Engsci 741: Inverse Problems Assignment

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Due: **Monday 8th October 11.59 pm** (submit via Canvas).

Question 1

Consider the standard Tikhonov form of the regularised least squares problem

$$\min_x ||Ax - y||^2 + \lambda||x||^2$$

where we will assume that A is $m \times n$ for $m < n$ and $\lambda > 0$ is the regularisation parameter.

- Rewrite this in the form of a new 'augmented' but 'standard' least squares problem.
- Hence explain why this form of regularisation can be thought of as helping us convert an underdetermined problem into an overdetermined problem.
- Justify the linear independence of the columns of the matrix in the resulting overdetermined problem.
- Use the above to derive an explicit expression for the 'Tikhonov inverse'. You may state/use the normal equations for standard least squares problems without proof.
- What solutions does the Tikhonov inverse give in the two limiting cases a) $\lambda \to 0$ and b) $\lambda \to \infty$? Justify your answers.

Question 2

Here we consider the 'inverse problem' of polynomial regression for data $\{(x_i, y_i)\},\ i = 1, .., m$. Suppose you have a forward model with three parameters:

$$y = \theta_1 + \theta_2 x + \theta_3 x^2$$

and four observations $(x_1, y_1), (x_2, y_2), (x_3, y_3), (x_4, y_4)$.

- Set up the problem to be 'solved' as a matrix equation of the form $A\theta = y$. Explain why, however, you would not generally expect this problem to be solvable in the standard sense.
- Write down the general expressions for both the *model (parameter) resolution* operator R_θ and the *data resolution* operator R_d a) in terms of A and its generalised inverse A^+ **and** b) in terms of the matrices of singular vectors U_r, V_r of the (reduced) SVD of A.
- Which of the resolution operators do you expect to be the identity matrix in the present problem and which not? Why?
- Give a simple example of U_r, V_r that would be compatible with the above given information. (Justify your answer!)
- Using Python/Matlab etc, verify your answers to the question about which resolution operators are the identity for the case where the forward mapping is given by:

$$A = \begin{bmatrix} 1. & 1. & -0.5 \\ 1. & 5. & -12.5 \\ 1. & 7. & -24.5 \\ 1. & 13. & -84.5 \end{bmatrix}.$$

Question 3

[Note: your answers to this question should be given in the form of Python/Matlab etc code and output produced from this. You should include your code in your submission.]

This problem concerns the so-called source history reconstruction problem: we want to recover the time history of the concentration of a pollutant at a known source site from later measurements. That is, we want to recover a *boundary condition* given measurements of concentrations at a series of locations at a future time.

This is illustrated in the figure below (see also the Aster et al. 'Inverse Problems and Parameter Estimation' section handout on Canvas under readings).

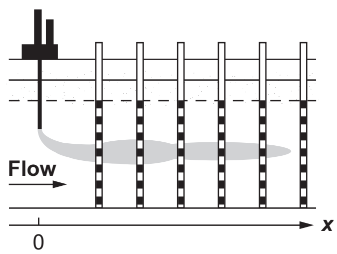

Figure 1: The source history recovery problem (from Aster et al. 'Inverse Problems and Parameter Estimation'). We measure the concentration at the vertical observation wells at some fixed future time T, and want to use this to recover the time history of the pollutant source.

A simple forward model for this problem is the advection-diffusion equation

$$\frac{\partial C}{\partial t} = D\frac{\partial^2 C}{\partial x^2} - v\frac{\partial C}{\partial x}$$

with boundary conditions

$$C(0,t) = C_{\text{in}}(t)$$

and

$$C(x,t) \to 0 \text{ as } x \to \infty$$

where D is the (known) diffusion coefficient, v is the (known) fluid velocity, and $C(x,t)$ is the pollutant concentration. Normally the boundary condition $C_{\text{in}}(t)$ would be taken as known, but here we will look to *invert* for it - i.e. solve an inverse problem!

It can be shown that the solution of the PDE above at time T can be expressed as

$$C(x,T) = \int_0^T k(x, T-t)C_{\text{in}}(t)dt$$

where the *kernel* k is given by

$$k(x, T-t) = \frac{x}{2\sqrt{\pi D(T-t)^3}} \exp\left(\frac{-[x - v(T-t)]^2}{4D(T-t)}\right).$$

Our goal is to recover the input history $C_{\text{in}}(t)$ at a fixed location, given a set of measurements $C(x,T)$ at a series of x locations taken at the same time T. Since the foward problem above takes the form of a (convolution) integral equation, we expect we will need to regularise the solution of the inverse problem.

We can think of the forward problem above as a mapping of a *series of measurements in time at a fixed x location* to a *series of measurements in space at a fixed future time.*

If we discretise space x into a grid of m (mid-)points x_i and t into a grid of n (mid-)points t_j, and we use the simple numerical integration rule

$$\int_0^T k(x, T-t) C_{\text{in}}(t) dt \approx \sum_{j=1}^{n} k(x_i, T-t_j) C_{\text{in}}(t_j) \Delta t$$

where Δt is the time interval between t_j grid points, then the forward problem becomes

$$Ka = b$$

where $K(i,j) = k(x_i, T-t_j)\Delta t$, a is the (time) vector of source concentrations, i.e. $C_{\text{in}}(t_j)$, of length n and b is the (spatial) vector of concentrations at a known time T, i.e. $C(x_i, T)$, with length m.

- Implement a function (or set of functions) in Python/Matlab etc that returns the above linear forward operator K given problem inputs $x_{\min}$, $x_{\max}$, $t_{\min}$, $t_{\max}$, m, n, T, D and v.
- Verify that an input source history of $C_{\text{in}}(t) = 3 + \sin(2\pi t/n)\sin(0.01t)$ (see left panel in figure below) gives, when operated on by your forward model for the settings given below, output source measurements at T that look like those shown in the right panel of the figure below.

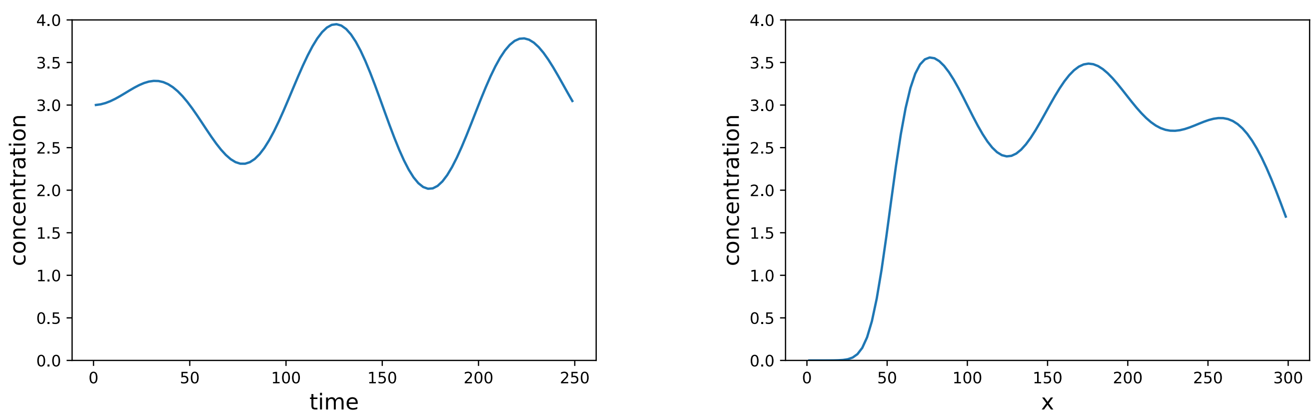

Figure 2: (L) Input signal. (R) Output from forward model.

Problem input settings: $x_{\min} = 0,\ x_{\max} = 300,\ t_{\min} = 0,\ t_{\max} = 250,\ m = 100,\ n = 100,\ D = 1,\ v = 1,\ T = 300$. We will assume everything is non-dimensionalised or expressed in appropriate units...

- Now create some synthetic data for an inverse problem by taking your output source measurement vector at T and adding a small amount of noise to each observation, e.g. add a realisation of normal noise to each output value using a normal distribution with mean 0.0 and standard deviation 0.01.

We can now attempt to recover an estimate of the original input source history given these measurements.

- First, show that the naive (unregularised) least squares solution produces bad results even though the noise is small.
- Next, solve the inverse problem properly, using a regularisation scheme of your choice, to recover an estimate of the original input source history. Produce a tradeoff curve for your choice of regularisation scheme (e.g. an L-curve) and use this to plot what you expect to be a) an underfitting solution, b) a good solution and c) an overfitting solution. (Note: you probably won't be able to *exactly* recover the truth - that's OK!). Then compare your results determined from the parameter choice method to the actual truth that we used to generate the data.