ECSE 343 Numerical Methods in Engineering

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Inner Product



$$\frac{u}{\theta}$$

$$\langle u, v \rangle = |u||v|\cos(\theta)$$

$$u = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_n \end{bmatrix} \qquad v = \begin{bmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{bmatrix}$$

$$\langle u, v \rangle = \sum_{i=1}^{n} u_i v_i$$

Inner Product



$$\theta$$

$$\langle a, b \rangle = |a||b|\cos(\theta)$$

$$b = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix} \qquad a = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}$$

$$\langle a,b\rangle = \sum_{i=1}^n a_i b_i = a^T b$$

Orthogonal Projection



$$\frac{b}{p}$$
 a

$$|\boldsymbol{p}| = |\boldsymbol{b}|\cos(\boldsymbol{\theta})$$

$$\langle a, b \rangle = |a||b|\cos(\theta)$$

$$|\boldsymbol{p}| = \frac{\langle \boldsymbol{a}, \boldsymbol{b} \rangle}{|\boldsymbol{a}|} = \frac{\boldsymbol{a}^T \boldsymbol{b}}{|\boldsymbol{a}|}$$

$$p = \widehat{a}|p|$$

 \widehat{a} is the unit vector in direction of a

$$\widehat{a} = \frac{a}{|a|}$$

$$p = \frac{a}{|a|} \frac{a^T b}{|a|} = \frac{aa^T}{|a||a|} b$$

$$\boldsymbol{p} = \frac{\boldsymbol{a}\boldsymbol{a}^T}{\boldsymbol{a}^T\boldsymbol{a}}\boldsymbol{b}$$

Orthogonal Projection



$$\boldsymbol{p} = \frac{\boldsymbol{a}\boldsymbol{a}^T}{\boldsymbol{a}^T\boldsymbol{a}}\boldsymbol{b}$$

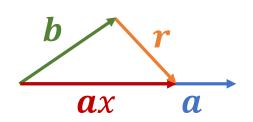
$$p = Pb$$

$$a = \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix}$$

$$P = \frac{aa^{T}}{a^{T}a}$$
Projection Matrix

Solution of One Equation





Find scalar x such that: ax = b

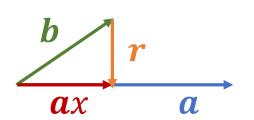
Impossible: $ax \neq b$ for all x

Minimize residual r = ax - b

i.e. minimize ||r|| = ||ax - b||

Solution of One Equation





Find scalar x such that: ax = b

Impossible: $ax \neq b$ for all x

Minimize $\mathbf{r} = \mathbf{a}x - \mathbf{b}$

i.e. minimize ||r|| = ||ax - b||

||r|| is minimum when $r \perp a$

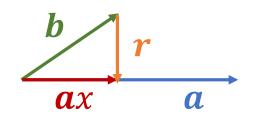
||r|| is minimum when $a^T r = 0$

||r|| is minimum when $a^T(ax - b) = 0$

 $\|r\|$ is minimum when $a^T a x = a^T b$

Solution of One Equation





$$\|r\|$$
 is minimum when $x = \frac{a^T b}{a^T a}$

 $\|r\|$ is minimum when ax is the orthogonal projection of b on a

The orthogonal projection of b on a is

$$p = ax = a\frac{a^Tb}{a^Ta} = \frac{aa^T}{a^Ta}b$$

Overdetermined System



$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ a_{41} & a_{42} & a_{43} \\ a_{51} & a_{52} & a_{53} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{bmatrix}$$
• 3 degrees of freedom (unknowns)
• 5 constraints (equations)
• Solution may or may not exist.

Least squares method: Can find approximate solution by

minimizing the residual: ||Ax - b||

$$\boldsymbol{x} = (\boldsymbol{A}^T \boldsymbol{A})^{-1} \, \boldsymbol{A}^T \boldsymbol{b}$$

Overdetermined Systems



$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ a_{41} & a_{42} & a_{43} \\ a_{51} & a_{52} & a_{53} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{bmatrix}$$

- Assume columns of A are linearly independent
- Columns of A form a 3D subspace Q of \mathbb{R}^5

Overdetermined Systems



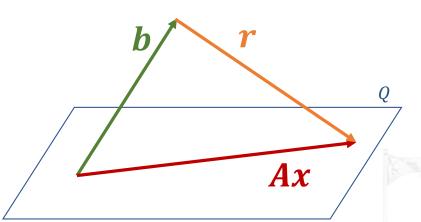
Find x such that: Ax = b

Impossible:

$$Ax \in Q$$
 $b \notin Q$

Minimize $\mathbf{r} = \mathbf{A}\mathbf{x} - \mathbf{b}$

i.e. minimize
$$||r|| = ||Ax - b||$$



Overdetermined Systems



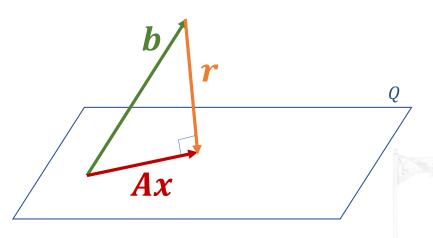
Minimize ||r|| = ||Ax - b||

$$\Rightarrow r \perp Q$$

$$\Rightarrow A^{T}(Ax - b) = 0$$

$$\Rightarrow \boxed{A^T A x = A^T b}$$

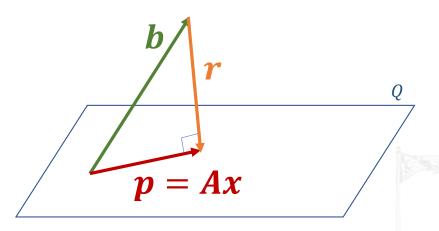
$$\Rightarrow x = (A^T A)^{-1} A^T b$$



Projection onto *Q*

$$x = (A^{T}A)^{-1}A^{T}b$$

$$p = Ax = A(A^{T}A)^{-1}A^{T}b$$
Projection Matrix



Overdetermined System



$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ a_{41} & a_{42} & a_{43} \\ a_{51} & a_{52} & a_{53} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{bmatrix}$$
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Consider n data points (t_i, y_i)

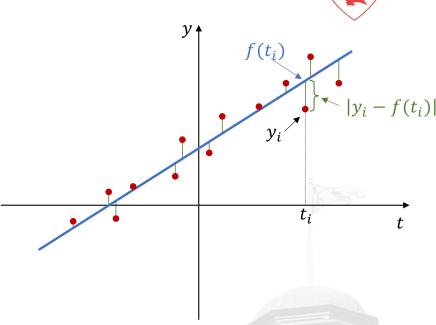
Approximate data with a model:

$$y = f(t) = a_o + a_1 t$$

 a_o and a_1 are the model parameters.

Choose the parameters to minimize:

$$e = \sum_{i=1}^{n} (f(t_i) - y_i)^2$$





Consider n data points (t_i, y_i)

$$y = f(t) = a_o + a_1 t$$

Choose the parameters to minimize: $e = \sum_{i=1}^{n} (f(t_i) - y_i)^2$

Let:
$$r \equiv \begin{bmatrix} f(t_1) - y_1 \\ \vdots \\ f(t_i) - y_i \\ \vdots \\ f(t_n) - y_n \end{bmatrix}$$
 Then: $e = r^T r = ||r||_2^2$

Then:
$$e=oldsymbol{r}^Toldsymbol{r}=\|oldsymbol{r}\|_2^2$$





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$$y = f(t) = a_o + a_1 t$$

$$r = \begin{bmatrix} f(t_1) - y_1 \\ \vdots \\ f(t_i) - y_i \\ \vdots \\ f(t_n) - y_n \end{bmatrix} = \begin{bmatrix} a_o + a_1 t_1 - y_1 \\ \vdots \\ a_o + a_1 t_i - y_i \\ \vdots \\ a_o + a_1 t_n - y_n \end{bmatrix} = \begin{bmatrix} 1 & t_1 \\ \vdots & \vdots \\ 1 & t_i \\ \vdots & \vdots \\ 1 & t_n \end{bmatrix} \begin{bmatrix} a_o \\ a_1 \end{bmatrix} - \begin{bmatrix} y_1 \\ \vdots \\ y_i \\ \vdots \\ y_n \end{bmatrix}$$

Minimize: $e = \mathbf{r}^T \mathbf{r} = ||\mathbf{r}||_2^2$

Overdetermined System



$$\begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \\ a_{41} & a_{42} & a_{43} \\ a_{51} & a_{52} & a_{53} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \end{bmatrix}$$
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$$\begin{bmatrix} 1 & t_1 \\ \vdots & \vdots \\ 1 & t_i \\ \vdots & \vdots \\ 1 & t_n \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_i \\ \vdots \\ y_n \end{bmatrix}$$

$$Ax = b$$

The parameters that result in a least squares approximation are the solution of:

$$A^T A x = A^T b$$



Consider n data points (t_i, y_i)

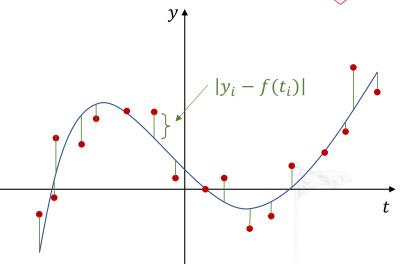
Approximate data with a model:

$$y = f(t) = a_0 + a_1 t + a_2 t^2 + a_3 t^3 + \cdots$$

 a_0 , a_1 , ... are the model <u>parameters</u>.

Choose the parameters to minimize:

$$e = \sum_{i=1}^{n} (f(t_i) - y_i)^2$$





Consider n data points (t_i, y_i)

$$y = f(t) = a_0 + a_1t + a_2t^2 + a_3t^3 + \cdots$$

 $y=f(t)=a_o+a_1t+a_2t^2+a_3t^3+\cdots$ Choose the parameters to minimize: $e=\sum_{i=1}^n(f(t_i)-y_i)^2$

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Then:
$$e = oldsymbol{r}^T oldsymbol{r} = \|oldsymbol{r}\|_2^2$$





Consider n data points (t_i, y_i)

$$y = f(t) = a_0 + a_1 t + a_2 t^2 + a_3 t^3$$

$$\mathbf{r} = \begin{bmatrix} f(t_1) - y_1 \\ \vdots \\ f(t_i) - y_i \\ \vdots \\ f(t_n) - y_n \end{bmatrix} = \begin{bmatrix} a_o + a_1 t_1 + a_2 t_1^2 + a_3 t_1^3 - y_1 \\ \vdots \\ a_o + a_1 t_i + a_2 t_i^2 + a_3 t_i^3 - y_i \\ \vdots \\ a_o + a_1 t_n + a_2 t_n^2 + a_3 t_n^3 - y_n \end{bmatrix}$$







Consider n data points (t_i, y_i)

$$y = f(t) = a_0 + a_1 t + a_2 t^2 + a_3 t^3$$

$$\boldsymbol{r} = \begin{bmatrix} f(t_1) - y_1 \\ \vdots \\ f(t_i) - y_i \\ \vdots \\ f(t_n) - y_n \end{bmatrix} = \begin{bmatrix} 1 & t_1 & t_1^2 & t_1^3 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & t_i & t_i^2 & t_i^3 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & t_n & t_n^2 & t_n^3 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} - \begin{bmatrix} y_1 \\ \vdots \\ y_i \\ \vdots \\ y_n \end{bmatrix}$$





$$\begin{bmatrix} 1 & t_1 & t_1^2 & t_1^3 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & t_i & t_i^2 & t_i^3 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & t_n & t_n^2 & t_n^3 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_i \\ \vdots \\ y_n \end{bmatrix}$$

$$Ax = b$$

The parameters that result in a least squares approximation are the solution of:

$$A^T A x = A^T b$$

Vandermonde Matrix



Γ1	t_1	t_{1}^{2}	t_{1}^{3}	• • •	t_1^m
	•	•	•		•
1	t_i	t_i^2	t_i^3	•••	t_i^m
 :	•	•	•		•
L1	t_n	t_n^2	t_n^3	• • •	$t_n^m \rfloor$

The Vandermonde Matrix is well known to be ill-conditioned

Conditioning of the Normal Equations



$$A^T A x = A^T b$$

$$\operatorname{cond}\{A^T A\} \cong \operatorname{cond}\{A\}^2$$

Can be very ill-conditioned.





$$\begin{bmatrix} 1 & t_1 & t_1^2 & t_1^3 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & t_i & t_i^2 & t_i^3 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & t_n & t_n^2 & t_n^3 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_i \\ \vdots \\ y_n \end{bmatrix}$$

$$Ax = b$$

- If the problem is ill-conditioned
- Impose an additional constraint that ||x|| is small.



$$Ax = b$$

The solution of $A^T A x = A^T b$

minimizes the residual: $\min_{x} ||Ax - b||_{2}^{2}$

Instead, minimize: $\min_{x} \{ \|Ax - b\|_{2}^{2} + \lambda^{2} \|x\|_{2}^{2} \}$



$$\begin{bmatrix} A \\ \lambda U \end{bmatrix} x = \begin{bmatrix} b \\ 0 \end{bmatrix}$$

$$r = \begin{bmatrix} A \\ \lambda U \end{bmatrix} x - \begin{bmatrix} b \\ 0 \end{bmatrix} = \begin{bmatrix} Ax - b \\ \lambda x \end{bmatrix}$$

$$||r||_2^2 = r^T r = ||Ax - b||_2^2 + \lambda^2 ||x||_2^2$$



$$\begin{bmatrix} \mathbf{A} \\ \lambda \mathbf{U} \end{bmatrix} \mathbf{x} = \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix}$$

Normal Equation:

$$\begin{bmatrix} \mathbf{A}^T & \lambda \mathbf{U} \end{bmatrix} \begin{bmatrix} \mathbf{A} \\ \lambda \mathbf{U} \end{bmatrix} \mathbf{x} = \begin{bmatrix} \mathbf{A}^T & \lambda \mathbf{U} \end{bmatrix} \begin{bmatrix} \mathbf{b} \\ \mathbf{0} \end{bmatrix}$$

$$\boldsymbol{x} = [\boldsymbol{A}^T$$

$$[\lambda U]$$

$$(A^TA + \lambda^2 U)x = A^Tb$$



Conditioning of the Normal Equations



$$A^T A x = A^T b$$

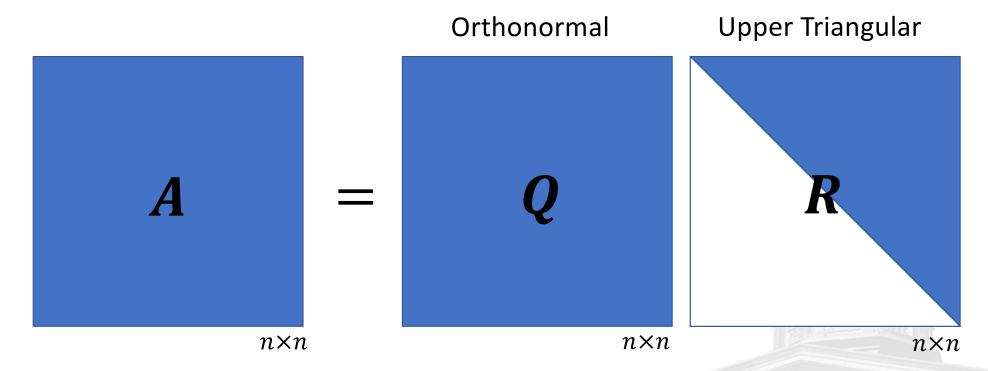
$$\operatorname{cond}\{A^T A\} \cong \operatorname{cond}\{A\}^2$$

Can be very ill-conditioned.

Can we avoid the Normal Equations?

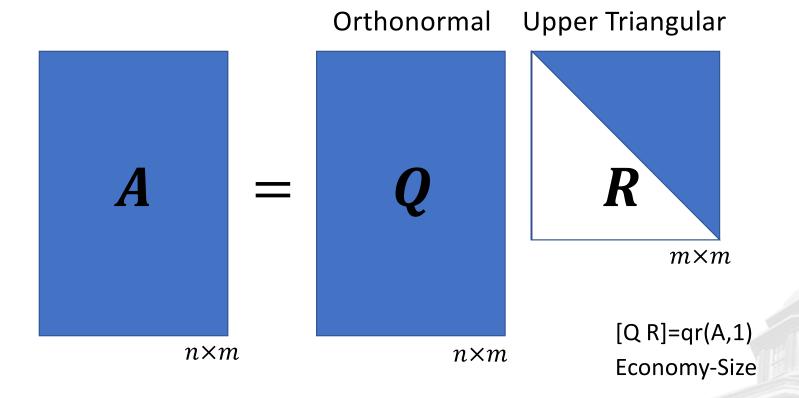
QR Decomposition





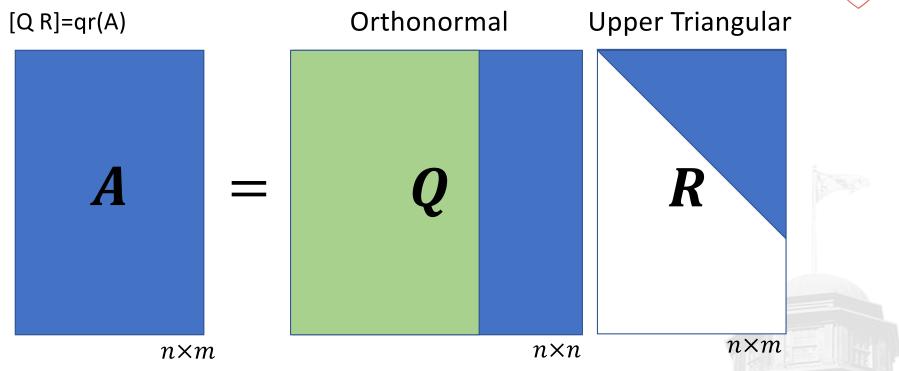
QR Decomposition





QR Decomposition





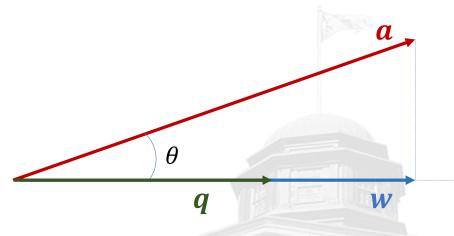
Projectors Review



$$\|q\|_{2} = 1$$

$$\langle \boldsymbol{a}, \boldsymbol{q} \rangle = \boldsymbol{q}^{T} \boldsymbol{a} = \|\boldsymbol{q}\|_{2} \|\boldsymbol{a}\|_{2} \cos(\theta) = \|\boldsymbol{a}\|_{2} \cos(\theta)$$

$$\boldsymbol{w} = \boldsymbol{q} \langle \boldsymbol{a}, \boldsymbol{q} \rangle = \boldsymbol{q} \boldsymbol{q}^{T} \boldsymbol{a}$$





Orthonormal

$$\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \cdots \begin{bmatrix} a_m \\ a_m \end{bmatrix} = \begin{bmatrix} q_1 \\ q_1 \end{bmatrix} \begin{bmatrix} q_2 \\ q_2 \end{bmatrix} \cdots \begin{bmatrix} q_m \\ q_m \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & r_{13} & \cdots & r_{1m} \\ r_{22} & r_{23} & \cdots & r_{2m} \\ r_{33} & \cdots & r_{3m} \\ \vdots & \vdots & \vdots \\ r_{mm} \end{bmatrix}$$

$$\boldsymbol{q}_i^T \boldsymbol{q}_j = \begin{cases} 1 ; i = j \\ 0 ; i \neq j \end{cases}$$



$$\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \cdots \begin{bmatrix} a_m \\ a_m \end{bmatrix} = \begin{bmatrix} q_1 \\ q_1 \end{bmatrix} \begin{bmatrix} q_2 \\ q_2 \end{bmatrix} \cdots \begin{bmatrix} q_m \\ q_m \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & r_{13} & \cdots & r_{1m} \\ r_{22} & r_{23} & \cdots & r_{2m} \\ r_{33} & \cdots & r_{3m} \\ \vdots & \vdots & \vdots \\ r_{mm} \end{bmatrix}$$

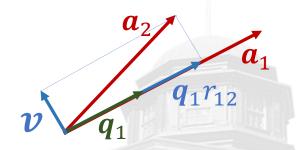
$$\left\| \mathbf{q}_{1} \right\| = \mathbf{q}_{1} r_{11}$$
 $\left\| \mathbf{q}_{1} \right\| = 1$
 $r_{11} = \left\| \mathbf{a}_{1} \right\|$
 $r_{11} = \left\| \mathbf{a}_{1} \right\|$
 $r_{11} = \left\| \mathbf{a}_{1} \right\|$





$$\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \cdots \begin{bmatrix} a_m \\ a_m \end{bmatrix} = \begin{bmatrix} q_1 \\ q_2 \end{bmatrix} \cdots \begin{bmatrix} q_m \\ q_m \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & r_{13} & \cdots & r_{1m} \\ r_{22} & r_{23} & \cdots & r_{2m} \\ r_{33} & \cdots & r_{3m} \\ \vdots & \vdots & \vdots \\ r_{mm} \end{bmatrix}$$

$$m{a}_2 = m{q}_1 r_{12} + m{q}_2 r_{22}$$
 $m{q}_1^T m{a}_2 = m{q}_1^T m{q}_1 r_{12} + m{q}_1^T m{q}_2 r_{22} = r_{12}$
 $m{v} = m{a}_2 - m{q}_1 r_{12} = m{q}_2 r_{22}$
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$$\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \cdots \begin{bmatrix} a_m \\ a_m \end{bmatrix} = \begin{bmatrix} q_1 \\ q_1 \end{bmatrix} \begin{bmatrix} q_2 \\ q_2 \end{bmatrix} \cdots \begin{bmatrix} q_m \\ q_m \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & r_{13} & \cdots & r_{1m} \\ r_{22} & r_{23} & \cdots & r_{2m} \\ & & & r_{33} & \cdots & r_{3m} \\ & & & \ddots & \vdots \\ & & & & r_{mm} \end{bmatrix}$$

$$||v = q_2 r_{22}|$$
 $||v||$ $||q_2|| = 1$ $||v||$ $||q_2|| = \frac{v}{r_{22}}$





$$\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \quad \cdots \quad \begin{bmatrix} a_m \\ a_m \end{bmatrix} = \begin{bmatrix} q_1 \\ q_2 \end{bmatrix} \quad \cdots \quad \begin{bmatrix} q_m \\ q_m \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & r_{13} & \cdots & r_{1m} \\ r_{22} & r_{23} & \cdots & r_{2m} \\ & & & r_{33} & \cdots & r_{3m} \\ & & & \ddots & \vdots \\ & & & & r_{mm} \end{bmatrix}$$

$$a_3 = q_1 r_{13} + q_2 r_{23} + q_3 r_{33}$$

$$\mathbf{q}_1^T \mathbf{a}_3 = r_{13}$$
$$\mathbf{q}_2^T \mathbf{a}_3 = r_{23}$$

$$v = a_3 - q_1 r_{13} - q_2 r_{23} = q_3 r_{33}$$



$$\begin{bmatrix} a_1 \\ a_2 \end{bmatrix} \cdots \begin{bmatrix} a_m \\ a_m \end{bmatrix} = \begin{bmatrix} q_1 \\ q_1 \end{bmatrix} \begin{bmatrix} q_2 \\ q_2 \end{bmatrix} \cdots \begin{bmatrix} q_m \\ q_m \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & r_{13} & \cdots & r_{1m} \\ r_{22} & r_{23} & \cdots & r_{2m} \\ & & & r_{33} & \cdots & r_{3m} \\ & & & \ddots & \vdots \\ & & & & r_{mm} \end{bmatrix}$$

$$||v| = q_3 r_{34}$$
 $||v|| = 1$ $||v||$ $||q_3|| = 1$ $||v||$ $||q_3|| = \frac{v}{r_{33}}$