Ex: $\vec{x}_1 = \begin{bmatrix}1\\1\\0\\0\end{bmatrix}$, $\vec{x}_2 = \begin{bmatrix}0\\1\\1\\0\end{bmatrix}$, $\vec{x}_3 = \begin{bmatrix}1\\1\\1\\1\end{bmatrix}$ - basis for $W = \text{Span}\{\vec{x}_1, \vec{x}_2, \vec{x}_3\} \subset \mathbb{R}^4$

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Q: find an orthog. basis for W

Sol: $\vec{v}_1 = \vec{x}_1 = \begin{bmatrix}1\\1\\0\\0\end{bmatrix}$

$$\vec{v}_2 = \vec{x}_2 - \frac{\vec{x}_2 \cdot \vec{v}_1}{\vec{v}_1 \cdot \vec{v}_1}\vec{v}_1 = \begin{bmatrix}0\\1\\1\\0\end{bmatrix} - \frac{1}{2}\begin{bmatrix}1\\1\\0\\0\end{bmatrix} = \begin{bmatrix}-1/2\\1/2\\1\\0\end{bmatrix} \xrightarrow[\text{rescaling}]{} \vec{v}_2' = \begin{bmatrix}-1\\1\\2\\0\end{bmatrix}$$

$$\vec{v}_3 = \vec{x}_3 - \frac{\vec{x}_3 \cdot \vec{v}_1}{\vec{v}_1 \cdot \vec{v}_1}\vec{v}_1 - \frac{\vec{x}_3 \cdot \vec{v}_2'}{\vec{v}_2' \cdot \vec{v}_2'}\vec{v}_2' = \begin{bmatrix}1\\1\\1\\1\end{bmatrix} - \frac{2}{2}\begin{bmatrix}1\\1\\0\\0\end{bmatrix} - \frac{2}{6}\begin{bmatrix}-1\\1\\2\\0\end{bmatrix} = \begin{bmatrix}1/3\\-1/3\\1/3\\1\end{bmatrix} \xrightarrow[\text{rescaling}]{} \vec{v}_3' = \begin{bmatrix}1\\-1\\1\\3\end{bmatrix}$$

Thus: $\left\{ \vec{v}_1 = \begin{bmatrix}1\\1\\0\\0\end{bmatrix}, \vec{v}_2' = \begin{bmatrix}-1\\1\\2\\0\end{bmatrix}, \vec{v}_3' = \begin{bmatrix}-1\\-1\\1\\3\end{bmatrix} \right\}$ - orthog. basis for W.

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Q: find an orthonormal basis for W from above

Sol: normalize $\vec{v}_1, \vec{v}_2', \vec{v}_3'$ to unit length: $\left\{ \vec{u}_1 = \frac{1}{\sqrt{2}}\begin{bmatrix}1\\1\\0\\0\end{bmatrix}, \vec{u}_2 = \frac{1}{\sqrt{6}}\begin{bmatrix}-1\\1\\2\\0\end{bmatrix}, \vec{u}_3 = \frac{1}{\sqrt{12}}\begin{bmatrix}1\\-1\\1\\3\end{bmatrix} \right\}$

- o/n basis for W.

QR factorization

THM (the QR factorization)
if A is an $m \times n$ mat. with LI columns, then A can be factored as $A = QR$ where Q is an $m\times n$ mat. whose columns form an o/n basis for Col A and R is an $n\times n$ upper triangular invertible mat. with positive diagonal entries.

Idea: $A = [\vec{x}_1 \cdots \vec{x}_n]$, $W = \underbrace{\text{Span}\{\vec{x}_1, \cdots \vec{x}_n\}}_{\text{Col}\,A} \subset \mathbb{R}^m \xrightarrow[\text{Gram-Schmidt}]{} \{\vec{u}_1, \dots, \vec{u}_n\}$ - o/n basis for W

$$\vec{x}_k = r_{1k}\vec{u}_1 + \dots + r_{k-1\,k}\vec{u}_{k-1} + \underbrace{r_{kk}}_{\|\vec{v}_k\| > 0}\vec{u}_k + 0\cdot\vec{u}_{k+1} + \dots + 0\cdot\vec{u}_n$$

$$\Rightarrow A = \underbrace{[\vec{u}_1 \cdots \vec{u}_n]}_{Q} \underbrace{\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ 0 & r_{22} & \cdots & r_{2n} \\ \vdots & 0 & \ddots & r \\ 0 & 0 & \cdots & r_{nn} \end{bmatrix}}_{R}$$

Ex: $A = \begin{bmatrix}1&0&1\\1&1&1\\0&1&1\\0&0&1\end{bmatrix}$ find the QR decomposition

Sol: $Q = [\vec{u}_1\, \vec{u}_2\, \vec{u}_3] = \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{12} \\ 1/\sqrt{2} & 1/\sqrt{6} & -1/\sqrt{12} \\ 0 & 2/\sqrt{6} & 1/\sqrt{12} \\ 0 & 0 & 3/\sqrt{12} \end{bmatrix}$

$A = QR \Rightarrow Q^TA = \underbrace{Q^TQ}_{I}R = R$

$$R = Q^TA = \begin{bmatrix} \sqrt{2} & 1/\sqrt{2} & \sqrt{2} \\ 0 & 3/\sqrt{6} & 2/\sqrt{6} \\ 0 & 0 & 4/\sqrt{12} \end{bmatrix}$$

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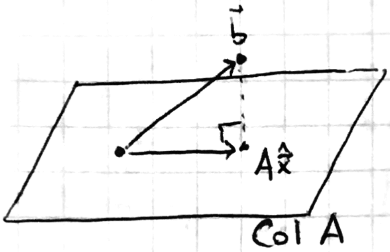
6.5. Least-squares problems

Consider $A\vec{x} = \vec{b}$ inconsistent system. Want $\hat{\vec{x}}$ s.t. $A\hat{\vec{x}}$ (approximation to $\vec{b}$) as close as possible to $\vec{b}$

for A $m\times n$ mat., $\vec{b} \in \mathbb{R}^m$, a least-squares solution 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

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

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

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

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

$\iff$ $A^T(\vec{b} - A\hat{\vec{x}}) = 0$ $\iff$ $\boxed{A^T A \hat{\vec{x}} = A^T\vec{b}}$

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

THM Set of least-squares solutions of $A\vec{x} = \vec{b}$ coincides with the (nonempty) set of solutions of the normal equations $A^T A \vec{x} = A^T \vec{b}$. (*)

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

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

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

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

Ex: in the example above, least-squares error $= \|\vec{b} - A\hat{\vec{x}}\|$
$$= \left\| \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} - \begin{bmatrix} 1 \\ 5/2 \\ 5/2 \end{bmatrix} \right\| = \left\| \begin{bmatrix} 0 \\ -1/2 \\ 1/2 \end{bmatrix} \right\| = \frac{\sqrt{2}}{2}$$

• LS solution can be non-unique.

THM Let A be $m \times n$ 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. independent

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: $A^TA=\begin{bmatrix}1 & 1\\2 & 2\end{bmatrix}\begin{bmatrix}1 & 2\\1 & 2\end{bmatrix}=\underbrace{\begin{bmatrix}2 & 4\\4 & 8\end{bmatrix}}_{\text{non-invertible}}$

$A^T\vec{b}=\begin{bmatrix}1 & 1\\2 & 2\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix}=\begin{bmatrix}1\\2\end{bmatrix}$ $\begin{bmatrix}2 & 4\\4 & 8\end{bmatrix}\underbrace{\begin{bmatrix}x_1\\x_2\end{bmatrix}}_{\hat{\vec{x}}}=\begin{bmatrix}1\\2\end{bmatrix}$

$\begin{bmatrix}2 & 4 & 1\\4 & 8 & 2\end{bmatrix}\sim\begin{bmatrix}1 & 2 & 1/2\\0 & 0 & 0\end{bmatrix}$ $\Rightarrow$ $\hat{\vec{x}}=\begin{bmatrix}1/2\\0\end{bmatrix}+x_2\begin{bmatrix}-2\\1\end{bmatrix}$ - non-unique LS solution.

x_2-free var.

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

Indeed: $\underbrace{A^TA}_{R^TQ^TQR}\hat{\vec{x}} = \underbrace{A^T\vec{b}}_{R^TQ^T\vec{b}}$ $\Big|\, R^{-1}(R^T)^{-1}$ $\Rightarrow$ $\hat{\vec{x}}=R^{-1}Q^T\vec{b}$.

$\underbrace{R^T}_{\text{invertible}}\underbrace{Q^TQ}_{I}R\hat{\vec{x}}$