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1 Optimal Iterative Sketching with the Subsampled Randomized Hadamard Transform

Based on [2].

The performance of iterative Hessian sketch (IHS) has only been studied empirically in existing literature. Lacotte et al. [2] show that for IHS with random matrices projected via refreshed (i.i.d.) truncated Haar matrices or subsampled randomized Hadamard transform (SRHT), the limiting rate of convergence is expected to be better than that of IHS with Gaussian random projections. Their other theoretical contributions include a closed form optimal (limiting) step size for IHS with Haar sketches, showing that momentum does not improve performance of IHS with refreshed Haar sketches, and an explicit formula for the second inverse moment of Haar sketches.

1.1 Background

1.1.1 Problem and method

Consider overdetermined least-squares problems of the form

$$\mathbf{b}^* = \arg \min_{\mathbf{b} \in \mathbb{R}^d} \left\{ f(\mathbf{b}) = \frac{1}{2} \|\mathbf{X}\mathbf{b} - \mathbf{y}\|^2 \right\}$$

where $\mathbf{X} \in \mathbb{R}^{n \times d}$ is a given data matrix with $n \geq d$ and $\text{rank}(\mathbf{X}) = d$ and $\mathbf{y} \in \mathbb{R}^n$ is a vector of observations. Iterative Hessian sketch is one iterative method for solving the problem where given step sizes $\{\alpha_t\}$ and momentum $\{\beta_t\}$, the solutions are iteratively updated by

$$\mathbf{b}_{t+1} = \mathbf{b}_t - \alpha_t H_t^{-1} \nabla f(\mathbf{b}_t) + \beta_t (\mathbf{b}_t - \mathbf{b}_{t-1}) .$$

The matrix H_t is an approximation of the Hessian $H = \mathbf{X}^\top \mathbf{X}$ and is given by $H_t = \mathbf{X}^\top \mathbf{S}_t^\top \mathbf{S}_t \mathbf{X}$ where $\mathbf{S}_0, \dots, \mathbf{S}_t, \dots$ are refreshed (i.i.d.) $m \times n$ sketching (random) matrices with $m \ll n$. The types of sketches discussed by Lacotte et al. [2] include

1. Gaussian sketches where $(\mathbf{S}_t)_{ij} \stackrel{\text{i.i.d.}}{\sim} N(0, m^{-1})$. Computing the matrix product $\mathbf{S}\mathbf{X}$ is $O(mnd)$ in general, which is larger than the cost of $O(nd^2)$ for direct method solvers when $m \geq d$.
2. truncated Haar sketches using Haar matrices \mathbf{S}_t where the rows are orthonormal. Generating the matrix requires $O(nm^2)$ using a Gram-Schmidt procedure which is larger than $O(nd^2)$.
3. subsampled randomized Hadamard transform where the sketch $\mathbf{S}\mathbf{X}$ can be obtained in $O(nd \log m)$ time. Like other orthogonal embeddings, the performance tends to be better than random projections with i.i.d. entries.

1.1.2 Random matrix theory and tools

Let $\{\mathbf{M}_n\}_n$ be a sequence of $n \times n$ Hermitian random matrices. The empirical spectral distribution (e.s.d.) of \mathbf{M}_n is the CDF of its eigenvalues $\lambda_1, \dots, \lambda_n$ given by $F_{\mathbf{M}_n}(x) = \frac{1}{n} \sum_{j=1}^n \mathbb{1}[\lambda_j \leq x]$ for $x \in \mathbb{R}$. The eigenvalues are random and so $F_{\mathbf{M}_n}$ is also random. The e.s.d. $F_{\mathbf{M}_n}$ converges weakly to the limiting spectral distribution (l.s.d.) of \mathbf{M}_n as $n \rightarrow \infty$.

For a probability measure μ with support on $[0, \infty)$, its Stieltjes transform is defined over the complex space of z outside the support of μ as

$$m_\mu(z) = \int \frac{1}{x - z} \mu(dx) .$$

The S -transform of μ is unique under certain conditions and is defined as the solution to the equation

$$m_\mu \left(\frac{z + 1}{z S_\mu(z)} \right) + z S_\mu(z) = 0 .$$

The η -transform is an alternative form of the Stieltjes transform defined for $z \in \mathbb{C} \setminus \mathbb{R}^-$ and given by

$$\eta_\mu(z) = \int \frac{1}{1+zx} \mu(dx) = \frac{1}{z} m_\mu\left(-\frac{1}{z}\right).$$

The Marchenko-Pastur theorem says that for a $m \times d$ matrix \mathbf{S} where $(\mathbf{S})_{ij} \stackrel{\text{i.i.d.}}{\sim} N(0, m^{-1})$, then as $m, d \rightarrow \infty$ with $\frac{m}{d} \rightarrow \rho \in (0, 1)$, $\mathbf{S}^\top \mathbf{S}$ has l.s.d. F_ρ with a Stieltjes transform that is the unique solution of a certain fixed point equation and with a density given by

$$\mu_\rho(x) = \frac{\sqrt{(1+\sqrt{\rho})^2 - x}_+(x - (1-\sqrt{\rho})^2)_+}{2\pi\rho x}$$

where $y_+ = \max\{0, y\}$.

For a random matrix \mathbf{X}_n in algebra \mathcal{A}_n of $n \times n$ matrices, the normalized trace operator

$$\tau_n(\mathbf{X}_n) = \frac{1}{n} \mathbb{E}[\text{trace}(\mathbf{X}_n)]$$

is a linear functional (and is analogous to expectations with scalar random variables; see Terry Tao's notes on free probability).

1.1.3 Other notation

Define the aspect ratios $\gamma = \lim_{n,d \rightarrow \infty} \frac{d}{n} \in (0, 1)$, $\xi = \lim_{n,m \rightarrow \infty} \frac{m}{n} \in (\gamma, 1)$ and $\rho_g = \frac{\gamma}{\xi} \in (0, 1)$ where subscript g refers to Gaussians and h refers to Haar or Hadamard. For a sequence $\{\mathbf{b}_t\}$, denote the error vector $\Delta_t = \mathbf{U}^\top \mathbf{X}(\mathbf{b}_t - \mathbf{b}^*)$ where \mathbf{U} is the $n \times d$ matrix of left singular vectors of \mathbf{X} . Note that $\|\Delta_t\|^2 = \|\mathbf{X}(\mathbf{b}_t - \mathbf{b}^*)\|^2$.

1.2 Sketching with Haar matrices

Theorem 3.1 (Optimal IHS with Haar sketches): for refreshed Haar matrices $\{\mathbf{S}_t\}$, step sizes $\alpha_t = \frac{\theta_{1,h}}{\theta_{2,h}}$ (defined in Lemma 3.2) and momentum parameters $\beta_t = 0$, the sequence of error vectors $\{\Delta_t\}$ satisfies

$$\rho_h = \left(\lim_{n \rightarrow \infty} \frac{\mathbb{E}\|\Delta_t\|^2}{\|\Delta_0\|^2} \right)^{\frac{1}{t}} = \rho_g \cdot \frac{\xi(1-\xi)}{\gamma^2 + \xi - 2\xi\gamma}.$$

For any step sizes $\{a_t\}$ and momentum parameters $\{\beta_t\}$,

$$\rho_h \leq \liminf_{t \rightarrow \infty} \left(\lim_{n \rightarrow \infty} \frac{\mathbb{E}\|\Delta_t\|^2}{\|\Delta_0\|^2} \right)^{\frac{1}{t}},$$

i.e., ρ_h is the optimal rate for Haar embeddings.

Theorem 3.1 says that using the optimal parameters (which has closed forms), the rate at any time step $t \geq 1$ is given by

$$\rho_h^t = \lim_{n \rightarrow \infty} \frac{\mathbb{E}\|\Delta_t\|^2}{\|\Delta_0\|^2}$$

with $\rho_h < \rho_g$. Momentum also does not provide benefits.

Lemma 3.2 (First two inverse moments of Haar sketches): let \mathbf{S} be a $m \times n$ Haar matrix, \mathbf{U} a $n \times d$ deterministic matrix with orthonormal columns. Then

$$\begin{aligned} \theta_{1,h} &= \lim_{n \rightarrow \infty} \frac{1}{d} \text{trace}(\mathbb{E}[(\mathbf{U}^\top \mathbf{S}^\top \mathbf{S} \mathbf{U})^{-1}]) = \frac{1-\gamma}{\xi-\gamma} \\ \theta_{2,h} &= \lim_{n \rightarrow \infty} \frac{1}{d} \text{trace}(\mathbb{E}[(\mathbf{U}^\top \mathbf{S}^\top \mathbf{S} \mathbf{U})^{-2}]) = \frac{(1-\gamma)(\gamma^2 + \xi - 2\gamma\xi)}{(\xi-\gamma)^3} \end{aligned}$$

(Note that $\theta_{i,h}$ is the average of the eigenvalues of $\mathbf{U}^\top \mathbf{S}^\top \mathbf{S} \mathbf{U}$ to the power of $-i$.)

Lacotte et al. [2] show that as the sketch size m increases relative to n , the convergence ratio of Haar sketches versus Gaussian projections scales as $\frac{\rho_h}{\rho_g} \approx (1 - \xi)$.

1.3 Sketching with SRHT matrices

Lacotte et al. [2] consider a version of SRHT where the transform $\mathbf{X} \mapsto \mathbf{S}\mathbf{X}$ first randomly permutes the rows of \mathbf{X} before applying the classical transform, i.e., $\mathbf{S} = \frac{1}{\sqrt{n}} \mathbf{B} \mathbf{H}_n \mathbf{D} \mathbf{P}$ where \mathbf{B} is a $n \times n$ diagonal matrix of i.i.d. Bernoulli random variables with success probability $\frac{m}{n}$, \mathbf{D} is a $n \times n$ diagonal matrix of i.i.d. sign random variables with uniform probability, and \mathbf{P} is a $n \times n$ uniformly distributed permutation matrix. \mathbf{H}_n is the $n \times n$ Walsh-Hadamard matrix where for $n = 2^p$ for $p \geq 1$, the matrix is defined recursively as

$$\mathbf{H}_n = \begin{bmatrix} \mathbf{H}_{\frac{n}{2}} & \mathbf{H}_{\frac{n}{2}} \\ \mathbf{H}_{\frac{n}{2}} & -\mathbf{H}_{\frac{n}{2}} \end{bmatrix}$$

with $\mathbf{H}_1 = 1$. Before applying the transformation to \mathbf{X} , the zero rows of \mathbf{S} are discarded and so \mathbf{S} is a $M \times n$ orthogonal matrix with $M \sim \text{Binomial}(\frac{m}{n}, n)$, and $\frac{M}{n} \rightarrow \xi$ as $n \rightarrow \infty$. Note that \mathbf{S} is still referred to as a $m \times n$ SRHT matrix.

Theorem 4.1 (IHS with SRHT sketches): suppose that \mathbf{b}_0 is random and that the error vector Δ_0 satisfies $\mathbb{E} [\Delta_0 \Delta_0^\top] = d^{-1} \mathbf{I}_d$. Then for refreshed SRHT matrices $\{\mathbf{S}_t\}$, step sizes $\alpha_t = \frac{\theta_{1,h}}{\theta_{2,h}}$ and momentum parameters $\beta_t = 0$, the sequence $\{\Delta_t\}$ satisfies

$$\rho_s = \left(\lim_{n \rightarrow \infty} \frac{\mathbb{E} [\|\Delta_t\|^2]}{\mathbb{E} [\|\Delta_0\|^2]} \right)^{\frac{1}{t}} = \rho_g \cdot \frac{\xi(1 - \xi)}{\gamma^2 + \xi - 2\xi\gamma} = \rho_h.$$

The additional initialization condition can be satisfied by picking \mathbf{b}_0 uniformly from the unit d -sphere \mathbf{S}^{d-1} and applying a random signed permutation and scaling to the columns of \mathbf{X} (TODO). The case of general Δ_0 or momentum $\beta_t \neq 0$ has not yet been explored.

Theorem 4.2 (Upper bound of SRHT error): for any \mathbf{b}_0 with refreshed SRHT matrices $\{\mathbf{S}_t\}$, step sizes $\alpha_t = \frac{\theta_{1,h}}{\theta_{2,h}}$ and momentum parameters $\beta_t = 0$, the sequence of error vectors $\{\Delta_t\}$ satisfies

$$\limsup_{n \rightarrow \infty} \left(\frac{\mathbb{E} [\|\Delta_t\|^2]}{d \mathbb{E} [\|\Delta_0\|^2]} \right)^{\frac{1}{t}} \leq \rho_h.$$

(Weaker by a factor of d , but is negligible for large t .)

Lemma 4.3 (First two inverse moments of SRHT sketches): let \mathbf{S} be a $m \times n$ SRHT matrix, \mathbf{S}_h a $m \times n$ Haar matrix and \mathbf{U} a $n \times d$ deterministic matrix with orthonormal columns. Then $\mathbf{U}^\top \mathbf{S}^\top \mathbf{S} \mathbf{U}$ and $\mathbf{U}^\top \mathbf{S}_h^\top \mathbf{S}_h \mathbf{U}$ have the same limiting spectral distribution and therefore the same two inverse moments.

1.4 Complexity analysis

Lacotte et al. [2] compare the (asymptotic) complexity of IHS with SRHT embeddings to that of the standard pre-conditioned conjugate gradient method. The latter uses a sketch $\mathbf{S}\mathbf{X}$ to compute a pre-conditioning matrix \mathbf{P} such that $\mathbf{X}\mathbf{P}^{-1}$ has a small condition number and solves the least squares problem $\min_{\mathbf{b}} \|\mathbf{X}\mathbf{P}^{-1}\mathbf{b} - \mathbf{y}\|^2$. The sketch size is prescribed to be $m \approx d \log d$, and the complexity to achieve $\|\Delta_t\|^2 \leq \epsilon$ scales as $C_c \asymp nd \log d + d^3 \log d + nd \log \epsilon^{-1}$ (cost of forming $\mathbf{S}\mathbf{X}$, factoring, and per-iteration cost times number of iterations, respectively). For IHS with SRHT, we can take $m \approx d$ which results in complexity $C_n \asymp (nd \log d + d^3 + nd) \log \epsilon^{-1}$. Treating $\log \epsilon^{-1}$ as constant independent of the dimensions, $\frac{C_n}{C_c} \asymp \frac{1}{\log d}$ as $n, m, d \rightarrow \infty$.

1.5 Numerical simulations

The main results of the numerical simulations by Lacotte et al. [2] (involving ill-conditioned matrices) include:

- IHS with refreshed Haar/SRHT embeddings (using optimal step size from Theorem 4.1 and finite sample approximations of ξ and γ) converge faster than IHS with refreshed Gaussian embeddings (using parameters α_t and β_t derived from previous work).
- Haar embeddings and SRHT embeddings perform similarly (though SRHT has a computational advantage).
- IHS with refreshed SRHT embeddings every iteration converge faster than the pre-conditioned conjugate gradient method. IHS with sketches refreshed at lower frequencies converge slower.

1.6 Appendix

1.6.1 B.2

- Distribution F_γ with density $\gamma\delta_1 + (1 - \gamma)\delta_0$
- Distribution F_ξ with density $\xi\delta_1 + (1 - \xi)\delta_0$
- System of equations

$$\begin{aligned}
\eta_C(z) &= \int \frac{1}{z\gamma(z)x + 1} F_\xi(dx) \\
&= \frac{\xi}{z\gamma(z) + 1} + 1 - \xi \\
\gamma(z) &= \int \frac{x}{\eta_C(z) + z\delta(z)x} F_\gamma(dx) \\
&= \frac{\gamma}{\eta_C(z) + z\delta(z)} \\
\delta(z) &= \int \frac{x}{z\gamma(z)x + 1} F_\xi(dx) \\
&= \frac{\xi}{z\gamma(z) + 1}
\end{aligned}$$

TODO

$$\eta_C(z) = (1 - \gamma) + \frac{\gamma}{\left(1 + z \left(1 + \frac{\xi - 1}{\eta_C(z)}\right)\right)}$$

1.7 Code

[GitHub](#)

2 Scratch notes

2.1 Random matrix theory

- Stieltjes transform:
<https://mathoverflow.net/questions/79109/intuitive-understanding-of-the-stieltjes-transform>
<https://terrytao.wordpress.com/2010/02/02/254a-notes-4-the-semi-circular-law/>
 Berkeley lecture notes: https://www.stat.berkeley.edu/~songmei/Teaching/STAT260_Spring2021/Lecture_notes/scribe_lecture17.pdf
 Distribution of sums of independent commutative r.v.'s can be quickly computed using characteristic function; analogous for distribution of sums of freely independent non-commutative r.v.'s is using the Stieltjes transform
 Stieltjes transform of e.s.d. of a random matrix is easy to compute [1]
- S -transform: under suitable conditions, the S -transform of the l.s.d. of a matrix product \mathbf{AB} is the product of the S -transforms of the l.s.d. of \mathbf{A} and the l.s.d. of \mathbf{B} [1]
- η -transform: purpose mainly to simplify long derivations involving Stieltjes transform [1]
- Free probability (non-commutative random variables, e.g., random matrices):
<https://terrytao.wordpress.com/2010/02/10/245a-notes-5-free-probability/>
 Light intro: <https://arxiv.org/pdf/1902.10763.pdf> [3]
 - Freeness between non-commutative random variables analogous to independence in commutative random variables
 - Semicircular distribution of free CLT analogous to Gaussian distribution of classical CLT; the asymptotic distributions of eigenvalues of Hermitian Gaussian random matrices (Wigner's semi-circle law); sub-Gaussian distribution
 Example: <https://mathworld.wolfram.com/WignersSemicircleLaw.html>
 - Cauchy transform = Stieltjes transform (or closely related)? Theorem 3 says that Cauchy transforms and probability measures on \mathbb{R} are in one-to-one correspondence
 - One method to construct Haar unitary matrices: take $n \times n$ random matrix with i.i.d. Gaussian random variables and apply the Gram-Schmidt procedure
- Marchenko-Pastur proof given in [1]

2.2 Newton's method

Problem: for f twice-differentiable, minimize

$$\min_{x \in \mathbb{R}} f(x) .$$

Second-order Taylor expansion around iterate x_t :

$$f(x_t + a) \approx f(x_t) + f'(x_t)a + \frac{1}{2}f''(x_t)a^2 .$$

If second derivative positive, minimum at derivative zero and so

$$f'(x_t) + f''(x_t)a = 0 \quad \Rightarrow \quad a = -\frac{f'(x_t)}{f''(x_t)} .$$

Newton update:

$$x_{t+1} = x_t + a = x_t - \frac{f'(x_t)}{f''(x_t)} .$$

2.3 Underdetermined least squares

Is there anything interesting about IHS in the underdetermined least squares case?

- For example, gradient descent in underdetermined least squares converges to the minimum norm solution (assuming solution initialized in orthogonal complement of null space of data matrix, i.e., row space).
[Implicit Regularization in Matrix Factorization](#); SE
- If $n \ll d$, does it make more sense to reduce the feature dimension, i.e., $\tilde{A} = AS$ for A $n \times d$, S $d \times m$, $m \ll d$? For fixed sketches? Otherwise are there any computational savings from sketching? Note $A^T A$ not invertible in this case but AA^T is.
[High-Dimensional Optimization in Adaptive Random Subspaces](#): uses right sketching matrix, works with AA^T .
[Effective Dimension Adaptive Sketching Methods for Faster Regularized Least-Squares Optimization](#): dual of underdetermined is overdetermined problem?
- Ridge regression allows for an unique solution.
[An Iterative, Sketching-based Framework for Ridge Regression](#)

2.4 Quantile regression

Are there problems for which IHS could perform better than conventional methods?

- Models conditional quantiles. Makes no assumptions about distribution of response nor homoscedasticity. Is equivariant to transformation. Need more data than linear regression and is computationally intensive.
[What is quantile regression](#)
[Five Things You Should Know about Quantile Regression](#)
[Quantile Regression](#)
[An Interior Point Algorithm for Nonlinear Quantile Regression](#)
[An Improved Interior Point Algorithm for Quantile Regression](#)

2.5 Related literature

- Extensions of IHS:
[Distributed Averaging Methods for Randomized Second Order Optimization](#)
[Iterative Hessian Sketch with Momentum](#) **TODO**: how does this work differ or not contradict the current work?
[Optimal Randomized First-Order Methods for Least-Squares Problems](#): extension of current work with non-refreshed sketches
[Adaptive Newton Sketch: Linear-time Optimization with Quadratic Convergence and Effective Hessian Dimensionality](#)
[Newton-LESS: Sparsification without Trade-offs for the Sketched Newton Update](#): sparse IHS?
[Asymptotics for Sketching in Least Squares](#): referenced paper in current work; compares one-step sketch matrices
- Applications:
[Randomized sketches for kernels: Fast and optimal nonparametric regression](#)
- Possibly helpful:
[On randomized sketching algorithms and the Tracy-Widom law](#)
[Practical sketching algorithms for low-rank matrix approximation](#)
[A Statistical Perspective on Randomized Sketching for Ordinary Least-Squares](#): complementary to 2016 IHS paper
[Efficient Matrix Sketching over Distributed Data: PCA?](#)
[Randomized Iterative Methods for Linear Systems](#): classical sketch
[Optimal approximate matrix product in terms of stable rank](#): error bounds on matrix approximations

- Related to expectation of solution?
High-Dimensional Optimization in Adaptive Random Subspaces
Randomized sketches for kernels: Fast and optimal nonparametric regression
- Underdetermined?
Effective Dimension Adaptive Sketching Methods for Faster Regularized Least-Squares Optimization:
refreshed embeddings does not improve on fixed embedding?
 - Faster Least Squares Optimization
 - Optimal Randomized First-Order Methods for Least-Squares Problems: first-order method with fixed sketches that provide better guarantees.

Input Sparsity Time Low-Rank Approximation via Ridge Leverage Score Sampling
An Iterative, Sketching-based Framework for Ridge Regression

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- [3] Xiang-Gen Xia. A simple introduction to free probability theory and its application to random matrices. *arXiv preprint arXiv:1902.10763*, 2019.