Orthogonal Polynomials and Spectral Algorithms

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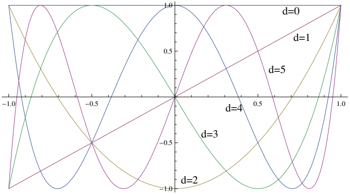

FOCS, Oct. 8, 2016

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μ-orthogonality

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

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μ-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 μ-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 $\mu(x) = \frac{1}{\sqrt{1-x^2}}$.

Orthgonal polynomials have many amazing properties

Monic μ-orthogonal polynomials satisfy 3-term recurrences

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

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

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Proof sketch

1. $\overbrace{p_{d+1} - xp_d}^{\text{degree } d} = \alpha_{d+1} p_d + \beta_d p_{d-1} + \sum_{i<d-1} \gamma_i p_i$

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Roots (corollaries)

- If $p_0, p_1, \ldots, p_d, \ldots$ are orthogonal w.r.t. $\mu : [a, b] \to \mathbb{R}_{\geq 0}$ then for each p_d, roots are distinct, real and lie in $[a, b]$.
- Roots of p_d and p_{d+1} also interlace!

Many and growing applications in TCS ...

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  Invariance principles, hardness of approximation *a la* Mossel, O'Donnell, Oleszkiewicz, ...

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  Spectral algorithms – *This talk*
- Extensions to multivariate and matrix polynomials
- **Several examples in this workshop ..**

The goal of today's talk

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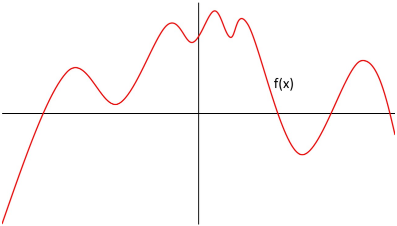
Approximation theory provides the right framework to study these questions – Borrows heavily from orthogonal polynomials!

Approximation Theory



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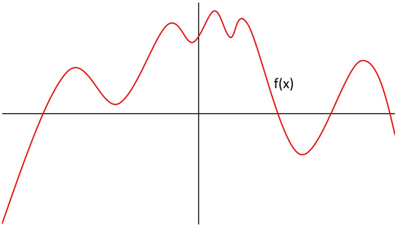

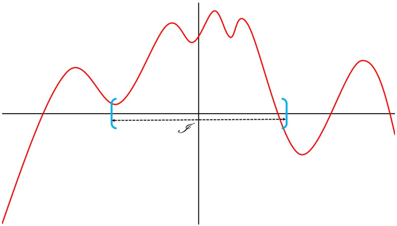

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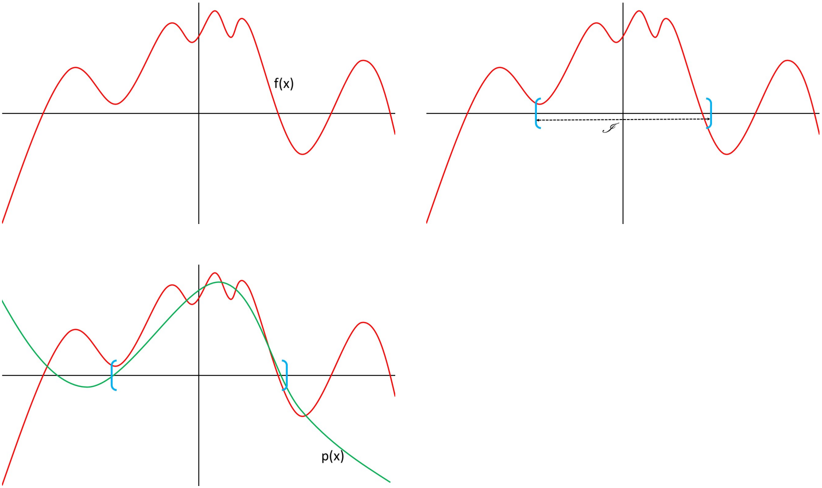

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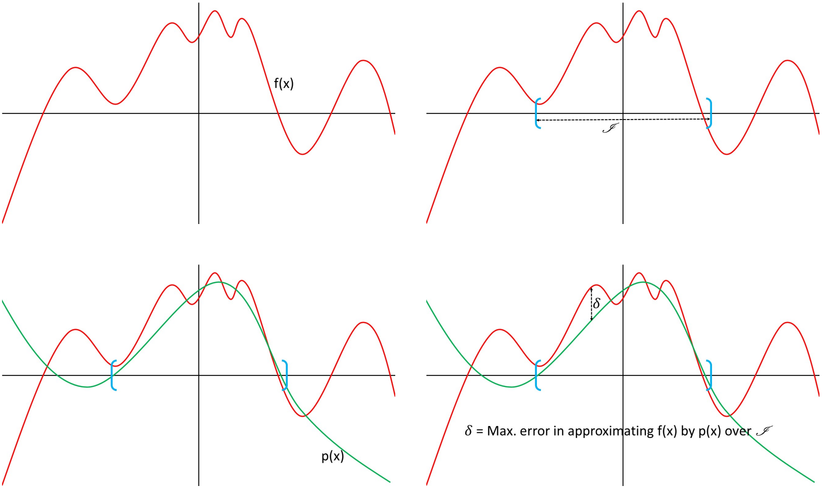

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$$\inf_{p,q \in \Sigma_d} \sup_{x \in \mathcal{I}} |f(x) - p(x)/q(x)|.$$

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- For our applications good enough approximations suffice.

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Compute $A^s v$ where A is symmetric with eigenvalues in $[-1, 1]$, v is a vector and s is a large positive integer.

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- The time to compute $\sum_{i=0}^{d} a_i A^i v$ is $O(md)$.
- $\|\sum_{i=0}^{d} a_i A^i v - A^s v\| \leq \delta \|v\|$ since
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How small can d be?

Example: Approximating the Monomial

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

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

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- **Quadratic speedup over the Power Method**: Given A, in time $\sim m/\sqrt{\delta}$ can compute a value $\mu \in [(1-\delta)\lambda_1(A), \lambda_1(A)]$.

Chebyshev Polynomials

Recall: Chebyshev polynomial orthogonal w.r.t. $\frac{1}{\sqrt{1-x^2}}$ over $[-1, 1]$

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Thus, $|T_d(x)| \leq 1$ for all $x \in [-1, 1]$.

Back to Approximating Monomials

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

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\begin{aligned}
x^{s+1} &= x \cdot \mathop{\mathbf{E}}_{Y_1,\ldots,Y_s} T_{D_s}(x) = \mathop{\mathbf{E}}_{Y_1,\ldots,Y_s}[x \cdot T_{D_s}(x)] \\
&= \mathop{\mathbf{E}}_{Y_1,\ldots,Y_s}[1/2(T_{D_s+1}(x) + T_{D_s-1}(x))] = \mathop{\mathbf{E}}_{Y_1,\ldots,Y_{s+1}}[T_{D_{s+1}}(x)].
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Thus, $\Pr\left[|D_s| \geq \sqrt{2s \log(2/\delta)}\right] \leq \delta$.

Key Claim: $\mathop{\mathbf{E}}_{Y_1,\ldots,Y_s}[T_{D_s}(x)] = x^s$.

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x^{s+1} &= x \cdot \mathop{\mathbf{E}}_{Y_1,\ldots,Y_s} T_{D_s}(x) = \mathop{\mathbf{E}}_{Y_1,\ldots,Y_s}[x \cdot T_{D_s}(x)] \\
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Our Approximation to x^s:

$$p_{s,d}(x) \stackrel{\text{def}}{=} \mathop{\mathbf{E}}_{Y_1,\ldots,Y_s}\left[T_{D_s}(x) \cdot 1_{|D_s| \leq d}\right] \quad \text{for} \quad d = \sqrt{2s \log(2/\delta)}.$$

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\sup_{x \in [-1,1]} |p_{s,d}(x) - x^s| &= \sup_{x \in [-1,1]} \left| \underset{Y_1,\ldots,Y_s}{\mathbf{E}} \left[T_{D_s}(x) \cdot 1_{|D_s| > d}\right] \right| \\
&\leq \underset{Y_1,\ldots,Y_s}{\mathbf{E}} \left[1_{|D_s|>d} \cdot \sup_{x \in [-1,1]} |T_{D_s}(x)|\right] \leq \underset{Y_1,\ldots,Y_s}{\mathbf{E}}\left[1_{|D_s|>d}\right] \leq \delta.
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A General Recipe?

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

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How far can polynomial approximations take us?

Lower Bounds for Polynomial Approximations

Bad News [see Sachdeva-V. 2014]

- Polynomial approx. to x^s on $[-1, 1]$ requires degree $\Omega(\sqrt{s})$.
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Bypass this barrier via rational functions!

Example: Approximating the Exponential

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

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

Rational Approximations with Negative Poles

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 $\mathrm{poly}(d)$ arithmetic operations, where all intermediate numbers use $\mathrm{poly}(d)$ 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 δ, we compute a vector u s.t. $\|\exp(-A)v - u\| \leq \delta$, in time $\tilde{O}\left(m \log\|A\| \log 1/\delta\right)$.

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

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Are Laplacian solvers necessary for the matrix exponential?

Matrix Inversion via Exponentiation

Belykin-Monzon 2010, Sachdeva-V. 2014

For $\varepsilon, \delta \in (0,1]$, there exist $\mathrm{poly}(\log(1/\varepsilon\delta))$ 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 $O(\mathrm{poly}(1/\delta\varepsilon))$, 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 $x^{-1} = \int_0^\infty e^{-xt} \mathrm{d}t$ naively **needs** $\mathrm{poly}(1/(\varepsilon\delta))$ terms.
- Substituting $t = e^y$ in the above integral obtains the identity $x^{-1} = \int_{-\infty}^{\infty} e^{-xe^y + y} \mathrm{d}y$.
- 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.