### Orthogonal Polynomials and Spectral Algorithms

#### Nisheeth K. Vishnoi





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### **Orthogonal Polynomials**

### $\mu$ -orthogonality

Polynomials p(x), q(x) are  $\mu$ -orthogonal w.r.t.  $\mu : \mathcal{I} \to \mathbb{R}_{\geq 0}$  if

$$\langle p,q\rangle_{\mu} := \int_{\mathbf{x}\in\mathcal{I}} p(\mathbf{x})q(\mathbf{x})d\mu(\mathbf{x}) = 0$$

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#### $\mu$ -orthogonal family

Start with  $1, x, x^2, \ldots, x^d, \ldots$  and apply Gram-Schmidt orthogonalization w.r.t.  $\langle \cdot, \cdot \rangle_{\mu}$  to obtain a  $\mu$ -orthogonal family  $p_0(x) = 1, p_1(x), p_2(x), \ldots, p_d(x), \ldots$ 

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#### Examples

- Legendre:  $\mathcal{I} = [-1, 1]$  and  $\mu(x) = 1$ .
- Hermite:  $\mathcal{I} = \mathbb{R}$  and  $\mu(x) = e^{-x^2/2}$ .
- Laguerre:  $\mathcal{I} = \mathbb{R}_{\geq 0}$  and  $\mu(x) = e^{-x}$ .
- Chebyshev (Type 1):  $\mathcal{I} = [-1, 1]$  and  $\mu(x) = \frac{1}{\sqrt{1-x^2}}$ .

Monic  $\mu$ -orthogonal polynomials satisfy 3-term recurrences

$$p_{d+1}(x) = (x - \alpha_{d+1})p_d + \beta_d p_{d-1}$$

for  $d \ge 0$  with  $p_{-1} = 0$ .



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# Proof sketch $\underbrace{degree \ d}_{p_{d+1} - xp_d} = \alpha_{d+1}p_d + \beta_d p_{d-1} + \sum_{i < d-1} \gamma_i p_i$

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### Roots (corollaries)

- If p<sub>0</sub>, p<sub>1</sub>,..., p<sub>d</sub>,... are orthogonal w.r.t. μ : [a, b] → ℝ<sub>≥0</sub> then for each p<sub>d</sub>, roots are distinct, real and lie in [a, b].
- Roots of  $p_d$  and  $p_{d+1}$  also interlace!

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- Extensions to multivariate and matrix polynomials
- Several examples in this workshop ...

Many spectral algorithms today rely on ability to quickly compute good approximations to matrix-function-vector products: e.g.,

- $A^{s}v, A^{-1}v, \exp(-A)v, ...$
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How to reduce the problem of computing these primitives to a **small number** of computations of the form Bu where B is a matrix closely related to A (often A itself) and u is some vector.

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**Approximation theory** provides the right framework to study these questions – Borrows heavily from orthogonal polynomials!









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#### Uniform (Chebyshev) Approximation by Polynomials/Rationals

For  $f : \mathbb{R} \mapsto \mathbb{R}$  and an interval  $\mathcal{I}$ , what is the closest a degree d polynomial/rational function can remain to f(x) **throughout**  $\mathcal{I}$ 

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$$\inf_{q \in \Sigma_d} \sup_{\mathbf{x} \in \mathcal{I}} |f(\mathbf{x}) - \frac{p(\mathbf{x})}{q(\mathbf{x})}|.$$

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- 150+ years of fascinating history, deep results and many applications.
- Interested in fundamental functions such as x<sup>s</sup>, e<sup>-x</sup> and 1/x over finite and infinite intervals such as [−1, 1], [0, n], [0,∞).
- For our applications good enough approximations suffice.

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$$\|\sum_{i=0}^{d} a_i A^i v - A^s v\| \le \delta \|v\|$$
 since  
• all the eigenvalues of A lie in  $[-1, 1]$ , and  
•  $p_{s,d}$  is  $\delta$ -close to  $x^s$  in the entire interval  $[-1, 1]$ .
# Algorithms/Numerical Linear Alg.- f(A)v, Eigenvalues, ...

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### How small can d be?

For any s, for any  $\delta > 0$ , and  $d \sim \sqrt{s \log(1/\delta)}$ , there is a polynomial  $p_{s,d}$  s.t.  $\sup_{x \in [-1,1]} |p_{s,d}(x) - x^s| \le \delta$ .

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- Conjugate Gradient Method: Given Ax = b with eigenvalues of A in (0, 1], one can find y s.t.  $\|y - A^{-1}b\|_A \le \delta \|A^{-1}b\|_A$  in time roughly  $m\sqrt{\kappa(A)\log 1/\delta}$ .

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- Quadratic speedup over the Power Method: Given A, in time ~ m/√δ can compute a value μ ∈ [(1 − δ)λ<sub>1</sub>(A), λ<sub>1</sub>(A)].

Recall: Chebyshev polynomial orthogonal w.r.t.  $\frac{1}{\sqrt{1-x^2}}$  over [-1,1] $T_{d+1}(x) = 2xT_d(x) - T_{d-1}(x)$ 

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Averaging Property

$$xT_d(x) = \frac{T_{d+1}(x) + T_{d-1}(x)}{2}$$

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#### **Boundedness Property**

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#### **Boundedness Property**

For any  $\theta$ , and any integer d,  $T_d(\cos \theta) = \cos(d\theta)$ . Thus,  $|T_d(x)| \le 1$  for all  $x \in [-1, 1]$ .

$$D_s \stackrel{\text{def}}{=} \sum_{i=1}^{s} Y_i$$
 where  $Y_1, \ldots, Y_s$  i.i.d.  $\pm 1$  w.p.  $\frac{1}{2} (D_0 \stackrel{\text{def}}{=} 0)$ .

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Thus,  $\Pr\left[ |D_s| \ge \sqrt{2s \log(2/\delta)} \right] \le \delta.$ 

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$$\begin{aligned} x^{s+1} &= x \cdot \sum_{Y_1, \dots, Y_s} T_{D_s}(x) = \sum_{Y_1, \dots, Y_s} [x \cdot T_{D_s}(x)] \\ &= \sum_{Y_1, \dots, Y_s} [1/2(T_{D_s+1}(x) + T_{D_s-1}(x))] = \sum_{Y_1, \dots, Y_{s+1}} [T_{D_{s+1}}(x)] \end{aligned}$$

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Our Approximation to  $x^s$ :

$$p_{s,d}(x) \stackrel{\text{def}}{=} \frac{\mathsf{E}}{\mathsf{Y}_1, \dots, \mathsf{Y}_s} \left[ \mathcal{T}_{D_s}(x) \cdot \mathbf{1}_{|D_s| \leq d} \right] \text{ for } d = \sqrt{2s \log\left(\frac{2}{\delta}\right)}.$$

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$$\begin{split} \sup_{x \in [-1,1]} |p_{s,d}(x) - x^{s}| &= \sup_{x \in [-1,1]} \left| \frac{\mathbf{E}}{\mathbf{Y}_{1,\dots,\mathbf{Y}_{s}}} \left[ T_{D_{s}}(x) \cdot \mathbf{1}_{|D_{s}| > d} \right] \right| \\ &\leq \frac{\mathbf{E}}{\mathbf{Y}_{1,\dots,\mathbf{Y}_{s}}} \left[ \mathbf{1}_{|D_{s}| > d} \cdot \sup_{x \in [-1,1]} |T_{D_{s}}(x)| \right] \leq \frac{\mathbf{E}}{\mathbf{Y}_{1,\dots,\mathbf{Y}_{s}}} \left[ \mathbf{1}_{|D_{s}| > d} \right] \leq \delta. \end{split}$$

Let f(x) be  $\delta$ -approximated by a Taylor polynomial  $\sum_{s=0}^{k} c_s x^s$ . Then, one may instead try the approx. (with suitably shifted  $p_{s,d}$ )  $\sum_{s=0}^{k} c_s p_{s,\sqrt{s \log 1/\delta}}(x)$ 

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#### Approximating the Exponential

For every b > 0, and  $\delta$ , there is a polynomial  $r_{b,\delta}$  s.t.  $\sup_{x \in [0,b]} |e^{-x} - r_{b,\delta}(x)| \le \delta$ ; degree  $\sim \sqrt{b \log 1/\delta}$ . (Taylor - $\Omega(b)$ .)

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### How far can polynomial approximations take us?

### Bad News [see Sachdeva-V. 2014]

- Polynomial approx. to  $x^s$  on [-1, 1] requires degree  $\Omega(\sqrt{s})$ .
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Markov's Theorem (inspired by a prob. of Mendeleev in Chemistry)

Any degree-*d* polynomial *p* s.t.  $|p(x)| \le 1$  over [-1, 1] must have its derivative  $|p^{(1)}(x)| \le d^2$  for all  $x \in [-1, 1]$ .

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### Bypass this barrier via rational functions!

For all integers  $d \ge 0$ , there is a degree-d polynomial  $S_d(x)$  s.t.  $\sup_{x \in [0,\infty)} \left| e^{-x} - \frac{1}{S_d(x)} \right| \le 2^{-\Omega(d)}.$ 

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How do we compute  $(S_d(A))^{-1} v$ ?

Factor  $S_d(x) = \alpha_0 \prod_{i=1}^d (x - \beta_i)$  and output  $\alpha_0 \prod_{i=1}^d (A - \beta_i I)^{-1} v$ .

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### Sachdeva-V. 2014

Moreover, the coefficients of  $p_d$  are bounded by  $d^{O(d)}$ , and can be approximated up to an error of  $d^{-\Theta(d)}$  using poly(d) arithmetic operations, where all intermediate numbers use poly(d) bits.
## Computing the Matrix Exponential- Summary

### Orecchia-Sachdeva-V. 2012, Sachdeva-V. 2014

Given an **SDD**  $A \succeq 0$ , a vector v with ||v|| = 1 and  $\delta$ , we compute a vector u s.t.  $||\exp(-A)v - u|| \le \delta$ , in time  $\tilde{O}(m \log ||A|| \log 1/\delta)$ .

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### Corollary [Orecchia-Sachdeva-V. 2012]

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#### SDD Solvers

Given Lx = b, L is SDD, and  $\varepsilon > 0$ , obtain a vector u s.t.,  $\|u - L^{-1}b\|_L \le \varepsilon \|L^{-1}b\|_L$ . Time required  $\tilde{O}(m \log 1/\varepsilon)$ 

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### Are Laplacian solvers necessary for the matrix exponential?

#### Belykin-Monzon 2010, Sachdeva-V. 2014

For  $\varepsilon, \delta \in (0, 1]$ , there exist  $\operatorname{poly}(\log(1/\varepsilon \delta))$  numbers  $0 < w_j, t_j$  s.t. for all symm.  $\varepsilon I \preceq A \preceq I, (1 - \delta)A^{-1} \preceq \sum_j w_j e^{-t_j A} \preceq (1 + \delta)A^{-1}$ .

- Weights  $w_j$  are  $O(\text{poly}(1/\delta \varepsilon))$ , we lose only a polynomial factor in the approximation error.
- For applications polylogarithmic dependence on both  $1/\delta$  and the condition number of  $A(1/\varepsilon$  in this case).
- Discretizing  $x^{-1} = \int_0^\infty e^{-xt} dt$  naively **needs** poly( $1/(\varepsilon \delta)$ ) terms.
- Substituting  $t = e^y$  in the above integral obtains the identity  $x^{-1} = \int_{-\infty}^{\infty} e^{-xe^y + y} dy$ .
- Discretizing this integral, we bound the error using the Euler-Maclaurin formula, Riemann zeta fn.; global error analysis!

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#### Thanks for your attention!

#### Reference

*Faster algorithms via approximation theory*. Sushant Sachdeva, Nisheeth K. Vishnoi. Foundations and Trends in TCS, 2014.