Subspace Learning

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Subspace Learning

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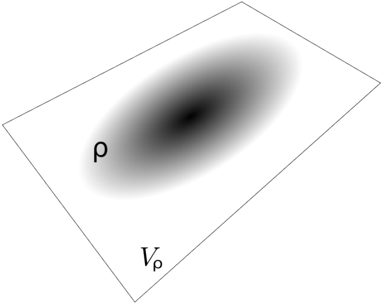
- $\mathcal{H}$: Hilbert Space
- ρ: probability distribution on $\mathcal{H}$
- $\operatorname{supp}\rho$: is the support of ρ
- $V_\rho = \overline{\operatorname{span}\{x \mid x \in \operatorname{supp}\rho\}}$
  "smallest" linear subspace containing $\operatorname{supp}\rho$



Problem How to "find" V_ρ given the examples $x_1, \ldots, x_n \sim \rho$?

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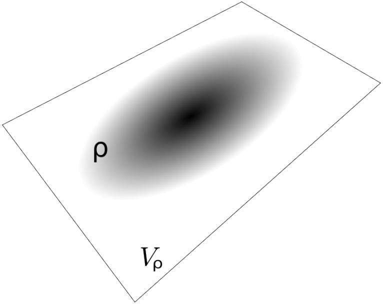

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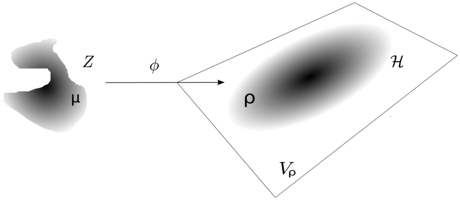
Setting: Why a Hilbert Space $\mathcal{H}$

- limit for high dimensional data
- embedded data $(Z, \mu) \xrightarrow{\phi} \mathcal{H}$



Example 1: PCA - Kernel PCA

PCA

V_ρ the smallest linear subspace of $\mathcal{H}$ that contains all the distribution

$$V_\rho = \operatorname*{argmin}_V dim(V) \quad \text{such that} \;\; var(V) = var(\mathcal{H})$$

Kernel PCA [Schölkopf 1997]

performs PCA on the data embedded in $\mathcal{H}$ by a feature map ϕ

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Example 2: Kernel Support Estimation

- $(Z, \mu),\ M = \operatorname{supp}\mu$
- $\phi : Z \to \mathcal{H},\ V_\rho = \overline{\operatorname{span}\{\phi(z) \mid Z \in M\}}$

If ϕ is *separating* [De Vito 2010]

$$M = \{z \in Z \mid \phi(z) \in V_\rho\}$$

Examples separating ϕs on $\mathbb{R}^d$

- Abel kernel, $\langle \phi(z), \phi(z') \rangle = \exp(-\gamma \|z - z'\|_{\ell_2})$
- the convex combination or the product of two separating kernels
- Gaussian kernel is NOT separating

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Problem definition

Given $x_1, \ldots, x_n$ drawn independently from ρ, find $\hat{V}$ such that

$$P\left(d(\hat{V}, V_\rho) > \epsilon\right) \leq \delta(\epsilon, n)$$

How to build $\hat{V}$?
Which distance d on linear subspaces?

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Covariance Lemma in the continuous case

$$V_\rho = \overline{\operatorname{span}\{u_i \mid i \geq 1\}}$$

where $Cu_i = \sigma_i u_i$ with $C : \mathcal{H} \to \mathcal{H}$ the covariance operator

$$C = \mathbb{E}_{x \sim \rho}[x \otimes x] - \mu \otimes \mu$$

Truncated estimator

Analogously we can define

$$\hat{V}^k = \operatorname{span}\{\hat{u}_i \mid 1 \leq i \leq k\}$$

where $\hat{C} u_i = \hat{\sigma}_i \hat{u}_i$ with $\hat{C} : \mathcal{H} \to \mathcal{H}$ the empirical covariance operator

$$\hat{C} = \frac{1}{n} \sum_{i=1}^{n} x_i \otimes x_i - \hat{\mu} \otimes \hat{\mu}$$

What is a good value of k?
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Which metric?

Let C be the covariance operator associated to the distribution ρ.

$$d_{\alpha,p,\rho}(U,V) = \|(P_U - P_V)C^{\alpha}\|_p$$

- C is the covariance operator of ρ
- P_U is the projection operator associated to the subspace U
- $\|\|_p$ is the p-Schatten norm, $\|A\|_p^p = \sum_{i \geq 1} \sigma_i^p$

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Metric for Kernel PCA

Reconstruction error:

$$R(V) = \mathbb{E}_{x\sim\rho}\left[\|x - P_V x\|^2_{\mathcal{H}}\right]$$

- Commonly used in literature [Shawe-Taylor 2005, Blanchard 2007]
- $R(V) = d^2_{\frac{1}{2},2,\rho}(V, V_\rho)$

note that $R(W) \leq R(V)$ when $V \subseteq W$

Metric for Support Estimation

When the feature map is separating, the support M is defined as

$$M = \{z \in Z \mid F_{V_\rho}(z) = 0\} \text{ with } F_{V_\rho}(z) = \operatorname{dist}_{V_\rho}(\phi(z))$$

The natural estimator studied in [De Vito 2010, De Vito 2012] is defined as

$$\hat{M} = \{z \in Z \mid F_{\hat{V}^k}(z) \leq \tau\} \text{ with } F_{\hat{V}^k}(z) = \operatorname{dist}_{\hat{V}^k}(\phi(z))$$

In order to study the convergence of the set $\hat{M}$ to M is of interest to bound the quantity

$$\sup_{z \in Z} |F_{V_\rho}(z) - F_{\hat{V}^k}(z)| \leq \left\|(P_{\hat{V}^k} - P_{V_\rho})C^\alpha\right\|_\infty = d_{\alpha,\infty,\rho}(\hat{V}^k, V_\rho)$$

where α depends on the eigenvalue decay of C.

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More on General metric

- $d_{\alpha,p,\rho}$ is a metric for $\Lambda(V_\rho)$, the collection of subspaces of V_ρ, where $0 \leq \alpha \leq 1$ and $1 \leq p \leq \infty$
- each $\hat{V}^k$ is a subspace of V_ρ thus $\hat{V}^k \in \Lambda(V_\rho)$
- $d_{\alpha,p,\rho}(V, W) \leq d_{\alpha,p,\rho}(U, W) \qquad U \subseteq V \subseteq W$

the metric $d_{a,p,\rho}$ allows to control a variety of metrics classically used to measure distance between sets [Beer 1993]

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Subspace Learning

Learning rate for the general metric

Theorem 1 (Rudi, Canas, Rosasco 2013)

With probability $1-\delta$

$$d_{\alpha,p,\rho}(\hat{V}^k, V_\rho) \leq 4t^\alpha \mathcal{N}_{\alpha p}(t)^\alpha$$

- $t = \max\{\sigma_k, \frac{9}{n}\log\frac{n}{\delta}\}$
- σ_k the k-th eigenvalue of C
- $\mathcal{N}_{\alpha p}(t) = \left\|C(C+tI)^{-1}\right\|_{\alpha p}$ a generalization of the effective dimension [Caponnetto 2005] (that is $\mathcal{N}(t) = \mathcal{N}_2(t)$)

tools from: spectral theory, Löwner partial orderings, concentrations bounds on operators [Tropp 2012]

Learning rate for the general metric

Assumption on the eigenvalue decay of C

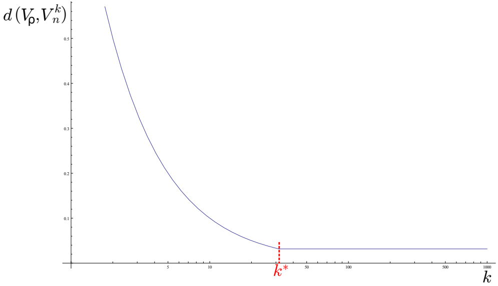
if we assume that $\sigma_m(C) \sim m^{-r}$ with $r > 1$ we have

$$d_{\alpha,p,\rho}(\hat{V}^k, V_\rho) \leq \begin{cases} Qk^{-r\alpha+\frac{1}{p}} & \text{if } k < k^* \qquad \text{(polynomial decay)} \\ Qk^{*-r\alpha+\frac{1}{p}} & \text{if } k \geq k^* \qquad \text{(plateau)} \end{cases}$$

with probability $1 - \delta$ and q, Q constants

$$k^* = \left(\frac{qn}{9 \log(n/\delta)} \right)^{\frac{1}{r}}$$

Learning Rates for Kernel PCA and Reconstruction error



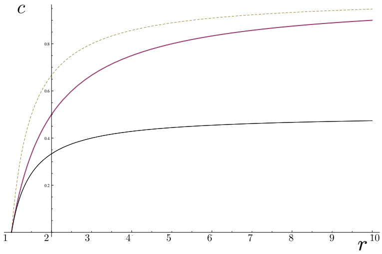
$$k^* = \left(\frac{n}{\log n}\right)^{\frac{1}{r}}$$

$$R(\hat{V}^k) = d_{\frac{1}{2},2,\rho}(\hat{V}^k, V_\rho)^2 \leq Q \begin{cases} k^{-\frac{r-1}{r}} & k < k^* \\ \left(\frac{\log n}{n}\right)^{\frac{r-1}{r}} & k \geq k^* \end{cases}$$

$$\text{where } \sigma_m(C) \sim m^{-r}, \ r > 1$$

Rates comparison on Kernel PCA

- [Blanchard 2007] (dotted line). Analysis for fixed k and reconstruction error. It makes assumptions on the fourth order. Learning rate $O(n^{-c})$ with $c = \frac{s(r-1)}{r-s+rs}$ where s is the fourth-moment eigenvalue decay.
- [Shawe-Taylor 2005] (black line) Analysis for fixed k and reconstruction error. Learning rate $O(n^{-c})$ with $c = \frac{r}{2(r-1)}$.
- *Our result for reconstruction error* (purple thick line). Learning rate $O(n^{-c})$ with $c = \frac{r}{r-1}$ where s is the fourth-moment eigenvalue decay.



Learning Rates for Kernel Support Estimation

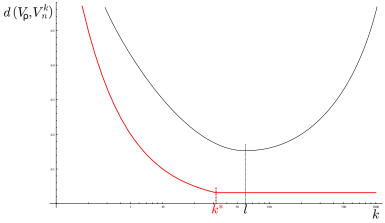
With probability $1 - \delta$

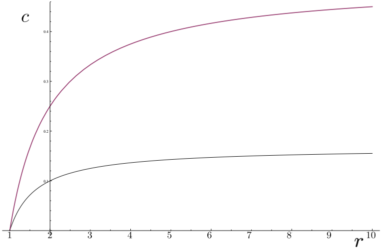
$$d_{\alpha,\infty,\rho}(\hat{V}^k, V_\rho) \leq Q \begin{cases} k^{-r\alpha} & k < k^* \\ \left(\frac{\log n}{n}\right)^{r\alpha} & k \geq k^* \end{cases}$$

where $k^* = \left(\frac{n}{\log n}\right)^{\frac{1}{r}}$ and $\sigma_m(C) \sim m^{-r},\ r > 1$

Rates comparison on Kernel Support Estimation

- [De Vito 2010, De Vito 2012] (black line on the left) It does not respect the monotonicity of the distance w.r.t. nested sets. (black line on the right) Learning rate $O(n^{-c})$ with $c = \frac{r-1}{2(3r-1)}$ with the worst case $\alpha = \frac{r-1}{2r}$
- *Our result* (red thick line). (red line on the left). It respect the monotonicity of the distance. (black line on the right) Learning rate $O(n^{-c})$ with $c = \frac{r-1}{2r}$ with the worst case $\alpha = \frac{r-1}{2r}$

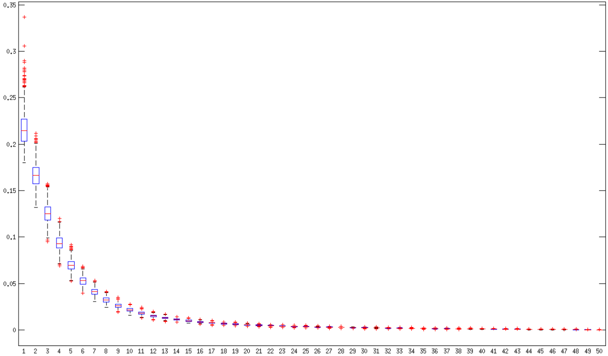




Subspace Learning

Experiments:Simulation on Kernel PCA(1)

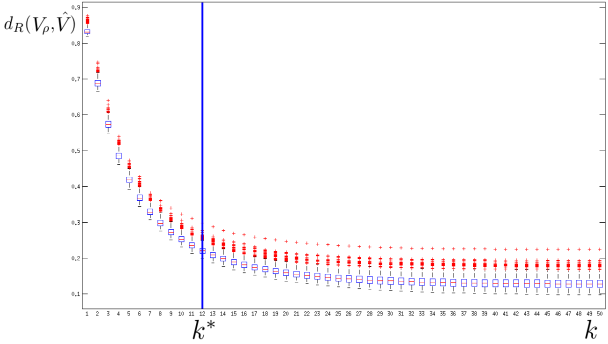
- μ uniform distribution on $[0, 1]$ with $Z = \mathbb{R}^2$
- $K(x, y) = \exp(-\gamma \|x - y\|_{\ell_1})$
- 1000 trials, each one of 1000 points independently drawn from μ



Eigenvalue decay of the associated empirical Covariance operator $\hat{C}$

Experiments:Simulation on Kernel PCA(2)

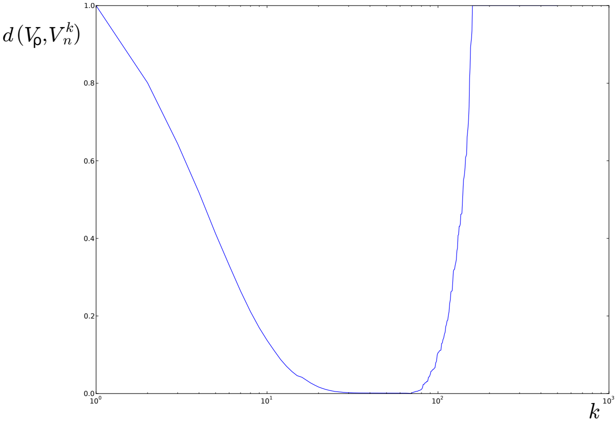
- the true covariance C can be computed analytically, it has polynomial decay $r = 2$.
- thus we can compute k^*
- the experiment shows the plateau behavior



Reconstruction error function of the number of the number of components k

Experiments: Numerical tradeoff in Kernel PCA (3)

- μ uniform distribution on $[0, 1]$ with $Z = \mathbb{R}^2$ with Gaussian kernel
- 1000 points independently drawn from μ
- computations performed on 32bits floating point precision



Reconstruction error with respect to the number of components k

Contribution

- Learning Rates for a wide range of metrics on linear subspaces
- Specific results for Kernel PCA and Spectral Support Estimation
- an optimal k^* for the truncated estimator

Future work

- Theoretical analysis on statistical/computational trade-off
- What happens with the noise?

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