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

Since $m \geq n$, the minimizer generally does not attain a zero residual $\mathbf{A} \mathbf{x} - \mathbf{b}$.

We can rewrite the optimization problem constraint via

$$
\mathbf{x}^* = \arg\min_{\mathbf{x} \in \mathbb{R}^n} \| \mathbf{A} \mathbf{x} - \mathbf{b} \|^2_2 = \arg\min_{\mathbf{x} \in \mathbb{R}^n} \left[ (\mathbf{A} \mathbf{x} - \mathbf{b})^T (\mathbf{A} \mathbf{x} - \mathbf{b}) \right]
$$

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

- The minimizer satisfies $\mathbf{U} \mathbf{\Sigma} \mathbf{V}^T \mathbf{x}^* \cong \mathbf{b}$ and consequently also satisfies $\mathbf{\Sigma} \mathbf{y}^* \cong \mathbf{d}$ where $\mathbf{y}^* = \mathbf{V}^T \mathbf{x}^*$ and $\mathbf{d} = \mathbf{U}^T \mathbf{b}$.

- The minimizer of the reduced problem is $\mathbf{y}^* = \mathbf{\Sigma}^\dagger \mathbf{d}$, 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 $A^T Ax = A^T b$:

  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.
Solving the Normal Equations

- 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:
  \[
  A^T A = LL^T
  \]
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 $A^T A = L L^T$, we can take $R = L^T$ and obtain $Q = AL^{-T}$, since

$$
\begin{bmatrix}
L^{-1} & A^T \\
Q^T & Q
\end{bmatrix} = I
$$

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 $R$, $\hat{R}$. 
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 $b_i = MGS(a_i, i - 1)$, where $MGS(d, 0) = d$ and

  $$ MGS(d, j) = MGS(d - \langle q_j, d \rangle q_j, j - 1) $$
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 $z$,

$$u = \frac{z \pm ||z||_2e_1}{||z \pm ||z||_2e_1||_2}$$
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 $||y||_2 = ||w||_2$. 