Dynamic Trace Estimation

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Implicit trace estimation

- A basic problem in linear algebra
  Given matrix $A \in \mathbb{R}^{n \times n}$ and access to A via matrix vector products $Av \in \mathbb{R}^n$, for $v \in \mathbb{R}^n$ (implicit access), approximate $\text{tr}(A) = \sum_{i=1}^{n} A_{ii}$.

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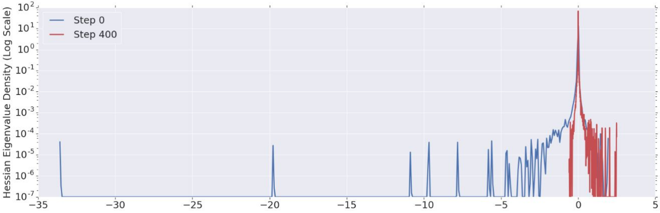

Figure 1: Ghorbani et al. [2019] analyze spectrum of Hessian for Resnet-32.

Implicit trace estimation

- For matrix functions $A = f(B)$, we can leverage iterative methods to approximate $Av = f(B)v$. (e.g. $A = B^{-1} / \exp(B) / \log(B)$). Typically, runtime is $O(n^2)$ compared to $O(n^3)$ for explicitly forming A.

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- Measure the computational cost in number of matrix-vector products required $Av_1, \ldots, Av_\ell$.

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- Approximate $\text{tr}(A)$ as $h_\ell(A) = \frac{1}{\ell}\sum_{i=1}^{\ell} g_i^T A g_i$ where entries in $g_i \in \mathbb{R}^n$ are random i.i.d. ± 1.

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- $h_\ell(A)$ approximates $\text{tr}(A)$ in expectation.

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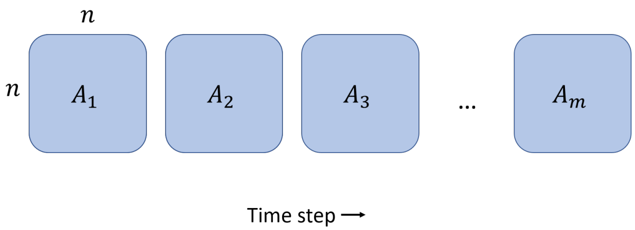
Main takeaways from the Hutchinson's estimator (Avron and Toledo [2011], Roosta-Khorasani and Ascher [2015], Cortinovis and Kressner [2020]):

- Variance of $h_\ell(A) \leq \frac{2}{\ell}\|A\|_F^2$
- For $\ell = O(\frac{\log(1/\delta)}{\epsilon^2})$, with high probability, $|h_\ell(A) - \text{tr}(A)| \leq \epsilon\|A\|_F$

Dynamic setting



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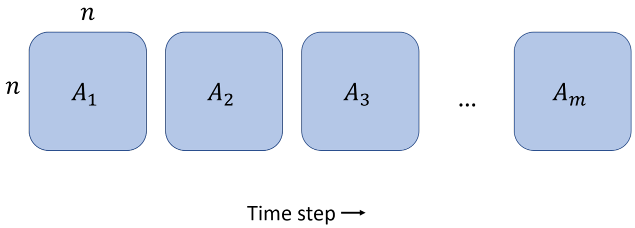

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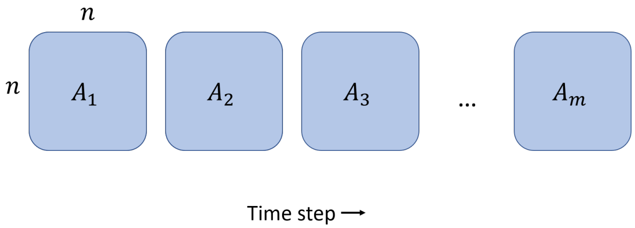

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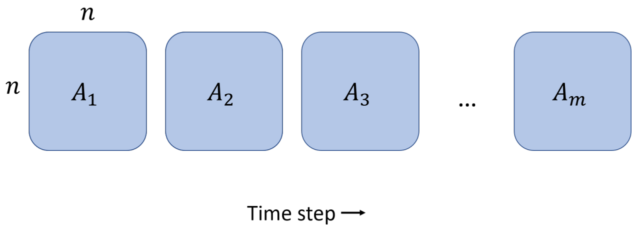

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Our result: Yes and can obtain *quadratic* improvements under certain assumptions!

Problem formulation

Problem (Dynamic trace estimation)

Let $A_1, ..., A_m$ be $n \times n$ symmetric matrices satisfying:

1. $\|A_i\|_F \leq 1$, *for all* $i \in [1, m]$.
2. $\|A_{i+1} - A_i\|_F \leq \alpha$, *for all* $i \in [1, m-1]$.

Given implicit matrix-vector multiplication access to each A_i in sequence, the goal is to compute trace approximations $t_1, \ldots, t_m$ for $tr(A_1), ..., tr(A_m)$ such that, for each $i \in 1, \ldots, m$,

$$\mathbb{P}[|t_i - tr(A_i)| \geq \epsilon] \leq \delta.$$

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t_2 = Reuse + Estimate

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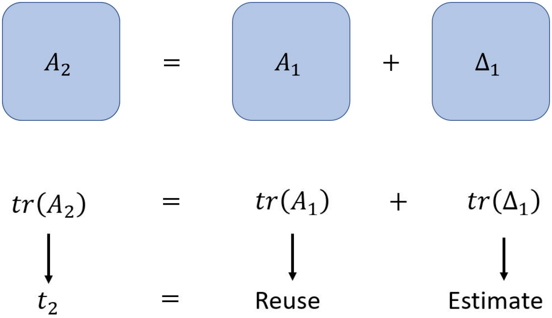
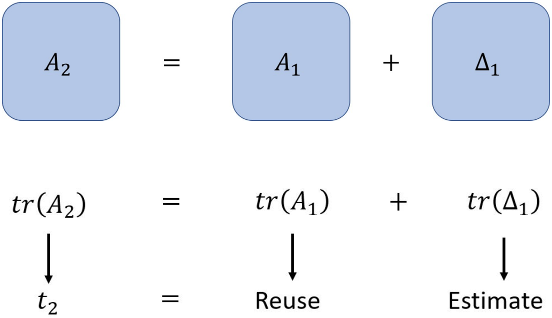


Observation: If $\|\Delta_i\|_F << \|A_i\|_F$, we should be able to accurately estimate $\text{tr}(\Delta_i)$ with a lot less matrix-vector products.



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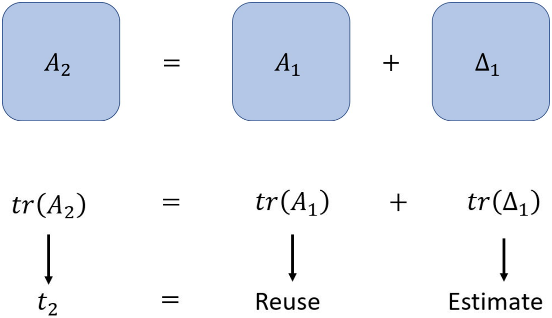

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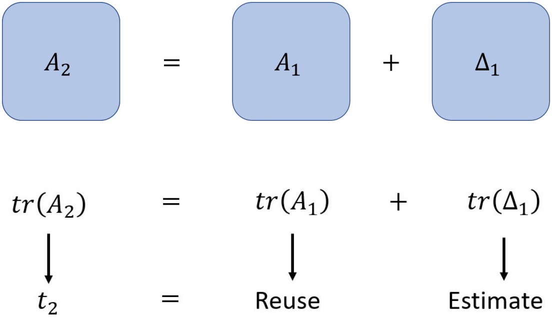

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- Multiplying by $(1-\gamma)$ reduces the variance of the leading term.

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For any $\epsilon, \delta, \alpha \in (0, 1)$, the DeltaShift algorithm solves Dynamic Trace Estimation problem with

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For $\alpha \approx \epsilon$, DeltaShift requires $O(\frac{\log(1/\delta)}{\epsilon})$ total matrix-vector products.

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- Note: We can reuse the same matrix-vector products used by trace estimation.

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For $\|A_i\|_* \leq 1$ and $\|A_{i+1} - A_i\|_* \leq \alpha$ for all i, DeltaShift++ solves dynamic trace estimation problem with

$$O\left(m \cdot \frac{\sqrt{\alpha/\delta}}{\epsilon} + \frac{\sqrt{1/\delta}}{\epsilon}\right)$$

total matrix-vector products with $A_1, A_2, ..., A_m$.

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We can estimate near-optimal γ for DeltaShift++ as well!

Let $K_A = \|A - A_k\|_F^2$

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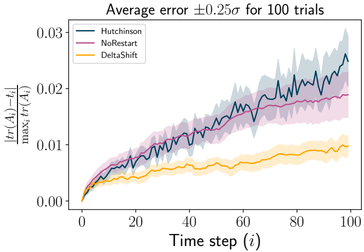
Similar to DeltaShift, we can reuse matrix-vector products from trace estimation!

Empirical results

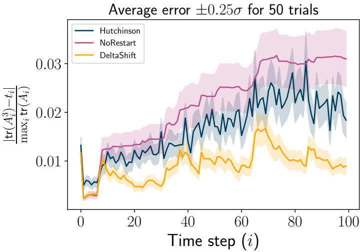
For the dynamic trace problem, we compare using the **same number of total matrix-products** for

- Hutchinson's estimator at each time step
- Estimate $\text{tr}(\Delta_i)$ at each time step and add to $\text{tr}(A_i)$ (NoRestart)
- DeltaShift

Empirical results



(a) Synthetic data with total matrix-vector products= $8 * 10^3$



(b) Graph data with total matrix-vector products= 10^4

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The three term recurrence relation for Chebyshev polynomials is:

$$T_0(H) = I, \qquad T_1(H) = H, \qquad T_{n+1}(H) = 2HT_n(H) - T_{n-1}(H).$$

Empirical results

Table 1: Average error for trace of polynomials of Hessian with learning rate 0.001 and total matrix-vector products = 2000

	Hutchinson	NoRestart	DeltaShift
$T_1(H)$	2.5E-02	3.7E-02	**1.7E-02**
$T_2(H)$	1.2E-06	1.7E-06	**8.0E-07**
$T_3(H)$	4.0E-02	4.1E-02	**3.1E-02**
$T_4(H)$	1.5E-06	1.7E-06	**1.0E-06**
$T_5(H)$	2.1E-02	4.3E-02	**1.9E-02**

Future work

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- Can we do better when Δ matrices have additional structure? Partial progress in form of DeltaShift++.

Thank you!