

Determination of regularization parameter in discrete linear ill-posed problem using DNN

- Examples: V2 -

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September 17, 2021

In this note, a couple of ill-posed problems are illustrated with numerical simulations. The goal of our work is to develop algorithms to estimate the optimal regularization parameters for each problem.

1 Cauchy problem for the backward heat equation

Consider the one-dimensional heat equation.

$$u_t = u_{xx}, \quad 0 < x < \pi, \quad t > 0 \quad (1a)$$

$$u(t, 0) = u(t, \pi) = 0, \quad t > 0 \quad (1b)$$

To solve this problem additional condition is required. In general, the initial condition is given,

$$u(0, x) = q(x), \quad 0 < x < \pi \quad (2)$$

Then u is uniquely solvable under suitable condition on q . Thus, we know the temperature at any time $t = T$, say,

$$u(T, x) = f(x), \quad 0 < x < \pi \quad (3)$$

The backward heat equation is an inverse problem to reconstruct the initial temperature q from the measurement of f . It is well-known that it is an ill-posed problem.

Numerical solutions

From the method of separation of variables, the general solution to (1) is given by

$$u(t, x) = \sum_{n=1}^{\infty} c_n e^{-n^2 t} \sin nx$$

We assume that $q, f \in L_0^2(0, \pi)$, which is a set of square integrable functions vanishing at the boundary. As

$$\mathcal{S} := \{\sin nx : 0 \leq x \leq \pi\}_{n=1}^{\infty} \quad (4)$$

is dense in L_0^2 , we have

$$\begin{aligned} q &= \sum_{n=1}^{\infty} q_n \sin nx, \\ f &= \sum_{n=1}^{\infty} f_n \sin nx, \end{aligned}$$

where

$$\begin{aligned} q_n &= \frac{2}{\pi} \int_0^{\pi} q(x) \sin nx dx, \\ f_n &= \frac{2}{\pi} \int_0^{\pi} f(x) \sin nx dx. \end{aligned}$$

The initial condition (2) gives that

$$u(0, x) = \sum_{n=1}^{\infty} c_n \sin nx = \sum_{n=1}^{\infty} q_n \sin nx,$$

or

$$c_n = q_n, \quad n = 1, 2, 3, \dots$$

Together with (3), we have

$$q_n e^{-n^2 T} = f_n, \quad n = 1, 2, 3, \dots \quad (5)$$

or

$$q_n = e^{n^2 T} f_n, \quad n = 1, 2, 3, \dots$$

Algorithm 1. *Backward heat equation*

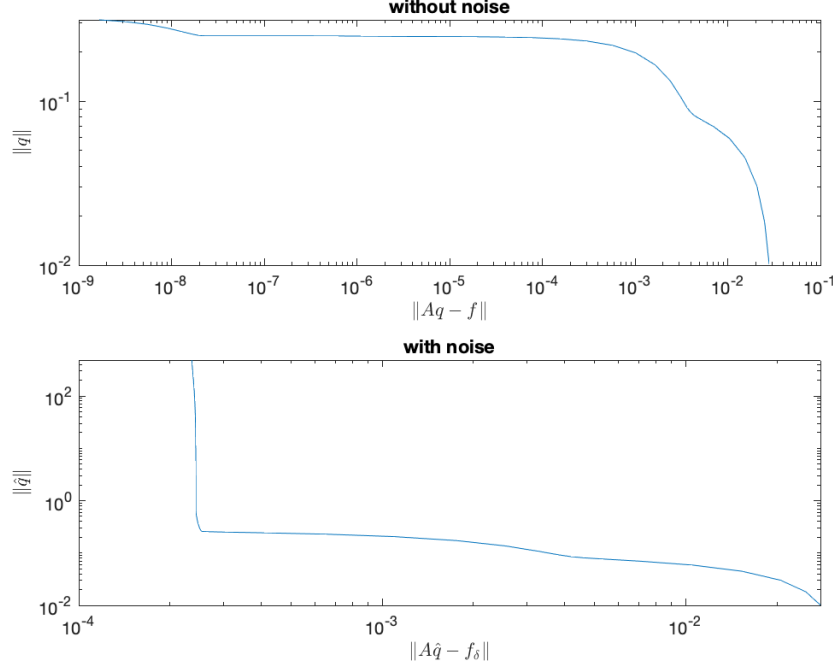


Figure 1: L-curves

1. Set T . Take N .
2. For a given $f \in L_0^2(0, \pi)$ compute $\{f_n\}_{n=1}^N$.
3. Solve

$$F = AQ \quad (6)$$

where $F = (f_1, \dots, f_N)^T$, $Q = (q_1, \dots, q_N)^T$, and $A = \text{diag}(e^{-T}, e^{-2^2T}, \dots, e^{-N^2T})$.

Note that we need a regularization scheme to solve (6) when F has a noise. We use Tikhonov regularization method with the parameter α .

Then approximation solution \hat{Q} is given by

$$\hat{Q} = (A^*A + \alpha I)^{-1}A^*F$$

or

$$\hat{q}_n = \frac{f_n}{\alpha e^{n^2T} + e^{-n^2T}}, \quad n = 1, 2, \dots, N.$$

Figure 1 shows that log-log plots for $\|Aq - f\|$ and $\|q\|$. Let $q = \sum_{n=1}^5 q_n \sin nx$. $\{q_n\}_{n=1}^5$ is randomly generated satisfying $\|q\| \leq \tau = 1$. (see 'generate_Q_rej.m').

Solve the direct problem to obtain F at the terminal time $T = 1$ by ‘*sol_act.m*’. Run ‘*noise_data.m*’ to get noisy data with noise level $\delta = 0.01$, denoted by nF or f_δ . Now we have one data set (Q, F, nF) from the direct problem solver. Conversely, we solve the inverse problem with the Tikhonov method by ‘*sol_Tik.m*’ with the various regularization parameter α . All procedures can be done by ‘*result_Lcurve.m*’. See the comments on it. We set $\text{min_al} = -20$ for Figure 1.

To obtain data set for training, see ‘*result_genData.m*’.

Task

- Understand the theory and algorithm
- Run (and modify) the appended codes with various parameters
- Generate data set
- Train a model, say \mathcal{M}_1 , with $\{(Q, F)\}$. What is the accuracy? Can we use \mathcal{M}_1 to solve $AQ = nF$, i.e., for the noisy data f_δ ?
- Train a model, say \mathcal{M}_2 for $\{nF\}$.
- Train a model to find the best regularization parameter.

2 Integral equation of the first kind

The standard form of the integral equation of the first kind with kernel K is given by

$$f(x) = \int_a^b K(x, y)u(y)dy. \quad (7)$$

We seek a function u satisfying (7) for a given f . In general, it is an ill-posed problem. Specifically, we consider the following problem.

$$f(x) = \int_0^\pi K(x, y)u(y)dy \quad (8)$$

where

$$K(x, y) := \begin{cases} \frac{1}{\pi}(\pi - x)y, & 0 \leq y \leq x \leq \pi \\ \frac{1}{\pi}(\pi - y)x, & 0 \leq x \leq y \leq \pi \end{cases}$$

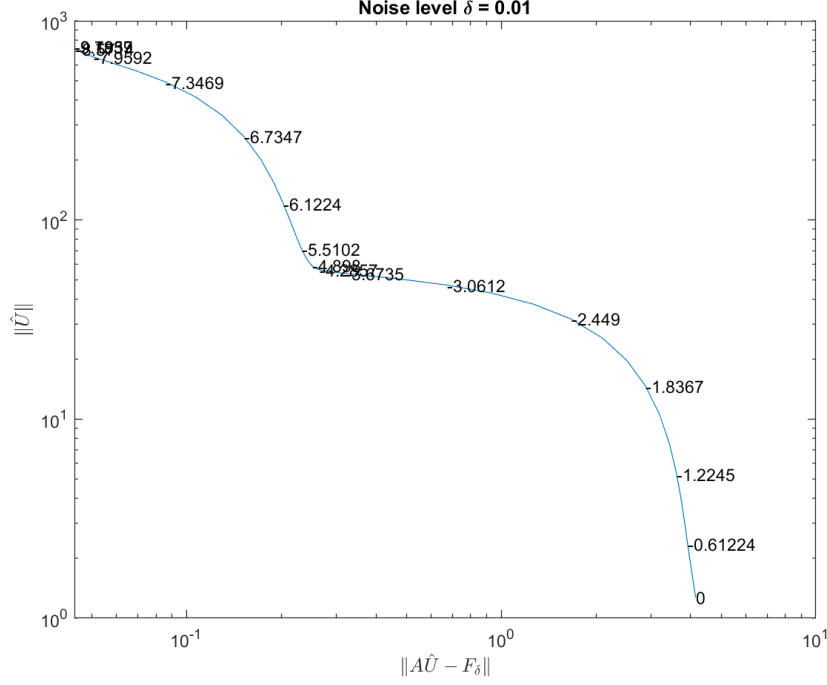


Figure 2: L-curves for the integral equation. Here, $N = 5$ and $\tau = 1$.

We are interested in solving (8) for any $f \in L_0^2(0, \pi) := \{f \in L^2 : f(0) = f(\pi) = 0\}$. Note that (8) can be converted to the second order differential equation;

$$f''(x) = -u(x), \quad 0 \leq x \leq \pi \quad (9a)$$

$$f(0) = f(\pi) = 0. \quad (9b)$$

We see that if f is not twice differentiable, u satisfying (9) does not exist in the classical sense. This may give the ill-posedness of (8). Nevertheless, we want to solve (or find approximation) (8) for a given $f \in L_0^2(0, \pi)$ numerically.

Numerical solutions

Let $\{0 = x_1, x_2, \dots, x_L = \pi\}$ be a partition for $[0, \pi]$ and set $y_i = x_i, i = 1, 2, \dots, L$. Then, at $x = x_j$

$$f(x_j) = \int_0^\pi K(x_j, y)u(y)dy.$$

Using numerical integration, we obtain

$$f(x_j) = \sum_{j=1}^L K(x_i, y_j)\omega_j u(y_j), \quad j = 1, 2, \dots, L.$$

Here, ω_j is a weight for the numerical integration. In vector notations, we rewrite

$$F = AU, \tag{10}$$

where

$$\begin{aligned} F_i &= f(x_i), \\ A_{ij} &= K(x_i, y_j)\omega_j, \\ U_j &= u(y_j). \end{aligned}$$

It is known that $\{\sin nx : n \in \mathbb{N}\}$ is basis for $L_0^2(0, \pi)$. Thus, we generate data set over $\{f = \sum_{n=1}^N Q_n \sin nx : \|f\|_2 \leq \tau\}$. Here, $\{Q_n\}$ is randomly generated. For a given f , the exact solution u is given by

$$u = \sum_{n=1}^N Q_n n^2 \sin nx$$

As for the numerical integration, we simply use the trapezoidal rule, which determines

$$\omega_j = \begin{cases} \Delta y/2 & j = 1, N \\ \Delta y & \text{else} \end{cases}$$

Also note that the first and last rows and columns of matrix A are vanished since $K(0, \cdot) = K(\pi, \cdot) = K(\cdot, 0) = K(\cdot, \pi) = 0$. Thus, A is singular. To solve (10), we may reformulate the equation by removing all the boundary vales or use regularization technique by taking into account $u \in L_0^2$. In the code, the second method is applied.

Figure 2 shows the L-curve for the associate integral equation. We plot the exact u and restored u from the Tikhonov regularization scheme with the best or near the best regularization parameter in Figure ?? . Also, we compare the regularization solution and solution obtained from (9) in Figure 4.

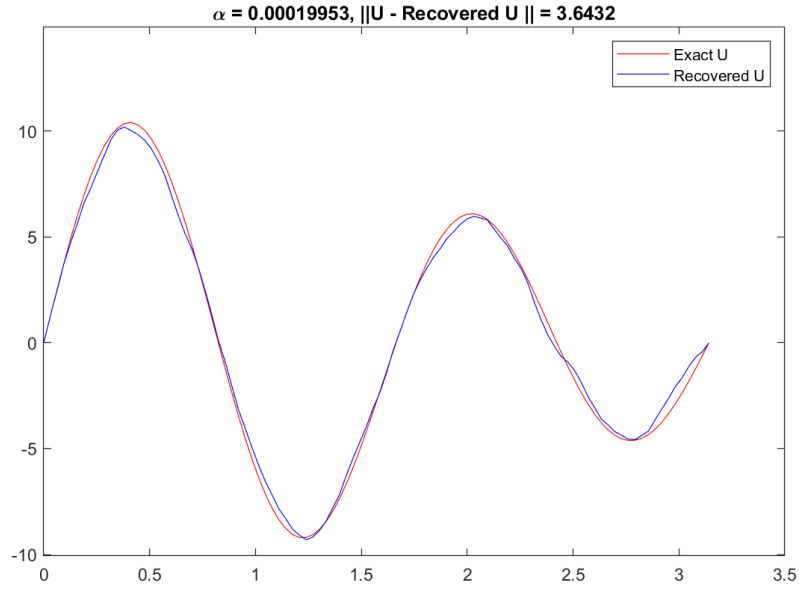


Figure 3: Exact solution and restored solution by Tikhonov regularization.

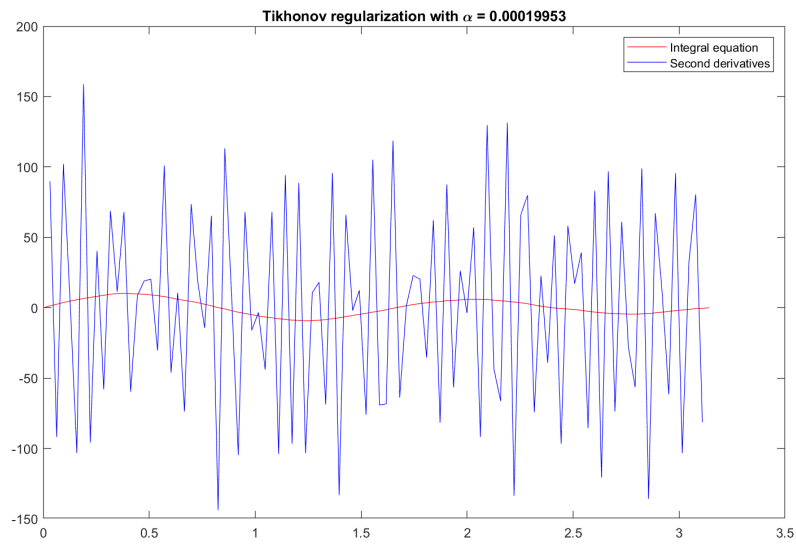


Figure 4: Restored solutions by Tikhonov regularization and numerical derivative for noisy data F .

3 Some scattering problems

Will be discussed.