Mathematics 327
SVD and least squares

Today we'll investigate how to solve least squares problems using singular value decompositions. Remember how this works: if we have an equation $A\mathbf{x} = \mathbf{b}$ that is inconsistent, we orthogonally project $\mathbf{b}$ onto $\mathrm{Col}(A)$ to obtain $\widehat{\mathbf{b}}$. We say that the least squares approximate solution to $A\mathbf{x} = \mathbf{b}$ is the vector $\widehat{\mathbf{x}}$ that satisfies $A\widehat{\mathbf{x}} = \widehat{\mathbf{b}}$.

1. Suppose that A is a matrix whose singular value decomposition is $A = U\Sigma V^T$ where $\Sigma = \begin{bmatrix} 5 & 0 \\ 0 & 2 \\ 0 & 0 \end{bmatrix}$.

   What are the dimensions of the matrices A, U and V?

   What is $\mathrm{rank}(A)$?

   Let's write $U = \begin{bmatrix} \mathbf{u}_1 & \mathbf{u}_2 & \mathbf{u}_3 \end{bmatrix}$. Which vectors of U form a basis for the column space of A?

   Form a matrix Q whose vectors form an orthonormal basis for $\mathrm{Col}(A)$. How is Q obtained from U?

   Think back to earlier in the course and explain the signficance of the matrices QQ^T and Q^TQ?

Explain why the least squares approximate solution to $A\mathbf{x} = \mathbf{b}$, satisfies $A\widehat{\mathbf{x}} = QQ^T\mathbf{b}$.

We will also form the matrix $\widehat{\Sigma}$, which is obtained from Σ by removing the bottom rows of zeroes:

$$\widehat{\Sigma} = \begin{bmatrix} 5 & 0 \\ 0 & 2 \end{bmatrix}.$$

What is Σ^{-1}?

Write the product $U\Sigma$ in terms of the columns of U. Then explain why $U\Sigma = Q\widehat{\Sigma}$.

Now we have $A = U\Sigma V^T = Q\widehat{\Sigma}V^T$ so that $A\widehat{\mathbf{x}} = QQ^T\mathbf{b}$ becomes

$$Q\widehat{\Sigma}V^T\widehat{\mathbf{x}} = QQ^T\mathbf{b}.$$

Multiply both sides of this equation on the left by Q^T and explain why $\widehat{\Sigma}V^T\widehat{\mathbf{x}} = Q^T\mathbf{b}$.

Explain why the least squares approximate solution of $A\mathbf{x} = \mathbf{b}$ is

$$\widehat{\mathbf{x}} = V\widehat{\Sigma}^{-1}Q^T\mathbf{b}.$$

2. Sage interlude: you can find the singular value decomposition of a matrix `A` using `A.SVD()`. One catch, however, is that you need to declare the matrix `A` to be a floating point matrix. You can do this with

   ```
   A = matrix(RDF, 2, 2, [1,2,2,1])
   ```

   where we have added `RDF` to tell Sage to interpret the matrix as floating point. You may ask Sage to store the results by saying

   ```
   U, Sigma, V = A.SVD()
   ```

   Remember that, if `M` is a matrix, you also have commands

   ```
   M.matrix_from_columns(list)
   ```

   ```
   M.matrix_from_rows(list).
   ```

3. Suppose that we would like to find the least squares approximate solution to $A\mathbf{x} = \mathbf{b}$ where

$$A = \begin{bmatrix} 1 & 4 \\ -3 & 3 \\ 5 & 1 \end{bmatrix}, \qquad \mathbf{b} = \begin{bmatrix} -16 \\ 28 \\ 6 \end{bmatrix}.$$

   Find the singular value decomposition of A.

   Find the matrices Q and $\widehat{\Sigma}$.

   Find the least squares approximate solution $\widehat{\mathbf{x}} = V\widehat{\Sigma}^{-1}Q^T\mathbf{b}$.

4. Find the line $y = \beta_0 + \beta_1 x$ that comes closest to passing through the points $(1, 1)$, $(2, 1)$, and $(3, 3)$ using a singular value decomposition.