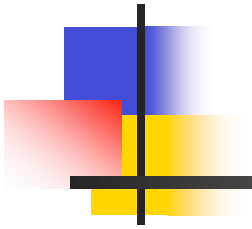

# (On the Nyström Method for) Approximating a Gram Matrix for Improved Kernel-Based Learning


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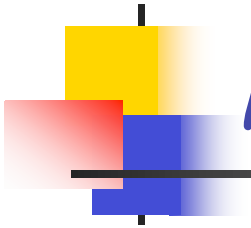


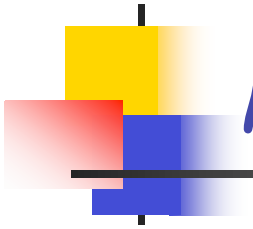
# Motivation (1 of 3)

Methods to extract linear structure from the data:

- Support Vector Machines (SVMs).
- Gaussian Processes (GPs).
- Singular Value Decomposition (SVD) and the related PCA.

Kernel-based learning methods to extract non-linear structure:

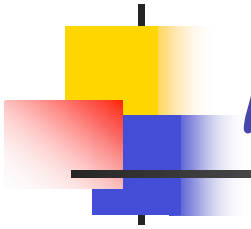
- Choose features to define a (dot product) space F.
- Map the data, X, to F by $\phi$: X→F.
- Do classification, regression, and clustering in F with linear methods.



# Motivation (2 of 3)

- Use dot products for information about mutual positions.
- Define the kernel or Gram matrix: $G_{ij}=k_{ij}=(\phi(X^{(i)}), \phi(X^{(j)}))$.
- Algorithms that are expressed in terms of dot products can be given the Gram matrix $G$ instead of the data covariance matrix $X^TX$.

- Note: Isomap, LLE, graph Laplacian eigenmaps, Hessian eigenmaps, SDE (dimensionality reduction methods for nonlinear manifolds) are kernel-PCA for particular Gram matrices.
- Note: for Mercer kernels, $G$ is SPSD.



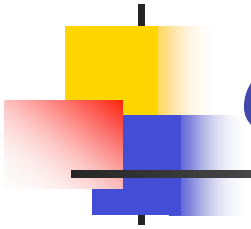
# Motivation (3 of 3)

If the Gram matrix $G$ -- $G_{ij}=k_{ij}=(\phi(X^{(i)}), \phi(X^{(j)}))$ -- is dense but (nearly) low-rank, then calculations of interest still need $O(n^2)$ space and $O(n^3)$ time:

- matrix inversion in GP prediction,
- quadratic programming problems in SVMs,
- computation of eigendecomposition of $G$.

Relevant recent work using low-rank methods:

- Achlioptas, McSherry, and Schölkopf, 2002, ``randomized kernels''.
- Williams and Seeger, 2001, the ``Nystrom method''.



# Overview

Our main algorithm:

- Randomized algorithm to approximate a Gram matrix.
- Low-rank approximation in terms of columns (and rows) of $G=X^TX$.

Our main quality-of-approximation theorem:

- Provably good approximation if nonuniform probabilities are used.

Discussion of the Nystrom method:

- Nystrom method for integral equations and matrix problems.
- Relationship to randomized SVD and CUR algorithms.

# Review of Linear Algebra

F-norm: $\|A\|_F^2 = \sum_{ij} A_{ij}^2$

2-norm: $\|A\|_2 = \sup_{x \in R^n,\ x \neq 0} \frac{\|Ax\|}{\|x\|}$

SVD: $A = U \Sigma V^T$

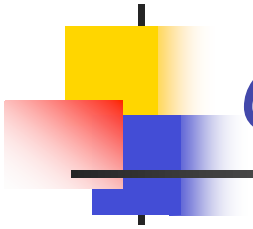
$A_k = U_k \Sigma_k V_k^T$

SPSD: $x^T A x \geq 0 \ \forall x \neq 0$

MPGI: $A^+ = V \Sigma^{-1} U^T$

$$\max_{t:1 \leq t \leq n} |\sigma_t(A+E) - \sigma_t(A)| \leq \|E\|_2$$

$$\sum_{k=1}^{n} (\sigma_k(A+E) - \sigma_k(A))^2 \leq \|E\|_F^2$$



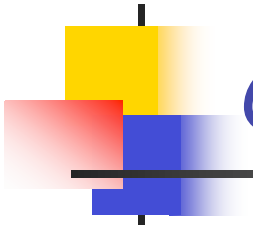
# Our Main Algorithm

**Input**: n x n SPSD matrix $G$, probabilities $\{p_i, 1=1,\ldots,n\}$, c <= n, and k <= c.

**Output**: n x c matrix $C$, and c x c matrix $W_k^+$ (s.t. $CW_k^+C^T \approx G$).

***Algorithm***:

- Pick c columns of $G$ in i.i.d. trials, with replacement and with respect to the probabilities $\{p_i\}$; let $\mathcal{I}$ be the set of indices of the sampled columns.
- Scale each sampled column (with index $i \in \mathcal{I}$) by dividing its by $\sqrt{cp_i}$.
- Let $C$ be the n x c matrix containing the rescaled sampled columns.
- Let $W$ be the c x c matrix of $G$ with entries $G_{ij}/c\sqrt{p_i\, p_j}$, $i,j \in \mathcal{I}$.
- Compute $W_k^+$.



# Our Main Theorem

Let $\varepsilon > 0$ and $\eta = 1 + \sqrt{8\log(1/\delta)}$.

Construct an approximation $CW_k^+C^T$ with our Main Algorithm by sampling $c$ columns of $G$ with probabilities $p_i = G_{ii}^2 / \Sigma_i G_{ii}^2$.

If $c >= 64k\eta^2/\varepsilon^4$, then w.h.p.:

$$||G-CW_k^+C^T||_F <= ||G-G_k||_F + \varepsilon \Sigma_i G_{ii}^2.$$

If $c >= 4\eta^2/\varepsilon^2$, then w.h.p.:

$$||G-CW_k^+C^T||_2 <= ||G-G_k||_2 + \varepsilon \Sigma_i G_{ii}^2.$$

# Notes About Our Main Result (1 of 2)

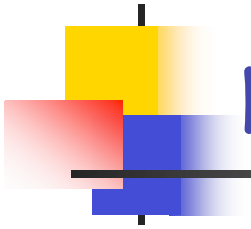
Note: the structural simplicity of our main result:

- $C$ consists of a small number of representative data points.
- $W$ consists of the induced subgraph defined by those points.

$$\begin{pmatrix} \quad G \quad \end{pmatrix} \approx \begin{pmatrix} \quad \tilde{G} \quad \end{pmatrix} = \begin{pmatrix} \quad C \quad \end{pmatrix} \begin{pmatrix} \quad W \quad \end{pmatrix}^{+} \begin{pmatrix} \quad C^{T} \quad \end{pmatrix}$$

Computational resource requirements:

- Assume the data X (or Gram matrix G) are stored externally.
- Algorithm performs two passes over the data.
- Algorithm uses O(n) additional scratch space and additional computation time.



# Notes About Our Main Result (2 of 2)

How to interpret the sampling probabilities?

If the sampling probabilities were:

$$p_i = ||G^{(i)}||^2/||G||_F^2$$

- they would provide a bias towards data points that are more ``important'' - longer and/or more representative.
- the additional error would be $\varepsilon||G||_F$ and not $\varepsilon \Sigma_i G_{ii}^2 = \varepsilon||X||_F^2$ (where $G=X^TX$).

Our sampling probabilities ignore correlations:

$$p_i = G_{ii}^2/ \Sigma_i G_{ii}^2 = ||X^{(i)}||^2/||X||_F^2$$

# Proof of Our Main Theorem (1 of 4)

Let $G = X^T X$ and let:

$$\begin{aligned} C &= GSD = X^T XSD \\ C_X &= XSD \\ &= \tilde{U}\tilde{\Sigma}\tilde{V}^T \\ W &= (SD)^T GSD = C_X^T C_X = \tilde{V}\tilde{\Sigma}^2\tilde{V}^T. \end{aligned}$$

Then:

$$\begin{aligned} CW_k^+ C^T &= GSD\,(W_k)^+\,(GSD)^T \\ &= X^T \hat{U}_k \hat{U}_k^T X. \end{aligned}$$

The error matrix is:

$$\begin{aligned} G - \tilde{G}_k &= X^T X - X^T \hat{U}_k \hat{U}_k^T X \\ &= \left(X - \hat{U}_k \hat{U}_k^T X\right)^T \left(X - \hat{U}_k \hat{U}_k^T X\right). \end{aligned}$$

# Proof of Our Main Theorem (2 of 4)

First, bound the spectral norm:

$$\begin{aligned}
\|G - \tilde{G}_k\|_2 &= \left\| \left(X - \hat{U}_k \hat{U}_k^T X\right)^T \left(X - \hat{U}_k \hat{U}_k^T X\right) \right\|_2 \\
&= \|X - \hat{U}_k \hat{U}_k^T X\|_2^2 \\
&\leq \|X - X_k\|_2^2 + 2\|XX^T - C_X C_X^T\|_2 \\
&\leq \|G - G_k\|_2 + 2\|E_{XX^T}\|_2.
\end{aligned}$$

Note: If k >= r = rank(W), then:

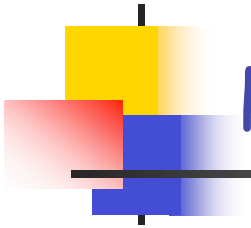
$$\|G - \tilde{G}_r\|_2 \leq \|E_{XX^T}\|_2$$

# Proof of Our Main Theorem (3 of 4)

Next, bound the Frobenius norm:

Let $E = XX^TXX^T - C_XC_X^TC_XC_X^T$. Then:

$$\begin{aligned}
\left\|G - \tilde{G}_k\right\|_F^2 &= \left\|X^TX - X^T\hat{U}_k\hat{U}_k^TX\right\|_F^2 \\
&= \left\|X^TX\right\|_F^2 - 2\left\|XX^T\hat{U}_k\right\|_F^2 + \left\|\hat{U}_k^TXX^T\hat{U}_k\right\|_F^2 \\
&\leq \left\|X^TX\right\|_F^2 - 2\left(\sum_{t=1}^{k}\sigma_t^4(C_X) - \sqrt{k}\left\|E\right\|_F\right) + \sum_{t=1}^{k}\sigma_t^4(C_X) + \sqrt{k}\left\|E\right\|_F \\
&= \left\|X^TX\right\|_F^2 - \sum_{t=1}^{k}\sigma_t^4(C_X) + 3\sqrt{k}\left\|E\right\|_F \\
&\leq \left\|X^TX\right\|_F^2 - \sum_{t=1}^{k}\sigma_t^2(X^TX) + 4\sqrt{k}\left\|E\right\|_F \\
&\leq \left\|G - G_k\right\|_F^2 + 4\sqrt{k}\left\|E\right\|_F,
\end{aligned}$$



# Proof of Our Main Theorem (4 of 4)

**Goal**: Approximate the product of two (or more) matrices. (DK,DKM,DM)

**Input**: m x n matrix $A$, number c <= n, and probabilities {p_i, i=1,…,n}

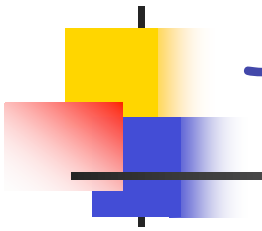
**Output**: m x c matrix $C$ (s.t. $CC^T \approx AA^T$)

**Algorithm**:

- Randomly sample c columns from $A$ according to $\{p_i\}$
- Rescale each column by $1/\sqrt{cp_{i\_t}}$ to form $C$

**Theorem**: Let $\eta = 1 + \sqrt{8\log(1/\delta)}$. If $p_i = |A^{(i)}|^2/||A||_F^2$ and c >=4 $\eta^2/\varepsilon^2$:

- $||AA^T-CC^T|| <= \varepsilon\ ||A||_F^2$
- $||AA^TAA^T-CC^TCC^T|| <= \varepsilon\ ||A||_F^4$



# The Nystrom Method (1 of 3)

Consider the eigenfunction problem:

$$\int_D K(t,s)\Phi(s)ds = \lambda\Phi(t)\ t \in D. \tag{1}$$

Discretize with a quadrature rule ($\{w_j\}$ are the weights and $\{s_j\}$ are the quadrature points):

$$\sum_{j=1}^{n} w_j k(x,s_j)\tilde{\phi}(s_j) = \tilde{\lambda}\tilde{\phi}(x). \tag{2}$$

Choose a set $\{x_i\}$ of Nyström points (often the same as $\{s_i\}$):

$$\sum_{j=1}^{n} w_j k(x_i,s_j)\tilde{\phi}(s_j) = \tilde{\lambda}\tilde{\phi}(x_i). \tag{3}$$

Extend the eigenvectors $\tilde{\phi}_m$ on the Nyström points to $\bar{\phi}_m(x)$ on $D$:

$$\bar{\phi}_m(x) = \frac{1}{\tilde{\lambda}_m}\sum_{j=1}^{n} w_j k(x,s_j)\tilde{\phi}_m(s_j). \tag{4}$$

$\bar{\phi}_m(x)$ is the *Nyström extension* of $\tilde{\phi}_m$ and it approximates $\Phi_m$.

# The Nystrom Method (2 of 3)

Partition an $m \times n$ matrix $A$ as:

$$A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}. \tag{1}$$

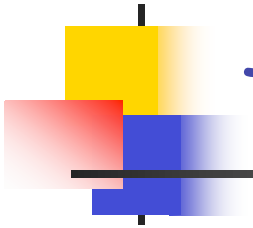
Let the SVD of $A_{11}$ be $A_{11} = \tilde{U}\tilde{\Sigma}\tilde{V}^T$. The Nyström extension of $\tilde{U}$ and $\tilde{V}$ gives:

$$\bar{U} = \begin{bmatrix} \tilde{U} \\ A_{21}\tilde{V}\tilde{\Sigma}^{-1} \end{bmatrix} \text{ and } \bar{V} = \begin{bmatrix} \tilde{V} \\ A_{12}^T\tilde{U}\tilde{\Sigma}^{-1} \end{bmatrix}. \tag{2}$$

Then, to approximate $A$ (via matrix completion), set $\tilde{A} = \bar{U}\tilde{\Sigma}\bar{V}^T$:

$$\tilde{A} = \begin{bmatrix} \tilde{U} \\ A_{21}\tilde{V}\tilde{\Sigma}^{-1} \end{bmatrix} \tilde{\Sigma} \begin{bmatrix} \tilde{V}^T & \tilde{\Sigma}^{-1}\tilde{U}^T A_{12} \end{bmatrix} \tag{3}$$

$$= \begin{bmatrix} A_{11} \\ A_{21} \end{bmatrix} A_{11}^{+} \begin{bmatrix} A_{11} & A_{12} \end{bmatrix}. \tag{4}$$



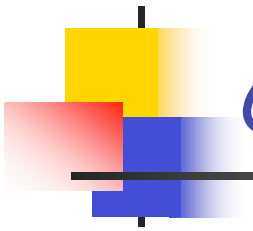
# The Nystrom Method (3 of 3)

Randomized SVD Algorithms (of Frieze, Kannan, and Vempala, and Drineas, Kannan, and Mahoney)

- Randomly sample columns (xor rows).
- Compute/approximate low-dimensional singular vectors.
- Nystrom-extend to approximate $H_k$, the high-dim. sing. vect.
- Bound $||A-H_kH_k^TA||_{2,F} <= ||A-A_k||_{2,F} + \varepsilon||A||_F$.

Randomized CUR Algorithms (of Drineas, Kannan, and Mahoney)

- Randomly sample columns and rows
- Bound $||A-CUR||_{2,F} <= ||A-A_k||_{2,F} + \varepsilon||A||_F$.
- Does not need or use the SPSD property



# Conclusion

Main Result: We randomly sample columns (biased towards longer columns) of a Gram matrix $G$ to get an approximation s.t.:

$$||G-CW_k^{+}C^T||_{2,F} <= ||G-G_k||_{2,F} + \varepsilon||X||_F^2.$$

Open problem: Sample with respect to probabilities that include correlations, preserve the SPSD property, and obtain bounds with an additional error of $\varepsilon||G||_F$. (Probably a corollary of general CUR.)