# DN2222
# Applied Numerical Methods
# - part 2:
# Numerical Linear Algebra

## Lecture 4
## Least Squares Problem
## &
## Singular Value Decomposition

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### Linear systems: $Ax = b$

- If $A$ is $n \times n$ and non-singular then $x = A^{-1}b$ uniquely.
- If $A$ is $m \times n$ and $m < n$ the problem is *underdetermined* (and thus usually have infinitely many solutions).
- If $A$ is $m \times n$ and $m > n$ the problem is *overdetermined* and then normally have no solution. This is the topic for today.
- We will try to find the "best approximate solution" to the overdetermined system.

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### Example 3.1 Ruhe p21

Given $m$ pairs of data points $(t_1, y_1), \dots (t_m, y_m)$ from a sample of radioactive decay. The intensity is modeled by

$$y = \sum_{j=1}^{n} \alpha_j \mathrm{e}^{-\lambda_j t}, \qquad \alpha_j, \lambda_j \geq 0$$

The residual is then

$$r = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_m \end{pmatrix} - \begin{pmatrix} \mathrm{e}^{-\lambda_1 t_1} & \cdots & \mathrm{e}^{-\lambda_n t_1} \\ \mathrm{e}^{-\lambda_1 t_2} & \cdots & \mathrm{e}^{-\lambda_n t_2} \\ \vdots & \vdots & \vdots \\ \mathrm{e}^{-\lambda_1 t_m} & \cdots & \mathrm{e}^{-\lambda_n t_m} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \alpha_n \end{pmatrix} = y - A(\lambda, t)x(\alpha)$$

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- $r = y - A(\lambda, t)x(\alpha)$
- The *residual*, $r$, is the difference between the *observation* vector $y$ and the product of the *design* or *system* matrix $A$ and the *parameter* vector $x$.
- The task at hand is to compute parameters $\alpha$ and $\lambda$ such that the residual is minimized in an appropriate norm.
- If the $\lambda$ are known and only the $\alpha$ need to be determined the system is linear, otherwise non-linear.

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### Choice of norm

- If the errors are independent we choose the Euclidian norm $||r||_2 = (r^T r)^{1/2} = (\sum_{i=1}^{m} r_i^2)^{1/2}$. It is the most common and we talk about the *least squares method.*

- If we want to minimze the maximal residual we use the infimum norm $||r||_\infty = \max_i |r_i|$. This is typical for polynomial interpolation.
- Another choice is the 1-norm $||r||_1 = \sum_i |r_i|$. This is typically used when avoidance of outliers is important.

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### Quiz

- Given the three data points $x = (1, 2, 3)$ and $y = (2, 3, 5)$. Determine the optimal line if the norm is chosen as

○ $||r||_2$

○ $||r||_\infty$

○ $||r||_1$

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### Surveyers work

- The least squares method was invented by Gauss trying to improve accuracy in the German surveyers and astronomers measurement.
- In 1974-78 the US National Geodetic Survey updated its database in the same manner - solving the biggest least squares problem ever: about 6 million equations and 400000 unknowns.

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### Solutions

- **Normal equations**. Fast but not very accurate. Adequate when the condition number is small.
- **QR decomposition**. Twice the amount of work but more accuarate. The standard method.
- **SVD**. Even more work but works even if $A$ is not full rank.

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### Normal equations

- To derive the normal equations we need to minimize $||r||_2^2 = r^T r = (b - Ax)^T (b - Ax)$
- Leads to $A^T Ax = A^T b$ or $x = (A^T A)^{-1} A^T b$
- Proof: Let $x' = x + e$ then

$$||Ax' - b||_2^2 = (Ax' - b)^T (Ax' - b) = (Ae + Ax - b)^T (Ae + Ax - b)$$

$$= (Ae)^T (Ae) + (Ax - b)^T (Ax - b) + 2(Ae)^T (Ax - b)$$

$$= ||Ae||_2^2 + ||Ax - b||_2^2 + 2e^T (A^T Ax - A^T b) = ||Ae||_2^2 + ||Ax - b||_2^2$$

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- This is equivalent to the Pythagorean theorem. The solution is optimized when the residual is orthogonal to the space spanned by the columns of $A$.

- Since $A^TA$ is symmetric and positive definite we can use Cholesky factorization. The cost for Cholesky is $\frac{1}{3}n^3$ and the cost for obtaining $A^TA$ from $A$ is $n^2m$.
- Since $m > n$ forming $A^TA$ dominates the cost!

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## QR Decomposition

- **Thm 3.1** (Dp107) Let $A$ be $m \times n$ with $m > n$ and rank($A$)=$n$. Then there exists a unique $m \times n$ orthogonal matrix $Q$ ($Q^TQ = I_n$) and a unique $n \times n$ upper triangular matrix $R$ with positive diagonal elements $r_{ii} > 0$ such that $A = QR$.
- First proof uses Gram-Schmidt orthogonalization process. If apply GS to the columns of $A = [a_1, a_2, \dots a_n$ one gets a sequence of orthonormal vectors $q_i$ obtained from a linear combination of $a_1$ to $a_i$.
- Unfortunately GS is numerically unstable in floating point arithmetic when the columns of $A$ are nearly dependent.
- Modified Gram-Schmidt (MGS) is more stable but could still end up with a $Q$ which is far from orthogonal.

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

- The cost for QR-decomposition is about $2n^2m - \frac{2}{3}n^3$, about twice the cost of normal equations if $m >> n$ and about the same if $m = n$.

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## Singular Value Decomposition

- SVD is used for many things, not only least squares.
- Thm 3.2 (Dp109) Let $A$ be an arbitrary $m \times n$ matrix with $m \geq n$. Then we can write $A = U\Sigma V^T$, where $U$ is an $m \times n$ such that $U^TU = I$, $V$ is an $n \times n$ such that $V^TV = I$, and $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_n)$, where $\sigma_1 \geq \sigma_2 \cdots \geq \sigma_n \geq 0$. The columns $u_1, \dots, u_n$ of $U$ are called left singular vectors. The columns $v_1, \dots, v_n$ of $V$ are called left singular vectors. The $\sigma_i$ are called singular values.
- Proof of Thm 3.2: We assume that SVD exists for an $(m-1) \times (n-1)$ matrix and then prove it for an $n \times m$. SVD has a large number of properties:
- If $A$ is symmetric, then $\sigma_i = |\lambda_i|$ and $v_i = sign(\lambda_i)u_i$.
- The eigenvalues of $A^TA$ are $\sigma_i^2$. The right singular vectors are the corresponding orthogonal eigenvectors.
- The eigenvalues of $AA^T$ are $\sigma_i^2$ and $m - n$ zeroes. The left singular vectors are the corresponding orthogonal eigenvectors.

- If $A$ has full rank, the least squares solution of $Ax = b$ is $x = V\Sigma^{-1}U^T b$.
- $||A||_2 = |\sigma_1|$.
- If $A$ is square and non-singular then $||A^{-1}||_2^{-1} = \sigma_n$ and $||A||_2||A^{-1}||_2 = \frac{\sigma_1}{\sigma_n}$.
- Suppose that $A$ is $m \times n$ and has rank $n$ with $m > n$, then $A^+ = (A^T A)^{-1}A^T = R^{-1}Q^T = V\Sigma^{-1}U^T$ is called the (Morse-Penrose) pseudo-inverse of $A$.
- If $m < n$ then $A^+ = A^T(AA^T)^{-1}$.

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**Rank Deficient least Squares Problems**

- What happens if $A$ is rank deficient (or nearly)?
- This occurs often, like signals in noisy data (Lab3), digital image restoration or compression, etc.
- Rank deficient problems are very ill-conditioned.
- Making an ill-conditioned problem well-conditioned by imposing extra conditions on the solution is called *regularization*.
- If $A$ is rank deficient the least squares solution is not unique.
- Prop 3.1 (Dp125) Let $A$ be an $m \times n$ matrix with rank($A$)=$r < n$. Then there is an $n - r$ dimensional set of vectors that all minimizes $||(||Ax - b)$.
- Proof: Let $z$ be such that $Az = 0$ then if $x$ minimizes $||Ax - b||$ then so does $x + z$.
- If, due to round-off, some $\sigma_i$ has a small value rather than zero, Then the unique solution is likely to be very large.
- Thus: If $A$ is nearly rank deficient ($\sigma_{min}$ is small) the solution $x$ is ill-conditioned and possibly very large.

Prop 3.3 (Dp126) When $A$ is exactly singular, the $x$ tht minimizes $||Ax - b||_2$ can be characterized as follows: Let $A = U\Sigma V^T$ have rank $r < n$. Then write

$$A = [U1, U2] \begin{bmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{bmatrix} [V1, V2]^T = U_1\Sigma_1 V_1^T$$

where $\Sigma_1$ is $r \times r$ and non-singular and $U_1$ and $V_1$ have $r$ columns. Let $\sigma = \sigma_{min}(\Sigma_1)$. Then:

- all solutions $x$ can be written as $x = V_1\Sigma_1^{-1}U_1^T b + V_2 z$, $z$ being any vector.

Proof: Choose $\tilde{U}$ such that $W = [U_1, U_2, \tilde{U}]$ is an orthogonal matrix.

$$||Ax - b||_2^2 = ||W^T(Ax - b)||_2^2 = || \begin{bmatrix} U_1^T \\ U_2^T \\ \tilde{U}^T \end{bmatrix} (U_1\Sigma_1 V_1^T x - b)||_2^2$$

$$= ||\Sigma_1 V_1^T x - U_1^T b||_2^2 + ||U_2^T b||_2^2 + ||\tilde{U}^T b||_2^2$$

Thus, $x$ is multiplied with $V_1$, anything with $V_2$ will add zero.

- the solution $x$ has minimal norm $||x||_2$ precisely when $z = 0$, in which case $x = V_1\Sigma_1^{-1}U_1^T b$ and $||x||_2 \leq ||b||_2/\sigma$.

  Proof: Since $V_1$ and $V_2$ are mutually orthogonal by Pythagoras

$$||x||_2^2 = ||V_1\Sigma_1^{-1}U_1^T b||_2^2 + ||V_2 z||_2^2$$

which is minimized when $z = 0$.

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- Changing $b$ into $b + \delta b$ can change the minimal norm solution $x$ by at most $||\delta b||_2/\sigma$

  Proof:

$$||V_1\Sigma_1^{-1}U_1^T \delta b||_2 \leq ||\Sigma_1^{-1}||_2||\delta b||_2 = ||\delta b||_2/\sigma$$

- The norm and condition number of the unique minimal norm solution $x$ depends on the smalleest non-zero singular value of $A$.
- This is the key to a practical algorithm!

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**Pseudoinverse for Rank Deficient matrix**

- Let $A = U\Sigma V^T = U_1\Sigma_1 V_1^T$ Then $A^+ = V_1\Sigma_1^{-1}U_1^T$ or $A^+ = V^T\Sigma^+ U$ where $\Sigma^+ = \begin{bmatrix} \Sigma_1 & 0 \\ 0 & 0 \end{bmatrix}^+ = \begin{bmatrix} \Sigma_1^{-1} & 0 \\ 0 & 0 \end{bmatrix}$
- So the least squares solution is always $x = A^+ b$. When $A$ is rank deficient, $x$ has minimum norm.
- So we need to know the rank of $A$ and the smallest singular value.

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**Example: Demmel p128**

$A = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$ has smallest nonzero eigenvalue 1. With $b = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ we get least square solution $x = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ with condition number $1/\sigma = 1$.

But if we have $A = \begin{pmatrix} 1 & 0 \\ 0 & \varepsilon \end{pmatrix}$ we have smallest nonzero eigenvalue $\varepsilon$ and $x = \begin{pmatrix} 1 \\ 1/\varepsilon \end{pmatrix}$ and condition number $1/\varepsilon$.

- The practical solution is to treat all $\sigma_i$ smaller than a tolerance (normally $O(\varepsilon) \cdot ||A||_2$) as zero.
- This is called *truncated SVD*
- A similar idea can be used in QR-decomposition, but it is less reliable.

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**Some review questions:**

- **Q45.** What is the range $R(A)$ of a matrix $A$? How do you find a basis for it by means of SVD?
- **Q50.** What is meant by a rank deficient matrix?
- **Q51.** How can we determine $A^{(k)}$, the matrix of rank $k$ closest to a given matrix $A$ using SVD?
- **Q53.** What are the advantages and disadvantages of replacing the matrix $A$ by a lower rank approximation $A^{(k)}$ when solving a least squares problem?