Augmented leverage score sampling

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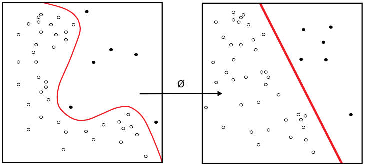
Problem statement

Computational expensive analysis of large datasets

- Large n which limits available computation per item
- Desired analysis is computationally expensive for n
- A subset of size $m \ll n$ is representative of the entire dataset

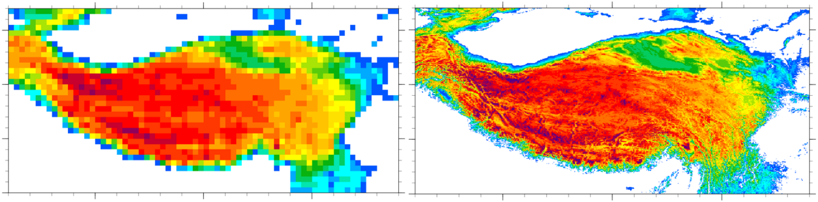
Example: kernel learning on large datasets



- Naive kernel based learning requires kernel (Gram) matrix $\mathbf{A^T A}$
  - $\mathcal{O}(n^2)$ + "analysis cost"
- Nyström approximation to the kernel matrix $\mathbf{A^T A}$
  - Select a subset $\mathbf{C}$ of size $m \ll n$
  - $\mathbf{A^T A}_{i,j} \approx \mathbf{A_i^T C (C^T C)^{-1} C^T A_j}$
  - $\mathcal{O}(m^2)$ + "analysis cost"
- Use on *resource limited machines* requires careful subset selection

[0] image from wikipedia.org

Example: multifidelity simulation



- Uncertainty analysis
  - Random parameter(s) of interest, $\eta \in \mathcal{D}$
  - n samples of $\eta \in \mathcal{D}$ to quantify uncertainty
- Multifidelity uncertainty analysis
  - High fidelity model: only $m \ll n$ simulations
  - Low fidelity model: run all n simulations
  - Representative subset of size m from n for high fidelity simulation
- Careful selection of subset important!

[0] images from www.ncl.ucar.edu

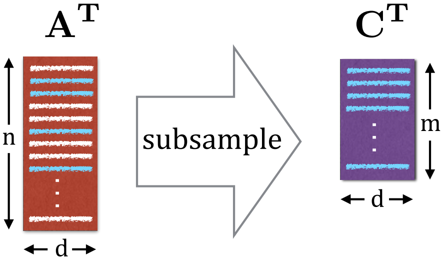
Problem statement

Definition

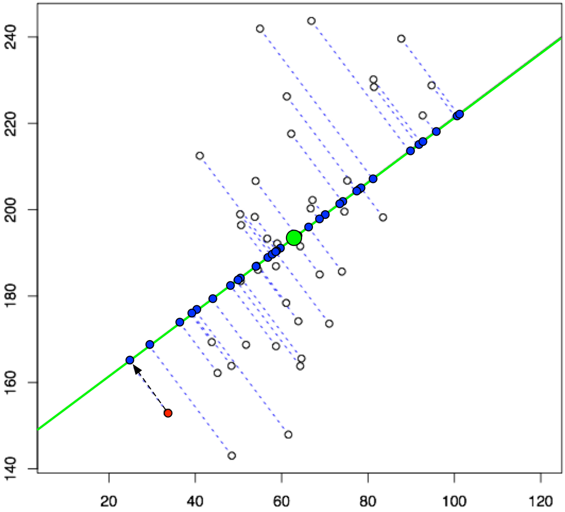
Column Subset Selection Problem. Let $\mathbf{A} \in \mathbb{R}^{d \times n}$. Find $m < n$ columns for $\mathbf{A}$ - denoted as $\mathbf{C} \in \mathbb{R}^{d \times m}$ that minimize

$$\|\mathbf{A} - \mathbf{C}\mathbf{C}^{\dagger}\mathbf{A}\|_{\eta}, \tag{1}$$

for $\eta \in \{F, 2\}$, and where $\mathbf{C}^{\dagger}$ denotes the Moore-Penrose pseudo-inverse.



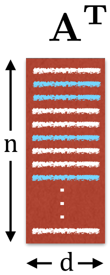
Problem statement: visually



Related work

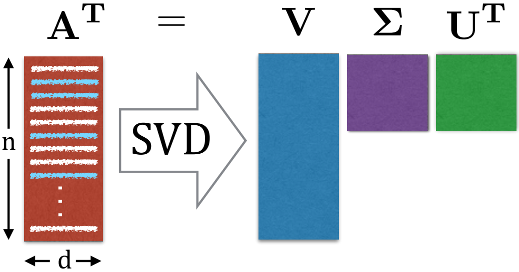
- Leverage sampling [Mahoney, 2011, Mahoney, 2010, Papailiopoulos et al., 2014, Boutsidis et al., 2014]
  - [Papailiopoulos et al., 2014] obtained a very similar bound for deterministic leverage sampling
- Greedy subset selection [Altschuler et al., 2016]
  - obtained a bound in a different form (relative to the optimal subset) for deterministic greedy subset selection
- CUR [Drineas et al., 2008]
  - [Drineas et al., 2008] uses leverage sampling
- Nyström approximation [Drineas and Mahoney, 2005, Gittens and Mahoney, 2013, Gittens, 2011]
  - [Drineas and Mahoney, 2005] uses uniform sampling

Deterministic leverage score sampling



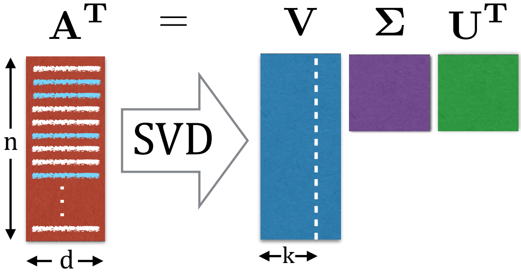
- data matrix $\mathbf{A} \in \mathbb{R}^{d \times n}$

Deterministic leverage score sampling



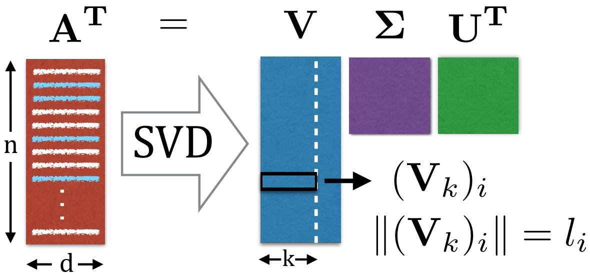
- singular value decomposition

Deterministic leverage score sampling



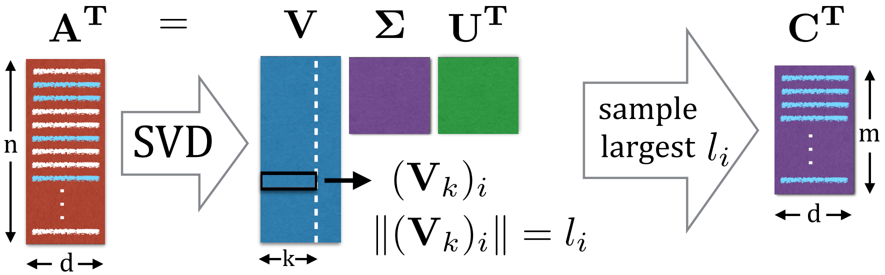
- best rank-k approximation

Deterministic leverage score sampling



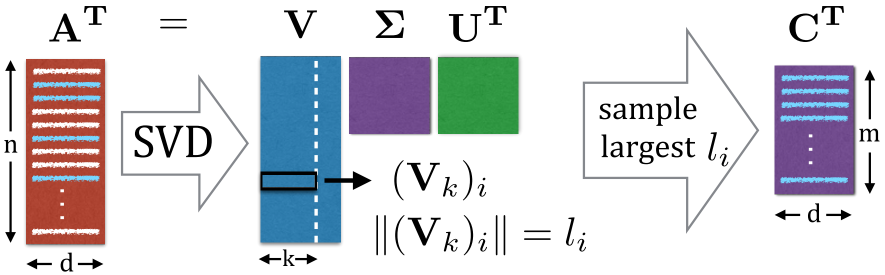
- norm of each row $\mathbf{V_k}$

Deterministic leverage score sampling



- Deterministic samples largest l_i values first

Deterministic leverage score sampling



- Probabilistic version samples with probability l_i

Leverage scores

Definition

Let $\mathbf{V_k} \in \mathbb{R}^{n \times k}$ contain the top k right singular vectors of a $d \times n$ matrix A with rank $\rho = \mathbf{rank}(\mathbf{A}) \geq k$. Then the (rank-k) leverage score of the i-th column of $\mathbf{A}$ is defined as

$$l_i^{(k)} = \|[\mathbf{V_k}]_{i,:}\|_2^2, \;\; i = 1, 2, \ldots, n. \tag{2}$$

Here, $[\mathbf{V_k}]_{i,:}$ denotes the i-th row of $\mathbf{V_k}$.

Leverage score bound

$$\|\mathbf{A} - \mathbf{C}\mathbf{C}^{\dagger}\mathbf{A}\|_{\zeta}^2 < (1 + 2\epsilon) \cdot \|\mathbf{A} - \mathbf{A_k}\|_{\zeta}^2. \tag{3}$$

for $\zeta \in \{2, F\}$, $\epsilon \in (0, .5)$, where $\mathbf{A_k}$ is the best rank-k approximation to $\mathbf{A}$ [Papailiopoulos et al., 2014].

CSSP Objective: data scale also important

$$\|\mathbf{A} - \mathbf{C}\mathbf{C}^{\dagger}\mathbf{A}\|_{\eta}$$
$$\|\mathbf{A} - \mathbf{C}(\mathbf{C}^{\mathbf{T}}(\mathbf{C}\mathbf{C}^{\mathbf{T}})^{-1})\mathbf{A}\|_{\eta}$$
$$\|\mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^{\mathbf{T}} - \mathbf{W}_{\mathbf{d}}\mathbf{W}_{\mathbf{d}}^{\mathbf{T}}\mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^{\mathbf{T}}\|_{\eta}$$
$$\|(\mathbf{U} - \mathbf{W}_{\mathbf{d}}\mathbf{W}_{\mathbf{d}}^{\mathbf{T}}\mathbf{U})\boldsymbol{\Sigma}\mathbf{V}^{\mathbf{T}}\|_{\eta}$$

where $\mathbf{A} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^{\mathbf{T}}$ and $\mathbf{C} = \mathbf{W}\boldsymbol{\Psi}\mathbf{H}^{\mathbf{T}}$ are the respective SVDs.

- Indictates the "unwhitened" data points $\boldsymbol{\Sigma}\mathbf{V}^{\mathbf{T}}$, not $\mathbf{V}^{\mathbf{T}}$
- This informs the core idea of an *augmented leverage score*

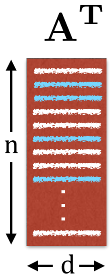
Proposed: augmented leverage score

Definition

Let $\mathbf{Y_k} = \mathbf{V_k \Sigma_k} \in \mathbb{R}^{n \times k}$ contain the top k singular values multiplied with the right singular vectors of a $d \times n$ matrix $\mathbf{A}$ with rank $\rho = \mathbf{rank}(\mathbf{A}) \geq k$. Then the (rank-k) augmented leverage score of the i–th column of $\mathbf{A}$ is defined as

$$\hat{l}_i^{(k)} = \|[\mathbf{Y_k}]_{i,:}\|_2^2, \;\; i = 1, 2, \ldots, n.$$

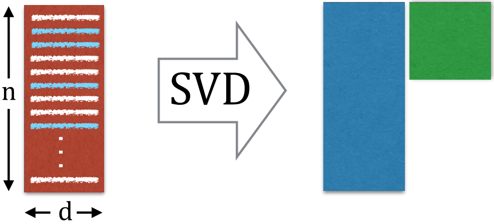
Augmented leverage score sampling



- data matrix $\mathbf{A} \in \mathbb{R}^{d \times n}$

Augmented leverage score sampling

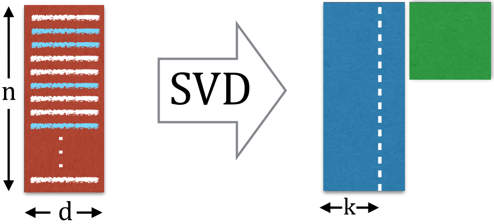
$$\mathbf{A^T} = \mathbf{V\Sigma U^T} = \mathbf{Y^T U^T}$$



- singular value decomposition, combine $\mathbf{V^T\Sigma} = \mathbf{Y^T}$

Augmented leverage score sampling

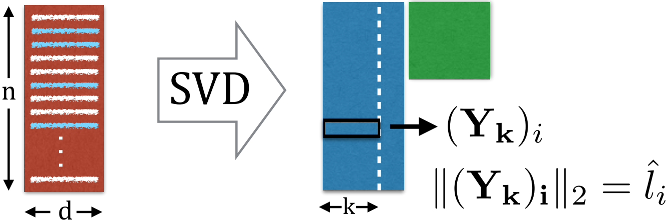
$$\mathbf{A}^{\mathbf{T}} = \mathbf{V\Sigma U}^{\mathbf{T}} = \mathbf{Y}^{\mathbf{T}}\mathbf{U}^{\mathbf{T}}$$



- best rank-k approximation

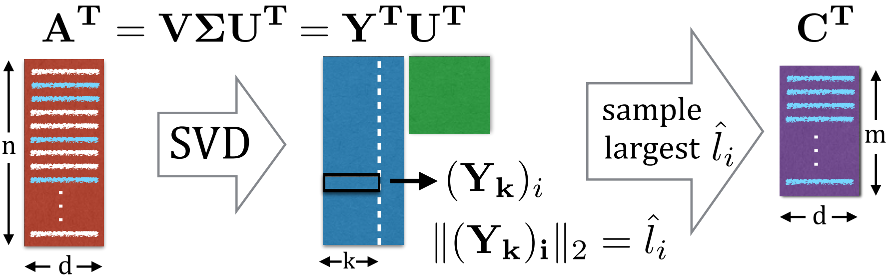
Augmented leverage score sampling

$$\mathbf{A^T} = \mathbf{V \Sigma U^T} = \mathbf{Y^T U^T}$$



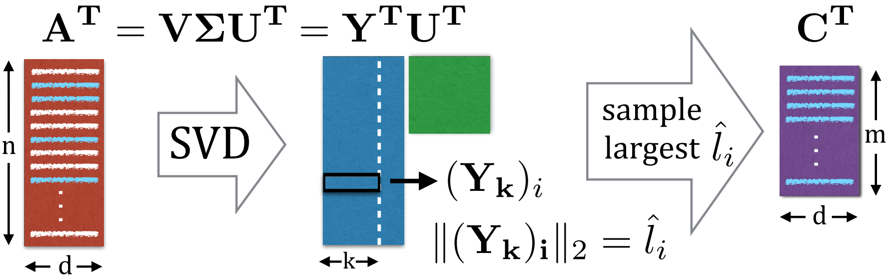
- norm of each row $\mathbf{Y_k}$

Augmented leverage score sampling



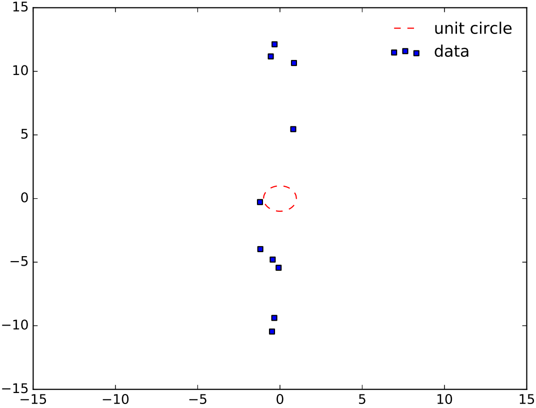
- Augmented samples largest $\hat{l}_i$ values first

Augmented leverage score sampling



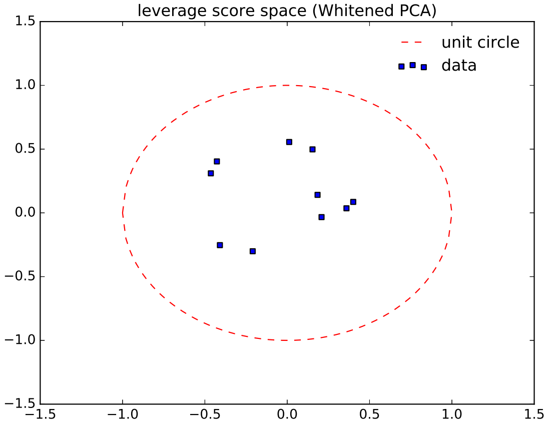
- Probabilistic version samples with probability $\hat{l}_i$

Leverage score: visual example



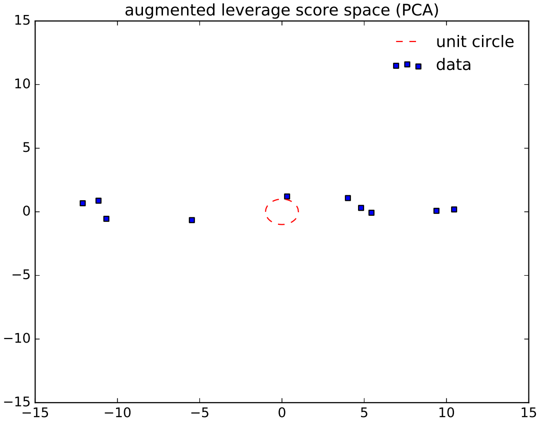
- samples from Gaussian with covariance $\begin{bmatrix} 1 & 0 \\ 0 & 10 \end{bmatrix}$

Leverage score: visual example



- $\mathbf{V}_{\mathbf{k}}^{\mathbf{T}} = \mathbf{\Sigma}_{\mathbf{k}}^{-1}\mathbf{U}_{\mathbf{k}}^{\mathbf{T}}\mathbf{A}$
- Norm sampling based on a whitened rank-k PCA projection

Augmented leverage score: visual example



- $\mathbf{\Sigma_k V_k^T = U_k^T A}$
- Norm sampling based on an (unwhitened) rank-k PCA projection

Augmented Leverage Score Sampling Algorithm

Input $\mathbf{A} \in \mathbb{R}^{d \times n}, k, \theta$
Compute $\mathbf{Y_k} = \mathbf{V_k}\hat{\mathbf{\Sigma}}_\mathbf{k} \in \mathbb{R}^{n \times k}$
for $i = 1, 2, \ldots, n$
    $\hat{l}_i^{(k)} = \|[\mathbf{Y_k}]_{i,:}\|_2^2$
end for
Sort $\hat{l}_i^{(k)}$ **in place**
Find index $m \in \{1, \ldots, n\}$ **such that:**

$$m = \arg\min_m \left(\sum_{i=1}^{m} \hat{l}_i^{(k)} > \theta \right).$$

If $m < k$**, set** $m = k$**.**
Output $\mathbf{S} \in \mathbb{R}^{n \times m}$**, s.t. AS has the top** m **columns of A.**

Bounds of augmented leverage score sampling

Theorem

Let $\theta = k \cdot \frac{\sigma_1^2}{\sigma_k^2} - \epsilon$ *for some* $\epsilon \in (0, 0.5)$, *and let* $\mathbf{S} \in \mathbb{R}^{n \times m}$ *be the sampling matrix from Augmented Leverage Score Sampling Algorithm, then, for* $\mathbf{C} = \mathbf{AS}$ *and* $\zeta = \{2, F\}$

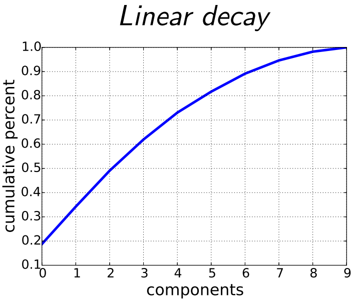
$$\|\mathbf{A} - \mathbf{C}\mathbf{C}^{\dagger}\mathbf{A}\|_{\zeta}^{2} < \frac{\sigma_1^2}{\sigma_k^2}(1 + 2\epsilon) \cdot \|\mathbf{A} - \mathbf{A_k}\|_{\zeta}^{2}. \tag{4}$$

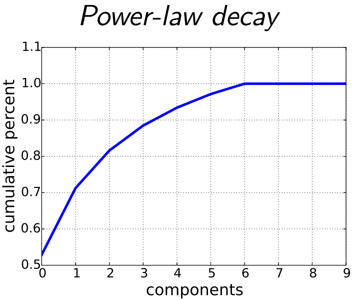
Experiments: synthetic data attributes

name	n	d	k
Synthetic linear decay	1000	10	9
Synthetic power law decay	1000	10	6

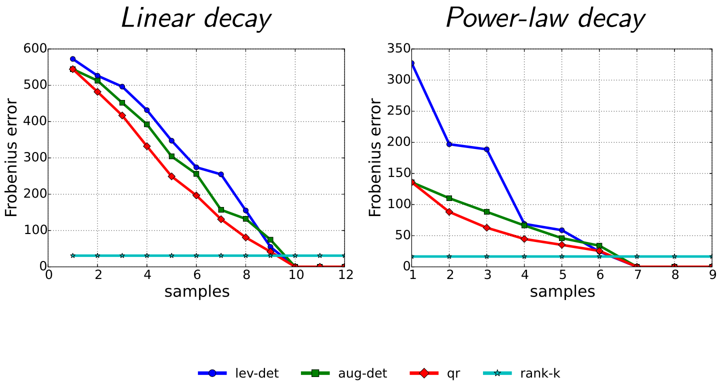
- n - number of columns
- d - dimension of each column
- k - number of PCA dimensions to preserve 90% of spectral energy

Experiments: synthetic data spectra

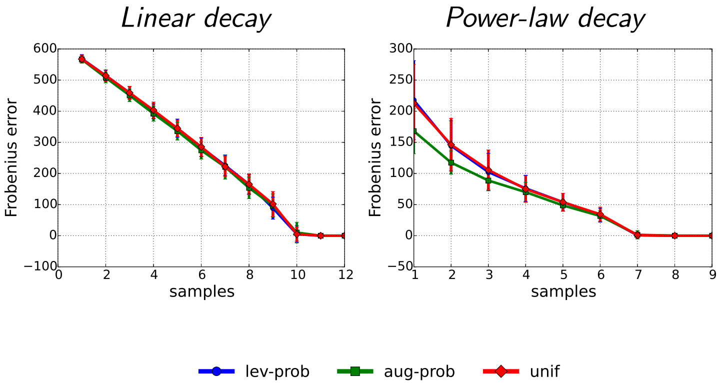




Experiments: synthetic data deterministic results



Experiments: synthetic data probabilistic results

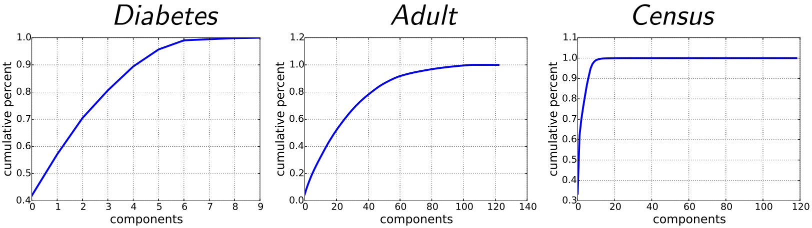


Experiments: real data attributes

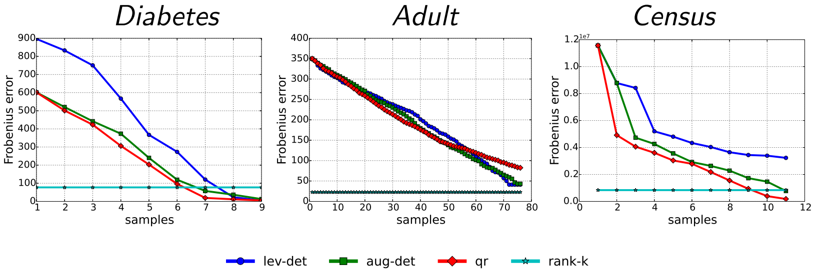
name	n	d	k
Diabetes	442	9	6
Adult	16281	123	73
Census	2273	119	8

- n - number of columns
- d - dimension of each column
- k - number of PCA dimensions to preserve 90% of spectral energy

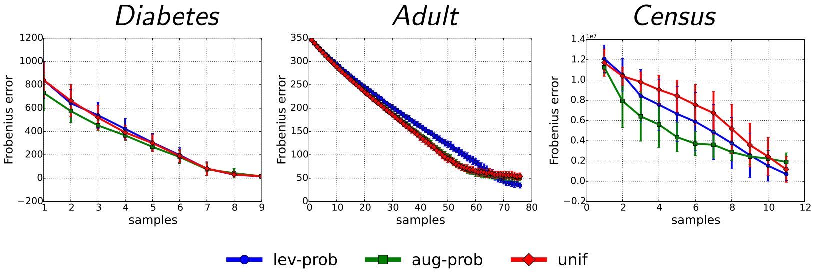
Experiments: real data spectra



Experiments: real data results



Experiments: real data results



Conclusion

- Proposed the *augmented leverage score* motivated by the CSSP objective
- Provided an initial error bound for deterministic augmented leverage score sampling
- Shown empricial results comparing the method on a variety of data sets
  - advantages for data sets with sharp spectral decay
  - shown advantages in both deterministic and probabilistic settings

Acknowledgments

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Thank you!

Questions?

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