

Notice $\mathbf{a} \in \mathbb{R}^n, \mathbf{Q} \in \mathbb{R}^{n \times n}, [\mathbf{I}_n - \mathbf{Q}\mathbf{Q}^T] \in \mathbb{R}^{n \times n}$ notice its semi-orthogonal condition $\mathbf{Q}^T \mathbf{Q} = \mathbf{I}_n$

Notice $\Rightarrow \mathbf{a}_j = \mathbf{Q} \mathbf{e}_j \Rightarrow \mathbf{Q} \mathbf{e}_1, \dots, \mathbf{Q} \mathbf{e}_n, \dots, \mathbf{Q} \mathbf{e}_n^T = \mathbf{Q} \mathbf{e}_j^T$

Let $\mathbf{R} = [\mathbf{r}_1 | \dots | \mathbf{r}_n] \in \mathbb{R}^{m \times n}$

$\mathbf{A} = \mathbf{Q} \mathbf{R} = \mathbf{Q} \begin{bmatrix} \mathbf{r}_1 & \dots & \mathbf{r}_n \\ 0 & \dots & 0 \end{bmatrix}$ notice its

upper-triangular

Full QR Decomposition

Consider full \mathbf{QR} decomposition $\mathbf{A} = [\mathbf{a}_1 | \dots | \mathbf{a}_n] \in \mathbb{R}^{m \times n}$ ($m \geq n$), i.e. $\mathbf{a}_1, \dots, \mathbf{a}_n \in \mathbb{R}^m$ are linearly independent

Apply QR decomposition to obtain:

$\text{ONB } \{\mathbf{q}_1, \dots, \mathbf{q}_n\} \in \mathbb{R}^m$ for $\mathbf{Q}(\mathbf{A})$

Semi-orthogonal $\mathbf{Q}_1 \in [\mathbf{q}_1 | \dots | \mathbf{q}_n] \in \mathbb{R}^{m \times n}$ and upper-triangular $\mathbf{R}_1 \in \mathbb{R}^{n \times n}$ where $\mathbf{A} = \mathbf{Q}_1 \mathbf{R}_1$

Compute basis extension to obtain remaining $\mathbf{q}_{n+1}, \dots, \mathbf{q}_m \in \mathbb{R}^m$ where $\{\mathbf{q}_1, \dots, \mathbf{q}_m\}$ is **ONB** for \mathbb{R}^m

Notice $\{\mathbf{q}_{n+1}, \dots, \mathbf{q}_m\}$ is **ONB** for $\mathbf{Q}(\mathbf{A})^\perp = \ker(\mathbf{A}^T)$

Let $\mathbf{Q}_2 = [\mathbf{q}_{n+1} | \dots | \mathbf{q}_m] \in \mathbb{R}^{m \times (m-n)}$ let $\mathbf{Q} = [\mathbf{Q}_1 | \mathbf{Q}_2] \in \mathbb{R}^{m \times m}$ let $\mathbf{R} = [\mathbf{R}_1 | \mathbf{0}_{(n-m) \times n}] \in \mathbb{R}^{m \times n}$

Then **full QR decomposition** is

$\mathbf{A} = \mathbf{Q} \mathbf{R} = [\mathbf{Q}_1 | \mathbf{Q}_2] \begin{bmatrix} \mathbf{R}_1 \\ \mathbf{0}_{(m-n) \times n} \end{bmatrix} = \mathbf{Q}_1 \mathbf{R}_1$

\mathbf{Q} is **orthogonal**, i.e. $\mathbf{Q}^{-1} = \mathbf{Q}^T$ so its a basis transformation

$\text{proj}_{\mathbf{Q}(\mathbf{A})}(\mathbf{Q}_1 \mathbf{Q}_1^T) = \text{proj}_{\mathbf{Q}(\mathbf{A})}(\mathbf{A} \mathbf{A}^T) = \mathbf{Q}_1 \mathbf{Q}_1^T$ are orthogonal projections onto $\mathbf{C}(\mathbf{A})$, $\mathbf{C}(\mathbf{A})^\perp = \ker(\mathbf{A}^T)$ respectively

Notice: $\mathbf{Q} \mathbf{Q}^T = \mathbf{I}_m = \mathbf{Q}_1 \mathbf{Q}_1^T + \mathbf{Q}_2 \mathbf{Q}_2^T$

Generalizable to $\mathbb{C} \in \mathbb{C}^{m \times n}$ by changing transpose to conjugate-transpose

Lines and hyperplanes in $\mathbb{E}^n(\mathbb{R}^n)$

Consider **standard Euclidean space $\mathbb{E}^n(\mathbb{R}^n)$** with standard basis $\{\mathbf{e}_1, \dots, \mathbf{e}_n\} \in \mathbb{R}^n$ with standard origin $\mathbf{0} \in \mathbb{R}^n$

A line $\mathbf{L} = \mathbf{Rn}(\mathbf{c})$ is characterized by direction $\mathbf{n} \in \mathbb{R}^n$ ($\mathbf{n} \neq \mathbf{0}$) and offset from origin $\mathbf{c} \in \mathbf{L}$

\mathbf{L} is a unit vector, i.e. $\|\mathbf{n}\| = \|\mathbf{c}\| = 1$

$\mathbf{c} \in \mathbf{L}$ is closest point to origin, i.e. $\mathbf{c} \perp \mathbf{n}$

If $\mathbf{c} \perp \mathbf{n}$ then \mathbf{L} is vector-subspace of \mathbb{R}^n i.e. $\mathbf{0} \in \mathbf{L}$ i.e. \mathbf{L} doesn't go through the origin

\mathbf{L} is affine-subspace of \mathbb{R}^n

If $\mathbf{c} \perp \mathbf{n}$ i.e. $\mathbf{L} = \mathbf{Rn}(\mathbf{c}) = \mathbf{L}$ is vector-subspace of \mathbb{R}^n i.e. $\mathbf{0} \in \mathbf{L}$ i.e. \mathbf{L} goes through the origin

\mathbf{L} has $\dim(\mathbf{L}) = 1$ and orthogonal basis (ONB) $\{\hat{\mathbf{n}}\}$

A hyperplane $\mathbf{P} = \mathbf{Rn}(\mathbf{n}) + \mathbf{c}$ where $\mathbf{x} = \mathbf{x} + \mathbf{c}$ where $\mathbf{x} \in \mathbf{R}^n, \mathbf{x} \perp \mathbf{n}$ is $\mathbf{x} \in \mathbf{R}^n | \mathbf{x} \cdot \mathbf{n} = \mathbf{c} \cdot \mathbf{n}$

characterized by normal $\mathbf{n} \in \mathbb{R}^n$ ($\mathbf{n} \neq \mathbf{0}$) and offset from origin $\mathbf{c} \in \mathbf{P}$

It represents an $(n-1)$ -dimensional slice of the n -dimensional space

It is customary that:

\mathbf{n} is a **unit vector**, i.e. $\|\mathbf{n}\| = \|\hat{\mathbf{n}}\| = 1$

$\mathbf{c} \in \mathbf{P}$ is **closest point to origin**, i.e. $\mathbf{c} \perp \mathbf{n}$

With those $\Rightarrow \mathbf{P} = \{\mathbf{x} \in \mathbb{R}^n | \mathbf{x} \cdot \mathbf{n} = \mathbf{c} \cdot \mathbf{n}\}$

If $\mathbf{c} \cdot \mathbf{n} = 0 \Rightarrow \mathbf{P}$ is not vector-subspace of \mathbb{R}^n i.e. $\mathbf{0} \notin \mathbf{P}$ i.e. \mathbf{P} doesn't go through the origin

\mathbf{P} is affine-subspace of \mathbb{R}^n

If $\mathbf{c} \cdot \mathbf{n} = 0$ i.e. $\mathbf{P} = \mathbf{Rn}(\mathbf{n}) \Rightarrow \mathbf{P}$ is vector-subspace of \mathbb{R}^n

i.e. $\mathbf{0} \in \mathbf{P}$ i.e. \mathbf{P} goes through the origin

\mathbf{P} has $\dim(\mathbf{P}) = n-1$

Notice $\mathbf{L} = \mathbf{Rn}(\mathbf{n})$ and $\mathbf{P} = \mathbf{Rn}(\mathbf{n})^\perp$ are orthogonal complements, so:

$\text{proj}_{\mathbf{L}} \cdot \hat{\mathbf{n}}^T$ is orthogonal projection onto \mathbf{L} (along \mathbf{P})

$\text{proj}_{\mathbf{P}} = \text{id}_{\mathbb{R}^n} - \text{proj}_{\mathbf{L}} = \mathbf{I}_n - \hat{\mathbf{n}} \hat{\mathbf{n}}^T$ is orthogonal projection onto \mathbf{P}^\perp (along \mathbf{L})

$\mathbf{L} = \text{im}(\text{proj}_{\mathbf{L}}) = \ker(\text{proj}_{\mathbf{P}})$ and $\mathbf{P} = \ker(\text{proj}_{\mathbf{L}}) = \text{im}(\text{proj}_{\mathbf{P}})$

$\mathbf{P} = \mathbf{Rn}(\mathbf{Rn}(\mathbf{n})^\perp)$ i.e. all vectors $\mathbf{v} \in \mathbf{Rn}(\mathbf{n})^\perp$ uniquely decomposed into $\mathbf{v} = \mathbf{v}_L + \mathbf{v}_P$

Householder Maps: reflections

Two points $\mathbf{x}, \mathbf{y} \in \mathbb{E}^n$ are reflections w.r.t hyperplane $\mathbf{P} = \mathbf{Rn}(\mathbf{n}) + \mathbf{c}$ if:

1- The translation $\tilde{\mathbf{y}} = \mathbf{y} - \mathbf{x}$ is parallel to normal \mathbf{n} i.e. $\tilde{\mathbf{y}} \perp \mathbf{n}$

2- Midpoint $\mathbf{m} = 1/2(\mathbf{x} + \mathbf{y}) \in \mathbf{P}$ lies on \mathbf{P} i.e. $\mathbf{m} \cdot \mathbf{n} = \mathbf{c} \cdot \mathbf{n}$

Suppose $\mathbf{P} = \mathbf{Rn}(\mathbf{n})$ goes through the origin with unit normal $\mathbf{u} \in \mathbb{R}^n$

Householder matrix $\mathbf{H} = \mathbf{I}_n - 2\mathbf{u}\mathbf{u}^T$ is reflection w.r.t hyperplane $\mathbf{P} = \mathbf{Rn}(\mathbf{u})$

Recall: let $\mathbf{L}_u = \mathbf{P}_u$

\mathbf{n}_k k th order partial derivative w.r.t \mathbf{x}_k of f of \dots of \mathbf{n}_1 1 th order partial derivative w.r.t \mathbf{x}_1 of f is:

$\text{proj}_{\mathbf{L}_u} = \mathbf{u}\mathbf{u}^T$ and $\text{proj}_{\mathbf{P}_u} = \mathbf{I}_n - \mathbf{u}\mathbf{u}^T \Rightarrow$

$\mathbf{H} = \text{proj}_{\mathbf{P}_u} - \text{proj}_{\mathbf{L}_u}$

Visualize as preserving component in \mathbf{P}_u then flipping component in \mathbf{L}_u

$\mathbf{H}^2 = \mathbf{I}$ is involutory, orthogonal and symmetric, i.e. $\mathbf{H}^T = \mathbf{H} = \mathbf{H}^{-1}$

Modified Gram-Schmidt

Go check Classical GS first, as this is just an alternative computation method

Let $\mathbf{P}_1, \dots, \mathbf{P}_n \in \mathbb{R}^{m \times n}$ be **projector** onto hyperplane $\mathbf{P}_1, \dots, \mathbf{P}_n$

$(\mathbf{R}\mathbf{q}_j)^\perp$ i.e. orthogonal compliment of line $\mathbf{R}\mathbf{q}_j$

Re-state: $\mathbf{u}_{j+1} = (\mathbf{I}_m - \mathbf{Q}_j \mathbf{Q}_j^T) \mathbf{a}_{j+1}$

$\mathbf{u}_{j+1} = (\mathbf{I}_m - \mathbf{P}_1 - \mathbf{P}_2 - \dots - \mathbf{P}_j) \mathbf{a}_{j+1}$

Projectors $\mathbf{P}_1, \dots, \mathbf{P}_n$ are iteratively applied to \mathbf{a}_{j+1} removing its components along $\mathbf{q}_1, \dots, \mathbf{q}_j$ then along \mathbf{q}_{j+1} and so on...

Let $\mathbf{u}_k = (\mathbf{I}_m - \mathbf{P}_1 - \mathbf{P}_2 - \dots - \mathbf{P}_j) \mathbf{a}_k$ i.e. \mathbf{a}_k without its components along $\mathbf{q}_1, \dots, \mathbf{q}_j$

Notice: $\mathbf{u}_j = \mathbf{u}_j^{(j-1)}$ thus $\mathbf{q}_j = \mathbf{u}_j = \mathbf{u}_j^{(j-1)} / \|\mathbf{u}_j\|$ where $r_{jj} = \|\mathbf{u}_j^{(j-1)}\|$

Iterative step:

$\mathbf{u}_j^{(j)} = (\mathbf{I}_m - \mathbf{P}_1 - \mathbf{P}_2 - \dots - \mathbf{P}_{j-1} - \mathbf{Q}_j \mathbf{Q}_j^T) \mathbf{q}_j$

i.e. each projection \mathbf{P}_j of MGS computes $\mathbf{P}_j \mathbf{u}_j^{(j-1)}$ (and projections under \mathbf{R}) in one go

At start of iteration $j=1$ we have ONB $\mathbf{q}_1, \dots, \mathbf{q}_{j-1} \in \mathbb{R}^m$ and residual $\mathbf{u}_j^{(j-1)} = \mathbf{u}_j^{(j-1)} \in \mathbb{R}^m$

Compute $r_{jj} = \|\mathbf{u}_j^{(j-1)}\| \Rightarrow \mathbf{q}_j = \mathbf{u}_j^{(j-1)} / r_{jj}$

For each $k \in \{j+1, \dots, n\}$ compute $r_{jk} = \mathbf{q}_j \cdot \mathbf{u}_k^{(j-1)} \Rightarrow \mathbf{u}_k^{(j)} = (\mathbf{u}_k^{(j-1)} - r_{jk} \mathbf{q}_j)$

It is customary that:

\mathbf{u}_j is a **unit vector**, i.e. $\|\mathbf{u}_j\| = \|\hat{\mathbf{u}}_j\| = 1$

NOTE: for $j=1 \Rightarrow \mathbf{q}_1, \dots, \mathbf{q}_{j-1} = \mathbf{0}$ i.e. none yet

By end of iteration $j=n$ we have **ONB** $\{\mathbf{q}_1, \dots, \mathbf{q}_n\} \in \mathbb{R}^m$

$\mathbf{A} = [\mathbf{a}_1 | \dots | \mathbf{a}_n] = [\mathbf{q}_1 | \dots | \mathbf{q}_n] \begin{bmatrix} r_{11} & \dots & r_{1n} \\ \vdots & \ddots & \vdots \\ 0 & \dots & r_{nn} \end{bmatrix} = \mathbf{Q} \mathbf{R}$

corresponds to thin QR decomposition

Where $\mathbf{A} \in \mathbb{R}^{m \times n}$ is full-rank, $\mathbf{Q} \in \mathbb{R}^{m \times n}$ is semi-orthogonal, and $\mathbf{R} \in \mathbb{R}^{n \times n}$ is upper-triangular

Classical vs. Modified Gram-Schmidt

These algorithms both compute thin QR decomposition

	Classical Gram-Schmidt	Modified Gram-Schmidt
1. for $j = 1$ to n do	1. for $j = 1$ to n do	1. for $j = 1$ to n do
2. $\mathbf{u}_j = \mathbf{a}_j$	2. $\mathbf{u}_j = \mathbf{a}_j$	2. $\mathbf{u}_j = \mathbf{a}_j$
3. end for	3. end for	3. end for
4. for $j = 1$ to n do	4. for $j = 1$ to n do	4. for $j = 1$ to n do
5. $\mathbf{u}_j = \mathbf{u}_j - r_{1j} \mathbf{q}_1$	5. $\mathbf{u}_j = \mathbf{u}_j - r_{1j} \mathbf{q}_1$	5. $\mathbf{u}_j = \mathbf{u}_j - r_{1j} \mathbf{q}_1$
6. end for	6. end for	6. end for
7. $\mathbf{u}_j = \ \mathbf{u}_j\ \mathbf{q}_j$	7. $\mathbf{u}_j = \ \mathbf{u}_j\ \mathbf{q}_j$	7. $\mathbf{u}_j = \ \mathbf{u}_j\ \mathbf{q}_j$
8. end for	8. end for	8. end for

Computes at j th step:

Classical GS $\Rightarrow j$ th column of \mathbf{Q} and the j th column of \mathbf{R}

Modified GS $\Rightarrow j$ th column of \mathbf{Q} and the j th row of \mathbf{R}

Both have **flop (floating-point operation)** count of $O(2mn^2)$

Householder method has $2(mn^2 - n^3/3)$ flops

Recall, but better numerical properties

Count: $\mathbf{Q}^T \mathbf{Q} = \mathbf{I}_n \Rightarrow$ check for loss of orthogonality with $\|\mathbf{I}_n - \mathbf{Q}^T \mathbf{Q}\|$ loss

Classical GS $\Rightarrow \|\mathbf{I}_n - \mathbf{Q}^T \mathbf{Q}\| = \text{Cond}(\mathbf{A})^2 \epsilon_{\text{mach}}$

Modified GS $\Rightarrow \|\mathbf{I}_n - \mathbf{Q}^T \mathbf{Q}\| = \text{Cond}(\mathbf{A}) \epsilon_{\text{mach}}$

NOTE: Householder method has $\|\mathbf{I}_n - \mathbf{Q}^T \mathbf{Q}\| \leq \epsilon_{\text{mach}}$

Multivariate Calculus

Consider $f: \mathbb{R}^n \rightarrow \mathbb{R}$

When clear write \mathbf{J}_f component of input as \mathbf{J} instead of \mathbf{x}_j

Level curve w.r.t. $\mathbf{c} \in \mathbb{R}$ is all points s.t. $f(\mathbf{x}) = \mathbf{c}$

Projecting level curves onto \mathbb{R}^n gives \mathbf{f} 's contour-map

\mathbf{f} is **backwards stable** if $\forall \mathbf{x} \in \mathbb{X} \exists \mathbf{x} \in \mathbf{X}$ s.t. $f(\mathbf{x}) = f(\tilde{\mathbf{x}})$

\mathbf{f} is **stable** if $\forall \mathbf{x} \in \mathbb{X} \exists \mathbf{x} \in \mathbf{X}$ s.t. $f(\mathbf{x}) = f(\tilde{\mathbf{x}})$

relative error $\Rightarrow \frac{\|f(\mathbf{x}) - f(\tilde{\mathbf{x}})\|}{\|f(\mathbf{x})\|} = O(\epsilon_{\text{mach}})$

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relative error $\Rightarrow \frac{\|f(\mathbf{x}) - f(\tilde{\mathbf{x}})\|}{\|f(\mathbf{x})\|} = O(\epsilon_{\text{mach}})$

absolute error $\Rightarrow \frac{\|f(\mathbf{x}) - f(\tilde{\mathbf{x}})\|}{\|f(\mathbf{x})\|} = O(\epsilon_{\text{mach}})$

relative error $\Rightarrow \frac{\|f(\mathbf{x}) - f(\tilde{\mathbf{x}})\|}{\|f(\mathbf{x})\|} = O(\epsilon_{\text{mach}})$

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relative error $\Rightarrow \frac{\|f(\mathbf{x}) - f(\tilde{\math$