3/30/2020

LAST TIME

- Gram-Schmidt: $W = \text{Span}\{\vec{x}_1, \dots, \vec{x}_p\} \rightsquigarrow$ orthog. basis $\{\vec{v}_1, \dots, \vec{v}_p\}$

$\vec{v}_1 = \vec{x}_1$

$\dots$

$$\vec{v}_k = \vec{x}_k - \text{proj}_{W_{k-1}} \vec{x}_k = \boxed{\vec{x}_k - \frac{\vec{x}_k \cdot \vec{v}_1}{\vec{v}_1 \cdot \vec{v}_1}\vec{v}_1 - \dots - \frac{\vec{x}_k \cdot \vec{v}_{k-1}}{\vec{v}_{k-1} \cdot \vec{v}_{k-1}}\vec{v}_{k-1}}$$

$W_{k-1} = \text{Span}\{\vec{x}_1, \dots, \vec{x}_{k-1}\} = \text{Span}\{\vec{v}_1, \dots, \vec{v}_{k-1}\}$

- QR factorization: $A = QR$

$A = [\vec{x}_1 \cdots \vec{x}_n]$ — lin indep. columns

$Q = [\vec{u}_1 \cdots \vec{u}_n]$ — normalized Gram-Schmidt basis for Col A

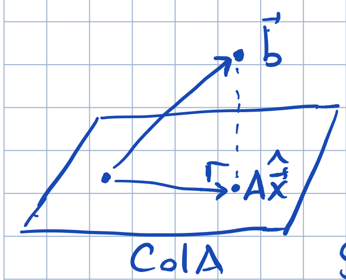
R — upper triangular

finding R: $\boxed{R = Q^T A}$

6.5 Least-squares problems

Consider $A\vec{x} = \vec{b}$ an <u>inconsistent</u> system. Want $\hat{\vec{x}}$ s.t. $A\hat{\vec{x}}$ as close as possible to $\vec{b}$ — approximation to $\vec{b}$

def for A $m \times n$ mat, $\vec{b} \in \mathbb{R}^m$, a <u>least-squares solution</u> of $A\vec{x} = \vec{b}$ is $\hat{\vec{x}} \in \mathbb{R}^n$ s.t. $\|\vec{b} - A\hat{\vec{x}}\| \leq \|\vec{b} - A\vec{x}\|$ for all $\vec{x} \in \mathbb{R}^n$.



Solution of the general least-squares problem

$\hat{\vec{b}} = \text{proj}_{\text{Col}A} \vec{b}$ — closest point to $\vec{b}$ on Col A.

So: $A\hat{\vec{x}} = \hat{\vec{b}} \implies \vec{b} - A\hat{\vec{x}}$ orthog. to Col A

$\iff \vec{a}_j \cdot (\vec{b} - A\hat{\vec{x}}) = 0, \ j = 1, \dots, n \qquad \iff A^T(\vec{b} - A\hat{\vec{x}}) = 0$

$A = [\vec{a}_1 \cdots \vec{a}_n]$

$\iff \boxed{A^T A \hat{\vec{x}} = A^T \vec{b}}$

— "normal equations" for $A\vec{x} = \vec{b}$

THM Set of least-squares solutions of $A\vec{x} = \vec{b}$ coincides with the (non-empty) set of solutions of the normal equations

$$\boxed{A^T A \hat{\vec{x}} = A^T \vec{b}}$$

Ex: $A = \begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 1 \end{bmatrix}$ $\quad \vec{b} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}$ $\quad$ Q: find the least-squares sol. of $A\vec{x} = \vec{b}$.

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Sol: $A^TA = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 3 & 2 \\ 2 & 2 \end{bmatrix}$, $(A^TA)^{-1} = \frac{1}{2}\begin{bmatrix} 2 & -2 \\ -2 & 3 \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ -1 & 3/2 \end{bmatrix}$

$A^T\vec{b} = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 1 & 1 \end{bmatrix}\begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} = \begin{bmatrix} 6 \\ 5 \end{bmatrix} \Rightarrow \hat{x} = (A^TA)^{-1}(A^T\vec{b}) = \begin{bmatrix} 1 & -1 \\ -1 & 3/2 \end{bmatrix}\begin{bmatrix} 6 \\ 5 \end{bmatrix} = \boxed{\begin{bmatrix} 1 \\ 3/2 \end{bmatrix}}$

- Distance from $\vec{b}$ to the approximation $A\hat{\vec{x}}$ is the "least-squares error" of the approximation

Ex: In the example above,

least-squares error $= \|\vec{b} - A\vec{x}\| = \left\| \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} - \begin{bmatrix} 1 \\ 5/2 \\ 5/2 \end{bmatrix} \right\| = \left\| \begin{bmatrix} 0 \\ -1/2 \\ 1/2 \end{bmatrix} \right\| = \boxed{\frac{\sqrt{2}}{2}}$

- LS solution can be non-unique.

THM. Let A be an $m\times n$ mat. The following are equivalent:

(a) eq. $A\vec{x} = \vec{b}$ has a unique LS sol. for each $\vec{b} \in \mathbb{R}^m$.

(b) columns of A are lin. indep.

(c) A^TA is invertible.

When these hold, LS solution is: $\hat{\vec{x}} = (A^TA)^{-1}A^T\vec{b}$

Ex: $A = \begin{bmatrix} 1 & 2 \\ 1 & 2 \end{bmatrix}$, $\vec{b} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ **LS sol:** $A^TA = \begin{bmatrix} 1 & 1 \\ 2 & 2 \end{bmatrix}\begin{bmatrix} 1 & 2 \\ 1 & 2 \end{bmatrix} = \begin{bmatrix} 2 & 4 \\ 4 & 8 \end{bmatrix}$

non-invertible!

$A^T\vec{b} = \begin{bmatrix} 1 \\ 2 \end{bmatrix}$

$\begin{bmatrix} 2 & 4 \\ 4 & 8 \end{bmatrix}\underbrace{\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}}_{\hat{\vec{x}}} = \begin{bmatrix} 1 \\ 2 \end{bmatrix} \rightsquigarrow \left[\begin{array}{cc|c} 2 & 4 & 1 \\ 4 & 8 & 2 \end{array}\right] \sim \left[\begin{array}{cc|c} 1 & 2 & \frac{1}{2} \\ 0 & 0 & 0 \end{array}\right]$

x_2-free var

$\Rightarrow \hat{\vec{x}} = \begin{bmatrix} 1/2 \\ 0 \end{bmatrix} + x_2\begin{bmatrix} -2 \\ 1 \end{bmatrix}$ non-unique LS solution

Alternative way:

THM If A $m\times n$ mat. with lin. indep. columns and $A = \underbrace{Q}_{\text{o/n col.}}\underbrace{R}_{\text{upper triang}}$ decomposition, then for each $\vec{b} \in \mathbb{R}^m$, the LS sol. of $A\vec{x} = \vec{b}$ is: $\hat{\vec{x}} = R^{-1}Q^T\vec{b}$

Indeed: $\underbrace{A^T A}_{R^T \underbrace{Q^T Q}_{I} R} \hat{\vec{x}} = \underbrace{A^T \vec{b}}_{R^T Q^T \vec{b}} \xrightarrow[R^{-1}(R^T)^{-1} \cdot]{} \boxed{\hat{\vec{x}} = R^{-1} Q^T \vec{b}}$

invertible

<u>Rem</u> In practice, instead of finding R^{-1}, it is easier to solve $\boxed{R \vec{x} = Q^T \vec{b}}$ by row reduction / back substitution.