

EE270

Large scale matrix computation, optimization and learning

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Randomized Linear Algebra

Lecture 7: Least Squares Optimization and Random Projections

Recap: Johnson Lindenstrauss Lemma

- Let $\epsilon \in (0, \frac{1}{2})$. Given any set of points $\{x_1, \dots, x_n\}$ in \mathbb{R}^d , there exists a map $S : \mathbb{R}^n \rightarrow \mathbb{R}^m$ with $m = \frac{9 \log(n)}{\epsilon^2 - \epsilon^3}$ such that

$$1 - \epsilon \leq \frac{\|Sx_i - Sx_j\|_2^2}{\|x_i - x_j\|_2^2} \leq 1 + \epsilon$$

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- ▶ Note that the target dimension m is **independent of the original dimension d** , and depends **only on the number of points n** and the accuracy parameter.

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- ▶ Note that the target dimension m is **independent of the original dimension d** , and depends **only on the number of points n** and the accuracy parameter.
- ▶ more surprises: picking an $m \times d$ random matrix $S = \frac{1}{\sqrt{m}} G$ with $G_{ij} \sim N(0, 1)$ standard normal works with high probability!

True ‘projections’: random subspaces also work

- ▶ Pick $S_{(i)}$ uniformly random on the unit sphere
- ▶ Pick $S_{(i+1)}$ uniformly random on the unit sphere and $\perp S_{(i)}, \dots, S_{(1)}$
- ▶ S is a projection matrix, which projects onto a uniformly random subspace

$$\mathbb{P} \left\{ \left| \|Su\|_2 - \sqrt{\frac{m}{d}} \right| > t \right\} \leq 2e^{-\frac{t^2 d}{2}}$$

- ▶ Applying union bound for all points $i, j = 1, \dots, d$ gives a similar result
- ▶ Random i.i.d. S matrices are easier to generate and approximately orthogonal: $\mathbb{E} S^T S = I$

Computationally cheaper random matrices

- ▶ Gaussian $S_{ij} = \frac{1}{\sqrt{m}} N(0, 1)$
- ▶ Rademacher

$$S_{ij} = \begin{cases} +\frac{1}{\sqrt{m}} & \text{with probability } \frac{1}{2} \\ -\frac{1}{\sqrt{m}} & \text{with probability } \frac{1}{2} \end{cases} \quad (1)$$

- ▶ Bernoulli-Rademacher

$$S_{ij} = \begin{cases} +\frac{\sqrt{3}}{\sqrt{m}} & \text{with probability } \frac{1}{6} \\ 0 & \text{with probability } \frac{2}{3} \\ -\frac{\sqrt{3}}{\sqrt{m}} & \text{with probability } \frac{1}{6} \end{cases} \quad (2)$$

- ▶ other sparse matrices (e.g. one non-zero per column)
- ▶ Fourier transform based matrices

Random projection for Approximate Matrix Multiplication

- ▶ Let the approximate product of AB be $C = AS^T SB$

$$\mathbb{P} [\|AB - C\|_F > 3\epsilon\|A\|_F\|B\|_F] \leq \delta$$

- ▶ Follows from JL Moment property
- ▶ $S \in \mathbb{R}^{m \times n} \sim \frac{1}{\sqrt{m}} \times \text{random i.i.d. sub-Gaussian, e.g., } \pm 1, \text{ or } N(0, 1) \text{ with } m = \frac{c_1}{\epsilon^2} \log \frac{1}{\delta}$
- ▶ $S \in \mathbb{R}^{m \times n} \sim \frac{1}{\sqrt{m}} \times \text{CountSketch matrix (one nonzero per column, which is } \pm 1 \text{ at a uniformly random location) with } m = \frac{c_2}{\epsilon^2 \delta}$
- ▶ $S \in \mathbb{R}^{m \times n} \sim \frac{1}{\sqrt{m}} \times \text{Fast JL Transform with } m = \frac{c_3}{\epsilon} \log \frac{1}{\delta}$

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- ▶ $S \in \mathbb{R}^{m \times n} \sim \frac{1}{\sqrt{m}} \times \text{Fast JL Transform with } m = \frac{c_3}{\epsilon} \log \frac{1}{\delta}$
- ▶ Sparse JL and Fast JL are more efficient
- ▶ advantages: doesn't require any knowledge about matrices A and B (**oblivious**)
- ▶ optimal sampling probabilities depend on the column/row norms of A and B

Least Squares Regression

- Predict the value of a continuous target variable y

$(a_1, b_1), \dots, (a_n, b_n)$

$a_i \in \mathbb{R}^d$ and $b_i \in \mathbb{R}$

- Linear regression $f(a) = x^T a + x_0$

$$A = \begin{bmatrix} a_1^T \\ \vdots \\ a_n^T \end{bmatrix} \quad b = \begin{bmatrix} b_1 \\ \vdots \\ b_n \end{bmatrix}$$

$\approx b$

Least Squares Regression

$$I = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$

- Predict the value of a continuous target variable y

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$a_i \in \mathbb{R}^d$ and $b_i \in \mathbb{R}$

- Linear regression $f(a) = x^T a + x_0$

$$\min_x \|Ax - b + x_0 I\|_2^2$$

- Performance measure: minimum sum of squares

$$\min_{x, x_0} \frac{1}{n} \sum_{i=1}^n (b_i - x^T a_i - x_0)^2$$

Least Squares Regression

- ▶ Predict the value of a continuous target variable y
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 $a_i \in \mathbb{R}^d$ and $b_i \in \mathbb{R}$
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- ▶ Performance measure: minimum sum of squares

$$\min_{x, x_0} \frac{1}{n} \sum_{i=1}^n (b_i - x^T a_i - x_0)^2$$

(Handwritten purple circle around the squared term with $\|x\|_2$ written inside)

- ▶ we can add a regularization term $\lambda \|x\|_2^2$

$$\min_{x, x_0} \frac{1}{n} \sum_{i=1}^n (b_i - x^T a_i - x_0)^2 + \lambda \|x\|_2^2$$

Ridge or Tikhonov

Least Squares Regression

- Loss function:

$$L(x, x_0) = \frac{1}{n} \sum_{i=1}^n (b_i - x^T a_i - x_0)^2 + \lambda \|x\|_2^2$$

- $\frac{\partial}{\partial x_0} L(x, x_0) = 0$

→ optimal $x_0^* = \frac{1}{n} \sum_{i=1}^n (y_i - x^T a_i) = \bar{b} - x^T \bar{a}$
where $\bar{a} = \sum_{i=1}^n a_i$ and $\bar{b} = \sum_{i=1}^n b_i$

- plugging x_0^* in $L(x, x_0)$

$$L(x, x_0^*) = \frac{1}{n} \sum_{i=1}^n (b_i - \bar{b} - x^T (a_i - \bar{a}))^2 + \lambda \|x\|_2^2$$

Least Squares Regression

- Loss function:

$$L(x, x_0) = \frac{1}{n} \sum_{i=1}^n (b_i - x^T a_i - x_0)^2 + \lambda \|x\|_2^2$$

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$$\text{optimal } x_0^* = \frac{1}{n} \sum_{i=1}^n (y_i - x^T a_i) = \bar{b} - x^T \bar{a}$$

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$$L(x, x_0^*) = \frac{1}{n} \sum_{i=1}^n (b_i - \bar{b} - x^T (a_i - \bar{a}))^2 + \lambda \|x\|_2^2$$

define centered data $\tilde{a}_i = a_i - \bar{a}$ and $\tilde{b}_i = b_i - \bar{b}$

$$\min_x \|\tilde{A}x - \tilde{b}\|_2^2 + n\lambda \|x\|_2^2$$

Least Squares Regression

- Loss function:

$$L(x, x_0) = \frac{1}{n} \sum_{i=1}^n (b_i - x^T a_i - x_0)^2 + \lambda \|x\|_2^2$$

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$$\text{where } \bar{a} = \sum_{i=1}^n a_i \text{ and } \bar{b} = \sum_{i=1}^n b_i$$

- plugging x_0^* in $L(x, x_0)$

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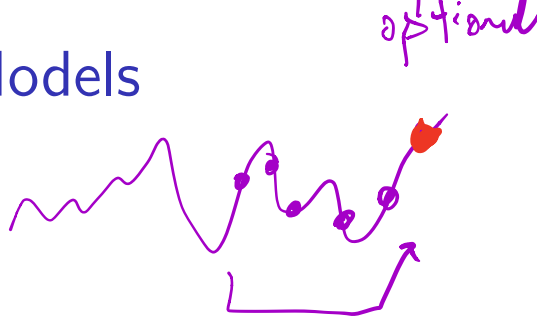
$$\text{define centered data } \tilde{a}_i = a_i - \bar{a} \text{ and } \tilde{b}_i = b_i - \bar{b}$$

$$\min_x \|\tilde{A}x - \tilde{b}\|_2^2 + n\lambda \|x\|_2^2$$

$$\frac{\partial}{\partial x} L(x, x_0^*) = 2\tilde{A}^T (\tilde{A}x^* - \tilde{b}) + 2n\lambda x^* = 0$$

$$\text{optimal solution } x^* = (\tilde{A}^T \tilde{A} + n\lambda I)^{-1} \tilde{A}^T \tilde{b}$$

Autoregressive Models



$$b[n] = a[n + 1] \approx \sum_k x_k a[n - k]$$



- ▶ AR(2) model : two non-zero filter coefficients

$$a[n + 1] = -x_0 a[n] - x_1 a[n - 1]$$

and error term $e_n = 0$

- ▶ Example: Sine wave $a[n] = \sin(\alpha n)$ satisfies AR(2) model



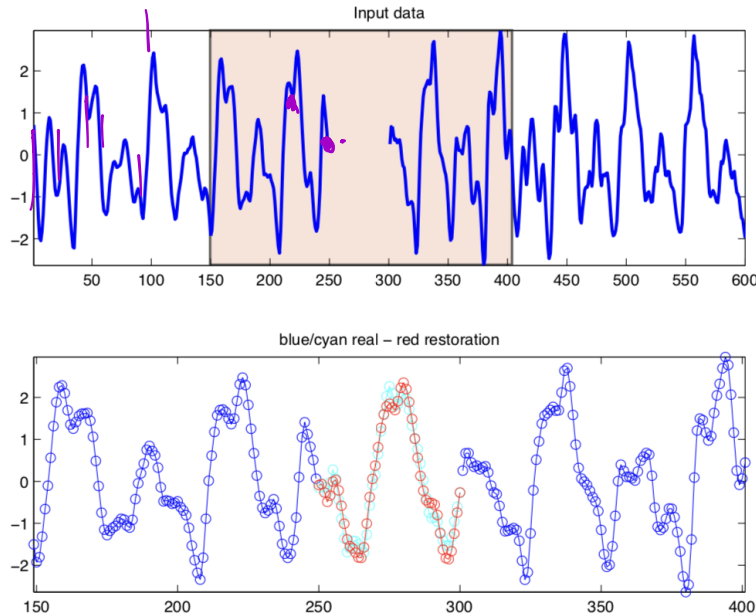
Autoregressive models

- We can predict future values using

$$b[n] = \sum_k a[n-k]x_k$$

1000

only $\parallel Ax=b$



d

n

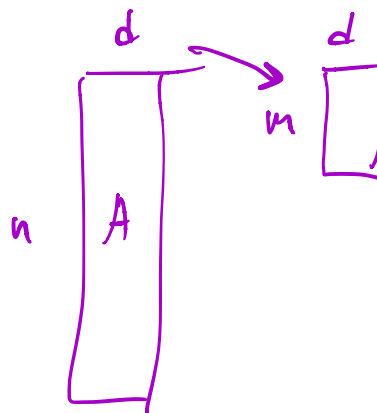
tail.

Least Squares Problems and Random Projection

- ▶ Given $A \in \mathbb{R}^{n \times d}$ and $b \in \mathbb{R}^d$
find the best linear fit $Ax \approx b$ according to

$$\min_{x \in \mathbb{R}^d} \|Ax - b\|_2^2$$

- ▶ no regularization, i.e., $\lambda = 0$
- ▶ If A is full column rank then
- ▶ $x_{LS} = (A^T A)^{-1} A^T b$



$$(A^T A)^{-1} \quad O(d^2 \text{ time})$$

$$\begin{array}{l} A^T A : O(nd^2) \leftarrow \text{large } n \\ d \times n \quad n \times d \end{array} \quad n d^2 > d^3 \quad n > d$$

Geometry

$$\min_{x \in \mathbb{R}^d} \|Ax - b\|_2^2$$

Normal
eq.

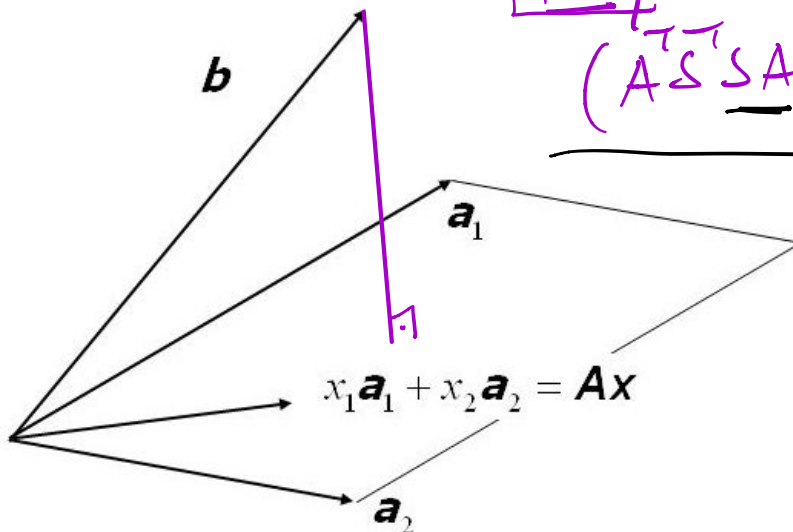
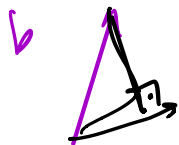
$$\begin{bmatrix} a_1^T a_1 & a_1^T a_2 \\ a_2^T a_1 & a_2^T a_2 \end{bmatrix}$$



$$\underbrace{A^T A} x = \underbrace{A^T b}$$

Idea: Randomized LS. solver

$$(\underbrace{A^T S^T S A}) x = \underbrace{A^T S^T S b}$$



Singular Value Decomposition

$$Ax = b$$
$$x \neq A^{-1}b$$

- ▶ Every $A \in \mathbb{R}^{n \times n}$ has a singular value decomposition

$$A = U\Sigma V^T$$

where $U \in \mathbb{R}^{n \times n}$ has orthonormal columns

Σ is diagonal with non-increasing non negative entries

V^T has orthonormal rows

- ▶ Pseudoinverse $A^\dagger = V\Sigma^{-1}U^T$

- ▶ Least Square solution

$$x_{LS} = \underbrace{(A^T A)^{-1} A^T}_{A^\dagger} b = A^\dagger b = V\Sigma^{-1}U^T b$$

Classical Methods for Least Squares

► Direct methods *exact*

→ *not efficient* ► Cholesky decomposition: Form $A^T A$ and decompose $A^T A = R^T R$ where R is upper triangular. Solve normal equations $(A^T A)^{-1} = (R^T R)^{-1} A^T b$

► QR decomposition: $A = QR$, solve $Rx = Q^T b$

$$QRx = b$$

► Singular Value Decomposition: $x_{LS} = V \Sigma^{-1} U^T b$

$$Rx = Q^T b$$

Direct methods have typically $O(nd^2)$ complexity

$$A^T A : O(nd^2)$$

► Indirect methods

► Gradient descent with momentum (Chebyshev iteration)

► Conjugate Gradient

we'll see + more

► Other iterative methods

Indirect methods have typically $O(\sqrt{\kappa} nd)$ complexity, where κ is the condition number $Ax : O(nd)$

$$\kappa = \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)}$$

Faster Least Squares Optimization: Random Projection

$$\mathbb{E} \left[\left(\bar{A}^T S^T S A \right) x \right] = \mathbb{E} \left[\bar{A}^T S^T b \right] \quad \text{approx. normal eq.}$$

$$\bar{A}^T A x = \bar{A}^T b \quad \text{if } S \sim \mathcal{O}(L)$$

► Left-sketching

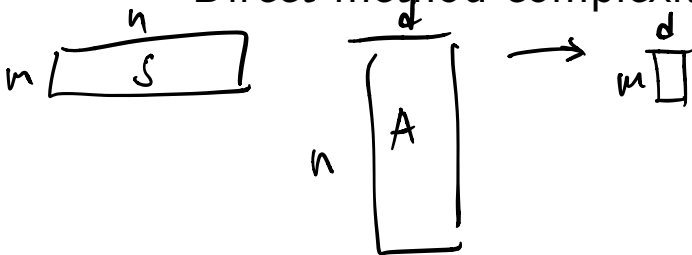
Form SA and Sb where $S \in \mathbb{R}^{m \times n}$ is a random projection matrix

► Solve the smaller problem

$$\min_{x \in \mathbb{R}^d} \|SAx - Sb\|_2^2$$

► using any classical method.

Direct method complexity md^2



Faster Least Squares Optimization: Random Projection

Right-sketching

$$\min_{y \in \mathbb{R}^m} \|A y - b\|_2^2$$

► Left-sketching

Form SA and Sb where $S \in \mathbb{R}^{m \times n}$ is a random projection matrix

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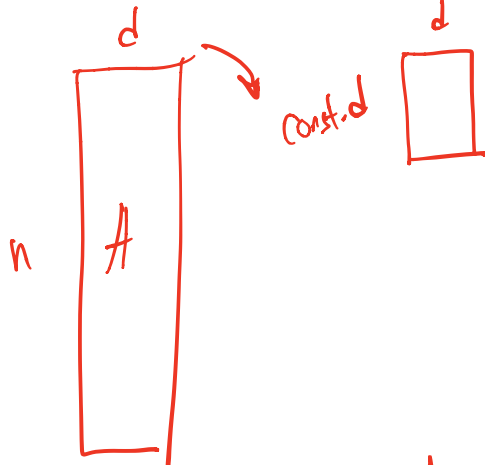
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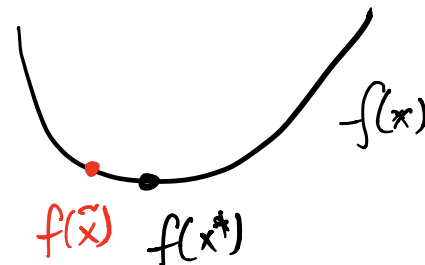
Approximation Result

ipd subGaussian
Count Sketch
Fast JL

► Let $S \in \mathbb{R}^{m \times d}$ be a Johnson-Lindenstrauss Embedding



$$x_{LS} = \arg \min_{x \in \mathbb{R}^d} \underbrace{\|Ax - b\|_2^2}_{f(x)}$$



$$\tilde{x} = \arg \min_{x \in \mathbb{R}^d} \|SAx - Sb\|_2^2$$

$\text{rank}(A) \leq d$

► If $m \geq \underbrace{\text{constant}}_1 \times \frac{\text{rank}(A)}{\epsilon^2}$ then,

► $f(x_{LS}) \leq f(\tilde{x}) \leq (1 + \epsilon^2)f(x_{LS})$

► $\|A(x_{LS} - \tilde{x})\|_2 \leq \epsilon$ with high probability

$> 1m$

$1 + \epsilon^2$

100

$$\begin{bmatrix} A_1 \\ \vdots \\ A_n \end{bmatrix} \begin{bmatrix} s_1 & \dots & s_B \end{bmatrix} \begin{bmatrix} A_1 \\ \vdots \\ A_n \end{bmatrix}$$

approximation $\sum s_i \cdot A_i$

$m = \frac{1}{0.01} \cdot \text{rank}(A) \Rightarrow 1.01$

Gaussian Sketch

- ▶ Let S be $\frac{1}{\sqrt{m}} \times$ i.i.d. Gaussian. $\mathbb{E}[S^T S] = I$

$$\tilde{x} = \arg \min_{x \in \mathbb{R}^d} \|SAx - Sb\|_2^2$$

- ▶ Is $\mathbb{E}[\tilde{x}]$ equal to x_{LS} ? Yes! $\mathbb{E} \tilde{x} = x_{LS}$

Questions?