen and al.

- Easy if we know the SVD of A
- Otherwise compute points on the L–curve and use interpolation
- However, computing a point on the L–curve is expensive
- Alternative, L–ribbon approximation (Calvetti, Golub and Reichel)

The L–ribbon

$$\|x_\mu\|^2 = c^T A(A^T A + \mu I)^{-2} A^T c$$

and

$$\begin{aligned} \|c - Ax_\mu\|^2 \;&=\; c^T c + c^T A(A^T A + \mu I)^{-1} A^T A(A^T A + \mu I)^{-1} A^T c \\ &\quad -2c^T A(A^T A + \mu I)^{-1} A^T c \end{aligned}$$

By denoting $K = A^T A$ and $d = A^T c$

$$\|c - Ax_\mu\|^2 = c^T c + d^T K(K + \mu I)^{-2} d - 2d^T (K + \mu I)^{-1} d$$

Define

$$\begin{aligned}\phi_1(t) &= (t+\mu)^{-2}\\ \phi_2(t) &= t(t+\mu)^{-2} - 2(t+\mu)^{-1}\end{aligned}$$

we are interested in $s_i = d^T \phi_i(K) d$, $i = 1, 2$

We can obtain bounds using the Golub–Kahan bidiagonalization algorithm

At iteration k, the algorithm computes a Jacobi matrix $J_k = B_k^T B_k$ and the Gauss rule gives

$$I_k^G(\phi_i) = \|d\|^2 (e^1)^T \phi_i(J_k) e^1$$

We can also use the Gauss–Radau rule with a prescribed node $a = 0$

$$I_k^{GR}(\phi_i) = \|d\|^2 (e^1)^T \phi_i(\hat{J}_k) e^1$$

$\hat{J}_k = \hat{B}_k^T \hat{B}_k$ where $\hat{B}_k$ is obtained from B_k by setting the last diagonal element $\delta_k = 0$

Theorem

$$I_k^G(\phi_1) \leq s_1 \leq I_k^{GR}(\phi_1)$$

where

$$\begin{aligned} I_k^G(\phi_1) &= \|d\|^2 (e^1)^T (B_k^T B_k + \mu I)^{-2} e^1 \\ I_k^{GR}(\phi_1) &= \|d\|^2 (e^1)^T (\hat{B}_k^T \hat{B}_k + \mu I)^{-2} e^1 \end{aligned}$$

$$I_k^{GR}(\phi_2) \leq s_2 \leq I_k^G(\phi_2)$$

where

$$I_k^G(\phi_2) = \|d\|^2 [(e^1)^T B_k^T B_k (B_k^T B_k + \mu I)^{-2} e^1 - 2(e^1)^T (B_k^T B_k + \mu I)^{-1} e^1]$$

$$I_k^{GR}(\phi_2) = \|d\|^2 [(e^1)^T \hat{B}_k^T \hat{B}_k (\hat{B}_k^T \hat{B}_k + \mu I)^{-2} e^1 - 2(e^1)^T (\hat{B}_k^T \hat{B}_k + \mu I)^{-1} e^1]$$

$$x^-(\mu) = \sqrt{I_k^G(\phi_1)}, \quad x^+(\mu) = \sqrt{I_k^{GR}(\phi_1)}$$

$$y^-(\mu) = \sqrt{c^T c + I_k^{GR}(\phi_2)}, \quad y^+(\mu) = \sqrt{c^T c + I_k^G(\phi_2)}$$

For a given value of $\mu > 0$ the bounds are

$$x^-(\mu) \le \|x_\mu\| \le x^+(\mu), \quad y^-(\mu) \le \|c - Ax_\mu\| \le y^+(\mu)$$

Calvetti, Golub and Reichel defined the L–ribbon as the union of rectangles for all $\mu > 0$

$$\bigcup_{\mu>0} \{ \{x(\mu), y(\mu)\} : x^-(\mu) \le x(\mu) \le x^+(\mu),\, y^-(\mu) \le y(\mu) \le y^+(\mu)\}$$

Then, we have to select a point (a value of μ) inside the L–ribbon

The L–curvature

Another possibility is to obtain bounds of the curvature (in log–log scale) and to look for the maximum

$$C_\mu = 2\frac{\rho''\eta' - \rho'\eta''}{((\rho')^2 + (\eta')^2)^{3/2}}$$

where $'$ denotes differentiation with respect to μ and

$$\begin{aligned}
\rho(\mu) &= \frac{1}{2}\log\|c - Ax_\mu\| = \log \mu^2 c^T \phi(AA^T)c \\
\eta(\mu) &= \frac{1}{2}\log\|x_\mu\| = \log c^T A\phi(A^T A)A^T c
\end{aligned}$$

where $\phi(t) = (t+\mu)^{-2}$

The first derivatives can be computed as

$$\begin{aligned}
\rho'(\mu) &= \frac{c^T A(A^T A + \mu I)^{-3} A^T c}{\mu c^T (AA^T + \mu I)^{-2} c} \\
\eta'(\mu) &= -\frac{c^T A(A^T A + \mu I)^{-3} A^T c}{c^T A(A^T A + \mu I)^{-2} A^T c}
\end{aligned}$$

The numerator is more complicated

$$\begin{aligned}
\rho'\eta'' - \rho''\eta' = \quad & \left(\frac{c^T A(A^T A + \mu I)^{-3} A^T c}{\mu c^T (AA^T + \mu I)^{-2} c \cdot c^T A(A^T A + \mu I)^{-2} A^T c} \right)^2 \\
& (c^T (AA^T + \mu I)^{-2} c \cdot c^T A(A^T A + \mu I)^{-2} A^T c \\
& + 2\mu c^T (AA^T + \mu I)^{-3} c \cdot c^T A(A^T A + \mu I)^{-2} A^T c \\
& - 2\mu c^T (AA^T + \mu I)^{-2} c \cdot c^T A(A^T A + \mu I)^{-3} A^T c)
\end{aligned}$$

Locating the corner of the L–curve

- Using the SVD (Hansen): `lc`
- Pruning algorithm (Hansen, Jensen and Rodriguez): `lp`
- Rotating the L–curve (GM): `lc1`
- Finding an interval where $\log \|x_\mu\|$ and $\log \|c - Ax_\mu\|$ are almost constant (GM): `lc2`

L-curve algorithms, Baart problem, $n = 100$

noise	meth	μ	$\|c - Ax\|$	$\|x - x_0\|$
10^{-3}	opt	$2.4990\ 10^{-8}$	$9.8720\ 10^{-4}$	$1.5080\ 10^{-1}$
	lc	$4.5414\ 10^{-9}$	$9.8524\ 10^{-4}$	$1.6030\ 10^{-1}$
	lp	$8.2364\ 10^{-9}$	$9.8545\ 10^{-4}$	$1.5454\ 10^{-1}$
	lc1	$6.3232\ 10^{-9}$	$9.8534\ 10^{-4}$	$1.5669\ 10^{-1}$
	lc2	$5.8203\ 10^{-12}$	$9.8463\ 10^{-4}$	$4.1492\ 10^{-1}$
		$4.1297\ 10^{-8}$	$9.8996\ 10^{-4}$	$1.5153\ 10^{-1}$

L-curve algorithms, `Phillips` problem, $n = 200$

noise	meth	μ	$\|c - Ax\|$	$\|x - x_0\|$
10^{-3}	`opt`	$8.5392\ 10^{-7}$	$9.9864\ 10^{-4}$	$7.3711\ 10^{-3}$
	`lc`	$7.1966\ 10^{-10}$	$8.5111\ 10^{-4}$	$5.3762\ 10^{-1}$
	`lp`	$4.5729\ 10^{-10}$	$8.3869\ 10^{-4}$	$6.8849\ 10^{-1}$
	`lc1`	$3.6084\ 10^{-10}$	$8.3172\ 10^{-4}$	$7.8603\ 10^{-1}$
	`lc2`	$1.0250\ 10^{-9}$	$8.6013\ 10^{-4}$	$4.4563\ 10^{-1}$
		$2.9147\ 10^{-7}$	$9.7098\ 10^{-4}$	$1.3595\ 10^{-2}$

L-ribbon

Ex	noise	nb it	μ	nb it no reorth.
`Baart`	10^{-7}	11	$6.0889\ 10^{-17}$	40
	10^{-5}	9	$6.1717\ 10^{-13}$	19
	10^{-3}	8	$6.3232\ 10^{-9}$	10
	10^{-1}	6	$7.2928\ 10^{-5}$	6
	10	5	$3.260\ 10^{-2}$	5

Generalized cross–validation

GCV comes from statistics (Golub, Heath and Wahba)

The regularized problem is written as

$$\min\{\|c - Ax\|^2 + m\mu\|x\|^2\}$$

where $\mu \geq 0$ is the regularization parameter and the matrix A is m by n

The GCV estimate of the parameter μ is the minimizer of

$$G(\mu) = \frac{\frac{1}{m}\|(I - A(A^T A + m\mu I)^{-1}A^T)c\|^2}{(\frac{1}{m}\mathrm{tr}(I - A(A^T A + m\mu I)^{-1}A^T))^2}$$

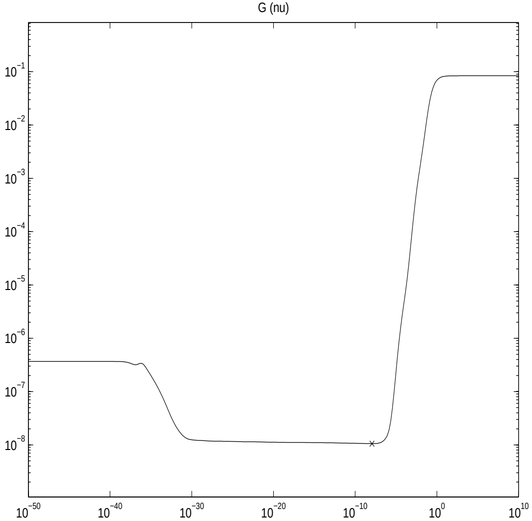
If we know the SVD of A and $m \geq n$ this can be computed as

$$G(\nu) = \frac{m\left\{\sum_{i=1}^{r} d_i^2 \left(\frac{\nu}{\sigma_i^2+\nu}\right)^2 + \sum_{i=r+1}^{m} d_i^2\right\}}{[m - n + \sum_{i=1}^{r} \frac{\nu}{\sigma_i^2+\nu}]^2}$$

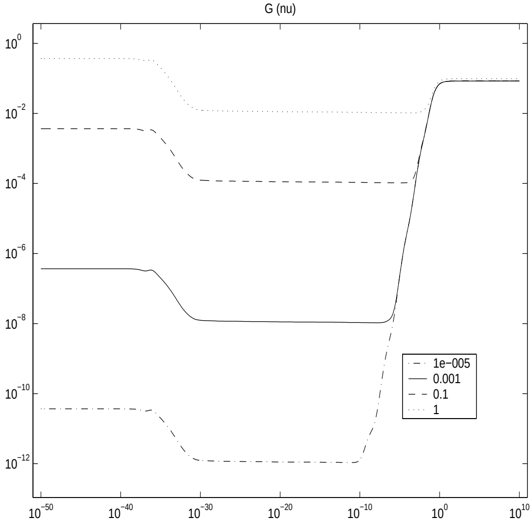
where $\nu = m\mu$

- G is almost constant when ν is very small or large, at least in log–log scale
- When $\nu \to \infty$, $G(\nu) \to \|c\|^2/m$
- When $\nu \to 0$ the situation is different wether $m = n$ or not

An example of GCV function



GCV function for the `Baart` problem, $m = n = 100$, $noise = 10^{-3}$



GCV functions for the Baart problem, $m = n = 100$ for different noise levels

The main problem is that the GCV function is usually quite flat near the minimum

For large problems we cannot use the SVD

- First we approximate the trace in the denominator $\longrightarrow \tilde{G}$
- Then using the Golub–Kahan bidiagonalization algorithms we can obtain bounds of all the terms in $\tilde{G}$
- Finally we have to locate the minimum of the lower and/or upper bounds

Proposition

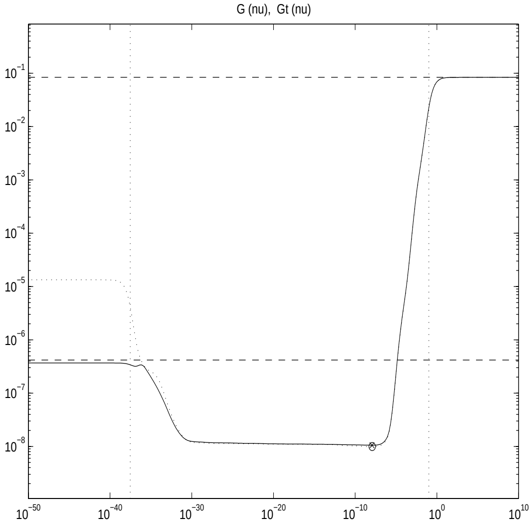
Let B be a symmetric matrix of order n with $\mathrm{tr}(B) \neq 0$
Let $\mathcal{Z}$ be a discrete random variable with values 1 and -1 with equal probability 0.5 and let z be a vector of n independent samples from $\mathcal{Z}$
Then $z^T Bz$ is an unbiased estimator of $\mathrm{tr}(B)$

$$E(z^T Bz) = \mathrm{tr}(B)$$

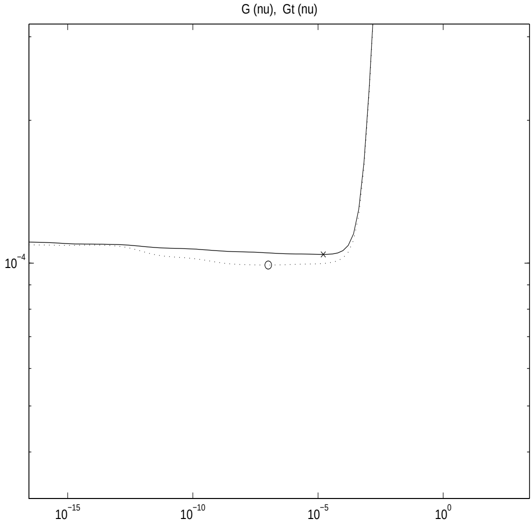
$$\mathrm{var}(z^T Bz) = 2 \sum_{i \neq j} b_{i,j}^2$$

where $E(\cdot)$ denotes the expected value and var denotes the variance

For GCV we just use one vector z



G (plain) and $\tilde{G}$ (dotted) functions for the Baart problem, $m = n = 100$, *noise* $= 10^{-3}$



G (plain) and $\tilde{G}$ (dotted) functions for the `Baart` problem, $m = n = 100$, $noise = 10^{-1}$

The Golub and Von Matt algorithm

Let $s_z(\nu) = z^T(A^TA + \nu I)^{-1}z$, where z is a random vector
Using Gauss and Gauss–Radau we can obtain

$$g_z(\nu) \leq s_z(\nu) \leq r_z(\nu)$$

We can also bound $s_c^{(p)}(\nu) = c^TA(A^TA + \nu I)^{-p}A^Tc, \quad p = 1, 2$
satisfying

$$g_c^{(p)}(\nu) \leq s_c^{(p)}(\nu) \leq r_c^{(p)}(\nu)$$

We want to compute approximations of

$$\tilde{G}(\mu) = m\frac{c^Tc - s_c^{(-1)}(\nu) - \nu s_c^{(-2)}(\nu)}{(m - n + \nu s_z(\nu))^2}$$

We define

$$L_0(\nu) = m\frac{c^Tc - r_c^{(-1)}(\nu) - \nu r_c^{(-2)}(\nu)}{(m - n + \nu r_z(\nu))^2}$$

$$U_0(\nu) = m\frac{c^Tc - g_c^{(-1)}(\nu) - \nu g_c^{(-2)}(\nu)}{(m - n + \nu g_z(\nu))^2}$$

These quantities L_0 and U_0 are lower and upper bounds for the estimate of $G(\mu)$

We can also compute estimates of the derivatives of L_0 and U_0

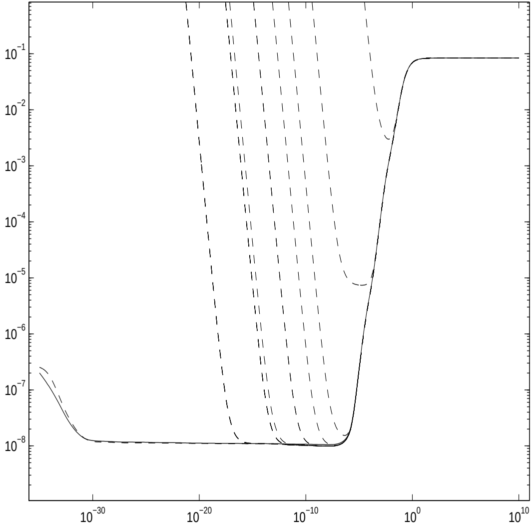
These bounds improve with the number of Lanczos iterations

- They first do $k_{min} = \lceil 3 \log \min(m, n) \rceil$ Lanczos iterations
- Then the global minimizer $\hat{\nu}$ of $U_0(\nu)$ is computed
- If one can find a ν such that $0 < \nu < \hat{\nu}$ and $L_0(\nu) > L_0(\hat{\nu})$, the algorithm stops and return $\hat{\nu}$
- Otherwise, the algorithm executes one more Lanczos iteration and repeats the convergence test

Von Matt computed the minimum of the upper bound:

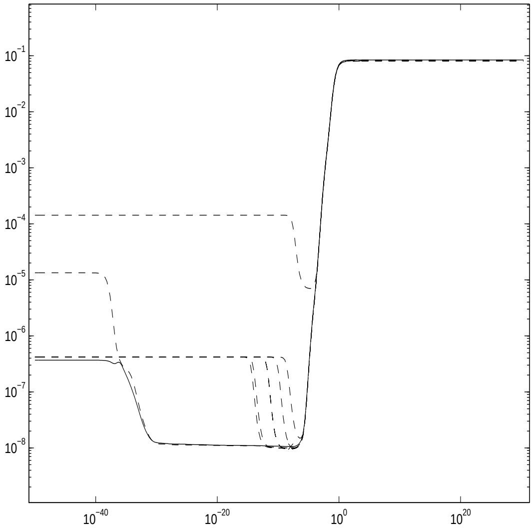
- By sampling the function on 100 points with an exponential distribution
- If the neighbors of the minimum do not have the same values, he looked at the derivative and sought for a local minimum in either the left or right interval depending on the sign of the derivative
- The local minimum is found by using bisection

The upper bound does not have the right asymptotic behavior when $m = n$ and $\nu \to 0$



G (plain) and $\tilde{G}$ (dashed) functions and upper bounds for the `Baart` problem, $m = n = 100$, $noise = 10^{-3}$

To obtain a better behavior we add a term $\|c\|^2$ to the denominator



G (plain) and $\tilde{G}$ (dashed) functions and upper bounds for the `Baart` problem, $m = n = 100$, $noise = 10^{-3}$

Optimization of the algorithm

- We choose a (small) value of ν (denoted as ν_0)
- When

$$\left|\frac{U_k^0(\nu_0) - U_{k-1}^0(\nu_0)}{U_{k-1}^0(\nu_0)}\right| \leq \epsilon_0$$

  we start computing the minimum of the upper bound

The algorithm for finding the minimum is modified as follows

- We work in log–log scale and compute only a minimizer of the upper bound
- We evaluate the numerator of the approximation by computing the SVD of B_k once per iteration
- We compute 50 samples of the function on a regular mesh
- We locate the minimum, say the point k, we then compute again 50 samples in the interval $[k-1\ \ k+1]$

- We use the Von Matt algorithm for computing a local minimum in this interval
- After locating a minimum ν_k with a value of the upper bound U_k^0 at iteration k, the stopping criteria is

$$\left|\frac{\nu_k - \nu_{k-1}}{\nu_{k-1}}\right| + \left|\frac{U_k^0 - U_{k-1}^0}{U_{k-1}^0}\right| \leq \epsilon$$

GCV algorithms, Baart problem

	noise	μ	$\|c - Ax\|$	$\|x - x_0\|$	t (s)
vm	10^{-7}	$9.6482\ 10^{-15}$	$9.8049\ 10^{-8}$	$5.9424\ 10^{-2}$	0.38
	10^{-5}	$9.7587\ 10^{-12}$	$9.8566\ 10^{-6}$	$6.5951\ 10^{-2}$	0.18
	10^{-3}	$1.2018\ 10^{-8}$	$9.8573\ 10^{-4}$	$1.5239\ 10^{-1}$	0.16
	10^{-1}	$1.0336\ 10^{-7}$	$9.8730\ 10^{-2}$	1.6614	–
gm-opt	10^{-7}	$1.0706\ 10^{-14}$	$9.8058\ 10^{-8}$	$5.9519\ 10^{-2}$	0.18
	10^{-5}	$1.0581\ 10^{-11}$	$9.8588\ 10^{-6}$	$6.5957\ 10^{-2}$	0.27
	10^{-3}	$1.3077\ 10^{-8}$	$9.8582\ 10^{-4}$	$1.5205\ 10^{-1}$	0.14
	10^{-1}	$1.1104\ 10^{-7}$	$9.8736\ 10^{-2}$	1.6227	–

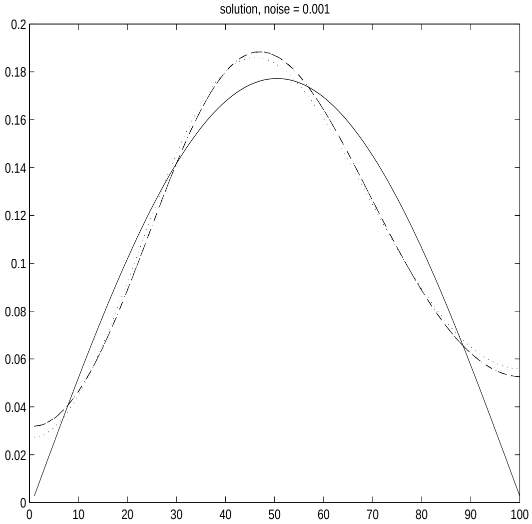
GCV algorithms, Phillips problem

	noise	μ	$\|c - Ax\|$	$\|x - x_0\|$	t (s)
vm	10^{-7}	$8.7929\ 10^{-11}$	$9.0162\ 10^{-8}$	$2.2391\ 10^{-4}$	29.50
	10^{-5}	$4.5432\ 10^{-9}$	$9.0825\ 10^{-6}$	$2.2620\ 10^{-3}$	6.09
	10^{-3}	$4.3674\ 10^{-7}$	$9.7826\ 10^{-4}$	$1.0057\ 10^{-2}$	1.14
	10^{-1}	$3.8320\ 10^{-5}$	$9.8962\ 10^{-2}$	$9.3139\ 10^{-2}$	0.16
gm-opt	10^{-7}	$1.6343\ 10^{-10}$	$1.1260\ 10^{-7}$	$2.2163\ 10^{-4}$	15.30
	10^{-5}	$5.3835\ 10^{-9}$	$9.1722\ 10^{-6}$	$2.1174\ 10^{-3}$	6.09
	10^{-3}	$4.1814\ 10^{-7}$	$9.7737\ 10^{-4}$	$1.0375\ 10^{-2}$	0.66
	10^{-1}	$4.1875\ 10^{-5}$	$9.9016\ 10^{-2}$	$9.0659\ 10^{-2}$	0.22

Comparisons of methods

Baart problem, $n = 100$

noise	meth	μ	$\|c - Ax\|$	$\|x - x_0\|$
10^{-3}	μ opt	$2.7826\ 10^{-8}$	$2.3501\ 10^{-3}$	$1.5084\ 10^{-1}$
	vm	$1.2018\ 10^{-8}$	$9.8573\ 10^{-4}$	$1.5239\ 10^{-1}$
	gm-opt	$1.3077\ 10^{-8}$	$9.8582\ 10^{-4}$	$1.5205\ 10^{-1}$
	gcv	$9.4870\ 10^{-9}$	$9.8554\ 10^{-4}$	$1.5362\ 10^{-1}$
	disc	$8.4260\ 10^{-8}$	$1.0000\ 10^{-3}$	$1.5556\ 10^{-1}$
	gr	$1.7047\ 10^{-7}$	$1.0235\ 10^{-3}$	$1.6373\ 10^{-1}$
	lc	$4.5414\ 10^{-9}$	$9.8524\ 10^{-4}$	$1.6028\ 10^{-1}$
	qo	$1.2586\ 10^{-8}$	$9.8450\ 10^{-4}$	$6.6072\ 10^{-1}$
	L-rib	$6.3232\ 10^{-9}$	$9.8534\ 10^{-4}$	$1.5669\ 10^{-1}$
	L-cur	$5.8220\ 10^{-9}$	$9.8531\ 10^{-4}$	$1.5749\ 10^{-1}$



Solutions for the Baart problem, $m = n = 100$, $noise = 10^{-3}$, solid=unperturbed solution, dashed=vm, dot–dashed=gm-opt

Phillips problem, $n = 200$

noise	meth	μ	$\|c - Ax\|$	$\|x - x_0\|$
10^{-5}	μ opt	$1.3725\ 10^{-7}$	$2.9505\ 10^{-14}$	$1.6641\ 10^{-3}$
	vm	$4.5432\ 10^{-9}$	$9.0825\ 10^{-6}$	$2.2620\ 10^{-3}$
	gm-opt	$5.3835\ 10^{-9}$	$9.1722\ 10^{-6}$	$2.1174\ 10^{-3}$
	gcv	$3.1203\ 10^{-9}$	$8.9283\ 10^{-6}$	$2.6499\ 10^{-3}$
	disc	$1.2107\ 10^{-8}$	$1.0000\ 10^{-5}$	$1.6873\ 10^{-3}$
	gr	$4.1876\ 10^{-8}$	$1.5784\ 10^{-5}$	$1.9344\ 10^{-3}$
	lc	$3.6731\ 10^{-14}$	$2.4301\ 10^{-6}$	$7.9811\ 10^{-1}$
	qo	$1.5710\ 10^{-8}$	$1.0542\ 10^{-5}$	$1.6463\ 10^{-3}$
	L-rib	$2.6269\ 10^{-14}$	$2.2118\ 10^{-6}$	$8.9457\ 10^{-1}$
	L-cur	$4.7952\ 10^{-14}$	$2.6093\ 10^{-6}$	$7.2750\ 10^{-1}$

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