Statistical Consistency of Kernel PCA with Random Features

Bharath K. Sriperumbudur

Department of Statistics, Pennsylvania State University

École Polytechnique
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(Joint work with Nicholas Sterge, PSU)

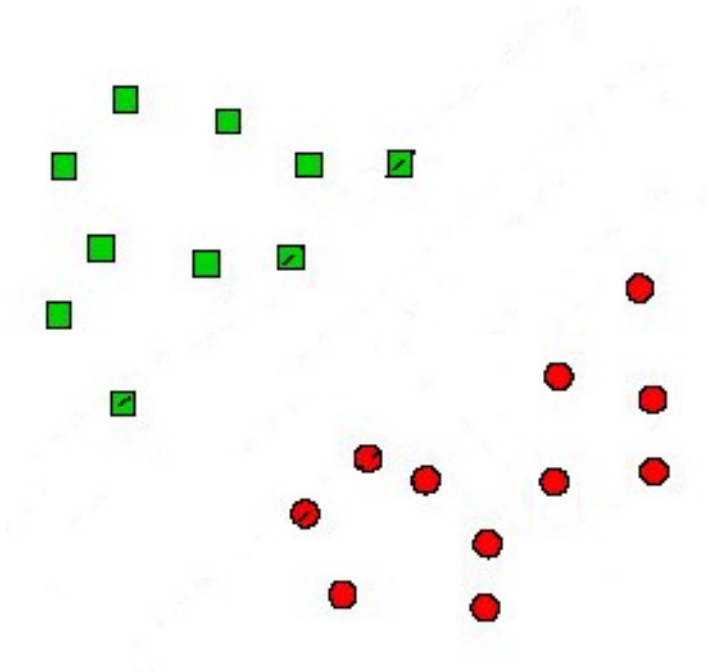
Outline

- Motivating example
  - Binary classification
  - Ridge regression
- Approximation methods
- Kernel PCA
  - Computational vs. statistical trade off

Motivating Example: Binary Classification

- Given: $D := \{(x_j, y_j)\}_{j=1}^{n}$, $x_j \in \mathcal{X}$, $y_j \in \{-1, +1\}$
- Goal: Learn a function $f : \mathcal{X} \to \mathbb{R}$ such that

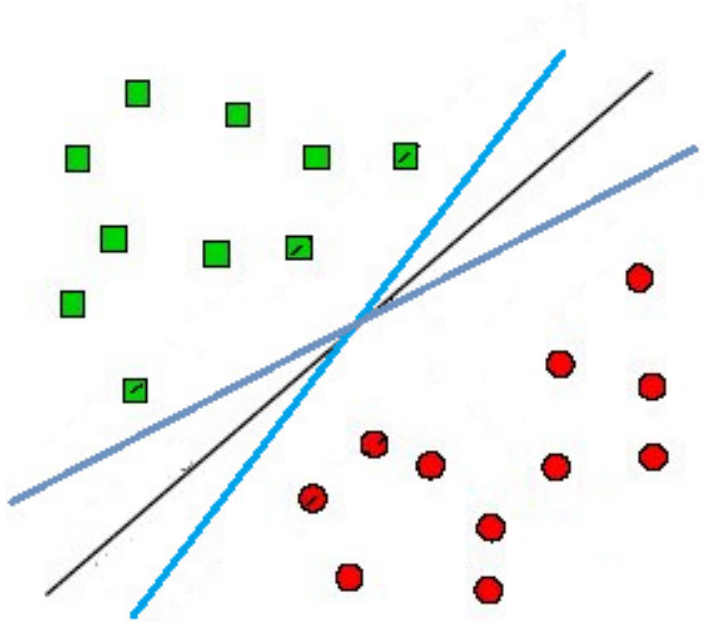
$$y_j = \text{sign}(f(x_j)), \forall\, j = 1, \ldots, n.$$



Linear Classifiers

- Linear classifier: $f_{w,b}(x) = \langle w, x \rangle_2 + b,\ w, x \in \mathbb{R}^d,\ b \in \mathbb{R}$
- Find $w \in \mathbb{R}^d$ and $b \in \mathbb{R}$ such that

$$y_j \left(\langle w, x_j \rangle_2 + b \right) \geq 0,\ \forall j = 1, \ldots, n.$$



- Fisher discriminant analysis, Support vector machine, Perceptron, ...

Nonlinear Classification: 1

- There is no linear classifier that separates red and blue regions.

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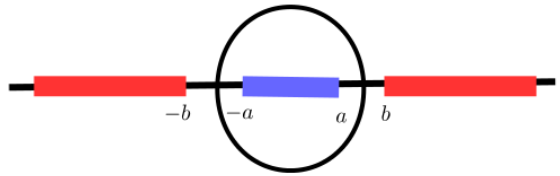

- There is no linear classifier that separates red and blue regions.
- However, the following function perfectly separates red and blue regions

$$f(x) = x^2 - r = \left\langle \underbrace{(1, -r)}_{w}, \underbrace{(x^2, 1)}_{\Phi(x)} \right\rangle_2 , \; a < r < b.$$

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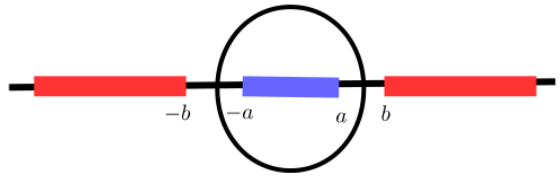

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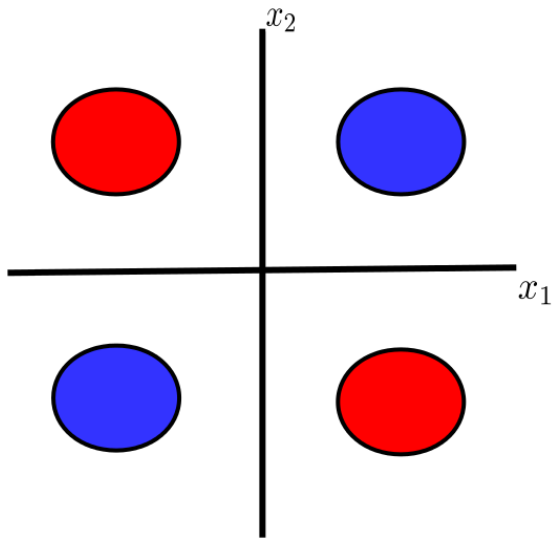
- By mapping $x \in \mathbb{R}$ to $\Phi(x) = (x^2, 1) \in \mathbb{R}^2$, the nonlinear classification problem is turned into a linear problem.
- We call Φ as the feature map.

Nonlinear Classification: 2



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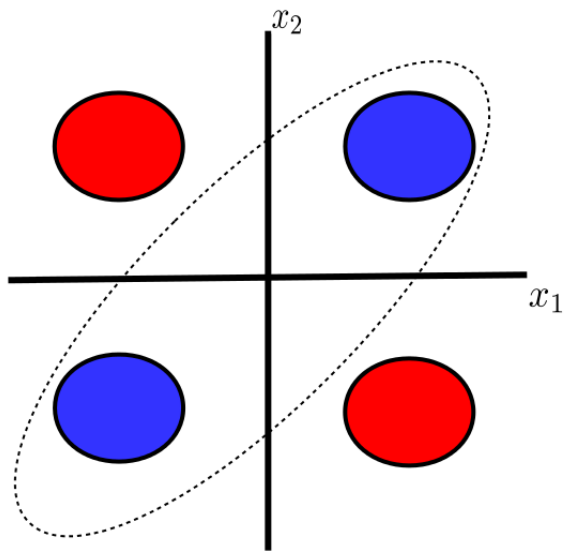

- There is no linear classifier that separates red and blue regions.
- A conic section, however, perfectly separates them

$$f(x) = ax_1^2 + bx_1x_2 + cx_2^2 + dx_1 + ex_2 + g$$
$$= \left\langle \underbrace{(a, b, c, d, e, g)}_{w}, \underbrace{(x_1^2, x_1x_2, x_2^2, x_1, x_2, 1)}_{\Phi(x)} \right\rangle_2 .$$

- $\Phi(x) \in \mathbb{R}^6$.

Motivating Example: Ridge regression

- Given: $\{(x_i, y_i)\}_{i=1}^n$ where $x_i \in \mathbb{R}^d$, $y_i \in \mathbb{R}$
- Task: Find a linear regressor $f = \langle w, \cdot \rangle_2$ s.t. $f(x_i) \approx y_i$,

$$\min_{w \in \mathbb{R}^d} \frac{1}{n} \sum_{i=1}^{n} (\langle w, x_i \rangle_2 - y_i)^2 + \lambda \|w\|_2^2 \quad (\lambda > 0)$$

- Solution: For $\mathbf{X} := (x_1, \ldots, x_n) \in \mathbb{R}^{d \times n}$ and $\mathbf{y} := (y_1, \ldots, y_n)^\top \in \mathbb{R}^n$,

$$w = \underbrace{\frac{1}{n} \left(\frac{1}{n} \mathbf{X}\mathbf{X}^\top + \lambda I_d \right)^{-1} \mathbf{X}\mathbf{y}}_{primal}$$

- Easy:

$$\left(\frac{1}{n} \mathbf{X}\mathbf{X}^\top + \lambda I_d \right) \mathbf{X} = \mathbf{X} \left(\frac{1}{n} \mathbf{X}^\top \mathbf{X} + \lambda I_n \right)$$

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Ridge regression

- Prediction: Given $t \in \mathbb{R}^d$

$$f(t) = \langle w, t \rangle_2 = \mathbf{y}^\top \mathbf{X}^\top \left(\mathbf{X}\mathbf{X}^\top + n\lambda I_d \right)^{-1} t$$
$$= \mathbf{y}^\top \left(\mathbf{X}^\top \mathbf{X} + n\lambda I_n \right)^{-1} \mathbf{X}^\top t$$

- How does $\mathbf{X}^\top \mathbf{X}$ look like?

$$\mathbf{X}^\top \mathbf{X} = \underbrace{\begin{bmatrix} \langle x_1, x_1 \rangle_2 & \langle x_1, x_2 \rangle_2 & \cdots & \langle x_1, x_n \rangle_2 \\ \langle x_2, x_1 \rangle_1 & \langle x_2, x_2 \rangle_2 & \cdots & \langle x_2, x_n \rangle_2 \\ \vdots & \langle x_i, x_j \rangle_2 & \ddots & \vdots \\ \langle x_n, x_1 \rangle_1 & \langle x_n, x_2 \rangle_2 & \cdots & \langle x_n, x_n \rangle_2 \end{bmatrix}}_{\text{Matrix of inner products: Gram Matrix}}$$

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Kernel Ridge regression

- Given: $\{(x_i, y_i)\}_{i=1}^n$ where $x_i \in \mathcal{X}$, $y_i \in \mathbb{R}$
- Task: Find a regressor $f \in \mathcal{H}$ (some feature space) s.t. $f(x_i) \approx y_i$.
- Idea: Map x_i to $\Phi(x_i)$ and do linear regression,

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} (\langle f, \Phi(x_i) \rangle_{\mathcal{H}} - y_i)^2 + \lambda \|f\|_{\mathcal{H}}^2 \quad (\lambda > 0)$$

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Remarks

- Kernel: A function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is called a kernel if there exists a Hilbert space $\mathcal{H}$ and a map $\Phi : \mathcal{X} \to \mathcal{H}$ such that

$$k(x, x') := \langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}, \quad \forall\, x, x' \in \mathcal{H}.$$

- A complete characterization is provided by Moore-Aronszajn Theorem (Aronszajn, 1950)

  A function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a kernel if and only if it is symmetric and positive definite.

- The primal formulation requires the knowledge of feature map Φ (and of course $\mathcal{H}$) and these could be infinite dimensional.

- The dual formulation is entirely determined by kernel evaluations, Gram matrix and $(k(x_i, t))_i$. But poor scalability: $O(n^3)$.

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Approximation Schemes

- Incomplete Cholesky factorization (e.g., (Fine and Scheinberg, JMLR 2001)
- Sketching (Yang et al., 2015)
- Sparse greedy approximation (Smola and Schölkopf, NIPS 2000)
- Nyström method (e.g., Williams and Seeger, NIPS 2001)
- Random Fourier features (e.g., Rahimi and Recht, NIPS 2008), ...

Random Fourier Approximation

- $\mathcal{X} = \mathbb{R}^d$; k be continuous and translation-invariant, i.e., $k(x, y) = \psi(x - y)$.
- Bochner's theorem: ψ is positive definite if and only if

$$k(x, y) = \int_{\mathbb{R}^d} e^{\sqrt{-1}\langle \omega, x-y \rangle_2} \, d\Lambda(\omega),$$

  where Λ is a finite non-negative Borel measure on $\mathbb{R}^d$.
  - k is symmetric and therefore Λ is a "symmetric" measure on $\mathbb{R}^d$.
- Therefore

$$k(x, y) = \int_{\mathbb{R}^d} \cos(\langle \omega, x - y \rangle_2) \, d\Lambda(\omega).$$

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Random Feature Approximation

(Rahimi and Recht, NIPS 2008): Draw $(\omega_j)_{j=1}^m \overset{i.i.d.}{\sim} \Lambda$.

$$k_m(x,y) = \frac{1}{m}\sum_{j=1}^{m} \cos\left(\langle \omega_j, x-y\rangle_2\right) = \langle \Phi_m(x), \Phi_m(y)\rangle_{\mathbb{R}^{2m}},$$

where

$$\Phi_m(x) = (\cos(\langle \omega_1, x\rangle_2), \ldots, \cos(\langle \omega_m, x\rangle_2), \sin(\langle \omega_1, x\rangle_2), \ldots, \sin(\langle \omega_m, x\rangle_2))^\top.$$

- Use the feature map idea with Φ_m, i.e., $x \mapsto \Phi_m(x)$ and apply your favorite linear method.

How good is the approximation?

(S and Szabó, NIPS 2016):

$$\sup_{x,y \in \mathscr{S}} |k_m(x,y) - k(x,y)| = O_{a.s.}\left(\sqrt{\frac{\log|\mathscr{S}|}{m}}\right)$$

Optimal convergence rate

- Other results are known but they are non-optimal (Rahimi and Recht, NIPS 2008; Sutherland and Schneider, UAI 2015).

Ridge Regression: Random Feature Approximation

- Given: $\{(x_i, y_i)\}_{i=1}^n$ where $x_i \in \mathcal{X}$, $y_i \in \mathbb{R}$
- Task: Find a regressor $w \in \mathbb{R}^{2m}$ s.t. $f(x_i) \approx y_i$.
- Idea: Map x_i to $\Phi_m(x_i)$ and do linear regression,

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} (\langle f, \Phi_m(x_i) \rangle_{\mathbb{R}^{2m}} - y_i)^2 + \lambda \|w\|_{\mathbb{R}^{2m}}^2 \quad (\lambda > 0)$$

- Solution: For $\Phi_m(\mathbf{X}) := (\Phi_m(x_1), \ldots, \Phi_m(x_n)) \in \mathbb{R}^{2m \times n}$ and $\mathbf{y} := (y_1, \ldots, y_n)^\top \in \mathbb{R}^n$,

$$f = \underbrace{\frac{1}{n} \left(\frac{1}{n} \Phi_m(\mathbf{X}) \Phi_m(\mathbf{X})^\top + \lambda I_{2m} \right)^{-1} \Phi_m(\mathbf{X}) \mathbf{y}}_{primal}$$

$$= \underbrace{\frac{1}{n} \Phi_m(\mathbf{X}) \left(\frac{1}{n} \Phi_m(\mathbf{X})^\top \Phi_m(\mathbf{X}) + \lambda I_n \right)^{-1} \mathbf{y}}_{dual}$$

Computation: $O(m^2 n)$.

Ridge Regression: Random Feature Approximation

- Given: $\{(x_i, y_i)\}_{i=1}^n$ where $x_i \in \mathcal{X}$, $y_i \in \mathbb{R}$
- Task: Find a regressor $w \in \mathbb{R}^{2m}$ s.t. $f(x_i) \approx y_i$.
- Idea: Map x_i to $\Phi_m(x_i)$ and do linear regression,

$$\min_{f \in \mathcal{H}} \frac{1}{n} \sum_{i=1}^{n} (\langle f, \Phi_m(x_i) \rangle_{\mathbb{R}^{2m}} - y_i)^2 + \lambda \|w\|_{\mathbb{R}^{2m}}^2 \quad (\lambda > 0)$$

- Solution: For $\Phi_m(\mathbf{X}) := (\Phi_m(x_1), \ldots, \Phi_m(x_n)) \in \mathbb{R}^{2m \times n}$ and $\mathbf{y} := (y_1, \ldots, y_n)^\top \in \mathbb{R}^n$,

$$f = \underbrace{\frac{1}{n} \left(\frac{1}{n} \Phi_m(\mathbf{X}) \Phi_m(\mathbf{X})^\top + \lambda I_{2m} \right)^{-1} \Phi_m(\mathbf{X}) \mathbf{y}}_{primal}$$

$$= \underbrace{\frac{1}{n} \Phi_m(\mathbf{X}) \left(\frac{1}{n} \Phi_m(\mathbf{X})^\top \Phi_m(\mathbf{X}) + \lambda I_n \right)^{-1} \mathbf{y}}_{dual}$$

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Computation: $O(m^2 n)$.

What happens statistically?

- (Rudi and Rosasco, 2016): If $m \geq n^{\alpha}$ where $\frac{1}{2} \leq \alpha < 1$ with α depending on the properties of the unknown true regressor, f^*, then

$$\mathcal{R}_{L,\mathbf{P}}(f_{m,n}) - \mathcal{R}_{L,\mathbf{P}}(f^*)$$

achieves the minimax optimal rate as obtained in the case with no approximation. Here L is the squared loss.

Computational gain with no statistical loss!!

- Goal: "Learn" a function $f : X \to Y$ given a set $D := \{(x_1, y_1), \ldots, (x_n, y_n)\}$ of input/output pairs drawn independently from an unknown probability distribution $\mathbf{P}$ on $X \times Y$.
- Loss function: $L : Y \times Y \to [0, \infty)$
- Risk functional:

$$\mathcal{R}_{L,\mathbf{P}}(f) := \int_{X \times Y} L(y, f(x))\, d\mathbf{P}(x, y).$$

Reproducing Kernel Hilbert Space

- A Hilbert space $\mathcal{H}$ of real-valued functions on $\mathcal{X}$ is said to be a reproducing kernel Hilbert space (RKHS) with $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ as the reproducing kernel, if
  - $\forall\, x \in \mathcal{X},\ k(\cdot, x) \in \mathcal{H}$;
  - $\forall x \in \mathcal{X},\ \forall\, f \in \mathcal{H},\ \langle f, k(\cdot, x)\rangle_{\mathcal{H}} = f(x)$.
- The reproducing kernel (r.k.) k of $\mathcal{H}$ is a kernel:

$$k(x, x') = \Big\langle \underbrace{k(\cdot, x)}_{\Phi(x)}, \underbrace{k(\cdot, x')}_{\Phi(x')} \Big\rangle_{\mathcal{H}}, \quad x, x' \in \mathcal{X}.$$

  We refer to $\Phi(x) = k(\cdot, x)$ as the canonical feature map.
- Every r.k. is a symmetric and positive definite function.

Kernels $\Leftrightarrow$ Positive definite & symmetric functions $\Leftrightarrow$ RKHS

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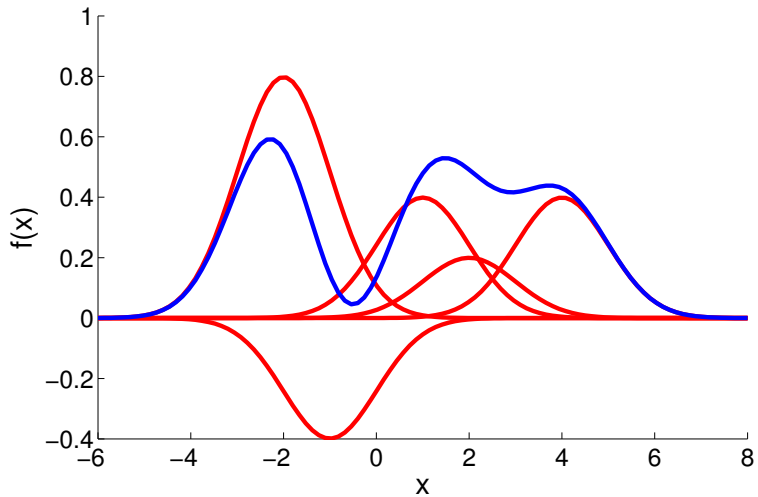
Functions in the RKHS

- $\mathcal{H} = \overline{\text{span}\{k(\cdot, x) : x \in \mathcal{X}\}}$ (linear span of kernel functions)
  - Example: $f(x) = \sum_{i=1}^{m} \alpha_i k(x, x_i)$ for arbitrary $m \in \mathbb{N}$, $\{\alpha_i\} \subset \mathbb{R}$, $x \in \mathcal{X}$ and $\{x_i\} \subset \mathcal{X}$.

$$k(x, y) = e^{-\|x-y\|^2/2\sigma^2}$$



Picture credit: A. Gretton

Properties of RKHS

- k is bounded if and only every $f \in \mathcal{H}$ is bounded.
- If $\int_{\mathcal{X}} \sqrt{k(x,x)}\, d\mu(x) < \infty$, then for every $f \in \mathcal{H}$, $\int_{\mathcal{X}} f(x)\, d\mu(x) < \infty$.
- Every $f \in \mathcal{H}$ is continuous if and only if $k(\cdot, x)$ is continuous for all $x \in \mathcal{X}$.
- Every $f \in \mathcal{H}$ is m-times continuously differentiable if k is m-times continuously differentiable.

k controls the properties of $\mathcal{H}$

Explicit Realization of RKHS

- $\mathcal{X} = \mathbb{R}^d$ and $k(x, y) = \psi(x - y)$ where ψ is a positive definite function.
- Assume ψ satisfies $\int_{\mathbb{R}^d} |\psi(x)|\, dx < \infty$. Denote $\hat{\psi}$ to be the Fourier transform of ψ.
- $$\mathcal{H} = \left\{ f \in L^2(\mathbb{R}^d) \cap C(\mathbb{R}^d) \Big| \int_{\mathbb{R}^d} \frac{|\hat{f}(\omega)|^2}{\hat{\psi}(\omega)}\, d\omega < \infty \right\}$$

  endowed with

$$\langle f, g \rangle_{\mathcal{H}} = (2\pi)^{-d/2} \int \frac{\hat{f}(\omega)\overline{\hat{g}(\omega)}}{\hat{\psi}(\omega)}\, d\omega$$

is an RKHS with k as the r.k.

(Wendland, 2005)

Gaussian RKHS

- Gaussian kernel:

$$k(x, y) = \psi(x - y) = e^{-\|x-y\|_2^2/\gamma^2},\ x, y \in \mathbb{R}^d$$

- Fourier transform:

$$\hat{\psi}(\omega) = \left(\frac{\gamma^2}{2}\right)^{d/2} e^{-\frac{\gamma^2\|\omega\|_2^2}{4}},\ \omega \in \mathbb{R}^d$$

-

$$\mathcal{H}_\gamma(\mathbb{R}^d) := \left\{ f \in L^2(\mathbb{R}^d) : \underbrace{\int_{\mathbb{R}^d} |\hat{f}(\omega)|^2 e^{\frac{\gamma^2\|\omega\|_2^2}{4}} d\omega}_{\|f\|_{\mathcal{H}_\gamma}^2} < \infty \right\}$$

Fast decay of $\hat{\psi} \Rightarrow$ Smooth $\mathcal{H}$

Sobolev RKHS

- Laplacian kernel:

$$k(x,y) = \psi(x-y) = \sqrt{\frac{\pi}{2}} e^{-|x-y|},\ x,y \in \mathbb{R}$$

- Fourier transform:

$$\hat{\psi}(\omega) = \frac{1}{1+|\omega|^2},\ \omega \in \mathbb{R}$$

-

$$\mathcal{H}_1^2(\mathbb{R}) := \left\{ f \in L^2(\mathbb{R}) \,:\, \underbrace{\int_{\mathbb{R}} |\hat{f}(\omega)|^2 (1+|\omega|^2)\, d\omega}_{\|f\|^2_{\mathcal{H}_1^2}} < \infty \right\}$$

Extension to $\mathbb{R}^d$: Matérn Kernel

Principal Component Analysis (PCA)

- Suppose $X \sim \mathbb{P}$ be a random variable in $\mathbb{R}^d$ with mean μ and covariance matrix Σ.
- Find a direction $w \in \{v : \|v\|_2 = 1\}$ such that

$$\mathrm{Var}[\langle w, X \rangle_2]$$

  is maximized.
- Find a direction $w \in \mathbb{R}^d$ such that

$$\mathbb{E}\|(X - \mu) - \langle w, (X - \mu) \rangle_2 w\|_2^2$$

  is minimized.
- The formulations are equivalent and the solution is the eigen vector of the covariance matrix Σ corresponding to the largest eigenvalue.
- Can be generalized to multiple directions (find a subspace...).
- Applications: dimensionality reduction.

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Kernel PCA

- Nonlinear generalization of PCA (Schölkopf et al., 1998).
- $X \mapsto \Phi(X)$ and apply PCA.
- Provides a low dimensional manifold (curves) in $\mathbb{R}^d$ to efficiently represent the data.
- Kernel PCA: Find $f \in \{g \in \mathcal{H} : \|g\|_{\mathcal{H}} = 1\}$ such that $\mathrm{Var}[f(X)]$ is maximized, i.e.,

$$f^* = \arg \sup_{\|f\|_{\mathcal{H}}=1} \mathbb{E}[f^2(X)] - \mathbb{E}^2[f(X)]$$

- Using the reproducing property $f(X) = \langle f, k(\cdot, X)\rangle_{\mathcal{H}}$, we obtain

$$\begin{aligned}\mathbb{E}[f^2(X)] = \mathbb{E}\langle f, k(\cdot, X)\rangle^2_{\mathcal{H}} &= \mathbb{E}\langle f, (k(\cdot, X) \otimes_{\mathcal{H}} k(\cdot, X))f\rangle_{\mathcal{H}} \\ &= \langle f, \mathbb{E}[k(\cdot, X) \otimes_{\mathcal{H}} k(\cdot, X)]f\rangle_{\mathcal{H}},\end{aligned}$$

  assuming $\int_{\mathcal{X}} k(x, x)\, d\mathbb{P}(x) < \infty$.

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where

$$\Sigma := \int_{\mathcal{X}} k(\cdot, x) \otimes_{\mathcal{H}} k(\cdot, x) \, d\mathbb{P}(x) - \mu_{\mathbb{P}} \otimes_{\mathcal{H}} \mu_{\mathbb{P}}$$

is the covariance operator (symmetric, positive and Hilbert-Schmidt) on $\mathcal{H}$.

- Spectral theorem:

$$\Sigma = \sum_{i \in I} \lambda_i \phi_i \otimes_{\mathcal{H}} \phi_i$$

  where I is either countable ($\lambda_i \to 0$ as $i \to \infty$) or finite.

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Empirical Kernel PCA

In practice, $\mathbb{P}$ is unknown but have access to $(X_i)_{i=1}^n \overset{i.i.d.}{\sim} \mathbb{P}$.

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- How to solve find $\hat{\phi}_i$ in practice?
- Sampling operator: $S : \mathcal{H} \to \mathbb{R}^n,\ f \mapsto \frac{1}{\sqrt{n}}(f(X_1), \ldots, f(X_n))$.
- Reconstruction operator: $S^* : \mathbb{R}^n \to \mathcal{H},\ \boldsymbol{\alpha} \mapsto \frac{1}{\sqrt{n}}\sum_{i=1}^n \alpha_i k(\cdot, X_i)$.

(Smale and Zhou et al., 2007)

- S^* is the adjoint (transpose) of S and they satisfy

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Empirical Kernel PCA: Random Features

- Empirical kernel PCA solves an $n \times n$ linear system: Complexity is $O(n^3)$.
- Use the idea of random features: $X \mapsto \Phi_m(X)$ and apply PCA.

$$\hat{w}^* := \arg \sup_{\|w\|=1} \widehat{\mathrm{Var}}[\langle w, \Phi_m(X) \rangle_2] = \langle w, \hat{\Sigma}_m w \rangle_2$$

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is a covariance matrix of size $2m \times 2m$.

- Eigen decomposition: $\hat{\Sigma}_m = \sum_{i=1}^{2m} \hat{\lambda}_{i,m} \hat{\phi}_{i,m} \hat{\phi}_{i,m}^\top$
- $\hat{w}^*$ is obtained by solving a $2m \times 2m$ eigensystem: Complexity is $O(m^3)$.

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Two notions:

- Reconstruction error (what does this depend on?)
- Convergence of eigenvectors (more generally, eigenspaces)

Eigenspace Convergence

What we have?

- Eigenvectors after approximation, $(\hat{\phi}_{i,m})_{i=1}^{2m}$: these form a subspace in $\mathbb{R}^{2m}$
- Population eigenfunctions $(\phi_i)_{i \in I}$ of Σ: these form a subspace in $\mathcal{H}$.
- How do we compare?
- We embed them in a common space before comparing. The common space is $L^2(\mathbb{P})$.

Eigenspace Convergence

- $\mathfrak{I} : \mathcal{H} \to L^2(\mathbb{P})$, $f \mapsto f - \int_{\mathcal{X}} f(x)\, d\mathbb{P}(x)$
- $\mathfrak{U} : \mathbb{R}^{2m} \to L^2(\mathbb{P})$, $\boldsymbol{\alpha} \mapsto \sum_{i=1}^{2m} \alpha_i \left(\Phi_{m,i} - \int_{\mathcal{X}} \Phi_{m,i}(x)\, d\mathbb{P}(x) \right)$ where

$$\Phi_m = (\cos(\langle \omega_1, \cdot \rangle_2), \ldots, \cos(\langle \omega_m, \cdot \rangle_2), \sin(\langle \omega_1, \cdot \rangle_2), \ldots, \sin(\langle \omega_m, \cdot \rangle_2))^\top.$$

Main results: (S and Sterge, 2017)

- $$\sum_{i=1}^{\ell} \| \mathfrak{I}\hat{\phi}_i - \mathfrak{I}\phi_i \|_{L^2(\mathbb{P})} = O_p\left(\frac{1}{\sqrt{n}}\right).$$

  Similar result holds in $\| \cdot \|_{\mathcal{H}}$ (Zwald et al., NIPS 2005)
- $$\sum_{i=1}^{\ell} \| \mathfrak{U}\hat{\phi}_{i,m} - \mathfrak{I}\phi_i \|_{L^2(\mathbb{P})} = O_p\left(\frac{1}{\sqrt{m}} + \frac{1}{\sqrt{n}}\right).$$

- Random features are not helpful from the point of view of eigenvector convergence (also holds for eigenspaces).
- May be useful in the reconstruction error convergence (in progress).

Eigenspace Convergence

- $\mathfrak{I} : \mathcal{H} \to L^2(\mathbb{P})$, $f \mapsto f - \int_{\mathcal{X}} f(x)\, d\mathbb{P}(x)$
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