QR Decompositions of Matrices

Some Essential Linear Algebra

The Cauchy-Schwarz inequality and the angle between vectors in $\mathbb{R}^n$

In these lectures $\langle x, y \rangle$ defines an inner product between vectors x, y of equal length such that $\langle x, y \rangle = y^T x$ if x and y are *both real* and $\langle x, y \rangle = y^* x$, otherwise.

The Cauchy-Schwarz inequality and the angle between vectors in $\mathbb{R}^n$

In these lectures $\langle x, y\rangle$ defines an inner product between vectors x, y of equal length such that $\langle x, y\rangle = y^T x$ if x and y are *both real* and $\langle x, y\rangle = y^* x$, otherwise.

The Cauchy-Schwarz inequality: Given any $x, y \in \mathbb{C}^n$,

$$|\langle x, y\rangle| \leq \|x\|_2 \|y\|_2$$

with equality holding if and only if $\{x, y\}$ is a linearly dependent set.

The Cauchy-Schwarz inequality and the angle between vectors in $\mathbb{R}^n$

In these lectures $\langle x, y \rangle$ defines an inner product between vectors x, y of equal length such that $\langle x, y \rangle = y^T x$ if x and y are *both real* and $\langle x, y \rangle = y^* x$, otherwise.

The Cauchy-Schwarz inequality: Given any $x, y \in \mathbb{C}^n$,

$$|\langle x, y \rangle| \leq \|x\|_2 \|y\|_2$$

with equality holding if and only if $\{x, y\}$ is a linearly dependent set.

If $x, y \in R^n$, then by the Cauchy-Schwarz inequality

$$-1 \leq \frac{\langle x, y \rangle}{\|x\|_2 \|y\|_2} \leq 1.$$

Hence $\theta = \arccos \frac{\langle x, y \rangle}{\|x\|_2 \|y\|_2}$ is called the angle between x and y.

The Cauchy-Schwarz inequality and the angle between vectors in $\mathbb{R}^n$

In these lectures $\langle x, y\rangle$ defines an inner product between vectors x, y of equal length such that $\langle x, y\rangle = y^T x$ if x and y are *both real* and $\langle x, y\rangle = y^* x$, otherwise.

The Cauchy-Schwarz inequality: Given any $x, y \in \mathbb{C}^n$,

$$|\langle x, y\rangle| \le \|x\|_2 \|y\|_2$$

with equality holding if and only if $\{x, y\}$ is a linearly dependent set.

If $x, y \in R^n$, then by the Cauchy-Schwarz inequality

$$-1 \le \frac{\langle x, y\rangle}{\|x\|_2 \|y\|_2} \le 1.$$

Hence $\theta = \arccos \frac{\langle x, y\rangle}{\|x\|_2 \|y\|_2}$ is called the angle between x and y.

Two vectors $x, y \in \mathbb{C}^n$ are said to be mutually orthogonal if $\langle x, y\rangle = 0$.

Orthogonal complements of sets

Let S be any nonempty subset of $\mathbb{F}^n$ where $\mathbb{F} = \mathbb{R}$ or $\mathbb{F} = \mathbb{C}$. Then the orthogonal complement of S is defined by

$$S^{\perp} := \{x \in \mathbb{F}^n : \langle x, y \rangle = 0 \text{ for all } y \in S\}.$$

Orthogonal complements of sets

Let S be any nonempty subset of $\mathbb{F}^n$ where $\mathbb{F} = \mathbb{R}$ or $\mathbb{F} = \mathbb{C}$. Then the orthogonal complement of S is defined by

$$S^\perp := \{x \in \mathbb{F}^n : \langle x, y \rangle = 0 \text{ for all } y \in S\}.$$

Examples:

1. In $\mathbb{C}^3$, $\{e_3\}^\perp = \operatorname{span}\{e_1, e_2\}$.
2. In $\mathbb{R}^4$, $\{e_2 + e_4\}^\perp = \operatorname{span}\{e_1, e_3, e_2 - e_4\}$.

Orthogonal complements of sets

Let S be any nonempty subset of $\mathbb{F}^n$ where $\mathbb{F} = \mathbb{R}$ or $\mathbb{F} = \mathbb{C}$. Then the orthogonal complement of S is defined by

$$S^\perp := \{x \in \mathbb{F}^n : \langle x, y \rangle = 0 \text{ for all } y \in S\}.$$

Examples:

1. In $\mathbb{C}^3$, $\{e_3\}^\perp = \operatorname{span}\{e_1, e_2\}$.
2. In $\mathbb{R}^4$, $\{e_2 + e_4\}^\perp = \operatorname{span}\{e_1, e_3, e_2 - e_4\}$.

Exercise: Let S be any nonempty subset of $\mathbb{F}^n$. Prove that

1. $S^\perp$ is always a *subspace* of $\mathbb{F}^n$.
2. $S^{\perp\perp} = \operatorname{span} S$.

Orthogonal complements of sets

Let S be any nonempty subset of $\mathbb{F}^n$ where $\mathbb{F} = \mathbb{R}$ or $\mathbb{F} = \mathbb{C}$. Then the orthogonal complement of S is defined by

$$S^\perp := \{x \in \mathbb{F}^n : \langle x, y \rangle = 0 \text{ for all } y \in S\}.$$

Examples:

1. In $\mathbb{C}^3$, $\{e_3\}^\perp = \operatorname{span}\{e_1, e_2\}$.
2. In $\mathbb{R}^4$, $\{e_2 + e_4\}^\perp = \operatorname{span}\{e_1, e_3, e_2 - e_4\}$.

Exercise: Let S be any nonempty subset of $\mathbb{F}^n$. Prove that

1. $S^\perp$ is always a *subspace* of $\mathbb{F}^n$.
2. $S^{\perp\perp} = \operatorname{span} S$.

Exercise: Given any $n \times n$ matrix A prove that $N(A)^\perp = R(A^T)$ where

$$N(A) = \{x \in \mathbb{F}^n : Ax = 0\}$$
$$R(A^T) = \{A^T x : x \in \mathbb{F}^n\}$$

with $\mathbb{F} = \mathbb{R}$ if A is real and $\mathbb{F} = \mathbb{C}$ if A is complex.

Sums and direct sums of subspaces

Sum of two subspaces: Given any two subspaces U, W of $\mathbb{F}^n$,

$$\mathbb{F}^n = U + W$$

if for every $x \in \mathbb{F}^n$, there exist $x_1 \in U$ and $x_2 \in W$ such that $x = x_1 + x_2$.

Sums and direct sums of subspaces

Sum of two subspaces: Given any two subspaces U, W of $\mathbb{F}^n$,

$$\mathbb{F}^n = U + W$$

if for every $x \in \mathbb{F}^n$, there exist $x_1 \in U$ and $x_2 \in W$ such that $x = x_1 + x_2$.

Examples:

1. $\mathbb{R}^4 = \operatorname{span}\{e_1, e_3, e_2 + e_4\} + \{[\alpha, 0, -\alpha, 0]^T : \alpha \in \mathbb{R}\}$.
2. $\mathbb{C}^4 = \operatorname{span}\{e_1, e_1 + e_3, e_2 - e_4\} + \operatorname{span}\{e_2, e_3\}$.

Sums and direct sums of subspaces

Sum of two subspaces: Given any two subspaces U, W of $\mathbb{F}^n$,

$$\mathbb{F}^n = U + W$$

if for every $x \in \mathbb{F}^n$, there exist $x_1 \in U$ and $x_2 \in W$ such that $x = x_1 + x_2$.

Examples:

1. $\mathbb{R}^4 = \mathrm{span}\,\{e_1, e_3, e_2 + e_4\} + \{[\alpha, 0, -\alpha, 0]^T : \alpha \in \mathbb{R}\}$.
2. $\mathbb{C}^4 = \mathrm{span}\,\{e_1, e_1 + e_3, e_2 - e_4\} + \mathrm{span}\,\{e_2, e_3\}$.

Theorem Let U and W be two subspaces of $\mathbb{F}^n$. such that $\mathbb{F}^n = U + W$. Then

$$\dim U + \dim W - \dim(U \cap W) = n,$$

and $\mathrm{span}\,(U \cup W) = U + W$.

Sums and direct sums of subspaces

Direct sum of two subspaces: Let U and W be subspaces of $\mathbb{F}^n$. Then $\mathbb{F}^n$ is the *direct* sum of U and W denoted by

$$\mathbb{F}^n = U \oplus W \tag{1}$$

if for every $x \in \mathbb{F}^n$, there exist *unique* $x_1 \in U$ and $x_2 \in W$ such that $x = x_1 + x_2$. The equation (1) is called a diect sum decomposition of $\mathbb{F}^n$.

Sums and direct sums of subspaces

Direct sum of two subspaces: Let U and W be subspaces of $\mathbb{F}^n$. Then $\mathbb{F}^n$ is the *direct* sum of U and W denoted by

$$\mathbb{F}^n = U \oplus W \tag{1}$$

if for every $x \in \mathbb{F}^n$, there exist *unique* $x_1 \in U$ and $x_2 \in W$ such that $x = x_1 + x_2$. The equation (1) is called a diect sum decomposition of $\mathbb{F}^n$.

Sums and direct sums of subspaces

Direct sum of two subspaces: Let U and W be subspaces of $\mathbb{F}^n$. Then $\mathbb{F}^n$ is the *direct* sum of U and W denoted by

$$\mathbb{F}^n = U \oplus W \qquad (1)$$

if for every $x \in \mathbb{F}^n$, there exist *unique* $x_1 \in U$ and $x_2 \in W$ such that $x = x_1 + x_2$. The equation (1) is called a diect sum decomposition of $\mathbb{F}^n$.

Examples:

1. $\mathbb{R}^4 = \mathrm{span}\{e_1, e_3, e_2 + e_4\} \oplus \{[\alpha, 0, -\alpha, 0]^T : \alpha \in \mathbb{R}\}$.
2. However $\mathbb{C}^4 = \mathrm{span}\{e_1, e_1 + e_3, e_2 - e_4\} + \mathrm{span}\{e_2, e_3\}$ is a sum that is not a direct sum.
3. Given any subspace U of $\mathbb{F}^n$, $\mathbb{F}^n = U \oplus U^{\perp}$.

Sums and direct sums of subspaces

Direct sum of two subspaces: Let U and W be subspaces of $\mathbb{F}^n$. Then $\mathbb{F}^n$ is the *direct* sum of U and W denoted by

$$\mathbb{F}^n = U \oplus W \tag{1}$$

if for every $x \in \mathbb{F}^n$, there exist *unique* $x_1 \in U$ and $x_2 \in W$ such that $x = x_1 + x_2$. The equation (1) is called a diect sum decomposition of $\mathbb{F}^n$.

Examples:

1. $\mathbb{R}^4 = \mathrm{span}\,\{e_1, e_3, e_2 + e_4\} \oplus \{[\alpha, 0, -\alpha, 0]^T : \alpha \in \mathbb{R}\}$.
2. However $\mathbb{C}^4 = \mathrm{span}\,\{e_1, e_1 + e_3, e_2 - e_4\} + \mathrm{span}\,\{e_2, e_3\}$ is a sum that is not a direct sum.
3. Given any subspace U of $\mathbb{F}^n$, $\mathbb{F}^n = U \oplus U^\perp$.

Theorem Suppose U, W are subspaces of $\mathbb{F}^n$ such that $\mathbb{F}^n = U + W$. Then $\mathbb{F}^n = U \oplus W$ if and only if $u + w = 0$ for $u \in U$, $w \in W$, implies that $u = w = 0$.

Sums and direct sums of subspaces

Direct sum of two subspaces: Let U and W be subspaces of $\mathbb{F}^n$. Then $\mathbb{F}^n$ is the *direct* sum of U and W denoted by

$$\mathbb{F}^n = U \oplus W \tag{1}$$

if for every $x \in \mathbb{F}^n$, there exist *unique* $x_1 \in U$ and $x_2 \in W$ such that $x = x_1 + x_2$. The equation (1) is called a diect sum decomposition of $\mathbb{F}^n$.

Examples:

1. $\mathbb{R}^4 = \operatorname{span}\{e_1, e_3, e_2 + e_4\} \oplus \{[\alpha, 0, -\alpha, 0]^T : \alpha \in \mathbb{R}\}$.
2. However $\mathbb{C}^4 = \operatorname{span}\{e_1, e_1 + e_3, e_2 - e_4\} + \operatorname{span}\{e_2, e_3\}$ is a sum that is not a direct sum.
3. Given any subspace U of $\mathbb{F}^n$, $\mathbb{F}^n = U \oplus U^\perp$.

Theorem Suppose U, W are subspaces of $\mathbb{F}^n$ such that $\mathbb{F}^n = U + W$. Then $\mathbb{F}^n = U \oplus W$ if and only if $u + w = 0$ for $u \in U$, $w \in W$, implies that $u = w = 0$.

Find more examples like example 2!

Projections

A linear map $P : \mathbb{F}^n \mapsto \mathbb{F}^n$ is called a *projection* if $P^2 = P$.

Projections

A linear map $P : \mathbb{F}^n \mapsto \mathbb{F}^n$ is called a *projection* if $P^2 = P$.

Example: $x \mapsto Ax$ for all $x \in \mathbb{R}^3$ where $A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \end{bmatrix}$.

In fact, any $n \times n$ idempotent matrix, ie., $A^2 = A$ defines a projection on $\mathbb{F}^n$.

Projections

A linear map $P : \mathbb{F}^n \mapsto \mathbb{F}^n$ is called a *projection* if $P^2 = P$.

Example: $x \mapsto Ax$ for all $x \in \mathbb{R}^3$ where $A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & -1 \\ 0 & 0 & 0 \end{bmatrix}$.

In fact, any $n \times n$ idempotent matrix, ie., $A^2 = A$ defines a projection on $\mathbb{F}^n$.

Exercises:

1. Given any projection P on $\mathbb{F}^n$, prove the following.
   (a) $\mathbb{F}^n = N(P) \oplus R(P)$.
   (b) $I - P$ is also a projection.
   (c) $N(P) = R(I - P)$ and $R(P) = N(I - P)$.
2. If U and V are subspaces of $\mathbb{F}^n$ such that $\mathbb{F}^n = U \oplus V$ then $P : \mathbb{F}^n \mapsto \mathbb{F}^n$ defined by $Px = x_1$ where $x = x_1 + x_2, x_1 \in U, x_2 \in V$, is a projection onto U, that is, $R(P) = U$.

Orthogonal projections

A linear map $P : \mathbb{F}^n \mapsto \mathbb{F}^n$ is called an *orthogonal projection* if $P^2 = P$ and $P^T = P$.

Orthogonal projections

A linear map $P : \mathbb{F}^n \mapsto \mathbb{F}^n$ is called an *orthogonal projection* if $P^2 = P$ and $P^T = P$.

Example: $x \mapsto Ax$ for all $x \in \mathbb{R}^3$ where $A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$.

In fact, any $n \times n$ idempotent symmetric matrix, defines an orthogonal projection on $\mathbb{F}^n$.

Orthogonal projections

A linear map $P : \mathbb{F}^n \mapsto \mathbb{F}^n$ is called an *orthogonal projection* if $P^2 = P$ and $P^T = P$.

Example: $x \mapsto Ax$ for all $x \in \mathbb{R}^3$ where $A = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix}$.

In fact, any $n \times n$ idempotent symmetric matrix, defines an orthogonal projection on $\mathbb{F}^n$.

Exercises:

1. Given any orthogonal projection P on $\mathbb{F}^n$, prove the following.
   (a) $I - P$ is also an orthogonal projection.
   (b) $N(P) = R(P)^\perp$.
   (c) $\mathbb{F}^n = R(P) \oplus R(P)^\perp$.
2. If U is a subspace of $\mathbb{F}^n$ such that $\mathbb{F}^n = U \oplus U^\perp$ then $P : \mathbb{F}^n \mapsto \mathbb{F}^n$ defined by $Px = x_1$ where $x = x_1 + x_2, x_1 \in U, x_2 \in U^\perp$, is an orthogonal projection onto U, that is $R(P) = U$.

Orthonormal sets and orthonormal bases

A nonempty subset $\{v_1, \ldots, v_m\}$ of $\mathbb{R}^n$ or $\mathbb{C}^n$ is said to be an *orthonormal set* if

$$\langle v_i, v_j \rangle = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases}$$

Orthonormal sets and orthonormal bases

A nonempty subset $\{v_1, \ldots, v_m\}$ of $\mathbb{R}^n$ or $\mathbb{C}^n$ is said to be an *orthonormal set* if

$$\langle v_i, v_j \rangle = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases}$$

Examples:

- The canonical basis $\{e_1, \ldots, e_n\}$ of $\mathbb{R}^n$ or $\mathbb{C}^n$ where e_i is the i^{th} column of I_n.
- $\left\{ \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \\ 0 \end{bmatrix}, \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\}$ in $\mathbb{R}^3$ or $\mathbb{C}^3$.

Orthonormal sets and orthonormal bases

A nonempty subset $\{v_1, \ldots, v_m\}$ of $\mathbb{R}^n$ or $\mathbb{C}^n$ is said to be an *orthonormal set* if

$$\langle v_i, v_j \rangle = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases}$$

Examples:

- The canonical basis $\{e_1, \ldots, e_n\}$ of $\mathbb{R}^n$ or $\mathbb{C}^n$ where e_i is the i^{th} column of I_n.
- $\left\{ \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \\ 0 \end{bmatrix}, \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\}$ in $\mathbb{R}^3$ or $\mathbb{C}^3$.

An orthonormal set is always a linearly independent set.

Orthonormal sets and orthonormal bases

A nonempty subset $\{v_1, \ldots, v_m\}$ of $\mathbb{R}^n$ or $\mathbb{C}^n$ is said to be an *orthonormal set* if

$$\langle v_i, v_j \rangle = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases}$$

Examples:

- The canonical basis $\{e_1, \ldots, e_n\}$ of $\mathbb{R}^n$ or $\mathbb{C}^n$ where e_i is the i^{th} column of I_n.
- $\left\{ \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \\ 0 \end{bmatrix}, \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\}$ in $\mathbb{R}^3$ or $\mathbb{C}^3$.

An orthonormal set is always a linearly independent set.

An *orthonormal basis* of $\mathbb{R}^n$ or $\mathbb{C}^n$ is an orthonormal set with n elements.

Orthonormal sets and orthonormal bases

A nonempty subset $\{v_1, \ldots, v_m\}$ of $\mathbb{R}^n$ or $\mathbb{C}^n$ is said to be an *orthonormal set* if

$$\langle v_i, v_j \rangle = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases}$$

Examples:

- The canonical basis $\{e_1, \ldots, e_n\}$ of $\mathbb{R}^n$ or $\mathbb{C}^n$ where e_i is the i^{th} column of I_n.
- $\left\{ \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \\ 0 \end{bmatrix}, \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\}$ in $\mathbb{R}^3$ or $\mathbb{C}^3$.

An orthonormal set is always a linearly independent set.

An *orthonormal basis* of $\mathbb{R}^n$ or $\mathbb{C}^n$ is an orthonormal set with n elements.

The canonical basis in $\mathbb{R}^n$ or $\mathbb{C}^n$ is a classic example of an orthonormal basis.

Orthonormal sets and orthonormal bases

A nonempty subset $\{v_1, \ldots, v_m\}$ of $\mathbb{R}^n$ or $\mathbb{C}^n$ is said to be an *orthonormal set* if

$$\langle v_i, v_j \rangle = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases}$$

Examples:

- The canonical basis $\{e_1, \ldots, e_n\}$ of $\mathbb{R}^n$ or $\mathbb{C}^n$ where e_i is the i^{th} column of I_n.
- $\left\{ \begin{bmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \\ 0 \end{bmatrix}, \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right\}$ in $\mathbb{R}^3$ or $\mathbb{C}^3$.

An orthonormal set is always a linearly independent set.

An *orthonormal basis* of $\mathbb{R}^n$ or $\mathbb{C}^n$ is an orthonormal set with n elements.

The canonical basis in $\mathbb{R}^n$ or $\mathbb{C}^n$ is a classic example of an orthonormal basis.

Any linearly independent subset of $\mathbb{R}^n$ or $\mathbb{C}^n$ may be converted to an orthonormal set via the process of Gram-Schmidt orthonormalisation.

Classical Gram Schmidt Orthonormalisation

Let $\{v_1, \ldots, v_m\}$ be an ordered set of linearly independent vectors in $\mathbb{R}^n$. The Classical Gram Schmidt (CGS) process finds an ordered orthonormal set of vectors $\{q_1, \ldots, q_m\}$ in $\mathbb{R}^n$ such that

$$\mathrm{span}\{v_1, \ldots, v_k\} = \mathrm{span}\{q_1, \ldots, q_k\}, \; k = 1, \ldots, m.$$

Classical Gram Schmidt Orthonormalisation

Let $\{v_1, \ldots, v_m\}$ be an ordered set of linearly independent vectors in $\mathbb{R}^n$. The Classical Gram Schmidt (CGS) process finds an ordered orthonormal set of vectors $\{q_1, \ldots, q_m\}$ in $\mathbb{R}^n$ such that

$$\operatorname{span}\{v_1, \ldots, v_k\} = \operatorname{span}\{q_1, \ldots, q_k\}, \;\; k = 1, \ldots, m.$$

Classical Gram Schmidt (CGS):

Step 1: $q_1 := v_1 / \|v_1\|_2$.

Step 2: $q_2 := \underbrace{(v_2 - (v_2^T q_1) q_1)}_{=:\hat{q}_2} / \|v_2 - (v_2^T q_1) q_1\|_2$.

Step k: Assuming that $q_1, \ldots, q_{k-1}$ are calculated as above,

$$q_k = \underbrace{\left(v_k - \sum_{i=1}^{k-1} (v_k^T q_i) q_i\right)}_{=:\hat{q}_k} / \|v_k - \Sigma_{i=1}^{k-1} (v_k^T q_i) q_i\|_2.$$

Classical Gram Schmidt Orthonormalisation

Let $\{v_1, \ldots, v_m\}$ be an ordered set of linearly independent vectors in $\mathbb{R}^n$. The Classical Gram Schmidt (CGS) process finds an ordered orthonormal set of vectors $\{q_1, \ldots, q_m\}$ in $\mathbb{R}^n$ such that

$$\mathrm{span}\{v_1, \ldots, v_k\} = \mathrm{span}\{q_1, \ldots, q_k\}, \ k = 1, \ldots, m.$$

Classical Gram Schmidt (CGS):

Step 1: $q_1 := v_1/\|v_1\|_2$.

Step 2: $q_2 := \underbrace{(v_2 - (v_2^T q_1)q_1)}_{=:\hat{q}_2} /\|v_2 - (v_2^T q_1)q_1\|_2$.

Step k: Assuming that $q_1, \ldots, q_{k-1}$ are calculated as above,

$$q_k = \underbrace{(v_k - \sum_{i=1}^{k-1}(v_k^T q_i)q_i)}_{=:\hat{q}_k} /\|v_k - \Sigma_{i=1}^{k-1}(v_k^T q_i)q_i\|_2.$$

Exercise: Show that CGS applied to the basis $\{e_1 + e_2, e_2, e_2 + e_3\}$ in $\mathbb{R}^3$ produces the ordered orthonormal basis

$$\{(e_1 + e_2)/\sqrt{2}, (e_2 - e_1)/\sqrt{2}, e_3\}.$$

Unitary/Orthogonal matrices

Unitary matrices are square matrices such that $Q^* = Q^{-1}$.
A real unitary matrix is called an orthogonal matrix.

Unitary/Orthogonal matrices

Unitary matrices are square matrices such that $Q^* = Q^{-1}$.
A real unitary matrix is called an orthogonal matrix.

Evidently, a square matrix Q is unitary (orthogonal) if and only if its columns form an orthonormal basis of $\mathbb{R}^n$ ($\mathbb{C}^n$).

Unitary/Orthogonal matrices

Unitary matrices are square matrices such that $Q^* = Q^{-1}$.
A real unitary matrix is called an orthogonal matrix.

Evidently, a square matrix Q is unitary (orthogonal) if and only if its columns form an orthonormal basis of $\mathbb{R}^n$ ($\mathbb{C}^n$).

They play a very important role in matrix computations due to their nice properties. In the following let Q be an $n \times n$ unitary matrix.

Unitary/Orthogonal matrices

Unitary matrices are square matrices such that $Q^* = Q^{-1}$.
A real unitary matrix is called an orthogonal matrix.

Evidently, a square matrix Q is unitary (orthogonal) if and only if its columns form an orthonormal basis of $\mathbb{R}^n$ ($\mathbb{C}^n$).

They play a very important role in matrix computations due to their nice properties. In the following let Q be an $n \times n$ unitary matrix.

- $\langle Qx, Qy \rangle = \langle x, y \rangle$ for all $x, y \in \mathbb{C}^n$.
- $\|Qx\|_2 = \|x\|_2$.
- $\|QB\|_2 = \|B\|_2$ for any $B \in \mathbb{C}^{n\times m}$.
- $\|Q\|_2 = 1$ and $\|Q\|_F = \sqrt{n}$.
- $\kappa_2(Q) = 1$.
- Q^*AQ is Hermitian if A is Hermitian.
- If A is real symmetric and Q is orthogonal, then Q^TAQ is also real symmetric.
- In the presence of rounding errors, $fl(QA) = Q(A + E)$ where $\|E\|_2/\|A\|_2$ is $O(u)$.

Unitary/Orthogonal matrices

Unitary matrices are square matrices such that $Q^* = Q^{-1}$.
A real unitary matrix is called an orthogonal matrix.

Evidently, a square matrix Q is unitary (orthogonal) if and only if its columns form an orthonormal basis of $\mathbb{R}^n$ ($\mathbb{C}^n$).

They play a very important role in matrix computations due to their nice properties. In the following let Q be an $n \times n$ unitary matrix.

- $\langle Qx, Qy \rangle = \langle x, y \rangle$ for all $x, y \in \mathbb{C}^n$.
- $\|Qx\|_2 = \|x\|_2$.
- $\|QB\|_2 = \|B\|_2$ for any $B \in C^{n \times m}$.
- $\|Q\|_2 = 1$ and $\|Q\|_F = \sqrt{n}$.
- $\kappa_2(Q) = 1$. Prove these properties!
- $Q^* AQ$ is Hermitian if A is Hermitian.
- If A is real symmetric and Q is orthogonal, then $Q^T AQ$ is also real symmetric.
- In the presence of rounding errors, $fl(QA) = Q(A + E)$ where $\|E\|_2 / \|A\|_2$ is $O(u)$.

Isometry

A matrix $Q \in \mathbb{C}^{n \times m}$, or $\mathbb{R}^{n \times m}$ with $n > m$, is said to be an isometry if $Q^* Q = I_m$.

Isometry

A matrix $Q \in \mathbb{C}^{n\times m}$, or $\mathbb{R}^{n\times m}$ with $n > m$, is said to be an isometry if $Q^*Q = I_m$.

Clearly a matrix Q with more rows than columns is an isometry if and only if its columns form an orthonormal set in $\mathbb{R}^n$ or $\mathbb{C}^n$.

Isometry

A matrix $Q \in \mathbb{C}^{n \times m}$, or $\mathbb{R}^{n \times m}$ with $n > m$, is said to be an isometry if $Q^* Q = I_m$.

Clearly a matrix Q with more rows than columns is an isometry if and only if its columns form an orthonormal set in $\mathbb{R}^n$ or $\mathbb{C}^n$.

Isometries have properties very similar to that of unitary matrices. Given an $n \times m$ isometry $Q = [q_1 \cdots q_m]$,

- $\langle Qx, Qy \rangle = \langle x, y \rangle$ for all $x, y \in \mathbb{C}^n$.
- $\|Qx\|_2 = \|x\|_2$.
- $\|QB\|_2 = \|B\|_2$ for any $B \in \mathbb{C}^{n \times m}$.
- $\|Q\|_2 = 1$ and $\|Q\|_F = \sqrt{m}$.
- $\kappa_2(Q) = 1$.
- In the presence of rounding errors, $fl(QA) = Q(A + E)$ where $\|E\|_2 / \|A\|_2$ is $O(u)$.
- QQ^* is the orthogonal projection onto $\mathrm{span}\,\{q_1, \ldots, q_m\}$, that is, $QQ^* v = v$ for all $v \in \mathrm{span}\,\{q_1, \ldots, q_m\}$ and $QQ^* w = 0$ for all $w \in \{q_1, \ldots, q_m\}^\perp$. Prove this!

Suggested resources for further study

- G. Strang, Linear Algebra and Its Applications, Cengage Learning, 4th Edition, 2006.
- J. Gilbert and L. Gilbert, Linear Algebra and Matrix Theory, Academic Press, 1995.
- MIT OCW on Linear Algebra.

QR decomposition of matrices

QR Decomposition: Given any matrix $A \in \mathbb{R}^{n \times m}$, $n \geq m$, there exists an orthogonal matrix $Q \in \mathbb{R}^{n \times n}$ and an upper triangular matrix $R \in \mathbb{R}^{n \times m}$ such that

$$A = QR. \tag{2}$$

The decomposition (2) is called a QR decomposition of A.

If $n > m$, then $R = \begin{bmatrix} R_1 \\ 0 \end{bmatrix}$ where $R_1 \in \mathbb{R}^{m \times m}$ is upper triangular.

In particular if $n = m$, then (2) takes the form $A = QR$ where R is a square upper triangular matrix.

If $A \in \mathbb{C}^{n \times m}$, $n \geq m$, then (2) holds with $\mathbb{R}$ replaced by $\mathbb{C}$, Q being a unitary matrix.

Condensed QR decomposition

Given $A \in \mathbb{R}^{n \times m}$ with $n > m$, if $A = QR$ be a QR decomposition of A with $R = \begin{bmatrix} R_1 \\ 0 \end{bmatrix}$, then partitioning $Q = [Q_1 \;\; Q_2]$ where $Q_1 \in \mathbb{R}^{n \times m}$, gives,

$$A = QR = [Q_1 \;\; Q_2] \begin{bmatrix} R_1 \\ 0 \end{bmatrix} = Q_1 R_1 .$$

This motivates the following theorem.

Theorem Given any $n \times m$ matrix A with $n > m$, there exists an isometry $Q \in \mathbb{R}^{n \times m}$ and an upper triangular matrix R such that

$$A = QR. \qquad ((3))$$

If $\operatorname{rank} A = m$, then R is nonsingular.

The decomposition in (3) is called a *condensed QR decomposition of A.*

Equivalence of CGS and condensed QR decomposition

CGS $\equiv$ condensed QR

Supose $\{v_1, \ldots, v_m\}$ is an ordered linearly independent subset of $\mathbb{R}^n$ and $\{q_1, \ldots, q_m\}$ is the output of CGS on $\{v_1, \ldots, v_m\}$.

CGS $\equiv$ condensed QR

Supose $\{v_1, \ldots, v_m\}$ is an ordered linearly independent subset of $\mathbb{R}^n$ and $\{q_1, \ldots, q_m\}$ is the output of CGS on $\{v_1, \ldots, v_m\}$. Then,

$$\underbrace{[v_1 \cdots v_m]}_{=:V} = \underbrace{[q_1 \cdots q_m]}_{=:Q} \underbrace{\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1m} \\ & r_{22} & \cdots & r_{2m} \\ & & \ddots & \vdots \\ & & & r_{mm} \end{bmatrix}}_{=:R}$$

where $r_{ij} = v_j^T q_i$ for $j > i$, $r_{jj} = \|\hat{q}_j\|_2$ and $r_{ij} = 0$ otherwise. Clearly, $V = QR$ is a condensed QR decomposition of V.

CGS $\equiv$ condensed QR

Supose $\{v_1, \ldots, v_m\}$ is an ordered linearly independent subset of $\mathbb{R}^n$ and $\{q_1, \ldots, q_m\}$ is the output of CGS on $\{v_1, \ldots, v_m\}$. Then,

$$\underbrace{[v_1 \cdots v_m]}_{=:V} = \underbrace{[q_1 \cdots q_m]}_{=:Q} \underbrace{\begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1m} \\ & r_{22} & \cdots & r_{2m} \\ & & \ddots & \vdots \\ & & & r_{mm} \end{bmatrix}}_{=:R}$$

where $r_{ij} = v_j^T q_i$ for $j > i$, $r_{jj} = \|\hat{q}_j\|_2$ and $r_{ij} = 0$ otherwise. Clearly, $V = QR$ is a condensed QR decomposition of V.

Exercise: Conversely if $V = QR$ be a condensed QR decomposition of $V = [v_1 \cdots v_m] \in \mathbb{R}^{n \times m}$ where $R = [r_{ij}]_{m \times m}$ with $r_{ii} > 0$ for all $i = 1, \ldots, m$, then the columns $q_1, \ldots, q_m$ of Q are equal to those obtained via CGS on the columns of V with

$$r_{ij} = \begin{cases} v_j^T q_i, & i < j, \\ \|\hat{q}_j\|_2, & i = j \\ 0, & \text{otherwise.} \end{cases}$$

Numerical issues associated with CGS and Modified Gram Schmidt (MGS)

Flop count and numerical issues of CGS

For each $k = 1, 2, \ldots, m$, computing,

$\hat{q}_k = v_k - \sum_{i=1}^{k-1} (v_k^T q_i) q_i \longrightarrow 4n(k-1)$ flops

$\|\hat{q}_k\|_2 \longrightarrow 2n$ flops and one square root.

So,

$$q_k = \frac{\hat{q}_k}{\|\hat{q}_k\|_2} \longrightarrow 4nk - n \text{ flops and one square root.}$$

Flop count and numerical issues of CGS

For each $k = 1, 2, \ldots, m$, computing,

$\hat{q}_k = v_k - \sum_{i=1}^{k-1} (v_k^T q_i) q_i \longrightarrow 4n(k-1)$ flops

$\|\hat{q}_k\|_2 \longrightarrow 2n$ flops and one square root.

So,

$q_k = \frac{\hat{q}_k}{\|\hat{q}_k\|_2} \longrightarrow 4nk - n$ flops and one square root.

Therefore the total cost of CGS is

$$\sum_{k=1}^{m} 4nk - n = 2nm^2 + O(nm) + O(m^2)$$

flops.

Flop count and numerical issues of CGS

For each $k = 1, 2, \ldots, m$, computing,

$\hat{q}_k = v_k - \sum_{i=1}^{k-1} (v_k^T q_i) q_i \longrightarrow 4n(k-1)$ flops

$\|\hat{q}_k\|_2 \longrightarrow 2n$ flops and one square root.

So,

$q_k = \frac{\hat{q}_k}{\|\hat{q}_k\|_2} \longrightarrow 4nk - n$ flops and one square root.

Therefore the total cost of CGS is

$$\sum_{k=1}^{m} 4nk - n = 2nm^2 + O(nm) + O(m^2)$$

flops.

The quality of the orthonormalisation is measured by *the departure from orthonormality* $\|I_m - Q^T Q\|_2$ of the computed Q.

It is considered to be good in the presence of rounding error if $\|I_m - Q^T Q\|_2$ is $O(u)$.

CGS is a poor performer in the presence of rounding error

The quality of orthonormalisation in CGS can be poor in the presence of rounding error.

Example: Consider the set of vectors $\{v_1, v_2, v_3\}$ where

$$v_1 := \begin{bmatrix} 1 \\ \epsilon \\ 0 \\ 0 \end{bmatrix}, \; v_2 := \begin{bmatrix} 1 \\ 0 \\ \epsilon \\ 0 \end{bmatrix}, \; v_3 := \begin{bmatrix} 1 \\ 0 \\ 0 \\ \epsilon \end{bmatrix},$$

where $\epsilon > 0$ is such that $\epsilon^2 < u$. Perform CGS on the set assuming that $fl(1 + \epsilon^2) = 1$ and there is no other rounding and report the departure from orthonormality.

CGS is a poor performer in the presence of rounding error

The quality of orthonormalisation in CGS can be poor in the presence of rounding error.

Example: Consider the set of vectors $\{v_1, v_2, v_3\}$ where

$$v_1 := \begin{bmatrix} 1 \\ \epsilon \\ 0 \\ 0 \end{bmatrix}, \; v_2 := \begin{bmatrix} 1 \\ 0 \\ \epsilon \\ 0 \end{bmatrix}, \; v_3 := \begin{bmatrix} 1 \\ 0 \\ 0 \\ \epsilon \end{bmatrix},$$

where $\epsilon > 0$ is such that $\epsilon^2 < u$. Perform CGS on the set assuming that $fl(1 + \epsilon^2) = 1$ and there is no other rounding and report the departure from orthonormality.

A modification to the CGS process which is theoretically equivalent to CGS called Modified Gram Schmidt(MGS) is seen to be superior in the presence of rounding error.

Modified Gram Schmidt(MGS)

Let $\{v_1, \ldots, v_m\}$ be a linearly independent subset of $\mathbb{R}^n$.
The first two steps of MGS and CGS are the same. Assume that q_1, q_2 are formed.

Step 3: Let

$$\begin{aligned} v_3^{(1)} &:= v_3 - (v_3^T q_1) q_1 \\ v_3^{(2)} &:= v_3^{(1)} - \{\left(v_3^{(1)}\right)^T q_2\} q_2 \\ \tilde{q}_3 &:= v_3^{(2)} / \|v_3^{(2)}\|_2. \end{aligned}$$

$v_3^{(2)}$ and $\tilde{q}_3$ are respectively the same as $\hat{q}_3$ and q_3 of CGS in theory.
This is because $\left(v_3^{(1)}\right)^T q_2 = v_3^T q_2$ in theory.

However, the computed q_1 and q_2 are not exactly orthogonal to each other. Also the computed $v_3^{(1)}$ is not exactly orthogonal to q_1. So the computed q_3 and $\tilde{q}_3$ are different.

Modified Gram Schmidt(MGS)

Continuing similarly till $\tilde{q}_1, \tilde{q}_2, \ldots, \tilde{q}_{k-1}$ have been found, let

Step k:

$$
\begin{aligned}
v_k^{(1)} &:= v_k - (v_k^T \tilde{q}_1)\tilde{q}_1 \\
v_k^{(2)} &:= v_k^{(1)} - \{\left(v_k^{(1)}\right)^T \tilde{q}_2\}\tilde{q}_2 \\
&\vdots \\
v_k^{(k-1)} &:= \underbrace{v_k^{(k-2)} - \{\left(v_k^{(k-2)}\right)^T \tilde{q}_{k-1}\}\tilde{q}_{k-1}}_{=\hat{q}_k \text{of CGS in theory}} \\
\tilde{q}_k &:= \underbrace{v_k^{(k-1)}/\|v_k^{(k-1)}\|_2}_{=q_k \text{ in theory}}
\end{aligned}
$$

Thus MGS produces the orthonormal set $\{\tilde{q}_1, \tilde{q}_2, \ldots, \tilde{q}_m\}$.

Modified Gram Schmidt(MGS)

Continuing similarly till $\tilde{q}_1, \tilde{q}_2, \ldots, \tilde{q}_{k-1}$ have been found, let

Step k:

$$
\begin{aligned}
v_k^{(1)} &:= v_k - (v_k^T \tilde{q}_1)\tilde{q}_1 \\
v_k^{(2)} &:= v_k^{(1)} - \{\left(v_k^{(1)}\right)^T \tilde{q}_2\}\tilde{q}_2 \\
&\vdots \\
v_k^{(k-1)} &:= \underbrace{v_k^{(k-2)} - \{\left(v_k^{(k-2)}\right)^T \tilde{q}_{k-1}\}\tilde{q}_{k-1}}_{=\hat{q}_k \text{of CGS in theory}} \\
\tilde{q}_k &:= \underbrace{v_k^{(k-1)}/\|v_k^{(k-1)}\|_2}_{=q_k \text{ in theory}}
\end{aligned}
$$

Thus MGS produces the orthonormal set $\{\tilde{q}_1, \tilde{q}_2, \ldots, \tilde{q}_m\}$.

Exercise: Prove that MGS produces an exactly orthonormal set when applied on the set of vectors $\{v_1, v_2, v_3\}$ considered earlier under the same assumptions with respect to rounding.

MGS $\equiv$ Condensed QR

Exercise: *Let* $\{v_1, \ldots, v_m\}$ *be a linearly independent subset of* $\mathbb{R}^n$. *For* $j = 1, \ldots, i-1$, *and* $i = 1, \ldots, m$, *let* $\tilde{q}_i$ *and* $v_i^{(j)}$ *be the vectors obtained via Modified Gram Schmidt.*
Let $\tilde{Q} = [\tilde{q}_1 \cdots \tilde{q}_m]$, $V = [v_1 \cdots v_m]$, *and* $\tilde{R} = [\tilde{r}_{ij}] \in \mathbb{R}^{m \times m}$ *be an upper triangular matrix with* $\tilde{r}_{ik} = \left(v_k^{(i)}\right)^T q_i$ *for* $1 \leq i \leq k-1$ *and* $\tilde{r}_{kk} = \|v_k^{(k-1)}\|_2$ *for* $k = 1, \ldots, m$. *Prove that*

$$V = \tilde{Q}\tilde{R}$$

is theoretically the same condensed QR decomposition of V *as the one via CGS and has the exact same flop count.*

MGS $\equiv$ Condensed QR

Exercise: *Let $\{v_1, \ldots, v_m\}$ be a linearly independent subset of $\mathbb{R}^n$. For $j = 1, \ldots, i-1$, and $i = 1, \ldots, m$, let $\tilde{q}_i$ and $v_i^{(j)}$ be the vectors obtained via Modified Gram Schmidt.*
Let $\tilde{Q} = [\tilde{q}_1 \cdots \tilde{q}_m]$, $V = [v_1 \cdots v_m]$, and $\tilde{R} = [\tilde{r}_{ij}] \in \mathbb{R}^{m\times m}$ be an upper triangular matrix with $\tilde{r}_{ik} = \left(v_k^{(i)}\right)^T q_i$ for $1 \le i \le k-1$ and $\tilde{r}_{kk} = \|v_k^{(k-1)}\|_2$ for $k = 1, \ldots, m$. Prove that

$$V = \tilde{Q}\tilde{R}$$

is theoretically the same condensed QR decomposition of V as the one via CGS and has the exact same flop count.

The computed $\tilde{Q}_c$ from MGS satisfies $\|I_m - \tilde{Q}_c^T\tilde{Q}_c\|_2 \approx \kappa_2(V)u$. [Higham, 96], [Björck, 96] So, orthonormalisation is poor if $\kappa_2(V)$ is large.

MGS $\equiv$ Condensed QR

Exercise: *Let $\{v_1, \ldots, v_m\}$ be a linearly independent subset of $\mathbb{R}^n$. For $j = 1, \ldots, i-1$, and $i = 1, \ldots, m$, let $\tilde{q}_i$ and $v_i^{(j)}$ be the vectors obtained via Modified Gram Schmidt.*
Let $\tilde{Q} = [\tilde{q}_1 \cdots \tilde{q}_m]$, $V = [v_1 \cdots v_m]$, and $\tilde{R} = [\tilde{r}_{ij}] \in \mathbb{R}^{m \times m}$ be an upper triangular matrix with $\tilde{r}_{ik} = \left(v_k^{(i)}\right)^T q_i$ for $1 \leq i \leq k-1$ and $\tilde{r}_{kk} = \|v_k^{(k-1)}\|_2$ for $k = 1, \ldots, m$. Prove that

$$V = \tilde{Q}\tilde{R}$$

is theoretically the same condensed QR decomposition of V as the one via CGS and has the exact same flop count.

The computed $\tilde{Q}_c$ from MGS satisfies $\|I_m - \tilde{Q}_c^T \tilde{Q}_c\|_2 \approx \kappa_2(V)u$. [Higham, 96], [Björck, 96] So, orthonormalisation is poor if $\kappa_2(V)$ is large.

Numerically CGS with one more re-orthogonalisation is done. The computed Q_c satisfies $\|I_m - Q_c^T Q_c\|_2 \approx cu$ for some small $c > 0$ if $\kappa_2(V) \ll 1/u$. [Giraud et. al., 2005]

QR decomposition by Rotators and Reflectors

The strategy to compute a QR decomposition

The strategy to compute a QR decomposition of A is to find some 'elementary' $n \times n$ matrices $Q_1, \ldots, Q_k$ that are orthogonal if A is real and unitary if A is complex such that

$$Q_k^\star \cdots Q_1^\star A \text{ is upper triangular.}$$

Here $\star = T$ is A is real and $\star =^*$ if A is complex.

This strategy will be elaborated for $A \in \mathbb{R}^{n \times m}$, $n \geq m$ although everything extends to the complex case as well with appropriate modifications.

Rotators

A real Givens (or plane) rotator is an orthogonal matrix $Q \in \mathbb{R}^{n \times n}$, of the form

$$Q = \begin{bmatrix} 1 & & & & & & & & & & \\ & \ddots & & & & & & & & & \\ & & 1 & & & & & & & & \\ & & & c & & & & -s & & & \\ & & & & 1 & & & & & & \\ & & & & & \ddots & & & & & \\ & & & & & & 1 & & & & \\ & & & s & & & & c & & & \\ & & & & & & & & 1 & & \\ & & & & & & & & & \ddots & \\ & & & & & & & & & & 1 \end{bmatrix}$$

where $c = cos\,\theta$, $s = \sin\,\theta$. Evidently, $QQ^T = I_n = Q^T Q$.

Rotators

Assuming that $i < j$ and $Q\{i,j\} = \begin{bmatrix} c & -s \\ s & c \end{bmatrix}$, if $y = Q^T x$ for $x = [x_1\ x_2\ \cdots\ x_n]^T \in \mathbb{R}^n$, then

$$\begin{bmatrix} y_i \\ y_j \end{bmatrix} = \begin{bmatrix} cx_i + sx_j \\ -sx_i + cx_j \end{bmatrix} \text{ with } y_k = x_k \text{ for } k \neq i \text{ or } j.$$

Rotators

Assuming that $i < j$ and $Q\{i,j\} = \begin{bmatrix} c & -s \\ s & c \end{bmatrix}$, if $y = Q^T x$ for $x = [x_1\ x_2\ \cdots\ x_n]^T \in \mathbb{R}^n$, then

$$\begin{bmatrix} y_i \\ y_j \end{bmatrix} = \begin{bmatrix} cx_i + sx_j \\ -sx_i + cx_j \end{bmatrix} \text{ with } y_k = x_k \text{ for } k \neq i \text{ or } j.$$

So if $\sqrt{x_i^2 + x_j^2} \neq 0$, then for, $c = \frac{x_i}{\sqrt{x_i^2+x_j^2}}$ and $s = \frac{x_j}{\sqrt{x_i^2+x_j^2}}$, $y_i = \sqrt{x_i^2 + x_j^2}$ and $y_j = 0$. In particular if $n = 2$,

$$Q^T \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} \sqrt{x_1^2 + x_2^2} \\ 0 \end{bmatrix}.$$

QR decomposition by Rotators

Let $A \in \mathbb{R}^{n\times m}$, $n \geq m$. Find Givens rotators $Q_1^{(1)}, Q_2^{(1)}, \ldots Q_{n-1}^{(1)}$ such that

$$(Q_{n-1}^{(1)})^T \cdots (Q_2^{(1)})^T (Q_1^{(1)})^T A(:,1) = \begin{bmatrix} \pm\|A(:,1)\|_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

where $A(:,1) = [a_{11}\; a_{21}\; \cdots\; a_{n1}]^T$ is the first column of A.

QR decomposition by Rotators

Let $A \in \mathbb{R}^{n\times m}$, $n \geq m$. Find Givens rotators $Q_1^{(1)}, Q_2^{(1)}, \ldots Q_{n-1}^{(1)}$ such that

$$(Q_{n-1}^{(1)})^T \cdots (Q_2^{(1)})^T (Q_1^{(1)})^T A(:,1) = \begin{bmatrix} \pm\|A(:,1)\|_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

where $A(:,1) = [a_{11}\ a_{21}\ \cdots\ a_{n1}]^T$ is the first column of A. Then,

$$(Q_{n-1}^{(1)})^T \cdots (Q_2^{(1)})^T (Q_1^{(1)})^T A = \underbrace{\begin{bmatrix} \pm\|A(:,1)\|_2 & a_{12}^{(1)} & \cdots & a_{1m}^{(1)} \\ 0 & a_{22}^{(1)} & \cdots & a_{2m}^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & a_{n2}^{(1)} & \cdots & a_{nm}^{(1)} \end{bmatrix}}_{=:A_1}$$

QR decomposition by Rotators

Next find Givens rotators $Q_1^{(2)}, Q_2^{(2)}, \ldots Q_{n-2}^{(2)}$ such that

$$(Q_{n-2}^{(2)})^T \cdots (Q_2^{(2)})^T (Q_1^{(2)})^T A_1(:,2) = \begin{bmatrix} a_{12}^{(1)} \\ \pm\|A_1(2:n,2)\|_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

where $A_1(2:n,2) = [a_{22}^{(1)}\; a_{23}^{(1)}\; \cdots\; a_{n2}^{(1)}]^T$ is the second column of A_1 from entries 2 to n.

QR decomposition by Rotators

Next find Givens rotators $Q_1^{(2)}, Q_2^{(2)}, \ldots Q_{n-2}^{(2)}$ such that

$$(Q_{n-2}^{(2)})^T \cdots (Q_2^{(2)})^T (Q_1^{(2)})^T A_1(:,2) = \begin{bmatrix} a_{12}^{(1)} \\ \pm\|A_1(2:n,2)\|_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

where $A_1(2:n,2) = [a_{22}^{(1)}\ a_{23}^{(1)}\ \cdots\ a_{n2}^{(1)}]^T$ is the second column of A_1 from entries 2 to n. Then,

$$(Q_{n-2}^{(2)})^T \cdots (Q_2^{(2)})^T (Q_1^{(2)})^T A_1 = \underbrace{\begin{bmatrix} \pm\|A(:,1)\|_2 & a_{12}^{(1)} & \cdots & a_{1m}^{(1)} \\ 0 & \pm\|A_1(2:n,2)\|_2 & \cdots & a_{2m}^{(2)} \\ 0 & 0 & \cdots & a_{3m}^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{nm}^{(2)} \end{bmatrix}}_{=:A_2}$$

QR decomposition by Rotators

Set

$$Q^{(k)} := Q_1^{(k)} \cdots Q_{n-k}^{(k)} \text{ for } k = 1, \ldots, p$$

where $p = m$ if $n > m$ and $p = n - 1$ otherwise. Then,

$$(Q^{(p)})^T \cdots (Q^{(1)})^T A =: R \in \mathbb{R}^{n\times m} \text{ is upper triangular.}$$

Setting $A_0 := A$, $R(i,i) = \pm\|A_{i-1}(i:n,i)\|_2$ for $i = 1, \ldots, m$.

So for the orthogonal matrix $Q := Q^{(1)} \cdots Q^{(p)}$, we have

$$Q^T A = R \Rightarrow A = QR.$$

QR decomposition by Rotators

Set

$$Q^{(k)} := Q_1^{(k)} \cdots Q_{n-k}^{(k)} \text{ for } k = 1, \ldots, p$$

where $p = m$ if $n > m$ and $p = n - 1$ otherwise. Then,

$$(Q^{(p)})^T \cdots (Q^{(1)})^T A =: R \in \mathbb{R}^{n \times m} \text{ is upper triangular.}$$

Setting $A_0 := A$, $R(i,i) = \pm \|A_{i-1}(i:n,i)\|_2$ for $i = 1, \ldots, m$.

So for the orthogonal matrix $Q := Q^{(1)} \cdots Q^{(p)}$, we have

$$Q^T A = R \Rightarrow A = QR.$$

Exercise: Given $A \in \mathbb{F}^{n \times m}$ where $\mathbb{F} = \mathbb{R}$ or $\mathbb{F} = \mathbb{C}$, and $n \geq m$, use mathematical induction to show that A has a QR decomposition.

Flop Count of finding R by Rotators

Total number of rotators used: $\Sigma_{k=1}^{p}(n-k)$.
Flop count of constructing each rotator: 5 flops and 1 square root.
Flop count of applying each rotator to a matrix with j columns: 6j flops.
So total flop count of finding R is

$$\underbrace{6\Sigma_{k=1}^{p}(n-k)(m-k)}_{\text{applying the rotators}}+\underbrace{(5+\alpha)\Sigma_{k=1}^{p}(n-k)}_{\text{creating the rotators}}.$$

Here α accounts for a square root and is usually about 8 flops.

Flop Count of finding R by Rotators

Total number of rotators used: $\Sigma_{k=1}^{p}(n-k)$.
Flop count of constructing each rotator: 5 flops and 1 square root.
Flop count of applying each rotator to a matrix with j columns: 6j flops.
So total flop count of finding R is

$$\underbrace{6\Sigma_{k=1}^{p}(n-k)(m-k)}_{\text{applying the rotators}} + \underbrace{(5+\alpha)\Sigma_{k=1}^{p}(n-k)}_{\text{creating the rotators}}.$$

Here α accounts for a square root and is usually about 8 flops.

Exercise: Show that the flop count for finding R of a QR decomposition of $A \in \mathbb{R}^{n\times m}$ by rotators is $3nm^2 - m^3 + O(nm) + O(m^2)$ if $n > m$ and $2n^3 + O(n^2)$ if $n = m$.

QR Decomposition by Householder Reflectors

Householder Reflectors

Let $u \in \mathbb{R}^n \setminus \{0\}$ and $H = \{u\}^\perp$. Then

$$\mathbb{R}^n = \mathrm{span}\{u\} \oplus H.$$

For each $x \in \mathbb{R}^n$ there exists unique $a \in \mathbb{R}$ and $v \in H$ (satisfying $v^T u = 0$) such that

$$x = au + v.$$

Householder Reflectors

Let $u \in \mathbb{R}^n \setminus \{0\}$ and $H = \{u\}^\perp$. Then

$$\mathbb{R}^n = \mathrm{span}\{u\} \oplus H.$$

For each $x \in \mathbb{R}^n$ there exists unique $a \in \mathbb{R}$ and $v \in H$ (satisfying $v^T u = 0$) such that

$$x = au + v.$$

Suppose $Q \in \mathbb{R}^{n \times n}$ such that $Qu = -u$ and $Qw = w$ for all $w \in H$. Then

$$Qx = -au + v$$

which is the reflection of x through H.

Householder Reflectors

Let $u \in \mathbb{R}^n \setminus \{0\}$ and $H = \{u\}^\perp$. Then

$$\mathbb{R}^n = \mathrm{span}\{u\} \oplus H.$$

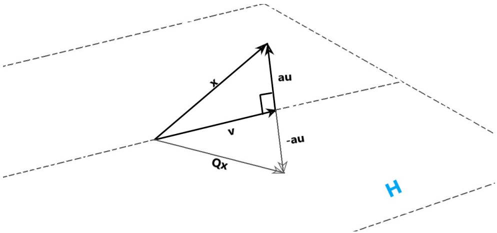
For each $x \in \mathbb{R}^n$ there exists unique $a \in \mathbb{R}$ and $v \in H$ (satisfying $v^T u = 0$) such that

$$x = au + v.$$

Suppose $Q \in \mathbb{R}^{n \times n}$ such that $Qu = -u$ and $Qw = w$ for all $w \in H$. Then

$$Qx = -au + v$$

which is the reflection of x through H.



Householder Reflectors

What is the form of Q?

Householder Reflectors

What is the form of Q?

$$Q = I_n - \frac{2}{\|u\|^2} uu^T \; !$$

Householder Reflectors

What is the form of Q?

$$Q = I_n - \frac{2}{||u||^2} u u^T \ !$$

This is called the Householder reflector associated with any multiple of u. Q is

Householder Reflectors

What is the form of Q?

$$Q = I_n - \frac{2}{||u||^2} uu^T \ !$$

This is called the Householder reflector associated with any multiple of u. Q is

- Symmetric

Householder Reflectors

What is the form of Q?

$$Q = I_n - \frac{2}{||u||^2} uu^T \; !$$

This is called the Householder reflector associated with any multiple of u. Q is

- Symmetric
- Orthogonal

Householder Reflectors

What is the form of Q?

$$Q = I_n - \frac{2}{\|u\|^2} uu^T \ !$$

This is called the Householder reflector associated with any multiple of u. Q is

- Symmetric
- Orthogonal
- an involution, i. e., $Q = Q^{-1}$.

Householder Reflectors

What is the form of Q?

$$Q = I_n - \frac{2}{\|u\|^2} uu^T \ !$$

This is called the Householder reflector associated with any multiple of u. Q is

- Symmetric
- Orthogonal
- an involution, i. e., $Q = Q^{-1}$.

Theorem Let $x, y \in \mathbb{R}^n$ such that $x \neq y$ and $\|x\|_2 = \|y\|_2$. Then there exists a unique Householder reflector $Q \in \mathbb{R}^{n \times n}$ such that $Qx = y$.

Householder Reflectors

What is the form of Q?

$$Q = I_n - \frac{2}{\|u\|^2} uu^T \ !$$

This is called the Householder reflector associated with any multiple of u. Q is

- Symmetric
- Orthogonal
- an involution, i. e., $Q = Q^{-1}$.

Theorem Let $x, y \in \mathbb{R}^n$ such that $x \neq y$ and $\|x\|_2 = \|y\|_2$. Then there exists a unique Householder reflector $Q \in \mathbb{R}^{n \times n}$ such that $Qx = y$.

Proof: Since $\|x\|_2 = \|y\|_2$, $(x-y)^T(x+y) = 0$. Let $u = \frac{1}{2}(x-y)$. Then $u \neq 0$ as $x \neq y$ and $v := \frac{1}{2}(x+y) \in \{u\}^\perp$. Now $x = u + v$ and the reflector $Q = I - \frac{2}{\|u\|_2^2} uu^T$ is such that $Qx = -u + v = y$. $\square$

Creating zeroes in vectors by using Householder Reflectors

Corollary Let $x \in \mathbb{R}^n \setminus \{0\}$. There exists a Householder reflector $Q = I_n - \gamma u u^T \in \mathbb{R}^{n \times n}$ such that $Qx = [-\tau \, 0 \, \cdots \, 0]^T$ where $\tau = \|x\|_2$ or $-\|x\|_2$. Also γ, u and τ can be computed in $O(n)$ flops.

Creating zeroes in vectors by using Householder Reflectors

Corollary Let $x \in \mathbb{R}^n \setminus \{0\}$. There exists a Householder reflector $Q = I_n - \gamma uu^T \in \mathbb{R}^{n\times n}$ such that $Qx = [-\tau\, 0 \, \cdots \, 0]^T$ where $\tau = \|x\|_2$ or $-\|x\|_2$. Also γ, u and τ can be computed in $O(n)$ flops.

Proof: Suppose $x = [x_1 \ \cdots \ x_n]^T$ and assume without loss of generality that $x_j \neq 0$ for some $j = 3, \ldots, n$. Let $y = [-\tau \ 0 \ \cdots \ 0]^T$ where $\tau = \mathrm{sign}(x_1)\|x\|_2$. The choice of the sign of τ avoids catastrophic cancellation in computing the first entry of $x - y$ wich is $x_1 + \tau$. As $x \neq y$ and $\|x\|_2 = \|y\|_2$, the Householder reflector $Q = I - \frac{2}{\|x-y\|_2^2}(x-y)(x-y)^T$ is such that $Qx = y$.

Suppose $u = \frac{1}{x_1+\tau}(x-y)$. Then $Q = I - \gamma uu^T$ where $\gamma = \frac{2}{\|u\|_2^2} = \frac{\tau + x_1}{\tau}$. Clearly, γ, u and τ can all be computed in $O(n)$ flops. $\square$

QR decomposition via Householder Reflectors

Let $A \in \mathbb{R}^{n \times m}$, $n \geq m$. Let Q_1 be a reflector such that

$$Q_1 A(:,1) = \begin{bmatrix} \pm\|A(:,1)\|_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix}.$$

Then,

$$Q_1 A = \underbrace{\begin{bmatrix} \pm\|A(:,1)\|_2 & a_{12}^{(1)} & \cdots & a_{1m}^{(1)} \\ 0 & a_{22}^{(1)} & \cdots & a_{2m}^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & a_{n2}^{(1)} & \cdots & a_{nm}^{(1)} \end{bmatrix}}_{=:A_1}$$

QR Decomposition by Reflectors

Let $Q_2 = \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & \underbrace{I_{n-1} - \frac{2}{\|u^{(2)}\|_2^2} u^{(2)} u^{(2)T}}_{:=\tilde{Q}_2} \end{array}\right]$ where

$$\tilde{Q}_2 A_1(2:n,2) = [\pm\|A_1(2:n,2)\|_2,\ 0, \cdots, 0]^T,$$

Then,

$$Q_2 A_1(:,2) = \begin{bmatrix} a_{12}^{(1)} \\ \pm\|A_1(2:n,2)\|_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix},$$

and

$$Q_2 A_1 = \underbrace{\begin{bmatrix} \pm\|A(:,1)\|_2 & a_{12}^{(1)} & a_{13}^{(1)} & \cdots & a_{1m}^{(1)} \\ 0 & \pm\|A_1(2:n,2)\|_2 & a_{23}^{(2)} & \cdots & a_{2m}^{(2)} \\ 0 & 0 & a_{33}^{(2)} & \cdots & a_{3m}^{(2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & a_{n3}^{(2)} & \cdots & a_{nm}^{(2)} \end{bmatrix}}_{=:A_2}$$

QR Decomposition by Reflectors

Thus there exist reflectors

$$Q_i = \left[\begin{array}{c|c} I_{i-1} & 0 \\ \hline 0 & I_{n-i+1} - \frac{2}{\|u^{(i)}\|_2^2} u^{(i)} u^{(i)T} \end{array}\right], i = 1, 2, \ldots, p,$$

(where $p = m$ if $n > m$ and $p = n - 1$ otherwise) such that

$$Q_p^T \cdots Q_2^T Q_1^T A = R \text{ is upper triangular}$$

Hence, $A = QR$ where $Q = Q_1 Q_2 \cdots Q_p$.

Flop count of computing the R of a QR Decomposition by Reflectors

Let $Q = I_n - \gamma uu^T$ be an $n \times n$ reflector and B be an $n \times m$ matrix. $W := QB = B - \gamma uu^T B$ may be computed in a number of ways.

Flop count of computing the R of a QR Decomposition by Reflectors

Let $Q = I_n - \gamma u u^T$ be an $n \times n$ reflector and B be an $n \times m$ matrix. $W := QB = B - \gamma u u^T B$ may be computed in a number of ways.

Bad idea :

$$\left(B - \left(\left((\gamma u)u^T\right) B\right)\right)$$

Find $v := \gamma u$. (Costs n flops)
Find $W := vu^T$. (Costs n^2 flops)
Find $G := WB$. (Costs $2n^2m$ flops)
Find $B - G$. (Cost nm flops)

Flop count of computing the R of a QR Decomposition by Reflectors

Let $Q = I_n - \gamma uu^T$ be an $n \times n$ reflector and B be an $n \times m$ matrix. $W := QB = B - \gamma uu^T B$ may be computed in a number of ways.

Bad idea :

$$\left(B - \left(\left((\gamma u)u^T\right) B\right)\right)$$

Find $v := \gamma u$. (Costs n flops)
Find $W := vu^T$. (Costs n^2 flops)
Find $G := WB$. (Costs $2n^2 m$ flops)
Find $B - G$. (Cost nm flops)

Total cost is $n^2(2m + 1) + nm + n$ flops.

Flop count of computing R of a QR Decomposition by Reflectors

But $W = B - \gamma u u^T B$ may also be computed as follows:

Good idea:

$$\left(B - \left((\gamma u)(u^T B)\right)\right)$$

Find $v := \gamma u$. (Costs n flops)
Find $w^T := u^T B$. (Costs $2nm$ flops)
Find $C := v w^T$. (Costs nm flops)
Find $W := B - C$. (Costs nm flops)

Flop count of computing R of a QR Decomposition by Reflectors

But $W = B - \gamma u u^T B$ may also be computed as follows:

Good idea:

$$\Big(B - \big((\gamma u)(u^T B)\big)\Big)$$

Find $v := \gamma u$. (Costs n flops)
Find $w^T := u^T B$. (Costs $2nm$ flops)
Find $C := v w^T$. (Costs nm flops)
Find $W := B - C$. (Costs nm flops)

Total cost is $4nm + n \approx 4nm$ flops.

Flop count of finding R of a QR Decomposition by Reflectors

Let $A \in \mathbb{R}^{n \times m}$, $n \geq m$. Finding reflector Q_1 such that

$$Q_1 A(:,1) = \begin{bmatrix} \pm\|A(:,1)\|_2 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

costs $O(n)$ flops.
Computing

$$Q_1 A = \underbrace{\begin{bmatrix} \pm\|A(:,1)\|_2 & a_{12}^{(1)} & \cdots & a_{1m}^{(1)} \\ 0 & a_{22}^{(1)} & \cdots & a_{2m}^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & a_{n2}^{(1)} & \cdots & a_{nm}^{(1)} \end{bmatrix}}_{=:A_1}$$

costs 4n(m-1) flops.

Flop count of finding R of a QR Decomposition by Reflectors

$$\text{Finding } Q_2 = \left[\begin{array}{c|c} 1 & 0 \\ \hline 0 & \underbrace{I_{n-1} - \frac{2}{\|u^{(2)}\|_2^2} u^{(2)} u^{(2)T}}_{:=\tilde{Q}_2} \end{array}\right] \text{ such that}$$

$$\tilde{Q}_2 A(2:n,2) = [\pm\|A(2:n,2)\|_2,\, 0, \cdots, 0]^T,$$

costs $O(n-1)$ flops. Computing,

$$Q_2 A_1 = \underbrace{\begin{bmatrix} \pm\|A(:,1)\|_2 & a_{12}^{(1)} & a_{13}^{(1)} & \cdots & a_{1m}^{(1)} \\ 0 & \pm\|A_1(2:n,2)\|_2 & a_{23}^{(2)} & \cdots & a_{2m}^{(2)} \\ 0 & 0 & a_{33}^{(2)} & \cdots & a_{3m}^{(2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & a_{n3}^{(2)} & \cdots & a_{nm}^{(2)} \end{bmatrix}}_{=:A_2}$$

costs 4(n-1)(m-2) flops.

Flop count of finding R of a QR Decomposition by Reflectors

Setting $p = n - 1$ if $n = m$ and $p = m$ if $n > m$, the total costs of finding the p reflectors is

$$\Sigma_{k=1}^{p} O(n-k+1) = \begin{cases} O(n^2) & \text{if } n = m, \\ O(nm) + O(m^2) & \text{if } n > m. \end{cases}$$

The cost of applying the p reflectors is $4\Sigma_{k=1}^{p}(n-k+1)(m-k)$.

Flop count of finding R of a QR Decomposition by Reflectors

Setting $p = n - 1$ if $n = m$ and $p = m$ if $n > m$, the total costs of finding the p reflectors is

$$\Sigma_{k=1}^{p} O(n-k+1) = \begin{cases} O(n^2) & \text{if } n = m, \\ O(nm) + O(m^2) & \text{if } n > m. \end{cases}$$

The cost of applying the p reflectors is $4\Sigma_{k=1}^{p}(n-k+1)(m-k)$.

Exercise: Show that the flop count of finding the R of a QR decomposition of $A \in \mathbb{R}^{n\times m}$ by reflectors is $2nm^2 - \frac{2}{3}m^3 + O(nm) + O(m^2)$ flops if $n > m$ and $\frac{4}{3}n^3 + O(n^2)$ flops if $n = m$.

Computing the Q of a Condensed QR decomposition via reflectors

Given $A \in \mathbb{R}^{n \times m}$, $n > m$, the flop count for finding the isometry Q of a condensed QR decomposition is equal to that of finding R if it is done efficiently.

Computing the Q of a Condensed QR decomposition via reflectors

Given $A \in \mathbb{R}^{n \times m}$, $n > m$, the flop count for finding the isometry Q of a condensed QR decomposition is equal to that of finding R if it is done efficiently.

Let $\hat{Q}$ be the orthogonal matrix in the full QR decomposition of A.

Then $\hat{Q} = Q_1 Q_2 \cdots Q_m$ and $Q = \left[\hat{Q}e_1 \cdots \hat{Q}e_m \right]$.

Computing the Q of a Condensed QR decomposition via reflectors

Given $A \in \mathbb{R}^{n \times m}$, $n > m$, the flop count for finding the isometry Q of a condensed QR decomposition is equal to that of finding R if it is done efficiently.

Let $\hat{Q}$ be the orthogonal matrix in the full QR decomposition of A. Then $\hat{Q} = Q_1 Q_2 \cdots Q_m$ and $Q = \left[\hat{Q} e_1 \cdots \hat{Q} e_m \right]$. Since,

$$Q_i = \left[\begin{array}{c|c} I_{i-1} & 0 \\ \hline 0 & I_{n-i+1} - \frac{2}{\|u^{(i)}\|_2^2} u^{(i)} u^{(i)T} \end{array} \right], i = 1, 2, \ldots, p,$$

$\hat{Q} e_k = Q_1 Q_2 \cdots Q_k e_k, \; k = 1, \ldots, m,$

Computing the Q of a Condensed QR decomposition via reflectors

Given $A \in \mathbb{R}^{n \times m}$, $n > m$, the flop count for finding the isometry Q of a condensed QR decomposition is equal to that of finding R if it is done efficiently.

Let $\hat{Q}$ be the orthogonal matrix in the full QR decomposition of A. Then $\hat{Q} = Q_1 Q_2 \cdots Q_m$ and $Q = \left[\hat{Q} e_1 \cdots \hat{Q} e_m \right]$. Since,

$$Q_i = \left[\begin{array}{c|c} I_{i-1} & 0 \\ \hline 0 & I_{n-i+1} - \frac{2}{\|u^{(i)}\|_2^2} u^{(i)} u^{(i)T} \end{array} \right], i = 1, 2, \ldots, p,$$

$\hat{Q} e_k = Q_1 Q_2 \cdots Q_k e_k,\ k = 1, \ldots, m$, and the flop count of finding Q is

$$\sum_{k=1}^{m} \sum_{j=1}^{k} 4(n - j + 1) = 2nm^2 - (2m^3)/3 + O(nm) + O(m^2)$$

which is equal to that of computing R.

Computing the Q of a Condensed QR decomposition via reflectors

Given $A \in \mathbb{R}^{n\times m}$, $n > m$, the flop count for finding the isometry Q of a condensed QR decomposition is equal to that of finding R if it is done efficiently.

Let $\hat{Q}$ be the orthogonal matrix in the full QR decomposition of A. Then $\hat{Q} = Q_1 Q_2 \cdots Q_m$ and $Q = \left[\hat{Q}e_1 \cdots \hat{Q}e_m\right]$. Since,

$$Q_i = \left[\begin{array}{c|c} I_{i-1} & 0 \\ \hline 0 & I_{n-i+1} - \frac{2}{\|u^{(i)}\|_2^2} u^{(i)} u^{(i)T} \end{array}\right], i = 1, 2, \ldots, p,$$

$\hat{Q}e_k = Q_1 Q_2 \cdots Q_k e_k,\ k = 1, \ldots, m$, and the flop count of finding Q is

$$\sum_{k=1}^{m} \sum_{j=1}^{k} 4(n - j + 1) = 2nm^2 - (2m^3)/3 + O(nm) + O(m^2)$$

which is equal to that of computing R.

Exercise: Prove that finding a QR decomposition of $A \in \mathbb{R}^{n\times n}$ costs $(8n^3)/3 + O(n^2)$ flops.

Practice exercises

Exercise: Let A be a $n \times n$ nonsingular real or complex matrix. Prove the following.

1. A has a unique QR decomposition such the diagonal entries of R are positive.
2. If $A = Q_1 R_1$ and $A = Q_2 R_2$ be two QR decompositions of A, and $A_1 := Q_1^* A Q_1$, and $A_2 := Q_2^* A Q_2$, then there exists a unitary diagonal matrix D, such that $A_2 = D^* A_1 D$.

Solve all problems on pages 206-210 and pages 236-239 of *Fundamentals of Matrix Computations,* by D. S. Watkins, (2nd edition).

Rank revealing QR decomposition

Given any matrix $A \in \mathbb{R}^{n\times m}$, $n \geq m$, with $\operatorname{rank} A = r(\leq m)$, there exists a permutation matrix P, an orthogonal matrix $Q \in \mathbb{R}^{n\times n}$ and a matrix $R = \begin{bmatrix} R_1 & R_2 \\ 0 & 0 \end{bmatrix}$ where $R_1 \in \mathbb{R}^{r\times r}$ is nonsingular and upper triangular and $R_2 \in \mathbb{R}^{r\times(m-r)}$ such that

$$AP = QR. \tag{3}$$

Such a decomposition is called a *column pivoted* or *rank revealing* decomposition of A as the size of R_1 'reveals' the rank of A.

If A is a complex matrix, then the above decomposition exists for a unitary matrix Q with $\mathbb{R}$ replaced by $\mathbb{C}$ throughout.

Computing rank revealing QR

Find an $m \times m$ permutation matrix P_1 such that the first column of AP_1 has the largest 2-norm among all the columns of A.

Computing rank revealing QR

Find an $m \times m$ permutation matrix P_1 such that the first column of AP_1 has the largest 2-norm among all the columns of A.
[Costs 2nm + m flops]

Computing rank revealing QR

Find an $m \times m$ permutation matrix P_1 such that the first column of AP_1 has the largest 2-norm among all the columns of A.
[Costs 2nm + m flops]

Then choose an $n \times n$ reflector Q_1 such that

$$Q_1 A P_1 = \underbrace{\begin{bmatrix} \pm\|AP_1(:,1)\|_2 & a_{12}^{(1)} & \cdots & a_{1m}^{(1)} \\ 0 & a_{22}^{(1)} & \cdots & a_{2m}^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & a_{n2}^{(1)} & \cdots & a_{nm}^{(1)} \end{bmatrix}}_{=:A_1}$$

Computing rank revealing QR

Find an $m \times m$ permutation matrix P_1 such that the first column of AP_1 has the largest 2-norm among all the columns of A.
[Costs 2nm + m flops]

Then choose an $n \times n$ reflector Q_1 such that

$$Q_1 A P_1 = \underbrace{\begin{bmatrix} \pm\|AP_1(:,1)\|_2 & a_{12}^{(1)} & \cdots & a_{1m}^{(1)} \\ 0 & a_{22}^{(1)} & \cdots & a_{2m}^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & a_{n2}^{(1)} & \cdots & a_{nm}^{(1)} \end{bmatrix}}_{=:A_1}$$

[Costs 4n(m-1) flops]

Computing rank revealing QR

Find an $m \times m$ permutation P_2 such that $A_1 P_2(2:n,2)$ has the largest 2-norms among the columns $A_1(2:n,k), k = 2, \ldots, m$.

Computing rank revealing QR

Find an $m \times m$ permutation P_2 such that $A_1 P_2(2:n,2)$ has the largest 2-norms among the columns $A_1(2:n,k), k = 2,\ldots,m$.
[Costs 2(n-1)(m-1) + m-1 flops]

Computing rank revealing QR

Find an $m \times m$ permutation P_2 such that $A_1 P_2(2:n,2)$ has the largest 2-norms among the columns $A_1(2:n,k), k = 2,\ldots,m$.
[Costs 2(n-1)(m-1) + m-1 flops]

Then choose an $n \times n$ reflector $Q_2 = \begin{bmatrix} 1 & 0 \\ 0 & \tilde{Q}_2 \end{bmatrix}$ where $\tilde{Q}_2$ is an $n-1 \times n-1$ reflector such that

$$Q_2 Q_1 A P_1 P_2 = Q_2 A_1 P_2 = \underbrace{\begin{bmatrix} \pm\|A(:,1)\|_2 & a_{12}^{(1)} & a_{13}^{(1)} & \cdots & a_{1m}^{(1)} \\ 0 & \pm\|A_1 P_2(2:n,2)\|_2 & a_{23}^{(2)} & \cdots & a_{2m}^{(2)} \\ 0 & 0 & a_{33}^{(2)} & \cdots & a_{3m}^{(2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & a_{n3}^{(2)} & \cdots & a_{nm}^{(2)} \end{bmatrix}}_{=:A_2}$$

Computing rank revealing QR

Find an $m \times m$ permutation P_2 such that $A_1 P_2(2:n,2)$ has the largest 2-norms among the columns $A_1(2:n,k), k = 2,\ldots,m$.
[Costs 2(n-1)(m-1) + m-1 flops]

Then choose an $n \times n$ reflector $Q_2 = \begin{bmatrix} 1 & 0 \\ 0 & \tilde{Q}_2 \end{bmatrix}$ where $\tilde{Q}_2$ is an $n-1 \times n-1$ reflector such that

$$Q_2 Q_1 A P_1 P_2 = Q_2 A_1 P_2 = \underbrace{\begin{bmatrix} \pm\|A(:,1)\|_2 & a_{12}^{(1)} & a_{13}^{(1)} & \cdots & a_{1m}^{(1)} \\ 0 & \pm\|A_1 P_2(2:n,2)\|_2 & a_{23}^{(2)} & \cdots & a_{2m}^{(2)} \\ 0 & 0 & a_{33}^{(2)} & \cdots & a_{3m}^{(2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & a_{n3}^{(2)} & \cdots & a_{nm}^{(2)} \end{bmatrix}}_{=:A_2}$$

[Costs 4(n-1)(m-2) flops]

Computing rank revealing QR

Continuing in this way,

$$Q_r Q_{r-1} \cdots Q_1 A P_1 P_2 \cdots P_r = \begin{bmatrix} R_1 & R_2 \\ 0 & 0 \end{bmatrix}$$

where R_1 is $r \times r$ an upper triangular and R_2 is an $r \times (m - r)$ matrix.

Computing rank revealing QR

Continuing in this way,

$$Q_r Q_{r-1} \cdots Q_1 A P_1 P_2 \cdots P_r = \begin{bmatrix} R_1 & R_2 \\ 0 & 0 \end{bmatrix}$$

where R_1 is $r \times r$ an upper triangular and R_2 is an $r \times (m-r)$ matrix.

The total flop count is

$$\underbrace{\Sigma_{k=1}^{r}(2n-2k+3)(m-k+1)}_{\text{pivoting}} + \underbrace{4\Sigma_{k=1}^{r}(n-k+1)(m-k)}_{\text{applying the reflectors}}$$

Computing rank revealing QR

Continuing in this way,

$$Q_r Q_{r-1} \cdots Q_1 A P_1 P_2 \cdots P_r = \begin{bmatrix} R_1 & R_2 \\ 0 & 0 \end{bmatrix}$$

where R_1 is $r \times r$ an upper triangular and R_2 is an $r \times (m-r)$ matrix.

The total flop count is

$$\underbrace{\Sigma_{k=1}^{r}(2n-2k+3)(m-k+1)}_{\text{pivoting}} + \underbrace{4\Sigma_{k=1}^{r}(n-k+1)(m-k)}_{\text{applying the reflectors}}$$

The cost of pivoting is comparable in order to the cost of applying the reflectors. If $r = m$, then the total cost is more than finding the R of the QR decomposition without pivoting.

Computing rank revealing QR

The following strategy can reduce the cost of pivoting.

Find the norms of the columns $A_1(2:n,k)$ for $k = 2,\ldots,m$ by noticing that

$$\|A_1(2:n,k)\|_2^2 = \begin{cases} \|A(:,k)\|_2^2 - |A(1,k)|^2 & \text{if } P_1(:,k) = e_k \\ \|A(:,1)\|_2^2 - |A(1,1)|^2 & \text{otherwise.} \end{cases}$$

[This costs 2(m-1) flops.]

Computing rank revealing QR

The following strategy can reduce the cost of pivoting.

Find the norms of the columns $A_1(2:n,k)$ for $k=2,\ldots,m$ by noticing that

$$\|A_1(2:n,k)\|_2^2 = \begin{cases} \|A(:,k)\|_2^2 - |A(1,k)|^2 & \text{if } P_1(:,k) = e_k \\ \|A(:,1)\|_2^2 - |A(1,1)|^2 & \text{otherwise.} \end{cases}$$

[This costs 2(m-1) flops.]

The remaining norms of columns may be calculated in a similar way. This reduces the cost of pivoting to $O(m^2)$ flops and the cost of finding the R and the P of the rank revealing QR decomposition $AP = QR$ of an $n \times m$ matrix A becomes $2nm^2 - \frac{2}{3}m^3 + O(nm) + O(m^2)$ flops.

Exercise: Show that in the QR decomposition with column pivoting of any $A \in \mathbb{F}^{n\times m}$, with $\mathbb{F} = \mathbb{R}$ or $\mathbb{C}$, and $n > m$, the diagonal entries of the $r \times r$ upper triangular matrix R_1 are real numbers arranged in decreasing order of magnitude, i.e., $|R(1,1)| \geq \cdots \geq |R(r,r)|$.

Computing rank revealing QR: numerical issues

In practice, the rank r of A will not be known and if $r < m$, then at some stage $p < m$, the computed R is of the form

$$\begin{bmatrix} R_1 & R_2 \\ 0 & R_3 \end{bmatrix}$$

where R_1 is upper triangular of size $p \times p$ and R_3 is an $n - p \times m - p$ matrix with entries that have very small absolute values.

Computing rank revealing QR: numerical issues

In practice, the rank r of A will not be known and if $r < m$, then at some stage $p < m$, the computed R is of the form

$$\begin{bmatrix} R_1 & R_2 \\ 0 & R_3 \end{bmatrix}$$

where R_1 is upper triangular of size $p \times p$ and R_3 is an $n - p \times m - p$ matrix with entries that have very small absolute values.

Here p may or may not be equal to the exact rank of A.

Computing rank revealing QR: numerical issues

In practice, the rank r of A will not be known and if $r < m$, then at some stage $p < m$, the computed R is of the form

$$\begin{bmatrix} R_1 & R_2 \\ 0 & R_3 \end{bmatrix}$$

where R_1 is upper triangular of size $p \times p$ and R_3 is an $n - p \times m - p$ matrix with entries that have very small absolute values.

Here p may or may not be equal to the exact rank of A.

In such a case if all entries of R_3 have absolute values less than a predetermined tolerance level, then those may be set to 0 and the process is over. Else, the next column pivoted QR steps may be performed.

Computing rank revealing QR: numerical issues

In practice, the rank r of A will not be known and if $r < m$, then at some stage $p < m$, the computed R is of the form

$$\begin{bmatrix} R_1 & R_2 \\ 0 & R_3 \end{bmatrix}$$

where R_1 is upper triangular of size $p \times p$ and R_3 is an $n - p \times m - p$ matrix with entries that have very small absolute values.

Here p may or may not be equal to the exact rank of A.

In such a case if all entries of R_3 have absolute values less than a predetermined tolerance level, then those may be set to 0 and the process is over. Else, the next column pivoted QR steps may be performed.

The first nonzero rows of the resulting R are called the *numerical rank* of R.

Computing rank revealing QR: numerical issues

In practice, the rank r of A will not be known and if $r < m$, then at some stage $p < m$, the computed R is of the form

$$\begin{bmatrix} R_1 & R_2 \\ 0 & R_3 \end{bmatrix}$$

where R_1 is upper triangular of size $p \times p$ and R_3 is an $n - p \times m - p$ matrix with entries that have very small absolute values.

Here p may or may not be equal to the exact rank of A.

In such a case if all entries of R_3 have absolute values less than a predetermined tolerance level, then those may be set to 0 and the process is over. Else, the next column pivoted QR steps may be performed.

The first nonzero rows of the resulting R are called the *numerical rank* of R.

In MATLAB the default tolerance level is $\epsilon n |R(1, 1)|$. This method of computing the numerical rank is however less reliable than the SVD method.