Numerical Methods in Economics

MIT Press, 1998

Notes for Chapter 6: Approximation Methods

October 20, 2010

Approximation Methods

- General Objective: Given data about a function $f(x)$ (which is difficult to compute) construct a simpler function $g(x)$ that approximates $f(x)$.

- Questions:

  - What data should be produced and used?
  - What family of "simpler" functions should be used?
  - What notion of approximation do we use?
  - How good can the approximation be?
  - How simple can a good approximation be?

- Comparisons with statistical regression

  - Both approximate an unknown function
  - Both use a finite amount of data
  - Statistical data is noisy; we assume here that data errors are small
  - Nature produces data for statistical analysis; we produce the data in function approximation
  - Our approximation methods are like experimental design with very small experimental error

Local Approximation Methods

- Use information about $f : R \to R$ only at a point, $x_0 \in R$, to construct an approximation valid near x_0
- Taylor Series Approximation

$$\begin{aligned} f(x) &\doteq f(x_0) + (x - x_0)\, f'(x_0) + \frac{(x - x_0)^2}{2}\, f''(x_0) + \cdots \\ &+ \frac{(x - x_0)^n}{n!}\, f^{(n)}(x_0) + \mathcal{O}(|x - x_0|^{n+1}) \\ &= p_n\,(x) + \mathcal{O}(|x - x_0|^{n+1}) \end{aligned} \tag{6.1.1}$$

- Power series: $\sum_{n=0}^{\infty} a_n z^n$
  - The *radius of convergence* is

$$r = \sup\{|z| : |\sum_{n=0}^{\infty} a_n z^n| < \infty\},$$

  - $\sum_{n=0}^{\infty} a_n z^n$ converges for all $|z| < r$ and diverges for all $|z| > r$.

- Complex analysis
  - $f : \Omega \subset C \to C$ on the complex plane C is *analytic* on Ω iff

$$\forall a \in \Omega \;\; \exists r, c_k \left(\forall \, \|z - a\| < r \left(f(z) = \sum_{k=0}^{\infty} c_k (z-a)^k \right) \right)$$

  - A *singularity of* f is any a s. t. f is analytic on $\Omega - \{a\}$ but not on Ω.
  - If f or any derivative of f has a singularity at $z \in C$, then the radius of convergence in C of $\sum_{n=0}^{\infty} \frac{(x-x_0)^n}{n!} f^{(n)}(x_0)$, is bounded above by $\| \, x_0 - z \, \|$.

- Example: $f(x) = x^\alpha$ where $0 < \alpha < 1$.
  - One singularity at $x = 0$
  - Radius of convergence for power series around $x = 1$ is 1.
  - Taylor series coefficients decline slowly:

$$a_k = \frac{1}{k!}\frac{d^k}{dx^k}(x^\alpha)|_{x=1} = \frac{\alpha(\alpha-1)\cdots(\alpha-k+1)}{1\cdot 2\cdot\cdots\cdot k}.$$

Table 6.1 (corrected): Taylor Series Approximation Errors for $x^{1/4}$

	Taylor series error				$x^{1/4}$
x N:	5	10	20	50	
3.0	5(−1)	8(1)	3(3)	1(12)	1.3161
2.0	1(−2)	5(−3)	2(−3)	8(−4)	1.1892
1.8	4(−3)	5(−4)	2(−4)	9(−9)	1.1583
1.5	2(−4)	3(−6)	1(−9)	0(−12)	1.1067
1.2	1(−6)	2(−10)	0(−12)	0(−12)	1.0466
.80	2(−6)	3(−10)	0(−12)	0(−12)	.9457
.50	6(−4)	9(−6)	4(−9)	0(−12)	.8409
.25	1(−2)	1(−3)	4(−5)	3(−9)	.7071
.10	6(−2)	2(−2)	4(−3)	6(−5)	.5623
.05	1(−1)	5(−2)	2(−2)	2(−3)	.4729

Rational Approximation

- Definition: A (m,n) Padé approximant of f at x_0 is a rational function

$$r(x) = \frac{p(x)}{q(x)},$$

where degree of p (q)is at most m (n), and

$$0 = \frac{d^k}{dx^k}(p - f\ q)\,(x_0), \quad k = 0, \cdots, m+n.$$

- Construction
  - Usually choose $m = n$ or $m = n+1$.
  - The $m+1$ coefficients of p and the $n+1$ coefficients of q must satisfy linear conditions

$$p^{(k)}\,(x_0) = (f\,q)^{(k)}\,(x_0), \quad k = 0, \cdots, m+n, \tag{6.1.2}$$

  - (6.1.2) plus $q(x_0) = 1$ forms $m+n+2$ linear conditions on the $m+n+2$ coefficients
  - Linear system may be singular; if so, reduce n or m by 1

- Example: (2,1) Pade approx. of $x^{1/4}$ at $x = 1$
  - Construct degree $m + n = 2 + 1 = 3$ Taylor series

$$t(x) = 1 + \frac{(x-1)}{4} - \frac{3(x-1)^2}{32} + \frac{7(x-1)^3}{128} \equiv t(x).$$

  - Find p_0, p_1, p_2, and q_1 such that

$$p_0 + p_1(x-1) + p_2(x-1)^2 - t(x)(1 + q_1(x-1)) = 0 \tag{6.1.3}$$

  - Combine coefficients of like powers in (6.1.3) implies

$$\frac{21 + 70x + 5x^2}{40 + 56x}. \tag{6.1.4}$$

- Pade approximation is often better; not limited by singularities

Log-Linearization, Log-Quadraticization

- Log-linear approximation

  – Suppose we have an equation

  $$f\,(x,\varepsilon) = 0$$

  that defines x in terms of ε.

  – Implicit differentiation implies

  $$\hat{x} = \frac{dx}{x} = -\frac{\varepsilon f_\varepsilon}{x f_x}\frac{d\varepsilon}{\varepsilon} = -\frac{\varepsilon f_\varepsilon}{x f_x}\;\varepsilon,$$

  – Since $\hat{x} = d(\ln x)$, log-linearization implies log-linear approximation

  $$\ln x - \ln x_0 \doteq -\frac{\varepsilon_0 f_\varepsilon(x_0,\varepsilon_0)}{x_0 f_x(x_0,\varepsilon_0)}(\ln\varepsilon - \ln\varepsilon_0). \tag{6.1.5}$$

  which implies

  $$x \doteq x_0 \exp\left(-\frac{\varepsilon_0 f_\varepsilon(x_0,\varepsilon_0)}{x_0 f_x(x_0,\varepsilon_0)}(\ln\varepsilon - \ln\varepsilon_0)\right), \tag{6.1.6}$$

- Generalization to nonlinear change of variables.
  - Suppose $Y(X)$ implicitly defined by $f(Y(X), X) = 0$.
  - Define $x = \ln X$ and $y = \ln Y$, then $y(x) = \ln Y(e^x)$.
  - $f(Y(X), X) = 0$ is equivalent to $f(e^{y(x)}, e^x) \equiv g(y(x), x) = 0$.
  - Implicit differentiation of $g(y(x), x) = 0$ implies $y'(x) = \frac{d \ln Y}{d \ln X}$ and (6.1.5)
  - $\ln Y(X) = y(x)$ also suggests the second-order approximation

$$\ln Y(X) = y(x) \doteq y(x_0) + y'(x)(x - x_0) + y''(x_0)\frac{(x - x_0)^2}{2}, \tag{6.1.7}$$

  - Can construct Padé expansions in terms of the logarithm.
  - There is nothing special about log function.
    - Take any monotonic $h(\cdot)$
    - Define $x = h(X)$ and $y = h(Y)$
    - Use the identity

$$\begin{aligned} f(Y, X) &= f(h^{-1}(h(Y)), h^{-1}(h(X))) \\ &= f(h^{-1}(y), h^{-1}(x)) \\ &\equiv g(y, x). \end{aligned}$$

      to generate expansions

$$\begin{aligned} y(x) &\doteq y(x_0) + y'(x)(x - x_0) + \ldots \\ Y(X) &\doteq h^{-1}\left(y(h(X_0)) + y'(h(X_0))(h(X) - h(X_0)) + \ldots\right) \end{aligned}$$

    - $h(z) = \ln z$ is natural for economists, but others may be better globally

Types of Approximation Methods

- Interpolation Approach: find a function from an n-dimensional family of functions which exactly fits n data items

- Lagrange polynomial interpolation

  - Data: $(x_i, y_i)\,, i = 1, .., n.$
  - Objective: Find a polynomial of degree $n-1$, $p_n(x)$, which agrees with the data, i.e.,

$$y_i = f(x_i),\ \ i = 1, .., n$$

  - Result: If the x_i are distinct, there is a unique interpolating polynomial

- Question: Suppose that $y_i = f(x_i)$. Does $p_n(x)$ converge to $f(x)$ as we use more points?
- Convergence Counterexample
  - Suppose
$$f(x) = \frac{1}{1+x^2}, \quad x_i : \text{uniform on } [-5, 5]$$
  - Degree 10 (11 points) result:

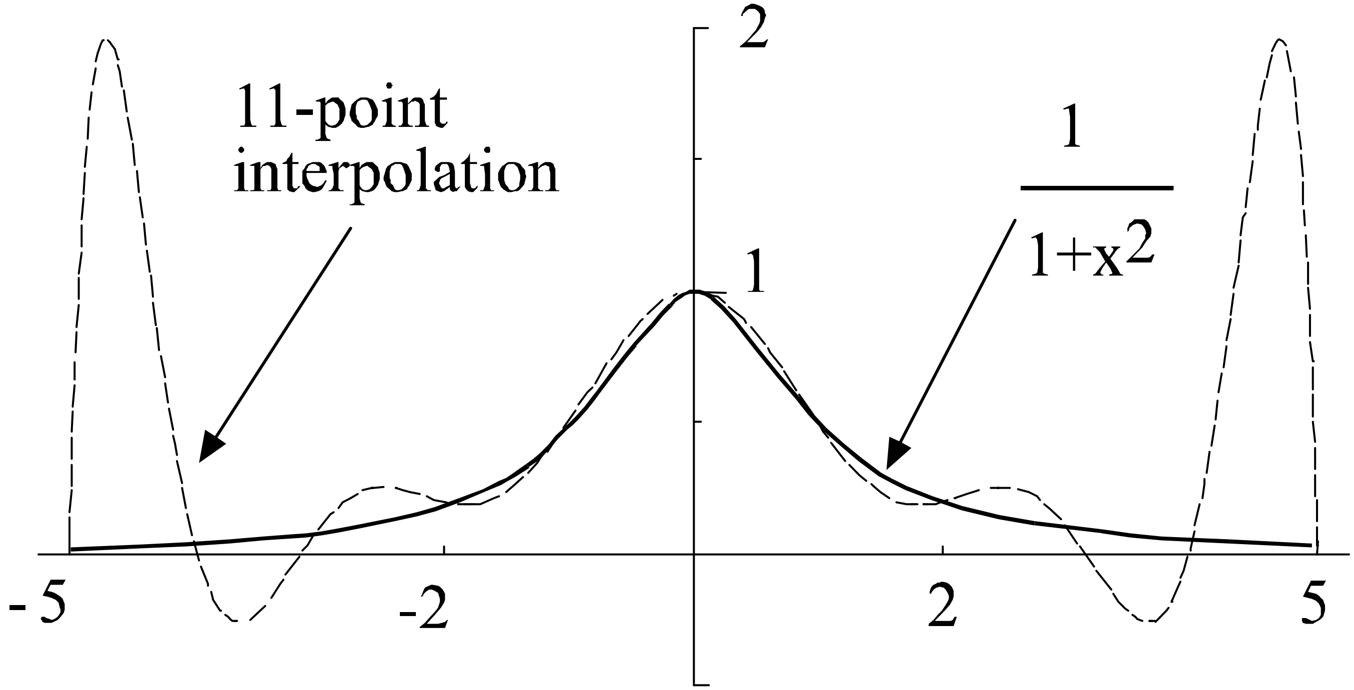


Figure 1:

- Hermite polynomial interpolation
  - Data: (x_i, y_i, y_i') , $i = 1, .., n$.
  - Objective: Find a polynomial of degree $2n - 1$, $p(x)$, which agrees with the data, i.e.,

$$y_i = p(x_i), \;\; i = 1, .., n$$
$$y_i' = p'(x_i), \;\; i = 1, .., n$$

  - Result: If the x_i are distinct, there is a unique interpolating polynomial
- Least squares approximation
  - Data: A function, $f(x)$.
  - Objective: Find a function $g(x)$ from a class G that best approximates $f(x)$, i.e.,

$$g = \arg\max_{g \in G} \|f - g\|^2$$

Orthogonal polynomials

- General orthogonal polynomials
  - Space: polynomials over domain D
  - weighting function: $w(x) > 0$
  - Inner product: $\langle f, g \rangle = \int_D f(x)g(x)w(x)dx$
  - Definition: $\{\phi_i\}$ is a family of orthogonal polynomials w.r.t $w(x)$ iff

$$\left\langle \phi_i, \phi_j \right\rangle = 0, \; i \neq j$$

  - We like to compute orthogonal polynomials using recurrence formulas

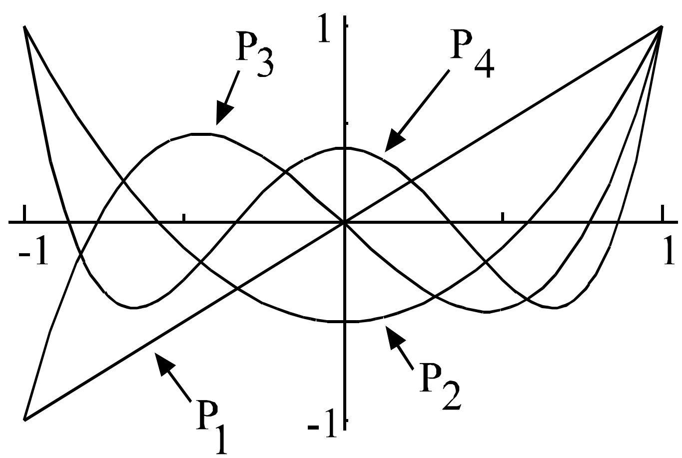
$$\begin{aligned}\phi_0(x) &= 1 \\ \phi_1(x) &= x \\ \phi_{k+1}(x) &= (a_{k+1}x + b_k)\, \phi_k(x) + c_{k+1}\phi_{k-1}(x)\end{aligned}$$

  - Approximation (assuming $\|\phi_i\| = 1$):

$$\begin{aligned}f(x) &= \sum_{i=0}^{\infty} a_i \phi_i \\ a_i &= \langle f, \phi_i \rangle = \int_D f(x)\phi_i(x)\, w(x)dx, \; i \neq j\end{aligned}$$

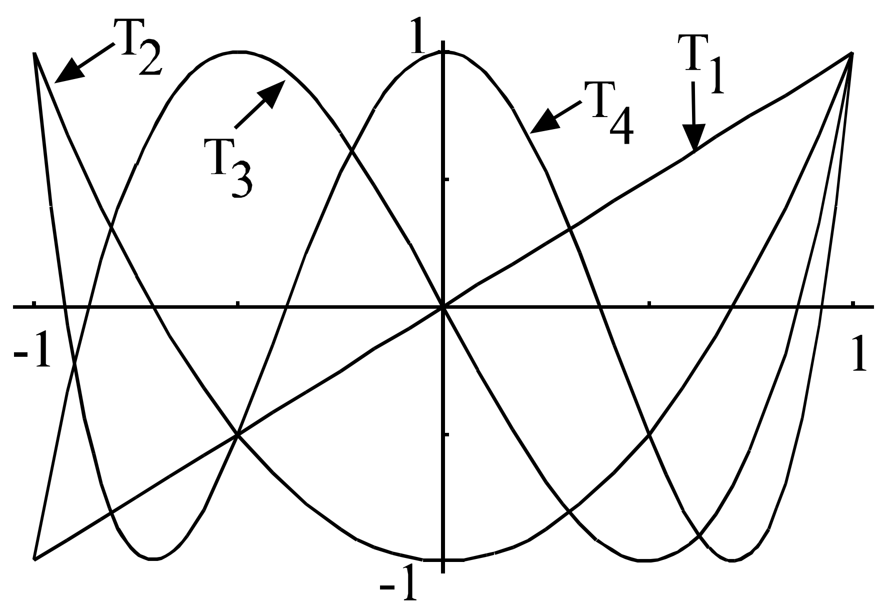
- Legendre polynomials
  - $[a, b] = [-1, 1]$
  - $w(x) = 1$
  - $P_n(x) = \frac{(-1)^n}{2^n n!} \frac{d^n}{dx^n} \left[(1 - x^2)^n\right]$
  - Recurrence formula:

$$
\begin{aligned}
P_0(x) &= 1 \\
P_1(x) &= x \\
P_{n+1}(x) &= \frac{2n+1}{n+1} \, x \, P_n(x) - \frac{n}{n+1} \, P_{n-1}(x),
\end{aligned}
$$



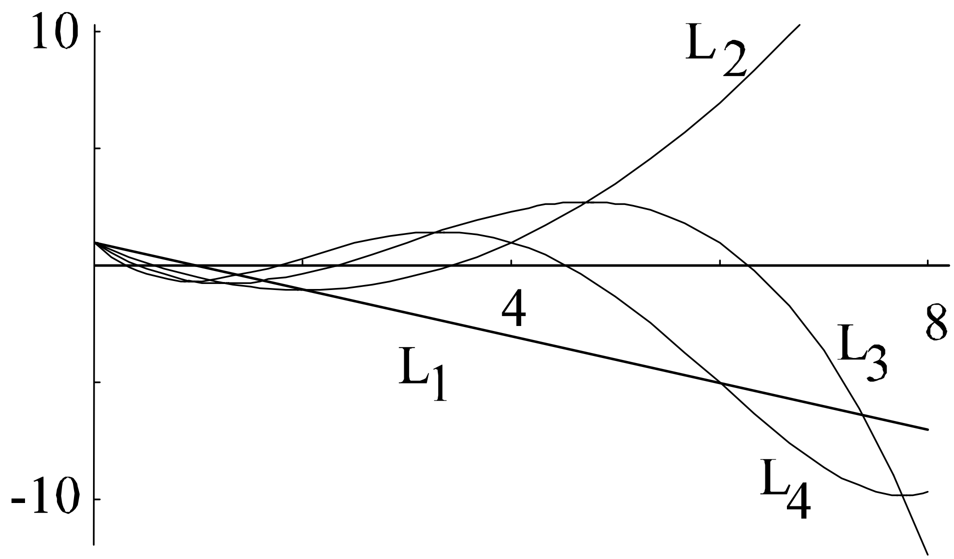
- Chebyshev polynomials
  - $[a, b] = [-1, 1]$
  - $w(x) = \left(1 - x^2\right)^{-1/2}$
  - $T_n(x) = \cos(n \cos^{-1} x)$
  - Recurrence formula:

$$T_0(x) = 1$$
$$T_1(x) = x$$
$$T_{n+1}(x) = 2x\, T_n(x) - T_{n-1}(x),$$



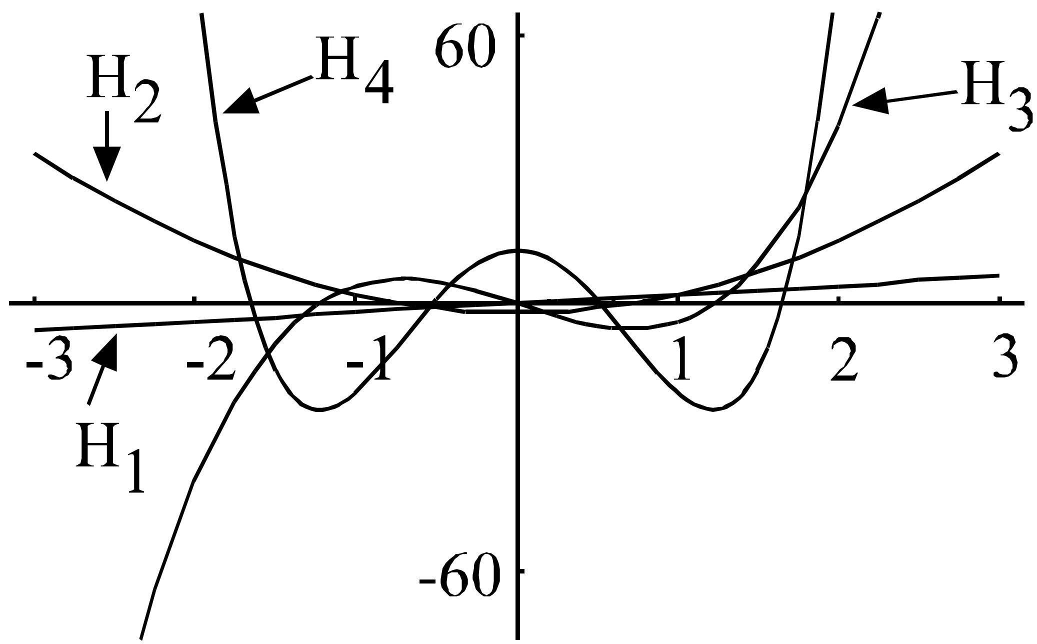
- Laguerre polynomials
  - $[a,b] = [0,\infty)$
  - $w(x) = e^{-x}$
  - $L_n(x) = \frac{e^x}{n!}\,\frac{d^n}{dx^n}\,(x^n\,e^{-x})$
  - Recurrence formula:

$$L_0(x) = 1$$
$$L_1(x) = 1 - x$$
$$L_{n+1}(x) = \frac{1}{n+1}\,(2n+1-x)\,L_n(x) - \frac{n}{n+1}\,L_{n-1}(x),$$



- Hermite polynomials
  - $[a,b] = (-\infty, \infty)$
  - $w(x) = e^{-x^2}$
  - $H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n} \left(e^{-x^2}\right)$
  - Recurrence formula:

$$
\begin{aligned}
H_0(x) &= 1 \\
H_1(x) &= 2x \\
H_{n+1}(x) &= 2x\, H_n(x) - 2n\, H_{n-1}(x).
\end{aligned}
$$



- General Orthogonal Polynomials
  - Few problems have the specific intervals and weights used in definitions
  - One must adapt interval through linear COV
    - If compact interval $[a, b]$ is mapped to $[-1, 1]$ by

$$y = -1 + 2\frac{x-a}{b-a}$$

then $\phi_i\left(-1 + 2\frac{x-a}{b-a}\right)$ are orthogonal over $x \in [a, b]$ with respect to $w\left(-1 + 2\frac{x-a}{b-a}\right)$ iff $\phi_i(y)$ are orthogonal over $y \in [-1, 1]$ w.r.t. $w(y)$

    - If half-infinite interval $[a, \infty]$ is mapped to $[0, \infty]$ by

$$y = \frac{x-a}{\lambda}$$
$$w(y) = e^{-y}$$

then $\phi_i\left(\frac{x-a}{\lambda}\right)$ are orthogonal over $x \in [a, \infty]$ w.r.t. $w\left(\frac{x-a}{\lambda}\right)$ iff $\phi_i(y)$ are orthogonal over $y \in [0, \infty]$ w.r.t. $w(y)$

    - If $[-\infty, \infty]$ is mapped to $[-\infty, \infty]$ by

$$y = (x - \mu) \Big/ \sqrt{\lambda}$$
$$w(y) = e^{-y^2}$$

then $\phi_i\left(\frac{x-\mu}{\sqrt{\lambda}}\right)$ are orthogonal over $x \in [a, \infty]$ w.r.t. $w\left(\frac{x-\mu}{\sqrt{\lambda}}\right)$ iff $\phi_i(y)$ are orthogonal over $y \in [0, \infty]$ w.r.t. $w(y)$

- Trigonometric polynomials and Fourier series
  - $\{\cos(n\theta), \sin(m\theta)\}$ are orthogonal on $[-\pi, \pi]$.
  - If f is continuous on $[-\pi, \pi]$ and $f(-\pi) = f(\pi)$, then

$$f(\theta) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \cos(n\theta) + \sum_{n=1}^{\infty} b_n \sin(n\theta)$$

    where the *Fourier coefficients* are

$$a_n = \frac{1}{\pi} \int_{\pi}^{\pi} f(\theta) \cos(n\theta) d\theta$$
$$b_n = \frac{1}{\pi} \int_{\pi}^{\pi} f(\theta) \sin(n\theta)\, d\theta,$$

  - A *trigonometric polynomial* is any function of the form in (6.4.4).
  - Convergence is uniform.
  - Excellent for approximating a smooth *periodic function*, i.e., $f : R \to R$ such that for some ω, $f(x) = f(x + \omega)$.
  - Not good for nonperiodic functions
    * Convergence is not uniform
    * Many terms are needed

Regression

- Data: (x_i, y_i) , $i = 1, .., n$.
- Objective: Find a function $f(x;\beta)$ with $\beta \in R^m$, $m \leq n$, with $y_i \doteq f(x_i), i = 1, .., n$.
- Least Squares regression:

$$\min_{\beta \in R^m} \sum \left(y_i - f\left(x_i;\beta\right)\right)^2$$

Chebyshev Regression

- Chebyshev Regression Data:
- (x_i, y_i) , $i = 1, .., n > m, x_i$ are the n zeroes of $T_n(x)$ adapted to $[a, b]$
- Chebyshev Interpolation Data:

(x_i, y_i) , $i = 1, .., n = m, x_i$ are the n zeroes of $T_n(x)$adapted to $[a, b]$

Algorithm 6.4: Chebyshev Approximation Algorithm in $\mathbb{R}^1$

- Objective: Given $f(x)$ defined on $[a, b]$, find a m-point degree n Chebyshev polynomial approximation $p(x)$
- Step 1: Compute the $m \geq n+1$ Chebyshev interpolation nodes on $[-1, 1]$:

$$z_k = -\cos\left(\frac{2k-1}{2m}\ \pi\right)\ ,\ \ k = 1, \cdots, m.$$

- Step 2: Adjust nodes to $[a, b]$ interval:

$$x_k = (z_k + 1)\left(\frac{b-a}{2}\right) + a, k = 1, ..., m.$$

- Step 3: Evaluate f at approximation nodes:

$$w_k = f(x_k)\ ,\ \ k = 1, \cdots, m.$$

- Step 4: Compute Chebyshev coefficients, $a_i, i = 0, \cdots, n$:

$$a_i = \frac{\sum_{k=1}^{m} w_k T_i(z_k)}{\sum_{k=1}^{m} T_i(z_k)^2}$$

  to arrive at approximation of $f(x, y)$ on $[a, b]$:

$$p(x) = \sum_{i=0}^{n} a_i T_i\left(2\frac{x-a}{b-a} - 1\right)$$

Minmax Approximation

- Data: $(x_i, y_i), i = 1, .., n.$
- Objective: L^∞ fit

$$\min_{\beta \in R^m} \max_i \|y_i - f(x_i; \beta)\|$$

- Problem: Difficult to compute

- Chebyshev minmax property

Theorem 1 *Suppose $f : [-1,1] \to R$ is C^k for some $k \geq 1$, and let I_n be the n-point (degree $n-1$) polynomial interpolation of f based at the zeroes of $T_n(x)$. Then*

$$\| f - I_n \|_\infty \leq \left(\frac{2}{\pi} \log(n+1) + 1 \right) \times \frac{(n-k)!}{n!} \left(\frac{\pi}{2} \right)^k \left(\frac{b-a}{2} \right)^k \| f^{(k)} \|_\infty$$

- Chebyshev interpolation:
  - converges in L^∞
  - essentially achieves minmax approximation
  - easy to compute
  - does *not* approximate f'

Splines

Definition 2 *A function $s(x)$ on $[a, b]$ is a spline of order n iff*

1. *s is C^{n-2} on $[a, b]$, and*
2. *there is a grid of points (called nodes) $a = x_0 < x_1 < \cdots < x_m = b$ such that $s(x)$ is a polynomial of degree $n-1$ on each subinterval $[x_i, x_{i+1}]$, $i = 0, \ldots, m-1$.*

Note: an order 2 spline is the piecewise linear interpolant.

- Cubic Splines
  - Lagrange data set: $\{(x_i,\, y_i) \mid i = 0,\, \cdots,\, n\}$.
  - Nodes: The x_i are the nodes of the spline
  - Functional form: $s(x) = a_i + b_i\, x + c_i\, x^2 + d_i\, x^3$ on $[x_{i-1},\, x_i]$
  - Unknowns: $4n$ unknown coefficients, $a_i, b_i, c_i, d_i, i = 1, \cdots n$.

- Conditions:
  - $2n$ interpolation and continuity conditions:

$$
\begin{aligned}
y_i = & a_i + b_i x_i + c_i x_i^2 + d_i x_i^3, \\
& i = 1, ., n \\
y_i = & a_{i+1} + b_{i+1} x_i + c_{i+1} x_i^2 + d_{i+1} x_i^3, \\
& i = 0, ., n-1
\end{aligned}
$$

  - $2n-2$ conditions from C^2 at the interior: for $i = 1, \cdots n-1$,

$$
\begin{aligned}
b_i + 2c_i x_i + 3d_i x_i^2 = & b_{i+1} + 2c_{i+1} x_i + 3d_{i+1} x_i^2 \\
2c_i + 6d_i x_i = & 2c_{i+1} + 6d_{i+1} x_i
\end{aligned}
$$

  - Equations (1–4) are $4n-2$ linear equations in $4n$ unknown parameters, a, b, c, and d.
  - construct 2 side conditions:
    * *natural spline:* $s'(x_0) = 0 = s'(x_n)$; it minimizes total curvature, $\int_{x_0}^{x_n} s''(x)^2 \, dx$, among solutions to (1-4).
    * *Hermite spline*: $s'(x_0) = y_0'$ and $s'(x_n) = y_n'$ (assumes extra data)
    * *Secant Hermite spline:* $s'(x_0) = (s(x_1) - s(x_0))/(x_1 - x_0)$ and $s'(x_n) = (s(x_n) - s(x_{n-1}))/(x_n - x_{n-1})$.
    * *not-a-knot*: choose $j = i_1, i_2$, such that $i_1 + 1 < i_2$, and set $d_j = d_{j+1}$.
  - Solve system by special (sparse) methods; see spline fit packages

- Quality of approximation

Theorem 3 *If* $f \in C^4[x_0, x_n]$ *and* s *is the Hermite cubic spline approximation to* f *on* $\{x_0, x_1, \cdots x_n\}$ *and* $h \geq \max_i\{x_i - x_{i-1}\}$*, then*

$$\| f - s \|_\infty \leq \frac{5}{384} \| f^{(4)} \|_\infty h^4$$

and

$$\| f' - s' \|_\infty \leq \left[\frac{\sqrt{3}}{216} + \frac{1}{24} \right] \| f^{(4)} \|_\infty h^3.$$

In general, order $k+2$ *splines with* n *nodes yield* $O(n^{-(k+1)})$ *convergence for* $f \in C^{k+1}[a, b]$*.*

- B-Splines: A basis for splines
  - Put knots at $\{x_{-k}, \cdots, x_{-1}, x_0, \cdots, x_n\}$.
  - Order 1 splines: step function interpolation spanned by

$$B_i^0(x) = \begin{cases} 0, & x < x_i, \\ 1, & x_i \le x < x_{i+1}, \\ 0, & x_{i+1} \le x, \end{cases}$$

  - Order 2 splines: piecewise linear interpolation and are spanned by

$$B_i^1(x) = \begin{cases} 0\ , & x \le x_i \text{ or } x \ge x_{i+2}, \\ \frac{x-x_i}{x_{i+1}-x_i}\ , & x_i \le x \le x_{i+1}, \\ \frac{x_{i+2}-x}{x_{i+2}-x_{i+1}}\ , & x_{i+1} \le x \le x_{i+2}. \end{cases}$$

    The B_i^1-spline is the tent function with peak at x_{i+1} and is zero for $x \le x_i$ and $x \ge x_{i+2}$.
  - Both B^0 and B^1 splines form cardinal bases for interpolation at the x_i's.
  - Higher-order B-splines are defined by the recursive relation

$$\begin{aligned} B_i^k(x) = & \left(\frac{x - x_i}{x_{i+k} - x_i}\right) B_i^{k-1}(x) \\ & + \left(\frac{x_{i+k+1} - x}{x_{i+k+1} - x_{i+1}}\right) B_{i+1}^{k-1}(x) \end{aligned}$$

Theorem 4 *Let S_n^k be the space of all order $k+1$ spline functions on $[x_0, x_n]$ with knots at $\{x_0, x_1, \cdots, x_n\}$. Then*

1. *The set*

$$\{B_i^k|_{[x_0,x_n]} \ : \ -k \le i \le n-1\}$$

forms a linearly independent basis for S_n^k, which has dimension $n+k$.

2. $B_i^k(x) \ge 0$ *and the support of* $B_i^k(x)$ *is* (x_i, x_{i+k+1}).

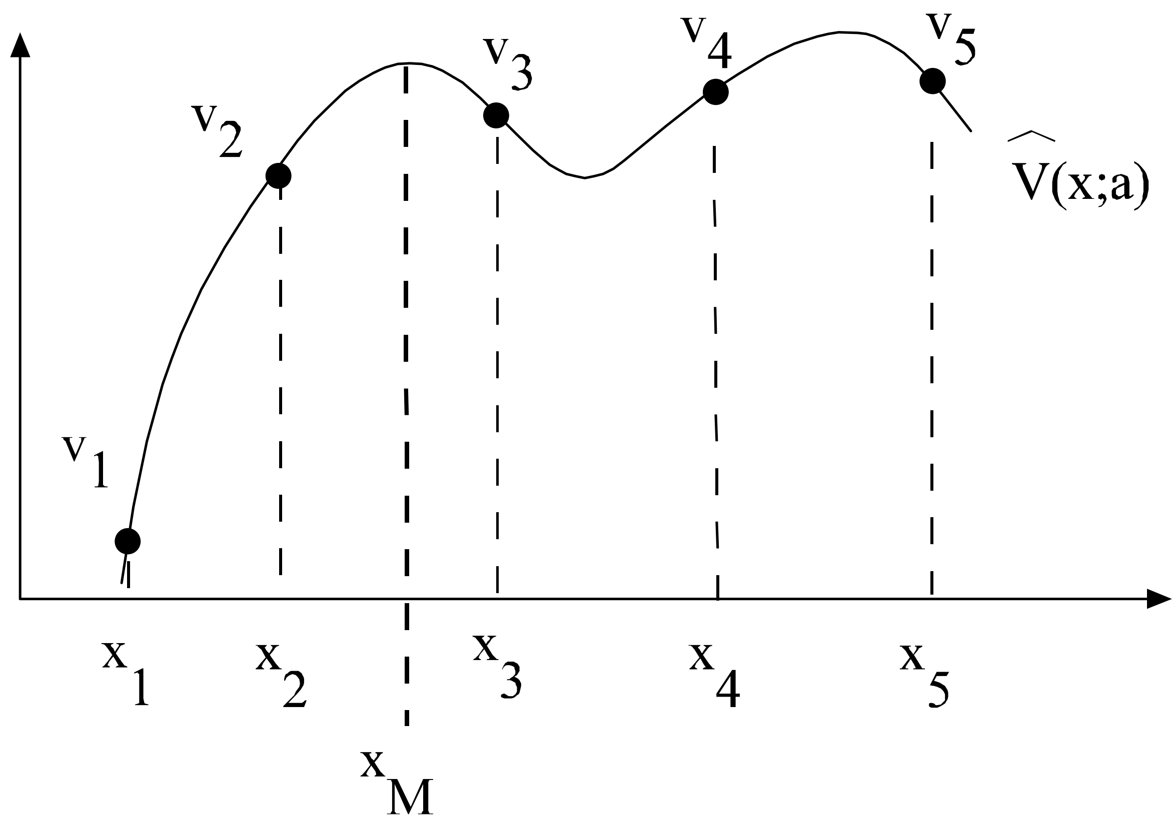
3. $\frac{d}{dx}\ (B_i^k(x)) = \left(\frac{k}{x_{i+k}-x_i}\right)\ B_i^{k-1}(x) - (\frac{k}{x_{i+k+1}-x_{i+1}})\ B_{i+1}^{k-1}(x)$.

4. *If we have Lagrange interpolation data, $(y_i, z_i), i = 1, \cdots, n+k$, and*

$$x_{i-k-1} < z_i < x_i\ ,\ \ 1 \le i \le n+k,$$

then there is an interpolant S in S_n^k such that $y = S(z_i),\ i = 1,..., n+k$.

- Shape-preservation
  - Concave (monotone) data may lead to nonconcave (nonmonotone) approximations.
  - Example



- Schumaker Procedure:

  1. Take level (and maybe slope) data at nodes x_i
  2. Add intermediate nodes $z_i^+ \in [x_i, x_{i+1}]$
  3. Run quadratic spline with nodes at the x and z nodes which intepolate data and preserves shape.
  4. Schumaker formulas tell one how to choose the z and spline coefficients (see book and correction at book's website)

- Many other procedures exist for one-dimensional problems
- Few procedures exist for two-dimensional problems
- Higher dimensions are difficult, but many questions are open.

- Spline summary:
  - Evaluation is cheap
    - Splines are locally low-order polynomial.
    - Can choose intervals so that finding which $[x_i, x_{i+1}]$ contains a specific x is easy.
    - Finding enclosing interval for general x_i sequence requires at most $\lceil \log_2 n \rceil$ comparisons
  - Good fits even for functions with discontinuous or large higher-order derivatives. E.g., quality of cubic splines depends only on $f^{(4)}(x)$, not $f^{(5)}(x)$.
  - Can use splines to preserve shape conditions

Multidimensional approximation methods

- Lagrange Interpolation
  - Data: $D \equiv \{(x_i, z_i)\}_{i=1}^N \subset R^{n+m}$, where $x_i \in R^n$ and $z_i \in R^m$
  - Objective: find $f : R^n \to R^m$ such that $z_i = f(x_i)$.
- Counterexample:
  - Interpolation nodes:

$$\{P_1, P_2, P_3, P_4\} \equiv \{(1,0), (-1,0), (0,1), (0,-1)\}$$

  - Use linear combinations of $\{1, x, y, xy\}$.
  - Data: $z_i = f(P_i), i = 1, 2, 3, 4$.
  - Interpolation form $f(x, y) = a + bx + cy + dxy$
  - Defining conditions form the singular system

$$\begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & -1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{pmatrix},$$

  - Task: Find combinations of interpolation nodes and spanning functions to produce a nonsingular (well-conditioned) interpolation matrix.

Tensor products

- General Approach:
  - If A and B are sets of functions over $x \in R^n$, $y \in R^m$, their tensor product is
  $$A \otimes B = \{\varphi(x)\psi(y) \mid \varphi \in A,\ \psi \in B\}.$$
  - Given a basis for functions of x_i, $\Phi^i = \{\varphi^i_k(x_i)\}_{k=0}^{\infty}$, the *n-fold tensor product* basis for functions of $(x_1, x_2, \ldots, x_n)$ is
  $$\Phi = \left\{ \prod_{i=1}^{n} \varphi^i_{k_i}(x_i) \mid k_i = 0, 1, \cdots,\ i = 1, \ldots, n \right\}$$
- Orthogonal polynomials and Least-square approximation
  - Suppose Φ^i are orthogonal with respect to $w_i(x_i)$ over $[a_i, b_i]$
  - Least squares approximation of $f(x_1, \cdots, x_n)$ in Φ is
  $$\sum_{\varphi \in \Phi} \frac{\langle \varphi, f \rangle}{\langle \varphi, \varphi \rangle} \varphi,$$
  where the product weighting function
  $$W(x_1, x_2, \cdots, x_n) = \prod_{i=1}^{n} w_i(x_i)$$
  defines $\langle \cdot, \cdot \rangle$ over $D = \prod_i [a_i, b_i]$ in
  $$\langle f(x), g(x) \rangle = \int_D f(x) g(x) W(x) dx.$$

Algorithm 6.4: Chebyshev Approximation Algorithm in $\mathbb{R}^2$

- Objective: Given $f(x,y)$ defined on $[a,b]\times[c,d]$, find the m-point degree n Chebyshev polynomial approximation $p(x,y)$
- Step 1: Compute the $m \geq n+1$ Chebyshev interpolation nodes on $[-1,1]$:
$$z_k = -\cos\left(\frac{2k-1}{2m}\ \pi\right)\ ,\ \ k=1,\cdots,m.$$
- Step 2: Adjust nodes to $[a,b]$ and $[c,d]$ intervals:
$$x_k = (z_k+1)\left(\frac{b-a}{2}\right)+a, k=1,...,m.$$
$$y_k = (z_k+1)\left(\frac{d-c}{2}\right)+c, k=1,...,m.$$
- Step 3: Evaluate f at approximation nodes:
$$w_{k,\ell} = f(x_k, y_\ell)\ ,\ \ k=1,\cdots,m.\ ,\ \ \ell=1,\cdots,m.$$
- Step 4: Compute Chebyshev coefficients, $a_{ij}, i,j=0,\cdots,n:$
$$a_{ij} = \frac{\sum_{k=1}^{m}\sum_{\ell=1}^{m} w_{k,\ell}T_i(z_k)T_j(z_\ell)}{\left(\sum_{k=1}^{m} T_i(z_k)^2\right)\left(\sum_{\ell=1}^{m} T_j(z_\ell)^2\right)}$$
to arrive at approximation of $f(x,y)$ on $[a,b]\times[c,d]$:
$$p(x,y) = \sum_{i=0}^{n}\sum_{j=0}^{n} a_{ij}T_i\left(2\frac{x-a}{b-a}-1\right)T_j\left(2\frac{y-c}{d-c}-1\right)$$

Multidimensional Splines

- B-splines: Multidimensional versions of splines can be constructed through tensor products; here B-splines would be useful.
- Summary
  - Tensor products directly extend one-dimensional methods to n dimensions
  - Curse of dimensionality often makes tensor products impractical

Complete polynomials

- Taylor's theorem for $\mathbb{R}^n$ produces the approximation

$$
\begin{aligned}
f(x) \doteq\, & f(x^0) \\
& + \textstyle\sum_{i=1}^{n} \frac{\partial f}{\partial x_i}(x^0)\ (x_i - x_i^0) \\
& + \frac{1}{2} \textstyle\sum_{i_1=1}^{n} \sum_{i_2=1}^{n} \frac{\partial^2 f}{\partial x_{i_1} \partial x_{i_k}}(x_0)(x_{i_1} - x_{i_1}^0)(x_{i_k} - x_{i_k}^0) \\
& \vdots
\end{aligned}
$$

  - For $k = 1$, Taylor's theorem for n dimensions used the linear functions

$$\mathcal{P}_1^n \equiv \{1, x_1, x_2, \cdots, x_n\}$$

  - For $k = 2$, Taylor's theorem uses

$$\mathcal{P}_2^n \equiv \mathcal{P}_1^n \cup \{x_1^2, \cdots, x_n^2, x_1 x_2, x_1 x_3, \cdots, x_{n-1} x_n\}.$$

    $\mathcal{P}_2^n$ contains some product terms, but not all; for example, $x_1 x_2 x_3$ is not in $\mathcal{P}_2^n$.

- In general, the kth degree expansion uses the *complete set of polynomials of total degree k in n variables.*

$$\mathcal{P}_k^n \equiv \{x_1^{i_1} \cdots x_n^{i_n} \mid \sum_{\ell=1}^{n} i_\ell \leq k,\ 0 \leq i_1, \cdots, i_n\}$$

- Complete orthogonal basis includes only terms with total degree k or less.

- Sizes of alternative bases

degree k	$\mathcal{P}_k^n$	Tensor Prod.
2	$1+n+n(n+1)/2$	3^n
3	$1+n+\frac{n(n+1)}{2}+n^2+\frac{n(n-1)(n-2)}{6}$	4^n

  - Complete polynomial bases contains fewer elements than tensor products.
  - Asymptotically, complete polynomial bases are as good as tensor products.
  - For smooth n-dimensional functions, complete polynomials are more efficient approximations

- Construction

  - Compute tensor product approximation, as in Algorithm 6.4
  - Drop terms not in complete polynomial basis (or, just compute coefficients for polynomials in complete basis).
  - Complete polynomial version is faster to compute since it involves fewer terms

Nonlinear approximation methods

- Neural Network Definitions:

  – A *single-layer* neural network is a function of form

$$F(x;\beta) \equiv h\left(\sum_{i=1}^{n} \beta_i g\left(x_i\right)\right)$$

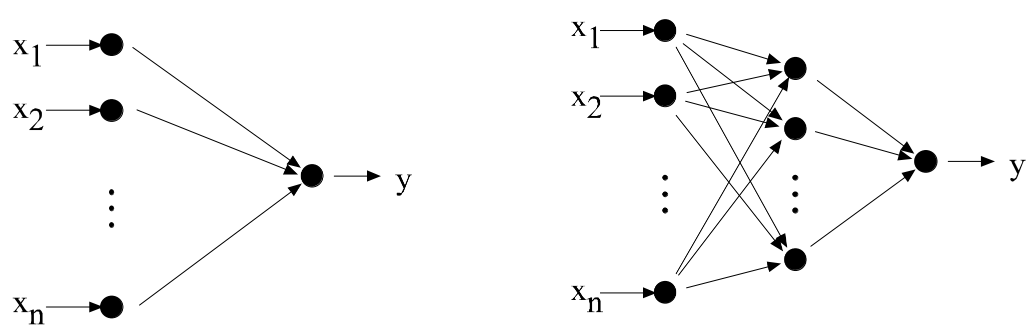
  where

  * $x \in R^n$ is the vector of inputs
  * h and g are scalar functions (e.g., $g(x) = x$)

  – A *single hidden-layer feedforward* neural network is a function of form

$$F(x;\beta,\gamma) \equiv f\left(\sum_{j=1}^{m} \gamma_j h\left(\sum_{i=1}^{n} \beta_i^j g\left(x_i\right)\right)\right),$$

  where h is called the *hidden-layer activation function.*



(a) (b)

- Neural Network Approximation: We form least-squares approximations by solving either

$$\min_{\beta} \sum_{j} \left(y_j - F(x^j;\beta)\right)^2$$

or

$$\min_{\beta,\gamma} \sum_{j} (y_j - F(x^j;\beta,\gamma))^2.$$

Theorem 5 : *(Universal approximation theorem) Let G be a continuous function, $G : R \rightarrow R$, such that either*

1. $\int_{-\infty}^{\infty} G(x)dx$ *is finite and nonzero and G is L^p for $1 \leq p < \infty$, or*
2. $G : R \rightarrow [0,1]$, *G nondecreasing,* $\lim_{x\rightarrow\infty} G(x) = 1$, *and* $\lim_{x\rightarrow-\infty} G(x) = 0$ *(i.e., G is a squashing function)*

Let $\Sigma^n(G)$ be the set of all possible single hidden-layer feedforward neural networks using, G as the hidden layer activation function; that is, of the form $\sum_{j=1}^{m} \beta_j G(w^j x + b_j)$ for $x, w^j \in R^n$ and scalar b_j. Let $f : R^n \rightarrow R$ be continuous. Then for all $\varepsilon > 0$, probability measures μ, and compact sets $K \subset R^n$, there is a $g \in \Sigma^n(G)$ such that

$$\sup_{x \in K} |f(x) - g(x)| \leq \varepsilon$$

and $\int_K |f(x) - g(x)| \, d\mu \quad \leq \varepsilon.$

Remark 6 *The logistic function is a popular squashing function.*

- Neural Networks are optimal in some sense:

Theorem 7 *(Barron's theorem) Neural nets are asymptotically the most efficient approximations for smooth functions of dimension greater than two.*

- Neural network summary:
  - flexible functional form
  - neural networks add squashing function to basic list of operations.
  - asymptotically efficient
  - difficult to solve necessary global optimization problem
  - do not know what points to use for approximation purposes
  - Just one example of possible nonlinear functional forms, all of which add some function besides multiplication and addition.

Approximation Methods: Summary

- Interpolation versus regression
  - Lagrange data uses level information only
  - Hermite data also uses slope information
  - Regression uses more points than coefficients
- One-dimensional problems
  - Smooth approximations
    * Orthogonal polynomial methods for nonperiodic functions
    * Fourier approximations for periodic functions
  - Less smooth approximations
    * Splines
    * Shape-preserving splines

- Multidimensional data
  - Tensor product methods have curse of dimension
  - Complete polynomials are more efficient
  - Neural networks are most efficient
- Approximation versus Statistics
  - Similarities:
    * both approximate unknown functions
    * both use finite amount of data
  - Differences
    * approximation uses error-free data, not noisy data
    * approximation generates data, not constrained by observations