CSE 392: Matrix and Tensor Algorithms for Data

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Supplement: Spectral sums

Outline

Spectral Sums

Given a symmetric positive semidefinite (PSD) matrix $\boldsymbol{A} \in \mathbb{R}^{d \times d}$ with eigen-decompostion $\boldsymbol{A} = \boldsymbol{U}\Lambda\boldsymbol{U}^T$ and eigenvalues $\{\lambda_i\}_{i=1}^d$, and desired function $f(\cdot)$, compute the *trace of the matrix function* $f(\boldsymbol{A}) = \boldsymbol{U}f(\Lambda)\boldsymbol{U}^\top$, i.e.,

$$\mathrm{Tr}(f(\boldsymbol{A})) = \sum_{i=1}^{d} f(\lambda_i).$$

- *Popular examples:* log-determinant ($\log(x)$), numerical rank (step function), spectral density $\delta(x - \lambda_i)$, Schatten p-norms ($x^{p/2}$), von Neumann Entropy ($x \log(x)$), Estrada index ($\exp(x)$), trace of matrix inverse ($\frac{1}{x}$).
- *Applications:* machine learning, graph signal processing, quantum algorithms, scientific computing, statistics, computational biology and physics.
- *Naive approaches :* Eigenvalue decomposition, Cholesky Decomposition, singular value decomposition (SVD).
  Cost: $O(d^3)$ or [Theory: $O(d^\omega)$ and $\omega = 2.373$].

Spectral Sums

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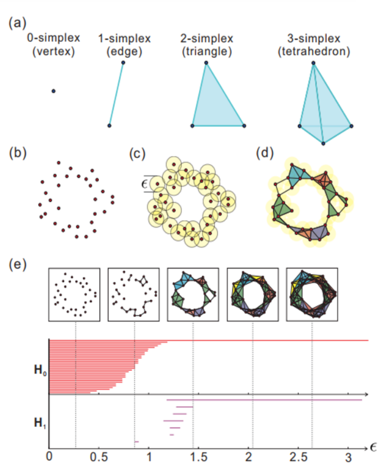
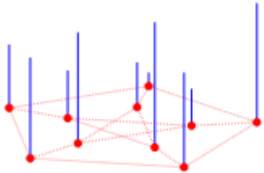
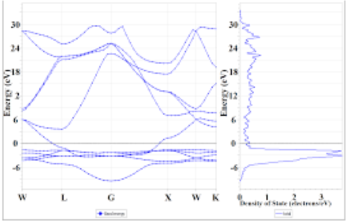
- Approximate the function using two approaches:
  1. Chebyshev polynomial approximation
  2. Lanczos quadrature method

Spectral Sums Applications

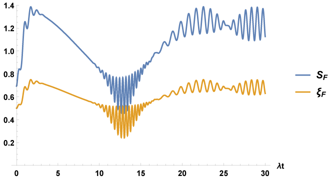


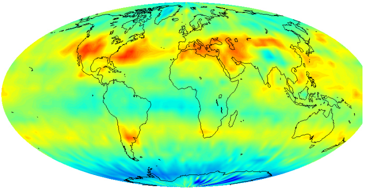


(b) Graph Signal Processing



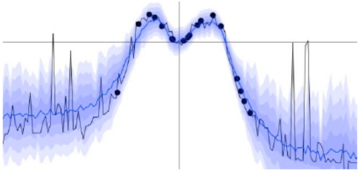
(c) Density of States



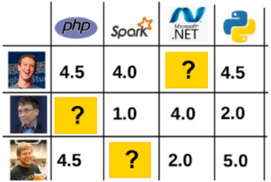


Matrix Functions in Machine Learning

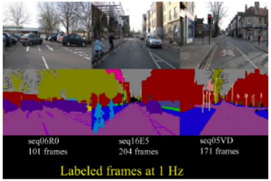
Matrix functions have been utilized in many machine learning problems:



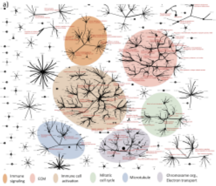
(a) Regression with Gaussian process



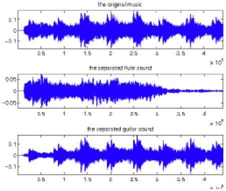
(b) Collaborative filtering for recommendation



(c) Image processing



(d) Gene expression



(e) Speech recognition

Can we estimate $\mathrm{Tr}(f(A))$ faster than matrix multiplication cost?

Discuss *fast scalable* methods with *theoretical guarantees* and perform *well in practice*.

Combine randomization with approximation theory!

Stochastic Chebyshev Method

Chebyshev polynomial approximation

Given a function $f : [-1, 1] \to \mathbb{R}$, a q degree **Chebyshev polynomial** approximation is given by:

$$f(x) \approx p_q(x) = \sum_{j=0}^{q} c_j T_j(x),$$

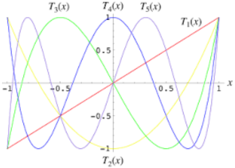
where $T_j(x)$ is the jth degree Chebyshev polynomial with $T_0(x) = 1, T_1(x) = x$,

$$T_{j+1}(x) = 2xT_j(x) - T_{j-1}(x),$$

and the (interpolation) coefficients,

$$c_j = \frac{2 - \delta_{j0}}{\pi} \int_{-1}^{1} \frac{f(x)T_j(x)}{\sqrt{1 - x^2}} dx \quad \text{or} \quad c_j = \frac{2 - \delta_{j0}}{q + 1} \sum_{k=0}^{q} f(x_k)T_j(x_k),$$

with Chebyshev nodes $x_k = \cos\left(\frac{\pi(k+1)/2}{q+1}\right)$.



Stochastic Chebyshev method

- $\boldsymbol{A}$ has spectrum in $[\lambda_{\min}, \lambda_{\max}]$, $\tilde{\boldsymbol{A}} = \left(\frac{2\boldsymbol{A}-(\lambda_{\max}+\lambda_{\min})I}{\lambda_{\max}-\lambda_{\min}}\right)$ spectrum in $[-1, 1]$.
- Approximate $\boldsymbol{x}_l^T f(\boldsymbol{A})\boldsymbol{x}_l \approx \boldsymbol{x}_l^T \boldsymbol{B}\boldsymbol{x}_l$, where $\boldsymbol{B} = \sum_{j=0}^{q} \tilde{c}_j T_j(\tilde{\boldsymbol{A}})$.
- Let $\boldsymbol{w}_l^{(j)} = T_j(\tilde{\boldsymbol{A}})\boldsymbol{x}_l$; with $\boldsymbol{w}_l^{(0)} = \boldsymbol{x}_l, \boldsymbol{w}_l^{(1)} = \tilde{\boldsymbol{A}}\boldsymbol{x}_l$, and

$$\boldsymbol{w}_l^{(j+1)} = 2\tilde{\boldsymbol{A}}\boldsymbol{w}_l^{(j)} - \boldsymbol{w}_l^{(j-1)}.$$

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$$\boldsymbol{w}_l^{(j+1)} = 2\tilde{\boldsymbol{A}}\boldsymbol{w}_l^{(j)} - \boldsymbol{w}_l^{(j-1)}.$$

  The **spectral sums** can be estimated as:

$$\mathrm{Tr}(f(A)) \approx \frac{1}{m}\sum_{l=1}^{m}\left[\sum_{j=0}^{q}\tilde{c}_j (v_l)^\top w_l^{(j)}\right]. \tag{1}$$

- **Computational cost**: $O(\mathrm{nnz}(\boldsymbol{A})mq)$.
- *Kernel Polynomial Method* - estimating spectral density [Lin et al.,2016] , Eigencount [Di Napoli et al., 2016], Numerical rank [Ubaru and Saad, 2016, Ubaru et al., 2017].
- *Theoretical analysis* for analytic functions and applications [Han et. al, 2017].

Stochastic Lanczos Quadrature

Stochastic Lanczos Quadrature

- The **Lanczos Quadrature** method by *Gene Golub* and his collaborators in a series of articles.
- Scalar (quadratic form) quantities $\boldsymbol{x}_l^\top f(\boldsymbol{A})\boldsymbol{x}_l$ as *Riemann-Stieltjes integral* problem, and employing *Gauss quadrature rule* to approximate this integral.
- With eigen-decomposition of A as $\boldsymbol{A} = \boldsymbol{U}\Lambda\boldsymbol{U}^\top$.

$$\boldsymbol{x}_l^\top f(\boldsymbol{A})\boldsymbol{x}_l = \boldsymbol{x}_l^\top \boldsymbol{U} f(\Lambda)\boldsymbol{U}^\top \boldsymbol{x}_l = \sum_{i=1}^{d} f(\lambda_i)\mu_i^2 = \int_a^b f(t)d\mu(t),$$

μ_i are components of $\boldsymbol{U}^\top \boldsymbol{x}_l$ and the measure $\mu(t)$ is a piecewise constant function

$$\mu(t) = \begin{cases} 0, & \text{if } t < a = \lambda_1, \\ \sum_{j=1}^{i} \mu_j^2, & \text{if } \lambda_i \le t < \lambda_{i+1}, \\ \sum_{j=1}^{d} \mu_j^2, & \text{if } b = \lambda_n \le t. \end{cases}$$

- Use Gauss quadrature rule:

$$\int_a^b f(t)d\mu(t) \approx \sum_{k=0}^{q} \omega_k f(\theta_k),$$

  $\{\omega_k\}$ are the weights and $\{\theta_k\}$ are the nodes of the q-point Gauss quadrature rule.
- Compute the nodes and the weights via. the *Lanczos algorithm*.

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- For $A \in \mathbb{R}^{d\times d}$ and $\boldsymbol{x}_l : \|\boldsymbol{x}_l\| = 1$, Lanczos algorithm forms $\boldsymbol{Z}_q^{(l)}$ orthonormal basis for *Krylov subspace*: $\text{Span}\{\boldsymbol{x}_l, \boldsymbol{A}\boldsymbol{x}_l, \dots, \boldsymbol{A}^q\boldsymbol{x}_l\}$,
  and tridiagonal matrix $\boldsymbol{T}_q^{(l)} = \boldsymbol{Z}_q^{(l)\top}\boldsymbol{A}\boldsymbol{Z}_q^{(l)}$.
- The columns $\boldsymbol{z}_j$ of $\boldsymbol{Z}_q^{(l)}$ are related as

$$\boldsymbol{z}_j = p_j(\boldsymbol{A})\boldsymbol{x}_0,\ j = 1, \dots, q,$$

  where $p_j(\cdot)$ are the Lanczos polynomials.
- These polynomials are orthogonal wrt. the measure $\mu(t)$; see Thm 4.2 in [Meurant, Golub, 2009].

Stochastic Lanczos Quadrature

- We approximate,
$$\boldsymbol{x}_l^\top f(\boldsymbol{A})\boldsymbol{x}_l \approx \sum_{k=0}^{q} (\tau_k^{(l)})^2 f(\theta_k^{(l)}) \quad \text{with} \quad (\tau_k^{(l)})^2 = \left[e_1^\top y_k^{(l)}\right]^2,$$
$(\theta_k^{(l)}, y_k^{(l)}), k = 0, 1, ..., q$ are eigenpairs of $\boldsymbol{T}_q^{(l)}$ corresponding to initial vectors $\boldsymbol{x}_l, l = 1, \ldots, m$.
- Matrix function trace estimation as,
$$\mathrm{Tr}(f(\boldsymbol{A})) \approx \frac{n}{m} \sum_{l=1}^{m} \left(\sum_{k=0}^{q} (\tau_k^{(l)})^2 f(\theta_k^{(l)}) \right). \tag{2}$$
- **Computational Cost:** $O(\mathrm{nnz}(\boldsymbol{A})mq)$.

Error Analysis

Theorem

Given a PSD matrix $\boldsymbol{A} \in \mathbb{R}^{d \times d}$ *with its eigenvalues in* $[\lambda_{\min}, \lambda_{\max}]$ *and condition number* $\kappa = \frac{\lambda_{\max}}{\lambda_{\min}}$, *a function* f *that is analytic inside this interval, and constants* $\epsilon, \eta \in (0, 1)$, *for SLQ parameters:*

- $q \geq \frac{\sqrt{\kappa}}{4} \log \frac{K}{\epsilon}$ *number of Lanczos steps, and*
- $m \geq \frac{24}{\epsilon^2} \log(2/\eta)$ *number of starting vectors,*

where $K = \frac{3\lambda_{\max}\sqrt{\kappa}M_\rho}{2m_\rho}$ *with* M_ρ *and* m_ρ *being the absolute maximum and minimum of the function in the interval,*

$$\Pr\left[\left|\mathrm{Tr}(f(\boldsymbol{A})) - \Gamma\right| \leq \epsilon \left|\mathrm{Tr}(f(\boldsymbol{A}))\right| \right] \geq 1 - \eta, \tag{3}$$

where Γ *is the output of the Stochastic Lanczos Quadrature method.*

S. Ubaru, Jie Chen, and Yousef Saad. SIAM Journal on Matrix Analysis and Applications, 38(4), 1075–1099, 2017.

Applications

Further Reading:

- *Applications of trace estimation techniques* by S. Ubaru and Y. Saad.
- *Approximating spectral sums of large-scale matrices using stochastic Chebyshev approximations* by s Insu Han, Dmitry Malioutov, Haim Avron, Jinwoo Shin.
- *Fast Estimation of* $\mathrm{Tr}(f(A))$ *via Stochastic Lanczos Quadrature*, by S. Ubaru, Jie Chen, and Yousef Saad.