Approximation of Functions

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Minimax problem

Least-squares Approximation

Orthogonal polynomials

Revisit Chebyshev polynomial

Comparison with Machine Learning Models

Weierstrass Theorem

- Worse-case scenario error measure: Inf norm
- ▶ Inf norm: $||f(x) p(x)||_{\infty} = \max_{a \le x \le b} |f(x) p(x)|$
- ▶ Weierstrass THM: Let f(x) be continuous on [a,b] and let $\epsilon>0$. Then \exists a polynomial p(x) s.t.

$$||f(x) - p(x)||_{\infty} \le \epsilon, a \le x \le b.$$

▶ **Question**: Why the polynomial fails in the Runge phenomenon?

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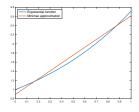
$$||f(x) - p(x)||_{\infty} \le \epsilon, a \le x \le b.$$

- Question: Why the polynomial fails in the Runge phenomenon?
- ▶ $||f^{(n)}(x)||_{\infty}$ increases fast w.r.t n
- Equispaced points error: $\|(x-x_0)\dots(x-x_n)\|_{\infty} \leq n! \left(\frac{b-a}{n}\right)^{n+1}$
- ► Polynomial is very powerful!
- Question: What is and how to find the best polynomial?



Minimax problem

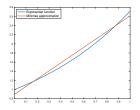
- Minimax problem $\min_{p_n} \|f p_n\|_{\infty}$
 - Given p_n , maximize $|f(x) p_n(x)|$
 - Find p_n , minimize $||f p_n||_{\infty}$
- ► E.g., $f(x) = e^x$, $p_n(x) = a + bx$, $x \in [0, 1]$



ightharpoonup arg $\max_x |f(x) - p_n(x)| =$

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- $\arg\max_{x} |f(x) p_n(x)| = 0, 1, \log(b), \|f g\|_{\infty} = \rho$
 - $e_1(0) = 1 a = \rho$
 - $e_1(\log(b)) = a + b\log(b) b = \rho = 1 a \Rightarrow a = \frac{e (e 1)\log(e 1)}{2}$
 - $e_1(1) = e a b = \rho = 1 a \Rightarrow b = e 1$
- ▶ THM: p_n minimizes $||f p_n||_{\infty}$ iff $\exists x_0 < \cdots < x_{n+1}$ s.t. $f(x_i) p_n(x_i) = \sigma(-1)^i ||f p_n||_{\infty}$, where σ is 1 or -1.

Near Minimax problem

- Minimax is too difficult, depends on f
- Interpolation error: $e_n = \left| \frac{f^{(n+1)}(\eta)}{(n+1)!} (x-x_0) \dots (x-x_n) \right|$
- ▶ Cannot control $f^{(n+1)}(x)$

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- ► Cannot control $f^{(n+1)}(x)$
- Near minimax: $\min_{x_0,\dots,x_n} |(x-x_0)\dots(x-x_n)|$
- ► Let $w_{n+1}(x) = (x x_0) \dots (x x_n)$
- ▶ THM: $w_{n+1}^*(x)$ is the solution iff $\exists \ a \leq \widetilde{x}_0 < \dots < \widetilde{x}_{n+1} \leq b$ s.t. $w_{n+1}^*(\widetilde{x}_i) = \sigma(-1)^i \|w_{n+1}\|_{\infty}$, where σ is 1 or -1.

Proof

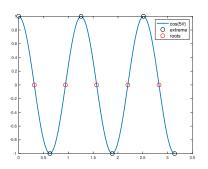
- ▶ **THM**: $w_{n+1}^*(x)$ is the solution iff $\exists a \leq \widetilde{x}_0 < \cdots < \widetilde{x}_{n+1} \leq b$ s.t. $w_{n+1}^*(\widetilde{x}_i) = \sigma(-1)^i ||w_{n+1}||_{\infty}$, where σ is 1 or -1.
- - ▶ Suppose q_n is a monic polynomial with $||q_{n+1}||_{\infty} < ||w_{n+1}^*||_{\infty}$
 - WLOG, assume $\sigma = 1$

 - $w_{n+1}^*(x) q_{n+1}(x)$ flips sign at least n+1 times $w_{n+1}^*(x) q_{n+1}(x)$ is a degree n polynomial (dominant term cancels)
 - $ightharpoonup IVT \Rightarrow n+1$ roots, contradiction
- **Question**: What function has such property?



Cosine function

 $ightharpoonup \cos((n+1)\theta)$ for $\theta \in [0,\pi]$



- **Extreme points:** $\theta_k = \frac{k\pi}{n+1}$, $0 \le k \le n+1$, $|\cos(\theta_k)| = 1$
- ▶ Roots: $\theta_k = \frac{(2k+1)\pi}{2n+2}$, $0 \le k \le n$



Find the polynomial

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- ▶ Roots: $\theta_k = \frac{(2k+1)\pi}{2n+2}$, $0 \le k \le n$
- ▶ But $cos(n\theta)$ is not a polynomial
- ▶ Suppose we focus on f(x) with $x \in [-1, 1]$
- ▶ Goal: find a function g(x) s.t.
 - $ightharpoonup \cos(n\theta)$ is a polynomial
 - $m{\theta} = g(x)$ s.t. $\cos(n\theta)$ has alternating extreme values
- Magic trick:

Find the polynomial

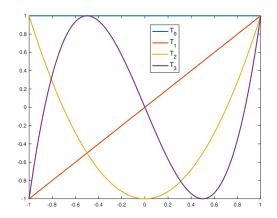
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 - $m{ heta} = g(x) ext{ s.t. } \cos(n\theta) ext{ has alternating extreme values}$
- Magic trick: $g(x) = \cos^{-1}(x)$
- $T_n(x) = \cos(n\cos^{-1}(x))$
 - $T_0(x) = \cos(0) = 1$
 - $ightharpoonup T_1(x) = x$
 - $T_{n\pm 1}(x) = \cos((n\pm 1)\theta) = \cos(n\theta)\cos(\theta) \mp \sin(n\theta)\sin(\theta)$
 - $T_{n+1}(x) + T_{n-1}(x) = 2\cos(n\theta)\cos(\theta) = 2T_n(x)x$
 - $T_{n+1}(x) = 2xT_n(x) T_{n-1}(x)$



Chebyshev polynomial

Chebyshev polynomial:

$$p_n(x) = \cos(n\theta) = \cos(n\cos^{-1}(x)), x \in [-1, 1]$$



Comparison

Chebyshev polynomial:

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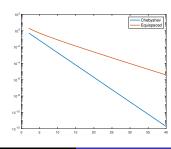
- **Extreme points**: $\theta_k = \frac{k\pi}{n+1}$, $0 \le k \le n+1$
- ▶ Error bound: $||(x-x_0)...(x-x_n)||_{\infty} \le$

Comparison

Chebyshev polynomial:

$$p_{n+1}(x) = \cos((n+1)\theta) = \cos((n+1)\cos^{-1}(x)), x \in [-1, 1]$$

- **Extreme points:** $\theta_k = \frac{k\pi}{n+1}$, $0 \le k \le n+1$
- First bound: $\|(x-x_0)\dots(x-x_n)\|_{\infty} \leq \frac{1}{2^{n-1}}$
 - \triangleright Extreme values: ± 1
 - $ightharpoonup T_0(x) = 1, T_1(x) = x$
 - Recurrence relationship: $T_{n+1}(x) = 2xT_n(x) T_{n-1}(x)$
- ▶ Equispaced points: $\|(x-x_0)\dots(x-x_n)\|_{\infty} \le n! \left(\frac{2}{n}\right)^{n+1}$
- ► Comparison:





Interpolation

- Chebyshev: $\cos((n+1)\theta) = \cos((n+1)\cos^{-1}(x)), x \in [-1, 1]$
- ▶ **Question**: how to interpolate a Chebyshev polynomial?

Interpolation

- ► Chebyshev: $\cos((n+1)\theta) = \cos((n+1)\cos^{-1}(x)), x \in [-1,1]$
- Question: how to interpolate a Chebyshev polynomial?
- $f(x) \approx p_n(x) = c_0 + c_1 x + \dots + c_n x^n$
- ▶ Roots: $\theta_k = \frac{(2k+1)\pi}{2n+2}$, $x_k = \cos(\theta_k)$, $0 \le k \le n$
- ightharpoonup Same way with different points: $\mathbf{Ac} = \mathbf{f}$

$$\begin{bmatrix} 1 & x_0 & \dots & x_0^n \\ 1 & x_1 & \dots & x_1^n \\ \vdots & \ddots & \ddots & \vdots \\ 1 & x_n & \dots & x_n^n \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ \vdots \\ c_n \end{bmatrix} = \begin{bmatrix} f(x_0) \\ f(x_1) \\ \vdots \\ f(x_n) \end{bmatrix}.$$

- ▶ Differentiation: same, $D = ABA^{-1}$
- ▶ Integration: same, $S = \widetilde{A}BA^{-1}$



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The least squares approximation problem

- ► Average error measurement: 2 norm
- Notation: $||g||_2 = \sqrt{\int_a^b |g(x)|^2} dx$
- ▶ Least squares approximation $\min_{p_n} \|f p_n\|_2^2$
- ► E.g. $f(x) = e^x$, $-1 \le x \le 1$, let $p_1(x) = c_0 + c_1 x$
- **Question**: How to minimize $r = ||f p_1(x)||_2^2$?

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- $0 = \frac{\partial r}{\partial c_0} = -2 \int_{-1}^1 e^x c_0 c_1 x \ dx$
- $0 = \frac{\partial r}{\partial c_1} = -2 \int_{-1}^{1} (e^x c_0 c_1 x) x \ dx$

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- $0 = \frac{\partial r}{\partial c_1} = -2 \int_{-1}^{1} (e^x c_0 c_1 x) x \ dx$
- $ightharpoonup c_0 = \frac{1}{2} \int_{-1}^1 e^x \ dx$
- $ightharpoonup c_1 = \frac{3}{2} \int_{-1}^1 x e^x \ dx$



General least squares problem

- $r = \int_a^b w(x)[f(x) p_n(x)]^2 dx$
- Examples:
 - $w(x) = 1, \ a \le x \le b$
 - $w(x) = \frac{1}{\sqrt{1-x^2}}, -1 \le x \le 1$
 - $w(x) = e^{-x^2}, -\infty < x < \infty$
- w(x) = 1 not necessarily always a good choice
- $\blacktriangleright \ w(x)$ allows different degrees of importance to different points
- Question: What are equations need to be solved?

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$$r(c_0, \dots, c_n) = \int_a^b w(x) \left[f(x) - \sum_{j=0}^n c_j x^j \right]^2 dx$$

- Question: How to solve this?



Solve the general least squares problem

► Form the linear system

Form the linear system
$$\begin{bmatrix} \int_a^b w(x) \ dx & \int_a^b w(x)x \ dx & \dots & \int_a^b w(x)x^n \ dx \\ \int_a^b w(x)x \ dx & \int_a^b w(x)x^2 \ dx & \dots & \int_a^b w(x)x^{n+1} \ dx \\ \vdots & & \ddots & \ddots & \vdots \\ \int_a^b w(x)x^n \ dx & \int_a^b w(x)x^{n+1} & \dots & \int_a^b w(x)x^{2n} \ dx \end{bmatrix} \begin{bmatrix} c_0 \\ c_1 \\ \vdots \\ c_n \end{bmatrix} = \begin{bmatrix} \int_a^b w(x)f(x) \ dx \\ \int_a^b w(x)f(x)x \ dx \\ \vdots \\ \int_a^b w(x)f(x)x^n \ dx \end{bmatrix}.$$

- Setting up the linear system requires a lot of integrals
- **Question**: Is there an alternative convenient way?



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Inner product

- ▶ Problem: Basis $\{x^n\}$ are very linearly dependent
- **Def**: **Inner product** of f and g:

$$(f,g) = \int_a^b w(x)f(x)g(x) \ dx.$$

- Properties:
 - $(\alpha f, g) = (f, \alpha g) = \alpha(f, g), \ \forall \alpha \in \mathbb{R}$
 - $(f_1 + f_2, g) = (f_1, g) + (f_2, g) \text{ and}$ $(f, g_1 + g_2) = (f, g_1) + (f, g_2)$
 - (f,g) = (g,f)
 - ► $(f, f) \ge 0$ and (f, f) = 0 iff f(x) = 0
- ▶ Def: Two norm: $\|f\|_2 = \sqrt{\int_a^b w(x) [f(x)]^2 \ dx} = \sqrt{(f,f)}$
- ▶ Lemma (Cauchy-Schwartz): $|(f,g)| \le ||f||_2 ||g_2||_2$
- Many properties in the textbook



Create orthogonal polynomials

- ▶ **Def**: f and g are **orthogonal** if (f,g) = 0
- ▶ **THM**: \exists a sequence of polynomials $\{\phi_n(x)|n\geq 0\}$ with $\deg(\phi_n)=n, \ \forall n, \ \text{and}$

$$(\phi_n, \phi_m) = 0, \quad \forall n \neq m, \quad n, m \ge 0.$$

In addition, if we require $(\phi_n, \phi_n) = 1$ and coefficients of x^n is positive, then the sequence $\{\phi_n\}$ is unique.

Question: Start with $1, x, \dots, x^n$, how to calculate it?

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- **Question**: Start with $1, x, \dots, x^n$, how to calculate it?
- Gram-Schmidt process:

$$\begin{split} \phi_0 &= \frac{1}{\|1\|_2}, \\ \phi_1 &= \frac{x - (\phi_0, x)\phi_0}{\|x - (\phi_0, x)\phi_0\|_2}, \\ \phi_2 &= \frac{x^2 - (\phi_0, x^2)\phi_0 - (\phi_1, x^2)\phi_1}{\|x^2 - (\phi_0, x^2)\phi_0 - (\phi_1, x^2)\phi_1\|_2}, \end{split}$$

Example

- ▶ Suppose w(x) = 1, [a, b] = [-1, 1]
- Question: How to calculate the first three orthogonal polynomials?

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- ▶ Suppose w(x) = 1, [a, b] = [-1, 1]
- Question: How to calculate the first three orthogonal polynomials?
- $(x, \phi_0)\phi_0 = \frac{1}{2} \int_{-1}^1 x \ dx = 0$
- $||x (x, \phi_0)\phi_0||_2^2 = \int_{-1}^1 x^2 \ dx = \frac{2}{3}$
- $(x^2, \phi_0)\phi_0 = \frac{1}{2} \int_{-1}^1 x^2 \ dx = \frac{1}{3}$
- $(x^2, \phi_1)\phi_1 = \frac{3}{2}x \int_{-1}^1 x^3 \ dx = 0$
- $||x^2 (x^2, \phi_0)\phi_0 (x^2, \phi_1)\phi_1||_2^2 = \int_{-1}^1 (x^2 \frac{1}{3})^2 dx = \frac{8}{45}$

QR decomposition

ightharpoonup Function version of QR?

QR decomposition

- Function version of QR?
- ► Gram-Schmidt: $\{1, x, \dots, x^n\} \Rightarrow \{\phi_0, \phi_1, \dots, \phi_n\}$

$$\mathbf{x}^T(x) = \begin{bmatrix} 1 & \dots & x^n \end{bmatrix}, \mathbf{q}^T(x) = \begin{bmatrix} \phi_0(x) & \dots & \phi_n(x) \end{bmatrix}$$

$$\mathbf{x}^T(x) = \begin{bmatrix} 1 & \dots & x^n \end{bmatrix} = \mathbf{q}^T(x)\mathbf{R}$$

$$x^k = c_0 \phi_0 + \dots + c_n \phi_n \Rightarrow c_i = (x^k, \phi_i)$$

$$(x^k, \phi_i) = 0 \text{ for } i > k$$

$$\mathbf{R} = \begin{bmatrix} (1, \phi_0) & (x, \phi_0) & \dots & (x^n, \phi_0) \\ 0 & (x, \phi_1) & \dots & (x^n, \phi_1) \\ \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \dots & (x^n, \phi_n) \end{bmatrix}$$

Relationship between two polynomials

Question: Relationships of coefficients?

Relationship between two polynomials

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- $p_n(x) = c_0 + \dots + c_n x^n = \begin{bmatrix} 1 & \dots & x^n \end{bmatrix} \begin{bmatrix} c_0 \\ \vdots \\ c_n \end{bmatrix} = \mathbf{x}^T(x)\mathbf{c}$
- $\mathbf{x}^T(x) = \mathbf{q}^T(x)\mathbf{R}$
- $p_n(x) = \mathbf{q}^T(x) \mathbf{R} \mathbf{c}$
- $q_n(x) = \mathbf{x}^T(x)\mathbf{R}^{-1}\mathbf{d}$



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Chebyshev polynomial

▶ **Def**: Chebyshev polynomial, $-1 \le x \le 1$

$$T_n(x) = \cos(n\theta) = \cos(n\cos^{-1}(x)).$$

- ▶ Chebyshev polynomial is orthogonal with $w(x) = \frac{1}{\sqrt{1-x^2}}$
- $T_m, T_n) = \int_{-1}^1 \frac{\cos(m \cos^{-1}(x)) \cos(n \cos^{-1}(x))}{\sqrt{1 x^2}} dx$

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- ► Change of variable: $x = \cos(\theta), dx = -\sin(\theta) d\theta$
- $(T_m, T_n) = \int_{\pi}^{0} \frac{\cos(m\theta)\cos(n\theta)}{\sqrt{1-\cos^2(\theta)}} (-\sin(\theta)) d\theta = \int_{0}^{\pi} \cos(m\theta)\cos(n\theta) d\theta$
- ► Recall: $2\cos(\theta)\cos(\eta) = \cos(\theta \eta) + \cos(\theta + \eta)$
- $(T_m, T_n) = \begin{cases} 0, & n \neq m, \\ \pi, & m = n = 0, \\ \frac{\pi}{2}, & n = m > 0. \end{cases}$



Chebyshev coefficients

$$f(x) = \frac{a_0}{2} + \sum_{i=1}^{n} a_i T_i(x)$$

Question: How are $\{a_i\}$ determined?

Chebyshev coefficients

- $f(x) = \frac{a_0}{2} + \sum_{i=1}^{n} a_i T_i(x)$
- **Question**: How are $\{a_i\}$ determined?
- $(T_j, f) = \frac{a_0}{2}(T_j, 1) + \sum_{i=1}^n a_i(T_j, T_i)$
- j = 0: $(T_0, f(x)) = \frac{a_0}{2}(T_0, T_0) = \frac{\pi}{2} \Rightarrow a_0 = \frac{2}{\pi}(T_0, f)$
- $j \neq 0 : (T_j, f(x)) = a_j(T_j, T_j) \Rightarrow a_j = \frac{2}{\pi}(T_j, f)$
- $a_j = \frac{2}{\pi} \int_{-1}^1 \frac{T_j(x)f(x)}{\sqrt{1-x^2}} \ dx = \frac{2}{\pi} \int_{-1}^1 \frac{\cos(j\cos^{-1}(x))f(x)}{\sqrt{1-x^2}} \ dx$
- $x = \cos(\theta), 0 \le \theta \le \pi$
- ► Cosine transform: $a_j = \frac{2}{\pi} \int_0^{\pi} f(\cos(\theta)) \cos(j\theta) \ d\theta$
- Question: How to discretize it?



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- $x = \cos(\theta), 0 \le \theta \le \pi$
- ► Cosine transform: $a_j = \frac{2}{\pi} \int_0^{\pi} f(\cos(\theta)) \cos(j\theta) \ d\theta$
- Question: How to discretize it?
- ► Chebyshev nodes: $x_k = \cos\left(\frac{2k+1}{2n+2}\pi\right)$, $0 \le k \le n$
- ▶ Discrete orthogonality: $\sum_{k=0}^{n} T_i(x_k) T_j(x_k) = K_i \delta_{i,j}$
- $ightharpoonup K_0=n+1$ and $K_i=rac{n+1}{2}$ for $1\leq i\leq n$



Least squares

- ▶ Consider orthogonal polynomials $T_j(x)$
- $p_n(x) = a_0 T_0(x) + \dots + a_n T_n(x)$
- $r = \|f p_n\|_2^2 = \int_{-1}^1 w(x) \left[f(x) \sum_{j=0}^n a_j T_j(x) \right]^2 dx$

- ▶ Inner product notation: $\sum_{j=0}^{n} a_j(T_j, T_k) = (f, T_k)$
- ▶ Orthogonality: $(T_j, T_k) = 0$ for $j \neq k$
- $a_k = \frac{(f, T_k)}{\|T_k\|_2^2}$
- $p_n^*(x) = \sum_{j=0}^n \frac{(f, T_j)}{\|T_j\|_2^2} T_j(x)$



Discrete cosine transform

- $p_n(x) = \frac{a_0}{2} + \sum_{j=1}^n a_j T_j(x)$
- $x_k = \cos\left(\frac{2k+1}{2n+2}\pi\right)$
- $ightharpoonup a_k = \frac{2}{n+1} \sum_{j=0}^n f(x_j) T_k(x_j)$
- $\theta_j = \frac{2j+1}{2N+2}\pi$
- **▶** Discrete cosine transform:

$$a_k = \frac{2}{n+1} \sum_{j=0}^n f(\cos(\theta_j)) \cos(n\theta_j)$$

Question: Matrix form



Connection with polynomial interpolation approach

- $f(x) \approx p_n(x) = \frac{a_0}{2} + \sum_{j=1}^n a_j T_j(x)$
- ▶ Chebyshev nodes: $x_k = \cos\left(\frac{2k+1}{2n+2}\pi\right) = \cos(\theta_k)$, $0 \le k \le n$
- ► $f(x_k) = p_n(x_k)$, **Aa** = **f**

$$\begin{bmatrix} \frac{1}{2} & \cos(\theta_0) & \dots & \cos(n\theta_0) \\ \frac{1}{2} & \cos(\theta_1) & \dots & \cos(n\theta_1) \\ \vdots & \ddots & \ddots & \vdots \\ \frac{1}{2} & \cos(\theta_n) & \dots & \cos(n\theta_n) \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} f(\cos(\theta_0)) \\ f(\cos(\theta_1)) \\ \vdots \\ f(\cos(\theta_n)) \end{bmatrix}$$

Orthogonality:

$$\mathbf{A}^T \mathbf{A} = \begin{bmatrix} \frac{n+1}{4} & 0 & \dots & 0 \\ 0 & \frac{n+1}{2} & \dots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & 0 & \dots & \frac{n+1}{2} \end{bmatrix}.$$



Differentiation and integration

- $f(x) = \frac{a_0}{2} + \sum_n a_n T_n(x)$
- $f'(x) = \frac{b_0}{2} + \sum_{n} b_n T_n(x)$
- Analytical computation:
 - Differentiation:

$$b_k = 2\sum_{\substack{j=k+1\\j+k \text{ odd}}} j \cdot a_j$$

► Integration:

$$c_k = \frac{1}{2k}(a_{k-1} - a_{k+1}), \ k \ge 1,$$

 $c_0 = 2(c_1 - c_2 + c_3 - \dots)$

- Matrix version:
 - ► A as the discrete cosine matrix
 - ▶ Differentiation matrix: $D = A^{-1}BA$
 - Integration matrix: $S = A^{-1}CA$



Minimax problem

Least-squares Approximation

Orthogonal polynomials

Revisit Chebyshev polynomia

Comparison with Machine Learning Models

Comparison

- Theoretical supports: both have universal approximation property
- Advantages:
 - Chebyshev is a near minimax approximation and nice analytical properties
 - ▶ ML empirically work well for high-dimensional problem
- Disadvantages:
 - Polynomial interpolations face with curse of dimensionality
 - Polynomial not good with complex geometries
 - ML models convergence slow

