Deep Learning, Neural Networks and Kernel Machines

Johan Suykens

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

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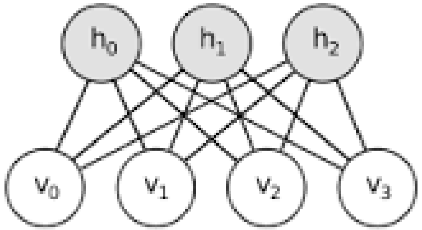
Part II: RBMs, kernel machines and deep learning

- Restricted Boltzmann Machines (RBM)
- Deep Boltzmann Machines (Deep BM)
- Restricted Kernel Machines (RKM)
- Deep RKM (see Part III)
- Generative RKM

Generative models: RBM, GAN and deep learning

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:

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

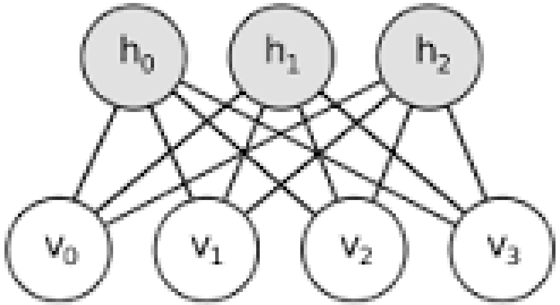
Joint distribution:

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

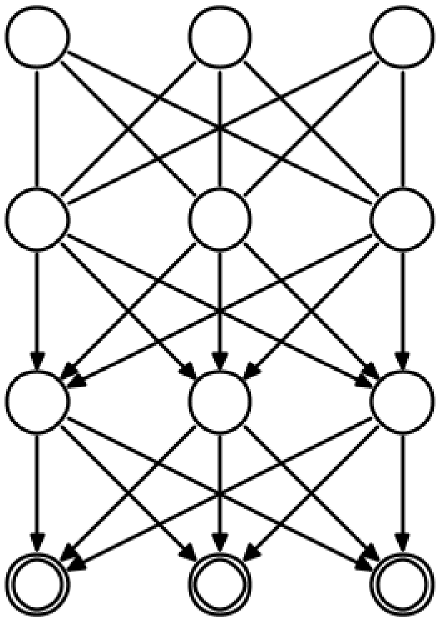
with partition function $Z(\theta) = \sum_v \sum_h \exp(-E(v, h; \theta))$

[Hinton, Osindero, Teh, Neural Computation 2006]

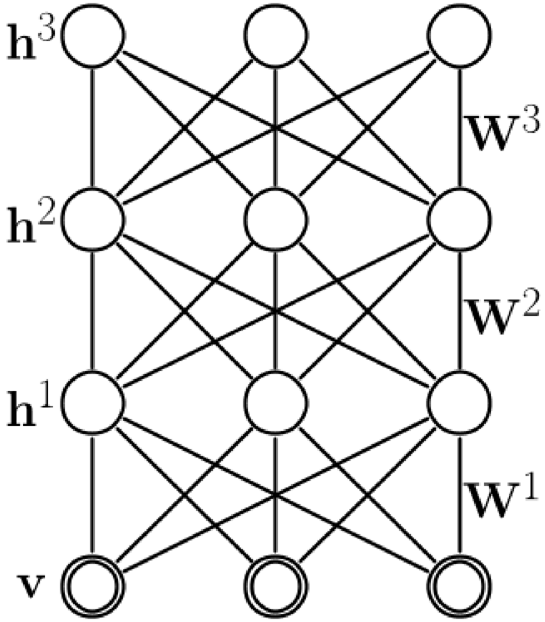
RBM and deep learning



Deep Belief Network



Deep Boltzmann Machine

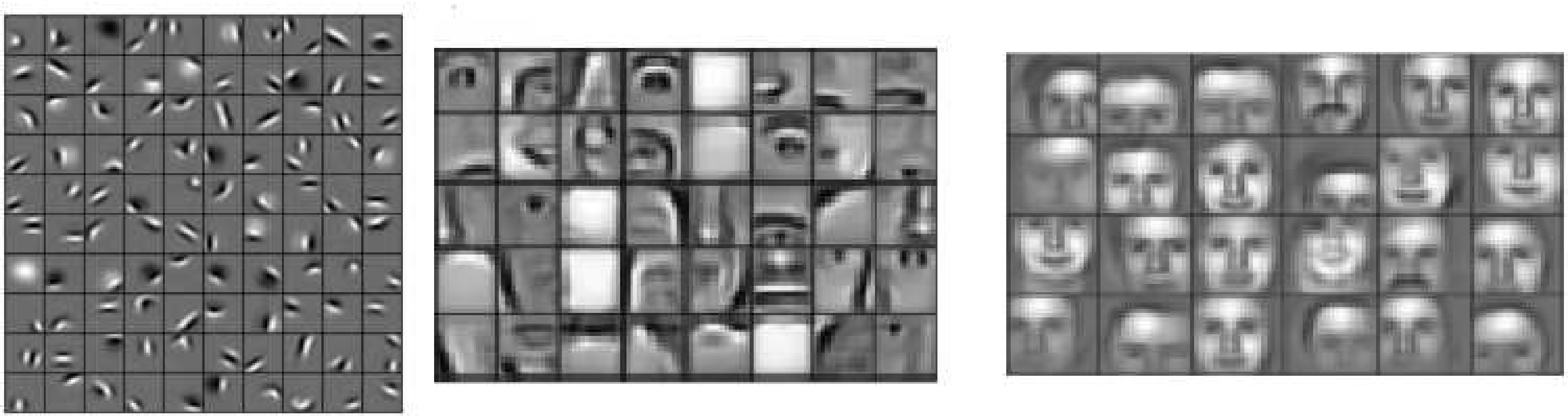


$p(v, h)$

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

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

Convolutional Deep Belief Networks



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

Energy function

- RBM:

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

- Deep Boltzmann machine (two layers):

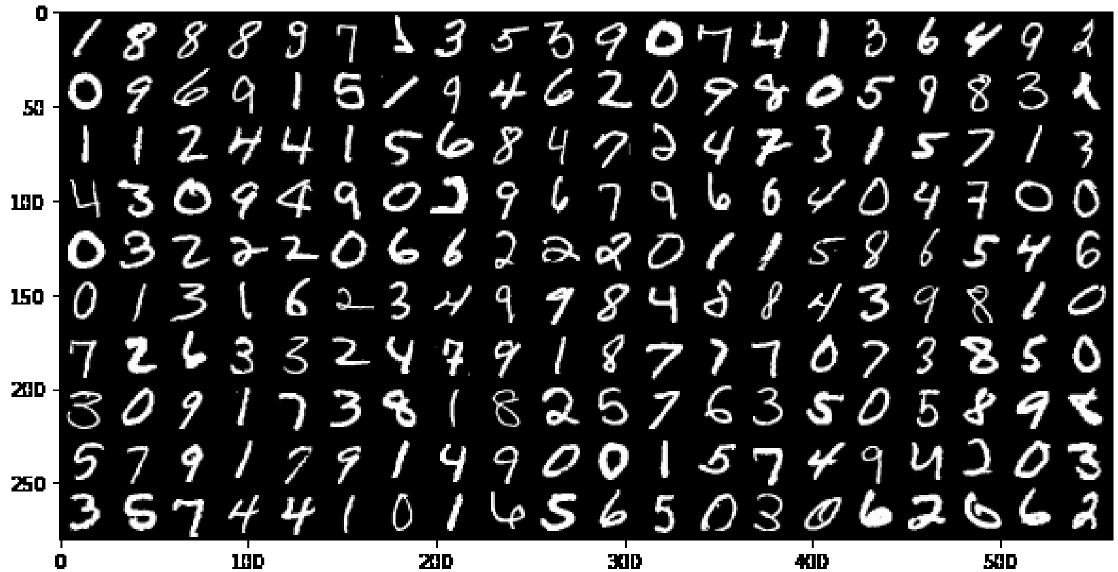
$$E = -v^T W^1 h^1 - {h^1}^T W^2 h^2$$

- Deep Boltzmann machine (three layers):

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

RBM: example on MNIST

MNIST training data:



Generating new images:

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

RBM training (1)

Thanks to the special bipartite structure, explicit **marginalization** is possible:

$$P(v;\theta) = \frac{1}{Z(\theta)} \sum_h \exp(-E(v,h;\theta)) = \frac{1}{Z(\theta)} \exp(b^T v) \prod_j (1+\exp(a_j + \sum_i W_{ij} v_j))$$

with $v_i \in \{0,1\}$, $h_i \in \{0,1\}$.

Conditional distributions:

$$P(h|v;\theta) = \prod_j p(h_j|v) \text{ with } p(h_j = 1|v) = \sigma(\sum_i W_{ij} v_i + a_j)$$

and

$$P(v|h;\theta) = \prod_i p(v_i|h) \text{ with } p(v_i = 1|h) = \sigma(\sum_j W_{ij} h_j + b_i)$$

with σ the sigmoid activation.

RBM training (2)

Given observations $\{v_n\}_{n=1}^N$, the **derivative of the log-likelihood** is

$$\begin{aligned}
\frac{1}{N}\sum_n \frac{\partial \log P(v_n;\theta)}{\partial W_{ij}} &= \mathbb{E}_{P_{\text{data}}}[v_i h_j] - \mathbb{E}_{P_{\text{model}}}[v_i h_j] \\
\frac{1}{N}\sum_n \frac{\partial \log P(v_n;\theta)}{\partial a_j} &= \mathbb{E}_{P_{\text{data}}}[h_j] - \mathbb{E}_{P_{\text{model}}}[h_j] \\
\frac{1}{N}\sum_n \frac{\partial \log P(v_n;\theta)}{\partial b_i} &= \mathbb{E}_{P_{\text{data}}}[v_i] - \mathbb{E}_{P_{\text{model}}}[v_i]
\end{aligned}$$

with

- **Data-dependent expectation** $\mathbb{E}_{P_{\text{data}}}[\cdot]$ (*form of Hebbian learning*): an expectation with respect to the data distribution $P_{\text{data}}(h, v; \theta) = P(h|v;\theta)P_{\text{data}}(v)$ with $P_{\text{data}}(v) = \frac{1}{N}\sum_n \delta(v - v_n)$ the empirical distribution.

- **Model's expectation** $\mathbb{E}_{P_{\text{model}}}[\cdot]$ (*unlearning*): an expectation with respect to the distribution defined by the model $P(v, h; \theta) = \frac{1}{Z(\theta)}\exp(-E(v, h; \theta))$.

RBM training (3)

Exact maximum likelihood learning is intractable (due to computation of $\mathbb{E}_{P_{\text{model}}}[\cdot]$). In practice, **Contrastive Divergence** (CD) algorithm [Hinton 2002]:

$$\Delta W = \alpha(\mathbb{E}_{P_{\text{data}}}[vh^T] - \mathbb{E}_{P_T}[vh^T])$$

with α learning rate and P_T a distribution defined by running a Gibbs chain initialized at the data for T full steps ($T = 1$, i.e. CD1 often in practice).

CD1 scheme:

1. Start Gibbs sampler $v^{(1)} := v_n$ and generate $h^{(1)} \sim P(h|v^{(1)})$
2. After obtaining $h^{(1)}$, generate $v^{(2)} \sim P(v|h^{(1)})$ (called fantasy data)
3. After obtaining $v^{(2)}$, generate $h^{(2)} \sim P(h|v^{(2)})$

with

$$\Delta W \propto (v_n {h^{(1)}}^T - v^{(2)} {h^{(2)}}^T)$$

Deep Boltzmann machine training (1)

Consider 3-layer Deep BM with **energy function** [Salakhutdinov 2015]:

$$E(v, h^1, h^2, h^3; \theta) = -v^T W^1 h^1 - {h^1}^T W^2 h^2 - {h^2}^T W^3 h^3$$

with unknown model parameters $\theta = \{W^1, W^2, W^3\}$.

The model assigns the following probability to a visible vector v:

$$P(v; \theta) = \frac{1}{Z(\theta)} \sum_{h^1, h^2, h^3} \exp(-E(v, h^1, h^2, h^3; \theta))$$

Deep Boltzmann machine training (2)

For training:

$$
\begin{aligned}
\frac{\partial \log P(v;\theta)}{\partial W^1} &= \mathbb{E}_{P_{\text{data}}}[v{h^1}^T] - \mathbb{E}_{P_{\text{model}}}[v{h^1}^T] \\
\frac{\partial \log P(v;\theta)}{\partial W^2} &= \mathbb{E}_{P_{\text{data}}}[h^1{h^2}^T] - \mathbb{E}_{P_{\text{model}}}[h^1{h^2}^T] \\
\frac{\partial \log P(v;\theta)}{\partial W^3} &= \mathbb{E}_{P_{\text{data}}}[h^2{h^3}^T] - \mathbb{E}_{P_{\text{model}}}[h^2{h^3}^T]
\end{aligned}
$$

Problem: the conditional distribution over the states of the hidden variables conditioned on the data is **no longer factorial**. For simplicity and speed one can **assume and impose a fully factorized distribution**, corresponding to a naive mean-field approximation [Salakhutdinov 2015].

Multimodal Deep Boltzmann Machine

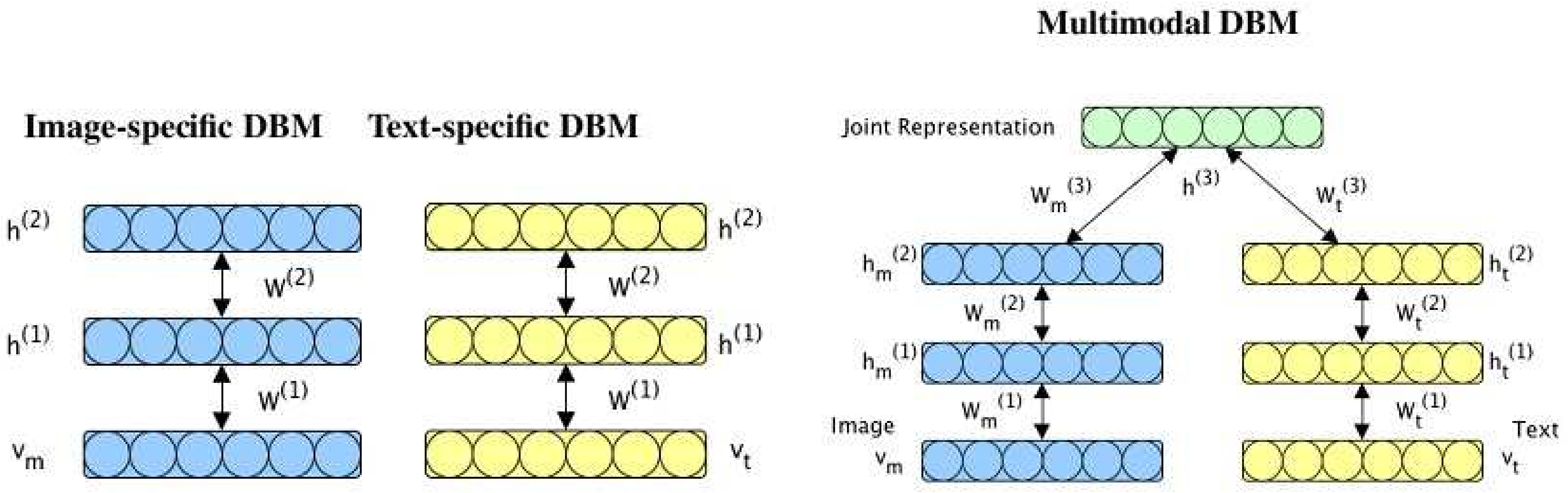


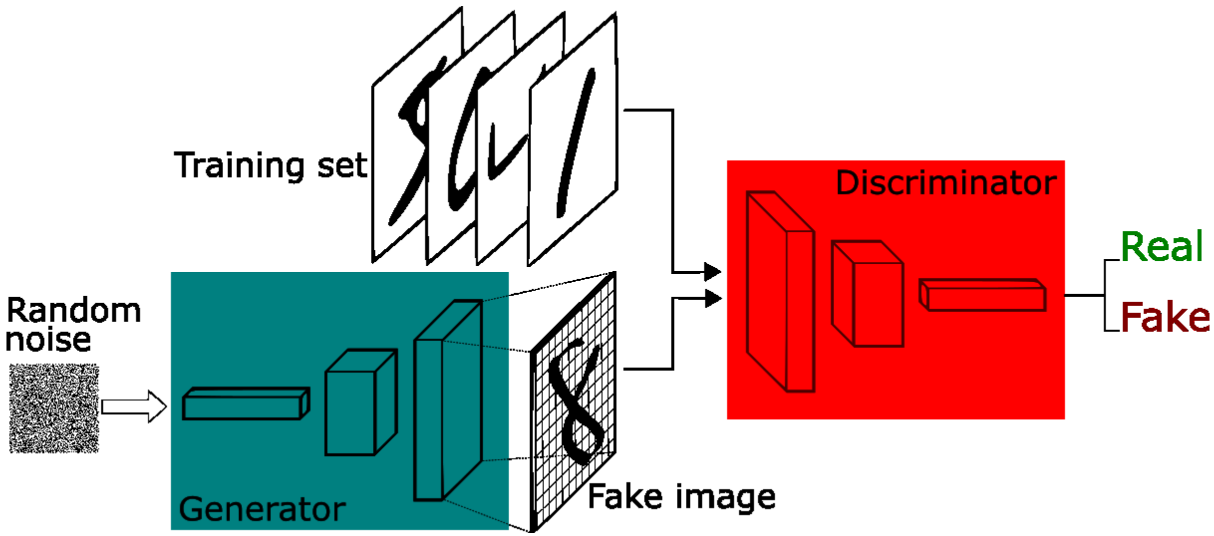
Figure 2: **Left:** Image-specific two-layer DBM that uses a Gaussian model to model the distribution over real-valued image features. **Middle:** Text-specific two-layer DBM that uses a Replicated Softmax model to model its distribution over the word count vectors. **Right:** A Multimodal DBM that models the joint distribution over image and text inputs.

From [Srivastava & Salakhutdinov 2014]

Generative Adversarial Network (GAN)

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

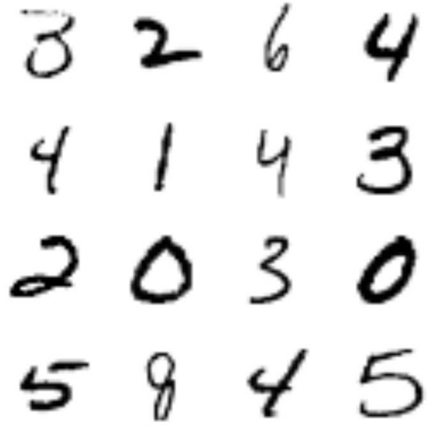
(Generator)	generate fake output examples from random noise
(Discriminator)	discriminate between fake examples and real examples.



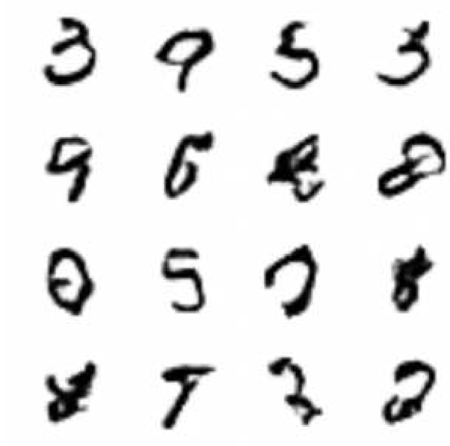
source: https://deeplearning4j.org/generative-adversarial-network

GAN: example on MNIST

MNIST training data:



GAN generated examples:



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

Kernel methods and deep learning

Kernel machines & deep learning

previous approaches:

- 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]
- other

Kernel machines & deep learning: New Challenges

- *new synergies* and *new foundations* between support vector machines & kernel methods and deep learning architectures?

- possible to extend primal and dual model representations (as occuring in SVM and LS-SVM models) *from shallow to deep architectures*?

- possible to handle *deep feedforward neural networks* and *deep kernel machines* within a common setting?

Kernel machines & deep learning: New Challenges

- *new synergies* and *new foundations* between support vector machines & kernel methods and deep learning architectures?
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→ new framework:

"Deep Restricted Kernel Machines" [Suykens, Neural Computation, 2017]

https://www.mitpressjournals.org/doi/pdf/10.1162/neco_a_00984

Restricted Kernel Machines

Restricted Kernel Machines (RKM)

Main characteristics:

- 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)

LS-SVM regression model: classical approach

LS-SVM regression model, given input & output data $x_i \in \mathbb{R}^d$, $y_i \in \mathbb{R}$

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

Solution in Lagrange multipliers α_i:

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

with $K(x_i, x_j) = \varphi(x_i)^T \varphi(x_j)$, $y_{1:N} = [y_1; ...; y_N]$
and $\hat{y} = \sum_i \alpha_i K(x, x_i) + b$.

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and $\hat{y} = \sum_i \alpha_i K(x, x_i) + b$.

$\rightarrow$ **How to achieve a representation with visible and hidden units?**

Conjugate feature duality

Property. For $\lambda > 0$, the following quadratic form property holds:

$$\frac{1}{2\lambda} e^T e \geq e^T h - \frac{\lambda}{2} h^T h, \quad \forall e, h \in \mathbb{R}^p$$

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Proof: This is verified by writing the quadratic form as

$$\frac{1}{2} \left[e^T \, h^T \right] \left[\begin{array}{cc} \frac{1}{\lambda} I & I \\ I & \lambda I \end{array} \right] \left[\begin{array}{c} e \\ h \end{array} \right] \geq 0, \; \forall e, h \in \mathbb{R}^p.$$

It is known that

$$Q = \left[\begin{array}{cc} A & B \\ B^T & C \end{array} \right] \geq 0$$

if and only if $A > 0$ and the Schur complement $C - B^T A^{-1} B \geq 0$.
This results into the condition $\frac{1}{2}(\lambda I - I(\lambda I) I) \geq 0$, which holds.

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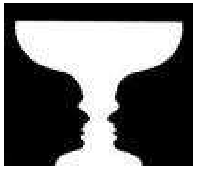
Note. One has

$$\frac{1}{2\lambda} e^T e = \max_h (e^T h - \frac{\lambda}{2} h^T h)$$



Model: living in two worlds ...

Original model:

$$\boxed{\hat{y} = W^T x + b, \; e = y - \hat{y}}$$

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

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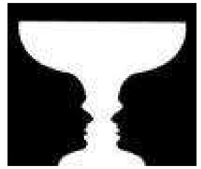

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$$\downarrow \quad \frac{1}{2\lambda} e^T e \geq e^T h - \frac{\lambda}{2} h^T h$$

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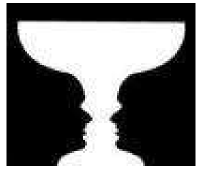

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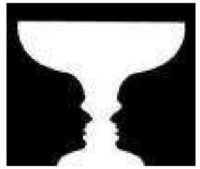
$$\downarrow \quad \frac{1}{2\lambda} e^T e \geq e^T h - \frac{\lambda}{2} h^T h$$

New representation:

$$\boxed{\hat{y} = \sum_j h_j x_j^T x + b}$$

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

Model: living in two worlds ...



Original model:

$$\boxed{\hat{y} = W^T \varphi(x) + b, \; e = y - \hat{y}}$$

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

$$\downarrow \quad \frac{1}{2\lambda} e^T e \geq e^T h - \frac{\lambda}{2} h^T h$$

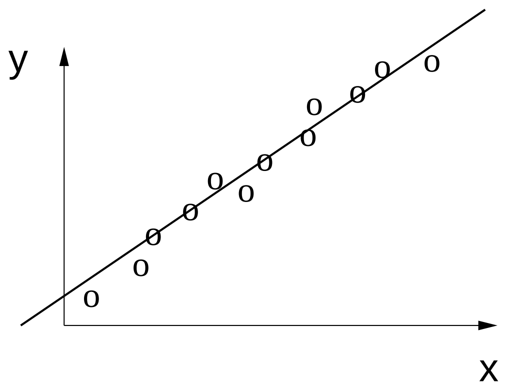
New representation:

$$\boxed{\hat{y} = \sum_j h_j K(x_j, x) + b}$$

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

Simplest example: line fitting

Given data: $\{(x_i, y_i)\}_{i=1}^{N}$, $x_i, y_i \in \mathbb{R}$

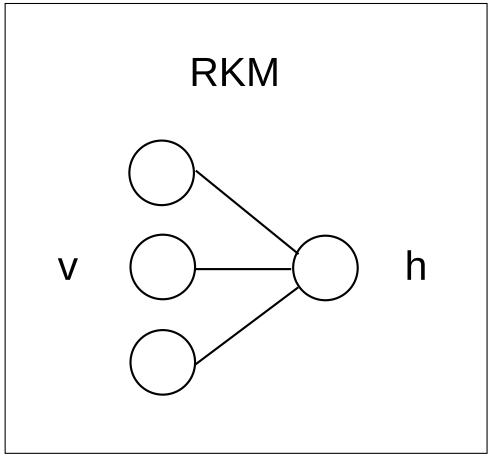


Linear model:

$$\hat{y} = wx + b, \ \ e = y - \hat{y}$$

RKM representation:

$$\hat{y} = \sum_i h_i x_i x + b$$



3 visible units: $v = [x; 1; -y]$
1 hidden unit: $h \in \mathbb{R}$

From LS-SVM to the RKM representation

Multi-output model $\hat{y} = W^T x + b$, $e = y - \hat{y}$

Objective in LS-SVM regression (linear case)

$$J = \frac{\eta}{2}\mathrm{Tr}(W^T W) + \frac{1}{2\lambda}\sum_{i=1}^{N} e_i^T e_i \ \text{ s.t. } e_i = y_i - W^T x_i - b, \forall i$$

From LS-SVM to the RKM representation

Multi-output model $\hat{y} = W^T x + b$, $e = y - \hat{y}$

Objective in LS-SVM regression (linear case)

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

From LS-SVM to the RKM representation

Multi-output model $\hat{y} = W^T x + b$, $e = y - \hat{y}$

Objective in LS-SVM regression (linear case)

$$
\begin{aligned}
J &= \frac{\eta}{2}\mathrm{Tr}(W^T W) + \frac{1}{2\lambda}\sum_{i=1}^{N} e_i^T e_i \;\; \text{s.t. } e_i = y_i - W^T x_i - b, \forall i \\
&\geq \sum_{i=1}^{N} e_i^T h_i - \frac{\lambda}{2}\sum_{i=1}^{N} h_i^T h_i + \frac{\eta}{2}\mathrm{Tr}(W^T W) \;\; \text{s.t. } e_i = y_i - W^T x_i - b, \forall i \\
&= \sum_{i=1}^{N} (y_i^T - x_i^T W - b^T) h_i - \frac{\lambda}{2}\sum_{i=1}^{N} h_i^T h_i + \frac{\eta}{2}\mathrm{Tr}(W^T W) \triangleq \underline{J}(h_i, W, b) \\
&= R_{\mathrm{RKM}}^{\mathrm{train}} - \frac{\lambda}{2}\sum_{i=1}^{N} h_i^T h_i + \frac{\eta}{2}\mathrm{Tr}(W^T W)
\end{aligned}
$$

Connection between RKM and RBM

- RKM & RBM: interpretation in terms of **visible and hidden units**

- RKM: **energy form** as in RBM:

$$
\begin{aligned}
R_{\mathrm{RKM}}^{\mathrm{train}} &= \sum_{i=1}^{N} R_{\mathrm{RKM}}(v_i, h_i) \\
&= -\sum_{i=1}^{N} (x_i^T W h_i + b^T h_i - y_i^T h_i) = \sum_{i=1}^{N} e_i^T h_i
\end{aligned}
$$

with $R_{\mathrm{RKM}}(v,h) = -v^T \tilde{W} h = -(x^T W h + b^T h - y^T h) = e^T h$.

- **Conjugate feature duality:** hidden features h_i are conjugated to the e_i and serve as dual variables.

From LS-SVM to RKM representation (2)

- Stationary points of $\underline{J}(h_i, W, b)$ (nonlinear case, feature map $\varphi(\cdot)$)

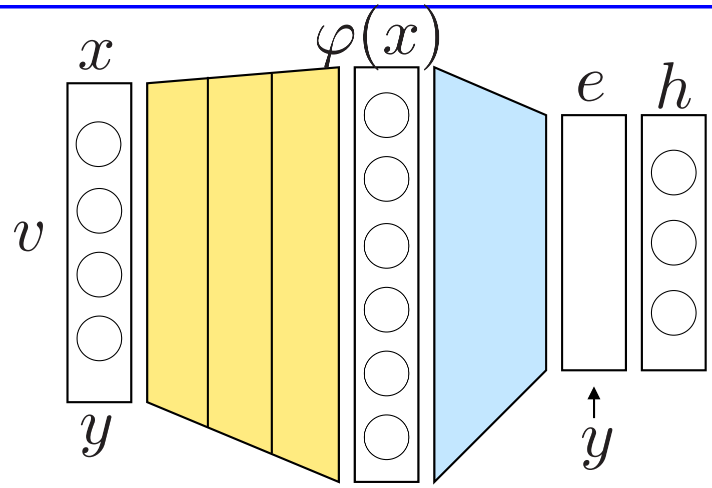
$$\left\{ \begin{array}{lll} \frac{\partial \underline{J}}{\partial h_i} = 0 & \Rightarrow & y_i = W^T \varphi(x_i) + b + \lambda h_i, \;\; \forall i \\ \frac{\partial \underline{J}}{\partial W} = 0 & \Rightarrow & W = \frac{1}{\eta} \sum_i \varphi(x_i) h_i^T \\ \frac{\partial \underline{J}}{\partial b} = 0 & \Rightarrow & \sum_i h_i = 0. \end{array} \right.$$

- Solution in h_i and b with positive definite kernel $K(x_i, x_j) = \varphi(x_i)^T \varphi(x_j)$

$$\left[\begin{array}{c|c} \frac{1}{\eta} K + \lambda I_N & 1_N \\ \hline 1_N^T & 0 \end{array} \right] \left[\begin{array}{c} H^T \\ \hline b^T \end{array} \right] = \left[\begin{array}{c} Y^T \\ \hline 0 \end{array} \right]$$

with $K = [K(x_i, x_j)]$, $H = [h_1 ... h_N]$, $Y = [y_1 ... y_N]$.

From LS-SVM to RKM representation (3)

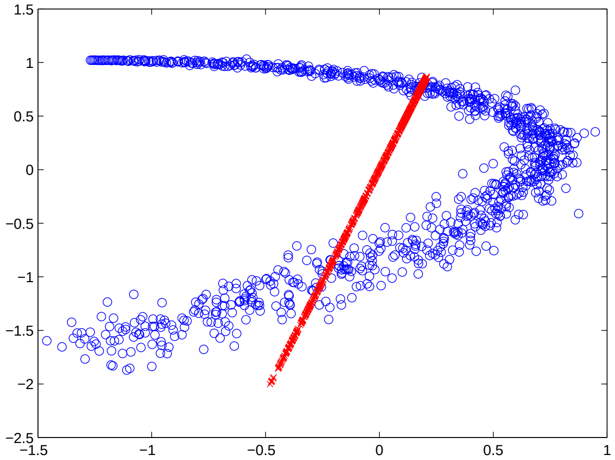


Note: $\varphi(x)$ can be multi-layered, visible units: $[\varphi(x); 1; -y]$
Conjugate feature duality: primal and dual model representations:

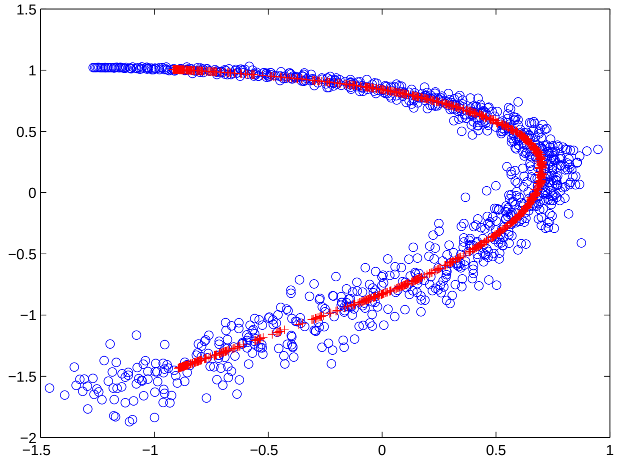
$$\mathcal{M} \begin{array}{l} \nearrow \quad (P)_{\mathrm{RKM}}: \quad \hat{y} = W^T \varphi(x) + b \\ \\ \searrow \quad (D)_{\mathrm{RKM}}: \quad \hat{y} = \frac{1}{\eta} \sum_j h_j K(x_j, x) + b. \end{array}$$

(large N, small d) versus (large d, small N)

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]

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

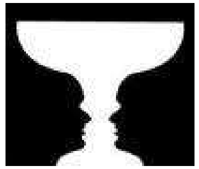
- Dual problem corresponds to kernel PCA

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

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

From KPCA to RKM representation



Model:

$$\boxed{e = W^T \varphi(x)}$$

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

$$\downarrow \quad - \frac{1}{2\lambda} e^T e \leq -e^T h + \frac{\lambda}{2} h^T h$$

RKM representation:

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

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

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

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

$$
\begin{cases}
\dfrac{\partial \overline{J}}{\partial h_i} = 0 \;\Rightarrow\; W^T\varphi(x_i) = \lambda h_i, \;\forall i \\[2ex]
\dfrac{\partial \overline{J}}{\partial W} = 0 \;\Rightarrow\; W = \dfrac{1}{\eta}\displaystyle\sum_i \varphi(x_i) h_i^T
\end{cases}
$$

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

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

Singular value decomposition

- Objective: given x_i, z_j row and column data of (non-square) matrix

$$J = -\frac{\eta}{2}\mathrm{Tr}(V^T W) + \frac{1}{2\lambda}\sum_{i=1}^{N} e_i^T e_i + \frac{1}{2\lambda}\sum_{j=1}^{M} r_j^T r_j \quad \text{s.t.} \quad \begin{aligned} e_i &= W^T \varphi(x_i), \forall i \\ r_j &= V^T \psi(z_j), \forall j \end{aligned}$$

- primal and dual representations (relates to non-symmetric kernels)

$$\mathcal{M} \begin{array}{l} \nearrow \quad (P)_{\mathrm{RKM}}: \quad \begin{aligned} \hat{e} &= W^T \varphi(x) \\ \hat{r} &= V^T \psi(z) \end{aligned} \\ \\ \searrow \quad (D)_{\mathrm{RKM}}: \quad \begin{aligned} \hat{e} &= \frac{1}{\eta}\sum_j h_{r_j} \psi(z_j)^T \varphi(x) \\ \hat{r} &= \frac{1}{\eta}\sum_i h_{e_i} \varphi(x_i)^T \psi(z) \end{aligned} \end{array}$$

Kernel probability mass function estimation

- Objective:

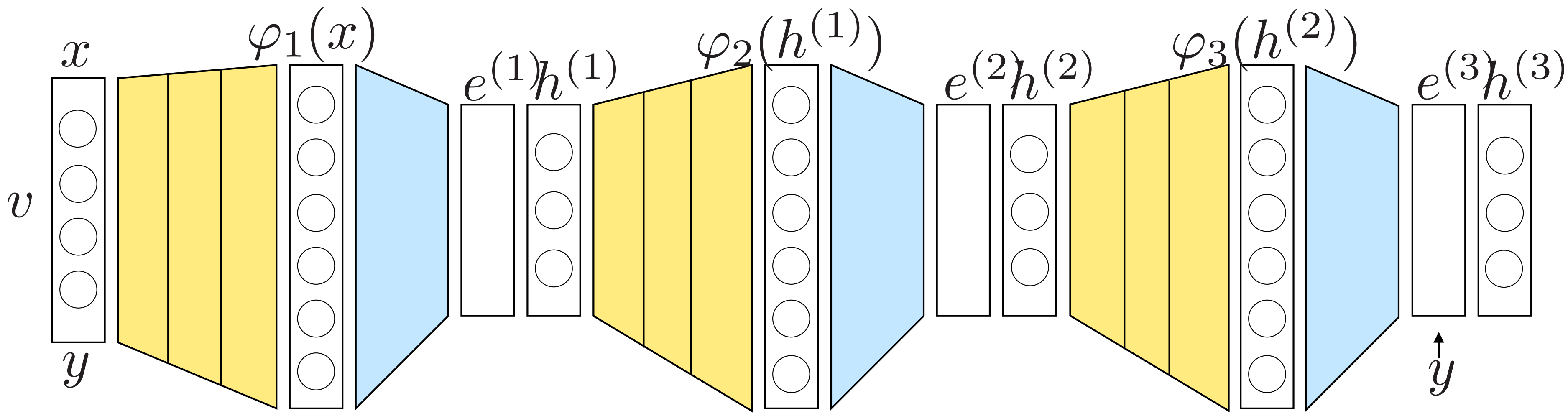
$$J = \sum_{i=1}^{N} (p_i - \varphi(x_i)^T w) h_i - \sum_{i=1}^{N} p_i + \frac{\eta}{2} w^T w$$

- primal and dual representations

$$\begin{array}{lll} & & (P)_{\mathrm{RKM}}: \quad p_i = w^T \varphi(x_i) \\ & \nearrow & \\ \mathcal{M} & & \\ & \searrow & \\ & & (D)_{\mathrm{RKM}}: \quad p_i = \dfrac{1}{\eta} \sum_j K(x_j, x_i) \end{array}$$

Deep Restricted Kernel Machines

Deep RKM: example



Deep RKM: KPCA + KPCA + LSSVM

Coupling of RKMs by taking sum of the objectives

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

Generative kernel PCA

RKM objective for training and generating (1)

- 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 objective function

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

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

[Schreurs & Suykens, ESANN 2018]

RKM objective for training and generating (2)

- **Training:** (clamp v)

$$\bar{J}_{\text{train}}(h_i, W) = -\sum_{i=1}^{N} v_i^{\mathrm{T}} W h_i + \frac{\lambda}{2}\sum_{i=1}^{N} h_i^{\mathrm{T}} h_i + \frac{\eta}{2}\mathrm{Tr}(W^{\mathrm{T}} W)$$

Stationary points:

$$\begin{array}{ll} \frac{\partial \bar{J}_{\text{train}}}{\partial h_i} = 0 & \Rightarrow W^{\mathrm{T}} v_i = \lambda h_i, \ \forall i \\ \frac{\partial \bar{J}_{\text{train}}}{\partial W} = 0 & \Rightarrow W = \frac{1}{\eta}\sum_{i=1}^{N} v_i h_i^{\mathrm{T}} \end{array}$$

Elimination of W:

$$\frac{1}{\eta} K H^{\mathrm{T}} = H^{\mathrm{T}} \Delta,$$

where $H = [h_1, \ldots, h_N] \in \mathbb{R}^{s \times N}$, $\Delta = \mathrm{diag}\{\lambda_1, \ldots, \lambda_s\}$ with $s \leq N$ the number of selected components and $K_{ij} = v_i^{\mathrm{T}} v_j$ the kernel matrix elements.

RKM objective for training and generating (3)

- **Generating:** (clamp h, W)

  Estimate distribution $p(h)$ from $h_i, i = 1, ..., N$ (or assumed normal).
  Obtain a new value $h^\star$.
  Generate in this way $v^\star$ from

$$\bar{J}_{\text{gen}}(v^\star) = -{v^\star}^{\mathrm{T}} W h^\star + \frac{1}{2} {v^\star}^{\mathrm{T}} v^\star$$

  Stationary points:

$$\frac{\partial \bar{J}_{\text{gen}}}{\partial v^\star} = 0$$

  This gives

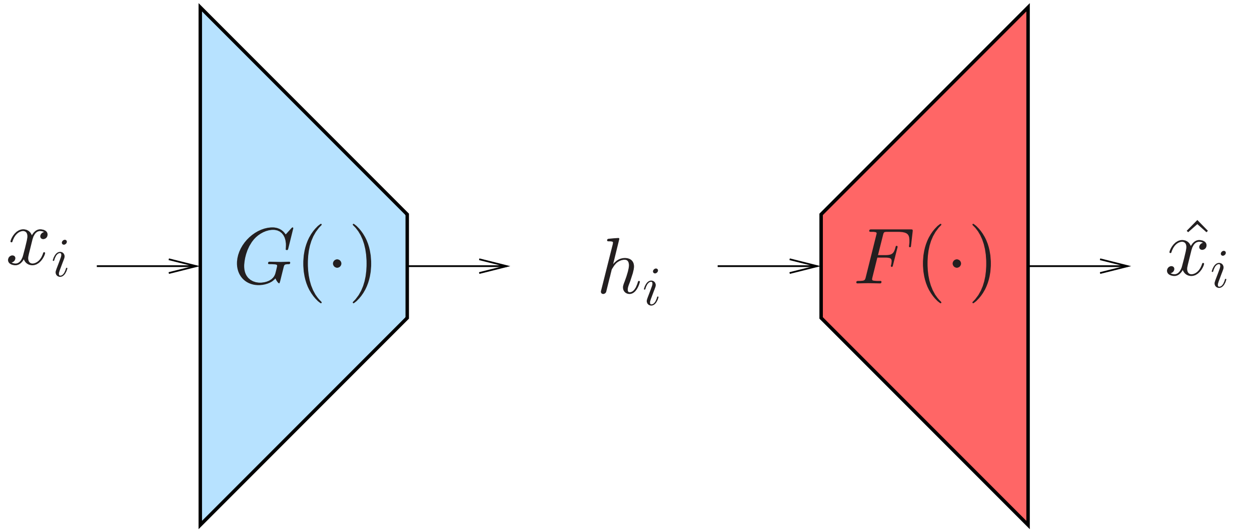
$$v^\star = W h^\star$$

Dimensionality reduction and denoising: linear case

- Given training data $v_i = x_i$ with $X \in \mathbb{R}^{d \times N}$, obtain hidden features $H \in \mathbb{R}^{s \times N}$:

$$\hat{X} = WH = (\frac{1}{\eta}\sum_{i=1}^{N} x_i h_i^T)H = \frac{1}{\eta}XH^T H$$

- Reconstruction error: $\|X - \hat{X}\|^2$



Dimensionality reduction and denoising: nonlinear case (1)

- New datapoint $x^\star$ generated from $h^\star$ by

$$\varphi(x^\star) = W h^\star = (\frac{1}{\eta} \sum_{i=1}^{N} \varphi(x_i) h_i^{\mathrm{T}}) h^\star$$

- Multiplying both sides by $\varphi(x_j)$ gives:

$$K(x_j, x^\star) = \frac{1}{\eta} (\sum_{i=1}^{N} K(x_j, x_i) h_i^{\mathrm{T}}) h^\star$$

On training data:

$$\hat{\Omega} = \frac{1}{\eta} \Omega H^{\mathrm{T}} H$$

with $H \in \mathbb{R}^{s \times N}, \Omega_{ij} = K(x_i, x_j) = \varphi(x_i)^T \varphi(x_j)$.

Dimensionality reduction and denoising: nonlinear case (2)

- Estimated value $\hat{x}$ for $x^\star$ by kernel smoother:

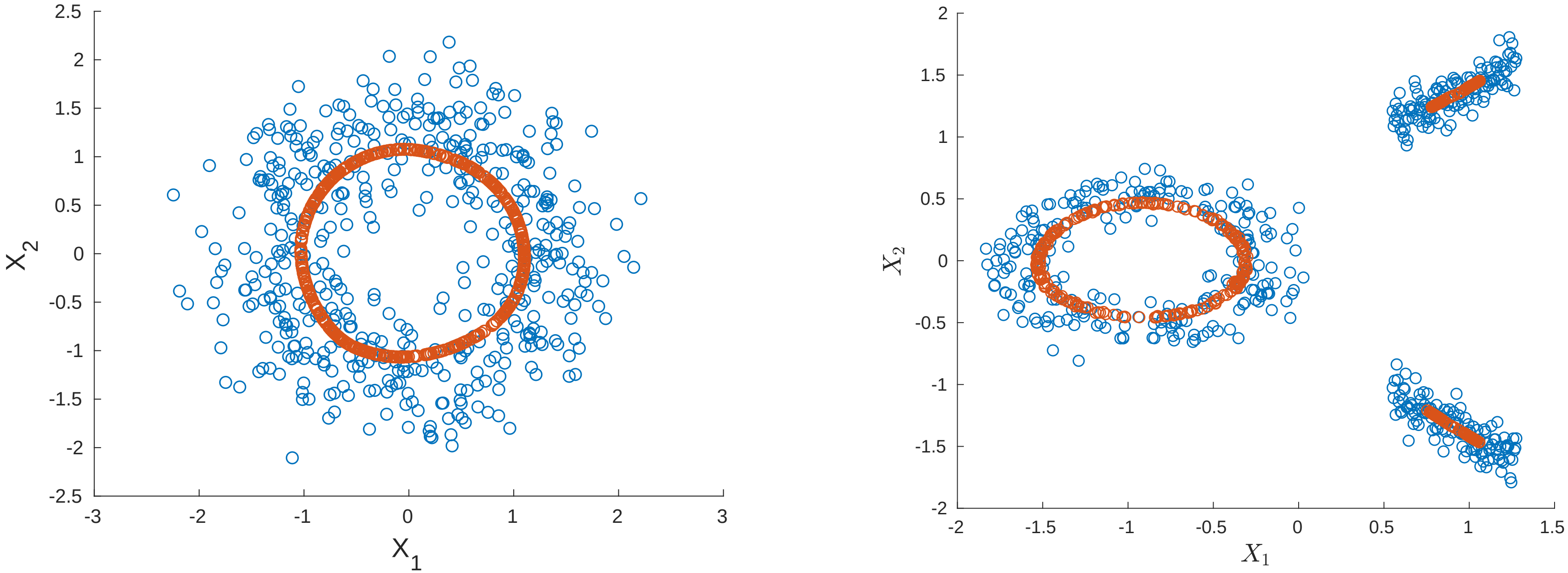
$$\hat{x} = \frac{\sum_{j=1}^{S} \tilde{K}(x_j, x^\star) x_j}{\sum_{j=1}^{S} \tilde{K}(x_j, x^\star)}$$

with $\tilde{K}(x_j, x^\star)$ (e.g. RBF kernel) the scaled similarity between 0 and 1, a design parameter $S \leq N$ (S closest points based on the similarity $\tilde{K}(x_j, x^\star)$).

[Schreurs & Suykens, ESANN 2018]

Example: denoising

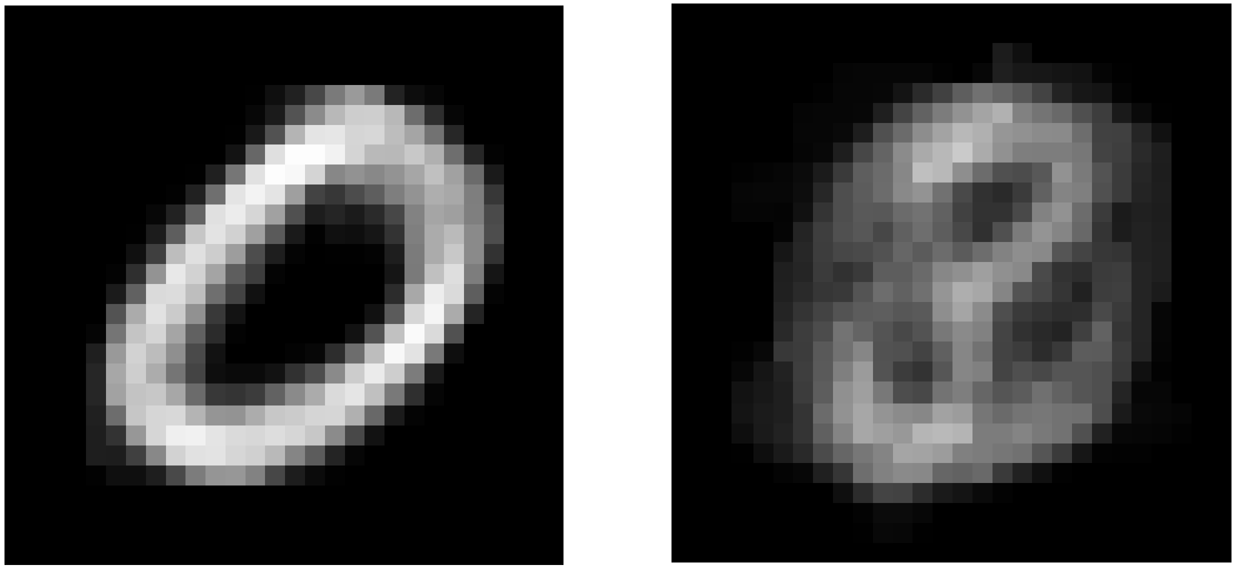
Synthetic data sets:



$X \in \mathbb{R}^{2\times 500}$ $(d = 2, N = 500)$
Kernel PCA using RBF kernel with $\tilde{\sigma}^2 = 1$ (left: $s = 2$; right: $s = 8$)
Kernel smoother: $S = 100$ closed points, $\tilde{\sigma}^2 = 0.2$

Example: generating new data

From MNIST data:

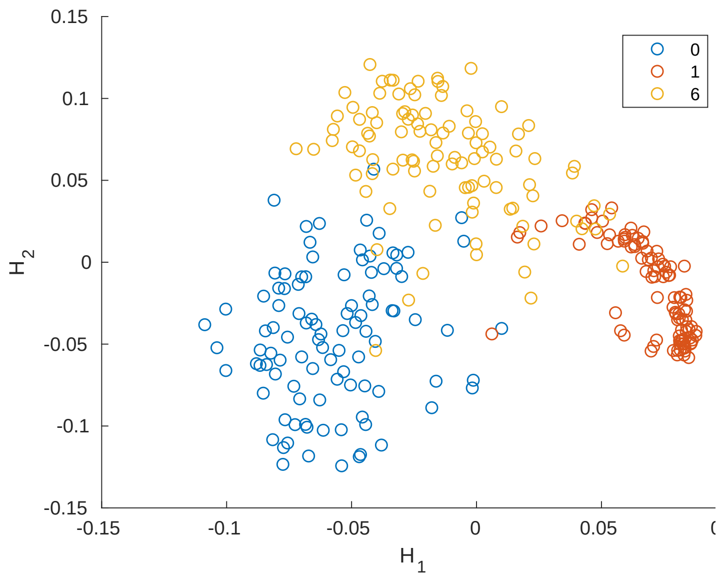


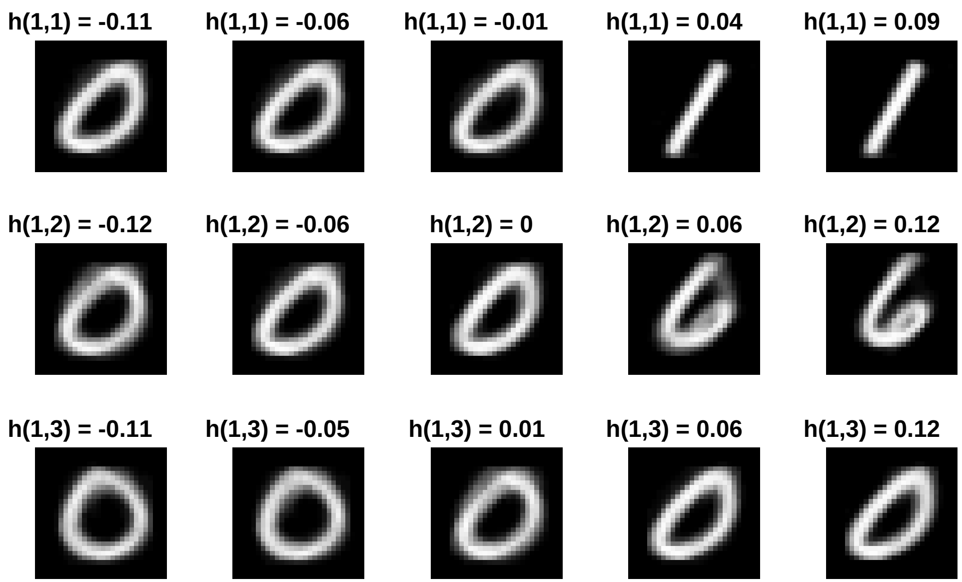
Training data: 50 images per digit; Kernel PCA (left: $s = 20$; right: $s = 50$)
Normal distribution fitted on h_i, used to generate $h^\star$
Kernel smoother: (left) $S = 10$ (digits 0); (right) $S = 100$ (digits 0,8)

[Schreurs & Suykens, ESANN 2018]

Towards explainable AI

Understanding the role of the hidden units:

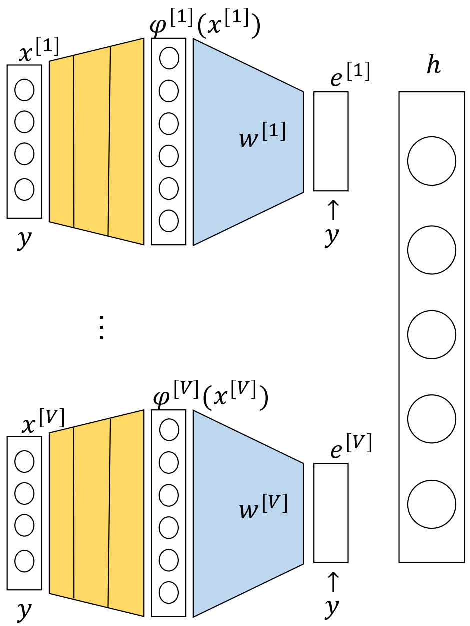


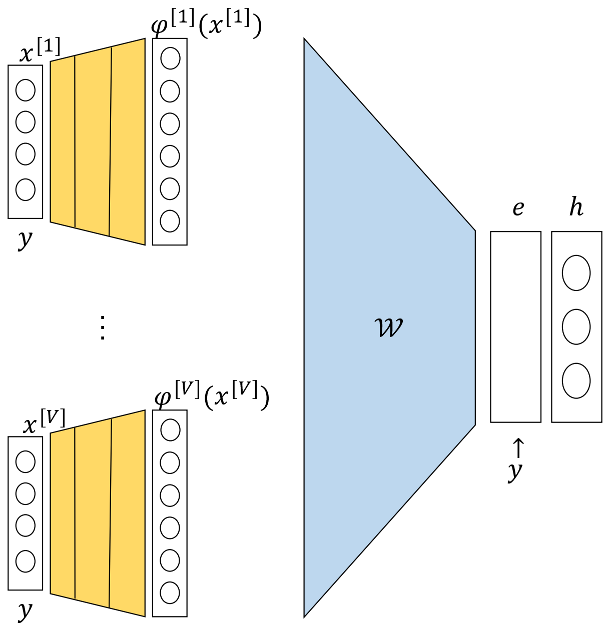


[figures by Joachim Schreurs]

Tensor-based RKM for Multi-view KPCA

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





[Houthuys & Suykens, ICANN 2018]

Generative RKM (1)

The objective

$$J_{\mathrm{train}}(h_i, V, U) = \sum_{i=1}^{N}(-\varphi_1(x_i)^T V h_i - \varphi_2(y_i)^T U h_i + \frac{\lambda_i}{2} h_i^T h_i) + \frac{\eta_1}{2}\mathrm{Tr}(V^T V) + \frac{\eta_2}{2}\mathrm{Tr}(U^T U)$$

results for **training** into the eigenvalue problem

$$(\frac{1}{\eta_1}K_1 + \frac{1}{\eta_2}K_2)H^T = H^T \Lambda$$

with $H = [h_1 ... h_N]$ and kernel matrices K_1, K_2 related to φ_1, φ_2.

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

Generative RKM (2)

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

$$J_{\text{generate}}(\varphi_1(x^\star), \varphi_2(y^\star)) = -\varphi_1(x^\star)^T V h^\star - \varphi_2(y^\star)^T U h^\star + \frac{1}{2}\varphi_1(x^\star)^T \varphi_1(x^\star) + \frac{1}{2}\varphi_2(y^\star)^T \varphi_2(y^\star)$$

giving

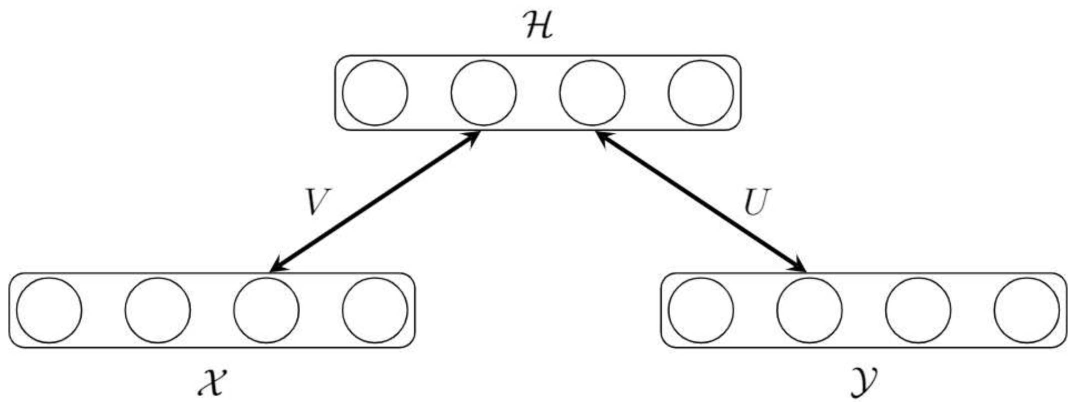
$$\varphi_1(x^\star) = \frac{1}{\eta_1}\sum_{i=1}^{N} \varphi_1(x_i) h_i^T h^\star, \;\; \varphi_2(y^\star) = \frac{1}{\eta_2}\sum_{i=1}^{N} \varphi_2(y_i) h_i^T h^\star.$$

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

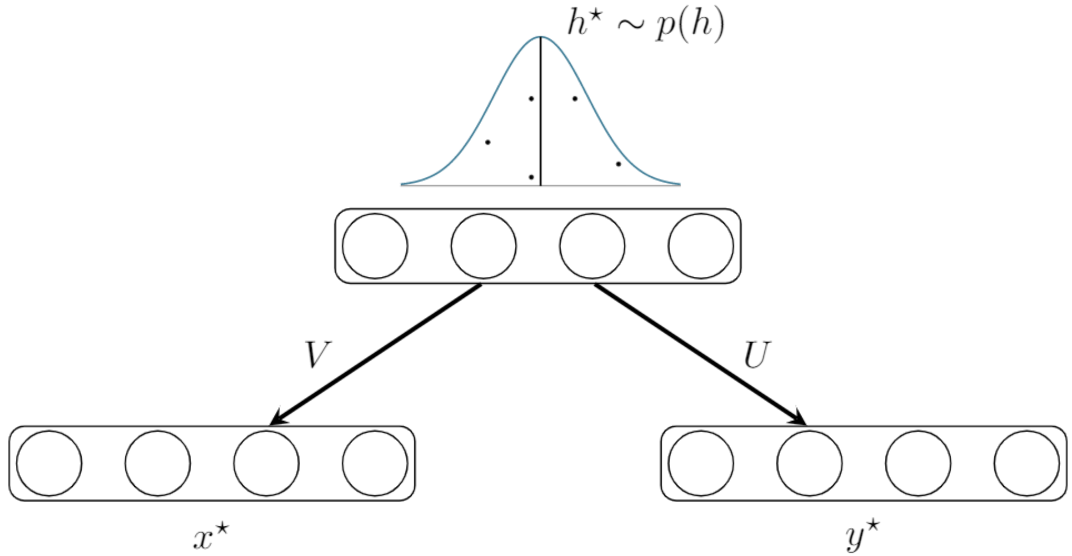
[Pandey, Schreurs & Suykens, 2019, arXiv:1906.08144]

Generative RKM (3)

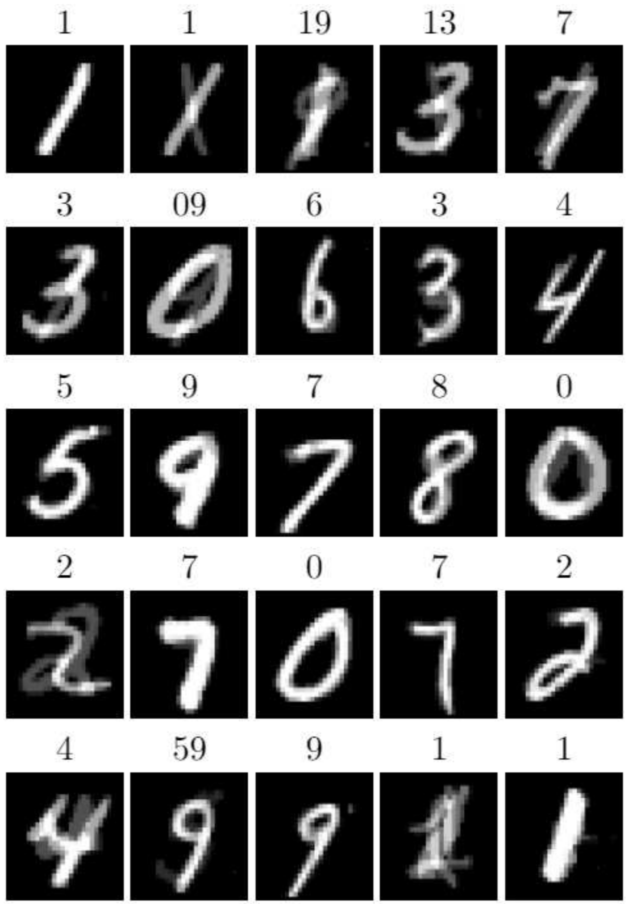
Train:



Generate:



Generative RKM (4)



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

Generative RKM (5)

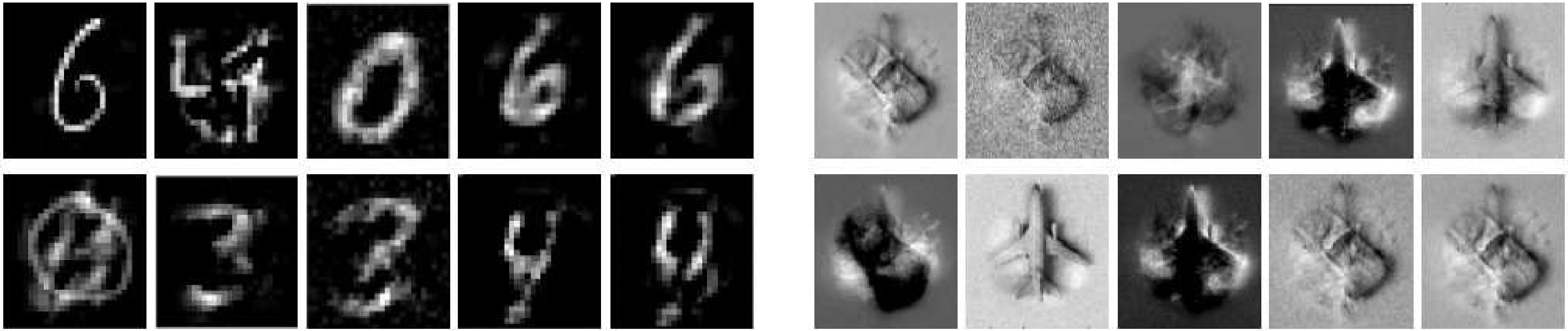


Figure: Image generation using neural networks as feature map:
(left) MNIST; (right) Small-NORB

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

Generative RKM (6)

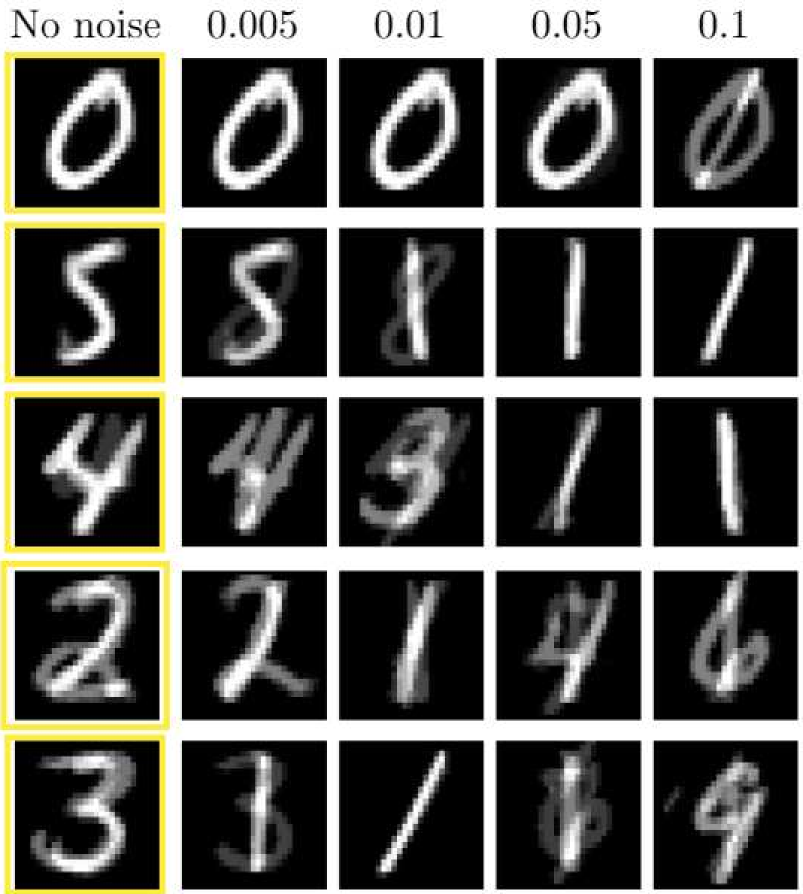


Figure: Targeted image generation through corresponding latent variable.

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

Conclusions

- From RBM to deep BM
- From RKM to deep RKM
- RKM and RBM representation: visible and hidden units
- RKM representation for LS-SVM, KPCA, SVD and others
- RKM representation obtained by conjugate feature duality
- Generative RKM

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NEW: ERC Advanced Grant E-DUALITY

Exploring duality for future data-driven modelling

Thank you