Lecture 6: Least Squares Problem, Householder and Serial Gram-Schmidt Orthogonalization Methods

Prof. Krishna R. Pattipati

Dept. of Electrical and Computer Engineering
University of Connecticut
Contact: krishna@engr.uconn.edu (860) 486-2890

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Outline of Lecture 6

- Why orthogonalization methods ?
- Least Squares Problem and its properties
- Householder transformation
- Gram-Schmidt orthogonalization
    - Serial (classical) Gram-Schmidt
    - Parallel (modified) Gram-Schmidt

Why Orthogonalization Methods ?

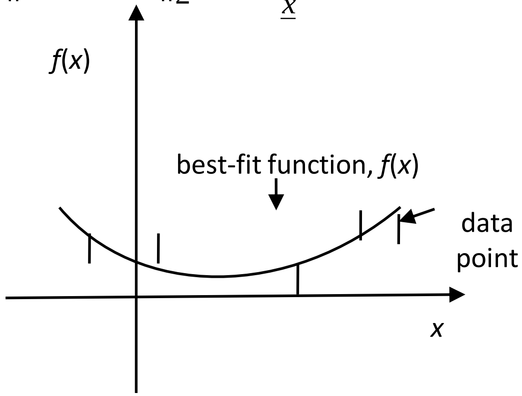
- Orthogonalization methods are ubiquitous in scientific computation
  - Used in Chebyshev orthogonal polynomials for function approximation (Lectures 2 and 3)
  - We like orthogonal descent directions in function minimization ⇒ conjugate directions (so-called *Q*-orthogonal directions (lecture 5))
  - Representation of random functions as weighted sum of orthogonal functions (e.g., Karhunen-Loeve expansion, sum of sinusoids or complex exponentials)
  - Orthogonal transformations: Householder, Gram-Schmidt, and Givens. Useful in Least Squares Estimation, Eigen value problems (QR), Lyapunov equations, and Riccati equations.
- To motivate the methods, consider a system of linear equations:

$A\underline{x} = \underline{b}$, A is $m \times n$, $m \gg n$

Least Squares Problem

- The Least Squares problem:

$$\min_{\underline{x}} \tfrac{1}{2}\|A\underline{x}-\underline{b}\|_2^2 = \min_{\underline{x}} \tfrac{1}{2}(A\underline{x}-\underline{b})^T(A\underline{x}-\underline{b})$$



Least squares estimate minimizes the vertical distance from the data points to the model

- Weighted Least Squares Problem:

$$\min_{\underline{x}} \tfrac{1}{2}\|A\underline{x}-\underline{b}\|_{V^{-1}}^2 = \min_{\underline{x}} \tfrac{1}{2}(A\underline{x}-\underline{b})^T V^{-1}(A\underline{x}-\underline{b})$$

where V is typically diagonal (i.e., V=diag($\sigma_1^2\ \sigma_2^2 \ldots \sigma_m^2$)). σ_i^2 is a measure of uncertainty (error) in the measurement b_i.

- Other Formulations

$$\left.\begin{array}{l}\min_{\underline{x}}\|A\underline{x}-\underline{b}\|_1\\ \min_{\underline{x}}\|A\underline{x}-\underline{b}\|_\infty\end{array}\right)$$ can be solved via Linear Programming (LP) .. Lecture 9

- 1-norm is less sensitive to the presence of "outliers" (bad data).

Example of Least Squares Problem- 1

- Example:
  - $b_i = x + e_i$
  - Criteria to be minimized

2-norm : $\min \sum_i (b_i - x)^2 \Rightarrow \hat{x}_2 =$ average of the b_i^S

1-norm : $\min \sum_i | b_i - x | \Rightarrow \hat{x}_1 =$ median of the b_i^S

∞-norm : $\min \max_i |b_i - x| \Rightarrow \hat{x}_\infty = \frac{1}{2}(\min_i \; b_i + \max_i \; b_i)$

- Consider the data set $\{b_i\}=\{1\ 2\ 3\ 5\ 8\}$

$$\hat{x}_2 = 3.8$$
$$\hat{x}_1 = 3$$
$$\hat{x}_\infty = 4.5$$

- Suppose that a mistake has been made and the last data point is thought to be 88 rather than 8. Then

$$\hat{x}_2 = 19.8$$
$\hat{x}_1 = 3$ the least affected by errors
$$\hat{x}_\infty = 44.5$$

Example of Least Squares Problem - 2

- We will use 2-norm in this and the next two lectures.
- Solution procedures for 1- and ∞- norm in Lecture 9.

❑ Why 2-norm:

- Because it is a twice continuously differentiable function
- Has nice statistical interpretation in terms of maximum likelihood estimation for Gaussian error models

❑ Example: Function approximation by a weighted sum of complex exponentials.

$$f(t) = \sum_{i=1}^{n} x_i e^{j\omega_i t}$$

- Suppose we sample the function at $t=0,T,2T,\ldots,(m\text{-}1)T$
- Then $f(kT) = \sum_{i=1}^{n} x_i e^{jk\omega_i T} = \sum_{i=1}^{n} x_i z^k;\; z = e^{j\omega_i T};\; k = 0,1,2,\ldots,(m-1)$
- The $(A, \underline{b})$ associated with the least squares problem are

$$A = \begin{bmatrix} 1 & 1 & \ldots & 1 \\ z_1 & z_2 & \ldots & z_n \\ z_1^2 & z_2^2 & \ldots & z_n^2 \\ \vdots & \vdots & & \vdots \\ z_1^{m-1} & z_2^{m-1} & \ldots & z_n^{m-1} \end{bmatrix};\; \underline{b} = \begin{bmatrix} f(0) \\ f(T) \\ f(2T) \\ \vdots \\ f((m-1)T) \end{bmatrix}$$

Rectangular Van der Monde Matrix

LS Problem Basics

- What do orthogonal transformations do for us?
  - Suppose have made an orthogonal transformation on A such that A is transformed into $Q^T A$

    $\Rightarrow \min_{\underline{x}} \frac{1}{2}\|Q^T A\underline{x} - Q^T \underline{b}\|_2^2$ is unchanged since $QQ^T = Q^T Q = I$
  - KEY IDEA: choose Q such that $Q^T A$ has nice form (e.g., upper Δ)
- What are the properties of LS solution?

$$\min J = \frac{1}{2}\left[\underline{x}^T A^T A \underline{x} - \underline{x}^T A^T \underline{b} - \underline{b}^T A^T \underline{x} + \underline{b}^T \underline{b}\right]$$

$$\partial J / \partial \underline{x} = 0 \Rightarrow A^T A \underline{x}_{LS} = A^T \underline{b}$$

$$\text{or } A^T[\underline{b} - A\underline{x}_{LS}] = \underline{0}$$

These are the so-called normal equations. Bad way to solve. We will come back to this later.

- $\underline{r} = \underline{b} - A\underline{x}_{LS}$ is called the residual vector = measurement - predicted measurement
- Recall the linear spaces associated with $A\underline{x} = \underline{b}$:
  - $R(A)$ = column space of $A \in R^m$
  - $N(A)$ = Null space of $A \in R^n$
- Linear spaces associated with
  - $R(A^T)$ = column space of $A \in R^n$
  - $N(A^T)$ = Null space of $A^T \in R^m$
- Know
  - $\dim(R(A)) + \dim(N(A^T)) = m$
  - $\dim(N(A)) + \dim(R(A^T)) = n$

Least Squares Solution Properties - 1

Orthogonal property of least squares

- $A^T \underline{r} = \underline{0} \Rightarrow \underline{r} \in N(A^T)$
- Since $R(A)$ is perpendicular to $N(A^T) \Rightarrow \underline{r}$ is perpendicular to $R(A)$
- $A\,\underline{x}_{LS} \Rightarrow$ linear combinations of columns of $A \in R(A)$
- Since $R(A)$ is perpendicular to $N(A^T)$

$$A\underline{x}_{LS} \in R(A) \perp \underline{r} \in N(A^T) \Rightarrow A\underline{x}_{LS} \perp \underline{r}$$

What does *LS* do?

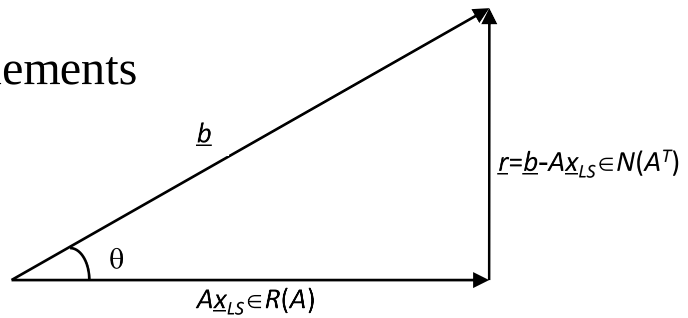
- Decomposes $\underline{b}$ into two **orthogonal** complements

  $A\,\underline{x}_{\mathrm{LS}} \in R(A)$ and $\underline{r} = \underline{b} - A\,\underline{x}_{LS} \in N(A^T)$

  $$\Rightarrow \|\underline{b}\|_2^2 = \|A\underline{x}_{LS}\|_2^2 + \|\underline{r}\|_2^2$$

  $$\cos\theta = \frac{\|A\underline{x}_{LS}\|_2}{\|\underline{b}\|_2}, \sin\theta = \frac{\|\underline{r}\|_2}{\|\underline{b}\|_2}$$

  For $m=n=\mathrm{Rank}(A)$ $\theta=0 \Rightarrow A\underline{x}_{LS} = \underline{b}$



- $A\underline{x}_{LS}$ is a "prediction" of what $\underline{b}$ is
- It is correct for full rank and $m \le n$ case
- If $m < n$ and full rank, $\exists$ an infinite # of solutions to $A\underline{x} = \underline{b}$

Least Squares Solution Properties - 2

- We will then ask for that $\underline{x}$ which has minimum 2-norm (i.e., smallest $\|x\|_2$ $\ni A\underline{x}=\underline{b}$).
- When rank$(A)=n$, $m>n$,

  $\underline{x}_{LS}=(A^TA)^{-1}A^T\underline{b}=A^{\dagger}\underline{b}$

  where $A^{\dagger}$= Moore-Penrose generalized (pseudo) inverse
- So, predicted measurement:

  $A\underline{x}_{LS}=A(A^TA)^{-1}A^T\underline{b}=AA^{\dagger}\underline{b}=P\underline{b}$

  where P~ projection matrix
- P is called Orthogonal projection onto $R(A)$ (very useful in constrained optimization)

$\Rightarrow \underline{r}=(I-P)\underline{b}$

❑ Properties of orthogonal Projections:

- $P=P^T$ (Symmetric)
- $P^2=P$ (idempotent)
- $(I-P)^2=(I-P)$ (idempotent)
- $PA=A$ or $(I-P)A=0$

$$\Rightarrow PA\underline{x}_{LS}=A\underline{x}_{LS}$$
$$(I-P)\,\underline{r} = (I-P)^2\underline{b} = \underline{r} \Rightarrow P\underline{r} = \underline{0}$$

Least Squares Solution Properties - 3

- Note 1: Standard deviation of the residuals is given by

$$\sigma_r = \frac{\|\underline{b} - A\underline{x}_{LS}\|_2}{\sqrt{m-n}} = \frac{\|\underline{r}\|_2}{\sqrt{m-n}}$$

  - 95% of the scaled residuals r_i/σ_r should lie in the interval [-2,2]. If not, there may be a problem with the data or model or both. See:
    - S. Chatterjee and B. Price, Regression Analysis by Example, Wiley: New York, 1977.
    - P. A. Belsey, E. Kuh and R. Welsh, Regression Diagnostics: Identifying Influential Data and Source of Collinearity, Wiley: New York, 1981.
- Note 2: $A^\dagger$ is defined for rank deficient cases also (See Lecture 7)
  - In the general case, $A^\dagger$ satisfies Moore-Penrose conditions:

$A A^\dagger A = A$; $AA^\dagger = (AA^\dagger)^T$; $A^\dagger A = (A^\dagger A)^T$; $A^\dagger A A^\dagger = A^\dagger$

$AA^\dagger \sim$ orthogonal projection onto $R(A) = P$

$A^\dagger A \sim$ orthogonal projection onto $R(A^T)$

$\underline{x}_{LS} = A^\dagger \underline{b} = A^\dagger A \underline{x}$;

$\Rightarrow A^\dagger A \underline{x}$ belongs to $R(A^T)$. This will become clear from the following SVD analysis

LS Solution & SVD

- Further insights into LS problem using SVD

$$A = U\Sigma V^T \qquad \Sigma = \begin{bmatrix} \Sigma_r & 0 \\ 0 & 0 \end{bmatrix} \qquad r = \text{rank of } A$$

$$= \sum_{i=1}^{r} \sigma_i \underline{u}_i \underline{v}_i^T \qquad \text{U}=(\underline{u}_1\ \underline{u}_2\ \ldots\ \underline{u}_m); \qquad \text{V}=(\underline{v}_1\ \underline{v}_2\ \ldots\ \underline{v}_n);$$

$$R(A)=(\underline{u}_1\ \underline{u}_2\ \ldots\ \underline{u}_r); \qquad R(A^T)=(\underline{v}_1\ \underline{v}_2\ \ldots\ \underline{v}_r);$$

$$N(A)=(\underline{v}_{r+1}\ \ldots\ \underline{v}_n); \qquad N(A^T)=(\underline{u}_{r+1}\ \ldots\ \underline{u}_m);$$

$$J = \|A\underline{x}-\underline{b}\|_2^2 = \|U^T A\underline{x} - U^T\underline{b}\|_2^2 = \|U^T AVV^T\underline{x} - U^T\underline{b}\|_2^2$$

$$\text{Let } \underline{y} = V^T\underline{x} \Rightarrow J = \|\Sigma\underline{y} - U^T\underline{b}\|_2^2 = \sum_{i=1}^{r}(\sigma_i y_i - \underline{u}_i^T\underline{b})^2 + \sum_{i=r+1}^{m}(\underline{u}_i^T\underline{b})^2$$

$$\Rightarrow \underline{y}_i = \begin{cases} \dfrac{\underline{u}_i^T\underline{b}}{\sigma_i}; & 1 \le i \le r \\ 0 & \text{otherwise} \end{cases}$$

$$\Rightarrow \underline{x} = V\underline{y} \Rightarrow \underline{x} = \sum_{i=1}^{r} y_i \underline{v}_i$$

- If $\underline{x}_{LS}$ solves the LS problem, then

$$\underline{x}_{LS} = \sum_{i=1}^{r}\left(\frac{\underline{u}_i^T\underline{b}}{\sigma_i}\right)\underline{v}_i \qquad \Rightarrow \underline{x}_{LS} \in R(A^T)$$

LS Solution Properties

$$\Rightarrow \quad A\underline{x}_{LS} = \sum_{k=1}^{r}\sum_{i=1}^{r}(\sigma_i \underline{u}_i \underline{v}_i^T)(\frac{\underline{u}_k^T \underline{b}}{\sigma_k})\underline{v}_k = \sum_{i=1}^{r} \underline{u}_i \underline{u}_i^T \underline{b} = \sum_{i=1}^{r} (\underline{u}_i^T \underline{b})\underline{u}_i \in R(A)$$

Note that Orthogonal Projection $P = \sum_{i=1}^{r} \underline{u}_i \underline{u}_i^T$ and $A\underline{x}_{LS} = P\underline{b}$

$$\Rightarrow \quad \underline{r} = \underline{b} - A\underline{x}_{LS} = \sum_{i=1}^{m} \underline{u}_i \underline{u}_i^T \underline{b} - \sum_{i=1}^{r} (\underline{u}_i^T \underline{b})\underline{u}_i = \sum_{i=r+1}^{m} (\underline{u}_i^T \underline{b})\underline{u}_i = (I-P)\underline{b} \in N(A^T)$$

$$J_{opt} = \sum_{i=r+1}^{m} (\underline{u}_i^T \underline{b})^2 = \|(I - AA^\dagger)\underline{b}\|_2^2 = \|(I-P)\underline{b}\|_2^2 = \|\underline{r}\|_2^2$$

$A\underline{x}_{LS} = P\underline{b}$ $\Rightarrow$ orthogonal projection onto $R(A)$

$\underline{x}_{LS} \in R(A^T) \Rightarrow A^\dagger A$ is orthogonal projection onto $R(A^T)$

Since $\underline{x}_{LS} = A^\dagger \underline{b} = A^\dagger A \underline{x}$

$A^\dagger = V\Sigma^\dagger U^T$

$\Sigma^\dagger = Diag(\sigma_1^{-1} \ \sigma_2^{-1} \ \ldots \ \sigma_r^{-1} \ 0 \ \ldots. \ 0)$

Also, $A^\dagger$ minimizes: (whenever A is full rank)

$$\min_X \|AX - I_m\|_F = \min_X tr\left[(AX - I_m)^T (AX - I_m)\right]$$

$$\Rightarrow \min_X tr\left[X^T A^T AX - X^T A^T - AX + I_m\right]$$

$$\Rightarrow A^T AX = A^T \Rightarrow X = (A^T A)^{-1} A^T = A^\dagger$$

How to Solve LS Problems?

- Let us return to the normal equations. $A^TA\,\underline{x}=A^T\,\underline{b}$.
  Assume full rank: Rank(A)=n
- One way:
  - Form Cholesky decomposition of $A^TA=LDL^T$ or SS^T and solve $S\underline{y}=A^T\underline{b}$; $S^T\underline{x}=\underline{y}$
- Problems
  - Must form $A^TA \approx O(n^3/2)$
  - Cholesky of $A^TA \approx O(n^3/6)$

$$Error \propto \kappa(A^TA) = \frac{\lambda_{\max}(A^TA)}{\lambda_{\min}(A^TA)} = \left[\frac{\sigma_{\max}(A)}{\sigma_{\min}(A)}\right]^2 = [\kappa(A)]^2$$

  - There exist other stable methods of solving $A\underline{x}=\underline{b}$ when $m \gg n$ and rank(A)=n
  - We will consider deficient rank case later in computing $A^\dagger$
- These stable methods are:
  - Householder
  - Gram-Schmidt (serial & Parallel) and
  - Givens orthogonalization methods.

Key Idea of Orthogonalization Methods

- Key idea of all three methods:
  - Find an $m \times n$ orthogonal matrix $Q \ni Q^T A = R = \begin{bmatrix} R_1 \\ 0 \end{bmatrix}$ where R_1 is upper $\Delta \Rightarrow A=QR$
  - Do the same thing to $\underline{b} \Rightarrow Q^T \underline{b} = \begin{matrix} n \\ m-n \end{matrix}\begin{bmatrix} \underline{c} \\ \underline{d} \end{bmatrix}$
  - Then

$$\left\|A\underline{x}-\underline{b}\right\|_2^2 = \left\|Q^T A\underline{x}-Q^T\underline{b}\right\|_2^2 = \left\|\begin{bmatrix} R_1 \\ 0 \end{bmatrix}\underline{x} - \begin{bmatrix} \underline{c} \\ \underline{d} \end{bmatrix}\right\|_2^2 = \left\|R_1\underline{x}-\underline{c}\right\|_2^2 + \left\|\underline{d}\right\|_2^2$$

$$\forall \underline{x} \in R^n$$

  - If rank(A)=n, R_1 is invertible $\Rightarrow \left\|A\underline{x}-\underline{b}\right\|_2^2 = \left\|\underline{d}\right\|_2^2$ if $\underline{x}_{LS} = R_1^{-1}\underline{b}$
- Householder transformations to compute R_1
  - Basic Idea: If have a vector $\underline{a}$=(a_1 a_2 … a_m)^T, then it is possible to find an orthogonal matrix W such that

$$W\begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \end{bmatrix} = \begin{bmatrix} \alpha \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

  - Since orthogonal matrices do not change the 2-norm, $\alpha = \pm\left\|a\right\|_2$

Householder Method

- Suppose we have a way of getting W. What does it mean in terms of solving the over determined system of equations $A\underline{x}=\underline{b}$ ($m>n$)
- Illustrative example: $m=6$, $n=4$

$$\begin{bmatrix} x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \\ x & x & x & x \end{bmatrix} \xrightarrow{W_1} \begin{bmatrix} \alpha & y & y & y \\ 0 & y & y & y \\ 0 & y & y & y \\ 0 & y & y & y \\ 0 & y & y & y \\ 0 & y & y & y \end{bmatrix} \xrightarrow{W_2} \begin{bmatrix} \alpha & y & y & y \\ 0 & \beta & * & * \\ 0 & 0 & * & * \\ 0 & 0 & * & * \\ 0 & 0 & * & * \\ 0 & 0 & * & * \end{bmatrix} \xrightarrow{W_3} \begin{bmatrix} \alpha & y & y & y \\ 0 & \beta & * & * \\ 0 & 0 & \gamma & z \\ 0 & 0 & 0 & z \\ 0 & 0 & 0 & z \\ 0 & 0 & 0 & z \end{bmatrix}$$

$$\xrightarrow{W_4} \begin{bmatrix} \alpha & y & y & y \\ 0 & \beta & * & * \\ 0 & 0 & \gamma & z \\ 0 & 0 & 0 & \Delta \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} R_1 \\ --- \\ 0 \end{bmatrix} \quad \Rightarrow W_4 W_3 W_2 W_1 A = R \Rightarrow Q^T A = R$$

❑ W=Householder matrix or Householder transformation (reflection matrix)

$$= \left[I - \frac{2\underline{u}\,\underline{u}^T}{\underline{u}^T\underline{u}} \right] = \left[I - 2\frac{\underline{u}}{\|\underline{u}\|_2}\frac{\underline{u}^T}{\|\underline{u}\|_2} \right] = \left[I - 2\underline{v}\,\underline{v}^T \right]; \ \underline{v} = \frac{\underline{u}}{\|\underline{u}\|_2} \quad \text{~unit vector}$$

$\Rightarrow W$ is symmetric $\Rightarrow W = W^T$

What does Householder Matrix do?

$\Rightarrow$ W is also orthogonal because

$$W^2 = I - 2\frac{\underline{u}\underline{u}^T}{\underline{u}^T\underline{u}} - 2\frac{\underline{u}\underline{u}^T}{\underline{u}^T\underline{u}} + 4\frac{\underline{u}\underline{u}^T\underline{u}^T\underline{u}}{(\underline{u}^T\underline{u})^2} = I$$

$W^{-1}=W=W^T \Rightarrow$ orthogonal

- So, Householder matrix W is ORTHOGONAL and SYMMETRIC

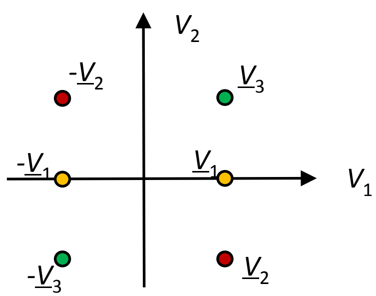
- What does W do? if $\underline{v} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$, $W = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$

$\Rightarrow$ $det\ W$ = -1 also $W\underline{v}_1 = -\underline{v}_1$

$$\underline{v}_2 = \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix} \Rightarrow W\underline{v}_2 = -\underline{v}_2 = \begin{bmatrix} -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix}$$

where

$$W = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} - 2\begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix}\frac{\begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{bmatrix}}{1} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$



$$\underline{v}_3 = \begin{bmatrix} \cos\theta \\ -\sin\theta \end{bmatrix},\ W = \begin{bmatrix} 1-2\cos^2\theta & 2\sin\theta\cos\theta \\ 2\sin\theta\cos\theta & 1-2\sin^2\theta \end{bmatrix} = \begin{bmatrix} -\cos 2\theta & \sin 2\theta \\ \sin 2\theta & \cos 2\theta \end{bmatrix}$$

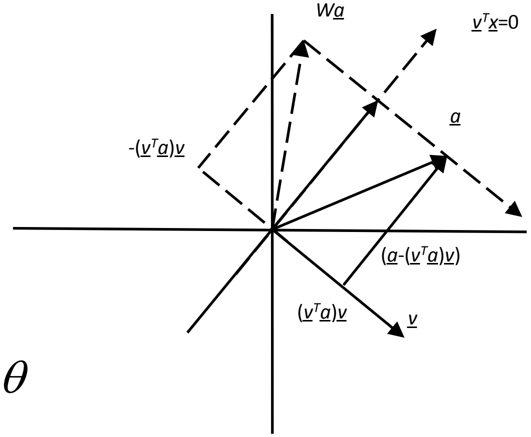
Properties of Householder Matrix

- What if we apply W to a general vector $\underline{a}$?

$$W\underline{a} = \underline{a} - \frac{2\underline{v}(\underline{v}^T\underline{a})}{\underline{v}^T\underline{v}} = \underline{a} - 2(\underline{v}^T\underline{a})\underline{v} = \underline{a} - (\underline{v}^T\underline{a})\underline{v} - (\underline{v}^T\underline{a})\underline{v}$$

Also, $\underline{a} = (\underline{a} - \underline{v}^T\underline{a}\,\underline{v}) + (\underline{v}^T\underline{a})\underline{v}$

Projection onto $\underline{v}^T\underline{x}=0$ Projection of $\underline{a}$ onto $\underline{v}$



- What does it mean?
  - To fix ideas, consider two dimensional case

$$\underline{v} = \begin{bmatrix} \cos\theta \\ -\sin\theta \end{bmatrix},\ \underline{a} = \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \Rightarrow \underline{v}^T\underline{a} = a_1\cos\theta - a_2\sin\theta$$

$$\underline{a} = \begin{bmatrix} a_1(1-\cos^2\theta) + a_2\sin\theta\cos\theta \\ a_1\sin\theta\cos\theta + a_2(1-\sin^2\theta) \end{bmatrix} + \begin{bmatrix} a_1\cos^2\theta - a_2\sin\theta\cos\theta \\ -a_1\sin\theta\cos\theta + a_2\sin^2\theta \end{bmatrix}$$

$$= \underline{c} + \underline{d}$$

  - $W\underline{a} = \underline{c} - \underline{d}$ mirror image on the otherside of $\underline{v}^T\underline{x}=0$
  - In n-dimensions, $\underline{v}^T\underline{x}=0$ is a plane

$\Rightarrow W\underline{a}$=mirror image of $\underline{a}$ on the other side of $\underline{v}^T\underline{x}=0$

  - If $\underline{a}$ lies on the plane (i.e., $\underline{v}^T\underline{a}=0$), then $W\underline{a} = \underline{a} \Rightarrow$ lies on the plane
  - So, $W\underline{v} = -\underline{v}$; $W\underline{a} = \underline{a}$ if $\underline{a} \ni \underline{v}^T\underline{a}=0 \Rightarrow \ni (n-1)$ such independent columns $\underline{a}$
  - $\Rightarrow \underline{\lambda}_i(w) = -1,1,1,\ldots,1 \Rightarrow |W| = -1$

Householder Method - 1

- What we want to do is to use W^S to change columns of A into columns of R
  - Suppose we want $W\,\underline{a} = \underline{r}$, then what should $\underline{v}$ be?

    $$\underline{a}=\underline{a}_v+\underline{a}_{\perp v},\ \underline{a}_v \parallel \underline{v}$$

  - Since $W\underline{a} = -\underline{a}_v + \underline{a}_{\perp v} \Rightarrow \underline{r} = \underline{a}_{\perp v} - \underline{a}_v$
  - $\underline{a} - \underline{r} = 2\underline{a}_v,\ \underline{r} = \underline{a}_{\perp v} - \underline{a}_v \Rightarrow \underline{a}-\underline{r} \parallel \underline{v}$
  - Also $\|\underline{a}\|_2 = \|\underline{r}\|_2$ since W is orthogonal
  - Want

    $$\underbrace{\begin{bmatrix} a_{11} \\ a_{21} \\ \vdots \\ a_{m1} \end{bmatrix}}_{\underline{a}} \rightarrow \underbrace{\begin{bmatrix} r_{11} \\ 0 \\ \vdots \\ 0 \end{bmatrix}}_{\underline{r}} = \underline{v} \parallel \begin{bmatrix} a_{11} - r_{11} \\ a_{21} \\ \vdots \\ a_{n1} \end{bmatrix}$$

  - This must be true because:

    $$W_1 = \left[I - 2\frac{\underline{u}\,\underline{u}^T}{\underline{u}^T\underline{u}} \right]$$

    $$W_1\underline{a} = \left[I - 2\frac{(\underline{a}-\underline{r})(\underline{a}-\underline{r})^T}{(\underline{a}-\underline{r})^T(\underline{a}-\underline{r})} \right]\underline{a} = \underline{a} - (\underline{a}-\underline{r})\frac{2(\underline{a}-\underline{r})^T\underline{a}}{(\underline{a}-\underline{r})^T(\underline{a}-\underline{r})} = \underline{r}$$

Householder Method - 2

- What is $\underline{u}^T\underline{u}=(\underline{a}-\underline{r})^T(\underline{a}-\underline{r})$
  - $(\underline{a}-\underline{r})^T\,\underline{a}-(\underline{a}-\underline{r})^T\,\underline{r} = \underline{a}^T\underline{a}+\underline{r}^T\underline{r}-2\underline{a}^T\underline{r} = 2\underline{a}^T\underline{u}$ (recall $\underline{a}^T\,\underline{a}=\underline{r}^T\underline{r}$)

  $=2[a_{11}(a_{11}-r_1)+(a_{21})^2+..+(a_{n1})^2]=2[(\|\underline{a}\|_2)^2-a_{11}r_{11}]$
  - To avoid round-off errors, select $r_{11}= -\text{sign}(a_{11})\,\|\underline{a}\|_2= -s_1$

  $\Rightarrow u_1=a_{11}-r_{11}=a_{11}+\text{sign}(a_{11})\,\|\underline{a}\|_2;\ u_i=a_{i1};\ i\geq 2$
  - Also, $\underline{u}^T\,\underline{u} = 2(\|\underline{a}_2\|^2+a_{11}s_1)=2s_1(s_1+a_{11})=2s_1\mu_1=2\beta_1$
  - To get the rest of the matrix (columns 2 to n)

$$W_1A=\left[I-2\frac{\underline{u}\underline{u}^T}{\underline{u}^T\underline{u}}\right]A=\left[I-\frac{\underline{u}\underline{u}^T}{\beta_1}\right]A=A-\underline{u}\left(\frac{\underline{u}^TA}{\beta_1}\right)$$

Where $\underline{u}^TA/\beta_1$ is a row vector and

$$W_1A=\begin{bmatrix} r_{11} & r_{12} & r_{13} & \dots & r_{1n} \\ 0 & \times & \times & \dots & \times \\ 0 & \times & \times & \dots & \times \\ 0 & \times & \times & \dots & \times \end{bmatrix}$$

- Next

$$W_2W_1A=\begin{bmatrix} r_{11} & r_{12} & r_{13} & \dots & r_{1n} \\ 0 & r_{22} & r_{23} & \dots & r_{2n} \\ 0 & 0 & \times & \dots & \times \\ 0 & 0 & \times & \dots & \times \end{bmatrix}$$

Householder Method - 3

- The $\underline{u}$ vector associated with W_2 will have

$$u_1 = 0$$

$$u_2 = a_{22} + s_2$$

$$s_2 = sign(a_{22})\left(\sum_{i=2}^{n} a_{i2}^2\right)^{\frac{1}{2}}$$

$$\beta_2 = a_{22}u_2$$

- Continue n steps to get $Q^T = W_n W_{n-1} \ldots W_1$ or $Q = W_1 W_2 \ldots W_n$

Example:

$$A = \begin{bmatrix} 3 & -1 \\ 0 & 0 \\ 4 & 7 \end{bmatrix}$$

$$\underline{u}_1 = \begin{bmatrix} 8 \\ 0 \\ 4 \end{bmatrix};\ W_1 = \begin{bmatrix} -\frac{3}{5} & 0 & -\frac{4}{5} \\ 0 & 1 & 0 \\ -\frac{4}{5} & 0 & \frac{3}{5} \end{bmatrix};\ W_1 A = \begin{bmatrix} -5 & -5 \\ 0 & 0 \\ 0 & 5 \end{bmatrix}$$

$$\underline{u}_2 = \begin{bmatrix} 5 \\ 5 \end{bmatrix};\ W_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & -1 & 0 \end{bmatrix};\ W_2 W_1 A = \begin{bmatrix} -5 & -5 \\ 0 & -5 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} R_{11} \\ 0 \end{bmatrix}$$

So, $R_{11} = \begin{bmatrix} -5 & -5 \\ 0 & -5 \end{bmatrix}$ and $Q = W_1 W_2 = \begin{bmatrix} -\frac{3}{5} & \frac{4}{5} & 0 \\ 0 & 0 & -1 \\ -\frac{4}{5} & -\frac{3}{5} & 0 \end{bmatrix}$

Householder Algorithm - 1

- Storage considerations: overwrite A with R and $\underline{u}$ vectors as follows

$$W_n W_{n-1} .. W_2 W_1 A = \begin{bmatrix} u_1^{(1)} & r_{12} & r_{13} & \dots & r_{1n} \\ u_2^{(1)} & u_2^{(2)} & r_{23} & \dots & r_{2n} \\ & & u_3^{(3)} & & \\ u_m^{(1)} & u_m^{(2)} & u_m^{(3)} & \dots & u_m^{(n)} \end{bmatrix}; \ \underline{d} = diag(R) = \begin{bmatrix} r_{11} \\ r_{22} \\ . \\ r_{nn} \end{bmatrix}; \ \beta = \begin{bmatrix} \beta_1 \\ \beta_2 \\ . \\ \beta_n \end{bmatrix}$$

…Since $\beta_i = u_i^{(i)} s_i = \left| u_i^{(i)} r_{ii} \right|$, need not store β_i^S

- Algorithm Householder

For k=1, 2, …, n DO

$$s = \operatorname{sgn}(a_{kk}) \sqrt{\sum_{i=k}^{n} a_{ii}^2}$$

$u_k = a_{kk} + s \Rightarrow$ can store in a_{kk} location

$u_i = a_{ik}$ for $i=k+1,\dots,n \Rightarrow$ don't do anything

$\beta_k = |s\, u_k|$

$d_k = -s$

Compute $z_i = \dfrac{\underline{a}_i^T \underline{u}}{\beta_k}$ for $i=k,\dots,n$

$a_{li} \leftarrow a_{li} - u_l z_i \quad i=k+1,\dots,n, \ l=k,\dots,n$

$\underline{b} \leftarrow \underline{b} - \underline{u}(\underline{u}^T \underline{b}/\beta)$

end DO

Householder Algorithm - 2

- Note: Q matrix can be computed off-line

  $Q = I$

  For k=1, 2, …, n DO

  $$Q \leftarrow Q - Q\frac{u^{(k)}u^{(k)T}}{|u_k^{(k)}d_k|}$$

  end DO

- To solve LS:
  - We have already formed $\underline{b}^{\text{new}} = Q^T \underline{b}$
  - So, use back substitution

  $$x_n = \frac{b_n^{new}}{d_n}$$

  For i=n-1,…, 1 DO

  $$x_i = \frac{\left(b_i^{new} - \sum_{j=i+1}^{n} a_{ij}x_j\right)}{d_i}$$

  end DO

Householder Example

- Example again:
  - Suppose
$$\underline{b} = \begin{bmatrix} 0 \\ 18 \\ 25 \end{bmatrix}$$
  - Then, the least squares solution is obtained via:
$$\begin{pmatrix} R_{11} \\ 0 \end{pmatrix} \underline{x}_{LS} = Q^T \underline{b} = \begin{bmatrix} -\frac{3}{5} & 0 & -\frac{4}{5} \\ \frac{4}{5} & 0 & -\frac{3}{5} \\ 0 & -1 & 0 \end{bmatrix} \begin{bmatrix} 0 \\ 18 \\ 25 \end{bmatrix} = \begin{bmatrix} -20 \\ -15 \\ -18 \end{bmatrix}$$
$$\Rightarrow \begin{bmatrix} -5 & -5 \\ 0 & -5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} -20 \\ -15 \end{bmatrix} \Rightarrow \underline{x}_{LS} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}$$
  - Residual at the solution $\underline{r} = \underline{b} - A\underline{x}_{LS} = \begin{bmatrix} 0 \\ 18 \\ 0 \end{bmatrix}$

$R(A)$ and $N(A^T)$ from Householder

- Computational load
  - Want R only: $n^2(m-n/3)$
  - Want R and $\underline{b}$ and $\underline{x}$: $n^2(m-n/3 + m\,n + O(n^2/2))$
  - Want R, $\underline{b}$, $\underline{x}$ and Q: $n^2(m-n/3) + m\,n + O(n^2/2) + 2[m^2n - mn^2 + n^3/3]$
- A nice feature of Householder method
  - Can get orthonormal basis for R^m
  - Given $(\underline{a}_1\ \underline{a}_2\ \ldots\ \underline{a}_n)$ where each $\underline{a}_i \in R^m$, find orthonormal basis for $R(A)$

    $$A = QR \Rightarrow (\underline{a}_1\ \underline{a}_2\ \ldots \underline{a}_m) = (Q\underline{r}_1\ Q\underline{r}_2\ \ldots Q\underline{r}_m) \Rightarrow \underline{a}_k = \sum_{i=1}^{k} r_{ik}\underline{q}_i$$
  - Since $\underline{q}_i$ are orthonormal

    $$r_{ik} = \underline{q}_i^T \underline{a}_k;\ i = 1, 2, \ldots, k$$

    $\underline{a}_1 = r_{11}\underline{q}_1$

    $\underline{a}_2 = r_{12}\underline{q}_1 + r_{22}\underline{q}_2$

    $\underline{a}_k = r_{1k}\underline{q}_1 + r_{2k}\underline{q}_2 + \ldots + r_{kk}\underline{q}_k$

    $\Rightarrow R(\underline{a}_1\ \ldots\ \underline{a}_k) = R(\underline{q}_1\ \ldots\ \underline{q}_k)$
  - So

    $R(A) = (\underline{q}_1\ \ldots \underline{q}_n)$

    $N(A^T) = (\underline{q}_{n+1}\ \ldots \underline{q}_m) = R(A)^{\perp}$

    = orthonormal basis for the null space of A^T

    = orthogonal complement of $R(A)$

Serial (Classical) Gram-Schmidt

- Example again

$$R(A) = \begin{bmatrix} \underline{q}_1 & \underline{q}_2 \end{bmatrix} = \begin{bmatrix} -0.6 & 0.8 \\ 0 & 0 \\ -0.8 & -0.6 \end{bmatrix}$$

$$N(A^T) = \underline{q}_3 = \begin{bmatrix} 0 \\ -1 \\ 0 \end{bmatrix}$$

- Gram-Schmidt orthogonalization procedure
  - Rank(A)=$n \Rightarrow r_{kk} \neq 0$ for k=1, 2, …, n
    $\Rightarrow$ can solve for $\underline{q}_k$ via $\underline{q}_k = \frac{1}{r_{kk}}\left[\underline{a}_k - \sum_{i=1}^{k-1} r_{ik}\underline{q}_i\right]$

    can think of $\underline{q}_k \parallel \left[\underline{a}_k - \sum_{i=1}^{k-1}(\underline{q}_i^T\underline{a}_k)\underline{q}_i\right]$ since $r_{ik} = \underline{q}_i^T\underline{a}_k$
  - This is precisely the classical Gram-Schmidt procedure for constructing an orthonormal basis ($\underline{q}_1 \ldots \underline{q}_n$) ∋ $\underline{q}_i^T\underline{q}_j=\delta_{ij}$ and span ($\underline{a}_1 \ldots \underline{a}_n$)
  - The procedure also computes $A=QR$ in the process

Classical Gram-Schmidt - 1

- Algorithm: Classical Gram-Schmidt

  For k=1, 2, …, n DO

  For i=1,k-1

  $r_{ik}=\underline{a}_i^T\underline{a}_k$

  $\underline{a}_k \leftarrow \underline{a}_k - r_{ik}\underline{a}_i$

  end DO

  end DO

  $$r_{kk} \leftarrow \left(\underline{a}_k^T \underline{a}_k\right)^{\frac{1}{2}}$$

  $$\underline{a}_k \leftarrow \frac{\underline{a}_k}{r_{kk}}$$

  end DO

  - At the k^{th} step, we determine k^{th} column of $\underline{Q}$ and k^{th} column of R. replaces A with Q
  - Can solve LS problem

    $A=QR \quad Q=m\times n;\ R=n\times n;\ Q^TQ=I_n$

    $A^TA\,\underline{x}=R^TQ^TQR\,\underline{x}=R^TQ^T\underline{b} \Rightarrow R^TR\,\underline{x}=R^T\underline{b}$

    $\Rightarrow R\underline{x}=\underline{b}$ since R is nonsingular
  - The algorithm behaves very badly numerically… severe loss of orthogonality

Classical Gram-Schmidt - 2

- One solution
  - Go through it a second time
  - Can show that r_{ik}^{s} add up
- Algorithm: Two-Step Gram-Schmidt

$R \leftarrow 0$

For k=1, 2, …, n DO

    For l=1, 2,… DO

        For i=1,k-1

            $s = \underline{a}_i^T \underline{a}_k$

            $\underline{a}_k \leftarrow \underline{a}_k - s\,\underline{a}_i$

            $r_{ik} \leftarrow r_{ik} + s$

        end DO

    end DO

    $r_{kk} \leftarrow \left(\underline{a}_k^T \underline{a}_k\right)^{\frac{1}{2}}$

    $\underline{a}_k \leftarrow \frac{\underline{a}_k}{r_{kk}}$

- end DO

- However ∃ a better method called: Modified Gram-Schmidt (MGS) ..(also called parallel Gram-Schmidt)

Motivating Parallel Gram-Schmidt

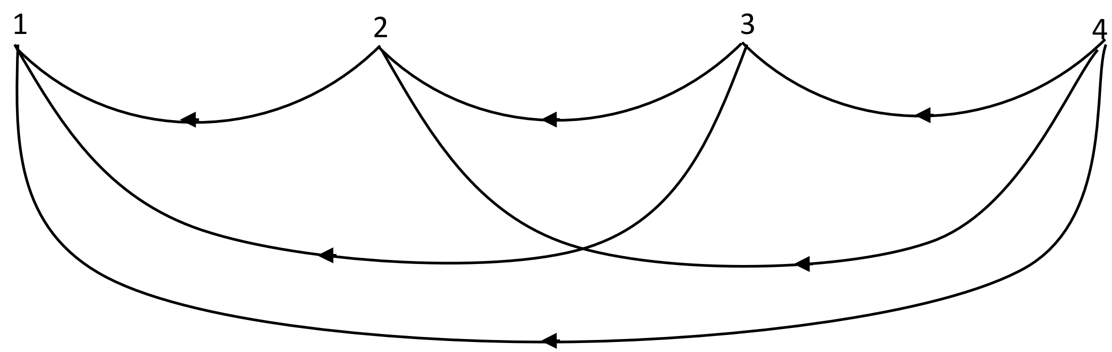
- To motivate the procedure, consider Serial (classical) Gram-Schmidt

$$\underline{q}_1 = \underline{a}_1;\ \underline{q}_1 = \frac{\underline{q}_1}{\|\underline{q}_1\|};\|\underline{q}_1\| = r_{11}$$

$$\underline{q}_2 = \underline{a}_2 - \underline{a}_2^T\underline{q}_1;\ \underline{q}_2 = \frac{\underline{q}_2}{\|\underline{q}_2\|};\|\underline{q}_2\| = r_{22};\ \underline{a}_2^T\underline{q}_1 = r_{12}$$

$$\underline{q}_3 = \underline{a}_3 - \underline{a}_3^T\underline{q}_1 - \underline{a}_3^T\underline{q}_2;\ \underline{q}_3 = \frac{\underline{q}_3}{\|\underline{q}_3\|};\|\underline{q}_3\| = r_{33};\ \underline{a}_3^T\underline{q}_1 = r_{13};\ \underline{a}_3^T\underline{q}_2 = r_{23}$$

$\Rightarrow$ Determine R one column at a time and orthogonalize $\underline{q}_k$ w.r.t. $\underline{q}_1, \underline{q}_2, \ldots, \underline{q}_{k-1}$, etc.

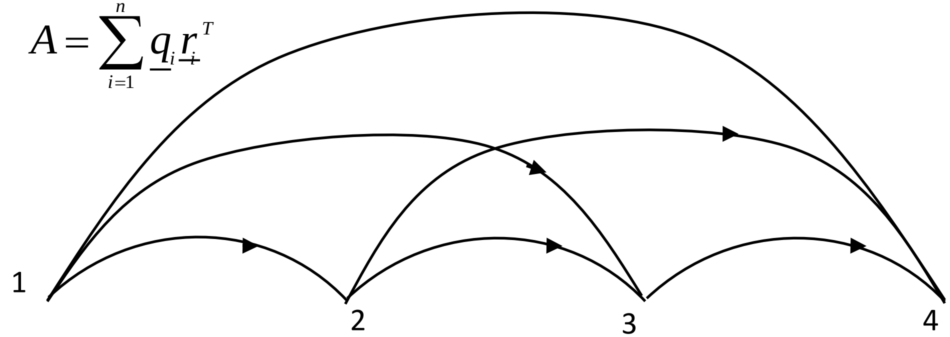


Result: $(\underline{a}_1\ \underline{a}_2\ \ldots\ \underline{a}_n) = [Q\underline{r}_1\ Q\underline{r}_2\ \ldots\ Q\ \underline{r}_n]$ **Backward looking**

Parallel Gram-Schmidt - 1

- In Parallel or modified Gram-Schmidt, we determine k^{th} column of Q and k^{th} row of R at the k^{th} step

  $\Rightarrow$ The procedure essentially writes A as a dyadic (or outer-product) sum $A = \sum_{i=1}^{n} \underline{q}_i \underline{r}_i^T$



Consider step k=1

We have $A^{(1)} = [\underline{a}_1 B] = \sum_{i=1}^{n} \underline{q}_i \underline{r}_i^T = \underline{q}_1 \underline{r}_1^T + \underline{q}_2 \underline{r}_2^T + \ldots + \underline{q}_n \underline{r}_n^T$ **Forward Looking**

$n \times n$ (n-1)non-zero columns   1 non-zero column

Set $r_{11} = \|\underline{a}_1\|_2 = (\underline{a}_1^T \underline{a}_1)^{1/2}$

$\underline{q}_1 = \underline{a}_1 / r_{11}$

recalling that $\underline{q}_i^T \underline{q}_j = \delta_{ij}$, we have

$\underline{q}_1^T [\underline{a}_1 B] = \underline{r}_1^T = (r_{11} \ldots r_{1n})$

$(\underline{q}_1^T \underline{a}_1 \;\; \underline{q}_1^T B) = \underline{r}_1^T \Rightarrow \underline{q}_1^T B = (r_{12} \ldots r_{1n})$

Parallel Gram-Schmidt - 2

Consequently, $r_{1k} = \underline{q}_1^T \underline{a}_k$, k=2, …, n

$$A - \underline{q}_1 \underline{r}_1^T = [\underline{a}_1 \,|\, B] - \underline{q}_1 \underline{r}_1^T = [0 \,|\, B - \underline{q}_1 (r_{12} \ldots r_{1n})]$$

⇒So, at step 2 we have

$$[0 \quad A^{(2)}] = A - \underline{q}_1 \underline{r}_1^T = \sum_{i=2}^{n} \underline{q}_i \underline{r}_i^T$$

$A^{(2)}$=[$\underline{z}$ B]; $\underline{z}$=new $\underline{a}_1$; B=new B

$r_{22}=\|\underline{z}\|_2$; $\underline{q}_2=\underline{z}/r_{22}$;

As before, $(r_{23} \ldots r_{2n})=\underline{q}_2^T B$

and $A^{(3)}=B-\underline{q}_2 (r_{23} \ldots r_{2n})$ since $\underline{q}_2 r_{22} = \underline{z}$

Next step, do with $[0 \quad 0 \quad A^{(3)}] = \sum_{i=3}^{n} \underline{q}_i \underline{r}_i^T$

- Note:
  - Can store Q in A
  - Do orthogonalization twice ⇒ r_{ki} from each iteration add up

Parallel Gram-Schmidt Algorithm

$R = 0$
For $k=1, 2, \ldots, n$ Do
$r_{kk} = (\underline{a}_k^T \underline{a}_k)^{1/2}$
    For $i=1, \ldots, m$ Do
        $a_{ik} = a_{ik} / r_{kk}$
    end DO
    For $l=1, 2$ DO
        For $j=k+1, \ldots, n$ Do

$$\alpha = \sum_{i=1}^{m} a_{ik} a_{ij} \Rightarrow \text{computing } \underline{q}_k^T \underline{a}_j$$

            For $i=1, \ldots, m$ Do
            $a_{ij} = a_{ij} - a_{ik}\,\alpha \Rightarrow$ computing $\underline{a}_j = \underline{a}_j - (\underline{q}_k^T \underline{a}_j)\, \underline{a}_j$
            end DO
        $r_{kj} = r_{kj} + \alpha$
        end DO
    end DO
end DO

- Requires $O(mn^2)$ operations per iteration.   Do it twice
- Householder $2(mn^2 - n^3/3)$ to get Q and R, but Householder has better accuracy

Summary

- Why orthogonalization methods ?
- Least Squares Problem and its properties
- Householder transformation
- Gram-Schmidt orthogonalization
  - – Serial (classical) Gram-Schmidt
  - – Parallel (modified) Gram-Schmidt