Need for approximation

- Function given
  - Approximate by a simpler function
    - For example, to integrate it
- Unknown function: only values at some points
  - Approximate by a function
    - Passing through all data points (Interpolation)
    - Capturing the general data trend (Regression)
  - Estimate the derivative or the integral
    - Derivative estimation, e.g., velocity from distance versus time data (Numerical Differentiation)
    - Integral estimation, e.g., area under a curve from y versus x data (Numerical Integration)

Approximation of functions

- Not very common, but simpler than “data” case
- Generally polynomials are used as approximating functions (or, if periodic, sine/cosine)
- First question: What should be the degree of the approximating polynomial?
  - Depends on the desired accuracy and required computational effort
- Second question: How do we quantify the “accuracy” or “error”?
- And finally: How do we obtain the “best” polynomial, i.e., the one with minimum error?

Approximation of functions

- Easiest method: Use Taylor's series.
  - Approximate *f(x)* over the interval (a,b) using an m^{th} degree polynomial, $f_m(x)$

$$f(x) = f(x_0) + (x - x_0) f'(x_0) + \frac{(x - x_0)^2}{2!} f''(x_0) + \ldots + \frac{(x - x_0)^m}{m!} f^{[m]}(x_0) + R_m$$

  - x_0 is some point in (a,b), midpoint may be best
  - R_m is the remainder, given by

$$R_m = \int_{x_0}^{x} \frac{(x - \chi)^m}{m!} f^{[m+1]}(\chi) d\chi = \frac{(x - x_0)^{m+1}}{(m+1)!} f^{[m+1]}(\zeta)$$

$$\zeta \in (x_0, x)$$

Taylor's Series: Example

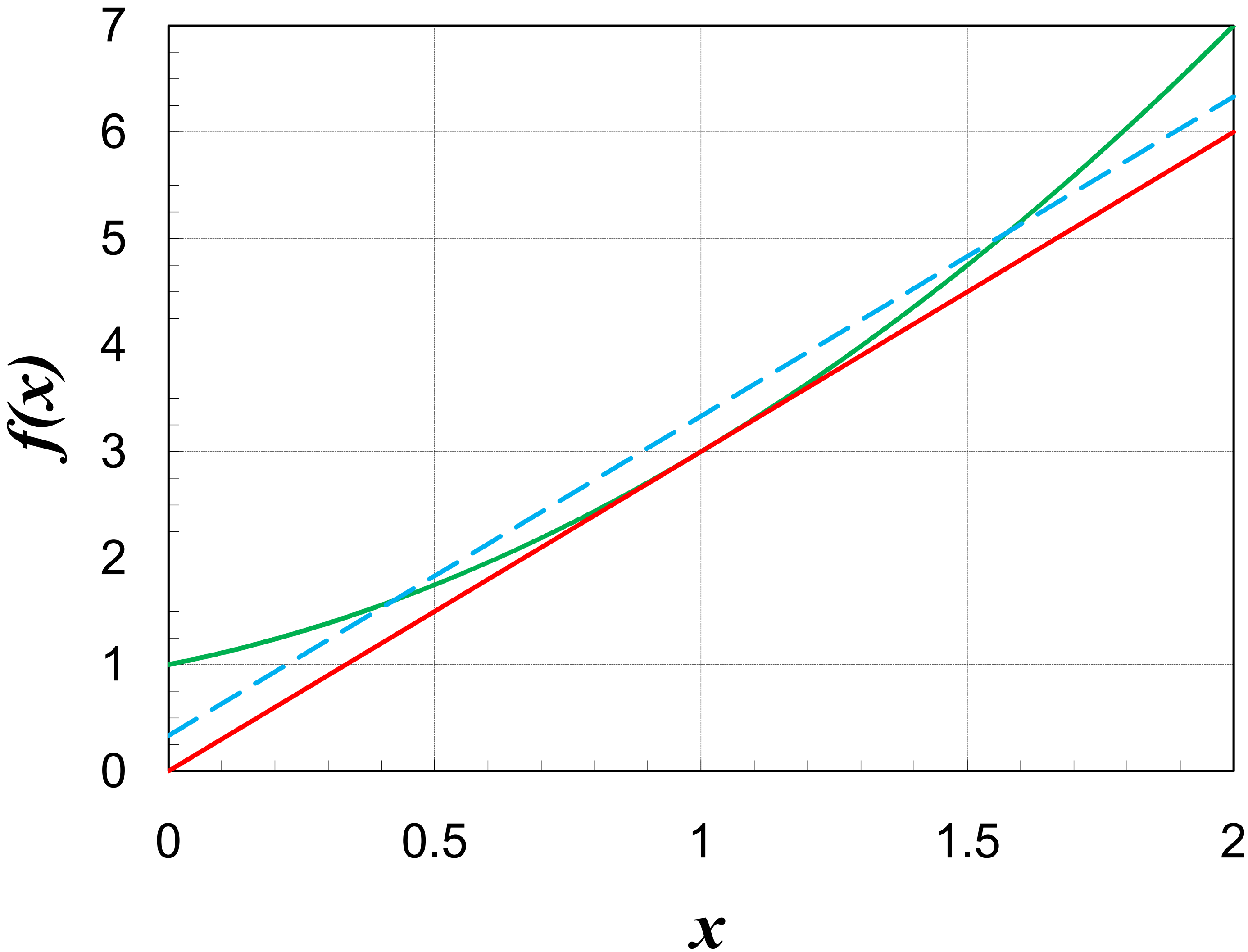
- Approximate $f(x)=1+x+x^2$ over the interval (0,2) using a linear function, $f_1(x)$
  - Choose $x_0=1$
  - Taylor's series:

$$f(x) = f(1) + (x-1)f'(1) + \frac{(x-1)^2}{2!} f''(\zeta); \zeta \in (1, x)$$

  - The linear approximation is

$$f_1(x) = 3 + 3(x-1) = 3x$$

  - And, since the second derivative is constant (=2), the error at any x is $(x-1)^2$



Taylor's series is not a very good fit! Other methods are needed.

Least Squares

- We treat the residual as an error term, $R_m = f(x) - f_m(x)$, and then minimize its "magnitude"
  - ➢ R_m is a function of x.
  - ➢ Magnitude may be taken as the integral over the domain (a,b)
  - ➢ To accommodate negative error, we square it
- The problem reduces to:

$$\text{Minimize} \int_a^b \left(f(x) - f_m(x) \right)^2 dx$$

$$\text{(Hence, the name "Least Squares")}$$

Least Squares: Formulation

- We could write $f_m(x)$ in the conventional form as

$$f_m(x) = c_0 + c_1 x + c_2 x^2 + \ldots + c_m x^m = \sum_{j=0}^{m} c_j x^j$$

- However, alternative forms may also be used:

$$f_m(x) = \sum_{j=0}^{m} c_j \left(x - x_0\right)^j; \quad f_m(x) = \sum_{j=0}^{m} c_j p_j; \quad f_m(x) = \sum_{j=0}^{m} c_j p_{m,j}$$

where, x_0 is a suitable point [e.g., (a+b)/2], p_j is a polynomial of degree j, and $p_{m,j}$ is a polynomial of degree m. The aim is to obtain the c's.

Least Squares: Formulation

- Examples, using a 2nd degree polynomial:

$$f_2(x) = c_0 + c_1 x + c_2 x^2$$

$$f_2(x) = c_0 + c_1\left(x-1\right) + c_2 (x-1)^2$$

$$f_2(x) = c_0 + c_1\left(1+x\right) + c_2\left(1+x+x^2\right)$$

$$f_2(x) = c_0\left(1+x+x^2\right) + c_1\left(1+2x+3x^2\right) + c_2\left(1+4x+9x^2\right)$$

Least Squares: Formulation

- We use a *general* form:

$$f_m(x) = \sum_{j=0}^{m} c_j \phi_j(x)$$

- ϕ's are known functions (here, polynomials) and the coefficients are chosen in such a way that the

error $\displaystyle\int_a^b \left(f(x) - \sum_{j=0}^{m} c_j \phi_j(x) \right)^2 dx$ is minimized.

Least Squares: Formulation

- Using the stationary point theorem, we take the derivative of the error w.r.t. each of the c's, and equate it to zero, to get a set of $m+1$ **linear** eqs.

$$\int_a^b 2\left(f(x) - \sum_{j=0}^{m} c_j \phi_j(x) \right)\left(-\phi_i(x)\right) dx = 0 \quad \text{for } i = 0,1,2,\ldots,m$$

- For a clearer presentation, we drop the (x) from the expressions and write

$$\int_a^b \left(f - \sum_{j=0}^{m} c_j \phi_j \right) \phi_i \, dx = 0 \quad \text{for } i = 0,1,2,\ldots,m$$

Least Squares: Inner product

- Analogous to vectors, for functions:

VECTORS		FUNCTIONS	
Norm	L_1, L_2, L_∞	Magnitude	$\frac{1}{b-a}\int_a^b \lvert f\rvert dx$ $\frac{1}{b-a}\sqrt{\int_a^b f^2 dx}$ $\lvert f\rvert_{\max}$ over (a,b)
Dot Product	$x.y$	Inner Product <*f*,*g*>	$\int_a^b f.g dx$
Orthogonality	$x.y$ =0	Orthogonality	<*f*,*g*> = 0

Least Squares: Normal Equations

- Using the inner product notation:

$$\left\langle \sum_{j=0}^{m} c_j \phi_j , \phi_i \right\rangle = \langle f , \phi_i \rangle \quad \text{for } i = 0,1,2,\ldots,m$$

- Or, concisely $[A]\{c\} = \{b\}$: Called the "Normal Equations"

in which,

$$a_{ij} = \left\langle \phi_i , \phi_j \right\rangle; b_i = \left\langle \phi_i , f \right\rangle;\ i, j = 0,1,2,\ldots,m$$

Normal Equations: Example

- Approximate $f(x)=1+x+x^2$ over the interval (0,2) using a linear function, $f_1(x)$
- Choose the linear function as $f_1(x)=c_0+c_1x$

=> $$\phi_0(x)=1; \phi_1(x)=x$$

$$a_{00}=\langle\phi_0,\phi_0\rangle=\int_0^2 1dx=2$$

$$a_{01}=a_{10}=\langle\phi_0,\phi_1\rangle=\int_0^2 xdx=2$$

$$a_{11}=\langle\phi_1,\phi_1\rangle=\int_0^2 x^2dx=\frac{8}{3}$$

Normal Equations: Example

- and $$b_0 = \langle \phi_0, f \rangle = \int_0^2 1 + x + x^2 dx = \frac{20}{3}$$

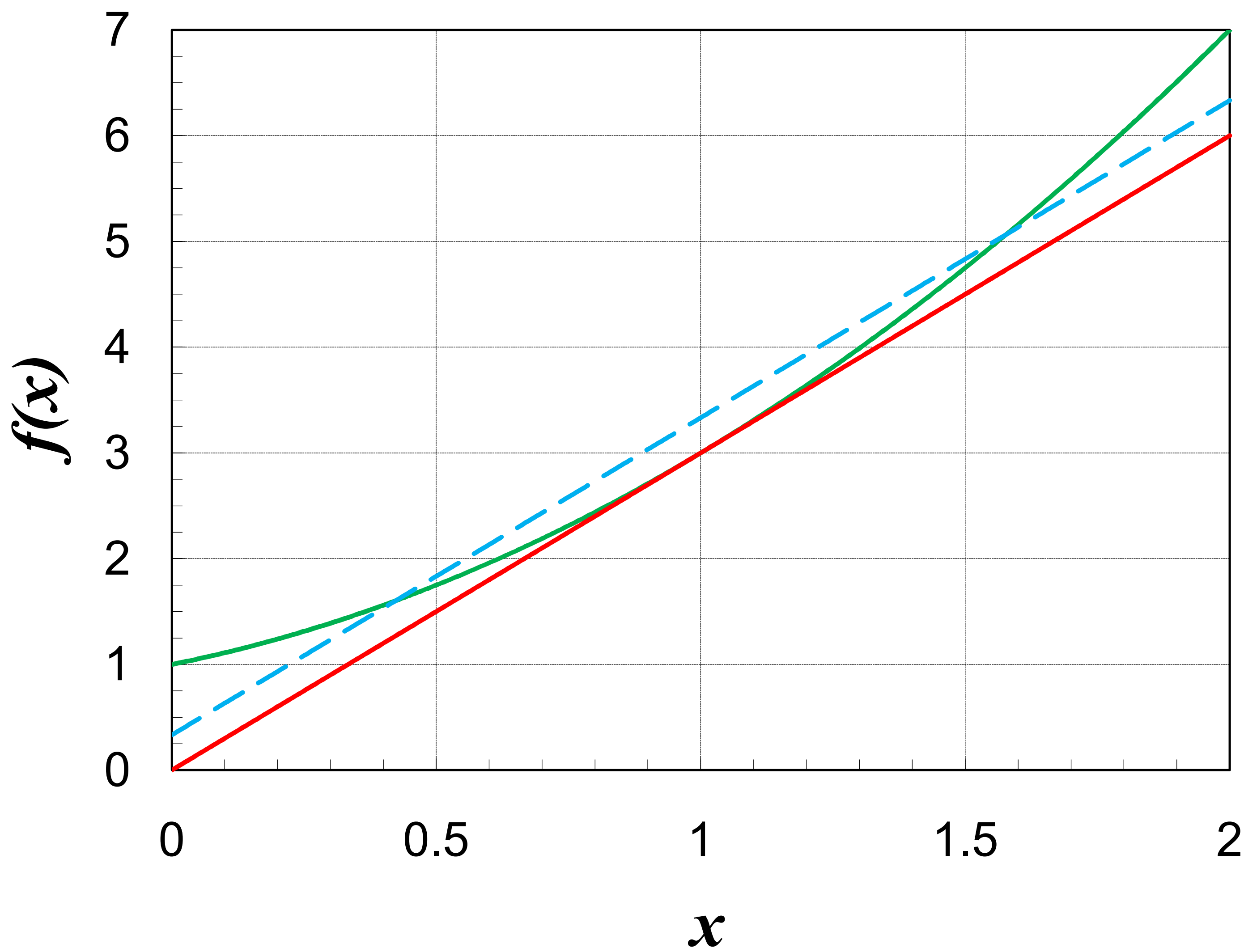
$$b_1 = \langle \phi_1, f \rangle = \int_0^2 x\left(1 + x + x^2\right) dx = \frac{26}{3}$$

- The normal equations are

$$\begin{bmatrix} 2 & 2 \\ 2 & 8/3 \end{bmatrix} \begin{Bmatrix} c_0 \\ c_1 \end{Bmatrix} = \begin{Bmatrix} 20/3 \\ 26/3 \end{Bmatrix}$$

$$\text{Solution}: \quad c_0 = \frac{1}{3}; c_1 = 3$$

- Therefore, $f_1(x)=1/3 + 3\,x$



Much better than Taylor's series in overall sense (NOT near 1 !)

Normal Equations: Diagonal form

- If the matrix A becomes diagonal, c is easily computed. Since we are free to choose the form of the basis functions (ϕ's), use "Orthogonal polynomials"
- Recall: $$a_{ij} = \langle \phi_i, \phi_j \rangle = \int_a^b \phi_i(x)\phi_j(x)dx$$
- Using the same example, over the domain (0,2)
- Choose ϕ_0=1 and ϕ_1 , a linear function orthogonal to it, = d_0 +d_1 x.
- Then: $$\int_0^2 (d_0 + d_1 x)dx = 0 \Rightarrow d_1 = -d_0$$

Normal Equations: Diagonal form

- d_0 is arbitrary, let us use 1 => $\phi_1 = 1 - x$
- The normal equations are:

$$\begin{bmatrix} 2 & 0 \\ 0 & 2/3 \end{bmatrix} \begin{Bmatrix} c_0 \\ c_1 \end{Bmatrix} = \begin{Bmatrix} 20/3 \\ -2 \end{Bmatrix}$$

Solution :

$$c_0 = \frac{10}{3}; c_1 = -3$$

- Therefore, $f_1(x) = 10/3 - 3\,(1 - x) = 1/3 + 3x$
- Same as before, but much easier to compute
- However, needs effort in finding the ϕ's, which depend on the range, i.e., a and b.

Orthogonal polynomials: Legendre

- If we standardize the domain, the orthogonal polynomials need to be computed only once

- Recall that there was an arbitrary constant

- If the standard domain of (−1,1) is chosen and the arbitrary constant is chosen to make ϕ =1 at x=1, we get the Legendre Polynomials, $P_n(x)$.

- If the problem specifies the domain (a,b) for the variable x*, the transformation

$$x = \frac{x^* - \frac{b+a}{2}}{\frac{b-a}{2}}$$

is used to standardize it.

Legendre polynomials

- $P_0(x)=1$.

- $P_1(x)$ should be a linear function orthogonal to $P_0(x)$ and should be equal to 1 at $x=1$

- Assume $P_1(x) = d_0 + d_1 x$

- Orthogonality: $\int_{-1}^{1}(d_0 + d_1 x)dx = 0 \Rightarrow d_0 = 0$

- Value at $x=1$ equal to 1 => $P_1(x) = x$

Legendre polynomials

- Similarly, assume $P_2(x) = d_0 + d_1\, x + d_2\, x^2$

- Orthogonality with P_0 gives $d_0 + d_2\,/3 = 0$; with P_1 gives $d_1 = 0$; and value at $x=1$ gives $d_0 + d_2 = 1$

- $P_2(x) = (-1+3x^2)/2$

- Similarly: $P_3(x) = (-3x+5x^3)/2$;

  $P_4(x) = (3-30x^2+35x^4)/8 \quad \ldots$

Legendre polynomials

- Recursive Formula

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

- Orthogonality

$$\left\langle P_i(x), P_j(x) \right\rangle = \int_{-1}^{1} P_i(x) P_j(x) dx = \begin{cases} 0 & i \neq j \\ \\ \dfrac{2}{2i+1} & i = j \end{cases}$$

Legendre polynomials: Example

- Approximate $f(x^*)=1+x^*+x^{*2}$ over the interval (0,2) using a linear function, $f_1(x^*)$
- First step: Normalization--- $x = \dfrac{x^* - \frac{b+a}{2}}{\frac{b-a}{2}} = x^* - 1$
- $f(x)=1+(x+1)+(x+1)^2 = 3+3x+x^2$
- $A = \begin{bmatrix} 2 & 0 \\ 0 & 2/3 \end{bmatrix} \qquad b = \begin{Bmatrix} 20/3 \\ 2 \end{Bmatrix}$
- Solution: $f_1(x)=10/3+3x$
- Convert back to original: $f_1(x^*)=10/3+3(x^*-1)$
- Same as before, $f_1(x^*)=1/3+3x^*$

Legendre polynomials: General Case

- For a general case, degree m:

$$A = \begin{bmatrix} 2 & & & & 0 \\ & 2/3 & & & \\ & & 2/5 & & \\ & 0 & & \ddots & \\ & & & & 2/(2m+1) \end{bmatrix}$$

$$b = \begin{Bmatrix} \langle 1, f(x) \rangle \\ \langle x, f(x) \rangle \\ \langle (3x^2 - 1)/2, f(x) \rangle \\ \vdots \\ \langle P_m(x), f(x) \rangle \end{Bmatrix}$$