Large Scale Kernel methods

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- MLRG

Outline

- Introduction to kernel methods
- Low rank approximation
  - Nystrom approximation
- Random Fourier Features
  - Random Kitchen Sink
  - Fastfood

Kernel

- Dataset $X \in R^{N \times D}$
  - N samples, D features
- A similarity function that takes two input vectors and spits out their similarity

$$K(X_i, X_j) = \phi(X_i) \cdot \phi(X_j)$$

- $\phi(X_i)$ is the feature representation of X_i in the higher dimensional space (possibly infinite)
  - Need not be explicitly computed
- Why kernels ?
  - $\phi(X_i) \cdot \phi(X_j)$ may have high dimensional complexity
  - $\phi(X_i) \cdot \phi(X_j)$ might be impossible to compute.
    - Gaussian Kernel: $\phi(X_j)$ projects X_j to infinite dimensions

Kernel

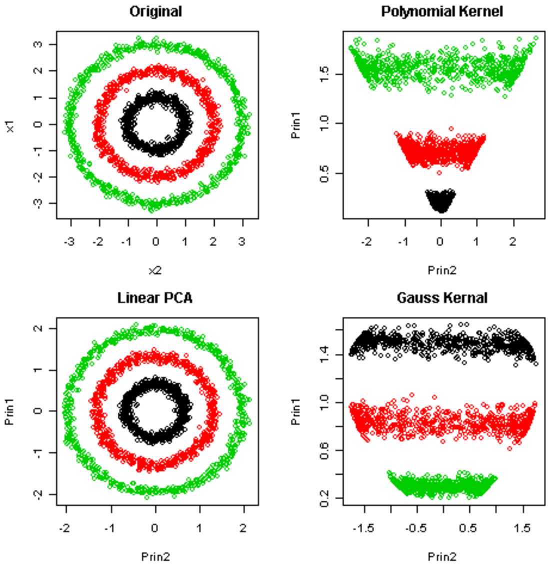


Figure 1:

Example

- Gaussian Kernel:
  - As, $K(X_i, X_j) = e^{-\frac{||X_i - X_j||^2}{2\sigma^2}}$
  - Also as, $K(X_i, X_j) = e^{-\frac{X_i \cdot X_j}{\sigma^2}}$
  - which is $K(X_i, X_j) = \sum_{n=0}^{\infty} \frac{(X_i \cdot X_j)^n}{\sigma^n n!}$
- Gaussian kernel is a combination of all polynomial kernels of degrees $n \geq 0$
- It's an infinite power series which converges

Kernel-based algorithms

- Dataset $X \in R^{N \times D}$, $y \in R^N$
  - N samples, D features
- SVMs, Kernel Ridge Regression, Gaussian Process Regression
- A Kernel matrix is a Gram matrix $K \in R^{N \times N}$
- Linear function expansion is

$$f(x) = \sum_i w_i K(X_i, X)$$

- Therefore, number of basis functions increases linearly in the number of observations
- Kernel Ridge Regression

$$w = [K + \lambda I]^{-1} zy$$

  - where $z_i = K(X_i, X)$
- Computational cost for large-scale problems
  - $\Omega(N^2)$ space.
  - $O(N^3)$ time for matrix inversion or SVD

Example

- Inverting a large matrix with $\mathrm{N} = 18\mathrm{M}$
- $K \approx 1300$ TB
- $320,000 \times 4$ GB RAM machines

Two main strategies

- Sampling-based low-rank approximation:
  - Compute and store only $T << N$ columns of K
  - Column-sampling using Nystrom method
- Explicit feature expansion (Fast feature extraction):
  - Fourier random features
  - Random Kitchen Sink, Fastfood

Original Nystrom Approximation

- Positive definite symmetric matrix $K \in R^{N \times N}$
- Computing the inverse - SVD on very large datasets can become prohibitive quickly for large N $O(N^3)$
- The Nystrom method is an efficient technique for the eigenvalue decomposition of large kernel matrices

Algorithm

- Input : Gram matrix K $\in RN \times N$
- Result : $\hat{K} \in R^{N \times N}$

1. Pick T columns of K in i.i.d trials, uniformly with replacement
2. Let I be the set of indices of the sampled columns
3. Let C be the $N \times T$ matrix containing the sampled columns
4. Let H be the $T \times T$ submatrix of K whose entries are K_{ij}, $i \in I$, $j \in I$
5. Return $\hat{K} = CH^{-1}C$

- Computes an approximation $\hat{K} \approx K$
- Computing SVD of H

$$O(T^3)$$

- Computing $\hat{K}$

$$O(N \cdot T \cdot k)$$

  - where k is the best rank-k approximation of K
  - $k \leq T$

Nyström Woodbury Approximation

- Kernel ridge regression

$$w = [K + \lambda I]^{-1} zy$$

- Computing $\underbrace{[K + \lambda I]^{-1}}_{O(N^3)}$
- Matrix inversion lemma

$$\begin{aligned}
(K + \lambda I)^{-1} &\approx (\hat{K} + \lambda I)^{-1} \\
&= (CH^{-1}C^T + \lambda I)^{-1} \\
&= \frac{1}{\lambda}(I - C(\lambda I + H^{-1}C^T C)^{-1} H^{-1} C^T) \\
&= \frac{1}{\lambda}(I - C\underbrace{(\lambda I + H^{-1}C^T C)^{-1}}_{O(T^3)} H^{-1} C^T)
\end{aligned}$$

- Inverting a $T \times T$ matrix instead

(Williams & Seeger, 2000)

Approximation Error

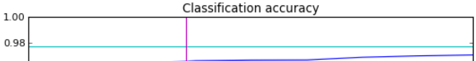
Drineas & Mahoney (2005)

Theorem 1:

- Let $\hat{K}$ be the best rank-k approximation of K
- Let $b = 1 + \sqrt{8 \log(1/\delta)}$
- Let ϵ be a small value larger than 0
- If $T \geq 4b^2/\epsilon^2$, then with probability at least $1 - \delta$

$$E[||K - \hat{K}||_F] \leq ||K - \hat{K}||_F + \epsilon \sum_{i=1}^{N} K_{ii}^2$$

- MNIST Dataset
  - 20000 taining examples and 10000 test examples.



Applications

- Examples
  - Spectral Clustering (Fowlkes et al., 2004).
  - Kernel Ridge Regression (Cortes, MM, and Talwalkar, AISTATS 2010).
  - Support Vector Machines (Fine and Scheinberg, 2001).
  - Kernel Logistic Regression (Karsmarker et al., 2007).
  - Manifold Learning (Kumar and Talwalkar, 2008)

Extensions on Nystrom

- We discussed unifom sampling of columns
- Other sampling methods include:
  - $l2$ norm of the columns
  - Non-uniformly $\propto$ diagonal elements K_{ii}
- Empirical results:
  - uniform sampling without replacement: best results and fastest for real-world datasets (Kumar, MM, and Talwalkar, 2009).
- Found to work great for sparse optimization

$$\min_{w} \frac{1}{2n} ||y - Kw||_2^2 + \lambda ||w||_1$$

2. Fourier Random Features

- Linear decision surface over the kernelized form,

$$f(x) = \sum_{i=1}^{N} w_i K(X_i, X)$$

- The Gram matrix K can be too large (10,000, 10,000)

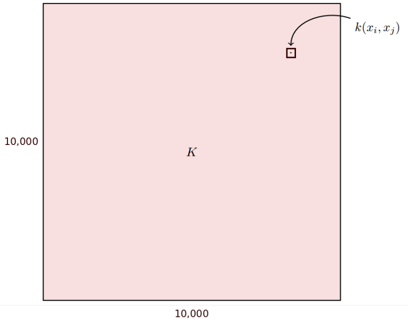


Figure 4:

2. Fourier Random Features

- Linear decision surface over the kernelized form,

$$f(x) = \sum_{i=1}^{N} w_i K(X_i, X)$$

- $K(X_i, X_j) = \phi(X_i) \cdot \phi(X_j)$
- Main Idea: Compute an approximated representation of $\phi(X_i)$
  - has $O(\log N)$ dimensional space
- Instead of computing $K \in R^{N \times N}$, compute $\phi(X) \in R^{N \times \log(N)}$
- For 10,000 images, $\log_{10}(10^4) = 4$
- Exact computation of $\phi(X)$

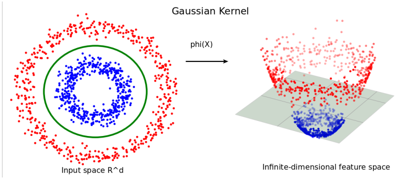


Figure 5:

2. Fourier Random Features

- Compute an approximation $\phi_z(X) \approx \phi(X)$ explicitly

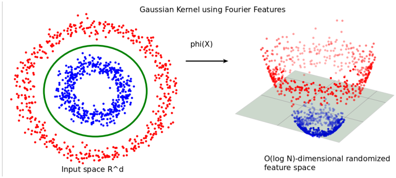


Figure 6:

- $K(X_i, X_j) = \phi(X_i) \cdot \phi(X_j)$
- Compute $\phi_z(X_i) \cdot \phi_z(X_j)$ such that

$$E_z[\phi_z(X_i)\phi_z(X_j)] = K(X_i, X_j)$$

2. Fourier Random Features

- Let K be a translation invariant kernel, that is,

$$K(X_i, X_j) = K(X_i - X_j, 0)$$

  - such as the gaussian kernel

- Bochner's Theorem: A kernel $K(X_i - X_j)$ is PSD iff $K(X_i - X_j)$ is the Fourier transform of a non-negative measure $p(z)$

$$K(X_i - X_j, 0) = \int_R e^{-iz(X_i - X_j)} p(z) dz$$

- where $p(z)$ is a positive finite measure which is when scaled is a proper probability distribution.

2. Fourier Random Features

- Therefore,

$$\begin{aligned}
k(X_i, X_j) &= k(X_i - X_j, 0) \\
&= \int_{R^d} p(z) e^{z(X_i - X_j)} dz \\
&\approx \frac{1}{T} \sum_{i=1}^{T} e^{jz_i(X_i - X_j)} && z_i \sim p(z) \ \text{iid, Monte-Carlo, } C \\
&= \frac{1}{T} \sum_{i=1}^{T} e^{jz_i X_i} e^{-jz_i X_j} \\
&= \frac{1}{\sqrt{T}} \phi_z(X_i) \frac{1}{\sqrt{(T)}} \phi_z(X_j)
\end{aligned}$$

2. Fourier Random Features

- To compute $e^{jz_i X_i}$, use the cosine identity

$$e^{\pm j\theta} = cos(\theta) \pm jsin(\theta)$$

- $k(X_i - X_j)$ is a real-value of $e^{iz_i(X_i - X_j)}$
- The real-value of $e^{i(X_i - X_j)Z}$ is $cos(X_i - X_j)Z$
- Two mapping of this exist as estimation:

1. $\phi_z(X) = [\cos(XZ) \quad \sin(XZ)]$
   - This is a vector
2. $\phi_z(X) = \sqrt{2}\cos(XZ + b)$
   - where b is drawn uniformly from $[0, 2\pi]$

Overall

- Let X be the dataset $\in R^{N \times D}$
- Let y be the target values $\in R^N$

1. Greedy Fitting

$$(W^\star, Z^\star) = \min_{W,Z} \| \sum_{i=1}^{T} w_i \phi_z(X_i) - y \|_F$$

2. Random Kitchen Sinks Fitting

$$z_1^\star, z_2^\star, ..., z_T^\star \sim p(w), \quad W^\star = \min_{W} || \sum_{i=1}^{T} w_i \phi_z(X_i) - y ||_F$$

1. Greedy method

- Inputs: y, probability measure μ
- Output $w_1, w_2, ..., w_T, z_1, z_2, ..., z_T$ so that

$$f(x) = \sum_{i=1}^{\infty} w_i \phi(x; z_i) \approx f_T(x) = \sum_{i=1}^{T} w_i \phi(x; z_i)$$

1. Initialize $f_0(x) = 0$
2. for $t = 1, 2, ..., T$
   - $(z_t, w_t) = arg\,\min_{w_t, z_t} ||(1 - w_t) f_{t-1} + \alpha_t \phi_{z_t}(x) - y||_F$
   - $f_t \leftarrow f_{t-1} + \alpha_t \phi_{z_t}(X)$

2. Random Kitchen Sink method

- Inputs: y, probability measure p
- Output $w_1, w_2, ..., w_T, z_1, z_2, ..., z_T$ so that

$$f(x) = \sum_{i=1}^{\infty} w_i \phi(x; z_i) \approx f_T(x) = \sum_{i=1}^{T} w_i \phi(x; z_i)$$

1. Draw $z_1, z_2, ...z_T \sim p(z)$
2. $w \leftarrow arg\min_w || \sum_{i=1}^{T} w_t \phi_z(X) - y||_F$

2. Random Kitchen Sink method in Python

```python
# Random Kitchen Sink method

# Fit a Gaussian Process using kernel approximation
import numpy as np

# Stage 1. Get the random features

# 1. N samples and D features
N, D = 100,50

# 2. Create Synthetic dataset
X = np.random.randn(N, D)
y = np.random.rand(N, 1)

# 3. Sample T from p(z)
T = 10
gamma = 1.
Z = (np.sqrt(2 * gamma) * np.random.randn(D, T))
```

Fastfood

D dimension, T random features, N datapoints

- Sample $D \times T$ random numbers : $Z \sim N(0, \sigma^{-2})$
- $\phi_z(X_i) = e^{(-iX_i Z)}$
- Computing the features $\phi_z(\cdot)$ for every datapoint is $O(NDT)$
- Fastfood - using Hadamard transform we can reduce the time complexity for computing the features to $O(\log(D)NT)$
- For images, if $D = 10,000$, $log_{10}(D) = 4$.

Fastfood

- Main idea: Compute $XZ \approx XV$
- V has similar properties to the Gaussian matrix Z

$$V = \frac{1}{\sigma\sqrt{N}} SHGPHB$$

- P is a N x N permutation matrix
- G is a diagonal random Gaussian
- B is a diagonal random $\{+1$, -1$\}$
- S is a diagonal random scaling
- H is Walsh- Hadamard matrix

More details

- Binary scaling matrix B:
  - It is a diagonal matrix with $Bii \in \pm 1$ drawn iid.
- Permutation P:
  - can be generated by sorting random numbers.
- Gaussian scaling matrix G:
  - This is a diagonal matrix whose elements $Gii\tilde{N}(0,1)$ are drawn iid from a Gaussian.
- Scaling matrix S:
  - Gaussian case S ensures that the length distribution of the row of V are independent of each other.

More details

- Main idea: Compute $XZ \approx XV$
- V has similar properties to the Gaussian matrix Z

$$V = \frac{1}{\sigma\sqrt{N}} SHGPHB$$

- S H G P H B produces pseudo-random Gaussian vectors
- S fixes the lengths to have the correct distribution

Fastfood in python

```
# Fast food

# Fit a Gaussian Process using kernel approximation
import numpy as np

# Stage 1. Get the random features

# 1. N samples and D features
N, D = 100,50

# 2. Create Synthetic dataset
X = np.random.randn(N, D)
y = np.random.rand(N, 1)

# 3. Sample T from p(w)
T = 10
gamma = 1.
```

Analysis - Random Kitchen sink

- Computing Features $\phi(x) = \frac{1}{\sqrt{T}} \exp(iZX)$
- Regression:

$$w = [\phi(x)^T \phi(x)]^{-1} \phi(x)^T y$$

- Train time complexity

$$O(\underbrace{NTD}_{\text{Computing Random Features}} + \underbrace{T^3}_{\text{Inverting Covariance matrix}} + \underbrace{T^2 N}_{\text{Multiplication}})$$

- Prediction: $y^* = w^T \phi(x^*)$
- Test time complexity: $O(\underbrace{N^* TD}_{\text{Computing Random Features}} + \underbrace{T^2 N^*}_{\text{Multiplication}})$

Analysis - FastFood

- Computing Features $\phi(x) = \frac{1}{\sqrt{T}} \exp(iVx) \approx \frac{1}{\sqrt{T}} \exp(iZx)$
- regression:

$$w = [\phi(x)^T \phi(x)]^{-1} \phi(x)^T y$$

- FF Train time compleixty
$$O(\underbrace{\log(N) TD}_{\text{Computing Random Features}} + \underbrace{T^3}_{\text{Inverting Covariance matrix}} + \underbrace{T^2 N}_{\text{Multiplication}})$$
- RKS Train time complexity
$$O(\underbrace{NTD}_{\text{Computing Random Features}} + \underbrace{T^3}_{\text{Inverting Covariance matrix}} + \underbrace{T^2 N}_{\text{Multiplication}})$$
- Prediction: $y^* = w^T \phi(x^*)$
- Test time complexity: $O(\underbrace{\log(D) TN^*}_{\text{Computing Random Features}} + \underbrace{T^2 N^*}_{\text{Multiplication}})$
- For images, if N = 10, 000, log10(N) = 4

Analysis - FastFood

We can lower the variance of the estimate of the kernel by concatenating D randomly chosen z_ω into one D-dimensional vector $\mathbf{z}$ and normalizing each component by $\sqrt{D}$. The inner product $\mathbf{z}(\mathbf{x})'\mathbf{z}(\mathbf{y}) = \frac{1}{D}\sum_{j=1}^{D} z_{\omega_j}(\mathbf{x})z_{\omega_j}(\mathbf{y})$ is a sample average of z_ω and is therefore a lower variance approximation to the expectation (2).

Since z_ω is bounded between $+\sqrt{2}$ and $-\sqrt{2}$ for a *fixed* pair of points $\mathbf{x}$ and $\mathbf{y}$, Hoeffding's inequality guarantees exponentially fast convergence in D between $\mathbf{z}(\mathbf{x})'\mathbf{z}(\mathbf{y})$ and $k(\mathbf{x}, \mathbf{y})$: $\Pr\left[|\mathbf{z}(\mathbf{x})'\mathbf{z}(\mathbf{y}) - k(\mathbf{x}, \mathbf{y})| \geq \epsilon\right] \leq 2\exp(-D\epsilon^2/4)$. Building on this observation, a much stronger assertion can be proven for every pair of points in the input space simultaneously:

Figure 7:

Method	Train Time	Test Time	Train Mem	Test Mem
Naive	$\mathcal{O}(N^2 D)$	$\mathcal{O}(ND)$	$\mathcal{O}(ND)$	$\mathcal{O}(ND)$
Low Rank	$\mathcal{O}(NTD)$	$\mathcal{O}(TD)$	$\mathcal{O}(TD)$	$\mathcal{O}(TD)$
Kitchen Sinks	$\mathcal{O}(NTD)$	$\mathcal{O}(TD)$	$\mathcal{O}(TD)$	$\mathcal{O}(TD)$
Fastfood	$\mathcal{O}(NT\log(D))$	$\mathcal{O}(T\log(D))$	$\mathcal{O}(T\log(D))$	$\mathcal{O}(T)$

Figure 8:

Analysis - FastFood

- MNIST Dataset
  - 20000 taining examples and 10000 test examples.