Unsupervised Representation Learning: Autoencoders, Factorization, and Sparse Coding

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Recap

We have talked about

- Basic DNNs (multi-layer feedforward)

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- Universal approximation theorems

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Models and applications

- Unsupervised representation learning: autoencoders and variants
- DNNs for spatial data: CNNs
- DNNs for sequential data: RNNs, LSTM
- Generative models: variational Autoencoders and GAN
- Interactive models: reinforcement learning

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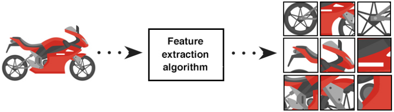
involve modification and composition of the basic DNNs

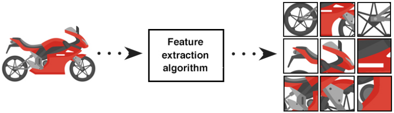
Feature engineering: old and new



Credit: [Elgendy, 2020]

Feature engineering: derive features for efficient learning

Feature engineering: old and new



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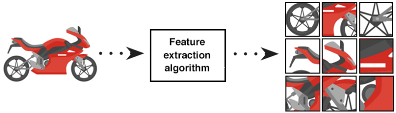
Feature engineering: derive features for efficient learning

Traditional learning pipeline

Feature engineering: old and new



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– feature extraction is "independent" of the learning models and tasks

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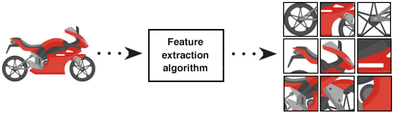

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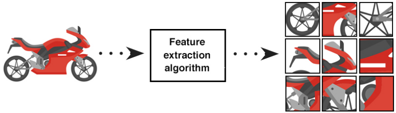

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Feature engineering: derive features for efficient learning

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Modern learning pipeline

– end-to-end DNN learning

Unsupervised representation learning

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(ICLR — International Conference on Learning Representation)

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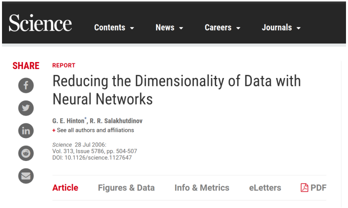
- **Historical**: Unsupervised representation learning key to the revival of deep learning (i.e., layerwise pretraining, [Hinton et al., 2006, Hinton, 2006])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Reducing the Dimensionality of Data with Neural Networks

G. E. Hinton*, R. R. Salakhutdinov
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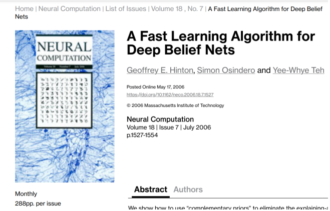
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NEURAL COMPUTATION

A Fast Learning Algorithm for Deep Belief Nets

Geoffrey E. Hinton, Simon Osindero and Yee-Whye Teh

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Abstract Authors

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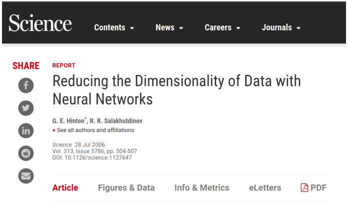

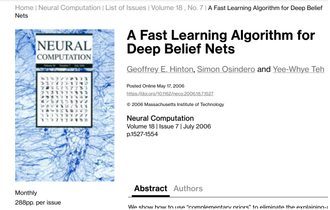

– **Practical**: Numerous advanced models built on top of the ideas in unsupervised representation learning (e.g., encoder-decoder networks)

Outline

PCA: the geometric picture

Principal component analysis (PCA)

- Assume $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n \in \mathbb{R}^D$ are zero-centered and write $\boldsymbol{X} = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_m]$
- $\boldsymbol{X} = \boldsymbol{U}\boldsymbol{S}\boldsymbol{V}^\intercal$, where $\boldsymbol{U}$ spans the column space (i.e., range) of $\boldsymbol{X}$
- Take top singular vectors $\boldsymbol{B}$ from $\boldsymbol{U}$, and obtain $\boldsymbol{B}^\intercal\boldsymbol{X}$

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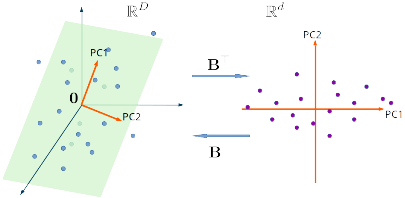

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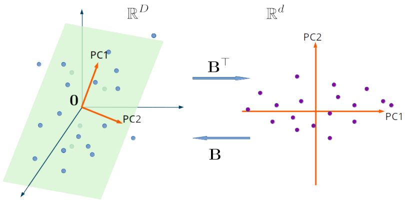

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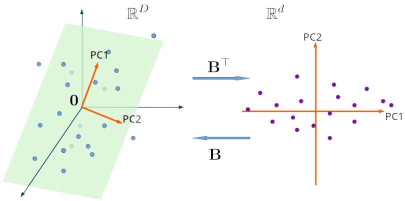

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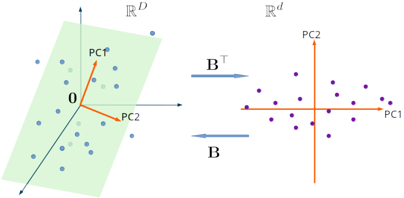

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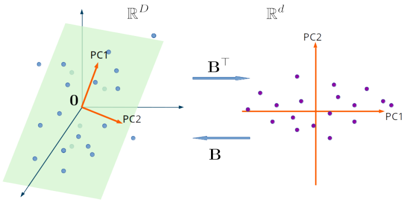

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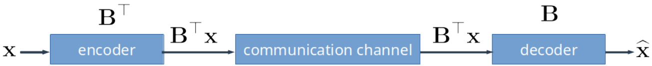
- $\widehat{\boldsymbol{x}} = \boldsymbol{B}\boldsymbol{B}^\intercal \boldsymbol{x} \approx \boldsymbol{x}$

Autoencoders

story in digital communications ...



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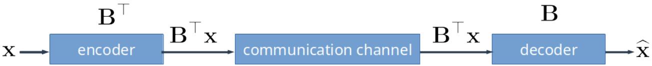

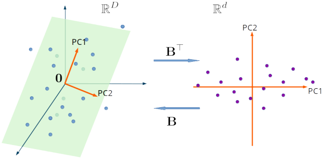

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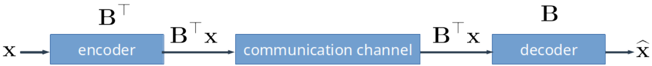
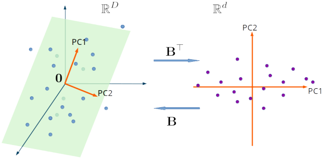
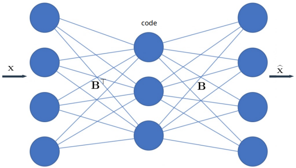




autoencoder: [Bourlard and Kamp, 1988, Hinton and Zemel, 1994]



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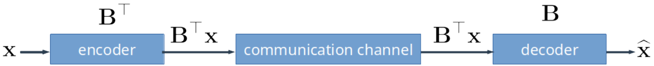

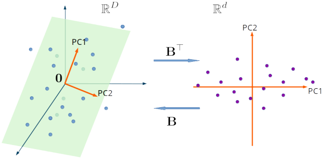

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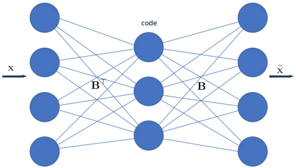

To find the basis $\boldsymbol{B}$, solve ($d \leq D$)

$$\min_{\boldsymbol{B} \in \mathbb{R}^{D \times d}} \sum_{i=1}^{m} \|\boldsymbol{x}_i - \boldsymbol{B}\boldsymbol{B}^\intercal \boldsymbol{x}_i\|_2^2$$

Autoencoders

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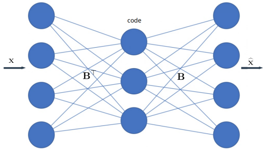

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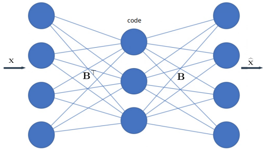

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$$\min_{\boldsymbol{B} \in \mathbb{R}^{D \times d}} \sum_{i=1}^{m} \|\boldsymbol{x}_i - \boldsymbol{B}\boldsymbol{B}^\top \boldsymbol{x}_i\|_2^2$$

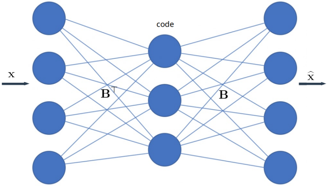
So the autoencoder is performing PCA!

One can even relax the weight tying:

$$\min_{\boldsymbol{B} \in \mathbb{R}^{D \times d}, \boldsymbol{A} \in \mathbb{R}^{d \times D}} \sum_{i=1}^{m} \|\boldsymbol{x}_i - \boldsymbol{B}\boldsymbol{A}^\top \boldsymbol{x}_i\|_2^2 \,,$$

which finds a basis (not necessarily orthonormal) $\boldsymbol{B}$ that spans the top singular space also [Baldi and Hornik, 1989], [Kawaguchi, 2016], [Lu and Kawaguchi, 2017].

Factorization



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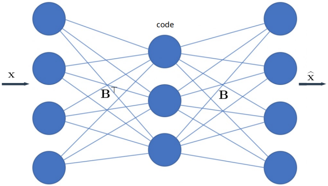

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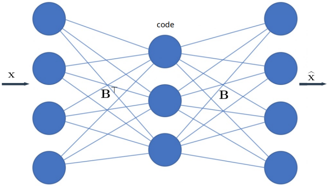

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Factorization: (or autoencoder without encoder)

$$\min_{\boldsymbol{B}\in\mathbb{R}^{D\times d}, \boldsymbol{Z}\in\mathbb{R}^{d\times m}} \sum_{i=1}^{m} \|\boldsymbol{x}_i - \boldsymbol{B}\boldsymbol{z}_i\|_2^2.$$

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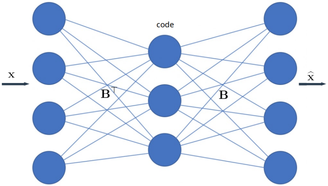

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All three formulations will find three different $\boldsymbol{B}$'s that span the same principal subspace [Tan and Mayrovouniotis, 1995, Li et al., 2020b, Li et al., 2020a, Valavi et al., 2020].

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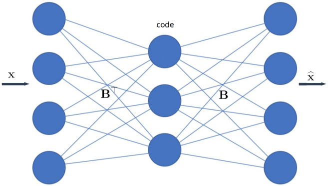

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Sparse coding

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What happens when we allow $d \geq D$?

Sparse coding

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What happens when we allow $d \geq D$? Underdetermined even if $\boldsymbol{B}$ is known.

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What happens when we allow $d \geq D$? Underdetermined even if $\boldsymbol{B}$ is known.

Sparse coding: assuming $\boldsymbol{z}_i$'s are sparse and $d \geq D$

$$\min_{\boldsymbol{B}\in\mathbb{R}^{D\times d},\boldsymbol{Z}\in\mathbb{R}^{d\times m}} \sum_{i=1}^{m} \|\boldsymbol{x}_i - \boldsymbol{B}\boldsymbol{z}_i\|_2^2 + \lambda \sum_{i=1}^{m} \Omega\left(\boldsymbol{z}_i\right)$$

where Ω promotes sparsity, e.g., $\Omega = \|\cdot\|_1$.

Sparse coding

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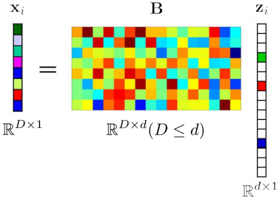

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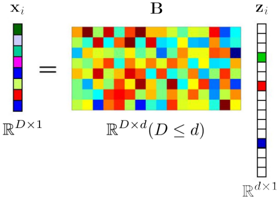

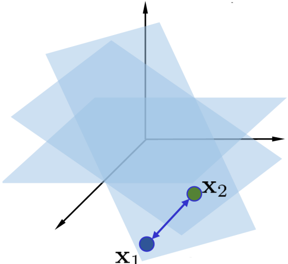

More on sparse coding

MENU **nature**

Letter | Published: 13 June 1996

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Bruno A. Olshausen & David J. Field

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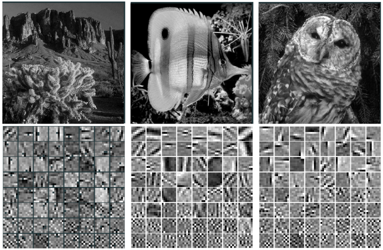

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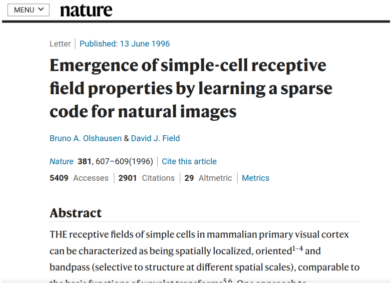
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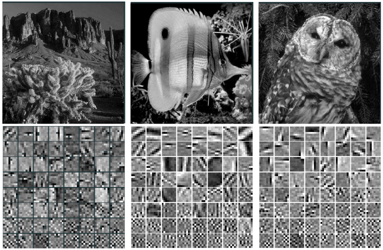
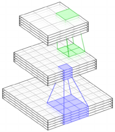


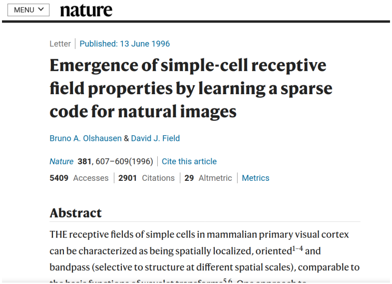
denoising

super resol.



recognition

More on sparse coding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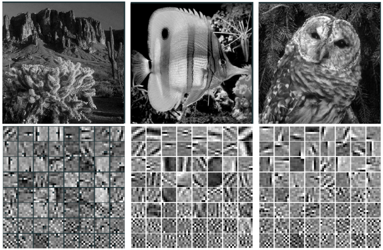

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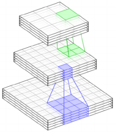
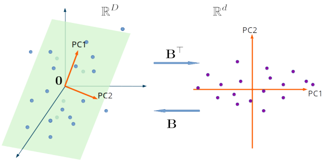


recognition

also known as **(sparse) dictionary learning** [Olshausen and Field, 1996, Mairal, 2014, Sun et al., 2017, Bai et al., 2018, Qu et al., 2019]

Outline

Quick summary of the linear models



PCA is effectively to identify the best-fit subspace to $\boldsymbol{x}_1, \dots, \boldsymbol{x}_m$

- $\boldsymbol{B}$ from $\boldsymbol{U}$ of $\boldsymbol{X} = \boldsymbol{U}\boldsymbol{S}\boldsymbol{V}^\intercal$
- autoencoder: $\min_{\boldsymbol{B} \in \mathbb{R}^{D \times d}} \sum_{i=1}^m \|\boldsymbol{x}_i - \boldsymbol{B}\boldsymbol{B}^\intercal \boldsymbol{x}_i\|_2^2$
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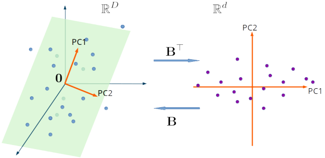

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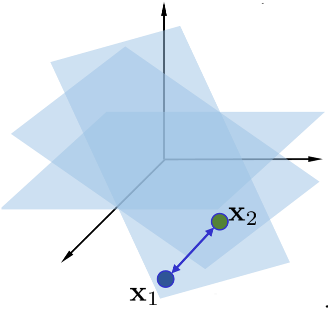

- when $d \geq D$, sparse coding/dictionary learning

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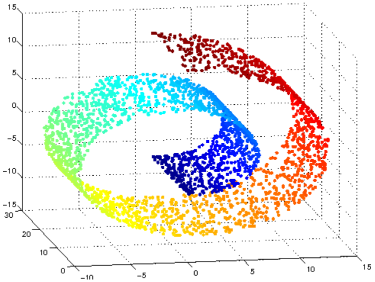
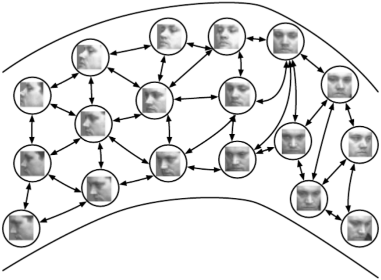
e.g., $\Omega = \|\cdot\|_1$

What about nonlinear data?





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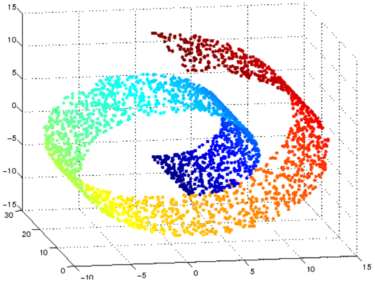

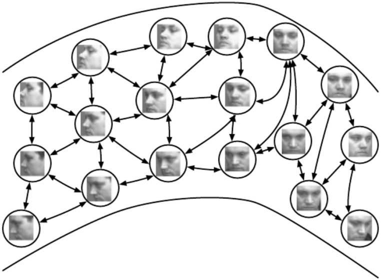

– Manifold, but not mathematically (i.e., differential geomety sense) rigorous

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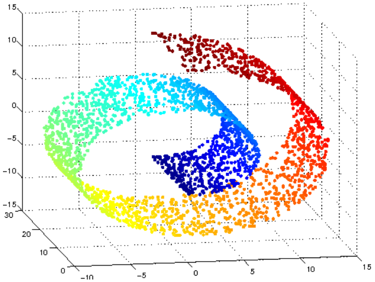

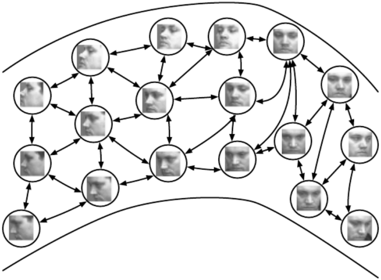

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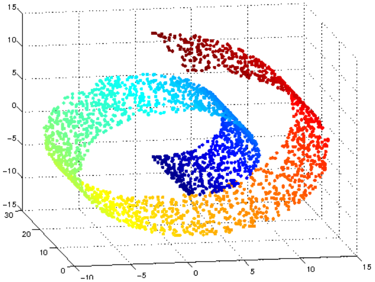
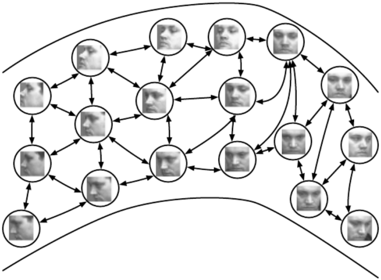


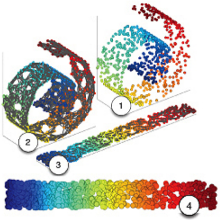


– Manifold, but not mathematically (i.e., differential geomety sense) rigorous

– **Working hypothesis for high-dimensional data**: practical data lie (approximately) on union of low-dimensional "manifolds". Why?

  * data generating processes often controlled by very few parameters

Manifold learning



Classic methods (mostly for visualization): .e.g.,

- ISOMAP [Tenenbaum, 2000]
- Locally-Linear Embedding [Roweis, 2000]
- Laplacian eigenmap [Belkin and Niyogi, 2001]
- t-distributed stochastic neighbor embedding (t-SNE) [van der Maaten and Hinton, 2008]

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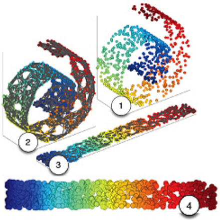

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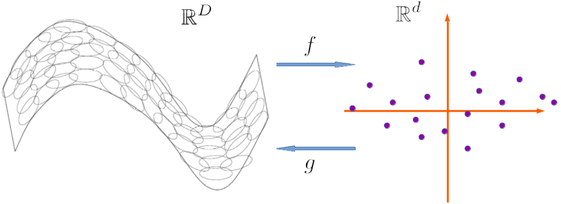
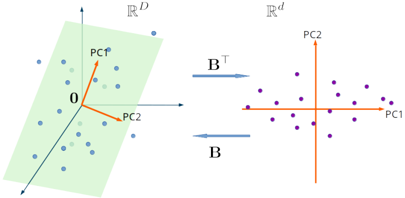
Nonlinear dimension reduction and representation learning:



From autoencoders to deep autoencoders



$$\min_{\boldsymbol{B} \in \mathbb{R}^{D \times d}} \sum_{i=1}^{m} \|\boldsymbol{x}_i - \boldsymbol{B}\boldsymbol{B}^\intercal \boldsymbol{x}_i\|_2^2$$

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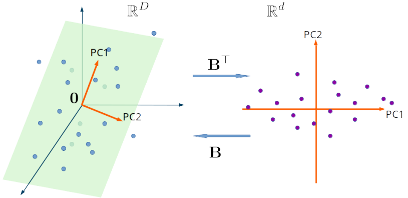

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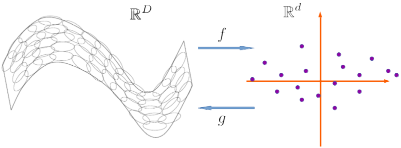
nonlinear generalization of the linear mappings:



deep autoencoders

$$\min_{\boldsymbol{V},\boldsymbol{W}} \sum_{i=1}^{m} \|\boldsymbol{x}_i - g_{\boldsymbol{V}} \circ f_{\boldsymbol{W}}(\boldsymbol{x}_i)\|_2^2$$

simply $\boldsymbol{A}^\intercal \to f_{\boldsymbol{W}}$ and $\boldsymbol{B} \to g_{\boldsymbol{V}}$

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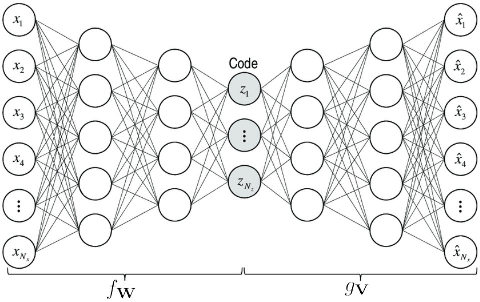
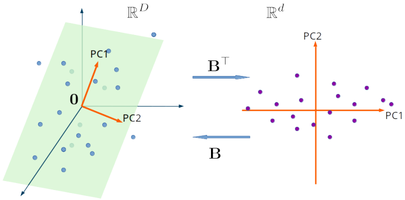


the landmark paper [Hinton, 2006]

From factorization to deep factorization



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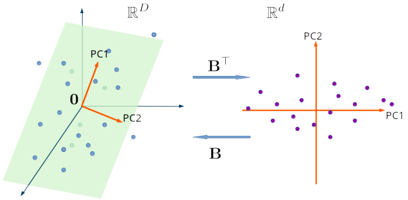

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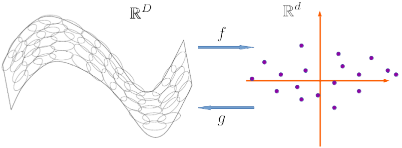

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simply $\boldsymbol{B} \to g_{\boldsymbol{V}}$

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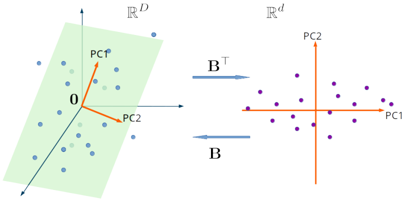

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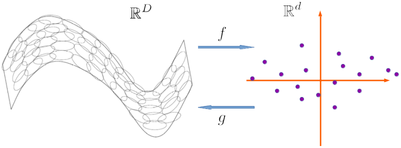

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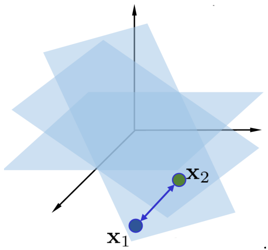
simply $\boldsymbol{B} \to g_{\boldsymbol{V}}$

[Tan and Mayrovouniotis, 1995, Fan and Cheng, 2018, Bojanowski et al., 2017, Park et al., 2019, Li et al., 2020b], also known as **deep decoder**.

From sparse coding to deep sparse coding



– when $d \geq D$, sparse coding/dictionary learning

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e.g., $\Omega = \|\cdot\|_1$

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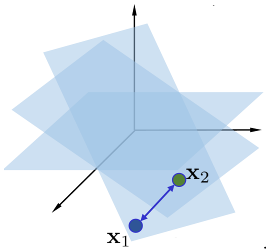

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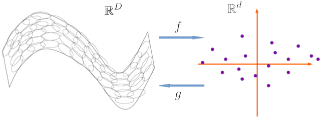
nonlinear generalization of the linear mappings: $(d \geq D)$

deep sparse coding/dictionary learning



$$\min_{\boldsymbol{V}, \boldsymbol{Z} \in \mathbb{R}^{d \times m}} \sum_{i=1}^{m} \|\boldsymbol{x}_i - g_{\boldsymbol{V}}(\boldsymbol{z}_i)\|_2^2 + \lambda \sum_{i=1}^{m} \Omega(\boldsymbol{z}_i)$$

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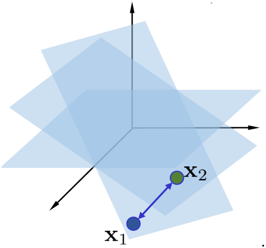

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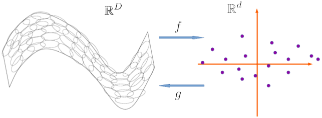

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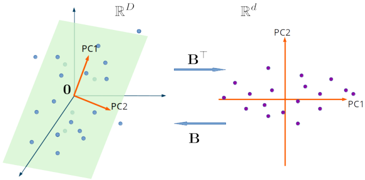
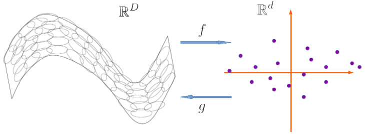
the 2nd also called **sparse autoencoder** [Ranzato et al., 2006].

Quick summary of linear vs nonlinear models





	linear models	nonlinear models
autoencoder	$\min_{\boldsymbol{B}} \sum_{i=1}^{m} \ell(\boldsymbol{x}_i, \boldsymbol{B}\boldsymbol{B}^\intercal \boldsymbol{x}_i)$ $\min_{\boldsymbol{B},\boldsymbol{A}} \sum_{i=1}^{m} \ell(\boldsymbol{x}_i, \boldsymbol{B}\boldsymbol{A}^\intercal \boldsymbol{x}_i)$	$\min_{\boldsymbol{V},\boldsymbol{W}} \sum_{i=1}^{m} \ell(\boldsymbol{x}_i, g_{\boldsymbol{V}} \circ f_{\boldsymbol{W}}(\boldsymbol{x}_i))$
factorization	$\min_{\boldsymbol{B},\boldsymbol{Z}} \sum_{i=1}^{m} \ell(\boldsymbol{x}_i, \boldsymbol{B}\boldsymbol{z}_i)$	$\min_{\boldsymbol{V},\boldsymbol{Z}} \sum_{i=1}^{m} \ell(\boldsymbol{x}_i, g_{\boldsymbol{V}}(\boldsymbol{z}_i))$
sparse coding	$\min_{\boldsymbol{B},\boldsymbol{Z}} \sum_{i=1}^{m} \ell(\boldsymbol{x}_i, \boldsymbol{B}\boldsymbol{z}_i)$ $+\lambda \sum_{i=1}^{m} \Omega(\boldsymbol{z}_i)$	$\min_{\boldsymbol{V},\boldsymbol{Z}} \sum_{i=1}^{m} \ell(\boldsymbol{x}_i, g_{\boldsymbol{V}}(\boldsymbol{z}_i))$ $+\lambda \sum_{i=1}^{m} \Omega(\boldsymbol{z}_i)$ $\min_{\boldsymbol{V},\boldsymbol{W}} \sum_{i=1}^{m} \ell(\boldsymbol{x}_i, g_{\boldsymbol{V}} \circ f_{\boldsymbol{W}}(\boldsymbol{x}_i))$ $+\lambda \sum_{i=1}^{m} \Omega(f_{\boldsymbol{W}}(\boldsymbol{x}_i))$

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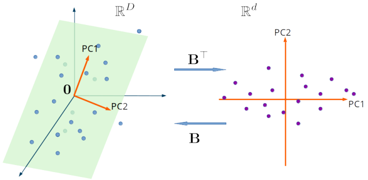

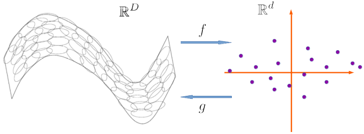

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ℓ can be general loss functions other than $\left\|\cdot\right\|_2$

Ω promotes sparsity, e.g., $\Omega = \left\|\cdot\right\|_1$

Outline

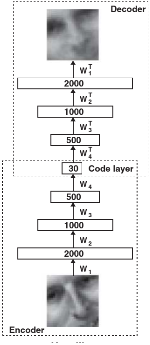
PCA for linear data

Extensions of PCA for nonlinear data

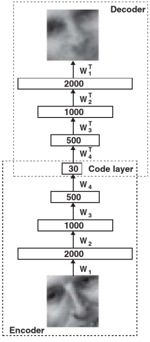
Application examples

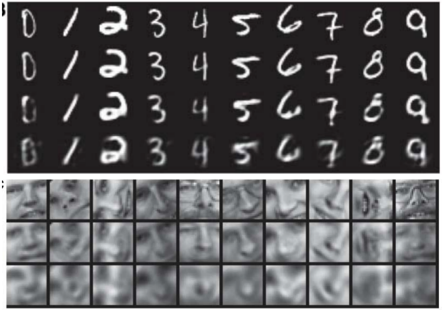
Suggested reading

Nonlinear dimension reduction



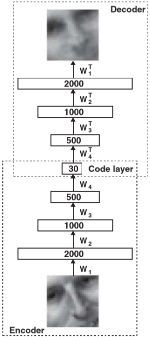
Nonlinear dimension reduction

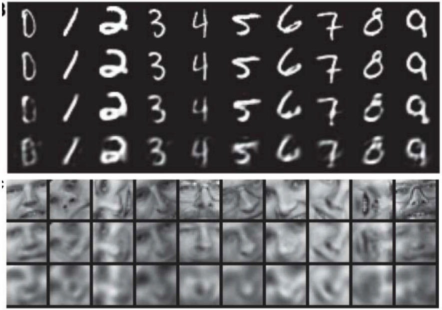




autoencoder vs. PCA vs. logistic PCA

Nonlinear dimension reduction





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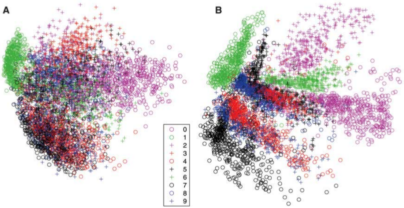

[Hinton, 2006]

Representation learning

Traditional learning pipeline

- feature extraction is "independent" of the learning models and tasks
- features are handcrafted and/or learned

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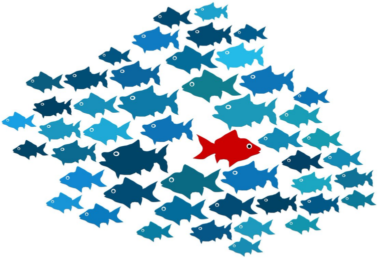
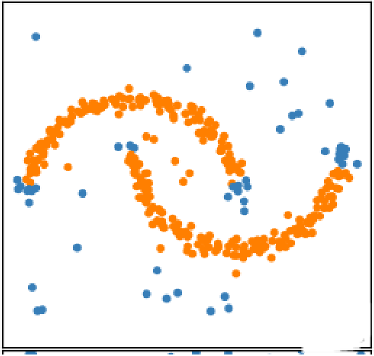
- semi-supervised (rich unlabeled data + little labeled data) learning

Outlier detection



(Credit: towardsdatascience.com)



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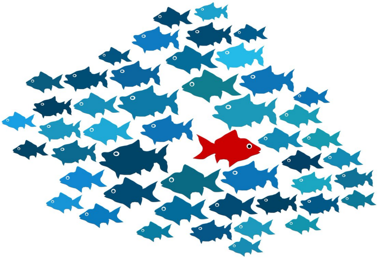

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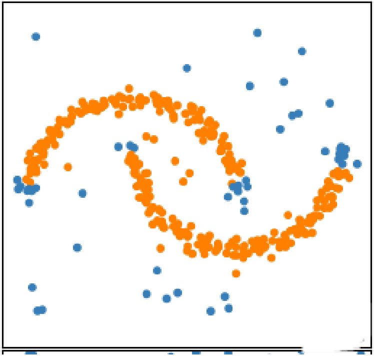

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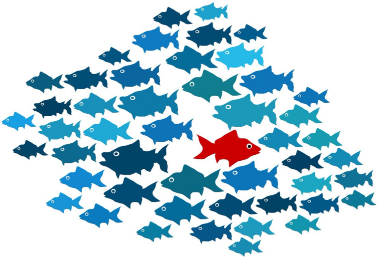

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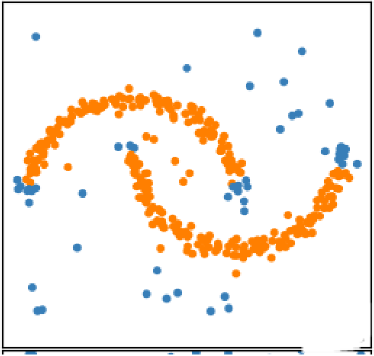

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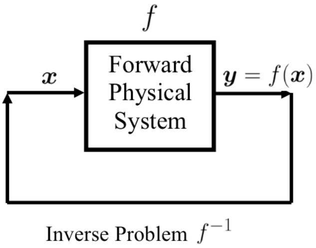
– for effective detection, better use ℓ that penalizes large errors less harshly than $\|\cdot\|_2^2$, e.g., $\ell\left(\boldsymbol{x}_i, g_{\boldsymbol{V}} \circ f_{\boldsymbol{W}}\left(\boldsymbol{x}_i\right)\right) = \left\|\boldsymbol{x}_i - g_{\boldsymbol{V}} \circ f_{\boldsymbol{W}}\left(\boldsymbol{x}_i\right)\right\|_2$ [Lai et al., 2019]

Deep generative prior



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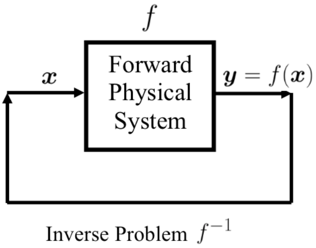

- **inverse problems**: given f and $\boldsymbol{y} = f(\boldsymbol{x})$, estimate $\boldsymbol{x}$
- often ill-posed, i.e., $\boldsymbol{y}$ doesn't contain enough info for recovery
- regularized formulation:

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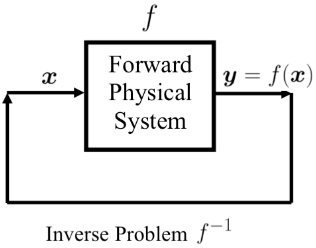

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Suppose $\boldsymbol{x}_1, \dots, \boldsymbol{x}_m$ come from the same manifold as $\boldsymbol{x}$

- train a deep factorization model on $\boldsymbol{x}_1, \dots, \boldsymbol{x}_m$: $\min_{\boldsymbol{V}, \boldsymbol{Z}} \sum_{i=1}^m \ell(\boldsymbol{x}_i, g_{\boldsymbol{V}}(\boldsymbol{z}_i))$
- $\boldsymbol{x} \approx g_{\boldsymbol{V}}(\boldsymbol{z})$ for a certain $\boldsymbol{z}$ so: $\min_{\boldsymbol{z}} \ \ell(\boldsymbol{y}, f \circ g_{\boldsymbol{V}}(\boldsymbol{z}))$. Some recent work even uses random $\boldsymbol{V}$, i.e., without training

[Ulyanov et al., 2018, Bora and Dimakis, 2017]

To be covered later

- convolutional encoder-decoder networks (i.e., segmentation, image processing, inverse problems)
- autoencoder sequence-to-sequence models (e.g., machine translation)
- variational autoencoders (generative models)

Outline

Suggested reading

- Representation Learning: A Review and New Perspectives (Bengio, Y., Courville, A., and Vincent, P.) [Bengio et al., 2013]
- Chaps 13–15 of Deep Learning [Goodfellow et al., 2017].
- Rethink autoencoders: Robust manifold learning [Li et al., 2020b]

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