# QR factorization

**Thm** (QR factorization)

If $A$ is an $m\times n$ matrix with lin. indep. columns, then $A$ can be factored as $A = QR$ where $Q$ is an $m\times n$ matrix whose columns form an o/n basis for $\operatorname{col}(A)$ and $R$ is an $n\times n$ upper-triangular invertible matrix with positive diagonal entries.

**Idea:** $A = [\vec{x}_1 \cdots \vec{x}_n]$   $W = \operatorname{col}(A) = \operatorname{Span}(\vec{x}_1, \dots, \vec{x}_n) \subset \mathbb{R}^m$

$$\Big\} \text{ Gram-Schmidt + normalization}$$

$$\{\vec{u}_1, \dots \vec{u}_n\} \text{ - o/n basis for } W$$

$$\vec{x}_k = \boxed{\operatorname{proj}_{W_{k-1}} x_k} + \boxed{\vec{v}_k} \quad \leftarrow \text{ from Gram-Schmidt}$$

$$= \boxed{r_{1k}\vec{u}_1 + \dots + r_{k-1\,k}\vec{u}_{k-1}} + \boxed{r_{kk}\vec{u}_k} + 0\cdot\vec{u}_{k+1} + \dots + 0\cdot\vec{u}_n$$

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

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**Ex:** 
$$A = \begin{array}{c} \begin{bmatrix} 1 & 0 & 1 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{bmatrix} \\ \begin{matrix} \uparrow & \uparrow & \uparrow \\ \vec{x}_1 & \vec{x}_2 & \vec{x}_3 \end{matrix} \end{array}$$

find QR factorization

- vectors from Ex*

**Sol:**
$$Q = \underbrace{[\vec{u}_1\ \vec{u}_2\ \vec{u}_3]}_{\substack{\text{normalized} \\ \text{G-S basis}}} = \boxed{\begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{6} & 1/\sqrt{12} \\ 1/\sqrt{2} & 1/\sqrt{6} & -1/\sqrt{12} \\ 0 & 2/\sqrt{6} & 1/\sqrt{12} \\ 0 & 0 & 3/\sqrt{12} \end{bmatrix}}$$

a short cut to get R: $A = QR \Rightarrow Q^T A = \underbrace{Q^T Q}_{I} R = R$

So, $R = Q^T A = \dots = \boxed{\begin{bmatrix} 2 & 1/\sqrt{2} & \sqrt{2} \\ 0 & 3/\sqrt{6} & 2/\sqrt{6} \\ 0 & 0 & 4/\sqrt{12} \end{bmatrix}}$

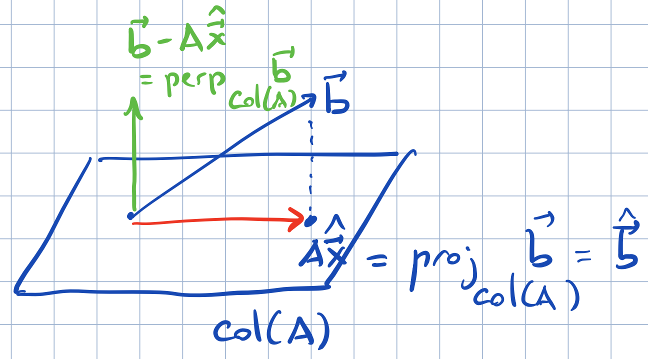
## Least squares solutions (Poole 7.3)

Let $A\vec{x} = \vec{b}$ be an inconsistent system. Want to find $\hat{\vec{x}}$ such that $\boxed{A\hat{\vec{x}}}$ is as close as possible to $\vec{b}$.

↑ approximation to $\vec{b}$

**def** For A an m×n matrix, $\vec{b} \in \mathbb{R}^m$, a least squares solution of $A\vec{x} = \vec{b}$ is $\hat{\vec{x}} \in \mathbb{R}^n$ s.t. $\|\vec{b} - A\hat{\vec{x}}\| \le \|\vec{b} - A\vec{x}\|$ for all $\vec{x} \in \mathbb{R}^n$

**Rem** textbook uses the notation $\bar{x}$, not $\hat{\vec{x}}$



## Solution of the general LS problem

$\hat{\vec{b}} = \text{proj}_{col(A)}\vec{b}$ - closest point to $\vec{b}$ on col(A)

So, $A\hat{\vec{x}} = \hat{\vec{b}} \Rightarrow \vec{b} - A\hat{\vec{x}}$ is orthogonal to col(A)

$\Leftrightarrow \vec{b} - A\hat{\vec{x}} \in (\text{col } A)^\perp = \text{null}(A^T) \Leftrightarrow A^T(\vec{b} - A\hat{\vec{x}}) = \vec{0}$

$\Leftrightarrow \boxed{A^T A \vec{x} = A^T \vec{b}}$ - "normal equations" for $A\vec{x} = \vec{b}$

**Thm** The set of least squares solutions of $A\vec{x} = \vec{b}$ coincides with the (non-empty) set of solutions of the normal equations $\boxed{A^T A \vec{x} = A^T \vec{b}}$

**Ex:** $A = \begin{bmatrix}1&0\\1&1\\1&1\end{bmatrix}$, $\vec{b} = \begin{bmatrix}1\\2\\3\end{bmatrix}$ Q: find LS solution of $A\vec{x}=\vec{b}$

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

$A^T\vec{b} = \begin{bmatrix}1&1&1\\0&1&1\end{bmatrix}\begin{bmatrix}1\\2\\3\end{bmatrix} = \begin{bmatrix}6\\5\end{bmatrix}$

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

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

In Ex above, LS error $= \|\vec{b} - A\hat{\vec{x}}\| = \left\|\begin{bmatrix}1\\2\\3\end{bmatrix} - \begin{bmatrix}1\\5/2\\5/2\end{bmatrix}\right\| = \left\|\begin{bmatrix}0\\-1/2\\1/2\end{bmatrix}\right\|$

$\left(A\hat{\vec{x}} = \begin{bmatrix}1&0\\1&1\\1&1\end{bmatrix}\begin{bmatrix}1\\3/2\end{bmatrix} = \begin{bmatrix}1\\5/2\\5/2\end{bmatrix}\right)$

$= \sqrt{0^2+(-\frac{1}{2})^2+(\frac{1}{2})^2} = \boxed{\frac{1}{\sqrt{2}}}$

- LS solution can be non-unique.

**Thm** Let $A$ be an $m\times n$ matrix. The following are equivalent:

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

(b) columns of $A$ are lin. independent

(c) $\underbrace{\underset{n\times m}{A^T}\ \underset{m\times n}{A}}_{n\times n}$ is invertible

When these hold, LS sol. 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!

$A^T\vec{b} = \begin{bmatrix}1&1\\2&2\end{bmatrix}\begin{bmatrix}1\\0\end{bmatrix} = \begin{bmatrix}1\\2\end{bmatrix}$

$\begin{bmatrix}2&4\\4&8\end{bmatrix}\begin{bmatrix}x_1\\x_2\end{bmatrix} = \begin{bmatrix}1\\2\end{bmatrix}$

aug. mat: $\left[\begin{array}{cc|c}2&4&1\\4&8&2\end{array}\right]\to\left[\begin{array}{cc|c}1&2&1/2\\0&0&0\\x_1&x_2&\end{array}\right]$   $x_1=\frac{1}{2}-2s$, $x_2=s$

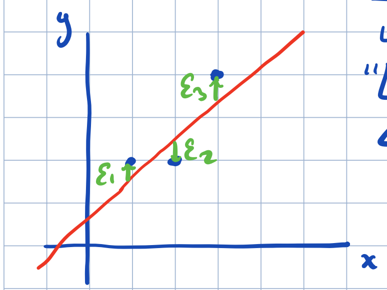
" s free

$$\boxed{\vec{x}=\begin{bmatrix}1/2\\0\end{bmatrix}+s\begin{bmatrix}-2\\1\end{bmatrix}}$$

– non-unique LS solution

## Application of LS solutions: LS approximation.

**Ex:** given data points $(1,2)$, $(2,2)$, $(3,4)$ find the line $y=a+bx$ which is the "best fit" for the points.



↑ want to have the "LS error"

$\Delta=\sqrt{\varepsilon_1^2+\varepsilon_2^2+\varepsilon_3^2}$

as small as possible

$$\left.\begin{aligned}\varepsilon_1&=2-(a+b\cdot 1)\\\varepsilon_2&=2-(a+b\cdot 2)\\\varepsilon_3&=4-(a+b\cdot 3)\end{aligned}\right\}\text{ errors}$$

So: we want a LS solution of $\underbrace{\begin{bmatrix}1&1\\1&2\\1&3\end{bmatrix}}_{A}\underbrace{\begin{bmatrix}a\\b\end{bmatrix}}_{\vec{x}}=\underbrace{\begin{bmatrix}2\\2\\4\end{bmatrix}}_{\vec{b}}$, $\begin{bmatrix}\varepsilon_1\\\varepsilon_2\\\varepsilon_3\end{bmatrix}=\vec{b}-A\vec{x}$

↑ "error vector"
– trying to minimize its norm

**normal eq.:** $\underbrace{A^TA}\hat{\vec{x}}=\underbrace{A^T\vec{b}}$

$$\begin{bmatrix}1&1&1\\1&2&3\end{bmatrix}\begin{bmatrix}1&1\\1&2\\1&3\end{bmatrix}\qquad\begin{bmatrix}1&1&1\\1&2&3\end{bmatrix}\begin{bmatrix}2\\2\\4\end{bmatrix}$$

$$\overset{\shortparallel}{\begin{bmatrix}3&6\\6&14\end{bmatrix}}\qquad\overset{\shortparallel}{\begin{bmatrix}8\\18\end{bmatrix}}$$

Aug. mat.: $\left[\begin{array}{cc|c}3&6&8\\6&14&18\end{array}\right]\to\left[\begin{array}{cc|c}1&2&8/3\\0&2&2\end{array}\right]\to\left[\begin{array}{cc|c}1&0&2/3\\0&1&1\end{array}\right]\Rightarrow\hat{\vec{x}}=\begin{bmatrix}\overset{a}{2/3}\\\underset{b}{1}\end{bmatrix}$

$\Rightarrow$ best fitting line: $y=\frac{2}{3}+x$
("least squares approximating line")

LS error: $\Delta=\|\vec{b}-A\hat{\vec{x}}\|=\left\|\begin{bmatrix}2\\2\\4\end{bmatrix}-\begin{bmatrix}5/3\\8/3\\11/3\end{bmatrix}\right\|=\left\|\begin{bmatrix}1/3\\-2/3\\1/3\end{bmatrix}\right\|=\frac{\sqrt{6}}{3}=\sqrt{\frac{2}{3}}$

$$A\hat{\vec{x}}=\begin{bmatrix}1&1\\1&2\\1&3\end{bmatrix}\begin{bmatrix}2/3\\1\end{bmatrix}=\begin{bmatrix}5/3\\8/3\\11/3\end{bmatrix}$$