# Matrix Approximations - II

Sanjiv Kumar, Google Research, NY EECS-6898, Columbia University - Fall, 2010

### Sampling Based Methods

#### So Far...

- Methods that primarily depend on matrix-vector products
- Not suitable when input matrix is large and dense
  - Kernel Matrix  $n = 20M \Rightarrow 1600 \text{ TB}$  200,000, 8GB machines!!
- Matrices may be so big that storage becomes a big problem
- One may want to reduce the computational cost significantly

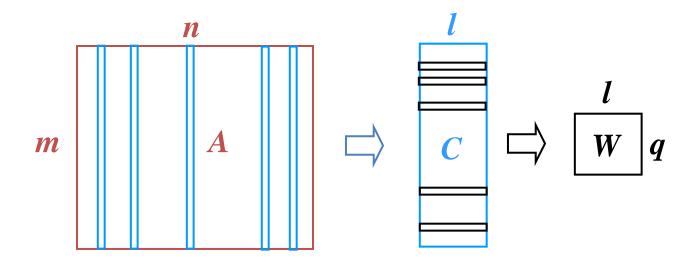
#### Sampling-Based Methods

- Sample a few columns or rows or both according to some distribution (without replacement in practice)
- Approximate the desired quantity by manipulating just the sampled vectors
  - No need to even create the entire matrix !!
- If done carefully, the error in approximation can be bounded

Can approximate multiplication, low-rank matrix, singular values, singular vectors

### Sampling Based Methods

#### Sample *l* columns/rows randomly



#### Main Issues

- How to sample columns and rows?
  - Uniformly?
  - From a fixed non-uniform distribution e.g., column/row norm?
  - From adaptive distribution: distribution changes after picking a sample subset
- What is the algorithm and how much error are we making?

### Overview

- 1. Approximate Matrix Multiplication
  - Sample columns of one matrix and rows from the other
- 2. Column-sampling methods for spectral decomposition
  - Methods that use decomposition of entire sampled columns
  - Methods that further sample the rows from the sampled columns
- 3. Low-rank approximation
  - Spectral reconstructions  $A_k = U_k \sum_k V_k^T$
  - Matrix Projection  $A_k = U_k U_k^T A$
- 4. Sampling Techniques
- 5. Ensemble Methods
  - How to combine multiple approximations to yield more accurate one

EECS6898 - Large Scale Machine Learning

We want to approximate

$$AB \approx CR$$

$$m \times n \ n \times p \ m \times l \ l \times p \qquad l << n$$

#### We want to approximate

$$AB \approx CR$$

$$m \times n \ n \times p \ m \times l \ l \times p \qquad l << n$$

#### Basic Idea

- 1. Sample *l* columns from *A* and form a submatrix *C*
- 2. Pick the corresponding rows from *B* and form a submatrix *R*

EECS6898 - Large Scale Machine Learning

- 3. Scale the submatrices appropriately
- 4. Output the multiplication of two scaled submatrices

#### We want to approximate

$$AB \approx CR$$

$$m \times n \ n \times p \ m \times l \ l \times p \qquad l << n$$

#### Algorithm

Given 
$$A, B, 1 \le l \le n, \{p_i\}_{i=1}^n$$
 s.t.  $\sum_i p_i = 1, p_i \ge 0$ 

fixed non-uniform distribution

#### We want to approximate

$$AB \approx CR$$

$$m \times n \ n \times p \ m \times l \ l \times p \qquad l << n$$

#### Algorithm

Sanjiv Kumar

Given 
$$A, B, 1 \le l \le n, \{p_i\}_{i=1}^n$$
 s.t.  $\sum_i p_i = 1, p_i \ge 0$ 

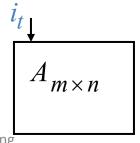
fixed non-uniform distribution

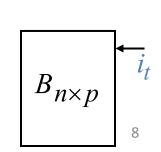
For 
$$t = 1,...,l$$

- Pick  $i_t \in \{1,...,n\}$  with  $P(i_t = k) = p_k$  independently, with replacement

- Set 
$$C^{(t)} = A^{(i_t)} / \sqrt{l p_{i_t}}$$
  $R_{(t)} = B_{(i_t)} / \sqrt{l p_{i_t}}$  row

Return C, R





in practice, without

replacement!

Standard proof strategy (based on concentration of measures)

#### Show

$$E[\|AB - CR\|_F^2] = \sum_{i=1}^n \sum_{j=1}^p E[(AB - CR)_{ij}^2] = \text{small quantity}$$

$$Var[\|AB - CR\|_F^2]$$
 is small for right choice of  $p_k$ 

We want to approximate  $AB = \sum_{t=1}^{n} A^{(t)} B_{(t)}$ 

$$CR = \sum_{t=1}^{l} C^{(t)} R_{(t)} = \sum_{t=1}^{l} \frac{1}{(l p_{i_t})} A^{(i_t)} B_{(i_t)}$$

Why is it a good approximation?

We want to approximate 
$$AB = \sum_{t=1}^{n} A^{(t)} B_{(t)}$$

$$CR = \sum_{t=1}^{l} C^{(t)} R_{(t)} = \sum_{t=1}^{l} \frac{1}{(l p_{i_t})} A^{(i_t)} B_{(i_t)}$$

EECS6898 – Large Scale Machine Learning

Why is it a good approximation?

Expectation 
$$E[(CR)_{ij}] = (AB)_{ij}$$

Variance 
$$Var[(CR)_{ij}] = \frac{1}{l} \sum_{k=1}^{n} \frac{A_{ik}^{2} B_{kj}^{2}}{p_{k}} - \frac{1}{l} (AB)_{ij}^{2}$$

We want to approximate  $AB = \sum_{t=1}^{n} A^{(t)} B_{(t)}$ 

$$CR = \sum_{t=1}^{l} C^{(t)} R_{(t)} = \sum_{t=1}^{l} \frac{1}{(l p_{i_t})} A^{(i_t)} B_{(i_t)}$$

Why is it a good approximation?

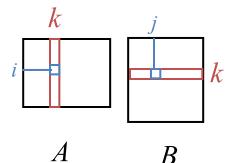
Expectation 
$$E[(CR)_{ij}] = (AB)_{ij}$$

Variance 
$$Var[(CR)_{ij}] = \frac{1}{l} \sum_{k=1}^{n} \frac{A_{ik}^{2} B_{kj}^{2}}{p_{k}} - \frac{1}{l} (AB)_{ij}^{2}$$

Variance 
$$Var[(CR)_{ij}] = \frac{1}{l} \sum_{k=1}^{n} \frac{A_{ik}^{2} B_{kj}^{2}}{p_{k}} - \frac{1}{l} (AB)_{ij}^{2}$$
Proof: Let 
$$X_{t} = \left(\frac{A^{(i_{t})} B_{(i_{t})}}{(l p_{i_{t}})}\right)_{ij}$$

$$E[X_{t}] = \sum_{k=1}^{n} p_{k} \frac{A_{ik} B_{kj}}{(l p_{k})} = \frac{1}{l} (AB)_{ij}$$

$$E[X_{t}^{2}] = \sum_{k=1}^{n} \frac{A_{ik}^{2} B_{kj}^{2}}{(l^{2} p_{k})}$$



We want to approximate 
$$AB = \sum_{t=1}^{n} A^{(t)} B_{(t)}$$

$$CR = \sum_{t=1}^{l} C^{(t)} R_{(t)} = \sum_{t=1}^{l} \frac{1}{(l p_{i_t})} A^{(i_t)} B_{(i_t)}$$

Why is it a good approximation? 
$$E[(CR)_{ij}] = (AB)_{ij}$$
 Variance 
$$Var[(CR)_{ij}] = \frac{1}{l} \sum_{k=1}^{n} \frac{A_{ik}^2 B_{kj}^2}{p_k} - \frac{1}{l} (AB)_{ij}^2$$
 Proof: Let 
$$X_t = \left(\frac{A^{(i_t)} B_{(i_t)}}{(l p_{i_t})}\right)_{ij} E[X_t] = \sum_{k=1}^{n} p_k \frac{A_{ik} B_{kj}}{(l p_k)} = \frac{1}{l} (AB)_{ij}$$
 Next, get 
$$E[X_t^2] = \sum_{k=1}^{n} \frac{A_{ik}^2 B_{kj}^2}{(l^2 p_k)}$$
 Var( $X_t$ ) =  $E[X_t^2] - E[X_t]^2$  Sanjiv Kumar 9/27/2010 EECS6898 - Large Scale Machine Learning 13

#### We want to find

$$E[\|AB - CR\|_F^2] = \sum_{i=1}^n \sum_{j=1}^p E[(AB - CR)_{ij}^2]$$

EECS6898 - Large Scale Machine Learning

EECS6898 - Large Scale Machine Learning

#### We want to find

$$E[\|AB - CR\|_{F}^{2}] = \sum_{i=1}^{n} \sum_{j=1}^{p} E[(AB - CR)_{ij}^{2}]$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{p} Var[(CR)_{ij}]$$

$$Var[(CR)_{ij}] = \frac{1}{l} \sum_{k=1}^{n} \frac{A_{ik}^{2} B_{kj}^{2}}{p_{k}} - \frac{1}{l} (AB)_{ij}^{2}$$

$$= \frac{1}{l} \sum_{k=1}^{n} \frac{1}{p_{k}} |A^{(k)}|^{2} |B_{(k)}|^{2} - \frac{1}{l} |AB|_{F}^{2}$$

#### We want to find

$$E[\|AB - CR\|_{F}^{2}] = \sum_{i=1}^{n} \sum_{j=1}^{p} E[(AB - CR)_{ij}^{2}]$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{p} Var[(CR)_{ij}]$$

$$Var[(CR)_{ij}] = \frac{1}{l} \sum_{k=1}^{n} \frac{A_{ik}^{2} B_{kj}^{2}}{p_{k}} - \frac{1}{l} (AB)_{ij}^{2}$$

$$= \frac{1}{l} \sum_{k=1}^{n} \frac{1}{p_{k}} |A^{(k)}|^{2} |B_{(k)}|^{2} - \frac{1}{l} |AB|_{F}^{2}$$

Find  $p_k$  that minimizes above  $p_k = \left|A^{(k)}\right| B_{(k)} \left|\sum_{k'=1}^n \left|A^{(k)}\right| B_{(k)}\right|$ 

with positivity and unit sum constraints

$$\frac{1}{l} \frac{\|B(k)\|}{\|B(k)\|} \frac{\|B(k)\|}{\|B(k)\|} = \frac{1}{l} \left( \sum_{k=1}^{n} |A^{(k)}\| B_{(k)} \right)^{2} - \frac{1}{l} \|AB\|_{F}^{2} \\
\leq \frac{1}{l} \|A\|_{F}^{2} \|B\|_{F}^{2}$$

### Theoretical Guarantee

Given 
$$A$$
,  $B$ ,  $1 \le l \le n$ ,  $\{p_i\}_{i=1}^n$  s.t.  $\sum_i p_i = 1$ ,  $p_i \ge 0$  and  $\beta \le 1$  if  $p_k \ge \beta \left|A^{(k)}\right| B_{(k)} \left| \sum_{k'=1}^n \left|A^{(k)}\right| B_{(k)} \right|$ 

then 
$$E[\|AB - CR\|_F^2] \le (1/\beta l) \|A\|_F^2 \|B\|_F^2$$

Let  $\delta \in (0,1)$  and  $\eta = 1 + \sqrt{(8/\beta)\log(1/\delta)}$ , then with probability at least  $1-\delta$ 

$$||AB - CR||_F^2 \le (\eta^2 / \beta l) ||A||_F^2 ||B||_F^2$$

Proof based on showing that changing one column/row does not change the product CR by much, and then applying concentration of measures: either Doob Martingale or Mcdiarmid's inequality

### Implementation Details

How to sample?

Uniform Random: just one pass over A and B

Data-dependent sampling: based on column/row norms of A and B

EECS6898 - Large Scale Machine Learning

- Two passes necessary
- First pass: compute and store  $A^{(k)}$  and  $B_{(k)}$  k = 1,...,n
- Second pass: sample from A and B with  $p_k = \alpha |A^{(k)}| |B_{(k)}|$

### Implementation Details

How to sample?

Uniform Random: just one pass over A and B

Data-dependent sampling: based on column/row norms of A and B

- Two passes necessary
- First pass: compute and store  $A^{(k)}$  and  $B_{(k)}$  k = 1,...,n
- Second pass: sample from A and B with  $p_k = \alpha \left| A^{(k)} \right| B_{(k)}$
- Special case  $B = A^T$

$$AA^T \approx CC^T$$
  $p_k = |A^{(k)}|^2 / ||A||_F^2$ 

$$E[\|AA^{T} - CC^{T}\|_{F}] \le (1/\sqrt{\beta l})\|A\|_{F}^{2}$$

### Overview

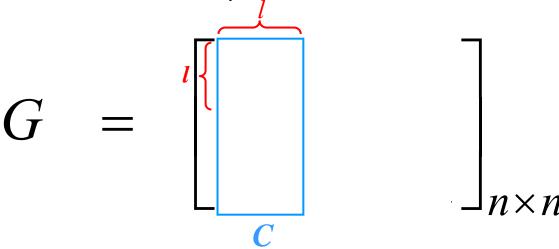
- 1. Approximate Matrix Multiplication
  - Sample columns of one matrix and rows from the other
- 2. Column-sampling methods for spectral decomposition
  - Methods that use decomposition of entire sampled columns
  - Methods that further sample the rows from the sampled columns
- 3. Low-rank approximation
  - Spectral reconstructions  $A_k = U_k \sum_k V_k^T$
  - Matrix Projection  $A_k = U_k U_k^T A$
- 4. Sampling Techniques
- 5. Ensemble Methods
  - How to combine multiple approximations to yield more accurate one

EECS6898 – Large Scale Machine Learning

## Approximate Spectral Decomposition

Let's focus on decomposition of a symmetric matrix - arise commonly in machine learning applications (other cases possible)

Sample *l* columns without replacement



- Column-Sampling Approximation SVD of C
- Nystrom Approximation SVD of W

## Column-Sampling Approximation

$$C = U_c \sum_{c} V_c^T \qquad O(nl^2)$$

$$n \times l \qquad n \times l \qquad l \times l \qquad l \times l$$

EECS6898 - Large Scale Machine Learning

## Column-Sampling Approximation

Suppose *l* columns were sampled uniformly

$$C = U_c \sum_c V_c^T \qquad O(nl^2)$$

$$\widetilde{U}_G = U_c = CV_c \sum_c^{-1}$$

$$\widetilde{\Sigma}_G = \sqrt{\frac{n}{l}} \, \Sigma_C$$

## Column-Sampling Approximation

Suppose *l* columns were sampled uniformly

$$C = U_c \sum_c V_c^T$$

$$0(nl^2)$$

$$n \sim 20M, l \sim 10K$$

$$\widetilde{U}_G = U_c = CV_c \sum_c^{-1}$$

$$\widetilde{\Sigma}_G = \sqrt{\frac{n}{l}} \Sigma_c$$

$$C^T C = V_c \sum_c^2 V_c^T$$

$$l \times l$$

$$O(nl^2)$$

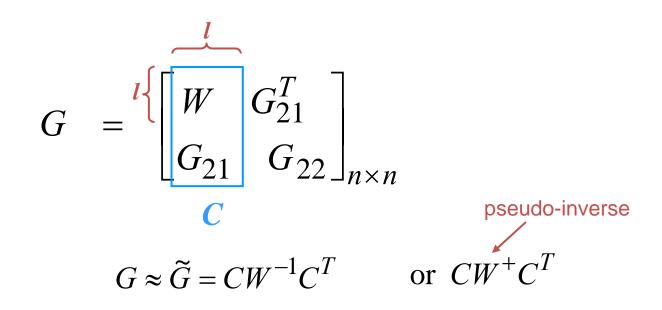
$$O(nl^2)$$

$$O(nl^2)$$

$$O(nl^3)$$
parallelize

For rank-k,  $k \le l$  reconstruction, pick top singular vectors and/or singular values!

EECS6898 – Large Scale Machine Learning



Reconstructs W and  $G_{21}$  i.e., C exactly!

$$G = \begin{bmatrix} W & G_{21}^T \\ G_{21} & G_{22} \end{bmatrix}_{n \times n}$$

$$C$$

$$G \approx \tilde{G} = CW^{-1}C^T$$

$$W = U_W \sum_W U_W^T \qquad O(l^3)$$

$$\tilde{\Sigma}_G = \frac{n}{l} \sum_W$$

EECS6898 - Large Scale Machine Learning

$$G = \begin{bmatrix} I \\ W \\ G_{21} \end{bmatrix} G_{21} \\ G_{22} \end{bmatrix}_{n \times n}$$

$$C$$

$$G \approx \tilde{G} = CW^{-1}C^{T}$$

$$W = U_{W} \sum_{W} U_{W}^{T} \qquad O(I^{3})$$

$$\tilde{\Sigma}_{G} = \frac{n}{l} \sum_{W}$$

$$\tilde{U}_{G} = \sqrt{\frac{l}{n}} CU_{W} \sum_{W}^{-1}$$

$$G = \begin{bmatrix} W & G_{21}^T \\ G_{21} & G_{22} \end{bmatrix}_{n \times n}$$

$$G \approx \widetilde{G} = CW^{-1}C^T$$

$$W = U_W \sum_W U_W^T$$

$$\widetilde{\Sigma}_G = \frac{n}{l} \Sigma_W$$

$$\widetilde{U}_G = \sqrt{\frac{l}{n}} C U_W \sum_{W}^{-1}$$

Not Orthonormal!

$$\widetilde{U}_G^T\widetilde{U}_G\neq I$$

For rank-k,  $k \le l$ reconstruction, pick top singular vectors and/or singular values!

## Nystrom Vs Column-Sampling

Spectral reconstruction: 
$$\tilde{G} = \tilde{U}_G \tilde{\Sigma}_G \tilde{U}_G^T$$

$$\widetilde{G}_{nys} = CW^{-1}C^{T}$$

$$\widetilde{G}_{col} = C\left[\left[\frac{l}{n}C^{T}C\right]^{1/2}\right]^{-1}C^{T}$$

EECS6898 - Large Scale Machine Learning

## Nystrom Vs Column-Sampling

Spectral reconstruction: 
$$\tilde{G} = \tilde{U}_G \tilde{\Sigma}_G \tilde{U}_G^T$$

$$\widetilde{G}_{nys} = CW^{-1}C^T$$

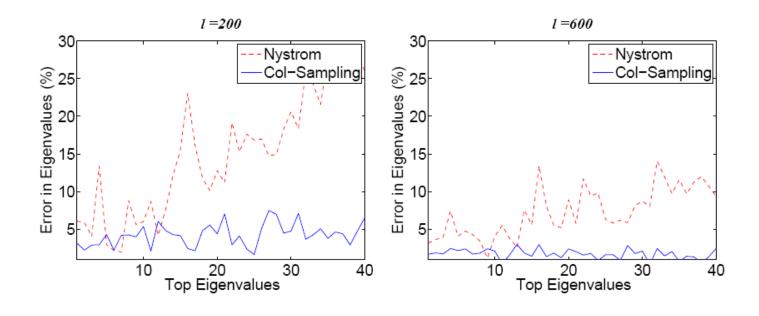
$$\widetilde{G}_{col} = C \left[ \left[ \frac{l}{n} C^T C \right]^{1/2} \right]^{-1} C^T$$

#### **Experimental Comparison**

- PIE-7K: 7K face images under different pose/illumination
- Linear kernel:  $k(x, y) = x^T y$
- G is a dense 7K x 7K symmetric positive semi-definite matrix
- Eigenvalues, eigenvectors, and low-rank approximations (spectralreconstruction)

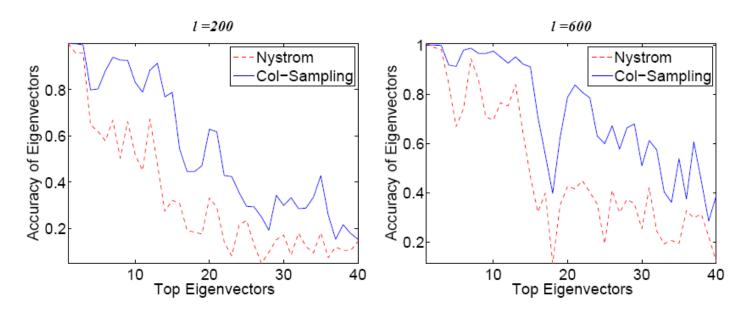
## Eigenvalues Comparison

#### % deviation from exact



## Eigenvectors Comparison

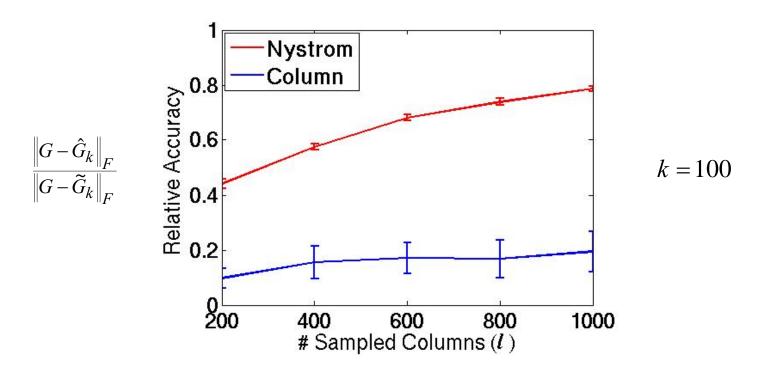
### Principal angle with exact



# Low-Rank Approximations

Spectral reconstruction:  $\widetilde{G}$ 

$$\widetilde{G}_k = \widetilde{U}_k \, \widetilde{\Sigma}_k \, \widetilde{U}_k^T$$

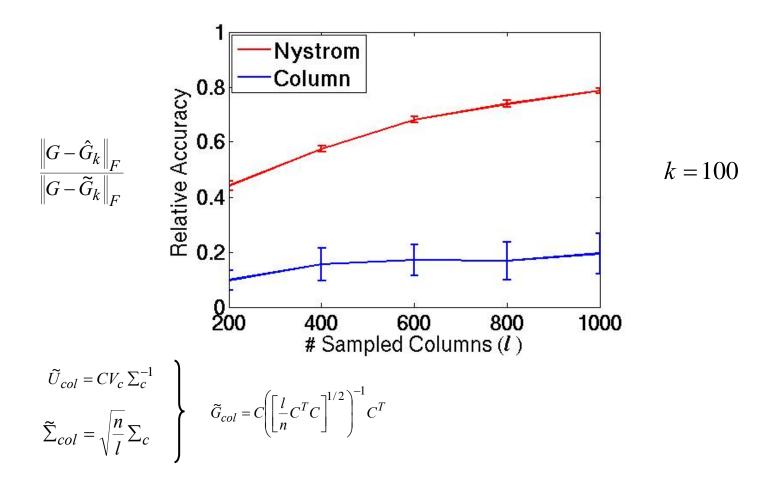


Nystrom gives better reconstruction than Col-Sampling!

# Low-Rank Approximations

Spectral reconstruction:  $\widetilde{G}_k = \widetilde{U}_k \widetilde{\Sigma}_k \widetilde{U}_k^T$ 

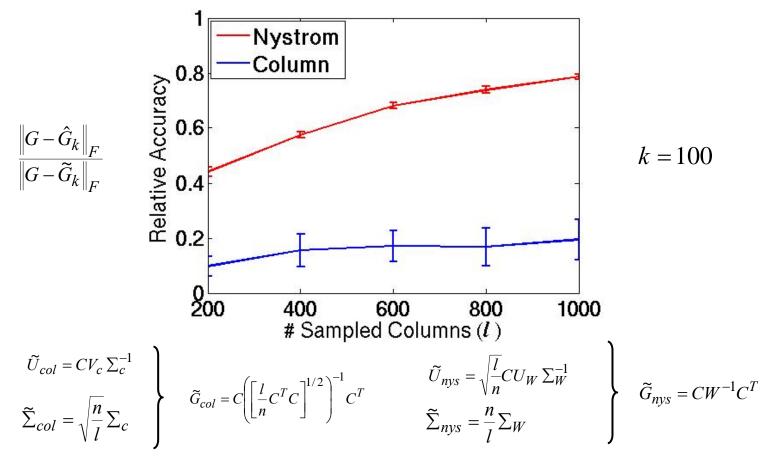
$$\widetilde{G}_k = \widetilde{U}_k \, \widetilde{\Sigma}_k \, \widetilde{U}_k^T$$



## Low-Rank Approximations

Spectral reconstruction:  $\widetilde{G}_k = \widetilde{U}_k \widetilde{\Sigma}_k \widetilde{U}_k^T$ 

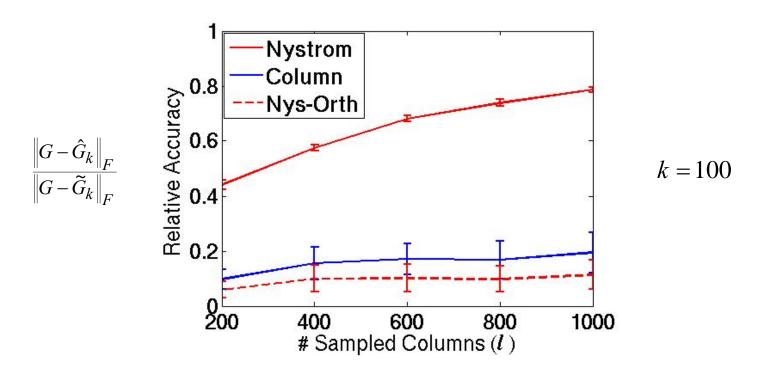
$$\widetilde{G}_k = \widetilde{U}_k \widetilde{\Sigma}_k \widetilde{U}_k^T$$



How about orthonormalized Nystrom eigenvectors?

# Orthogonalized Nystrom

Spectral reconstruction:  $\widetilde{G}_k = \widetilde{U}_k \widetilde{\Sigma}_k \widetilde{U}_k^T$ 



Nystrom-orthogonal gives worse reconstruction than Nystrom!

$$G_k = U_k \sum_k U_k^T = U_k U_k^T G = G U_k U_k^T$$

$$\tilde{G}_k = \tilde{U}_k \tilde{U}_k^T G \neq \tilde{U}_k \sum_k \tilde{U}_k^T$$

EECS6898 - Large Scale Machine Learning

$$G_k = U_k \sum_k U_k^T = U_k U_k^T G = G U_k U_k^T$$

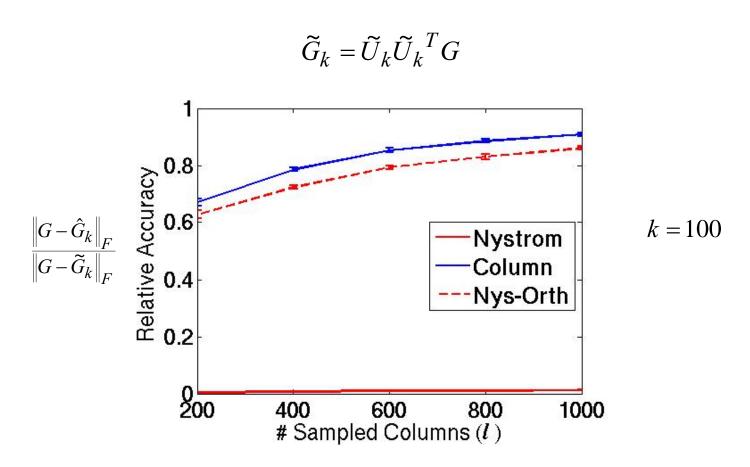
$$\widetilde{G}_k = \widetilde{U}_k \widetilde{U}_k^T G \neq \widetilde{U}_k \sum_k \widetilde{U}_k^T$$

$$\widetilde{G}_{col} = C(C^T C)^{-1} C^T G$$

$$\widetilde{G}_{col} = C(C^T C)^{-1} C^T G$$

$$\widetilde{G}_{nys} = C\left(\frac{l}{n}W^{-2}\right)C^T G$$

Reconstructs *C* exactly!



Col-Sampling gives better Reconstruction than Nystrom!

If k = l, Col-Sampling and Nystrom-orthogonal give the same answer!

Why does Col-sampling perform better than Nystrom?

Theorem: The matrix projection reconstruction for both Nystrom and Colsampling is of the form  $\tilde{G}_k = U_c R U_c^T G$ , where R is SPSD. Col-sampling gives the lowest reconstruction error (in Frobenius norm) among all such approximations when k = l.

EECS6898 – Large Scale Machine Learning

#### Why does Col-sampling perform better than Nystrom?

Theorem: The matrix projection reconstruction for both Nystrom and Colsampling is of the form  $\tilde{G}_k = U_c R U_c^T G$ , where R is SPSD. Col-sampling gives the lowest reconstruction error (in Frobenius norm) among all such approximations when k = l.

Partial proof: Let's look at the difference between any generic approx of the above form vs col-sampling approximation

$$E - E_{col} = \|G - U_c R U_c^T G\|_F^2 - \|G - U_c U_c^T G\|_F^2$$
 For col-sampling,  $R = I$ 
$$= Tr[G^T (U_c R^2 U_c^T - 2U_c R U_c^T + U_c U_c^T)G]$$
  $\|A\|_F^2 = Tr[A^T A]$ 

#### Why does Col-sampling perform better than Nystrom?

Theorem: The matrix projection reconstruction for both Nystrom and Colsampling is of the form  $\tilde{G}_k = U_c R U_c^T G$ , where R is SPSD. Col-sampling gives the lowest reconstruction error (in Frobenius norm) among all such approximations when k = l.

Partial proof: Let's look at the difference between any generic approx of the above form vs col-sampling approximation

$$E - E_{col} = \left\| G - U_c R U_c^T G \right\|_F^2 - \left\| G - U_c U_c^T G \right\|_F^2 \qquad \text{For col-sampling, } R = I$$

$$= Tr[G^T (U_c R^2 U_c^T - 2U_c R U_c^T + U_c U_c^T)G] \qquad \|A\|_F^2 = Tr[A^T A]$$

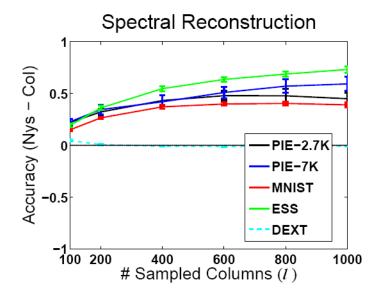
$$= Tr[(R - I)U_c^T G)^T (R - I)U_c^T G)]$$

$$\geq 0 \qquad \qquad Tr[A^T A] \geq 0$$

# Low-Rank Approx: Spectral Reconstruction

Why does Nystrom perform better than Col-sampling?

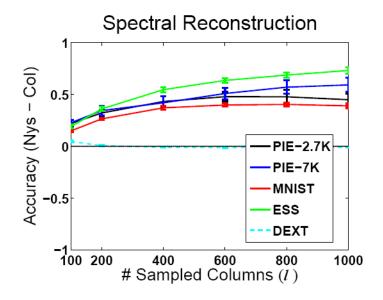
Unfortunately no clean theorem! Depends on the data spectrum!



# Low-Rank Approx: Spectral Reconstruction

Why does Nystrom perform better than Col-sampling?

Unfortunately no clean theorem! Depends on the data spectrum!

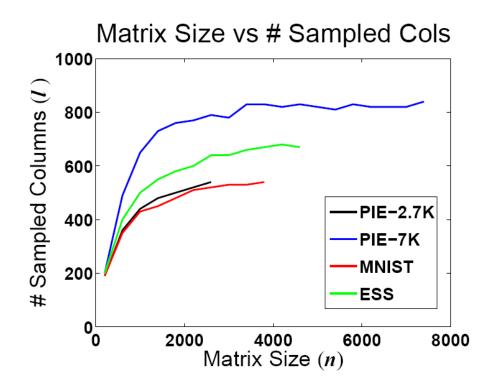


Theorem: Suppose,  $r = \operatorname{rank}(G) = \operatorname{rank}(W), r \le k \le l$ , then Nystrom approximation gives exact Spectral Reconstruction. In contrast, Colsampling gives the same result iff it reduces to Nystrom form, i.e.,

$$W = ((l/n)C^TC)^{1/2}$$

# How many columns are needed?

#### Columns needed to get 75% relative accuracy



### Formal Statements

Formal procedures for Nystrom and Col-sampling methods

EECS6898 - Large Scale Machine Learning

**Bounds on Errors** 

#### Algorithm

Given  $A, 1 \le k \le l \le n, \{p_i\}_{i=1}^n \text{ s.t. } \sum_i p_i = 1, p_i \ge 0$ 

Output  $\tilde{U}_k, \; \tilde{\Sigma}_k$ 

#### Algorithm

Given 
$$A, 1 \le k \le l \le n, \{p_i\}_{i=1}^n$$
 s.t.  $\sum_i p_i = 1, p_i \ge 0$ 

Output  $\widetilde{U}_k$ ,  $\widetilde{\Sigma}_k$ 

For t = 1, ..., l

- Pick  $i_t \in \{1,...,n\}$  with  $P(i_t = k) = p_k$  independently, with replacement fixed non-uniform distribution
- Set  $C^{(t)} = A^{(i_t)} / \sqrt{l p_i}$

Compute  $C^TC$  and decompose  $C^TC = V_c^T \Sigma_c^2 V_c$ 

Return 
$$\widetilde{\Sigma}_k = \Sigma_{c,k}$$
 and  $\widetilde{U}_k = U_{c,k} = CV_{c,k}\Sigma_{c,k}^{-1}$ 

#### Bound on error

$$\left\|A - \widetilde{U}_k \widetilde{U}_k^T A\right\|_F^2 \leq \left\|A - A_k\right\|_F^2 + 2\sqrt{k} \left\|AA^T - CC^T\right\|_F^2$$
 best rank-k matrix:  $A_k = U_k U_k^T A$  matrix-multiplication bound

EECS6898 - Large Scale Machine Learning

#### Bound on error

$$\left\|A - \widetilde{U}_k \widetilde{U}_k^T A\right\|_F^2 \leq \left\|A - A_k\right\|_F^2 + 2\sqrt{k} \left\|AA^T - CC^T\right\|_F^2$$
 best rank-k matrix:  $A_k = U_k U_k^T A$  matrix-multiplication bound

If 
$$p_i \ge \beta \left|A^{(i)}\right|^2 / \left\|A\right\|_F^2$$
,  $\beta \le 1$ ,  $\eta = 1 + \sqrt{(8/\beta)\log(1/\delta)}$  and  $l \ge 4k/\beta \varepsilon^2$ 

with probability at least  $(1-\delta)$ 

$$\left\|A - \widetilde{U}_k \widetilde{U}_k^T A\right\|_F^2 \le \left\|A - A_k\right\|_F^2 + \varepsilon \left\|A\right\|_F^2$$

#### Bound on error

$$\left\|A - \widetilde{U}_k \widetilde{U}_k^T A\right\|_F^2 \leq \left\|A - A_k\right\|_F^2 + 2\sqrt{k} \left\|AA^T - CC^T\right\|_F^2$$
 best rank-k matrix:  $A_k = U_k U_k^T A$  matrix-multiplication bound

If 
$$p_i \ge \beta |A^{(i)}|^2 / ||A||_F^2$$
,  $\beta \le 1$ ,  $\eta = 1 + \sqrt{(8/\beta) \log(1/\delta)}$  and  $l \ge 4k/\beta \varepsilon^2$ 

with probability at least  $(1-\delta)$ 

overestimate! In practice, much smaller

$$\left\|A - \widetilde{U}_k \widetilde{U}_k^T A\right\|_F^2 \le \left\|A - A_k\right\|_F^2 + \varepsilon \left\|A\right\|_F^2$$

Matrix-projection view

### Nystrom Method

Originally developed as a tool for numerical integration. When applied to eigenfunction estimation problem with quadrature rule, it allows extrapolation on full domain.

EECS6898 - Large Scale Machine Learning

#### **Algorithm**

Given 
$$G$$
,  $1 \le k \le l \le n$ ,  $\{p_i\}_{i=1}^n$  s.t.  $\sum_i p_i = 1$ ,  $p_i \ge 0$ 

Output  $\widetilde{G}_k$ 

### Nystrom Method

Originally developed as a tool for numerical integration. When applied to eigenfunction estimation problem with quadrature rule, it allows extrapolation on full domain.

#### Algorithm

Given 
$$G$$
,  $1 \le k \le l \le n$ ,  $\{p_i\}_{i=1}^n$  s.t.  $\sum_i p_i = 1$ ,  $p_i \ge 0$ 

Output  $\widetilde{G}_k$ 

- Pick  $i \in I \subset \{1,...,n\}$  with  $P(i=k) = p_k$  independently, with replacement fixed non-uniform distribution
- Set  $C = [G^{(i)} / \sqrt{l p_i}]$
- Select corresponding rows of  ${\it C}$  and form  ${\it W}$  such that each entry is

$$W_{ij} = G_{ij} / l \sqrt{p_i p_j} \qquad i, j \in I$$

Return 
$$\widetilde{G}_k = CW_k^{-1}C^T$$

## Nystrom Method

#### Bound on error

If 
$$p_i = G_{ii}^2 / \sum_i G_{ii}^2$$
,  $\eta = 1 + \sqrt{8\log(1/\delta)}$  and  $l \ge 64k\eta^2 / \varepsilon^4$ 

with probability at least  $(1-\delta)$ 

$$\|G - CW^{-1}C^T\|_F \le \|G - G_k\|_F + \varepsilon \sum_{i=1}^n G_{ii}^2$$

best rank-k matrix: $G_k = U_k \Sigma_k U_k^T$  matrix-multiplication bound

### Overview

- 1. Approximate Matrix Multiplication
  - Sample columns of one matrix and rows from the other
- 2. Column-sampling methods for spectral decomposition
  - Methods that use decomposition of entire sampled columns
  - Methods that further sample the rows from the sampled columns
- 3. Low-rank approximation
  - Spectral reconstructions  $A_k = U_k \sum_k V_k^T$
  - Matrix Projection  $A_k = U_k U_k^T A$
- 4. Sampling Techniques
- 5. Ensemble Methods
  - How to combine multiple approximations to yield more accurate one

EECS6898 – Large Scale Machine Learning

## Sampling Techniques

#### Fixed-Distribution Sampling methods

- Pick the columns randomly with equal probability
- Pick the columns proportional to their L<sub>2</sub> norm
- Pick the columns proportional to their diagonal entries

#### Advantages

- Uniform sampling very fast (constant time and space) and has been shown to work well in practice
- Data-dependent methods also provide fast sampling

#### Disadvantages

- L<sub>2</sub>-norm based methods need one pass through the entire matrix
- Expensive for large scale applications since each entry of the matrix is to be reconstructed  $\rightarrow O(n^2)$

EECS6898 – Large Scale Machine Learning

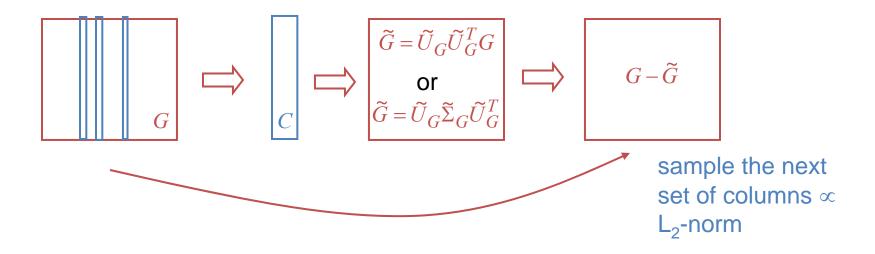
### Adaptive Sampling Techniques

Distribution over columns changes each time a column subset is picked

#### Basic Idea

Sanjiv Kumar

- Reconstruct the matrix given all the samples selected so far
- Find out reconstruction error for each column
- Pick the columns proportional to the reconstruction error



57

### Adaptive Sampling Techniques

Distribution over columns changes each time a column subset is picked

#### Basic Idea

- Reconstruct the matrix given all the samples selected so far
- Find out reconstruction error for each column
- Pick the columns proportional to the reconstruction error

#### Issues

- Usually much better than the fixed-distribution sampling methods
- Quite expensive for large scale applications
- Each entry of the matrix is to be reconstructed many times iteratively  $\rightarrow O(ln^2)$

Tighter Error Bound 
$$l \ge kt/\varepsilon$$

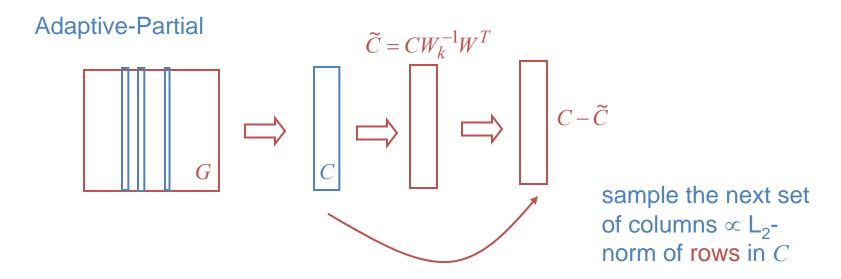
$$\left\|A - \widetilde{U}_k \widetilde{U}_k^T A\right\|_F^2 \le (1/1 - \varepsilon) \left\|A - A_k\right\|_F^2 + \varepsilon^t \left\|A\right\|_F^2$$

### Adaptive Sampling Techniques

Distribution over columns changes each time a column subset is picked

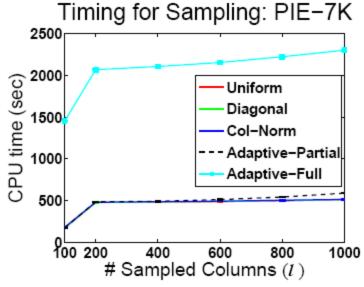
#### Basic Idea

- Reconstruct the matrix given all the samples selected so far
- Find out reconstruction error for each column
- Pick the columns proportional to the reconstruction error



## Experiments - Sampling Methods

l	11 1	1		1	1	Adapt-Full
	PIE-2.7K	$67.2 (\pm 1.1)$	$62.1 (\pm 0.9)$	$59.7 (\pm 1.0)$	$70.4 (\pm 0.9)$	72.6 $(\pm 1.0)$
	PIE-7K	$57.5 (\pm 1.1)$	$50.8 (\pm 1.9)$	$56.8 (\pm 1.6)$	$62.8 (\pm 0.9)$	$64.3 \ (\pm 0.7)$
400	MNIST	$67.4 (\pm 0.7)$	$67.4 (\pm 0.4)$	$65.3 (\pm 0.5)$	69.3 $(\pm 0.7)$	$69.2 (\pm 0.7)$
	ESS	$61.0 (\pm 1.7)$	$61.5 (\pm 1.5)$	$57.5 (\pm 1.9)$	$65.0\ (\pm 1.0)$	$63.9 (\pm 0.9)$
	PIE-2.7K	84.1 (±0.5)	$77.8 (\pm 0.6)$	$73.9 (\pm 1.0)$	$86.5 (\pm 0.4)$	$87.7 \ (\pm 0.4)$
	PIE-7K	$73.8 (\pm 1.2)$	$64.9 (\pm 1.8)$	$71.8 (\pm 3.0)$	$78.5 \ (\pm 0.5)$	$74.1 (\pm 0.6)$
800	MNIST	$83.3 (\pm 0.3)$	$83.0 (\pm 0.3)$	$80.4 (\pm 0.4)$	84.2 $(\pm 0.4)$	$80.7 (\pm 0.5)$
	ESS	$78.1 (\pm 1.0)$	$79.2 (\pm 0.9)$	$75.4 (\pm 1.2)$	$80.6~(\pm 1.1)$	$74.8 \ (\pm 0.8)$



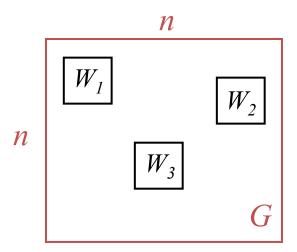
### Overview

- 1. Approximate Matrix Multiplication
  - Sample columns of one matrix and rows from the other
- 2. Column-sampling methods for spectral decomposition
  - Methods that use decomposition of entire sampled columns
  - Methods that further sample the rows from the sampled columns
- 3. Low-rank approximation
  - Spectral reconstructions  $A_k = U_k \sum_k V_k^T$
  - Matrix Projection  $A_k = U_k U_k^T A$
- 4. Sampling Techniques
- 5. Ensemble Methods
  - How to combine multiple approximations to yield more accurate one

EECS6898 – Large Scale Machine Learning

#### So far...

Nytrom Method picks a single square (usually noncontiguous) matrix from A



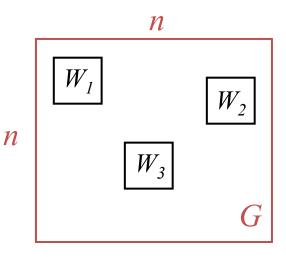
- Can we pick more such blocks and combine results to get better accuracy?
  - If yes, how to combine the results?
  - Computational cost ?

Yes, it is possible...

Pick *lp* columns without replacement: Divide into *p* sets

$$\widetilde{G}_r = C_r W_r^+ C_r^T$$
 for  $r = 1, ..., p$ 

Each  $C_r$  is non-overlapping



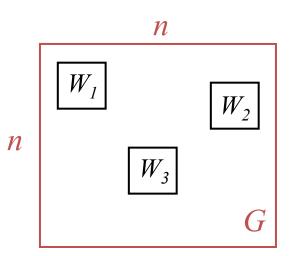
Yes, it is possible...

Pick *lp* columns without replacement: Divide into *p* sets

$$\widetilde{G}_r = C_r W_r^+ C_r^T$$
 for  $r = 1, ..., p$ 

Each  $C_r$  is non-overlapping

$$\widetilde{G} = \sum_{r=1}^{p} \mu_r \widetilde{G}_r$$



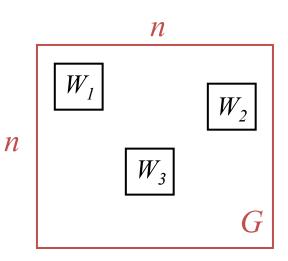
Yes, it is possible...

Pick *lp* columns without replacement: Divide into *p* sets

$$\widetilde{G}_r = C_r W_r^+ C_r^T$$
 for  $r = 1,..., p$ 

Each  $C_r$  is non-overlapping

$$\widetilde{G} = \sum_{r=1}^{p} \mu_r \widetilde{G}_r$$
 mixture weights



- How to compute mixture weights?
  - simplest choice:  $\mu_r = 1/p$

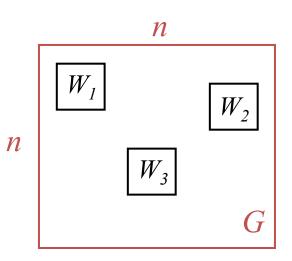
Yes, it is possible...

Pick *lp* columns without replacement: Divide into *p* sets

$$\widetilde{G}_r = C_r W_r^+ C_r^T$$
 for  $r = 1, ..., p$ 

Each  $C_r$  is non-overlapping

$$\widetilde{G} = \sum_{r=1}^{p} \mu_r \widetilde{G}_r$$
 mixture weights

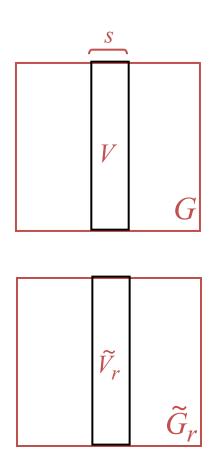


- How to compute mixture weights?
  - simplest choice:  $\mu_r = 1/p$
  - Learn using "training data"
  - Sample s columns separate from previous lp columns, and measure error in reconstructing those by each "expert" in ensemble

## Learning of Mixture Weights

#### Error in reconstruction for an expert

$$\varepsilon_r = \left\| V - \widetilde{V}_r \right\|_F$$
 for  $r = 1, ..., p$ 



## Learning of Mixture Weights

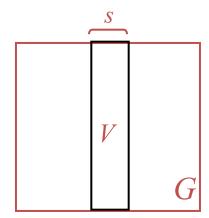
Error in reconstruction for an expert

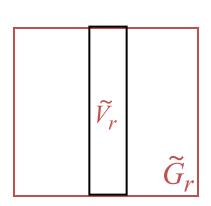
$$\varepsilon_r = \left\| V - \widetilde{V}_r \right\|_F$$
 for  $r = 1, ..., p$ 

**Exponential weighting** 

$$\mu_r = \exp(-\eta \varepsilon_r)/Z$$
 for  $\eta > 0$ 

Z is a normalizing constant such that  $\sum_r \mu_r = 1$ 





## Learning of Mixture Weights

#### Error in reconstruction for an expert

$$\varepsilon_r = \left\| V - \widetilde{V}_r \right\|_F$$
 for  $r = 1, ..., p$ 

#### **Exponential** weighting

$$\mu_r = \exp(-\eta \varepsilon_r)/Z$$
 for  $\eta > 0$ 

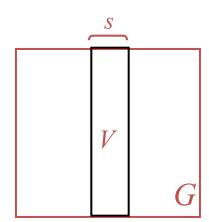
Z is a normalizing constant such that  $\sum_{r} \mu_{r} = 1$ 

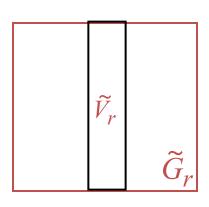
#### Linear (Ridge) Regression

Try to find weights that best reconstruct V

$$\mu = [\mu_1, \dots, \mu_p]^T$$

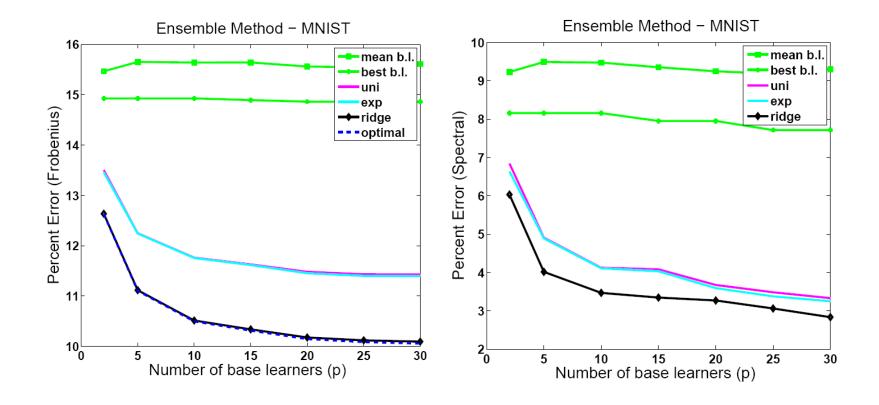
$$\hat{\mu} = \arg\min_{\mu} \left( \left\| \sum_r \mu_r \widetilde{V}_r - V \right\|_F^2 + \lambda \|\mu\|_2^2 \right)$$





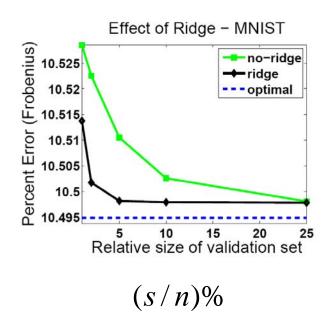
## Examples

- MNIST dataset: n = 4000, s = 20, k = 50
- Optimal weights: linear regression with s = n

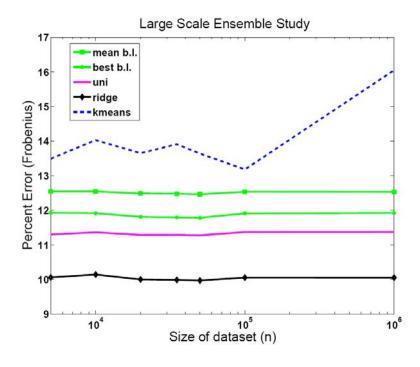


## Examples

- How important is ridge penalty?
- Large-scale comparison



#### SIFT-1M dataset



Fixed-time experiment

$$k = 50, p = 10, s = 2$$

71

### References

- A. Frieze, R. Kannan and S. Vempala, Fast Monte-Carlo Algorithms for finding low-rank approximations, Proceedings of the Foundations of Computer Science, 1998.
- P. Drineas and M. W. Mahoney, On the Nystrom method for approximating a Gram matrix for improved kernel-based learning, Journal of Machine Learning Research, 2005.
- 3. P. Drineas and R. Kannan, M. Mahoney, Fast Monte Carlo Algorithms for Matrices I: Approximating Matrix Multiplication, SIAM Journal on Computing, 2006.
- P. Drineas, R. Kannan, and M. W. Mahoney, Fast monte carlo algorithms for matrices II: 4. computing a low rank approximation to a matrix, SIAM Journal on Computing, 36(1), 2006.
- 5. Amit Deshpande, Santosh Vempala, Grant Wang, Matrix Approximation and Projective Clustering via Volume Sampling. Theory of Computing and SODA 2006.
- A. Talwalkar, S. Kumar and H. A. Rowley, Large-Scale Manifold Learning, *IEEE Computer Vision* and Pattern Recognition (CVPR), 2008.
- S. Kumar, M. Mohri and A. Talwalkar, Sampling Techniques for the Nystrom Method, Twelfth International Conference on Artificial Intelligence and Statistics (AISTATS), 2009.
- S. Kumar, M. Mohri and A. Talwalkar, On Sampling-based Approximate Spectral Decomposition, 8. International Conference on Machine Learning (ICML), 2009.
- S. Kumar, M. Mohri and A. Talwalkar, Ensemble Nystrom Method *Neural Information Processing* Systems (NIPS), 2009.

EECS6898 – Large Scale Machine Learning

11. M. Li, J.T. Kwok, B. Lu, Making large-scale Nystrom approximation possible. Proceedings of the Twenty-Seventh International Conference on Machine Learning (ICML), June 2010.