Least Squares Problems.

We are interested in solving the problem

$$Ax = b \text{ when } b \notin \text{Im} A$$

In this case, we are trying to solve the problem in the sense

$$\min \|Ax - b\|_2$$ or "least squares".

Suppose $A$ has full column rank and $A$ is $m \times n$. We start by finding the point where $\nabla \|Ax - b\|_2$ vanishes.

Now

$$\|Ax - b\|_2 = (Ax - b)^T (Ax - b)$$
Thus we want $\|Ax-b\|_2 \cdot v = 0$ for all $v$.

\[
\lim_{\epsilon \to 0} (A(x+\epsilon v) - b)^T (A(x+\epsilon v) - b) - (Ax-b)^T (Ax-b) = \epsilon
\]

\[
= \lim_{\epsilon \to 0} (Ax-b + \epsilon Av)^T (Ax-b + \epsilon Av) - (Ax-b)^T (Ax-b) = \epsilon
\]

\[
= \lim_{\epsilon \to 0} 2\epsilon (Av)^T (Ax-b) + \epsilon^2 (Av^T) Av = \epsilon
\]

\[
= 2(Av)^T (Ax-b)
\]

\[
= 2v^T (A^T A x - A^T b) = 0.
\]

Of course, this is true for all $v \Rightarrow A^T A x = A^T b$

This $(n \times m)(m \times n) = n \times n$ system is called the normal equations. Note: this matrix $A^T A$ is positive definite and, hence, nonsingular.
Why is this the global min? We complete the square: suppose $x$ satisfies $A^TAx = A^Tb$ and we write $x' = x + e$. Then

$$(Ax'-b)^T(Ax'-b) = (Ae+Ax-b)^T(Ae+Ax-b)$$

$$= Ae^TAe + (Ax-b)^T(Ax-b) + 2e^T(Ae)^T(Ax-b)$$

$$= ||Ae||_2^2 + ||Ax-b||_2^2 + 2e(A^TAx-A^Tb)$$

$$= ||Ae||_2^2 + ||Ax-b||_2^2$$

This is clearly minimized when $e=0$.

What do we do to solve the normal equations? We first note that $m \geq n$ (the system overdetermined).
Now $A^TA$ is spd, so we can use Cholesky decomposition ($\frac{1}{3}n^3 + O(n^2)$) flops. But just computing $A^TA$ takes $\sim n^2m > n^3$ operations!

We also note that

$$x(A^TA) = x(A)^2$$

so we have potential stability problems for ill-conditioned matrices. **Underline**

Now what do we do then? We first introduce a new matrix decomposition.
Theorem. If $A$ is $m \times n$ with $m \geq n$ and $A$ has full column rank, then there exists a unique $m \times n$ orthogonal matrix $Q$ and a unique $n \times n$ upper triangular $R$ with positive diagonals so $A = QR$.

Proof. Consider the columns $A_1, \ldots, A_n$ of $A$. By assumption, they span an $n$-dimensional subspace of $\mathbb{R}^m$.

Apply Gram-Schmidt. The resulting orthonormal vectors $q_i$ are the cols of $Q$. Further

$$A_i = r_{ii} q_i + r_{i(i-1)} q_{i-1} + \ldots + r_{i1} q_1$$

by the Gram-Schmidt construction.
The $r_{ij}$ are the entries in $R$. 0

How does this look as an algorithm?

for $i = 1$ to $n$

\[ q_i = \alpha \frac{a_i}{\|a_i\|_2} \]

for $j = 1$ to $i-1$

\[ r_{ji} = q_j^T a_i \text{ Classical Gram-Schmidt} \]
\[ r_{ji} = q_j^T q_i \text{ Modified Gram-Schmidt} \]

\[ q_i = q_i - r_{ji} q_j \]

end

\[ r_{ii} = \|q_i\|_2 \]

\[ q_i = q_i / r_{ii} \]

end
The flop count here is

$$\sum_{i=1}^{n} i \cdot (2^3 m) \approx \frac{3mn^2}{2}$$

Suppose we had such a decomposition. Then if $x$ solves our problem,

$$A^T A x = A^T b$$

$$x = (A^T A)^{-1} A^T b$$

$$= (R^T Q R Q R)^{-1} R^T Q b$$

$$= (R^T R)^{-1} R^T Q b$$

$$= R^{-1} R^T R Q b$$

$$= R^{-1} Q^T b$$

or

$$R x = Q^T b$$, which we can solve by forward substitution.
Here is a third technique which will prove really useful.

**Theorem. (SVD)** Let $A$ be any $m \times n$ matrix, with $m \geq n$. Then we can write

$$A = U \Sigma V^T$$

where $U$ and $V$ are orthogonal, $U$ is $m \times n$, $V$ is $n \times n$ and $\Sigma$ is a diagonal matrix with entries

$$\sigma_{11} \geq \sigma_{22} \geq \ldots \geq \sigma_{nn} \geq 0$$

The columns of $U$ and $V$ are called **left** and **right singular vectors** while the $\sigma_i$ are **singular values**.
The claim here is simple and striking!

"Any matrix is diagonal in suitably chosen orthogonal coordinates on its range and domain"
Proof. We use induction on $m$ and $n$, assuming the SVD exists for $(m-1) \times (n-1)$ matrices. We may assume $A \neq 0$.

Since $m \geq n$, the base case is $n = 1$, $m$ arbitrary ($A$ is a column vector). We have

\[
A = U \Sigma V^T
\]

\[
= \left( \frac{1}{\|A\|_2} A \right) [\|A\|_2] [1]
\]

For the inductive step, choose $v$ so $\|v\|_2 = 1$ and $\|A\|_2 = \|Av\|_2 > 0$. (This exists by definition of the matrix 2-norm.) Let $u = \frac{Av}{\|Av\|_2}$. Now complete $u$ to an orthogonal basis of $\mathbb{R}^n$, forming
an orthogonal matrix $U = [u, \tilde{U}]$. We can do the same with $V = [v, \tilde{V}]$.

Now

$$U^T A V = \begin{bmatrix} u^T \\ \tilde{U}^T \end{bmatrix} A \begin{bmatrix} v \\ \tilde{V} \end{bmatrix}$$

$$= \begin{bmatrix} u^T A \\ \tilde{U}^T A \end{bmatrix} \begin{bmatrix} v \\ \tilde{V} \end{bmatrix}$$

$$= \begin{bmatrix} u^T A v & u^T A \tilde{V} \\ \tilde{U}^T A v & \tilde{U}^T A \tilde{V} \end{bmatrix}$$

We know

$$u^T A v = \left(\frac{Av}{\|Av\|_2}\right)^T A v = \frac{\|Av\|_2^2}{\|Av\|_2} = \|Av\|_2^2 = \|A\|_2^2$$

call this value $\sigma$. Now

$$\tilde{U}^T A v = \tilde{U}^T u \cdot \|Av\|_2 = 0$$

(since $u$ is orthogonal to remaining cols of $\tilde{U}$).
Now consider $u^T \tilde{A} \tilde{V}$.

We claim $u^T \tilde{A} \tilde{V} = 0$. To see this, first observe

$$\|A\|_2 = \|U^T A V\|_2$$

since $U$ and $V$ are orthogonal matrices.

Now observe that $\|U^T A V\|_2 = \|(U^T A V)^T\|_2$.

Now

$$\| (U^T A V)^T e_1 \|_2 = \|[1, \ldots, 0]^T U^T A V\|_2$$

$$= \|[0 \ u^T A \tilde{V}]\|_2 = \sqrt{0^2 + \|u^T A \tilde{V}\|_2^2}$$

But this is equal to $\|A\|_2 = 0$ (tracing back through our chain of inequalities), so $\|u^T A \tilde{V}\|_2 = 0$ and $u^T A \tilde{V} = 0$. 
We now know

\[ U^T A V = \begin{bmatrix} \sigma & 0 \\ 0 & \tilde{U}^T \tilde{V} \end{bmatrix} = \begin{bmatrix} \sigma & 0 \\ 0 & \tilde{A} \end{bmatrix}. \]

Applying inductive hypothesis to \( \tilde{A} \), we can write \( \tilde{A} = U_1 \Sigma_1 V_1^T \) where then

\[ U^T A V = \begin{bmatrix} \sigma & 0 \\ 0 & u_1 \Sigma_1 v_1^T \end{bmatrix} \]

\[ = \begin{bmatrix} 1 & 0 \\ 0 & u_1 \Sigma_1 \end{bmatrix} \begin{bmatrix} \sigma & 0 \\ 0 & \Sigma_1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & v_1 \end{bmatrix}^T \]

So

\[ \tilde{A} = (U \begin{bmatrix} 1 & 0 \\ 0 & u_1 \end{bmatrix}) (\begin{bmatrix} \sigma & 0 \\ 0 & \Sigma_1 \end{bmatrix}) (\begin{bmatrix} 1 & 0 \\ 0 & v_1 \end{bmatrix})^T \]

which is the svd. \( \Box \)
The SVD has a lot of useful properties which we can prove here.

Theorem. Let $\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^T$ be the SVD of $\mathbf{A}$ where $\mathbf{A}$ is an $m \times n$ matrix with $m \geq n$.

1. If $\mathbf{A}$ is symmetric with eigenvalues $\lambda_i$ and orthonormal eigenvectors $\mathbf{u}_i$, then

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{U}^T$$

where $\sigma_i = \|\lambda_i\|_1$ and $\mathbf{v}_i = \text{sign}(\lambda_i) \mathbf{u}_i$ is an SVD of $\mathbf{A}$ (here we need the convention $\text{sign}(0) = 1$).

2. The eigenvalues of $\mathbf{A}^T\mathbf{A}$ are $\sigma_i^2$. The right singular vectors $\mathbf{v}_i$ are the corresponding eigenvectors.
3. The eigenvectors of $AA^T$ (m×m) are the $\sigma_i^2$ and mn zeros. The left singular vectors $u_i$ are eigenvectors for the $\sigma_i$.

4. If $H = \begin{bmatrix} 0 & A^T \\ A & 0 \end{bmatrix}$ where $A$ is square and $U\Sigma V^T$ is the SVD of $A$. The eigenvalues of $H$ are $\pm \sigma_i$ with unit eigenvectors $\frac{1}{\sqrt{2}} \begin{bmatrix} u_i \\ v_i \end{bmatrix}$.

5. If $A$ has full rank, the solution to $\min_x \|Ax - b\|_2$ is $x = U\Sigma^{-1}V^T b$.

6. $\|A\|_2 = \sigma_1$. If $A$ is square and nonsingular, $\|A^{-1}\|_2 = \frac{1}{\sigma_n}$ and $\|A\|_2 \|A^{-1}\|_2 = \frac{\sigma_1}{\sigma_n}$.
7. Suppose some of the \( \sigma_i \) are 0, so \( \sigma_1 > \ldots > \sigma_r > 0, \sigma_{r+1} = \ldots = \sigma_n = 0 \). Then \( \text{rank } A = r \) and

\[
\ker A = \text{span}(v_{r+1}, \ldots, v_n)
\]

while

\[
\text{Im } A = \text{span}(u_1, \ldots, u_r).
\]

8. Let \( S^{n-1} \) be the unit sphere in \( \mathbb{R}^n \). Then the image \( A S^{n-1} \) is an ellipsoid centered at the origin with axes \( \sigma_i u_i \).

9. If \( V = [v_1, \ldots, v_n] \) and \( U = [u_1, \ldots, u_n] \), so \( A = U \Sigma V^T = \sum_{i=1}^{\infty} \sigma_i u_i v_i^T \), where each \( u_i v_i^T \) is a rank 1 matrix. Then a rank \( k \) matrix closest to \( A \) (in \( \| \cdot \|_2 \)) is \( A_k = \sum_{i=1}^{k} \sigma_i u_i v_i^T \).
Further

\[ \| A - A_k \|_2 = \sigma_{k+1} \].

We can also write \( A_k \) as \( U \Sigma_k V^T \) where \( \Sigma_k \) is a diagonal matrix:

\[
\begin{pmatrix}
\sigma_1 & \cdots & 0 \\
0 & \ddots & 0 \\
\vdots & \ddots & \ddots \\
0 & \cdots & 0
\end{pmatrix}
\]

Proof.

1. Suppose \( A = U \Sigma V^T \). Then suppose \( A x = U \Sigma V^T x = \text{the SVD of } A \).

Now if \( x = v_i \), then since \( V^T V = V^{-1} \)

\[
A v_i = U \Sigma V^{-1} v_i
\]

\[
= U \Sigma e_i \\
= U \sigma_i e_i = \sigma_i U v_i.
\]
So if \( u_i \) is an eigenvector of \( A \) with eigenvalue \( \lambda_i \), then if \( U, V \) are as in claim

\[
U \Sigma V_u^T = U \Sigma V^{* \Sigma^{-1}}
\]

\[
= U \Sigma (\frac{\text{sign} \lambda_1}{\text{sign} \lambda_1} \ldots \frac{\text{sign} \lambda_n}{\text{sign} \lambda_n}) V^{* \Sigma^{-1}}
\]

\[
= U \Sigma (\frac{\text{sign} \lambda_1}{\text{sign} \lambda_1} \ldots \frac{\text{sign} \lambda_n}{\text{sign} \lambda_n}) e_i
\]

\[
= U \lambda_i e_i = \lambda_i u_i = A u_i.
\]

Thus \( U \Sigma V^T = A \). Now \( U, V \) are orthogonal, \( \Sigma \) diagonal, positive, as desired.

2. We check

\[
A^T A = V \Sigma U^T U \Sigma V^T
\]

\[
= V \Sigma^2 V^T
\]

as before, \( v_i \) are eigenvectors w/evals \( \sigma_i^2 \).
3. Choose \( \tilde{U} \) so \([U \tilde{U}]\) is \((m \times m)\) and orthogonal. Then
\[
AA^T = U \Sigma V^T V \Sigma U^T
\]
\[
= U \Sigma^2 U^T
\]
\[
= \begin{bmatrix} U & \tilde{U} \end{bmatrix} \begin{bmatrix} \Sigma^2 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} U & \tilde{U} \end{bmatrix}^T
\]

But as before, this means \( U_i, \tilde{U}_i \) are the eigenvectors of \( AA^T \).

4. Homework.

5. \( \|Ax - b\|_2^2 = \|U \Sigma V^T x - b\|_2^2 \).

Now \( A \) has full rank, so \( \Sigma \) does as well, and \( \Sigma \) is invertible. So let \([U \tilde{U}]\) be square \((m \times m)\) and orthogonal as above.
Now
\[ \| U \Sigma V^T x - b \|_2^2 = \| [\hat{u}^T] (U \Sigma V^T x - b) \|_2^2 \]
\[ = \| [\Sigma V^T x - U^T b] \|_2^2 \]
\[ = \| \Sigma V^T x - U^T b \|_2^2 + \| \Sigma b \|_2^2 \]

This is minimized
We can't change \( \hat{U}^T b \) (which is just the projection of \( b \) to the subspace orthogonal to the column space of \( U \)).
But we can minimize this by choosing \( x \) so
\[ \Sigma V^T x - U^T b = 0 \]
or
\[ x = V \Sigma^{-1} U^T b. \]
7. Choose an \( m \times (m-n) \) matrix \( \tilde{U} \) so that \([ U \; \tilde{U} ]\) is square, orthogonal as before. Call this \( \hat{U} \). Now \( \hat{U}, V \) are nonsingular and so

\[
\text{rank } A = \text{rank } \hat{U}AV
\]

\[
= \text{rank } [ U \; \tilde{U} ] U\Sigma V^T V
\]

\[
= \text{rank } [ \Sigma \; \tilde{U} \Sigma ] = \text{rank } [ \Sigma \; 0 ]
\]

\[
= \text{rank } \Sigma = r.
\]

Further, if \( \hat{\Sigma} = [ \Sigma \; 0 ] \) then \( \text{Ker } \hat{\Sigma} \) is clearly the subspace spanned by \( e_{n+1}, \ldots, e_n \). These are the images of \( v_{n+1}, \ldots, v_n \) under \( V^T \), so that must be \( \text{Ker } A \).
Now the image of \( A \) is then
\[
U \text{ span } (e_2, \ldots, e_r) = \text{ span } (u_1, \ldots, u_r).
\]

8. We may as well write \( S^{n-1} \) as
\[
\mathbb{S} \{ q \mid \Sigma q_i^2 = 1 \}
\]

since the matrix \( V \) is orthogonal.
This maps by \( \Sigma \) to an ellipsoid of
the axes of length \( \sigma_i \). Multiplying
by \( U \) rotates each axis \( \sigma_i e_i \) to
\( \sigma_i u_i \), as claimed.

9. \( A_k \) certainly has rank \( k \). Suppose
\( B \) is another rank \( k \) matrix. Now
\[
\text{span } (v_2, \ldots, v_{km}) \cap \ker B
\]
has dimension at least 1, so let \( h \)
be a unit vector in intersection. Now
\[ \| A - B \|_2^2 \geq \| (A - B) h \|_2^2 \]
\[ = \| A h \|_2^2 \]
\[ = \| U \Sigma V^T h \|_2^2 \]
\[ = \| \Sigma (V^T h) \|_2^2 \]

We know he span\( (v_1, \ldots, v_{n+1}) \) so \( V^T h \) is in \( \text{span}(e_1, \ldots, e_{n+1}) \). Each coordinate of \( V^T h \) gets scaled by some \( \sigma_i \) with \( i = 1, \ldots, n+1 \), by ordering of \( \sigma_i \), we have all these at least \( \sigma_{n+1} \). So

\[ \| \Sigma (V^T h) \|_2^2 \geq \sigma_{n+1}^2 \| V^T h \|_2^2 = \sigma_{n+1}^2 \].

The min is clearly achieved if \( V^T h = e_{n+1} \).
We now check

\[ \| A - A_k \|_2 = \left\| \sum_{i=k+1}^{n} \sigma_i u_i v_i^T \right\|_2 \]

\[ = \left\| U \begin{bmatrix} 0 & 
\sigma_{k+1} & 
\cdots & 
\sigma_{n} 
\end{bmatrix} V^T \right\|_2 \]

\[ = \sigma_{k+1}. \]

We now make a definition.

Definition. Suppose A is mxn with m \geq n and A has full rank. Further, suppose \( A = QR = U\Sigma V^T \) as QR and SVD decompositions.

We define the Moore-Penrose pseudoinverse

\( A^+ = (A^T A)\left( A^T A \right)^{-1} A^T = V\Sigma^{-1} U^T \)

\[ = R^{-1} Q^T. \]

If m < n, \( A^+ = A^T (AA^T)^{-1} \).
We can tie all our least squares methods together with the formula

\[ x \text{ solves } \min_{x} \|Ax-b\|_2 \iff x = A^+ b. \]