Numerical Analysis and Optimization
Academic Year 2021-2022

Numerical Linear Algebra Homework Project 2: Least Squares, Orthogonalization, and the SVD

Problem 1

The following problem frequently arises in the fitting of experimental data, and in the approximation of a given function. Suppose we are given m pairs of data points $(x_1, y_1), (x_2, y_2), \dots, (x_m, y_m)$. The problem of discrete approximation (in the least squares sense) is to find a linear combination of prescribed functions $\phi_1, \phi_2, \dots, \phi_n$ whose values at the points $x_i \in [a, b]$, $1 \le i \le m$, approximate the values $y_1, y_2, \dots, y_m$ as well as possible. More precisely, the problem is to find a function of the form $f(x) = \alpha_1\phi_1(x) + \cdots + \alpha_n\phi_n(x)$ such that

$$\sum_{i=1}^{m}[y_i - f(x_i)]^2 \le \sum_{i=1}^{m}[y_i - g(x_i)]^2 \tag{1}$$

for all functions $g \in \mathrm{Span}(\phi_1, \phi_2, \dots, \phi_n)$.

Note that usually the number m of "observations" (x_i, y_i) is (much) greater than the number n of basis functions ϕ_k used to approximate the data. In the remainder we assume $m > n$.

1. Formulate problem (1) as a linear least squares problem. That is, find a matrix $A = (a_{ij}) \in \mathbb{R}^{m\times n}$ and a right-hand side vector $\mathbf{b} \in \mathbb{R}^m$ such that problem (1) can be written as

$$\|\mathbf{b} - A\mathbf{x}\|_2 = \min$$

   where $\mathbf{x} = [\alpha_1\, \alpha_2\, \dots\, \alpha_n]^T$.

2. Suppose now that we take $\phi_k(x) = x^{k-1}$, $1 \le k \le n$. Write A out explicitly (the resulting matrix is called a *Vandermonde-type* matrix). Assuming that $x_i \ne x_j$ for $i \ne j$, show that A has full rank: $\mathrm{rank}(A) = n$. (**Hint**: Use the fact that a nonzero polynomial of degree n cannot have more than n roots).

3. Consider the problem of finding the best fit with a quadratic function $f(x) = \alpha_1 + \alpha_2 x + \alpha_3 x^2$ for the following data:

x_i	8	10	12	16	20	30	40	60	100
y_i	0.88	1.22	1.64	2.72	3.96	7.66	11.96	21.56	43.16

   Write a Matlab code that solves the corresponding least squares problem in two ways, first by solving the normal equations and then by (pivoted) QR factorization. The code should first form the matrices A and $C = A^TA$ and the right-hand sides $\mathbf{b}$ and $\mathbf{d} = A^T\mathbf{b}$; then the Cholesky algorithm should be used to solve $C\mathbf{x} = \mathbf{d}$. Use `chol` to compute the Cholesky factorization of C and `format long` to display the computed solution with 15 digits. Next, compute the solution using the pivoted QR factorization: this is just the backslash operator applied to the overdetermined system $A\mathbf{x} = \mathbf{b}$. Plot the data points and the graph of the quadratic approximation in a Matlab (x,y)-plot. Finally, compare the results obtained with the two approaches.

4. A good approximate solution $\hat{\mathbf{x}}$ of the previous problem is given by $\hat{\alpha}_1 = -1.919$, $\hat{\alpha}_2 = 0.2782$, and $\hat{\alpha}_3 = 0.001739$. Compute the residual $\mathbf{r} = \mathbf{d} - C\hat{\mathbf{x}}$ corresponding to this approximate solution. Explain your finding. **Hint**: use the fact that

$$\kappa^{-1}\frac{\|\mathbf{r}\|_2}{\|\mathbf{d}\|_2} \le \frac{\|\mathbf{x} - \hat{\mathbf{x}}\|_2}{\|\mathbf{x}\|_2} \le \kappa\frac{\|\mathbf{r}\|_2}{\|\mathbf{d}\|_2} \tag{2}$$

   where $\kappa := \|C\|_2\|C^{-1}\|_2$. Here C is any nonsingular $n \times n$ matrix and $\hat{\mathbf{x}}$ is an approximate solution to $C\mathbf{x} = \mathbf{d}$. Keep in mind that equality is possible on either side of (2).

Problem 2

1. Let $A \in \mathbb{R}^{m\times n}$, with $\mathrm{rank}(A) = n$, let $A = QR$ be the (full) QR factorization of A, with $Q \in \mathbb{R}^{m\times m}$ orthogonal and $R \in \mathbb{R}^{m\times n}$ upper trapezoidal. Also, let $A = Q_1R_1$ be the reduced QR factorization of A with $Q_1 \in \mathbb{R}^{m\times n}$ having orthonormal columns and $R_1 \in \mathbb{R}^{m\times m}$ upper triangular. Show that R_1 is nonsingular, and that the columns $\mathbf{q}_1 \ldots, \mathbf{q}_n$ of Q_1 form an orthonormal basis for $\mathrm{Ran}(A)$, the column space of A. Also, find an orthonormal basis for $\mathrm{Null}(A^T)$, the null space of A^T.

2. Use $\beta = 10$ and $t = 3$ digit arithmetic to compute (by hand) A^TA where

$$A = \begin{bmatrix} 1.07 & 1.10 \\ 1.07 & 1.11 \\ 1.07 & 1.15 \end{bmatrix}.$$

   Note that A has full rank. Is the computed A^TA positive definite?

3. Now use $\beta = 10$ and $t = 3$ digit arithmetic to compute (by hand) the QR factorization of the same matrix A by means of Householder transformations. Be as efficient as possible. Discuss your results.

4. Let $A \in \mathbb{R}^{m\times n}$, with $\mathrm{rank}(A) = n$, and let $\mathbf{b} \in \mathbb{R}^m$. Let $A = Q_1R_1$ be a reduced QR decomposition of A, where $Q_1 \in \mathbb{R}^{m\times n}$ has orthonormal columns and $R_1 \in \mathbb{R}^{n\times n}$ is upper triangular and nonsingular. Show that a reduced QR factorization of the augmented matrix $A_+ = [\,A \quad \mathbf{b}\,]$ is given by

$$A_+ = [\,Q_1 \quad \mathbf{q}_{n+1}\,] \begin{bmatrix} R_1 & \mathbf{z} \\ 0 & \rho \end{bmatrix}$$

   where $\mathbf{z} = Q_1^T\mathbf{b}$. Also, show that $|\rho| = \|\mathbf{b} - A\mathbf{x}^*\|_2$ where $\mathbf{x}^*$ is the solution to the least squares problem $\|\mathbf{b} - A\mathbf{x}\|_2 = \min$.

Problem 3

1. Let $A \in \mathbb{R}^{m\times n}$, with singular value decomposition $A = U\Sigma V^T$ and $\mathrm{rank}(A) = n$. Express the singular values and singular vectors of the following matrices in terms of those of A:
   (a) $(A^TA)^{-1}$,
   (b) $(A^TA)^{-1}A^T$,
   (c) $A(A^TA)^{-1}$,
   (d) $A(A^TA)^{-1}A^T$.

2. Let

$$A = \begin{bmatrix} 1 & 2 \\ 0 & 2 \end{bmatrix}.$$

   Compute (by hand) the singular values of A and the spectral condition number $\kappa_2(A)$. Also, draw the image of the unit ball (here it's just the unit circle) under the linear transformation $\mathbf{y} = A\mathbf{x}$.

3. Let

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix} \quad \text{and} \quad \mathbf{b} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}.$$

   Find the minimum norm solution to $\|\mathbf{b} - A\mathbf{x}\|_2 = \min$.

4. Let

$$A = \begin{bmatrix} -4 & -2 & -4 & -2 \\ 2 & -2 & 2 & 1 \\ -800 & 200 & -800 & -401 \end{bmatrix}.$$

   Using Matlab, determine the singular values of A, the rank of A, and the Moore-Penrose pseudoinverse A^+. Also, compute $\kappa_2(A)$.

5. For the matrix A in the previous problem, determine the best rank-1 and rank-2 approximations of A, denoted A_1 and A_2. What is $\kappa_2(A_2)$?

6. Let $R = (r_{ij})$ be the $n \times n$ upper triangular matrix with $r_{ii} = 1$ and $r_{ij} = -1$ for $j > i$. Plot the singular values of R for $n = 10$, $n = 20$, $n = 50$ and $n = 100$. Also, tabulate the spectral condition number $\kappa_2(R)$ for all n from 1 to 60. What can be said about the numerical rank of R as n grows?

Instructions:

- The use of Matlab is highly recommended, but not mandatory.
- Only neatly typed assignments will be accepted (preferably using LaTeX). Include tables and plots whenever appropriate, as well as a copy of all your scripts and the output of your runs. Make sure plots are readable, if necessary rescaling the axes or using (semi-)logarithmic scales.