CS 498ABD: Algorithms for Big Data

Fast Approximate Regression

Lecture 21 Nov 10, 2022

Linear least squares/Regression

Linear least squares: Given $A \in \mathbb{R}^{n \times d}$ and $b \in \mathbb{R}^{d}$ find x to minimize $||Ax - b||_2$.

Interesting when $n \gg d$ the over constrained case when there is no solution to Ax = b and want to find best fit.

Geometrically Ax is a linear combination of columns of A. Hence we are asking what is the vector z in the column space of A that is closest to vector b in ℓ_2 norm.

Closest vector to \boldsymbol{b} is the projection of \boldsymbol{b} into the column space of \boldsymbol{A} so it is "obvious" geometrically. How do we find it?

Linear least squares/Regression

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Closest vector to **b** is the projection of **b** into the column space of **A** so it is "obvious" geometrically. How do we find it? Find an orthonormal basis z_1, z_2, \ldots, z_r for the columns of **A**. Compute projection **c** as $\mathbf{c} = \sum_{j=1}^r \langle \mathbf{b}, \mathbf{z}_j \rangle \mathbf{z}_j$ and output answer as $||\mathbf{b} - \mathbf{c}||_2$.

Linear least square/Regression and SVD

Linear least squares: Given $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$ find x to minimize $||Ax - b||_2$.

Closest vector to **b** is the projection of **b** into the column space of **A** so it is "obvious" geometrically. Find an orthonormal basis z_1, z_2, \ldots, z_r for the columns of **A**. Compute projection **b'** as $b' = \sum_{i=1}^{r} \langle b, z_j \rangle z_j$ and output answer as $||b - b'||_2$.

Finding the basis is the expensive part. Recall SVD gives v_1, v_2, \ldots, v_r which form a basis for the *row* space of A but then $u_1^T, u_2^T, \ldots, u_m^T$ form a basis for the *column* space of A. Hence SVD gives us all the information to find b'. In fact we have

$$\min_{\mathbf{x}} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2 = \sum_{i=r+1}^m \langle u_i^T, \mathbf{b} \rangle^2$$

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Subspace Embedding

Question: Suppose we have linear subspace E of \mathbb{R}^n of dimension d. Can we find a projection $\Pi : \mathbb{R}^n \to \mathbb{R}^k$ such that for *every* $x \in E$, $\|\Pi x\|_2 = (1 \pm \epsilon) \|x\|_2$?

- Not possible if k < d.
- Possible if k = d. Pick Π to be an orthonormal basis for E.
 Disadvantage: This requires knowing E and computing orthonormal basis which is slow.

What we really want: *Oblivious* subspace embedding ala JL based on random projections

Oblivious Supspace Embedding

Theorem

Suppose **E** is a linear subspace of \mathbb{R}^n of dimension **d**. Let Π be a DJL matrix $\Pi \in \mathbb{R}^{k \times n}$ with $k = O(\frac{d}{\epsilon^2} \log(1/\delta))$ rows. Then with probability $(1 - \delta)$ for every $x \in E$,

$$\|rac{1}{\sqrt{k}} \Pi x\|_2 = (1\pm\epsilon) \|x\|_2.$$

In other words JL Lemma extends from one dimension to arbitrary number of dimensions in a graceful way.

Linear least squares via Subspace embeddings

Let a_1, a_2, \ldots, a_d be the columns of A and let E be the subspace spanned by $\{a_1, a_2, \ldots, a_d, b\}$

E has dimension at most d + 1.

Use subspace embedding on E. Applying JL matrix Π with $k = O(\frac{d}{\epsilon^2})$ rows we reduce a_1, a_2, \ldots, a_d, b to $a'_1, a'_2, \ldots, a'_d, b'$ which are vectors in \mathbb{R}^k .

Solve $\min_{x' \in \mathbb{R}^d} \| \mathbf{A}' \mathbf{x}' - \mathbf{b}' \|_2$

Faster Linear least squares via Subspace embeddings

Let a_1, a_2, \ldots, a_d be the columns of A and let E be the subspace spanned by $\{a_1, a_2, \ldots, a_d, b\}$

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Solve $\min_{x' \in \mathbb{R}^d} \| \mathbf{A}' x' - \mathbf{b}' \|_2$

Claim: Answer is a $(1 + O(\epsilon))$ -approximation to original problem if Π is a $(1 + \epsilon)$ -approximate subspace embedding.

Faster Linear least squares via Subspace embeddings

Apply subspace embedding Π to A, b to obtain A', b'

Solve $\min_{x' \in \mathbb{R}^d} \| \mathbf{A}' x' - \mathbf{b}' \|_2$

Claim: Answer is a $(1 + O(\epsilon))$ -approximation to original problem if Π is a $(1 + \epsilon)$ -approximate subspace embedding.

Advantage: Reduces **A** from $n \times d$ to $k \times d$ where $k = O(d/\epsilon^2)$. Use any fast approximate regression method on A', b' as a black box.

Disadvantage: Dependence of $1/\epsilon^2$ is high if one wants to choose small ϵ . In particular if **n** and **d** are large and comparable.

Accelerating Iterative Solvers via Sketching

- Iterative solvers that converge to solution are very common in numerical linear algebra. Each iteration is fast and goal is to reduce number of iterations
- Typically the number of iterations depends on how well-behaved the data is. An example is the *condition number* of the matrix.
- Iterative solvers can be sped up by *pre-conditioning* to make data well-behaved.

Goal: show that sketching techniques such as oblivious supspace embeddings can be viewed as preconditioning tools. Demonstrate on least squares regression.

Gradient Descent

Let $f : \mathbb{R}^d \to \mathbb{R}$ be a real-valued differentiable function. Recall $\nabla f(x)$ is the gradient of f at x which is a vector in \mathbb{R}^d with $(\nabla f(x))_i = \frac{\partial f}{\partial x_i}$. Gradient descent is a common search technique to find a local minimum/optimum of f in the unconstrained setting. A local optimum is a point x where $\nabla f(x) = 0$. When f is a convex function then any local optimum is a global optimum. There are many variants of gradient descent. Simplest one is based on having only access to the gradient and works with a fixed step size η .

GradientDescent (f, η) : Choose a good strating point $x^{(0)} \in \mathbb{R}$ For t = 1 to T to $x^{(t)} \leftarrow x^{(t-1)} - \eta \nabla f(x^{(t-1)})$ Output $x^{(T)}$

Gradient Descent

The choice of η (step size) is important for convergence and it depends on the smoothness of the function. If the gradient changes very rapidly it is difficult to find a local minimum since we may overshoot. An important parameter in the analysis is the smoothness which upper bounds the rate of change of the gradient.

Definition

f is L-smooth if $\|\nabla f(x) - \nabla f(y)\|_2 \le L \|x - y\|_2$ for all x, y.

One can show that GD converges if $\eta \leq 1/L$. Convergence is much faster if the function is in addition *strongly* convex.

Convex functions

Definition

A real-valued continuous function $f : \mathbb{R}^d \to \mathbb{R}$ is convex over a domain $D \subseteq \mathbb{R}^d$ if for all $x, y \in D$ and for all $\theta \in [0, 1]$, $f(\theta x + (1 - \theta)y) \leq \theta f(x) + (1 - \theta)f(y)$.

We will be interested in differentiable functions and twice-differentiable functions.

Fact: Differentiable function f is convex iff $f(x) \ge f(x_0) + (x - x_0)^T \nabla f(x_0)$ for all $x, x_0 \in D$.

f at any point x_0 lies above the tangent at point x_0 .

f is strictly convex if $f(x) > f(x_0) + (x - x_0)^T \nabla f(x_0)$ for all x, x_0 .

Convex functions

Suppose f is twice differentiable function. $H(x) = \nabla^2 f(x)$ is the Hessian of f at x. It is a $d \times d$ symmetric matrix where $H(x)_{i,j} = H(x)_{j,i} = \frac{\partial^2 f}{\partial x_i \partial x_j}$.

Fact: Twice-differentiable function f is convex iff $\nabla^2 f(x) \succeq 0$, that is, it is a positive semi-definite matrix. Alternatively, $y^T (\nabla^2 f(x)) y \ge 0$ for all y, x.

A real-symmetric matrix has all real eigen values and hence H(x) has real eigen-values for all twice-differentiable functions. When $H(x) \succeq 0$ (psd matrix) all the eigen-values are non-negative which means that the function's curvature is non-negative in all directions and hence bowl shaped (convex).

Strongly convex functions

Definition

A differentiable function f is strongly convex with parameter μ if $f(x) \ge f(x_0) + (\nabla f(x) - \nabla f(x_0))^T (x - x_0) + \frac{\mu}{2} ||x - x_0||_2^2$ for all $x, x_0 \in D$. Equivalently, $(\nabla f(x) - \nabla f(x_0))^T (x - x_0) \ge \mu ||x - x_0||_2^2$.

Fact: Twice differentiable f is strongly convex with parameter μ iff $\lambda_{\min}(H(x)) \ge \mu$ for all x where $\lambda_{\min}(H(x))$ is the smallest eigen-value of H(x).

Fact: f is strongly convex with parameter μ iff the function $g(x) = f(x) - \frac{\mu}{2} ||x||_2^2$ is convex.

Regression as convex optimization problem

Consider

$$f(\mathbf{x}) = \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2 = \mathbf{x}^{\mathsf{T}}\mathbf{A}^{\mathsf{T}}\mathbf{A}\mathbf{x} - 2\mathbf{x}^{\mathsf{T}}\mathbf{A}\mathbf{b} + \|\mathbf{b}\|_2^2$$

The gradient is easy to compute explicitly:

$$\nabla f(x) = 2A^T A x - 2Ab$$

One can see that the Hessian $\nabla^2 f(x) = 2A^T A$ and since $A^T A$ is psd it also shows that f is convex

Setting gradient to 0 one can see that the optimum solution value is $x^* = (A^T A)^{-1} A b$. Even though we have an explicit solution, iterative methods are preferred since maxtrix multiplication and computing the inverse are expensive.

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Smoothness of regression

Suppose $f(x) = ||Ax - b||_2^2 = x^T A^T A x - 2x^T A b + ||b||_2^2$. It is a convex function with gradient $\nabla f(x) = 2A^T A x - 2Ab$.

For x, y we have $\|\nabla f(x) - \nabla f(y)\|_2 = 2\|A^T A(x - y)\|_2$. It follows that

$$\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|_2 \le 2\sigma_1^2 \|\mathbf{x} - \mathbf{y}\|_2$$

where σ_1 is the top singular value of **A**.

Thus, for the regression problem, f is L-smooth where $L = 2\sigma_1^2$.

Condition number of a matrix

Suppose $f(x) = ||Ax - b||_2^2 = x^T A^T A x - 2x^T A b + ||b||_2^2$. It is a convex function with gradient $\nabla f(x) = 2A^T A x - 2Ab$.

Let $\sigma_{\max}(\mathbf{A}) = \sup_{\|\mathbf{x}\|_2=1} \|\mathbf{A}\mathbf{x}\|_2$ and let $\sigma_{\min}(\mathbf{A}) = \inf_{\|\mathbf{x}\|_2=1} \|\mathbf{A}\mathbf{x}\|_2$.

Definition

The condition number of **A**, denoted by $\kappa(\mathbf{A})$, is $\frac{\sigma_{\max}(\mathbf{A})}{\sigma_{\min}(\mathbf{A})}$.

Recall that $\lambda_{\min}(H(x))$ is the strong convexity parameter of f. For regression $2A^TA$ is the Hessian and hence $\lambda_{\min}(A^TA) = \sigma_{\min}^2$. Thus $\kappa(A) = L/\mu$ where L is the smoothness parameter and μ is the strong convexity parameter.

Gradient descent convergence when condition number is small

It is known that gradient descent converges very fast when L/μ is bounded. We state a lemma that captures this in a special case of regression while also making an additional assumption.

Lemma

Suppose all singular vectors of **A** are in the range $[1-1/\sqrt{2}, 1+1/\sqrt{2}]$. If we do gradient descent for regression with $\eta = 1/2$ then for all $t \ge 0$ we have

$$\|\mathbf{A}\mathbf{x}^{(t+1)} - \mathbf{A}\mathbf{x}^*\|_2 \le 2^{-t} \|\mathbf{A}\mathbf{x}^{(0)} - \mathbf{A}\mathbf{x}^*\|_2$$

In other words the error of the vector $\mathbf{x}^{(t)}$ after t steps goes down exponentially with t when compared to the initial error.

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Gradient descent convergence when condition number is small

The lemma in the previous slide is a special case of a more general theorem about convergence of gradient descent for strongly convex functions. For a direct proof of the stated lemma for regression in previous slide see Nelson's notes.

Lemma

Suppose f is an L-smooth and μ -strongly convex function. Gradient descent with $\eta \leq 1/L$ satisfies the property that

$$\|x^{(t)} - x^*\|_2^2 \le (1 - \alpha \mu)^t \|x^{(0)} - x^*\|_2^2.$$

Implication for Regression

Lemma shows that if condition number of A is small then gradient descent converges very fast. In particular if we have a good starting point $x^{(0)}$ such that $||Ax^{(0)} - b||_2 \le c ||Ax^* - b||$ for some constant c then gradient descent has the following property.

Lemma

After
$$\mathbf{t} = O(\log(\mathbf{c}/\epsilon))$$
 steps we have
 $\|\mathbf{A}\mathbf{x}^{(t)} - \mathbf{b}\|_2 \le (1+\epsilon)\|\mathbf{A}\mathbf{x}^* - \mathbf{b}\|.$

To see this we observe via triangle inequality and lemma,

 $\begin{aligned} \|Ax^{(t)} - b\|_2 &\leq \|Ax^{(t)} - Ax^*\|_2 + \|Ax^* - b\|_2 \leq 2^{-t} \|Ax^{(0)} - Ax^*\|_2 + \|Ax^* - b\|_2. \end{aligned}$ By triangle inequality

 $\|\mathbf{A}\mathbf{x}^{(0)} - \mathbf{A}\mathbf{x}^*\|_2 \le \|\mathbf{A}\mathbf{x}^{(0)} - \mathbf{b}\|_2 + \|\mathbf{A}\mathbf{x}^* - \mathbf{b}\|_2.$

Putting together

 $\|Ax^{(t)} - b\|_2 \le 2^{-t} \|Ax^{(0)} - b\|_2 + (1 + 2^{-t}) \|Ax^* - b\|_2 \le (1 + O(\epsilon)) \|Ax^* - b\|_2$

Oblivious Subspace Embeddings Again

Suppose we use α -approximate oblivious subspace embedding for the columns a_1, a_2, \ldots, a_d via a $k \times n$ sketch matrix Π . Thus we obtain $A' = \Pi A$. Previously we used $\alpha = (1 + \epsilon)$ and solved the regression problem $\min_{x' \in \mathbb{R}^d} ||A'x' - b'||_2$ where $b' = \Pi b$. This required k to be $\Theta(d/\epsilon^2)$. Now we instead use $\alpha = (1 + \epsilon_0)$ for some fixed constaint ϵ_0 (say 1/4).

Let $A' = \prod A = U' \Sigma' (V')^T$ where we compute SVD of A'. Note U' is an orthonormal basis for the columns of A'. Let $R = V' (\Sigma')^{-1}$.

Claim

The singular values of **AR** are in the range $[1 - \epsilon_0, 1 + \epsilon_0]$.

Oblivious Subspace Embeddings Again

Claim

The singular values of **AR** are in the range $[1 - \epsilon_0, 1 + \epsilon_0]$.

To see this consider any vector z:

 $\|z\|_2 = \|U'z\|_2 = \|\Pi ARz\|_2 = (1 \pm \epsilon_0) \|ARz\|_2.$

The first equality is from ortonormality of U', and second ineq is since Π is a $(1 + \epsilon_0)$ -approximate OBSE.

Claim

The column space of **A** and **AR** are the same since **V**' is orthonormal and Σ' is a diagonal matrix.

Thus solving $\min_{x} ||Ax - b||_{2}$ is same as solving $\min_{y} ||ARy - b||_{2}$. If y^{*} is solution to latter problem then $x^{*} = Ry^{*}$ is a solution to the original problem.

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Oblivious Subspace Embeddings Again

The previous two claims imply that gradient descent on AR will converge very fast since its condition number if small and moreover a solution to $\min_{y} ||ARy - b||_2$ allows us to recover a solution to the original regression problem with the same approximation quality.

Since Π is constant factor approximate OBSE, we can use the SVD $U'\Sigma'(V')^{\tau}$ of ΠA to obtain a constant factor approximate starting solution $x^{(0)}$ to start the gradient descent. This implies that the number of iterations required for an eventual $(1 + \epsilon)$ -approximation is $O(\log(1/\epsilon))$. Each iteration requires computing $ARx^{(t)}$.

Computing $ARx^{(t)}$ can be done in $O(d^2 + nnz(A))$ where nnz(A) is the number of non-zeroes in A.

Summarizing the algorithm

Input A, b where A is $n \times d$ matrix and $b \in \mathbb{R}^n$ with $n \geq d$

- Use $(1 + \epsilon_0)$ -approximate OBSE embedding $k \times n$ matrix Π with k = O(d) and compute $A' = \Pi A$ (use fast JL)
- Compute SVD $U'\Sigma'(V')^{T}$ of A' and let $R = V'(\Sigma')^{-1}$
- Use SVD to compute a good starting solution for $y^{(0)}$ for the problem min_y $||ARy b||_2$
- Use gradient descent for solving $\min_{y} ||ARy b||_2$ with starting solution $y^{(0)}$ and terminate in $t = O(\log(1/\epsilon))$ iterations
- Output $Ry^{(t)}$

We have reduced dependence on ϵ by using ϵ_0 approximate OBSE for some fixed ϵ_0 and then using gradient descent which has much better dependence on ϵ . For high accurate solutions this is an advantage.

Part I

Proof of GD Convergence for Strongly Convex Functions

Convergence of GD

Recall strong convexity implies that

$$f(y) \ge f(x) + (\nabla f(x))^T (y - x) + \frac{\mu}{2} ||y - x||_2^2$$

We need a very useful lemma.

Lemma

Suppose f is μ -strongly convex then it also satisfies the Polyak-Lojasiewicz condition that $\|\nabla f(x)\|_2^2 \ge 2\mu(f(x) - f(x^*)).$

Intuition: strongly convex means function is has a strong curvature. Thus, the farther x is from x^* (where gradient is 0) the larger the gradient.

Properties from smoothness

Lemma

Suppose **f** is **L**-smooth. Then

1
$$f(y) - f(x) - (\nabla f(x))^T (y - x) \le \frac{L}{2} ||x - y||_2^2$$

2 $f(x - \frac{1}{L} \nabla f(x)) - f(x) \le -\frac{1}{2L} ||\nabla f(x)||_2^2$

Corollary

Suppose f is L-smooth then $\|\nabla f(x)\|_2^2 \leq 2L(f(x) - f(x^*))$.

Follows from part (2) of Lemma since

$$f(x^*) - f(x) \le f(x - \frac{1}{L} \nabla f(x)) - f(x) \le -\frac{1}{2L} \|\nabla f(x)\|_2^2$$

Properties from smoothness

Suppose f is L-smooth. Then $f(y) - f(x) - (\nabla f(x))^T (y - x) \le \frac{L}{2} ||x - y||_2^2$.

Consider univariate function $g(\cdot)$ where $g(t) = f(x + t(y - x)) - (\nabla f(x))^T (x + t(y - x))$. Note that $g(0) = f(x) - (\nabla f(x))^T x$ and $g(1) = f(y) - (\nabla f(x))^T y$.

$$g(1) - g(0) = \int_0^1 g'(t) dt = \int_0^1 (\nabla f(x + t(y - x)) - \nabla f(x))^T (y - x) dt$$

$$\leq \int_0^1 \| (\nabla f(x + t(y - x)) - \nabla f(x)) \| \| (y - x) \| dt$$

$$\leq \int_0^1 Lt \| y - x \|^2 dt = \frac{L}{2} \| y - x \|^2.$$

We used smoothness to go from second to third line.

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Properties from smoothness

Second part: $f(x - \frac{1}{L}\nabla f(x)) - f(x) \le -\frac{1}{2L} \|\nabla f(x)\|_2^2$

Using first part with $\mathbf{y} = \mathbf{x} - \frac{1}{L} \nabla f(\mathbf{x})$,

$$f(x - \frac{1}{L}\nabla f(x)) - f(x) - (\nabla f(x))^{\mathsf{T}}(-\frac{1}{L}\nabla f(x)) \leq \frac{L}{2} \|\frac{1}{L}\nabla f(x)\|_2^2$$

Simplifying and rearranging terms gives the desired property.

Polyak-Lojasiewicz condition

We don't need this but it is a nice contrast to the previous lemma.

Lemma

Suppose f is μ -strongly convex then it also satisfies the Polyak-Lojasiewicz condition that $\|\nabla f(x)\|_2^2 \ge 2\mu(f(x) - f(x^*)).$

Applying strong convexity with $y = x^*$ and rearranging

$$\begin{aligned} f(x) - f(x^*) &\leq (\nabla f(x))^T (x - x^*) - \frac{\mu}{2} \|x - x^*\|_2^2 \\ &= \frac{1}{2\mu} \|\nabla f(x)\|_2^2 - \frac{1}{2} \|\sqrt{\mu} (x - x^*) - \frac{1}{\sqrt{\mu}} \nabla f(x)\|_2^2 \\ &\leq \frac{1}{2\mu} \|\nabla f(x)\|_2^2. \end{aligned}$$

Rearranging gives the desired claim.

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Proof of convergence of GD for strongly convex functions

Lemma

Suppose **f** is an **L**-smooth and μ -strongly convex function. Gradient descent with $\eta \leq 1/L$ satisfies the property that $\|x^{(t)} - x^*\|_2^2 \leq (1 - \alpha \mu)^t \|x^{(0)} - x^*\|_2^2$.

Suffices to prove the following

$$\|x^{(t+1)} - x^*\|_2^2 \le (1 - \alpha \mu) \|x^{(t)} - x^*\|_2^2$$

and apply it repeatedly.

Proof contd

$$\begin{aligned} \|x^{(t+1)} - x^*\|_2^2 &= \|x^{(t)} - \eta \nabla f(x^{(t)}) - x^*\|_2^2 \quad \text{from GD algorithm} \\ &= \|x^{(t)} - x^*\|_2^2 - 2\eta (\nabla f(x^{(t)}))^T (x^{(t)} - x^*) + \eta^2 \|\nabla f(x^{(t)})\|_2^2 \\ &\leq (1 - \alpha \mu) \|x^{(t)} - x^*\|_2^2 - 2\eta (f(x^{(t)}) - f(x^*)) + 2\eta^2 L \|\nabla f(x^{(t)})\|_2^2 \quad (\text{strong convexity ineq}) \\ &\leq (1 - \alpha \mu) \|x^{(t)} - x^*\|_2^2 - 2\eta (f(x^{(t)}) - f(x^*)) + 2\eta^2 L (f(x^{(t)}) - f(x^*)) \quad (\text{smoothness corollary}) \\ &\leq (1 - \alpha \mu) \|x^{(t)} - x^*\|_2^2 - 2\eta (1 - \eta L) (f(x^{(t)}) - f(x^*)) \\ &\leq (1 - \alpha \mu) \|x^{(t)} - x^*\|_2^2 \quad (\text{since } \eta \leq 1/L \text{ and } f(x^{(t)}) - f(x^*)) \end{aligned}$$