Introduction to inverse and ill-posed problems: QR and SVD. Solution of rank-deficient problems. Lecture 5

QR Decomposition

THEOREM QR decomposition. *Let A be m-by-n with $m \geq n$. Suppose that A has full column rank. Then there exist a unique m-by-n orthogonal matrix $Q(Q^TQ = I_n)$ and a unique n-by-n upper triangular matrix R with positive diagonals $r_{ii} > 0$ such that $A = QR$.*

Proof. Can be two proofs of this theorem: using the Gram-Schmidt orthogonalization process and using the Householder reflections. The first proof: this theorem is a restatement of the Gram-Schmidt orthogonalization process [P. Halmos. Finite Dimensional Vector Spaces. Van Nostrand, New York, 1958]. If we apply Gram-Schmidt to the columns a_i of $A = [a_1, a_2, \ldots, a_n]$ from left to right, we get a sequence of **orthonormal vectors** (if they are orthogonal and unit vectors) q_1 through q_n spanning the same space: these orthogonal vectors are the columns of Q. Gram-Schmidt also computes coefficients $r_{ji} = q_j^T a_i$ expressing each column a_i as a linear combination of q_1 through q_i: $a_i = \sum_{j=1}^{i} r_{ji} q_j$. The r_{ji} are just the entries of R.

ALGORITHM *The classical Gram-Schmidt (CGS) and modified Gram-Schmidt (MGS) Algorithms for factoring* $A = QR$:

for $i = 1$ *to* n */* compute* i*th columns of* Q *and* R **/*
$q_i = a_i$
for $j = 1$ *to* $i - 1$ */* subtract component in* q_j *direction from* a_i **/*

$$\begin{cases} r_{ji} = q_j^T a_i & CGS \\ r_{ji} = q_j^T q_i & MGS \end{cases}$$

$q_i = q_i - r_{ji} q_j$
end for
$r_{ii} = \|q_i\|_2$
if $r_{ii} = 0$ */** a_i *is linearly dependent on* $a_1, \ldots, a_{i-1}$ **/*
quit
end if
$q_i = q_i / rii$
end for

If A has full column rank, r_{ii} will not be zero.

Notes:

- Unfortunately, CGS is numerically unstable in floating point arithmetic when the columns of A are nearly linearly dependent.
- MGS is more stable and will be used in algorithms later in this course but may still result in Q being far from orthogonal ($\|Q^TQ - I\|$ being far larger than ε) when A is ill-conditioned
- Literature on this subject:

Å. Björck. Solution of Equations volume 1 of Handbook of Numerical Analysis, chapter Least Squares Methods. Elsevier/North Holland, Amsterdam, 1987.

Å. Björck. Least squares methods. Mathematics Department Report, Linkoping University, 1991.

Å. Björck. Numerical Methods for Least Squares Problems. SIAM, Philadelphia, PA, 1996.

N. J. Higham. Accuracy and Stability of Numerical Algorithms. SIAM, Philadelphia, PA, 1996.

We will derive the formula for the x that minimizes $||Ax - b||_2$ using the decomposition $A = QR$ in three slightly different ways. First, we can always choose $m - n$ more **orthonormal vectors** $\tilde{Q}$ so that $[Q, \tilde{Q}]$ is a square orthogonal matrix and thus $\tilde{Q}^T Q = 0$ (for example, we can choose any $m - n$ more independent vectors $\tilde{X}$ that we want and then apply QR Algorithm to the n-by-n nonsingular matrix $[Q, \tilde{X}]$). Then

$$
\begin{aligned}
||Ax - b||_2^2 &= ||[Q, \tilde{Q}]^T (Ax - b)||_2^2 \\
&= \left\| \begin{bmatrix} Q^T \\ \tilde{Q}^T \end{bmatrix} (QRx - b) \right\|_2^2 \\
&= \left\| \begin{bmatrix} I^{n \times n} \\ O^{(m-n) \times n} \end{bmatrix} Rx - \begin{bmatrix} Q^T b \\ \tilde{Q}^T b \end{bmatrix} \right\|_2^2 \\
&= \left\| \begin{bmatrix} Rx - Q^T b \\ -\tilde{Q}^T b \end{bmatrix} \right\|_2^2 \\
&= \left\| Rx - Q^T b \right\|_2^2 + ||\tilde{Q}^T b||_2^2 \geq ||\tilde{Q}^T b||_2^2.
\end{aligned}
$$

We can solve $Rx - Q^T b = 0$ for x, since A and R have the same rank, n, and so R is nonsingular. Then $x = R^{-1} Q^T b$, and the minimum value of $||Ax - b||_2$ is $||\tilde{Q}^T b||_2$.

Here is a second, slightly different derivation that does not use the matrix $\tilde{Q}$. Rewrite $Ax - b$ as

$$\begin{aligned} Ax - b &= QRx - b = QRx - (QQ^T + I - QQ^T)b \\ &= Q(Rx - Q^T b) - (I - QQ^T)b. \end{aligned}$$

Note that the vectors $Q(Rx - Q^T b)$ and $(I - QQ^T)b$ are orthogonal, because $(Q(Rx - Q^T b))^T((I - QQ^T)b) = (Rx - Q^T b)^T [Q^T (I - QQ^T)]b = (Rx - Q^T b)^T [0] b = 0$. Therefore, by the Pythagorean theorem,

$$\begin{aligned} \|Ax - b\|_2^2 &= \|Q(Rx - Q^T b)\|_2^2 + \|(I - QQ^T)b\|_2^2 \\ &= \|Rx - Q^T b\|_2^2 + \|(I - QQ^T)b\|_2^2. \end{aligned}$$

where we have used $\|Qy\|_2^2 = \|y\|_2^2$. This sum of squares is minimized when the first term is zero, i.e., $x = R^{-1} Q^T b$.

Finally, here is a third derivation that starts from the normal equations solution:

$$
\begin{aligned}
x &= (A^TA)^{-1}A^Tb \\
&= (R^TQ^TQR)^{-1}R^TQ^Tb = (R^TR)^{-1}R^TQ^Tb \\
&= R^{-1}R^{-T}R^TQ^Tb = R^{-1}Q^Tb.
\end{aligned}
$$

Singular values

The singular values, or s-numbers of a compact operator $T : X \rightarrow Y$ acting between Hilbert spaces X and Y, are the square roots of the eigenvalues of the nonnegative self-adjoint operator $T^*T : X \rightarrow X$ (where T^* denotes the adjoint of T).

$$\sigma(T) = \sqrt{\lambda(T^*T)}.$$

The singular values are nonnegative real numbers, usually listed in decreasing order $(s_1(T), s_2(T), ...)$. If T is self-adjoint, then the largest singular value $s1(T)$ is equal to the operator norm of T.
In the case of a normal matrix A (or $A^*A = AA^*$, when A is real then $A^TA = AA^T$), the spectral theorem can be applied to obtain unitary diagonalization of A as $A = U\Lambda U^*$. Therefore, $\sqrt{A^*A} = U|\Lambda|U^*$ and so the singular values are simply the absolute values of the eigenvalues.

Singular Value Decomposition

THEOREM SVD. *Let A be an arbitrary m-by-n matrix with $m \geq n$. Then we can write $A = U\Sigma V^T$, where U is m-by-n and satisfies $U^T U = I$, V is n-by-n and satisfies $V^T V = I$, and $\Sigma = diag(\sigma_1, \ldots, \sigma_n)$, where $\sigma_1 \geq \cdots \geq \sigma_n \geq 0$. The columns $u_1, \ldots, u_n$ of U are called left singular vectors. The columns $v_1, \ldots, v_n$ of V are called right singular vectors. The σ_i are called singular values. (If $m < n$, the SVD is defined by considering A^T.)*

THEOREM *Let* $A = U\Sigma V^T$ *be the SVD of the m-by-n matrix* A, *where* $m \geq n$. *(There are analogous results for* $m < n$.)

- 1. Suppose that A is symmetric, with eigenvalues λ_i and orthonormal eigenvectors u_i. i.e., $A = U\Lambda U^T$ is an eigendecomposition of A, with $\Lambda = diag(\lambda_1, \ldots, \lambda_n)$, and $U = [u_1, \ldots, u_n]$, and $UU^T = I$. Then an SVD of A is $A = U\Sigma V^T$, where $\sigma_i = |\lambda_i|$ and $\upsilon_i = sign(\lambda_i) u_i$, where $sign(0) = 1$.
- 2. The eigenvalues of the symmetric matrix A^TA are σ_i^2. The right singular vectors υ_i are corresponding orthonormal eigenvectors.
- 3. The eigenvalues of the symmetric matrix AA^T are σ_i^2 and $m - n$ zeroes. The left singular vectors u_i are corresponding orthonormal eigenvectors for the eigenvalues σ_i^2. One can take any $m - n$ other orthogonal vectors as eigenvectors for the eigenvalue 0.

- 4. Let $H = \begin{bmatrix} 0 & A^T \\ A & 0 \end{bmatrix}$, where A is square and $A = U\Sigma V^T$ is the SVD of A. Let $\Sigma = diag(\sigma_1, \dots, \sigma_n)$, $U = [u_1, \dots, u_n]$, and $V = [\upsilon_1, \dots, \upsilon_n]$. Then the 2n eigenvalues of H are $\pm\sigma_i$, with corresponding unit eigenvectors $\frac{1}{\sqrt{2}} \begin{bmatrix} \upsilon_i \\ \pm u_i \end{bmatrix}$.
- 5. If A has full rank, the solution of $\min_x \|Ax - b\|_2$ is $x = V\Sigma^{-1}U^T b$.
- 6. $\|A\|_2 = \sigma_1$. If A is square and nonsingular, then $\|A^{-1}\|_2^{-1} = \sigma_n$ and $\|A\|_2 \cdot \|A^{-1}\|_2 = \frac{\sigma_1}{\sigma_n}$.
- 7. Write $V = [\upsilon_1, \upsilon_2, \dots, \upsilon_n]$ and $U = [u_1, u_2, \dots, u_n]$, so $A = U\Sigma V^T = \sum_{i=1}^n \sigma_i u_i \upsilon_i^T$ (a sum of rank-1 matrices). Then a matrix of rank $k < n$ closest to A (measured with $\| \cdot \|_2$) is $A_k = \sum_{i=1}^k \sigma_i u_i \upsilon_i^T$ and $\|A - A_k\|_2 = \sigma_{k+1}$. We may also write $A_k = U\Sigma_k V^T$ where $\Sigma_k = diag(\sigma_1, \dots, \sigma_k, 0, \dots, 0)$.

Proof.

1. **Suppose that** A **is symmetric, with eigenvalues** λ_i **and orthonormal eigenvectors** u_i**. In other words** $A = U\Lambda U^T$ **is an eigendecomposition of** A**, with** $\Lambda = diag(\lambda_1, \ldots, \lambda_n)$**, and** $U = [u_1, \ldots, u_n]$**, and** $UU^T = I$**. Then an SVD of** A **is** $A = U\Sigma V^T$**, where** $\sigma_i = |\lambda_i|$ **and** $\upsilon_i = sign(\lambda_i)u_i$ **, where** $sign(0) = 1$**.**

This is true by the definition of the SVD.

2. **The eigenvalues of the symmetric matrix $A^T A$ are σ_i^2. The right singular vectors υ_i are corresponding orthonormal eigenvectors.**
$A^T A = V \Sigma U^T U \Sigma V^T = V \Sigma^2 V^T$. This is an eigendecomposition of $A^T A$, with the columns of V the eigenvectors and the diagonal entries of Σ^2 the eigenvalues.

3. **The eigenvalues of the symmetric matrix AA^T are σ_i^2 and $m-n$ zeroes. The left singular vectors u_i are corresponding orthonormal eigenvectors for the eigenvalues σ_i^2. One can take any $m-n$ other orthogonal vectors as eigenvectors for the eigenvalue 0.**

Choose an m-by-$(m-n)$ matrix $\tilde{U}$ so that $[U, \tilde{U}]$ is square and orthogonal. Then write

$$AA^T = U\Sigma V^T V\Sigma U^T = U\Sigma^2 U^T = \left[U, \tilde{U}\right] \cdot \begin{bmatrix} \Sigma^2 & 0 \\ 0 & 0 \end{bmatrix} \cdot \left[U, \tilde{U}\right]^T.$$

This is an eigendecomposition of AA^T.

4. **Let** $H = \begin{bmatrix} 0 & A^T \\ A & 0 \end{bmatrix}$**, where** A **is square and** $A = U\Sigma V^T$ **is the SVD of** A**. Let** $\Sigma = diag(\sigma_1, \ldots, \sigma_n)$**,** $U = [u_1, \ldots, u_n]$**, and** $V = [\upsilon_1, \ldots, \upsilon_n]$**. Then the 2n eigenvalues of** H **are** $\pm\sigma_i$**, with corresponding unit eigenvectors** $\frac{1}{\sqrt{2}} \begin{bmatrix} \upsilon_i \\ \pm u_i \end{bmatrix}$**.**

We substitute $A = U\Sigma V^T$ into H to get: $H = \begin{bmatrix} 0 & V\Sigma U^T \\ U\Sigma V^T & 0 \end{bmatrix}$

Choose orthogonal matrix G such that

$$G = \frac{1}{\sqrt{2}} \begin{bmatrix} V & V \\ U & -U \end{bmatrix}$$

It is orthogonal since $I = GG^T = \frac{1}{2} \begin{bmatrix} VV^T + VV^T & 0 \\ 0 & UU^T + UU^T \end{bmatrix}$

Then we observe that

$$G \begin{bmatrix} \Sigma & 0 \\ 0 & \Sigma \end{bmatrix} G^T = \begin{bmatrix} 0 & V\Sigma U^T \\ U\Sigma V^T & 0 \end{bmatrix} = H$$

Then using the spectral theorem we can conclude that the $2n$ eigenvalues of H are $\pm\sigma_i$, with corresponding eigenvectors $\frac{1}{\sqrt{2}} \begin{bmatrix} v_i \\ \pm u_i \end{bmatrix}$.

5. **If** A **has full rank, the solution of** $\min_x \|Ax - b\|_2$ **is** $x = V\Sigma^{-1}U^T b$**.**
$\|Ax - b\|_2^2 = \|U\Sigma V^T x - b\|_2^2$. Since A has full rank, so does Σ, and thus Σ is invertible. Now let $[U, \tilde{U}]$ be square and orthogonal as above so

$$
\begin{aligned}
\|U\Sigma V^T x - b\|_2^2 &= \left\| \begin{bmatrix} U^T \\ \tilde{U}^T \end{bmatrix} (U\Sigma V^T x - b) \right\|_2^2 \\
&= \left\| \begin{bmatrix} \Sigma V^T x - U^T b \\ -\tilde{U}^T b \end{bmatrix} \right\|_2^2 \\
&= \|\Sigma V^T x - U^T b\|_2^2 + \|\tilde{U}^T b\|_2^2 .
\end{aligned}
$$

This is minimized by making the first term zero, i.e., $x = V\Sigma^{-1}U^T b$.

6. $\|A\|_2 = \sigma_1$. **If** A **is square and nonsingular, then** $\|A^{-1}\|_2^{-1} = \sigma_n$ **and** $\|A\|_2 \cdot \|A^{-1}\|_2 = \frac{\sigma_1}{\sigma_n}$.
It is clear from its definition that the two-norm of a diagonal matrix is the largest absolute entry on its diagonal. Thus, by property of the norm,
$\|A\|_2 = \|U^T AV\|_2 = \|U^T U\Sigma V^T V\|_2 = \|\Sigma\|_2 = \sigma_1$ and
$\|A^{-1}\|_2 = \|V^T A^{-1} U\|_2 = \|\Sigma^{-1}\|_2 = \sigma_n^{-1}$.
Remark: $\|A^{-1}\|_2 = \|V^T A^{-1} U\|_2 = \|V^T (U\Sigma V^T)^{-1} U\|_2 = \|\Sigma^{-1}\|_2 = \sigma_n^{-1}$.

7. Write $V = [v_1, v_2, \ldots, v_n]$ and $U = [u_1, u_2, \ldots, u_n]$, so $A = U\Sigma V^T = \sum_{i=1}^{n} \sigma_i u_i v_i^T$ (a sum of rank-1 matrices). Then a matrix of rank $k < n$ closest to A (measured with $||\cdot||_2$) is $A_k = \sum_{i=1}^{k} \sigma_i u_i v_i^T$ and $||A - A_k||_2 = \sigma_{k+1}$. We may also write $A_k = U\Sigma_k V^T$ where $\Sigma_k = diag(\sigma_1, \ldots, \sigma_k, 0, \ldots, 0)$.

7. Write $V = [\upsilon_1, \upsilon_2, \ldots, \upsilon_n]$ and $U = [u_1, u_2, \ldots, u_n]$, so $A = U\Sigma V^T = \sum_{i=1}^n \sigma_i u_i \upsilon_i^T$ (a sum of rank-1 matrices). Then a matrix of rank $k < n$ closest to A (measured with $\|\cdot\|_2$) is $A_k = \sum_{i=1}^k \sigma_i u_i \upsilon_i^T$ and $\|A - A_k\|_2 = \sigma_{k+1}$. We may also write $A_k = U\Sigma_k V^T$ where $\Sigma_k = diag(\sigma_1, \ldots, \sigma_k, 0, \ldots, 0)$.
A_k has rank k by construction and

$$\|A - A_k\|_2 = \left\| \sum_{i=1}^n \sigma_i u_i \upsilon_i^T - \sum_{i=1}^k \sigma_i u_i \upsilon_i^T \right\|$$

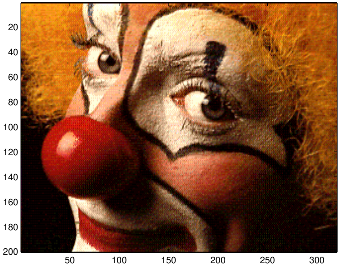
$$= \left\| \sum_{i=k+1}^n \sigma_i u_i \upsilon_i^T \right\| = \left\| U \begin{bmatrix} 0 & & & \\ & \sigma_{k+1} & & \\ & & \ddots & \\ & & & \sigma_n \end{bmatrix} V^T \right\|_2 = \sigma_{k+1}.$$

It remains to show that there is no closer rank k matrix to A. Let B be any rank k matrix, so its null space has dimension $n - k$. The space spanned by $\{\upsilon_1, ..., \upsilon_{k+1}\}$ has dimension $k + 1$. Since the sum of their dimensions is $(n - k) + (k + 1) > n$, these two spaces must overlap. Let h be a unit vector in their intersection. Then

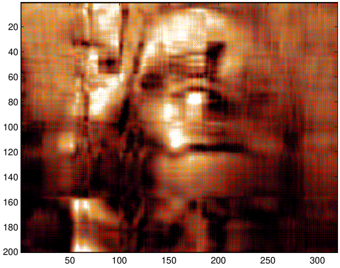
$$\begin{aligned}\|A - B\|_2^2 &\geq \left\|(A - B)h\right\|_2^2 = \|Ah\|_2^2 = \left\|U\Sigma V^T h\right\|_2^2 \\ &= \left\|\Sigma(V^T h)\right\|_2^2 \geq \sigma_{k+1}^2 \left\|V^T h\right\|_2^2 = \sigma_{k+1}^2.\end{aligned}$$

□

Example of application of linear systems: image compression using SVD



a) Original image



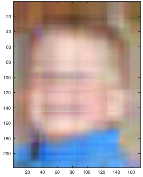
b) Rank k=20 approximation

Example of application of linear systems: image compression using SVD in Matlab

See path for other pictures:
/matlab-2012b/toolbox/matlab/demos
load clown.mat;
Size(X) = $m \times n = 320 \times 200$ pixels.
[U,S,V] = svd(X);
colormap(map);
k=20;
image(U(:,1:k)*S(1:k,1:k)*V(:,1:k)');
Now: size(U)= $m \times k$, size(V)= $n \times k$.

Image compression using SVD in Matlab

a) Original image



b) Rank k=4 approximation

b) Rank k=5 approximation

c) Rank k=6 approximation

d) Rank k=10 approximation

d) Rank k=15 approximation

Example of application of linear systems: image compression using SVD for arbitrary image

To get image on the previous slide, I took picture in jpg-format and loaded it in Matlab. You can also try to use following matlab code for your own pictures:

```
A = imread('Child.jpg'); // Real size of A: size(A) ans= 218 171 3
DDA=im2double(A); //convert from 'uint8' fromat to double format
figure(1); image(DDA);
//size of DDA will be (1:m,1:n,1:3)
[U1,S1,V1] = svd(DDA(:,:,1)); // we perform SVD for every 3 entries of DDA
[U2,S2,V2] = svd(DDA(:,:,2));
[U3,S3,V3] = svd(DDA(:,:,3));
k=15; //number of approximations: this number you can change
svd1 = U1(:,1:k)*S1(1:k,1:k)*V1(:,1:k)'; //compute new approximated matrices svd1, svd2, svd3
svd2 = U2(:,1:k)*S2(1:k,1:k)*V2(:,1:k)';
svd3 = U3(:,1:k)*S3(1:k,1:k)*V3(:,1:k)';
DDAnew = zeros(size(DDA));
DDAnew(:,:,1) = svd1; DDAnew(:,:,2) = svd2; DDAnew(:,:,3) = svd3;

figure(2); image(DDAnew);
```

Matrix norm. Induced norm

If vector norms on K_m and K_n are given (K is field of real or complex numbers), then one defines the corresponding induced norm or operator norm on the space of m-by-n matrices as the following maxima:

$$\begin{aligned} ||A|| &= \max\{||Ax|| : x \in K^n \text{ with } ||x|| = 1\} \\ &= \max\left\{\frac{||Ax||}{||x||} : x \in K^n \text{ with } x \neq 0\right\}. \end{aligned}$$

If $m = n$ and one uses the same norm on the domain and the range, then the induced operator norm is a sub-multiplicative matrix norm.

Condition number of the square matrix

Condition number of the square matrix in any induced norm

$$k(A) = cond(A) = \|A\| \cdot \|A^{-1}\|$$

Example

$$A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}; \; A^T = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}; \; A^T A - \lambda I = \begin{bmatrix} 1-\lambda & 0 \\ 0 & 1-\lambda \end{bmatrix} = 0;$$

$\lambda_1 = 1, \; \lambda_2 = 1; \; \|A\|_2 = \max \sqrt{\lambda(A^T A)} = \max(1,1) = 1.$

In this example,

$$A^{-1} = A; \|A^{-1}\|_2 = 1; k(A) = cond(A) = \|A\| \cdot \|A^{-1}\| = 1.$$

Perturbation Theory for the Least Squares Problem

When A is not square, we define its condition number with respect to the 2-norm to be

$$k_2(A) \equiv \sigma_{max}(A)/\sigma_{min}(A)$$

This reduces to the usual condition number when A is square. The next theorem justifies this definition.

THEOREM *Suppose that A is m-by-n with $m \geq n$ and has full rank. Suppose that x minimizes $\|Ax - b\|_2$. Let $r = Ax - b$ be the residual. Let $\tilde{x}$ minimize $\|(A + \delta A)\tilde{x} - (b + \delta b)\|_2$. Assume $\epsilon \equiv \max(\frac{\|\delta A\|_2}{\|b\|_2}, \frac{\|\delta b\|_2}{\|b\|_2}) < \frac{1}{k_2(A)} = \frac{\sigma_{min}(A)}{\sigma_{max}(A)}$. Then*

$$\frac{\|\tilde{x} - x\|}{\|x\|} \leq \epsilon \cdot \left\{ \frac{2 \cdot k_2(A)}{\cos\theta} + \tan\theta \cdot k_2^2(A) \right\} + O(\epsilon^2) \equiv \epsilon \cdot k_{LS} + O(\epsilon^2),$$

where $\sin\theta = \frac{\|r\|_2}{\|b\|_2}$. In other words, θ is the angle between the vectors b and Ax and measures whether the residual norm $\|r\|_2$ is large (near $\|b\|$) or small (near 0). k_{LS} is the condition number for the least squares problem.

Sketch of Proof. Expand $\tilde{x} = ((A + \delta A)^T (A + \delta A))^{-1} (A + \delta A)^T (b + \delta b)$ in powers of δA and δb. Then remove all non-linear terms, leave the linear terms for δA and δb. □

Rank-deficient Least Squares Problems

Proposition

Let A be m by n with $m \geq n$ and rank $A = r < n$. Then there is an $n - r$ dimensional set of vectors that minimize $||Ax - b||_2$.

Proof

Let $Az = 0$. Then of x minimizes $||Ax - b||_2$ then $x + z$ also minimizes $||A(x + z) - b||_2$.

This means that the least-squares solution is not unique.

Moore-Penrose pseudoinverse for a full rank A

Definition

Suppose that A is m by n with $m > n$ and has full rank with $A = QR = U\Sigma V^T$ being a QR and SVD decompositions of A, respectively. Then

$$A^+ \equiv (A^T A)^{-1} A^T = R^{-1} Q^T = V\Sigma^{-1} U^T$$

is called the Moore-Penrose pseudoinverse of A. If $m < n$ then $A^+ \equiv A^T (AA^T)^{-1}$.

The pseudoinverse of A allows write solution of the full-rank overdetermined least squares problem as $x = A^+ b$. If A is square and a full rank then this formula reduces to $x = A^{-1} b$. The A^+ is computed as *pinv(A)* in Matlab.

$$A^+ \equiv (A^T A)^{-1} A^T = ((QR)^T QR)^{-1} (QR)^T = (R^T Q^T QR)^{-1} (QR)^T$$
$$= (R^T R)^{-1} R^T Q^T = R^{-1} Q^T;$$

$$A^+ \equiv (A^T A)^{-1} A^T = ((U \Sigma V^T)^T U \Sigma V^T)^{-1} \cdot (U \Sigma V^T)^T$$
$$= (V \Sigma U^T U \Sigma V^T)^{-1} V \Sigma U^T = (V \Sigma^2 V^T)^{-1} V \Sigma U^T = V \Sigma^{-1} U^T$$

Moore-Penrose pseudoinverse for rank-deficient A

Definition

Suppose that A is m by n with $m > n$ and is rank-deficient with rank $r < n$. Let $A = U\Sigma V^T = U_1\Sigma_1 V_1^T$ being a SVD decompositions of A such that

$$\mathrm{A} = [\mathrm{U}_1, U_2]\left[\begin{array}{c|c} \Sigma_1 & 0 \\ \hline 0 & 0 \end{array}\right][V_1, V_2]^T = U_1\Sigma_1 V_1^T$$

Here, $size(\Sigma_1) = r \times r$ and is nonsingular, U_1 and V_1 have r columns. Then

$$A^+ \equiv V_1\Sigma_1^{-1}U_1^T$$

is called the Moore-Penrose pseudoinverse for rank-deficient A. The solution of the least-squares problem is always $x = A^+b$, when A is rank-deficient then x has minimum norm.

The next proposition states that if A is nearly rank deficient then the solution x of $Ax = b$ will be ill-conditioned and very large.

Proposition

Let $\sigma_{min} > 0$ is the smallest singular value of the nearly rank deficient A. Then

- 1. If x minimizes $\|Ax - b\|_2$, then $\|x\|_2 \geq \frac{|u_n^T b|}{\sigma_{min}}$ where u_n is the last column of U in SVD decomposition of $A = U \Sigma V^T$.
- 2. Changing b to $b + \delta b$ can change x to $x + \delta x$ where $\|\delta x\|_2$ can be estimated as $\frac{\|\delta b\|_2}{\sigma_{min}}$, or the solution is very ill-conditioned.

Proof

1: We have that for the case of full-rank matrix A the solution of $Ax = b$ is given by $x = (U \Sigma V^T)^{-1} b = V \Sigma^{-1} U^T b$. The matrix $A^+ = V \Sigma^{-1} U^T$ is Moore-Penrose pseodoinverse of A. Thus, we can write also this solution as $x = V \Sigma^{-1} U^T b = A^+ b$.

Then taking norms from both sides of above expression we have:

$$\|x\|_2 = \|\Sigma^{-1} U^T b\|_2 \geq |(\Sigma^{-1} U^T b)_n| = \frac{|u_n^T b|}{\sigma_{min}}, \tag{1}$$

where $|(\Sigma^{-1} U^T b)_n|$ is the n-th column of this product.
2. We apply now (1) for $\|x + \delta x\|$ instead of $\|x\|$ to get:

$$\begin{aligned} \|x + \delta x\|_2 = \|\Sigma^{-1} U^T (b + \delta b)\|_2 &\geq |(\Sigma^{-1} U^T (b + \delta b))_n| \\ = \frac{|u_n^T (b + \delta b)|}{\sigma_{min}} &= \frac{|u_n^T b + u_n^T \delta b|}{\sigma_{min}}. \end{aligned} \tag{2}$$

We observe that $\frac{|u_n^T b|}{\sigma_{min}} + \frac{|u_n^T \delta b|}{\sigma_{min}} \leq \|x + \delta x\|_2 \leq \|x\|_2 + \|\delta x\|_2$.
Choosing δb parallel to u_n and applying again (1) for estimation of $\|x\|_2$ we have

$$\|\delta x\|_2 \geq \frac{\|\delta b\|_2}{\sigma_{min}}. \tag{3}$$

In the next proposition we prove that the minimum norm solution x is unique and may be well-conditioned if the smallest nonzero singular value is not too small.

Proposition

When A is exactly singular, then x that minimize $\|Ax - b\|_2$ can be characterized as follows. Let $A = U\Sigma V^T$ have rank $r < n$. Write svd of A as

$$A = [U_1, U_2] \left[\begin{array}{c|c} \Sigma_1 & 0 \\ \hline 0 & 0 \end{array} \right] [V_1, V_2]^T = U_1 \Sigma_1 V_1^T$$

Here, $size(\Sigma_1) = r \times r$ and is nonsingular, U_1 and V_1 have r columns. Let $\sigma = \sigma_{min}(\Sigma_1).Then$

- 1. All solutions x can be written as $x = V_1 \Sigma_1^{-1} U_1^T + V_2 z$
- 2. The solution x has minimal norm $\|x\|_2$ when $z = 0$. Then $x = V_1 \Sigma_1^{-1} U_1^T$ and $\|x\|_2 \leq \frac{\|b\|_2}{\sigma}$.
- 3. Changing b to $b + \delta b$ can change x as $\frac{\|\delta b\|_2}{\sigma}$.

Proof

We choose the matrix $\tilde{U}$ such that $[U, \tilde{U}] = [U_1, U_2, \tilde{U}]$ be an $m \times m$ orthogonal matrix. Then

$$\begin{aligned}
\|Ax - b\|_2^2 &= \|[U_1, U_2, \tilde{U}]^T (Ax - b)\|_2^2 \\
&= \left\| \begin{bmatrix} U_1^T \\ U_2^T \\ \tilde{U}^T \end{bmatrix} (U_1 \Sigma_1 V_1^T x - b) \right\|_2^2 \\
&= \|[I^{r\times r}, O^{m\times(n-r)}, 0^{m\times m-n}]^T (\Sigma_1 V_1^T x - [U_1, U_2, \tilde{U}]^T \cdot b)\|_2^2 \\
&= \|[\Sigma_1 V_1^T x - U_1^T b; -U_2^T b; -\tilde{U}^T b]^T\|_2^2 \\
&= \|\Sigma_1 V_1^T x - U_1^T b\|_2^2 + \|U_2^T b\|_2^2 + \|\tilde{U}^T b\|_2^2
\end{aligned}$$

1. Then $\|Ax - b\|_2$ is minimized when $\Sigma_1 V_1^T x - U_1^T b = 0$. We can also write that the vector $x = (\Sigma_1 V_1^T)^{-1} U_1^T b + V_2 z$ or $x = V_1 \Sigma_1^{-1} U_1^T b + V_2 z$ is also solution of this minimization problem, because $V_1^T V_2 z = 0$ since columns of V_1 and V_2 are orthogonal.

2. Since columns of V_1 and V_2 are orthogonal, then by Pythagorean theorem we have that $\|x\|_2^2 = \|V_1 \Sigma_1^{-1} U_1^T b\|^2 + \|V_2 z\|^2$ which is minimized for $z = 0$.
3. Changing b to δb in the expression above we have:

$$\|V_1 \Sigma_1^{-1} U_1^T \delta b\|_2 \leq \|V_1 \Sigma_1^{-1} U_1^T\|_2 \cdot \|\delta b\|_2 = \|\Sigma_1^{-1}\|_2 \cdot \|\delta b\|_2 = \frac{\|\delta b\|_2}{\sigma}, \qquad (4)$$

where σ is smallest nonzero singular value of A. In this proof we used properties of the norm: $\|QAZ\|_2 = \|A\|_2$ if Q, Z are orthogonal.

How to solve rank-deficient least squares problems using QR decomposition with pivoting

QR decomposition with pivoting is cheaper but can be less accurate than SVD technique for solution of rank-deficient least squares problems.
If A has a rank $r < n$ with independent r columns QR decomposition can look like that

$$A = QR = Q \cdot \begin{bmatrix} R_{11} & R_{12} \\ 0 & 0 \\ 0 & 0 \end{bmatrix}.$$

(5)

with nonzingular R_{11} is of the size $r \times r$ and R_{12} is of the size $r \times (n - r)$.
We can try to get

$$R = \begin{bmatrix} R_{11} & R_{12} \\ 0 & R_{22} \\ 0 & 0 \end{bmatrix}, \quad (6)$$

where elements of R_{22} are very small and are of the order $\varepsilon \|A\|_2$.

If we set $R_{22} = 0$ and choose $[Q, \tilde{Q}]$ which is square and orthogonal then we will minimize

$$
\begin{aligned}
\|Ax - b\|_2^2 &= \left\| \begin{bmatrix} Q^T \\ \tilde{Q}^T \end{bmatrix} (Ax - b) \right\|_2^2 \\
&= \left\| \begin{bmatrix} Q^T \\ \tilde{Q}^T \end{bmatrix} (QRx - b) \right\|_2^2 \\
&= \left\| \begin{bmatrix} \text{Rx - } Q^T b \\ \text{- } \tilde{Q}^T \text{ b} \end{bmatrix} \right\|_2^2 \\
&= \|Rx - Q^T b\|_2^2 + \|\tilde{Q}^T b\|_2^2 .
\end{aligned}
\tag{7}
$$

Here we again used properties of the norm: $\|QAZ\|_2 = \|A\|_2$ if Q, Z are orthogonal.

Let us now decompose $Q = [Q_1, Q_2]$ with $x = [x_1, x_2]^T$ and

$$R = \begin{bmatrix} R_{11} & R_{12} \\ 0 & 0 \end{bmatrix} \tag{8}$$

such that equation (7) becomes

$$\begin{aligned} \|Ax - b\|_2^2 &= \left\| \begin{bmatrix} R_{11} & R_{12} \\ 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} - \begin{bmatrix} Q_1^T b \\ Q_2^T b \end{bmatrix} \right\|_2^2 + \|\tilde{Q}^T b\|_2^2 \\ &= \|R_{11} x_1 + R_{12} x_2 - Q_1^T b\|_2^2 + \|Q_2^T b\|_2^2 + \|\tilde{Q}^T b\|_2^2. \end{aligned} \tag{9}$$

We take now derivative with respect to x to get $(\|Ax - b\|_2^2)'_x = 0$. We see that minimum is achieved when

$$x = \begin{bmatrix} R_{11}^{-1}(Q_1^T b - R_{12} x_2) \\ x_2 \end{bmatrix} \tag{10}$$

for any vector x_2. If R_{11} is well-conditioned and $R_{11}^{-1} R_{12}$ is small than the choice $x_2 = 0$ will be good one.

The described method is not reliable for all rank-deficient least squares problems. This is because R can be nearly rank deficient for the case when no R_{22} is small. In this case can help QR decomposition with column pivoting: we factorize $AP = QR$ with permutation matrix P. To compute this permutation we do as follows:
1. In all columns from 1 to n at step i we select from the unfinished decomposition of part A in columns i to n and rows i to m the column with largest norm and exchange it with i-th column.
2. Then compute usual Householder transformation to zero out column i in entries $i+1$ to m.
Recent research is devoted to more advanced algorithms called rank-revealing QR algorithms which detects rank more faster and more efficient.

C. Bischof, Incremental condition estimation, *SIAM J.Matrix Anal.Appl.*, 11:312-322, 1990.
T.Chan, Rank revealing QR factorizations, *Linear Algebra Applications*, 88/89:67-82, 1987.