Neural Networks and Kernel Machines: the best of both worlds

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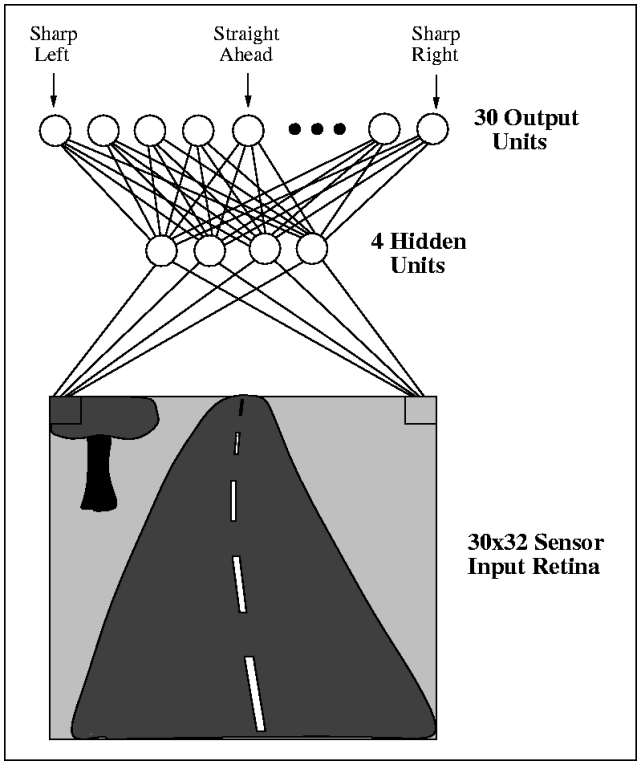
Overview

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

Introduction

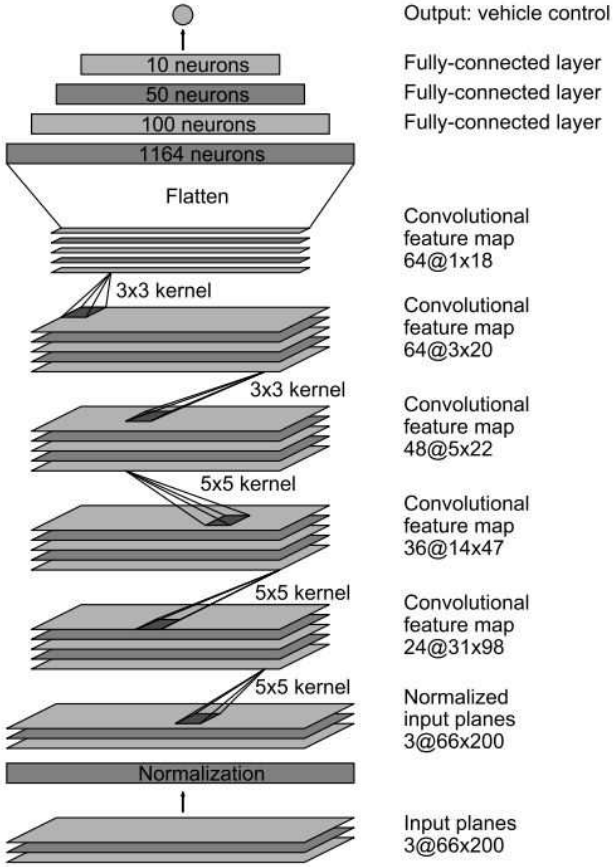
Self-driving cars and neural networks

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



(27 million connections)

Waymo / Google Self-Driving Car

Tesla Autopilot

Uber

nuTonomy

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

Convolutional neural networks

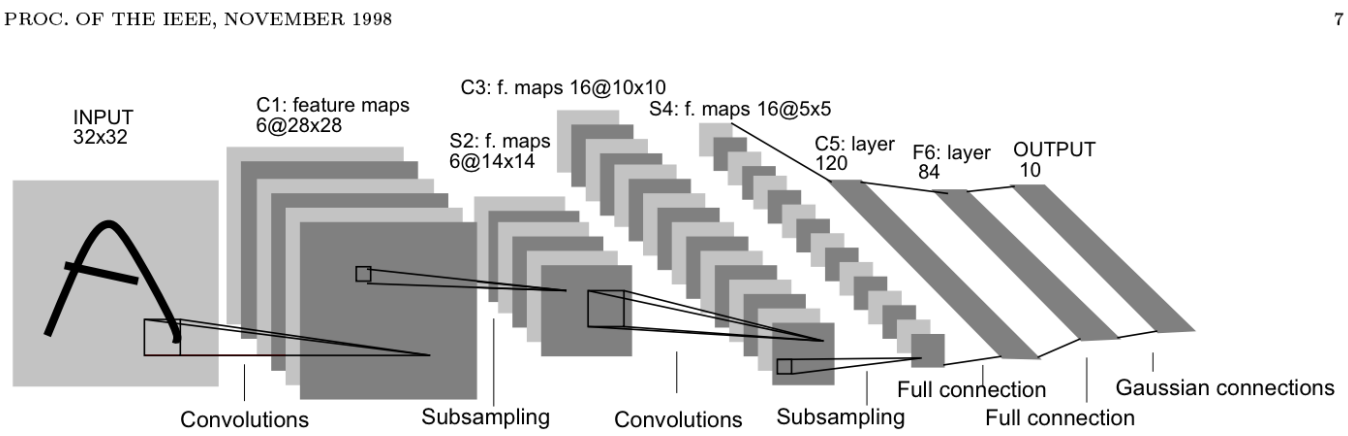


Fig. 2. Architecture of LeNet-5, a Convolutional Neural Network, here for digits recognition. Each plane is a feature map, i.e. a set of units whose weights are constrained to be identical.

[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

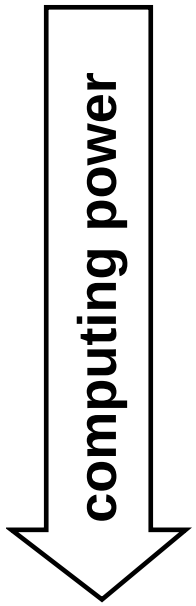
Historical context

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

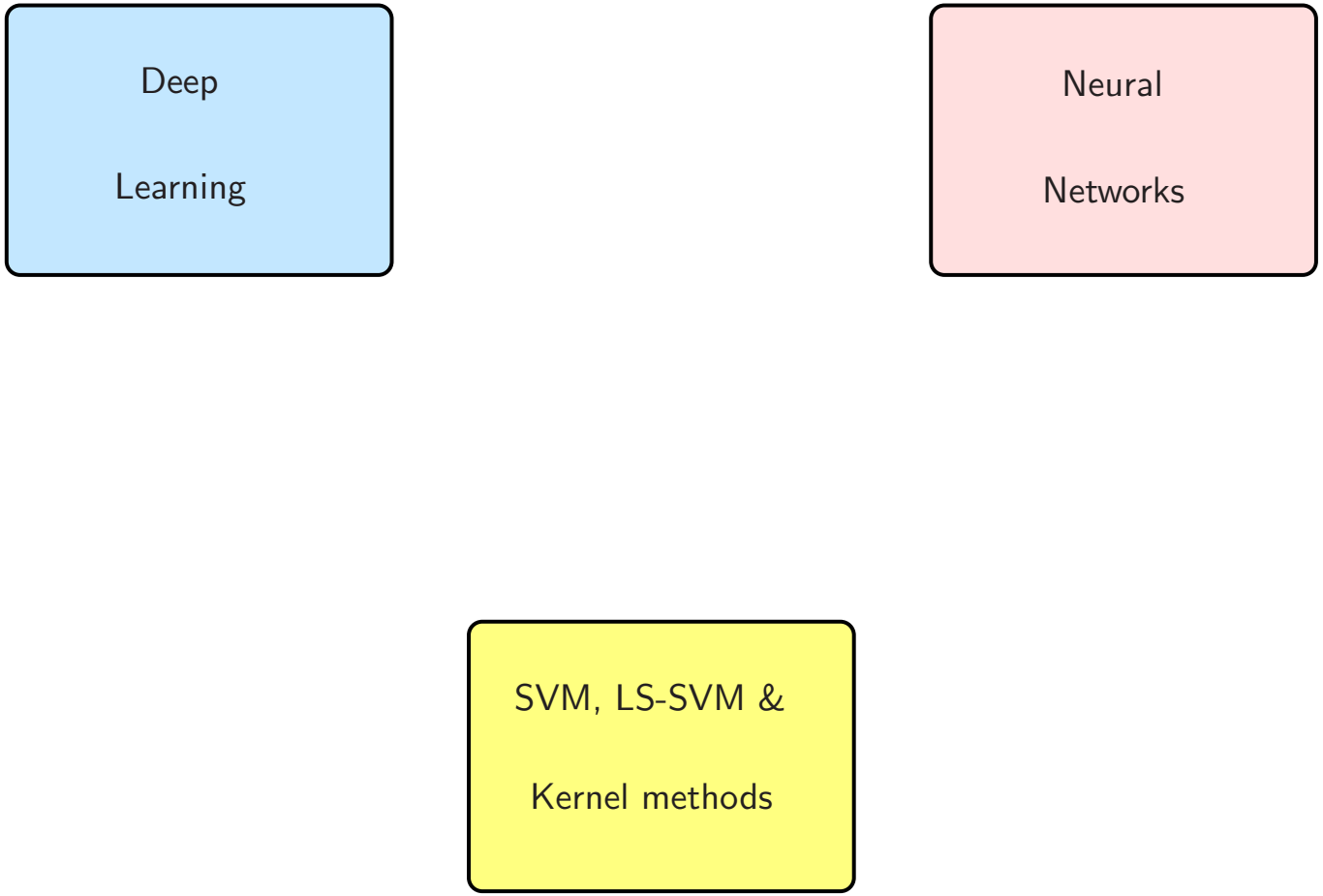
1986 Rumelhart et al.: error backpropagating neural networks
→ *booming of neural network universal approximators*

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

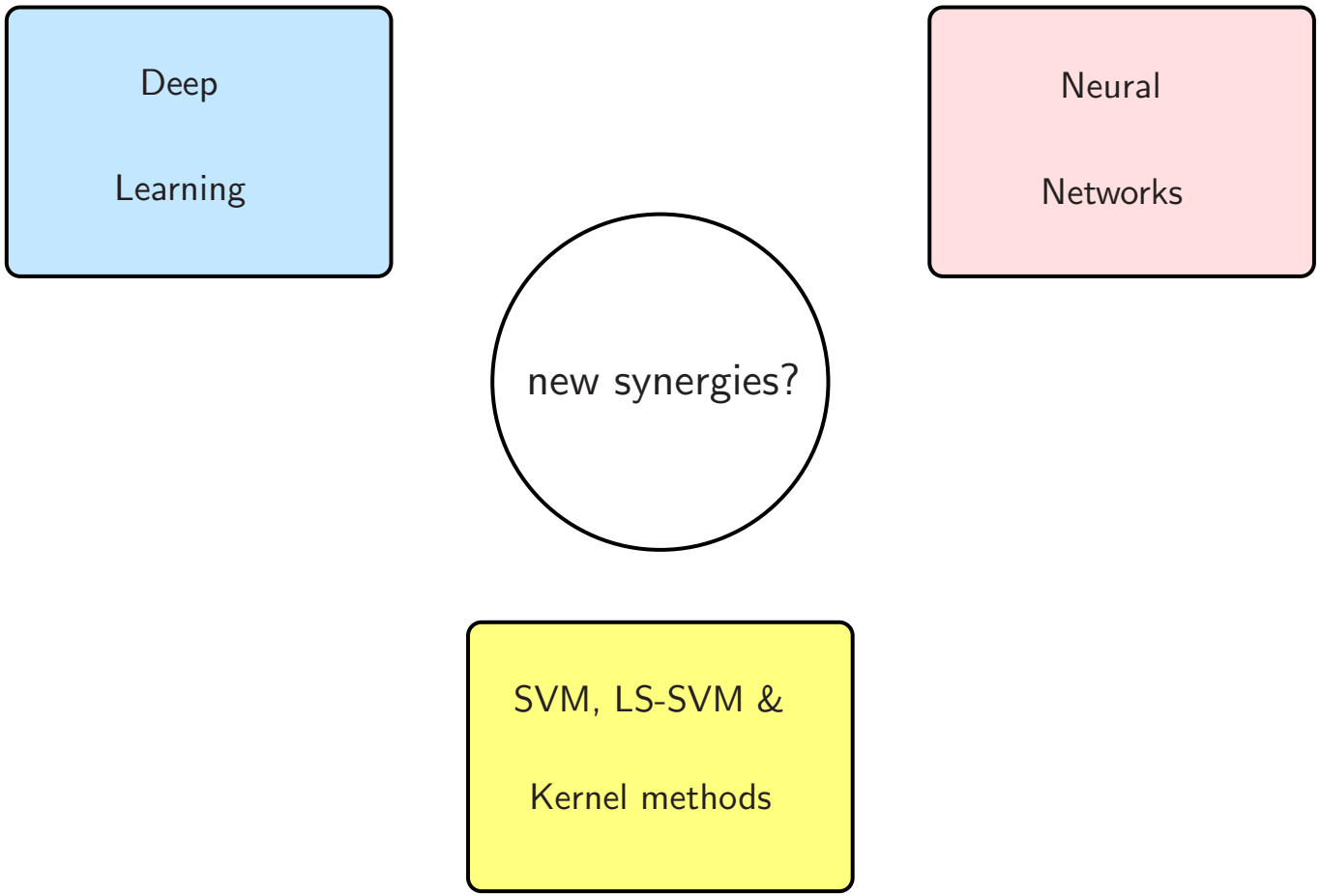
1998 LeCun et al.: convolutional neural networks
2006 Hinton et al.: deep belief networks
2010 Bengio et al.: stacked autoencoders
→ *booming of deep neural networks*



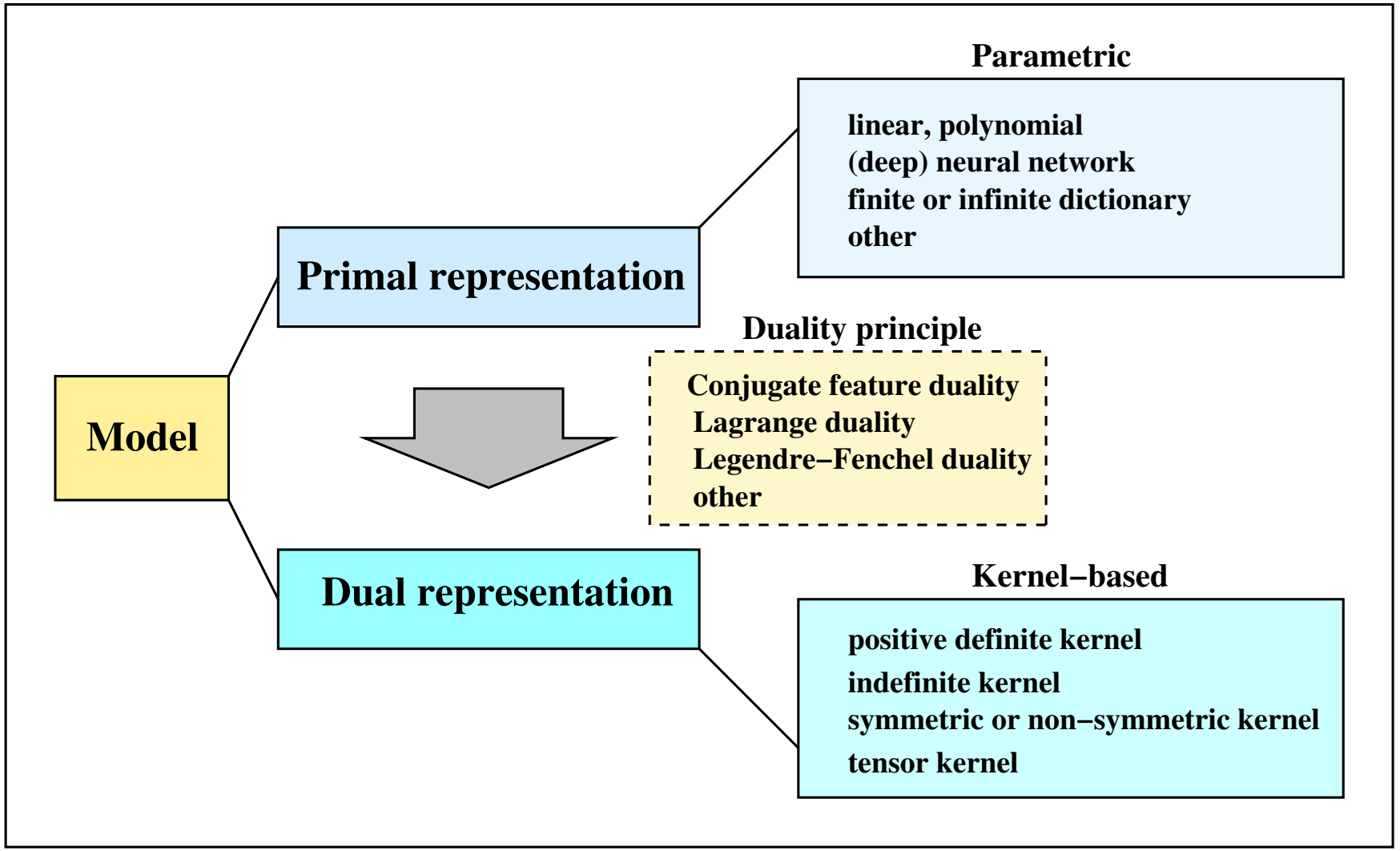
Different paradigms



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:

$$\begin{aligned} \min_{w,b,e} \quad & \tfrac{1}{2} w^T w + \gamma \tfrac{1}{2} \textstyle\sum_i e_i^2 \\ \text{subject to} \quad & e_i = y_i - w^T x_i - b, \quad i = 1, ..., N \end{aligned}$$

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 α, 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?

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training set $\{(x_i, y_i)\}_{i=1}^N$

Model

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

$$(D): \quad \hat{y} = \sum_i \alpha_i \, x_i^T x + b, \qquad \alpha \in \mathbb{R}^N$$

Linear model: solving in primal or dual?

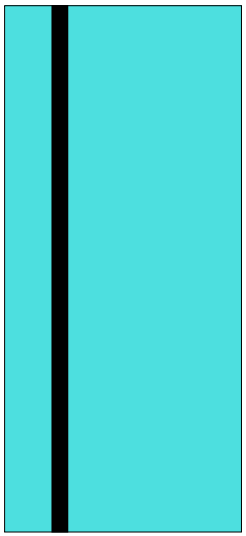
few inputs, many data points: $d \ll N$

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 φ **or** positive definite K):

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

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

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

Least Squares Support Vector Machines: "core models"

- Regression

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

- Classification

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

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

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

- Kernel canonical correlation analysis/partial least squares

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

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

Sparsity: through regularization or loss function

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

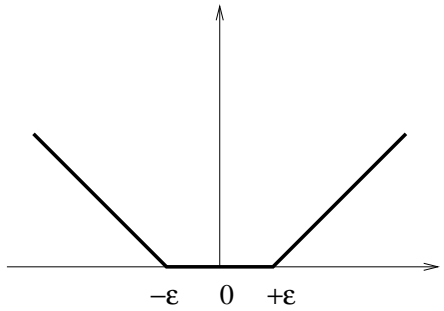
$$\min \sum_j |w_j| + \gamma \sum_i e_i^2$$

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

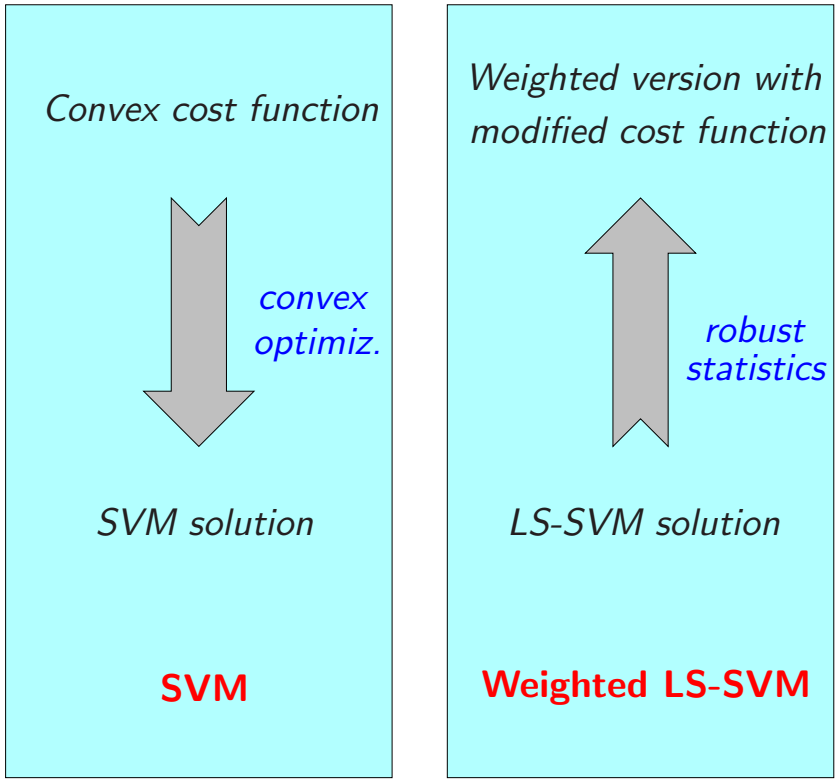
- through loss function: model $\hat{y} = \sum_i \alpha_i K(x, x_i) + b$

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

$\Rightarrow$ sparse α (e.g. SVM)

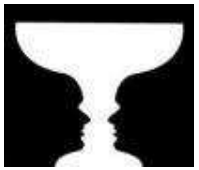


Weighted versions and robustness

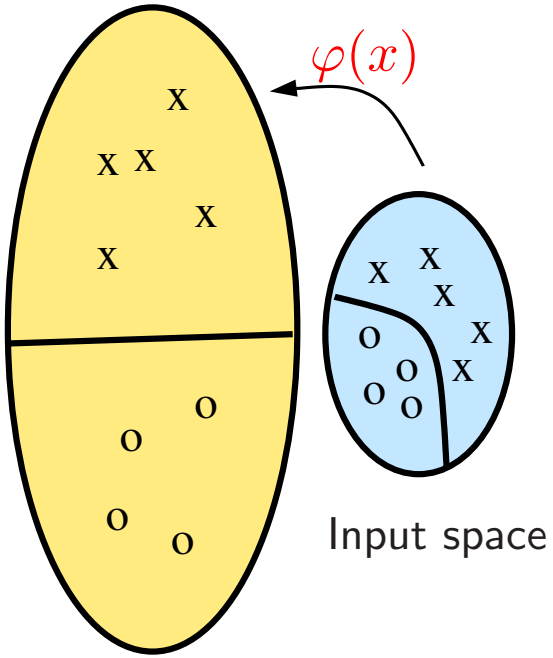


- Weighted LS-SVM: $\min_{w,b,e} \frac{1}{2} w^T w + \gamma \frac{1}{2} \sum_{i=1}^{N} v_i e_i^2 \ \text{s.t.} \ y_i = w^T \varphi(x_i) + b + e_i, \forall i$

  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]



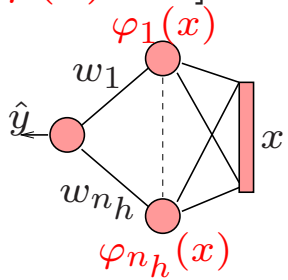
SVMs and neural networks



Primal space

Parametric

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



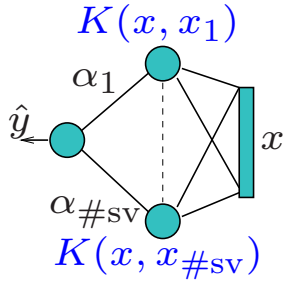
Parametric

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

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 $K(x, z) = \exp(-\|x - z\|_2^2/\sigma^2)$
- χ^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]

Data fusion with kernels (1)

- **Multiple kernel learning** in SVM:
  Comparison of different norms in combining data sources:

$$\begin{aligned} \min_{\alpha} \max_{\theta} \quad & \alpha^T (\sum_{j=1}^{p} \theta_j Q_j) \alpha \\ \text{subject to} \quad & Q_j \succeq 0, j = 1, ..., p \\ & \alpha \in \mathcal{C} \\ & \theta_j \geq 0, j = 1, ..., p \\ & \|\theta\|_m = 1 \end{aligned}$$

  including the cases $m = 1, 2, \infty$.

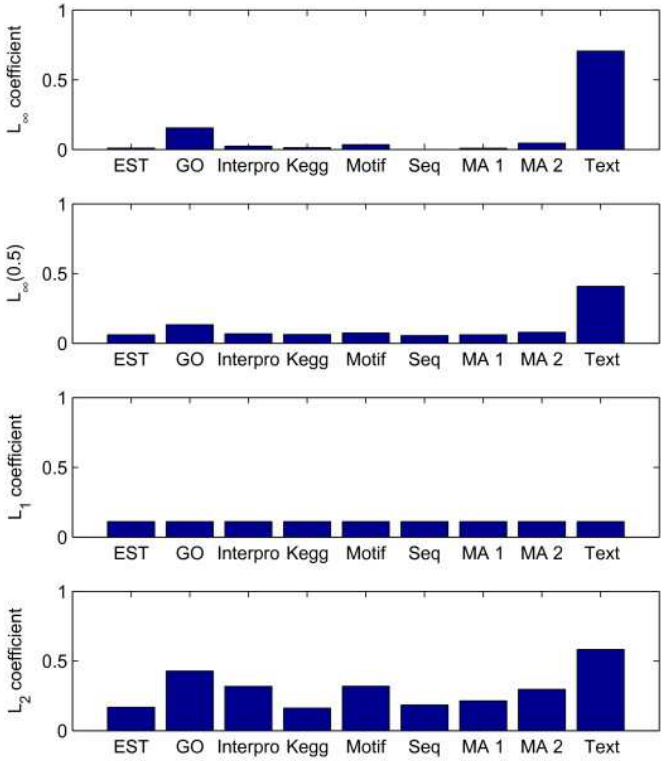
- **Non-sparse** 2-norm combination typically yields better results

  [Yu S., Falck T., Daemen A., Tranchevent L., Suykens J., De Moor B., Moreau Y., BMC Bioinformatics, 2010]

Data fusion with kernels (2)

- Experiment: disease gene prioritization
- Combined kernels from 9 heterogeneous genomic sources
- Average coefficients of 20 repetitions
- 3 most important data-sources ranked by L_∞: Text, GO, Motif
- L_2 method shows the same ranking on the 3 best data sources
- L_2 method gives a more refined ranking

(notation: L_n with $n = \frac{m}{m-1}$)



[Yu S., Falck T., Daemen A., Tranchevent L., Suykens J., De Moor B., Moreau Y., BMC Bioinformatics, 2010]

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 ϵ-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]

Banach spaces: tensor kernels

- Regression problem:

$$\begin{array}{cc} \min\limits_{(w,b,e)\in \ell^r(\mathbb{K})\times\mathbb{R}\times\mathbb{R}^N} & \rho(\|w\|_r) + \frac{\gamma}{N}\sum_{i=1}^N L(e_i) \\ \text{subject to} & y_i = \langle w, \varphi(x_i)\rangle + b + e_i\,, \forall i = 1, ..., N \end{array}$$

  with $r = \frac{m}{m-1}$ for even $m \geq 2$, ρ convex and even.

  For m large this approaches ℓ^1 regularization.

- **Tensor-kernel representation**

$$\hat{y} = \langle w, \varphi(x)\rangle_{r,r^*} + b = \frac{1}{N^{m-1}} \sum_{i_1,\ldots,i_{m-1}=1}^{N} u_{i_1}\ldots u_{i_{m-1}} K(x_{i_1}, \ldots, x_{i_{m-1}}, x) + b$$

[Salzo & Suykens, arXiv 1603.05876 AA2020; Salzo, Suykens, Rosasco, AISTATS 2018]

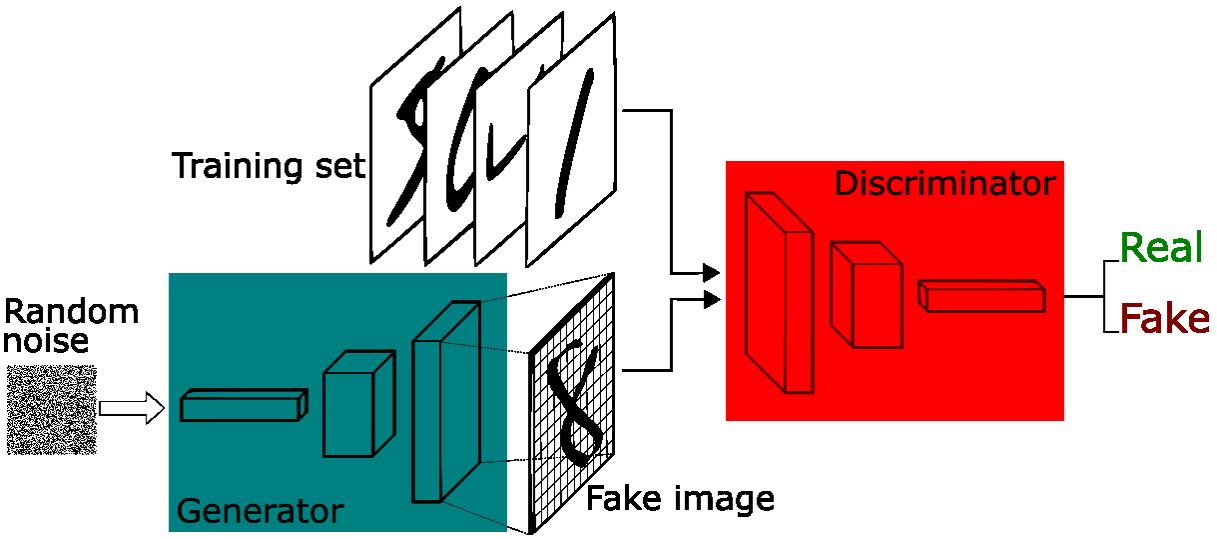
related: RKBS [Zhang 2013; Fasshauer et al. 2015]

Generative models

Generative Adversarial Network (GAN)

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

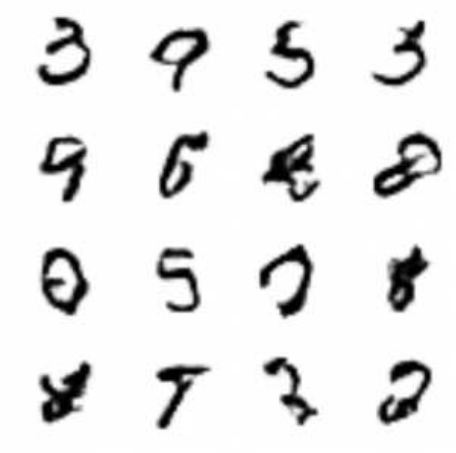
(Generator) generate fake output examples from random noise
(Discriminator) discriminate between fake examples and real examples.



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

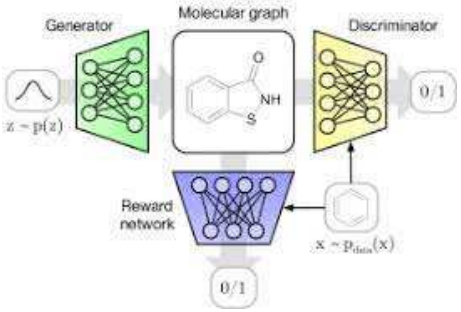
GAN: examples

- GAN generated examples on MNIST:

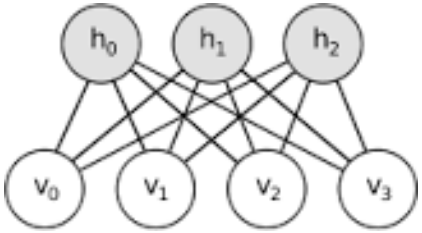


source: https://www.kdnuggets.com/2016/07/mnist-generative-adversarial-model-keras.html

- **Drug development: designing molecules**, e.g.
  MolGAN [De Cao & Kipf, 2018]
  Mol-CycleGAN [Maziarka1 et al., 2020]
  L-MolGAN [Tsujimoto et al., 2021]



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]

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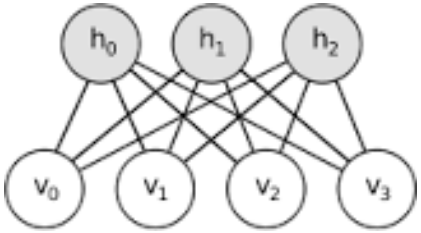

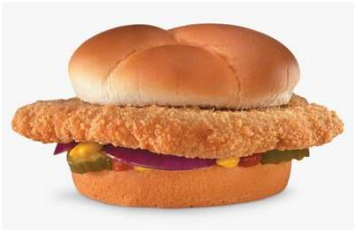

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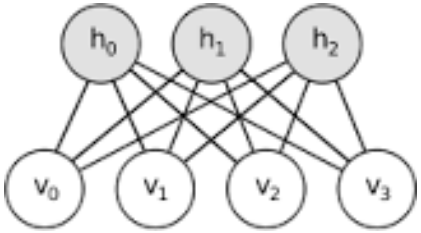

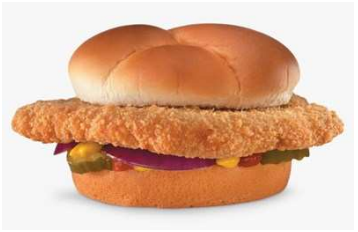

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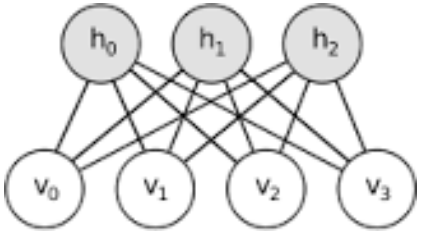
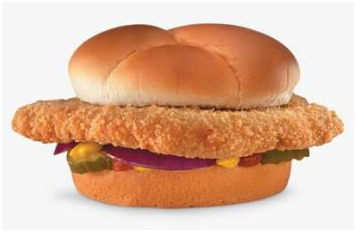
Restricted Boltzmann Machines (RBM)





- 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:

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

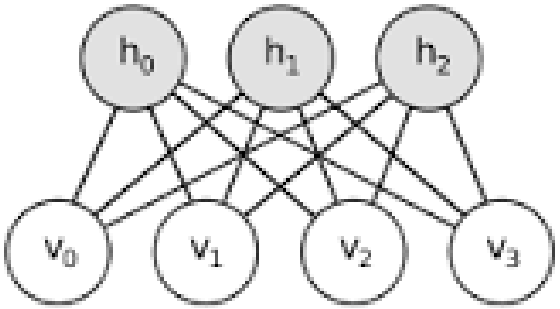
Joint distribution:

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

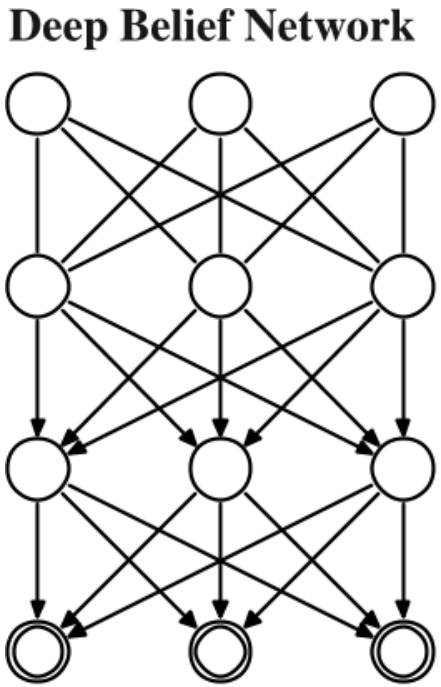
with partition function $Z(\theta) = \sum_v \sum_h \exp(-E(v,h;\theta))$

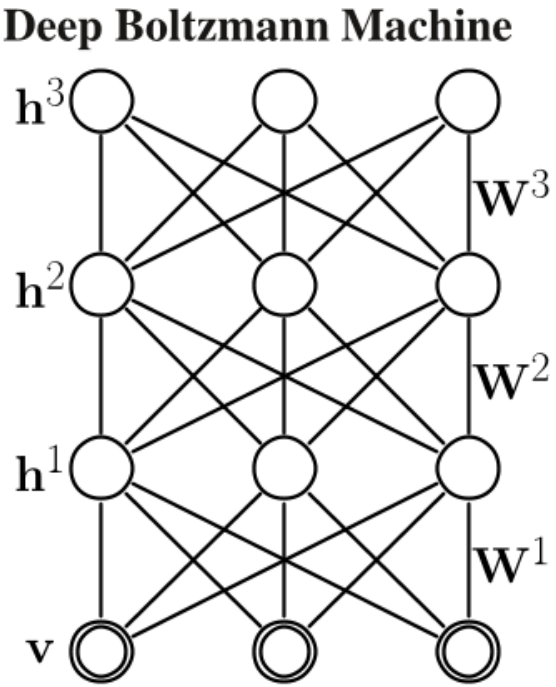
[Hinton, Osindero, Teh, Neural Computation 2006]

RBM and deep learning



$p(v, h)$



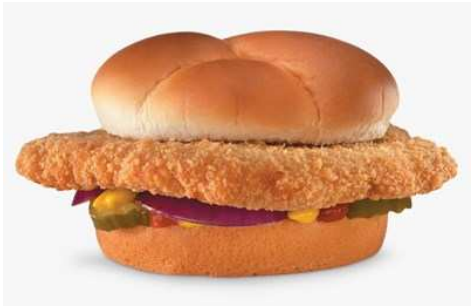


$p(v, h^1, h^2, h^3, ...)$

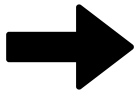
[Hinton et al., 2006; Salakhutdinov, 2015]

in other words ...

"sandwich"



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

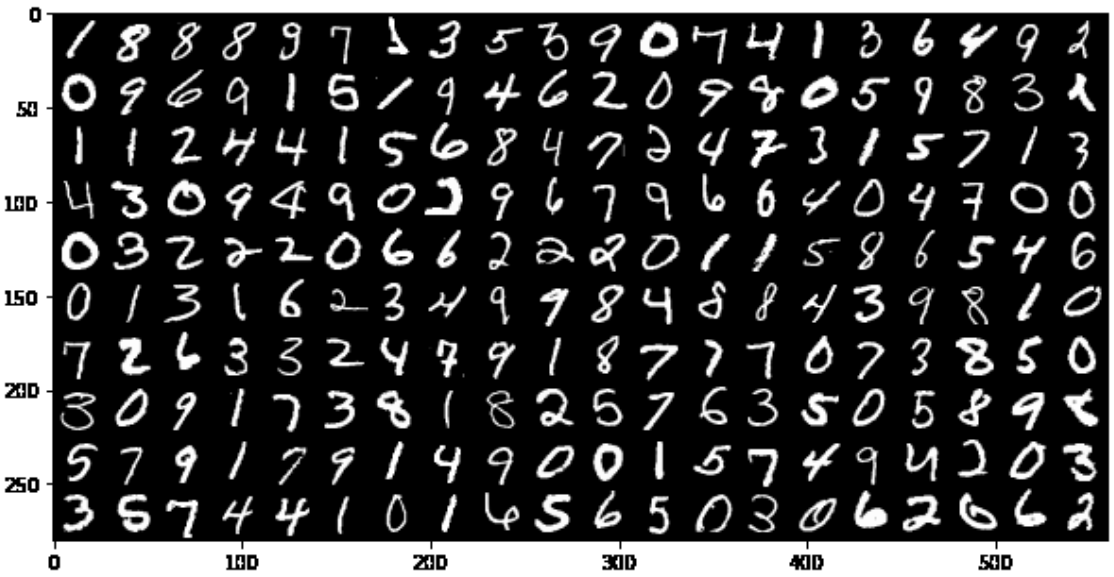


"deep sandwich"

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

RBM: example on MNIST

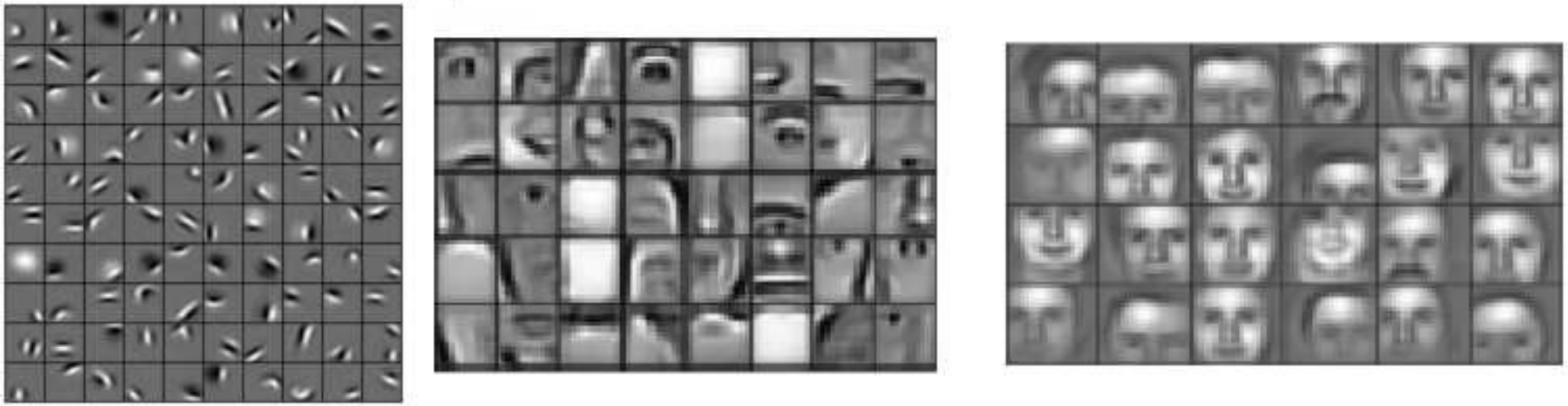
MNIST training data:



Generating new images:

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

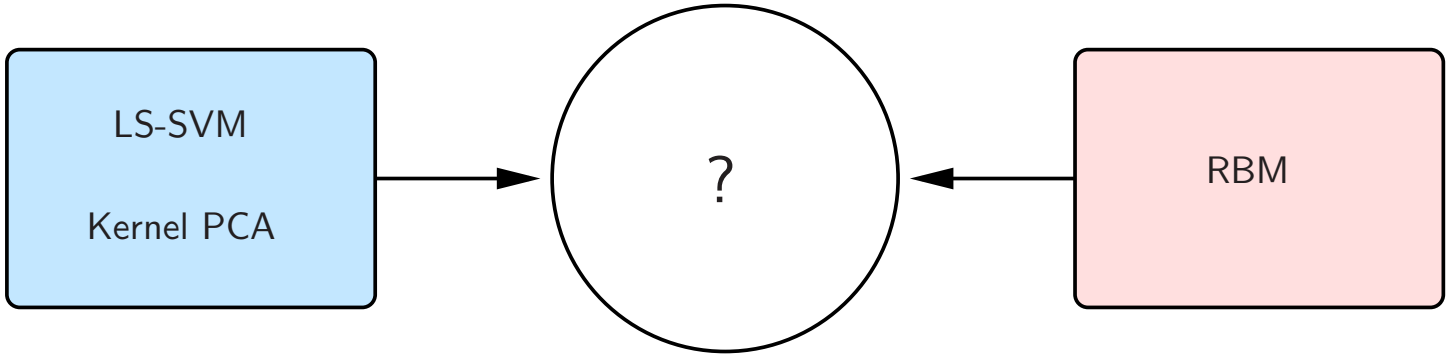
Convolutional Deep Belief Networks



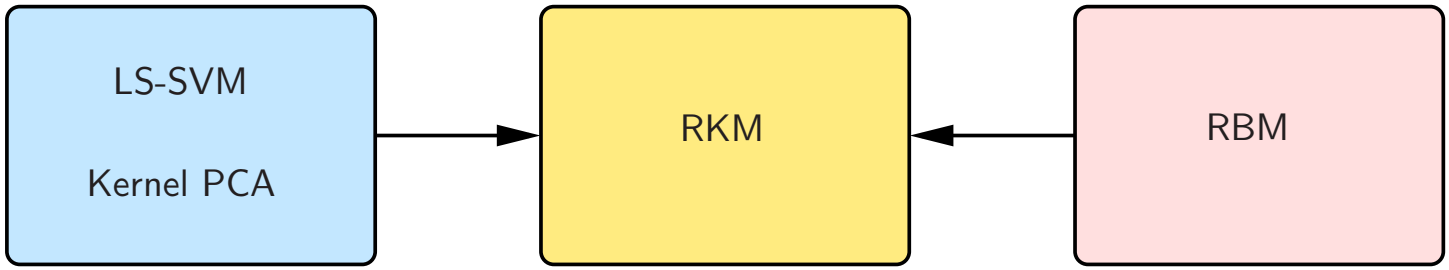
Unsupervised Learning of Hierarchical Representations with Convolutional Deep Belief Networks [Lee et al. 2011]

Restricted kernel machines

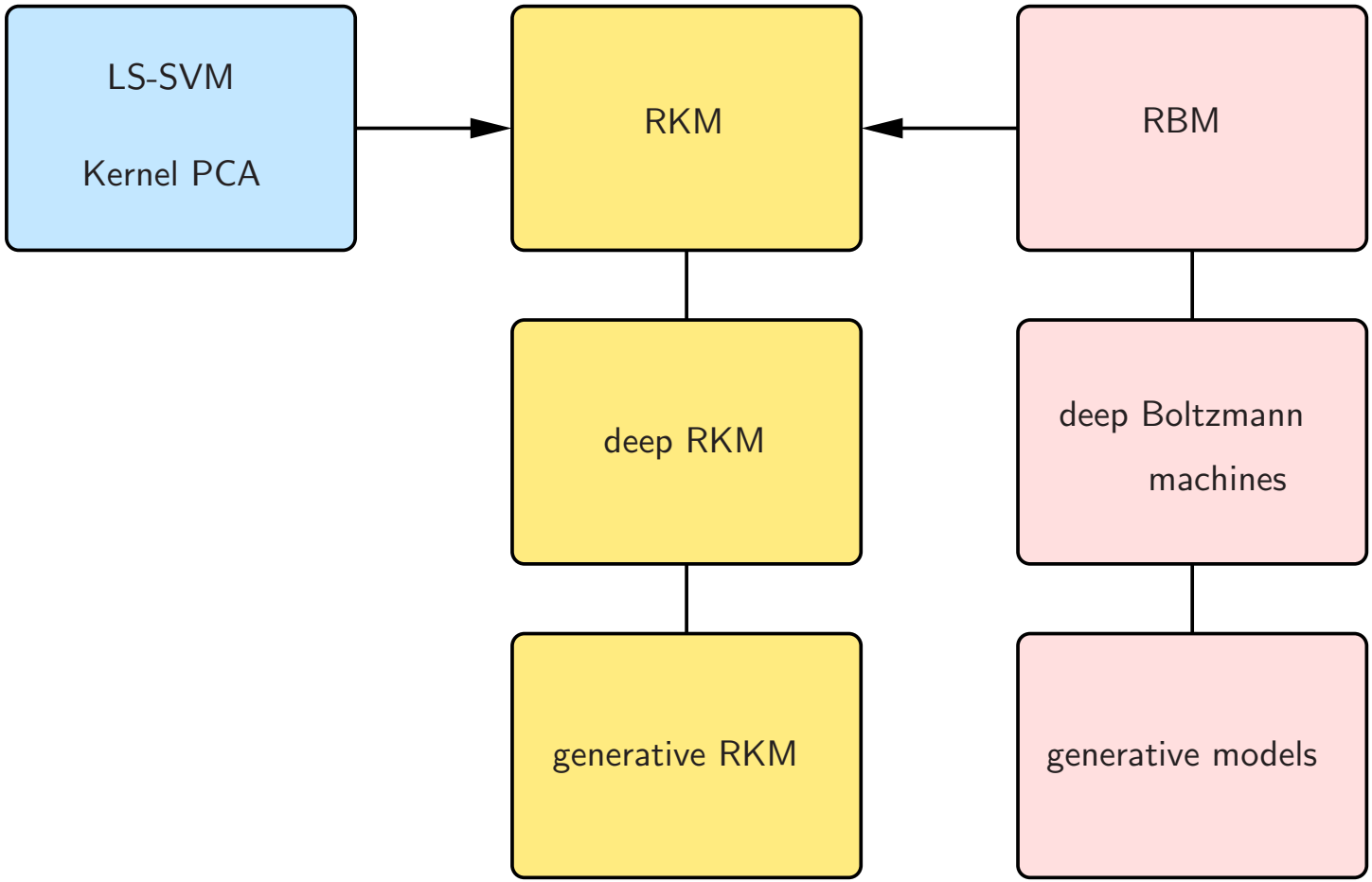
New connections



New connections



New connections



Restricted Kernel Machines (RKM)

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

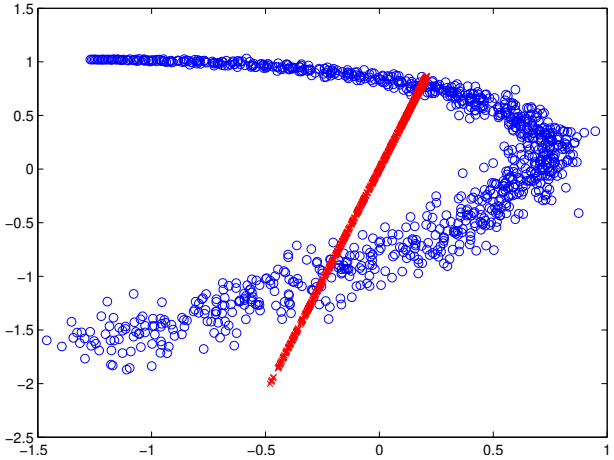
- Restricted Kernel Machine (**RKM**) representations for
  - LS-SVM regression/classification
  - Kernel PCA
  - Matrix SVD
  - Parzen-type models
  - other

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

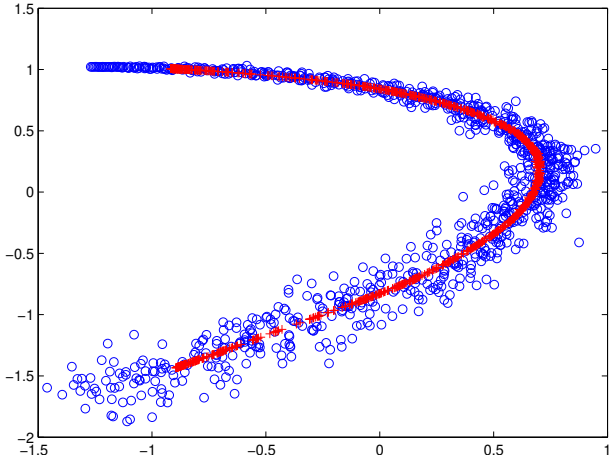
- Deep Restricted Kernel Machines (Deep RKM)

[Suykens, Neural Computation, 2017]

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 (Lagrange duality) 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]

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:

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

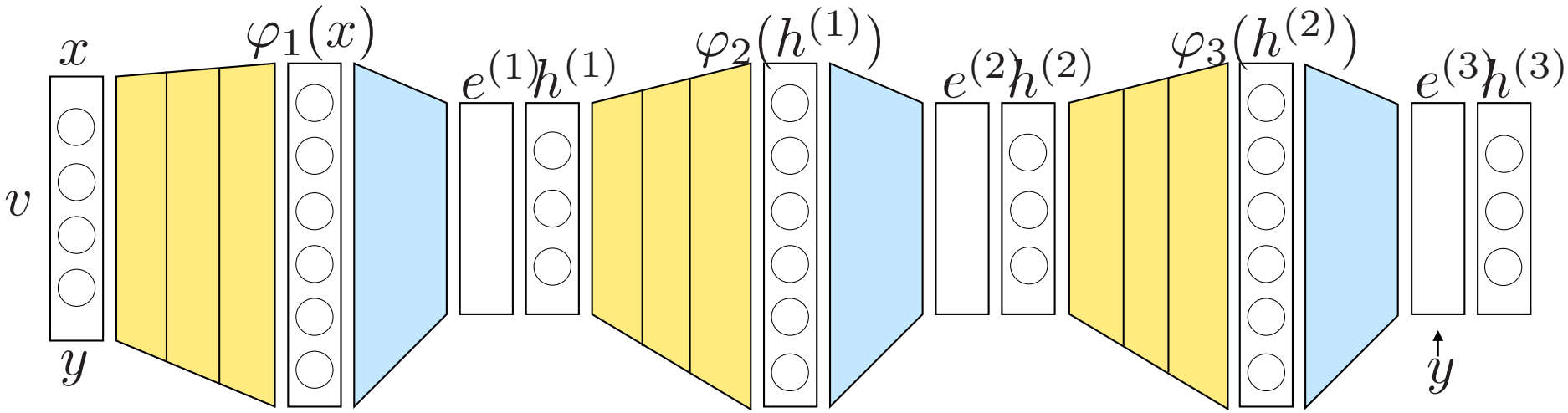
where $H = [h_1 ... h_N] \in \mathbb{R}^{s \times N}$ and $\Lambda = \mathrm{diag}\{\lambda_1, ..., \lambda_s\}$ with $s \leq N$

- 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



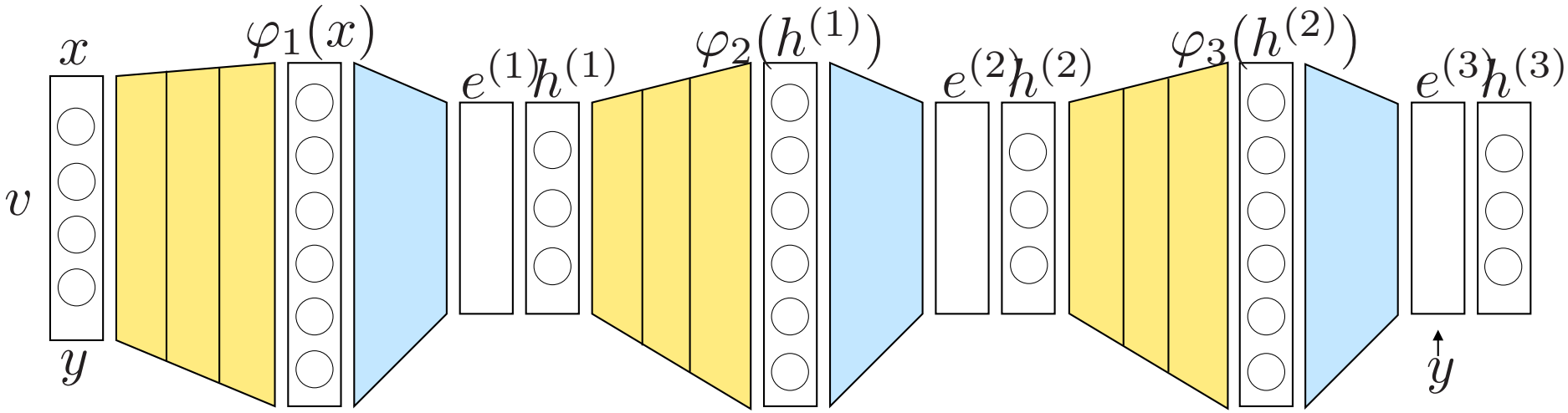
Deep RKM: KPCA + KPCA + LSSVM [Suykens, 2017]

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 ...



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

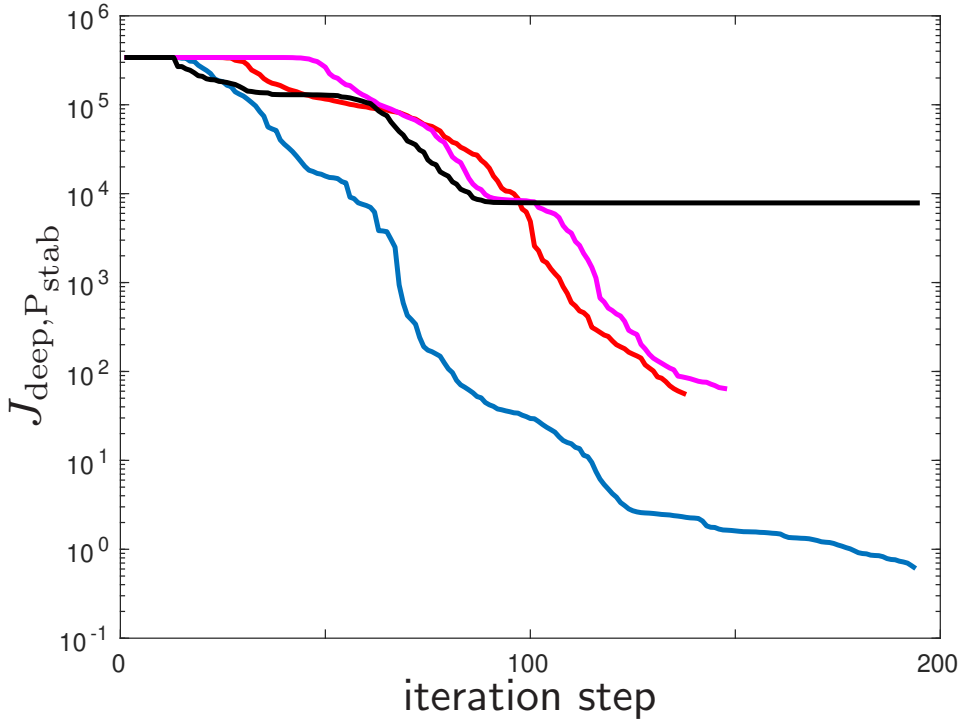
Primal and dual model representations

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

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_{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)

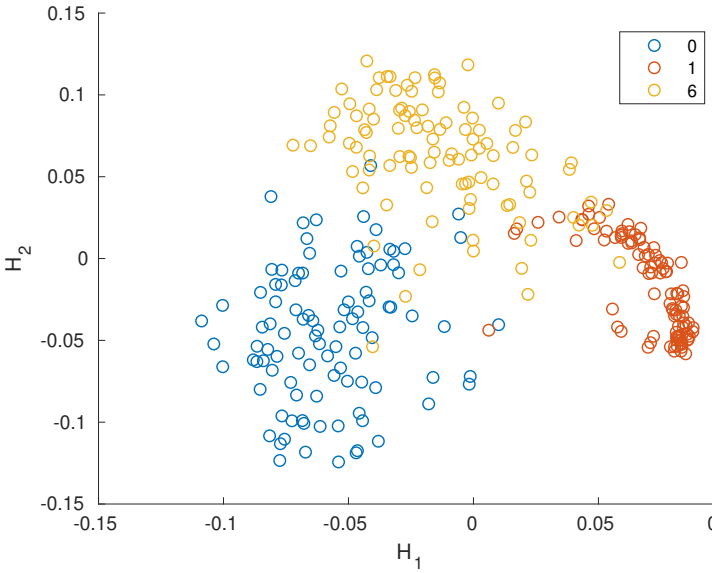
$$\bar{J}(v, h, W) = -v^{\mathrm{T}} W h + \frac{\lambda}{2} h^{\mathrm{T}} h + \frac{1}{2} v^{\mathrm{T}} v + \frac{\eta}{2} \mathrm{Tr}(W^{\mathrm{T}} W)$$

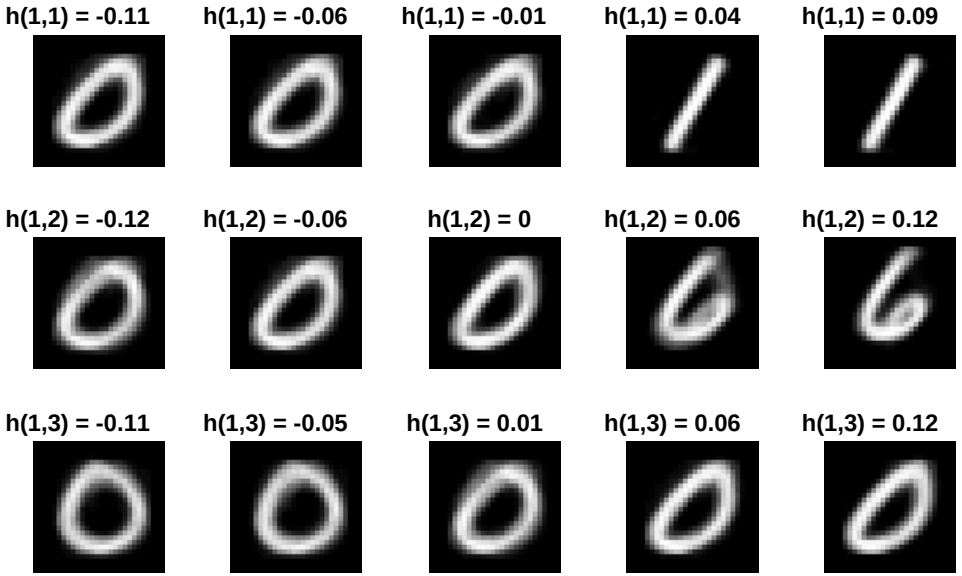
Training: clamp v $\rightarrow$ $\bar{J}_{\mathrm{train}}(h, W)$
Generating: clamp h, W $\rightarrow$ $\bar{J}_{\mathrm{gen}}(v)$

[Schreurs & Suykens, ESANN 2018]

Explainable AI: latent space exploration

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

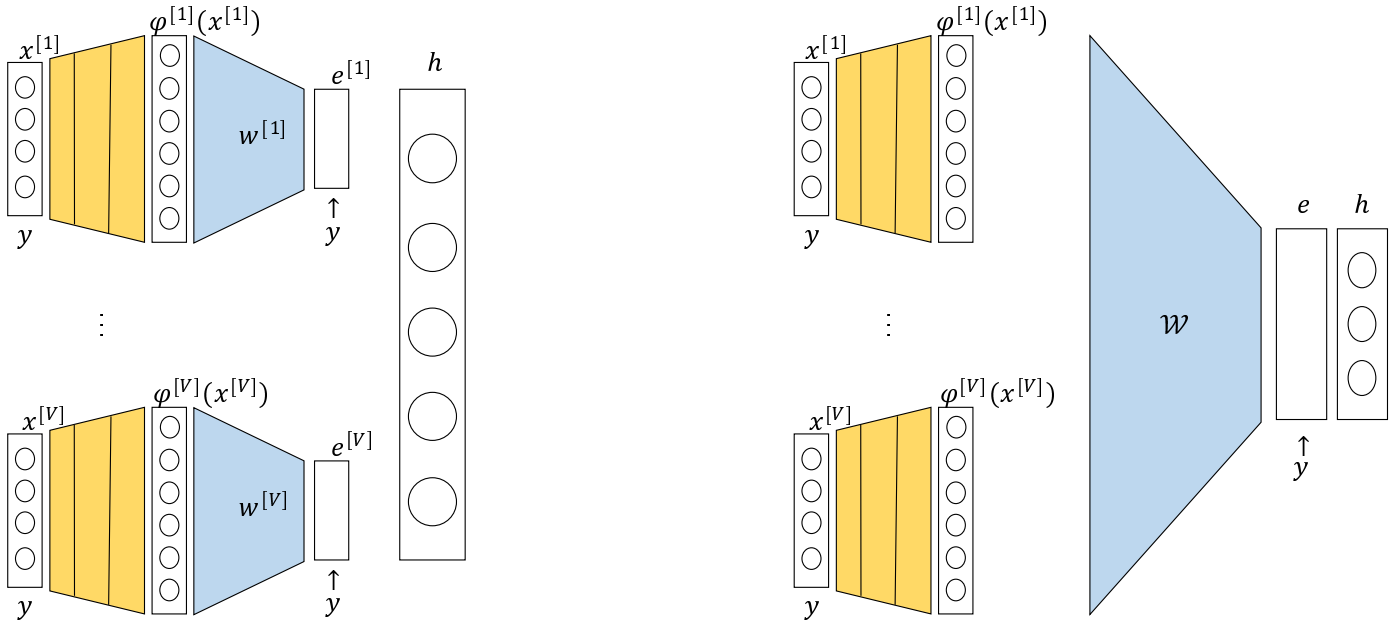




[figures by Joachim Schreurs]

Tensor-based RKM for Multi-view KPCA

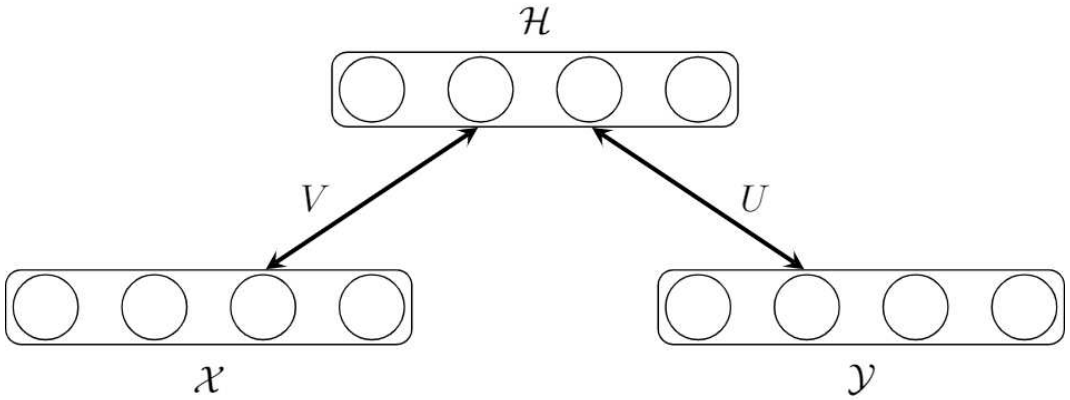
$$\min \langle \mathcal{W}, \mathcal{W} \rangle - \sum_{i=1}^{N} \left\langle \Phi_{(i)}, \mathcal{W} \right\rangle h_i + \lambda \sum_{i=1}^{N} h_i^2 \quad \text{with} \quad \Phi_{(i)} = \varphi^{[1]}(x_i^{[1]}) \otimes \ldots \otimes \varphi^{[V]}(x_i^{[V]})$$



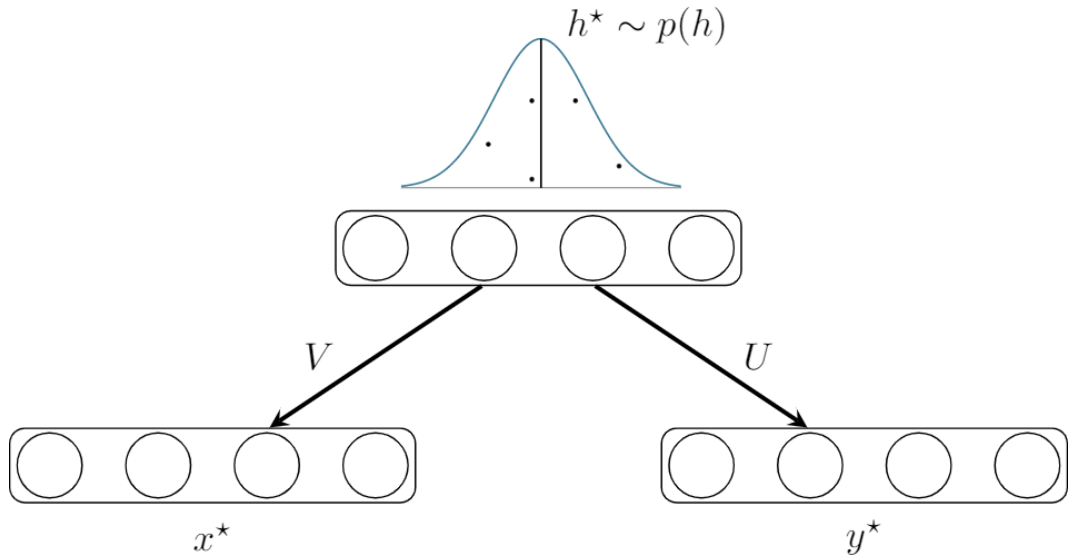
[Houthuys & Suykens, ICANN 2018]

Generative RKM (Gen-RKM) (1)

Train:

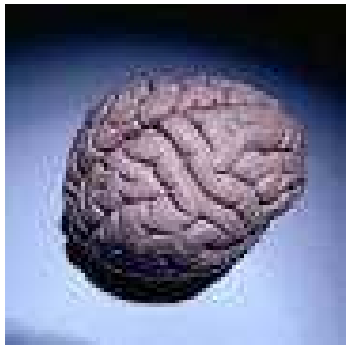


Generate:

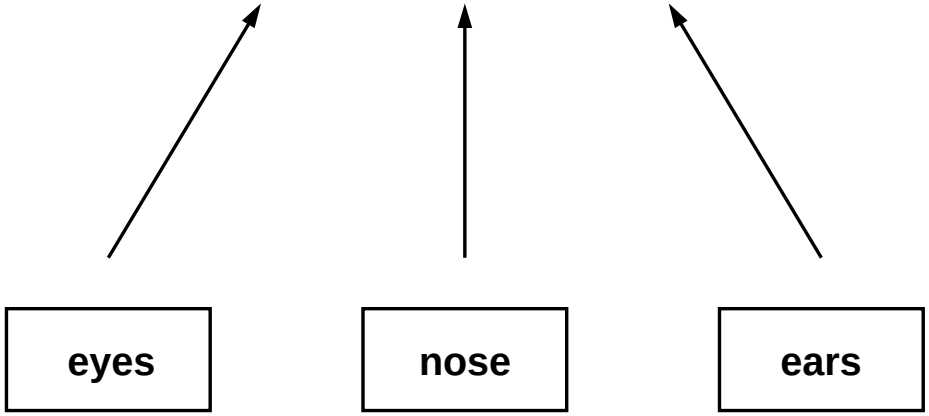


[Pandey, Schreurs & Suykens, 2019, arXiv:1906.08144]

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 ϕ_1, ϕ_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

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

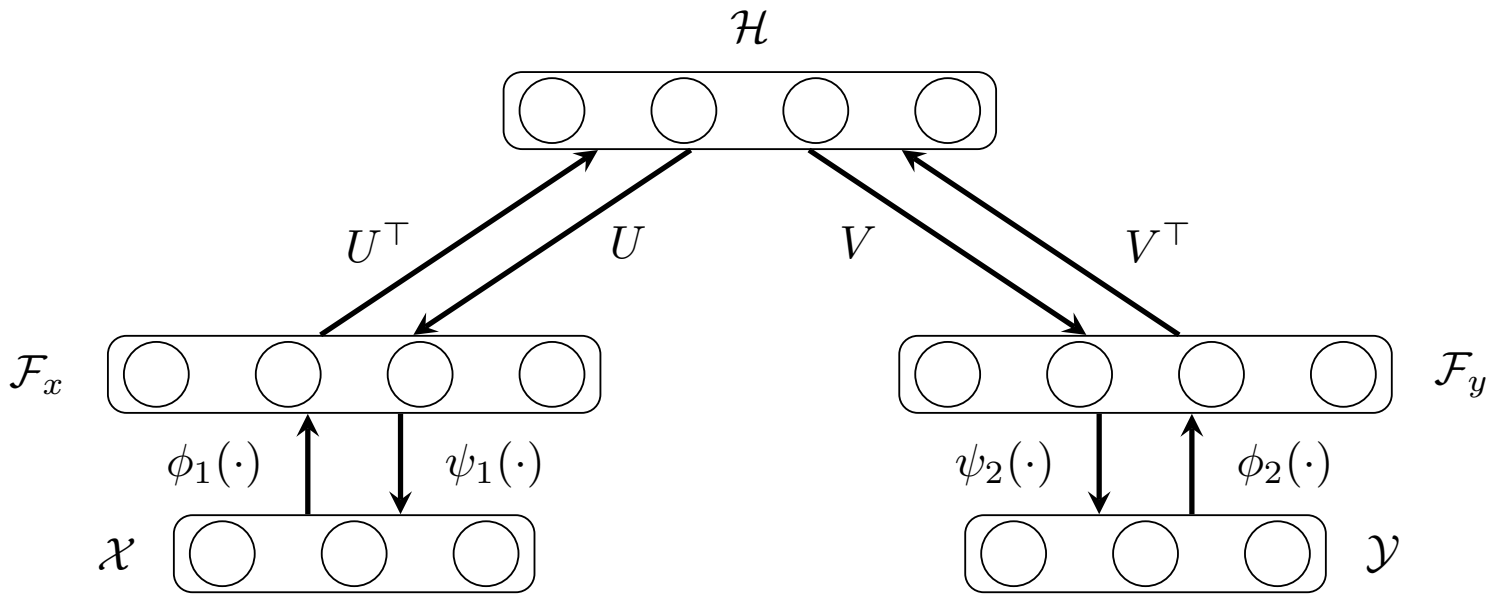
giving

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

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 ϕ_1, ϕ_2 are the feature maps ($\mathcal{F}_x$ and $\mathcal{F}_y$ represent the feature-spaces) corresponding to the two data sources. While ψ_1, ψ_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]:

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

with reconstruction errors

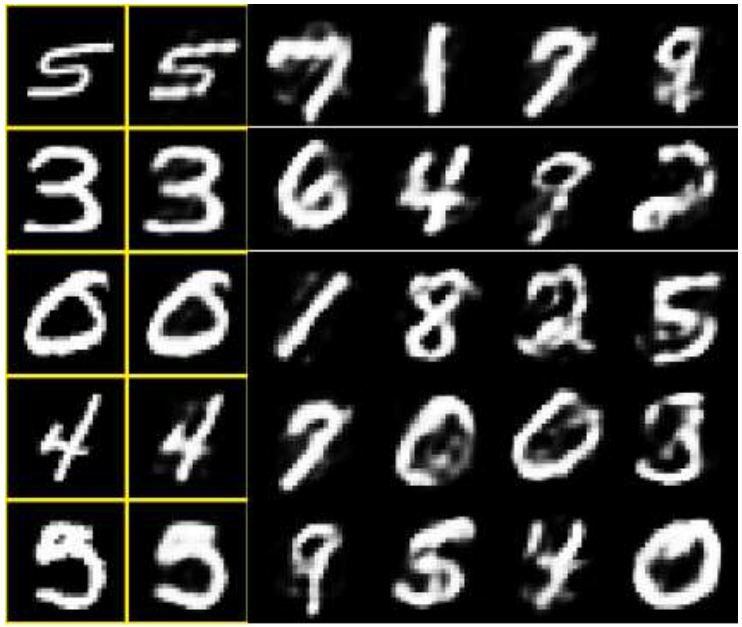
$$\begin{aligned}\mathcal{L}_1(\boldsymbol{x}_i^\star, \psi_{1_{\boldsymbol{\zeta}_1}}(\phi_{1_{\boldsymbol{\theta}_1}}(\boldsymbol{x}_i^\star))) &= \tfrac{1}{N}\|\boldsymbol{x}_i^\star - \psi_{1_{\boldsymbol{\zeta}_1}}(\phi_{1_{\boldsymbol{\theta}_1}}(\boldsymbol{x}_i^\star))\|_2^2, \\ \mathcal{L}_2(\boldsymbol{y}_i^\star,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

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

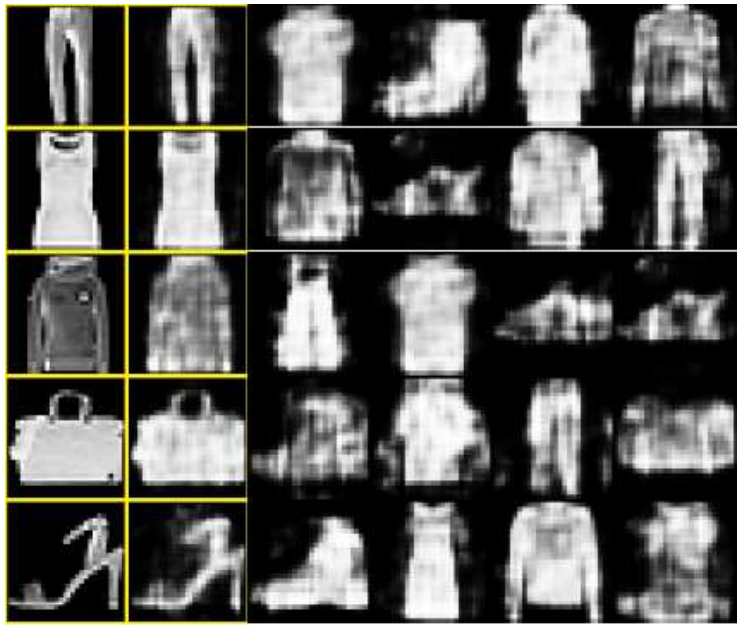
$$\begin{bmatrix} \frac{1}{\eta_1}\Phi_{\boldsymbol{x}}\Phi_{\boldsymbol{x}}^\top & \frac{1}{\eta_1}\Phi_{\boldsymbol{x}}\Phi_{\boldsymbol{y}}^\top \\ \frac{1}{\eta_2}\Phi_{\boldsymbol{y}}\Phi_{\boldsymbol{x}}^\top & \frac{1}{\eta_2}\Phi_{\boldsymbol{y}}\Phi_{\boldsymbol{y}}^\top \end{bmatrix} \begin{bmatrix}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

Hence, joint feature learning and subspace learning.

Gen-RKM: examples



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, Neural Networks 2021]

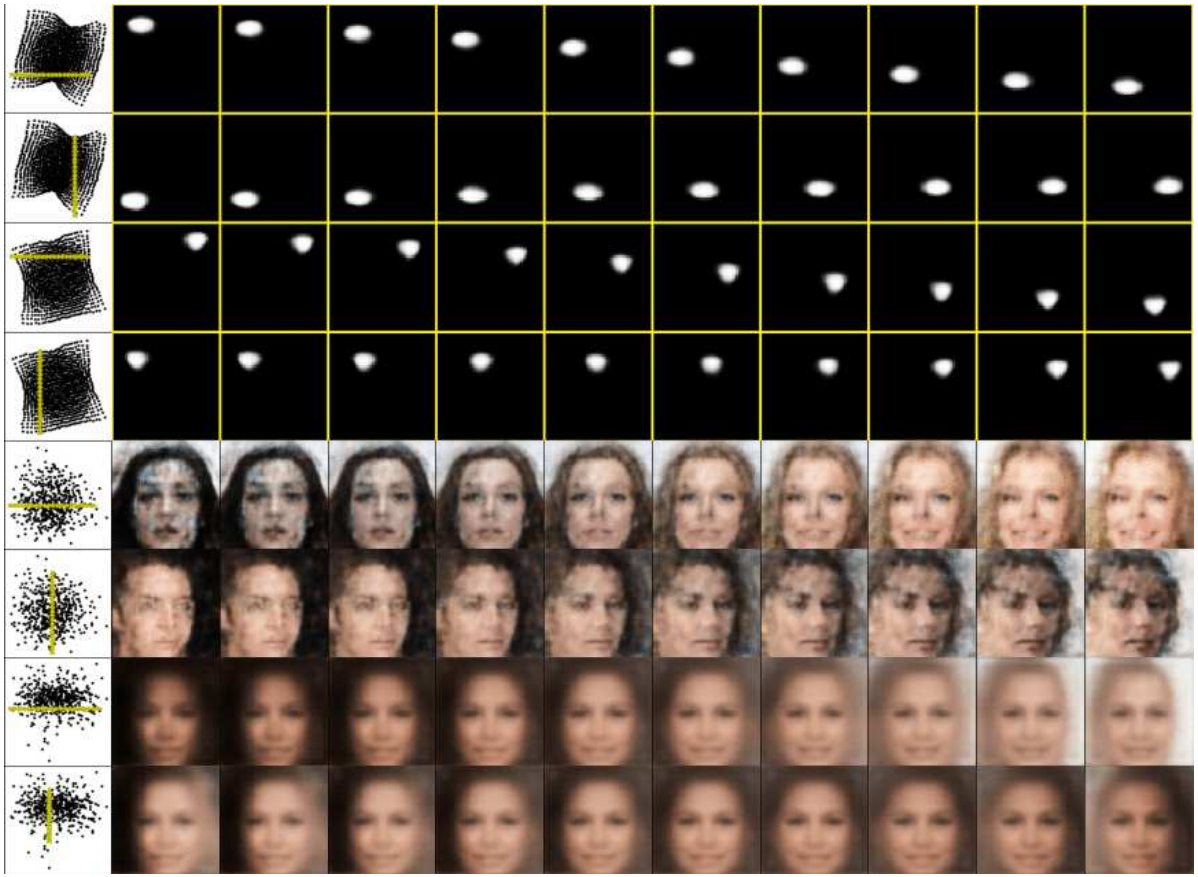
Gen-RKM: multi-view generation)

CelebA

Multi-view generation on CelebA dataset showing images and attributes

[Pandey, Schreurs & Suykens, Neural Networks 2021]

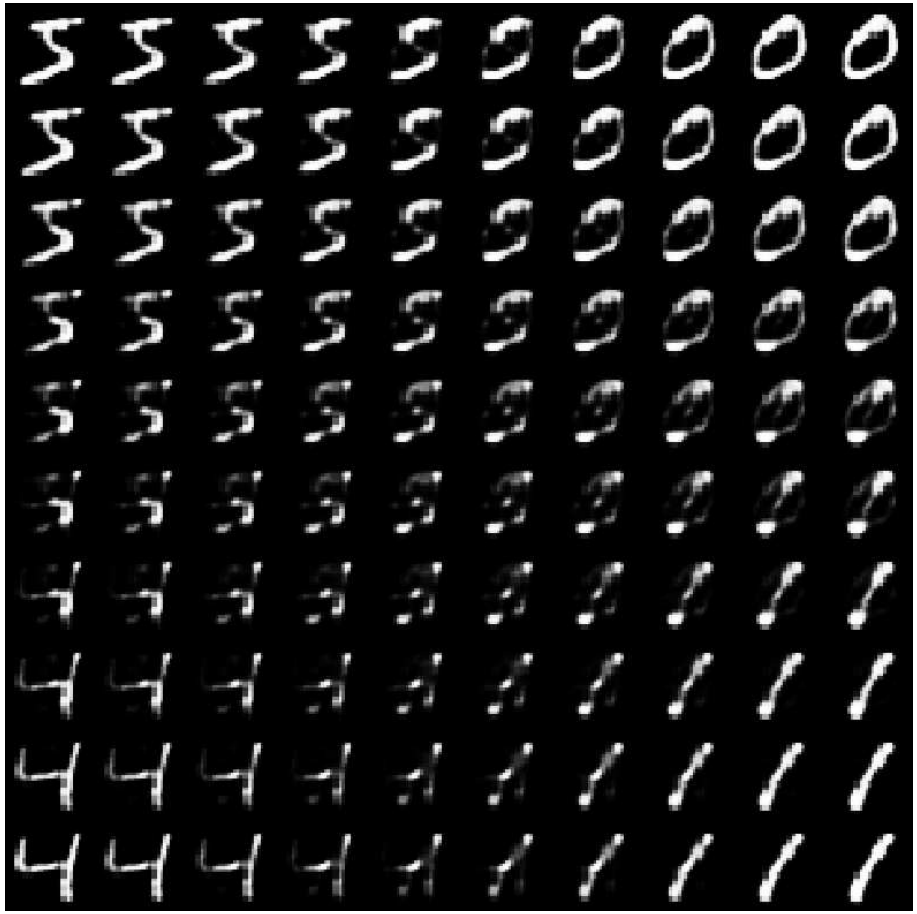
Gen-RKM: latent space exploration (1)



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

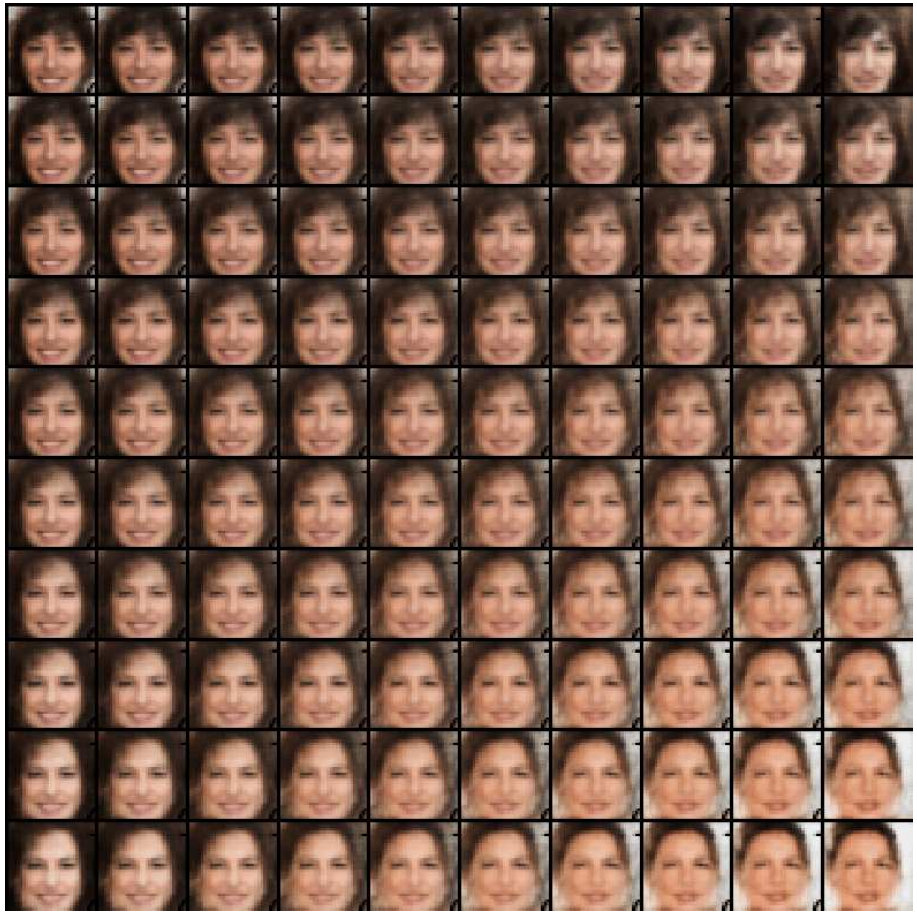
Explainability: changing one single neuron's hidden feature changes the hair color while preserving face structure! [Pandey, Schreurs & Suykens, Neural Networks 2021]

Gen-RKM: latent space exploration (2)



MNIST reconstructed images by bilinear-interpolation in latent space
[Pandey, Schreurs & Suykens, Neural Networks 2021]

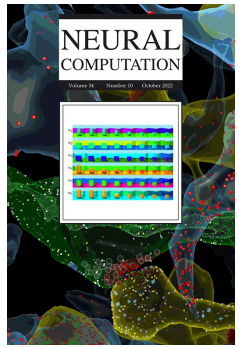
Gen-RKM: latent space exploration (3)



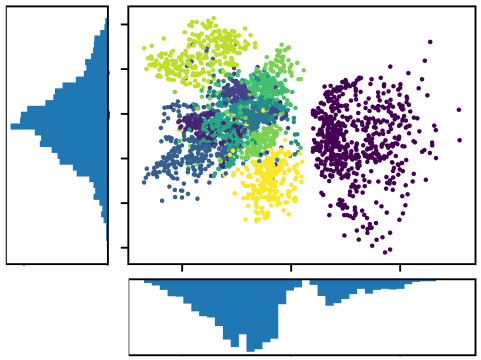
CelebA reconstructed images by bilinear-interpolation in latent space
[Pandey, Schreurs & Suykens, Neural Networks 2021]

Gen-RKM - traversals along principal components

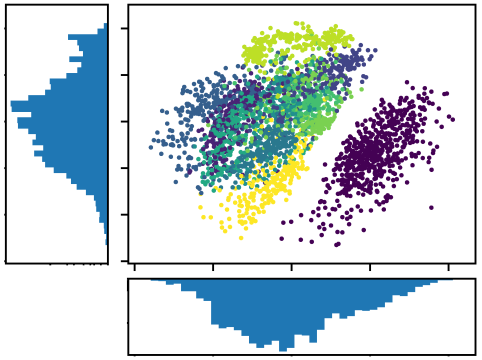
Disentangled Representation Learning &
Generation with Manifold Optimization
[Pandey, Fanuel, Schreurs & Suykens, Neural Computation, 2022]



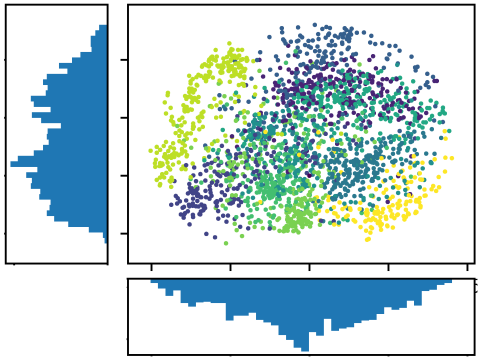
Robust Gen-RKM



VAE



Gen-RKM



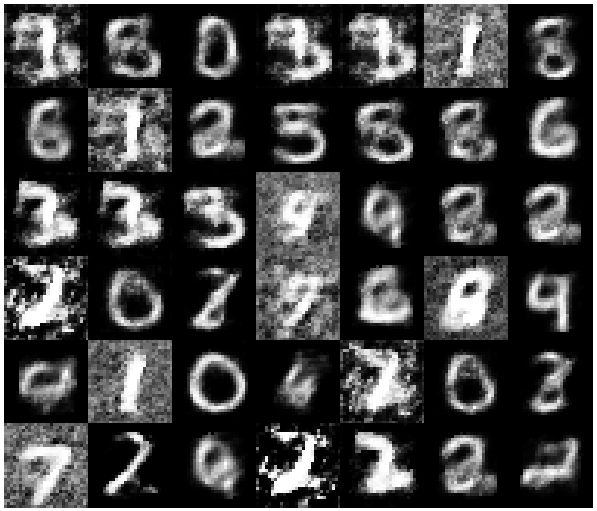
Robust Gen-RKM

- 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

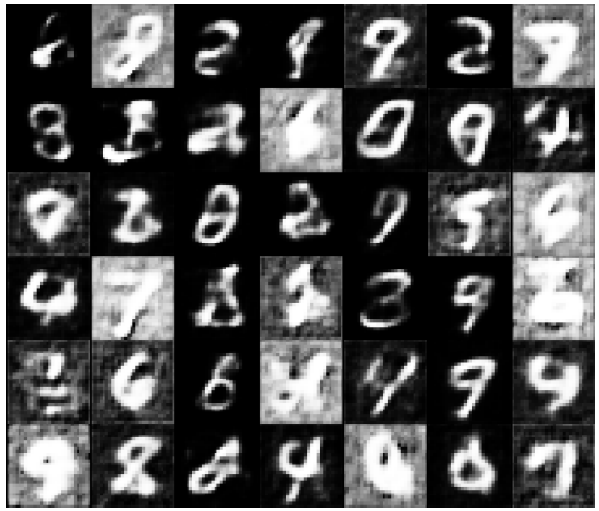
Weighted conjugate feature duality: $\frac{1}{2\lambda}e^T De + \frac{\lambda}{2}h^T D^{-1}h \geq e^T h$

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

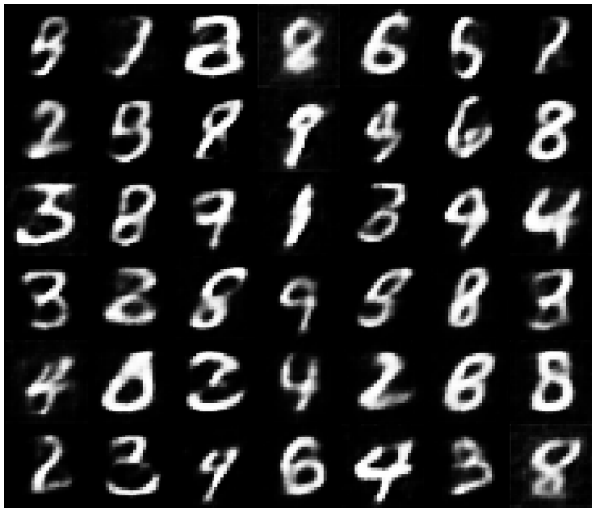
Robust Gen-RKM - Robust generation



VAE



Gen-RKM



Robust Gen-RKM

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

Deep unsupervised learning

Unsupervised learning of disentangled representations in deep restricted kernel machines with **orthogonality constraints**

$$\min_{W_1,W_2,H^{(1)},H^{(2)}} \quad \begin{aligned} &-\sum_i \varphi_1(x_i)^T W_1 h_i^{(1)} + \tfrac{\lambda_1}{2}\sum_i {h_i^{(1)}}^T h_i^{(1)} + \tfrac{1}{2}\mathrm{Tr}(W_1^T W_1) \\ &-\sum_i \varphi_2(h_i^{(1)})^T W_2 h_i^{(2)} + \tfrac{\lambda_2}{2}\sum_i {h_i^{(2)}}^T h_i^{(2)} + \tfrac{1}{2}\mathrm{Tr}(W_2^T W_2) \end{aligned}$$

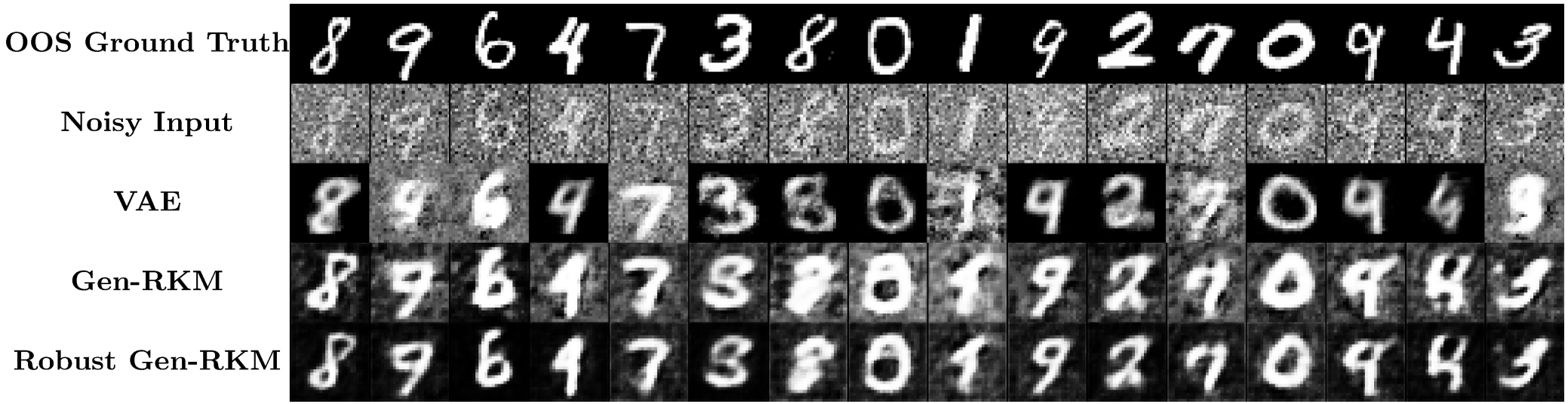
subject to

$$\begin{bmatrix} H^{(1)} \\ H^{(2)} \end{bmatrix} \begin{bmatrix} H^{(1)} & H^{(2)} \end{bmatrix} = I$$

with $H^{(1)} = [h_1^{(1)} ... h_N^{(1)}]$ and $H^{(2)} = [h_1^{(2)} ... h_N^{(2)}]$.

[F. Tonin, P. Patrinos, J.A.K. Suykens, Neural Networks 2021 - arXiv:2011.12659]

Robust Gen-RKM - Robust denoising



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

RKM references and software

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

Recurrent RKM

- Objective for **Recurrent RKM** [Pandey et al., 2022]:

$$J = -\sum_t \varphi(x_t)^T W h_t - \sum_t \sum_l h_{t-l}^T h_t + \frac{1}{2} h_t^T \Lambda h_t + \frac{1}{2} \mathrm{Tr} W^T W$$

- Results into a sequence $\{h_t\}$ in the latent space from which the future of the time-series is predicted.

- $\{h_t\}$ follows from the solution to an eigenvalue problem.

- Related work on recurrent temporal RBM [Sutskever et al., 2008; Osogami, 2019]

[A. Pandey, H. De Meulemeester, H. De Plaen, B. De Moor, J.A.K. Suykens, Recurrent Restricted Kernel Machines for Time-series Forecasting, ESANN 2022]

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

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Exploring duality for future data-driven modelling

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