A Framework for Statistical Inference via Randomized Algorithms

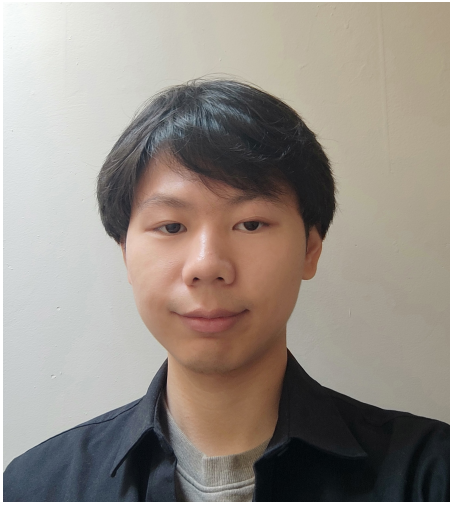
Edgar Dobriban, University of Pennsylvania
joint work with Zhixiang Zhang and Sokbae Lee

February 25, 2024

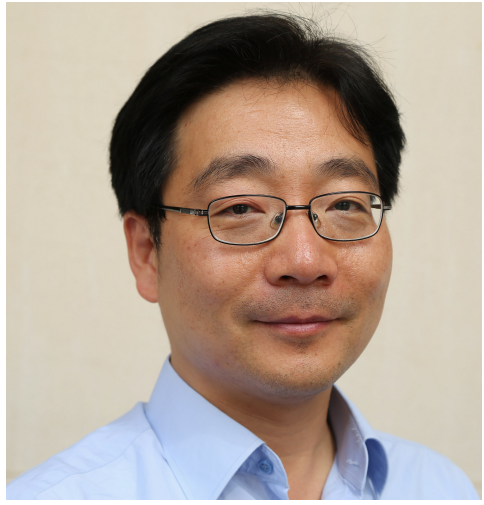
Research Interests

- the efficient statistical analysis of large complex datasets using advanced tools, such as those from random matrix theory
  - dimension reduction, PCA: [1], [2], [3], [4], [5], [6]
  - statistically principled prediction sets: [1], [2]
  - distribution shift and heterogeneity: [1], [2], [3]
  - multiple testing: [1], [2], [3]
  - high-dimensional regression: [1], [2]
  - statistical inference via randomized algorithms
  - invariance-based randomization tests
- the foundations of modern machine learning, including deep learning
  - uncertainty quantification: [1], [2], [3], [4], [5]
  - sketching and random projections: [1], [2], [3], [4], [5], [6]
  - data augmentation and symmetry: [1], [2], [3], [4]
  - distributed learning: [1], [2], [3]
  - (stochastic) gradient descent and flow: [1], [2], [3]
  - fairness: [1], [2]
  - overparametrization
  - retraining of ML models

Collaborators on This Project



Zhixiang Zhang



Sokbae Lee

Overview

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Randomized Algorithms

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- A randomized algorithm uses external randomness in its steps
  - Stochastic optimization
  - Monte Carlo methods (MCMC, ...)
  - Random projection/sketching methods

How Randomness Improves Algorithms

Quanta magazine

Unpredictability can help computer scientists solve otherwise intractable problems.

Random Projections in Science

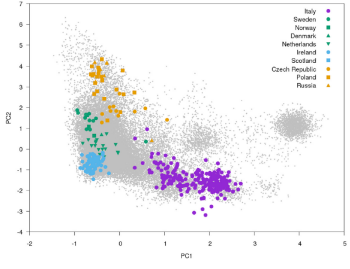
ARTICLE

Fast Principal-Component Analysis Reveals Convergent Evolution of *ADH1B* in Europe and East Asia

Kevin J. Galinsky,[1,2,*] Gaurav Bhatia,[2,3] Po-Ru Loh,[2,3] Stoyan Georgiev,[4] Sayan Mukherjee,[5] Nick J. Patterson,[2,6] and Alkes L. Price[1,2,3,6,*]

Searching for genetic variants with unusual differentiation between subpopulations is an established approach for identifying signals of natural selection. However, existing methods generally require discrete subpopulations. We introduce a method that infers selection using principal components (PCs) by identifying variants whose differentiation along top PCs is significantly greater than the null distribution of genetic drift. To enable the application of this method to large datasets, we developed the FastPCA software, which employs recent advances in random matrix theory to accurately approximate top PCs while reducing time and memory cost from quadratic to linear in the number of individuals, a computational improvement of many orders of magnitude. We apply FastPCA to a cohort of 54,734 European Americans, identifying 5 distinct subpopulations spanning the top 4 PCs.

456 The American Journal of Human Genetics *98*, 456–472, March 3, 2016



[Galinsky et al., 2016]: FastPCA, $n = 54,734$, $p = 162,335$

CAMBRIDGE

978-1-108-41498-2 — Advances in Economics and Econometrics

CHAPTER 1

Opportunities and Challenges: Lessons from Analyzing Terabytes of Scanner Data

Serena Ng

This paper seeks to better understand what makes big data analysis different, what we can and cannot do with existing econometric tools, and what issues need to be dealt with in order to work with the data efficiently. As a case study, I set out to extract any business cycle information that might exist in four terabytes of weekly scanner data. The main challenge is to handle the volume, variety, and characteristics of the data within the constraints of our computing environment. Scalable and efficient algorithms are available to ease the computation burden, but they often have unknown statistical properties and are not designed for the purpose of efficient estimation or optimal inference. As well, economic data have unique characteristics that generic algorithms may not accommodate. There is a need for computationally efficient econometric methods as big data is likely here to stay.

[Ng, 2017]: Nielsen scanner data: Four terabytes.

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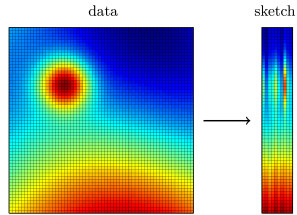

From U.S. Department of Energy Randomized Algorithms Workshop

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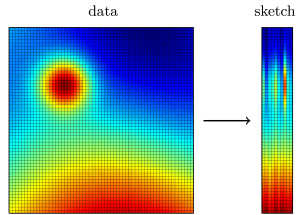

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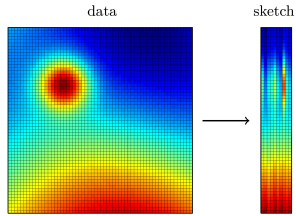

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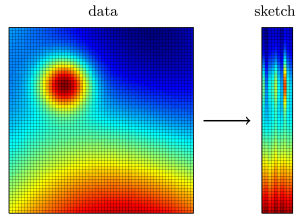

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- Challenge: How to be "responsibly reckless"—Jack Dongarra, Turing Award Lecture '21

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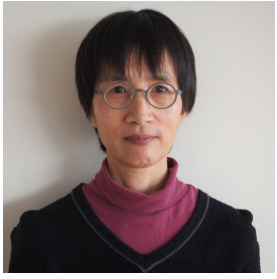
- Sketched least squares in fixed dimension:
  - CLTs for some sketches [Ahfock et al., 2021, Bartan and Pilanci, 2022];
  - bootstrap for some sketches under conditions [Lopes et al., 2018];
  - heteroskedastic linear models [Lee and Ng, 2022].

Miles Lopes

Michael Mahoney



Serena Ng

Mert Pilanci

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- Aim to develop a general framework for statistical inference when using randomized methods.
  - Require minimal assumptions: general data/algorithms

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  - Require minimal assumptions: general data/algorithms
- Illustrate with examples (Today, least squares).

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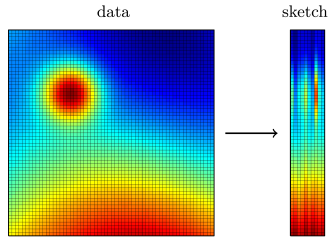

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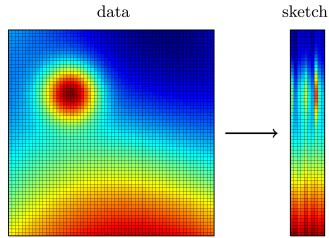

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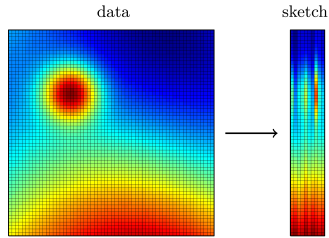

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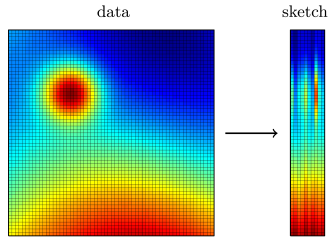

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  - S_m: random sketching/projection matrix,
  - Observed data $Z_m : (\tilde{X}_m, \tilde{y}_m) = (S_m X, S_m y)$,

Goal: Constructing a Confidence Region

- Goal: construct confidence region $C_m = C_m(Z_m)$ for θ such that

$$P_{S_m}(\theta \in C_m) \geqslant 1 - \alpha.$$

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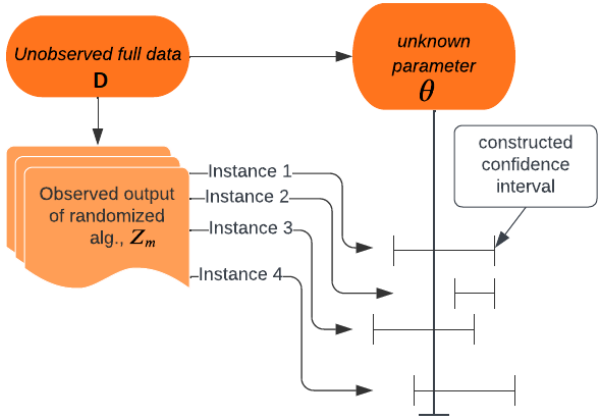
- The randomness is from S_m only.



Classical Pivotal Inference

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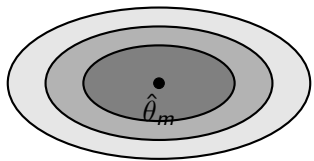
- To construct a confidence region, start from an estimator $\hat{\theta}_m = \hat{\theta}_m(Z_m)$ of θ
- Recall classical pivotal inference:
  - If pivot $\hat{T}_m(\hat{\theta}_m - \theta)$ has a known distribution J for a known matrix $\hat{T}_m = \hat{T}_m(Z_m)$,
  - Then for a set Γ such that $J(\Gamma) \geqslant 1 - \alpha$, can take

$$C_m = \hat{\theta}_m - \hat{T}_m{}^{-1}\Gamma.$$

Clearly $P_{S_m}(\theta \in C_m) \geqslant 1 - \alpha$.



C_m: Linear transform of Γ, centered at $\hat{\theta}_m$.

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- More generally, asymptotics: Establish $\hat{T}_m(\hat{\theta}_m - \theta) \Rightarrow J$,
- Meaning: asymptotically, estimator makes errors in a predictable way
- If J is known, pivotal method has asymptotic coverage;

More General Methods for Inference

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More General Methods for Inference

- What if J is not known?
- Taking inspiration from subsampling [Politis and Romano, 1994, Politis et al., 1999], propose "sub-randomization"

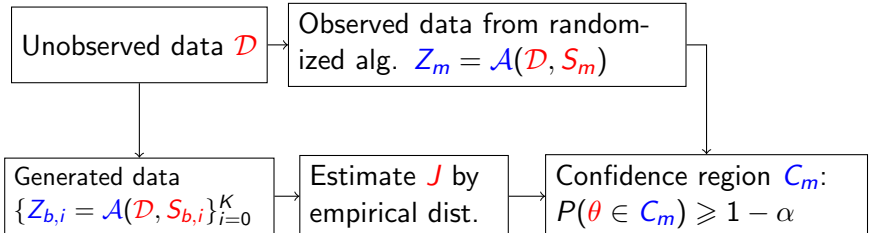
Dimitris Politis

Joseph Romano

Michael Wolf

Sub-randomization

- Generate $K+1$ i.i.d. smaller datasets $Z_{b,i} = \mathcal{A}(\mathcal{D}, S_{b,i})$, for $i = 0, \ldots, K$, with i.i.d. $S_{b,i}$ and $b < m$, by running the randomized algorithm.



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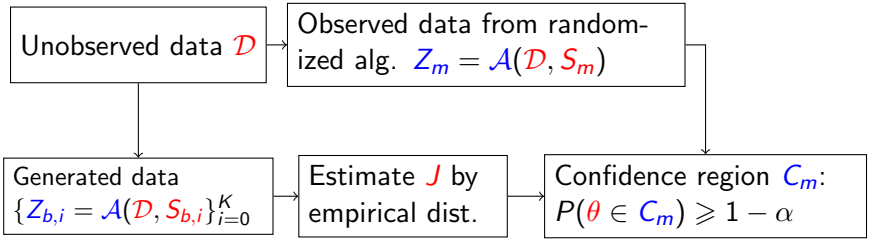


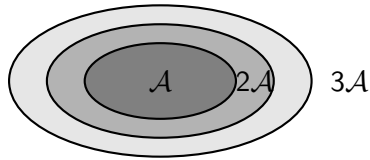
- Estimate J (where $\hat{T}_m(\hat{\theta}_m - \theta) \approx J$) by the empirical distribution of $\hat{\theta}_b(Z_{b,i})$, $i = 1, \ldots, K$, letting

$$\hat{J}(\cdot) = \frac{1}{K} \sum_{i=1}^{K} I\left(\widehat{T}_b(Z_{b,0}) \left[\hat{\theta}_b(Z_{b,i}) - \hat{\theta}_m(Z_m)\right] \in \cdot\right).$$

Scaling a set

- **Definition.** For a closed convex set $\mathcal{B}$, and probability dist. P, s.t. $P(x \cdot \mathcal{B}) \to 1$ as $x \to \infty$, define the scaling

$$\Gamma_P := \inf\{x \geqslant 0 : P(x \cdot \mathcal{B}) \geqslant 1 - \alpha\} \cdot \mathcal{B}$$



Sub-randomization: General result

- Let $\tilde{J}_m$ be the distribution of $\hat{T}_m(Z_m)(\hat{\theta}_m - \theta)$
- **Condition**: asymptotically, estimator makes errors in a predictable way (for both m and b)

$$\tilde{J}_m \Rightarrow J \text{ and } \tilde{J}_b \Rightarrow J.$$

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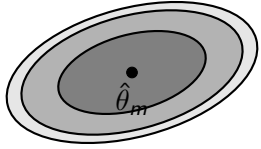
  Do not need to know J; only that it exists.
- Recall problem index n, large output size m, small output size b, number of runs K
- **Theorem.** When $n, m, b, K \to \infty$, if $(\widehat{T}_m(Z_m) - \widehat{T}_b(Z_b))^{-1}$ exists w.p. $\to 1$, and Γ_J is a continuity set of J,

$$C_m = \hat{\theta}_m - \left(\widehat{T}_m(Z_m) - \widehat{T}_b(Z_b)\right)^{-1} \Gamma_{\hat{J}}$$

  is an asymptotically valid confidence set: $\liminf_{n\to\infty} P(\theta \in C_m) \geqslant 1 - \alpha$.



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- If for some T_m, $T_m(\hat{\theta}_m - \theta_n) \Rightarrow \mathcal{N}(0, I_p)$, we can develop a simpler *plug-in method*

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- Compute $\hat{\theta}_{m,i} = \hat{\theta}_m(Z_{m,i})$ for $i \in [K]$ and let $\hat{\theta}^*_{K,m} = K^{-1} \sum_{i=1}^K \hat{\theta}_{m,i}$. Let

$$\widehat{\Sigma}_K = K^{-1} \sum_{i=1}^K (\hat{\theta}_{m,i} - \hat{\theta}^*_{K,m})(\hat{\theta}_{m,i} - \hat{\theta}^*_{K,m})^\top, \text{ and } \widehat{T}_K = \widehat{\Sigma}_K^{1/2}.$$

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- **Theorem.** Let $m, n, K \to \infty$, s.t. for $A_{m,n} = T_m(\hat{\theta}_m - \theta_n)$, $\mathbb{E}A_{m,n} \to 0$, $\mathbb{E}A_{m,n}A_{m,n}^\top \to I_p$, and Var $\left[(v^\top A_{m,n})^2\right]$ is bounded over m, n and $v \in \mathbb{R}^p$ with $\|v\| = 1$. Then, for an $1 - \alpha$-probability set Γ under $\mathcal{N}(0, I_p)$,

$$P_{Z_m}\left(\theta_n \in \hat{\theta}_m - \widehat{T}_K^{-1}\Gamma\right) \to_P 1 - \alpha.$$

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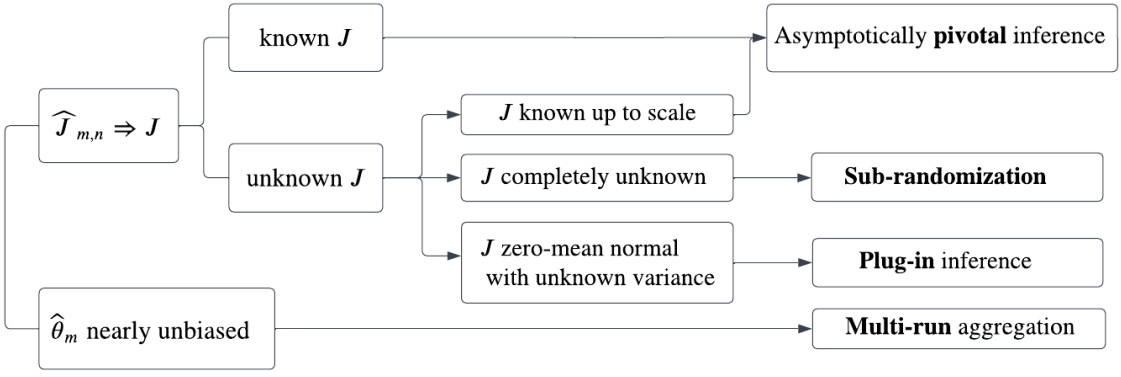
- **Theorem.** Let $b, n, K \to \infty$, and suppose there is $a > 0$ such that $\mathbb{E}|v^\top \hat{\theta}_b|^{2+a}$ is uniformly bounded over b, n and all $v \in \mathbb{R}^p$ with $\|v\| = 1$. Let $\lambda_b = \lambda_{\min}\left(\mathrm{Cov}\left[\hat{\theta}_b\right]\right)$, and suppose that $\|\mathbb{E}\hat{\theta}_b - \theta_n\| = o(K^{-1/2}{\lambda_b}^{1/2})$. Then,

$$P\left(\theta_n \in \frac{1}{K}\sum_{i=1}^{K}\hat{\theta}_{b,i} - \frac{1}{K^{1/2}}\widehat{T}_{K,b}^{-1}\Gamma\right) \to 1-\alpha.$$

Summary of inference methods via randomized algorithms



Overview

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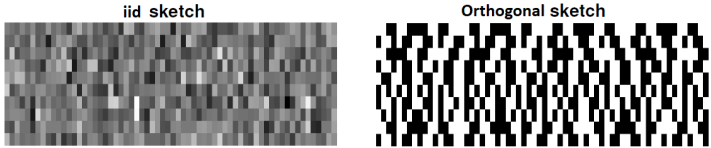

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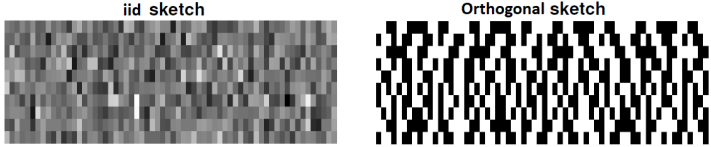

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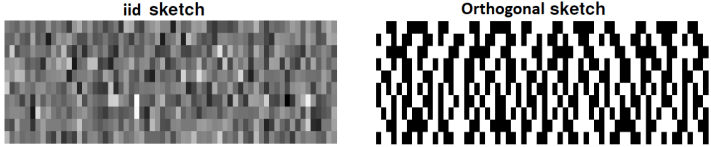

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- Later: partial sketching, iterative sketching: sketch-and-project, ...

Statistical Inference in Sketch-and-solve OLS

- Consider $c^\top \hat{\beta}_m$ for some fixed sequence of $c \in \mathbb{R}^p$.
- We aim to show asymptotic normality:

$$\tau_m \sigma^{-1}(c^\top \hat{\beta}_m - c^\top \beta) \Rightarrow \mathcal{N}(0, 1).$$

  where τ_m and $\sigma = \sigma(\mathcal{D})$ depend on the type of sketch.
- Implies that sub-randomization, plug-in inference, and aggregation (using additional bias bound) can be used, with $\hat{T}_m$ replaced by τ_m
- Asymptotically pivotal inference can also be used if we can estimate σ

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- **Theorem.** For i.i.d. sketching, when all moments of the entries of the sketching matrices are bounded, $\mathbb{E}|S_{1,1}|^l \leqslant C_l$ for any $(C_l)_{l \geqslant 1}$ with $C_l < \infty$, we have asymptotic normality with $\tau_m = (m-p)^{1/2}$, and

$$\sigma^2 = \frac{m-p}{m}(\kappa_4 - 3)\sum_{k=1}^{n}[c^\top (X^\top X)^{-1} x_k \varepsilon_k]^2 + c^\top (X^\top X)^{-1} c \|\varepsilon\|^2.$$

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- Gaussian case: Recall that $X = U\Lambda V^\top$, and $U_\perp$ is an orthogonal complement of U; then

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- Let $q(\theta) = m^{1/2}(c^\top \hat{\beta}_m(\theta) - c^\top \beta)$. Find the characteristic function $\mathbb{E}e^{itq(\pi/2)}$.

Proof idea for i.i.d. case continued

- We show that for any bounded complex-valued function f with bounded derivatives up to the fifth order, we have the ODE

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$$\frac{d\mathbb{E}g(\theta)}{d\theta} = \left(\frac{d\mathbb{E}\psi}{d\theta} + (\mathbb{E}\psi)2t^2(\kappa_4 - 3)\sin^3\theta\cos\theta\Psi\right)$$
$$\times \exp\left\{t^2(\kappa_4 - 3)\sin^4\theta\Psi/2\right\} = o(1),$$

  thus $\mathbb{E}g(\pi/2) = \mathbb{E}g(0)$ (matching Gaussian case).

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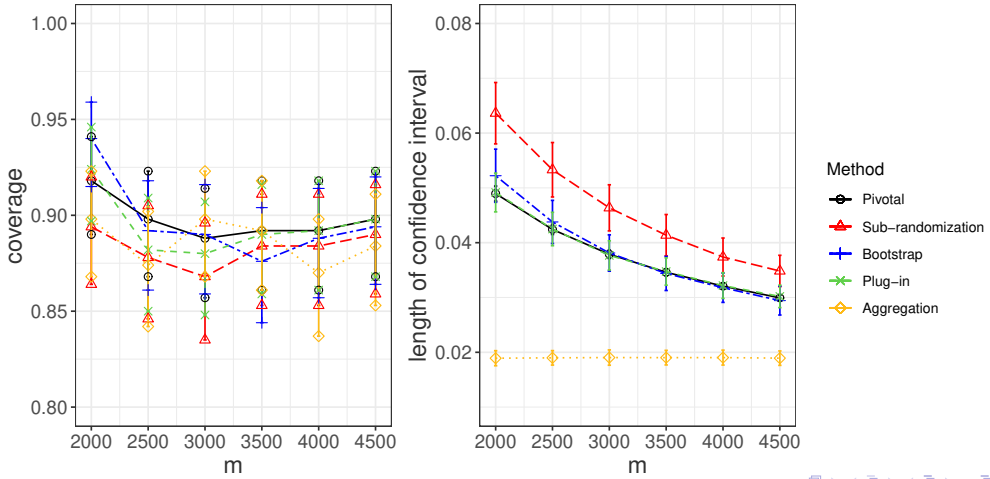
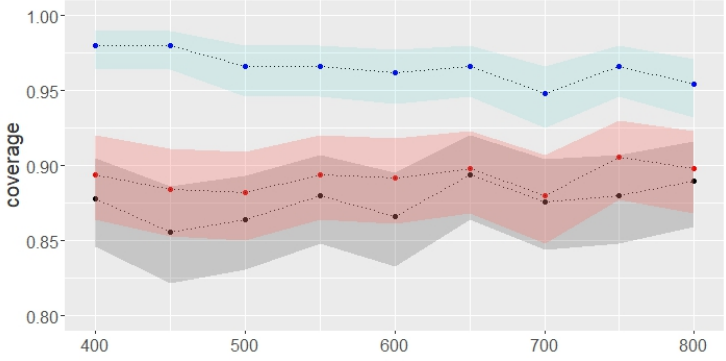
- With $n = 8,000$, $p = 500$, $b = 600$ and $K = 100$, find coverage of Hadamard sketching 90% intervals for the first coordinate of β; and 95% Clopper-Pearson interval for coverage



Empirical Data Example

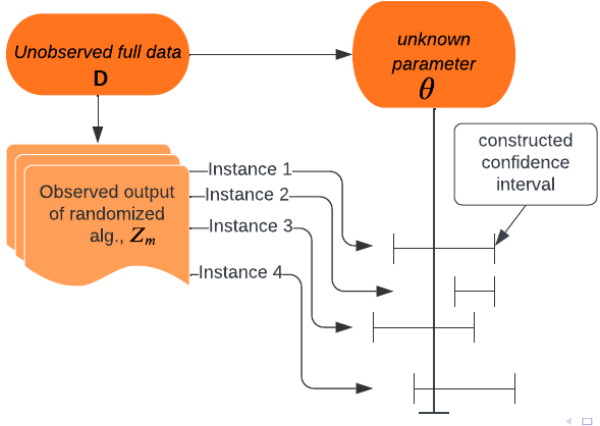
- Use subset of HGDP data, with $n = 1043$ indiv., $p = 200$ SNPs, $b = 300$, $K = 100$; Hadamard sketching.
- Show coverage of 90% intervals for the first coordinate of β; and 95% Clopper-Pearson interval for coverage

Pivotal method (black); sub-randomization (red); bootstrap (blue).



Summary

- A framework for statistical inference when using randomized algorithms
  - Requires showing $\widehat{T}_m(\hat{\theta}_m - \theta)$ has a limit distribution (sometimes more: normal limit, small bias)
- Example: Sketching in least squares. Aggregation is the "best" of the methods considered.
  - Allow broad classes of projections, algorithms
  - Handle growing data dimension



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- Pivotal: ✓

Partial Sketching

- **Theorem.** Asymptotic normality holds for Haar/Hadamard partial sketching. The plug-in estimators estimate Σ' (below) consistently.

τ_m, Σ for asymptotic distribution of $\hat{\beta}_m^{(\mathrm{pa})}$ when p is fixed

	τ_m	Σ'
i.i.d. ($\kappa_4 = 3$)	$m^{1/2}$	$(X^\top X)^{-1}\|X\beta\|^2 + \beta\beta^\top$
Haar	$\left(\frac{mn}{n-m}\right)^{1/2}$	$(X^\top X)^{-1}\|X\beta\|^2 + \beta\beta^\top$
Hadamard	$\left(\frac{mn}{n-m}\right)^{1/2}$	$(X^\top X)^{-1}\|X\beta\|^2 + 2\beta\beta^\top$

The asymptotic variances of $\hat{\beta}_m^{(\mathrm{pa})}$ differ slightly for Haar and Hadamard.

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- **Theorem.** For i.i.d. sketching,

$$m^{T/2}\left(\hat{\beta}_{T,m,n} - \beta\right) \Rightarrow V\Lambda^{-1}\left(\prod_{i=T}^{1} \mathcal{G}_i\right) U^\top y,$$

where $\mathcal{G}_i$ are i.i.d. symmetric zero-mean Gaussian, and for $j_1 \leq k_1$, $j_2 \leq k_2$

$$\mathrm{Cov}\left[(\mathcal{G}_i)_{j_1 k_1}, (\mathcal{G}_i)_{j_2 k_2}\right] = \delta_{j_1 j_2}\delta_{k_1 k_2} + \delta_{j_1 k_2}\delta_{k_1 j_2} + (\kappa_4 - 3) \lim_{n\to\infty} \sum_{\ell=1}^{n} U_{\ell,j_1} U_{\ell,k_1} U_{\ell,j_2} U_{\ell,k_2}.$$

- Sub-randomization & pivotal can be used.

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- **Theorem.** For i.i.d. sketching, $\alpha_m = \frac{m-p}{m}$, $\tau_m = (m-p)^{1/2}$,

$$\sigma'^2 = \frac{m-p}{m}(\kappa_4 - 3) \sum_{k=1}^{n} \left[c^\top (X^\top X)^{-1} x_k (y_k - \varepsilon_k) \right]^2 + \left[\|X\beta\|^2 c^\top (X^\top X)^{-1} c + (c^\top \beta)^2 \right].$$

Growing p, Partial Sketching

We aim to show

$$\tau_m \sigma'^{-1} \left(\alpha_m c^\top \hat{\beta}_m^{(\mathrm{pa})} - c^\top \beta \right) \Rightarrow \mathcal{N}(0,1).$$

- **Theorem.** For i.i.d. sketching, $\alpha_m = \frac{m-p}{m}$, $\tau_m = (m-p)^{1/2}$,

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- **Theorem.** For Haar sketching, $\alpha_m = \frac{n(m-p)}{m(n-p)}$, $\tau_m = \left(\frac{(m-p)(n-p)}{n-m} \right)^{1/2}$,

$$\sigma'^2 = \left[\|X\beta\|^2 c^\top (X^\top X)^{-1} c + (c^\top \beta)^2 \right].$$

- Sub-randomization & pivotal can be used.

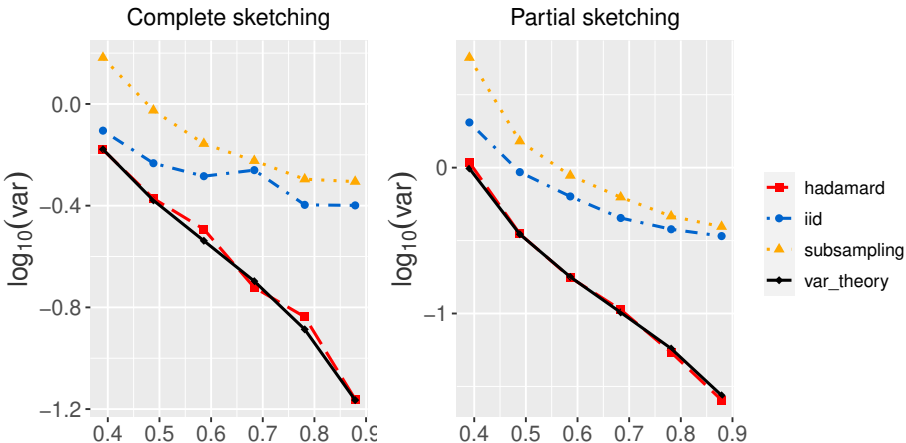
Numerical Experiments: Variance prediction

- Take $n = 2,048, p = 500$; m ranging from 800 to 1,800

Numerical Experiments: Variance prediction

- Take $n = 2,048, p = 500$; m ranging from 800 to 1,800
- Generate (then fix) the data X with i.i.d. $\mathcal{N}(0,1)$ entries; and y from Unif(0,1)

Log of variance of $\sqrt{m}c^\top \hat{\beta}_m$.



Numerical Experiments: Coverage

- Generate synthetic data, with $n = 8,000$ and $p = 500$ (as in Lopes et al. [2018]).

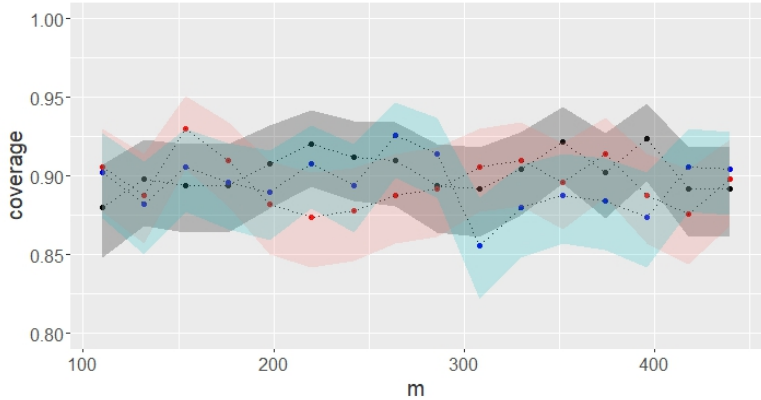
Numerical Experiments: Coverage

- Generate synthetic data, with $n = 8,000$ and $p = 500$ (as in Lopes et al. [2018]).
- $X = U\Lambda V^\top$, where
  - U consists of the left singular vectors of a matrix with i.i.d. $t_2(0, \Sigma)$, $\Sigma_{i,j} = 2 \times 0.5^{|i-j|}$ rows,
  - Λ is a diagonal matrix with entries uniformly spaced between 0.1 and 1,
  - V is the right singular matrix of a $p \times p$ standard Gaussian matrix.
- $y = Xb + \delta$, where $b = (\mathbf{1}_{0.2p}, t\mathbf{1}_{0.6p}, \mathbf{1}_{0.2p})$ with $t = 0.1$, and $\delta \sim \mathcal{N}(0, 0.01^2 I)$.

Empirical Data, fixed dimension

- Use "cpusmall" dataset, with $n = 8293, p = 11$, $b = 50$, $K = 100$, S_m (and $S_{b,i}$) be Hadamard sketching matrices, find coverage of 90% intervals for the first coordinate of β; and 95% Clopper-Pearson interval for coverage

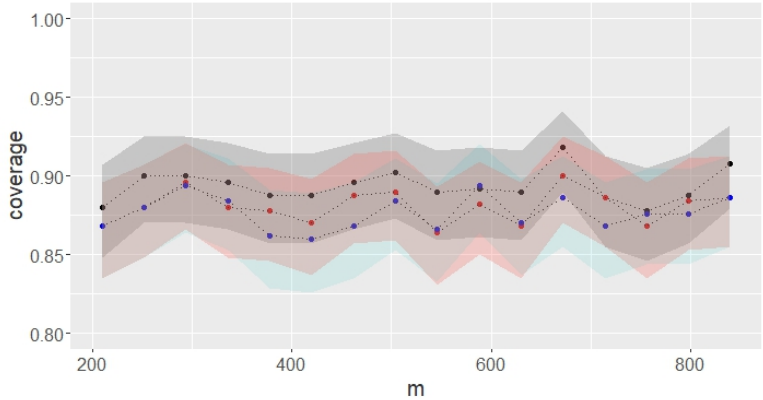
Pivotal method (black); sub-randomization (red); bootstrap (blue).



Empirical Data, fixed dimension

- Use "nycflight13" dataset, with $n = 60448, p = 21$, $b = 100$, $K = 100$, S_m (and $S_{b,i}$) be Hadamard sketching matrices, find coverage of 90% intervals for the first coordinate of β; and 95% Clopper-Pearson interval for coverage

Pivotal method (black); sub-randomization (red); bootstrap (blue).



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