CS 450: Numerical Analysis
Linear Least Squares

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1 These slides have been drafted by Edgar Solomonik as lecture templates and supplementary material for the book “Scientific Computing: An Introductory Survey” by Michael T. Heath (slides).
Linear Least Squares

- Find $x^* = \arg\min_{x \in \mathbb{R}^n} ||Ax - b||_2$ where $A \in \mathbb{R}^{m \times n}$:

  Since $m \geq n$, the minimizer generally does not attain a zero residual $Ax - b$.

  We can rewrite the optimization problem constraint via

  $$x^* = \arg\min_{x \in \mathbb{R}^n} ||Ax - b||_2^2 = \arg\min_{x \in \mathbb{R}^n} (Ax - b)^T(Ax - b)$$

- Given the SVD $A = U \Sigma V^T$ we have $x^* = V \Sigma^\dagger U^T b$, where $\Sigma^\dagger$ contains the reciprocal of all nonzeros in $\Sigma$

  >> The minimizer satisfies $U \Sigma V^T x^* \cong b$ and consequently also satisfies

  $$\Sigma y^* \cong d \text{ where } y^* = V^T x^* \text{ and } d = U^T b.$$  

  >> The minimizer of the reduced problem is $y^* = \Sigma^\dagger d$, so $y_i = d_i/\sigma_i$ for $i \in \{1, \ldots, n\}$ and $y_i = 0$ for $i \in \{n + 1, \ldots, m\}$.  


Consider fitting a line to a collection of points, then perturbing the points:

- If our line closely fits all of the points, a small perturbation to the points will not change the ideal fit line (least squares solution) much. Note that, if a least squares solution has a very small residual, any other solution with a residual close to as small, should be close to parallel to this solution.
- When the points are distributed erratically and do not admit a reasonable linear fit, then the least squares solution has a large residual, and totally different lines may exist with a residual nearly as small. For example, if the points are in a ball around the origin, any linear fit has the same residual. A tiny perturbation could then perturb the least squares solution to be perpendicular to the original.

LLS is ill-posed for any $A$, unless we consider solving for a particular $b$.

- If $b$ is entirely outside the span of $A$ then any perturbation to $A$ or $b$ can completely defines the new solution. Similarly, if most of $b$ is outside the span of $A$, a perturbation can cause the solution to fluctuate wildly.
- On other hand, if for a particular $b$ we can find a solution with (near-)zero residual, a small relative perturbation to $b$ or $A$ will have an effect similar to that of a linear system perturbation (growth bounded by $\kappa(A) = \sigma_{\text{max}}/\sigma_{\text{min}}$).

Demo: Polynomial fitting via the normal equations
Normal Equations

- Normal equations are given by solving $A^T Ax = A^T b$:
  
  If $A^T Ax = A^T b$ then
  
  
  $$(U\Sigma V^T)^T U \Sigma V^T x = (U\Sigma V^T)^T b$$
  
  $$\Sigma^T \Sigma V^T x = \Sigma^T U^T b$$
  
  $$V^T x = (\Sigma^T \Sigma)^{-1} \Sigma^T U^T b = \Sigma^\dagger U^T b$$
  
  $$x = V \Sigma^\dagger U^T b = x^*$$

- However, solving the normal equations is a more ill-conditioned problem than the original least squares algorithm

  Generally we have $\kappa(A^T A) = \kappa(A)^2$ (the singular values of $A^T A$ are the squares of those in $A$). Consequently, solving the least squares problem via the normal equations may be unstable because it involves solving a problem that has worse conditioning than the initial least squares problem.
If $A$ is full-rank, then $A^T A$ is symmetric positive definite (SPD):

- Symmetry is easy to check $(A^T A)^T = A^T A$.
- $A$ being full-rank implies $\sigma_{\text{min}} > 0$ and further if $A = U \Sigma V^T$ we have
  \[ A^T A = V^T \Sigma^2 V \]
  which implies that rows of $V$ are the eigenvectors of $A^T A$ with eigenvalues $\Sigma^2$ since $A^T A V^T = V^T \Sigma^2$.

Since $A^T A$ is SPD we can use Cholesky factorization, to factorize it and solve linear systems:

\[ A^T A = LL^T \]
QR Factorization

- If \( A \) is full-rank there exists an orthogonal matrix \( Q \) and a unique upper-triangular matrix \( R \) with a positive diagonal such that \( A = QR \)
  
  - Given \( A^T A = LL^T \), we can take \( R = L^T \) and obtain \( Q = AL^{-T} \), since 
    
    \[
    L^{-1} A^T L A^{-T} = I \implies Q^T Q = I \]
    
    implies that \( Q \) has orthonormal columns.

- A reduced QR factorization (unique part of general QR) is defined so that \( Q \in \mathbb{R}^{m \times n} \) has orthonormal columns and \( R \) is square and upper-triangular.
  
  A full QR factorization gives \( Q \in \mathbb{R}^{m \times m} \) and \( R \in \mathbb{R}^{m \times n} \), but since \( R \) is upper triangular, the latter \( m - n \) columns of \( Q \) are only constrained so as to keep \( Q \) orthogonal. The reduced QR factorization is given by taking the first \( n \) columns \( Q \) and \( \hat{Q} \) the upper-triangular block of \( R \), \( \hat{R} \) giving \( A = \hat{Q} \hat{R} \).

- We can solve the normal equations (and consequently the linear least squares problem) via reduced QR as follows

\[
A^T A x = A^T b \quad \Rightarrow \quad \hat{R}^T \hat{Q}^T \hat{Q} \hat{R} x = \hat{R}^T \hat{Q}^T b \quad \Rightarrow \quad \hat{R} x = \hat{Q}^T b
\]
Gram-Schmidt Orthogonalization

► Classical Gram-Schmidt process for QR:
The Gram-Schmidt process orthogonalizes a rectangular matrix, i.e. it finds a set of orthonormal vectors with the same span as the columns of the given matrix. If $a_i$ is the $i$th column of the input matrix, the $i$th orthonormal vector ($i$th column of $Q$) is

$$q_i = b_i / \|b_i\|_2,$$

where

$$b_i = a_i - \sum_{j=1}^{i-1} \langle q_j, a_i \rangle q_j.$$  

► Modified Gram-Schmidt process for QR:
Better numerical stability is achieved by orthogonalizing each vector with respect to each previous vector in sequence (modifying the vector prior to orthogonalizing to the next vector), so $b_i = \text{MGS}(a_i, i - 1)$, where \( \text{MGS}(d, 0) = d \) and

$$\text{MGS}(d, j) = \text{MGS}(d - \langle q_j, d \rangle q_j, j - 1)$$  

Demo: Gram-Schmidt–The Movie
Demo: Gram-Schmidt and Modified Gram-Schmidt
A Householder transformation $Q = I - 2uu^T$ is an orthogonal matrix defined to annihilate entries of a given vector $z$, so $||z||_2 Q e_1 = z$:

- Householder QR achieves unconditional stability, by applying only orthogonal transformations to reduce the matrix to upper-triangular form.
- Householder transformations (reflectors) are orthogonal matrices, that reduce a vector to a multiple of the first elementary vector, $\alpha e_1 = Q z$.
- Because multiplying a vector by an orthogonal matrix preserves its norm, we must have that $|\alpha| = ||z||_2$.
- As we will see, this transformation can be achieved by a rank-1 perturbation of identify of the form $Q = I - 2uu^T$ where $u$ is a normalized vector.
- Householder matrices are both symmetric and orthogonal implying that $Q = Q^T = Q^{-1}$.

Imposing this form on $Q$ leaves exactly two choices for $u$ given $z$, $u = \frac{z \pm ||z||_2 e_1}{||z \pm ||z||_2 e_1||_2}$.
Applying Householder Transformations

- The product $x = Qw$ can be computed using $O(n)$ operations if $Q$ is a Householder transformation

\[ x = (I - 2uu^T)w = w - 2\langle u, w \rangle u \]

- Householder transformations are also called *reflectors* because their application reflects a vector along a hyperplane (changes sign of component of $w$ that is parallel to $u$)

  - $I - uu^T$ would be an elementary projector, since $\langle u, w \rangle u$ gives component of $w$ pointing in the direction of $u$ and

  \[ x = (I - uu^T)w = w - \langle u, w \rangle u \]

  *subtracts it out.*

  - On the other hand, Householder reflectors give

  \[ y = (I - 2uu^T)w = w - 2\langle u, w \rangle u = x - \langle u, w \rangle u \]

  which reverses the sign of that component, so that $||y||_2 = ||w||_2$.
Givens Rotations

- Householder reflectors reflect vectors, Givens rotations rotate them
  - Householder matrices reflect vectors across a hyperplane, by negating the sign of the vector component that is perpendicular to the hyperplane (parallel to $\mathbf{u}$)
  - Any vector can be reflected to a multiple of an elementary vector by a single Householder rotation (in fact, there are two rotations, resulting in a different sign of the resulting vector)
  - Givens rotations instead rotate vectors by an axis of rotation that is perpendicular to a hyperplane spanned by two elementary vectors
  - Consequently, each Givens rotation can be used to zero-out (annihilate) one entry of a vector, by rotating it so that the component of the vector pointing in the direction of the axis corresponding to that entry, points into a different axis

- Givens rotations are defined by orthogonal matrices of the form

$$\begin{bmatrix} c & s \\ -s & c \end{bmatrix}$$

- Given a vector $\begin{bmatrix} a \\ b \end{bmatrix}$ we define $c$ and $s$ so that

$$\begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \sqrt{a^2 + b^2} \\ 0 \end{bmatrix}$$

- Solving for $c$ and $s$, we get

$$c = \frac{a}{\sqrt{a^2 + b^2}}, \quad s = \frac{b}{\sqrt{a^2 + b^2}}$$
We can apply a Givens rotation to a pair of matrix rows, to eliminate the first nonzero entry of the second row.

\[
\begin{bmatrix}
I & c & s \\
-s & I & c \\
& & I
\end{bmatrix}
\begin{bmatrix}
\vdots \\
a \\
\vdots \\
b \\
\vdots \\
0 \\
\vdots
\end{bmatrix}
= \begin{bmatrix}
\vdots \\
\sqrt{a^2 + b^2} \\
0
\end{bmatrix}
\]

Thus, \(n(n - 1)/2\) Givens rotations are needed for QR of a square matrix.

- Each rotation modifies two rows, which has cost \(O(n)\).
- Overall, Givens rotations cost \(2n^3\), while Householder QR has cost \((4/3)n^3\).
- Givens rotations provide a convenient way of thinking about QR for sparse matrices, since nonzeros can be successively annihilated, although they introduce the same amount of fill (new nonzeros) as Householder reflectors.
Suppose we want to solve a linear system or least squares problem with a (nearly) rank deficient matrix $A$.

- A rank-deficient (singular) matrix satisfies $Ax = 0$ for some $x \neq 0$.
- Rank-deficient matrices must have at least one zero singular value.
- Matrices are said to be deficient in numerical rank if they have extremely small singular values.
- The solution to both linear systems (if it exists) and least squares is not unique, since we can add to it any multiple of $x$.

Rank-deficient least squares problems seek a minimizer $x$ of $||Ax - b||_2$ of minimal norm $||x||_2$.

- If $A$ is a diagonal matrix (with some zero diagonal entries), the best we can do is $x_i = b_i/a_{ii}$ for all $i$ such that $a_{ii} \neq 0$ and $x_i = 0$ otherwise.
- We can solve general rank-deficient systems and least squares problems via $x = A^\dagger b$ where the pseudoinverse is

$$A^\dagger = V\Sigma^\dagger U^T, \quad \sigma_i^\dagger = \begin{cases} 1/\sigma_i : \sigma_i > 0 \\ 0 : \sigma_i = 0 \end{cases}$$
Truncated SVD

- After floating-point rounding, rank-deficient matrices typically regain full-rank but have nonzero singular values on the order of $\epsilon_{\text{mach}}\sigma_{\text{max}}$
  - Very small singular values can cause large fluctuations in the solution
  - To ignore them, we can use a pseudoinverse based on the truncated SVD which retains singular values above an appropriate threshold
  - Alternatively, we can use Tykhonov regularization, solving least squares problems of the form $\min_x \|Ax - b\|_2^2 + \alpha\|x\|_2^2$, which are equivalent to the augmented least squares problem
    \[
    \begin{bmatrix}
    A \\
    \sqrt{\alpha}I
    \end{bmatrix}
    x \approx
    \begin{bmatrix}
    b \\
    0
    \end{bmatrix}
    \]

- By the Eckart-Young-Mirsky theorem, truncated SVD also provides the best low-rank approximation of a matrix (in 2-norm and Frobenius norm)
  - The SVD provides a way to think of a matrix as a sum of outer-products $\sigma_i u_i v_i^T$ that are disjoint by orthogonality and the norm of which is $\sigma_i$
  - Keeping the $r$ outer products with largest norm provides the best rank-$r$ approximation
QR with Column Pivoting

- QR with column pivoting provides a way to approximately solve rank-deficient least squares problems and compute the truncated SVD
  - We seek a factorization of the form $QR = AP$ where $P$ is a permutation matrix that permutes the columns of $A$
  - For $n \times n$ matrix $A$ of rank $r$, the bottom $r \times r$ block of $R$ will be 0
  - To solve least squares, we can solve the rank-deficient triangular system $Ry = Q^Tb$ then compute $x = Py$

- A pivoted QR factorization can be used to compute a rank-$r$ approximation
  - To compute QR with column pivoting,
    1. pivot the column of largest norm to be the leading column,
    2. form and apply a Householder reflector $H$ so that $HA = \begin{bmatrix} \alpha & b \\ 0 & B \end{bmatrix}$,
    3. proceed recursively (go back to step 1) to pivot the next column and factorize $B$
  - Computing the SVD of the first $r$ columns of $AP^T$ generally (but not always) gives the truncated SVD
  - Halting after $r$ steps leads to a cost of $O(n^2r)$