Hutch++

Optimal Stochastic Trace Estimation

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Implicit Trace Estimation

Basic problem in linear algebra:

- Given access to a \( n \times n \) matrix \( A \) only through a Matrix-Vector Multiplication Oracle

\[
x \xrightarrow{\text{input}} \text{ORACLE} \xrightarrow{\text{output}} Ax
\]

- Goal is to approximate \( \text{tr}(A) = \sum_{i=1}^{n} A_{ii} = \sum_{i=1}^{n} \lambda_i \)

Main Question: How many matrix-vector multiplication queries \( Ax_1, \ldots, Ax_m \) are required to compute \( \text{tr}(A) \)?

\(^1x_i\) can be chosen adaptively, based on the results \( Ax_1, \ldots, Ax_{i-1} \)
Application: Trace of a Function of a Matrix

- Suppose $B$ is the adjacency matrix for graph $G$. Then $\frac{1}{6} \text{tr}(B^3)$ counts the number of triangles in $G$.
  - Computing $B^3$ directly takes $O(n^3)$ time
  - Computing $B^3x$ takes $O(n^2)$ time
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Other functions of interest: $\text{tr}(e^B)$, $\text{tr}(\ln(\Sigma))$, etc.

Computing $f(B)x$ is often much faster than computing $f(B)$ directly
- Especially if we only need very few $x$ vectors
Background: Matrix-Vector Oracle

Algorithms:

- Krylov Methods, Sketching Methods, Streaming Methods, etc.
- See also: *Implicit Matrix Methods*, *Matrix-Free Methods*
- Useful framework for algorithmic lower bounds
  - Allows us to prove optimality in a very general setting
The classical approach to trace estimation:

**Hutchinson 1991, Girard 1987**

1. Draw $x_1, \ldots, x_m \in \mathbb{R}^n$ with i.i.d. uniform $\{+1,-1\}$ entries
2. Return $\tilde{T} = \frac{1}{m} \sum_{i=1}^{m} x_i^T A x_i$

**Avron, Toledo 2011, Roosta, Ascher 2015**

If $m = O\left(\frac{\log(1/\delta)}{\varepsilon^2}\right)$, then with probability $1 - \delta$,

$$|\tilde{T} - \text{tr}(A)| \leq \varepsilon \|A\|_F$$
Background: Hutchinson’s Estimator

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If $m = O\left(\frac{\log(1/\delta)}{\varepsilon^2}\right)$, then with probability $1 - \delta$,

$$|\tilde{T} - \text{tr}(A)| \leq \varepsilon \|A\|_F$$

- If $A$ is PSD, then $\|A\|_F \leq \text{tr}(A)$, so that

$$\left(1 - \varepsilon\right) \text{tr}(A) \leq \tilde{T} \leq \left(1 + \varepsilon\right) \text{tr}(A)$$
Contribution: \(O(1/\varepsilon)\) vectors is optimal

**Theorems**

1. For PSD \(A\) and \(m = O\left(\frac{\log(1/\delta)}{\varepsilon}\right)\), with probability \(1 - \delta\),

\[
(1 - \varepsilon) \text{tr}(A) \leq \text{Hutch}++(A) \leq (1 + \varepsilon) \text{tr}(A)
\]

2. For any \(b\)-bit precision oracle, \(\tilde{\Omega}(1/\varepsilon b)\) possibly adaptive queries are necessary.

3. For any infinite precision oracle, \(\Omega(1/\varepsilon)\) non-adaptive queries are necessary.

For the rest of the talk, \(A\) is always PSD.
Contribution: $O(1/\varepsilon)$ vectors is optimal

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For the rest of the talk, $A$ is always PSD.

```matlab
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
```
Contribution: $O(1/\varepsilon)$ vectors is optimal

Theorems

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Hutchinson’s Estimator
Versus the Top Few Eigenvalues
Let’s return to the result for Hutchinson’s Estimator:

\[ |\tilde{T} - \text{tr}(A)| \leq O\left(\frac{1}{\sqrt{m}}\right) \|A\|_F \]
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\[ |\tilde{T} - \text{tr}(\mathbf{A})| \approx O\left(\frac{1}{\sqrt{m}}\right)\|\mathbf{A}\|_F \leq O\left(\frac{1}{\sqrt{m}}\right) \text{tr}(\mathbf{A}) = \varepsilon \text{tr}(\mathbf{A}) \]

○ When does Hutchinson’s Estimator truly need \( O\left(\frac{1}{\varepsilon^2}\right) \) queries?
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- When does Hutchinson’s Estimator truly need \(O\left(\frac{1}{\varepsilon^2}\right)\) queries?
- When is the bound \(\|A\|_F \leq \text{tr}(A)\) tight?
Hutchinson Analysis

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  - Property of norms: \(\|v\|_2 \approx \|v\|_1\) only if \(v\) is nearly sparse
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- When is the bound \(\|v\|_2 \leq \|v\|_1\) tight?
  - Property of norms: \(\|v\|_2 \approx \|v\|_1\) only if \(v\) is nearly sparse
- Hutchinson only requires \(O\left(\frac{1}{\varepsilon^2}\right)\) queries if \(A\) has a few large eigenvalues
Idea: Explicitly estimate the top few eigenvalues of A. Use Hutchinson’s for the rest.
Helping Hutchinson’s Estimator

Idea: Explicitly estimate the top few eigenvalues of \( A \). Use Hutchinson’s for the rest.

1. Find a good rank-\( k \) approximation \( \tilde{A}_k \)
2. Notice that \( \text{tr}(A) = \text{tr}(\tilde{A}_k) + \text{tr}(A - \tilde{A}_k) \)
3. Compute \( \text{tr}(\tilde{A}_k) \) exactly
4. Compute \( \tilde{T} \approx \text{tr}(A - \tilde{A}_k) \) with Hutchinson’s Estimator
5. Return \( \text{Hutch}^{++}(A) = \text{tr}(\tilde{A}_k) + \tilde{T} \)
Let $A_k$ be the best rank-$k$ approximation of $A$.

**Lemma (Sarlos 2006, Woodruff 2014)**

Let $S \in \mathbb{R}^{n \times m}$ have i.i.d. uniform $\pm 1$ entries, $Q = \text{orth}(AS)$, and $\tilde{A}_k = AQQ^T$. Then, with probability $1 - \delta$, 

$$\|A - \tilde{A}_k\|_F \leq 2\|A - A_k\|_F$$

so long as $S$ has $m = O(k + \log(1/\delta))$ columns.
Finding a Good Low-Rank Approximation

Let \( A_k \) be the best rank-\( k \) approximation of \( A \).

### Lemma (Sarlos 2006, Woodruff 2014)

Let \( S \in \mathbb{R}^{n \times m} \) have i.i.d. uniform ±1 entries, \( Q = \text{orth}(AS) \), and \( \tilde{A}_k = AQQ^T \). Then, with probability \( 1 - \delta \),

\[
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\]

so long as \( S \) has \( m = O(k + \log(1/\delta)) \) columns.

We can compute the trace of \( \tilde{A}_k \) with \( m \) queries and \( O(mn) \) space:

\[
\text{tr}(\tilde{A}_k) = \text{tr}(AQQ^T) = \text{tr}(Q^T(AQ))
\]
Complete Analysis

Lemma: $\|A - A_k\|_F \leq \frac{1}{\sqrt{k}} \text{tr}(A)$

Proof. Note that $\lambda_{k+1} \leq \frac{1}{k} \sum_{i=1}^{k} \lambda_i \leq \frac{1}{k} \text{tr}(A)$. 
Lemma: $\|A - A_k\|_F \leq \frac{1}{\sqrt{k}} \text{tr}(A)$

Proof. Note that $\lambda_{k+1} \leq \frac{1}{k} \sum_{i=1}^{k} \lambda_i \leq \frac{1}{k} \text{tr}(A)$. Then,

$$\|A - A_k\|_F^2 = \sum_{i=k+1}^{n} \lambda_i^2 \leq \lambda_{k+1} \sum_{i=k+1}^{n} \lambda_i \leq \left(\frac{1}{k} \text{tr}(A)\right) \cdot \text{tr}(A)$$
**Lemma:** \( \|A - A_k\|_F \leq \frac{1}{\sqrt{k}} \text{tr}(A) \)

**Proof.** Note that \( \lambda_{k+1} \leq \frac{1}{k} \sum_{i=1}^{k} \lambda_i \leq \frac{1}{k} \text{tr}(A) \). Then,

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\]

- Formalizes our earlier intuition
- Replaces the earlier bound \( \|A\|_F \leq \text{tr}(A) \)
- Similar to standard compressed sensing result:

\[
\text{For all } v \in \mathbb{R}^d, \text{ there exists } k\text{-sparse } \tilde{v} \text{ such that } \\
\|v - \tilde{v}\|_2 \leq \frac{1}{\sqrt{k}} \|v\|_1
\]
Complete Analysis

Using rank-$k$ approximation and $\ell$ sample for Hutchinson’s.
Using rank-$k$ approximation and $\ell$ sample for Hutchinson’s.

1. We can only make an error in the Hutchinson’s step:

$$|\text{tr}(A) - \text{Hutch}^{++}(A)| = |\text{tr}(A - \tilde{A}_k) - \tilde{T}|$$
Using rank-\(k\) approximation and \(\ell\) sample for Hutchinson’s.

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2. Guarantees for Hutchinson’s and Low-Rank Approximation:

\[
|\text{tr}(A - \tilde{A}_k) - \tilde{T}| \leq O\left(\frac{1}{\sqrt{\ell}}\right)\|A - \tilde{A}_k\|_F \leq O\left(\frac{1}{\sqrt{\ell}}\right) \cdot 2\|A - A_k\|_F
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Using rank-\(k\) approximation and \(\ell\) sample for Hutchinson’s.

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3. Use the lemma from the last slide:

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|\text{tr}(A) - \text{Hutch}^{++}(A)| \leq O\left(\frac{1}{\sqrt{k\ell}}\right) \text{tr}(A)
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Using rank-$k$ approximation and $\ell$ sample for Hutchinson’s.

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$$|\text{tr}(A) - \text{Hutch}^{++}(A)| \leq O\left(\frac{1}{\sqrt{k \ell}}\right)\text{tr}(A)$$

4. If $k = \ell = O\left(\frac{1}{\varepsilon}\right)$, then $|\text{tr}(A) - \text{Hutch}^{++}(A)| \leq \varepsilon \text{tr}(A)$ □
Lower Bound: Communication Complexity
Really rich area of theoretical computing

Gap-Hamming Problem

Let Alice and Bob each have vectors $s, t \in \{+1, -1\}^n$. Using as few bits of communication as possible, they must decide if

$$\langle s, t \rangle \geq \sqrt{n} \quad \text{or if} \quad \langle s, t \rangle \leq -\sqrt{n}$$

Chakrabarti, Regev 2012

Any (possibly adaptive) protocol between Alice and Bob must use $\Omega(n)$ bits to solve the Gap-Hamming problem with probability $\geq \frac{2}{3}$. 
Suppose the Matrix-Vector Oracle for $A$ only accepts queries with entries that use $b$ bits of precision

- (e.g. the entries of $x$ are integers between $-2^b$ and $2^b$).

**Theorem**

Any (possibly adaptive) algorithm that estimates $\text{tr}(A)$ to relative error $\varepsilon$ with probability $\geq \frac{2}{3}$ must use $\Omega\left(\frac{1}{\varepsilon(b+\log(1/\varepsilon))}\right)$ queries.

Proof Idea: Simulate a $m$-query trace-estimation algorithm to solve a $n$-bit Gap-Hamming problem
Let $Z = S + T$ and $A = Z^T Z$, so that $\text{tr}(A) = \|Z\|_F^2 = \|s + t\|_2^2 = 2n - 2\langle s, t \rangle$.

If Alice and Bob can estimate $\text{tr}(A)$ to error $\left(1 \pm \frac{1}{\sqrt{n}}\right)$, they can solve the Gap-Hamming problem (so $\varepsilon = \frac{1}{\sqrt{n}}$).
A Reduction to Trace Estimation

Let $Z = S + T$ and $A = Z^T Z$, so that

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For any precision $b$ vector $x$, Alice and Bob can compute $Ax$ with $O(\sqrt{n}(\log(n) + b))$ bits of communication.
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They can simulate any $m$-query trace estimation algorithm with $O(m \cdot \sqrt{n}(\log(n) + b))$ bits of communication.
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Gap-Hamming Lower bound: $m \geq \Omega\left(\frac{n}{\sqrt{n}(\log(n)+b)}\right)$.
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Gap-Hamming Lower bound: $m \geq \Omega\left(\frac{n}{\sqrt{n}(\log(n) + b)}\right)$

Substitute $\varepsilon = \frac{1}{\sqrt{n}}$: $m \geq \Omega\left(\frac{1}{\varepsilon(b + \log(1/\varepsilon))}\right)$
Lower Bound:
Statistical Hypothesis Testing
Design distributions $\mathcal{P}_0$ and $\mathcal{P}_1$ over PSD matrices such that

1. A trace estimator can distinguish $\mathcal{P}_0$ from $\mathcal{P}_1$
   - If $A_0 \sim \mathcal{P}_0$ and $A_1 \sim \mathcal{P}_1$
   - With high probability, $\text{tr}(A_0) \leq (1 - 2\varepsilon) \text{tr}(A_1)$
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2. No estimator can distinguish $\mathcal{P}_0$ from $\mathcal{P}_1$ with $\Omega\left(\frac{1}{\varepsilon}\right)$ queries
   - Nature samples $i \sim \{0, 1\}$, and $A \sim \mathcal{P}_i$
   - Any estimator that correctly guesses $i$ with probability $\geq \frac{3}{4}$ must use $\Omega\left(\frac{1}{\varepsilon}\right)$ queries
Design distributions $\mathcal{P}_0$ and $\mathcal{P}_1$ over PSD matrices such that

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   - Nature samples $i \sim \{0, 1\}$, and $A \sim \mathcal{P}_i$
   - Any estimator that correctly guesses $i$ with probability $\geq \frac{3}{4}$ must use $\Omega(\frac{1}{\varepsilon})$ queries

The design of $\mathcal{P}_0$ and $\mathcal{P}_1$ should reflect what structure makes trace estimation hard!
Designing a Hard Instance

What would the hardest input for Hutch++ be?

![Graph showing eigenvalues with hard instances marked as $O(\frac{1}{\epsilon})$ eigenvalues and the rest being zero.](image-url)
Designing a Hard Instance

What would the hardest input for Hutch++ be?

- Hutch++ only makes errors with Hutchinson’s estimator on $\text{tr}(\mathbf{A} - \tilde{\mathbf{A}}_k)$

![Diagram showing eigenvalues of $A - A_k$]

- $O\left(\frac{1}{\epsilon}\right)$ eigenvalues (computable with $O\left(\frac{1}{\epsilon}\right)$ queries)
- Eigenvalues of $A - A_k$ (hardest input for Hutchinson’s)
Designing a Hard Instance

What would the hardest input for Hutch++ be?

- Hutch++ only makes errors with Hutchinson’s estimator on $\text{tr}(A - \tilde{A}_k)$
- For what $A$ would Hutchinson’s estimator have difficulty estimating $\text{tr}(A - A_k)$?
What would the hardest input for Hutch++ be?

- Hutch++ only makes errors with Hutchinson’s estimator on \( \text{tr}(\mathbf{A} - \tilde{\mathbf{A}}_k) \)
- For what \( \mathbf{A} \) would Hutchinson’s estimator have difficulty estimating \( \text{tr}(\mathbf{A} - \mathbf{A}_k) \)?
  - Hutchinson’s estimator needs many samples when \( \mathbf{A} - \mathbf{A}_k \) has concentrated eigenvalues
What would the hardest input for Hutch++ be?

- Hutch++ only makes errors with Hutchinson’s estimator on \(\text{tr}(A - \tilde{A}_k)\).
- For what \(A\) would Hutchinson’s estimator have difficulty estimating \(\text{tr}(A - A_k)\)?
  - Hutchinson’s estimator needs many samples when \(A - A_k\) has concentrated eigenvalues.
- \(A\) has \(k = O(\frac{1}{\epsilon})\) large eigenvalues. The rest are zero.
Designing a Hard Instance

Formally, for large enough integer $d$,

<table>
<thead>
<tr>
<th>$\mathcal{P}_0$</th>
<th>$A = G^T G$ for $G \in \mathbb{R}^{d \times \left(\frac{1}{\epsilon}\right)}$ Gaussian</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\mathcal{P}_1$</td>
<td>$A = G^T G$ for $G \in \mathbb{R}^{d \times \left(\frac{1}{\epsilon} + 1\right)}$ Gaussian</td>
</tr>
</tbody>
</table>
Experiments
Synthetic Experiments

Results on synthetic matrix $\mathbf{A}$ with spectrum $\lambda_i = i^{-c}$ for different values of $c$:

(a) Fast Eigenvalue Decay ($c = 2$)

(b) Medium Eigenvalue Decay ($c = 1.5$)

(c) Slow Eigenvalue Decay ($c = 1$)

(d) Very Slow Eigenvalue Decay ($c = 0.5$)
Hutch++ works well empirically for many non-PSD matrices.

Let $B$ be the (indefinite) adjacency matrix of an undirected graph $G$, $\frac{1}{6} \text{tr}(B^3)$ is exactly equal to the number of triangles in $G$.

Figure: $A = B^3$ for arXiv.org citation network and Wikipedia voting network.
Open Questions

- **In progress:** Lower bounds for e.g. $\text{tr}(A^3)$, $\text{tr}(e^A)$, $\text{tr}(A^{-1})$

- What about inexact oracles? We often approximate $f(A)x$ with iterative methods. How accurate do these computations need to be?

- Extend to include row/column sampling? This would encapsulate e.g. SGD/SCD.
THANK YOU

Code available at
github.com/RaphaelArkadyMeyerNYU/hutchplusplus