MATH 076 - Computational Inverse Problems

Carter Kruse, July 26, 2023

Homework 2

Instructions

This homework assignment is split into two sections: written questions and computational questions. For the written questions, you are **not** permitted to use a calculator or any other computational tools. For the computational questions, you are asked to use a coding language of your choice to perform the tasks requested. You may make use any code posted to our course's Canvas page. **Please show all of your work.** If you have any questions or uncertainties, please reach out to your instructor.

Written Questions

1) Suppose $\boldsymbol{x} \in \mathbb{R}^n$, $A \in \mathbb{R}^{m \times n}$, $m \geq n$, is full rank, $\boldsymbol{b} \in \mathbb{R}^m$, and $\lambda > 0$. Recall that the Tikhonov regularization problem is given as

$$\boldsymbol{x}_\lambda = \min_{\boldsymbol{x}} \|A\boldsymbol{x} - \boldsymbol{b}\|_2^2 + \lambda^2 \|\boldsymbol{x}\|_2^2$$

In class, we discussed how this can be re-written as

$$\boldsymbol{x}_\lambda = \min_{\boldsymbol{x}} \left\| \begin{bmatrix} A \\ \lambda \mathbb{I}_n \end{bmatrix} \boldsymbol{x} - \begin{bmatrix} \boldsymbol{b} \\ \boldsymbol{0} \end{bmatrix} \right\|_2^2$$

Prove that the solution is

$$\boldsymbol{x}_\lambda = \left(A^T A + \lambda^2 \mathbb{I}_n\right)^{-1} A^T \boldsymbol{b}$$

Hint: Find the associated normal equations.

The Tikhonov regularization problem is given as

$$\boldsymbol{x}_\lambda = \min_{\boldsymbol{x}} \|A\boldsymbol{x} - \boldsymbol{b}\|_2^2 + \lambda^2 \|\boldsymbol{x}\|_2^2$$

where $\boldsymbol{x} \in \mathbb{R}^n$, $A \in \mathbb{R}^{m \times n}$, $m \geq n$, is full rank, $\boldsymbol{b} \in \mathbb{R}^m$, and $\lambda > 0$.

Let us consider the way that this expression may be re-written:

$$\boldsymbol{x}_\lambda = \min_{\boldsymbol{x}} \left\| \begin{bmatrix} A \\ \lambda \mathbb{I}_n \end{bmatrix} \boldsymbol{x} - \begin{bmatrix} \boldsymbol{b} \\ \boldsymbol{0} \end{bmatrix} \right\|_2^2$$

Now, we perform a similar method to that covered in class, which is outlined on the following page:

Consider $\min_{\boldsymbol{x}} \|A\boldsymbol{x} - \boldsymbol{b}\|_2^2$ where $A \in \mathbb{R}^{m\times n}, \boldsymbol{x} \in \mathbb{R}^n, \boldsymbol{b} \in \mathbb{R}^m, m \geq n$. A is assumed to be full rank.

$$\begin{aligned}
&\min_{\boldsymbol{x}} \left((A\boldsymbol{x} - \boldsymbol{b})^T (A\boldsymbol{x} - \boldsymbol{b}) \right) \\
&\min_{\boldsymbol{x}} \left(\left(\boldsymbol{x}^T A^T - \boldsymbol{b}^T\right) (A\boldsymbol{x} - \boldsymbol{b}) \right) \\
&\min_{\boldsymbol{x}} \left(\boldsymbol{x}^T A^T A\boldsymbol{x} - \boldsymbol{b}^T A\boldsymbol{x} - \boldsymbol{x}^T A^T \boldsymbol{b} + \boldsymbol{b}^T\boldsymbol{b} \right) \\
&\min_{\boldsymbol{x}} \left(\boldsymbol{x}^T A^T A\boldsymbol{x} - \boldsymbol{b}^T A\boldsymbol{x} - \boldsymbol{x}^T A^T \boldsymbol{b} \right) \\
&\min_{\boldsymbol{x}} \left(\boldsymbol{x}^T A^T A\boldsymbol{x} - 2\boldsymbol{x}^T A^T \boldsymbol{b} \right)
\end{aligned}$$

Recall that for a given $f(\boldsymbol{x})$,

$$\nabla f(\boldsymbol{x}) = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \cdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}$$

We have $\nabla \left(\boldsymbol{x}^T A^T A\boldsymbol{x}\right)$. Let $G = A^T A$.

$$\begin{aligned}
\nabla \left(\boldsymbol{x}^T G\boldsymbol{x}\right) &= \nabla \left(\begin{pmatrix} x_1, \ldots, x_n \end{pmatrix} \begin{pmatrix} g_{1,1}, \ldots, g_{1,n} \\ \cdots \quad \cdots \quad \cdots \\ g_{n,1}, \ldots, g_{n,n} \end{pmatrix} \begin{pmatrix} x_1 \\ \cdots \\ x_n \end{pmatrix} \right) \\
&= 2A^T A\boldsymbol{x}
\end{aligned}$$

Similarly, we have the following:

$$\nabla \left(2\boldsymbol{x}^T A^T \boldsymbol{b}\right) = 2A^T\boldsymbol{b}$$

Setting the gradient of the initial expression equal to zero, we find the following:

$$\begin{aligned}
2A^T A\boldsymbol{x} &= 2A^T\boldsymbol{b} \\
A^T A\boldsymbol{x} &= A^T\boldsymbol{b} \\
\boldsymbol{x} &= \left(A^T A\right)^{-1} A^T\boldsymbol{b}
\end{aligned}$$

Using this method, we may determine the solution $\boldsymbol{x}_\lambda$ as follows:

$$\boldsymbol{x}_\lambda = \min_{\boldsymbol{x}} \left(\boldsymbol{x}^T A^T A\boldsymbol{x} - 2\boldsymbol{x}^T A^T\boldsymbol{b} + \lambda^2 \boldsymbol{x}^T\boldsymbol{x} \right)$$

By taking $\nabla f(\boldsymbol{x})$ and setting it equal to zero, we find the following:

$$2A^T A\boldsymbol{x}_\lambda - 2A^T\boldsymbol{b} + 2\lambda^2\boldsymbol{x}_\lambda = \boldsymbol{0}$$

Now, we may solve for the solution to the Tikhonov regularization problem, $\boldsymbol{x}_\lambda$.

$$2A^T A\boldsymbol{x}_\lambda - 2A^T\boldsymbol{b} + 2\lambda^2\boldsymbol{x}_\lambda = \boldsymbol{0}$$

$$\begin{aligned}
\left(A^T A - \lambda^2\mathbb{I}_n\right)\boldsymbol{x}_\lambda - A^T\boldsymbol{b} &= \boldsymbol{0} \\
\left(A^T A - \lambda^2\mathbb{I}_n\right)\boldsymbol{x}_\lambda &= A^T\boldsymbol{b}
\end{aligned}$$

At this point, we may take the inverse to find the solution, as expected:

$$\boldsymbol{x}_\lambda = \left(A^T A - \lambda^2\mathbb{I}_n\right)^{-1} A^T\boldsymbol{b}$$

2) Suppose we have a random variable $\boldsymbol{\varepsilon} \in \mathbb{R}^n$ such that the elements ε_i, $i = 1, \ldots, n$ are each uniformly distributed on the interval $\left[-\eta\sqrt{3}, \eta\sqrt{3}\right]$, where $\eta > 0$. Prove that $\boldsymbol{\varepsilon}$ is white noise, i.e. show

$$\operatorname{cov}(\boldsymbol{\varepsilon}) = \eta^2 \mathbb{I}_n$$

When solving problems with real, measured data, there may be a component of noise. When dealing with a discrete problem $A\boldsymbol{x} = \boldsymbol{b}$, the "perturbation" of the right hand side takes the form of noise (more or less random variations caused by measurement errors, etc).

In this case, the random variable $\boldsymbol{\varepsilon} \in \mathbb{R}^n$ includes elements ε_i, $i = 1, \ldots, n$ that are each uniformly distributed on the interval $\left[-\eta\sqrt{3}, \eta\sqrt{3}\right]$, where $\eta > 0$. Given that $E[\boldsymbol{x}]$ represents the "expected value" of a variable, the covariance may be defined as follows:

$$\operatorname{cov}(\boldsymbol{x}) = E\left[(\boldsymbol{x} - E[\boldsymbol{x}])(\boldsymbol{x} - E[\boldsymbol{x}])^T\right]$$

Now, as each ε_i is *uniformly* distributed on the interval $\left[-\eta\sqrt{3}, \eta\sqrt{3}\right]$, we know $E[\varepsilon_i] = 0$ (for $i = 1, \ldots, n$), and thus $E[\boldsymbol{\varepsilon}] = \mathbf{0}$. This is because the interval has an average value of zero ($\mu = 0$, as the interval is "centered" around zero).

Hence, we may observe the following:

$$\operatorname{cov}(\boldsymbol{\varepsilon}) = E\left[(\boldsymbol{\varepsilon} - E[\boldsymbol{\varepsilon}])(\boldsymbol{\varepsilon} - E[\boldsymbol{\varepsilon}])^T\right] = E\left[\boldsymbol{\varepsilon}\boldsymbol{\varepsilon}^T\right]$$

To represent the covariance in matrix form, let us consider the different rows and columns of the matrix, say M. For $i, j = 1, \ldots n$, we have the following:

$$M_{i,j} = E[\varepsilon_i \varepsilon_j]$$

In the case where $i \neq j$, the entry in the matrix M is zero. Given that ε_i and ε_j are independent, alongside the previous assumption that $E[\varepsilon_i] = 0$, the expected value may be written as follows.

$$E[\varepsilon_i \varepsilon_j] = E[\varepsilon_i] E[\varepsilon_j] = 0$$

In the case where $i = j$, the entry in the matrix M is η^2. This will be demonstrated as follows. We start with the following:

$$M_{i,i} = E\left[\varepsilon_i^2\right]$$

From this point, we may apply the integral definition of expected value, as follows:

$$M_{i,i} = \int_{-\infty}^{\infty} \varepsilon_i^2 \pi(\varepsilon_i)\, d\varepsilon_i$$

In this expression $\pi(\varepsilon_i) = 1$ represents the probability density function. Given that the random variable $\boldsymbol{\varepsilon} \in \mathbb{R}^n$ is uniformly distributed on the interval $\left[-\eta\sqrt{3}, \eta\sqrt{3}\right]$, this may be expressed using the following form (a and b represent the interval bounds):

$$\frac{1}{b-a} \int_a^b \varepsilon_i^2 \, d\varepsilon_i$$

Thus, we have the following:

$$
\begin{aligned}
M_{i,i} &= \frac{1}{2\eta\sqrt{3}} \int_{-\eta\sqrt{3}}^{\eta\sqrt{3}} \varepsilon_i^2 \, d\varepsilon_i \\
&= \frac{1}{2\eta\sqrt{3}} \left[\frac{1}{3}\varepsilon_i^3\right]_{-\eta\sqrt{3}}^{\eta\sqrt{3}} \\
&= \eta^2
\end{aligned}
$$

As such, the diagonal elements of the matrix M are given as η^2, so the covariance matrix for $\boldsymbol{\varepsilon}$ is the scaled identity matrix. This demonstrates that $\boldsymbol{\varepsilon}$ is white noise, i.e. $\operatorname{cov}(\boldsymbol{\varepsilon}) = \eta^2 \mathbb{I}_n$. $\square$

Aside: The book mentions that a white-noise vector $\boldsymbol{\varepsilon}$ is not required to have elements from a Gaussian distribution. The requirement is that $cov(\boldsymbol{\varepsilon}) = \eta^2 \mathbb{I}_n$. This is the case if the elements ε_i of $\boldsymbol{\varepsilon}$ are uncorrelated and from the same uniform distribution in the interval $\left[-\eta\sqrt{3}, \eta\sqrt{3}\right]$.

3) Suppose $\boldsymbol{x} \in \mathbb{R}^n$, $A \in \mathbb{R}^{m\times n}$, $m \geq n$, is full rank, $\boldsymbol{b} \in \mathbb{R}^m$, $\lambda > 0$, and $\boldsymbol{x}_0 \in \mathbb{R}^n$. Consider the generalized Tikhonov minimization problem given by

$$\boldsymbol{x}^* = \min_{\boldsymbol{x}} \|A\boldsymbol{x} - \boldsymbol{b}\|_2^2 + \lambda^2 \|\boldsymbol{x} - \boldsymbol{x}_0\|_2^2$$

Find the solution $\boldsymbol{x}^*$ to the above.

To find the solution $\boldsymbol{x}^*$, let us start with the generalized Tikhonov minimization problem, given by

$$\boldsymbol{x}^* = \min_{\boldsymbol{x}} \|A\boldsymbol{x} - \boldsymbol{b}\|_2^2 + \lambda^2 \|\boldsymbol{x} - \boldsymbol{x}_0\|_2^2$$

To express this as a singular norm, let us consider the method used previously to express the Tikhonov regularization problem. Recall the following:

> Suppose $\boldsymbol{x} \in \mathbb{R}^n$, $A \in \mathbb{R}^{m\times n}$, $m \geq n$, is full rank, $\boldsymbol{b} \in \mathbb{R}^m$, and $\lambda > 0$. The Tikhonov regularization problem is given as
>
> $$\boldsymbol{x}_\lambda = \min_{\boldsymbol{x}} \|A\boldsymbol{x} - \boldsymbol{b}\|_2^2 + \lambda^2 \|\boldsymbol{x}\|_2^2$$
>
> In class, we discussed how this can be re-written as
>
> $$\boldsymbol{x}_\lambda = \min_{\boldsymbol{x}} \left\| \begin{bmatrix} A \\ \lambda \mathbb{I}_n \end{bmatrix} \boldsymbol{x} - \begin{bmatrix} \boldsymbol{b} \\ \boldsymbol{0} \end{bmatrix} \right\|_2^2$$
>
> Prove that the solution is
>
> $$\boldsymbol{x}_\lambda = \left(A^T A + \lambda^2 \mathbb{I}_n\right)^{-1} A^T \boldsymbol{b}$$
>
> *Hint: Find the associated normal equations.*

Now, we may apply a similar method to re-write the generalized Tikhonov minimization problem. Given $\boldsymbol{x} \in \mathbb{R}^n$, $A \in \mathbb{R}^{m\times n}$, $m \geq n$, is full rank, $\boldsymbol{b} \in \mathbb{R}^m$, $\lambda > 0$, and $\boldsymbol{x}_0 \in \mathbb{R}^n$,

$$\begin{aligned}
\boldsymbol{x}^* &= \min_{\boldsymbol{x}} \|A\boldsymbol{x} - \boldsymbol{b}\|_2^2 + \lambda^2 \|\boldsymbol{x} - \boldsymbol{x}_0\|_2^2 \\
&= \min_{\boldsymbol{x}} \|A\boldsymbol{x} - \boldsymbol{b}\|_2^2 + \|\lambda\left(\boldsymbol{x} - \boldsymbol{x}_0\right)\|_2^2 \\
&= \min_{\boldsymbol{x}} \left\| \begin{bmatrix} A\boldsymbol{x} - \boldsymbol{b} \\ \lambda\left(\boldsymbol{x} - \boldsymbol{x}_0\right) \end{bmatrix} \right\|_2^2 = \min_{\boldsymbol{x}} \left\| \begin{bmatrix} A\boldsymbol{x} - \boldsymbol{b} \\ \lambda\boldsymbol{x} - \lambda\boldsymbol{x}_0 \end{bmatrix} \right\|_2^2 \\
&= \min_{\boldsymbol{x}} \left\| \begin{bmatrix} A \\ \lambda \mathbb{I}_n \end{bmatrix} \boldsymbol{x} - \begin{bmatrix} \boldsymbol{b} \\ \lambda\boldsymbol{x}_0 \end{bmatrix} \right\|_2^2
\end{aligned}$$

At this point, we mirror the steps taken to solve the Tikhonov regularization problem in Q1. Recall that for $\min_{\boldsymbol{x}} \|A\boldsymbol{x} - \boldsymbol{b}\|_2^2$, the normal equations are $A^T A\boldsymbol{x} = A^T\boldsymbol{b}$. Thus,

$$\begin{bmatrix} A \\ \lambda \mathbb{I}_n \end{bmatrix}^T \begin{bmatrix} A \\ \lambda \mathbb{I}_n \end{bmatrix} \boldsymbol{x}^* = \begin{bmatrix} A \\ \lambda \mathbb{I}_n \end{bmatrix}^T \begin{bmatrix} \boldsymbol{b} \\ \lambda\boldsymbol{x}_0 \end{bmatrix}$$

By expanding the terms and taking the inverse, this implies the following:

$$\left(A^T A + \lambda^2 \mathbb{I}_n\right) \boldsymbol{x}^* = \left(A^T\boldsymbol{b} + \lambda^2 \boldsymbol{x}_0\right) \qquad \to \qquad \boldsymbol{x}^* = \left(A^T A + \lambda^2 \mathbb{I}_n\right)^{-1} \left(A^T\boldsymbol{b} + \lambda^2 \boldsymbol{x}_0\right)$$

Describe a situation in which this may be a more desirable objective function than the regular Tikhonov solution.

The generalized Tikhonov minimization problem given by

$$\boldsymbol{x}^* = \min_{\boldsymbol{x}} \|A\boldsymbol{x} - \boldsymbol{b}\|_2^2 + \lambda^2 \|\boldsymbol{x} - \boldsymbol{x}_0\|_2^2$$

where $\boldsymbol{x} \in \mathbb{R}^n$, $A \in \mathbb{R}^{m \times n}$, $m \geq n$, is full rank, $\boldsymbol{b} \in \mathbb{R}^m$, $\lambda > 0$, and $\boldsymbol{x}_0 \in \mathbb{R}^n$ may be a more desirable objective function than the regular Tikhonov solution in the case where we aim to encourage solutions of $\boldsymbol{x}$ close to the chosen value of $\boldsymbol{x}_0$.

In other words, the regular Tikhonov solution is a specific case of the generalized Tikhonov minimization solution, with $\boldsymbol{x}_0 = 0$. In the regular Tikhonov case, the term $\|\boldsymbol{x}\|_2^2$ measures regularity of the solution, with λ as the regularization parameter than controls the weighting. Specifically, the regularization ensures that values of $\boldsymbol{x}$ close to zero (small values) are considered.

By changing x_0 to be non-zero, the Tikhonov solution encourages solutions of $\boldsymbol{x}$ close to the chosen value of $\boldsymbol{x}_0$.

Perhaps this would be useful when we know the solution $\boldsymbol{x}$ should be close to $\boldsymbol{x}_0$, yet we still aim to consider goodness of fit (according to the data), using the term $\|A\boldsymbol{x} - \boldsymbol{b}\|_2^2$. The regularization parameter $\lambda > 0$ allows us to control these objectives, given the different components of the model for the data.

4) Zou and Hastie, in their 2005 paper *Regularization and Variable Selection via the Elastic Net*, introduced the elastic net minimization problem. The elastic net can be seen as a sort of generalization of the L1 regularization problem, and it is given as

$$\boldsymbol{x}^\star = \min_{\boldsymbol{x}} \|A\boldsymbol{x} - \boldsymbol{b}\|_2^2 + \lambda_1\|\boldsymbol{x}\|_1 + \lambda_2\|\boldsymbol{x}\|_2^2$$

where $A \in \mathbb{R}^{m\times n}$, $\boldsymbol{x} \in \mathbb{R}^n$, $b \in \mathbb{R}^m$, and $\lambda_1, \lambda_2 > 0$.

In the original work, a few reasons were given as to why one may want to use the elastic net formulation instead of the classic L1 regularization problem. Please summarize one of these reasons in your own words.

The 2005 paper *Regularization and Variable Selection via the Elastic Net* by Zou and Hastie proposes the elastic net, a new regularization and variable selection method.

According to the paper, "real world data and a simulation study show that the elastic net often outperforms the lasso while enjoying a similar sparsity of representation." Further, the paper states that the elastic net "encourages a grouping effect, where strongly correlated predictors tend to be in or out of the model together."

The limitations of the lasso are provided as follows:

- "In the $p > n$ case, the lasso selects at most n variables before it saturates, because of the nature of the convex optimization problem."
  - "This seems to be a limiting feature for a variable selection method."
  - "Moreover, the lasso is not well-defined unless the bound on the L1 norm of coefficients is smaller than a certain value."
- "If there is a group of variables among which the pairwise correlations are very high, then the lasso tends to select only one variable from the group and does not care which one is selected."
- "For usual $n > p$ situations, if there are high correlations between predictors, it has been empirically observed that the prediction performance of the lasso is dominated by ridge regression."

In other words, the elastic net formulation eliminates the limitations of the classic L1 regularization problem.

By allowing for the grouping of highly-correlated variables, the elastic net formulation (instead of the classic L1 regularization problem) encourages applications involving characteristics that are closely related.

Further, in situations where there are relatively few observations compared to the number of predictors, the elastic net formulation is superior in accuracy to the lasso as a variable selection method.

Show how the elastic net can be re-written as a classic L1 regularization problem, i.e. find $\tilde{A}$, $\tilde{\boldsymbol{b}}$, and $\tilde{\lambda}$ such that

$$\boldsymbol{x}^\star = \min_{\boldsymbol{x}} \left\| \tilde{A}\boldsymbol{x} - \tilde{b} \right\|_2^2 + \tilde{\lambda}\|\boldsymbol{x}\|_1$$

The elastic net minimization problem (as a sort of generalization of the L1 regularization problem) is given as

$$\boldsymbol{x}^\star = \min_{\boldsymbol{x}} \|A\boldsymbol{x} - \boldsymbol{b}\|_2^2 + \lambda_1\|\boldsymbol{x}\|_1 + \lambda_2\|\boldsymbol{x}\|_2^2$$

where $A \in \mathbb{R}^{m\times n}$, $\boldsymbol{x} \in \mathbb{R}^n$, $\boldsymbol{b} \in \mathbb{R}^m$, and $\lambda_1, \lambda_2 > 0$.

To express this as a classic L1 regularization problem, let us consider the method used previously to express the Tikhonov regularization problem. Recall the following:

> Suppose $\boldsymbol{x} \in \mathbb{R}^n$, $A \in \mathbb{R}^{m\times n}$, $m \geq n$, is full rank, $\boldsymbol{b} \in \mathbb{R}^m$, and $\lambda > 0$. The Tikhonov regularization problem is given as
>
> $$\boldsymbol{x}_\lambda = \min_{\boldsymbol{x}} \|A\boldsymbol{x} - \boldsymbol{b}\|_2^2 + \lambda^2\|\boldsymbol{x}\|_2^2$$
>
> In class, we discussed how this can be re-written as
>
> $$\boldsymbol{x}_\lambda = \min_{\boldsymbol{x}} \left\| \begin{bmatrix} A \\ \lambda\mathbb{I}_n \end{bmatrix} \boldsymbol{x} - \begin{bmatrix} \boldsymbol{b} \\ \boldsymbol{0} \end{bmatrix} \right\|_2^2$$

Now, we may apply a similar method to re-write the elastic net as a classic L1 regularization problem. Given $A \in \mathbb{R}^{m\times n}$, $\boldsymbol{x} \in \mathbb{R}^n$, $\boldsymbol{b} \in \mathbb{R}^m$, and $\lambda_1, \lambda_2 > 0$.

$$\begin{aligned} \boldsymbol{x}^\star &= \min_{\boldsymbol{x}} \|A\boldsymbol{x} - \boldsymbol{b}\|_2^2 + \lambda_1\|\boldsymbol{x}\|_1 + \lambda_2\|\boldsymbol{x}\|_2^2 \\ &= \min_{\boldsymbol{x}} \left\| \begin{bmatrix} A \\ \sqrt{\lambda_2}\mathbb{I}_n \end{bmatrix} \boldsymbol{x} - \begin{bmatrix} \boldsymbol{b} \\ \boldsymbol{0} \end{bmatrix} \right\|_2^2 + \lambda_1\|\boldsymbol{x}\|_1 \end{aligned}$$

Thus, we are able to find $\tilde{A}$, $\tilde{\boldsymbol{b}}$, and $\tilde{\lambda}$ such that

$$\boldsymbol{x}^\star = \min_{\boldsymbol{x}} \left\| \tilde{A}\boldsymbol{x} - \tilde{\boldsymbol{b}} \right\|_2^2 + \tilde{\lambda}\|\boldsymbol{x}\|_1$$

The following values are the solution:

$$\tilde{A} = \begin{bmatrix} A \\ \sqrt{\lambda_2}\mathbb{I}_n \end{bmatrix} \qquad \tilde{\boldsymbol{b}} = \begin{bmatrix} \boldsymbol{b} \\ \boldsymbol{0} \end{bmatrix} \qquad \tilde{\lambda} = \lambda_1$$

Computational Questions

View *Matlab* Code