

APPROXIMATION METHODS

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Approximation Methods

- ▶ General Objective: Given data about $f(x)$ construct simpler $g(x)$ to approximate $f(x)$.
- ▶ Questions:
 - ▶ What data should be produced and used?
 - ▶ What family of “simpler” functions should be used?
 - ▶ What notion of approximation do we use?
- ▶ Comparisons with statistical regression
 - ▶ Both approximate an unknown function and use a finite amount of data
 - ▶ Statistical data is noisy but we assume data errors are small
 - ▶ Nature produces data for statistical analysis but we produce the data in function approximation

Interpolation Methods

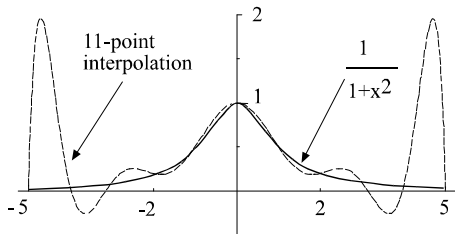
- ▶ Interpolation: find $g(x)$ from an n -dimensional family of functions to exactly fit n data points
- ▶ Lagrange polynomial interpolation
 - ▶ Data: $(x_i, y_i), i = 1, \dots, n$.
 - ▶ Objective: Find a polynomial of degree $n - 1$, $p_n(x)$, which agrees with the data, i.e.,

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

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

- ▶ Does $p_n(x)$ converge to $f(x)$ as we use more points?
- ▶ No! Consider

$$f(x) = \frac{1}{1+x^2}$$
$$x_i = -5, -4, \dots, 3, 4, 5$$



- ▶ Why does this fail? because there are zero degrees of freedom? bad choice of points? bad function?

▶ Hermite polynomial interpolation

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

$$y_i = p(x_i), i = 1, \dots, n$$

$$y'_i = p'(x_i), i = 1, \dots, n$$

- ▶ 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.,

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

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

$$\langle \phi_i, \phi_j \rangle = 0, \quad i \neq j$$

- ▶ We can compute orthogonal polynomials using recurrence formulas

$$\phi_0(x) = 1$$

$$\phi_1(x) = x$$

$$\phi_{k+1}(x) = (a_{k+1}x + b_k)\phi_k(x) + c_{k+1}\phi_{k-1}(x)$$

► Chebyshev polynomials

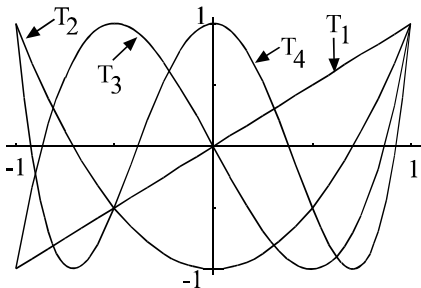
- $[a, b] = [-1, 1]$ and $w(x) = (1 - x^2)^{-1/2}$
- $T_n(x) = \cos(n \cos^{-1} x)$
- Recursive definition

$$T_0(x) = 1$$

$$T_1(x) = x$$

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

► Graphs



▶ General intervals

- ▶ Few problems have the specific intervals and weights used in definitions
- ▶ One must adapt the polynomials to fit the domain through linear COV:

- ▶ Define the linear change of variables that maps the compact interval $[a, b]$ to $[-1, 1]$

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

- ▶ The polynomials $\phi_i^*(x) \equiv \phi_i\left(-1 + 2 \frac{x-a}{b-a}\right)$ are orthogonal over $x \in [a, b]$ with respect to the weight $w^*(x) \equiv \left(-1 + 2 \frac{x-a}{b-a}\right)$ iff the $\phi_i(y)$ are orthogonal over $y \in [-1, 1]$ w.r.t. $w(y)$

Regression

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

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

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

- ▶ Objective: Given $f(x)$ on $[a, b]$, find Chebyshev poly approx $p(x)$
- ▶ Step 1: Define $m \geq n + 1$ Chebyshev interpolation nodes on $[-1, 1]$:

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

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

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

- ▶ Step 3: Evaluate f at approximation nodes:

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

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

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

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

Minmax Approximation

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

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

- ▶ Problem: Difficult to compute
- ▶ Chebyshev minmax property

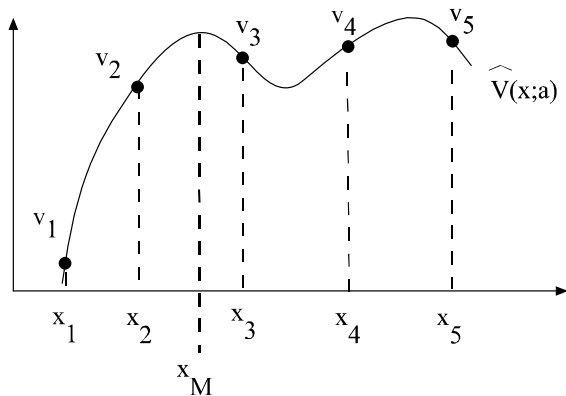
Suppose $f : [-1, 1] \rightarrow \mathbb{R}$ is C^k for some $k \geq 1$, and let I_n be the degree n polynomial interpolation of f based at the zeroes of $T_{n+1}(x)$. Then

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

- ▶ Chebyshev interpolation:
 - ▶ converges in L^∞ ; essentially achieves minmax approximation
 - ▶ works even for C^2 and C^3 functions
 - ▶ easy to compute
 - ▶ does *not* necessarily approximate f' well

Shape Issues

- ▶ Approximation methods and shape
 - ▶ Concave (monotone) data may lead to nonconcave (nonmonotone) approximations.
 - ▶ Shape problems destabilize value function iteration



Shape-preserving polynomial approximation

- ▶ Least squares Chebyshev approximation that preserves increasing concave shape with Lagrange data (x_i, v_i)

$$\begin{aligned} \min_{c_j} \quad & \sum_{i=1}^m \left(\sum_{j=0}^n c_j \phi_j(x_i) - v_i \right)^2 \\ \text{s.t.} \quad & \sum_{j=1}^n c_j \phi_j'(x_i) > 0, \\ & \sum_{j=1}^n c_j \phi_j''(x_i) < 0, \quad i = 1, \dots, m. \end{aligned}$$

- ▶ Least squares Chebyshev approximation preserving increasing concave shape with Hermite data (x_i, v_i, v'_i)

$$\begin{aligned} \min_{c_j} \quad & \sum_{i=1}^m \left(\sum_{j=0}^n c_j \phi_j(x_i) - v_i \right)^2 + \lambda \sum_{i=1}^m \left(\sum_{j=0}^n c_j \phi'_j(x_i) - v'_i \right)^2 \\ \text{s.t.} \quad & \sum_{j=1}^n c_j \phi'_j(x_i) > 0, \quad i = 1, \dots, m, \\ & \sum_{j=1}^n c_j \phi''_j(x_i) < 0, \quad i = 1, \dots, m. \end{aligned}$$

where λ is some parameter.

L1 Shape-preserving approximation

- ▶ L1 increasing concave approximation

$$\begin{aligned} \min_{c_j} \quad & \sum_{i=1}^m \left| \sum_{j=1}^n c_j \phi_j(x_i) - v_i \right| \\ \text{s.t.} \quad & \sum_{j=1}^n c_j \phi_j'(z_k) \geq 0, \quad k = 1, \dots, K \\ & \sum_{j=1}^n c_j \phi_j''(z_k) \leq 0, \quad k = 1, \dots, K \end{aligned}$$

- ▶ NOTE: We impose shape on a set of points, z_k , possibly different, and generally larger, from the approximation points, x_i .

- ▶ This looks like a nondifferentiable problem, but it is not when we rewrite it as

$$\begin{aligned} \min_{c_j, \lambda_i} \quad & \sum_{i=1}^m \lambda_i \\ \text{s.t.} \quad & \sum_{j=1}^n c_j \phi_j'(z_k) \geq 0, \quad k = 1, \dots, K \\ & \sum_{j=1}^n c_j \phi_j''(z_k) \leq 0, \quad k = 1, \dots, K \\ -\lambda_i \leq \quad & \sum_{j=1}^n c_j \phi_j(x_i) - v_i \leq \lambda_i, \quad i = 1, \dots, m \\ 0 \leq \quad & \lambda_i, \quad i = 1, \dots, m \end{aligned}$$

- ▶ Use possibly different points for shape constraints; generally you want more shape checking points than data points.
- ▶ Mathematical justification: semi-infinite programming
- ▶ Many other procedures exist for one-dimensional problems, but few procedures exist for two-dimensional problems

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 $f : R^n \rightarrow R^m$ such that $z_i = f(x_i)$.
- ▶ Need to choose nodes carefully.
- ▶ 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 , $\Phi^i = \{\varphi_k^i(x_i)\}_{k=0}^{\infty}$, the n -fold tensor product basis for functions of (x_1, x_2, \dots, x_n) is

$$\Phi = \left\{ \prod_{i=1}^n \varphi_{k_i}^i(x_i) \mid k_i = 0, 1, \dots, i = 1, \dots, n \right\}$$

- ▶ 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 $f(x_1, \dots, x_n)$ in Φ is

$$\sum_{\varphi \in \Phi} \frac{\langle \varphi, f \rangle}{\langle \varphi, \varphi \rangle} \varphi,$$

where the product weighting function

$$W(x_1, x_2, \dots, x_n) = \prod_{i=1}^n w_i(x_i)$$

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 its Chebyshev polynomial approximation $p(x, y)$

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

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

$$y_k = (z_k + 1)\left(\frac{d-c}{2}\right) + c, \quad k = 1, \dots, m.$$

$$w_{k,\ell} = f(x_k, y_\ell), \quad k = 1, \dots, m, \quad \ell = 1, \dots, m.$$

$$p(x, y) = \sum_{i=0}^n \sum_{j=0}^n a_{ij} T_i\left(2\frac{x-a}{b-a} - 1\right) T_j\left(2\frac{y-c}{d-c} - 1\right)$$

Polynomials

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

$$f(x) \doteq f(x^0) + \sum_{i=1}^n \frac{\partial f}{\partial x_i}(x^0) (x_i - x_i^0) \\ + \frac{1}{2} \sum_{i_1=1}^n \sum_{i_2=1}^n \frac{\partial^2 f}{\partial x_{i_1} \partial x_{i_2}}(x_0)(x_{i_1} - x_{i_1}^0)(x_{i_2} - x_{i_2}^0) + \dots$$

- ▶ For $k = 1$, Taylor's theorem for n dimensions used the linear functions $\mathcal{P}_1^n \equiv \{1, x_1, x_2, \dots, x_n\}$
- ▶ For $k = 2$, Taylor's theorem uses $\mathcal{P}_2^n \equiv \mathcal{P}_1^n \cup \{x_1^2, \dots, x_n^2, x_1 x_2, x_1 x_3, \dots, x_{n-1} x_n\}$.
- ▶ In general, the k th degree expansion uses the *complete set of polynomials of total degree k in n variables*.

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

- ▶ 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
- Almost as accurate as tensor product; in general, degree $k + 1$ complete is better than degree k tensor product but uses far fewer terms.

Shape Issues

- ▶ Much harder in higher dimensions
- ▶ No general method
- ▶ The L2 and L1 methods generalize to higher dimensions.
 - ▶ The constraints will be restrictions on directional derivatives in many directions
 - ▶ There will be many constraints
 - ▶ But, these will be linear constraints
 - ▶ L1 reduces to linear programming; we can now solve huge LP problems, so don't worry.