Least squares and QR factorization

linalg 5

$A \in \mathbb{R}^{m \times n}$, $m > n$, full rank

minimize $\| A\vec{x} - \vec{b} \|$ over all $\vec{x} \in \mathbb{R}^n$

* one solution: solve $A^T A \vec{x} = A^T \vec{b}$

  BAD NUMERICALLY

  $\kappa(A^T A)$ tends to be large.

* New approach QR factorization

Write $A = QR$ where Q is an <u>orthogonal</u> matrix and R is upper Δ.

Will discuss how to do this later.

Q orthogonal means $Q^T = Q^{-1}$

<u>THM</u> Assume Q is orthogonal. Then for any $\vec{v}$, we have $\|Q\vec{v}\| = \|\vec{v}\|$ (norm preserving)

<u>Proof</u>: $\|Q\vec{v}\|^2 = (Q\vec{v})^T(Q\vec{v}) = \vec{v}^T \overbrace{Q^T Q}^{I} \vec{v} = \vec{v}^T\vec{v} = \|\vec{v}\|^2$

If Q is orthogonal then so is Q^T.

$\vec{r} = A\vec{x} - \vec{b} = QR\vec{x} - \vec{b}$

Because $\vec{r}$ and $Q^T\vec{r} = R\vec{x} - Q^T\vec{b}$

have same length, following problems are equivalent:

minimize $\|A\vec{x} - \vec{b}\| \iff$ minimize $\|R\vec{x} - Q^T\vec{b}\|$

Generic 4x3 example

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ a_{41} & a_{42} & a_{43} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}$$

$$A\vec{x} = \vec{b}$$

$$R\vec{x} = \vec{w} = Q^T \vec{b}$$

$$\begin{pmatrix} r_{11} & r_{12} & r_{13} \\ 0 & r_{22} & r_{23} \\ 0 & 0 & r_{33} \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{pmatrix} = \begin{pmatrix} q_{11} & q_{12} & q_{13} & q_{14} \\ q_{21} & q_{22} & q_{23} & q_{24} \\ q_{31} & q_{32} & q_{33} & q_{34} \\ q_{41} & q_{42} & q_{43} & q_{44} \end{pmatrix}^T \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}$$

$$\|R\vec{x}-\vec{w}\| = \left\| \begin{pmatrix} r_{11} & r_{12} & r_{13} \\ 0 & r_{22} & r_{23} \\ 0 & 0 & r_{33} \\ \hline 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} - \begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ \hline w_4 \end{pmatrix} \right\|$$

$$\left\| \begin{pmatrix} r_{11}x_1 + r_{12}x_2 + r_{13}x_3 - w_1 \\ r_{22}x_2 + r_{23}x_3 - w_2 \\ r_{33}x_3 - w_3 \\ \hline -w_4 \end{pmatrix} \right\|$$

$+$ solve $\begin{pmatrix} r_{11} & r_{12} & r_{13} \\ & r_{22} & r_{23} \\ & & r_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix}$ best we can do

$$\begin{pmatrix} 1 & -1 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 3 \\ 11 \end{pmatrix}$$

$$V\vec{c} = \vec{y}$$

$$\underbrace{\begin{pmatrix} 1 & -1 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \end{pmatrix}}_{A} = \underbrace{\begin{pmatrix} \frac{1}{2} & -\frac{3}{2\sqrt{5}} & \frac{1}{2} & -\frac{1}{2\sqrt{5}} \\ \frac{1}{2} & -\frac{1}{2\sqrt{5}} & -\frac{1}{2} & \frac{3}{2\sqrt{5}} \\ \frac{1}{2} & \frac{1}{2\sqrt{5}} & -\frac{1}{2} & -\frac{3}{2\sqrt{5}} \\ \frac{1}{2} & \frac{3}{2\sqrt{5}} & \frac{1}{2} & \frac{1}{2\sqrt{5}} \end{pmatrix}}_{Q} \underbrace{\begin{pmatrix} 2 & 1 & 3 \\ 0 & \sqrt{5} & \sqrt{5} \\ 0 & 0 & 2 \\ 0 & 0 & 0 \end{pmatrix}}_{R}$$

$$\begin{pmatrix} 2 & 1 & 3 \\ 0 & \sqrt{5} & \sqrt{5} \\ 0 & 0 & 2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\ -\frac{3}{2\sqrt{5}} & -\frac{1}{2\sqrt{5}} & \frac{1}{2\sqrt{5}} & \frac{3}{2\sqrt{5}} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} & \frac{1}{2} \\ -\frac{1}{2\sqrt{5}} & \frac{3}{2\sqrt{5}} & -\frac{3}{2\sqrt{5}} & \frac{1}{2\sqrt{5}} \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 3 \\ 11 \end{pmatrix} = \begin{pmatrix} 8 \\ \frac{16}{\sqrt{5}} \\ 4 \\ \frac{2}{\sqrt{5}} \end{pmatrix}$$

Solve

$$\begin{pmatrix} 2 & 1 & 3 \\ 0 & \sqrt{5} & \sqrt{5} \\ 0 & 0 & 2 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} 8 \\ \frac{16}{\sqrt{5}} \\ 4 \end{pmatrix}$$

$$c_3 = 2$$

$$\sqrt{5}\, c_2 + 2\sqrt{5} = \frac{16}{\sqrt{5}}$$

$$c_2 = \frac{6}{5}$$

$$2c_1 + \frac{6}{5} + 6 = 8$$

$$c_1 = \frac{2}{5}$$