

# 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

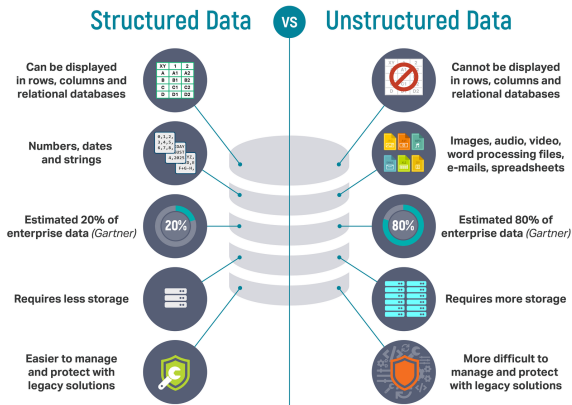
## **Now** Generative/unsupervised/self-supervised/reinforcement learning

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

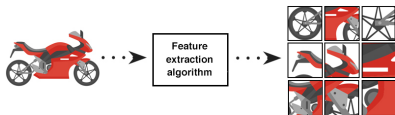


Credit: <https://lawtomated.com/>

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

- structured data 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: [Elgendy, 2020]

## Traditional learning pipeline



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

## Modern learning pipeline

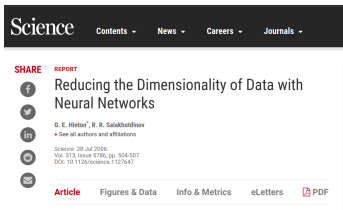


- end-to-end DNN learning

# 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](#)])



Science Contents - News - Careers - Journals -

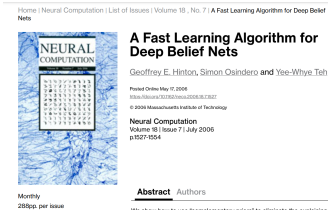
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**Reducing the Dimensionality of Data with Neural Networks**

G. E. Hinton<sup>1</sup>, R. R. Salakhutdinov<sup>2</sup>  
+ See all authors and affiliations

Science 29 Jul 2006  
Vol. 313, Issue 5746, pp. 504-507  
DOI: 10.1126/science.1127647

Article Figures & Data Info & Metrics eLetters PDF



Home | Neural Computation | List of Issues | Volume 18, No. 7 | A Fast Learning Algorithm for Deep Belief Nets

**NEURAL COMPUTATION**

**A Fast Learning Algorithm for Deep Belief Nets**

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

Printed Online May 17, 2006  
ISSN: 0899-7667  
© 2006 Massachusetts Institute of Technology

Neural Computation  
Volume 18 | Issue 7, July 2006  
p.1527-1554

Monthly  
288pp. per issue

Abstract Authors

We show how to use "stochastic restricted Boltzmann machines" to allocate the available

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

PCA for linear data

Autoencoder: extensions of PCA for nonlinear data

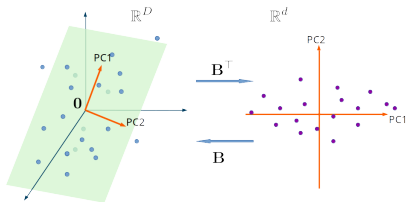
Applications of autoencoder

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  $\mathbf{x}_1, \dots, \mathbf{x}_m$

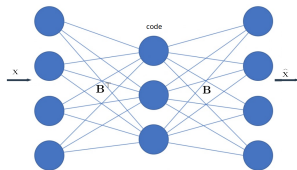
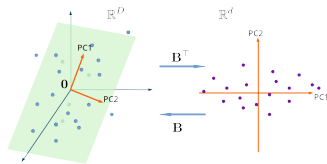
- $\mathbf{B}$  has orthonormal columns, i.e.,  $\mathbf{B}^\top \mathbf{B} = \mathbf{I}$  ( $\mathbf{B}\mathbf{B}^\top \neq \mathbf{I}$  when  $D \neq d$ )
- sample to representation:  
 $\mathbf{x} \mapsto \mathbf{x}' \doteq \mathbf{B}^\top \mathbf{x}$  ( $\mathbb{R}^D \rightarrow \mathbb{R}^d$ ,  
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:** [Bourlard and Kamp, 1988, Hinton and Zemel, 1994]



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

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

or:

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

– **Encoding:**

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

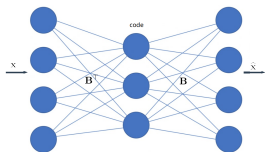
– **Decoding:**

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



# Autoencoders

autoencoder:



To find the basis  $B$ , solve

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

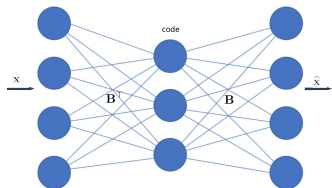
So the autoencoder is performing PCA!

One can even relax the weight tying:

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

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,

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

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)

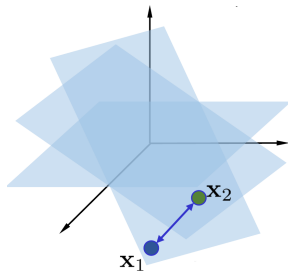
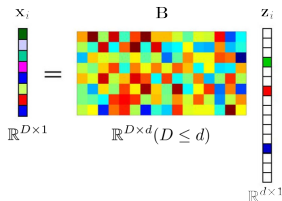
$$\min_{B \in \mathbb{R}^{D \times d}, z'_i s \in \mathbb{R}^d} \sum_{i=1}^m \|x_i - Bz_i\|_2^2.$$

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

**Sparse coding (i.e., dictionary learning):** assuming  $z_i$ 's are sparse and  $d \geq D$

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

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



# 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

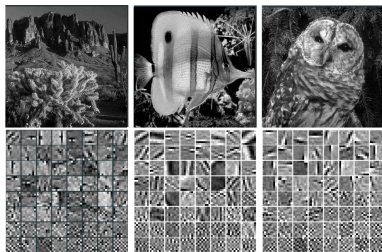
Bruno A. Olshausen & David J. Field

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

5409 Accesses | 2901 Citations | 29 Altmetric | [Metrics](#)

### Abstract

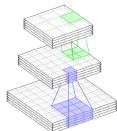
THE receptive fields of simple cells in mammalian primary visual cortex can be characterized as being spatially localized, oriented<sup>1-4</sup> and bandpass (selective to structure at different spatial scales), comparable to



denoising



super resol.



recognition

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

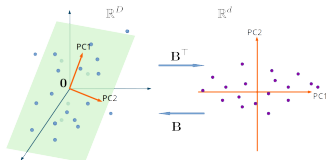
PCA for linear data

Autoencoder: extensions of PCA for nonlinear data

Applications of autoencoder

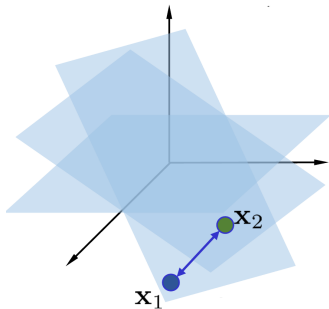
Self-supervised learning (SSL)

# Quick summary of the linear models



PCA is effectively to identify  
the best-fit subspace to

$$\mathbf{x}_1, \dots, \mathbf{x}_m$$



–  $B$  from  $V$  of  $X = USV^T$

– autoencoder:

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

– autoencoder:

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

– factorization:

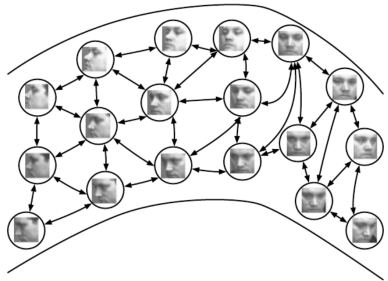
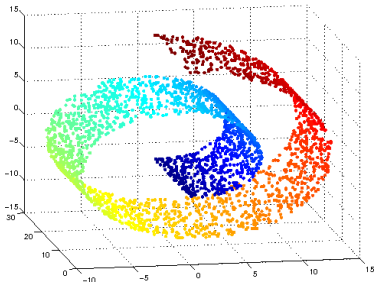
$$\min_{B \in \mathbb{R}^{D \times d}, \mathbf{z}'_i \in \mathbb{R}^d} \sum_{i=1}^m \|\mathbf{x}_i - B\mathbf{z}'_i\|_2^2$$

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

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

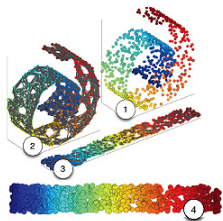
e.g.,  $\Omega = \|\cdot\|_1$

# 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

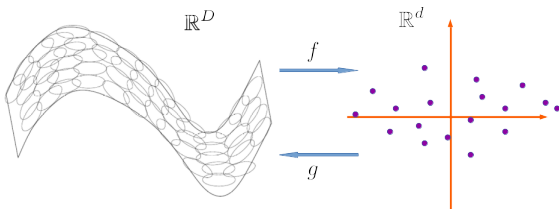
# Manifold learning



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

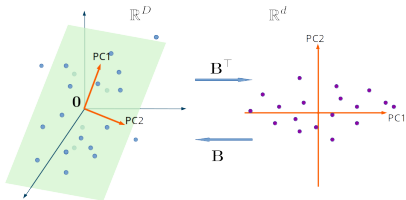
- ISOMAP [Tenenbaum, 2000]
- Locally-linear embedding [Roweis, 2000]
- Laplacian eigenmap [Belkin and Niyogi, 2001]
- t-distributed stochastic neighbor embedding (t-SNE) [van der Maaten and Hinton, 2008]

Nonlinear dimension reduction and representation learning



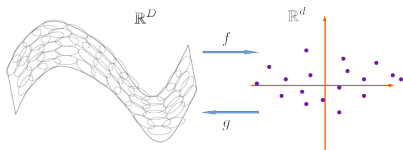


# From autoencoders to deep autoencoders



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

nonlinear generalization of the linear mappings:



**deep autoencoders**

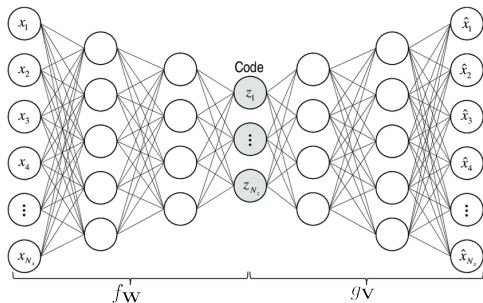
$$\min_{V, W} \sum_{i=1}^m \|\mathbf{x}_i - gV \circ fW(\mathbf{x}_i)\|_2^2$$

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

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

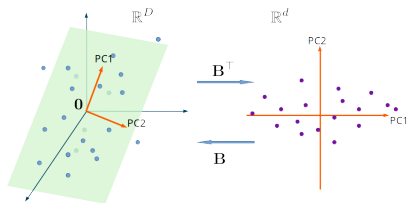
# Deep autoencoders

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



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

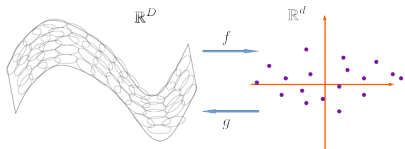
# From factorization to deep factorization



factorization

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

nonlinear generalization of the linear mappings:



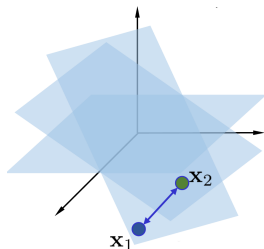
deep factorization

$$\min_{V, z'_i \in \mathbb{R}^d} \sum_{i=1}^m \|\mathbf{x}_i - gV(z'_i)\|_2^2$$

simply  $B \rightarrow gV$

[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



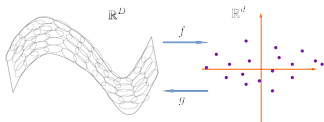
- when  $d \geq D$ , sparse coding/dictionary learning

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

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

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

## deep sparse coding/dictionary learning

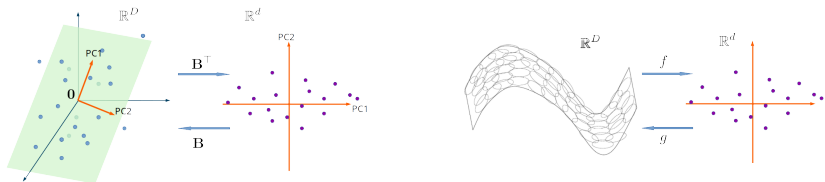


$$\min_{V, z'_i s \in \mathbb{R}^d} \sum_{i=1}^m \|\mathbf{x}_i - gV(z_i)\|_2^2 + \lambda \sum_{i=1}^m \Omega(z_i)$$

$$\min_{V, W} \sum_{i=1}^m \|\mathbf{x}_i - gV \circ f_W(\mathbf{x}_i)\|_2^2 + \sum_{i=1}^m \Omega(f_W(\mathbf{x}_i))$$

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

# Quick summary of linear vs nonlinear models



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

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

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

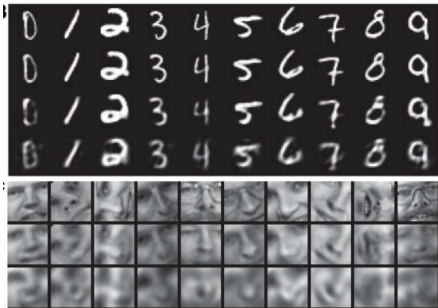
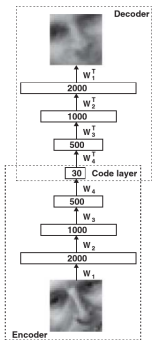
PCA for linear data

Autoencoder: extensions of PCA for nonlinear data

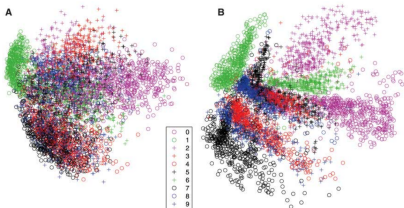
Applications of autoencoder

Self-supervised learning (SSL)

# Nonlinear dimension reduction



autoencoder vs. PCA vs. logistic PCA



[Hinton, 2006]

# Representation learning

## Traditional learning pipeline



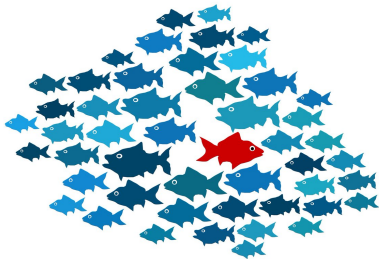
- feature extraction is “independent” of the learning models and tasks
- features are handcrafted and/or learned

## Use the low-dimensional codes as features/representations

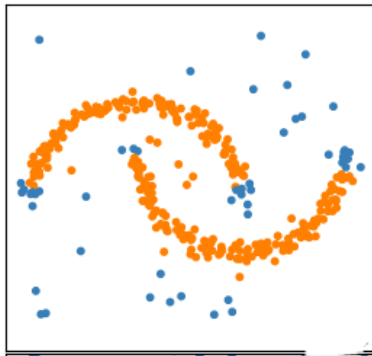
- task agnostic
- less overfitting
- semi-supervised (rich unlabeled data + little labeled data) learning



# Outlier detection

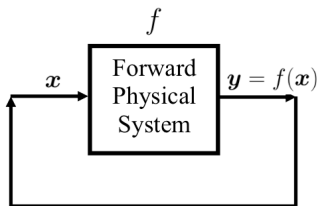


(Credit: towardsdatascience.com)



- 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  $\ell$  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  $\Omega$  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]

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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?

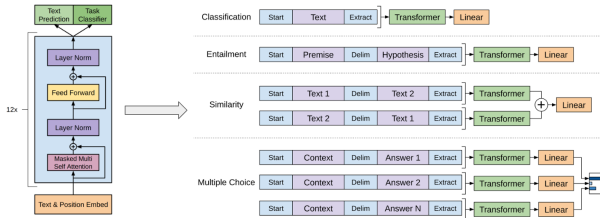
- labeling is expensive
- unlabeled data can be abundant
- supervised learning are task-specific (despite transfer learning)

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 modelir**  $p[x^{(t+1)} | x^{(0)}, \dots, x^{(t)}]$

**Finetuning:** on task-specific  
supervised data



# SSL: contrastive learning

learning embedding/representation that respects certain predefined constraints/goals

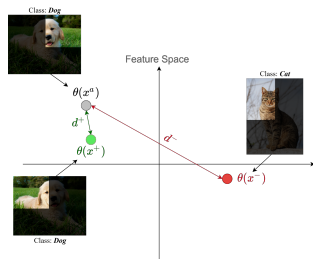
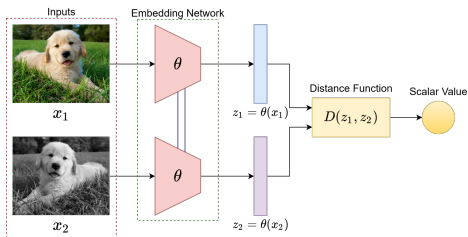
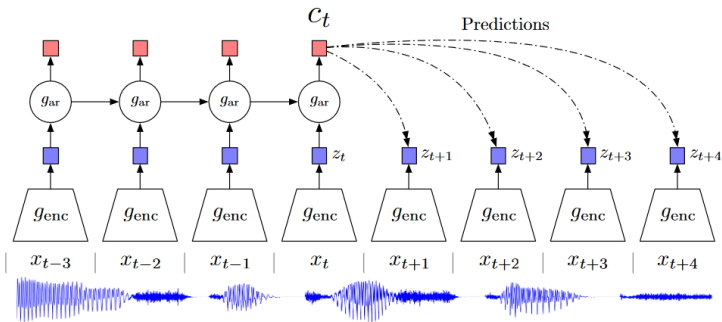


Image credit:

<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](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/>

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