LARGE-SCALE KERNEL METHODS

MDI 341, MS Big Data, Télécom ParisTech

Aurélien Bellet

Inria Lille

March 20, 2017

OUTLINE

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REMINDER ON KERNEL METHODS

NOTATIONS

- Training observations $x_1, \ldots, x_n \in \mathcal{X}$
- For now, we assume $\mathcal{X} \subset \mathbb{R}^p$
- Training labels $y_1, \ldots, y_n \in \{-1, 1\}$
- Linear classifier with parameters $w \in \mathbb{R}^p$, $b \in \mathbb{R}$:

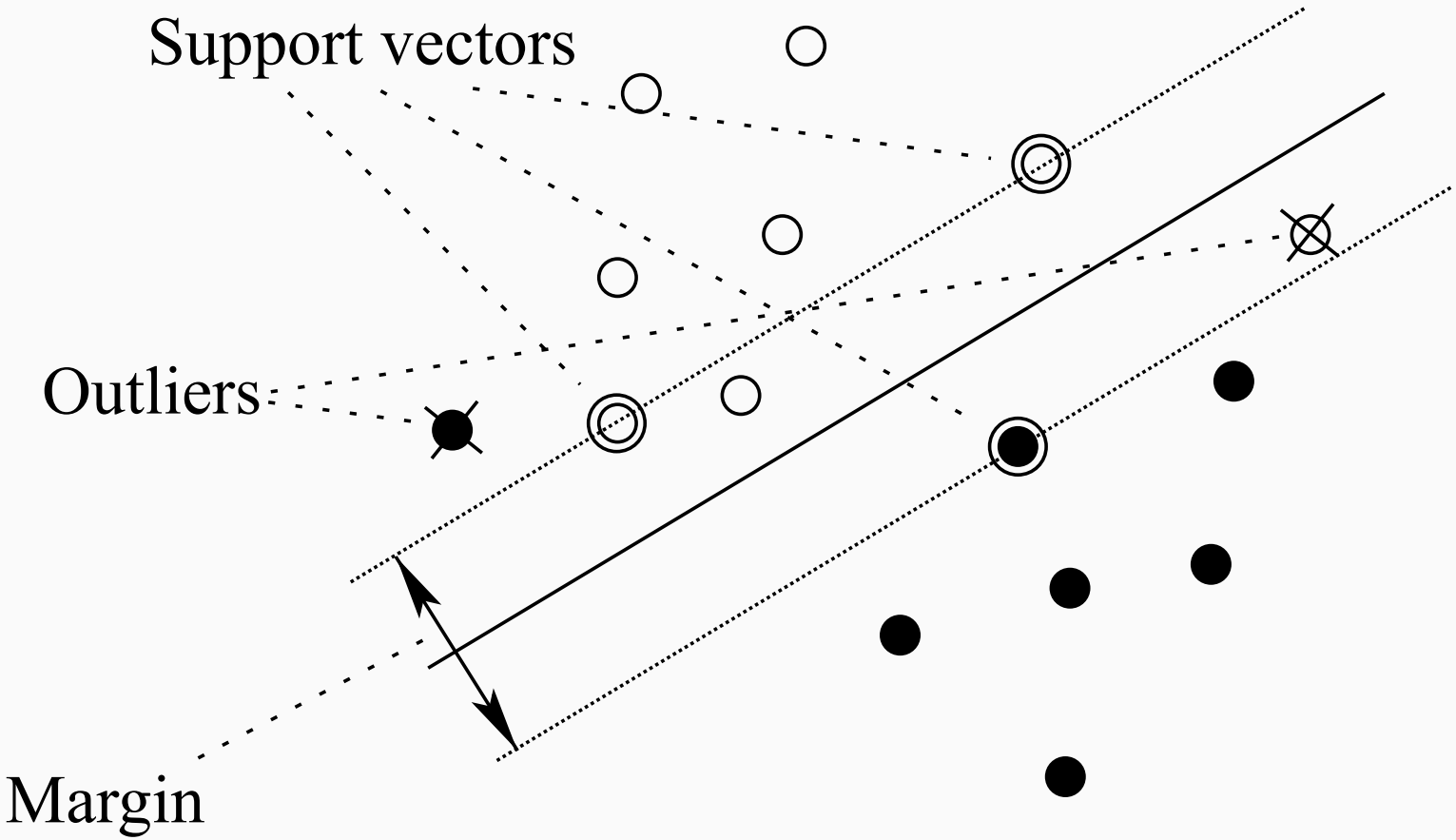
$$f(x) = \text{sign}(w^T x + b)$$

SVM: primal formulation

$$\begin{aligned} \min_{\boldsymbol{w}\in\mathbb{R}^p, b\in\mathbb{R}, \boldsymbol{\xi}\in\mathbb{R}^n} \quad & \frac{1}{2}\|\boldsymbol{w}\|_2^2 \quad + \quad C\sum_{i=1}^{n}\xi_i \\ \text{s.t.} \quad & y_i(\boldsymbol{w}^T\boldsymbol{x}+b) \geq 1-\xi_i \quad i=1,\ldots,n \\ & \xi_i \geq 0 \quad i=1,\ldots,n \end{aligned}$$

- Key principle: margin maximization
- Convex optimization problem

SUPPORT VECTOR MACHINES: PRIMAL

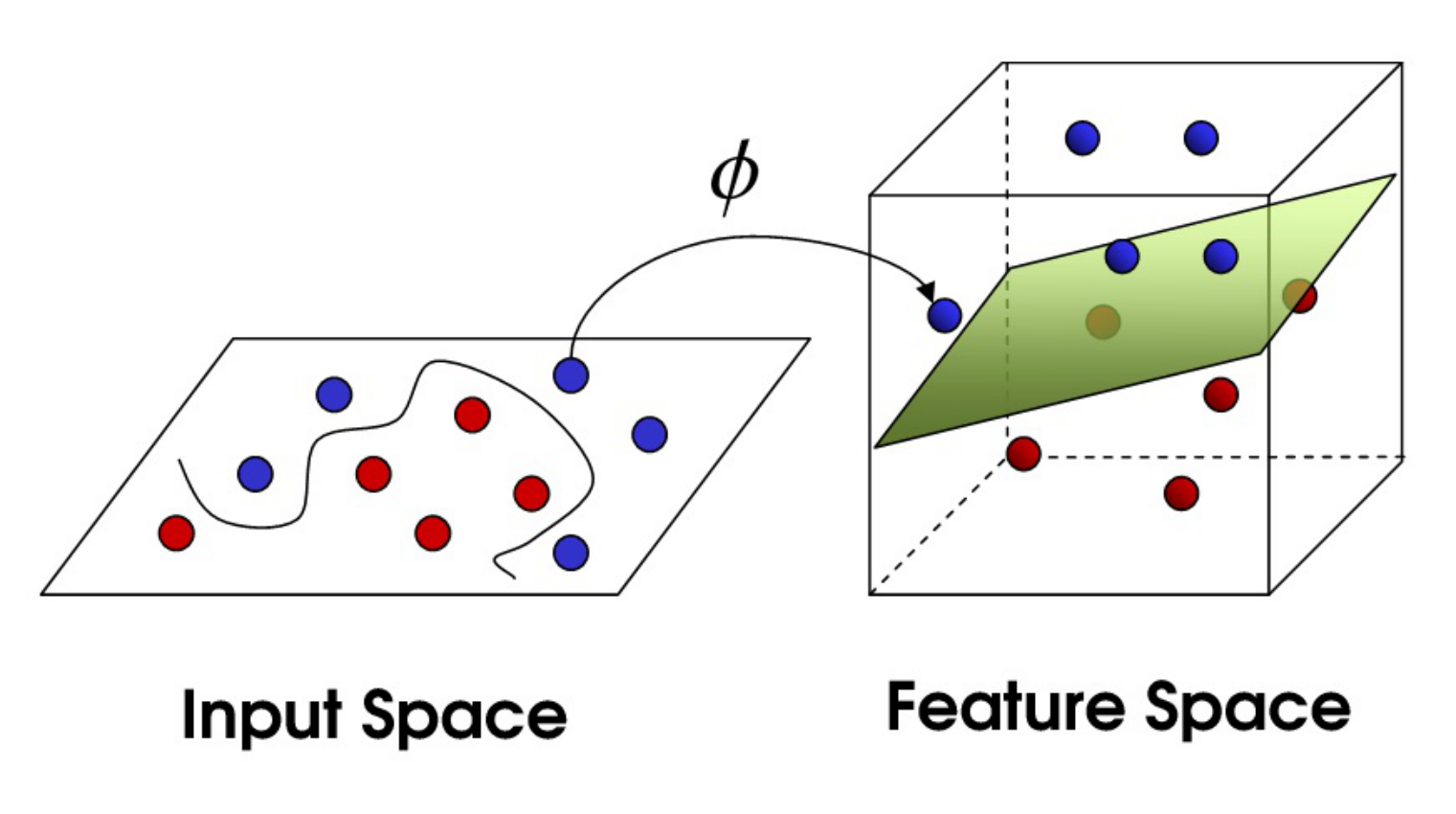


SVM: Lagrange dual formulation

$$\begin{aligned} \max_{\boldsymbol{\alpha} \in \mathbb{R}^n} \quad & \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \boldsymbol{x}_i^T \boldsymbol{x}_j \\ \text{s.t.} \quad & 0 \leq \alpha_i \leq C \quad i = 1, \ldots, n \\ & \sum_{i=1}^{n} \alpha_i y_i = 0 \end{aligned}$$

- Also convex
- We have $\boldsymbol{w} = \sum_{i=1}^{n} \alpha_i y_i \boldsymbol{x}_i$ and thus

$$f(\boldsymbol{x}) = \text{sign} \left(\sum_{i=1}^{n} \alpha_i y_i \boldsymbol{x}^T \boldsymbol{x}_i \right)$$


ϕ
Input Space
Feature Space

Definition (Kernel function)

A symmetric function $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a *kernel* if there exists a mapping function $\phi : \mathcal{X} \to \mathbb{H}$ from the instance space $\mathcal{X}$ to a Hilbert space $\mathbb{H}$ such that K can be written as an inner product in $\mathbb{H}$:

$$K(x, x') = \langle \phi(x), \phi(x') \rangle .$$

Equivalently, K is a *kernel* if it is symmetric positive semi-definite (PSD), i.e.,

$$\sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j K(x_i, x_j) \geq 0$$

for all finite sequences of $x_1, \ldots, x_n \in \mathcal{X}$ and $c_1, \ldots, c_n \in \mathbb{R}$.

Kernel SVM formulation

$$\max_{\boldsymbol{\alpha} \in \mathbb{R}^n} \quad \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j K(\boldsymbol{x}_i, \boldsymbol{x}_j)$$

$$\text{s.t.} \quad 0 \leq \alpha_i \leq C \quad i = 1, \ldots, n$$

$$\sum_{i=1}^{n} \alpha_i y_i = 0$$

- We have $\boldsymbol{w} = \sum_{i=1}^{n} \alpha_i y_i \phi(\boldsymbol{x}_i)$ and thus

$$f(\boldsymbol{x}) = \text{sign} \left(\sum_{i=1}^{n} \alpha_i y_i K(\boldsymbol{x}, \boldsymbol{x}_i) \right)$$

KERNELS: EXAMPLES

- Kernels between vectors
  - Linear kernel: $K(\boldsymbol{x}, \boldsymbol{x}') = \boldsymbol{x}^T \boldsymbol{x}'$
  - Polynomial kernel: $K(\boldsymbol{x}, \boldsymbol{x}') = (\boldsymbol{x}^T \boldsymbol{x}' + c)^d$
  - Gaussian RBF kernel: $K(\boldsymbol{x}, \boldsymbol{x}') = \exp(-\gamma \|\boldsymbol{x} - \boldsymbol{x}'\|_2^2)$
  - Laplace RBF kernel: $K(\boldsymbol{x}, \boldsymbol{x}') = \exp(-\gamma \|\boldsymbol{x} - \boldsymbol{x}'\|_1)$
- Kernels on structured data
  - Many string, tree and graph kernels [Gärtner, 2003]
  - Frameworks to design structured kernels: convolution kernels [Haussler, 1999], mapping kernels [Shin and Kuboyama, 2008]
- Use closure properties to build new kernels from existing ones
  - Sums, positive combinations, etc

KERNELS: APPLICATIONS

- Kernels allow to obtain nonlinear variants for many linear machine learning algorithms
- A few examples
  - SVM
  - Ridge regression
  - PCA
  - CCA
  - K-Means
- Today's topic: scalability of kernel methods
  - Identify general issues
  - Study general solutions

SCALABILITY ISSUES

TRAINING TIME COMPLEXITY

- All kernel methods rely on the Gram matrix $\boldsymbol{G} \in \mathbb{R}^{n \times n}$

$$\boldsymbol{G} = \begin{pmatrix} K(\boldsymbol{x}_1, \boldsymbol{x}_1) & K(\boldsymbol{x}_1, \boldsymbol{x}_2) & \cdots & K(\boldsymbol{x}_1, \boldsymbol{x}_n) \\ K(\boldsymbol{x}_2, \boldsymbol{x}_1) & K(\boldsymbol{x}_2, \boldsymbol{x}_2) & \cdots & K(\boldsymbol{x}_2, \boldsymbol{x}_n) \\ \vdots & \vdots & \ddots & \vdots \\ K(\boldsymbol{x}_n, \boldsymbol{x}_1) & K(\boldsymbol{x}_n, \boldsymbol{x}_2) & \cdots & K(\boldsymbol{x}_n, \boldsymbol{x}_n) \end{pmatrix}$$

- Assuming complexity of one kernel evaluation is constant
  - Constructing $\boldsymbol{G}$ takes $O(n^2)$ time
  - If we need to invert $\boldsymbol{G}$ (e.g., Kernel Ridge Regression): $O(n^3)$ time
- **Training time of popular algorithms:** $O(n^2)$ or $O(n^3)$
- This is infeasible for large n

TEST TIME COMPLEXITY

- Kernel methods are nonparametric: the learned model relies on the training data points
- To process a test point $\boldsymbol{x}$, one generally needs to evaluate the kernel between $\boldsymbol{x}$ and the training points
  - For instance in SVM:

$$f(\boldsymbol{x}) = \text{sign}\left(\sum_{i=1}^{n} \alpha_i y_i K(\boldsymbol{x}, \boldsymbol{x}_i)\right)$$

  - Number of support vectors grows linearly with n [Steinwart, 2003]
- **Prediction time of kernel methods:** $O(n)$
- This is slow when n is large

SCALING UP KERNEL METHODS

- Today we will study two techniques which can be used to scale up any kernel method
- Random Kernel Features: approximate kernel function / map
- Nyström Approximation: approximate Gram matrix
- Both methods are very popular and successful in practice
- Still an active area of research

RANDOM KERNEL FEATURES

Kernel SVM : primal formulation

$$\min_{\boldsymbol{w},b} \quad \frac{1}{2}\|\boldsymbol{w}\|_2^2 \quad + \quad C\sum_{i=1}^{n}\left[y_i(\boldsymbol{w}^T\phi(\boldsymbol{x})+b)\right]_+$$

where $[a]_+ = \max(0, 1-a)$ is the hinge loss function

- When $\phi(\boldsymbol{x})$ is known and finite-dimensional (e.g., linear kernel)
  - Training time linear in n (see e.g., [Shalev-Shwartz et al., 2011])
  - Prediction complexity independent of n
- But $\phi(\boldsymbol{x})$ is usually unknown and potentially infinite-dimensional
- In this case we can only solve the problem in dual form
  - Training time quadratic or cubic in n
  - Prediction complexity linear in n

FEATURE MAP APPROXIMATION

- **Idea:** find a finite-dimensional feature map $\hat{\phi}(x) \in \mathbb{R}^c$ such that

$$\left\langle \hat{\phi}(x), \hat{\phi}(x') \right\rangle \approx K(x, x')$$

- We can then solve in primal form to get $w \in \mathbb{R}^c$ and $b \in \mathbb{R}$
- We can predict using

$$f(x) = \text{sign}(w^T \hat{\phi}(x) + b)$$

- If $c \ll n^2$, training is much faster
- If $c \ll n$, prediction is also much faster

Definition (Shift-invariant kernel)

Let $K : \mathbb{R}^p \times \mathbb{R}^p \to \mathbb{R}$ be a positive definite kernel. K is said to be *shift-invariant* if for any $\boldsymbol{a} \in \mathbb{R}^p$ and any $(\boldsymbol{x}, \boldsymbol{x'}) \in \mathbb{R}^p \times \mathbb{R}^p$

$$K(\boldsymbol{x} - \boldsymbol{a}, \boldsymbol{x}' - \boldsymbol{a}) = K(\boldsymbol{x}, \boldsymbol{x}').$$

For simplicity we denote $K(\boldsymbol{x}, \boldsymbol{x}') = K(\boldsymbol{x} - \boldsymbol{x}')$.

- Examples of shift-invariant kernels
  - Gaussian RBF kernel: $K(\boldsymbol{x} - \boldsymbol{x}') = \exp(-\gamma \|\boldsymbol{x} - \boldsymbol{x}'\|_2^2)$
  - Laplace kernel: $K(\boldsymbol{x} - \boldsymbol{x}') = \exp(-\gamma \|\boldsymbol{x} - \boldsymbol{x}'\|_1)$

Bochner's theorem

Theorem (Bochner's theorem, see [Rahimi and Recht, 2007])

A continuous shift-invariant kernel $K(\boldsymbol{x}, \boldsymbol{x}') = K(\boldsymbol{x} - \boldsymbol{x}')$ is positive definite if and only if $K(\boldsymbol{\delta})$ is the Fourier transform of a nonnegative measure. In particular, if K is properly scaled, we have

$$K(\boldsymbol{x} - \boldsymbol{x}') = \int_{\mathbb{R}^p} P(\boldsymbol{\omega}) e^{i\boldsymbol{\omega}^T \boldsymbol{x}} e^{-i\boldsymbol{\omega}^T \boldsymbol{x}'} d\boldsymbol{\omega},$$

where $P(\boldsymbol{\omega})$ is a real-valued probability density function over $\mathbb{R}^p$.

BOCHNER'S THEOREM

Developing the result of Bochner's theorem:

$$
\begin{aligned}
K(x - x') &= \int_{\mathbb{R}^p} P(\omega) e^{i\omega^T x} e^{-i\omega^T x'} d\omega \\
&= \int_{\mathbb{R}^p} P(\omega) \cos(\omega^T x - \omega^T x') d\omega && (1) \\
&= \int_{\mathbb{R}^p} P(\omega) \left(\cos(\omega^T x) \cos(\omega^T x') + \sin(\omega^T x) \sin(\omega^T x') \right) d\omega && (2) \\
&= \int_{\mathbb{R}^p} \int_{b=0}^{2\pi} \frac{P(\omega)}{2\pi} 2 \cos(\omega^T x + b) \cos(\omega^T x' + b) d\omega db && (3) \\
&= \mathbb{E}_{\omega \sim P, b \sim \mathcal{U}(0,2\pi)} \left[\sqrt{2} \cos(\omega^T x + b) \sqrt{2} \cos(\omega^T x' + b) \right] && (4)
\end{aligned}
$$

(1): $K(x - x'), P(\omega) \in \mathbb{R}$ so we can ignore imaginary part

(2) and (3): use sum of angles formulas

BOCHNER'S THEOREM

- We have obtained

$$K(\boldsymbol{x} - \boldsymbol{x}') = \mathbb{E}_{\boldsymbol{\omega} \sim P, b \sim \mathcal{U}(0, 2\pi)} \left[\sqrt{2} \cos(\boldsymbol{\omega}^T \boldsymbol{x} + b) \sqrt{2} \cos(\boldsymbol{\omega}^T \boldsymbol{x}' + b) \right]$$

- K can thus be written as an expectation over $\boldsymbol{\omega}$ drawn from the distribution P

- If we know P for the kernel K of interest, we can approximate K by random sampling

RANDOM KERNEL FEATURES: METHOD

1. Set number of random kernel features c
2. Draw $\boldsymbol{\omega}_1, \ldots, \boldsymbol{\omega}_c \sim P(\boldsymbol{\omega})$ and $b_1, \ldots, b_c \sim \mathcal{U}(0, 2\pi)$
3. Map training points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in \mathbb{R}^p$ to their random kernel features $\hat{\phi}(\boldsymbol{x}_1), \ldots, \hat{\phi}(\boldsymbol{x}_n) \in \mathbb{R}^c$ where

$$\hat{\phi}_j(\boldsymbol{x}) = \sqrt{\frac{2}{c}} \cos(\boldsymbol{\omega}_j^T \boldsymbol{x} + b_j), \quad j \in \{1, \ldots, c\}$$

4. Train linear model (such as linear SVM) on transformed data $\hat{\phi}(\boldsymbol{x}_1), \ldots, \hat{\phi}(\boldsymbol{x}_n) \in \mathbb{R}^c$

RANDOM KERNEL FEATURES: EXAMPLES

- For the Gaussian RBF kernel, P is a Gaussian distribution

$$P^{rbf}(\boldsymbol{\omega}) = \mathcal{N}(0, 2\gamma \mathbf{I}_p)$$

- For the Laplace kernel, P is a Cauchy distribution

$$P^{lap}(\boldsymbol{\omega}) = \prod_p \frac{1}{\pi(1 + \omega_p^2/2\gamma)}$$

Theorem ([Rahimi and Recht, 2007])

Let $c \geq 1$ and $\hat{\phi} : \mathbb{R}^p \to \mathbb{R}^c$ be the feature map obtained by drawing $\boldsymbol{\omega}_1, \ldots, \boldsymbol{\omega}_c$ from $P(\boldsymbol{\omega})$. Then we have with high probability:

$$\sup_{x, x' \in \mathcal{X}} \left| \left\langle \hat{\phi}(x), \hat{\phi}(x') \right\rangle - K(x, x') \right| \leq O\left(\sqrt{\frac{p}{c}} \right)$$

- Kernel approximation error uniformly decreases in $O(\sqrt{1/c})$
- Can also bound generalization error [Rahimi and Recht, 2008]

ADDITIONAL COMMENTS

- Example of large-scale application: acoustic models for speech recognition [Lu et al., 2016]
  - Trained on 50 hours of speech with $c = 500K$ random features
  - Performance comparable to deep neural nets
- Random features exist for other kernels, such as dot product kernels (including polynomial kernels) [Kar and Karnick, 2012]
- Techniques to speed up prediction further [Le et al., 2013]
  - From $O(cp)$ to $O(c \log p)$ time
- Easy to combine multiple kernels by stacking their random features [Lu et al., 2014]

NYSTRÖM APPROXIMATION

LOW-RANK APPROXIMATION

- Let us consider the Gram matrix $\boldsymbol{G} \in \mathbb{R}^{n \times n}$ $(G_{ij} = K(\boldsymbol{x}_i, \boldsymbol{x}_j))$
- When n is large, could approximate $\boldsymbol{G}$ with a matrix of rank $k \leq n$
- Consider the spectral decomposition of $\boldsymbol{G}$

$$\boldsymbol{G} = \boldsymbol{U} \boldsymbol{\Lambda} \boldsymbol{U}^T$$

  - $\boldsymbol{U} = [\boldsymbol{u}_1, \ldots, \boldsymbol{u}_n]^T \in \mathbb{R}^{n \times n}$ the set of eigenvectors
  - $\boldsymbol{\Lambda} = \text{diag}(\lambda_1, \ldots, \lambda_n)$ the eigenvalues $(\lambda_1 \geq \cdots \geq \lambda_n)$

- Best rank-k approximation $\boldsymbol{G}_k \in \mathbb{R}^{n \times n}$ is given by

$$\boldsymbol{G}_k = \boldsymbol{U}_k \boldsymbol{\Lambda}_k \boldsymbol{U}_k^T$$

where $\boldsymbol{U}_k = [\boldsymbol{u}_1, \ldots, \boldsymbol{u}_k]^T \in \mathbb{R}^{n \times k}$ and $\boldsymbol{\Lambda}_k = \text{diag}(\lambda_1, \ldots, \lambda_k)$

NYSTRÖM APPROXIMATION

- In the context of kernel methods this is useless
  - We still need to construct $\boldsymbol{G}$: $O(n^2)$ time
  - And compute its k-thresholded spectral decomposition: between $O(n^2)$ and $O(n^3)$ depending on the value of k
- Alternative: Nyström approximation [Drineas and Mahoney, 2005]
  1. Sample a set $\mathcal{I}$ of c indices uniformly in $\{1, \ldots, n\}$
  2. Compute $\boldsymbol{C} \in \mathbb{R}^{n \times c}$ with $\boldsymbol{C}_{i,j} = K(\boldsymbol{x}_i, \boldsymbol{x}_j)$ for $i \in \{1, \ldots, n\}$ and $j \in \mathcal{I}$
  3. Form reduced Gram matrix $\tilde{\boldsymbol{G}} \in \mathbb{R}^{c \times c}$ with $\tilde{\boldsymbol{G}}_{i,j} = K(\boldsymbol{x}_i, \boldsymbol{x}_j)$ for $i, j \in \mathcal{I}$
  4. Compute $\tilde{\boldsymbol{G}}_k \in \mathbb{R}^{c \times c}$, the best rank-$k$ approximation of $\tilde{\boldsymbol{G}}$ ($k \leq c$)
  5. Final Gram matrix approximation $\hat{G} \in \mathbb{R}^{n \times n}$

$$\boldsymbol{G}_{nys} \in \mathbb{R}^{n \times n} = \boldsymbol{C} \tilde{\boldsymbol{G}}_k^{+} \boldsymbol{C}^T$$

  where $\tilde{\boldsymbol{G}}_k^{+}$ is the pseudoinverse of $\tilde{\boldsymbol{G}}_k$

- Time complexity is $O(c^3 + nck)$

Theorem ([Drineas and Mahoney, 2005])

Let $G \in \mathbb{R}^{n \times n}$ be the Gram matrix. Let G_k be its best rank-k approximation and G_{nys} be its Nyström approximation. We have with high probability:

$$\|G - G_{nys}\|_F \leq \|G - G_k\|_F + O\left(\sqrt{\frac{n}{c}}\right)$$

- If c is large enough, G_{nys} is nearly as good as G_k
- Some nonuniform sampling techniques have been proposed, but uniform sampling tends to work best in practice [Kumar et al., 2009]

EXPLICIT FEATURE MAP

- G_{nys} can be used directly to speed up training algorithms
- It can also be used to generate an explicit feature map an in RKF
- Denote $\tilde{G}_k = \tilde{U}_k \tilde{\Lambda}_k \tilde{U}_k^T$
- Approximate feature map $\hat{\phi}(x) \in \mathbb{R}^k$ is given by

$$\hat{\phi}(x) = k_{x,\mathcal{I}} \tilde{U}_k \tilde{\Lambda}_k^{-1/2}$$

where $k_{x,\mathcal{I}} = [K(x, x_i)]_{i \in \mathcal{I}}$

CONCLUSION

NYSTRÖM APPROXIMATION *VS.* RANDOM KERNEL FEATURES

- Both methods have a $O(1/\sqrt{c})$ convergence rate (c: # of random features for RKF, # of random columns for Nyström)
- Nyström' approximation guarantee is adaptive to the data, while RKF is data-independent
  - In fact, Nyström can achieve $O(1/c)$ convergence when eigengap of $\boldsymbol{G}$ is large [Yang et al., 2012]
- At equal number of random samples (features/columns)
  - Nyström tends to achieve better performance
  - But RKF are generally cheaper to generate (no spectral decomposition or matrix inversion needed)
- Lacks a solid large-scale comparison

CONCLUSION

- Kernel methods: general class of nonlinear algorithms
- Training and prediction time scales badly with n
- Two general techniques to make kernel methods scalable: Random Kernel Features and Nyström approximation
- We can then take advantage of existing fast solvers for linear algorithms

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