

LARGE-SCALE KERNEL METHODS

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1. Reminder on Kernel Methods
2. Scalability Issues
3. Random Kernel Features
4. Nyström Approximation
5. Conclusion

REMINDER ON KERNEL METHODS

- Training observations $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathcal{X}$
- For now, we assume $\mathcal{X} \subset \mathbb{R}^p$
- Training labels $y_1, \dots, y_n \in \{-1, 1\}$
- Linear classifier with parameters $\mathbf{w} \in \mathbb{R}^p, b \in \mathbb{R}$:

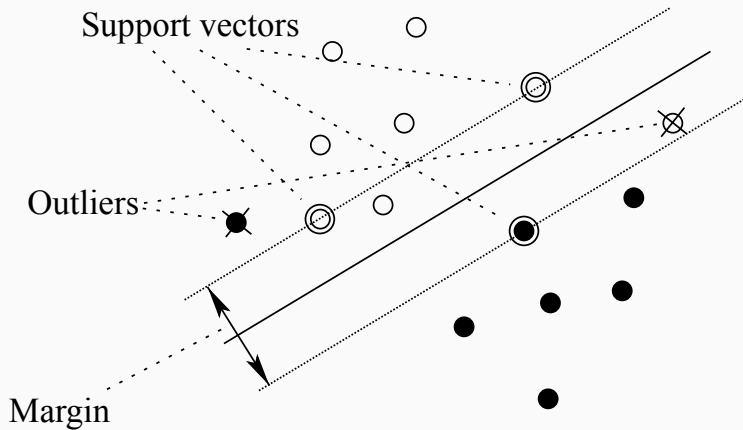
$$f(\mathbf{x}) = \text{sign}(\mathbf{w}^T \mathbf{x} + b)$$

SVM: primal formulation

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

- Key principle: **margin maximization**
- Convex optimization problem

SUPPORT VECTOR MACHINES: PRIMAL



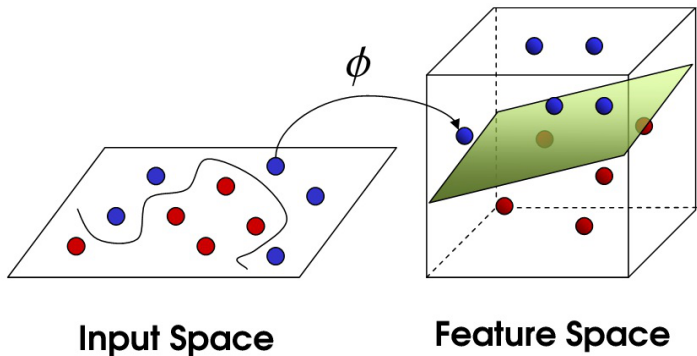
SVM: Lagrange dual formulation

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

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

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

- Note: b can be deduced from support vectors



Definition (Kernel function)

A symmetric function $K : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}$ is a *kernel* if there exists a mapping function $\phi : \mathcal{X} \rightarrow \mathbb{H}$ 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} :

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

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

$$\sum_{i=1}^n \sum_{j=1}^n c_i c_j K(\mathbf{x}_i, \mathbf{x}_j) \geq 0$$

for all finite sequences of $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathcal{X}$ and $c_1, \dots, c_n \in \mathbb{R}$.

Kernel SVM formulation

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

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

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

- Kernels between vectors
 - Linear kernel: $K(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T \mathbf{x}'$
 - Polynomial kernel: $K(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^T \mathbf{x}' + c)^d$
 - Gaussian RBF kernel: $K(\mathbf{x}, \mathbf{x}') = \exp(-\gamma \|\mathbf{x} - \mathbf{x}'\|_2^2)$
 - Laplace RBF kernel: $K(\mathbf{x}, \mathbf{x}') = \exp(-\gamma \|\mathbf{x} - \mathbf{x}'\|_1)$
- 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 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

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

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

- Assuming complexity of one kernel evaluation is constant
 - Constructing \mathbf{G} takes $O(n^2)$ time
 - If we need to invert \mathbf{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

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

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

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

- 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

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

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

- When $\phi(\mathbf{x})$ 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 $\phi(\mathbf{x})$ 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

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

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

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

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

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

Definition (Shift-invariant kernel)

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

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

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

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

BOCHNER'S THEOREM

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

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

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

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

BOCHNER'S THEOREM

Developing the result of Bochner's theorem:

$$\begin{aligned} K(\mathbf{x} - \mathbf{x}') &= \int_{\mathbb{R}^p} P(\boldsymbol{\omega}) e^{i\boldsymbol{\omega}^T \mathbf{x}} e^{-i\boldsymbol{\omega}^T \mathbf{x}'} d\boldsymbol{\omega} \\ &= \int_{\mathbb{R}^p} P(\boldsymbol{\omega}) \cos(\boldsymbol{\omega}^T \mathbf{x} - \boldsymbol{\omega}^T \mathbf{x}') d\boldsymbol{\omega} \end{aligned} \quad (1)$$

$$= \int_{\mathbb{R}^p} P(\boldsymbol{\omega}) \left(\cos(\boldsymbol{\omega}^T \mathbf{x}) \cos(\boldsymbol{\omega}^T \mathbf{x}') + \sin(\boldsymbol{\omega}^T \mathbf{x}) \sin(\boldsymbol{\omega}^T \mathbf{x}') \right) d\boldsymbol{\omega} \quad (2)$$

$$= \int_{\mathbb{R}^p} \int_{b=0}^{2\pi} \frac{P(\boldsymbol{\omega})}{2\pi} 2 \cos(\boldsymbol{\omega}^T \mathbf{x} + b) \cos(\boldsymbol{\omega}^T \mathbf{x}' + b) d\boldsymbol{\omega} db \quad (3)$$

$$= \mathbb{E}_{\boldsymbol{\omega} \sim P, b \sim \mathcal{U}(0, 2\pi)} \left[\sqrt{2} \cos(\boldsymbol{\omega}^T \mathbf{x} + b) \sqrt{2} \cos(\boldsymbol{\omega}^T \mathbf{x}' + b) \right] \quad (4)$$

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

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

- We have obtained

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

- K can thus be written as an expectation over $\boldsymbol{\omega}$ drawn from the distribution P
- If we know how to sample from P (the Fourier transform of K), we can approximate K by random sampling

RANDOM KERNEL FEATURES: EXAMPLES

- P is given by the (scaled) Fourier transform of $K(\Delta)$

$$P(\omega) = \frac{1}{(2\pi)^p} \int_{\mathbb{R}^p} K(\Delta) e^{-i\omega^T \Delta} d\Delta$$

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

$$\begin{aligned} p^{rbf}(\omega) &= \frac{1}{(2\pi)^p} \int_{\mathbb{R}^p} e^{-\gamma \|\Delta\|_2^2} e^{-i\omega^T \Delta} d\Delta \\ &= \frac{1}{\sqrt{(2\pi)^p 2\gamma}} \int_{\mathbb{R}^p} \frac{1}{\sqrt{(2\pi)^p \frac{1}{2\gamma}}} e^{-\gamma \|\Delta\|_2^2} e^{-i\omega^T \Delta} d\Delta \\ &= \frac{1}{\sqrt{(2\pi)^p 2\gamma}} e^{-\frac{\|\omega\|_2^2}{4\gamma}} = \mathcal{N}(0, 2\gamma \mathbf{I}_p) \end{aligned}$$

- For the **Laplace kernel**, P is a Cauchy distribution

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

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

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

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

Theorem ([Rahimi and Recht, 2007])

Let $c \geq 1$ and $\hat{\phi} : \mathbb{R}^p \rightarrow \mathbb{R}^c$ be the feature map obtained by drawing $\omega_1, \dots, \omega_c$ from $P(\omega)$. Then we have with high probability:

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

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

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

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

- $\mathbf{U} = [\mathbf{u}_1, \dots, \mathbf{u}_n]^T \in \mathbb{R}^{n \times n}$ the set of eigenvectors
- $\mathbf{\Lambda} = \text{diag}(\lambda_1, \dots, \lambda_n)$ the eigenvalues ($\lambda_1 \geq \dots \geq \lambda_n$)
- **Best rank- k approximation** $\mathbf{G}_k \in \mathbb{R}^{n \times n}$ is given by

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

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

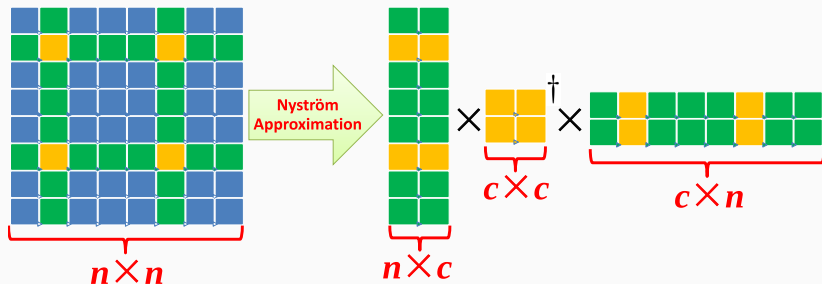
- In the context of kernel methods this is useless
 - We still need to construct \mathbf{G} : $O(n^2)$ time
 - We need to compute its k -thresholded spectral decomposition \mathbf{G}_k : $O(n^2)$ to $O(n^3)$ time depending on the value of k
- **Goal:** find good approximation $\hat{\mathbf{G}}_k$ of \mathbf{G}_k in $O(n)$ time

NYSTRÖM APPROXIMATION

- Nyström approximation [Drineas and Mahoney, 2005]:

$$\hat{G}_k = CW^\dagger C^T$$

where $C \in \mathbb{R}^{n \times c}$, $W \in \mathbb{R}^{c \times c}$ and W^\dagger is the pseudo-inverse of W



- For intuition: think of approximation of distances between cities

NYSTRÖM APPROXIMATION: GENERAL ALGORITHM

1. Sample a set \mathcal{I} of c indices uniformly in $\{1, \dots, n\}$
2. Compute $\mathbf{C} \in \mathbb{R}^{n \times c}$ with $\mathbf{C}_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$ for $i \in \{1, \dots, n\}$ and $j \in \mathcal{I}$
3. Form matrix $\mathbf{W} \in \mathbb{R}^{c \times c}$ with $\mathbf{W}_{ij} = K(\mathbf{x}_i, \mathbf{x}_j)$ for $i, j \in \mathcal{I}$
4. Compute $\mathbf{W}_k \in \mathbb{R}^{c \times c}$, the best rank- k approximation of \mathbf{W} ($k \leq c$)
5. Final rank k approximation of \mathbf{G} :

$$\hat{\mathbf{G}}_k = \mathbf{C} \mathbf{W}_k^\dagger \mathbf{C}^T \in \mathbb{R}^{n \times n}$$

where \mathbf{W}_k^\dagger is the Moore-Penrose pseudoinverse of \mathbf{W}_k

Time complexity: $O(c^3 + nck)$

Theorem ([Drineas and Mahoney, 2005])

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

$$\|\mathbf{G} - \hat{\mathbf{G}}_k\|_F \leq \|\mathbf{G} - \mathbf{G}_k\|_F + O\left(\sqrt{\frac{n}{c}}\right)$$

- If c is large enough, $\hat{\mathbf{G}}_k$ is nearly as good as \mathbf{G}_k
- Setting $k < c$ removes the noise contained in smallest eigenvalues of \mathbf{W}
- Some nonuniform sampling techniques have been proposed, but uniform sampling tends to work best in practice
[Kumar et al., 2009]

NYSTRÖM APPROXIMATION: EXPLICIT FEATURE MAP

- $\hat{\mathbf{G}}_k$ can be used directly to speed up training algorithms
- It can also be used to generate an explicit feature map as in RKF
- Recall that $\hat{\mathbf{G}}_k = \mathbf{C}\mathbf{W}_k^\dagger\mathbf{C}^T$, denote $\mathbf{W}_k^\dagger = \mathbf{V}_k\mathbf{\Sigma}_k\mathbf{V}_k^T$
- For training points we have an explicit feature map given by:

$$\hat{\phi}(\mathbf{x}_i) = \mathbf{C}_i\mathbf{V}_k\mathbf{\Sigma}_k^{1/2}$$

- Natural extension to unseen points:

$$\hat{\phi}(\mathbf{x}) = \mathbf{k}_{\mathbf{x},\mathcal{I}}\mathbf{V}_k\mathbf{\Sigma}_k^{1/2}$$

where $\mathbf{k}_{\mathbf{x},\mathcal{I}} = [K(\mathbf{x}, \mathbf{x}_i)]_{i \in \mathcal{I}} \in \mathbb{R}^c$

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 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)

- 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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