LEAST SQUARE PROBLEMS, QR DECOMPOSITION, AND SVD DECOMPOSITION

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ABSTRACT. We review basics on least square problems. The material is mainly taken from books [2, 1, 3].

We consider an overdetermined system $Ax = b$ where $A_{m\times n}$ is a tall matrix, i.e., $m > n$. We have more equations than unknowns and in general cannot solve it exactly.

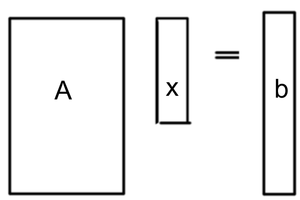

FIGURE 1. An overdetermined system.

1. FUNDAMENTAL THEOREM OF LINEAR ALGEBRA

Let $A_{m\times n} : \mathbb{R}^n \to \mathbb{R}^m$ be a matrix. Consider four subspaces associated to A:

- $N(A) = \{x \in \mathbb{R}^n, Ax = 0\}$
- $C(A) =$ the subspace spanned by column vectors of A
- $N(A^T) = \{y \in \mathbb{R}^m, y^T A = 0\}$
- $C(A^T)$ the subspace spanned by row vectors of A

The fundamental theorem of linear algebra [2] is:

$$N(A) = C(A^T)^{\perp}, \qquad N(A^T) = C(A)^{\perp}.$$

In words, the null space is the *orthogonal complement* of the row space in $\mathbb{R}^n$. The left null space is the *orthogonal complement* of the column space in $\mathbb{R}^m$. The column space $C(A)$ is also called the range of A. It is illustrated in the following figure.

Therefore $Ax = b$ is solveable if and only if b is in the column space (the range of A). Looked at indirectly. $Ax = b$ requires b to be perpendicular to the left null space, i.e., $(b, y) = 0$ for all $y \in \mathbb{R}^m$ such that $y^T A = 0$.

The real action of $A : \mathbb{R}^n \to \mathbb{R}^m$ is between the row space and column space. From the row space to the column space, A is actually invertible. Every vector b in the column space comes from exactly one vector x_r in the row space.

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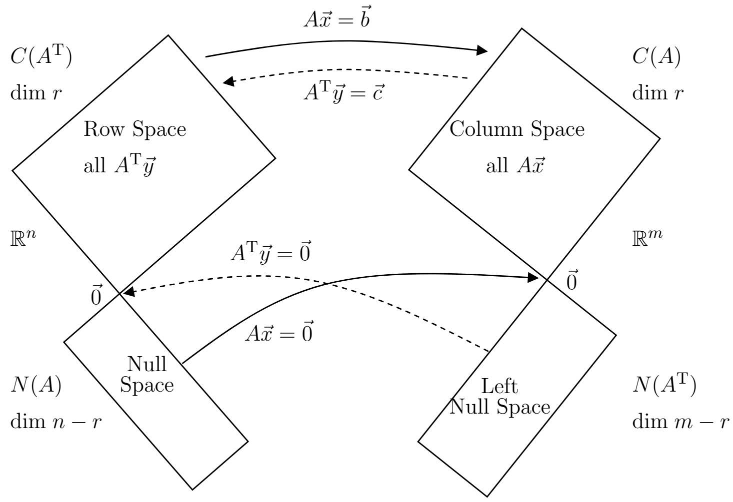

FIGURE 2. Fundamental theorem of linear algebra.

2. LEAST SQUARES PROBLEMS

How about the case $b \notin C(A)$? We consider the following equivalent facts:

(1) Minimize the square of the l^2-norm of the residual, i.e.,

$$\min_{x \in \mathbb{R}^n} \|b - Ax\|^2 \tag{1}$$

(2) Find the projection of b in $C(A)$;

(3) $b - Ax$ must be perpendicular to the space $C(A)$.

By the fundament theorem of linear algebra, $b - Ax$ is in the left null space of A, i.e., $(b - Ax)^T A = 0$ or equivalently $A^T(Ax - b) = 0$. We then get the normal equation

$$A^T A x = A^T b. \tag{2}$$

One can easily derive the normal equation (2) by consider the first order equation of the minimization problem (1).

The least square solution

$$x = A^\dagger b := (A^T A)^{-1} A^T b,$$

and the projection of b to $C(A)$ is given by

$$Ax = A(A^T A)^{-1} A^T b.$$

The operator $A^\dagger := (A^T A)^{-1} A^T$ is called the *Moore-Penrose pseudo-inverse* of A.

3. PROJECTION MATRIX

The projection matrix to the column space of A is

$$P = A(A^T A)^{-1} A^T : \mathbb{R}^m \to C(A).$$

Its orthogonal complement projection is given by

$$I - P = I - A(A^T A)^{-1} A^T : \mathbb{R}^m \to N(A^T).$$

In general a projector or idempotent is a square matrix P that satisfies

$$P^2 = P.$$

When $v \in C(P)$, then applying the projector results in v itself, i.e. P restricted to the range space of P is identity.

For a projector P, $I - P$ is also a projector and is called the complementary projector to P. We have the complementary result

$$C(I - P) = N(P), \quad N(I - P) = C(P).$$

An orthogonal projector P is a projector P such that $(v - Pv) \perp C(P)$. Algebraically an orthogonal projector is any projector that is symmetric, i.e., $P^T = P$. An orthogonal projector can be always written in the form

$$P = QQ^T,$$

where the columns of Q are orthonormal. The projection $Px = Q(Q^T x)$ can be interpret as: $c = Q^T x$ is the coefficient vector and Qc is expanding Px in the orthonormal basis defined by column vectors of Q.

Notice that $Q^T Q$ is the $n \times n$ identity matrix, whereas QQ^T is an $m \times m$ matrix. It is the identity mapping for vectors in the column space of Q and maps the orthogonal complement of $C(Q)$, which is the nullspace of Q^T, to zero.

An important special case is the rank-one orthogonal projector which can be written as

$$P = qq^T, \quad P^{\perp} = I - qq^T.$$

for a unit vector q and for a general vector a

$$P = \frac{aa^T}{a^T a}, \quad P^{\perp} = I - \frac{aa^T}{a^T a}.$$

Example 3.1. Consider Stokes equation with $B = -\mathrm{div}$. Here B is a long-thin matrix and can be thought as A^T. Then the projection to divergences free space, i.e., $N(B)$ is given by $P = I - B^T (BB^T)^{-1} B$.

Example 3.2. Note that the default orthogonality is with respect to the l_2 inner product. Let $V_H \subset V$ be a subspace and $I_H : V_H \hookrightarrow V$ be the natural embedding. For an SPD matrix A, the A-orthogonal projection $P_H : V \to V_H$ is

$$P_H = I_H (I_H^T A I_H)^{-1} I_H^T A,$$

which is symmetric in the $(\cdot, \cdot)_A$ inner product.

4. QR Decomposition

The least square problem $Qx = b$ for a matrix Q with orthonormal columns is ver easy to solve: $x = Q^T b$. For a general matrix, we try to change to the orthogonal case.

4.1. **Gram-Schmidt Algorithm.** Given a tall matrix A, we can apply a procedure to turn it into a matrix with orthogonal columns. The idea is very simple. Suppose we have orthogonal columns $Q_{j-1} = (q_1, q_2, \ldots, q_{j-1})$, take a_j, the j-th column of A, we project a_j to the orthogonal complement of the column space of Q_{j-1}. The formula is

$$P_{C^{\perp}(Q_{j-1})} a_j = (I - Q_{j-1} Q_{j-1}^T) a_j = a_j - \sum_{i=1}^{j-1} q_i (q_i^T a_j).$$

After that we normalize $P_{C^{\perp}(Q_{j-1})} a_j$.

4.2. **QR decomposition.** The G-S procedure leads to a factorization

$$A = QR,$$

where Q is an orthogonal matrix and R is upper triangular. Think the matrix times a vector as a combination of column vectors of the matrix using the coefficients given by the vector. So R is upper triangular since the G-S procedure uses the previous orthogonal vectors only.

It can be also thought of as the coefficient vector of the column vector of A in the orthonormal basis given by Q. We emphasize that:

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(3) QR factorization is as important as LU factorization.

LU is for solving $Ax = b$ for square matrices A. QR simplifies the least square solution to the over-determined system $Ax = b$. With QR factorization, we can get

$$Rx = Q^T b,$$

which can be solved efficiently since R is upper triangular.

5. Stable Methods for QR Decomposition

The original G-S algorithm is not numerically stable. The obtained matrix Q may not be orthogonal due to the round-off error especially when column vectors are nearly dependent. Modified G-S is more numerically stable. Householder reflection enforces the orthogonality into the procedure.

5.1. **Modified Gram-Schmidt Algorithm.** Consider the upper triangular matrix $R = (r_{ij})$, G-S algorithm is computing r_{ij} column-wise while modified G-S is row-wise. Recall that in the j-th step of G-S algorithm, we project the vector a_j to the orthogonal complement of the spanned by $(q_1, q_2, \ldots, q_{j-1})$. This projector can be written as the composition of

$$P_j = P^{\perp}_{q_{j-1}} \cdots P^{\perp}_{q_2} P^{\perp}_{q_1}.$$

Once q_1 is known, we can apply $P^{\perp}_{q_1}$ to all column vectors from $2 : n$ and in general when q_i is computed, we can update $P^{\perp}_{q_i} v_j$ for $j = i+1 : n$.

Operation count: there are $n^2/2$ entries in R and each entry r_{ij} requires $4m$ operations. So the total operation is $4mn^2$. Roughly speaking, we need to compute the n^2 pairwise inner product of n column vectors and each inner product requires m operation. So the operation is $\mathcal{O}(mn^2)$.

5.2. **Householder Triangulation.** We can summarize

- Gram-Schmit: triangular orthogonalization $AR_1R_2...R_n = Q$
- Householder: orthogonal triangularization $Q_n...Q_1A = R$

The orthogonality of Q matrix obtained in Householder method is enforced.

One step of Houserholder algorithm is the Householder reflection which changes a vector x to ce_1. The operation should be orthogonal so the projection to e_1 is not a choice. Instead the reflection is since it is orthogonal.

It is a reflection so the norm should be preserved, i.e., the point on the e_1 axis is either $\|x\|e_1$ or $-\|x\|e_1$. For numerical stability, we should chose the point which is not too close to x. So the reflection point is $x^T = -\text{sign}(x_1)\|x\|e_1$.

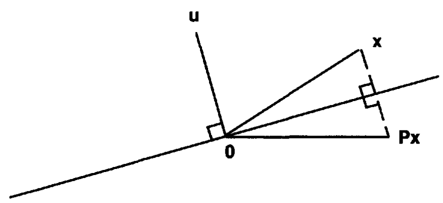

FIGURE 3. Householder reflection

With the reflection point, we can form the normal vector $v = x - x^T = x + \mathrm{sign}(x_1)\|x\|e_1$ and the projection to v is $P_v = v(v^T v)^{-1} v^T$ and the reflection is given by

$$I - 2P_v.$$

The reflection is applied to the lower part column vectors $A(k : m, k : n)$ and in-place implementation is possible.

6. SVD

For a tall matrix $A_{m\times n}$, there exist orthonormal matrix $U_{m\times n}$ and $V_{n\times n}$ and a diagonal matrix $\Sigma_{n\times n} = \mathrm{diag}(\sigma_1, \sigma_2, \cdots, \sigma_n)$ such that

$$A_{m\times n} = U_{m\times n}\Sigma_{n\times n}V_{n\times n}^T,$$

which is called the Singular Value Decomposition of A and the numbers σ_i are called singular values.

By direct computation, we know σ_i^2 is an eigenvalue of $A^T A$ and AA^T. More precisely

$$A^T A = V\Sigma U^T U\Sigma V^T = V\Sigma^2 V^T.$$

So V is formed by n-eigenvectors of $A^T A$ and $\Sigma^2 = \mathrm{diag}(\lambda_1, \ldots, \lambda_n)$. Similarly U formed by eigenvectors of AA^T. Notice that the rank of $m \times m$ matrix AA^T is at most n, i.e., at most n non-zero eigenvalues. We can extend U by adding orthonormal eigenvectors of the zero eigenvalue of AA^T and denote by $\bar{U}$. The $n \times n$ matrix Σ can be extended to $\bar{\Sigma}_{m\times n}$ by adding zero rows. So another form of SVD decomposition is

$$A_{m\times n} = \bar{U}_{m\times m}\bar{\Sigma}_{m\times n}V_{n\times n}^T.$$

If we treat A is a mapping from $\mathbb{R}^n \to \mathbb{R}^m$, the geometrical interpretation of SVD is: in the correct coordinate, the mapping is just the scaling of the axis vectors. Thus a circle in $\mathbb{R}^n$ is embedded into $\mathbb{R}^m$ as an ellipse.

If we let $U^{(i)}$ and $V^{(i)}$ to denote the i-th column vectors of U and V, respectively. We can rewrite the SVD decomposition as a decomposition of A into rank one matrices:

$$A = \sum_{i=1}^{n} \sigma_i U^{(i)} (V^{(i)})^T.$$

If we sort the singular values in decent order: $\sigma_1 \geq \sigma_2 \cdots \geq \sigma_n$, for $k \leq n$, the best rank k approximation, denoted by A_k, is given by

$$A_k = \sum_{i=1}^{k} \sigma_i U^{(i)} (V^{(i)})^T.$$

And

$$\|A - A_k\|_2 = \left\| \sum_{i=k+1}^{n} \sigma_i U^{(i)} (V^{(i)})^T . \right\| = \sigma_{k+1}.$$

It can proved A_k is the best one in the sense that

$$\|A - A_k\|_2 = \min_{X, \operatorname{rank}(X) = k} \|A - X\|_2.$$

When the rank of A is r, then $\sigma \neq 0, \sigma_{r+1} = \sigma_{r+2} = \cdots = \sigma_n = 0$ and we can reduce U to a $m \times r$ matrix and Σ, V to $r \times r$.

7. Methods for Solving Least Square Problems

Given a tall matrix $A_{m\times n}, m > n$, the least square problem $Ax = b$ can be solved by the following methods

(1) Solve the normal equation $A^T Ax = A^T b$
(2) Find QR factorization $A = QR$ and solve $Rx = Q^T b$.
(3) Find SVD factorization $A = U\Sigma V^T$ and solve $x = V\Sigma^{-1}U^T b$.

Which method to use?

- Simple answer: QR approach is the 'daily used' method for least square problems.
- Detailed answer: In terms of speed, 1 is the fastest one. But the condition number is squared and thus less stable. QR factorization is more stable but the cost is almost doubled. The SVD approach is more appropriate when A is rank-deficient.

References

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[3] L. N. Trefethen and D. Bau III. *Numerical linear algebra*, volume 50. Siam, 1997.