University of Wrocław: Algorithms for Big Data (Spring'22)

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Lecture 7: Regression, Low Rank Approximation

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1 Linear Regression

In a regression problem we have predictor variables a_1, \ldots, a_d and a measured variable b. In linear regression, we assume there is a relation $b \approx \sum_i a_i x_i$ for some $x_1, \ldots, x_d \in \mathbb{R}$.

We assume we received n batches $(a_{i,1}, \ldots, a_{i,d}, b_i), i = 1..n$. In the least square method we minimize the cost function

$$\sum_{i} (a_{i,1}x_1 + \dots a_{i,d}x_d - b_i)^2.$$

Formally:

Definition 1. On the input we have $A = \mathbb{R}^{n \times d}$ and $b \in \mathbb{R}^n$. Least square linear regression asks for $x \in \mathbb{R}^d$ so that

$$||Ax - b||_2$$

is minimized.

1.1 Exact solution

Assume b = Ax' + b' where b' is orthogonal to colsp(A) (column space of A) and Ax' is projection of b onto colsp(A). Then (by Pythagorean theorem)

$$||Ax - b||_2^2 = ||A(x - x') - b'||_2^2 = ||A(x - x')||_2^2 + ||b'||_2^2$$

which is minimized when x = x'. The condition of Ax' being projection is equivalent to

$$A^T(Ax'-b) = A^Tb' = 0$$

so equivalently we have a following condition

$$A^T A x' = A^T b. (1)$$

If $(A^T A)$ is invertible (its rank is d), we can simply compute

$$x' = (A^T A)^{-1} A^T b.$$

Definition 2. Let $A = U\Sigma V^T$ be SVD of A. Let Σ^{\dagger} be defined as diagonal matrix where $\Sigma_{i,i}^{\dagger} = \frac{1}{\Sigma_{i,i}}$ if $\Sigma_{i,i} \neq 0$ and 0 otherwise. We then call $A^{\dagger} = V\Sigma^{\dagger}U^T$ a pseudoinverse of A.

Theorem 3. $x' = A^{\dagger}b$ satisfies condition (1) and has minimal L_2 norm among all the solutions.

Proof. First part:

$$A^TAx' = A^TAA^{\dagger}b = (V\Sigma^TU^T)(U\Sigma V^T)(V\Sigma^{\dagger}U^T)b = V\Sigma^T\Sigma\Sigma^{\dagger}U^Tb = V\Sigma^TU^Tb = A^Tb$$

(note, $\Sigma^T \Sigma \Sigma^{\dagger} = \Sigma^T$ even though $\Sigma \Sigma^{\dagger} \neq I$ generally).

Second part: any solution is of the form

$$x'' = A^{\dagger}b + z$$

where $A^TAz = 0$, or equivalently $V\Sigma^T\Sigma V^Tz = 0$ or $\Sigma^T\Sigma V^Tz = 0$ (since V is orthonormal) or $\Sigma V^Tz = 0$ (since $\text{Ker}(\Sigma^T\Sigma) = \text{Ker}(\Sigma)$) or $V^Tz \in \text{Ker}(\Sigma)$ or $z \in V \cdot \text{Ker}(\Sigma)$.

We have $A \dagger b = V \Sigma^{\dagger} U^T b \in V \cdot \operatorname{Im}(\Sigma^{\dagger}) = V \cdot \operatorname{Im}(\Sigma)$.

Since $\operatorname{Ker}(\Sigma) \perp \operatorname{Im}(\Sigma^{\dagger})$, and since V is orthonormal, $V \cdot \operatorname{Ker}(\Sigma) \perp V \cdot \operatorname{Im}(\Sigma^{\dagger})$. So by the Pythagorean theorem,

$$||x''||_2^2 = ||A^{\dagger}b||_2^2 + ||z||_2^2 \ge ||A^{\dagger}b||_2^2$$

which proves optimality.

Downside: time to compute SVD is $\mathcal{O}(\min(n^2d, nd^2))$ which can be prohibitive.

1.2 Approximate solution

Instead of solving exact regression, we pick a projection $\Pi \in \mathbb{R}^{m \times n}$ and solve a problem of smaller dimensionality (m instead of n), where we have ΠA and Πb instead of A and b:

minimize
$$\|\Pi Ax - \Pi b\|_2$$

It is enough to use subspace embedding Π for space spanned on columns of A + single vector b. Thus we can pick oblivious subspace embedding for $m = \mathcal{O}(d/\varepsilon^2)$, and have

$$\forall_{x \in \mathbb{R}^d} ||Ax - b||_2 \le ||\Pi Ax - \Pi b||_2 \le (1 + \varepsilon) ||Ax - b||_2.$$

Thus minimizing projected problem provides $1 + \varepsilon$ approximation to original regression problem. Total computation time is $\mathcal{O}(mn + \min(m^2d, md^2)) = \mathcal{O}(nd/\varepsilon^2 + d^3/\varepsilon^2)$.

2 Low rank approximation

Consider input matrix $A \in \mathbb{R}^{n \times d}$. The goal of the low-rank approximation is the following: find B such that B has small rank and $B \approx A$.

Denote such $B = C \times D$, where $C \in \mathbb{R}^{n \times k}$ and $D \in \mathbb{R}^{k \times d}$. Motivation (assume k is small)

- B requires much less space to store: nk + kd vs nd.
- matrix-vector multiplication involving B is much faster: $B \cdot v$ takes $\mathcal{O}(nk + kd)$ time vs $\mathcal{O}(nd)$ time of $A \cdot v$.
- matrix-matrix multiplication: for $X \in \mathbb{R}^{d \times m}$, $B \cdot X$ takes $\mathcal{O}(kdm + nkm)$, vs $\mathcal{O}(ndm)$ time of $A \cdot X$
- ullet A might have low-rank natural structure but we measured it with noise. Then B is the denoising of A

2.1 Exact solution

We are looking at

$$\arg\min_{B:\operatorname{rank}(B)\leq k}\|A-B\|$$

and denote it as A_k , best rank-k approximation of A.

How to find such A_k ? Following theorem holds for both $\|\cdot\|_F$ and $\|\cdot\|_2$ norms.

Theorem 4 (Eckart-Young theorem). Consider SVD of $A = U\Sigma V^T$. Let Σ_k be Σ where only k largest in absolute value singular values are preserved, and every other value is zeroed.

$$A_k = U\Sigma_k V^T \tag{2}$$

Unfortunately the time is dominated by SVD computation $\mathcal{O}(\min(nd^2, n^2d))$.

2.2 Approximate solution - projection

Approximate low rank approximation: we are looking for rank-k A'_k such that:

$$||A'_k - A||_F = (1 \pm \varepsilon)||A_k - A||.$$

Obtaining good approximate solution is possible for this problem, using the same framework: we project our problem to smaller dimension and hope that solution in reduced dimension approximates good solution to original problem.

Specifically, we use projection matrix $S \in \mathbb{R}^{m \times n}$, for small m. So $m = \mathcal{O}(k/\varepsilon)$ (note, m is independent of dimensions of A, and depends on desired rank k).

First, we show that it is ok to limit ourselves to following:

Theorem 5.

$$\min_{Y: rank(Y) \le k} ||YSA - A||_F \le (1+\varepsilon)||A - A_k||_F$$

that is it is enough to limit ourselves to rank-k matrices in a row-space of SA.

Proof. Consider the regression problem:

$$\min_{X} \|A_k X - A\|_F$$

We have¹

$$||SA_kX - SA||_F = (1 \pm \varepsilon)||A_kX - A||_F.$$

Left side is minimized for $X = (SA_k)^{\dagger}SA$ (see exercises), while right side is always at least $||A_k - A||_F$ (since A_kX is rank at most k and A_k was the best approximation of A for rank-k), so

$$||SA_k(SA_k)^{\dagger}SA - SA||_F = (1 \pm \varepsilon)||A_k - A||_F$$

and since S is an affine embedding, we can skip S on the left side at the cost of an extra $1 \pm \varepsilon$ factor. Thus we see that it is enough to set $Y = A_k(SA_k)^{\dagger}$ to have proper guarantees, and such Y is of rank at most k.

¹we picked S dimension to have a property of affine embedding: an approximate norm preserving projection for matrices, proof of this fact is outside of scope of this lecture

We choose a second affine embedding $R \in \mathbb{R}^{n \times m}$, so that

$$||YSAR - AR||_F = (1 \pm \varepsilon)||YSA - A||_F.$$

And so we reduced our problem to a following form: find rank-k Y that minimizes

$$||YSAR - AR||_F$$

and output YSA (preferably in a factorized form).

We now observe that², by pythagorean theorem and properties of projections:

$$||YSAR - A||_F^2 = ||YSAR - A(SAR)^{\dagger}SAR||_F^2 + ||A(SAR)^{\dagger}SAR - A||_F^2$$

thus we need to find rank-k Y that minimizes

$$||YSAR - A(SAR)^{\dagger}SAR||_F$$

however if Y is rank $\leq k$, then so is YSAR, so it is enough to find rank-k Z that minimizes:

$$||Z - A(SAR)^{\dagger}SAR||_F$$

and (by the structure of optimization problem) have Z = YSAR guaranteed. Now we can apply Eckart-Young theorem to $A(SAR)^{\dagger}SAR$. It requires SVD, but the matrix we run it on is of dimension $n \times m$ so the cost is $nm^2 = n\frac{k^2}{\varepsilon^2}$. Thus we obtain Z = CD where $C \in \mathbb{R}^{n \times k}$ and $D \in \mathbb{R}^{k \times m}$, and we can output $Z(SAR)^{\dagger}SA = C(D(SAR)^{\dagger}SA)$ with factors being C and $D(SAR)^{\dagger}SA$. Relevant computations of SA, SAR and $(SAR)^{\dagger}$ are all tractable (in time $n\frac{k^2}{\varepsilon^2}$).

3 Sparse Fourier

Fourier transform: signal \rightarrow frequencies.

Definition 6. Assume $a=(a_0,\ldots,a_{n-1})$ is a signal. Let ω be n-th root of unity, that is $\omega=e^{-\frac{2\pi}{n}}$. Let F be such that $F_{ij}=\frac{1}{\sqrt{n}}\omega^{ij}$. Then $\hat{a}=Fa$ is a (Discrete) Fourier transform of a.

DFT can be computed in $\mathcal{O}(n \log n)$ time. However, for some applications this time can already be prohibitive. Consider a following scenario (of signal compression):

- Take input signal a and compute \hat{a} .
- Let \hat{a}_k be \hat{a} with only k largest magnitude elements kept (rest is zeroed).
- Output $a_k = F^{-1}\hat{a}_k$.

If we consider complexity measure of Fourier support $fs(a) = \|\hat{a}\|_0$ that is number of non-zero Fourier coefficients, then actually there is

$$a_k = \arg\min_{x: fs(x) < k} ||a - x||_2$$

(proof: exercise)

²to project b to subspace of Ax we need to set $x = A^{\dagger}b$, similarly to project to subspace xA we need to set $x = bA^{\dagger}$, and this generalizes to matrices, see exercise

If we assume that a comes from real-life scenarios (photos, audio recording), then it should have only few "strong" frequencies, rest is noise. Since a_k has much simpler representation (namely, \hat{a}_k which takes $\mathcal{O}(k \log n)$ bits), this is a lossy compression scheme.

How do we compute \hat{a}_k efficiently? (Assumption is that we have random access to a, otherwise just reading the input would dominate the computation time.)

Simpler question: can we recover \hat{a} if we know that $fs(a) = ||\hat{a}||_0 \le k$ (so there are only k non-zero frequencies)?