ESO 208A: Computational Methods in Engineering

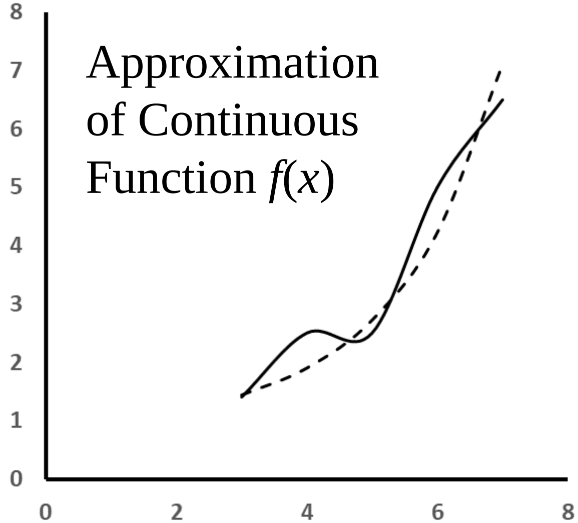
Theory of Approximation

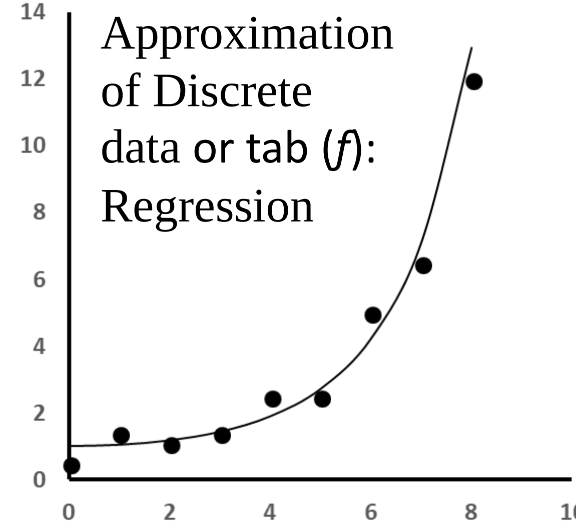
Saumyen Guha

Department of Civil Engineering
IIT Kanpur

Approximation of Functions

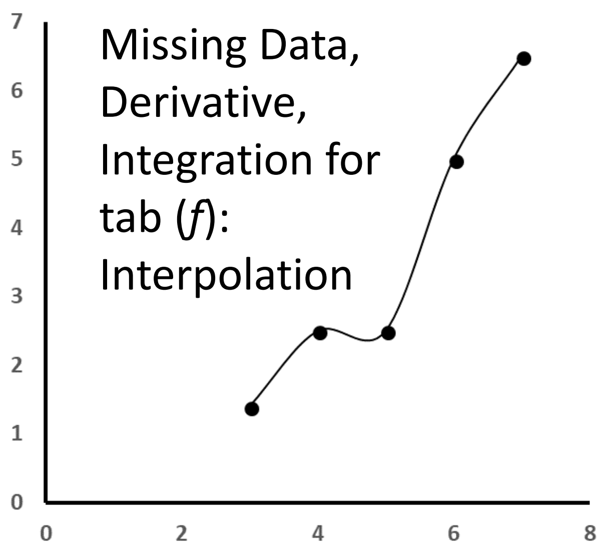
- ✓ Forms the basis for all numerical methods of interest in engineering and science – cannot emphasize enough!
  - ✓ Function approximation: monotone, periodic, pwc, etc.
  - ✓ Discrete and Fast Fourier Transform
  - ✓ Regression
  - ✓ Interpolation
  - ✓ Numerical Differentiation
  - ✓ Numerical Integration
  - ✓ Solution of ODE and PDE: both finite difference and finite element

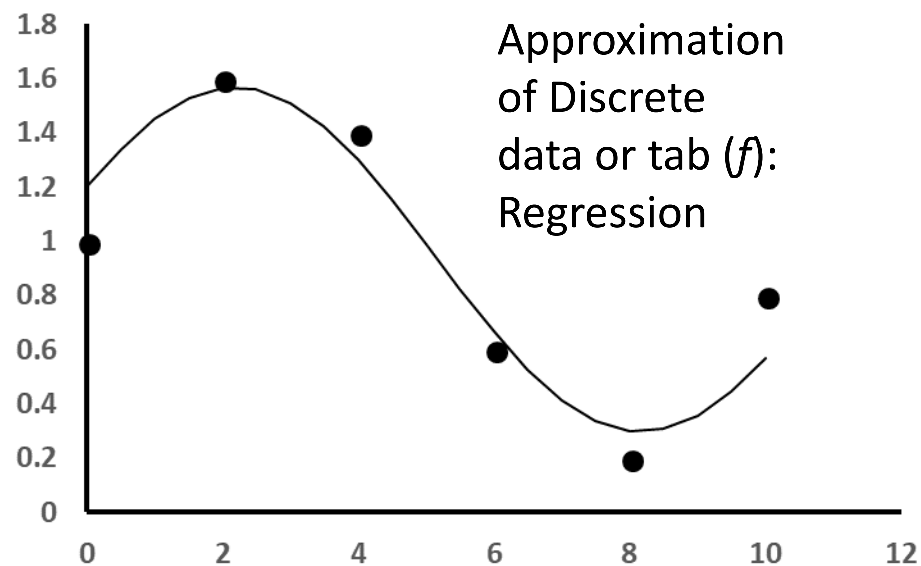




Complicated Analytical Function, Analog Signal from a measuring device

Discrete measurements of continuous experiments or phenomena





Approximation of Functions

We shall divide the approximation problems into five parts:

- ✓ Least square approximation of continuous function using various basis polynomials
- ✓ Least square approximation of discrete functions or Regression
- ✓ Orthogonal basis functions
- ✓ Approximation of periodic functions
- ✓ Interpolation

Approximation of Functions

Why polynomial basis ?

Weierstrass Approximation Theorem:

For every continuous and real valued function $f(x)$ in $[a, b]$ and $\varepsilon > 0$, there exists a polynomial $p(x)$ such that,

$$\|f(x) - p(x)\| < \varepsilon$$

When not to use polynomial basis?

- ✓ If the functional form or the model is known
- ✓ Sharp front
- ✓ Periodic function

Function Space vs. Vector Space

Polynomial $p(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$

- Completely defined by the vector $\{a_0, a_1, \ldots a_n\}$: belongs to $(n + 1)$ dimensional vector space
- $(n + 1)$ dimensional function space: space of all polynomials of degree n

Example:

- $n = 1$ is the space of all straight lines (basis functions are 1 and x)
- $n = 2$ is the space of all quadratics (basis functions are 1, x, x^2)

Norm and Seminorm

A real valued function is called a norm on a vector space if it is defined everywhere on the space and satisfies the following conditions:

- ✓ $\|f\| > 0$ for $f \neq 0$; $\|f\| = 0$ iff $f = 0\ \forall x \in [a,b]$
- ✓ $\|\alpha f\| = |\alpha|\|f\|$ for a real α
- ✓ $\|f + g\| \leq \|f\| + \|g\|$

✓ L_p-Norm: $\|f\|_p = \left(\int_a^b |f(x)|^p\, dx\right)^{1/p}$

- ✓ $p = 2$: Euclidean or L_2 norm, $\|f\|_2 = \left(\int_a^b |f(x)|^2\, dx\right)^{1/2}$
- ✓ $p \to \infty$: $\|f\|_\infty = \max_{x\in[a,b]} |f(x)|$
- ✓ Weighted Euclidean Norm: $\|f\|_{2,w} = \left(\int_a^b |f(x)|^2\, w(x)dx\right)^{1/2}$
- ✓ Euclidean seminorm: $\|\text{tab}\,(f)\|_{2,G} = \left(\sum_{j=0}^{n} \left|f(x_j)\right|^2\right)^{1/2}$

Inner Product

The inner product of two real-valued continuous functions $f(x)$ and $g(x)$ is denoted by $\langle f, g\rangle$ and is defined as:

$$\langle f, g\rangle = \begin{cases} \int_a^b f(x)g(x)w(x)dx & \text{(Continuous Case)} \\ \sum_{i=0}^{n} f(x_i)g(x_i)w_i & \text{(Discrete Case)} \end{cases}$$

- ✓ Properties of Inner Product:
  - ✓ Commutativity: $\langle f, g\rangle = \langle g, f\rangle$
  - ✓ Linearity: $\langle (c_1 f + c_2\, g), \varphi\rangle = c_1\langle f, \varphi\rangle + c_2\langle g, \varphi\rangle$
  - ✓ Positivity: $\langle f, f\rangle \geq 0$
  - ✓ $\langle f, f\rangle = (\|f\|_2)^2$

Basis Functions: Linear Independence

A sequence of $(n + 1)$ functions $\{\varphi_0, \varphi_1, \varphi_2, \cdots \varphi_n\}$ are linearly independent if,

$$\sum_{j=0}^{n} c_j \varphi_j = 0 \implies c_j = 0 \quad \forall j$$

- ✓ This sequence of functions builds (or spans) an $(n + 1)$-dimensional linear subspace
- ✓ From the Definition of Norm:

$$\left\| \sum_{j=0}^{n} c_j \varphi_j \right\| = 0 \quad \text{is true only if } c_j = 0 \quad \forall j$$

- ✓ Linearity of inner product:

$$\left\langle \sum_{j=0}^{n} c_j \varphi_j , \varphi_k \right\rangle = \sum_{j=0}^{n} c_j \langle \varphi_j(x), \varphi_k(x) \rangle$$

Orthogonal Functions

- ✓ Two real-valued continuous functions *f*(*x*) and *g*(*x*) are said to be *orthogonal* if $\langle f, g \rangle = 0$
- ✓ A finite or infinite sequence of functions $\{\varphi_0, \varphi_1, \varphi_2, \cdots \varphi_n, \cdots\}$ make an *orthogonal system* if $\langle \varphi_i, \varphi_j \rangle = 0$ for all $i \neq j$ and $\|\varphi_i\| \neq 0$ for all i.
- ✓ In addition, if $\|\varphi_i\| = 1$, the sequence of functions is called an *orthonormal system*
- ✓ *Pythagorean Theorem* for functions: $\langle f, g \rangle = 0 \Longrightarrow \|f + g\|^2 = \|f\|^2 + \|g\|^2$
  - ✓ $\|f + g\|^2 = \langle (f + g), (f + g) \rangle = \langle f, f \rangle + \langle f, g \rangle + \langle g, f \rangle + \langle g, g \rangle = \|f\|^2 + 0 + 0 + \|g\|^2$
- ✓ Generalized for *orthogonal system*: $\left\|\sum_{j=0}^{n} c_j \varphi_j\right\|^2 = \sum_{j=0}^{n} c_j^2 \left\|\varphi_j\right\|^2$

Least Square Problem

Let $f(x)$ be a continuous real-valued function in (a, b) that is to be approximated by $p(x)$, a linear combination of a system of $(n + 1)$ linearly independent functions $\{\varphi_0, \varphi_1, \varphi_2, \cdots \varphi_n\}$ as shown below:

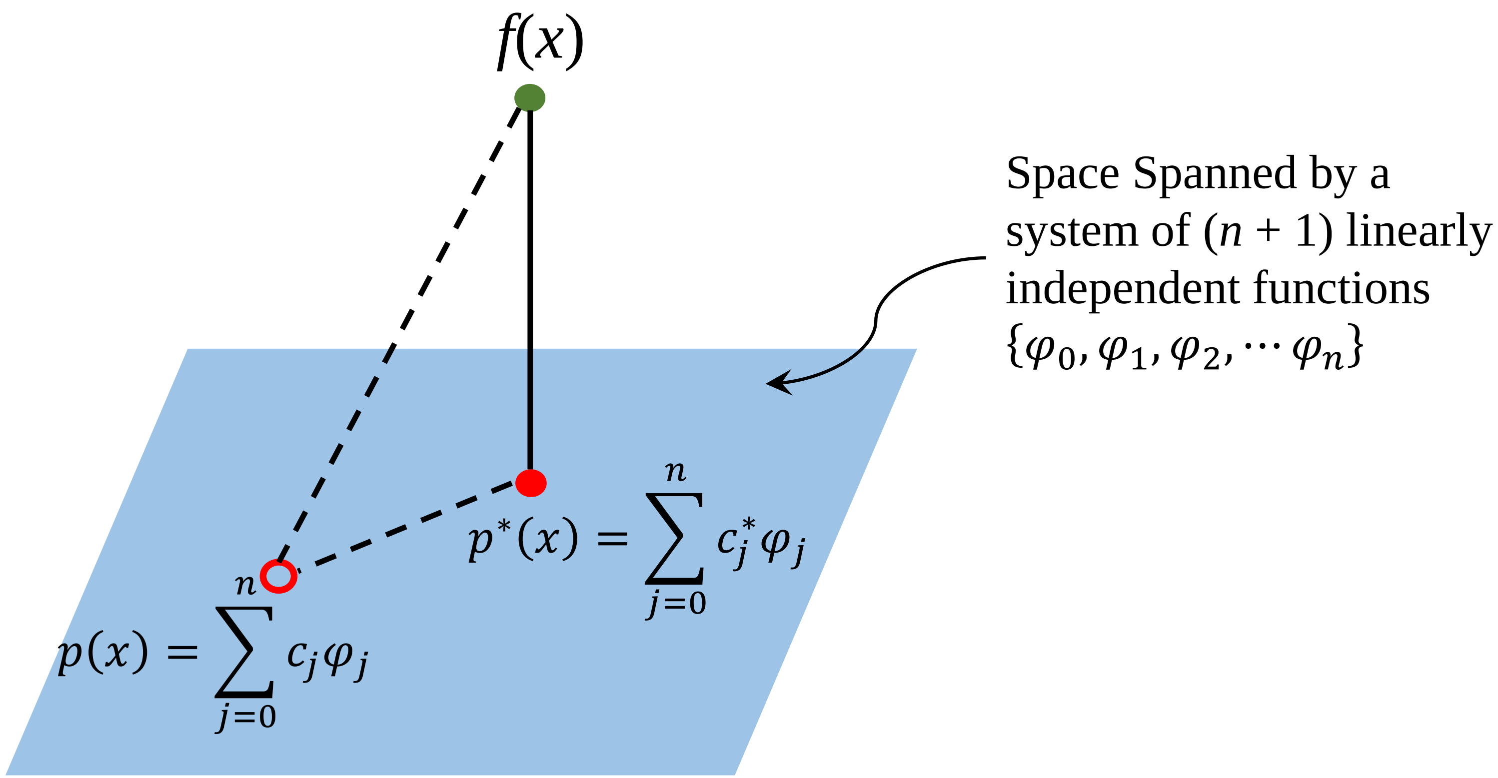
$$p(x) = \sum_{j=0}^{n} c_j \varphi_j(x)$$

Determine the coefficients $c_j = c_j^*$ such that, a weighted *Euclidean norm* or *seminorm* of error $p(x) - f(x)$ becomes as small as possible.

- ✓ $\|p(x) - f(x)\|^2 = \int_a^b |p(x) - f(x)|^2 \, dx$ is minimum when $c_j = c_j^*$
- ✓ $\|p(x) - f(x)\|^2 = \sum_{i=1}^{m} |p(x_i) - f(x_i)|^2$ is minimum when $c_j = c_j^*$

Least Square Solution: $p^*(x) = \sum_{j=0}^{n} c_j^* \varphi_j(x)$

Schematic of Least Square Solution



Solution: $\langle (f(x) - p^*(x)), \varphi_k \rangle = 0$ for $k = 0, 1, 2, \ldots n$

Least Square Solution: Proof

When $\{\varphi_0, \varphi_1, \varphi_2, \cdots \varphi_n\}$ are linearly independent, the least square problem has a unique solution:

$$p^*(x) = \sum_{j=0}^{n} c_j^* \varphi_j(x)$$

where, $p^*(x) - f(x)$ is orthogonal to all φ_j's, $j = 0, 1, 2, \ldots n$.

We need to prove:

- ✓ $\|p^*(x) - f(x)\|^2$ is minimum when $p^*(x) - f(x)$ is orthogonal to all φ_j's, $j = 0, 1, 2, \ldots n$
- ✓ **existence** and **uniqueness** of the least square solution

Least Square Solution: Proof

Let $\{c_0, c_1, c_2, \cdots c_n\}$ be another sequence of coefficients with $c_j \neq c_j^*$ for at least one j, then

$$\sum_{j=0}^{n} c_j \varphi_j(x) - f(x) = \sum_{j=0}^{n} \left(c_j - c_j^*\right) \varphi_j(x) + \left(p^*(x) - f(x)\right)$$

If $p^*(x) - f(x)$ is orthogonal to all φ_j's, it is also orthogonal to their linear combination $\sum_{j=0}^{n} \left(c_j - c_j^*\right) \varphi_j(x)$. According to Pythagorean theorem, we have:

$$\left\| \sum_{j=0}^{n} c_j \varphi_j(x) - f(x) \right\|^2 = \left\| \sum_{j=0}^{n} \left(c_j - c_j^*\right) \varphi_j(x) \right\|^2 + \|p^*(x) - f(x)\|^2$$

$$> \|p^*(x) - f(x)\|^2$$

Therefore, if $p^*(x) - f(x)$ is orthogonal to all φ_j's, then $p^*(x)$ is the solution of the least square problem.

Least Square Solution: Normal Equations

If $\{\varphi_0, \varphi_1, \varphi_2, \cdots \varphi_n\}$ are linearly independent, solution to the least square problem is:

$$\langle (p^*(x) - f(x)), \varphi_k(x) \rangle = 0 \quad k = 0, 1, 2, \cdots n$$

$$\text{where,} \qquad p^*(x) = \sum_{j=0}^{n} c_j^* \varphi_j(x)$$

Therefore,

$$\left\langle \left(\sum_{j=0}^{n} c_j^* \varphi_j(x) - f(x) \right), \varphi_k(x) \right\rangle = 0 \quad k = 0, 1, 2, \cdots n$$

$$\sum_{j=0}^{n} c_j^* \langle \varphi_j(x), \varphi_k(x) \rangle = \langle f(x), \varphi_k(x) \rangle \qquad k = 0, 1, 2, \cdots n$$

Normal Equations!

Least Square Solution: Normal Equations

$$\sum_{j=0}^{n} c_j^* \left\langle \varphi_j(x), \varphi_k(x) \right\rangle = \langle f(x), \varphi_k(x) \rangle; \quad k = 0, 1, 2, \cdots n$$

$$\begin{array}{lr}
c_0^*\langle \varphi_0, \varphi_0 \rangle + c_1^*\langle \varphi_1, \varphi_0 \rangle + c_2^*\langle \varphi_2, \varphi_0 \rangle + \cdots + c_n^*\langle \varphi_n, \varphi_0 \rangle = \langle f, \varphi_0 \rangle & k = 0 \\
c_0^*\langle \varphi_0, \varphi_1 \rangle + c_1^*\langle \varphi_1, \varphi_1 \rangle + c_2^*\langle \varphi_2, \varphi_1 \rangle + \cdots + c_n^*\langle \varphi_n, \varphi_1 \rangle = \langle f, \varphi_1 \rangle & k = 1 \\
c_0^*\langle \varphi_0, \varphi_2 \rangle + c_1^*\langle \varphi_1, \varphi_2 \rangle + c_2^*\langle \varphi_2, \varphi_2 \rangle + \cdots + c_n^*\langle \varphi_n, \varphi_2 \rangle = \langle f, \varphi_2 \rangle & k = 2 \\
\quad \vdots \quad + \quad \vdots \quad + \quad \vdots \quad + \cdots + \quad \vdots \quad = \quad \vdots & \\
c_0^*\langle \varphi_0, \varphi_n \rangle + c_1^*\langle \varphi_1, \varphi_n \rangle + c_2^*\langle \varphi_2, \varphi_n \rangle + \cdots + c_n^*\langle \varphi_n, \varphi_n \rangle = \langle f, \varphi_n \rangle & k = n
\end{array}$$

Moreover, if $\{\varphi_0, \varphi_1, \varphi_2, \cdots \varphi_n\}$ is an orthogonal system:

$$c_k^* = \frac{\langle f, \varphi_k \rangle}{\langle \varphi_k, \varphi_k \rangle} \qquad k = 0, 1, 2, \cdots n$$

Least Square Solution: Existence and Uniqueness

$$\sum_{j=0}^{n} c_j^* \langle \varphi_j(x), \varphi_k(x) \rangle = \langle f(x), \varphi_k(x) \rangle; \quad k = 0, 1, 2, \cdots n$$

$$\begin{array}{lr}
c_0^* \langle \varphi_0, \varphi_0 \rangle + c_1^* \langle \varphi_1, \varphi_0 \rangle + c_2^* \langle \varphi_2, \varphi_0 \rangle + \cdots + c_n^* \langle \varphi_n, \varphi_0 \rangle = \langle f, \varphi_0 \rangle & k = 0 \\
c_0^* \langle \varphi_0, \varphi_1 \rangle + c_1^* \langle \varphi_1, \varphi_1 \rangle + c_2^* \langle \varphi_2, \varphi_1 \rangle + \cdots + c_n^* \langle \varphi_n, \varphi_1 \rangle = \langle f, \varphi_1 \rangle & k = 1 \\
c_0^* \langle \varphi_0, \varphi_2 \rangle + c_1^* \langle \varphi_1, \varphi_2 \rangle + c_2^* \langle \varphi_2, \varphi_2 \rangle + \cdots + c_n^* \langle \varphi_n, \varphi_2 \rangle = \langle f, \varphi_2 \rangle & k = 2 \\
\quad \vdots \quad + \quad \vdots \quad + \quad \vdots \quad + \cdots + \quad \vdots \quad = \quad \vdots & \\
c_0^* \langle \varphi_0, \varphi_n \rangle + c_1^* \langle \varphi_1, \varphi_n \rangle + c_2^* \langle \varphi_2, \varphi_n \rangle + \cdots + c_n^* \langle \varphi_n, \varphi_n \rangle = \langle f, \varphi_n \rangle & k = n
\end{array}$$

Solution to the normal equations exist and is unique **unless the following homogenous system has a nontrivial solution** for $\{c_0^*, c_1^*, \cdots c_n^*\}$, *i.e.*, $c_j^* \neq 0$ for at least one *j*:

$$\sum_{j=0}^{n} c_j^* \langle \varphi_j(x), \varphi_k(x) \rangle = 0$$

Least Square Solution: Existence and Uniqueness

Solution to the normal equations exist and is unique unless the following homogenous system has a nontrivial solution for $\{c_0^*, c_1^*, \cdots c_n^*\}$, *i.e.*, $c_j^* \neq 0$ for at least one *j*:

$$\sum_{j=0}^{n} c_j^* \langle \varphi_j(x), \varphi_k(x) \rangle = 0$$

This would lead to

$$\left\| \sum_{j=0}^{n} c_j^* \varphi_j \right\|^2 = \left\langle \sum_{j=0}^{n} c_j^* \varphi_j, \sum_{k=0}^{n} c_k^* \varphi_k \right\rangle = \sum_{k=0}^{n} \sum_{j=0}^{n} \langle \varphi_j, \varphi_k \rangle c_j^* c_k^* = \sum_{k=0}^{n} 0.\, c_k^* = 0$$

which contradicts that the $\{\varphi_0, \varphi_1, \varphi_2, \cdots \varphi_n\}$ are linearly independent.

Least Square Solution: Example (Continuous)

Approximate the function $f(x) = 1/(1 + x^2)$ for x in [0, 1] using a straight line.

The basis functions are: $\varphi_0(x) = \varphi_0 = 1;\ \ \varphi_1(x) = \varphi_1 = x;\ \ p^*(x) = \sum_{j=0}^{1} c_j^* \varphi_j(x)$

$$c_0^*\langle\varphi_0, \varphi_0\rangle + c_1^*\langle\varphi_1, \varphi_0\rangle = \langle f, \varphi_0\rangle$$
$$c_0^*\langle\varphi_0, \varphi_1\rangle + c_1^*\langle\varphi_1, \varphi_1\rangle = \langle f, \varphi_1\rangle$$

$$\langle\varphi_0, \varphi_0\rangle = \int_0^1 (1)(1)\,dx = 1;\ \langle\varphi_0, \varphi_1\rangle = \langle\varphi_1, \varphi_0\rangle = \int_0^1 (x)(1)\,dx = \frac{1}{2} = 0.5$$

$$\langle\varphi_1, \varphi_1\rangle = \int_0^1 (x)(x)\,dx = \frac{1}{3};\ \langle f, \varphi_0\rangle = \int_0^1 \frac{1}{1+x^2}(1)\,dx = \frac{\pi}{4}$$

$$\langle f, \varphi_1\rangle = \int_0^1 \frac{1}{1+x^2}(x)\,dx = \frac{\ln 2}{2}$$

Least Square Solution: Example (Continuous)

$$c_0^*\langle\varphi_0,\varphi_0\rangle + c_1^*\langle\varphi_1,\varphi_0\rangle = \langle f,\varphi_0\rangle$$
$$c_0^*\langle\varphi_0,\varphi_1\rangle + c_1^*\langle\varphi_1,\varphi_1\rangle = \langle f,\varphi_1\rangle$$

$$\begin{bmatrix} 1 & 0.5 \\ 0.5 & 1/3 \end{bmatrix}\begin{bmatrix} c_0^* \\ c_1^* \end{bmatrix} = \begin{bmatrix} \pi/4 \\ \ln 2/2 \end{bmatrix}$$

$$c_0^* = \frac{\begin{vmatrix} \pi/4 & 0.5 \\ \ln 2/2 & 1/3 \end{vmatrix}}{\begin{vmatrix} 1 & 0.5 \\ 0.5 & 1/3 \end{vmatrix}} = 1.062$$

$$c_1^* = \frac{\begin{vmatrix} 1 & \pi/4 \\ 0.5 & \ln 2/2 \end{vmatrix}}{\begin{vmatrix} 1 & 0.5 \\ 0.5 & 1/3 \end{vmatrix}} = -0.5535$$

$$p^*(x) = \sum_{j=0}^{1} c_j^*\varphi_j(x) = 1.062 - 0.5535x$$

Least Square Solution: Example (Continuous)

Approximate the function $f(x) = 1/(1 + x^2)$ for x in [0, 1] using a 2nd order polynomial.

The basis functions are: $\varphi_0 = 1;\quad \varphi_1 = x;\quad \varphi_2 = x^2;\quad p^*(x) = \sum_{j=0}^{2} c_j^* \varphi_j$

$$c_0^*\langle\varphi_0,\varphi_0\rangle + c_1^*\langle\varphi_1,\varphi_0\rangle + c_2^*\langle\varphi_2,\varphi_0\rangle = \langle f,\varphi_0\rangle$$
$$c_0^*\langle\varphi_0,\varphi_1\rangle + c_1^*\langle\varphi_1,\varphi_1\rangle + c_2^*\langle\varphi_2,\varphi_1\rangle = \langle f,\varphi_1\rangle$$
$$c_0^*\langle\varphi_0,\varphi_2\rangle + c_1^*\langle\varphi_1,\varphi_2\rangle + c_2^*\langle\varphi_2,\varphi_2\rangle = \langle f,\varphi_2\rangle$$

Additional inner products to be evaluated are:

$$\langle\varphi_0,\varphi_2\rangle = \langle\varphi_2,\varphi_0\rangle = \int_0^1 (x^2)(1)\,dx = \frac{1}{3}$$

$$\langle\varphi_1,\varphi_2\rangle = \langle\varphi_2,\varphi_1\rangle = \int_0^1 (x^2)(x)\,dx = \frac{1}{4} = 0.25; \langle\varphi_2,\varphi_2\rangle = \int_0^1 (x^2)(x^2)\,dx = \frac{1}{5} = 0.2$$

$$\langle f,\varphi_2\rangle = \int_0^1 \frac{1}{1+x^2}(x^2)\,dx = 1 - \frac{\pi}{4}$$

Least Square Solution: Example (Continuous)

$$c_0^*\langle\varphi_0,\varphi_0\rangle + c_1^*\langle\varphi_1,\varphi_0\rangle + c_2^*\langle\varphi_2,\varphi_0\rangle = \langle f,\varphi_0\rangle$$
$$c_0^*\langle\varphi_0,\varphi_1\rangle + c_1^*\langle\varphi_1,\varphi_1\rangle + c_2^*\langle\varphi_2,\varphi_1\rangle = \langle f,\varphi_1\rangle$$
$$c_0^*\langle\varphi_0,\varphi_2\rangle + c_1^*\langle\varphi_1,\varphi_2\rangle + c_2^*\langle\varphi_2,\varphi_2\rangle = \langle f,\varphi_2\rangle$$

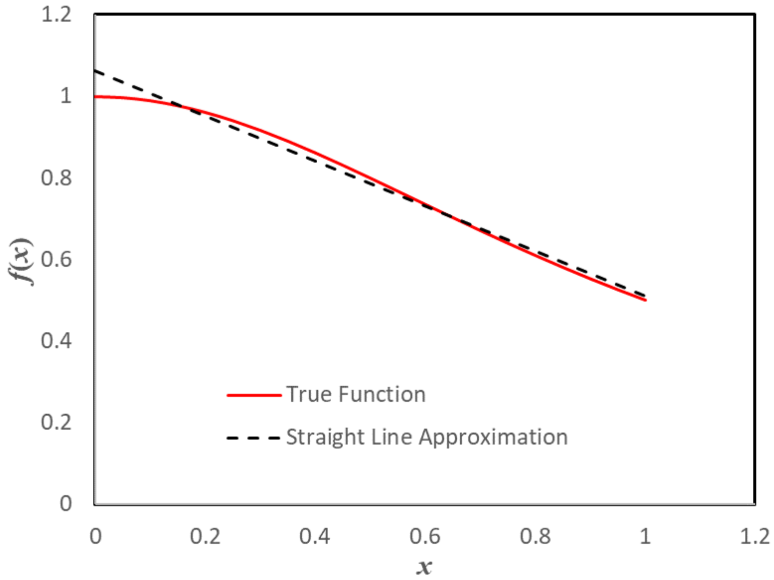
$$\begin{bmatrix} 1 & 0.5 & 1/3 \\ 0.5 & 1/3 & 0.25 \\ 1/3 & 0.25 & 0.2 \end{bmatrix}\begin{bmatrix} c_0^* \\ c_1^* \\ c_2^* \end{bmatrix} = \begin{bmatrix} \pi/4 \\ \ln 2/2 \\ 1-\pi/4 \end{bmatrix}$$

Solving by Gauss Elimination:

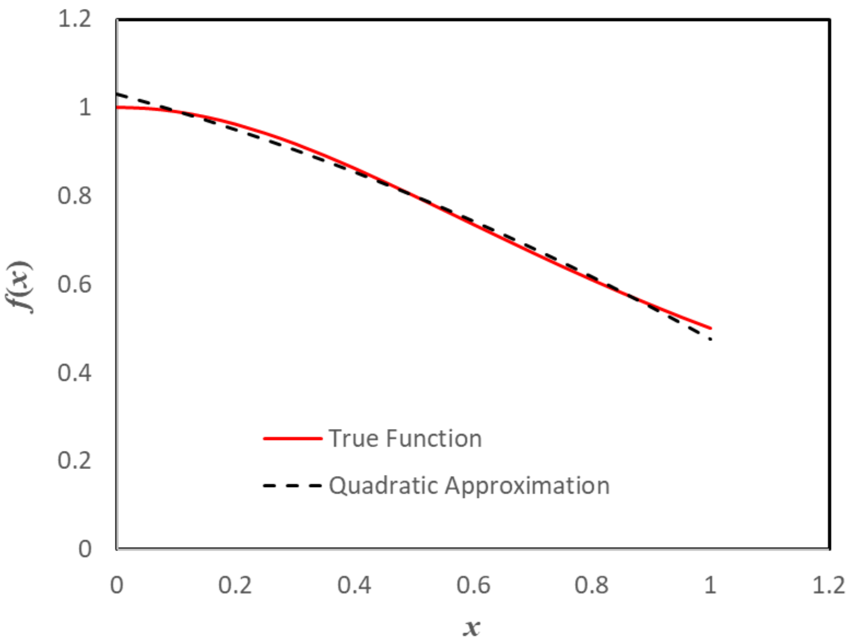
$$c_0^* = 1.030; \qquad c_1^* = -0.3605; \qquad c_2^* = -0.1930$$

$$p^*(x) = \sum_{j=0}^{2} c_j^*\varphi_j(x) = 1.03 - 0.3605x - 0.193x^2$$

Least Square Solution: Example (Continuous)



How do you judge how good the fit is or how do you compare fit of two polynomials?



Estimate $\|p^*(x) - f(x)\|_\infty$.
Two options:

- Analytical (+ numerical)
- Numerical (+ visual)

Discrete Data

- ✓ $(n + 1)$ observations or data pairs $[(x_0, y_0), (x_1, y_1), (x_2, y_2) \ldots (x_n, y_n)]$
- ✓ $(m + 1)$ basis functions: $\{\varphi_0, \varphi_1, \varphi_2, \cdots \varphi_m\}$
- ✓ Approximating polynomial: $p(x) = \sum_{j=0}^{m} c_j \varphi_j(x)$

$$c_0\varphi_0(x_0) + c_1\varphi_1(x_0) + c_2\varphi_2(x_0) + \cdots + c_m\varphi_m(x_0) = y_0$$
$$c_0\varphi_0(x_1) + c_1\varphi_1(x_1) + c_2\varphi_2(x_1) + \cdots + c_m\varphi_m(x_1) = y_1$$
$$\vdots$$
$$c_0\varphi_0(x_n) + c_1\varphi_1(x_n) + c_2\varphi_2(x_n) + \cdots + c_m\varphi_m(x_n) = y_n$$

- ✓ n equations, m unknowns:
  - ✓ **$m < n$: over-determined system, least square regression**
  - ✓ $m = n$: unique solution, interpolation
  - ✓ $m > n$: under-determined system

Least Square Solution: Example (Discrete Data)

Variation of Ultimate Shear Strength (y) with curing Temperature (x) for a certain rubber compound was reported (*J. Quality Technology*, 1971, pp. 149-155) as:

***x*, *in* ^{o}C**	**138**	**140**	**144.5**	**146**	**148**	**151.5**	**153.5**	**157**
y, in psi	770	800	840	810	735	640	590	560

Fit a linear and a quadratic regression model to the data.

For the linear model, the basis functions and the polynomial are:

$$\varphi_0(x) = \varphi_0 = 1;\ \ \varphi_1(x) = \varphi_1 = x;\ \ p^*(x) = \sum_{j=0}^{1} c_j^* \varphi_j(x)$$

$$c_0^*\langle\varphi_0, \varphi_0\rangle + c_1^*\langle\varphi_1, \varphi_0\rangle = \langle f, \varphi_0\rangle$$

$$c_0^*\langle\varphi_0, \varphi_1\rangle + c_1^*\langle\varphi_1, \varphi_1\rangle = \langle f, \varphi_1\rangle$$

Given vectors: ***x*** = [138, 140, 144.5, 146, 148, 151.5, 153.5, 157] and

y* = *f(x) = [770, 800, 840, 810, 735, 640, 590, 560]

No. of data points, m = 8. Denote elements of ***x*** and ***y*** as x_i and y_i, respectively.

Least Square Solution: Example (Discrete Data)

$$\langle \varphi_0, \varphi_0 \rangle = \sum_{i=1}^{m} (1)(1) = 8; \quad \langle \varphi_1, \varphi_1 \rangle = \sum_{i=1}^{m} (x_i)(x_i) = \sum_{i=1}^{m} x_i^2 = 173907.75$$

$$\langle \varphi_1, \varphi_0 \rangle = \langle \varphi_0, \varphi_1 \rangle = \sum_{i=1}^{m} (1)(x_i) = \sum_{i=1}^{m} x_i = 1178.5$$

$$\langle f, \varphi_0 \rangle = \sum_{i=1}^{m} (y_i)(1) = 5745; \quad \langle f, \varphi_1 \rangle = \sum_{i=1}^{m} (y_i)(x_i) = 842125$$

$$c_0^* \langle \varphi_0, \varphi_0 \rangle + c_1^* \langle \varphi_1, \varphi_0 \rangle = \langle f, \varphi_0 \rangle$$
$$c_0^* \langle \varphi_0, \varphi_1 \rangle + c_1^* \langle \varphi_1, \varphi_1 \rangle = \langle f, \varphi_1 \rangle$$

$$\begin{bmatrix} 8 & 1178.5 \\ 1178.5 & 173907.75 \end{bmatrix} \begin{bmatrix} c_0^* \\ c_1^* \end{bmatrix} = \begin{bmatrix} 5745 \\ 842125 \end{bmatrix} \quad \Longrightarrow \quad c_0^* = 2773.50; \quad c_1^* = -13.9525$$

$$p^*(x) = \sum_{j=0}^{1} c_j^* \varphi_j(x) = 2773.5 - 13.9525x$$

Least Square Solution: Example (Discrete Data)

For the quadratic model, the basis functions and the polynomial are:

$\varphi_0 = 1; \quad \varphi_1 = x; \quad \varphi_2 = x^2; \quad p^*(x) = \sum_{j=0}^{2} c_j^* \varphi_j$

$$c_0^*\langle\varphi_0, \varphi_0\rangle + c_1^*\langle\varphi_1, \varphi_0\rangle + c_2^*\langle\varphi_2, \varphi_0\rangle = \langle f, \varphi_0\rangle$$
$$c_0^*\langle\varphi_0, \varphi_1\rangle + c_1^*\langle\varphi_1, \varphi_1\rangle + c_2^*\langle\varphi_2, \varphi_1\rangle = \langle f, \varphi_1\rangle$$
$$c_0^*\langle\varphi_0, \varphi_2\rangle + c_1^*\langle\varphi_1, \varphi_2\rangle + c_2^*\langle\varphi_2, \varphi_2\rangle = \langle f, \varphi_2\rangle$$

Additional inner products to be evaluated are:

$$\langle\varphi_0, \varphi_2\rangle = \langle\varphi_2, \varphi_0\rangle = \sum_{i=1}^{m} (1)\left(x_i^2\right) = 173907.75$$

$$\langle\varphi_1, \varphi_2\rangle = \langle\varphi_2, \varphi_1\rangle = \sum_{i=1}^{m} (x_i)\left(x_i^2\right) = \sum_{i=1}^{m} x_i^3 = 25707160$$

$$\langle\varphi_2, \varphi_2\rangle = \sum_{i=1}^{m} \left(x_i^2\right)\left(x_i^2\right) = \sum_{i=1}^{m} x_i^4 = 3806534454$$

$$\langle f, \varphi_2\rangle = \sum_{i=1}^{m} (y_i)\left(x_i^2\right) = 123643297.5$$

Least Square Solution: Example (Discrete Data)

$$c_0^*\langle\varphi_0,\varphi_0\rangle + c_1^*\langle\varphi_1,\varphi_0\rangle + c_2^*\langle\varphi_2,\varphi_0\rangle = \langle f,\varphi_0\rangle$$
$$c_0^*\langle\varphi_0,\varphi_1\rangle + c_1^*\langle\varphi_1,\varphi_1\rangle + c_2^*\langle\varphi_2,\varphi_1\rangle = \langle f,\varphi_1\rangle$$
$$c_0^*\langle\varphi_0,\varphi_2\rangle + c_1^*\langle\varphi_1,\varphi_2\rangle + c_2^*\langle\varphi_2,\varphi_2\rangle = \langle f,\varphi_2\rangle$$

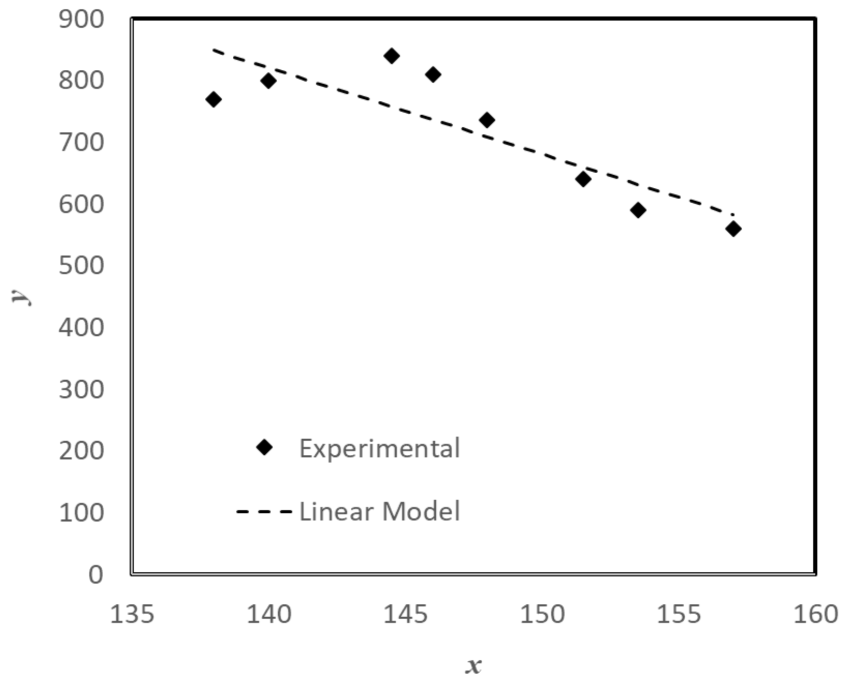
$$\begin{bmatrix} 8 & 1178.5 & 173907.75 \\ 1178.5 & 173907.75 & 25707160 \\ 173907.75 & 25707160 & 3806534454 \end{bmatrix} \begin{bmatrix} c_0^* \\ c_1^* \\ c_2^* \end{bmatrix} = \begin{bmatrix} 5745 \\ 842125 \\ 123643297.5 \end{bmatrix}$$

Solving by Gauss Elimination:

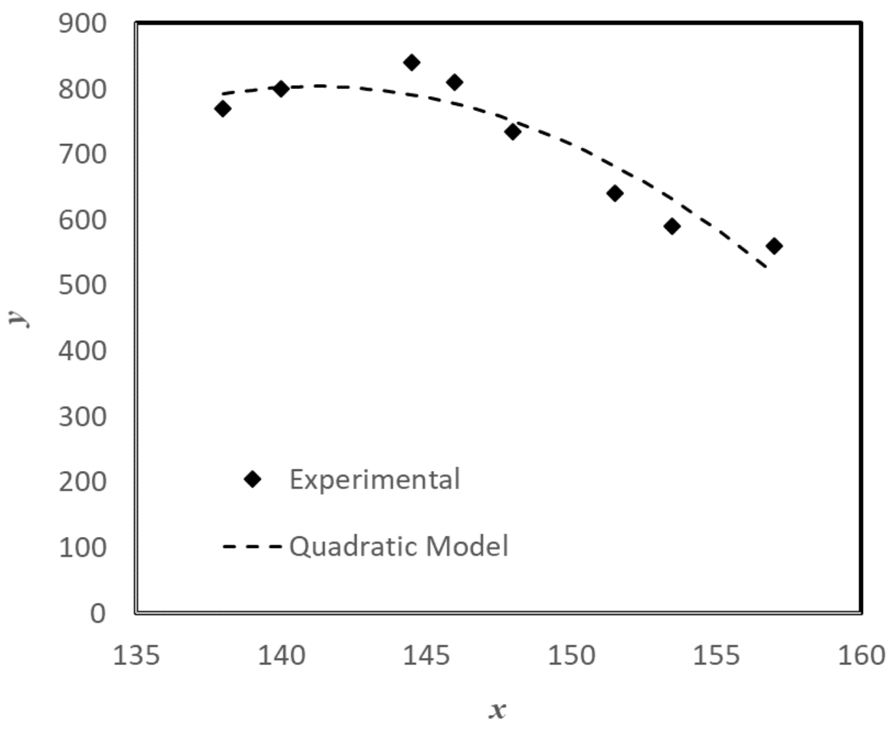
$c_0^* = -21935.4;$ $c_1^* = 322.103;$ $c_2^* = -1.14067$

$$p^*(x) = \sum_{j=0}^{2} c_j^*\varphi_j(x) = -21935.4 + 322.103x - 1.14067x^2$$

Least Square Solution: Example (Discrete Data)

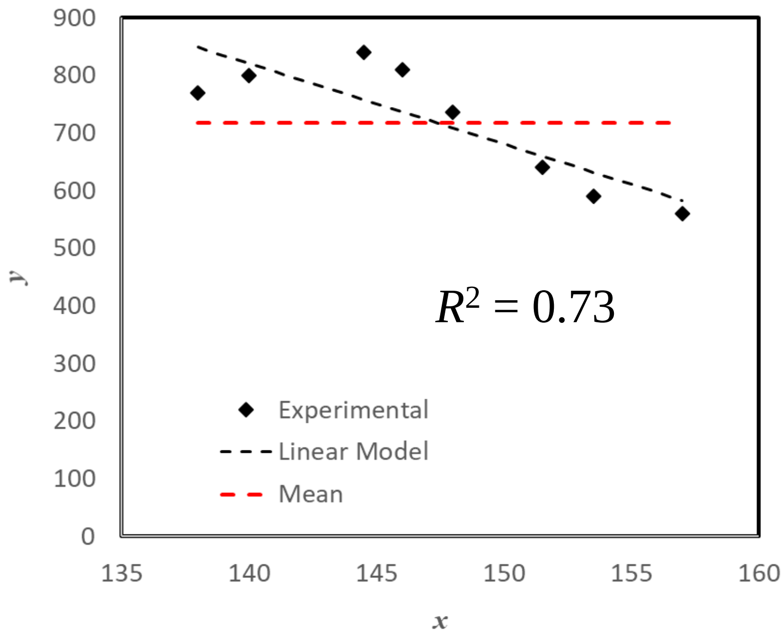


How do you judge how good the fit is or how do you compare fit of two polynomials?



Square of errors!

Least Square Solution: Example (Discrete Data)



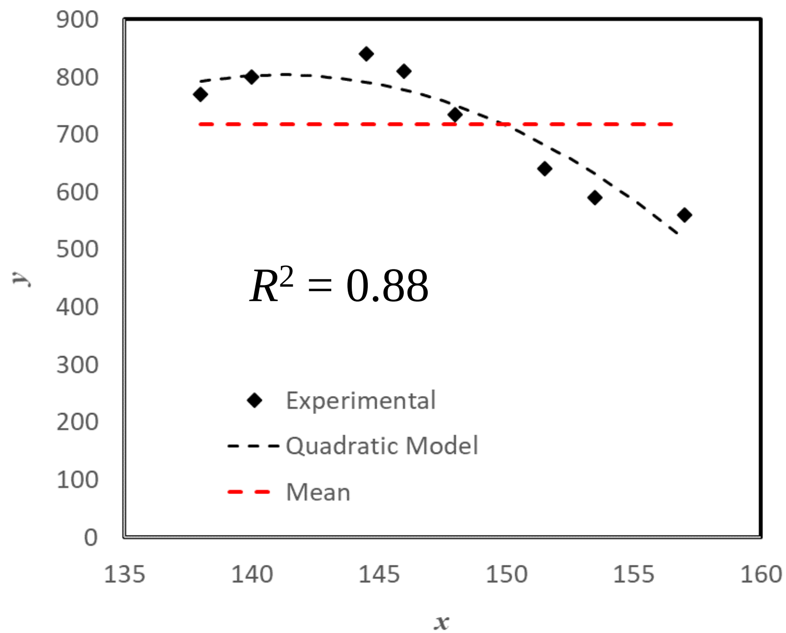
Denote: $y_i = f(x_i)$, $\quad \widehat{y}_i = p^*(x_i)$

$$\mu_y = \frac{\sum_{i=0}^{m} y_i}{m+1}, \qquad \sigma_t^2 = \sum_{i=0}^{m} \left(y_i - \mu_y\right)^2$$

$$\varepsilon^2 = \sum_{i=0}^{m} (y_i - \widehat{y}_i)^2$$

Coefficient of regression r or R is given by:

$$r^2 = \frac{\sigma_t^2 - \varepsilon^2}{\sigma_t^2}$$



Additional Points

- You can do multiple regression using the same frame work.
- Linearize some non-linear equations
- Evaluate Integrals using Numerical Methods for Integration for functions that are not easy to integrate using analytical means!

ESO 208A: Computational Methods in Engineering

Orthogonal Basis, Periodic Functions

Saumyen Guha

Department of Civil Engineering
IIT Kanpur

Least Square Solution: Normal Equations

$$\sum_{j=0}^{n} c_j^* \langle \varphi_j(x), \varphi_k(x) \rangle = \langle f(x), \varphi_k(x) \rangle; \quad k = 0, 1, 2, \cdots n$$

If $\{\varphi_0, \varphi_1, \varphi_2, \cdots \varphi_n\}$ is an orthogonal system:

$$c_k^* = \frac{\langle f, \varphi_k \rangle}{\langle \varphi_k, \varphi_k \rangle} \qquad k = 0, 1, 2, \cdots n$$

Let us explore orthogonal systems of basis functions!

Orthogonal Polynomials: Tchebycheff

Consider the Equality:

$$\cos(n+1)\varphi + \cos(n-1)\varphi = 2\cos\varphi\cos n\varphi \qquad n \geq 1$$

- ✓ $n = 1$: $\cos 2\varphi = 2\cos^2\varphi - 1$
- ✓ $n = 2$: $\cos 3\varphi = 2\cos\varphi\cos 2\varphi - \cos\varphi = 4\cos^3\varphi - 3\cos\varphi$
- ✓ Define: $x = \cos\varphi$, $\varphi \in [0, \pi]$ and $T_n(x) = \cos n\varphi = \cos(n\cos^{-1}x)$
- ✓ Recursion Formula: $T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x)$
- ✓ Example: $T_0(x) = 1$; $T_1(x) = x$; $T_2(x) = 2x^2 - 1$
- ✓ Symmetry: $T_n(-x) = (-1)^n T_n(x)$
- ✓ Leading Coefficient: 2^{n-1} for $n \geq 1$ and 1 for $n = 0$

$T_n(x)$ constitutes an orthogonal family of polynomials in [-1, 1]!

Orthogonal Polynomials: Tchebycheff

✓ $T_n(x)$ has n zeros in [-1, 1] called the **Tchebycheff abscissae**:

$$x_k = \cos\left(\frac{2k+1}{n}\frac{\pi}{2}\right) \qquad k = 0, 1, 2 \cdots (n-1)$$

$$\left(\text{Follows from } \cos n\varphi = 0 \ \text{ for } \ \varphi = \frac{2k+1}{n}\frac{\pi}{2}\right)$$

✓ $T_n(x)$ has n+1 **extrema** in [-1, 1]:

$$x_j = \cos\left(\frac{j\pi}{n}\right); \ \ T_n(x_j) = (-1)^j \qquad j = 0, 1, 2 \cdots n$$

$$\left(\text{Follows from } |\cos n\varphi| \ \text{ has maxima at } \ \varphi = \frac{j\pi}{n}\right)$$

Orthogonal Polynomials: Tchebycheff

Orthogonality (continuous):

$$\langle T_m(x), T_n(x)\rangle = \int_0^{\pi} \cos m\varphi \cos n\varphi \, d\varphi$$

$$= \int_{-1}^{1} T_m(x) T_n(x) \frac{1}{\sqrt{1-x^2}} dx$$

$$= \begin{cases} 0 & \text{if } \; m \neq n \\ \dfrac{\pi}{2} & \text{if } \; m = n \neq 0 \\ \pi & \text{if } \; m = n = 0 \end{cases}$$

For arbitrary $f(x)$, $a \le x \le b$: $x = \frac{b+a}{2} + \frac{b-a}{2}\xi \qquad -1 \le \xi \le 1$

Orthogonal Polynomials: Tchebycheff

Orthogonality (discrete): For $0 \le m \le N$ and $0 \le n \le N$

$$\langle T_m(x), T_n(x) \rangle = \sum_{k=0}^{N} T_m(x_k) T_n(x_k)$$

$$= \begin{cases} 0 & \text{if } \; i \neq j \\ \frac{1}{2}(N+1) & \text{if } \; i = j \neq 0 \\ (N+1) & \text{if } \; i = j = 0 \end{cases}$$

where, $\{x_k\}$ are the zeros of $T_{N+1}(x)$

Orthogonal Polynomials: Legendre

Solution of the Legendre's equation (for *n* non-negative:

$$\frac{d}{dx}\left[(1-x^2)\frac{d\varphi}{dx}\right] + n(n+1)\varphi = 0 \qquad -1 \le x \le 1$$

- ✓ Solutions are an orthogonal set of polynomials given by:

$$P_0(x) = 1; \qquad P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}[(x^2-1)^n]$$

- ✓ Bonnet's recursive relation for $n \geq 2$:

$$P_n(x) = \frac{2n-1}{n} x P_{n-1}(x) - \frac{n-1}{n} P_{n-2}(x)$$

- ✓ Examples:

$P_0(x) = 1;\;\; P_1(x) = x;\;\; P_2(x) = \frac{1}{2}(3x^2-1);\;\; P_3(x) = \frac{1}{2}(5x^3-3x)$

Orthogonal Polynomials: Legendre

✓ Symmetry: $P_n(-x) = (-1)^n P_n(x)$

✓ Orthogonality (continuous):

$$\langle P_m(x), P_n(x) \rangle = \begin{cases} 0 & \text{if } \ m \neq n \\ \dfrac{2}{2n+1} & \text{if } \ m = n \end{cases}$$

$$\omega(x) = 1; \qquad |P_n(x)| \leq 1$$

For discrete data: equidistant data points.

Orthonormal Polynomials: Gram

For Equidistant Discrete Data:

- ✓ For $-1 \leq x \leq 1$, a net of (n + 1) equidistant points are given by:

$$x_k = -1 + \frac{2k}{n} \quad \text{for} \quad k = 0, 1, 2, \cdots n$$

- ✓ On this net, the orthonormal set of polynomials $\{G_m(x)\}_{m=0}^{n}$ are given by:

$$G_{-1}(x) = 0; \qquad G_0(x) = \frac{1}{\sqrt{n+1}}; \qquad G_{m+1}(x) = \alpha_m x G_m(x) - \frac{\alpha_m}{\alpha_{m-1}} G_{m-1}(x)$$

$$\alpha_m = \frac{n}{m+1}\sqrt{\frac{4(m+1)^2 - 1}{(n+1)^2 - (m+1)^2}} \qquad\qquad m = 0, 1, 2, \cdots n-1$$

- ✓ Example (for n = 5):

$$G_0(x) = \frac{1}{\sqrt{6}}; \qquad G_1(x) = \frac{5x}{\sqrt{70}}; \qquad G_2(x) = \frac{25}{16}\sqrt{\frac{3}{7}}x^2 - \frac{5}{16}\sqrt{\frac{7}{3}}$$

Orthonormal Polynomials: Gram

- ✓ Orthogonality:

$$\langle G_i(x), G_j(x) \rangle = \sum_{k=0}^{n} G_i(x_k) G_j(x_k) = \begin{cases} 0 & \text{if } \; i \neq j \\ 1 & \text{if } \; i = j \end{cases}$$

- ✓ When $m << n^{1/2}$, $G_m(x)$ are very similar to the Legendre polynomials
- ✓ When $n << m^{1/2}$, $G_m(x)$ have very large oscillations between the net points, large maximum norm in [-1, 1]
- ✓ When fitting a polynomial to *equidistant* data, one should never choose m larger than ~ $2n^{1/2}$

Least Square Solution: Example (Continuous)

Approximate the function $f(x) = 1/(1 + x^2)$ for x in [0, 1] using a 2nd order polynomial using Legendre polynomials.

For Legendre polynomials, use $x = (z + 1)/2$ such that for x in [0, 1], z is in [-1, 1]

The function is: $f(z) = 4/(5 + 2z + z^2)$

The basis functions are: $\varphi_0 = 1$; $\varphi_1 = z$; $\varphi_2 = \frac{1}{2}(3z^2 - 1)$; $p^*(z) = \sum_{j=0}^{2} c_j^* \varphi_j$

$$\langle f, \varphi_0 \rangle = \int_{-1}^{1} \frac{4}{5 + 2z + z^2} dz = \frac{\pi}{2} = 1.5708$$

$$\langle f, \varphi_1 \rangle = \int_{-1}^{1} \frac{4z}{5 + 2z + z^2} dz = 2 \ln 2 - \frac{\pi}{2} = -0.1845$$

$$\langle f, \varphi_2 \rangle = \int_{-1}^{1} \frac{4\frac{1}{2}(3z^2 - 1)}{5 + 2z + z^2} dz = 12 - 6 \ln 2 - \frac{5\pi}{2} = -0.1286 \times 10^{-1}$$

$$c_0^* = \frac{1.5708}{2} = 0.7854; c_1^* = \frac{-0.1845}{2/3} = -0.2768; c_2^* = \frac{-0.1286 \times 10^{-1}}{2/5} = -0.3216 \times 10^{-1}$$

Least Square Solution: Example (Continuous)

$$c_0^* = \frac{1.5708}{2} = 0.7854; c_1^* = \frac{-0.1845}{2/3} = -0.2768; c_2^* = \frac{-0.1286 \times 10^{-1}}{2/5}$$
$$= -0.3216 \times 10^{-1}$$

$$p^*(z) = \sum_{j=0}^{2} c_j^* \varphi_j(z) = 0.7854 - 0.2768z - 0.3216 \times 10^{-1} \times \tfrac{1}{2}(3z^2 - 1)$$
$$= 0.8015 - 0.2768z - 0.4824 \times 10^{-1} z^2$$

If you now use, $z = 2x - 1$

$$p^*(x) = 0.8015 - 0.2768(2x - 1) - 0.4824 \times 10^{-1}(2x - 1)^2$$
$$= 1.030 - 0.3605x - 0.193x^2$$

Least square polynomial is unique! It does not depend on the basis!

Periodic Functions

A function of period *p*:

$$f(x + p) = f(x) \text{ for all } x$$

We shall study functions of period 2π

$$0 \le x \le 2\pi \qquad \text{or} \qquad -\pi \le x \le \pi$$

For any function $f(x)$ with a period p, transform $t = 2\pi x/p$

Allow functions to have complex values.

Definition: Inner product of two complex-valued functions *f* and *g* of period 2π

$$\langle f, g\rangle = \int_0^{2\pi} f(x)\bar{g}(x)\,dx \qquad (Continuous)$$

$$= \sum_{m=0}^{M} f(x_m)\bar{g}(x_m)\,; \quad x_m = \frac{2\pi m}{M+1} \qquad (Discrete)$$

Periodic Orthogonal Basis Functions

$$\phi_k(x) = e^{ikx}; \qquad 0 \le x \le 2\pi \quad \text{or} \quad -\pi \le x \le \pi$$
$$k = 0, \pm 1, \pm 2, \cdots \pm \infty$$

Continuous Case:

$$\langle \phi_j, \phi_k \rangle = \int_{-\pi}^{\pi} e^{ijx} e^{-ikx}\, dx = \begin{cases} 0 & \text{if } \ j \neq k \\ 2\pi & \text{if } \ j = k \end{cases}$$

Discrete Case: $x_m = \frac{2\pi m}{M+1}$

$$\langle \phi_j, \phi_k \rangle = \sum_{m=0}^{M} e^{ijx_m} e^{-ikx_m} = \sum_{m=0}^{M} \exp\left[i(j-k)\frac{2\pi m}{M+1} \right]$$

$$= \begin{cases} M+1 & \text{if} \quad \dfrac{j-k}{M+1} \ \text{is an integer} \\ 0 & \text{Otherwise} \end{cases}$$