MACHINE LEARNING II

Kernel PCA

kPCA derivation

As in the original space, in feature space, the covariance matrix can be diagonalized and we can find the eigenvectors and eigenvalues that satisfy:

$$C_\phi v^i = \lambda_i v^i$$

Primal eigenvalue problem

But finding the eigenvectors v of C_ϕ may not possible, as we do not have the feature space.

=> Formulate everything as a dot product and use kernel trick!

kPCA Solution to Dual Problem

Eigenvalue problem of the form:

$$K\alpha^i = M\lambda_i\alpha^i, \qquad K: \text{ Gram Matrix}$$

The solutions to the dual eigenvalue problem are given by all the eigenvectors $\alpha^1,...,\alpha^M$ with non-zero eigenvalues $\lambda_1,...,\lambda_M$.

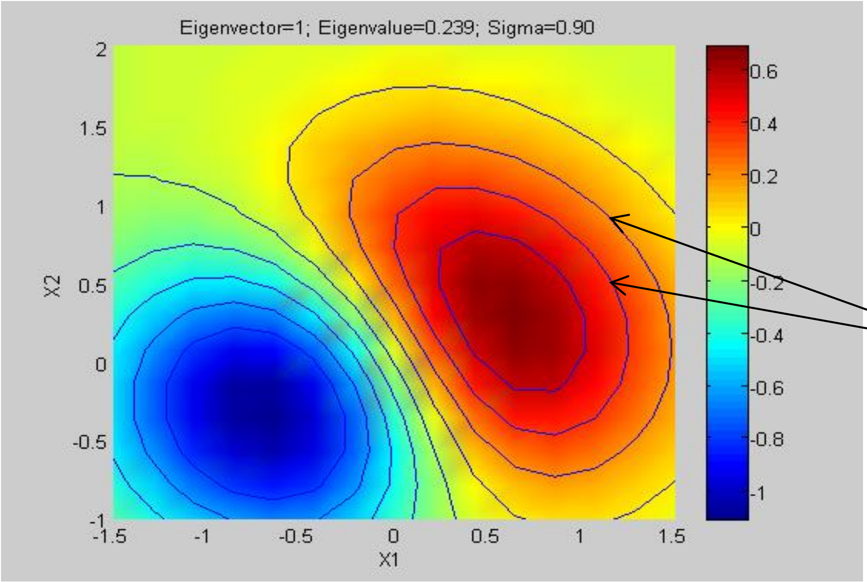
Constructing the kPCA projections

We cannot see the projections in feature space!

We can only compute the projections of each point onto each eigenvector.

Projection of query point x onto eigenvector v^i:

$$\left\langle v^i, \phi(x) \right\rangle = \frac{1}{\lambda_i M} \sum_{j=1}^{M} \alpha_j^i k\left(x^j, x\right)$$



Isolines group points with equal projection:

All points $x, s.t.$: $\left\langle v^i, \phi(x) \right\rangle = cst.$

kPCA Exercise 1.1

Projection of query point x onto eigenvector v^i:

$$\langle v^i, \phi(x) \rangle = \frac{1}{\lambda_i M} \sum_{j=1}^{M} \alpha_j^i k\left(x^j, x\right)$$

Using the RBF kernel: $k\left(x, x'\right) = e^{-\frac{\|x-x'\|^2}{\sigma^2}}$

Consider a 2 – dimensional data – space, with two datapoints:

a) How many dual eigenvectors do you have and what is their dimension?

b) Compute the eigenvectors and draw the isolines for the projections on each eigenvector.

HINT: kPCA requires data to be centered in feature space

This leads to the following transformation (see suppl. exercises)

$$\tilde{\mathbf{K}}_{ij} = \mathbf{K}_{ij} - \frac{1}{M}\sum_{k=1}^{M}\mathbf{K}_{ik} - \frac{1}{M}\sum_{k=1}^{M}\mathbf{K}_{kj} + \frac{1}{M^2}\sum_{k,l=1}^{M}\mathbf{K}_{kl}$$

kPCA Exercise 1.1

$$K = \begin{bmatrix} 1 & k(x^1, x^2) \\ k(x^2, x^1) & 1 \end{bmatrix}$$

After centering $\tilde{K} = \begin{bmatrix} a & b \\ b & a \end{bmatrix} = \begin{bmatrix} a & -a \\ -a & a \end{bmatrix}$

$$a = -b = \frac{1}{2} - \frac{k\left(x^1, x^2\right)}{2}$$

$$\tilde{\mathbf{K}}_{ij} = \mathbf{K}_{ij} - \frac{1}{M}\sum_{k=1}^{M}\mathbf{K}_{ik} - \frac{1}{M}\sum_{k=1}^{M}\mathbf{K}_{kj} + \frac{1}{M^2}\sum_{k,l=1}^{M}\mathbf{K}_{kl}$$

1: Compute Dual eigenvectors $\alpha^1 = \frac{1}{\sqrt{2}}[1, 1]^T$ and $\alpha^2 = \frac{1}{\sqrt{(2)}}[1, -1]^T$

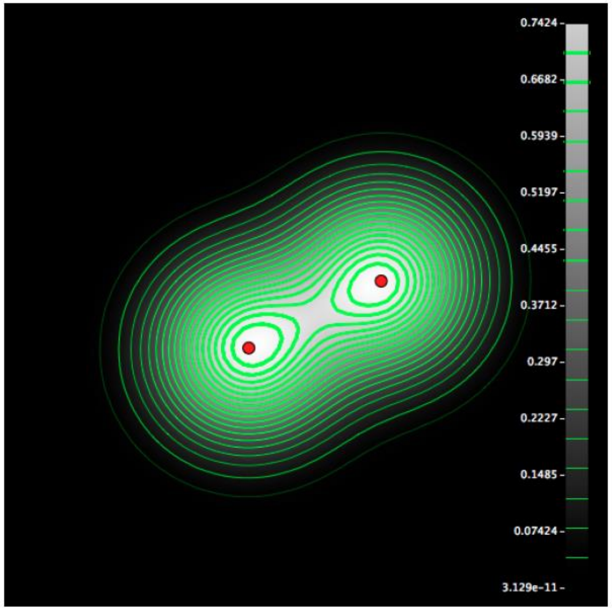
2. Projection of query point x onto eigenvector v^i: $\left\langle v^i, \phi(x)\right\rangle = \frac{1}{\lambda_i M}\sum_{j=1}^{M}\alpha_j^i k\left(x^j, x\right)$

1st eigenvector v^1: $\langle v^1, \phi(x)\rangle = \alpha_1^1 k(x^1, x) + \alpha_1^2 k(x^2, x) = \frac{1}{\sqrt{2}}k(x^1, x) + \frac{1}{\sqrt{2}}k(x^2, x)$

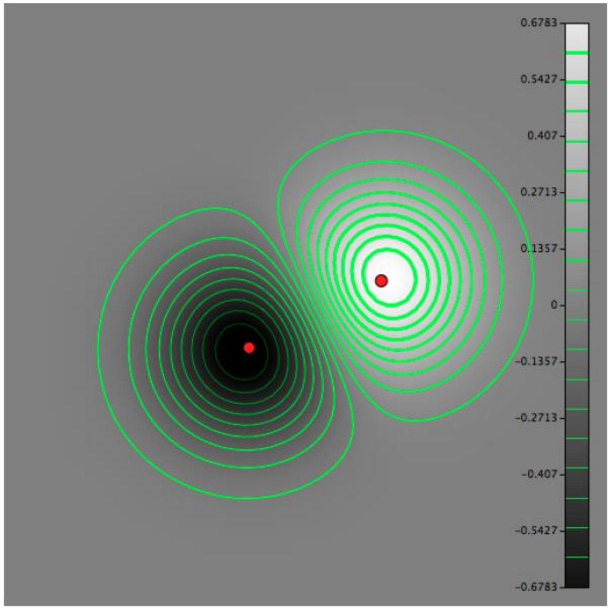
2nd eigenvector v^2: $\langle v^2, \phi(x)\rangle = \alpha_2^1 k(x^1, x) + \alpha_2^2 k(x^2, x) = \frac{1}{\sqrt{2}}k(x^1, x) - \frac{1}{\sqrt{2}}k(x^2, x)$

kPCA Exercise 1.1

3: Draw the isolines



Projection on first eigenvector



Projection on second eigenvector

1st eigenvector v^1: $$\langle v^1, \phi(x)\rangle = \alpha_1^1 k(x^1, x) + \alpha_1^2 k(x^2, x) = \frac{1}{\sqrt{2}} k(x^1, x) + \frac{1}{\sqrt{2}} k(x^2, x)$$

2nd eigenvector v^2: $$\langle v^2, \phi(x)\rangle = \alpha_2^1 k(x^1, x) + \alpha_2^2 k(x^2, x) = \frac{1}{\sqrt{2}} k(x^1, x) - \frac{1}{\sqrt{2}} k(x^2, x)$$

kPCA Exercise 1.2

Projection of query point x onto eigenvector v^i:

$$\langle v^i, \phi(x) \rangle = \frac{1}{\lambda_i M} \sum_{j=1}^{M} \alpha_j^i k\left(x^j, x\right)$$

homogeneous polynomial kernel with p=1 and p=2:

$$k(x, x') = \langle x, x' \rangle^p$$

Consider a 2 – dimensional data – space, with two datapoints:
Compute the eigenvectors and draw the isolines for the projections on each eigenvector.

kPCA Exercise 1.2: solution

$$K = \begin{bmatrix} k(x^1,x^1) & k(x^1,x^2) \\ k(x^2,x^1) & k(x^2,x^2) \end{bmatrix} \text{ (before centering)}$$

$$\tilde{\mathbf{K}}_{ij} = \mathbf{K}_{ij} - \frac{1}{M}\sum_{k=1}^{M}\mathbf{K}_{ik} - \frac{1}{M}\sum_{k=1}^{M}\mathbf{K}_{kj} + \frac{1}{M^2}\sum_{k,l=1}^{M}\mathbf{K}_{kl}$$

After centering $\tilde{K} = \begin{bmatrix} a & b \\ b & a \end{bmatrix}, \qquad a = -b$

$$a = -\frac{1}{2}k(x^1,x^2) + \frac{1}{4}\left(k(x^1,x^1)+k(x^2,x^2)\right),\ b = \frac{1}{2}k(x^1,x^2) - \frac{1}{4}\left(k(x^1,x^1)+k(x^2,x^2)\right)$$

$$a = -\frac{1}{2}\left(\|x^1\|\|x^2\|\cos(\theta)\right)^p + \frac{1}{4}\sum_{i=1}^{2}\|x^i\|^p,\ b = \frac{1}{2}\left(\|x^1\|\|x^2\|\cos(\theta)\right)^p - \frac{1}{4}\sum_{i=1}^{2}\|x^i\|^p$$

Dual eigenvectors are: $\alpha^1 = \frac{1}{\sqrt{2}}[-1\ 1]^T \quad \alpha^2 = \frac{1}{\sqrt{2}}[1\ \ 1]^T$

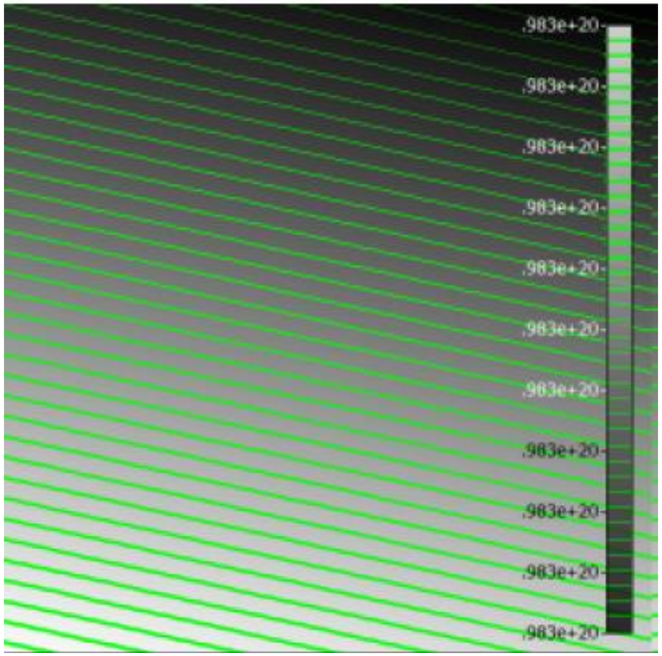
Projections on eigenvectors: $\langle v^1, \phi(x)\rangle = \frac{1}{\sqrt{2}}k(x^2,x) - \frac{1}{\sqrt{2}}k(x^1,x)$ $\quad \langle v^2, \phi(x)\rangle = \frac{1}{\sqrt{2}}k(x^1,x) + \frac{1}{\sqrt{2}}k(x^2,x)$

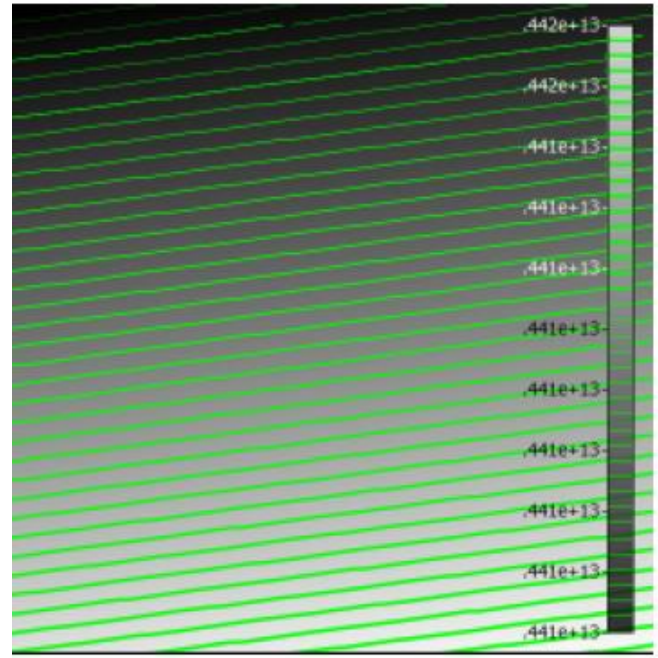
$p = 1$, the isolines are lines perpendicular to the combination of vector points.

$p = 2, 4, 6,$ etc generate ellipses and variants on these (see kernel lecture)

$p = 3, 5, 7,$ etc generate hyperbolas and variants on these (see kernel lecture)

kPCA Exercise 1.2: solution





For the particular case where the two vector points are colinear or anticolinear, or when they are orthogonal, the solution is a set of lines orthogonal to the two vector points.

For orthogonal vectors, $K = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, and the dual eigenvectors are $\alpha^1 = [0\ 1]^T, \alpha^2 = [1\ 0]^T$

$$\left\langle v^1, \phi(x) \right\rangle = k\left(x^1, x\right) = \left(\left(x^1\right)^T x\right)^p \quad \text{and} \quad \left\langle v^2, \phi(x) \right\rangle = k\left(x^2, x\right) = \left(\left(x^1\right)^T x\right)^p$$

kPCA Exercise 1.3

Projection of query point x onto eigenvector v^i:

$$\left\langle v^i, \phi(x) \right\rangle = \frac{1}{\lambda_i M} \sum_{j=1}^{M} \alpha_j^i k\left(x^j, x\right)$$

Consider a 2 – dimensional data – space, with 3 equidistant datapoints:
Compute the eigenvectors and draw the isolines for the projections on each eigenvector, when using:

a) RBF kernel

b) Homogeneous polynomial kernel

What happens if the points are not equidistant?

kPCA Exercise 1.3: solution

$$K = \begin{bmatrix} 1 & k(x^1, x^2) & k(x^1, x^3) \\ k(x^2, x^1) & 1 & k(x^2, x^3) \\ k(x^3, x^1) & k(x^3, x^2) & 1 \end{bmatrix}$$

Points equidistant: $k\left(x^1, x^2\right) = k\left(x^1, x^3\right) = k\left(x^2, x^3\right) = b$

$$K = \begin{bmatrix} 1 & b & b \\ b & 1 & b \\ b & b & 1 \end{bmatrix} \Rightarrow \tilde{K} = \frac{1}{3}\begin{bmatrix} 2-2b & b-1 & b-1 \\ b-1 & 2-2b & b-1 \\ b-1 & b-1 & 2-2b \end{bmatrix}$$

Dual eigenvectors

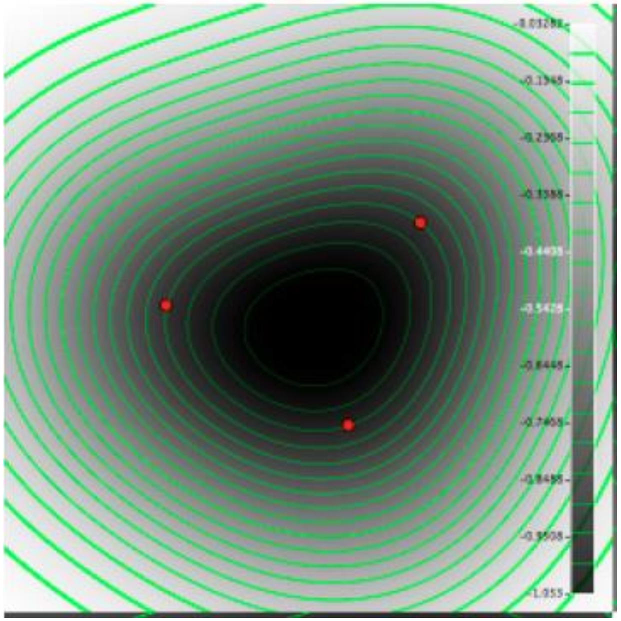
$$\alpha^1 = \frac{1}{\sqrt{3}}[1 \ \ 1 \ \ 1]^T$$

$$\alpha^2 = \frac{1}{\sqrt{2}}[0 \ \ 1 \ \ -1]^T$$

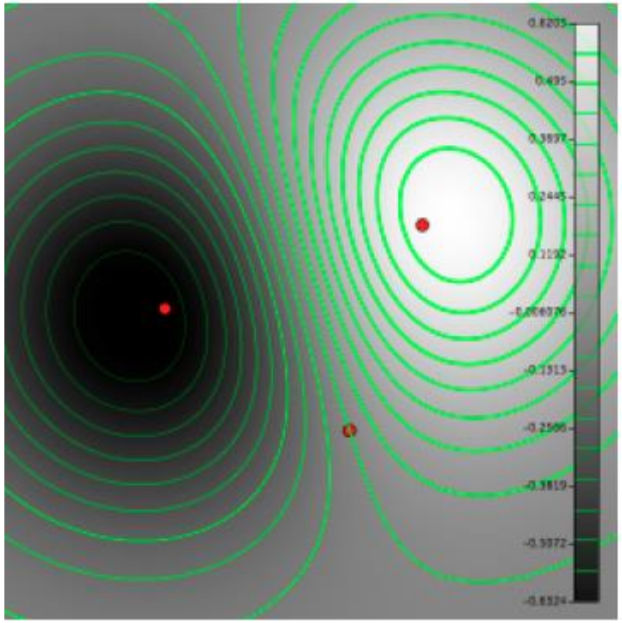
$$\alpha^3 = \sqrt{\frac{2}{3}}[1 \ \ -1/2 \ \ -1/2]^T$$

kPCA Exercise 1.3: solution

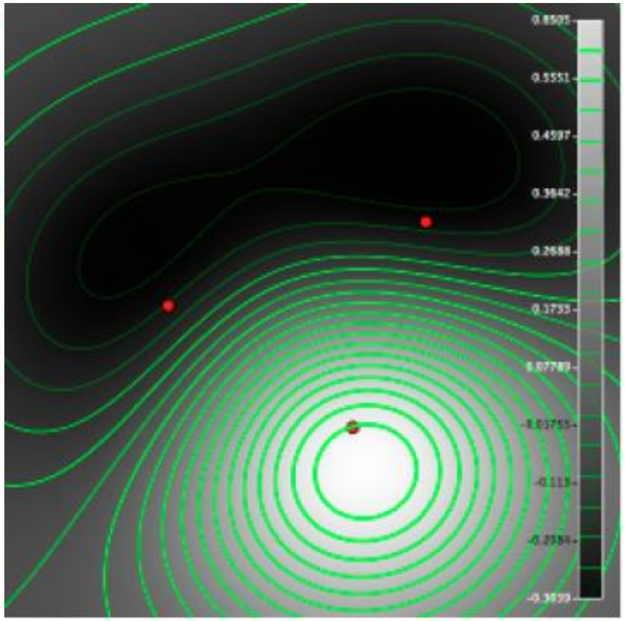
Projections on dual eigenvectors with RBF



$$\alpha^1 = \frac{1}{\sqrt{3}}[1 \;\; 1 \;\; 1]^T$$



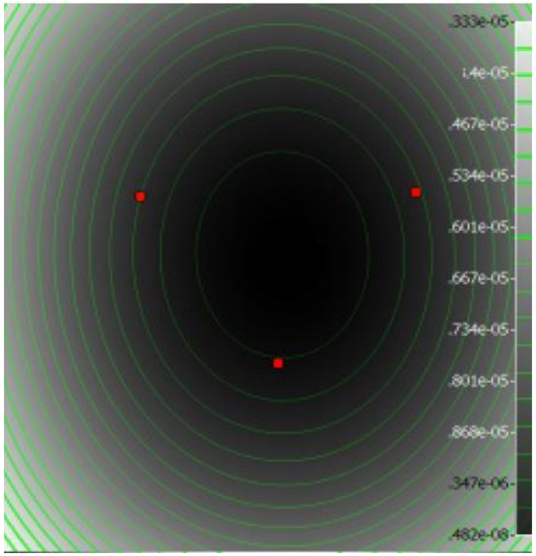
$$\alpha^2 = \frac{1}{\sqrt{2}}[0 \;\; 1 \;\; -1]^T$$

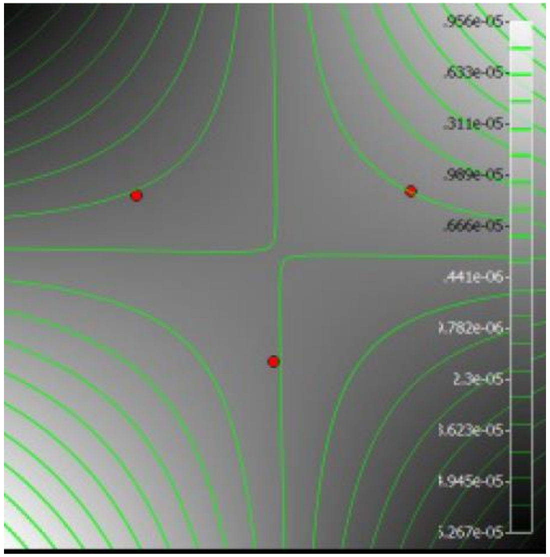


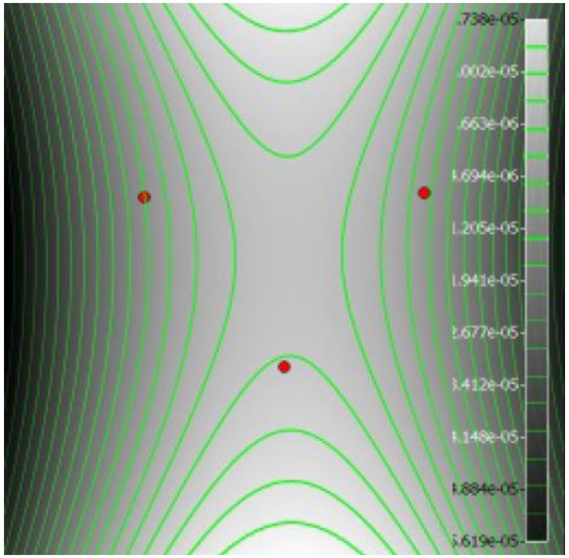
$$\alpha^3 = \sqrt{\frac{2}{3}}[1 \;\; -1/2 \;\; -1/2]^T$$

kPCA Exercise 1.3: solution

Projections on dual eigenvectors with polynomial of order 2







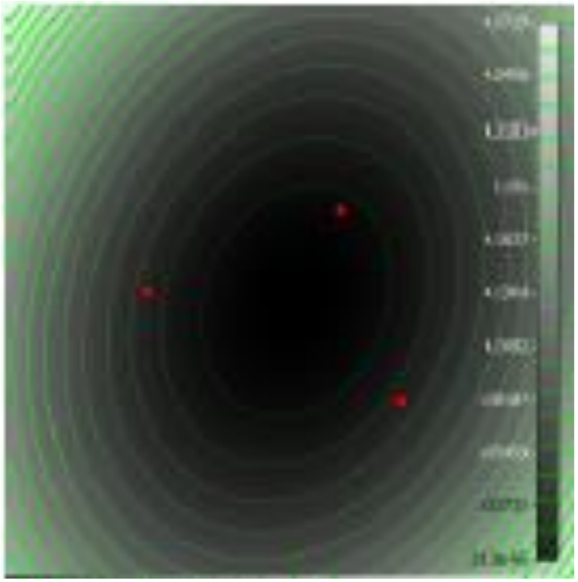
$$\alpha^1 = \frac{1}{\sqrt{3}}[1 \;\; 1 \;\; 1]^T$$

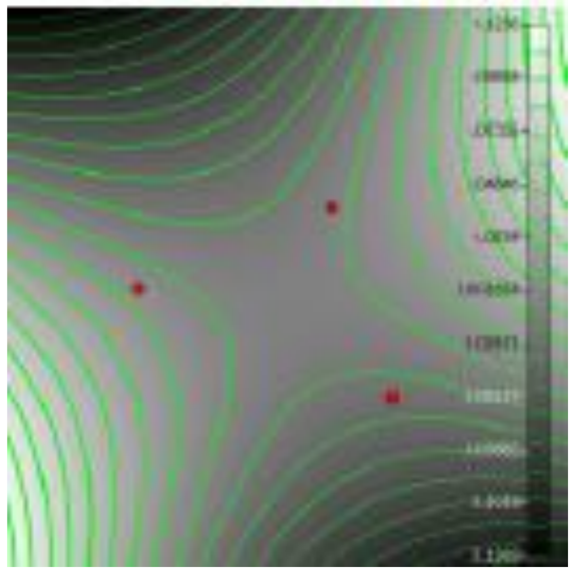
$$\alpha^2 = \frac{1}{\sqrt{2}}[0 \;\; 1 \;\; -1]^T$$

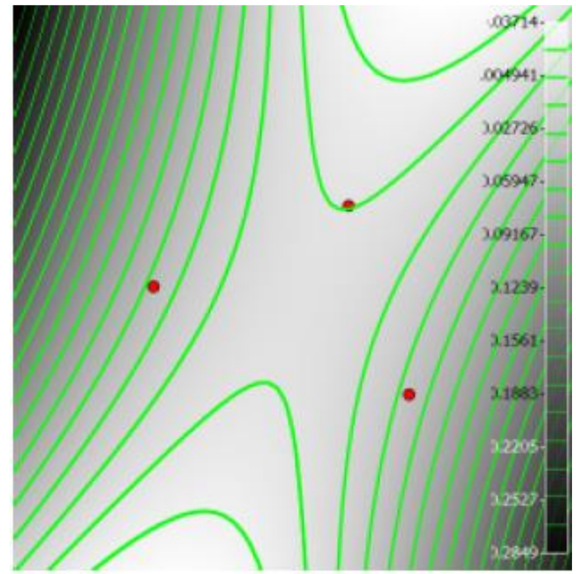
$$\alpha^3 = \sqrt{\frac{2}{3}}[1 \;\; -1/2 \;\; -1/2]^T$$

kPCA Exercise 1.3: solution

Projections on dual eigenvectors with polynomial of order 2





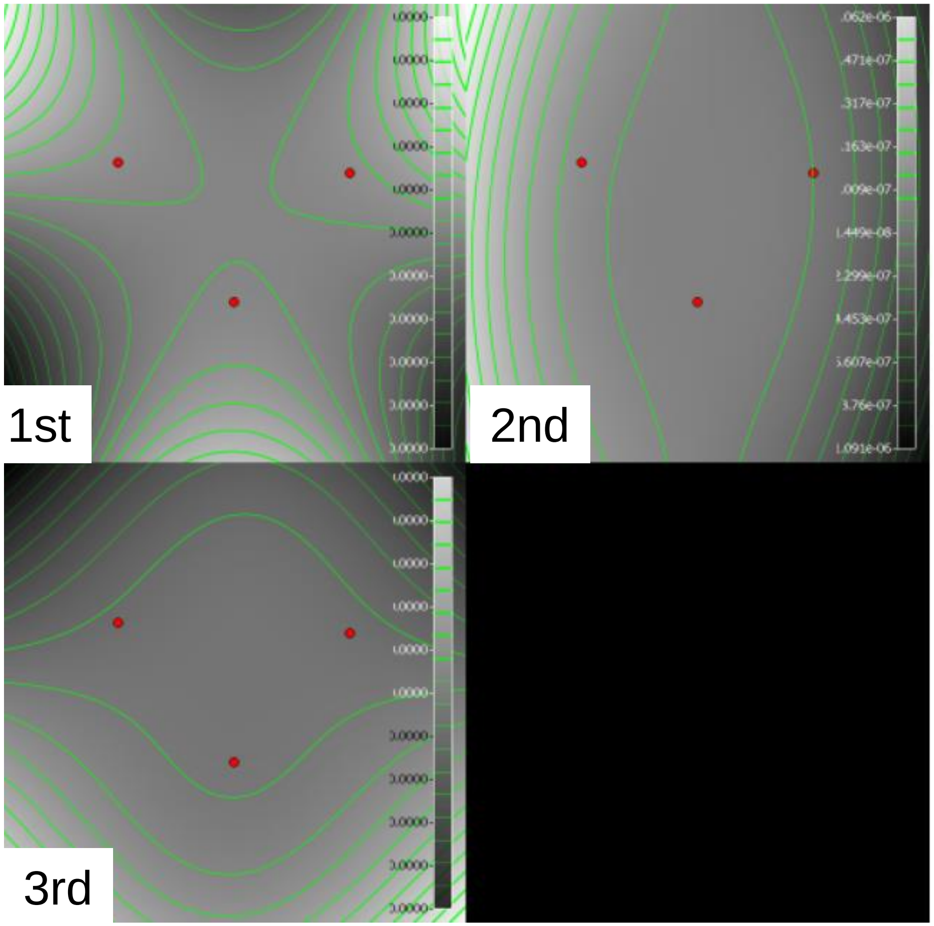


$$\alpha^1 = \frac{1}{\sqrt{3}}[1 \;\; 1 \;\; 1]^T \qquad \alpha^2 = \frac{1}{\sqrt{2}}[0 \;\; 1 \;\; -1]^T \qquad \alpha^3 = \sqrt{\frac{2}{3}}[1 \;\; -1/2 \;\; -1/2]^T$$

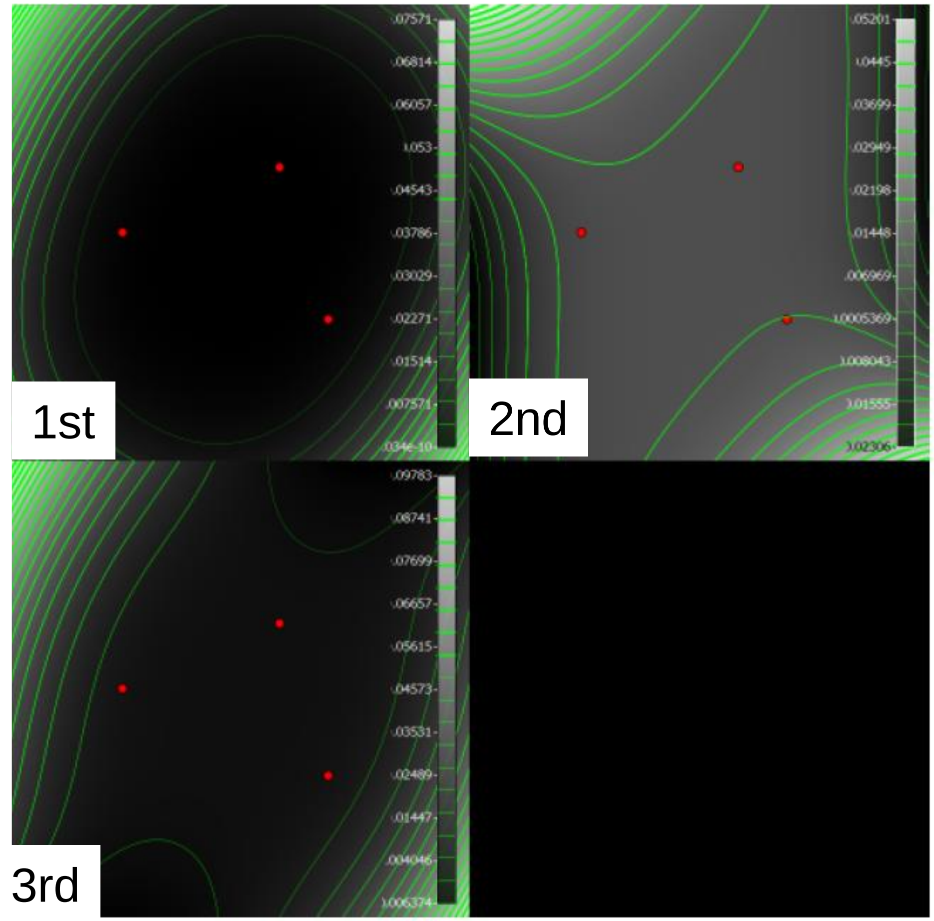
Observe how the ellipse and hyperbolas align with the points' spatial distribution.

kPCA Exercise 1.3: solution

Dual eigenvectors remain identical even when the kernel is of higher order

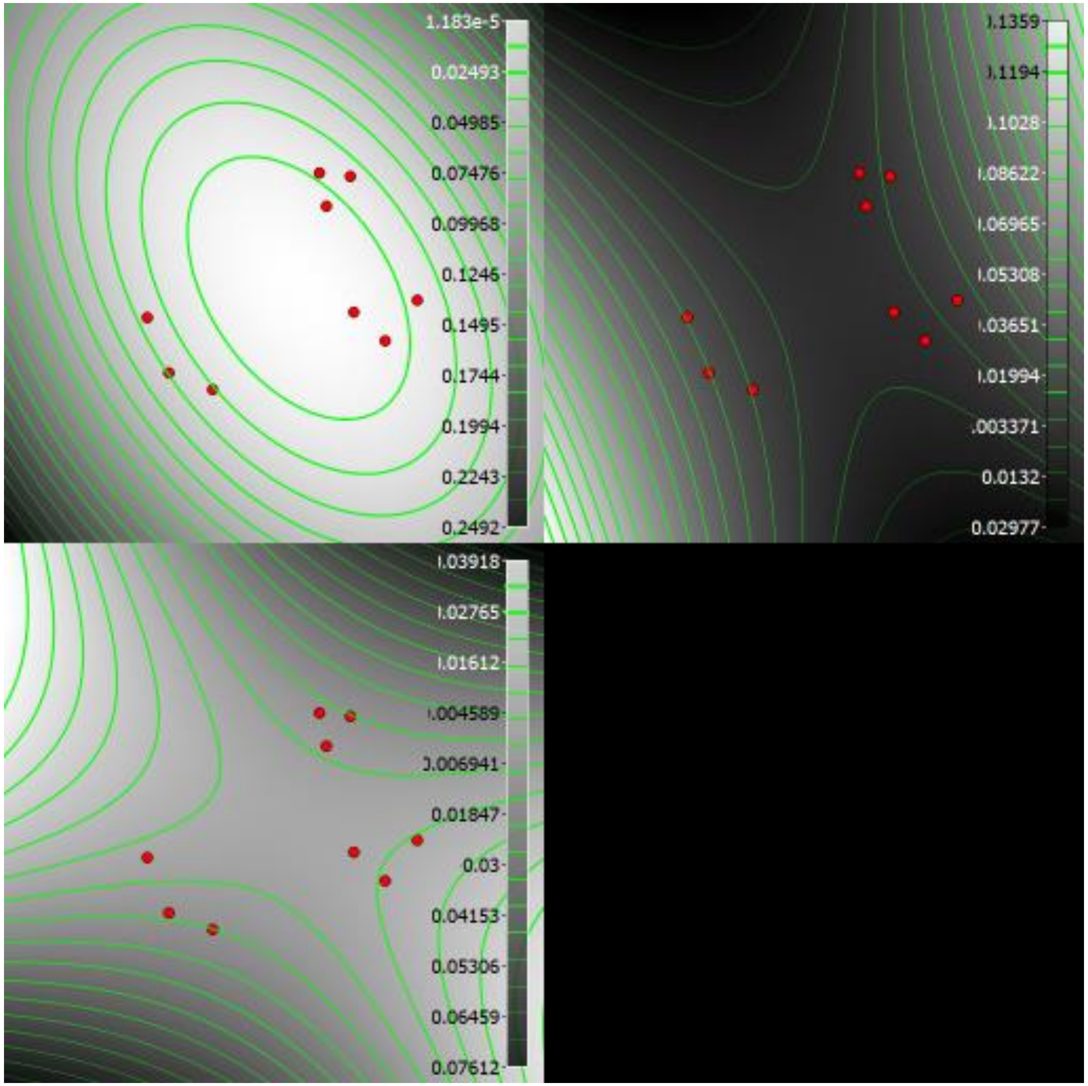


P=3



P=4

kPCA Exercise 1.3: solution



Adding more datapoints affects only the direction of the ellipse and hyperbolas but not the shape as the projections are solely a combination of the addition of several polynomial or RBF kernels.