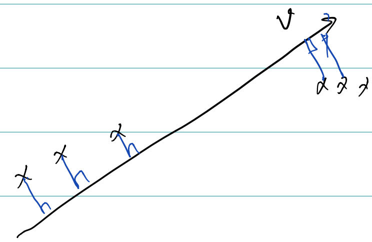
Principal Component Analysis



$v^T \cdot x_1 \quad v^T x_2 \quad \cdots \quad v^T x_n$ 内积为投影

$v^T \cdot 0 = 0$ 均值投影

$s^2 = \sum_{i=1}^{n} (v^T x_i - 0)^2 = \sum (v^T x_i)(v^T x_i)^T$ 分散程度.

$= \sum v^T x_i \cdot x_i^T v.$

$= v^T C \cdot v.$

$C = \sum_{i=1}^{n} x_i x_i^T.$

$v = \underset{\|v\|=1}{\arg\max}\ v^T C^T v$

拉格朗日:

$f(v, \lambda) = v^T C v - \lambda (v^T v - 1)$

$\frac{\partial f}{\partial v} = 2Cv - 2\lambda v = 0 \Rightarrow Cv = \lambda v$

$\frac{\partial f}{\partial \lambda} = v^T v - 1 = 0 \Rightarrow v^T v = 1$

则 $s^2 = \lambda$ ← 可以找到最大方向

kernel-based PCA

- $$C = \frac{1}{N}\sum_{i=1}^{N}\phi(x_i)\,\phi(x_i)^T = \frac{1}{N}[\phi(x_1), \cdots, \phi(x_N)]\begin{bmatrix}\phi(x_1)^T \\ \vdots \\ \phi(x_N)^T\end{bmatrix}$$

If $X^T = [\phi(x_1), \cdots, \phi(x_N)]$

then

$$C = \frac{1}{N}X^TX$$

kernel

- $$K = XX^T = \underset{n\times 1}{\begin{bmatrix}\phi(x_1)^T \\ \vdots \\ \phi(x_N)^T\end{bmatrix}}\underset{1\times n}{[\phi(x_1), \cdots, \phi(x_N)]}$$

$$= \begin{bmatrix}\phi(x_1)^T\phi(x_1) & \cdots & \phi(x_1)^T\phi(x_N) \\ \phi(x_N)^T\phi(x_1) & \cdots & \phi(x_N)^T\phi(x_N)\end{bmatrix}$$

$$= \begin{bmatrix}k(x_1, x_1) & \cdots & k(x_1, x_N) \\ \vdots & & \\ k(x_N, x_1) & \cdots & k(x_N, x_N)\end{bmatrix}$$

已知，易得

$$(XX^T)u = \lambda u$$

特征值同

$$X^T(XX^T)u = \lambda X^Tu \Rightarrow (X^TX)(X^Tu) = \lambda(X^Tu).$$

归一化，$\|v\|=1$

$$v = \frac{1}{\|X^Tu\|}X^Tu = \frac{1}{\sqrt{u^TXX^Tu}}\cdot X^Tu$$

特征向量

$$= \frac{1}{\sqrt{u^T(\lambda u)}}\cdot X^Tu = \frac{1}{\sqrt{\lambda}}X^Tu.$$

未知 已知

投影坐标

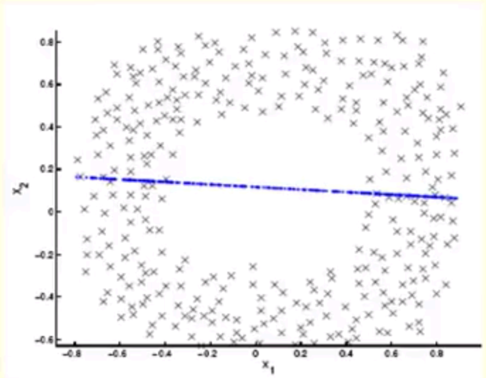
$$v^T\phi(x') = \left(\frac{1}{\sqrt{\lambda}}X^Tu\right)^T\phi(x') = \frac{1}{\sqrt{\lambda}}u^TX\phi(x')$$

$$= \frac{1}{\sqrt{\lambda}}u^T\begin{bmatrix}\phi(x_1)^T \\ \vdots \\ \phi(x_N)^T\end{bmatrix}\cdot\phi(x') = \frac{1}{\sqrt{\lambda}}u^T\begin{bmatrix}k(x_1, x') \\ \vdots \\ k(x_N, x')\end{bmatrix}$$

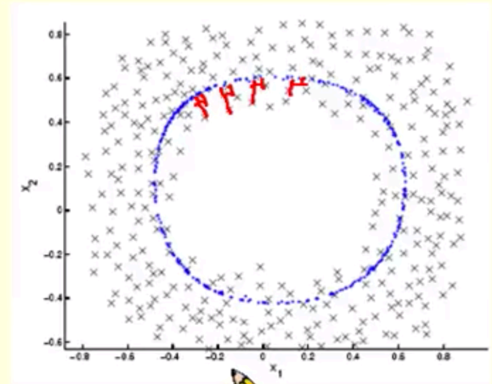
已知 已知 已知

计算核PCA，①找到特征值，定方向；②找到x'在特征维上的投影坐标.

案例



PCA



KPCA