Notes for Math 571 – Numerical Linear Algebra

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Chapter 1

1.1 Rank of Matrices

1.2 Cauchy-Schwarz

1.3 Projection Matrices, Gram-Schmidt Process

Suppose we have a plane of dimension $n-1$ and a direction orthogonal to it. A unit vector q with $q^T q = 1$.

Through a q a dim is specified as well as the $n-1$ dimensional plane orthogonal to it.

Given x we want to decompose it as $y+z$ with

1. y parallel to q
2. z orthogonal to q

We note $q^T z = 0$. So

$$
\begin{aligned}
x &= \alpha a + z \\
q^T z &= \alpha q^T q = \alpha \\
x &= q(q^T x) + z
\end{aligned}
$$

If $x = y + z$ is the decomposition of x then

$$
\begin{aligned}
y &= q(q^T x) = (qq^T)x \\
z &= x - (qq^T)x
\end{aligned}
$$

The matrix qq^T is a projection matrix. Applied to x it gives the component along q. If

$p = qq^T$ then P_x = component of x along q. $(I - P)x$ = component of x along the plane orthogonal to q.

(All projection are orthogonal throughout the class.)

Let us try to understand P.

1. What is the rank of P? $\operatorname{rank} P = 1$. (all columns multiples of q)
2. Eigenvalues and eigenvectors of P?

   $Pq = q$. Suppose $x \perp q$ then $Px = 0$. And eigenvalue $= 1$, eigenvalue $= 0$ with multiplicity $n - 1$.
3. $P^2 = P$. $(qq^T)(qq^T) = q(q^T q)q^T = qq^T$. $P^2 = Px$ for all $x \implies P^2 = P$.
4. $(I - P)^2 = I - P$.
5. $P(I - P) = 0$.

Given x and unit vector q, how many operations to compute $(I - P)x = x - q(q^T x)$?

1. $q^T x$ takes n multiplications and $n - 1$ additions
2. $q(q^T x)$ takes n multiplications
3. $x - q(q^T x)$ takes n subtractions

In total it takes $4n - 1$ or $4n$ arithmetic operations.

Suppose q_1 and q_2 are unit vectors with $q_1 \perp q_2$. Then which matrix projects to $\langle q_1, q_2\rangle$, the plane spanned by q_1 and q_2?

$P = P_1 + P_2$ with $P_1 = q_1 q^T$, $P_2 = q_2 q_2^T$.

Definition 1.3.1. $q_1, \ldots, q_k$ is called an orthonormal set of vectors if

1. $q_i q_i^T = 1$ for all i,
2. $q_i^T q_j = 0$ for all $i \neq q$.

$Q = \begin{pmatrix} | & & | \\ q_1 & \cdots & q_k \\ | & & | \end{pmatrix} \in \mathbb{R}^{n,k}$ is a matrix with orthonormal columns.

If $q_1, \ldots, q_k$ are orthonormal then

$$P = q_1 q_1^T + q_2 q_2^T + \ldots + q_x q_x^T$$

projects to $\langle q_1, \ldots, q_k\rangle$.

P can be expressed as $P = QQ^T$ where $Q \in \mathbb{R}^{n,k}$ with q_j as its columns.

What is the interpretation of $Q^T x$? $Q^T x$ gives the coefficients when the projection of x to $\langle q_1, \ldots, q_k \rangle$ is written as a linear combination of q_j.

What is $Q^T Q$? Identity matrix. Columns of Q forms as orthogonal set iff $Q^T Q = I$.

1. What is $I - QQ^T$? Projection to $\langle q_1, \ldots, q_k \rangle^\perp = (n-k)$ dim plane orthogonal to $\langle q_1, \ldots, q_k \rangle$.
2. $\operatorname{rank}(QQ^T) = k$.
3. $\operatorname{rank}(I - QQ^T) = n - k$.

Definition 1.3.2. A matrix $Q \in \mathbb{R}^{n,n}$ with orthonormal columns is called an orthogonal matrix. The columns of an orthogonal matrix Q form an orthogonal basis.

1. $QQ^T = \mathrm{id}$ since $QQ^T x = x$ for all x (projection to the whole space.)
2. What is the interpretation of $Q^T x$? The coefficients for x as linear combinations of columns of Q.
3. $Q^T Q$ still equal to identity.
4. The rows of Q also form an orthonormal basis.
5. $Q^{-1} = Q^T$.

<u>Classical Gram-Schmidt Process</u>

Suppose $A \in \mathbb{R}^{n,k}$ with $n \geq k$ and $\operatorname{rank} A = k$. Let $a_1, \ldots, a_k$ be the columns of A. The Gram-Schmidt process generates an orthonormal set q_1 through q_k such that

1. $\langle q_1 \rangle = \langle a_1 \rangle$,
2. $\langle q_1, q_2 \rangle = \langle a_1, a_2 \rangle$,

$\vdots$

k. $\langle q_1, q_2, \ldots, q_k \rangle = \langle a_1, a_2, \ldots, a_k \rangle$.

An algorithm for computing $q_1, \ldots, q_k$:

$$
\begin{aligned}
q_1 &= \frac{a_1}{\|a_1\|} = \frac{a_1}{(a_1^T a_1)} \\
\tilde{q_2} &= a_2 - P_1 a_2 = a_2 - q_1(q_1^T a_2), q_2 = \frac{\tilde{q_2}}{\|q_2\|} \\
&\vdots \\
\tilde{q_k} &= a_k - \sum_{i=1}^{k-1} P_i a_k = a_k - \sum_{i=1}^{k-1} q_i q_i^T a_k, q_k = \frac{\tilde{q_k}}{\|q_k\|}.
\end{aligned}
$$

Expression of Gram-Schmidt as $A = QR$ with R upper triangles. Suppose $q_1, \dots, q_k$ are computed by applying Gram-Schmidt to the columns of A.

Let Q be the matrix whose columns are $q_1, \dots, q_k$. Both A and Q are $n \times k$.

$$\begin{aligned} A &= Q(k \times k \text{ matrix}) \\ &= QR. \end{aligned}$$

Every column of A is expressed as a linear combination of $q_1, \dots, q_k$.

What are the entries of R?

Note that $a_j = q_1(q_1^T a_j) + \dots + a_j(a_j^T a_j)$ because $a_j \in \langle q_1, \dots, q_j \rangle$. Write $a_j = q_1 r_{1j} + \dots + a_j r_{ij}$. Thus

$$r_{ij} = \begin{cases} q_i^T a_j & i \leq j, \\ 0 & i > j. \end{cases}$$

During Gram=Schmidt process these coefficients are computed

$$\begin{aligned} r_{ij} &= q_i^T a_j, \quad i < j \\ r_{jj} &= \|\tilde{q}_j\| \end{aligned}$$

<u>APPLICATION OF CLASSICAL GRAM-SCHMIDT</u>

Think of $a_1, \dots, a_k$ as defining a $k-$dim parallelepiped in $\mathbb{R}^n$. What is the volume of the parallelepiped defined by $a_1, \dots, a_k$?

$\prod r_{ii}$.

<u>NOTE</u> Classical Gram-Schmidt (CGS) is not numerically stable. More precisely, when A has near rank efficiency, then CGS does not behave well.

We can use modified Gram-Schmidt (MGS):

Lemma 1.3.1. *If $q_1, \dots, q_j$ are an orthonormal set and $P_1, \dots, P_j$ are corresponding projections, then*

$$I - P_1 - \dots - P_j = (I - P_j) \dots (I - P_2)(I - P_1)$$

(Projection one at a time (RHS) vs. project at once (LHS))

Proof. $P_i P_j = 0$ if $i \neq j$. Expand RHS and we are done. ∎

MGS has step j given by $\tilde{q}_j = (I - P_{j-1}) \dots (I - P_1) a_j, q_j = \frac{\tilde{q}_j}{\|q_j\|}$.

In CGS, $A = QR$ with $a_j = q_i r_{ij} + \dots + q_j r_{jj}$. $r_{ij} = q_i^T a_j i \neq j, \|\tilde{q}_j\|$.

$q_i^T a_j$ are not available as intermediate quantities in MGS.

$$\begin{aligned}
\tilde{q}_j &= (I - P_{j-1}) \dots (I - P_1) a_j \\
a_{j,1} &= (I - P_1) a_j \quad (= a_j - P_1 a_j) \\
a_{j,2} &= (I - P_2) a_{j,1} \quad (= a_j - P_2 a_j - P_1 a_j \text{ mathematically}) \\
a_{j,3} &= (I - P_3) a_{j,2} \quad (= a_j - P_3 a_j - P_2 a_j - P_1 a_j \text{ mathematically}) \\
&\vdots
\end{aligned}$$

In practice the rounding error will accumulate differently, which makes MGS stable.

So

$$\begin{aligned}
r_{i,j} &= q_i^T a_{j,i-1} \\
&= q_i^T (I - P_1 - \dots - P_{i-1}) a_i \\
&= q_i^T a_j
\end{aligned}$$

Operations count for MGS (or CGS): In step j we have the following:

$$\begin{aligned}
a_{j,1} &= (I - P_1) a_j \\
a_{j,2} &= (I - P_2) a_{j,1} \\
&\vdots \\
a_{j,j-1} &= (I - P_{j-1}) a_{j,j-2} \\
q_j &= \frac{a_{j,j-1}}{\|a_{j,j-1}\|}
\end{aligned}$$

To count operations, recall that $(I - P)x$ requires $4n$ operations.

$$(I - P)x = x - q(q^T x)$$

$2n-1$ for $q^T x$, n for $q(q^T x)$, n for $x - q(q^T x)$. Operation count for step i is $(4n)(j-1) + 3n$.

The total count is

$$\sum_{j=1}^{k} (4n-1)(j-1) + 3n = (4n-1)\frac{k(k-1)}{2} 3nk = 2nk^2 \text{ leading terms}$$

Also:

$$\sum_{j=1}^{k} 4nj = 4n \sum_{i=1}^{k} j = 4n \int_0^k x \mathrm{d}x = 4nk^2.$$

1.4 Applications of MGS and QR Factorization

1.4.1 Solution of $Ax = b$ for $A \in \mathbb{R}^{m,n}, \operatorname{rank}(A) = n$

$$QRx = b \implies Rx = Q^T b$$

Now $Rx = \tilde{b}$ can be solved by back substitution.

Operation count for solving $Ax = b$ using QR.

1. calculating $QR : 2n^3$
2. $\tilde{b} = Q^T b, 2n^2 - n$
3. solving $Rx = \tilde{b}$ using back substitution: n^2.

Linear system solved using Gaussian elimination with partial pivoting is n^3.

1.4.2 Connection with Volumes and QR

Let a_1 and a_2 be vectors in $\mathbb{R}^m$. They will define a parallelogram as follows.

1.4.3 Determinants