

Unsupervised Representation Learning: Autoencoders, Factorization, and Sparse Coding

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Recap

We have talked about

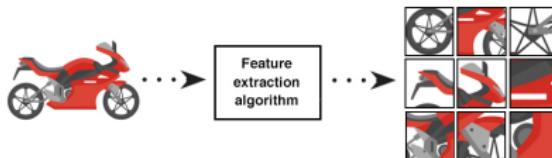
- Basic DNNs (multi-layer feedforward)
- Universal approximation theorems
- Numerical optimization and training DNNs

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

involve modification and composition of the basic DNNs

Feature engineering: old and new



Feature engineering: derive features for **efficient** learning

Credit: [Elgendi, 2020]

Traditional learning pipeline



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

Modern learning pipeline



- end-to-end DNN learning

Unsupervised representation learning

Learning feature/representation without task information (e.g., labels)
(ICLR — International Conference on Learning Representation)

Why not jump into the end-to-end learning?

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

The screenshot shows the Science journal website. At the top, there are navigation links for 'Contents', 'News', 'Careers', and 'Journals'. Below this, a 'SHARE' section includes social media icons for Facebook, Twitter, LinkedIn, and Email. The main title of the article is 'Reducing the Dimensionality of Data with Neural Networks' by G. E. Hinton, R. R. Salakhutdinov. Below the title, it says 'See all authors and affiliations'. The article is from 'Science' 29 April 2006; Vol. 311, Issue 5786, pp. 594-597; DOI: 10.1126/science.1127647. To the right, there is a thumbnail image of the journal cover for 'NEURAL COMPUTATION' featuring a blue neural network diagram. The journal's masthead 'NEURAL COMPUTATION' is visible above the image. Below the image, it says 'Monthly' and '288pp. per issue'. On the far right, there is a summary section with 'Abstract' and 'Authors' links.

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

Outline

PCA for linear data

Extensions of PCA for nonlinear data

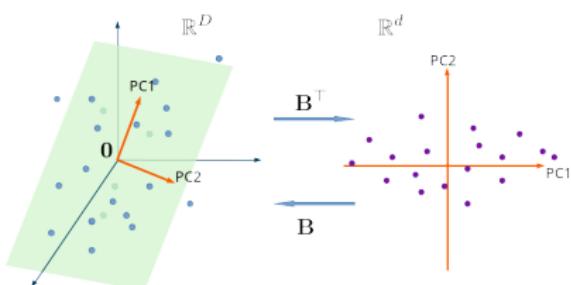
Application examples

Suggested reading

PCA: the geometric picture

Principal component analysis (PCA)

- Assume $x_1, \dots, x_n \in \mathbb{R}^D$ are zero-centered and write $\mathbf{X} = [x_1, \dots, x_m]$
- $\mathbf{X} = \mathbf{U}\mathbf{S}\mathbf{V}^\top$, where \mathbf{U} spans the column space (i.e., range) of \mathbf{X}
- Take top singular vectors \mathbf{B} from \mathbf{U} , and obtain $\mathbf{B}^\top \mathbf{X}$



PCA is effectively to identify the best-fit subspace to x_1, \dots, x_m

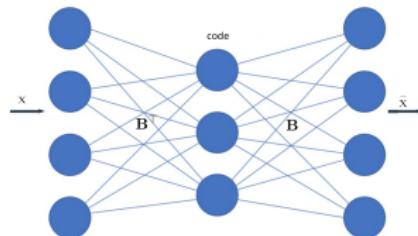
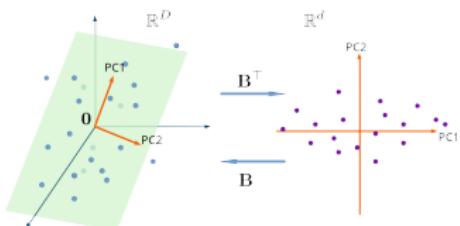
- \mathbf{B} has orthonormal columns, i.e., $\mathbf{B}^\top \mathbf{B} = \mathbf{I}$ ($\mathbf{B}\mathbf{B}^\top \neq \mathbf{I}$ when $D \neq d$)
- sample to representation:
 $x \mapsto x' \doteq \mathbf{B}^\top x$ ($\mathbb{R}^D \rightarrow \mathbb{R}^d$, dimension reduction)
- representation to sample:
 $x' \mapsto \hat{x} \doteq \mathbf{B}x'$ ($\mathbb{R}^d \rightarrow \mathbb{R}^D$)
- $\hat{x} = \mathbf{B}\mathbf{B}^\top x \approx x$

Autoencoders

... story in digital communications ...



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



– **Encoding:**

$$x \mapsto x' = B^\top x$$

– **Decoding:**

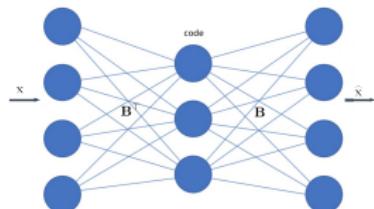
$$x' \mapsto BB^\top x = \hat{x}$$

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

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

Autoencoders

autoencoder:



To find the basis B , solve

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

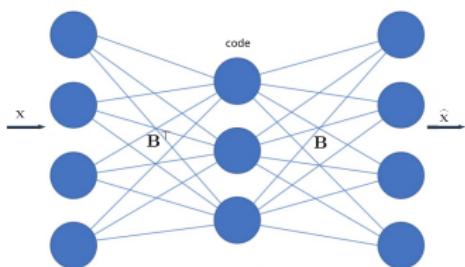
So the autoencoder is performing PCA!

One can even relax the weight tying:

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

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

Factorization



To perform PCA,

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

But: the basis B and the representations/codes z_i 's are all we care about

Factorization: (or autoencoder without encoder)

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

All three formulations will find three **different** B 's that span the **same** principal subspace [Tan and Mayrovouniotis, 1995, Li et al., 2020b, Li et al., 2020a, Valavi et al., 2020]. They're all doing PCA!

Sparse coding

Factorization: (or autoencoder without encoder)

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

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

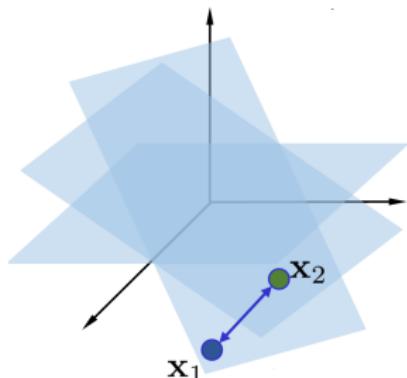
Sparse coding: assuming \mathbf{z}_i 's are sparse and $d \geq D$

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

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

$$\mathbf{x}_i = \mathbf{B} \mathbf{z}_i$$

$\mathbb{R}^{D \times 1} \quad \mathbb{R}^{D \times d} (D \leq d) \quad \mathbb{R}^{d \times 1}$



More on sparse coding

MENU ▾ nature

Letter | Published: 13 June 1996

Emergence of simple-cell receptive field properties by learning a sparse code for natural images

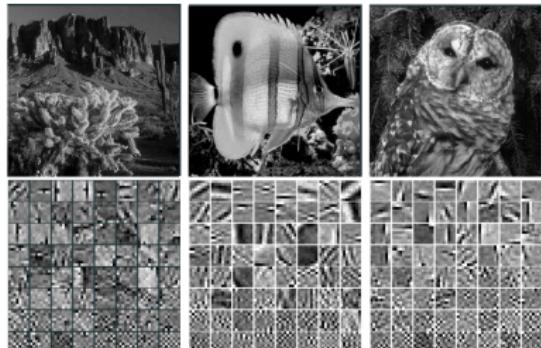
Bruno A. Olshausen & David J. Field

Nature 381, 607–609(1996) | Cite this article

5409 Accesses | 2901 Citations | 29 Altmetric | Metrics

Abstract

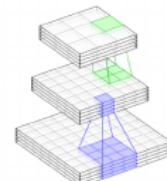
THE receptive fields of simple cells in mammalian primary visual cortex can be characterized as being spatially localized, oriented^{1–4} and bandpass (selective to structure at different spatial scales), comparable to



denoising



super resol.



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

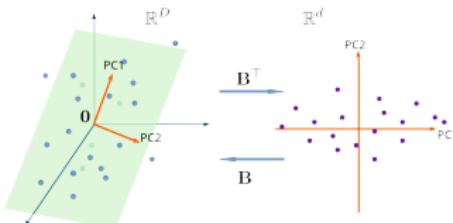
PCA for linear data

Extensions of PCA for nonlinear data

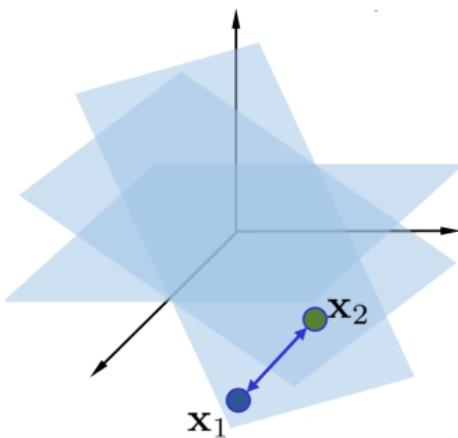
Application examples

Suggested reading

Quick summary of the linear models



PCA is effectively to identify the best-fit subspace to x_1, \dots, x_m



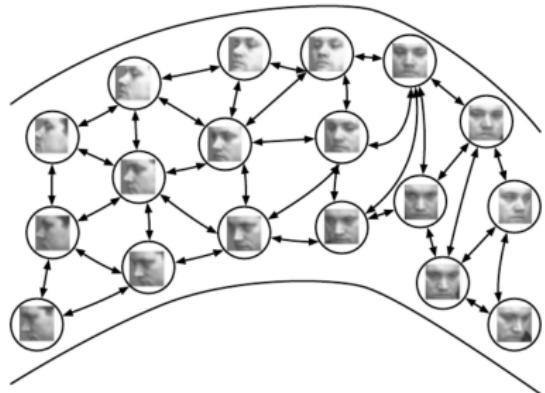
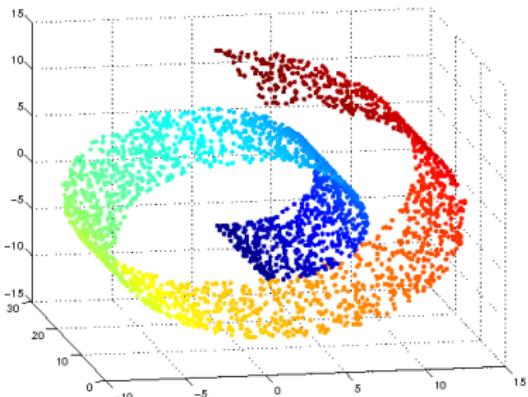
- B from U of $X = USV^\top$
- autoencoder:
$$\min_{B \in \mathbb{R}^{D \times d}} \sum_{i=1}^m \|x_i - BB^\top x_i\|_2^2$$
- autoencoder:
$$\min_{B \in \mathbb{R}^{D \times d}, A \in \mathbb{R}^{d \times D}} \sum_{i=1}^m \|x_i - BA^\top x_i\|_2^2$$
- factorization:
$$\min_{B \in \mathbb{R}^{D \times d}, Z \in \mathbb{R}^{d \times m}} \sum_{i=1}^m \|x_i - Bz_i\|_2^2$$

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

$$\min_{B \in \mathbb{R}^{D \times d}, Z \in \mathbb{R}^{d \times m}} \sum_{i=1}^m \|x_i - Bz_i\|_2^2 + \lambda \sum_{i=1}^m \Omega(z_i)$$

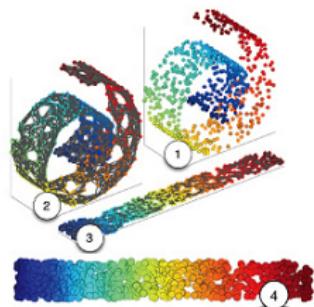
e.g., $\Omega = \|\cdot\|_1$

What about nonlinear data?



- Manifold, but not mathematically (i.e., differential geometry 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

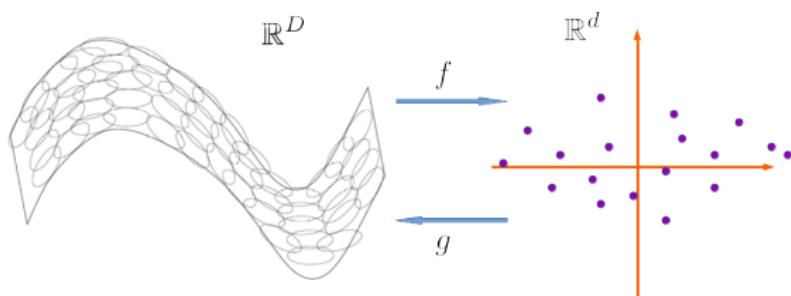
Manifold learning



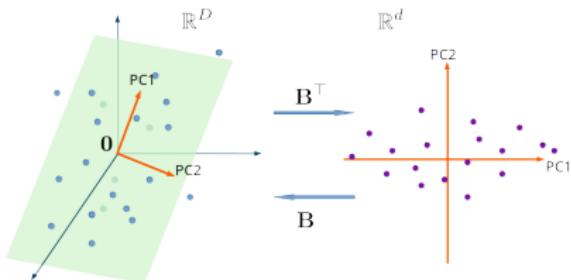
Classic methods (mostly for visualization): .e.g.,

- 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]

Nonlinear dimension reduction and representation learning:

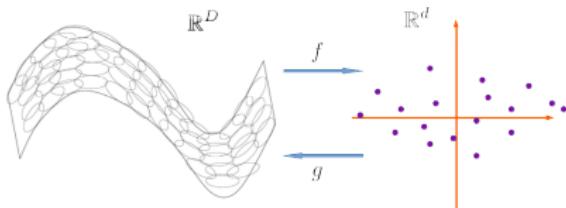


From autoencoders to deep autoencoders



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

nonlinear generalization of the linear mappings:



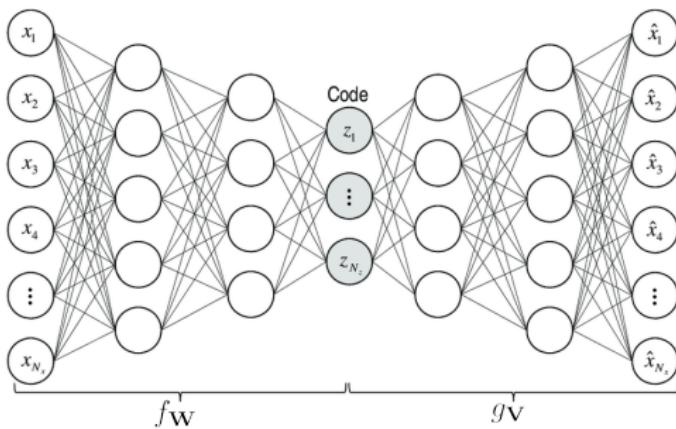
deep autoencoders

$$\min_{V, W} \sum_{i=1}^m \|x_i - g_V \circ f_W(x_i)\|_2^2$$

simply $A^\top \rightarrow f_W$ and $B \rightarrow g_V$

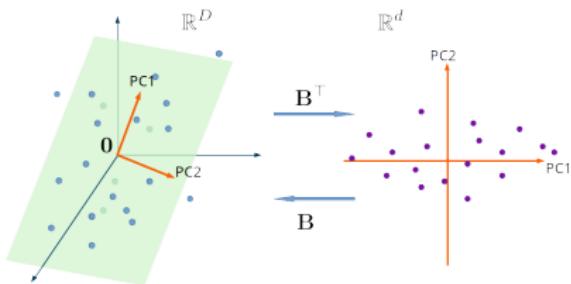
Deep autoencoders

$$\min_{V, W} \sum_{i=1}^m \|x_i - g_V \circ f_W(x_i)\|_2^2$$



the landmark paper [[Hinton, 2006](#)]

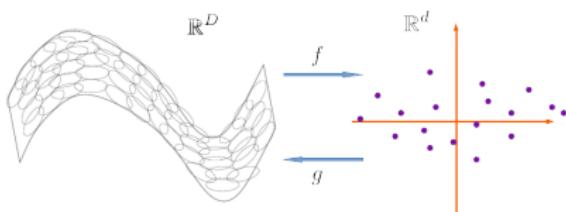
From factorization to deep factorization



factorization

$$\min_{B \in \mathbb{R}^{D \times d}, Z \in \mathbb{R}^{d \times m}} \sum_{i=1}^m \|x_i - Bz_i\|_2^2$$

nonlinear generalization of the linear mappings:



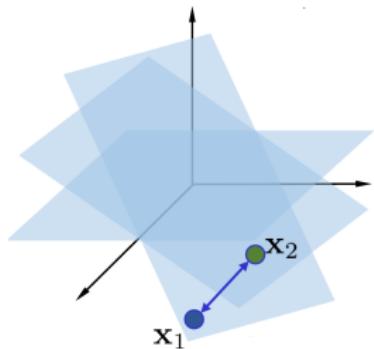
deep factorization

$$\min_{V, Z \in \mathbb{R}^{d \times m}} \sum_{i=1}^m \|x_i - g_V(z_i)\|_2^2$$

simply $B \rightarrow g_V$

[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



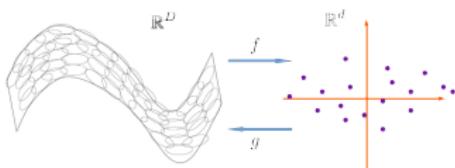
- when $d \geq D$, sparse coding/dictionary learning

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

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

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

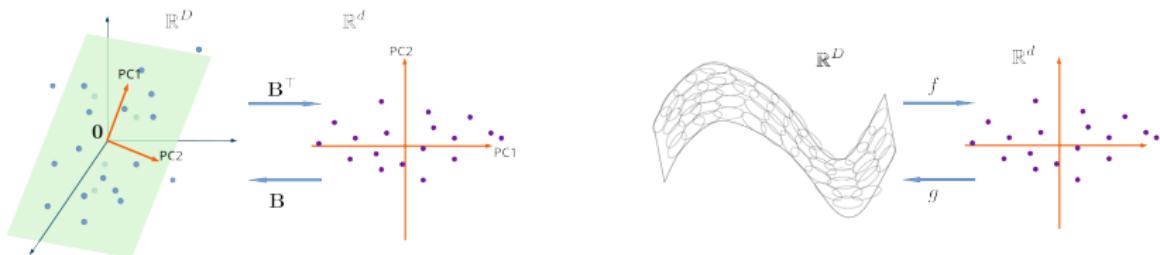
deep sparse coding/dictionary learning



$$\min_{\mathbf{V}, \mathbf{Z} \in \mathbb{R}^{d \times m}} \sum_{i=1}^m \|\mathbf{x}_i - \mathbf{g}\mathbf{v}(\mathbf{z}_i)\|_2^2 + \lambda \sum_{i=1}^m \Omega(\mathbf{z}_i)$$
$$\min_{\mathbf{V}, \mathbf{W}} \sum_{i=1}^m \|\mathbf{x}_i - \mathbf{g}\mathbf{v} \circ f_{\mathbf{W}}(\mathbf{x}_i)\|_2^2 + \sum_{i=1}^m \Omega(f_{\mathbf{W}}(\mathbf{x}_i))$$

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

Quick summary of linear vs nonlinear models



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

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

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

Outline

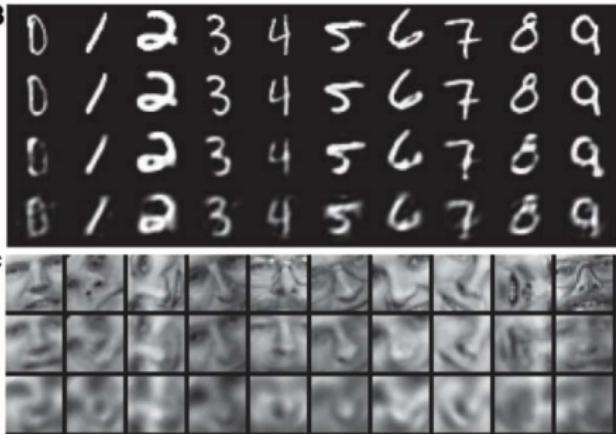
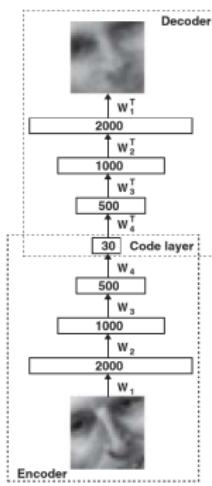
PCA for linear data

Extensions of PCA for nonlinear data

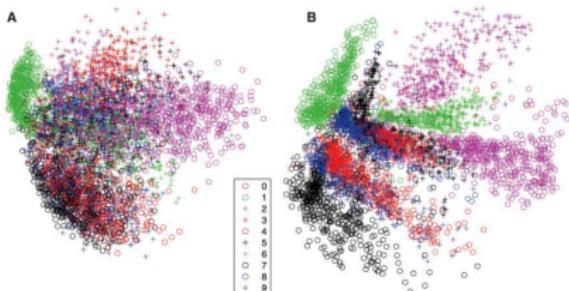
Application examples

Suggested reading

Nonlinear dimension reduction



autoencoder vs. PCA vs. logistic PCA



[Hinton, 2006]

Representation learning

Traditional learning pipeline

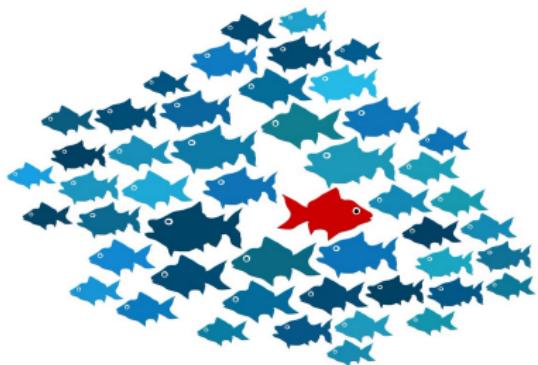


- feature extraction is “independent” of the learning models and tasks
- features are handcrafted and/or learned

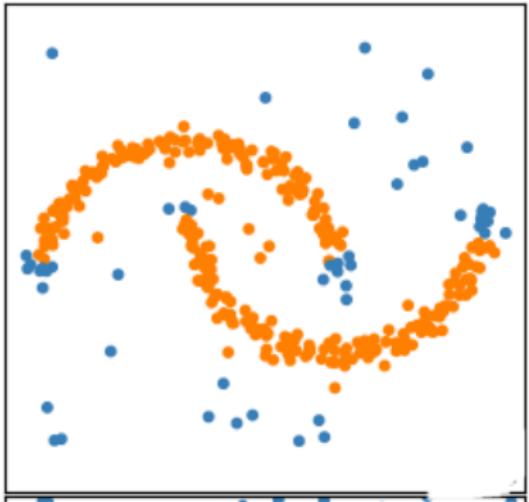
Use the low-dimensional codes as features/representations

- task agnostic
- less overfitting
- semi-supervised (rich unlabeled data + little labeled data) learning

Outlier detection

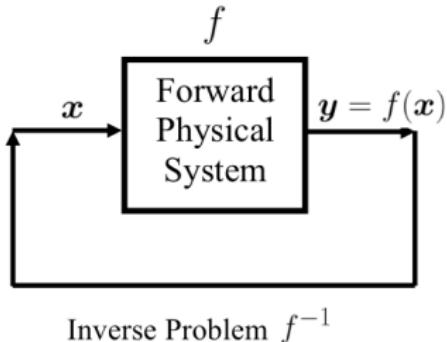


(Credit: towardsdatascience.com)



- idea: outliers don't obey the manifold assumption — the reconstruction error $\ell(\mathbf{x}_i, g_V \circ f_W(\mathbf{x}_i))$ is large after autoencoder training
- for effective detection, better use ℓ that penalizes large errors less harshly than $\|\cdot\|_2^2$, e.g., $\ell(\mathbf{x}_i, g_V \circ f_W(\mathbf{x}_i)) = \|\mathbf{x}_i - g_V \circ f_W(\mathbf{x}_i)\|_2$
[Lai et al., 2019]

Deep generative prior



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

$$\min_{\mathbf{x}} \ell(\mathbf{y}, f(\mathbf{x})) + \lambda \Omega(\mathbf{x})$$

where Ω contains extra info about \mathbf{x}

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

- train a deep factorization model on $\mathbf{x}_1, \dots, \mathbf{x}_m$:
$$\min_{\mathbf{V}, \mathbf{z}} \sum_{i=1}^m \ell(\mathbf{x}_i, g_{\mathbf{V}}(\mathbf{z}_i))$$
- $\mathbf{x} \approx g_{\mathbf{V}}(\mathbf{z})$ for a certain \mathbf{z} so: $\min_{\mathbf{z}} \ell(\mathbf{y}, f \circ g_{\mathbf{V}}(\mathbf{z}))$. Some recent work even uses random \mathbf{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)

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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](#)]

References i

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