Solving Least Squares
Normal Equations

• Let $\tilde{A}$ have full column rank, and be size $mxn$ with $m \geq n$

• Diagonal (nonzero) weighting $A = D\tilde{A}$ does not change the rank/size
  • but changes the answer when $D \neq I$ and $m \neq n$

• Minimizing $\|r\|_2 = \|b - Ac\|_2$ leads to the normal equations $A^TAc = A^Tb$ for the critical point

• Since $A^TA$ is SPD, $A^TAc = A^Tb$ has a unique solution obtainable via fast/efficient SPD solvers

• When $b$ is in the range of $A$, the unique solution to $A^TAc = A^Tb$ makes $r = 0$, and is thus the unique solution to $Ac = b$
  • When $A$ is square ($m = n$), and full rank, then $b$ is always in the range of $A$
Condition Number

• Compare $A = U\Sigma V^T$ and $A^T A = V \Sigma^T \Sigma V^T = V \Lambda V^T$ where $\Lambda = \Sigma^T \Sigma$ is a diagonal size $nxn$ matrix of singular values squared

• Since the singular values of $A^T A$ are the square of those in $A$, the condition number $\frac{\sigma_{\text{max}}}{\sigma_{\text{min}}}$ of $A^T A$ is also squared (compared to $A$)
  • Thus, solving the normal equations requires twice the precision (e.g. $(10^7)^2 = 10^{14}$)
  • It takes twice as much precision to get the same number of significant digits!

• The normal equations should only be used as a last resort (when there are no other options)

• However, (like the SVD) it is a great tool for theoretical purposes
  • I.e. can transform any full column rank matrix into an SPD system
Understanding Least Squares

- When $A = U\Sigma V^T$ has full column rank, $\Sigma = \begin{pmatrix} \hat{\Sigma} \\ 0 \end{pmatrix}$ with $\hat{\Sigma}$ a size $n \times n$ diagonal matrix of (strictly) positive singular values
  - The $0$ submatrix is size $(m - n) \times n$ and doesn't exist when $m = n$
- Note: $A^T A = V \Sigma^T \Sigma V^T = V \hat{\Sigma}^2 V^T$ and $(A^T A)^{-1} = V \hat{\Sigma}^{-2} V^T$
- So $c = (A^T A)^{-1} A^T b = V \hat{\Sigma}^{-2} V^T V \Sigma^T U^T b = V (\hat{\Sigma}^{-1} \ 0) U^T b$
- $Ac = U\Sigma V^T V (\hat{\Sigma}^{-1} \ 0) U^T b = U \begin{pmatrix} \hat{\Sigma} \\ 0 \end{pmatrix} (\hat{\Sigma}^{-1} \ 0) U^T b = U \begin{pmatrix} I_{nxn} & 0 \\ 0 & 0 \end{pmatrix} U^T b$
- $r = b - Ac = U I_{mxm} U^T b - U \begin{pmatrix} I_{nxn} & 0 \\ 0 & 0 \end{pmatrix} U^T b = U \begin{pmatrix} 0 & 0 \\ 0 & I_{(m-n)x(m-n)} \end{pmatrix} U^T b$
Understanding Least Squares

• Recall: from SVD slides (unit 3):
  • The columns of $U$ corresponding to “nonzero” singular values form an orthonormal basis for the range of $A$
  • The remaining columns of $U$ form an orthonormal basis for the (unattainable) space perpendicular to the range of $A$

• Since $A$ only has $n$ singular values, only the first $n$ columns of $U$ (which has $m$ columns) span the range of $A$

• Writing \( \begin{pmatrix} \hat{b}_r \\ \hat{b}_z \end{pmatrix} = U^T b \) separates $\hat{b}_r$ (which is size $n \times 1$) in the range of $A$ from $\hat{b}_z$ (which is size $(m - n) \times 1$) orthogonal to the range of $A$

• Then (from the last slide): $c = V \hat{\Sigma}^{-1} \hat{b}_r$, $Ac = U \begin{pmatrix} \hat{b}_r \\ 0 \end{pmatrix}$, and $r = U \begin{pmatrix} 0 \\ \hat{b}_z \end{pmatrix}$
Orthogonal Matrices (and the L2 norm)

• Recall (from unit 3):
  • **Orthogonal matrices** have orthonormal columns (an orthonormal basis), so their transpose is their inverse. They preserve inner products, and thus are rotations, reflections, and combinations thereof

  \[
  QQ^T = Q^TQ = I \\
  \]

• An orthogonal \( \hat{Q} \) has \( \hat{Q}\hat{Q}^T = \hat{Q}^T\hat{Q} = I \)

• So, \( \|\hat{Q}r\|_2 = \sqrt{\hat{Q}r \cdot \hat{Q}r} = \sqrt{r^T\hat{Q}^T\hat{Q}r} = \sqrt{r^Tr} = \|r\|_2 \)

• Similarly, \( \|\hat{Q}^Tr\|_2 = \sqrt{\hat{Q}^Tr \cdot \hat{Q}^Tr} = \sqrt{r^T\hat{Q}\hat{Q}^Tr} = \sqrt{r^Tr} = \|r\|_2 \)

• That is, orthogonal transformations preserve Euclidean distance
Understanding Least Squares

• $r = U \begin{pmatrix} 0 \\ \hat{b}_z \end{pmatrix}$ with orthogonal $U$ implies $\|r\|_2 = \|\hat{b}_z\|_2$

• Consider the diagonalized SVD view of $Ac = b$ when $A$ has full rank:

$$U \Sigma V^T c = b \quad \text{or} \quad \begin{pmatrix} \hat{\Sigma} \\ 0 \end{pmatrix} \hat{c} = \begin{pmatrix} \hat{b}_r \\ \hat{b}_z \end{pmatrix}$$

• The first block row gives $c = V \hat{\Sigma}^{-1} \hat{b}_r$, which is the least squares solution

• The second block row is $0 = \hat{b}_z$, and the norm of the residual for this block row is $\|\hat{b}_z\|_2$, which is identical to $\|r\|_2$

• The SVD approach gives the same (minimum residual) least squares solution
Recall: Gram-Schmidt (Unit 5)

- Orthogonalizes a set of vectors
- For each new vector, subtract its (weighted) dot product overlap with all prior vectors, making it orthogonal to them
- A-orthogonal Gram-Schmidt uses an A-weighted dot/inner product
- Given vector $\mathbf{S}^q$, subtract out the A-overlap with $s^1$ to $s^{q-1}$ so that the resulting vector $s^q$ has $\langle s^q, s^{\hat{q}} \rangle_A = 0$ for $\hat{q} \in \{1, 2, \ldots, q - 1\}$
- That is, $s^q = \mathbf{S}^q - \sum_{\hat{q}=1}^{q-1} \frac{\langle \mathbf{S}^q, s^{\hat{q}} \rangle_A}{\langle s^{\hat{q}}, s^{\hat{q}} \rangle_A} s^{\hat{q}}$ where the two non-normalized $s^{\hat{q}}$ both require division by their norm (and $\langle s^{\hat{q}}, s^{\hat{q}} \rangle_A = \|s^{\hat{q}}\|_A^2$)
- Proof: $\langle s^q, s^{\hat{q}} \rangle_A = \langle \mathbf{S}^q, s^{\hat{q}} \rangle_A - \frac{\langle \mathbf{S}^q, s^{\hat{q}} \rangle_A}{\langle s^{\hat{q}}, s^{\hat{q}} \rangle_A} \langle s^{\hat{q}}, s^{\hat{q}} \rangle_A = 0$
Gram-Schmidt QR Factorization

- From $A$, create a full rank $Q$ with orthonormal columns
- For each column $a_k$, subtract the overlap with all prior columns in $Q$ and make unit length:

\[
q_k = \frac{a_k - \sum_{k=1}^{k-1} <a_k, q_{\hat{k}} > q_{\hat{k}}}{\|a_k - \sum_{k=1}^{k-1} <a_k, q_{\hat{k}} > q_{\hat{k}}\|_2}
\]

- Define $r_{\hat{k}k} = < a_k, q_{\hat{k}} >$ for $k > \hat{k}$, and $r_{kk} = \|a_k - \sum_{k=1}^{k-1} <a_k, q_{\hat{k}} > q_{\hat{k}}\|_2$
- Then $q_k = \frac{a_k - \sum_{k=1}^{k-1} r_{\hat{k}k} q_{\hat{k}}}{r_{kk}}$, and thus $a_k = r_{kk} q_k + \sum_{\hat{k}=1}^{k-1} r_{\hat{k}k} q_{\hat{k}} = \sum_{\hat{k}=1}^{k} r_{\hat{k}k} q_{\hat{k}}$
- That is, $A = QR$ where $R$ is upper triangular and $Q^T Q = I$
Gram-Schmidt QR (Example)

• Example: \( A = QR \) with upper triangular \( R \)

\[
\begin{pmatrix}
3 & -3 & 3 \\
2 & -1 & 1 \\
2 & -3 & 3 \\
2 & -3 & 5 \\
\end{pmatrix} = \begin{pmatrix}
3/5 & 0 & 0 \\
2/5 & 1/2 & 1/2 \\
2/5 & -1/2 & -1/2 \\
2/5 & -1/2 & 1/2 \\
\end{pmatrix} \begin{pmatrix}
5 & -5 & 5 \\
0 & 2 & -4 \\
0 & 0 & 2 \\
\end{pmatrix}
\]

• Note that \( Q^T Q = I_{3 \times 3} \) since the columns of \( Q \) are orthonormal

• However, \( QQ^T \neq I_{5 \times 5} \) and \( Q \) is only a subset of an orthogonal matrix
Not Good for Large Matrices

• Gram-Schmidt has too much numerical drift for large matrices
• Don’t use Gram-Schmidt to find $A = QR$ with upper triangular $R$ and $Q^T Q = I$
• But it does provide a good conceptual way to think about $A = QR$
QR Factorization

• Consider $A = QR$ with upper triangular $R$ and $Q^TQ = I$
• $Q$ is size $mxn$ (just like $A$) with $n$ orthonormal columns
• Let $\tilde{Q}$ be the matrix with $m - n$ orthonormal columns that span the space perpendicular to the range of $Q$
• Then, the size $m \times m$ matrix $\hat{Q} = (Q \quad \tilde{Q})$ is orthogonal
• So $\|r\|_2 = \|\hat{Q}^T r\|_2 = \left\| \begin{pmatrix} Q^T \\ \tilde{Q}^T \end{pmatrix} \begin{pmatrix} b - QRC \end{pmatrix} \right\|_2 = \left\| \begin{pmatrix} Q^Tb - Rc \\ \tilde{Q}^Tb \end{pmatrix} \right\|_2$
• Only the first (block) row varies with $c$, so $\|r\|_2$ is minimized by solving $Rc = Q^Tb$
• Since $R$ is upper triangular, $Rc = Q^Tb$ can be solved via back-substitution
Householder Transform

- Let unit normal $\hat{v}$ implicitly define a plane orthogonal to it.
- Then, $H = I - 2\hat{v}\hat{v}^T$ reflects vectors across that plane.
- $Ha = a - 2(\hat{v}^Ta)\hat{v}$
- $H$ is orthogonal with $H = H^T = H^{-1}$
- Don’t form the full $H$
- Instead, apply it via the definition of $\hat{v}$
Householder Transform

- Choose directions $v_k = a - Ha$ in a manner that zeroes out elements

- E.g. $v_k = \begin{pmatrix} a_1 \\ \vdots \\ a_{k-1} \\ a_k \\ a_{k+1} \\ \vdots \\ a_n \end{pmatrix} - \begin{pmatrix} a_1 \\ \vdots \\ a_{k-1} \\ \gamma \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \hat{a}_k - \gamma \hat{e}_k$ where $\hat{a}_k = \begin{pmatrix} 0 \\ \vdots \\ 0 \\ a_k \\ a_{k+1} \\ \vdots \\ a_n \end{pmatrix}$

- $Ha$ should be the same length as $a$ (i.e. a reflection), so $\|\gamma\|_2 = \|\hat{a}_k\|_2$

- Then, $v_k = \hat{a}_k \pm \|\hat{a}_k\|_2 \hat{e}_k$, which is subsequently normalized to $\hat{v}_k = \frac{v_k}{\|v_k\|_2}$

- For robustness, $v_k = \hat{a}_k + S(a_k)\|\hat{a}_k\|_2 \hat{e}_k$ where $S(a_k) = \pm 1$ is the sign function
Householder Transform (Example)

- Consider $a = \begin{pmatrix} 2 \\ 1 \\ 2 \end{pmatrix}$ in the formulation $v_k = \hat{a}_k + S(a_k)\|\hat{a}_k\|_2 \hat{e}_k$

- Here $\hat{a}_1 = \begin{pmatrix} 2 \\ 1 \\ 2 \end{pmatrix}$, $v_1 = \begin{pmatrix} 2 \\ 1 \\ 2 \end{pmatrix} + S(2)\sqrt{9} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 5 \\ 1 \\ 2 \end{pmatrix}$, $\hat{v}_1 = \frac{1}{\sqrt{30}} \begin{pmatrix} 5 \\ 1 \\ 2 \end{pmatrix}$

- So $H_1 a = a - 2(\hat{v}_1^T a) \hat{v}_1 = \begin{pmatrix} 2 \\ 1 \\ 2 \end{pmatrix} - 2 \begin{pmatrix} 15 \\ 15 \end{pmatrix} \begin{pmatrix} 5 \\ 1 \\ 2 \end{pmatrix} = \begin{pmatrix} -3 \\ 0 \\ 0 \end{pmatrix}$
Householder Transform (QR)

- For each column of \( A \), construct the Householder transform that zeroes out entries below the diagonal

- Then \( H_n H_{n-1} \cdots H_2 H_1 A = \begin{pmatrix} R \\ 0 \end{pmatrix} \) and \( H_n H_{n-1} \cdots H_2 H_1 b = \begin{pmatrix} \tilde{b}_r \\ \tilde{b}_z \end{pmatrix} \)

- Apply \( H_k \) efficiently using \( \hat{v}_k \) and to apply it to all columns \( \geq k \)
  - It doesn’t affect columns \(< k\) (because of all the zeros at the top of \( \hat{v}_k \))

- Note: \( H_n \) is required to get zeroes at the bottom of the last column

- Letting \( \tilde{Q}^T = H_n H_{n-1} \cdots H_2 H_1 \) gives \( \tilde{Q}^T A = \begin{pmatrix} R \\ 0 \end{pmatrix} \) or \( A = \tilde{Q} \begin{pmatrix} R \\ 0 \end{pmatrix} \)

- And \( \|r\|_2 = \|\tilde{Q}^T r\|_2 = \|\tilde{Q}^T (b - \hat{Q} \begin{pmatrix} R \\ 0 \end{pmatrix} c)\|_2 = \|\left(\begin{pmatrix} \tilde{b}_r \\ \tilde{b}_z \end{pmatrix} - \begin{pmatrix} Rc \\ 0 \end{pmatrix}\right)\|_2 \)

- So, minimize \( \|r\|_2 \) to \( \|\tilde{b}_z\|_2 \) by solving \( Rc = \tilde{b}_r \)