

Unsupervised and Self-Supervised Learning

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Our roadmap

Covered: Fundamentals

Fundamental belief: universal approximation theorem

Basics of numerical optimization

Training DNNs: basic methods and tricks

Covered: Structured data: images, sequences, graphs

Work with images: convolutional neural networks & applications

Work with sequences: recurrent neural networks & applications

Working with graphs: graph neural networks & applications

Transformers, large-language models, and foundation models

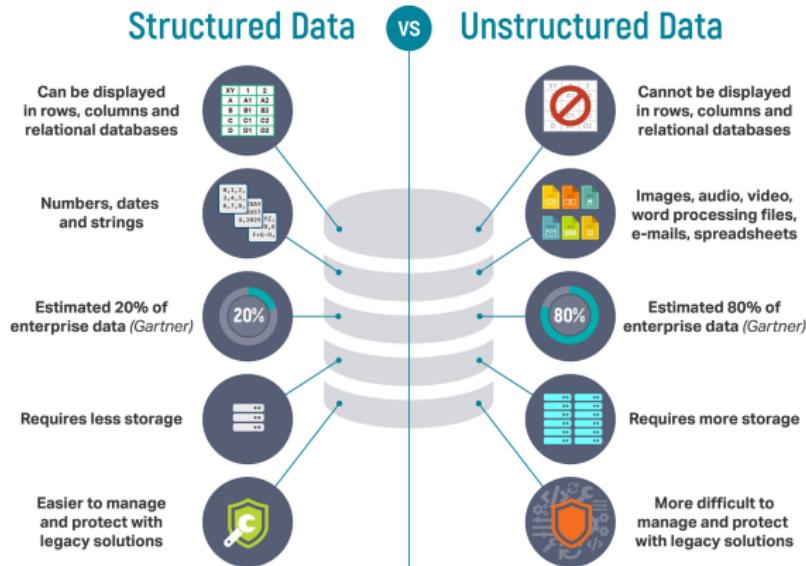
Now Generative/unsupervised/self-supervised/reinforcement learning

Learning representation without labels: dictionary learning, autoencoders, self-supervised learning

Learning probability distributions: generative models

(won't cover) Gaming time: deep reinforcement learning

Structured vs. unstructured data

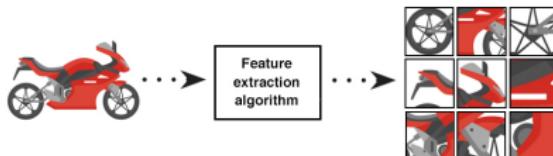


Credit: <https://lawtomated.com/>

[structured-data-vs-unstructured-data-what-are-they-and-why-care/](https://lawtomated.com/structured-data-vs-unstructured-data-what-are-they-and-why-care/)

- structured data also called **tabular data**
- structured data often directly fed into classical ML tools
- the success of DL mostly lies at **learning useful features/patterns from unstructured data**, i.e., **representation learning**

Feature engineering for unstructured data: 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)

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

The screenshot shows a journal article from the journal *Neural Computation*. The article is titled "A Fast Learning Algorithm for Deep Belief Nets" and is authored by Geoffrey E. Hinton, Simon Osindero, and Yee-Whye Teh. It was published online on May 17, 2006, with the DOI <https://doi.org/10.1162/neco.2006.18.7.17647>. The journal is described as "A Monthly Journal of Computational Neuroscience". The article abstract is partially visible.

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

Outline

PCA for linear data

Autoencoder: extensions of PCA for nonlinear data

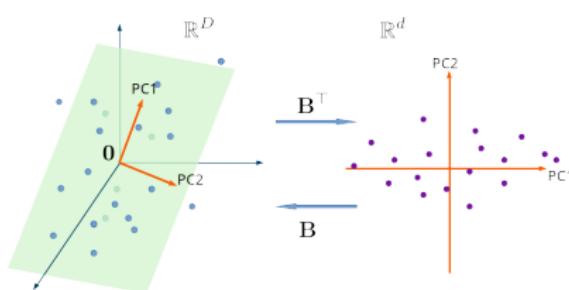
Applications of autoencoder

Self-supervised learning (SSL)

PCA: the geometric picture

Principal component analysis (PCA)

- $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^D$ zero-centered and write $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_m]^\top \in \mathbb{R}^{m \times D}$
- Compact SVD $\mathbf{X} = \mathbf{U}\mathbf{S}\mathbf{V}^\top$, where $\mathbf{V} \in \mathbb{R}^{D \times r}$ spans the row space of \mathbf{X}
- Take top right singular vectors \mathbf{B} from \mathbf{V} , and obtain $\mathbf{X}\mathbf{B}$



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

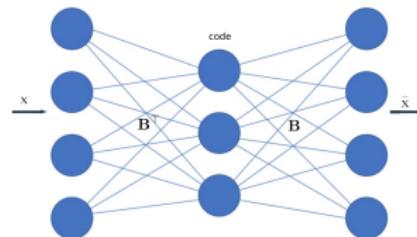
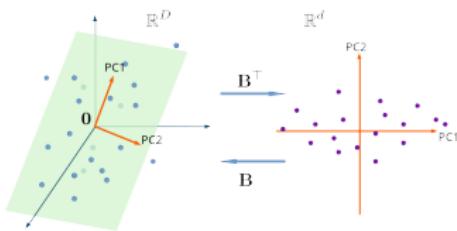
- \mathbf{B} has orthonormal columns, i.e., $\mathbf{B}^\top \mathbf{B} = \mathbf{I}$ ($\mathbf{B}\mathbf{B}^\top \neq \mathbf{I}$ when $D \neq d$)
- sample to representation:
 $\mathbf{x} \mapsto \mathbf{x}' \doteq \mathbf{B}^\top \mathbf{x}$ ($\mathbb{R}^D \rightarrow \mathbb{R}^d$, dimension reduction)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

Autoencoders

... story in digital communications ...



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



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

– **Encoding:**

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

– **Decoding:**

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

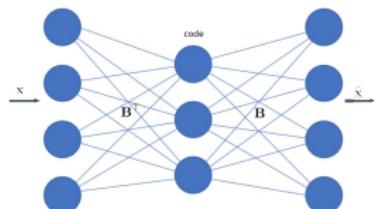
$$\min_{B \in \mathbb{R}^{D \times d}} \sum_{i=1}^m \|x_i - BB^\top x_i\|_2^2$$

or:

$$\min_{B \in \mathbb{R}^{D \times d}} \|\mathbf{X} - \mathbf{X}BB^\top\|_F^2$$

Autoencoders

autoencoder:



To find the basis B , solve

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

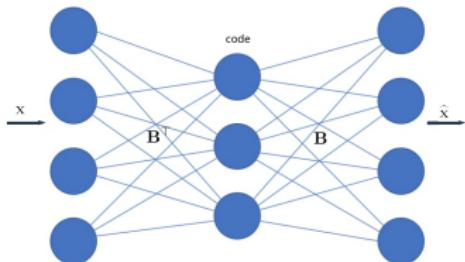
So the autoencoder is performing PCA!

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)

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

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)

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

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

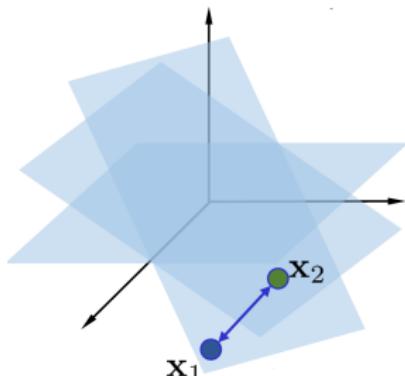
Sparse coding (i.e., dictionary learning): assuming \mathbf{z}_i 's are sparse and $d \geq D$

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

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

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

$\mathbf{x}_i \in \mathbb{R}^{D \times 1}$ $\mathbf{B} \in \mathbb{R}^{D \times d} (D \leq d)$ $\mathbf{z}_i \in \mathbb{R}^{d \times 1}$



More on sparse coding (dictionary learning)

MENU ▾ nature

Letter | Published: 13 June 1996

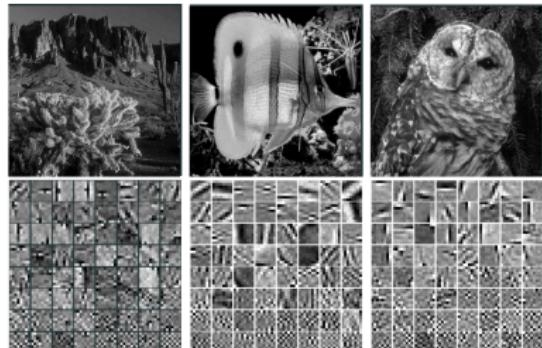
Emergence of simple-cell receptive field properties by learning a sparse code for natural images

Bruno A. Olshausen & David J. Field

Nature 381, 607–609(1996) | Cite this article
5409 Accesses | 2901 Citations | 29 Altmetric | Metrics

Abstract

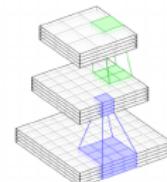
THE receptive fields of simple cells in mammalian primary visual cortex can be characterized as being spatially localized, oriented^{1–4} and bandpass (selective to structure at different spatial scales), comparable to



denoising



super resol.



recognition

References: [Olshausen and Field, 1996, Mairal, 2014, Sun et al., 2017, Bai et al., 2018, Qu et al., 2019]

Outline

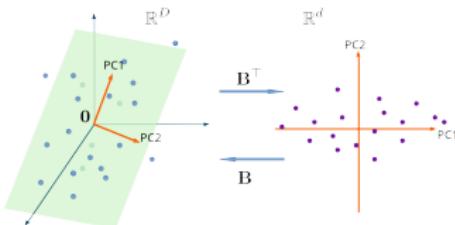
PCA for linear data

Autoencoder: extensions of PCA for nonlinear data

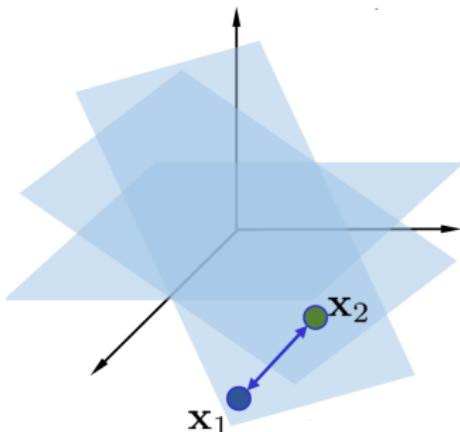
Applications of autoencoder

Self-supervised learning (SSL)

Quick summary of the linear models



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



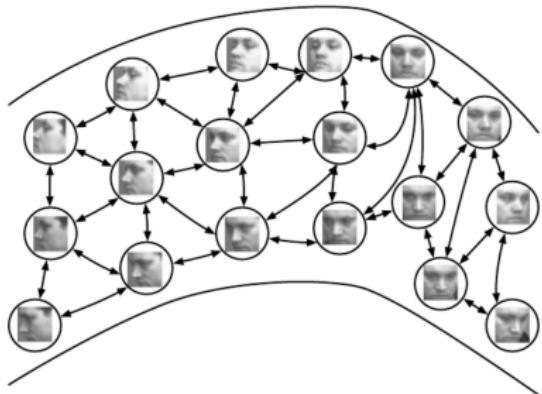
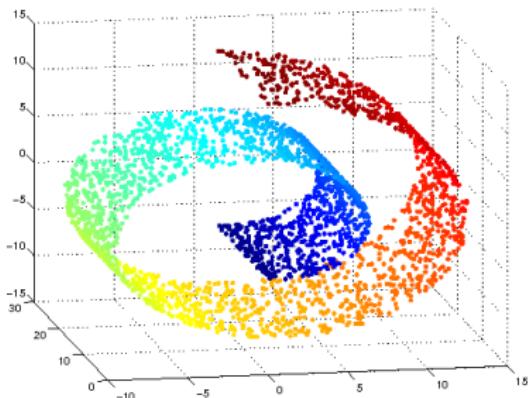
- B from V of $X = USV^\top$
- autoencoder:
 $\min_{B \in \mathbb{R}^{D \times d}} \sum_{i=1}^m \|x_i - BB^\top x_i\|_2^2$
- autoencoder:
 $\min_{B \in \mathbb{R}^{D \times d}, A \in \mathbb{R}^{D \times d}} \sum_{i=1}^m \|x_i - BA^\top x_i\|_2^2$
- factorization:
 $\min_{B \in \mathbb{R}^{D \times d},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

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

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

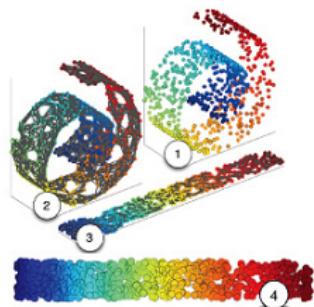
e.g., $\Omega = \|\cdot\|_1$

What about nonlinear data?



- Manifold, but not mathematically (i.e., differential geometry sense) rigorous
- **(No. 1?) 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

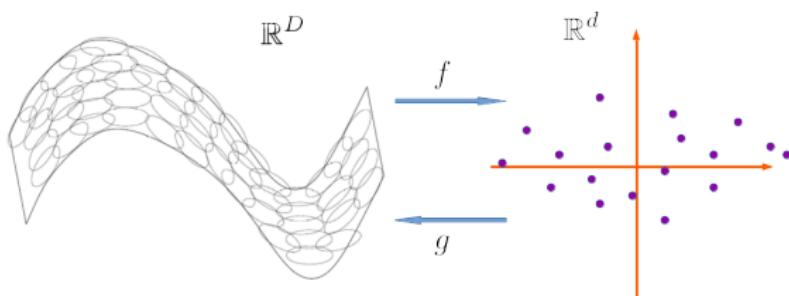
Manifold learning



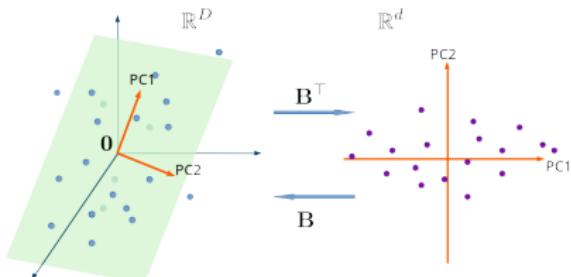
Classic methods (mostly for visualization): e.g.,

- 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

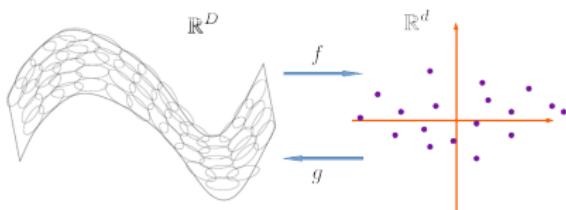


From autoencoders to deep autoencoders



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

nonlinear generalization of the linear mappings:



deep autoencoders

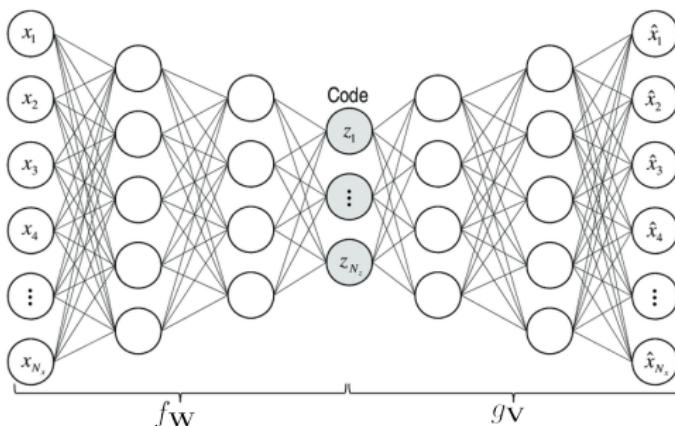
$$\min_{V, W} \sum_{i=1}^m \|x_i - g_V \circ f_W(x_i)\|_2^2$$

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

A side question: why not calculate “nonlinear basis”?

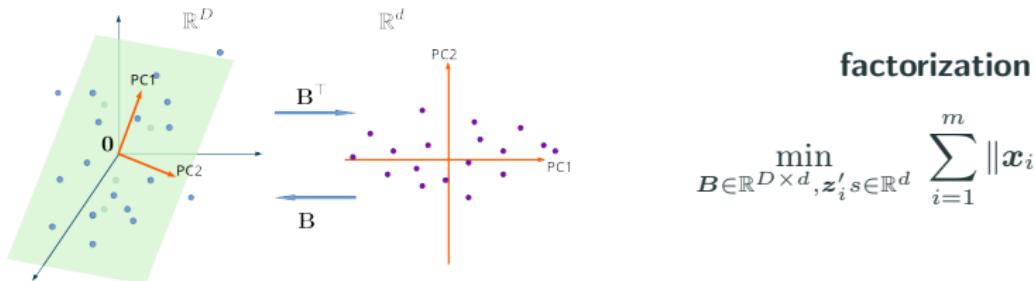
Deep autoencoders

$$\min_{\mathbf{V}, \mathbf{W}} \sum_{i=1}^m \| \mathbf{x}_i - \mathbf{g}_{\mathbf{V}} \circ \mathbf{f}_{\mathbf{W}} (\mathbf{x}_i) \|_2^2$$



the landmark paper [Hinton, 2006] ... that introduced **pretraining**

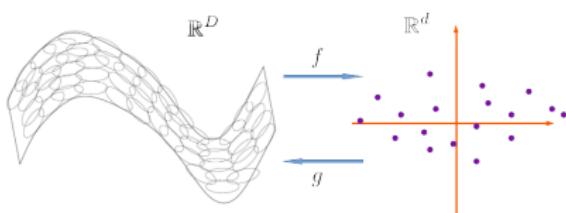
From factorization to deep factorization



factorization

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

nonlinear generalization of the linear mappings:



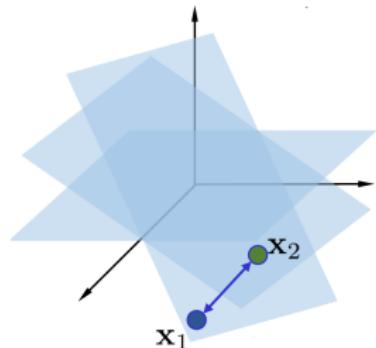
deep factorization

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

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



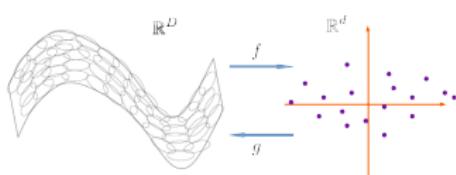
- when $d \geq D$, sparse coding/dictionary learning

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

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

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

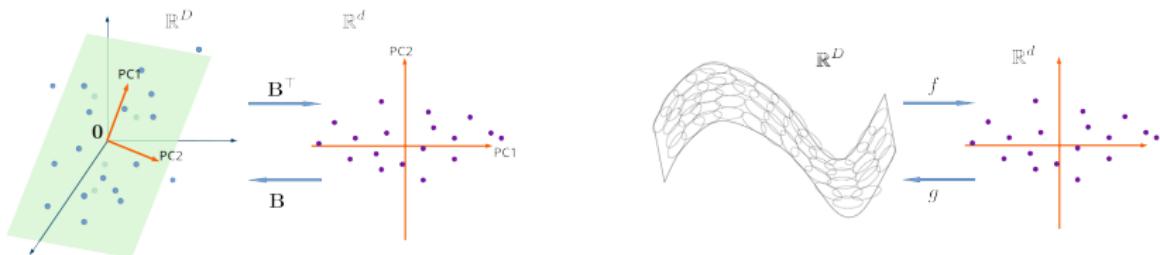
deep sparse coding/dictionary learning



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

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

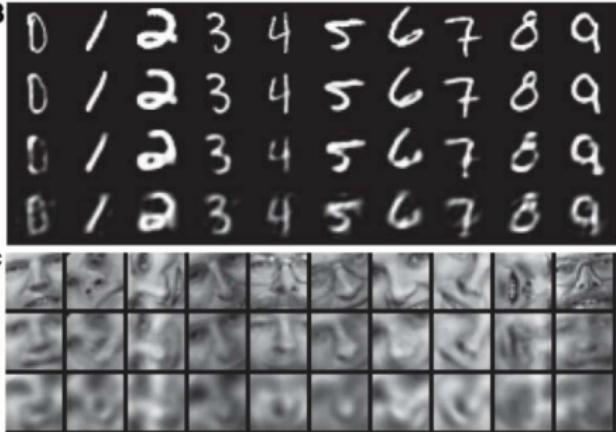
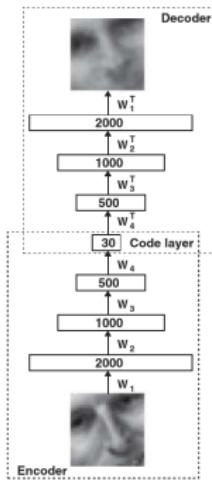
PCA for linear data

Autoencoder: extensions of PCA for nonlinear data

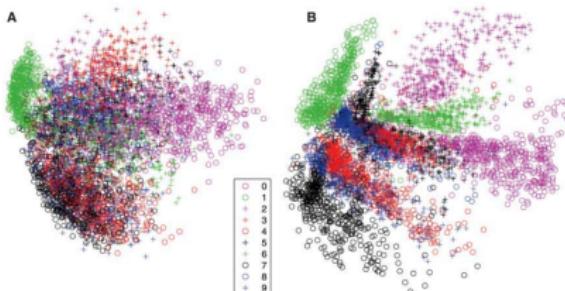
Applications of autoencoder

Self-supervised learning (SSL)

Nonlinear dimension reduction



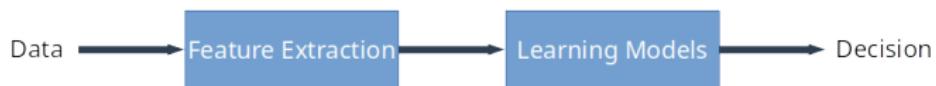
autoencoder vs. PCA vs. logistic PCA



[Hinton, 2006]

Representation learning

Traditional learning pipeline

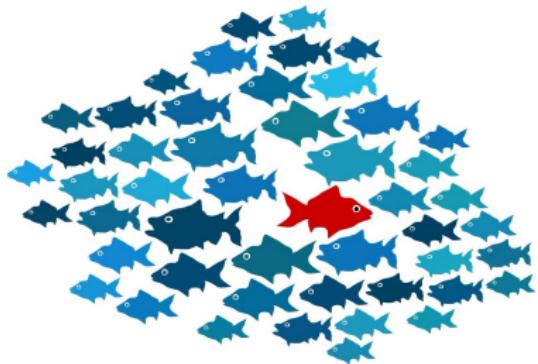


- feature extraction is “independent” of the learning models and tasks
- features are handcrafted and/or learned

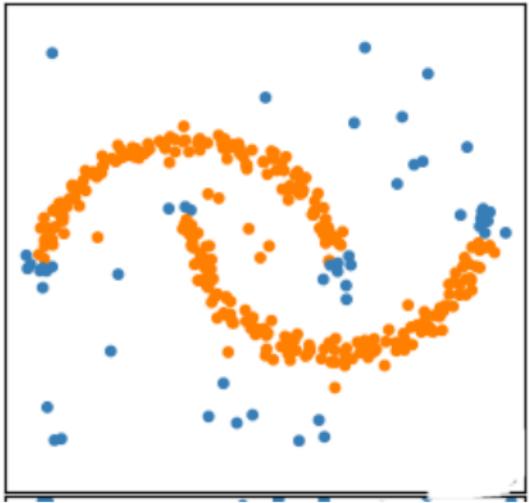
Use the low-dimensional codes as features/representations

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

Outlier detection

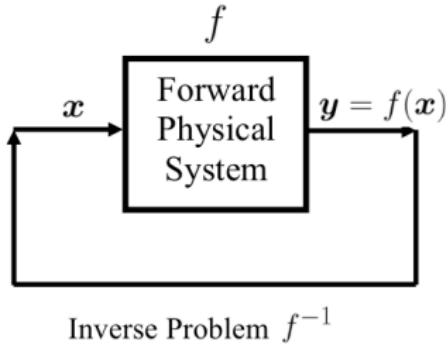


(Credit: towardsdatascience.com)



- 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 $\mathbf{y} \approx f(\mathbf{x})$, estimate \mathbf{x}
- often ill-posed, i.e., \mathbf{y} doesn't contain enough info for recovery
- **regularized data-fitting** 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

See: [Pan et al., 2020, Ulyanov et al., 2018, Bora et al., 2017,
Wang et al., 2021, Zhuang et al., 2022]

Outline

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Autoencoder: extensions of PCA for nonlinear data

Applications of autoencoder

Self-supervised learning (SSL)

SSL: marriage of supervised and unsupervised learning

Why not supervised learning?

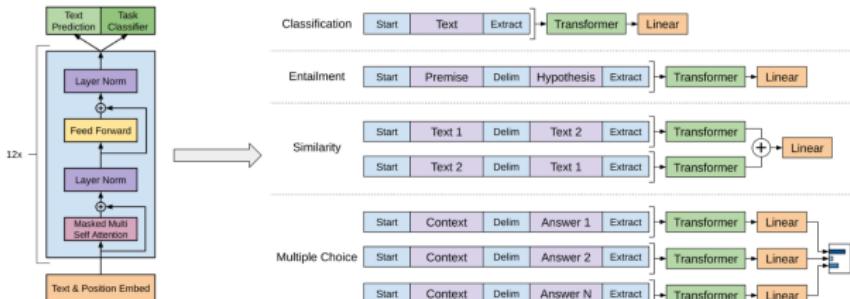
- labeling is expensive
- unlabeled data can be abundant
- supervised learning are task-specific (despite transfer learning)

What's self-supervised learning?

- like unsupervised learning: no task-specific labels
- like supervised learning: trained on tasks defined on the unlabeled data

Pretraining: (transformer-based)
decoder-only architectures pretrained
on **language model** $\mathbb{P} [x^{(t+1)} | x^{(t)}, \dots, x^{(1)}]$

Finetuning: on task-specific
supervised data



SSL: contrastive learning

learning embedding/representation that respects certain predefined constraints/goals

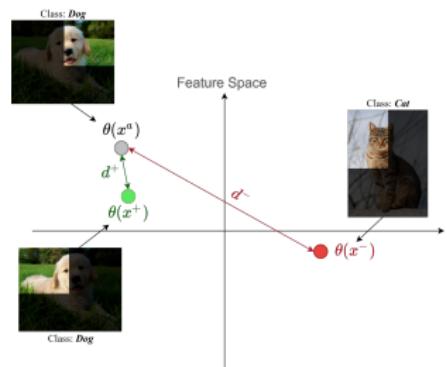
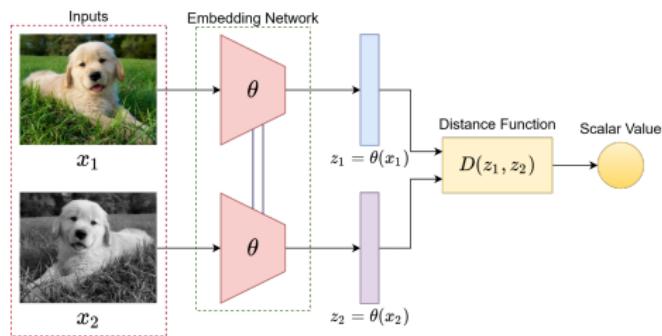
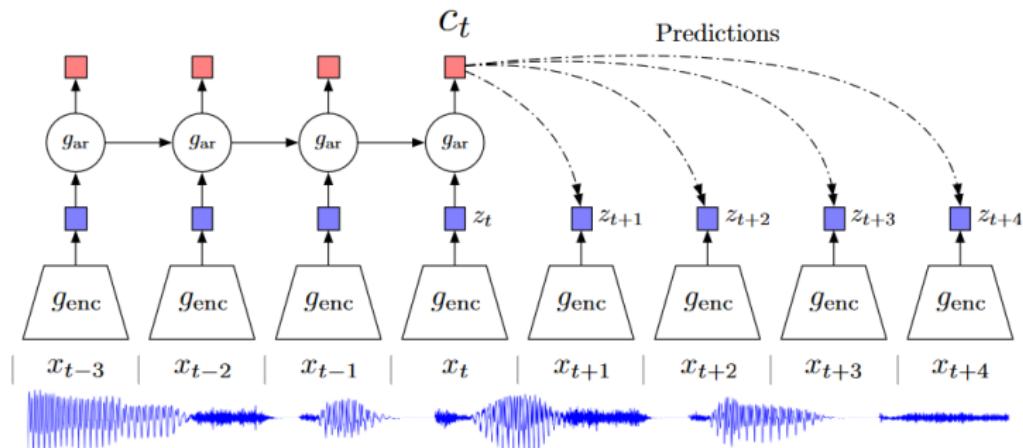


Image credit:

<https://www.v7labs.com/blog/self-supervised-learning-guide>

SSL: sequential prediction



Language modeling is a special case

Image credit:

<https://www.v7labs.com/blog/self-supervised-learning-guide>

More about self-supervised learning

- Awesome Self-Supervised Learning
<https://github.com/jason718/awesome-self-supervised-learning>
- A Cookbook of Self-Supervised Learning
<https://arxiv.org/abs/2304.12210>
- Know Your Self-supervised Learning: A Survey on Image-based Generative and Discriminative Training <https://arxiv.org/abs/2305.13689>
- https://cs229.stanford.edu/notes2021spring/notes2021spring/cs229_lecture_selfsupervision_final.pdf
- Self-Supervised Representation Learning <https://lilianweng.github.io/posts/2019-11-10-self-supervised/>

References i

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