Machine/Statistical Learning

PCA and Kernel PCA

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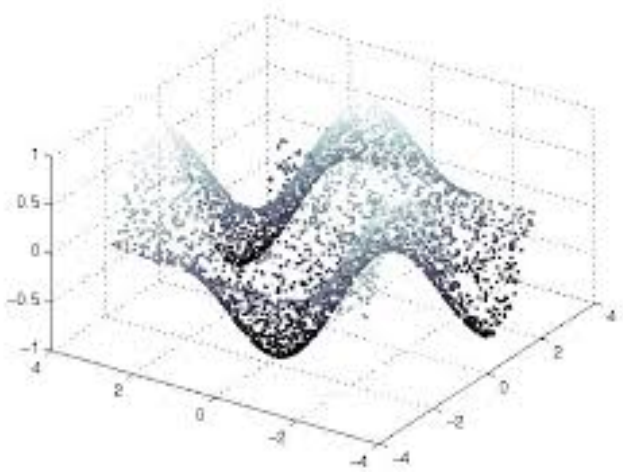

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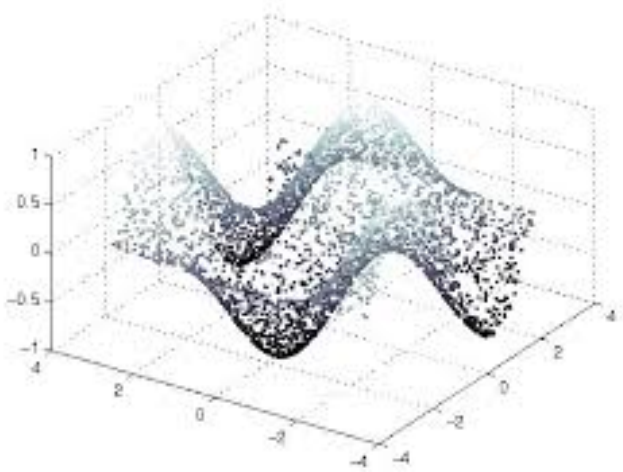
- dimension reduction $\rightarrow$ noise reduction : noise "visits" all possible dimensions



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- Statistical methods, dictionary learning
- Filtering (linear/non linear)
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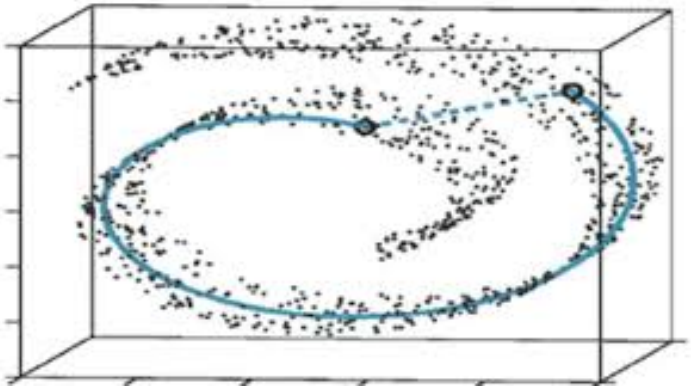

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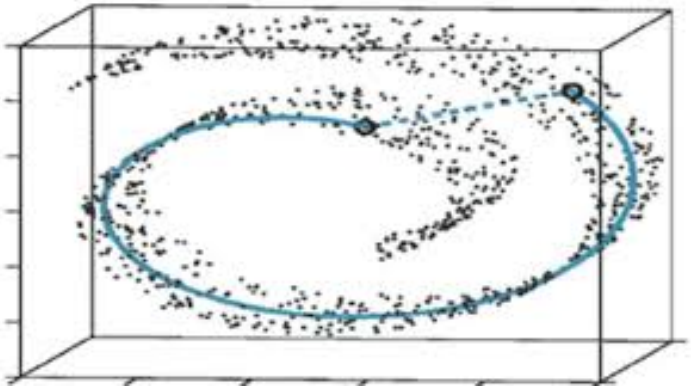

☞ Finding/learning **data representation** ("features extraction") is somehow the core of modern ML. **PCA is a foundational idea**.

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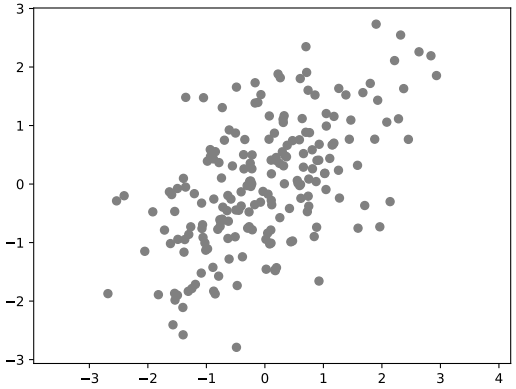

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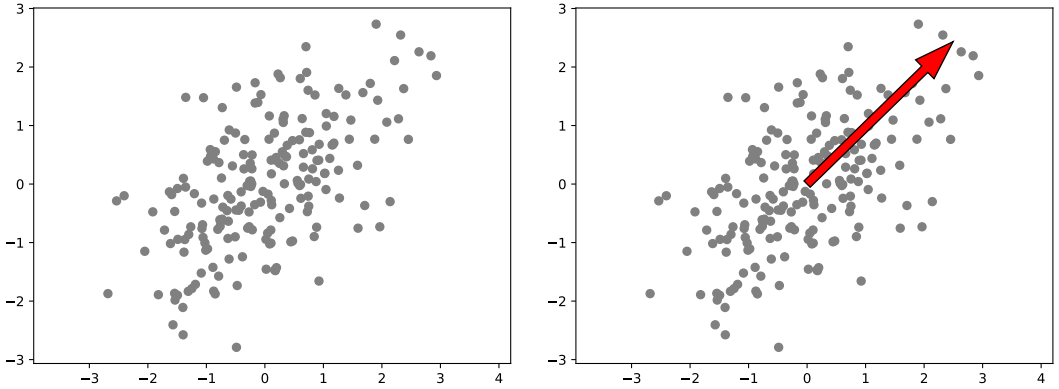

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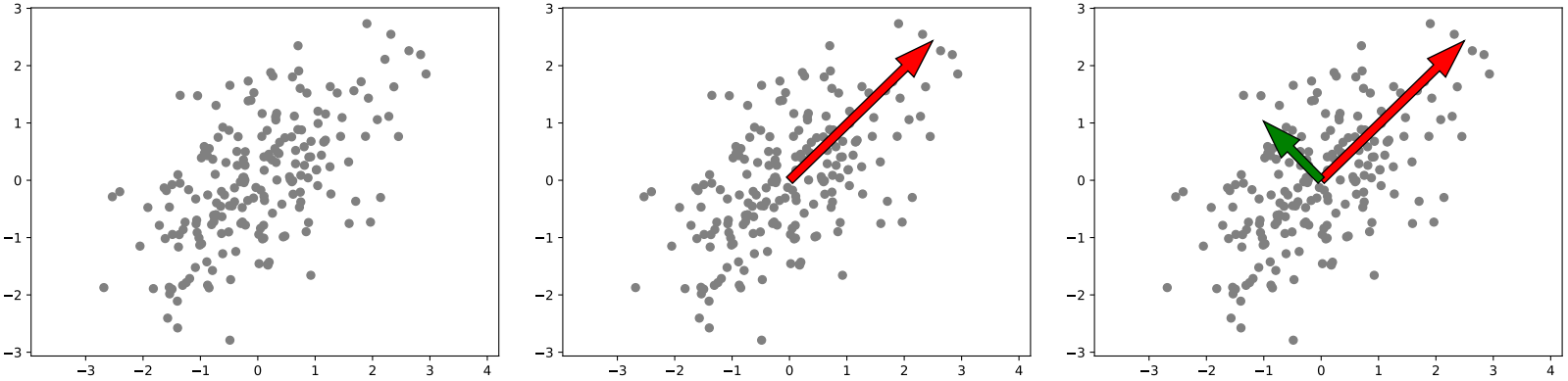

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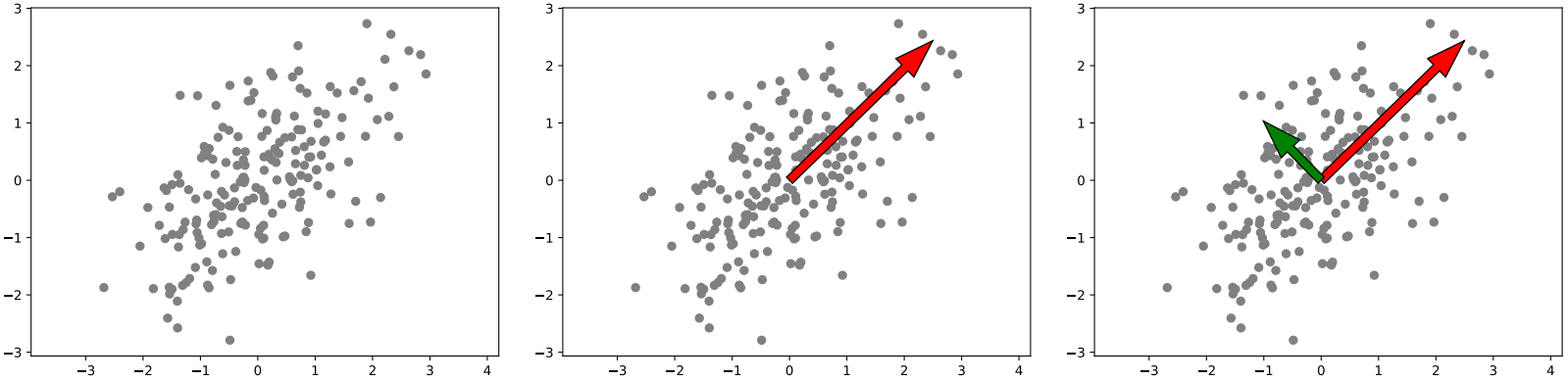
- Find p orthonormal vectors $v_1, \ldots, v_p$ where $p \ll d$ such that :



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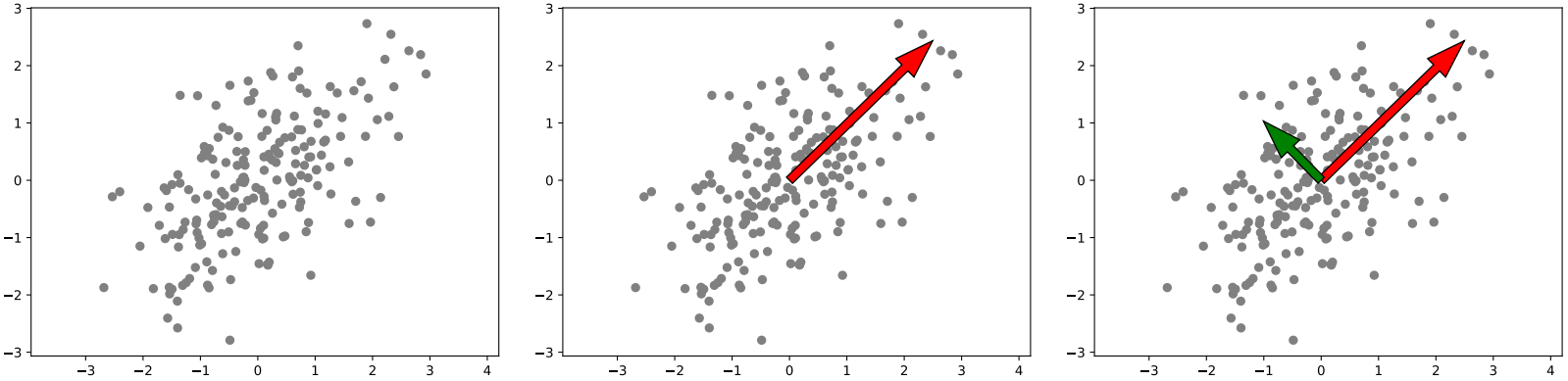

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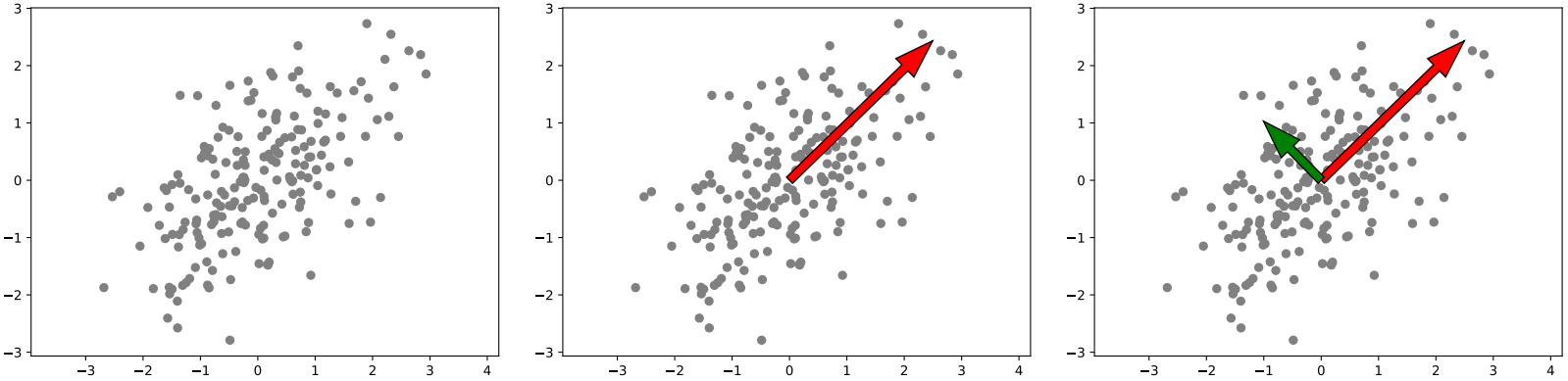

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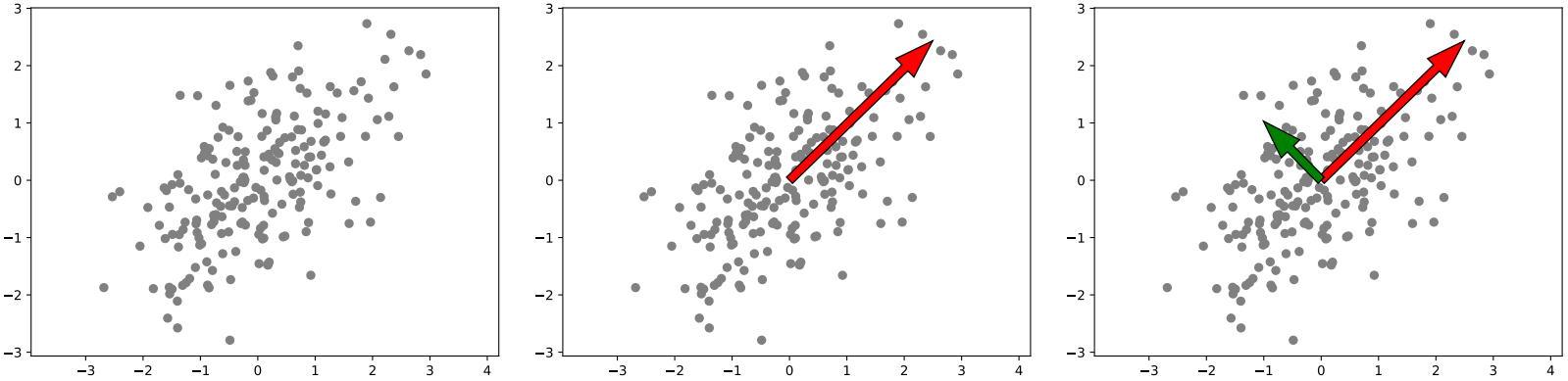

Computing PCA

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$$\nabla_v \mathcal{L} = 2\Sigma v - 2\lambda v$$

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1. Compute empirical mean : $\hat{\mu} = \frac{1}{n}\sum_{i=1}^{n} x_i$ (cost $O(nd)$)
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Remark : SVD

Taking X_c the matrix of centered data $x_i - \hat{\mu}$, such that $\hat{\Sigma} = X_c^\top X_c/(n-1)$, and the Singular Value Decomposition

$$X_c = U\Gamma V^\top \qquad \text{(cost } O(nd^2 + d^3))$$

we have directly $\hat{\Sigma} = V\Gamma^2 V^\top/(n-1)$. SVD is often "more convenient" (more algorithms available, more stable, etc.)

PCA : remarks

Standardization matter

- Often center and "whiten" data to unit norm column $\tilde{x}_i = \text{diag}(1/\sigma_k)(x_i - \hat{\mu})$
- The low-dimensional representation of x is $z = [\tilde{x}^\top v_k]_k \in \mathbb{R}^p$. Don't forget the same pre-processing ! ! Scikit-learn does it automatically.

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Model selection

Popular criterion : increase p until the "explained variance"

$$\frac{\sum_{k=1}^{p} \lambda_k}{\sum_{k=1}^{d} \lambda_k}$$

is close enough to 1. But computing full SVD may be too costly ! Myriad of other strategies.

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- Properties :
  - the matrix Σ is rank $n < d$, it has only n non-zero eigenvalues.
  - Same non-zero eigenvalues as full-rank S.
  - Given v_i, $X_c v_i$ is an eigenvector of S, and given u_i, $X_c^\top v_i$ is an eigenvector of Σ. Not necessarily normalized ! !
- The decomposition can be done on S instead ! Cost $O(n^3)$. Given u_i with $\|u_i\| = 1$, v_i can be recovered (after normalization $\|v_i\| = 1$) as

$$v_i = \frac{1}{\sqrt{(n-1)\lambda_i}} X_c^T u_i$$

Kernel PCA

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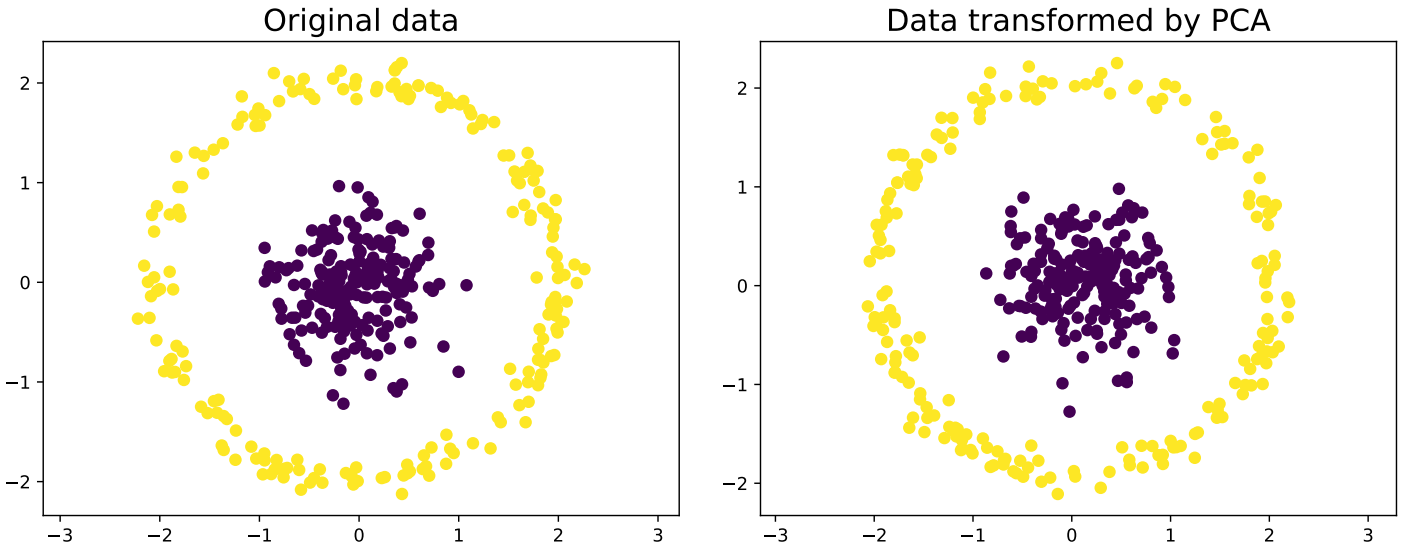

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- (High-dim) PCA **depends only on the inner products between samples**.
- We can improve PCA by transforming the data into a higher-dimensional space $\Phi(x_i) \in \mathcal{H}$, as long as we know how to compute $\langle \Phi(x), \Phi(x') \rangle_{\mathcal{H}}$

Some properties of Kernel function

Definition (Positive semi-definite kernel)

A symmetric kernel $k : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is said to be positive semi-definite (psd) iff

$$\forall n \in \mathbb{N}, \quad \forall \xi_1 \dots \xi_n \in \mathbb{R}, \quad \forall \mathrm{x}_1 \dots \mathrm{x}_n \in \mathbb{R}^d, \sum_{i,j}^{n} \xi_i \xi_j k(\mathrm{x}_i, \mathrm{x}_j) \geq 0$$

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But the converse is also true ! !

Theorem (Mercer Theorem)

For every positive semi-definite kernel k, there exists a Hilbert space $\mathcal{H}$ and a feature map $\phi : \mathbb{R}^d \to \mathcal{H}$ such that $k(x, x') = \langle \phi(x), \phi(x') \rangle_{\mathcal{H}}$.

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It is possible to choose $\mathcal{H}$ as a space of functions, such that $k(\cdot, x) \in \mathcal{H}$, and $\langle f, k(\cdot, x) \rangle_{\mathcal{H}} = f(x)$. It is called the Reproducing Kernel Hilbert Space (RKHS) associated to k.

Operations on kernels

Let k_1 and k_2 be psd, and $\lambda_{1,2} > 0$ then :

1. $\lambda_1 k_1$, (multiplication by a positive scalar)
2. $\lambda_1 k_1 + \lambda_2 k_2$, (sum of kernels),
3. $k_1 k_2$, (product of kernels),
4. $\exp(k_1)$, (exponential of kernel),
5. $(\mathrm{x}_i, \mathrm{x}_j) \mapsto g(\mathrm{x}_i) g(\mathrm{x}_j) k_1(\mathrm{x}_i, \mathrm{x}_j)$, with $g : \mathbb{R}^d \to \mathbb{R}$, (multiplication by a function)

are all positive semi-definite, hence valid kernels.

☞ These operations allow us to create more complicated kernels by combining simple ones.

Choosing the Kernel function

Usual kernel functions

- Linear kernel ($\mathcal{F} \equiv \mathbb{R}^d$) : $k(x, x') = x^T x'$
- Polynomial kernel (dimension of $\mathcal{F}$ increases with the order d)

$$k(x, x') = (x^T x')^d \quad \text{or} \quad (x^T x' + 1)^d$$

- Gaussian radial function ($\mathcal{F}$ with infinite dimension)

$$k(x, x') = \exp\left(-\gamma ||x - x'||^2\right)$$

- Neural net kernel ($\mathcal{F}$ with infinite dimension)

$$k(x, x') = \tanh\left(\kappa_1 x^T x' + \kappa_2\right)$$

☞ standard practice is to estimate the optimal kernel parameters by cross-validation

Kernel PCA

Idea

Replace $x_i^\top x_j$ with $k(x_i, x_j) = \langle \Phi(x_i), \Phi(x_j) \rangle_{\mathcal{H}} \ldots$

☞ Just replace $S = \frac{1}{n-1} X_c X_c^\top$ with $S_K = \frac{1}{n-1} K$, where $K = [k(x_i, x_j)]_{ij}$.

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- It is generally impossible to compute $v_k = \frac{\sum_i \Phi(x_i)(u_k)_i}{\sqrt{(n-1)\lambda_k}}$ since it is in $\mathcal{H}$...
- ... however for any x we can compute the projection on the components $\langle \Phi(x), v_k \rangle_{\mathcal{H}} = \frac{1}{\sqrt{(n-1)\lambda_k}} \sum_i k(x, x_i)(u_k)_i$

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Centering

- Recall that we have assumed $\hat{\mu} = 0$, or equivalently, we work with $\tilde{x} = x - \hat{\mu}$.
- In the kernel space, we would like to work with $\tilde{\Phi}(x) = \Phi(x) - \frac{1}{n} \sum_i \Phi(x_i)$.
- The inner product becomes $\langle \tilde{\Phi}(x), \tilde{\Phi}(x') \rangle_{\mathcal{H}} = k(x, x') - \frac{1}{n} \sum_i [k(x, x_i) + k(x', x_i)] + \frac{1}{n^2} \sum_{ij} k(x_i, x_j)$

Kernel PCA summary

Kernel PCA

1. Construct the normalized Kernel Matrix

$$\tilde{K} = K - UK - KU + UKU$$

where $U = 1_{n \times n}/n$.

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3. The projection of x is $z_k = \langle \tilde{\Phi}(x), v_k \rangle$ with $v_k = \frac{\sum_i (u_k)_i \tilde{\Phi}(x_i)}{\sqrt{\lambda_k (n-1)}}$, i.e.

$$z_k = \frac{\tilde{K}_x^\top u_k}{\sqrt{\lambda_k (n-1)}}$$

   where $K_x = [k(x, x_i)]_i$ and $\tilde{K}_x = K_x - UK_x - K\frac{1_n}{n} + UK\frac{1_n}{n}$.

Example of KPCA