Hutch++

Optimal Stochastic Trace Estimation

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Trace Estimation

- Goal: Estimate trace of $d \times d$ matrix $\boldsymbol{A}$:

$$\mathrm{tr}(\boldsymbol{A}) = \sum_{i=1}^{d} \boldsymbol{A}_{ii} = \sum_{i=1}^{d} \lambda_i$$

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- Instead, $\boldsymbol{B}$ is in memory and $\boldsymbol{A} = f(\boldsymbol{B})$:

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- If $\boldsymbol{A} = f(\boldsymbol{B})$, then we can often compute $\boldsymbol{A}\mathbf{x}$ quickly
- Goal: Estimate $\mathrm{tr}(\boldsymbol{A})$ by computing $\boldsymbol{A}\mathbf{x}_1, \ldots \boldsymbol{A}\mathbf{x}_k$

Formal Problem Statement

Implicit Matrix Trace Estimation: Estimate $\mathrm{tr}(\boldsymbol{A})$ with as few Matrix-Vector products $\boldsymbol{A}\mathbf{x}_1, \dots, \boldsymbol{A}\mathbf{x}_m$ as possible.

$$(1-\varepsilon)\,\mathrm{tr}(\boldsymbol{A}) \leq \tilde{\mathrm{tr}}(\boldsymbol{A}) \leq (1+\varepsilon)\,\mathrm{tr}(\boldsymbol{A}) \qquad \text{w.p. } 1-\delta$$

Our Contributions

For PSD matrix trace estimation,

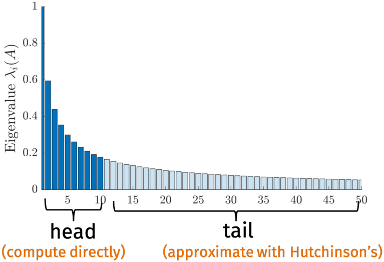
- Hutch++ algorithm, which uses $\tilde{O}(\frac{1}{\varepsilon})$ matrix-vector products.
  - Improves prior rate of $\tilde{O}(\frac{1}{\varepsilon^2})$
  - Empirically works well
  - Matching $\Omega(\frac{1}{\varepsilon})$ Lower Bound

Only 5 lines of code:

```
function T = hutchplusplus(A, m)
    S = 2*randi(2,size(A,1),m/3);
    G = 2*randi(2,size(A,1),m/3);
    [Q,~] = qr(A*S,0);
    G = G - Q*(Q'*G);
    T = trace(Q'*A*Q) + 1/size(G,2)*trace(G'*A*G);
end
```

[1] $\tilde{O}$ notation only hide logarithmic dependence on the failure probability.

Hutch++ Intuition



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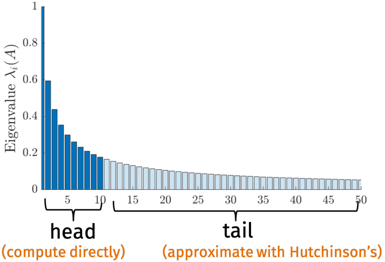

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1. Find a good rank-k approximation $\tilde{\boldsymbol{A}}_k$
2. Compute $\tilde{T} \approx \mathrm{tr}(\boldsymbol{A} - \tilde{\boldsymbol{A}}_k)$ with m steps of Hutchinson's
3. Return Hutch++$(\boldsymbol{A}) = \mathrm{tr}(\tilde{\boldsymbol{A}}_k) + \tilde{T}$

THANK YOU

Code available at

github.com/RaphaelArkadyMeyerNYU/hutchplusplus