Householder Reflectors and Givens Rotations

Why orthogonality is fine

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Gram-Schmidt as Triangular Orthogonalization

- Gram-Schmidt multiplies with triangular matrices to make columns orthogonal, for example at the first step:

$$\begin{bmatrix} v_1 & v_2 & \cdots & v_n \end{bmatrix} \begin{bmatrix} \frac{1}{r_{11}} & \frac{-r_{12}}{r_{11}} & \frac{-r_{13}}{r_{11}} & \cdots \\ & 1 & & \\ & & 1 & \\ & & & \ddots \end{bmatrix} = \begin{bmatrix} q_1 & v_2^{(2)} & \cdots & v_n^{(2)} \end{bmatrix}$$

- After all the steps we get a product of triangular matrices

$$A \underbrace{R_1 R_2 \ldots R_n}_{\hat{R}^{-1}} = \hat{Q}$$

- “Triangular orthogonalization”

Householder Triangularization

- The Householder method multiplies by unitary matrices to make columns triangular, for example at the first step:

$$Q_1 A = \begin{bmatrix} r_{11} & \times & \cdots & \times \\ 0 & \times & \cdots & \times \\ 0 & \times & \cdots & \times \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \times & \cdots & \times \end{bmatrix}$$

- After all the steps we get a product of orthogonal matrices

$$\underbrace{Q_n \ldots Q_2 Q_1}_{Q^*} A = R$$

- "Orthogonal triangularization"

Introducing Zeros

- Q_k introduces zeros below the diagonal in column k
- Preserves all the zeros previously introduced

$$
\underset{A}{\begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix}}
\xrightarrow{Q_1}
\underset{Q_1 A}{\begin{bmatrix} \times & \times & \times \\ \mathbf{0} & \times & \times \\ \mathbf{0} & \times & \times \\ \mathbf{0} & \times & \times \\ \mathbf{0} & \times & \times \end{bmatrix}}
\xrightarrow{Q_2}
\underset{Q_2 Q_1 A}{\begin{bmatrix} \times & \times & \times \\ & \times & \times \\ & \mathbf{0} & \times \\ & \mathbf{0} & \times \\ & \mathbf{0} & \times \end{bmatrix}}
\xrightarrow{Q3}
\underset{Q_3 Q_2 Q_1 A}{\begin{bmatrix} \times & \times & \times \\ & \times & \times \\ & & \times \\ & & \mathbf{0} \\ & & \mathbf{0} \end{bmatrix}}
$$

Householder Reflectors

- Let Q_k be of the form

$$Q_k = \begin{bmatrix} I & 0 \\ 0 & F \end{bmatrix}$$

  where I is $(k-1) \times (k-1)$ and and F is $(m-k+1) \times (m-k+1)$
- Create Householder reflector F that introduces zeros:

$$x = \begin{bmatrix} \times \\ \times \\ \vdots \\ \times \end{bmatrix} \qquad Fx = \begin{bmatrix} \|x\| \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \|x\| \, e_1$$

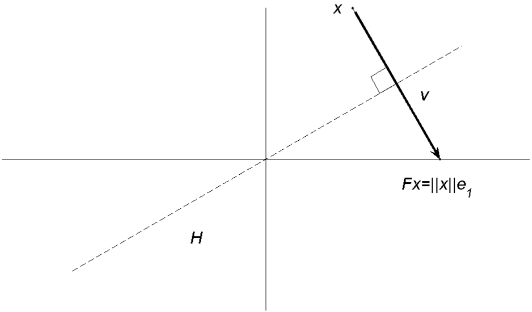
Householder Reflectors-Idea

- Idea: Reflect across hyperplane H orthogonal to $v = \|x\|_2 e_1 - x$, by the unitary matrix

$$F = I - 2\frac{vv^*}{v^*v}$$

- Compare with projector

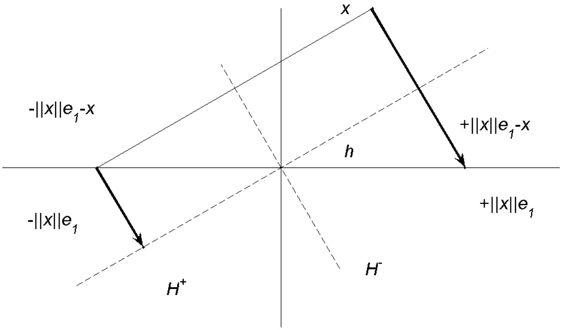
$$P_{\perp v} = I - \frac{vv^*}{v^*v}$$



Choice of Reflector

- We can choose to reflect to any multiple z of $\|x\|\, e_1$ with $|z| = 1$
- Better numerical properties with large $\|v\|$, for example $v = \mathrm{sign}(x_1)\,\|x\|\, e_1 + x$

- Note: $\mathrm{sign}(0) = 1$, but in MATLAB, `sign(0)==0`



The Householder Algorithm

- Compute the factor R of a QR factorization of $m \times n$ matrix A $(m \geq n)$
- Leave result in place of A, store reflection vectors v_k for later use

Algorithm: Householder QR Factorization

for $k := 1$ **to** n **do**

$x := A_{k:m,k}$;

$v_k := \operatorname{sign}(x_1)\|x\|_2 e_1 + x$;

$v_k := v_k / \|v_k\|_2$;

$A_{k:m,k:n} = A_{k:m,k:n} - 2v_k\left(v_k^* A_{k:m,k:n}\right)$

Applying or Forming Q

- Compute $Q^* b = Q_n \dots Q_2 Q_1 b$ and $Qx = Q_1 Q_2 \dots Q_n x$ implicitly
- To create Q explicitly, apply to $x = I$

Algorithm: Implicit Calculation of $Q^* b$

for $k := 1$ **to** n **do**

$b_{k:m} = b_{k:m} - 2v_k \left(v_k^* b_{k:m} \right);$

Algorithm: Implicit Calculation of Qx

for $k := n$ **downto** 1 **do**

$x_{k:m} = x_{k:m} - 2v_k \left(v_k^* x_{k:m} \right);$

Operation Count -Householder QR

- Most work done by

$$A_{k:m,k:n} = A_{k:m,k:n} - 2v_k \left(v_k^* A_{k:m,k:n}\right)$$

- Operations per iteration:
  - $2(m-k)(n-k)$ for the dot products $v_k^* A_{k:m,k:n}$
  - $(m-k)(n-k)$ for the outer product $2v_k(\cdots)$
  - $(m-k)(n-k)$ for the subtraction $A_{k:m,k:n} - \cdots$
  - $4(m-k)(n-k)$ total
- Including the outer loop, the total becomes

$$\sum_{k=1}^{n} 4(m-k)(n-k) = 4\sum_{k=1}^{n} \left(mn - k\left(m+n\right) + k^2\right)$$

$$\sim 4mn^2 - 4(m+n)n^2/2 + 4n^3/3 = 2mn^2 - 2n^3/3$$

Givens Rotations

- Alternative to Householder reflectors
- A Givens rotation $R = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$ rotates $x \in \mathbb{R}^2$ by θ
- To set an element to zero, choose $\cos\theta$ and $\sin\theta$ so that

$$\begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} x_i \\ x_j \end{bmatrix} = \begin{bmatrix} \sqrt{x_i^2 + x_j^2} \\ 0 \end{bmatrix}$$

or

$$\cos\theta = \frac{x_i}{\sqrt{x_i^2 + x_j^2}}, \qquad \sin\theta = \frac{-x_j}{\sqrt{x_i^2 + x_j^2}}$$

Givens QR

- Introduce zeros in column from bottom and up

$$
\begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix}
\xrightarrow{(3,4)}
\begin{bmatrix} \times & \times & \times \\ \times & \times & \times \\ \boldsymbol{\times} & \boldsymbol{\times} & \boldsymbol{\times} \\ \mathbf{0} & \boldsymbol{\times} & \boldsymbol{\times} \end{bmatrix}
\xrightarrow{(2,3)}
\begin{bmatrix} \times & \times & \times \\ \boldsymbol{\times} & \boldsymbol{\times} & \boldsymbol{\times} \\ \mathbf{0} & \boldsymbol{\times} & \boldsymbol{\times} \\ & \times & \times \end{bmatrix}
\xrightarrow{(1,2)}
$$

$$
\begin{bmatrix} \boldsymbol{\times} & \boldsymbol{\times} & \boldsymbol{\times} \\ \mathbf{0} & \boldsymbol{\times} & \boldsymbol{\times} \\ & \times & \times \\ & \times & \times \end{bmatrix}
\xrightarrow{(3,4)}
\begin{bmatrix} \times & \times & \times \\ & \times & \times \\ & \boldsymbol{\times} & \boldsymbol{\times} \\ & \mathbf{0} & \boldsymbol{\times} \end{bmatrix}
\xrightarrow{(2,3)}
\begin{bmatrix} \times & \times & \times \\ & \boldsymbol{\times} & \boldsymbol{\times} \\ & \mathbf{0} & \boldsymbol{\times} \\ & & \times \end{bmatrix}
\xrightarrow{(3,4)} R
$$

- Flop count $3mn^2 - n^3$ (or 50% more than Householder QR)

Figure: Alston S. Householder (1904-1993), American mathematician. Important contributions to mathematical biology and mainly to numerical linear algebra. His well known book "The Theory of Matrices in Numerical Analysis" has a great impact on development of numerical analysis and computer science.

Figure: James Wallace Givens (1910-1993) Pioneer of numerical linear algebra and computer science

Figure: Gatlinburg Conference