Error Estimation for Randomized Numerical Linear Algebra via the Bootstrap

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- Randomized methods can be competitive with highly optimized software (e.g. LAPACK)
- In exchange for reduced cost, randomized solutions also come with (random) approximation error.

Trading off computational cost and accuracy

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- However, such guarantees typically have limitations:
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  - conservative or unknown constants
  - ignore unique problem structure

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- **Our approach:** Estimate error via bootstrap.
  1. Randomized matrix multiplication (MM)
  2. Randomized least squares (LS)

Part I: Error estimation for matrix multiplication

Review of randomized MM

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Ordinary matrix multiplication has cost $\mathcal{O}(nd^2)$.

This cost can be a major bottleneck if matrix multiplication is used repeatedly in the analysis of large datasets.

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Recall that A and B each have a very large number of rows n.

One way to speed up the computation of $A^\top B$ is to use smaller matrices, called "sketches" $\tilde{A}$ and $\tilde{B}$, each having t rows, where $d \ll t \ll n$.

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The sketching matrix is generated randomly, satisfying $\mathbb{E}[S^\top S] = \mathbf{I}_{n\times n}$. Hence,

$$\mathbb{E}[\tilde{A}^\top \tilde{B}] = \mathbb{E}[A^\top S^\top SB] = A^\top B.$$

(Many sophisticated types of S matrices have been proposed, but we omit these details.)

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Usually the rows $\mathbf{s}_1, \ldots, \mathbf{s}_t$ are (nearly) i.i.d., and so as t becomes large, LLN suggests $S^\top S \approx \mathbf{I}_{n\times n}$, giving

$$\tilde{A}^\top \tilde{B} \; = \; A^\top S^\top S B \; \approx \; A^\top B.$$

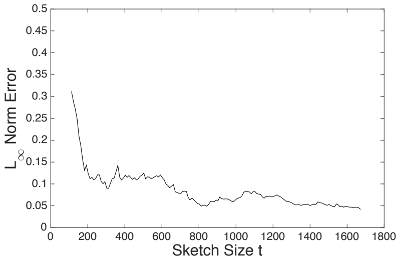
However, the cost of sketching grows proportionally with t.

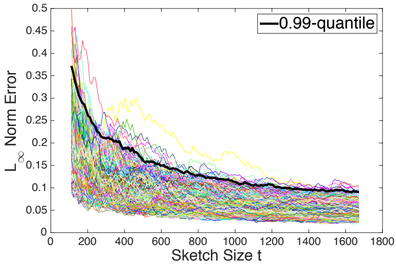
How does error depend on sketch size?

Consider the error

$$\varepsilon_t \ := \ \left\|\tilde{A}^\top \tilde{B} - A^\top B\right\|, \tag{1}$$

which is a random variable, since the sketches $\tilde{A}$ and $\tilde{B}$ are random.





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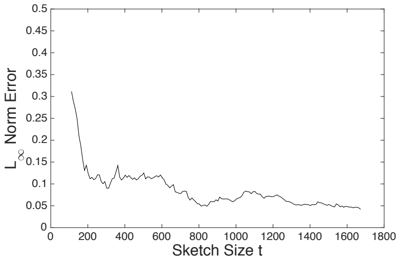
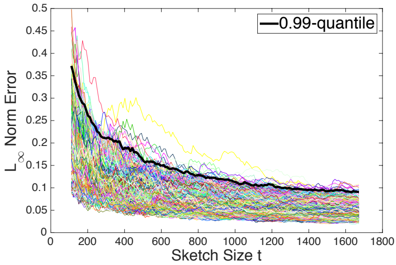


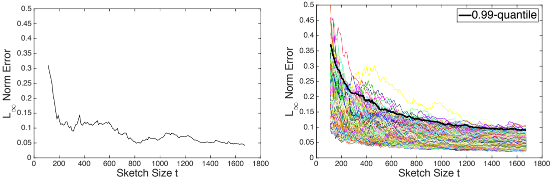


Note: The user is not able to see these curves in practice.

How does error depend on sketch size?

Let $q_{1-\alpha}(t)$ be the $(1-\alpha)$-quantile of ε_t.

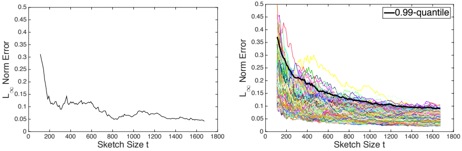
This is the tightest upper bound on ε_t that holds w.p. at least $1-\alpha$.



If the user knew the function $q_{1-\alpha}(t)$, they could know two things:

1. How accurate $\tilde{A}^\top \tilde{B}$ is likely to be for any given t.
2. How large t needs to be in order to achieve a given degree of accuracy.

Estimating the error quantiles



Problem formulation:

- We want to estimate the thick black curve $q_{1-\alpha}(t)$ from only one run of sketching. (i.e. just $\tilde{A}$ and $\tilde{B}$)
- It's not clear this is even possible, because $q_{1-\alpha}(t)$ reflects variation over many runs.
- We are computationally constrained: Any method we come up with should be cheap, so that it does not defeat the purpose of sketching.
- Also note that in practice, the user gets to see none of the curves above.

Intuition for bootstrap

- If we could generate samples of $\|\tilde{A}^\top \tilde{B} - A^\top B\|$, we would be done.

- For instance, if we could generate 100 samples, then we could take the 99th largest to estimate $q_{.99}(t)$.

- However, this is not possible since we don't know $A^\top B$.

- The bootstrap gives a way to generate "pseudo-samples" of $\|\tilde{A}^\top \tilde{B} - A^\top B\|$ using only the observed matrices $\tilde{A}$ and $\tilde{B}$.

Bootstrap procedure

Input: a positive integer m and the sketches $\tilde{A}$ and $\tilde{B}$.

For $l = 1, \ldots, m$ **do**

1. Draw a vector $(i_1, \ldots, i_t)$ by sampling t numbers with replacement from $\{1, \ldots, t\}$.

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Return: $\widehat{q}_{1-\alpha}(t) \longleftarrow$ the $(1-\alpha)$-quantile of the values $\varepsilon_1^*, \ldots, \varepsilon_m^*$.

Speeding things up with extrapolation

The CLT indicates that $q_{1-\alpha}(t)$ should decay like $1/\sqrt{t}$.

Hence, we can bootstrap small "initial sketches" with t_0 rows, and then use

$$\widehat{q}_{1-\alpha}^{\,\text{ext}}(t) := \tfrac{\sqrt{t_0}}{\sqrt{t}}\,\widehat{q}_{1-\alpha}(t_0).$$

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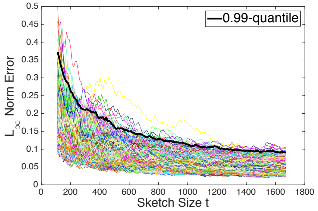

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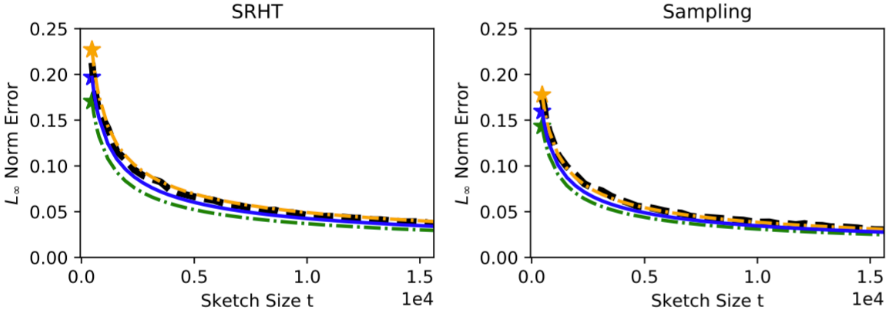
Empirically, merely $m = 20$ produces good results! (plots given later).

Also, we take $\frac{t}{t_0} \geq 20$ in many experiments.

Empirical performance

MNIST data: computing $A^\top A$ with $A \in \mathbb{R}^{60,000\times 780}$.

- initial sketch size $t_0 = 390$
- bootstrap samples $m = 20$



Comments on theoretical results

- It is possible to measure the quality of the estimator $\widehat{q}_{1-\alpha}(t)$ in terms of the Lévy-Prohorov metric between $\mathcal{L}(\sqrt{t}\varepsilon_t)$ and $\mathcal{L}(\sqrt{t}\varepsilon_t^*|S)$.

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- Proof makes use of recent ideas on the "multiplier bootstrap" method in the high-dimensional statistics literature, as well as sharp constants in Rosenthal's inequality.

Part II: Error estimation for randomized least squares

Review of randomized LS

Consider a deterministic matrix $A \in \mathbb{R}^{n \times d}$ and vector $b \in \mathbb{R}^n$, with $n \gg d$.

The exact solution $x_{\text{opt}} := \underset{x \in \mathbb{R}^d}{\operatorname{argmin}} \|Ax - b\|_2$ is too costly to compute.

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We focus on two particular randomized LS algorithms:

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1. **Classic Sketch (CS).** (Drineas et al, 2006)

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2. **Iterative Hessian Sketch (IHS).** (Pilanci & Wainwright 2016)

$$\widehat{x}_{i+1} := \underset{x \in \mathbb{R}^d}{\operatorname{argmin}} \left\{ \tfrac{1}{2} \|\tilde{A}(x - \widehat{x}_i)\|_2^2 + \langle A^\top (A\widehat{x}_i - b)\,,\, x \rangle \right\}, \qquad i = 1, \dots, k.$$

Problem formulation (error estimation)

We will estimate the errors of the random solutions $\tilde{x}$ and $\widehat{x}_k$ in terms of high-probability bounds.

Let $\|\cdot\|$ denote any norm on $\mathbb{R}^d$, and let $\alpha \in (0,1)$ be fixed.

Goal: Compute numerical estimates $q_{1-\alpha}(t)$ and $\widehat{q}_{1-\alpha}(t,k)$, such that the bounds

$$\|\tilde{x} - x_{\text{opt}}\| \leq \tilde{q}_{1-\alpha}(t)$$

$$\|\widehat{x}_k - x_{\text{opt}}\| \leq \widehat{q}_{1-\alpha}(t,k)$$

each hold with probability at least $1-\alpha$.

Intuition for the bootstrap

Key idea: Artificially generate a bootstrapped solution $\tilde{x}^*$ such that the fluctuations of $\tilde{x}^* - \tilde{x}$ are statistically similar to the fluctuations of $\tilde{x} - x_{\text{opt}}$.

In the "bootstrap world", $\tilde{x}$ plays the role of x_{opt}, and $\tilde{x}^*$ plays the role of $\tilde{x}$.

The bootstrap sample $\tilde{x}^*$ is the LS solution obtained by "perturbing" $\tilde{A}$ and $\tilde{b}$.

(The same intuition also applies to the IHS solution $\widehat{x}_k$.)

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Note: A similar algorithm works for IHS.

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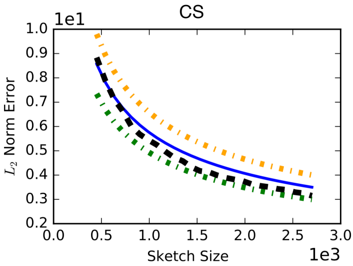
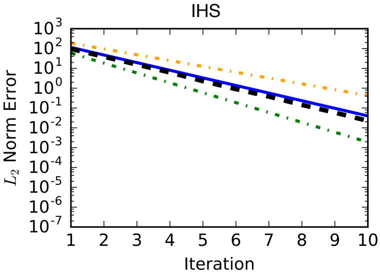
5. Error estimates can be extrapolated (similar to MM context).

Empirical performance

'YearPredictionMSD' data from LIBSVM: $n \approx 5 \times 10^5$ and $d = 90$

- **CS:** fix initial sketch size $t_0 = 5d$ and extrapolate on $t \gg t_0$
- **IHS:** fix sketch size $t = 10d$ and extrapolate on number of iterations
- bootstrap samples $m = 20$





Comments on theoretical results

- Main result shows that under certain asymptotic assumptions

$$\liminf_{n\to\infty} \mathbb{P}\Big(\|\tilde{x} - x_{\text{opt}}\| \leq \tilde{q}_{1-\alpha}(t)\Big) \;\geq 1-\alpha,$$

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- The most difficult part of the proof concerns the IHS algorithm which is iterative. This leads to analyzing the distribution of $\widehat{x}_k$ conditionally on the previous iterates, and this requires approximations that hold "uniformly" over past iterates.

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- Numerical performance is encouraging, and is supported by theoretical guarantees.

Recent work

- *A Bootstrap Method for Error Estimation in Randomized Matrix Multiplication*
  arxiv:1708.01945
- *Error Estimation for Randomized Least-Squares Algorithms via the Bootstrap*
  ICML 2018, and arxiv:1803.08021
- *Estimating the Algorithmic Variance of Randomized Ensembles via the Bootstrap*
  The Annals of Statistics (to appear) 2018

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