# Deep Learning and Kernel Machines

**Johan Suykens**

KU Leuven, ESAT-STADIUS
Kasteelpark Arenberg 10
B-3001 Leuven (Heverlee), Belgium
Email: johan.suykens@esat.kuleuven.be
http://www.esat.kuleuven.be/stadius/

**VISUM 2020, Porto, July 2020**
**Computer Vision and Machine Learning Summer School**

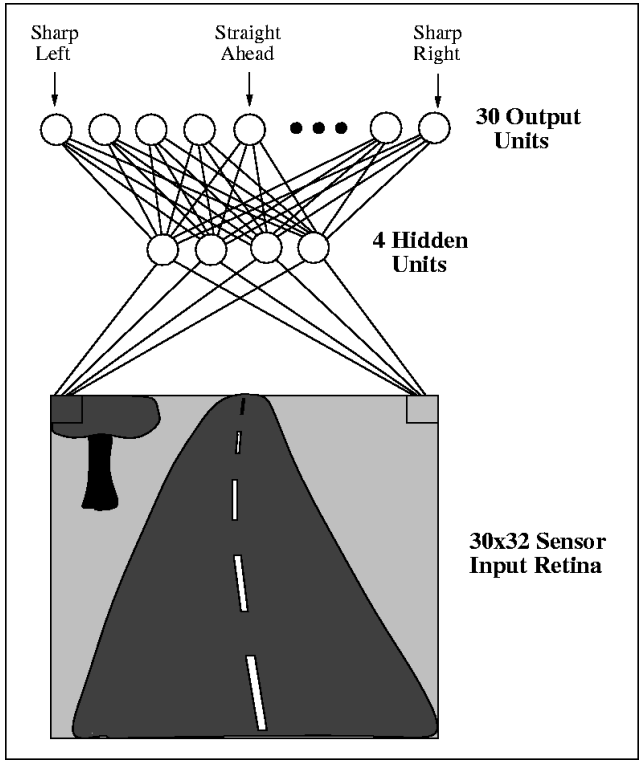
# Overview

- Introduction
- Function estimation and model representations
- Least squares support vector machines (LS-SVM) as core models
- Kernel spectral clustering (KSC)
- Restricted kernel machines (RKM), generative models
- Deep learning and kernel machines: new synergies
- Conclusions

# *Introduction*

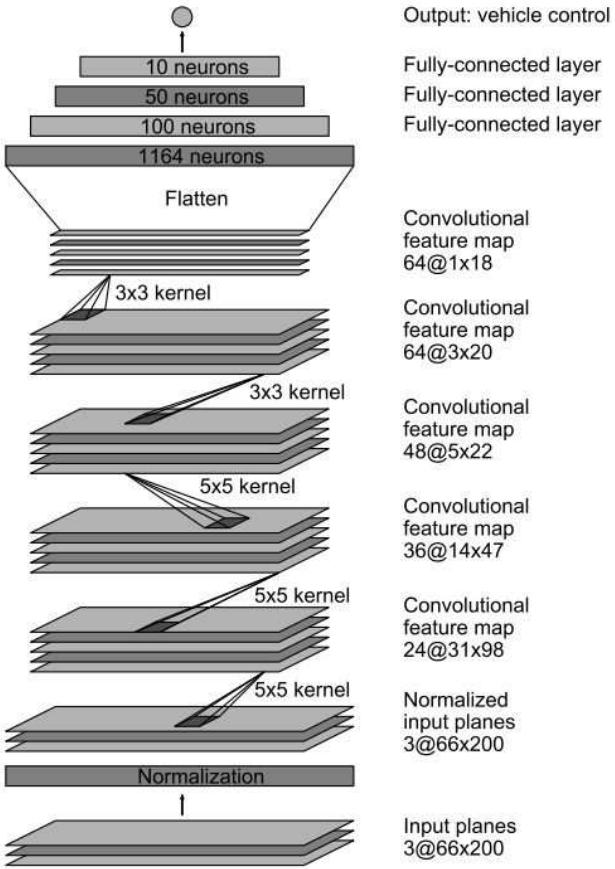
# Self-driving cars and neural networks

in the early days of neural networks:




ALVINN (Autonomous Land Vehicle In a Neural Network)
[Pomerleau, Neural Computation 1991]

# Self-driving cars and deep learning




Waymo / Google Self-Driving Car

Tesla Autopilot


Uber


nuTonomy

(27 million connections)

from: [selfdrivingcars.mit.edu (Lex Fridman et al.), 2017]

# Convolutional neural networks



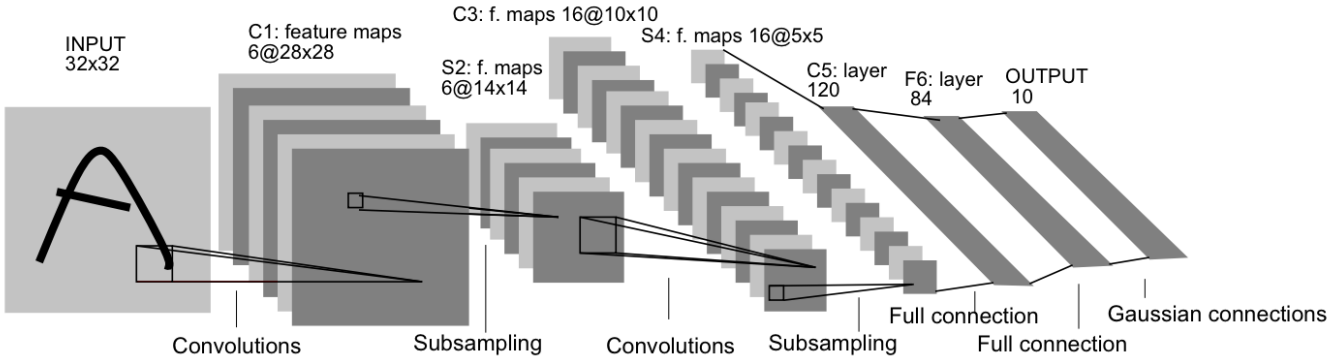



Fig. 2. Architecture of LeNet-5, a Convolutional Neural Network, here for digits recognition. Each plane is a feature map, i.e. a set of units whose weights are constrained to be identical.

[LeCun et al., Proc. IEEE 1998]

Further advanced architectures:

| | |
|---|---|
| Alexnet (2012): | 5 convolutional layers, 3 fully connected |
| VGGnet (2014): | 19 layers |
| GoogLeNet (2014): | 22 layers |
| ResNet (2015): | 152 layers |

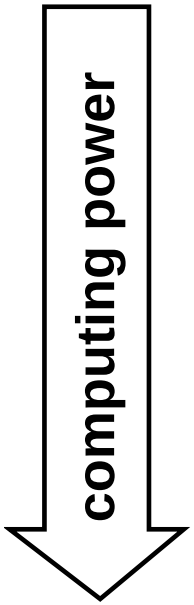
# Historical context

1942 McCulloch & Pitts: mathematical model for neuron
1958 Rosenblatt: perceptron learning
1960 Widrow & Hoff: adaline and lms learning rule
1969 Minsky & Papert: limitations of perceptron

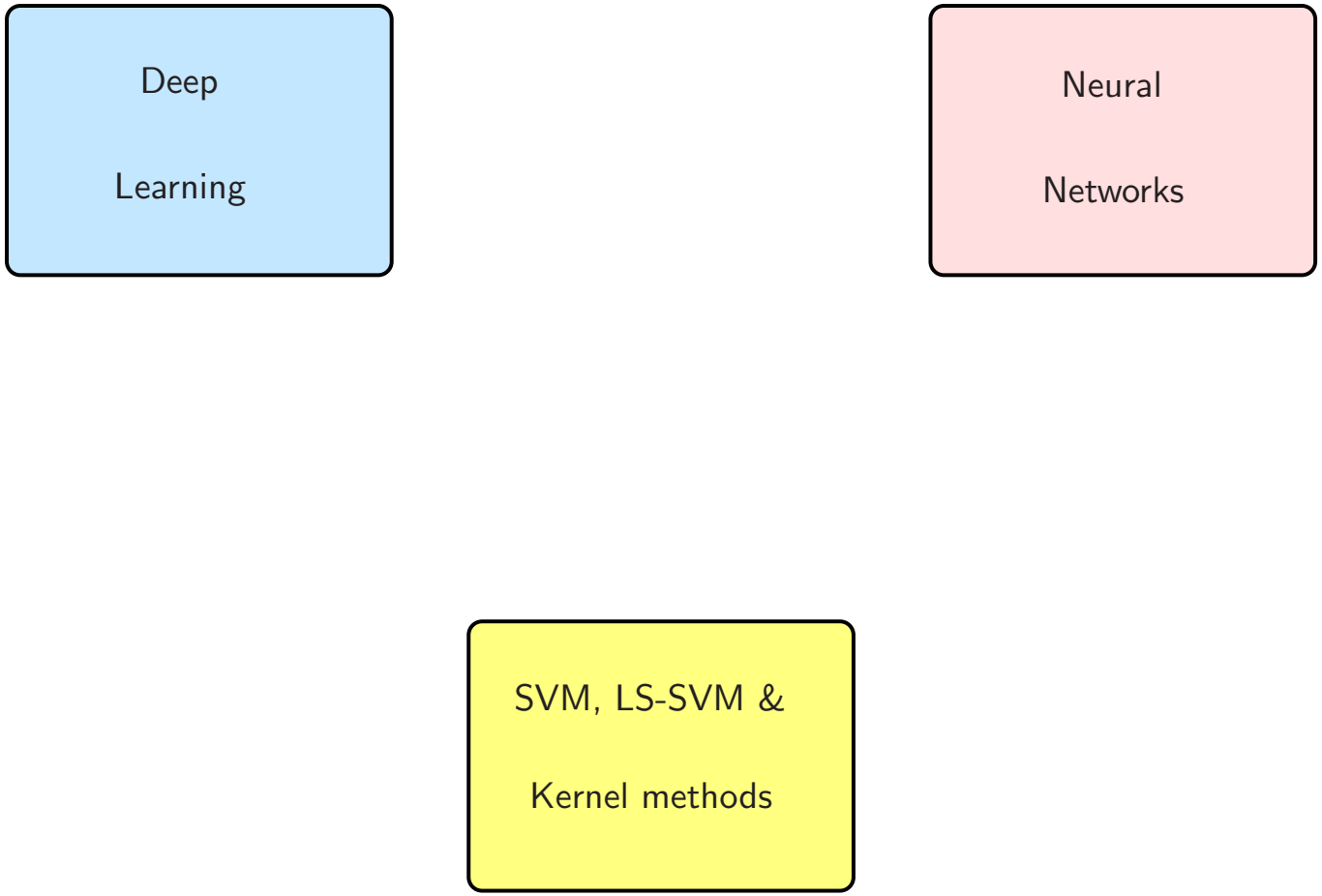
1986 Rumelhart et al.: error backpropagating neural networks
→ *booming of neural network universal approximators*

1992 Vapnik et al.: support vector machine classifiers
→ *convex optimization, kernel machines*

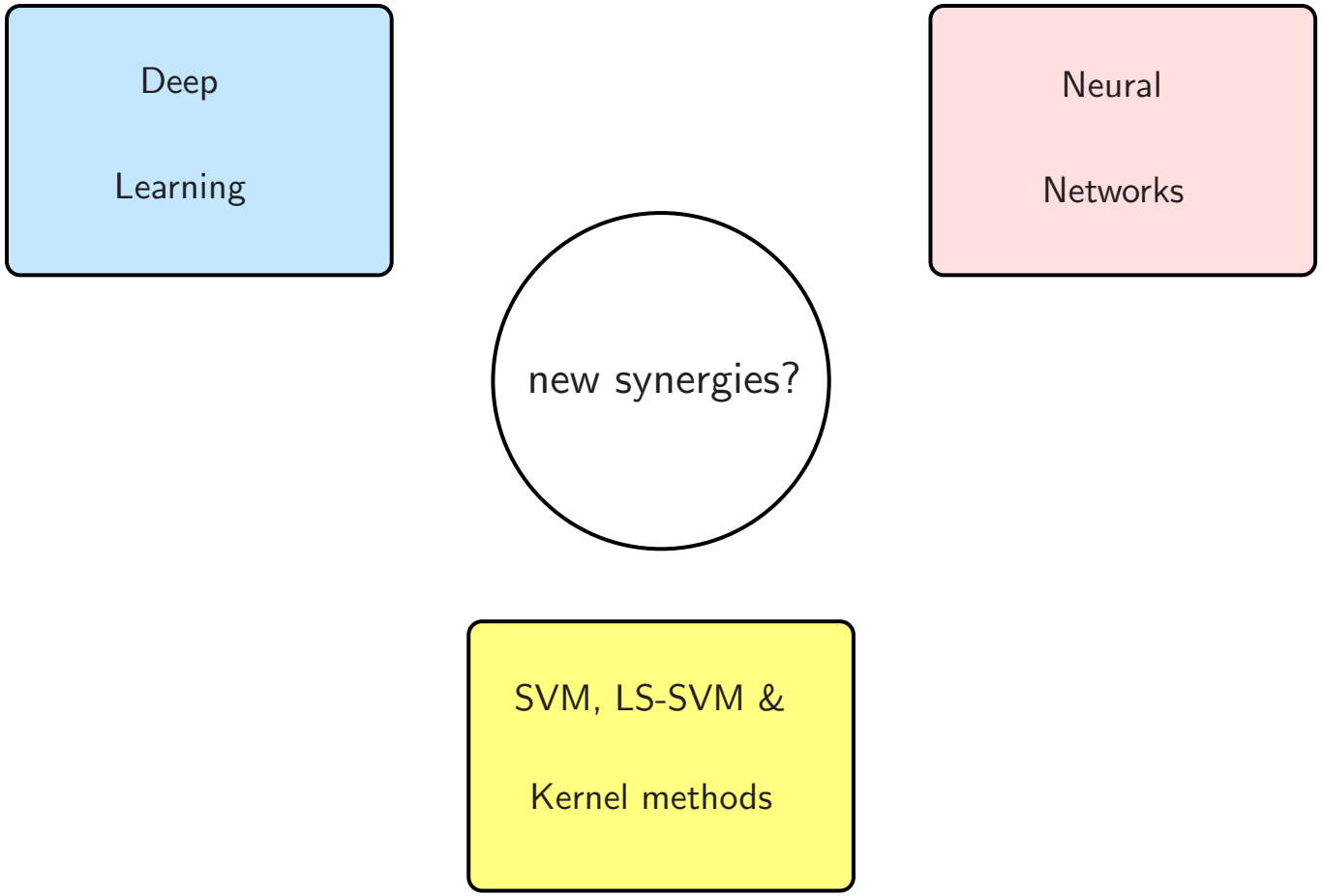
1998 LeCun et al.: convolutional neural networks
2006 Hinton et al.: deep belief networks
2010 Bengio et al.: stacked autoencoders
→ *booming of deep neural networks*



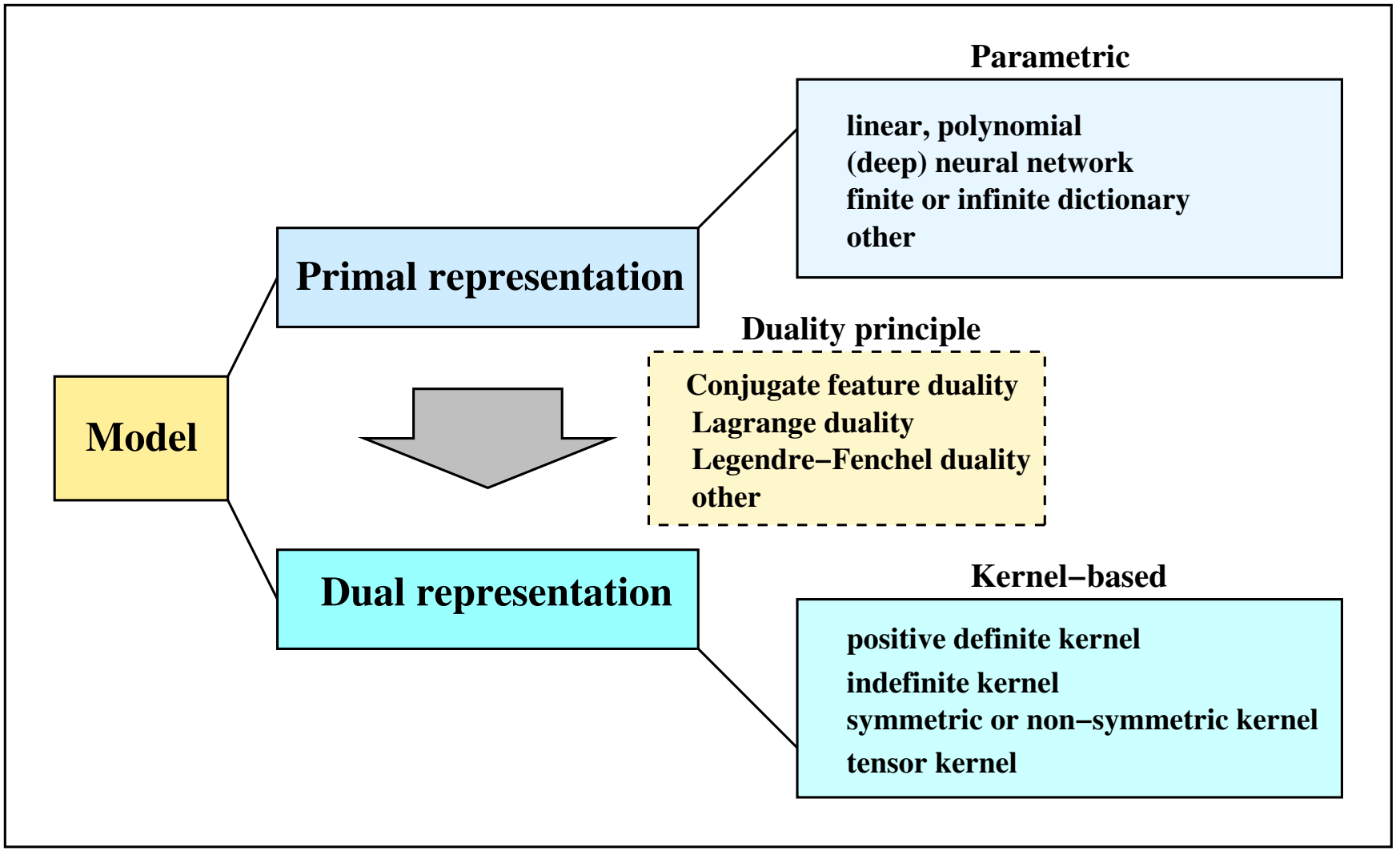
# Different paradigms



# Different paradigms



# Towards a unifying picture




[Suykens 2017]

*Function estimation and model representations*

# Linear function estimation (1)

- Given $\{(x_i, y_i)\}_{i=1}^N$ with $x_i \in \mathbb{R}^d$, $y_i \in \mathbb{R}$, consider $\hat{y} = f(x)$ where $f$ is parametrized as

$$\hat{y} = w^T x + b$$

  with $\hat{y}$ the estimated output of the linear model.

- Consider estimating $w, b$ by

$$\min_{w,b} \frac{1}{2} w^T w + \gamma \frac{1}{2} \sum_{i=1}^{N} (y_i - w^T x_i - b)^2$$

  $\rightarrow$ one can directly solve in $w, b$

# Linear function estimation (2)

- ... or write as a constrained optimization problem:

$$\begin{array}{ll} \min\limits_{w,b,e} & \frac{1}{2}w^T w + \gamma\frac{1}{2}\sum_i e_i^2 \\ \text{subject to} & e_i = y_i - w^T x_i - b, \quad i = 1, ..., N \end{array}$$

Lagrangian: $\mathcal{L}(w, b, e_i, \alpha_i) = \frac{1}{2}w^T w + \gamma\frac{1}{2}\sum_i e_i^2 - \sum_i \alpha_i(e_i - y_i + w^T x_i + b)$

- From optimality conditions:

$$\hat{y} = \sum_i \alpha_i \, x_i^T x + b$$

where $\alpha, b$ follows from solving a linear system

$$\left[\begin{array}{c|c} 0 & 1_N^T \\ \hline 1_N & \Omega + I/\gamma \end{array}\right] \left[\begin{array}{c} b \\ \hline \alpha \end{array}\right] = \left[\begin{array}{c} 0 \\ \hline y \end{array}\right]$$

with $\Omega_{ij} = x_i^T x_j$ for $i, j = 1, ..., N$ and $y = [y_1; ...; y_N]$.

# Linear model: solving in primal or dual?

inputs $x \in \mathbb{R}^d$, output $y \in \mathbb{R}$
training set $\{(x_i, y_i)\}_{i=1}^N$

$$(P): \quad \hat{y} = w^T x + b, \qquad w \in \mathbb{R}^d$$

Model $\nearrow$

# Linear model: solving in primal or dual?

inputs $x \in \mathbb{R}^d$, output $y \in \mathbb{R}$
training set $\{(x_i, y_i)\}_{i=1}^N$

$$\text{Model} \begin{cases} \nearrow & (P): \quad \hat{y} = w^T x + b, \qquad w \in \mathbb{R}^d \\ \searrow & (D): \quad \hat{y} = \sum_i \alpha_i \, x_i^T x + b, \qquad \alpha \in \mathbb{R}^N \end{cases}$$

# Linear model: solving in primal or dual?

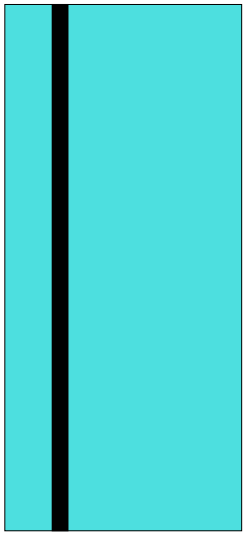
**few inputs, many data points:** $d \ll N$

**primal**: $w \in \mathbb{R}^d$

dual: $\alpha \in \mathbb{R}^N$ (large kernel matrix: $N \times N$)

# Linear model: solving in primal or dual?

**many inputs, few data points:** $d \gg N$



primal: $w \in \mathbb{R}^d$

**dual**: $\alpha \in \mathbb{R}^N$ (small kernel matrix: $N \times N$)

# Feature map and kernel

From linear to nonlinear model:

$$\text{Model} \begin{cases} \nearrow & (P): \quad \hat{y} = w^T \varphi(x) + b \\ \searrow & (D): \quad \hat{y} = \sum_i \alpha_i \, K(x_i, x) + b \end{cases}$$

Mercer theorem (one can **either** choose $\varphi$ **or** positive definite $K$):

$$K(x, z) = \varphi(x)^T \varphi(z)$$

Feature map $\varphi$, Kernel function $K(x, z)$ (e.g. linear, polynomial, RBF, ...)

- SVMs: feature map and positive definite kernel [Cortes & Vapnik, 1995]
- Neural networks: consider hidden layer as feature map [Suykens & Vandewalle, 1999]
- Least squares support vector machines [Suykens et al., 2002]: $L_2$ loss and regularization

# Least Squares Support Vector Machines: "core models"

- Regression

$$\min_{w,b,e} w^T w + \gamma \sum_i e_i^2 \quad \text{s.t.} \quad y_i = w^T \varphi(x_i) + b + e_i, \quad \forall i$$

- Classification

$$\min_{w,b,e} w^T w + \gamma \sum_i e_i^2 \quad \text{s.t.} \quad y_i(w^T \varphi(x_i) + b) = 1 - e_i, \quad \forall i$$

- Kernel pca $(V = I)$, Kernel spectral clustering $(V = D^{-1})$

$$\min_{w,b,e} -w^T w + \gamma \sum_i v_i e_i^2 \quad \text{s.t.} \quad e_i = w^T \varphi(x_i) + b, \quad \forall i$$

- Kernel canonical correlation analysis/partial least squares

$$\min_{w,v,b,d,e,r} w^T w + v^T v + \nu \sum_i (e_i - r_i)^2 \text{ s.t. } \begin{cases} e_i &= w^T \varphi^{(1)}(x_i) + b \\ r_i &= v^T \varphi^{(2)}(y_i) + d \end{cases}$$

[Suykens & Vandewalle, 1999; Suykens et al., 2002; Alzate & Suykens, 2010]

# Sparsity: through regularization or loss function

- through regularization: model $\hat{y} = w^T x + b$

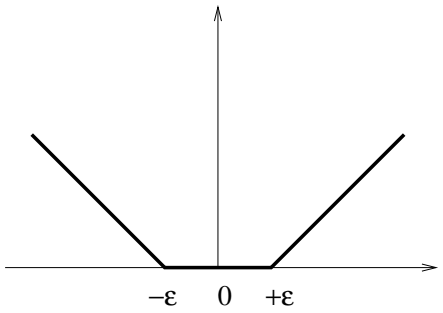
$$\min \sum_j |w_j| + \gamma \sum_i e_i^2$$

$\Rightarrow$ sparse $w$ (e.g. Lasso)

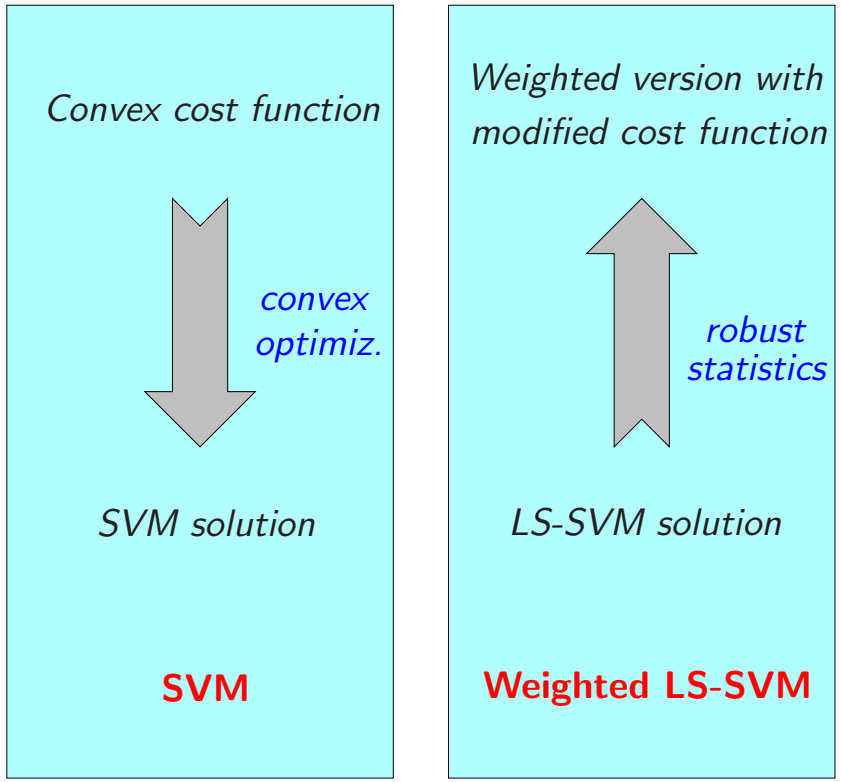
- through loss function: model $\hat{y} = \sum_i \alpha_i K(x, x_i) + b$

$$\min \; w^T w + \gamma \sum_i L(e_i)$$

$\Rightarrow$ sparse $\alpha$ (e.g. SVM)



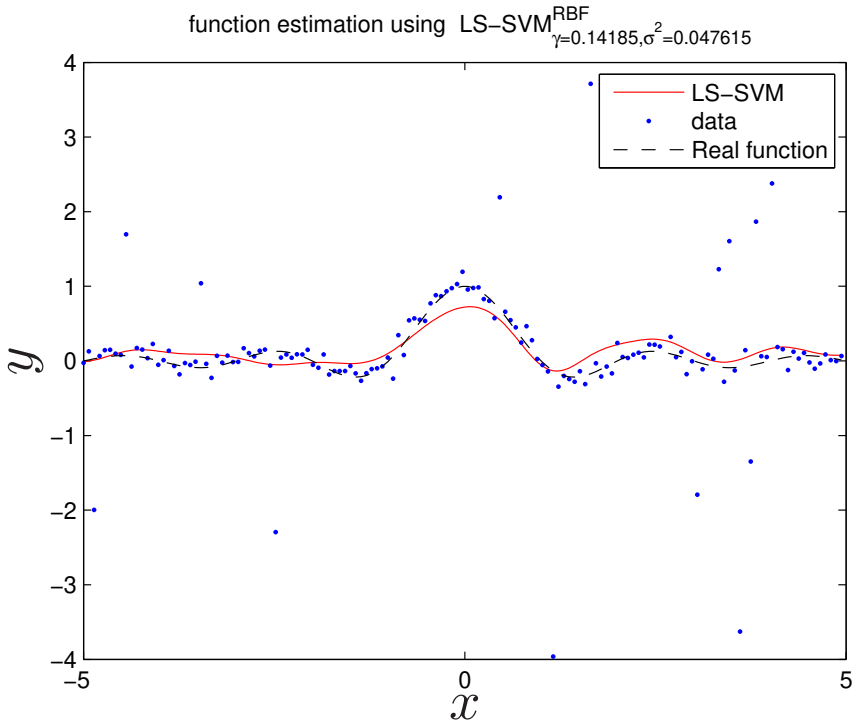
# Weighted versions and robustness

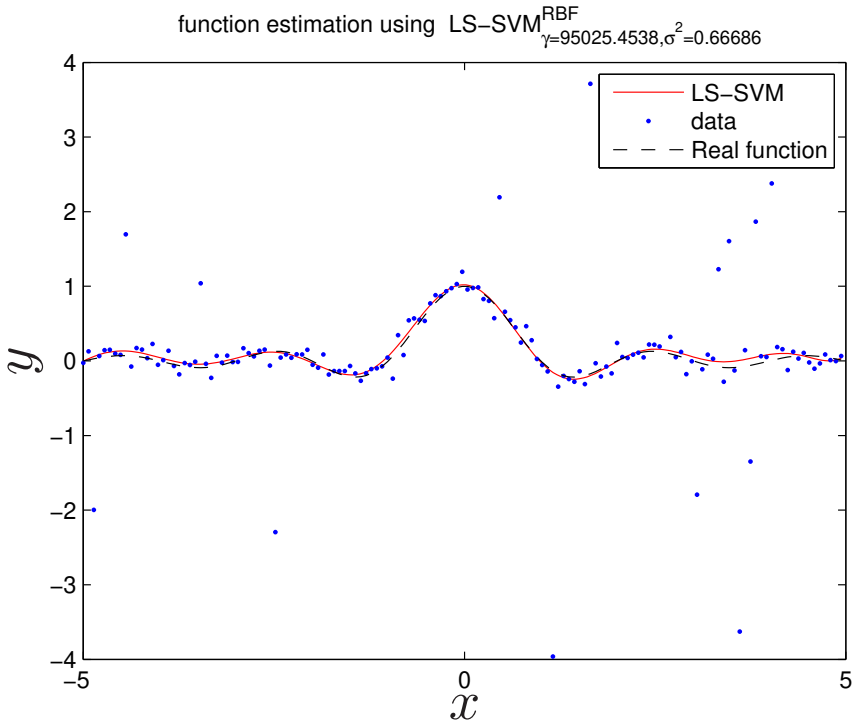



- Weighted LS-SVM: $\min_{w,b,e} \frac{1}{2} w^T w + \gamma \frac{1}{2} \sum_{i=1}^{N} v_i e_i^2 \ \text{s.t.} \ y_i = w^T \varphi(x_i) + b + e_i, \ \forall i$

  with $v_i$ determined from $\{e_i\}_{i=1}^N$ of unweighted LS-SVM [Suykens et al., 2002].
  Robustness and stability [Debruyne et al., JMLR 2008, 2010].
- SVM solution by applying iteratively weighted LS [Perez-Cruz et al., 2005]

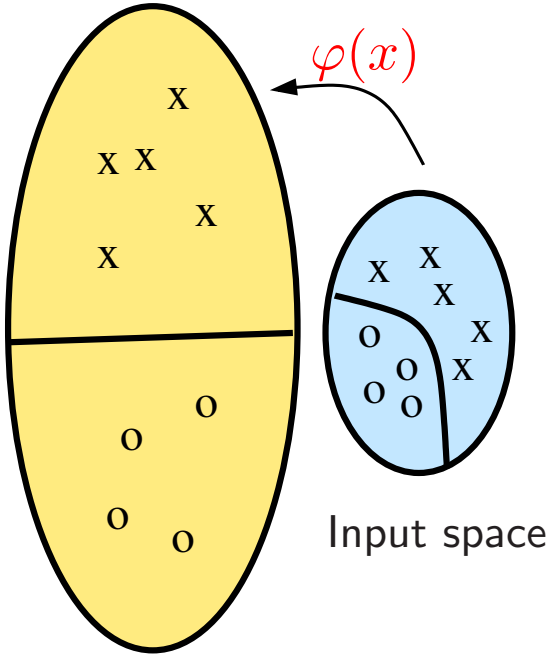
# Example: robust regression using weighted LS-SVM




using LS-SVMlab v1.8 http://www.esat.kuleuven.be/sista/lssvmlab/

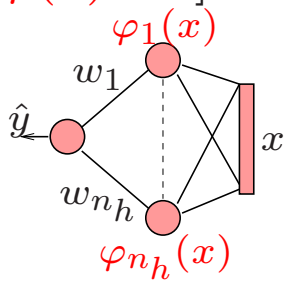
# SVMs and neural networks




## Primal space

Parametric

$$\hat{y} = \text{sign}[w^T \varphi(x) + b]$$



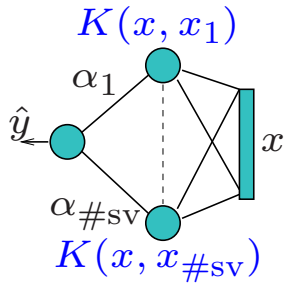

Parametric

$K(x_i, x_j) = \varphi(x_i)^T \varphi(x_j)$ **("Kernel trick")**

## Dual space

Nonparametric

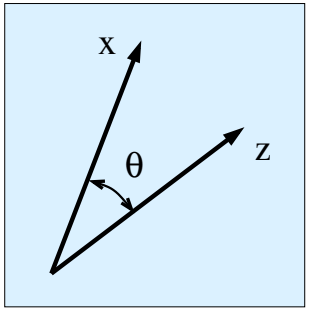
$$\hat{y} = \text{sign}[\sum_{i=1}^{\#\text{sv}} \alpha_i y_i K(x, x_i) + b]$$




Non−parametric

[Suykens et al., 2002]

# Wider use of the "kernel trick"




- **Angle between vectors:** (e.g. correlation analysis)
  Input space:

$$\cos\theta_{xz} = \frac{x^T z}{\|x\|_2 \|z\|_2}$$

  Feature space:

$$\cos\theta_{\varphi(x),\varphi(z)} = \frac{\varphi(x)^T \varphi(z)}{\|\varphi(x)\|_2 \|\varphi(z)\|_2} = \frac{K(x,z)}{\sqrt{K(x,x)}\sqrt{K(z,z)}}$$

- **Distance between vectors:** (e.g. for "kernelized" clustering methods)
  Input space:

$$\|x - z\|_2^2 = (x-z)^T(x-z) = x^T x + z^T z - 2x^T z$$

  Feature space:

$$\|\varphi(x) - \varphi(z)\|_2^2 = K(x,x) + K(z,z) - 2K(x,z)$$

# Interpretation of kernel-based models

Decision making: classification problem (e.g. apples versus tomatoes)
Input data $x_i \in \mathbb{R}^d$ and class labels $y_i \in \{-1, +1\}$. $N$ training data.

SVM or LS-SVM classifier: given a new $x$ (e.g.  ), obtain

$$\hat{y} = \text{sign}[\sum_i \alpha_i y_i K(x, x_i) + b]$$

with $x_i$ for $i = 1, ..., N$:

Here $K(x, x_i)$ characterizes the similarity between $x$ and $x_i$.
The bias term $b$ can be related to prior class probabilities (Ethics & AI !).

# Kernels

Wide range of positive definite kernel functions possible:

- linear $K(x, z) = x^T z$
- polynomial $K(x, z) = (\eta + x^T z)^d$
- radial basis function $K(x, z) = \exp(-\|x - z\|_2^2/\sigma^2)$
- $\chi^2$ kernel (on images)
- Wasserstein exponential kernels (optimal transport)
- splines, wavelets
- string kernel
- Fisher kernels, kernels from graphical models
- kernels for dynamical systems
- graph kernels
- data fusion kernels
- additive kernels (good for explainability)
- other

[Schölkopf & Smola, 2002; Shawe-Taylor & Cristianini, 2004; Jebara et al., 2004; other]

# Function estimation in RKHS

- Find function $f$ such that [Wahba, 1990; Evgeniou et al., 2000]

$$\min_{f \in \mathcal{H}_K} \frac{1}{N} \sum_{i=1}^{N} L(y_i, f(x_i)) + \lambda \|f\|_K^2$$

  with $L(\cdot, \cdot)$ the loss function. $\|f\|_K$ is norm in RKHS $\mathcal{H}_K$ defined by $K$.

- Representer theorem: for convex loss function, solution of the form

$$f(x) = \sum_{i=1}^{N} \alpha_i K(x, x_i)$$

  Reproducing property $f(x) = \langle f, K_x \rangle_K$ with $K_x(\cdot) = K(x, \cdot)$

- Sparse representation by hinge and $\epsilon$-insensitive loss [Vapnik, 1998]

# Krein spaces: indefinite kernels

- LS-SVM for indefinite kernel case:

$$\min_{w_+,w_-,b,e} \frac{1}{2}(w_+^T w_+ - w_-^T w_-) + \frac{\gamma}{2}\sum_{i=1}^{N} e_i^2 \text{ s.t. } y_i = w_+^T\varphi_+(x_i) + w_-^T\varphi_-(x_i) + b + e_i, \forall i$$

and **indefinite kernel** $K(x_i, x_j) = K_+(x_i, x_j) - K_-(x_i, x_j)$
with positive definite kernels $K_+, K_-$

$$K_+(x_i, x_j) = \varphi_+(x_i)^T\varphi_+(x_j) \text{ and } K_-(x_i, x_j) = \varphi_-(x_i)^T\varphi_-(x_j)$$

- also: KPCA with indefinite kernel [X. Huang et al. 2017], KSC and semi-supervised learning [Mehrkanoon et al., 2018]

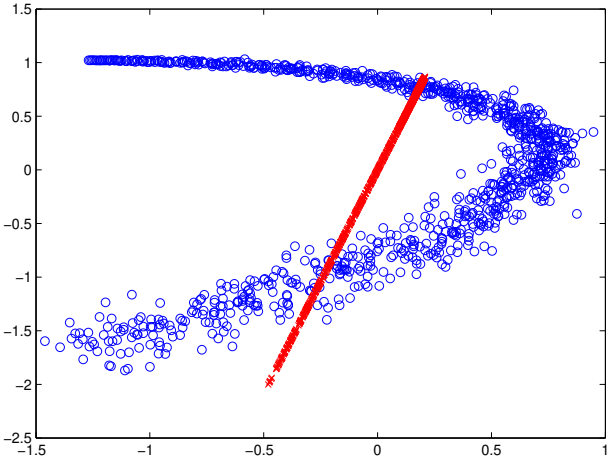
[X. Huang, Maier, Hornegger, Suykens, ACHA 2017]

[Mehrkanoon, X. Huang, Suykens, Pattern Recognition, 2018]

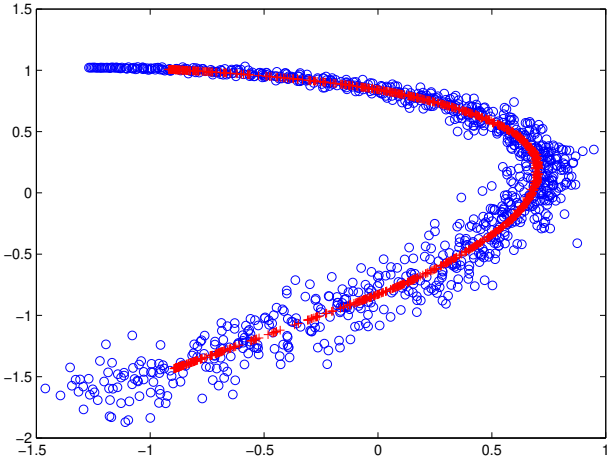
Related work of RKKS: [Ong et al 2004; Haasdonk 2005; Luss 2008; Loosli et al. 2015]

# *Kernel spectral clustering*

# Kernel principal component analysis (KPCA)




*linear PCA*




*kernel PCA (RBF kernel)*

**Kernel PCA** [Schölkopf et al., 1998]:
take eigenvalue decomposition of the kernel matrix

$$\begin{bmatrix} K(x_1, x_1) & \dots & K(x_1, x_N) \\ \vdots & & \vdots \\ K(x_N, x_1) & \dots & K(x_N, x_N) \end{bmatrix}$$

(applications in dimensionality reduction and denoising)

# Kernel PCA: classical LS-SVM approach

- Primal problem: [Suykens et al., 2002]: **model-based** approach

$$\min_{w,b,e} \ \frac{1}{2}w^T w - \frac{1}{2}\gamma \sum_{i=1}^{N} e_i^2 \ \text{ s.t. } \ e_i = w^T \varphi(x_i) + b, \ i = 1, ..., N.$$

- Dual problem corresponds to kernel PCA

$$\Omega^{(c)}\alpha = \lambda\alpha \ \text{ with } \ \lambda = 1/\gamma$$

with $\Omega_{ij}^{(c)} = (\varphi(x_i) - \hat{\mu}_\varphi)^T(\varphi(x_j) - \hat{\mu}_\varphi)$ the *centered kernel matrix* and $\hat{\mu}_\varphi = (1/N)\sum_{i=1}^{N} \varphi(x_i)$.

- Interpretation:
  1. pool of candidate components (objective function equals zero)
  2. select relevant components

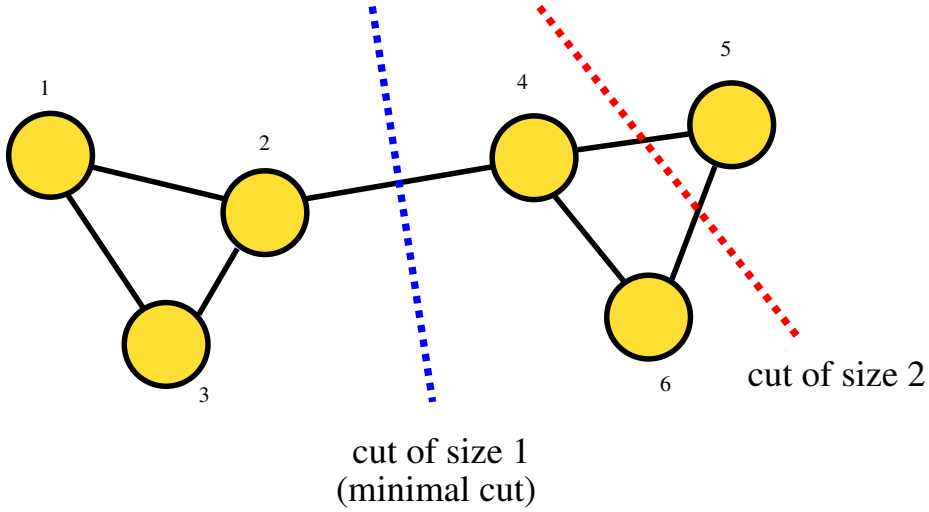
- Robust and sparse versions [Alzate & Suykens, 2008]

# Spectral graph clustering (1)

**Minimal cut**: given the graph $\mathcal{G} = (V, E)$, find clusters $\mathcal{A}_1, \mathcal{A}_2$

$$\min_{q_i \in \{-1,+1\}} \frac{1}{2} \sum_{i,j} w_{ij}(q_i - q_j)^2$$

with cluster membership indicator $q_i$ ($q_i = 1$ if $i \in \mathcal{A}_1$, $q_i = -1$ if $i \in \mathcal{A}_2$) and $W = [w_{ij}]$ the weighted adjacency matrix.



# Spectral graph clustering (2)

- **Min-cut** spectral clustering problem

$$\min_{\tilde{q}^T\tilde{q}=1} \tilde{q}^T L \tilde{q}$$

with $L = D - W$ the unnormalized graph Laplacian, degree matrix $D = \mathrm{diag}(d_1, ..., d_N)$, $d_i = \sum_j w_{ij}$, giving

$$L\tilde{q} = \lambda\tilde{q}.$$

Cluster member indicators: $\hat{q}_i = \mathrm{sign}(\tilde{q}_i - \theta)$ with threshold $\theta$.

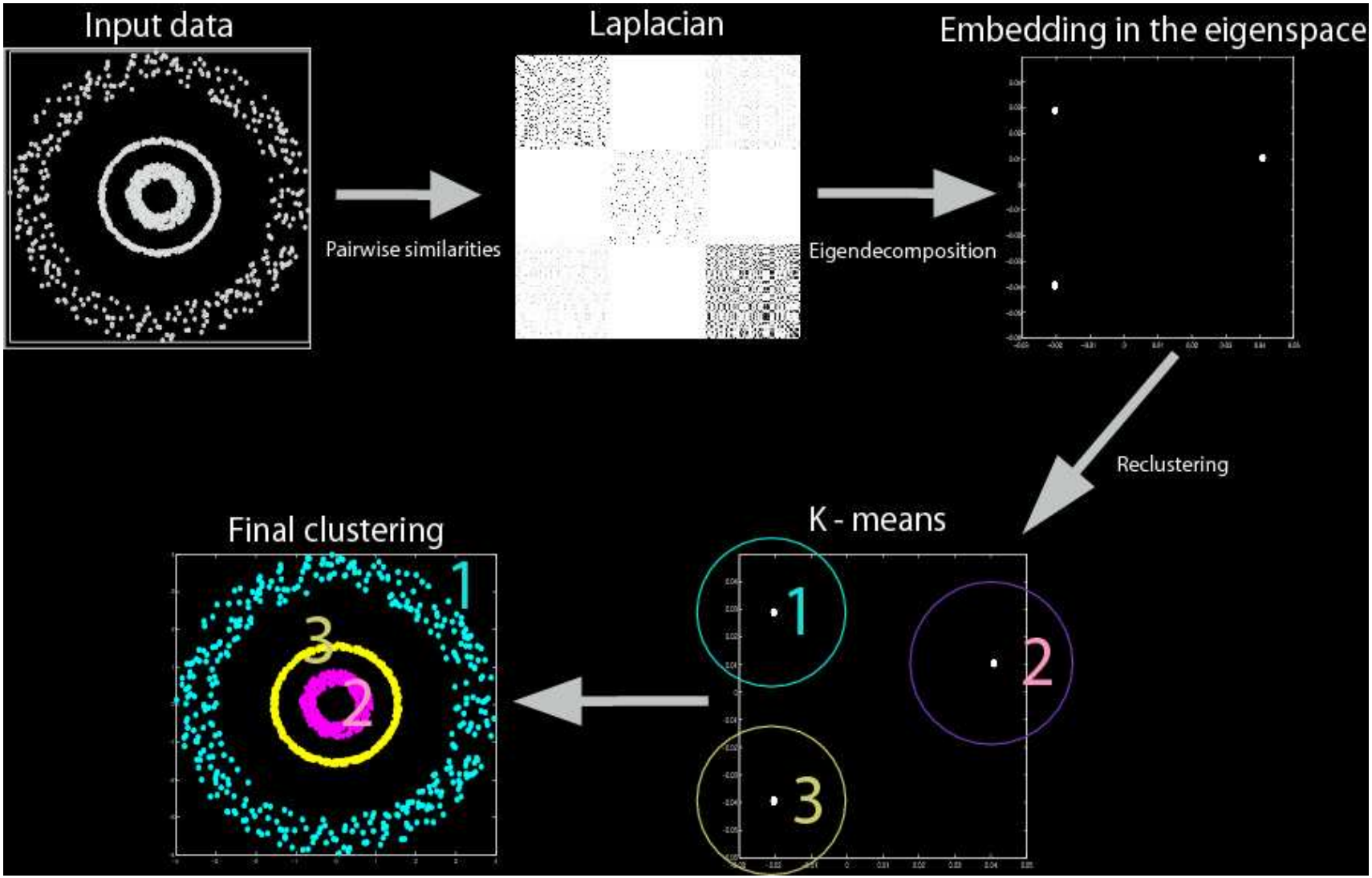
- **Normalized cut**

$$L\tilde{q} = \lambda D\tilde{q}$$

[Fiedler, 1973; Shi & Malik, 2000; Ng et al. 2002; Chung, 1997; von Luxburg, 2007]

- **Discrete version** to continuous problem (Laplace operator)
[Belkin & Niyogi, 2003; von Luxburg et al., 2008; Smale & Zhou, 2007]

# Spectral clustering + K-means



# Kernel Spectral Clustering (KSC): case of two clusters

- **Primal problem:** training on given data $\{x_i\}_{i=1}^N$

$$\begin{array}{ll} \min\limits_{w,b,e} & \frac{1}{2}w^Tw - \gamma\frac{1}{2}e^TVe \\ \text{subject to} & e_i = w^T\varphi(x_i) + b, \quad i = 1, ..., N \end{array}$$

  with weighting matrix $V$ and $\varphi(\cdot) : \mathbb{R}^d \to \mathbb{R}^h$ the feature map.

- **Dual:**

$$VM_V\Omega\alpha = \lambda\alpha$$

  with $\lambda = 1/\gamma$, $M_V = I_N - \frac{1}{1_N^TV1_N}1_N1_N^TV$ weighted centering matrix, $\Omega = [\Omega_{ij}]$ kernel matrix with $\Omega_{ij} = \varphi(x_i)^T\varphi(x_j) = K(x_i, x_j)$

-

[Alzate & Suykens, IEEE-PAMI, 2010]

# Kernel Spectral Clustering (KSC): case of two clusters

- **Primal problem:** training on given data $\{x_i\}_{i=1}^N$

$$\begin{array}{ll} \min\limits_{w,b,e} & \frac{1}{2}w^Tw - \gamma\frac{1}{2}e^TVe \\ \text{subject to} & e_i = w^T\varphi(x_i) + b, \quad i = 1, ..., N \end{array}$$

  with weighting matrix $V$ and $\varphi(\cdot) : \mathbb{R}^d \to \mathbb{R}^h$ the feature map.

- **Dual:**

$$VM_V\Omega\alpha = \lambda\alpha$$

  with $\lambda = 1/\gamma$, $M_V = I_N - \frac{1}{1_N^TV1_N}1_N1_N^TV$ weighted centering matrix, $\Omega = [\Omega_{ij}]$ kernel matrix with $\Omega_{ij} = \varphi(x_i)^T\varphi(x_j) = K(x_i, x_j)$

- Taking $V = D^{-1}$ with degree matrix $D = \text{diag}\{d_1, ..., d_N\}$ and $d_i = \sum_{j=1}^N \Omega_{ij}$ relates to random walks algorithm.

[Alzate & Suykens, IEEE-PAMI, 2010]

# Lagrangian and conditions for optimality

- Lagrangian:

$$\mathcal{L}(w,b,e;\alpha) = \frac{1}{2}w^T w - \gamma\frac{1}{2}\sum_{i=1}^{N} v_i e_i^2 + \sum_{i=1}^{N}\alpha_i(e_i - w^T\varphi(x_i) - b)$$

- Conditions for optimality:

$$\begin{cases} \dfrac{\partial\mathcal{L}}{\partial w} = 0 & \Rightarrow \quad w = \sum_i \alpha_i\varphi(x_i) \\ \dfrac{\partial\mathcal{L}}{\partial b} = 0 & \Rightarrow \quad \sum_i \alpha_i = 0 \\ \dfrac{\partial\mathcal{L}}{\partial e_i} = 0 & \Rightarrow \quad \alpha_i = \gamma v_i e_i, \ \ i = 1,...,N \\ \dfrac{\partial\mathcal{L}}{\partial \alpha_i} = 0 & \Rightarrow \quad e_i = w^T\varphi(x_i) + b, \ \ i = 1,...,N \end{cases}$$

- Eliminate $w, b, e$, write solution in Lagrange multipliers $\alpha_i$.

# Kernel spectral clustering: more clusters

- Case of $k$ clusters: additional sets of constraints

$$
\begin{aligned}
\min_{w^{(l)},e^{(l)},b_l} \quad & \frac{1}{2}\sum_{l=1}^{k-1} w^{(l)^T} w^{(l)} - \frac{1}{2}\sum_{l=1}^{k-1} \gamma_l e^{(l)^T} D^{-1} e^{(l)} \\
\text{subject to} \quad & e^{(1)} = \Phi_{N\times n_h} w^{(1)} + b_1 1_N \\
& e^{(2)} = \Phi_{N\times n_h} w^{(2)} + b_2 1_N \\
& \vdots \\
& e^{(k-1)} = \Phi_{N\times n_h} w^{(k-1)} + b_{k-1} 1_N
\end{aligned}
$$

  where $e^{(l)} = [e_1^{(l)}; ...; e_N^{(l)}]$ and $\Phi_{N\times n_h} = [\varphi(x_1)^T; ...; \varphi(x_N)^T] \in \mathbb{R}^{N\times n_h}$.

- **Dual problem**: $M_D \Omega \alpha^{(l)} = \lambda D \alpha^{(l)}$, $l = 1, ..., k-1$.

[Alzate & Suykens, IEEE-PAMI, 2010]

# Primal and dual model representations

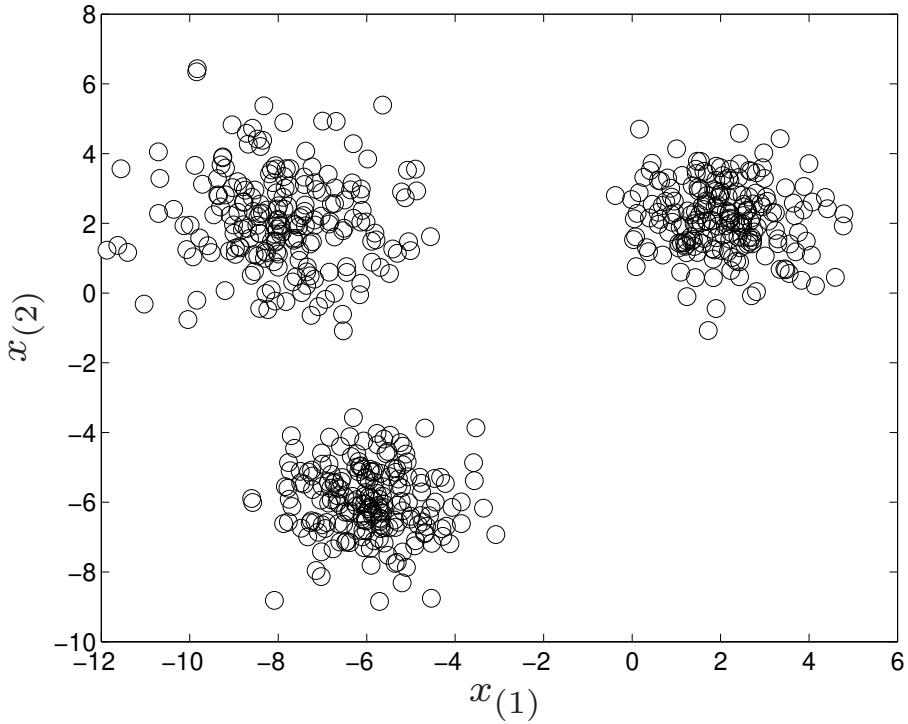
$k$ clusters
$k-1$ sets of constraints (index $l = 1, ..., k-1$)

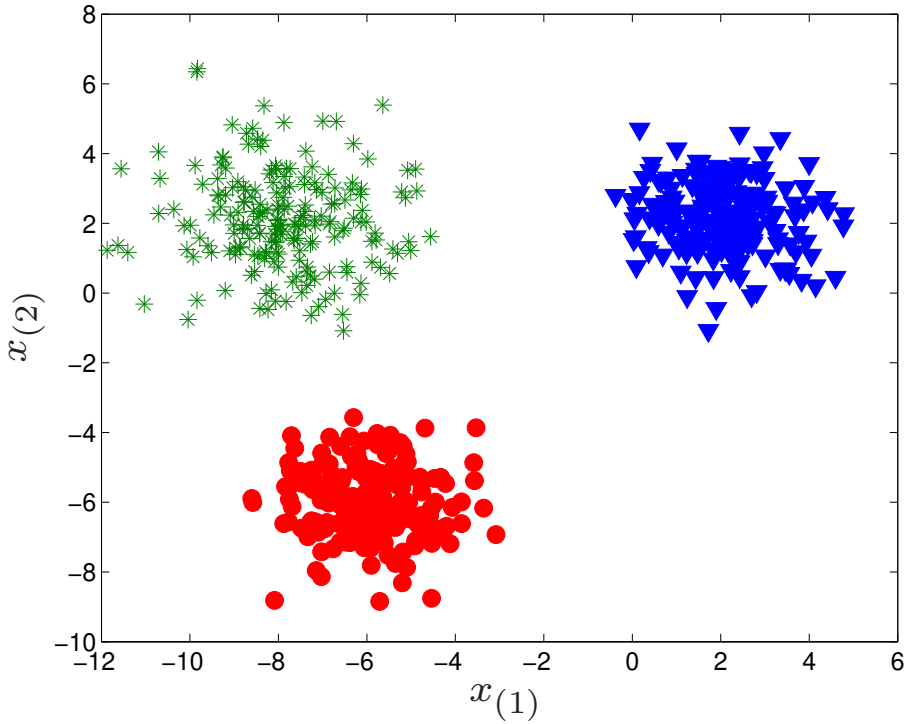
$$\mathcal{M} \begin{cases} \nearrow & (P): \quad \text{sign}[\hat{e}_*^{(l)}] = \text{sign}[{w^{(l)}}^T \varphi(x_*) + b_l] \\ \searrow & (D): \quad \text{sign}[\hat{e}_*^{(l)}] = \text{sign}[\sum_j \alpha_j^{(l)} K(x_*, x_j) + b_l] \end{cases}$$

# Advantages of kernel-based setting

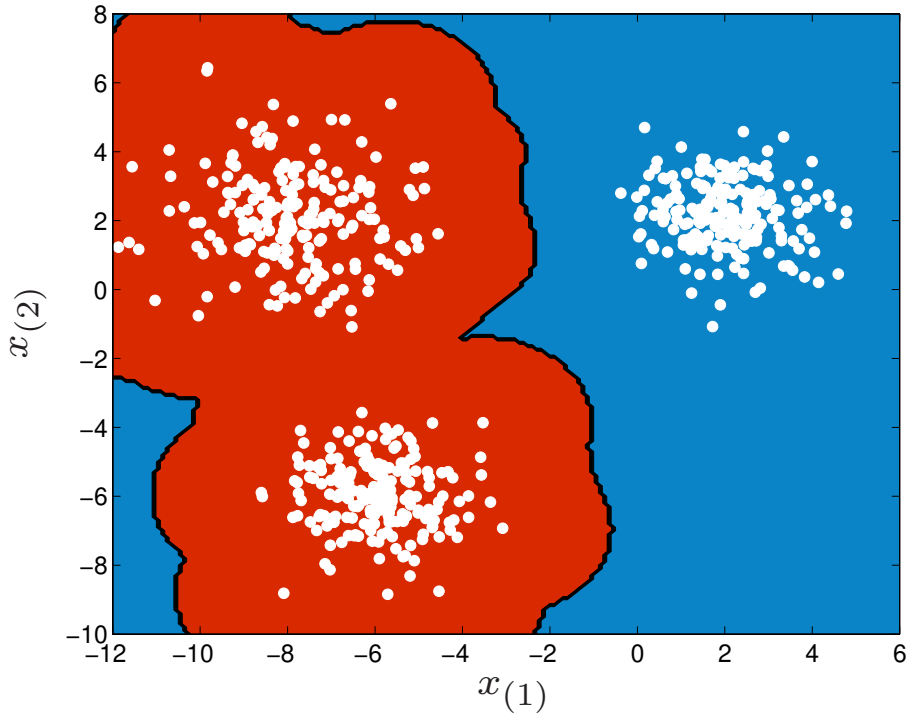
- **model-based** approach
- **out-of-sample extensions**, applying model to new data
- consider **training, validation and test data**
  (training problem corresponds to eigenvalue decomposition problem)
- model selection procedures
- **sparse representations and large scale methods**

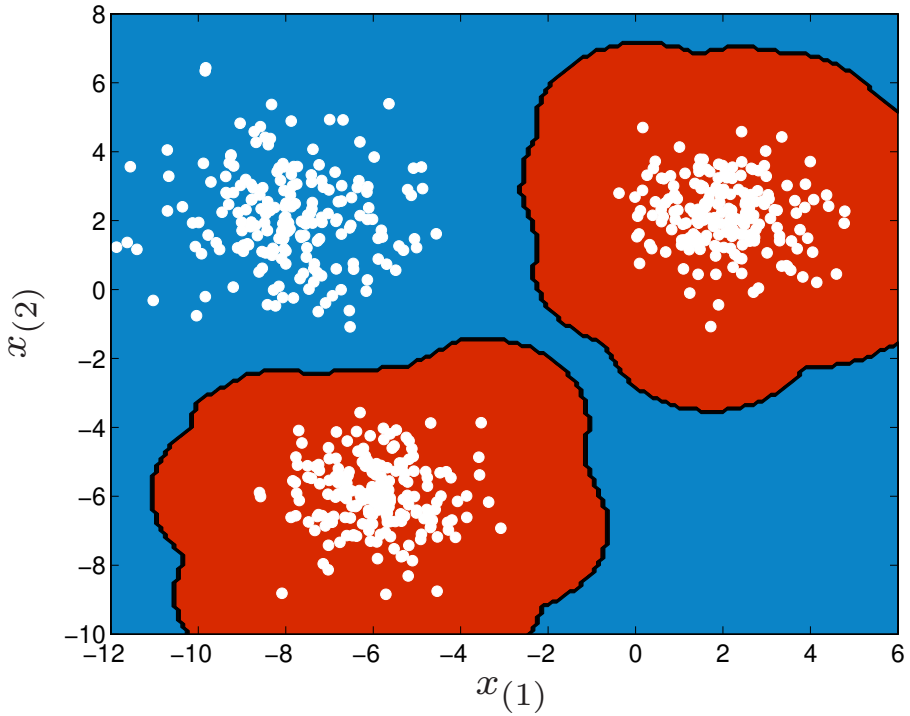
# Out-of-sample extension and coding



# Out-of-sample extension and coding



# Piecewise constant eigenvectors and extension (1)

- **Definition.** [Meila & Shi, 2001] Vector $\alpha$ is called *piecewise constant* relative to a partition $(\mathcal{A}_1, ..., \mathcal{A}_k)$ iff $\alpha_i = \alpha_j \ \forall x_i, x_j \in \mathcal{A}_p, p = 1, ..., k$.

- **Proposition.** [Alzate & Suykens, 2010] Assume

  (i) a training set $\mathcal{D} = \{x_i\}_{i=1}^N$ and validation set $\mathcal{D}^v = \{x_m^v\}_{m=1}^{N_v}$ i.i.d. sampled from the same underlying distribution;
  (ii) a set of $k$ clusters $\{\mathcal{A}_1, ..., \mathcal{A}_k\}$ with $k > 2$;
  (iii) an isotropic kernel function such that $K(x, z) = 0$ when $x$ and $z$ belong to different clusters;
  (iv) the eigenvectors $\alpha^{(l)}$ for $l = 1, ..., k-1$ are piecewise constant.

  Then validation set points belonging to the same cluster are *collinear* in the $k-1$ dimensional subspace spanned by the columns of $E^v \in \mathbb{R}^{N_v \times (k-1)}$ where $E^v_{ml} = e_m^{(l)} = \sum_{i=1}^N \alpha_i^{(l)} K(x_i, x_m^v) + b_l$.

# Piecewise constant eigenvectors and extension (2)

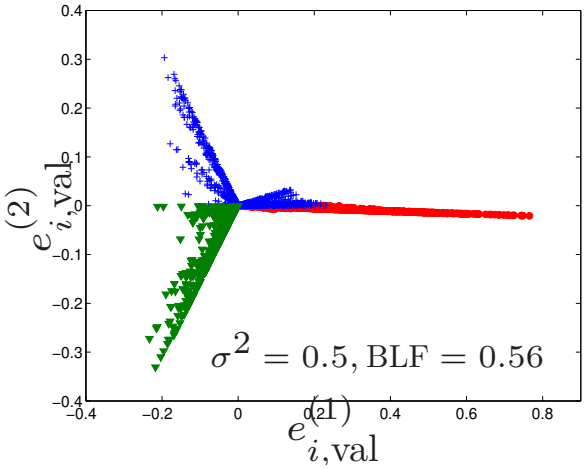
- **Key aspect of the proof:** for $x_* \in \mathcal{A}_p$ one has

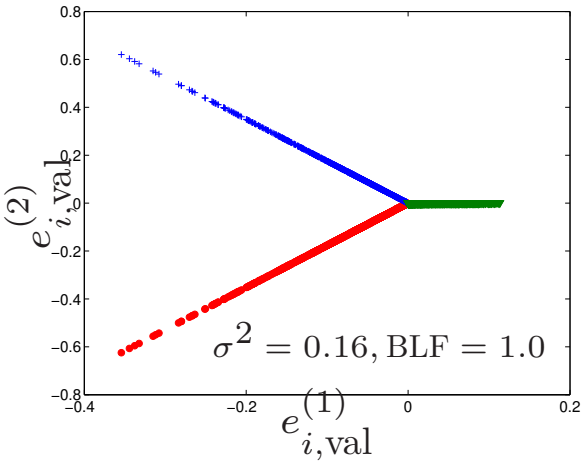
$$\begin{aligned} e_*^{(l)} &= \sum_{i=1}^N \alpha_i^{(l)} K(x_i, x_*) + b^{(l)} \\ &= c_p^{(l)} \sum_{i \in \mathcal{A}_p} K(x_i, x_*) + \sum_{i \notin \mathcal{A}_p}^N \alpha_i^{(l)} K(x_i, x_*) + b^{(l)} \\ &= c_p^{(l)} \sum_{i \in \mathcal{A}_p} K(x_i, x_*) + b^{(l)} \end{aligned}$$

- **Model selection** to determine kernel parameters and $k$:
  Looking for line structures in the space $(e_i^{(1)}, e_i^{(2)}, ..., e_i^{(k-1)})$,
  evaluated on validation data (aiming for good generalization)

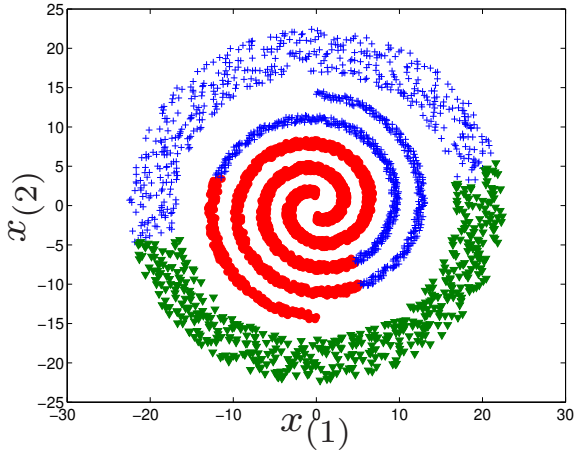
- **Choice kernel:**
  Gaussian RBF kernel
  $\chi^2$-kernel for images

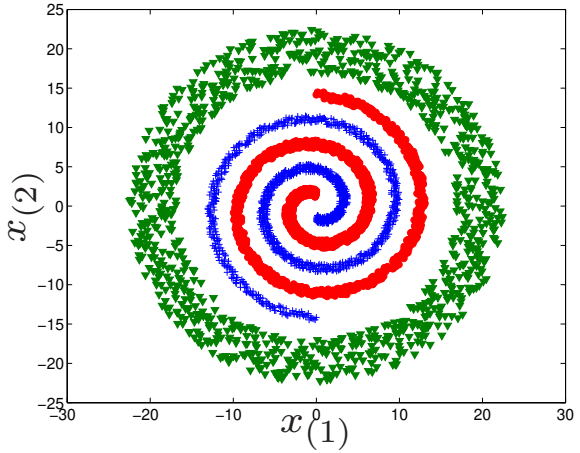
# Model selection (looking for lines): toy problem 1



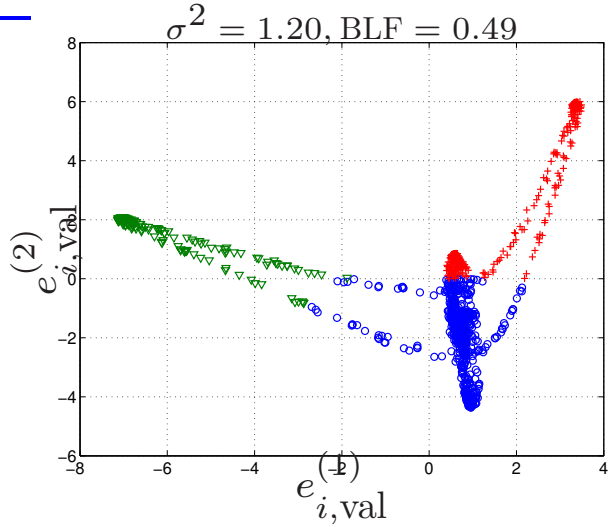

validation set

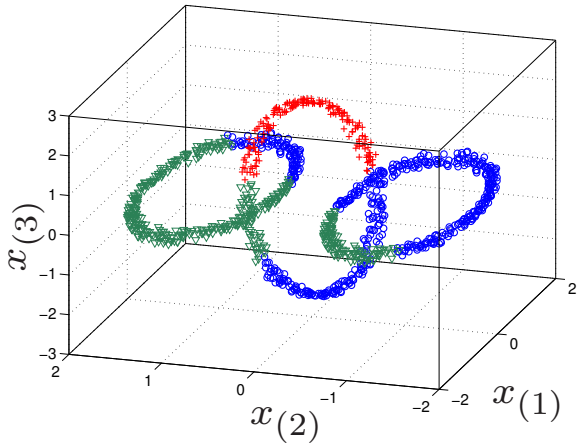


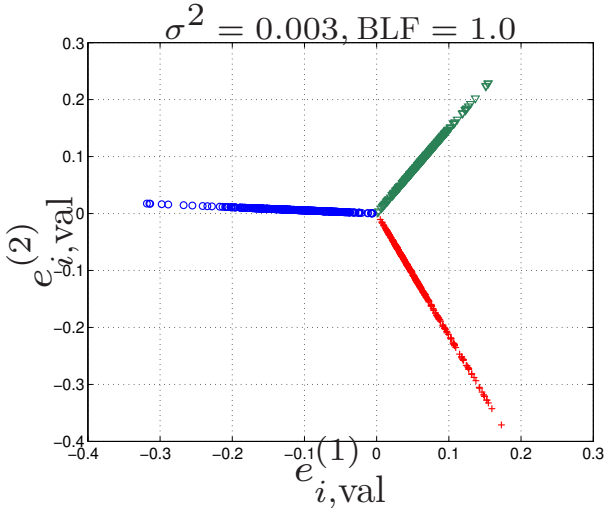




train + validation + test data

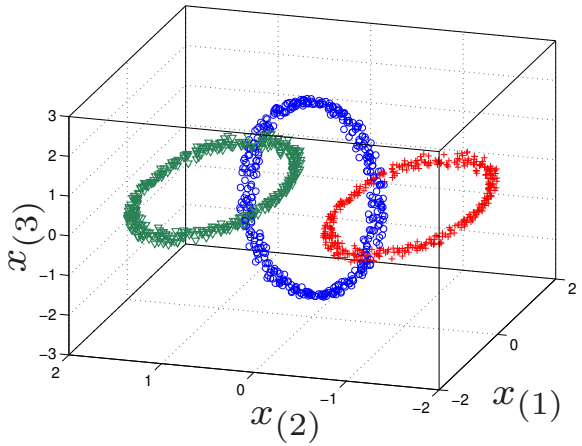
# Model selection (looking for lines): toy problem 2



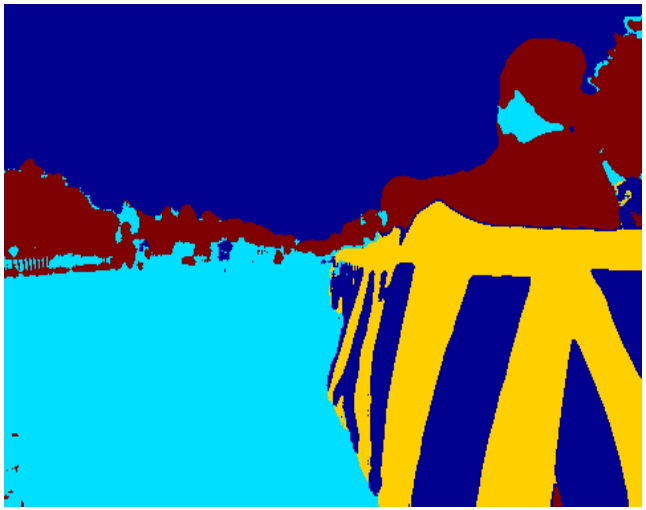



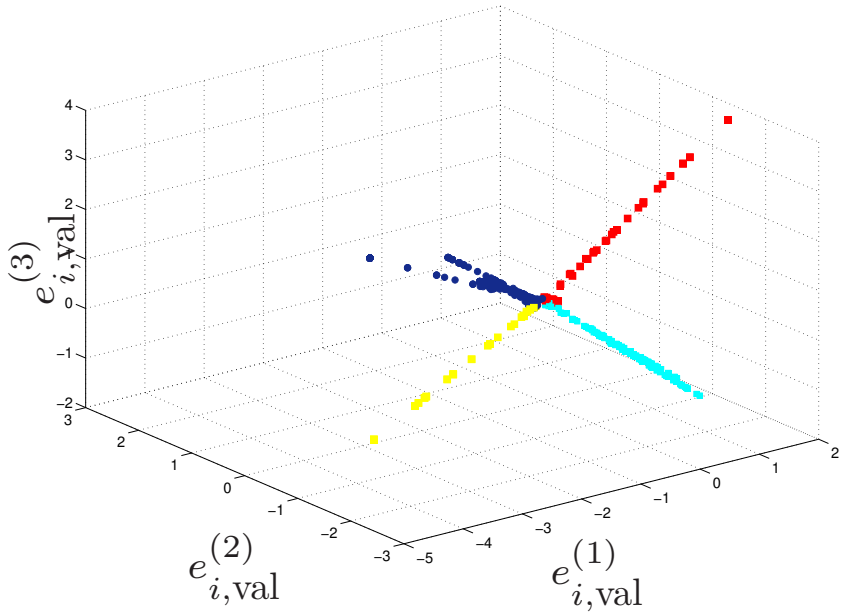

validation set

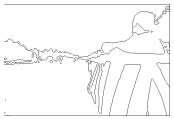
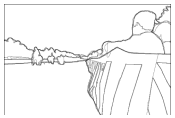
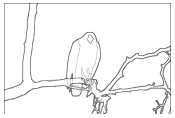
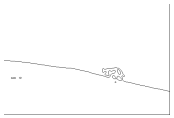
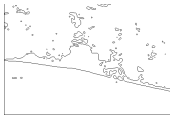
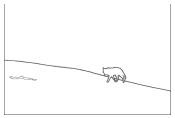
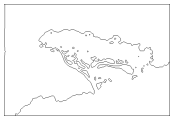
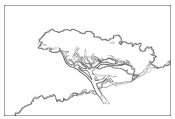
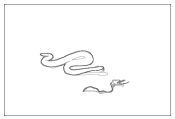
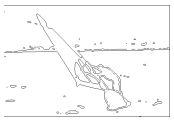
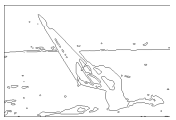
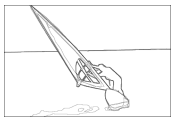
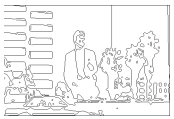
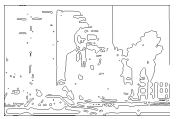
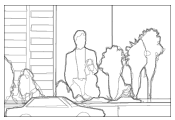
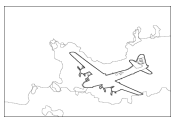
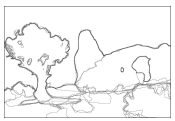
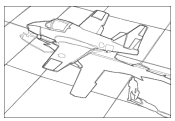



train + validation + test data

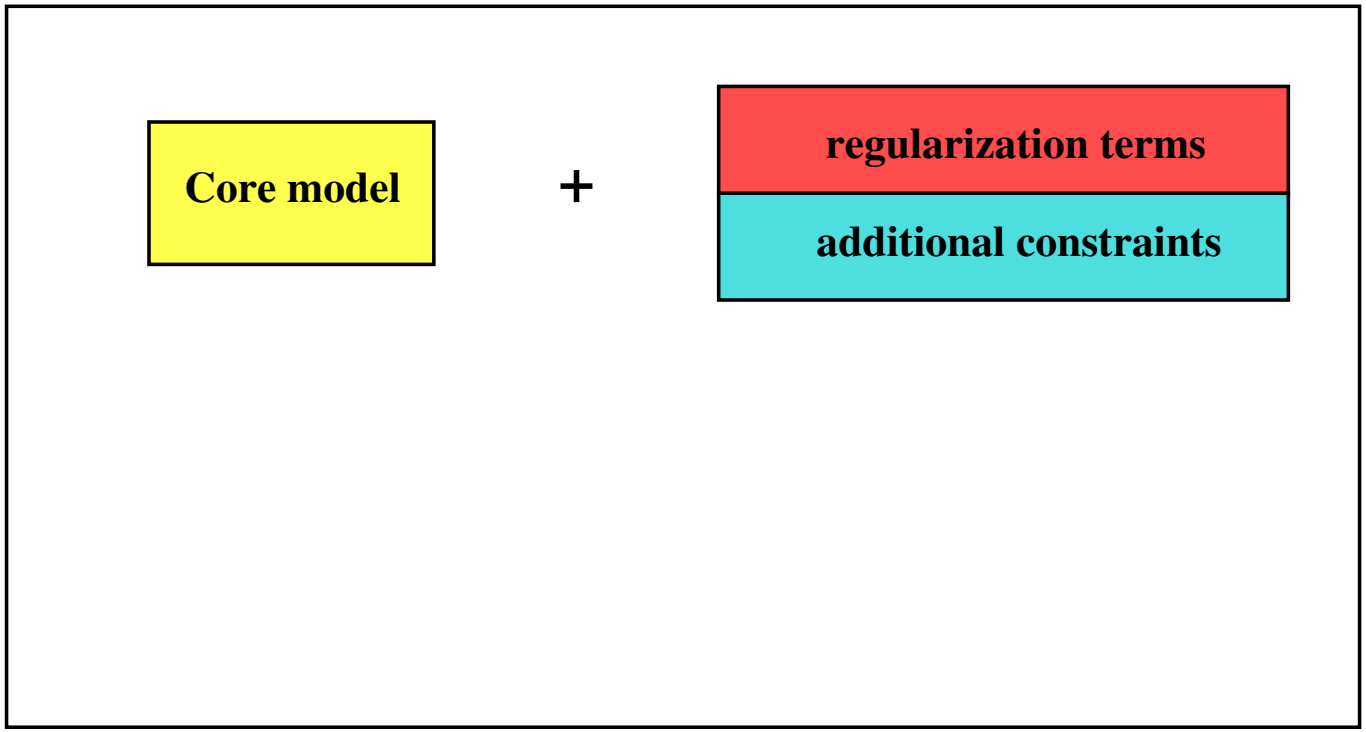
# Example: image segmentation (looking for lines)



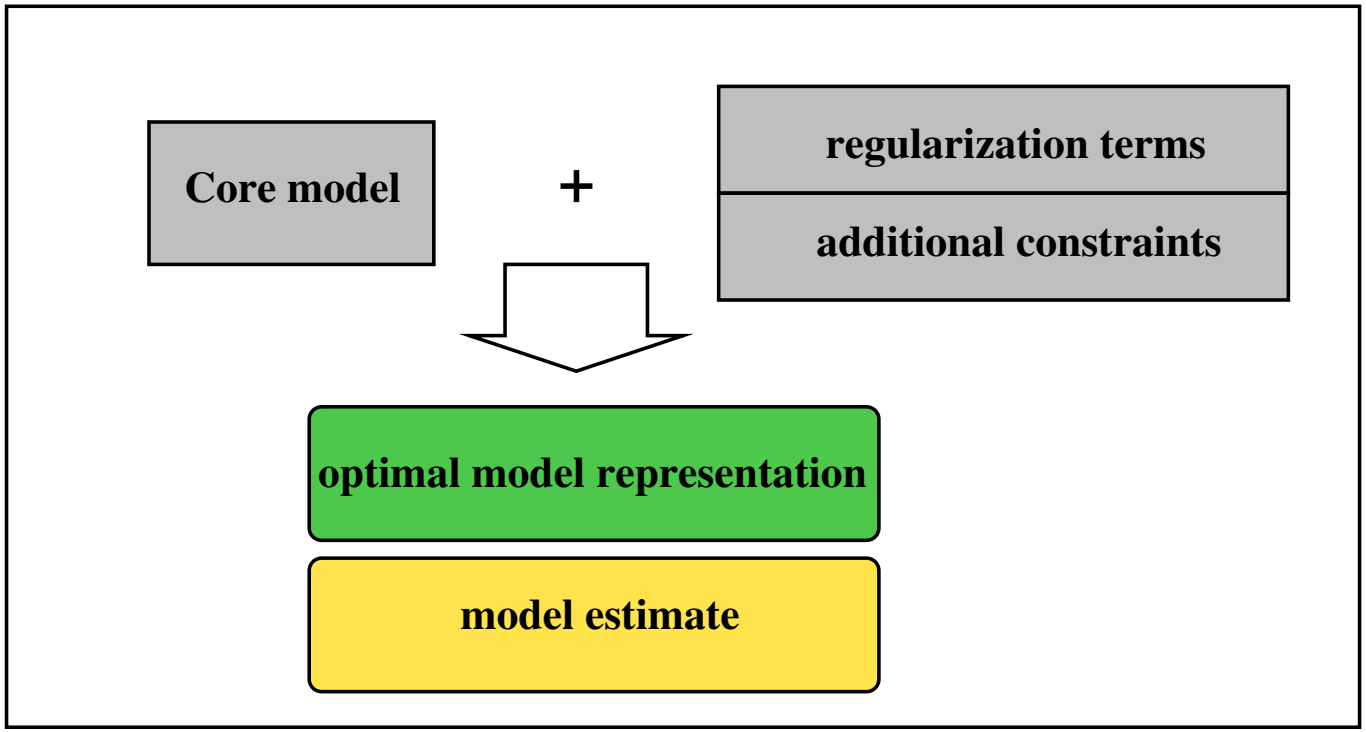


| Image ID | Image | Proposed method | Nyström method | Human |
|---|---|---|---|---|
| 145086 |  |  |  |  |
| 42049 |  |  |  |  |
| 167062 |  |  |  |  |
| 147091 |  |  |  |  |
| 196073 |  |  |  |  |
| 62096 |  |  |  |  |
| 119082 |  |  |  |  |
| 3096 |  |  |  |  |
| 295087 |  |  |  |  |
| 37073 |  |  |  |  |

# Core models + constraints



# Core models + constraints



# Kernel spectral clustering: adding prior knowledge

- Pair of points $x_\dagger, x_\ddagger$: $c = 1$ must-link, $c = -1$ cannot-link

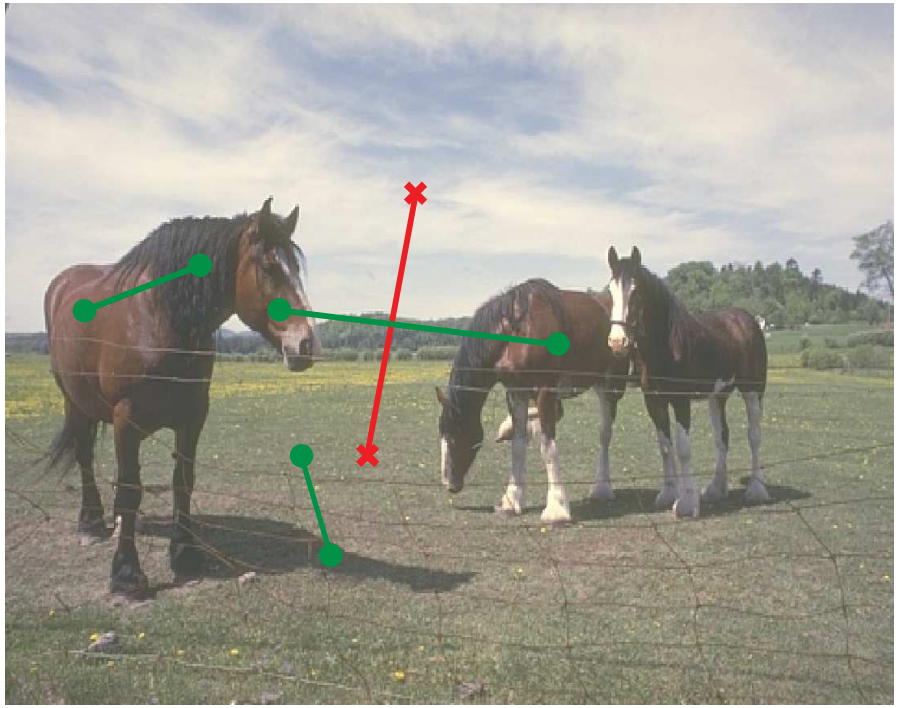
- Primal problem [Alzate & Suykens, IJCNN 2009]

$$
\begin{aligned}
\min_{w^{(l)}, e^{(l)}, b_l} \quad & -\frac{1}{2}\sum_{l=1}^{k-1} {w^{(l)}}^T w^{(l)} + \frac{1}{2}\sum_{l=1}^{k-1} \gamma_l {e^{(l)}}^T D^{-1} e^{(l)} \\
\text{subject to} \quad & e^{(1)} = \Phi_{N\times n_h} w^{(1)} + b_1 1_N \\
& \vdots \\
& e^{(k-1)} = \Phi_{N\times n_h} w^{(k-1)} + b_{k-1} 1_N \\
& {w^{(1)}}^T \varphi(x_\dagger) = c {w^{(1)}}^T \varphi(x_\ddagger) \\
& \vdots \\
& {w^{(k-1)}}^T \varphi(x_\dagger) = c {w^{(k-1)}}^T \varphi(x_\ddagger)
\end{aligned}
$$

- Dual problem: yields rank-one downdate of the kernel matrix

# Adding prior knowledge

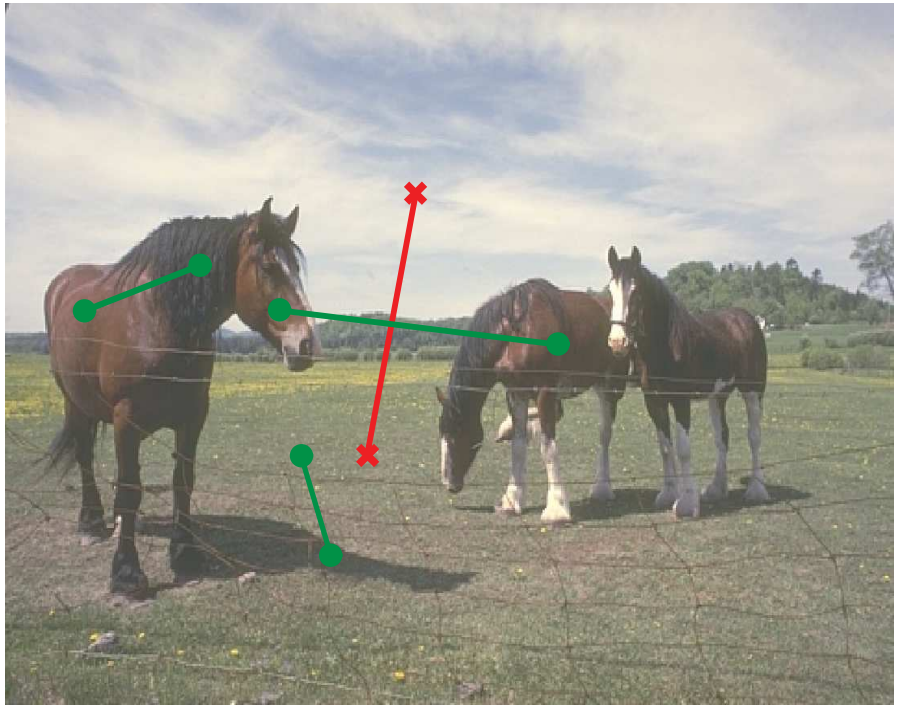
original image



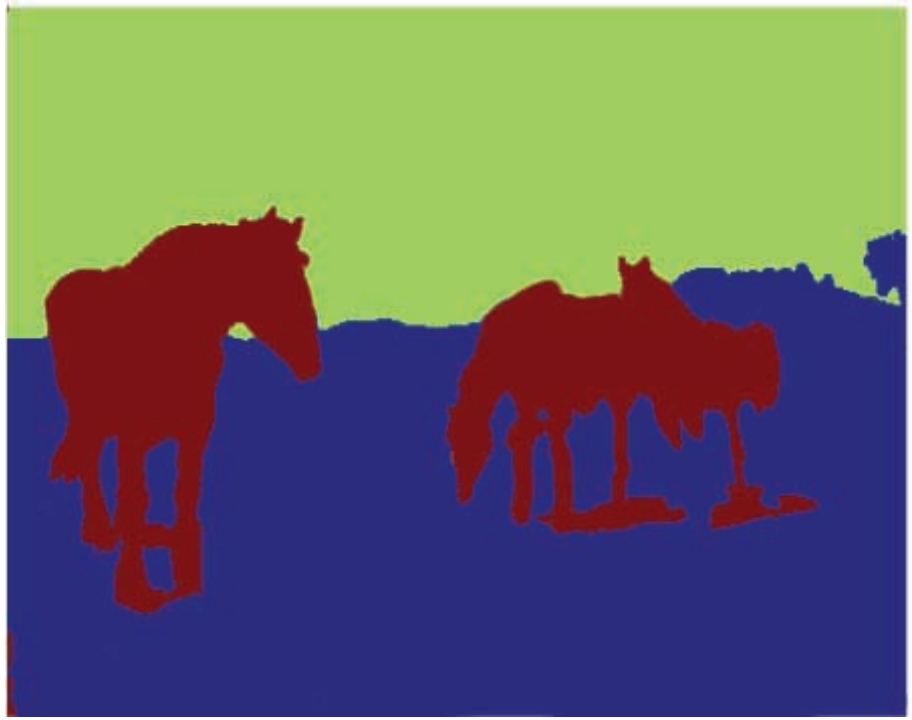
without constraints

# Adding prior knowledge

original image



with constraints



# Semi-supervised learning using KSC (1)

- $N$ unlabeled data, but additional labels on $M - N$ data
  $\mathcal{X} = \{x_1, ..., x_N, x_{N+1}, ..., x_M\}$

- Kernel spectral clustering as core model (binary case [Alzate & Suykens, WCCI 2012], multi-way/multi-class [Mehrkanoon et al., TNNLS 2015])

$$\begin{aligned} \min_{w,e,b} \quad & \frac{1}{2} w^T w - \gamma \frac{1}{2} e^T D^{-1} e + \rho \frac{1}{2} \sum_{m=N+1}^{M} (e_m - y_m)^2 \\ \text{subject to} \quad & e_i = w^T \varphi(x_i) + b, \; i = 1, ..., M \end{aligned}$$

  Dual solution is characterized by a linear system. Suitable for clustering as well as classification.

- Other approaches in semi-supervised learning and manifold learning, e.g. [Belkin et al., 2006]

# Semi-supervised learning using KSC (2)

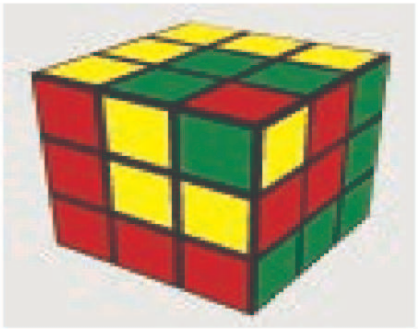
| Dataset | size | $n_L/n_U$ | test (%) | FS semi-KSC | RD semi-KSC | Lap-SVMp |
|---|---|---|---|---|---|---|
| Spambase | 4597 | 368/736 | 919 (20%) | $0.885 \pm 0.01$ | $0.883 \pm 0.01$ | $0.880 \pm 0.03$ |
| Satimage | 6435 | 1030/1030 | 1287 (20%) | $0.864 \pm 0.006$ | $0.831 \pm 0.009$ | $0.834 \pm 0.007$ |
| Ring | 7400 | 592/592 | 1480 (20%) | $0.975 \pm 0.005$ | $0.974 \pm 0.005$ | $0.972 \pm 0.006$ |
| Magic | 19020 | 761/1522 | 3804 (20%) | $0.836 \pm 0.006$ | $0.829 \pm 0.006$ | $0.827 \pm 0.005$ |
| Cod-rna | 331152 | 1325/1325 | 66230 (20%) | $0.957 \pm 0.006$ | $0.947 \pm 0.008$ | $0.951 \pm 0.001$ |
| Covertype | 581012 | 2760/2760 | 29050 (5%) | $0.715 \pm 0.005$ | $0.684 \pm 0.008$ | $0.697 \pm 0.001$ |
| | | 2760/27600 | | $0.729 \pm 0.04$ | $0.709 \pm 0.05$ | – |
| | | 2760/82800 | | $0.739 \pm 0.04$ | $0.716 \pm 0.03$ | – |
| | | 2760/138000 | | $0.742 \pm 0.05$ | $0.723 \pm 0.06$ | – |

FS semi-KSC: Fixed-size semi-supervised KSC
RD semi-KSC: other subset selection related to [Lee & Mangasarian, 2001]
Lap-SVM: Laplacian support vector machine [Belkin et al., 2006]

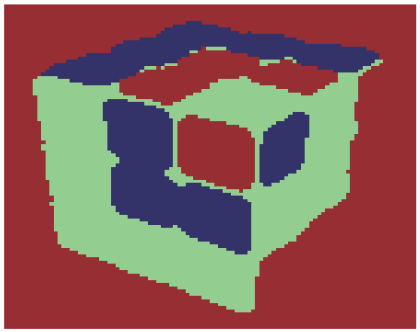
[Mehrkanoon & Suykens, 2014]

# Semi-supervised learning using KSC (3)

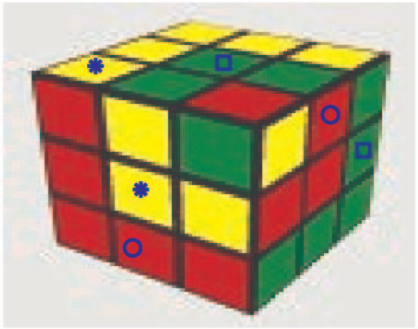
original image



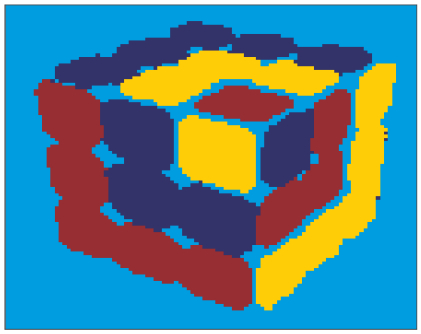
KSC



given a few labels

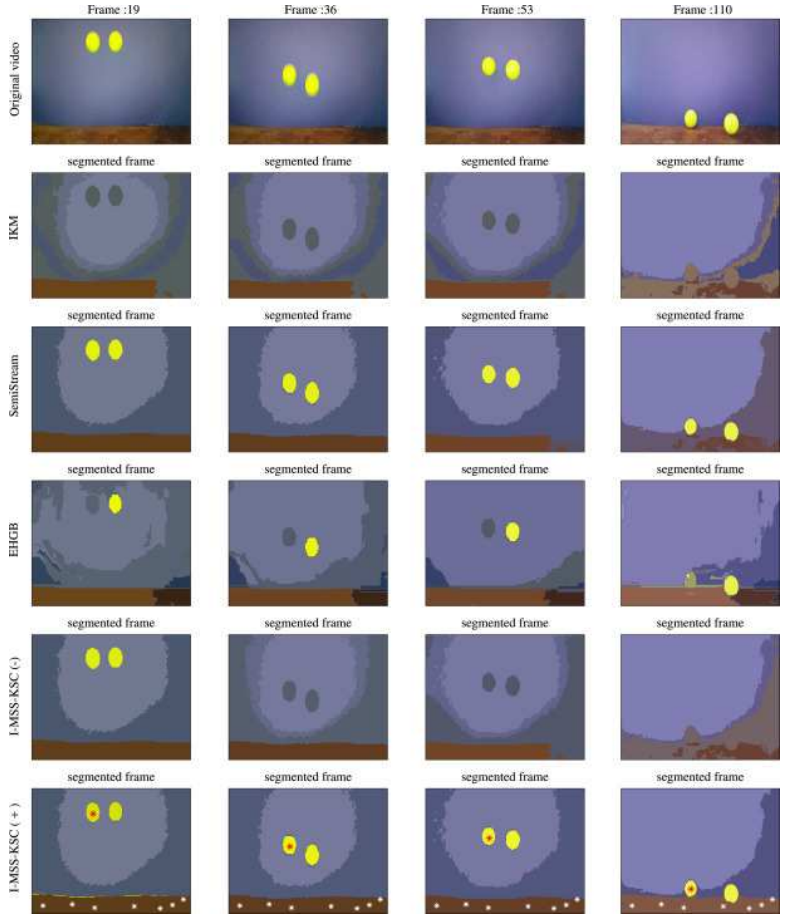


semi-supervised KSC



[Mehrkanoon, Alzate, Mall, Langone, Suykens, IEEE-TNNLS, 2015]

# Semi-supervised learning using KSC (4)




KSC regularized by Kalman filtering for on-line video segmentation:

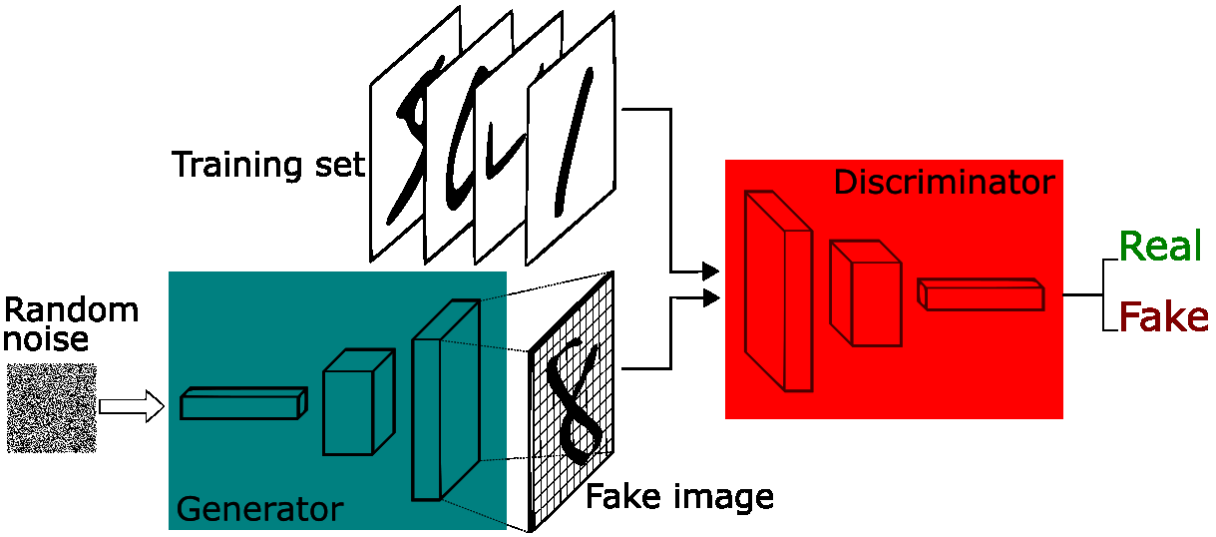
Mehrkanoon S., Agudelo M., Suykens J.A.K, "Incremental multi-class semi-supervised clustering regularized by Kalman filtering", *Neural Networks*, vol. 71, Nov. 2015, pp. 88-104.

# *Generative models*

# Generative Adversarial Network (GAN)

Generative Adversarial Network (GAN) [Goodfellow et al., 2014]
Training of two competing models in a zero-sum game:

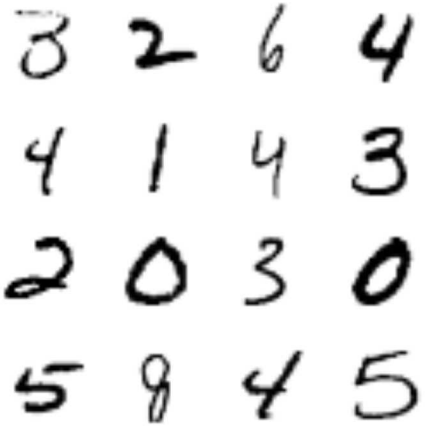
(Generator) generate fake output examples from random noise
(Discriminator) discriminate between fake examples and real examples.



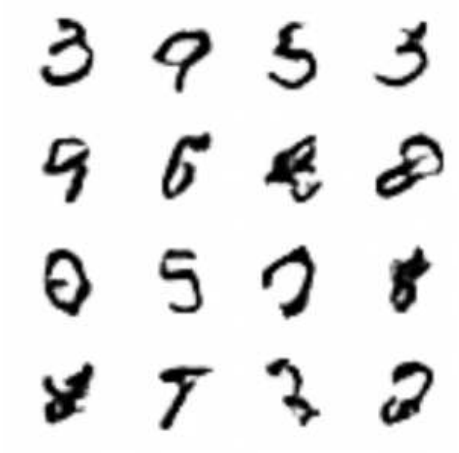

source: https://deeplearning4j.org/generative-adversarial-network

# GAN: example on MNIST

MNIST training data:

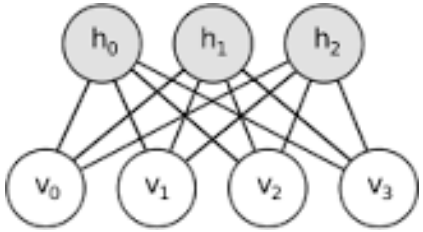


GAN generated examples:



source: https://www.kdnuggets.com/2016/07/mnist-generative-adversarial-model-keras.html

# Restricted Boltzmann Machines (RBM)




- Markov random field, bipartite graph, stochastic binary units
  Layer of visible units $v$ and layer of hidden units $h$
  **No hidden-to-hidden connections**
- Energy:

$$E(v, h; \theta) = -v^T W h - c^T v - a^T h \quad \text{with} \quad \theta = \{W, c, a\}$$

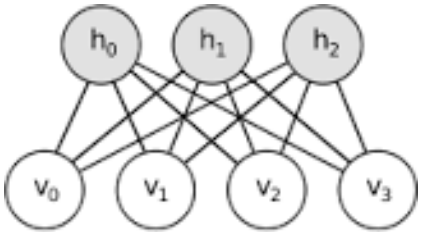
Joint distribution:

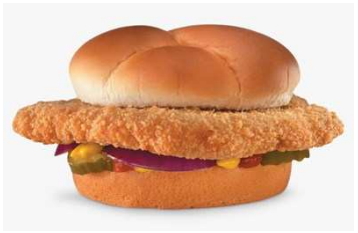
$$P(v, h; \theta) = \frac{1}{Z(\theta)} \exp(-E(v, h; \theta))$$

with partition function $Z(\theta) = \sum_v \sum_h \exp(-E(v, h; \theta))$

[Hinton, Osindero, Teh, Neural Computation 2006]

# Restricted Boltzmann Machines (RBM)



- Markov random field, bipartite graph, stochastic binary units
  Layer of visible units $v$ and layer of hidden units $h$
  **No hidden-to-hidden connections**
- Energy:

$$E(v, h; \theta) = -v^T W h - c^T v - a^T h \quad \text{with} \quad \theta = \{W, c, a\}$$

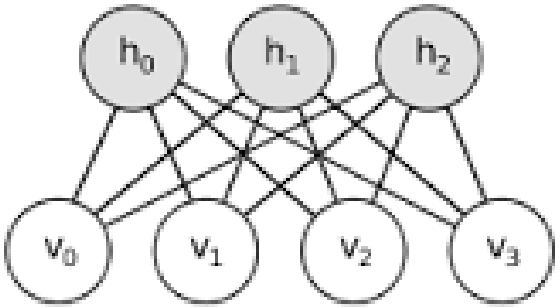
Joint distribution:

$$P(v, h; \theta) = \frac{1}{Z(\theta)} \exp(-E(v, h; \theta))$$

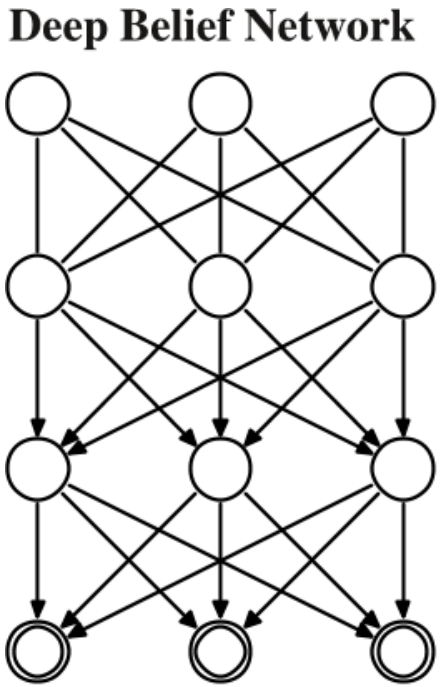
with partition function $Z(\theta) = \sum_v \sum_h \exp(-E(v, h; \theta))$

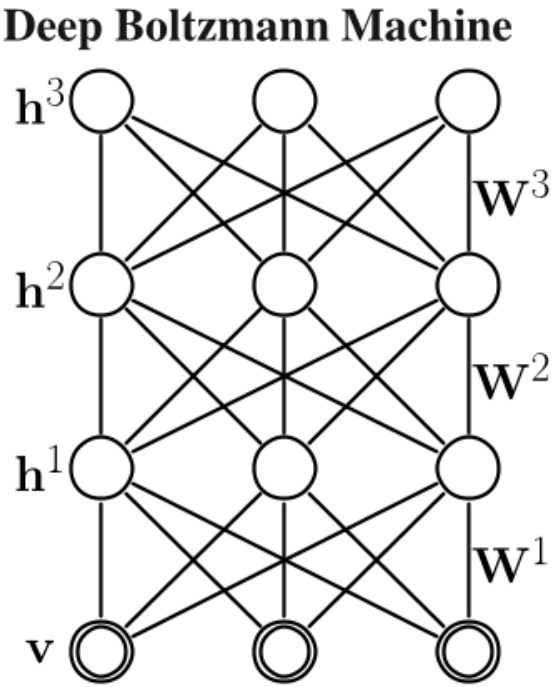
[Hinton, Osindero, Teh, Neural Computation 2006]

# RBM and deep learning




$p(v, h)$



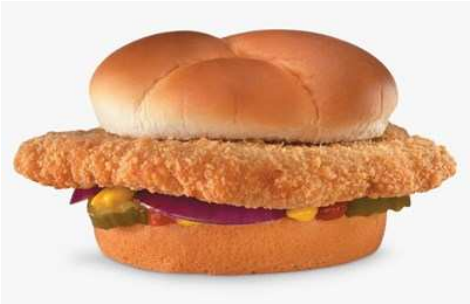




$p(v, h^1, h^2, h^3, ...)$

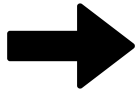
[Hinton et al., 2006; Salakhutdinov, 2015]

# in other words ...

*"sandwich"*



$$E = -v^T W h$$

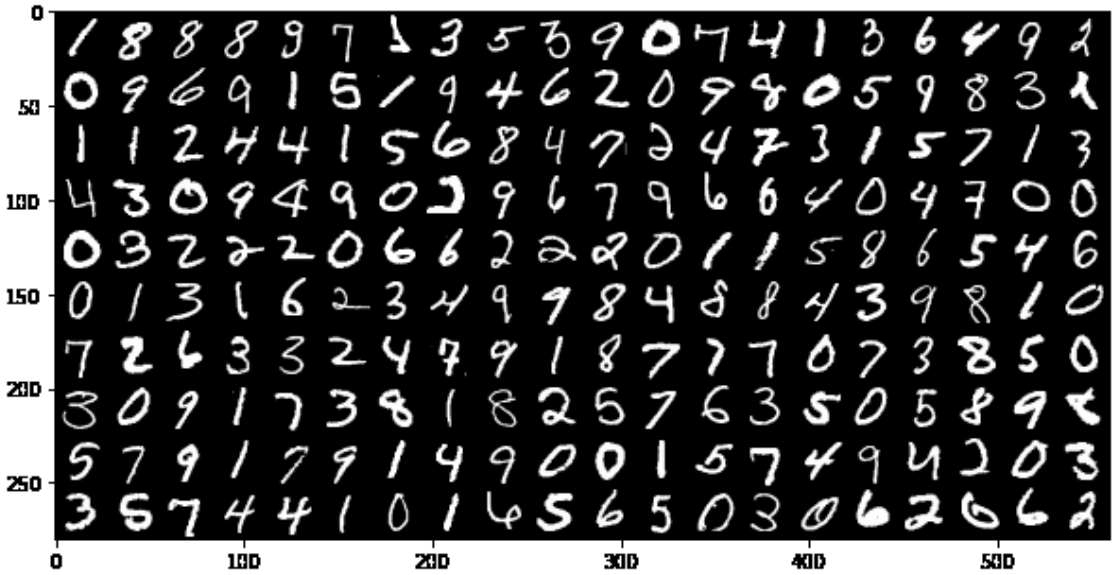


*"deep sandwich"*

$$E = -v^T W^1 h^1 - h^{1T} W^2 h^2 - h^{2T} W^3 h^3$$

# RBM: example on MNIST

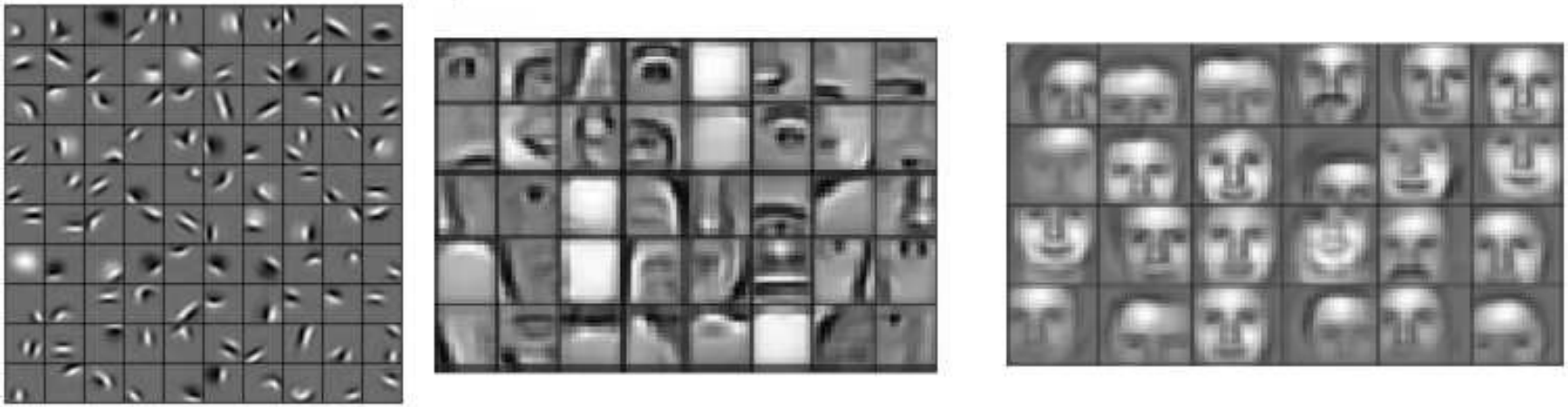
MNIST training data:




Generating new images:


source: https://www.kaggle.com/nicw102168/restricted-boltzmann-machine-rbm-on-mnist

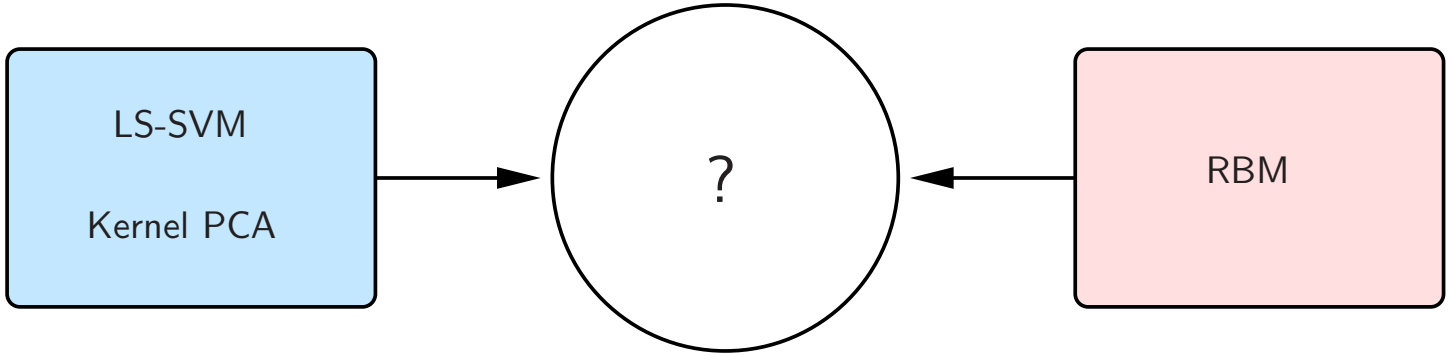
# Convolutional Deep Belief Networks



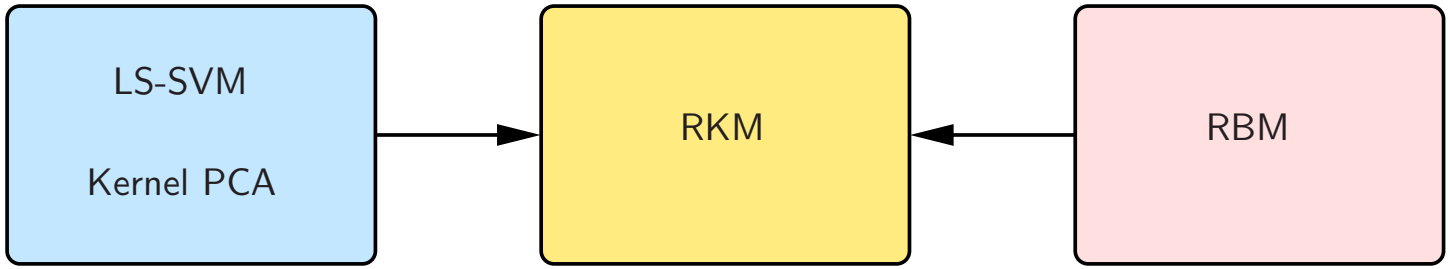
Unsupervised Learning of Hierarchical Representations with Convolutional Deep Belief Networks [Lee et al. 2011]

# *Restricted kernel machines*

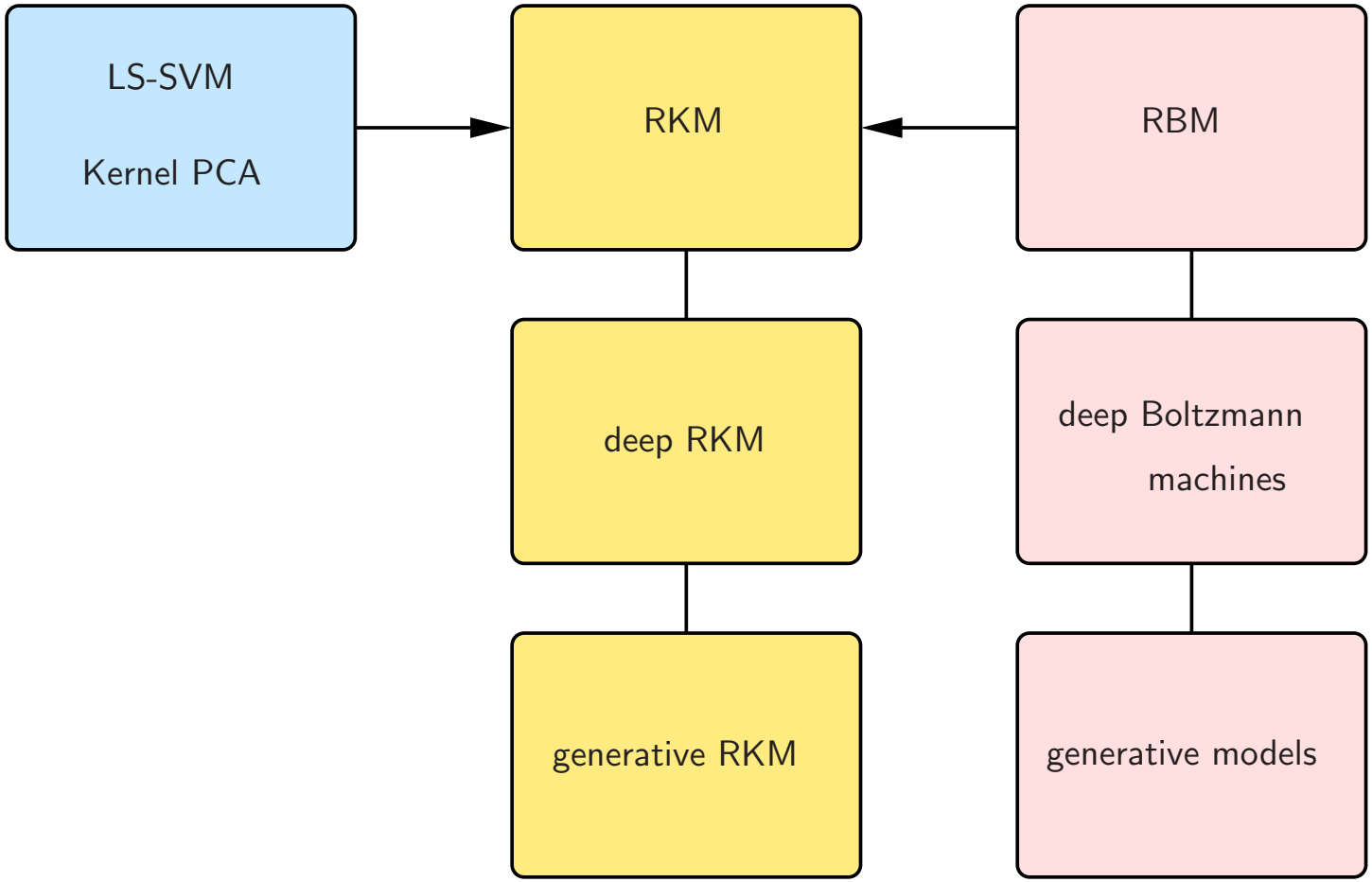
# New connections



# New connections



# New connections



# Restricted Kernel Machines (RKM)

- Kernel machine interpretations in terms of **visible and hidden units** (similar to Restricted Boltzmann Machines (**RBM**))

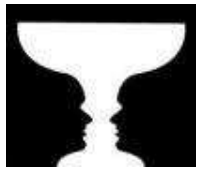
- Restricted Kernel Machine (**RKM**) representations for
  - LS-SVM regression/classification
  - Kernel PCA
  - Matrix SVD
  - Parzen-type models
  - other

- Based on principle of **conjugate feature duality** (with hidden features corresponding to dual variables)

- Deep Restricted Kernel Machines (Deep RKM)

[Suykens, Neural Computation, 2017]

# From KPCA to RKM representation (1)



Model:

$e = W^T \varphi(x)$

objective $J$
$=$ regularization term $\mathrm{Tr}(W^T W)$
- $(\frac{1}{\lambda})$ variance term $\sum_i e_i^T e_i$

$\downarrow$ use property $e^T h \leq \frac{1}{2\lambda} e^T e + \frac{\lambda}{2} h^T h$

RKM representation:

$e = \sum_j h_j K(x_j, x)$

obtain $J \leq \overline{J}(h_i, W)$
solution from stationary points of $\overline{J}$:
$\frac{\partial \overline{J}}{\partial h_i} = 0$, $\frac{\partial \overline{J}}{\partial W} = 0$

# From KPCA to RKM representation (2)

- Objective

$$
\begin{aligned}
J &= \frac{\eta}{2}\mathrm{Tr}(W^TW) - \frac{1}{2\lambda}\sum_{i=1}^{N} e_i^T e_i \text{ s.t. } e_i = W^T\varphi(x_i), \forall i \\
&\leq -\sum_{i=1}^{N} e_i^T h_i + \frac{\lambda}{2}\sum_{i=1}^{N} h_i^T h_i + \frac{\eta}{2}\mathrm{Tr}(W^TW) \text{ s.t. } e_i = W^T\varphi(x_i), \forall i \\
&= -\sum_{i=1}^{N} \varphi(x_i)^T W h_i + \frac{\lambda}{2}\sum_{i=1}^{N} h_i^T h_i + \frac{\eta}{2}\mathrm{Tr}(W^TW) \triangleq \overline{J}
\end{aligned}
$$

- Stationary points of $\overline{J}(h_i, W)$:

$$
\begin{cases}
\dfrac{\partial \overline{J}}{\partial h_i} = 0 \quad \Rightarrow \quad W^T\varphi(x_i) = \lambda h_i, \ \forall i \\
\dfrac{\partial \overline{J}}{\partial W} = 0 \quad \Rightarrow \quad W = \dfrac{1}{\eta}\sum_i \varphi(x_i) h_i^T
\end{cases}
$$

# From KPCA to RKM representation (3)

- Elimination of $W$ gives the eigenvalue decomposition:

$$\frac{1}{\eta} K H^T = H^T \Lambda$$

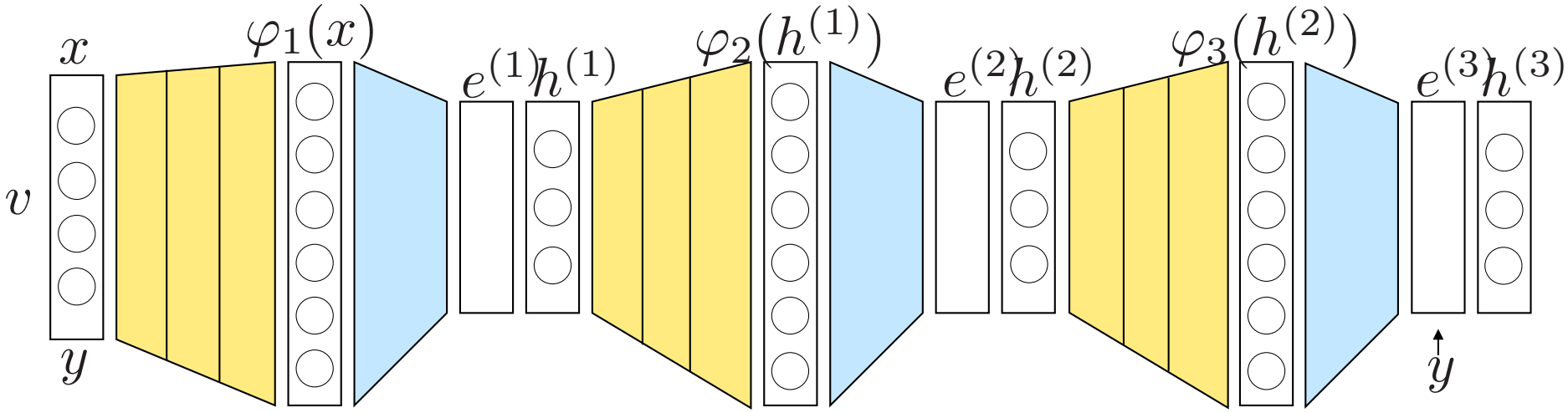
where $H = [h_1 ... h_N] \in \mathbb{R}^{s \times N}$ and $\Lambda = \mathrm{diag}\{\lambda_1, ..., \lambda_s\}$ with $s \leq N$

- Primal and dual model representations

$$\mathcal{M} \begin{cases} \nearrow & (P)_{\mathrm{RKM}}: \quad \hat{e} = W^T \varphi(x) \\ \searrow & (D)_{\mathrm{RKM}}: \quad \hat{e} = \frac{1}{\eta} \sum_j h_j K(x_j, x). \end{cases}$$

# *Deep Restricted Kernel Machines*

# Deep RKM: example



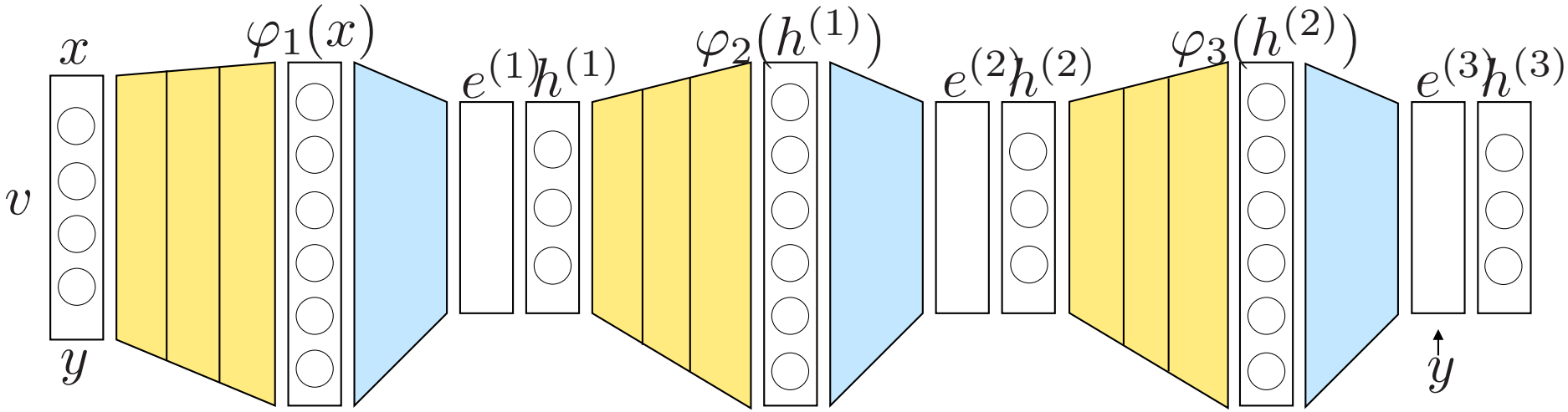

Deep RKM: KPCA + KPCA + LSSVM [Suykens, 2017]

Coupling of RKMs by taking sum of the objectives

$$J_{\text{deep}} = \overline{J}_1 + \overline{J}_2 + \underline{J}_3$$

Multiple *levels* and multiple *layers* per level.

# in more detail ...




$$
\begin{aligned}
J_{\text{deep}} \quad = \quad & -\sum_{i=1}^{N} \varphi_1(x_i)^T W_1 h_i^{(1)} + \frac{\lambda_1}{2} \sum_{i=1}^{N} {h_i^{(1)}}^T h_i^{(1)} + \frac{\eta_1}{2} \text{Tr}(W_1^T W_1) \\
& -\sum_{i=1}^{N} \varphi_2(h_i^{(1)})^T W_2 h_i^{(2)} + \frac{\lambda_2}{2} \sum_{i=1}^{N} {h_i^{(2)}}^T h_i^{(2)} + \frac{\eta_2}{2} \text{Tr}(W_2^T W_2) \\
& +\sum_{i=1}^{N} (y_i^T - \varphi_3(h_i^{(2)})^T W_3 - b^T) h_i^{(3)} - \frac{\lambda_3}{2} \sum_{i=1}^{N} {h_i^{(3)}}^T h_i^{(3)} + \frac{\eta_3}{2} \text{Tr}(W_3^T W_3)
\end{aligned}
$$

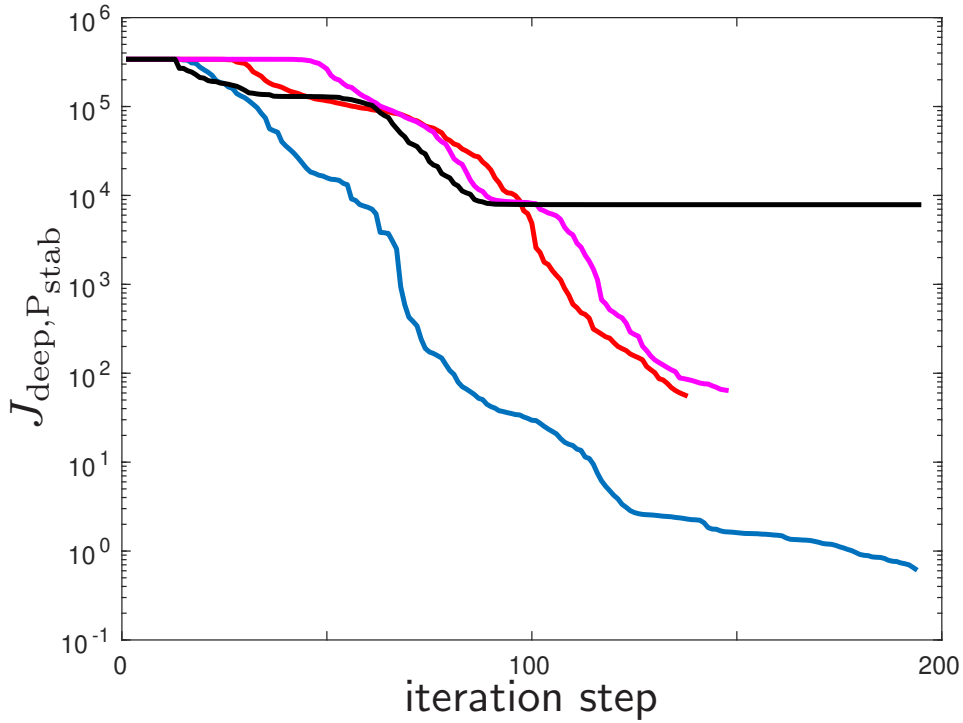
# Primal and dual model representations

$$
\mathcal{M} \begin{cases} \nearrow & (P)_{\text{DeepRKM}}: \quad \begin{aligned} \hat{e}^{(1)} &= W_1^T \varphi_1(x) \\ \hat{e}^{(2)} &= W_2^T \varphi_2(\Lambda_1^{-1} \hat{e}^{(1)}) \\ \hat{y} &= W_3^T \varphi_3(\Lambda_2^{-1} \hat{e}^{(2)}) + b \end{aligned} \\ \searrow & (D)_{\text{DeepRKM}}: \quad \begin{aligned} \hat{e}^{(1)} &= \frac{1}{\eta_1} \sum_j h_j^{(1)} K_1(x_j, x) \\ \hat{e}^{(2)} &= \frac{1}{\eta_2} \sum_j h_j^{(2)} K_2(h_j^{(1)}, \Lambda_1^{-1} \hat{e}^{(1)}) \\ \hat{y} &= \frac{1}{\eta_3} \sum_j h_j^{(3)} K_3(h_j^{(2)}, \Lambda_2^{-1} \hat{e}^{(2)}) + b \end{aligned} \end{cases}
$$

The framework can be used for training deep feedforward neural networks and deep kernel machines [Suykens, 2017].

(Other approaches: e.g. kernels for deep learning [Cho & Saul, 2009], mathematics of the neural response [Smale et al., 2010], deep gaussian processes [Damianou & Lawrence, 2013], convolutional kernel networks [Mairal et al., 2014], multi-layer support vector machines [Wiering & Schomaker, 2014])

# Training process




Objective function (logarithmic scale) during training on the ion data set:

- black color: level 3 objective only
- $J_{\mathrm{deep}}$ for $c_{\mathrm{stab}} = 1$, 10, 100 (blue, red, magenta color) in stabilization term

# *Generative RKM*

# RKM objective for training and generating

- RBM energy function

$$E(v, h; \theta) = -v^{\mathrm{T}} W h - c^{\mathrm{T}} v - a^{\mathrm{T}} h$$

with model parameters $\theta = \{W, c, a\}$

- RKM "super-objective" function (for training and for generating)

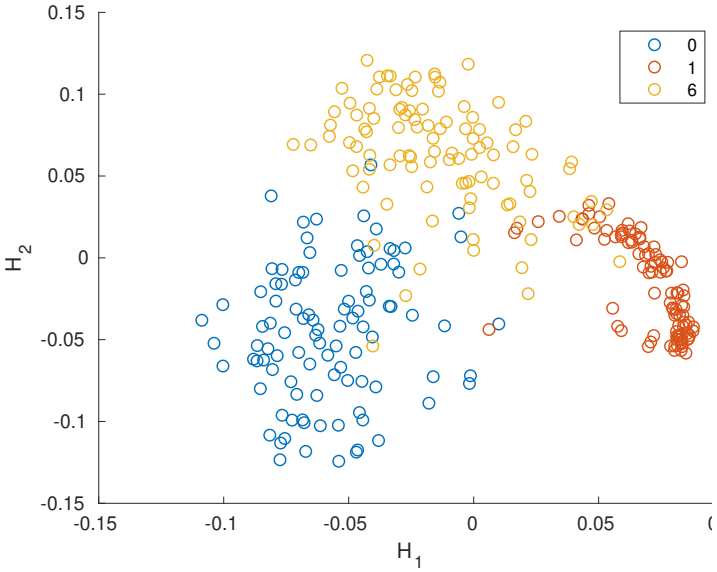
$$\bar{J}(v, h, W) = -v^{\mathrm{T}} W h + \frac{\lambda}{2} h^{\mathrm{T}} h + \frac{1}{2} v^{\mathrm{T}} v + \frac{\eta}{2} \mathrm{Tr}(W^{\mathrm{T}} W)$$

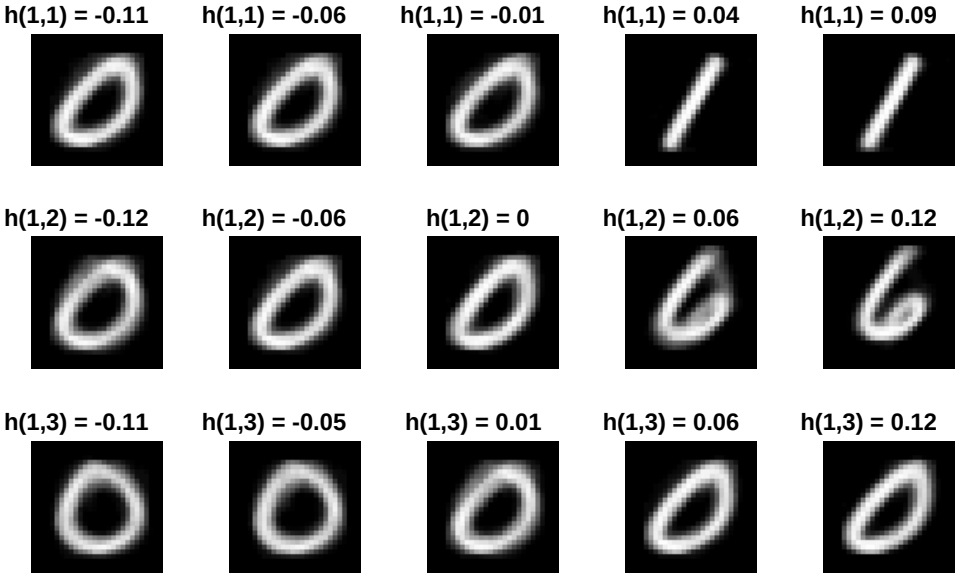
| | | | |
|---|---|---|---|
| **Training:** | clamp $v$ | $\rightarrow$ | $\bar{J}_{\mathrm{train}}(h, W)$ |
| **Generating:** | clamp $h, W$ | $\rightarrow$ | $\bar{J}_{\mathrm{gen}}(v)$ |

[Schreurs & Suykens, ESANN 2018]

# Explainable AI: latent space exploration (1)

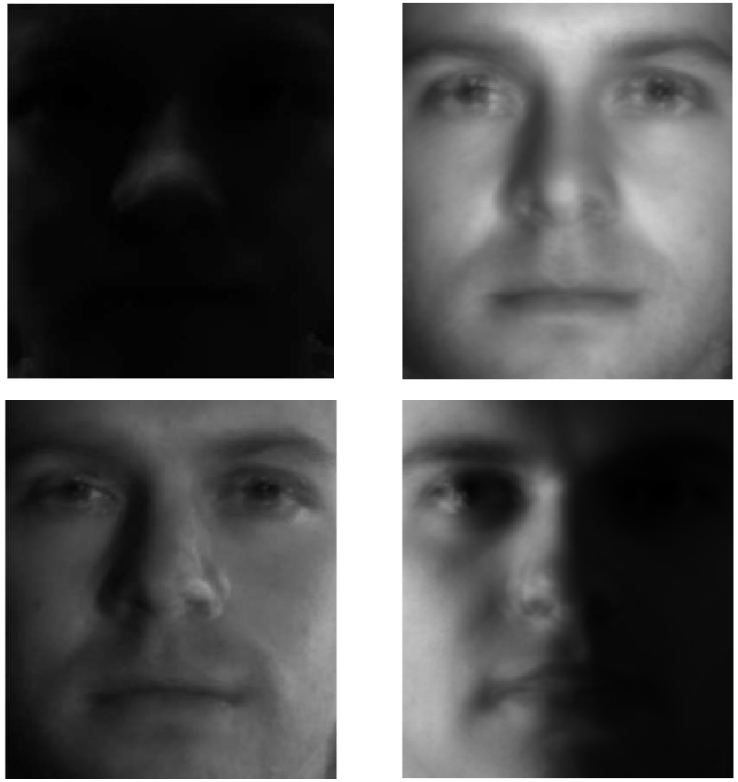
hidden units: exploring the **whole continuum**:

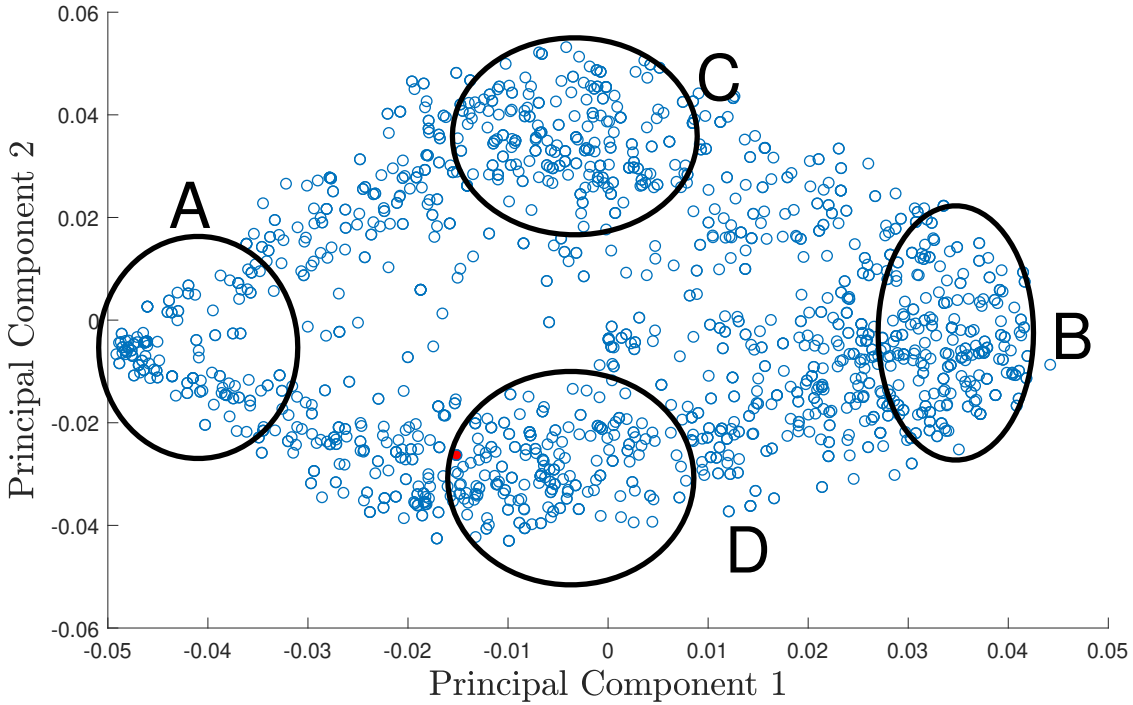



[figures by Joachim Schreurs]

# Explainable AI: latent space exploration (2)



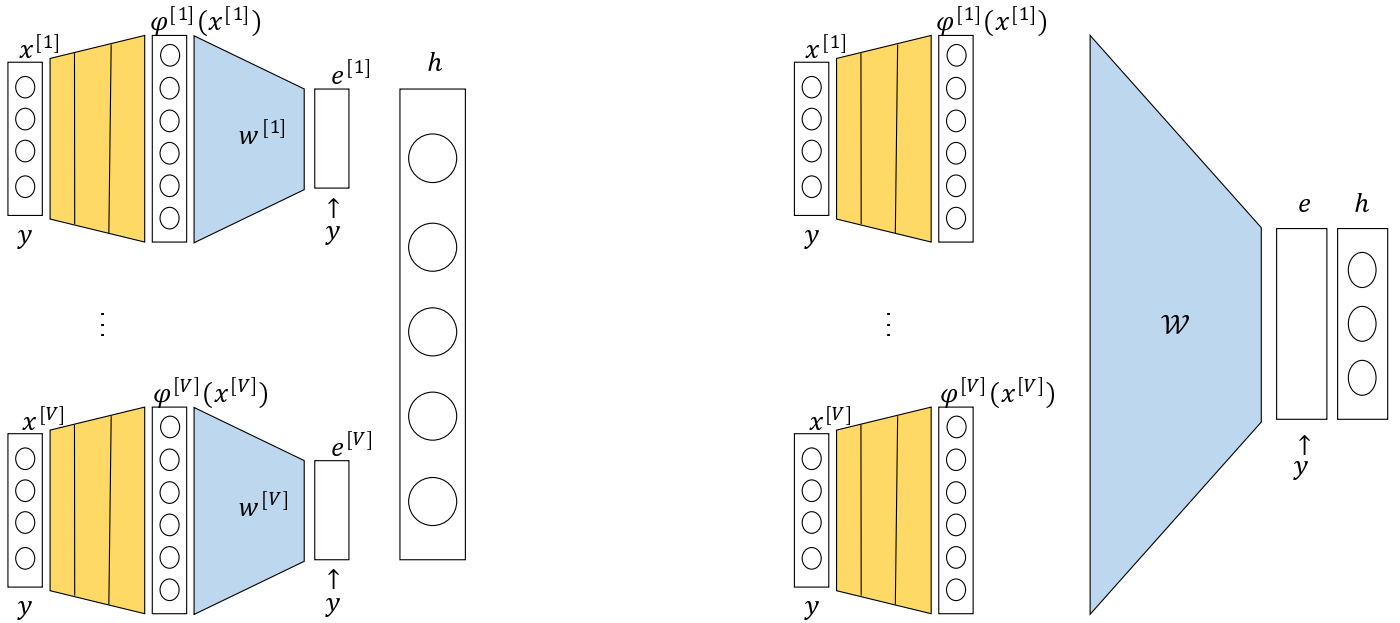



Yale Face database - generated faces from different regions A,B,C,D

[Winant, Schreurs, Suykens, BNAIC 2019]

# Tensor-based RKM for Multi-view KPCA

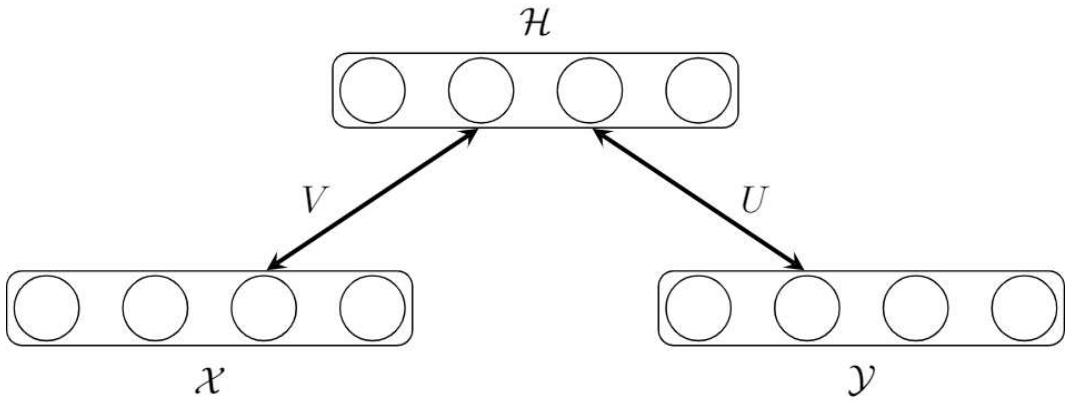
$$\min \langle \mathcal{W}, \mathcal{W} \rangle - \sum_{i=1}^{N} \left\langle \Phi_{(i)}, \mathcal{W} \right\rangle h_i + \lambda \sum_{i=1}^{N} h_i^2 \quad \text{with} \quad \Phi_{(i)} = \varphi^{[1]}(x_i^{[1]}) \otimes \ldots \otimes \varphi^{[V]}(x_i^{[V]})$$



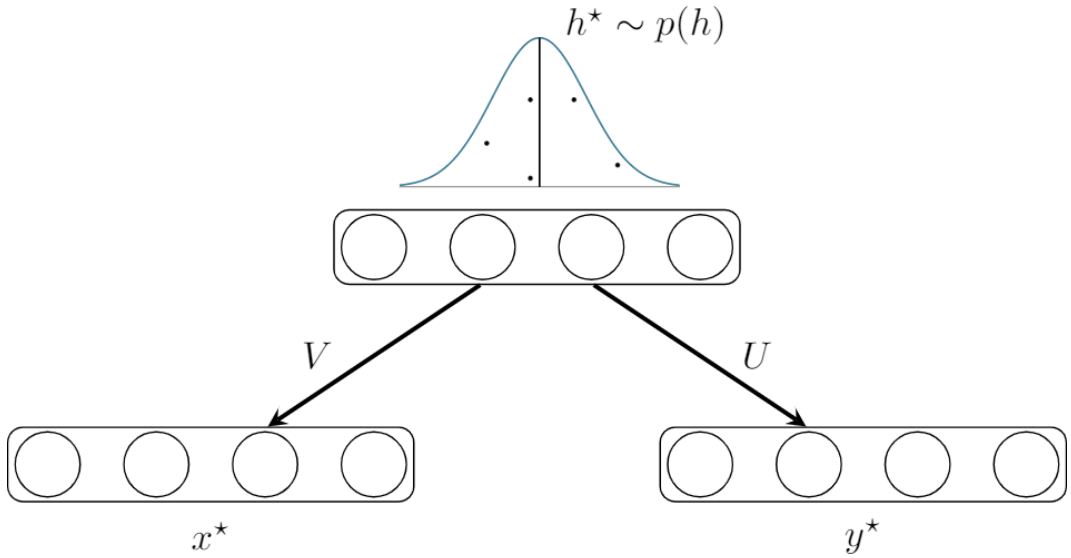

[Houthuys & Suykens, ICANN 2018]

# Generative RKM (Gen-RKM) (1)

**Train:**

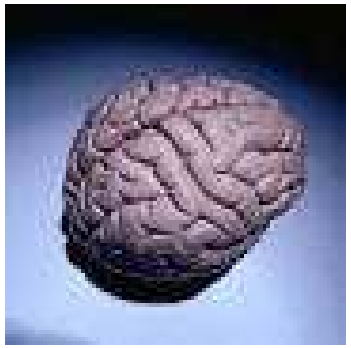



**Generate:**

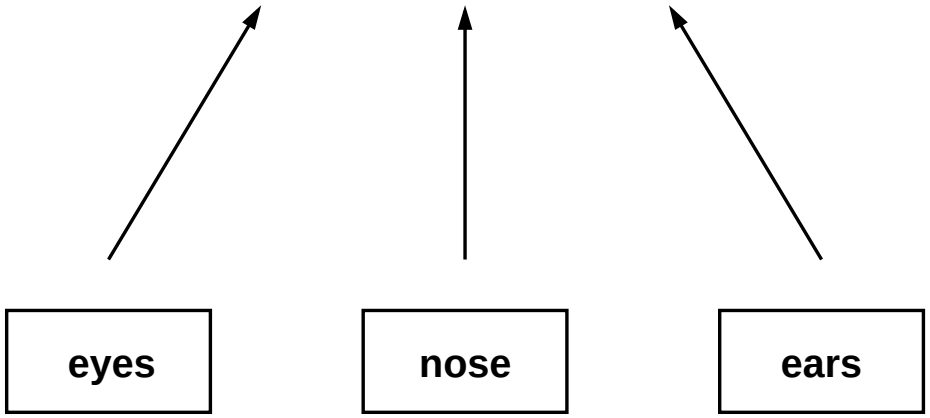



[Pandey, Schreurs & Suykens, 2019, arXiv:1906.08144]

# Analogy with the human brain



*shared feature representation*




*multimodal data*

# Gen-RKM (2)

The objective

$$J_{\text{train}}(\boldsymbol{h}_i, \boldsymbol{U}, \boldsymbol{V}) = \sum_{i=1}^{N} \left(-\phi_1(\boldsymbol{x}_i)^T \boldsymbol{U} \boldsymbol{h}_i - \phi_2(\boldsymbol{y}_i)^T \boldsymbol{V} \boldsymbol{h}_i + \frac{\lambda}{2} \boldsymbol{h}_i^T \boldsymbol{h}_i\right) + \frac{\eta_1}{2}\text{Tr}(\boldsymbol{U}^T\boldsymbol{U}) + \frac{\eta_2}{2}\text{Tr}(\boldsymbol{V}^T\boldsymbol{V})$$

results for **training** into the eigenvalue problem

$$(\frac{1}{\eta_1}\boldsymbol{K}_1 + \frac{1}{\eta_2}\boldsymbol{K}_2)\boldsymbol{H}^T = \boldsymbol{H}^T\boldsymbol{\Lambda}$$

with $\boldsymbol{H} = [\boldsymbol{h}_1 ... \boldsymbol{h}_N]$ and kernel matrices $\boldsymbol{K}_1, \boldsymbol{K}_2$ related to $\phi_1, \phi_2$.

[Pandey, Schreurs & Suykens, 2019, arXiv:1906.08144]

# Gen-RKM (3)

**Generating** data is based on a newly generated $\boldsymbol{h}^\star$ and the objective

$$J_{\text{gen}}(\phi_1(\boldsymbol{x}^\star), \varphi_2(\boldsymbol{y}^\star)) = -\phi_1(\boldsymbol{x}^\star)^T \boldsymbol{V} \boldsymbol{h}^\star - \phi_2(\boldsymbol{y}^\star)^T \boldsymbol{U} \boldsymbol{h}^\star + \frac{1}{2}\phi_1(\boldsymbol{x}^\star)^T \phi_1(\boldsymbol{x}^\star) + \frac{1}{2}\phi_2(\boldsymbol{y}^\star)^T \phi_2(\boldsymbol{y}^\star)$$

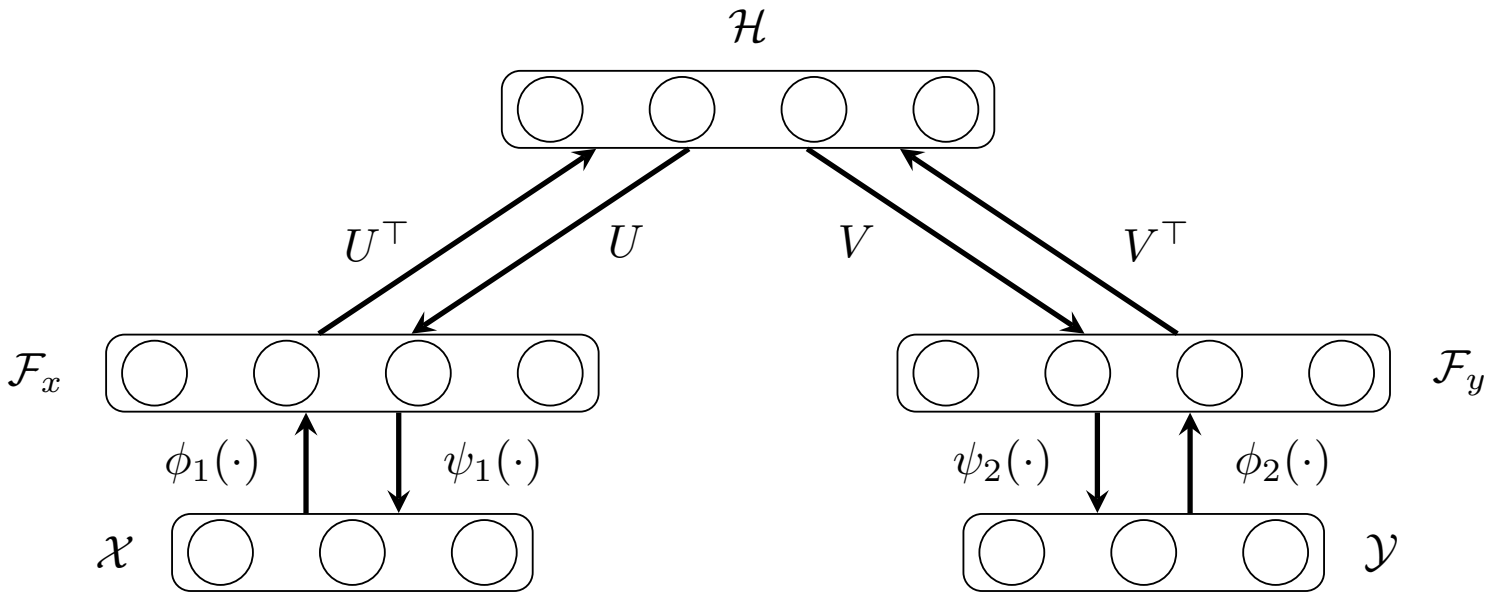
giving

$$\phi_1(\boldsymbol{x}^\star) = \frac{1}{\eta_1}\sum_{i=1}^{N} \phi_1(\boldsymbol{x}_i)\boldsymbol{h}_i^T \boldsymbol{h}^\star, \;\; \phi_2(\boldsymbol{y}^\star) = \frac{1}{\eta_2}\sum_{i=1}^{N} \phi_2(\boldsymbol{y}_i)\boldsymbol{h}_i^T \boldsymbol{h}^\star.$$

For generating $\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}$ one can either work with the kernel smoother or work with an explicit feature map using a (deep) neural network or CNN.

[Pandey, Schreurs & Suykens, 2019, arXiv:1906.08144]

# Gen-RKM (4)




Gen-RKM schematic representation modeling a common subspace $\mathcal{H}$ between two data sources $\mathcal{X}$ and $\mathcal{Y}$. The $\phi_1$, $\phi_2$ are the feature maps ($\mathcal{F}_x$ and $\mathcal{F}_y$ represent the feature-spaces) corresponding to the two data sources. While $\psi_1$, $\psi_2$ represent the pre-image maps. The interconnection matrices $U, V$ model dependencies between latent variables and the mapped data sources.

[Pandey, Schreurs & Suykens, 2019, arXiv:1906.08144]

# Gen-RKM: implicit feature map (choose kernel)

Obtain

$$\boldsymbol{k}_{\boldsymbol{x}^\star} = \frac{1}{\eta_1}\boldsymbol{K}_1\boldsymbol{H}^\top\boldsymbol{h}^\star, \quad \boldsymbol{k}_{\boldsymbol{y}^\star} = \frac{1}{\eta_2}\boldsymbol{K}_2\boldsymbol{H}^\top\boldsymbol{h}^\star,$$

with $\boldsymbol{k}_{\boldsymbol{x}^\star} = [k(\boldsymbol{x}_1, \boldsymbol{x}^\star), \ldots, k(\boldsymbol{x}_N, \boldsymbol{x}^\star)]^\top$.

Using the kernel-smoother:

$$\hat{\boldsymbol{x}} = \psi_1\left(\phi_1(\boldsymbol{x}^\star)\right) = \frac{\sum_{j=1}^{n_r}\tilde{k}_1(\boldsymbol{x}_j, \boldsymbol{x}^\star)\boldsymbol{x}_j}{\sum_{j=1}^{n_r}\tilde{k}_1(\boldsymbol{x}_j, \boldsymbol{x}^\star)}, \quad \hat{\boldsymbol{y}} = \psi_2\left(\phi_2(\boldsymbol{y}^\star)\right) = \frac{\sum_{j=1}^{n_r}\tilde{k}_2(\boldsymbol{y}_j, \boldsymbol{y}^\star)\boldsymbol{y}_j}{\sum_{j=1}^{n_r}\tilde{k}_2(\boldsymbol{y}_j, \boldsymbol{y}^\star)},$$

with $\tilde{k}_1(\boldsymbol{x}_i, \boldsymbol{x}^\star)$ and $\tilde{k}_2(\boldsymbol{y}_i, \boldsymbol{y}^\star)$ the scaled similarities between $0$ and $1$.
$n_r$ is the number of closest points based on the similarity defined by kernels $\tilde{k}_1$ and $\tilde{k}_2$.

# Gen-RKM: choose explicit (CNN) feature map

Parametrized feature maps: $\phi_{\boldsymbol{\theta}}(\cdot)$, $\psi_{\boldsymbol{\zeta}}(\cdot)$ (e.g. CNN and transposed CNN).

Overall objective function, using a stabilization mechanism [Suykens, 2017]:

$$\begin{aligned}\min_{\boldsymbol{\theta}_1,\boldsymbol{\theta}_2,\boldsymbol{\zeta}_1,\boldsymbol{\zeta}_2} \mathcal{J}_c \;=\; & \mathcal{J}_{\text{train}} + \tfrac{c_{\text{stab}}}{2}\mathcal{J}^2_{\text{train}} \\ & + \tfrac{c_{\text{acc}}}{2N}\left(\sum_{i=1}^{N}\left[\mathcal{L}_1(\boldsymbol{x}_i^\star, \psi_{1_{\boldsymbol{\zeta}_1}}(\phi_{1_{\boldsymbol{\theta}_1}}(\boldsymbol{x}_i^\star))) + \mathcal{L}_2(\boldsymbol{y}_i^\star, \psi_{2_{\boldsymbol{\zeta}_2}}(\phi_{2_{\boldsymbol{\theta}_2}}(\boldsymbol{y}_i^\star)))\right]\right)\end{aligned}$$

with reconstruction errors

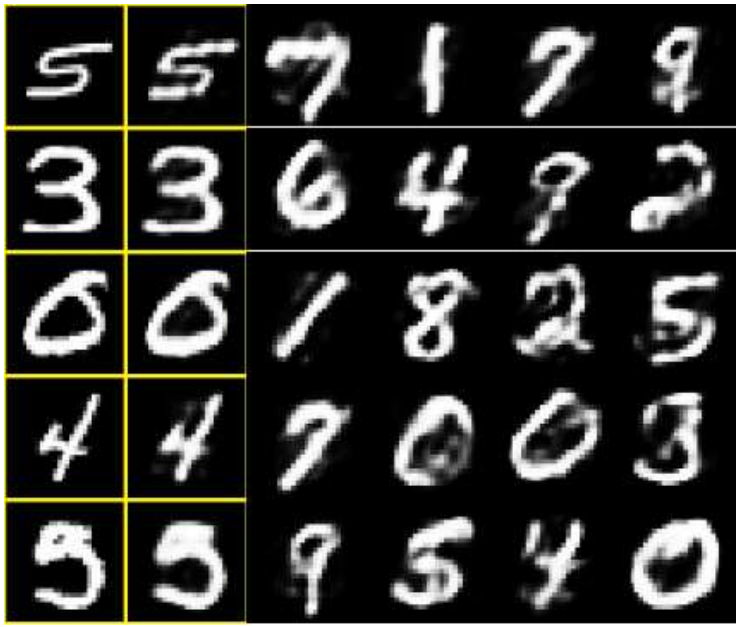
$$\begin{aligned}\mathcal{L}_1(\boldsymbol{x}_i^\star, \psi_{1_{\boldsymbol{\zeta}_1}}(\phi_{1_{\boldsymbol{\theta}_1}}(\boldsymbol{x}_i^\star))) &= \tfrac{1}{N}\|\boldsymbol{x}_i^\star - \psi_{1_{\boldsymbol{\zeta}_1}}(\phi_{1_{\boldsymbol{\theta}_1}}(\boldsymbol{x}_i^\star))\|_2^2, \\ \mathcal{L}_2(\boldsymbol{y}_i^\star, \psi_{2_{\boldsymbol{\zeta}_2}}(\phi_{2_{\boldsymbol{\theta}_2}}(\boldsymbol{y}_i^\star))) &= \tfrac{1}{N}\|\boldsymbol{y}_i^\star - \psi_{2_{\boldsymbol{\zeta}_2}}(\phi_{2_{\boldsymbol{\theta}_2}}(\boldsymbol{y}_i^\star))\|_2^2\end{aligned}$$

and with $\Phi_{\boldsymbol{x}} = [\phi_1(\boldsymbol{x}_1), \ldots, \phi_1(\boldsymbol{x}_N)], \Phi_{\boldsymbol{y}} = [\phi_2(\boldsymbol{y}_1), \ldots, \phi_2(\boldsymbol{y}_N)]$, $U, V$ from

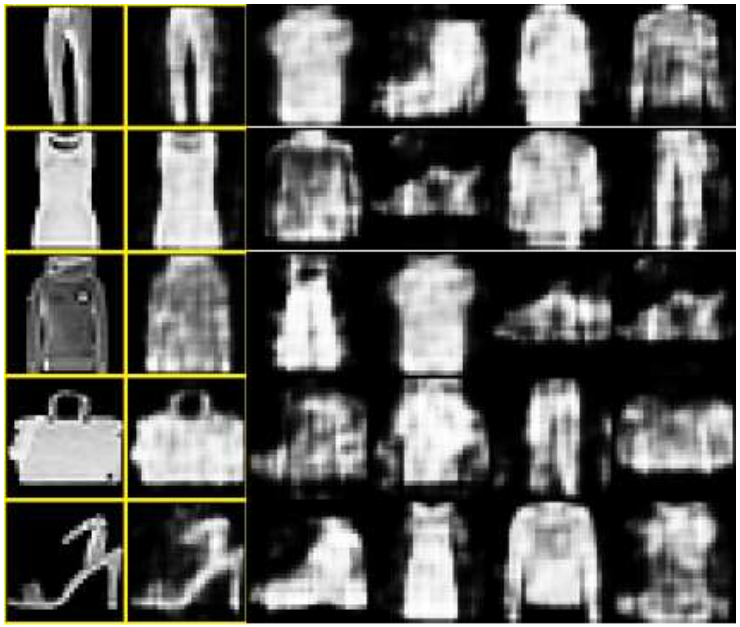
$$\begin{bmatrix} \frac{1}{\eta_1}\Phi_{\boldsymbol{x}}\Phi_{\boldsymbol{x}}^\top & \frac{1}{\eta_1}\Phi_{\boldsymbol{x}}\Phi_{\boldsymbol{y}}^\top \\ \frac{1}{\eta_2}\Phi_{\boldsymbol{y}}\Phi_{\boldsymbol{x}}^\top & \frac{1}{\eta_2}\Phi_{\boldsymbol{y}}\Phi_{\boldsymbol{y}}^\top \end{bmatrix} \begin{bmatrix} U \\ V \end{bmatrix} = \begin{bmatrix} U \\ V \end{bmatrix} \Lambda.$$

Hence, joint feature learning and subspace learning.

# Gen-RKM: examples (1)



MNIST

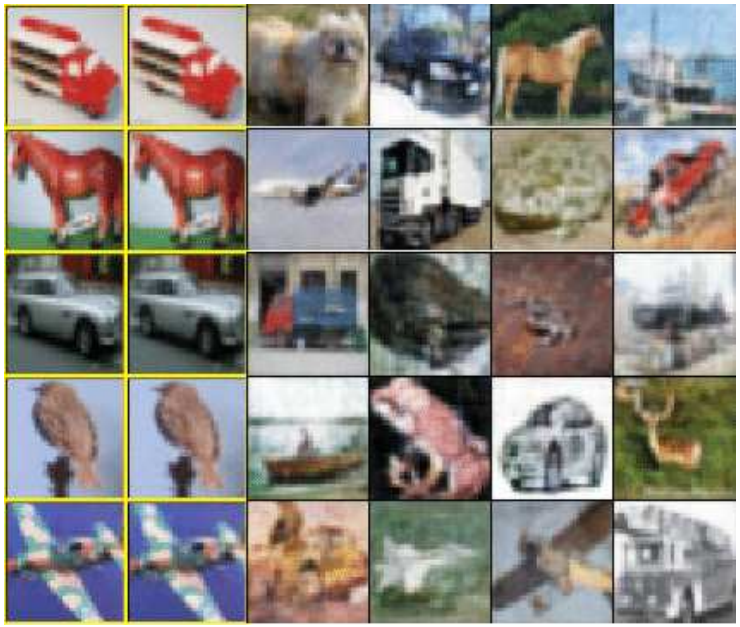


Fashion-MNIST

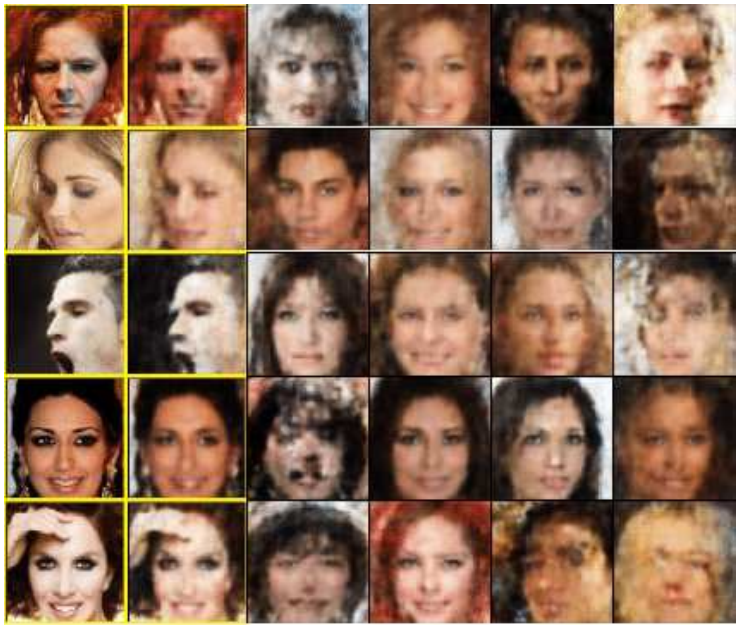
Generated samples from the model using CNN as explicit feature map in the kernel function. The yellow boxes show training examples and the adjacent boxes show the reconstructed samples. The other images (columns 3-6) are generated by random sampling from the fitted distribution over the learned latent variables.

[Pandey, Schreurs & Suykens, 2019, arXiv:1906.08144]

# Gen-RKM: examples (2)



CIFAR-10



CelebA

Generated samples from the model using CNN as explicit feature map in the kernel function. The yellow boxes show training examples and the adjacent boxes show the reconstructed samples. The other images (columns 3-6) are generated by random sampling from the fitted distribution over the learned latent variables.

[Pandey, Schreurs & Suykens, 2019, arXiv:1906.08144]

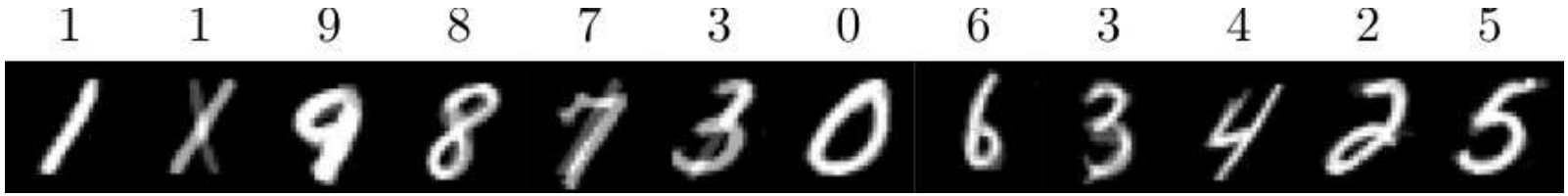
# Gen-RKM: multi-view generation (1)


CelebA

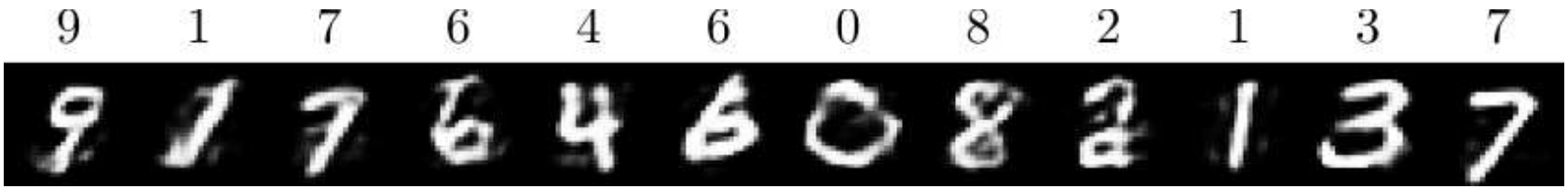
Multi-view generation on CelebA dataset showing images and attributes

[Pandey, Schreurs & Suykens, 2019, arXiv:1906.08144]

# Gen-RKM: multi-view generation (2)




MNIST: Implicit feature maps with Gaussian kernel + generation by kernel-smoother



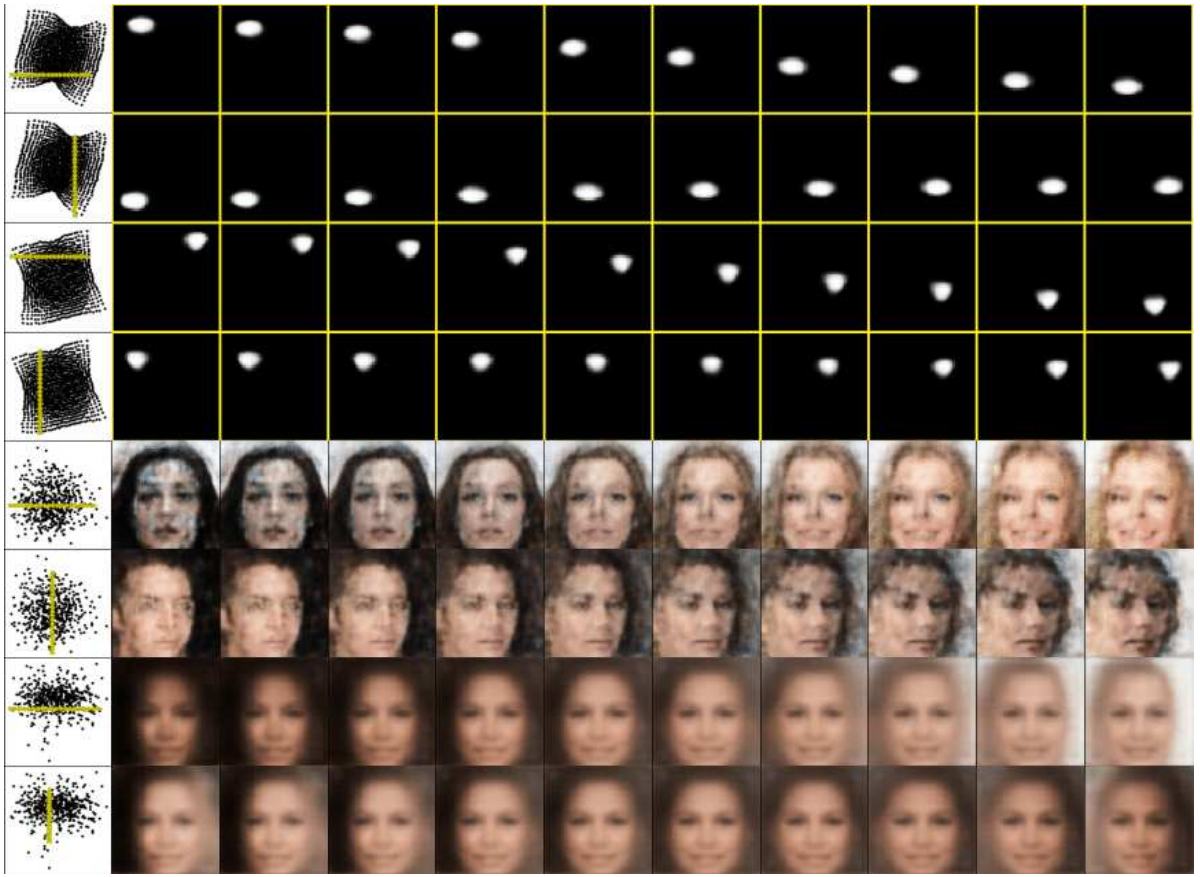

MNIST: Explicit feature maps using Convolutional Neural Networks


CIFAR-10: Explicit feature maps using CNNs + Transposed CNNs

Multi-view Generation (images and labels) using implicit and explicit feature maps

[Pandey, Schreurs & Suykens, 2019, arXiv:1906.08144]

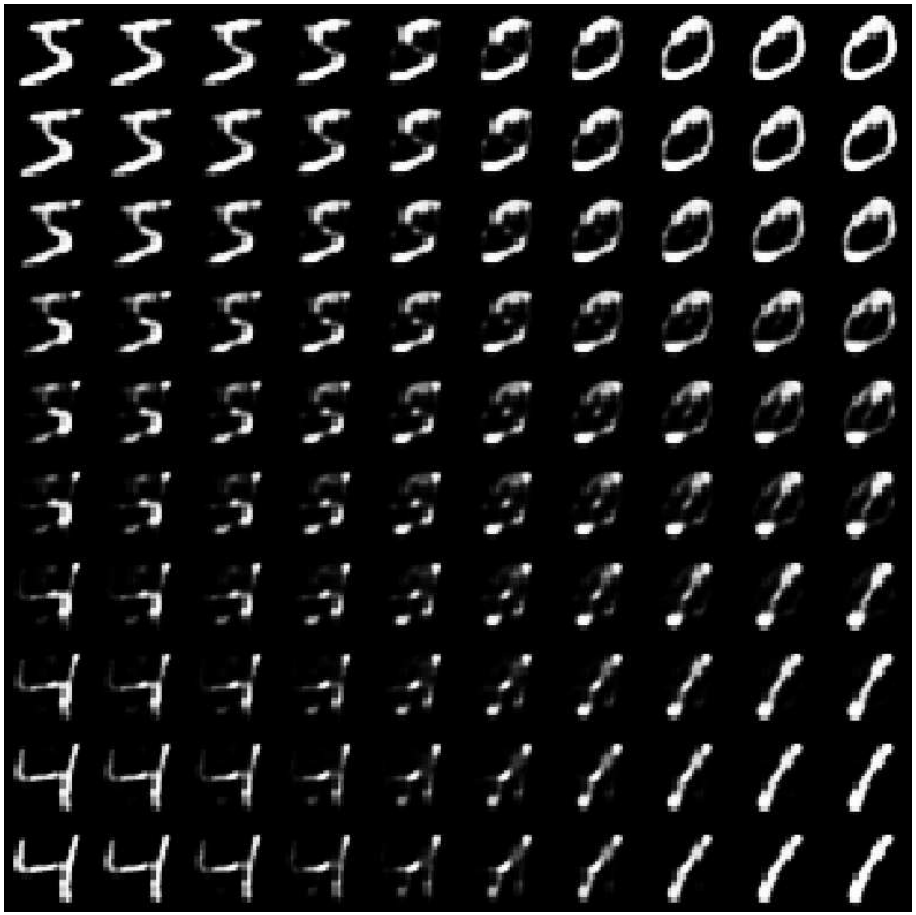
# Gen-RKM: latent space exploration (1)



Exploring the learned **uncorrelated-features** by traversing along the eigenvectors

**Explainability:** changing one single neuron's hidden feature changes the hair color while preserving face structure! [Pandey, Schreurs & Suykens, 2019, arXiv:1906.08144]

# Gen-RKM: latent space exploration (2)



MNIST reconstructed images by bilinear-interpolation in latent space
[Pandey, Schreurs & Suykens, 2019, arXiv:1906.08144]

# Gen-RKM: latent space exploration (3)

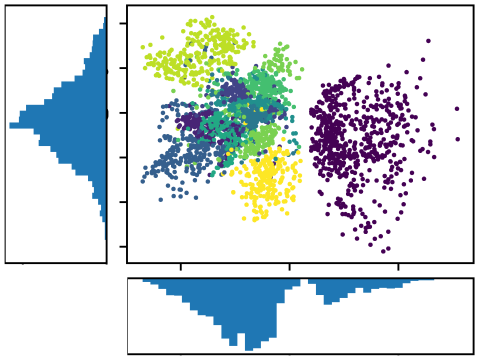
CelebA reconstructed images by bilinear-interpolation in latent space
[Pandey, Schreurs & Suykens, 2019, arXiv:1906.08144]

# Gen-RKM - traversals along principal components

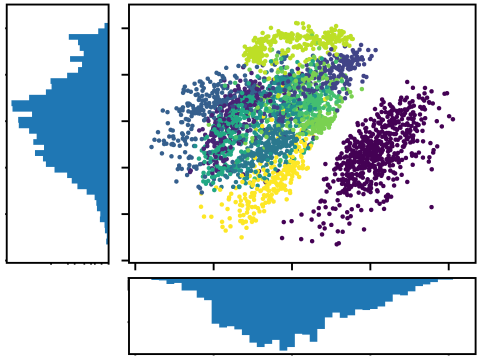

Disentangled Representation Learning and Generation with Manifold Optimization

[Pandey, Fanuel, Schreurs & Suykens, 2019, arXiv:2006.07046]

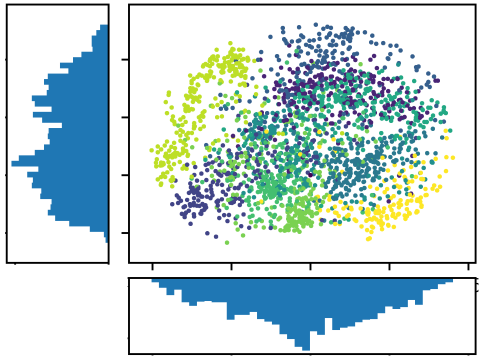
# Robust Gen-RKM



VAE



Gen-RKM



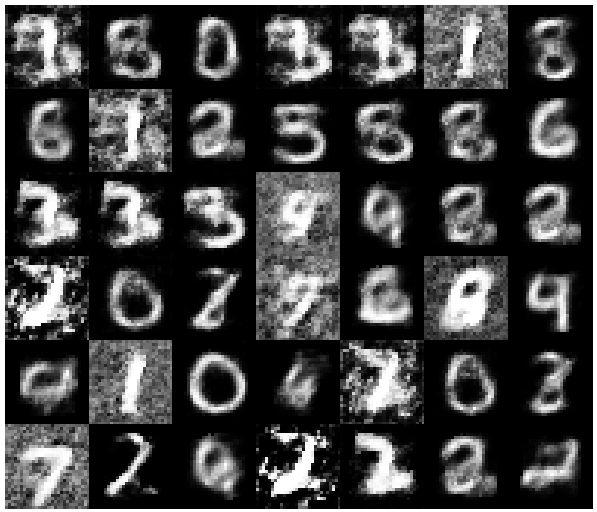
Robust Gen-RKM

- VAE and Gen-RKM: presence of outliers distorts the distribution of the latent variables
- Robust Gen-RKM: down-weighting of the outliers makes close to Gaussian distribution

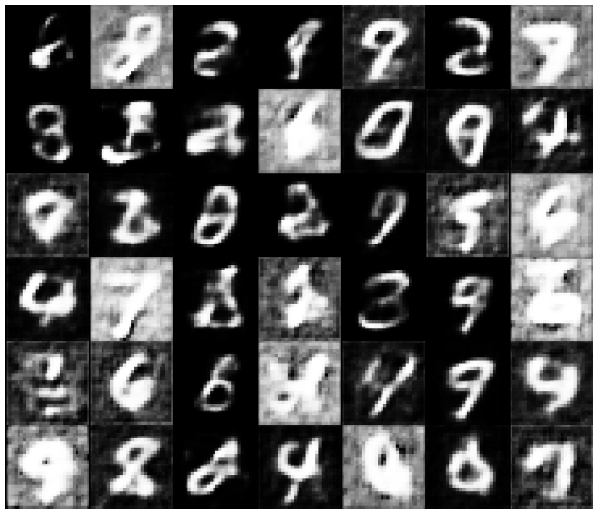
Weighted conjugate feature duality: $\frac{1}{2\lambda}e^T De + \frac{\lambda}{2}h^T D^{-1}h \geq e^T h$

[Pandey, Schreurs & Suykens, 2019, arXiv:2002.01180, LOD 2020]

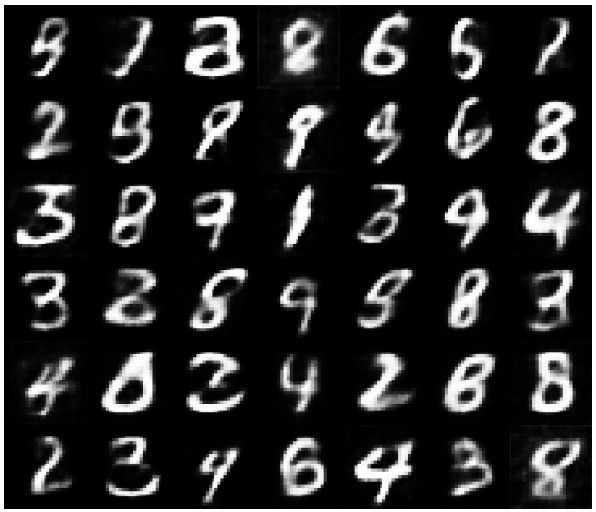
# Robust Gen-RKM - Robust generation



VAE



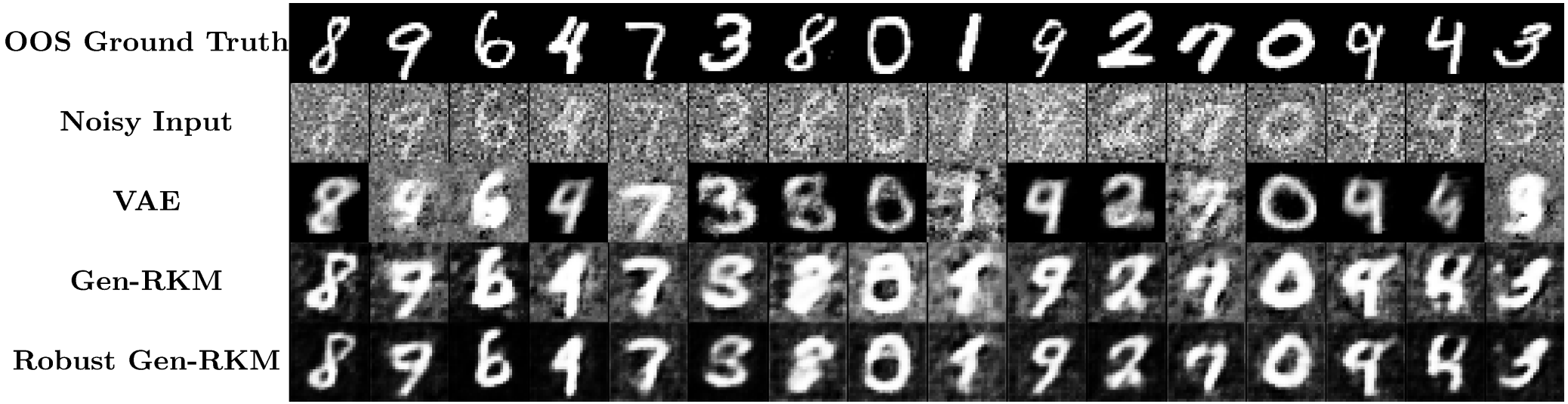
Gen-RKM



Robust Gen-RKM

[Pandey, Schreurs & Suykens, 2019, arXiv:2002.01180, LOD 2020]

# Robust Gen-RKM - Robust denoising




[Pandey, Schreurs & Suykens, 2019, arXiv:2002.01180, LOD 2020]

# RKM references and software

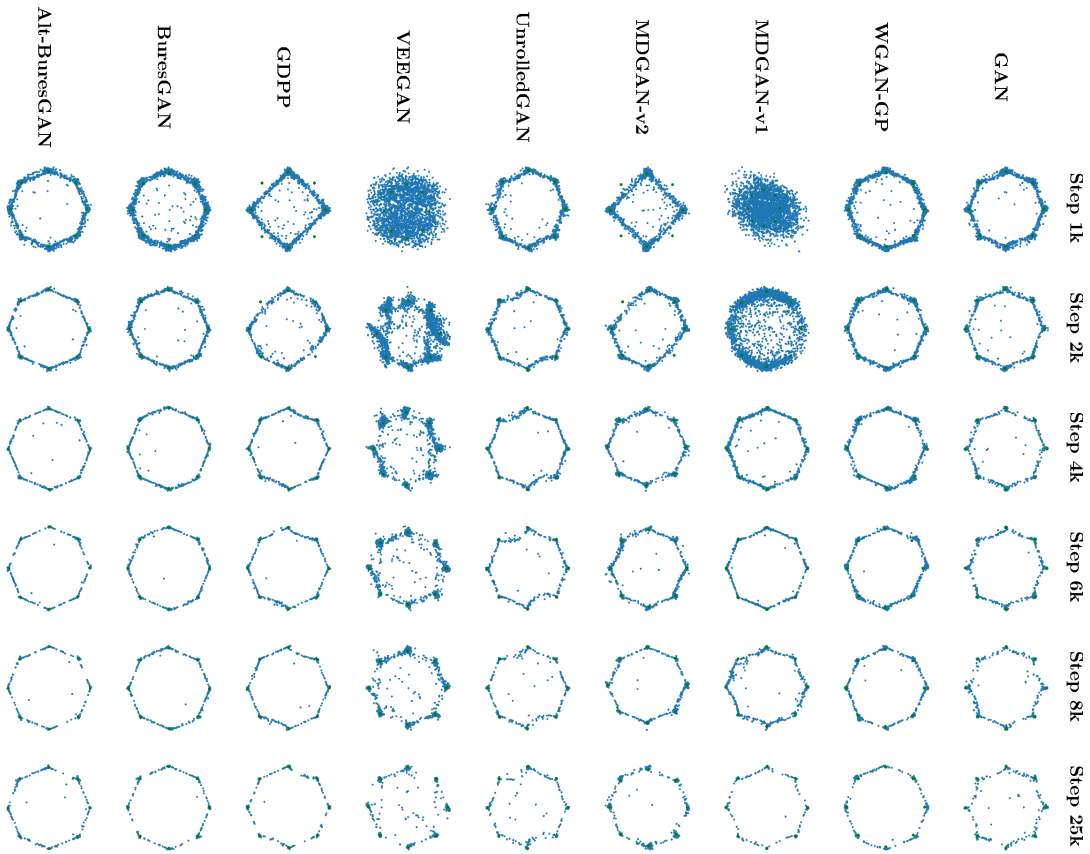

- Suykens J.A.K., "Deep Restricted Kernel Machines using Conjugate Feature Duality", *Neural Computation*, vol. 29, no. 8, pp. 2123-2163, Aug. 2017. https://www.mitpressjournals.org/doi/pdf/10.1162/neco_a_00984
- Houthuys L., Suykens J.A.K., "Tensor Learning in Multi-View Kernel PCA",*International Conference on Artificial Neural Networks 2018 (ICANN 2018)*, Rhodes, Greece, Oct. 2018, pp. 205-215.
- Schreurs J., Suykens J.A.K., "Generative Kernel PCA", *European Symposium on Artificial Neural Networks (ESANN 2018)*, Bruges, Belgium, Apr. 2018, pp. 129-134.
- Pandey A., Schreurs J., Suykens J.A.K., Generative Restricted Kernel Machines, arXiv:1906.08144
- Pandey A., Fanuel M., Schreurs J., Suykens J.A.K., Disentangled Representation Learning and Generation with Manifold Optimization, arXiv:2006.07046
- Pandey A., Schreurs J., Suykens J.A.K., Robust Generative Restricted Kernel Machines using Weighted Conjugate Feature Duality, arXiv:2002.01180, *LOD 2020*.


**Software:** see https://www.esat.kuleuven.be/stadius/E/software.php

# Future challenges

- efficient algorithms and implementations for large data
- extension to other loss functions and regularization schemes
- multimodal data, tensor models, coupling schemes
- models for deep clustering and semi-supervised learning
- choice kernel functions, invariances and symmetry properties
- deep generative models
- optimal transport
- synergies between neural networks, deep learning and kernel machines

# BuresGAN (1)




Bures Metric for Taming Mode Collapse in Generative Adversarial Networks

Computation of Bures distance in either *feature space or kernel space*

[De Meulemeester H., Schreurs J., Fanuel M., De Moor B., Suykens J.A.K., arXiv:2006.09096]

# BuresGAN (2)

Stacked MNIST

CIFAR-10

CIFAR-100

Generated samples from a trained BuresGAN: high-quality images and preserving diversity.

[De Meulemeester H., Schreurs J., Fanuel M., De Moor B., Suykens J.A.K., arXiv:2006.09096]

# Conclusions

- function estimation: **parametric versus kernel-based**
- **primal and dual** model representations
- **neural network interpretations** in primal and dual
- RKM: **new connections** between RBM, kernel PCA and LS-SVM
- **deep kernel machines**
- **generative models**
- **explainability:** latent space exploration, understanding the role of each individual neuron

# Acknowledgements (1)


- Current and former co-workers at ESAT-STADIUS:

  C. Alzate, Y. Chen, J. De Brabanter, K. De Brabanter, B. De Cooman, L. De Lathauwer, H. De Meulemeester, B. De Moor, H. De Plaen, Ph. Dreesen, M. Espinoza, T. Falck, M. Fanuel, Y. Feng, B. Gauthier, X. Huang, L. Houthuys, V. Jumutc, Z. Karevan, R. Langone, F. Liu, R. Mall, S. Mehrkanoon, G. Nisol, M. Orchel, A. Pandey, P. Patrinos, K. Pelckmans, S. RoyChowdhury, S. Salzo, J. Schreurs, M. Signoretto, Q. Tao, F. Tonin, J. Vandewalle, T. Van Gestel, S. Van Huffel, C. Varon, Y. Yang, and others

- Many other people for joint work, discussions, invitations, organizations

- Support from ERC AdG E-DUALITY, ERC AdG A-DATADRIVE-B, KU Leuven, OPTEC, IUAP DYSCO, FWO projects, IWT, Flanders AI

# Acknowledgements (2)


KATHOLIEKE UNIVERSITEIT
LEUVEN

FWO
VLAANDEREN

# Acknowledgements (3)


NEW: ERC Advanced Grant E-DUALITY

Exploring duality for future data-driven modelling

# Thank you