Randomized linear algebra



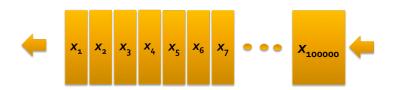
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Outline

- Approximate matrix multiplication
- Least squares approximation
- Low-rank matrix approximation
- Graph sparsification

Main reference: "Lecture notes on randomized linear algebra," Michael W. Mahoney, 2016

Efficient large-scale data processing



When processing large-scale data (in particular, streaming data), we desire methods that can be performed with

- a few (e.g. one or two) passes of data
- limited memory (so impossible to store all data)
- low computational complexity

Key idea: dimension reduction via random sketching

- random sampling: randomly downsample data
 - o often relies on information of data
- random projection: rotates / projects data onto lower dimensions
 - often data-agnostic

Approximate matrix multiplication

Matrix multiplication: a fundamental algebra task

Given $m{A} \in \mathbb{R}^{m imes n}$ and $m{B} \in \mathbb{R}^{n imes p}$, compute or approximate $m{A}m{B}$

Algorithm 1.1 Vanilla algorithm for matrix multiplication

- 1: **for** $i = 1, \dots, m$ **do**
- 2: for $k=1,\cdots,n$ do
- 3: $M_{i,k} = A_{i,:}B_{:,k}$
- 4: return M

Computational complexity: O(mnp), or $O(n^3)$ if m=n=p

For simplicity, we will assume m=n=p unless otherwise noted.

Faster matrix multiplication?

- Strassen algorithms: exact matrix multiplication
 - Computational complexity $\approx O(n^{2.8})$
 - o For various reasons, rarely used in practice
- Approximate solution?

A simple randomized algorithm

View AB as sum of rank-one matrices (or outer products)

$$oldsymbol{AB} = \sum_{i=1}^n oldsymbol{A}_{:,i} oldsymbol{B}_{i,:}$$

Idea: randomly sample r rank-one components

Algorithm 1.2 Basic randomized algorithm for matrix multiplication

- 1: for $l=1,\cdots,r$ do
- 2: Pick $i_l \in \{1,\cdots,n\}$ i.i.d. with prob. $\mathbb{P}\{i_l=k\}=p_k$
- 3: return

$$\boldsymbol{M} = \sum_{l=1}^{r} \frac{1}{r p_{i_l}} \boldsymbol{A}_{:,l} \boldsymbol{B}_{l,:}$$

• $\{p_k\}$: importance sampling probabilities

A simple randomized algorithm

Rationale: M is unbiased estimate of AB, i.e.

$$\mathbb{E}\left[\boldsymbol{M}\right] = \sum_{l=1}^{r} \sum_{k} \mathbb{P}\left\{i_{l} = k\right\} \frac{1}{rp_{k}} \boldsymbol{A}_{:,k} \boldsymbol{B}_{k,:}$$
$$= \sum_{k} \boldsymbol{A}_{:,k} \boldsymbol{B}_{k,:} = \boldsymbol{A} \boldsymbol{B}$$

Clearly, approximation error (e.g. $\|AB - M\|$) depends on $\{p_k\}$.

Importance sampling probabilities

• Uniform sampling $(p_k \equiv \frac{1}{n})$: one can choose sampling set before looking at data, so it's implementable via one pass over data

Intuitively, one may prefer biasing towards larger rank-1 components

• Nonuniform sampling

$$p_k = \frac{\|\boldsymbol{A}_{:,k}\|_2 \|\boldsymbol{B}_{k,:}\|_2}{\sum_l \|\boldsymbol{A}_{:,l}\|_2 \|\boldsymbol{B}_{l,:}\|_2}$$

 $\circ \ \{p_k\}$ can be computed using one pass and O(n) memory

Optimal sampling probabilities?

Let's measure approximation error by $\mathbb{E}\left[\|m{M}-m{A}m{B}\|_{\mathrm{F}}^2
ight].$

As it turns out, $\mathbb{E}\left[\|oldsymbol{M}-oldsymbol{A}oldsymbol{B}\|_{\mathrm{F}}^2
ight]$ is minimized by

$$p_k = \frac{\|\mathbf{A}_{:,k}\|_2 \|\mathbf{B}_{k,:}\|_2}{\sum_l \|\mathbf{A}_{:,l}\|_2 \|\mathbf{B}_{l,:}\|_2}$$
(1.1)

Thus, we call (1.1) optimal sampling probabilities .

Justification of optimal sampling probabilities

Since $\mathbb{E}[M] = AB$, one has

$$\mathbb{E}\left[\|\boldsymbol{M} - \boldsymbol{A}\boldsymbol{B}\|_{\mathrm{F}}^{2}\right] = \mathbb{E}\left[\sum_{i,j} \left(M_{i,j} - \boldsymbol{A}_{i,:}\boldsymbol{B}_{:,j}\right)^{2}\right] = \sum_{i,j} \mathsf{Var}[M_{i,j}]$$

$$= \frac{1}{r} \sum_{k} \sum_{i,j} \frac{A_{i,k}^{2} B_{k,j}^{2}}{p_{k}} - \frac{1}{r} \sum_{i,j} \left(\boldsymbol{A}_{i,:}\boldsymbol{B}_{:,j}\right)^{2} \quad \text{(check)}$$

$$= \frac{1}{r} \sum_{k} \frac{1}{p_{k}} \|\boldsymbol{A}_{:,k}\|_{2}^{2} \|\boldsymbol{B}_{k,:}\|_{2}^{2} - \frac{1}{r} \|\boldsymbol{A}\boldsymbol{B}\|_{\mathrm{F}}^{2}. \tag{1.2}$$

In addition, Cauchy-Schwarz yields $(\sum_k p_k) \left(\sum_k \frac{\alpha_k}{p_k}\right) \geq \left(\sum_k \sqrt{\alpha_k}\right)^2$, with equality attained if $p_k \propto \sqrt{\alpha_k}$. This implies

$$\mathbb{E}\left[\|\boldsymbol{M} - \boldsymbol{A}\boldsymbol{B}\|_{\mathrm{F}}^2\right] \geq \frac{1}{r} \left(\sum_{k} \|\boldsymbol{A}_{:,k}\|_2 \|\boldsymbol{B}_{k,:}\|_2\right)^2 - \frac{1}{r} \|\boldsymbol{A}\boldsymbol{B}\|_{\mathrm{F}}^2,$$

where lower bound is achieved when $p_k \propto \|\mathbf{A}_{::k}\|_2 \|\mathbf{B}_{k::}\|_2$.

Error concentration

Practically, one often hopes that approximation error is absolutely controlled most of the time. In other words, we desire a method whose estimate is sufficiently close to truth with very high probability

For approximate matrix multiplication, two error metrics are of particular interest

- ullet Frobenius norm bound: $\|oldsymbol{M}-oldsymbol{A}oldsymbol{B}\|_{ ext{F}}$
- ullet spectral norm bound: $\|M-AB\|$

invoke concentration of measure results to control these errors

Asymptotic notation

ullet $f(n) \lesssim g(n)$ or f(n) = O(g(n)) means

$$\lim_{n \to \infty} \frac{|f(n)|}{|g(n)|} \ \leq \ \operatorname{const}$$

• $f(n) \gtrsim g(n)$ or $f(n) = \Omega(g(n))$ means

$$\lim_{n \to \infty} \frac{|f(n)|}{|g(n)|} \ \geq \ \operatorname{const}$$

• $f(n) \asymp g(n)$ or $f(n) = \Theta(g(n))$ means

$$\operatorname{const}_1 \leq \lim_{n \to \infty} \frac{|f(n)|}{|g(n)|} \leq \operatorname{const}_2$$

• f(n) = o(g(n)) means

$$\lim_{n \to \infty} \frac{|f(n)|}{|g(n)|} = 0$$

A hammer: matrix Bernstein inequality

Theorem 1.1 (Matrix Bernstein inequality)

Let $\left\{ oldsymbol{X}_l \in \mathbb{R}^{d_1 imes d_2} \right\}$ be a sequence of independent zero-mean random matrices. Assume each random matrix satisfies $\| oldsymbol{X}_l \| \leq R$. Define $V := \max \left\{ \left\| \mathbb{E} \left[\sum_{l=1}^L oldsymbol{X}_l oldsymbol{X}_l^{ op} \right] \right\|, \left\| \mathbb{E} \left[\sum_{l=1}^L oldsymbol{X}_l^{ op} oldsymbol{X}_l \right] \right\| \right\}$. Then,

$$\mathbb{P}\left\{\left\|\sum_{l=1}^{L} \boldsymbol{X}_{l}\right\| \geq \tau\right\} \leq (d_{1} + d_{2}) \exp\left(\frac{-\tau^{2}/2}{V + R\tau/3}\right)$$

- moderate-deviation regime (τ is not too large): sub-Gaussian tail behavior $\exp(-\tau^2/V)$
- large-deviation regime (τ is large): sub-exponential tail behavior $\exp(-\tau/R)$ (slower decay)

A hammer: matrix Bernstein inequality

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$$\mathbb{P}\left\{\left\|\sum_{l=1}^{L} \boldsymbol{X}_{l}\right\| \geq \tau\right\} \leq (d_{1} + d_{2}) \exp\left(\frac{-\tau^{2}/2}{V + R\tau/3}\right)$$

• an alternative form (exercise): with prob. $1 - O((d_1 + d_2)^{-10})$,

$$\left\| \sum_{l=1}^{L} \boldsymbol{X}_{l} \right\| \lesssim \sqrt{V \log(d_1 + d_2)} + R \log(d_1 + d_2)$$

Frobenius norm error of matrix multiplication

Theorem 1.2

Suppose $p_k \geq \frac{\beta \|\mathbf{A}_{:,k}\|_2 \|\mathbf{B}_{k,:}\|_2}{\sum_l \|\mathbf{A}_{:,l}\|_2 \|\mathbf{B}_{l,:}\|_2}$ for some quantity $0 < \beta \leq 1$. If $r \gtrsim \frac{\log n}{\beta}$, then

$$\|oldsymbol{M} - oldsymbol{A}oldsymbol{B}\|_{ ext{F}} \lesssim \sqrt{rac{\log n}{eta r}} \|oldsymbol{A}\|_{ ext{F}} \|oldsymbol{B}\|_{ ext{F}}$$

with prob. exceeding $1 - O(n^{-10})$

Proof of Theorem 1.2

Clearly, $\text{vec}(\boldsymbol{M}) = \sum_{l=1}^r \boldsymbol{X}_l$, where $\boldsymbol{X}_l = \sum_{k=1}^n \frac{1}{rn_k} \boldsymbol{A}_{:,k} \otimes \boldsymbol{B}_{k,:}^{\top} \mathbb{1} \left\{ i_l = k \right\}$. These matrices $\{\boldsymbol{X}_l\}$ obey

$$\|\boldsymbol{X}_{l}\|_{2} \leq \max_{k} \frac{1}{rp_{k}} \|\boldsymbol{A}_{:,k}\|_{2} \|\boldsymbol{B}_{k,:}\|_{2} \approx \frac{1}{\beta r} \sum_{k=1}^{n} \|\boldsymbol{A}_{:,k}\|_{2} \|\boldsymbol{B}_{k,:}\|_{2} := R$$

$$\mathbb{E}\left[\sum_{l=1}^{r} \|\boldsymbol{X}_{l}\|_{2}^{2}\right] = r \sum_{k=1}^{n} \mathbb{P}\left\{i_{l} = k\right\} \frac{\|\boldsymbol{A}_{:,k}\|_{2}^{2} \|\boldsymbol{B}_{k,:}\|_{2}^{2}}{r^{2}p_{k}^{2}} \leq \underbrace{\frac{\left(\sum_{k=1}^{n} \|\boldsymbol{A}_{k,:}\|_{2} \|\boldsymbol{B}_{k,:}\|_{2}\right)^{2}}{\beta r}}_{:=V}$$

Invoke matrix Bernstein to arrive at

$$\begin{split} \|\boldsymbol{M} - \boldsymbol{A}\boldsymbol{B}\|_{\mathrm{F}} &= \left\| \sum_{l=1}^r \left(\boldsymbol{X}_l - \mathbb{E}[\boldsymbol{X}_l] \right) \right\|_2 \lesssim \sqrt{V \log n} + R \log n \\ & \asymp \sqrt{\frac{\log n}{\beta r}} \left(\sum_{k=1}^n \|\boldsymbol{A}_{k,:}\|_2 \|\boldsymbol{B}_{k,:}\|_2 \right) \leq \sqrt{\frac{\log n}{\beta r}} \|\boldsymbol{A}\|_{\mathrm{F}} \|\boldsymbol{B}\|_{\mathrm{F}} \text{ (Cauchy-Schwarz)} \end{split}$$

Spectral norm error of matrix multiplication

Theorem 1.3

Suppose $p_k \geq \frac{\beta \|A_{:,k}\|_2^2}{\|A\|_{\mathrm{F}}^2}$ for some quantity $0 < \beta \leq 1$, and $r \gtrsim \frac{\|A\|_{\mathrm{F}}^2}{\beta \|A\|^2 \log n}$. Then the estimate M returned by Algorithm 1.2 obeys

$$\|oldsymbol{M} - oldsymbol{A} oldsymbol{A}^ op \| \lesssim \sqrt{rac{\log n}{eta r}} \|oldsymbol{A}\|_{ ext{F}} \|oldsymbol{A}\|_{ ext{F}}$$

with prob. exceeding $1 - O(n^{-10})$

$$ullet$$
 If $r\gtrsim \underbrace{\frac{\|m{A}\|_{
m F}^2}{\|m{A}\|^2}}_{ ext{stable rank}} rac{\log n}{arepsilon^2eta}$, then $\|m{M}-m{A}m{A}^ op\|\lesssim arepsilon\|m{A}\|^2$

ullet can be generalized to approximate AB (Magen, Zouzias '11)

Proof of Theorem 1.3

Write $M = \sum_{l=1}^r Z_l$, where $Z_l = \sum_{k=1}^n \frac{1}{rp_k} A_{:,k} A_{:,k}^{\top} \mathbb{1} \{i_l = k\}$. These matrices satisfy

$$\begin{split} \|\boldsymbol{Z}_{l}\|_{2} &\leq \max_{k} \frac{\|\boldsymbol{A}_{:,k}\|_{2}^{2}}{rp_{k}} \asymp \frac{1}{r} \sum_{k=1}^{n} \|\boldsymbol{A}_{:,k}\|_{2}^{2} = \frac{1}{\beta r} \|\boldsymbol{A}\|_{F}^{2} := R \\ \left\| \mathbb{E} \left[\sum_{l=1}^{r} \boldsymbol{Z}_{l} \boldsymbol{Z}_{l}^{\top} \right] \right\| &= \left\| r \sum_{k=1}^{n} \mathbb{P} \left\{ i_{l} = k \right\} \frac{\|\boldsymbol{A}_{:,k}\|_{2}^{2}}{r^{2} p_{k}^{2}} \boldsymbol{A}_{:,k} \boldsymbol{A}_{:,k}^{\top} \right\| \\ &= \frac{1}{\beta r} \|\boldsymbol{A}\|_{F}^{2} \|\boldsymbol{A}\boldsymbol{A}^{\top}\| \\ &\leq \frac{1}{\beta r} \|\boldsymbol{A}\|_{F}^{2} \|\boldsymbol{A}\|^{2} := V \end{split}$$

Invoke matrix Bernstein to conclude that

Matrix multiplication with one-sided information

What if we can only use information about A?

For example, suppose $p_k \geq \frac{\beta \|\mathbf{A}_{:,k}\|_2^2}{\|\mathbf{A}\|_{\mathrm{F}}^2}$. In this case, matrix Bernstein inequality does NOT yield sharp concentration. But we can still use Markov's inequality to get some bound

Matrix multiplication with one-sided information

More precisely, when $p_k \geq \frac{\beta \|A_{i,k}\|_2^2}{\|A\|_{\mathbf{p}}^2}$, it follows from (1.2) that

$$\mathbb{E}\left[\|\boldsymbol{M} - \boldsymbol{A}\boldsymbol{B}\|_{\mathrm{F}}^{2}\right] = \frac{1}{r} \sum_{k} \frac{1}{p_{k}} \|\boldsymbol{A}_{:,k}\|_{2}^{2} \|\boldsymbol{B}_{k,:}\|_{2}^{2} - \frac{1}{r} \|\boldsymbol{A}\boldsymbol{B}\|_{\mathrm{F}}^{2}$$

$$\leq \frac{1}{\beta r} \left(\sum_{k} \|\boldsymbol{B}_{k,:}\|_{2}^{2} \right) \|\boldsymbol{A}\|_{\mathrm{F}}^{2}$$

$$= \frac{\|\boldsymbol{A}\|_{\mathrm{F}}^{2} \|\boldsymbol{B}\|_{\mathrm{F}}^{2}}{\beta r}$$

Hence, Markov's inequality yields that with prob. at least $1 - \frac{1}{\log n}$,

$$\|M - AB\|_{\mathrm{F}}^2 \le \frac{\|A\|_{\mathrm{F}}^2 \|B\|_{\mathrm{F}}^2 \log n}{\beta r}$$
 (1.3)

Least squares approximation

Least squares (LS) problems

Given $A \in \mathbb{R}^{n \times d}$ $(n \gg d)$ and $b \in \mathbb{R}^d$, find the "best" vector s.t. $Ax \approx b$, i.e.

$$\mathsf{minimize}_{oldsymbol{x} \in \mathbb{R}^d} \quad \|oldsymbol{A} oldsymbol{x} - oldsymbol{b}\|_2$$

If A has full column rank, then

$$oldsymbol{x}_\mathsf{ls} = (oldsymbol{A}^ op oldsymbol{A})^{-1} oldsymbol{A}^ op oldsymbol{b} = oldsymbol{V}_A oldsymbol{\Sigma}_A^{-1} oldsymbol{U}_A^ op oldsymbol{b}$$

where $\boldsymbol{A} = \boldsymbol{U}_{A}\boldsymbol{\Sigma}_{A}\boldsymbol{V}_{A}^{\top}$ is SVD of \boldsymbol{A} .

Methods for solving LS problems

Direct methods: computational complexity $O(nd^2)$

- Cholesky decomposition: compute upper triangular matrix R s.t. $A^{\top}A = R^{\top}R$, and solve $R^{\top}Rx = A^{\top}b$
- ullet QR decomposition: compute QR decomposition A=QR (Q: orthonormal; R: upper triangular), and solve $Rx=Q^ op b$

Iterative methods: computational complexity $O(\frac{\sigma_{\max}(\pmb{A})}{\sigma_{\min}(\pmb{A})}\|\pmb{A}\|_0\log\frac{1}{\varepsilon})$

conjugate gradient ...

Randomized least squares approximation

Basic idea: generate sketching / sampling matrix Φ (e.g. via random sampling, random projection), and solve instead

$$ilde{oldsymbol{x}}_{\mathsf{ls}} = rg\min_{oldsymbol{x} \in \mathbb{R}^d} \quad \|oldsymbol{\Phi}(oldsymbol{A}oldsymbol{x} - oldsymbol{b})\|_2$$

Goal: find Φ s.t.

$$egin{array}{ll} ilde{x}_{\mathsf{ls}} &pprox \ x_{\mathsf{ls}} \ \|A ilde{x}_{\mathsf{ls}} - oldsymbol{b}\|_2 &pprox \ \|Ax_{\mathsf{ls}} - oldsymbol{b}\|_2 \end{array}$$

Which sketching matrices enable good approximation?

We will start with two deterministic conditions that promise reasonably good approximation (Drineas et al '11)

Which sketching matrices enable good approximation?

Let $oldsymbol{A} = oldsymbol{U}_A oldsymbol{\Sigma}_A oldsymbol{V}_A^ op$ be SVD of $oldsymbol{A}$...

• Condition 1 (approximate isometry)

$$\sigma_{\min}^2(\mathbf{\Phi} U_A) \ge \frac{1}{\sqrt{2}} \tag{1.4}$$

- \circ says that ΦU_A is approximate isometry / rotation
- $\circ~1/\sqrt{2}$ can be replaced by other positive constants

Which sketching matrices enable good approximation?

Let $oldsymbol{A} = oldsymbol{U}_A oldsymbol{\Sigma}_A oldsymbol{V}_A^ op$ be SVD of $oldsymbol{A}$...

• Condition 2 (approximate orthogonality)

$$\left\| \boldsymbol{U}_{A}^{\top} \boldsymbol{\Phi}^{\top} \boldsymbol{\Phi} (\boldsymbol{A} \boldsymbol{x}_{\mathsf{ls}} - \boldsymbol{b}) \right\|_{2}^{2} \leq \frac{\varepsilon}{2} \|\boldsymbol{A} \boldsymbol{x}_{\mathsf{ls}} - \boldsymbol{b}\|_{2}^{2}$$
 (1.5)

- \circ says that ΦU_A is roughly orthogonal to $\Phi\underbrace{(Ax_{ extsf{ls}}-b)}_{=(U_AU_+^T-I)b}$
- \circ even though this condition depends on b, one can find Φ satisfying this condition without using any information about b

Can these conditions be satisfied?

Two extreme examples

1. $\Phi = I$, which satisfies

$$\begin{cases} \sigma_{\min}\left(\mathbf{\Phi} \boldsymbol{U}_{A}\right) &= \sigma_{\min}\left(\boldsymbol{U}_{A}\right) = 1 \\ \left\|\boldsymbol{U}_{A}^{\top} \mathbf{\Phi}^{\top} \mathbf{\Phi}\left(\boldsymbol{A} \boldsymbol{x}_{\mathsf{ls}} - \boldsymbol{b}\right)\right\|_{2} &= \left\|\boldsymbol{U}_{A}^{\top} \left(\boldsymbol{I} - \boldsymbol{U}_{A} \boldsymbol{U}_{A}^{\top}\right) \boldsymbol{b}\right\|_{2} = 0 \end{cases}$$

o easy to construct; hard to solve subsampled LS problem

Can these conditions be satisfied?

Two extreme examples

2. $oldsymbol{\Phi} = oldsymbol{U}_A^ op$, which satisfies

$$\begin{cases} \sigma_{\min} \left(\mathbf{\Phi} \mathbf{U}_A \right) &= \sigma_{\min} \left(\mathbf{I} \right) = 1 \\ \left\| \mathbf{U}_A^{\top} \mathbf{\Phi}^{\top} \mathbf{\Phi} \left(\mathbf{A} \mathbf{x}_{\mathsf{ls}} - \mathbf{b} \right) \right\|_2 &= \left\| \mathbf{U}_A^{\top} \left(\mathbf{I} - \mathbf{U}_A \mathbf{U}_A^{\top} \right) \mathbf{b} \right\|_2 = 0 \end{cases}$$

 \circ hard to construct (i.e. compute U_A); easy to solve subsampled LS problem

Quality of approximation

We'd like to assess quality of approximation w.r.t. both fitting error and estimation error

Lemma 1.4

Under Conditions 1-2, solution \tilde{x}_{ls} to subsampled LS problem obeys

(i)
$$\|A\tilde{x}_{ls} - b\|_2 \le (1 + \varepsilon) \|Ax_{ls} - b\|_2$$

(ii)
$$\| ilde{m{x}}_{\mathsf{ls}} - m{x}_{\mathsf{ls}}\|_2 \leq rac{\sqrt{arepsilon}}{\sigma_{\min}(m{A})} \|m{A}m{x}_{\mathsf{ls}} - m{b}\|_2$$

Proof of Lemma 1.4(i)

Subsampled LS problem can be rewritten as

$$egin{aligned} \min_{oldsymbol{x} \in \mathbb{R}^d} \|oldsymbol{\Phi} oldsymbol{b} - oldsymbol{\Phi} oldsymbol{A} oldsymbol{x}\|_2^2 &= \min_{oldsymbol{\Delta} \in \mathbb{R}^d} ig\|oldsymbol{\Phi} oldsymbol{b} - oldsymbol{\Phi} oldsymbol{A} oldsymbol{x}|_{\mathsf{s}}^2 + oldsymbol{\Delta} ig\|_2^2 \ &= \min_{oldsymbol{z} \in \mathbb{R}^d} ig\|oldsymbol{\Phi} ig(oldsymbol{b} - oldsymbol{A} oldsymbol{x}|_{\mathsf{s}}) - oldsymbol{\Phi} oldsymbol{D} oldsymbol{\Delta} oldsymbol{Z} ig\|_2^2. \end{aligned}$$

Therefore, optimal solution z_{ls} obeys

$$oldsymbol{z}_\mathsf{ls} = oldsymbol{(U_A^ op \Phi^ op \Phi U_A)}^{-1} oldsymbol{(U_A^ op \Phi^ op)} \Phi(oldsymbol{b} - oldsymbol{A} oldsymbol{x}_\mathsf{ls}).$$

Combine Conditions 1-2 to obtain

$$\|\boldsymbol{z}_{\mathsf{ls}}\|_2^2 \leq \left\| \left(\boldsymbol{U}_A^\top \boldsymbol{\Phi}^\top \boldsymbol{\Phi} \boldsymbol{U}_A\right)^{-1} \right\|^2 \left\| \boldsymbol{U}_A^\top \boldsymbol{\Phi}^\top \boldsymbol{\Phi} (\boldsymbol{b} - \boldsymbol{A} \boldsymbol{x}_{\mathsf{ls}}) \right\|_2^2 \leq \varepsilon \|\boldsymbol{b} - \boldsymbol{A} \boldsymbol{x}_{\mathsf{ls}}\|_2^2$$

Proof of Lemma 1.4(i) (cont.)

Previous bounds further yield

$$\begin{split} \left\| \boldsymbol{b} - \boldsymbol{A} \tilde{\boldsymbol{x}}_{\mathsf{ls}} \right\|_{2}^{2} &= \left\| \underbrace{\boldsymbol{b} - \boldsymbol{A} \boldsymbol{x}_{\mathsf{ls}}}_{\perp \boldsymbol{U}_{A}} + \underbrace{\boldsymbol{A} \boldsymbol{x}_{\mathsf{ls}} - \boldsymbol{A} \tilde{\boldsymbol{x}}_{\mathsf{ls}}}_{\in \mathsf{range}(\boldsymbol{U}_{A})} \right\|_{2}^{2} \\ &= \left\| \boldsymbol{b} - \boldsymbol{A} \boldsymbol{x}_{\mathsf{ls}} \right\|_{2}^{2} + \left\| \boldsymbol{A} \boldsymbol{x}_{\mathsf{ls}} - \boldsymbol{A} \tilde{\boldsymbol{x}}_{\mathsf{ls}} \right\|_{2}^{2} \\ &= \left\| \boldsymbol{b} - \boldsymbol{A} \boldsymbol{x}_{\mathsf{ls}} \right\|_{2}^{2} + \left\| \boldsymbol{U}_{A} \boldsymbol{z}_{\mathsf{ls}} \right\|_{2}^{2} \\ &\leq \left\| \boldsymbol{b} - \boldsymbol{A} \boldsymbol{x}_{\mathsf{ls}} \right\|_{2}^{2} + \left\| \boldsymbol{z}_{\mathsf{ls}} \right\|_{2}^{2} \\ &\leq \left(1 + \varepsilon \right) \left\| \boldsymbol{b} - \boldsymbol{A} \boldsymbol{x}_{\mathsf{ls}} \right\|_{2}^{2} \end{split}$$

Finally, we conclude proof by recognizing that $\sqrt{1+\varepsilon} \le 1+\varepsilon$.

Proof of Lemma 1.4(ii)

From proof of Lemma 1.4(i), we know $Ax_{\rm ls} - A\tilde{x}_{\rm ls} = U_Az_{\rm ls}$ and $\|z_{\rm ls}\|_2^2 \leq \varepsilon \|b - Ax_{\rm ls}\|_2^2$. These reveal that

$$egin{aligned} \|oldsymbol{x}_{\mathsf{ls}} - ilde{oldsymbol{x}}_{\mathsf{ls}}\|_2^2 &\leq rac{\|oldsymbol{A}(oldsymbol{x}_{\mathsf{ls}} - ilde{oldsymbol{x}}_{\mathsf{ls}})\|_2^2}{\sigma_{\min}^2(oldsymbol{A})} \ &= rac{\|oldsymbol{U}_A oldsymbol{z}_{\mathsf{ls}}\|_2^2}{\sigma_{\min}^2(oldsymbol{A})} \ &\leq rac{\|oldsymbol{b} - oldsymbol{A} oldsymbol{x}_{\mathsf{ls}}\|_2^2}{\sigma_{\min}^2(oldsymbol{A})} \end{aligned}$$

Quality of approximation (cont.)

By making further assumption on $m{b}$, we can connect error bound with $\|m{x}_{\mathsf{ls}}\|_2$

Lemma 1.5

Suppose $\|U_A U_A^{\top} b\|_2 \ge \gamma \|b\|_2$ for some $0 < \gamma \le 1$. Under Conditions 1-2, solution \tilde{x}_{ls} to subsampled LS problem obeys

$$\|\boldsymbol{x}_{\mathsf{ls}} - \tilde{\boldsymbol{x}}_{\mathsf{ls}}\|_2 \leq \sqrt{\varepsilon} \, \kappa(\boldsymbol{A}) \sqrt{\gamma^{-2} - 1} \|\boldsymbol{x}_{\mathsf{ls}}\|_2$$

where $\kappa(A)$: condition number of A

• $\|U_A U_A^{\top} b\|_2 \ge \gamma \|b\|_2$ says a nontrivial fraction of energy of b lies in range(A)

Proof of Lemma 1.5

Since
$$oldsymbol{b} - oldsymbol{A} oldsymbol{x}_{ ext{ls}} = (oldsymbol{I} - oldsymbol{U}_A oldsymbol{U}_A^{ op}) oldsymbol{b}$$
, one has
$$\begin{split} \| oldsymbol{b} - oldsymbol{A} oldsymbol{x}_{ ext{ls}} \|_2^2 &= \| (oldsymbol{I} - oldsymbol{U}_A oldsymbol{U}_A^{ op}) oldsymbol{b} \|_2^2 \\ &= \| oldsymbol{b} \|_2^2 - \| oldsymbol{U}_A oldsymbol{U}_A^{ op} oldsymbol{b} \|_2^2 \\ &\leq \left(\gamma^{-2} - 1 \right) \| oldsymbol{A} oldsymbol{x}_{ ext{ls}} \|_2^2 & (\text{since } \| oldsymbol{U}_A oldsymbol{U}_A^{ op} oldsymbol{b} \|_2) \\ &\leq \left(\gamma^{-2} - 1 \right) \| oldsymbol{A} oldsymbol{x}_{ ext{ls}} \|_2^2 & (\text{since } \| oldsymbol{A} oldsymbol{U}_A^{ op} oldsymbol{b} \|_2) \\ &\leq \left(\gamma^{-2} - 1 \right) \sigma_{\max}^2(oldsymbol{A}) \| oldsymbol{x}_{ ext{ls}} \|_2^2 \end{split}$$

This combined with Lemma 1.4(ii) concludes proof.

Connection with approximate matrix multiplication

Condition 1 can be guaranteed if

$$\|\boldsymbol{U}_{A}^{\top}(\boldsymbol{\Phi}^{\top}\boldsymbol{\Phi})\boldsymbol{U}_{A} - \underbrace{\boldsymbol{U}_{A}^{\top}\boldsymbol{U}_{A}}_{=\boldsymbol{I}}\| \leq 1 - \frac{1}{\sqrt{2}}$$

Condition 2 can be guaranteed if

$$\left\| \boldsymbol{U}_{A}^{\top} (\boldsymbol{\Phi}^{\top} \boldsymbol{\Phi}) (\boldsymbol{A} \boldsymbol{x}_{\mathsf{ls}} - \boldsymbol{b}) - \underbrace{\boldsymbol{U}_{A}^{\top} (\boldsymbol{A} \boldsymbol{x}_{\mathsf{ls}} - \boldsymbol{b})}_{=\boldsymbol{U}_{A}^{\top} (\boldsymbol{I} - \boldsymbol{U}_{A} \boldsymbol{U}_{A}^{\top}) \boldsymbol{b} = \boldsymbol{0}} \right\|_{2}^{2} \leq \frac{\varepsilon}{2} \underbrace{\|\boldsymbol{U}_{A}\|^{2}}_{=1} \|\boldsymbol{A} \boldsymbol{x}_{\mathsf{ls}} - \boldsymbol{b}\|_{2}^{2}$$

Both conditions can be viewed as approximating matrix multiplication (by designing $\Phi\Phi^{ op}$)

A (slow) random projection strategy

Gaussian sampling: let $\Phi \in \mathbb{R}^{r \times n}$ be composed of i.i.d. Gaussian entries $\mathcal{N}(0, \frac{1}{r})$

- Conditions 1-2 are satisfied with high prob. if $r \gtrsim \frac{d \log d}{\varepsilon}$ (exercise)
- implementing Gaussian sketching is expensive (computing ΦA takes time $\Omega(nrd) = \Omega(nd^2\log d)$)

Another random subsampling strategy

Let's begin with Condition 1 and try Algorithm 1.2 with optimal sampling probabilities ...

Another random subsampling strategy

Leverage scores of A are defined to be $||(U_A)_{:,i}||_2$ $(1 \le i \le n)$

Nonuniform random subsampling: set $\Phi \in \mathbb{R}^{r \times n}$ to be a (weighted) random subsampling matrix s.t.

$$\mathbb{P}\left(\mathbf{\Phi}_{i,:} = \frac{1}{\sqrt{rp_k}} \mathbf{e}_k^{\top}\right) = p_k, \quad 1 \le k \le n$$

with $p_k \propto \|(\boldsymbol{U}_A)_{i,:}\|_2^2$

still slow: needs to compute (exactly) leverage scores

Fast and data-agnostic sampling

Can we design data-agnostic sketching matrix Φ (i.e. independent of A, b) that allows fast computation while satisfying Conditions 1-2?

Subsampled randomized Hadamard transform (SRHT)

An SRHT matrix $\mathbf{\Phi} \in \mathbb{R}^{r \times n}$ is

$$\Phi = RHD$$

- $D \in \mathbb{R}^{n \times n}$: diagonal matrix, whose entries are random $\{\pm 1\}$
- $H \in \mathbb{R}^{n \times n}$: Hadamard matrix (scaled by $1/\sqrt{n}$ so it's orthonormal)
- $R \in \mathbb{R}^{r \times n}$: uniform random subsampling

$$\mathbb{P}\left(\boldsymbol{R}_{i,:} = \sqrt{\frac{n}{r}} \boldsymbol{e}_k^{\top}\right) = \frac{1}{n}, \quad 1 \le k \le n$$

Subsampled randomized Hadamard transform

Key idea of SRHT:

- use HD to "uniformize" leverage scores (so that $\{\|(HDU_A)_{i,:}\|_2\}$ are more-or-less identical)
- subsample rank-one components uniformly at random

Uniformization of leverage scores

Lemma 1.6

For any fixed matrix $U \in \mathbb{R}^{n \times d}$, one has

$$\max_{1 \le i \le n} \left\| (\boldsymbol{H} \boldsymbol{D} \boldsymbol{U})_{i,:} \right\|_2 \lesssim \frac{\log n}{\sqrt{n}} \| \boldsymbol{U} \|_{\mathrm{F}}$$

with prob. exceeding $1 - O(n^{-9})$

ullet HD preconditions U with high prob.; more precisely,

$$\frac{\|(\boldsymbol{H}\boldsymbol{D}\boldsymbol{U})_{i,:}\|_{2}^{2}}{\sum_{l=1}^{n}\|(\boldsymbol{H}\boldsymbol{D}\boldsymbol{U})_{l,:}\|_{2}^{2}} = \frac{\|(\boldsymbol{H}\boldsymbol{D}\boldsymbol{U})_{i,:}\|_{2}^{2}}{\|\boldsymbol{U}\|_{F}^{2}} \lesssim \frac{\log^{2}n}{n}$$
(1.6)

Proof of Lemma 1.6

For any fixed matrix $\boldsymbol{U} \in \mathbb{R}^{n \times d}$, one has

$$(\boldsymbol{H}\boldsymbol{D}\boldsymbol{U})_{i,:} = \sum_{j=1}^{n} \underbrace{h_{i,j}D_{j,j}}_{\mathsf{random on } \{\pm \frac{1}{\sqrt{n}}\}} \boldsymbol{U}_{j,:},$$

which clearly satisfies $\mathbb{E}\left[(HDU)_{i,:}\right]=\mathbf{0}$. In addition,

$$V := \mathbb{E}\left[\sum_{j=1}^{n} \|h_{i,j} D_{j,j} U_{j,:}\|_{2}^{2}\right] = \frac{1}{n} \sum_{j=1}^{n} \|U_{j,:}\|_{2}^{2} = \frac{1}{n} \|U\|_{F}^{2}$$

$$B := \max_{j} \|h_{i,j} D_{j,j} U_{j,:}\|_{2} = \frac{1}{\sqrt{n}} \max_{j} \|U_{j,:}\|_{2} \leq \frac{1}{\sqrt{n}} \|U\|_{F}$$

Invoke matrix Bernstein to demonstrate that with prob. $1 - O(n^{-10})$,

$$\|(\boldsymbol{H}\boldsymbol{D}\boldsymbol{U})_{i,:}\|_{2} \lesssim \sqrt{V \log n} + B \log n \lesssim \frac{\log n}{\sqrt{n}} \|\boldsymbol{U}\|_{\mathrm{F}}$$

Theoretical guarantees for SRHT

When uniform subsampling is adopted, one has $p_k=1/n$. In view of Lemma 1.6,

$$p_k \ge \beta \frac{\|(\boldsymbol{H}\boldsymbol{D}\boldsymbol{U}_A)_{i,:}\|_2^2}{\sum_{l=1}^n \|(\boldsymbol{H}\boldsymbol{D}\boldsymbol{U}_A)_{l,:}\|_2^2}$$

with $\beta \simeq \log^{-2} n$. Apply Theorem 1.3 to yield

$$\|\boldsymbol{U}_{A}^{\top}\boldsymbol{\Phi}^{\top}\boldsymbol{\Phi}\boldsymbol{U}_{A} - \boldsymbol{I}\| = \|\boldsymbol{U}_{A}^{\top}\boldsymbol{\Phi}^{\top}\boldsymbol{\Phi}\boldsymbol{U}_{A} - \boldsymbol{U}_{A}^{\top}\boldsymbol{U}_{A}\|$$

$$= \|(\boldsymbol{U}_{A}^{\top}\boldsymbol{D}^{\top}\boldsymbol{H}^{\top})\boldsymbol{R}^{\top}\boldsymbol{R}(\boldsymbol{H}\boldsymbol{D}\boldsymbol{U}_{A}) - (\boldsymbol{U}_{A}^{\top}\boldsymbol{D}^{\top}\boldsymbol{H}^{\top})(\boldsymbol{H}\boldsymbol{D}\boldsymbol{U}_{A})\|$$

$$\leq 1/2$$

when $r \gtrsim \frac{\|HDU_A\|_{\mathrm{F}}^2}{\|HDU_A\|^2} \frac{\log n}{\beta} \asymp d \log^3 n$. This establishes Condition 1

Theoretical guarantees for SRHT

Similarly, Condition 2 is satisfied with high prob. if $r \gtrsim \frac{d \log^3 n}{\varepsilon}$ (exercise)

Back to least squares approximation

Preceding analysis suggests following algorithm

Algorithm 1.3 Randomized LS approximation (uniform sampling)

- 1: Pick $r\gtrsim \frac{d\log^3 n}{\varepsilon}$, and generate $m{R}\in\mathbb{R}^{r imes n}$, $m{H}\in\mathbb{R}^{n imes n}$ and $m{D}\in\mathbb{R}^{n imes n}$ (as desribed before)
- 2: return $\tilde{x} = (RHDA)^{\dagger}RHDb$

computational complexity:

$$O\bigg(\underbrace{nd\log\frac{n}{\varepsilon}}_{\text{compute HDA}} + \underbrace{\frac{d^3\log^3n}{\varepsilon}}_{\text{solve subsampled LS }(rd^2)}\bigg)$$

An alternative approach: nonuniform sampling

Key idea of Algorithm 1.3 is to uniformize leverage scores followed by uniform sampling

Alternatively, one can also start by estimating leverage scores, and then apply nonuniform sampling accordingly

Fast approximation of leverage scores

Key idea: apply SRHT (or other fast Johnson-Lindenstrass transform) in appropriate places

$$egin{aligned} \|oldsymbol{U}_{i,:}\|_2^2 &= \|oldsymbol{e}_i^ op oldsymbol{U}\|_2^2 = \|oldsymbol{e}_i^ op oldsymbol{U}oldsymbol{U}^ op\|_2^2 \ &= \|oldsymbol{e}_i^ op oldsymbol{A}oldsymbol{A}^\dagger oldsymbol{\Phi}_1^ op\|_2^2 \end{aligned}$$

where $\Phi_1 \in \mathbb{R}^{r_1 \times n}$ is SRHT matrix

Issue: AA^{\dagger} is expensive to compute; can we compute $AA^{\dagger}\Phi_1^{\top}$ in a fast manner?

Aside: pseudo inverse

Let $\Phi \in \mathbb{R}^{r \times n}$ be SRHT matrix with sufficiently large $r \gg \frac{d \operatorname{poly} \log n}{\varepsilon^2}$. With high prob., one has (check Mahoney's lecture notes)

$$\|(\mathbf{\Phi} \mathbf{U}_A)^{\dagger} - (\mathbf{\Phi} \mathbf{U}_A)^{\top}\| \leq \varepsilon$$

and
$$(oldsymbol{\Phi} oldsymbol{A})^\dagger = oldsymbol{V}_{\!A} oldsymbol{\Sigma}_A^{-1} (oldsymbol{\Phi} oldsymbol{U}_A)^\dagger$$

These mean

$$\begin{aligned} \boldsymbol{A}(\boldsymbol{\Phi}\boldsymbol{A})^{\dagger} &= \boldsymbol{U}_{A}\boldsymbol{\Sigma}_{A}\boldsymbol{V}_{A}^{\top}\boldsymbol{V}_{A}\boldsymbol{\Sigma}_{A}^{-1}(\boldsymbol{\Phi}\boldsymbol{U}_{A})^{\dagger} \approx \boldsymbol{U}_{A}\boldsymbol{\Sigma}_{A}\boldsymbol{V}_{A}^{\top}\boldsymbol{V}_{A}\boldsymbol{\Sigma}_{A}^{-1}(\boldsymbol{\Phi}\boldsymbol{U}_{A})^{\top} \\ &= \boldsymbol{U}_{A}\boldsymbol{U}_{A}^{\top}\boldsymbol{\Phi}^{\top} = \boldsymbol{A}\boldsymbol{A}^{\dagger}\boldsymbol{\Phi} \end{aligned}$$

Fast approximation of leverage scores

Continuing our key idea: apply SRHT (or other fast Johnson-Lindenstrass transform) in appropriate places

$$egin{aligned} \|oldsymbol{U}_{i,:}\|_2^2 &pprox \|oldsymbol{e}_i^ op oldsymbol{A}(oldsymbol{\Phi}_1 oldsymbol{A})^\dagger \|_2^2 \ &pprox \|oldsymbol{e}_i^ op oldsymbol{A}(oldsymbol{\Phi}_1 oldsymbol{A})^\dagger oldsymbol{\Phi}_2\|_2^2 \end{aligned}$$

where $\Phi_1 \in \mathbb{R}^{r_1 \times n}$ and $\Phi_2 \in \mathbb{R}^{r_1 \times r_2}$ $(r_2 \asymp \mathsf{poly} \log n)$ are both SRHT matrices

Fast approximation of leverage scores

Algorithm 1.4 Leverage scores approximation

- 1: Pick $r_1 \gtrsim \frac{d \log^3 n}{\varepsilon}$ and $r_2 \asymp \operatorname{poly} \log n$
- 2: Compute $\Phi_1 A \in \mathbb{R}^{r_1 \times d}$ and its QR decompsotion, and let $R_{\Phi_1 A}$ be the "R" matrix from QR
- 3: Construct $oldsymbol{\Psi} = oldsymbol{A} oldsymbol{R}_{\Phi_1 A}^{-1} oldsymbol{\Phi}_2$
- 4: return $\ell_i = \|\mathbf{\Psi}_{i,:}\|_2$
 - computational complexity: $O\left(\frac{nd\mathsf{poly}\log n}{\varepsilon^2} + \frac{d^3\mathsf{poly}\log n}{\varepsilon^2}\right)$

Least squares approximation (nonuniform sampling)

Algorithm 1.5 Randomized LS approximation (nonuniform sampling)

- 1: Run Algorithm 1.4 to compute approximate leverage scores $\{\ell_k\}$, and set $p_k \propto \ell_k^2$
- 2: Randomly sample $r\gtrsim \frac{d\mathsf{poly}\log n}{\varepsilon}$ rows of \boldsymbol{A} and elements of \boldsymbol{b} using $\{p_k\}$ as sampling probabilities, rescaling each by $1/\sqrt{rp_k}$. Let $\boldsymbol{\Phi}\boldsymbol{A}$ and $\boldsymbol{\Phi}\boldsymbol{b}$ be the subsampled matrix and vector
- 3: return $\tilde{m{x}}_{\mathsf{ls}} = rg \min_{m{x} \in \mathbb{R}^d} \| m{\Phi} m{A} m{x} m{\Phi} m{b} \|_2$

informally, Algorithm 1.5 returns a reasonably good solution with prob. $1 - O(1/\log n)$

Low-rank matrix approximation

Low-rank matrix approximation

Question: given a matrix $A \in \mathbb{R}^{n \times n}$, how to find a rank-k matrix that well approximates A

ullet One can compute SVD of $oldsymbol{A} = oldsymbol{U} oldsymbol{\Sigma} oldsymbol{V}^{ op}$, then return

$$oldsymbol{A}_k = oldsymbol{U}_k oldsymbol{U}_k^ op oldsymbol{A}$$

where U_k consists of top-k singular vectors

- In general, takes time $O(n^3)$, or $O(kn^2)$ (by power methods)
- Can we find faster algorithms if we only want "good approximation"?

Randomized low-rank matrix approximation

Strategy: find a matrix C (via, e.g., subsampling columns of A), and return

$$CC^{\dagger}A$$
 project A onto column space of C

Question: how well can $CC^{\dagger}A$ approximate A?

A simple paradigm

Algorithm 1.6

- 1: **input:** data matrix $A \in \mathbb{R}^{n \times n}$, subsampled matrix $C \in \mathbb{R}^{n \times r}$
- 2: **return** H_k as top-k left singular vectors of C

• As we will see, quality of approximation depends on size of

$$AA^{\top} - CC^{\top}$$

connection with matrix multiplication

Quality of approximation (Frobenius norm)

One can also connect spectral-norm error with product of matrices

Lemma 1.7

The output of Algorithm 1.6 satisfies

$$\|\boldsymbol{A} - \boldsymbol{H}_k \boldsymbol{H}_k^{\top} \boldsymbol{A}\|_{\mathrm{F}}^2 \leq \|\boldsymbol{A} - \boldsymbol{U}_k \boldsymbol{U}_k^{\top} \boldsymbol{A}\|_{\mathrm{F}}^2 + 2\sqrt{k} \|\boldsymbol{A} \boldsymbol{A}^{\top} - \boldsymbol{C} \boldsymbol{C}^{\top}\|_{\mathrm{F}}$$

where $U_k \in \mathbb{R}^{n \times k}$ contains top-k left singular vectors of $oldsymbol{A}$

- ullet This holds for any C
- Approximation error depends on the error in approximating product of two matrices

Proof of Lemma 1.7

To begin with, since H_k is orthonormal, one has

$$\left\| \boldsymbol{A} - \boldsymbol{H}_k \boldsymbol{H}_k^{\top} \boldsymbol{A} \right\|_{\mathrm{F}}^2 = \left\| \boldsymbol{A} \right\|_{\mathrm{F}}^2 - \left\| \boldsymbol{H}_k^{\top} \boldsymbol{A} \right\|_{\mathrm{F}}^2$$

Next, letting $\boldsymbol{h}_i = (\boldsymbol{H}_k)_{::i}$ yields

$$\begin{aligned} \left| \left\| \boldsymbol{H}_{k}^{\top} \boldsymbol{A} \right\|_{\mathrm{F}}^{2} - \sum_{i=1}^{k} \sigma_{i}^{2}(\boldsymbol{C}) \right| &= \left| \sum_{i=1}^{k} \left\| \boldsymbol{A}^{\top} \boldsymbol{h}_{i} \right\|_{2}^{2} - \sum_{i=1}^{k} \left\| \boldsymbol{C} \boldsymbol{h}_{i} \right\|_{2}^{2} \right| \\ &= \left| \sum_{i=1}^{k} \left\langle \boldsymbol{h}_{i} \boldsymbol{h}_{i}^{\top}, \boldsymbol{A} \boldsymbol{A}^{\top} - \boldsymbol{C} \boldsymbol{C}^{\top} \right\rangle \right| \\ &= \left| \left\langle \boldsymbol{H}_{k} \boldsymbol{H}_{k}^{\top}, \boldsymbol{A} \boldsymbol{A}^{\top} - \boldsymbol{C} \boldsymbol{C}^{\top} \right\rangle \right| \\ &\leq \left\| \boldsymbol{H}_{k} \boldsymbol{H}_{k}^{\top} \right\|_{\mathrm{F}} \left\| \boldsymbol{A} \boldsymbol{A}^{\top} - \boldsymbol{C} \boldsymbol{C}^{\top} \right\|_{\mathrm{F}} \\ &\leq \sqrt{k} \| \boldsymbol{A} \boldsymbol{A}^{\top} - \boldsymbol{C} \boldsymbol{C}^{\top} \right\|_{\mathrm{F}} \end{aligned}$$

Proof of Lemma 1.7

In addition,

$$\begin{split} &\left|\sum_{i=1}^{k}\sigma_{i}^{2}(\boldsymbol{C})-\sum_{i=1}^{k}\sigma_{i}^{2}(\boldsymbol{A})\right| = \left|\sum_{i=1}^{k}\left\{\sigma_{i}(\boldsymbol{C}\boldsymbol{C}^{\top})-\sigma_{i}(\boldsymbol{A}\boldsymbol{A}^{\top})\right\}\right| \\ &\leq \sqrt{k}\sqrt{\sum_{i=1}^{n}\left\{\sigma_{i}(\boldsymbol{C}\boldsymbol{C}^{\top})-\sigma_{i}(\boldsymbol{A}\boldsymbol{A}^{\top})\right\}^{2}} \quad \text{(Cauchy-Schwarz)} \\ &\leq \sqrt{k}\left\|\boldsymbol{C}\boldsymbol{C}^{\top}-\boldsymbol{A}\boldsymbol{A}^{\top}\right\|_{\mathrm{F}} \quad \text{(Wielandt-Hoffman inequality)} \end{split}$$

Finally, one has
$$\|\boldsymbol{A} - \boldsymbol{U}_k \boldsymbol{U}_k^{\top} \boldsymbol{A}\|_{\mathrm{F}}^2 = \|\boldsymbol{A}\|_{\mathrm{F}}^2 - \sum_{i=1}^k \sigma_i^2(\boldsymbol{A})$$
.

Combining above results establishes the claim

Quality of approximation (spectral norm)

Lemma 1.8

The output of Algorithm 1.6 satisfies

$$\|\boldsymbol{A} - \boldsymbol{H}_k \boldsymbol{H}_k^{\top} \boldsymbol{A}\|^2 \le \|\boldsymbol{A} - \boldsymbol{U}_k \boldsymbol{U}_k^{\top} \boldsymbol{A}\|^2 + 2\|\boldsymbol{A} \boldsymbol{A}^{\top} - \boldsymbol{C} \boldsymbol{C}^{\top}\|$$

where $U_k \in \mathbb{R}^{n \times k}$ contains top-k left singular vectors of A

Proof of Lemma 1.8

First of all,

$$egin{aligned} egin{aligned} egin{aligned\\ egin{aligned} egi$$

Additionally, for any $m{x} \perp m{H}_k$,

$$egin{aligned} \left\|oldsymbol{x}^ op oldsymbol{A}
ight\|_2^2 &= \left|oldsymbol{x}^ op oldsymbol{C}^ op oldsymbol{x} + oldsymbol{x}^ op oldsymbol{C}oldsymbol{C}^ op oldsymbol{x} + oldsymbol{z}^ op oldsymbol{C}oldsymbol{C}^ op oldsymbol{x} + oldsymbol{z}^ op oldsymbol{C}oldsymbol{C}^ op oldsymbol{x} + oldsymbol{z}^ op oldsymbol{C}oldsymbol{C}^ op oldsymbol{z} + oldsymbol{z}^ op oldsymbol{C}oldsymbol{C}^ op oldsymbol{Z} + oldsymbol{Z} oldsymbol{A}oldsymbol{A}^ op - oldsymbol{C}oldsymbol{C}^ op oldsymbol{Z} \\ &\leq \sigma_{k+1} oldsymbol{A}oldsymbol{A}^ op oldsymbol{D} + oldsymbol{Z} oldsymbol{A}oldsymbol{A}^ op - oldsymbol{C}oldsymbol{C}^ op oldsymbol{Z} \\ &\leq \sigma_{k+1} oldsymbol{A}oldsymbol{A}^ op oldsymbol{D} + oldsymbol{Z} oldsymbol{A}oldsymbol{A}oldsymbol{A}^ op - oldsymbol{C}oldsymbol{C}^ op oldsymbol{Z} \\ &= oldsymbol{A}oldsymbol{A}oldsymbol{A}oldsymbol{A}oldsymbol{A}^ op oldsymbol{C} oldsymbol{C} oldsymbol{Z} \\ &= oldsymbol{A}oldsymbol{A}oldsymbol{A}oldsymbol{A}oldsymbol{A} oldsymbol{A} oldsymbol{C} oldsymbol{C} \\ &= oldsymbol{A}oldsymbol{A}oldsymbol{A}oldsymbol{A} oldsymbol{A} oldsymbol{A} oldsymbol{A} oldsymbol{A} oldsymbol{A} \\ &= oldsymbol{A}oldsymbol{A}oldsymbol{A} oldsymbol{A} oldsymbol{A} oldsymbol{A} oldsymbol{A} oldsymbol{A} oldsymbol{A} \\ &= oldsymbol{A} oldsymbol{A} oldsymbol{A} oldsymbol{A} oldsymbol{A} oldsymbol{A} oldsymbol{A} oldsymbol{A} oldsymbol{A} \\ &= oldsymbol{A} oldsymbol{$$

This concludes the proof.

Back to low-rank matrix approximation

To ensure $AA^{\top} - CC^{\top}$ is small, we can do random subsampling / projection as before. For example:

Algorithm 1.7

- 1: **for** $l = 1, \dots, r$ **do**
- 2: Pick $i_l \in \{1,\cdots,n\}$ i.i.d. with prob. $\mathbb{P}\{i_l=k\}=p_k$
- 3: Set $C_{:,l} = \frac{1}{\sqrt{rp_{i_l}}} A_{:,l}$
- 4: **return** H_k as top-k left singular vectors of C

Back to low-rank matrix approximation

Invoke Theorems 1.2 and 1.3 to see that with high prob.:

• If $r \gtrsim \frac{k \log n}{\beta \varepsilon^2}$, then

$$\|\boldsymbol{A} - \boldsymbol{H}_k \boldsymbol{H}_k^{\top} \boldsymbol{A}\|_{\mathrm{F}}^2 \le \|\boldsymbol{A} - \boldsymbol{U}_k \boldsymbol{U}_k^{\top} \boldsymbol{A}\|_{\mathrm{F}}^2 + \varepsilon \|\boldsymbol{A}\|_{\mathrm{F}}^2$$
(1.7)

• If $r \gtrsim \frac{\|A\|_{\mathrm{F}}^2}{\|A\|^2} \frac{\log n}{\beta \varepsilon^2}$, then

$$\|\boldsymbol{A} - \boldsymbol{H}_k \boldsymbol{H}_k^{\top} \boldsymbol{A}\|^2 \le \|\boldsymbol{A} - \boldsymbol{U}_k \boldsymbol{U}_k^{\top} \boldsymbol{A}\|^2 + \varepsilon \|\boldsymbol{A}\|^2$$
 (1.8)

An improved multi-pass algorithm

Algorithm 1.8 Multi-pass randomized SVD

- 1: $S = \{\}$
- 2: for $l=1,\cdots,t$ do
- 3: $oldsymbol{E}_l = oldsymbol{A} oldsymbol{A}_{\mathcal{S}} oldsymbol{A}_{\mathcal{S}}^{\dagger} oldsymbol{A}$
- 4: Set $p_k \ge \frac{\beta \|(E_l)_{:,k}\|_2^2}{\|E_l\|_{\mathrm{E}}^2}$, $1 \le k \le n$
- 5: Randomly select r column indices with sampling prob. $\{p_k\}$ and append to $\mathcal S$
- 6: **return** $C = A_{\mathcal{S}}$

An improved multi-pass algorithm

Theorem 1.9

Suppose $r \gtrsim \frac{k \log n}{\beta \varepsilon^2}$. With high prob.,

$$\|\boldsymbol{A} - \boldsymbol{C}\boldsymbol{C}^{\dagger}\boldsymbol{A}\|_{\mathrm{F}}^{2} \leq \frac{1}{1-arepsilon} \|\boldsymbol{A} - \boldsymbol{U}_{k}\boldsymbol{U}_{k}^{\top}\|_{\mathrm{F}}^{2} + arepsilon^{t} \|\boldsymbol{A}\|_{\mathrm{F}}^{2}$$

Proof of Theorem 1.9

We will prove it by induction. Clearly, the claim holds for t=1 (according to (1.7)). Assume

$$\left\| \underbrace{\boldsymbol{A} - \boldsymbol{C}^{t-1} (\boldsymbol{C}^{t-1})^{\dagger} \boldsymbol{A}}_{:=\boldsymbol{E}_{t}} \right\|_{\mathrm{F}}^{2} \leq \frac{1}{1-\varepsilon} \|\boldsymbol{A} - \boldsymbol{U}_{k} \boldsymbol{U}_{k}^{\top} \boldsymbol{A} \|_{\mathrm{F}}^{2} + \varepsilon^{t-1} \|\boldsymbol{A}\|_{\mathrm{F}}^{2},$$

and let Z be the matrix of the columns of E_t included in the sample. In view of (1.7),

$$\left\| \boldsymbol{E}_t - \boldsymbol{Z} \boldsymbol{Z}^{\dagger} \boldsymbol{E}_t \right\|_{\mathrm{F}}^2 \leq \left\| \boldsymbol{E}_t - (\boldsymbol{E}_t)_k \right\|_{\mathrm{F}}^2 + \varepsilon \| \boldsymbol{E}_t \|_{\mathrm{F}}^2,$$

with $(E_t)_k$ the best rank-k approximation of E_t . Combining the above two inequalities yields

$$\left\| \boldsymbol{E}_{t} - \boldsymbol{Z} \boldsymbol{Z}^{\dagger} \boldsymbol{E}_{t} \right\|_{F}^{2} \leq \left\| \boldsymbol{E}_{t} - (\boldsymbol{E}_{t})_{k} \right\|_{F}^{2}$$

$$+ \frac{\varepsilon}{1 - \varepsilon} \left\| \boldsymbol{A} - \boldsymbol{U}_{k} \boldsymbol{U}_{k}^{\top} \boldsymbol{A} \right\|_{F}^{2} + \varepsilon^{t} \|\boldsymbol{A}\|_{F}^{2}$$

$$(1.9)$$

Proof of Theorem 1.9 (cont.)

If we can show that

$$E_t - ZZ^{\dagger}E_t = A - C^t(C^t)^{\dagger}A \tag{1.10}$$

$$\|\boldsymbol{E}_t - (\boldsymbol{E}_t)_k\|_{\mathrm{F}}^2 \le \|\boldsymbol{A} - \boldsymbol{A}_k\|_{\mathrm{F}}^2$$
 (1.11)

then substitution into (1.9) yields

$$\begin{aligned} \left\| \boldsymbol{A} - \boldsymbol{C}^{t} (\boldsymbol{C}^{t})^{\dagger} \boldsymbol{A} \right\|_{\mathrm{F}}^{2} &\leq \| \boldsymbol{A} - \boldsymbol{A}_{k} \|_{\mathrm{F}}^{2} + \frac{\varepsilon}{1 - \varepsilon} \| \boldsymbol{A} - \boldsymbol{A}_{k} \|_{\mathrm{F}}^{2} + \varepsilon^{t} \| \boldsymbol{A} - \boldsymbol{A}_{k} \|_{\mathrm{F}}^{2} \\ &= \frac{1}{1 - \varepsilon} \| \boldsymbol{A} - \boldsymbol{A}_{k} \|_{\mathrm{F}}^{2} + \varepsilon^{t} \| \boldsymbol{A} - \boldsymbol{A}_{k} \|_{\mathrm{F}}^{2} \end{aligned}$$

We can then use induction to finish proof

Proof of Theorem 1.9 (cont.)

It remains to justify (1.10) and (1.11).

To begin with, (1.10) follows from the definition of E_t and the fact $ZZ^\dagger C^{t-1}(C^{t-1})^\dagger=0$, which gives

$$oldsymbol{C}^t(oldsymbol{C}^t)^\dagger = oldsymbol{C}^{t-1}(oldsymbol{C}^{t-1})^\dagger + oldsymbol{Z}oldsymbol{Z}^\dagger$$

Proof of Theorem 1.9 (cont.)

To show (1.11), note that $(E_t)_k$ is best rank-k approximation of E_t . This gives

$$egin{aligned} \|oldsymbol{E}_t - (oldsymbol{E}_t)_k\|_{ ext{F}}^2 &= \left\| \left(oldsymbol{I} - oldsymbol{C}^{t-1} (oldsymbol{C}^{t-1})^\dagger
ight) oldsymbol{A} - \left(\left(oldsymbol{I} - oldsymbol{C}^{t-1} (oldsymbol{C}^{t-1})^\dagger
ight) oldsymbol{A} - \left(oldsymbol{I} - oldsymbol{C}^{t-1} (oldsymbol{C}^{t-1})^\dagger
ight) oldsymbol{A}_k \|_{ ext{F}}^2 \\ &= \left\| \left(oldsymbol{I} - oldsymbol{C}^{t-1} (oldsymbol{C}^{t-1})^\dagger
ight) oldsymbol{A} - oldsymbol{A}_k
ight) \right\|_{ ext{F}}^2 \\ &= \left\| \left(oldsymbol{I} - oldsymbol{C}^{t-1} (oldsymbol{C}^{t-1})^\dagger
ight) oldsymbol{A} - oldsymbol{A}_k
ight) \right\|_{ ext{F}}^2 \\ &\leq \left\| oldsymbol{A} - oldsymbol{A}_k
ight\|_{ ext{F}}^2 , \end{aligned}$$

where A_k is best rank-k approximation of A. Substitution into (1.9) establishes the claim for t

Multiplicative error bounds

So far, our results read

$$\|m{A}-m{C}m{C}^{\dagger}m{A}\|_{\mathrm{F}}^2 \leq \|m{A}-m{A}_k\|_{\mathrm{F}}^2 + \mathsf{additive}$$
 error $\|m{A}-m{C}m{C}^{\dagger}m{A}\|^2 \leq \|m{A}-m{A}_k\|^2 + \mathsf{additive}$ error

In some cases, one might prefer multiplicative error guarantees, e.g.

$$\|\boldsymbol{A} - \boldsymbol{C}\boldsymbol{C}^{\dagger}\boldsymbol{A}\|_{\mathrm{F}} \leq (1+\varepsilon)\|\boldsymbol{A} - \boldsymbol{A}_k\|_{\mathrm{F}}$$

Two types of matrix decompositions

ullet CX decomposition: let $C\in\mathbb{R}^{n imes r}$ consist of r columns of $oldsymbol{A}$, and return

$$\hat{A} = CX$$

for some matrix $\boldsymbol{X} \in \mathbb{R}^{r \times n}$

• CUR decomposition: let $C \in \mathbb{R}^{n \times r}$ (resp. $R \in \mathbb{R}^{r \times n}$) consist of r columns (resp. rows) of A, and return

$$\hat{A} = CUR$$

for some matrix $\boldsymbol{U} \in \mathbb{R}^{r \times r}$

Generalized least squares problem

$$\mathsf{minimize}_{oldsymbol{X}} \quad \|oldsymbol{B} - oldsymbol{A} oldsymbol{X}\|_{\mathrm{F}}^2$$

where X is matrix (rather than vector)

- ullet generalization of over-determined ℓ_2 regression
- ullet optimal solution: $oldsymbol{X}^{\mathsf{ls}} = oldsymbol{A}^{\dagger} oldsymbol{B}$
- ullet if $\mathrm{rank}(oldsymbol{A}) \leq k$, then $oldsymbol{X}^{\mathsf{ls}} = oldsymbol{A}_k^\dagger oldsymbol{B}$

Generalized least squares approximation

Randomized algorithm: construct a optimally weighted subsampling matrix $\Phi \in \mathbb{R}^{r \times n}$ with $r \gtrsim \frac{k^2}{\epsilon^2}$ and compute

$$ilde{X}^{\mathsf{ls}} = (\mathbf{\Phi} A)^{\dagger} \mathbf{\Phi} B$$

Then informally, with high probability,

$$\begin{split} & \|\boldsymbol{B} - \boldsymbol{A}\tilde{\boldsymbol{X}}^{\mathsf{ls}}\|_{\mathrm{F}} \leq (1 + \epsilon) \left\{ \min_{\boldsymbol{X}} \|\boldsymbol{B} - \boldsymbol{A}\boldsymbol{X}\|_{\mathrm{F}} \right\} \\ & \|\boldsymbol{X}^{\mathsf{ls}} - \tilde{\boldsymbol{X}}^{\mathsf{ls}}\|_{\mathrm{F}} \leq \frac{\epsilon}{\sigma_{\min}(\boldsymbol{A}_k)} \left\{ \min_{\boldsymbol{X}} \|\boldsymbol{B} - \boldsymbol{A}\boldsymbol{X}\|_{\mathrm{F}} \right\} \end{split}$$

Randomized algorithm for CX decomposition

$\begin{tabular}{ll} \textbf{Algorithm 1.9} & \textbf{Randomized algorithm for constructing CX matrix decompositions} \end{tabular}$

- 1: Compute / approximate sampling probabilities $\{p_i\}_{i=1}^n$, where $p_i=\frac{1}{k}\|(\pmb{U}_{A,k})_{:,i}\|_2^2$
- 2: Use sampling probabilities $\{p_i\}$ to construct a rescaled random sampling marix $\mathbf{\Phi}$
- 3: Construct $oldsymbol{C} = oldsymbol{A} oldsymbol{\Phi}^ op$

Theoretical guarantees

Theorem 1.10

Suppose $r \gtrsim \frac{k \log k}{arepsilon^2}$, then Algorithm 1.9 yields

$$\|\boldsymbol{A} - \boldsymbol{C}\boldsymbol{C}^{\dagger}\boldsymbol{A}\|_{\mathrm{F}} \leq (1+\varepsilon)\|\boldsymbol{A} - \boldsymbol{A}_k\|_{\mathrm{F}}$$

Proof of Theorem 1.10

$$\begin{split} \|\boldsymbol{A} - \boldsymbol{C} \underbrace{\boldsymbol{C}^{\dagger} \boldsymbol{A}}_{:=\boldsymbol{X}^{\text{ls}}} \\ &= \|\boldsymbol{A} - (\boldsymbol{A} \boldsymbol{\Phi}^{\top}) (\boldsymbol{A} \boldsymbol{\Phi}^{\top})^{\dagger} \boldsymbol{A} \|_{\mathrm{F}} \\ &\leq \|\boldsymbol{A} - (\boldsymbol{A} \boldsymbol{\Phi}^{\top}) (\boldsymbol{P}_{A_{k}} \boldsymbol{A} \boldsymbol{\Phi}^{\top})^{\dagger} \boldsymbol{P}_{A_{k}} \boldsymbol{A} \|_{\mathrm{F}} \quad (\boldsymbol{P}_{A_{k}} := \boldsymbol{U}_{k} \boldsymbol{U}_{k}^{\top}) \\ &\qquad \qquad \text{since } \boldsymbol{X}^{\text{ls}} := \boldsymbol{C}^{\dagger} \boldsymbol{A} \text{ minimizes } \|\boldsymbol{A} - \boldsymbol{C} \boldsymbol{X} \|_{\mathrm{F}} \\ &= \|\boldsymbol{A} - (\boldsymbol{A} \boldsymbol{\Phi}^{\top}) (\boldsymbol{A}_{k} \boldsymbol{\Phi}^{\top})^{\dagger} \boldsymbol{A}_{k} \|_{\mathrm{F}} \\ &\leq (1 + \varepsilon) \|\boldsymbol{A} - \boldsymbol{A} \boldsymbol{A}_{k}^{\dagger} \boldsymbol{A}_{k} \|_{\mathrm{F}} \\ &= (1 + \varepsilon) \|\boldsymbol{A} - \boldsymbol{A}_{k} \|_{\mathrm{F}} \end{split}$$

Randomized linear algebra