Fall 2017:
Computational and Variational Methods for Inverse Problems
GEO 391/CSE 397/ME 397/ORI 397
Assignment 1 (due Sept. 27, 2017)

In this assignment we will build on the inverse heat equation problem considered in class. You will first derive expressions for the eigenvalues and eigenvectors of the *discretized* parameter-to-observable map $\boldsymbol{F}$ and then you will compare two methods for the selection of the regularization parameter α (L-curve and Morozov discrepancy) to the optimal choice of the regularization parameter (which you will be able to do since you know the true initial condition). The Jupyter notebook required for this assignment can be downloaded from https://uvilla.github.io/inverse17/. It is the one entitled *Inverse problem prototype*. Make sure to download the latest version, since we fixed a few typos. Also, if you have not yet done so, please register on our Piazza website at https://piazza.com/utexas/fall2017/geo391cse397me397ori397.

Problem 1

Recall the inverse problem for the 1D heat equation discussed in class. Here we attempt to reconstruct the initial temperature field from the observed temperature field at a later time T. As we have seen, this problem is (severely) ill-posed, and in this problem we will study the nature of the ill-posedness.

Let $u(x,t)$ denote the temperature field and $u(x,0) = m(x)$ the initial temperature profile. Given the length of the rod L, the thermal diffusivity $k > 0$, the final time T, and homogeneous Dirichlet boundary conditions ($u(0,t) = u(L,t) = 0$), the *parameter-to-observable map* $\mathcal{F}(m)$ can be written as

$$\mathcal{F}(m) = u(x,T),$$

where $u(x,T)$ denotes the solution at the final time T of the heat equation

$$\begin{cases} \frac{\partial u}{\partial t} - k\frac{\partial^2}{\partial x^2}u = 0 & 0 < x < L, \;\; 0 < t \le T, \\ u(x,0) = m(x) & 0 < x < L, \\ u(0,t) = u(L,t) = 0 & 0 < t \le T. \end{cases}$$

We discretize the problem using 2nd order centered finite differences in space and implicit Euler in time. We denote with $h = \frac{L}{n_x}$ the mesh size and with $\Delta t = \frac{T}{n_t}$ the time step used in the discretization. Then the $(n_x - 1) \times (n_x - 1)$ matrix $\boldsymbol{F}$, arising from the discretization of the parameter-to-observable map $\mathcal{F}$, takes the form

$$\boldsymbol{F}\boldsymbol{m} = (\boldsymbol{I} + \Delta t \boldsymbol{K})^{-n_t}\boldsymbol{m},$$

where the discretized diffusion operator $\boldsymbol{K}$ is an $(n_x - 1) \times (n_x - 1)$ matrix given by

$$\boldsymbol{K} = \frac{k}{h^2}\begin{bmatrix} 2 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & \dots & \dots & \dots & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 2 \end{bmatrix},$$

and $\boldsymbol{m}$ is an $n_x - 1$ vector representing the discretized parameter field we wish to invert for (i.e., the initial condition).

a) Verify that the eigenvalues λ_n and corresponding eigenfunctions v_n of the continuous map $\mathcal{F}$ are given by

$$\lambda_n = e^{-kT\left(\frac{\pi n}{L}\right)^2}, \quad v_n = \sqrt{\frac{2}{L}} \sin\left(n\,\pi \frac{x}{L}\right).$$

b) Derive the expression for the eigenvalues and eigenvectors of the parameter-to-observable matrix $\boldsymbol{F}$ using the fact that the eigenvalues μ_n of $\boldsymbol{K}$ are given by

$$\mu_n = k\frac{4}{h^2}\sin^2\left(\frac{\pi\, n}{2n_x}\right), \quad n = 1, 2, \ldots, n_x - 1,$$

and the jth component of the corresponding eigenvector $\boldsymbol{u}_n$ is given by

$$[\boldsymbol{u}_n]_j = \sqrt{\frac{2}{L}}\sin\left(n\,\frac{\pi}{L}\,j\,h\right), \quad n = 1, 2, \ldots, n_x - 1.$$

c) Set $T = 1$, $L = 1$, $n_x = 200$, and $n_t = 100$, and plot the decay of the eigenvalues of both the continuous ($\mathcal{F}$) and the discrete ($\boldsymbol{F}$) parameter-to-observable maps as a function of n. Do this for the following values of k: 0.0001, 0.001, 0.01, 0.1, 1.0 (all on the same plot).

d) Set $L = 1$, $k = 0.01$ and $T = 0.1$; plot the decay of the discrete eigenvalues as a function of n for different resolutions in the space and time discretization. Use $(n_x, n_t) = (20, 20), (40, 40), (80, 80), (160, 160)$. What do you observe as you increase the resolution?

Problem 2

Consider the same inverse heat equation problem as in **Problem 1** with $L = 1$, $T = 0.1$, $k = 0.01$. Discretize the problem using $n_x = 200$ intervals in space and $n_t = 100$ time steps. As initial condition use the (discrete version of) the true initial temperature profile

$$m_{\text{true}} = \max(0, 1 - |1 - 4x|) + 100\,x^{10}(1 - x)^2.$$

Use the code below to implement the above function in Python:

```
import numpy as np
x = np.arange(1,n_x, dtype=np.float64)*h
m_true = np.maximum( np.zeros_like(x), 1. - np.abs(1. - 4.*x)) \
        + 100.*np.power(x,10)*np.power(1.-x,2)
```

Add normally distributed noise[1] $\boldsymbol{n}$ with mean zero and variance $\sigma^2 = 10^{-4}$. The resulting noisy observation of the final time temperature profile is $\boldsymbol{d} = \boldsymbol{F}\boldsymbol{m} + \boldsymbol{n}$.

[1]Python provides the function `randn` through the `numpy.random` library.

a) Use the truncated singular value decomposition[2] filter (TSVD) with $\alpha = 0.0001, 0.001, 0.01, 0.1, 1$ to compute the regularized reconstructions $\boldsymbol{m}_\alpha^{\mathsf{TSVD}}$.

b) Use the Tikhonov filter with the same values for α for the reconstructions $\boldsymbol{m}_\alpha^{\mathsf{Tikh}}$.

c) Determine the (approximate) optimal value of the regularization parameter α in the Tikhonov regularization using the L-curve criterion.

d) Determine the (approximate) optimal value of the regularization parameter α in the Tikhonov regularization using Morozov's discrepancy criterion, i.e., find the largest value of α such that

$$\|\boldsymbol{F}\boldsymbol{m}_\alpha - \boldsymbol{d}\| \leq \delta$$

where $\delta = \|\boldsymbol{n}\|$ and $\boldsymbol{m}_\alpha$ is the solution of the Tikhonov-regularized inverse problem with regularization parameter α.

e) Plot the L_2 norm error in the reconstruction, $\|\boldsymbol{m}_{\mathsf{true}} - \boldsymbol{m}_\alpha\|$, as a function of α, where $\boldsymbol{m}_\alpha$ is the Tikhonov regularized solution. Which value of α (approximately) minimizes this error? Compare the "optimal" values of α obtained in parts c, d, and e of this problem and comment on any differences.

Problem 3 (Optional)

Consider now inverse heat equation problem with adiabatic (i.e. no heat flux) boundary conditions at the extremities of the rod,

$$k\frac{\partial u}{\partial x}\bigg|_{x=0} = k\frac{\partial u}{\partial x}\bigg|_{x=L} = 0.$$

Let $L = 1$, $T = 0.1$, $k = 0.01$ and discretize the problem using $n_x = 200$ intervals in space and $n_t = 100$ time steps. As initial condition use the (discrete version of) the true initial temperature profile

$$m_{\mathsf{true}} = x^2(1-x)^2(1 + 0.1\sin(20\pi x)),$$

and add normally distributed noise $\boldsymbol{n}$ with mean zero and variance $\sigma^2 = 10^{-4}$. The resulting noisy observation of the final time temperature profile is $\boldsymbol{d} = \boldsymbol{F}\boldsymbol{m} + \boldsymbol{n}$.

a) Modify the code to prescribe the different type of boundary conditions. Numerically compute and plot the eigenvalues and eigenvectors of the discretized problem.

b) Determine the (approximately) optimal value of the regularization parameter α in the Tikhonov-regularized solution using the L-curve criterion.

c) Which value of α minimizes the L_2 norm of the difference between the true image and the Tikhonov-regularized reconstruction? How does this value compare to the α yielded by the L-curve?

[2] Python provides the function `svd` to compute the singular value decomposition of a matrix through the `numpy.linalg` library.