CS 450: Numerical Analysis¹
Linear Least Squares

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¹These 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
    \[
    \Sigma y^* \cong d \quad \text{where} \quad y^* = V^T x^* \text{ and } d = U^T b.
    \]

  - 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 \( i \in \{n + 1, \ldots, m\} \).
Conditioning of Linear Least Squares

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 $\kappa(A) = \sigma_{\text{max}} / \sigma_{\text{min}}$).
Normal Equations

- **Normal equations** are given by solving $A^T A x = A^T b$:

  If $A^T A x = A^T b$ 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 $\begin{bmatrix} L^{-1}A^T & AL^{-T} \end{bmatrix} = I$ 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

$$A^T Ax = A^T b \quad \Rightarrow \quad \hat{R}^{T} \hat{Q}^{T} \hat{Q} \hat{R} x = \hat{R}^{T} \hat{Q}^{T} b \quad \Rightarrow \quad \hat{R} x = \hat{Q}^{T} b$$
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

  \[
  q_i = \frac{b_i}{\|b_i\|_2}, \quad \text{where} \quad b_i = a_i - \sum_{j=1}^{i-1} \langle q_j, a_i \rangle q_j.
  \]

- **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

  \[
  \text{MGS}(d, j) = \text{MGS}(d - \langle q_j, d \rangle q_j, j - 1)
  \]
A Householder transformation $Q = I - 2uu^T$ is an orthogonal matrix defined to annihilate entries of a given vector $z$, so $\|z\|_2Qe_1 = z$:

- 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, $\alpha e_1 = Qz$.
- 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 $\|y\|_2 = \|w\|_2$. 

**Activity:** Householder QR
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
  \[
  c = \frac{a}{\sqrt{a^2 + b^2}}, \quad s = \frac{b}{\sqrt{a^2 + b^2}}
  \]
QR via Givens Rotations

- We can apply a Givens rotation to a pair of matrix rows, to eliminate the first nonzero entry of the second row

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

- 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

**Demo:** Relative cost of matrix factorizations
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

$$A^\dagger = V \Sigma^\dagger U^T \quad \sigma^\dagger_i = \begin{cases} 1/\sigma_i : \sigma_i > 0 \\ 0 : \sigma_i = 0 \end{cases}$$
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 Tikhonov regularization, solving least squares problems of the form $\min_x ||Ax - b||_2^2 + \alpha ||x||^2$, 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 $Ry = Q^T b$ 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 $O(n^2 r)$