Numerical Methods

Course # PHY 203

Chapter #: 6: Least-Square Approximation

Lecture # 9.2: Polynomial Data Fitting

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- Discrete Least Squares: This is a method to solve an over-determined linear system.
- Recall that an over determined linear system is defined by the linear equation

$$Ax = b$$

where A is an $m \times n$ matrix with $m > n$, x is an $n \times 1$ column vector and b is an $m \times 1$ constant column vector.

- Since A is no longer a square matrix, we can not invert and solve the linear system. The basic idea is to make a square matrix out of A, and then solve the system.
- We multiply by A^T, and find:

$$\boxed{(A^T A)x = A^T b}$$

which are known as the `normal equations.

$A^T = n \times m$ & $A = m \times n$

$A^T A = (n \times m)(m \times n) = n \times n$

$A^T b = (n \times m)(m \times 1) = (n \times 1)$

- Here now $(A^T A)$ is an $n \times n$ square matrix. If the $\det(A^T A) \neq 0$, then $A^T A$ is invertible, and we can approximately solve the linear system.
- It is an approximate solution because we are solving for n number of unknown variables that satisfies m number of conditions and here $m > n$.

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- Theorem: The matrix $A^T A$ is invertible iff the columns of A are linearly independent, in which case $Ax = b$ has a unique least-squares solutions

$$\boxed{x = (A^T A)^{-1} A^T b.} \Rightarrow \text{solution } \det(A^T A) \neq 0$$

- Example: Polynomial Data fitting.

  An overdetermined system arise if we try to fit a polynomial

$$p_n(x) = a_0 + a_1 x + \cdots + a_n x^n$$

  to a function $f(x)$ at $m + 1$ nodes $x_0, x_1, \cdots, x_m$ with $m > n$. IN the natural basis, we can write:

$$p_n(x_0) = a_0 + a_1 x_0 + \cdots + a_n x_0^n = f(x_0)$$
$$p_n(x_1) = a_0 + a_1 x_1 + \cdots + a_n x_1^n = f(x_1)$$
$$\vdots$$
$$\vdots$$
$$p_n(x_m) = a_0 + a_1 x_m + \cdots + a_n x_m^n = f(x_m)$$

At the nodes

$p_n(x_0) = f(x_0)$

$p_n(x_1) = f(x_1)$

$\vdots$

$\boxed{m > n}$

- In matrix form, we can write,

x = unknown

Vandermonde matrix

A

$$\underbrace{\begin{pmatrix} 1 & x_0 & \cdots & x_0^n \\ 1 & x_1 & \cdots & x_1^n \\ 1 & x_2 & \cdots & x_2^n \\ \vdots & \vdots & & \vdots \\ 1 & x_m & \cdots & x_m^n \end{pmatrix}}_{m\times n} \underbrace{\begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{pmatrix}}_{n\times 1} = \underbrace{\overbrace{\begin{pmatrix} f(x_0) \\ f(x_1) \\ f(x_2) \\ \vdots \\ f(x_m) \end{pmatrix}}^{\vec{b}}}_{m\times 1} \Rightarrow Ax = b$$

- Here A in an $m \times n$ matrix. To solve we multiply from left by A^T such that $(A^T A)$ is now an $n \times n$ square matrix.
- The right-hand side in now a constant matrix of order $n \times 1$.

$$\boxed{A^T b = (n\times m)\,(m\times 1) = n \times 1}$$

- If $A^T A$ is invertible, the above linear system can be solved by Gaussian elimination method, or by QR-decomposition method (see next lecture). LU decom.
- If n is 2 or 3, we can also find the inverse matrix, and solve.

- Let us fit a least-squares $\boxed{\text{straight-line}}$ to the data: $f(-3) = f(0) = 0$, and $f(6) = 2$.
- Solution: Here $n = 1$, because we are fitting a straight line. Therefore,

$$\boxed{p_1(x) = a_0 + a_1 x} \Rightarrow a_0 = ?\ \&\ a_1 = ??$$

- And we have three nodes: $x_0 = -3, x_1 = 0, x_2 = 6$. So, $m = 2$. $(\therefore m > n)$.
- At the nodes we, have the following:

$$p_1(x_0) = a_0 + a_1 x_0 = f(x_0)$$
$$p_1(x_1) = a_0 + a_1 x_1 = f(x_1)$$
$$p_1(x_2) = a_0 + a_1 x_2 = f(x_2)$$

- In matric form, we write after using the values of the nodes and their functions:

$$A(3\times 2) = \underbrace{\begin{pmatrix} 1 & -3 \\ 1 & 0 \\ 1 & 6 \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} a_0 \\ a_1 \end{pmatrix}}_{x\ = 2\times 1} = \underbrace{\begin{pmatrix} 0 \\ 0 \\ 2 \end{pmatrix}}_{b\ (m\times 1)}$$

- Multiplying by A^T from left, we find:

$$\underbrace{\begin{pmatrix} 1 & 1 & 1 \\ -3 & 0 & 6 \end{pmatrix}}_{A^T=(2\times 3)} \overbrace{\begin{pmatrix} 1 & -3 \\ 1 & 0 \\ 1 & 6 \end{pmatrix}}^{A} \overbrace{\begin{pmatrix} a_0 \\ a_1 \end{pmatrix}}^{x} = \overbrace{\begin{pmatrix} 1 & 1 & 1 \\ -3 & 0 & 6 \end{pmatrix}}^{A^T} \overbrace{\begin{pmatrix} 0 \\ 0 \\ 2 \end{pmatrix}}^{b}$$

$$\Downarrow$$

$$\boxed{\begin{pmatrix} 3 & 3 \\ 3 & 45 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \end{pmatrix} = \begin{pmatrix} 2 \\ 12 \end{pmatrix}} \leftarrow A^T b$$

- Here: $A^T A = \begin{pmatrix} 3 & 3 \\ 3 & 45 \end{pmatrix}$ and $\det(A^T T) = 126 \neq 0$. The inverse is

$$\boxed{(A^T A)^{-1} = \frac{1}{126} \begin{pmatrix} 45 & -3 \\ -3 & 3 \end{pmatrix}}$$

- Therefore: $\begin{pmatrix} a_0 \\ a_1 \end{pmatrix} = \frac{1}{126} \begin{pmatrix} 45 & -3 \\ -3 & 3 \end{pmatrix} \begin{pmatrix} 2 \\ 12 \end{pmatrix} = \boxed{\begin{pmatrix} 3/7 \\ 5/21 \end{pmatrix}} \Longrightarrow \boxed{a_0 = \frac{3}{7}, a_1 = \frac{5}{21}}.$

- Hence, the solution is: $\boxed{p_1(x) = \frac{3}{7} + \frac{5}{21} x.}$