Matrix Sketching as a Tool in Numerical Algebra

Chengtao Li

Massachusetts Institute of Technology ctli@mit.edu

December 1, 2015

Overview

- Introduction
 - Motivating Example
 - General Pattern
 - Sketching Matrices
- 2 Column Subset Selection Problem
- 3 CUR decomposition
- 4 Spectral Sparsification
- Remarks



Linear Regression

• Have: $A \in \mathbb{R}^{n \times d}$, $b \in R^n$.

• Want: Find $x \in \mathbb{R}^d$ s.t. Ax and b as close as possible

Linear Regression

- Have: $A \in \mathbb{R}^{n \times d}$, $b \in R^n$.
- Want: Find $x \in \mathbb{R}^d$ s.t. Ax and b as close as possible
- Objective: $\min_{x} ||Ax b||_{p}$

Linear Regression cont.

- For p = 2, minimize Euclidean distances btw Ax and b.
- Solution: $(A^{\top}A)x^* = A^{\top}b$.

Linear Regression cont.

- For p = 2, minimize Euclidean distances btw Ax and b.
- Solution: $(A^{\top}A)x^* = A^{\top}b$.
- Problem: Overly constrained, Massive datasets at least $O(nd^2)$

To Circumvent

- Use *Sketching Techniques* to improve upon the time complexities.
- Relaxation: find x s.t. $||Ax b||_p \le (1 + \varepsilon)||Ax^* b||_p$

Other Examples

- Matrix Low-rank Approximation
- Matrix Product Approximation
- Kernel Methods
- Social Networks

Matrix Sketching Framework

- Specify $r \ll n$
- ② Sample a random matrix $S \in \mathbb{R}^{r \times n}$
- Solve the problem with the sketched matrices.

Matrix Sketching Framework

- **①** Specify $r \ll n$
- ② Sample a random matrix $S \in \mathbb{R}^{r \times n}$
- 3 Solve the problem with the sketched matrices.

In linear regression, the sketched regression problem becomes

$$\min_{x} \|(SA)x - (Sb)\|_2 \tag{1.1}$$

• How to choose $r \ll n$?

- How to choose $r \ll n$?
- From what distribution should we sample S?

- How to choose $r \ll n$?
- From what distribution should we sample S?
- Approximation bounds?

- How to choose $r \ll n$?
- **②** From what distribution should we sample *S*?
- Approximation bounds?
- Efficiency?

- How to choose $r \ll n$?
- From what distribution should we sample S?
- Approximation bounds?
- Efficiency?
- Optional) Optimality?

Different forms of Sketching Matrix S:

- Projection Matrix (JL-style)
- Selection Matrix (Our focus)

Different forms of Sketching Matrix S:

- Projection Matrix (JL-style)
- Selection Matrix (Our focus)
- Why Selection?
 - Interpretability
 - Preserves Sparsity/Structure

 Given a matrix A, select a small number of columns from A so that the selected columns serve as a good "snapshot" or "summarization" of A.

- Given a matrix A, select a small number of columns from A so that the selected columns serve as a good "snapshot" or "summarization" of A.
- Writing in math language: Let $A \in \mathbb{R}^{n \times m}$ be a huge matrix, sample |C| = c columns of A so as to approximate A as $A_C A_C^{\dagger} A$.

- Given a matrix A, select a small number of columns from A so that the selected columns serve as a good "snapshot" or "summarization" of A.
- Writing in math language: Let $A \in \mathbb{R}^{n \times m}$ be a huge matrix, sample |C| = c columns of A so as to approximate A as $A_C A_C^{\dagger} A$.
- Intuition

Objective

The objective function is to choose columns $C \subseteq [m]$ to minimize matrix norm:

$$\min_{C \subseteq [m]} \|A - A_C A_C^{\dagger} A\|_{\xi} \tag{2.1}$$

where ξ ∈ {2, F, *}.

Types of Error Bounds:

Additive Bounds:

$$||A - A_C A_C^{\dagger} A||_{\xi} \le ||A - A_k||_{\xi} + \varepsilon ||A||_{\xi}$$
 (2.2)

Types of Error Bounds:

• Additive Bounds:

$$||A - A_C A_C^{\dagger} A||_{\xi} \le ||A - A_k||_{\xi} + \varepsilon ||A||_{\xi}$$
 (2.2)

Relative Bounds:

$$||A - A_C A_C^{\dagger} A||_{\xi} \le (1 + \varepsilon)||A - A_k||_{\xi}$$
 (2.3)

Types of Error Bounds:

Additive Bounds:

$$||A - A_C A_C^{\dagger} A||_{\xi} \le ||A - A_k||_{\xi} + \varepsilon ||A||_{\xi}$$
 (2.2)

Relative Bounds:

$$||A - A_C A_C^{\dagger} A||_{\xi} \le (1 + \varepsilon)||A - A_k||_{\xi}$$
 (2.3)

Required to hold either in expectation or with high probability.

Optimal Column Selection (Guruswami & Sinop'12)

• Lower bounds: there exists a matrix M for which the best error achieved by a low rank matrix, whose columns are restricted to belong to the span of $r \geq k/\varepsilon$ columns of M, is at least $1 + \varepsilon - o(1)$ times the best rank-k approximation

Optimal Column Selection (Guruswami & Sinop'12)

- Lower bounds: there exists a matrix M for which the best error achieved by a low rank matrix, whose columns are restricted to belong to the span of $r \geq k/\varepsilon$ columns of M, is at least $1 + \varepsilon o(1)$ times the best rank-k approximation
- Optimal Result: $k/\varepsilon + k 1$ columns is sufficient for achieving $(1+\varepsilon)$ bound (match the lower bound up to lower order terms).

Volume Sampling on A

- Ground set G = [n]
- Select $S \subseteq G$ where |S| = k:

$$\Pr(S \subseteq G) \propto det(A_S A_S^{\top})$$
 (2.4)

Algorithm:

- **1** Sample S where |S| = c according to volume sampling
- 2 Approximate A by $A_S A_S^{\dagger} A$

Algorithm:

- **1** Sample S where |S| = c according to volume sampling
- 2 Approximate A by $A_S A_S^{\dagger} A$

Optimality:

• For $c \geq k$, we have

$$E_S[\|A - A_S A_S^{\dagger} A\|_F^2] \le \frac{c+1}{c+1-k} \|A - A_k\|_F^2$$
 (2.5)

Practical Issues:

Practical Issues:

• Running Time: $O(cm^2n)$

Practical Issues:

- Running Time: $O(cm^2n)$;
- Derandomization

Practical Issues:

- Running Time: $O(cm^2n)$;
- Derandomization

Another notable method:

Near-Optimal Column Selection (Boutsidis et.al.), selects $2k\varepsilon^{-1}(1+o(1))$ columns for reconstruction, runs in $O(mnk+nk^2)/\varepsilon^{2/3}$

- Given a matrix A, select a small number of columns and rows from A so that selected columns and rows serve as a good "snapshot" or "summarization" of A.
- Writing in math language: Let $A \in \mathbb{R}^{n \times m}$ sample |C| = c columns and |R| = r rows and calculate U so that we approximate A with $A_C U A^R$.
- Intuition

Objective

The objective is to choose columns $C \subseteq [m]$, $R \subseteq [n]$ and $U \in \mathbb{R}^{c \times r}$ so as to minimize matrix norm:

$$\min_{C,U,R} \|A - A_C U A^R\|_{\xi} \tag{3.1}$$

where ξ ∈ {2, F, *}.

Observation: Fixing C and R, and for $\xi = F$, have

$$\arg\min_{U} \|A - A_C U A^R\| = A_C^{\dagger} A (A^R)^{\dagger}$$
 (3.2)

Thus, usually the objective becomes:

$$\min_{C,R} \|A - A_C A_C^{\dagger} A (A^R)^{\dagger} A^R \|_F \tag{3.3}$$

Adaptive Sampling:

Given matrix $A \in \mathbb{R}^{n \times m}$ and let A_C be already selected columns of A. Define the residual $B = A - A_C A_C^{\dagger} A$. The adaptive sampling is to sample from distribution defined as

$$p_i = \|b_i\|_2^2 / \|B\|_F^2 \tag{3.4}$$

Theorem 5 (The Adaptive Sampling Algorithm) Given a matrix $\mathbf{A} \in \mathbb{R}^{m \times n}$ and a matrix $\mathbf{C} \in \mathbb{R}^{m \times c}$ such that $\operatorname{rank}(\mathbf{C}) = \operatorname{rank}(\mathbf{C}\mathbf{C}^{\dagger}\mathbf{A}) = \rho \ (\rho \le c \le n)$. We let $\mathbf{R}_1 \in \mathbb{R}^{r_1 \times n}$ consist of r_1 rows of \mathbf{A} , and define the residual $\mathbf{B} = \mathbf{A} - \mathbf{A}\mathbf{R}_1^{\dagger}\mathbf{R}_1$. Additionally, for $i = 1, \dots, m$, we define

$$p_i = \|\mathbf{b}^{(i)}\|_2^2 / \|\mathbf{B}\|_F^2.$$

We further sample r_2 rows i.i.d. from \mathbf{A} , in each trial of which the i-th row is chosen with probability p_i . Let $\mathbf{R}_2 \in \mathbb{R}^{r_2 \times n}$ contain the r_2 sampled rows and let $\mathbf{R} = [\mathbf{R}_1^T, \mathbf{R}_2^T]^T \in \mathbb{R}^{(r_1 + r_2) \times n}$. Then we have

$$\mathbb{E}\|\mathbf{A} - \mathbf{C}\mathbf{C}^{\dagger}\mathbf{A}\mathbf{R}^{\dagger}\mathbf{R}\|_{F}^{2} \leq \|\mathbf{A} - \mathbf{C}\mathbf{C}^{\dagger}\mathbf{A}\|_{F}^{2} + \frac{\rho}{r_{2}}\|\mathbf{A} - \mathbf{A}\mathbf{R}_{1}^{\dagger}\mathbf{R}_{1}\|_{F}^{2},$$

where the expectation is taken w.r.t. \mathbf{R}_2 .



A general framework

- Select $c \geq C(k, \varepsilon)$ columns (A_C) of A and $r_1 = c$ rows (A^{R_1}) with some CSSP method
- Select $r_2 = c/\varepsilon$ additional rows (A^{R_2}) with adaptive sampling with respect to $A A A(A^{R_1})^{\dagger}A^{R_1}$
- Let $R = R_1 \cup R_2$, construct $U = (A_C)^{\dagger} A (A_R)^{\dagger}$

Plug in and Play!

Plug in and Play!

- Plug in near-optimal CSSP
 - $c = \frac{2k}{\epsilon}(1 + o(1))$ columns
 - $r = \frac{c}{\varepsilon}(1+\varepsilon)$ rows
 - Running time:

$$O((m+n)k^3\varepsilon^{-2/3}+mk^2\varepsilon^{-2}+nk^2\varepsilon^{-4})+T_M(mnk/\varepsilon).$$

Plug in and Play!

- Plug in near-optimal CSSP
 - $c = \frac{2k}{\epsilon}(1 + o(1))$ columns
 - $r = \frac{c}{\varepsilon}(1+\varepsilon)$ rows
 - Running time:

$$O((m+n)k^3\varepsilon^{-2/3}+mk^2\varepsilon^{-2}+nk^2\varepsilon^{-4})+T_M(mnk/\varepsilon).$$

- Plug in optimal CSSP:
 - $c = k\varepsilon^{-1}(1 + o(1))$ columns
 - $r = c\varepsilon^{-1}(1+\varepsilon)$ rows

Problem

Let $A \in \mathbb{R}^{n \times m}$, we want to sample a set of re-weighted columns of A (with selection rescaled matrix S such that the spectrum of AS is similar to that of A. Specifically, we want

$$(1 - \varepsilon)AA^{\top} \leq AS(AS)^{\top} \leq (1 + \varepsilon)AA^{\top}$$
 (4.1)

Sampling with Statistical Leverage Score

• Statistical leverage score for the i-th column A_i is

$$p_i = A_i^{\top} (AA^{\top})^{\dagger} A_i \tag{4.2}$$

Sampling with Statistical Leverage Score

• Statistical leverage score for the i-th column A_i is

$$p_i = A_i^{\top} (AA^{\top})^{\dagger} A_i \tag{4.2}$$

• Theorem (Spielman & Srivastava): If we independently sample $O(n\varepsilon^{-2}\log n)$ columns of A with probability proportional to p_i and rescale with $1/p_i$, with probability 1-1/n we have

$$(1 - \varepsilon)AA^{\top} \leq AS(AS)^{\top} \leq (1 + \varepsilon)AA^{\top}$$
 (4.3)

Sampling with Statistical Leverage Score

• Statistical leverage score for the i-th column A_i is

$$p_i = A_i^{\top} (AA^{\top})^{\dagger} A_i \tag{4.2}$$

• Theorem (Spielman & Srivastava): If we independently sample $O(n\varepsilon^{-2}\log n)$ columns of A with probability proportional to p_i and rescale with $1/p_i$, with probability 1-1/n we have

$$(1 - \varepsilon)AA^{\top} \leq AS(AS)^{\top} \leq (1 + \varepsilon)AA^{\top}$$
 (4.3)

• Running time: $\tilde{O}(m(\log n)\varepsilon^{-2})$.



Remarks: Optimality

- Optimal CSSP: $O(\frac{k}{\varepsilon})$ columns
- \bullet Optimal CUR: $O(\frac{k}{\varepsilon})$ columns and $O(\frac{k}{\varepsilon})$ rows
- Optimal Spectral Sparsification: $O(\frac{k}{\varepsilon^2})$ columns

Introduction Column Subset Selection Problem CUR decomposition Spectral Sparsification Remarks

Thanks! Questions?