## Sketching as a Tool for Numerical Linear Algebra

# David WoodruffIBM Almaden

#### Massive data sets

#### Examples

- Internet traffic logs
- Financial data
- etc.

#### Algorithms

- Want nearly linear time or less
- Usually at the cost of a randomized approximation

#### Regression

 Statistical method to study dependencies between variables in the presence of noise.

#### Linear Regression

 Statistical method to study linear dependencies between variables in the presence of noise.

#### Linear Regression

 Statistical method to study linear dependencies between variables in the presence of noise.

#### Example

• Ohm's law  $V = R \cdot I$ 



#### **Example Regression**

#### Linear Regression

 Statistical method to study linear dependencies between variables in the presence of noise.

#### Example

- Ohm's law  $V = R \cdot I$
- Find linear function that best fits the data



#### Linear Regression

 Statistical method to study linear dependencies between variables in the presence of noise.

#### Standard Setting

- One measured variable b
- A set of predictor variables a1,..., ad
- Assumption:

$$b = x_0 + a_1 x_1 + ... + a_d x_d + \varepsilon$$

- ε is assumed to be noise and the x<sub>i</sub> are model parameters we want to learn
- Can assume  $x_0 = 0$
- Now consider n observations of b

#### Matrix form

**Input:** n×d-matrix A and a vector b=(b<sub>1</sub>,..., b<sub>n</sub>) n is the number of observations; d is the number of predictor variables

**Output:** x<sup>\*</sup> so that Ax\* and b are close

Consider the over-constrained case, when n À d

Can assume that A has full column rank

#### Least Squares Method

- Find x\* that minimizes  $|Ax-b|_2^2 = \Sigma (b_i \langle A_{i^*}, x \rangle)^2$
- A<sub>i\*</sub> is i-th row of A
- Certain desirable statistical properties

#### Method of least absolute deviation (I<sub>1</sub> -regression)

- Find x\* that minimizes  $|Ax-b|_1 = \Sigma |b_i \langle A_{i^*}, x \rangle|$
- Cost is less sensitive to outliers than least squares

#### Geometry of regression

- We want to find an x that minimizes |Ax-b|p
- The product Ax can be written as

$$A_{1}x_{1} + A_{2}x_{2} + ... + A_{d}x_{d}$$

where  $A_{*i}$  is the i-th column of A

- This is a linear d-dimensional subspace
- The problem is equivalent to computing the point of the column space of A nearest to b in Ip-norm

Solving least squares regression via the normal equations

- How to find the solution x to min<sub>x</sub> |Ax-b|<sub>2</sub>?
- Normal Equations:  $A^TAx = A^Tb$

• 
$$x = (A^T A)^{-1} A^T b$$

Solving I<sub>1</sub> -regression via linear programming

• Minimize  $(1,...,1) \cdot (\alpha_{+} + \alpha_{-})$ 

• Subject to:

$$A x + \alpha + - \alpha - = b$$
$$\alpha_{+}, \alpha - \geq 0$$

Generic linear programming gives poly(nd) time

### Talk Outline

Sketching to speed up Least Squares Regression

Sketching to speed up Least Absolute Deviation ( $I_1$ ) Regression

Sketching to speed up Low Rank Approximation

How to find an approximate solution x to  $min_x |Ax-b|_2$ ?

Goal: output x' for which  $|Ax'-b|_2 \cdot (1+\epsilon) \min_x |Ax-b|_2$  with high probability

Draw S from a k x n random family of matrices, for a value k << n

Compute S\*A and S\*b

Output the solution x' to  $min_{x'} |(SA)x-(Sb)|_2$ 

#### How to choose the right sketching matrix S?

Recall: output the solution x' to  $min_{x'} |(SA)x-(Sb)|_2$ 

Lots of matrices work

S is  $d/\epsilon^2 x$  n matrix of i.i.d. Normal random variables

Computing S\*A may be slow...



How to choose the right sketching matrix S? [S]

S is a Johnson Lindenstrauss Transform

 $S = P^*H^*D$ 

D is a diagonal matrix with +1, -1 on diagonals

H is the Hadamard transform

P just chooses a random (small) subset of rows of H\*D

S\*A can be computed much faster

Even faster sketching matrices [CW,MM,NN]

CountSketch matrix

Define k x n matrix S, for  $k = d^2/\epsilon^2$ 

S is really sparse: single randomly chosen non-zero entry per column



#### Talk Outline

Sketching to speed up Least Squares Regression

Sketching to speed up Least Absolute Deviation (I<sub>1</sub>) Regression

Sketching to speed up Low Rank Approximation

### Sketching to solve I<sub>1</sub>-regression

How to find an approximate solution x to  $min_x |Ax-b|_1$ ?

Goal: output x' for which  $|Ax'-b|_1 \cdot (1+\epsilon) \min_x |Ax-b|_1$  with high probability

Natural attempt: Draw S from a k x n random family of matrices, for a value k << n

Compute S\*A and S\*b

Output the solution x' to  $min_{x'} |(SA)x-(Sb)|_1$ 

Turns out this does not work!

### Sketching to solve I<sub>1</sub>-regression [SW]

Why doesn't outputting the solution x' to  $min_{x'}$  |(SA)x-(Sb)|<sub>1</sub> work?

Don't know of k x n matrices S with small k for which if x' is solution to  $min_x |(SA)x-(Sb)|_1$  then  $|Ax'-b|_1 \cdot (1+\epsilon) min_x |Ax-b|_1$  with high probability

Instead: can find an S so that  $|Ax^{\prime}-b|_{1} \cdot (d \log d) \min_{x} |Ax-b|_{1}$ 

S is a matrix of i.i.d. Cauchy random variables

### Cauchy random variables



They don't have a mean and have infinite variance

Ratio of two independent Normal random variables is Cauchy

### Sketching to solve I<sub>1</sub>-regression

How to find an approximate solution x to  $min_x |Ax-b|_1$ ?

Want x' for which if x' is solution to  $min_x |(SA)x-(Sb)|_1$ , then  $|Ax'-b|_1 \cdot (1+\epsilon) min_x |Ax-b|_1$  with high probability

For d log d x n matrix S of Cauchy random variables:  $|Ax^{-b}|_{1} \cdot (d \log d) \min_{x} |Ax-b|_{1}$ 

For this "poor" solution x', let b' = Ax'-b

Might as well solve regression problem with A and b'

### Sketching to solve I<sub>1</sub>-regression

Main Idea: Compute a QR-factorization of S\*A

Q has orthonormal columns and  $Q^*R = S^*A$ 

A\*R<sup>-1</sup> turns out to be a "well-conditioning" of original matrix A

Compute  $A^*R^{-1}$  and sample  $d^{3.5}/\epsilon^2$  rows of  $[A^*R^{-1}, b^2]$  where the i-th row is sampled proportional to its 1-norm

Solve regression problem on the (reweighted) samples

### Sketching to solve I<sub>1</sub>-regression [MM]

Most expensive operation is computing S\*A where S is the matrix of i.i.d. Cauchy random variables

All other operations are in the "smaller space"

Can speed this up by choosing S as follows:



### Further sketching improvements [WZ]

Can show you need a fewer number of sampled rows in later steps if instead choose S as follows

Instead of diagonal of Cauchy random variables, choose diagonal of reciprocals of exponential random variables



#### Talk Outline

Sketching to speed up Least Squares Regression

Sketching to speed up Least Absolute Deviation ( $I_1$ ) Regression

Sketching to speed up Low Rank Approximation

A is an n x n matrix

Typically well-approximated by low rank matrix E.g., only high rank because of noise

Want to output a rank k matrix A', so that  $|A-A'|_{F} \cdot (1+\epsilon) |A-A_k|_{F}$ , w.h.p., where  $A_k = \operatorname{argmin}_{rank \ k \ matrices \ B} |A-B|_{F}$ 

For matrix C,  $|C|_{F} = (\Sigma_{i,j} C_{i,j}^{2})^{1/2}$ 

#### Solution to low-rank approximation is

- Given n x n input matrix A Most time-consuming
- Compute S\*A using a sketching matrix S with k << n step is computing S\*A rows. S\*A takes random line a computing of fows A

A S can be matrix of i.i.d. Normals S can be a Fast Johnson Lindenstrauss Matrix S can be a CountSketch matrix SA Project rows of A onto SA approximation to points inside of SA. Caveat: projecting the points onto SA is slow [CW]

Current algorithm:

- 1. Compute S\*A (easy)
- 2. Project each of the rows onto S\*A
- 3. Find best rank-k approximation of projected points inside of rowspace of S\*A (easy)

Bottleneck is step 2

Turns out if you compute (AR)(S\*A\*R)<sup>-</sup>(SA), this is a good low-rank approximation

Uses generalized regression:  $min_X |X(SA)-A|_{F^2}$ 

#### Conclusion

Gave fast sketching-based algorithms for numerical linear algebra problems

Least Squares Regression

Least Absolute Deviation (I1) Regression

Low Rank Approximation

Sketching also provides "dimensionality reduction"

Communication-efficient solutions for these problems