QR factorization by Gram-Schmidt orthogonalization process

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Outline

- Classical Gram-Schmidt orthogonalization scheme (CGS)
- Modified Gram-Schmidt ortrhogonalization scheme (MGS)
- QR factorization by Gram-Schmidt orthogonalization

Orthogonal decomposition

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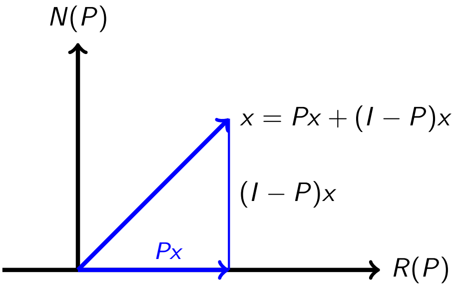

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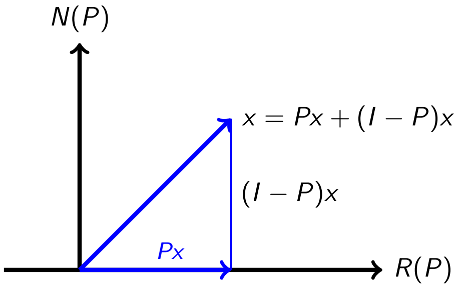

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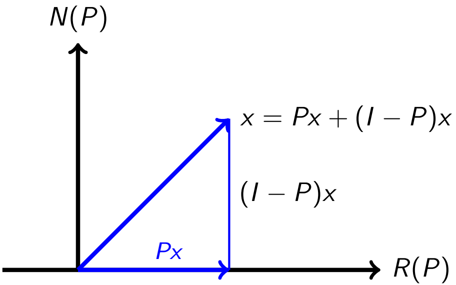

As (I-P)x belongs to N(P) and u belongs to R(P), and they are perpendicular,

Thus, if $P := uu^*$ with $u^*u = 1$ then $Px = uu^*x = \langle x, u\rangle u$ and $(I - P)x \perp u$.

More generally, if $U := \begin{bmatrix} u_1 & \cdots & u_m \end{bmatrix}$ is an isometry then $P := UU^*$ is an orthogonal projection

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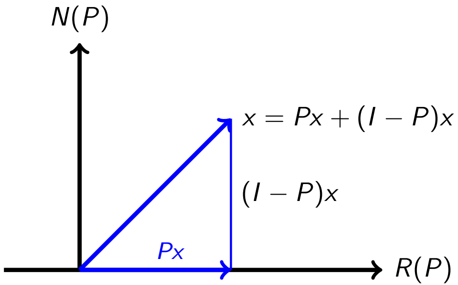

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More generally, if $U := \begin{bmatrix} u_1 & \cdots & u_m \end{bmatrix}$ is an isometry then $P := UU^*$ is an orthogonal projection such that $R(P) = R(U)$ and $(I-P)x \perp \{u_1, \ldots, u_m\}$ for any $x \in \mathbb{C}^n$.

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This yields the classical Gram-Schmidt orthonormal process: Define

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Does this mean (I - [u1 u2] [u1 u2]*)x3 is orthogonal to both u1 and u2?, => YES

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Let $x_1, \ldots, x_m$ be linearly indepedent vectors in $\mathbb{C}^n$. Then there exist orthonormal vectors $v_1, \ldots, v_m$ in $\mathbb{C}^n$ such that

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Assume it is singular and contradict.

Classical Gram-Schmidt scheme (CGS)

Equating the columns we have

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\begin{aligned}
x_1 &= v_1 r_{11} \Rightarrow r_{11} = \|x_1\|_2 \text{ and } v_1 := x_1/r_{11} \\
x_2 &= v_1 r_{12} + v_2 r_{22} \Rightarrow r_{12} = \langle x_2, v_1 \rangle, r_{22} := \|x_2 - \langle x_2, v_1 \rangle v_1\|_2
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and $v_2 := (x_2 - \langle x_2, v_1 \rangle v_1)/r_{22}$, where $\langle x, y \rangle = y^* x$.

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The classical Gram-Schmidt method constructs orthonormal vectors $v_1, \ldots, v_n$ as follows. Define

$$\begin{aligned} v_1 &:= \frac{x_1}{\|x_1\|_2}, \\ v_j &:= \frac{x_j - v_1 v_1^* x_j - \cdots - v_{j-1} v_{j-1}^* x_j}{\|x_j - v_1 v_1^* x_j - \cdots - v_{j-1} v_{j-1}^* x_j\|_2},\ j = 2 : n. \end{aligned}$$

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Then $v_1, \ldots, v_n$ are orthonormal, that is, $v_i^* v_j = 0$ for $i \neq j$ and $\|v_j\|_2 = 1$ for $j = 1 : n$. Note that $\|x_j - v_1 v_1^* x_j - \cdots - v_{j-1} v_{j-1}^* x_j\|_2 \neq 0$ as the vectors $x_1, \ldots, x_j$ are linearly independent.

Proof?

Classical Gram-Schmidt scheme (CGS)

Setting $r_{11} := \|x_1\|_2$ and $r_{jj} := \|x_j - v_1 v_1^* x_j - \cdots - v_{j-1} v_{j-1}^* x_j\|_2$, we have

$$\begin{aligned} x_1 &= v_1 r_{11}, \\ x_j &= v_1 v_1^* x_j + \cdots + v_{j-1} v_{j-1}^* x_j + v_j r_{jj}, \quad j = 2 : n. \end{aligned}$$

Setting $r_{kj} := v_k^* x_j$, in matrix notation, we have

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$$\begin{aligned} \begin{bmatrix} x_1 & \cdots & x_j \end{bmatrix} &= \begin{bmatrix} v_1 & \cdots & v_j \end{bmatrix} \begin{bmatrix} r_{11} & v_1^* x_2 & \cdots & v_1^* x_j \\ & r_{22} & \cdots & v_2^* x_j \\ & & \ddots & \vdots \\ & & & r_{jj} \end{bmatrix} \\ &= \begin{bmatrix} v_1 & \cdots & v_j \end{bmatrix} \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1j} \\ & r_{22} & \cdots & r_{2j} \\ & & \ddots & \vdots \\ & & & r_{jj} \end{bmatrix} \quad \text{for } \; j = 1 : n. \end{aligned}$$

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The CGS computes QR factorization $X = QR$ in which the j-th columns of Q and R are determined at the j-th step.

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Algorithm: CGS (Classical Gram-Schmidt algorithm)
Input: Linearly indendent vectors $x_1, \ldots, x_n$
Output: Orthonormal vectors $v_1, \ldots, v_n$

---

for $i = 1\colon n$
  $v_i := x_i$
  for $j = 1\colon i-1$
    $r_{ji} := v_j^* x_i$
    $v_i := v_i - v_j r_{ji}$
  end
$r_{ii} := \|v_i\|_2$
if $r_{ii} = 0$ then quit else
$v_i := v_i / r_{ii}$
end

Example

Consider $x_1 := \begin{bmatrix} 1 & 0 & 1 \end{bmatrix}^\top, x_2 := \begin{bmatrix} 2 & 1 & 0 \end{bmatrix}^\top$ and $\begin{bmatrix} 0 & 1 & 1 \end{bmatrix}^\top$. Then by the Gram-Schmidt process, we have $r_{11} := \|x_1\|_2 = \sqrt{2}$ which gives

$$v_1 := \frac{x_1}{r_{11}} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}.$$

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$$v_1 := \frac{x_1}{r_{11}} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}.$$

Next, we have $r_{12} := v_1^\top x_2 = \sqrt{2}$ and

$$\begin{aligned} q_2 &:= x_2 - v_1 v_1^\top x_2 = \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix} - \frac{\sqrt{2}}{\sqrt{2}} \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix}, \\ v_2 &:= \frac{q_2}{r_{22}} = \frac{1}{\sqrt{3}} \begin{bmatrix} 1 \\ 1 \\ -1 \end{bmatrix}, \text{ where } r_{22} := \|q_2\|_2 = \sqrt{3}. \end{aligned}$$

Example

Finally, $r_{13} := v_1^\top x_3 = 1/\sqrt{2}$ and $r_{23} := v_2^\top x_3 = 0$. Hence we have

$$\begin{aligned} q_3 &:= x_3 - v_1 v_1^\top x_3 - v_2 v_2^\top x_3 = \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix} - \frac{1}{2}\begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix} = \frac{1}{2}\begin{bmatrix} -1 \\ 2 \\ 1 \end{bmatrix}, \\ v_3 &:= \frac{q_3}{r_{33}} = \frac{1}{\sqrt{6}}\begin{bmatrix} -1 \\ 2 \\ 1 \end{bmatrix}, \quad \text{where } r_{33} := \|q_3\|_3 = \frac{\sqrt{6}}{2}. \end{aligned}$$

Setting $A := \begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}$ and $Q := \begin{bmatrix} v_1 & v_2 & v_3 \end{bmatrix}$, we have the QR factorization of A

$$\underbrace{\begin{bmatrix} 1 & 2 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix}}_{A} = \underbrace{\begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{3}} & \frac{-1}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{3}} & \frac{2}{\sqrt{6}} \\ \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{3}} & \frac{1}{\sqrt{6}} \end{bmatrix}}_{Q} \underbrace{\begin{bmatrix} \sqrt{2} & \sqrt{2} & \frac{1}{\sqrt{2}} \\ 0 & \sqrt{3} & 0 \\ 0 & 0 & \frac{\sqrt{6}}{2} \end{bmatrix}}_{R}. \blacksquare$$

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$$I - v_1 v_1^* - \cdots - v_{j-1} v_{j-1}^* = (I - v_1 v_1^*)(I - v_2 v_2^*) \cdots (I - v_{j-1} v_{j-1}^*).$$

Hence the CGS can be rewritten as

$$\begin{aligned} v_1 &:= \frac{x_1}{\|x_1\|_2}, \\ v_j &:= \frac{(I - v_{j-1} v_{j-1}^*) \cdots (I - v_1 v_1^*) x_j}{\|(I - v_{j-1} v_{j-1}^*) \cdots (I - v_1 v_1^*) x_j\|_2}, \; j = 2 : n. \end{aligned}$$

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CGS versus MGS

The tables below illustrate the essential difference between CGS and MGS steps.

Step	CGS Algorithm		
1.	$v_1 := \frac{x_1}{\|x_1\|_2}$	x_2	x_3
2.	v_1	$v_2 := \frac{(I - v_1 v_1^*)x_2}{\|(I - v_1 v_1^*)x_2\|_2}$	x_3
3.	v_1	v_2	$v_3 := \frac{(I - v_1 v_1^* - v_2 v_2^*)x_3}{\|(I - v_1 v_1^* - v_2 v_2^*)x_3\|_2}$

Step	MGS Algorithm		
1.	$v_1 := \frac{x_1}{\|x_1\|_2}$	$(I - v_1 v_1^*)x_2$	$(I - v_1 v_1^*)x_3$
2.	v_1	$v_2 := \frac{(I - v_1 v_1^*)x_2}{\|(I - v_1 v_1^*)x_2\|_2}$	$(I - v_2 v_2^*)(I - v_1 v_1^*)x_3$
3.	v_1	v_2	$v_3 := \frac{(I - v_2 v_2^*)(I - v_1 v_1^*)x_3}{\|(I - v_2 v_2^*)(I - v_1 v_1^*)x_3\|_2}$

Modified Gram-Schmidt Scheme (MGS)

Algorithm: MGS (Modified Gram-Schmidt algorithm)
Input: Linearly indendent vectors $x_1, \ldots, x_n$
Output: Orthonormal vectors $v_1, \ldots, v_n$

---

for $j = 1 \colon n$
  $q_j \colon = x_j$
end
for $i = 1 \colon n$
  $r_{ii} \colon = \|q_i\|_2$
  $v_i \colon = \dfrac{q_i}{r_{ii}}$ (if $r_{ii} \neq 0$ else quit)
  for $j = i + 1 \colon n$
    $r_{ij} \colon = v_i^* q_j$
    $q_j \colon = q_j - r_{ij} v_i$
  end
end

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It can be proved that the isometry Q produced by the MGS algorithm satisfies

$$\|\mathtt{Q}' * \mathtt{Q} - \mathtt{eye}(\mathtt{n}, \mathtt{n})\|_2 \approx \mathbf{u} * \mathtt{cond}(\mathtt{A}),$$

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However if $\mathtt{cond}(\mathtt{A})$ satisfies $1 \ll \mathtt{cond}(\mathtt{A}) \ll 1/\mathbf{u}$, then $\mathbf{u} * \mathtt{cond}(\mathtt{V}) \ll 1$ and in such a case MGS will return a Q which is quite close to being an isometry.

Example

Consider the matrix $A := \begin{bmatrix} 1 & 1 & 1 \\ \epsilon & 0 & 0 \\ 0 & \epsilon & 0 \\ 0 & 0 & \epsilon \end{bmatrix}$. Then $\mathrm{cond}(A) = \dfrac{\sqrt{3+\epsilon^2}}{\epsilon}$.

If $\epsilon = \sqrt{\mathbf{u}}$ then $\mathbf{u}\,\mathrm{cond}(A) \approx \sqrt{3}\sqrt{\mathbf{u}}$.

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Assume that $\epsilon^2 < \mathbf{u}$. Then, in finite precision arithmetic, Q_{CS} produced by CGS and Q_{MS} produced by MGS are given by

$$Q_{\mathrm{CS}} = \begin{bmatrix} u_1 & u_2 & u_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ \epsilon & \frac{-1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} \end{bmatrix} \text{ and } Q_{\mathrm{MS}} = \begin{bmatrix} v_1 & v_2 & v_3 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ \epsilon & \frac{-1}{\sqrt{2}} & \frac{-1}{\sqrt{6}} \\ 0 & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{6}} \\ 0 & 0 & \frac{\sqrt{2}}{\sqrt{3}} \end{bmatrix}.$$

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Example

Now, consider the matrix $A := \begin{bmatrix} 1 & 1 & 1 \\ \epsilon & 0 & 0 \\ 0 & \epsilon & 0 \\ 0 & 0 & \epsilon \end{bmatrix}$ and choose $\epsilon = .5 \times 10^{-8}$.

Computing QR factorization $A = QR$ using CGS, MGS and Householder QR factorization in MATLAB yields

Error	cgs	mgs	qr
$\|Q^*Q - I\|_2$	5.0000e − 01	4.0825e − 09	2.2888e − 16
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The last column shows that Q is an isometry up to working precision showing that qr is backward stable. We have $\mathrm{cond}(A) = 3.5 \times 10^8$.

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For MGS $\|Q^*Q - I\|_2 \approx \mathrm{cond}(A)\mathbf{u}$. Hence MGS is conditionally backward stable. But Q computed by CGS is not an isometry and hence CGS is an unstable algorithm. ■

CGS versus MGS in finite precision arithmetic

The CGS and MGS are not equivalent in finite precison arithmetic because the equality

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In finite precision arithmetic, P_j may not be an orthogonal projection. Therefore, the computed $v_j = (I - P_{j-1})x_j / \|(I - P_{j-1})x_j\|_2$ may fail to be orthogonal to $v_1, \ldots, v_{j-1}$.

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By contrast, Q_j is an orthogonal projection in finite precision arithmetic and hence

$$v_j = \frac{(I - Q_{j-1}) \cdots ((I - Q_2)((I - Q_1)x_j))}{\|(I - Q_{j-1}) \cdots ((I - Q_2)((I - Q_1)x_j))\|_2}$$

when computed incrementally as in the case of MGS is likely to be orthogonal to $v_1, \ldots, v_{j-1}$.