Deep Learning – Autoencoder Models

INTELLIGENT SYSTEMS FOR PATTERN RECOGNITION (ISPR)

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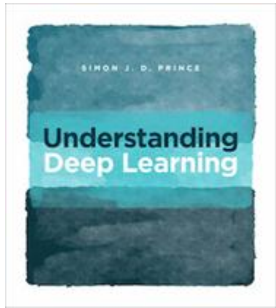
Module Outline

- Foundational models
  - Deep Autoencoders and RBM
  - Convolutional Neural Networks
  - Gated Recurrent Networks (LSTM, GRU, …)
  - Coding lectures: Keras/TF and Pytorch
- Advanced models
  - Advanced recurrent models (multiscale memories, …)
  - Advanced sequential models (seq-to-seq, …)
  - Attention and memory (Transformers, Neural Turing machines, …)

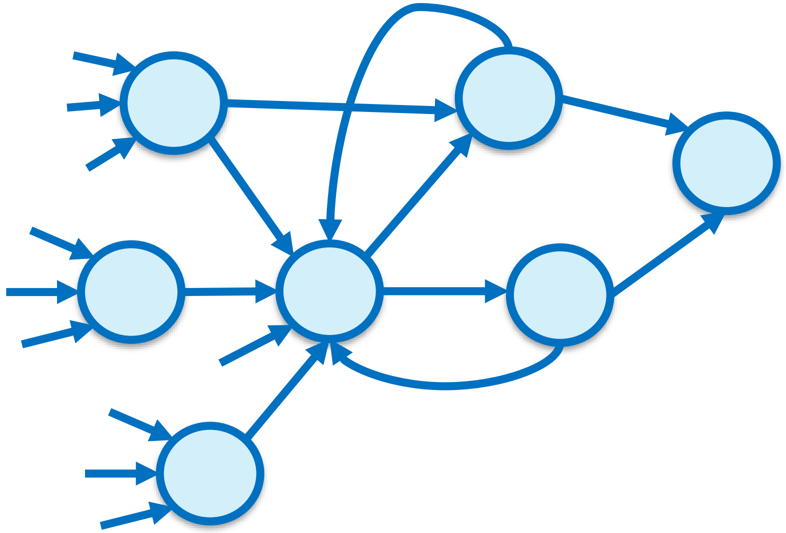
More advanced topics in the generative DL module and in the final module

Reference Book



Simon J.D. Prince, Understanding Deep Learning, MIT Press (2023)

Module's Prerequisites



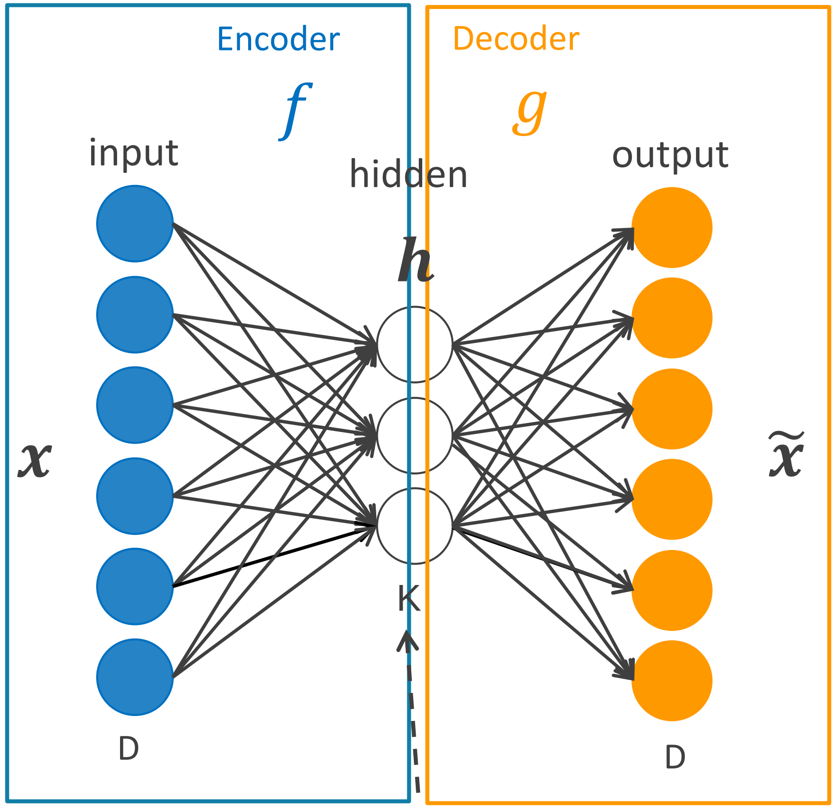
- Formal model of neuron
- Neural network
  - Feed-forward
  - Recurrent
- Cost function optimization
  - Backpropagation/SGD
  - Regularization
- Neural network hyper-parameters and model selection

Lecture Outline

Autoencoders a.k.a. The first and the latest deep learning model

- Autoencoders and dimensionality reduction
- Deep neural autoencoders
  - Sparse
  - Denoising
  - Contractive
- Deep generative-based autoencoders
  - Deep Belief Networks
  - Deep Boltzmann Machines
- Application Examples

Basic Autoencoder (AE)



Latent space projection
(again)

- Train a model to reconstruct the input
- Passing through some form of information bottleneck
  - $K \ll D$, or?
  - $\boldsymbol{h}$ sparsely active
- Train by loss minimization

  $L(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = L(\boldsymbol{x}, g(f(\boldsymbol{x})))$

Neural Autoencoders

Generally, we would like to train nonlinear AEs, with possibly $K > D$, that do not learn trivial identity

- Regularized autoencoders
  - Sparse AE
  - Denoising AE
  - Contractive AE
- Autoencoders with dropout layers

Sparse Autoencoder

Add a term to the cost function to penalize $\boldsymbol{h}$ (want the number of active units to be small)

$$J_{SAE}(\theta) = \sum_{x \in S} (L(\boldsymbol{x}, \widetilde{\boldsymbol{x}}) + \lambda \Omega(\boldsymbol{h}))$$

Typically

$$\Omega(\boldsymbol{h}) = \Omega(f(\boldsymbol{x})) = \sum_j \left| h_j(\boldsymbol{x}) \right|$$

Probabilistic Interpretation (Oh No, Again!)

Training with regularization is (akin to) MAP inference

$$\max \log P(\boldsymbol{h}, \boldsymbol{x}) = \max\,(\log P(\boldsymbol{x}|\boldsymbol{h}) + \log P(\boldsymbol{h}))$$

Likelihood

Prior

$$P(\boldsymbol{h}) = \frac{\lambda}{2}\exp(-\frac{\lambda}{2}|\boldsymbol{h}|_1) \Rightarrow \Omega(\boldsymbol{h}) = \lambda||\boldsymbol{h}||_1$$

Laplace

Denoising Autoencoder (DAE)

Train the AE to minimize the function

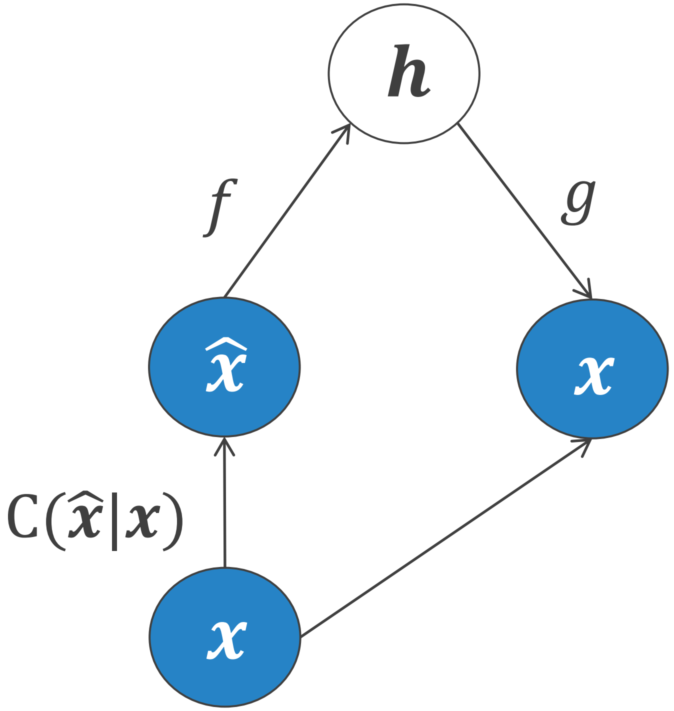
$$L(\boldsymbol{x}, g(f(\hat{\boldsymbol{x}})))$$

where $\hat{\boldsymbol{x}}$ is a version of original input $\boldsymbol{x}$ corrupted by some noise process $C(\hat{\boldsymbol{x}}|\boldsymbol{x})$

Key Intuition - Learned representations should be robust to partial destruction of the input

Another Interpretation…

…yes, exactly the one you are thinking of



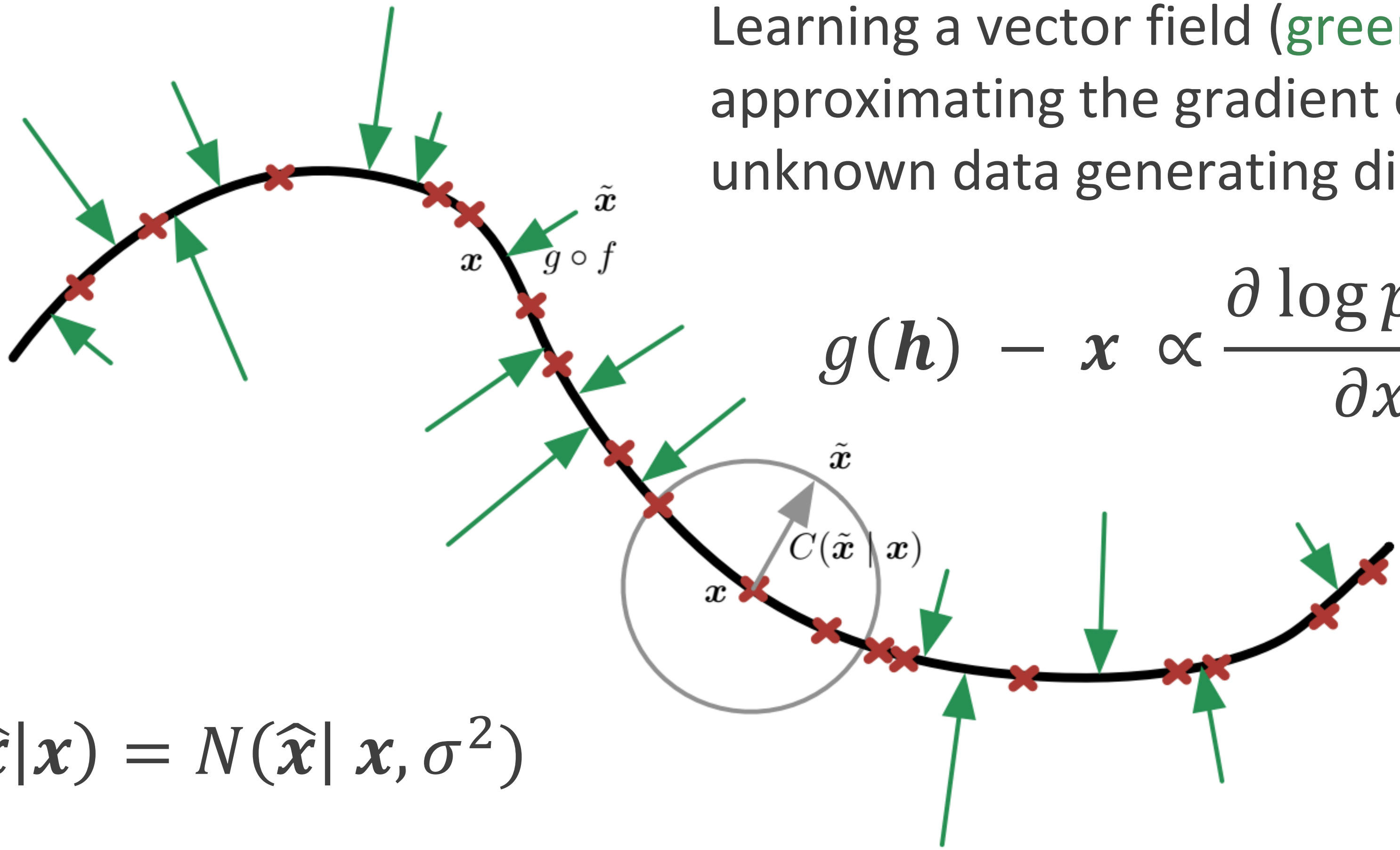
Learns the denoising distribution

$$P(\boldsymbol{x}|\tilde{\boldsymbol{x}})$$

By minimizing

$$-\log P_d(\boldsymbol{x}|\boldsymbol{h} = f(\tilde{\boldsymbol{x}}))$$

DAE as Manifold Learning

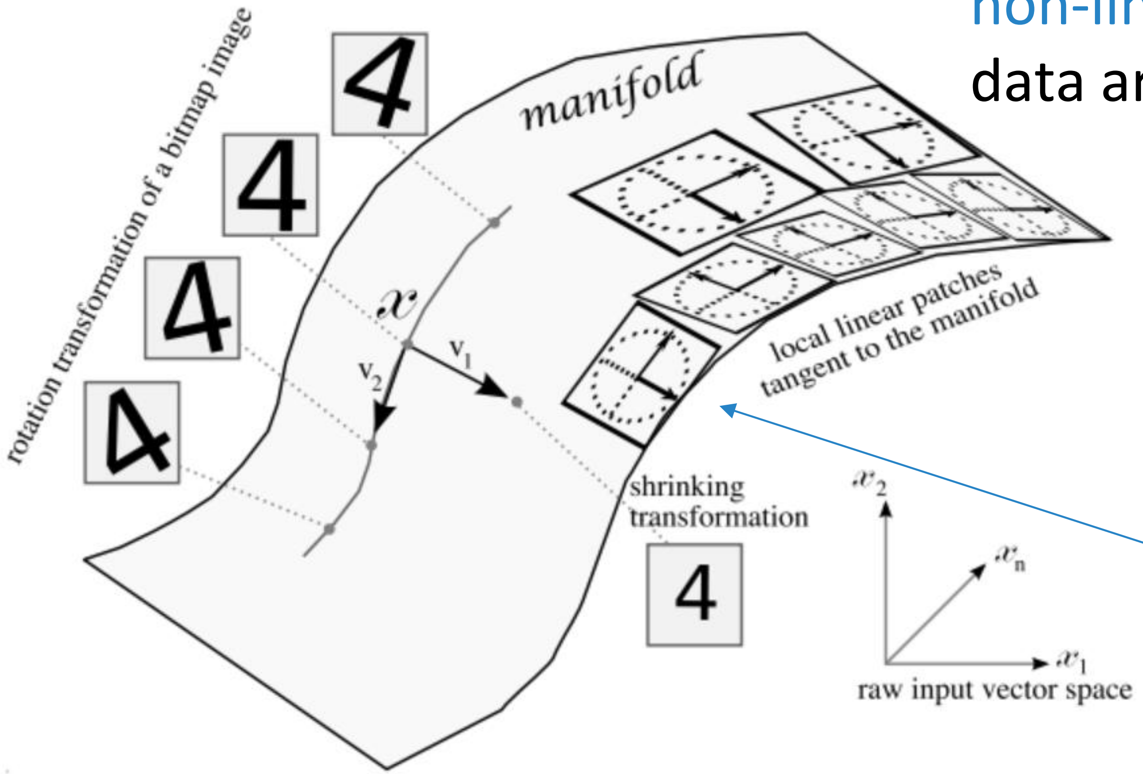


Learning a vector field (green arrows) approximating the gradient of the unknown data generating distribution

$$g(\boldsymbol{h}) - \boldsymbol{x} \propto \frac{\partial \log p(\boldsymbol{x})}{\partial x}$$

$$C(\widehat{\boldsymbol{x}}|\boldsymbol{x}) = N(\widehat{\boldsymbol{x}}|\,\boldsymbol{x}, \sigma^2)$$

The Manifold Assumption



Assume data lies on a lower dimensional non-linear manifold since variables in data are typically dependent

Regularized AE can afford to represent only variations that are needed to reconstruct training examples

AE mapping is sensitive only to changes in manifold direction

Yoshua Bengio, Learning Deep Architectures for AI, Foundations and Trends in Machine Learning, 2009.

Contractive Autoencoder

Penalize **encoding function** for input sensitivity

$$J_{CAE}(\theta) = \sum_{x \in S} (L(\boldsymbol{x}, \tilde{\boldsymbol{x}}) + \lambda \Omega(\boldsymbol{h}))$$

$$\Omega(\boldsymbol{h}) = \Omega(f(\boldsymbol{x})) = \left\| \frac{\partial f(\boldsymbol{x})}{\partial \boldsymbol{x}} \right\|_F$$

You can as well penalize on higher order derivatives

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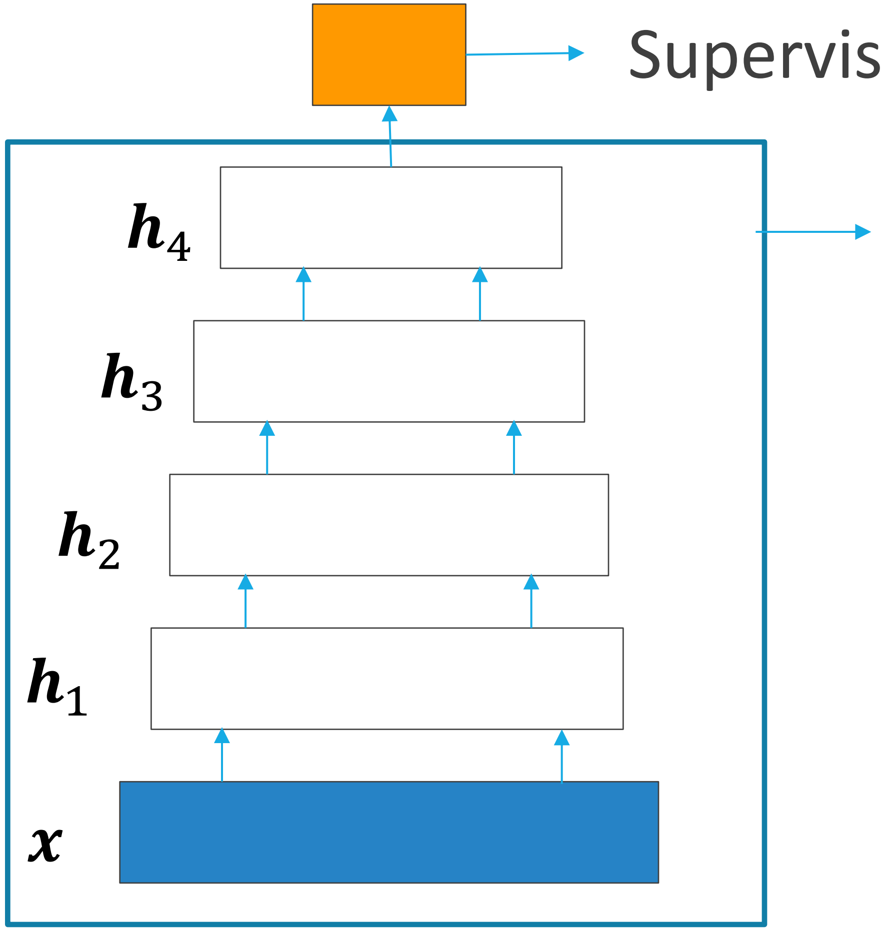
Deep Autoencoder (AE)



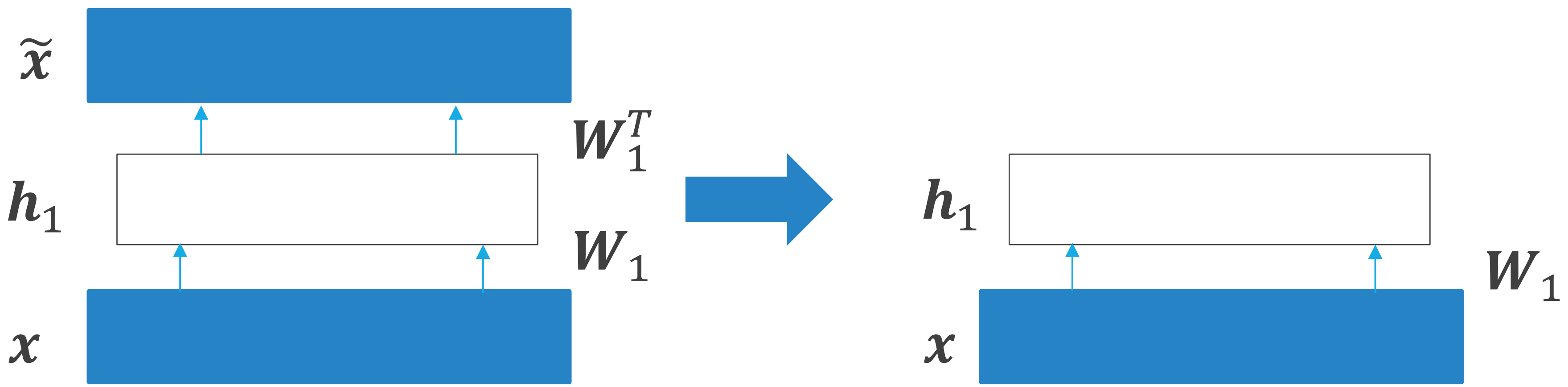
Supervised learning

- Unsupervised training
- Hierarchical autoencoder
- Extracts a representation of inputs that facilitates
  - Data visualization, exploration, indexing,…
  - Realization of a supervised task

Unsupervised Layerwise Pretraining

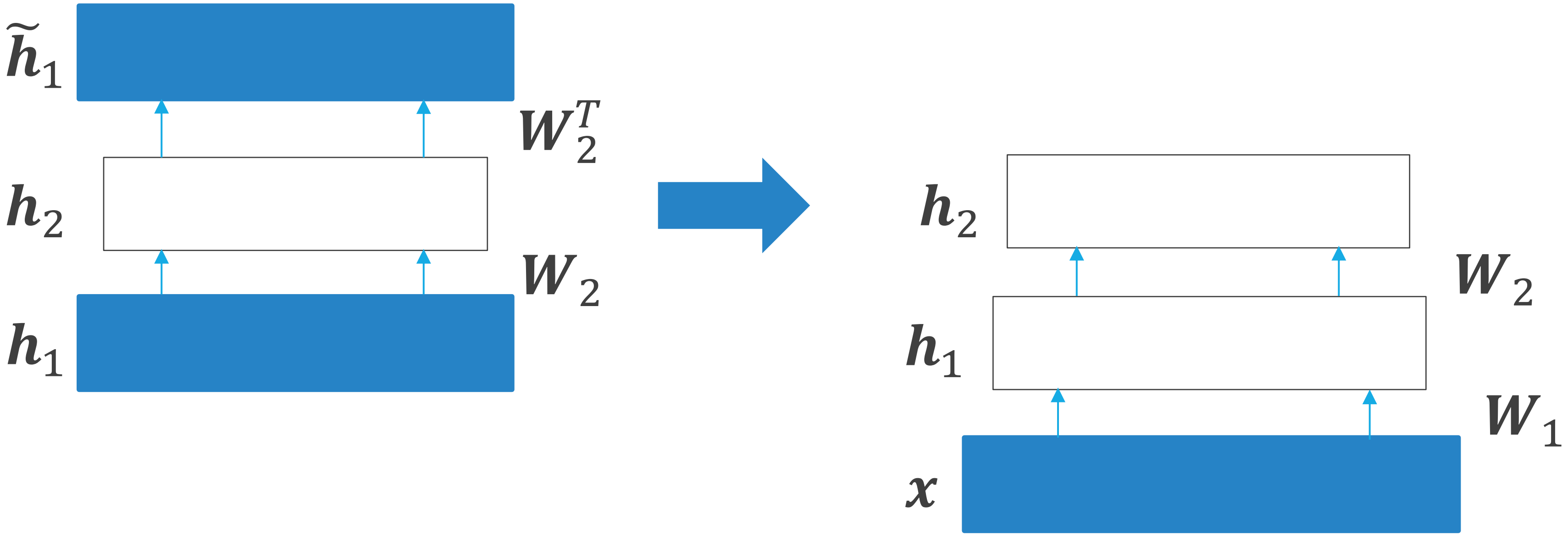
Incremental unsupervised construction of the Deep AE

Any form of AE, e.g. those shown in previous slides



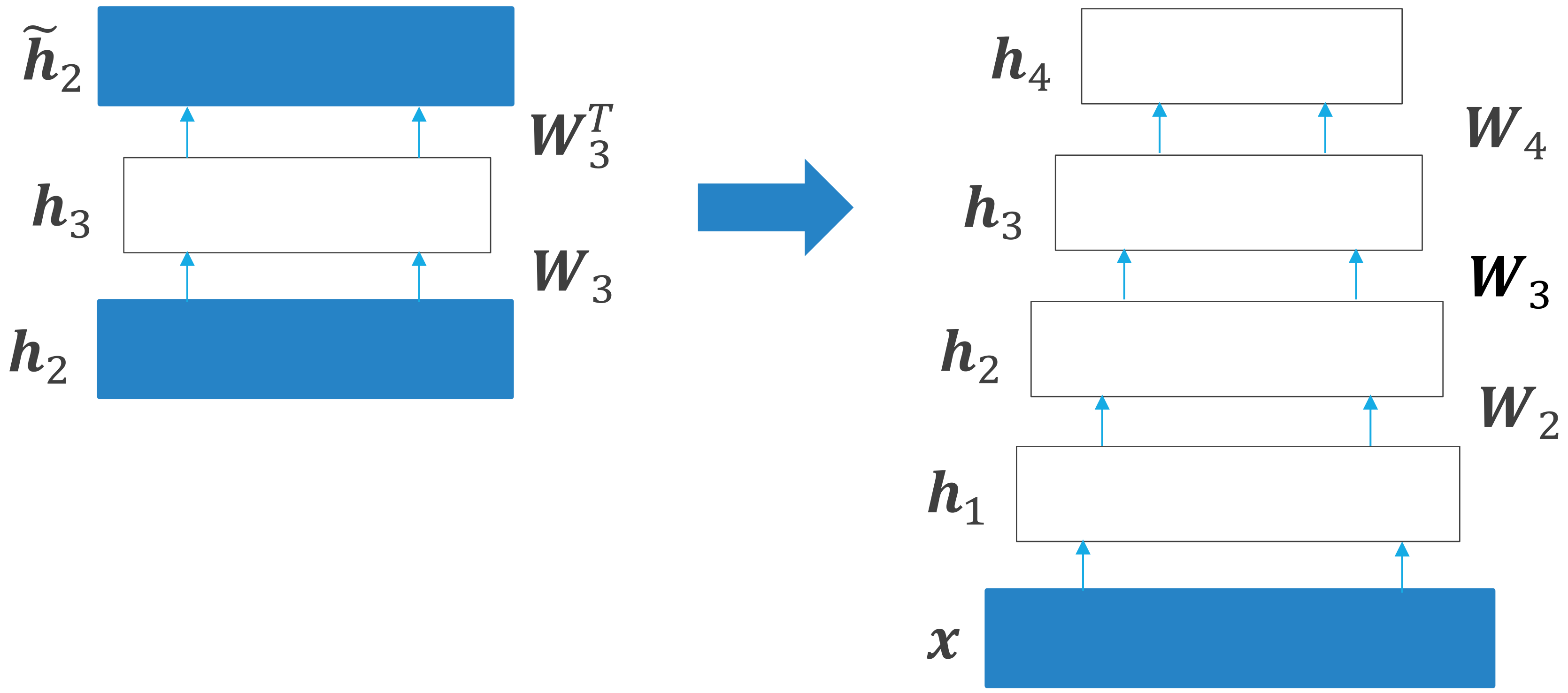
Unsupervised Layerwise Pretraining

Incremental unsupervised construction of the Deep AE



Unsupervised Layerwise Pretraining

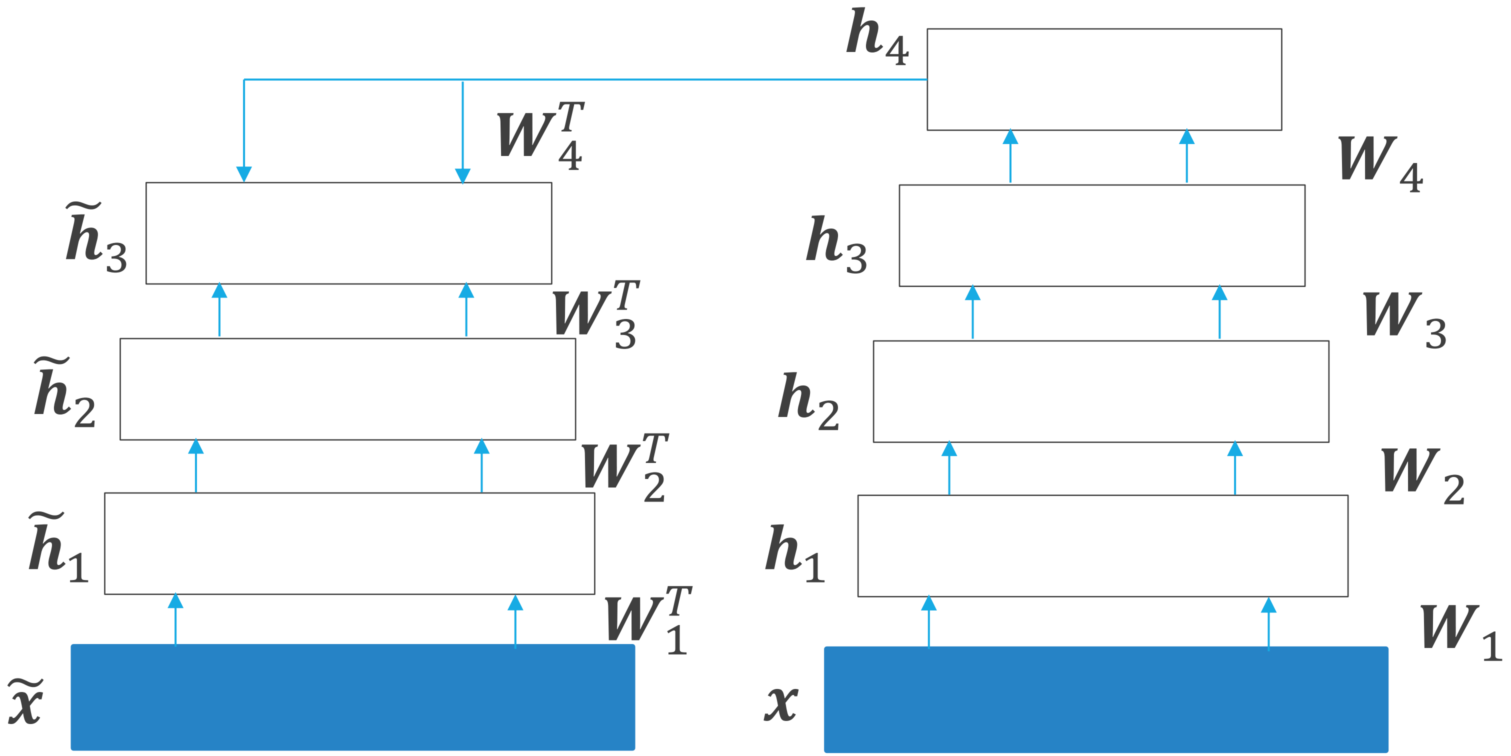
Incremental unsupervised construction of the Deep AE



Optional Fine Tuning

Fine tune the whole autoencoder to optimize input reconstruction

You can use backpropagation, but it remains an unsupervised task

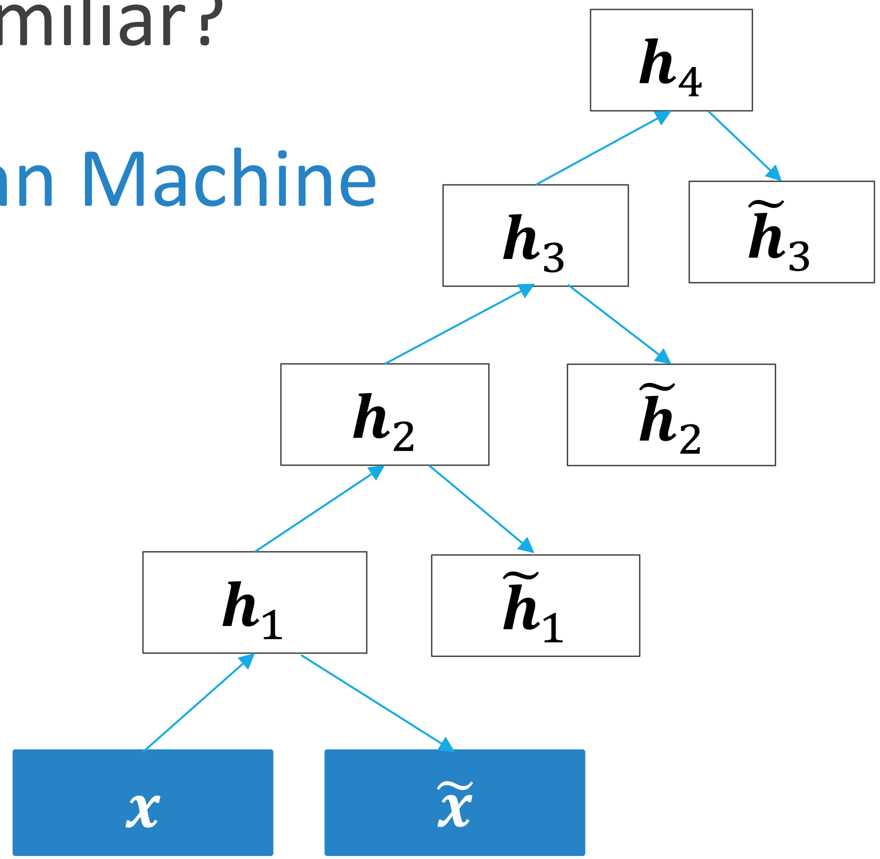


Rearranging the Graphics

Does it look like something familiar?

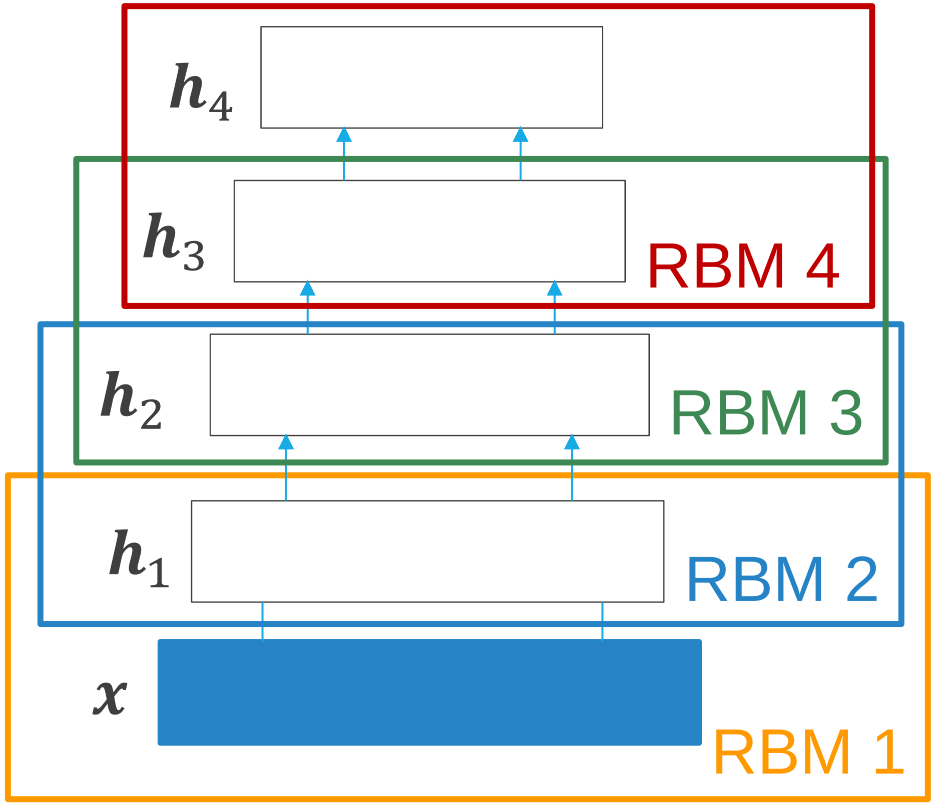
A layered Restricted Boltzmann Machine

Can use RBM to perform layerwise pretraining and learn the matrices $\boldsymbol{W}_i$



Deep Belief Network (DBN)

A stack of pairwise RBM



IMPORTANT NOTE

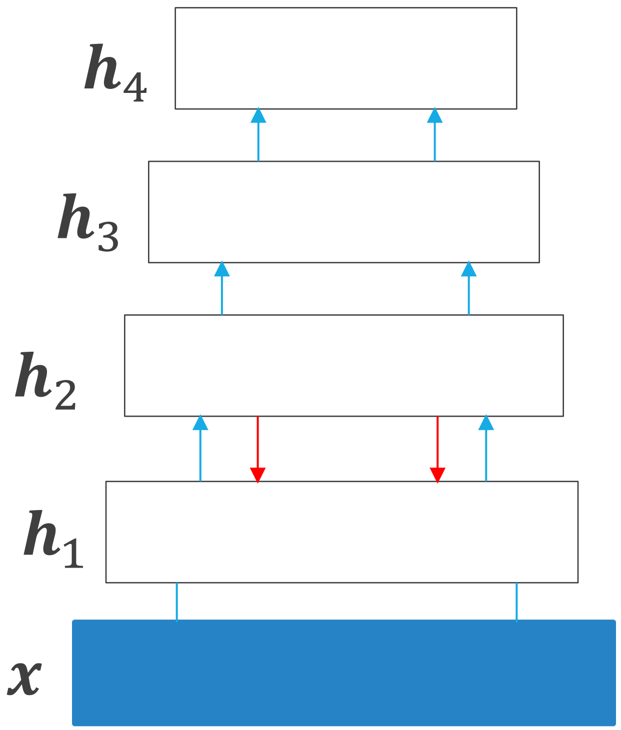
A DBM is a deep autoencoder

but it is NOT a deep RBM

It is (mostly) directed!

Deep Boltzmann Machine (DBM)

How do we get this?



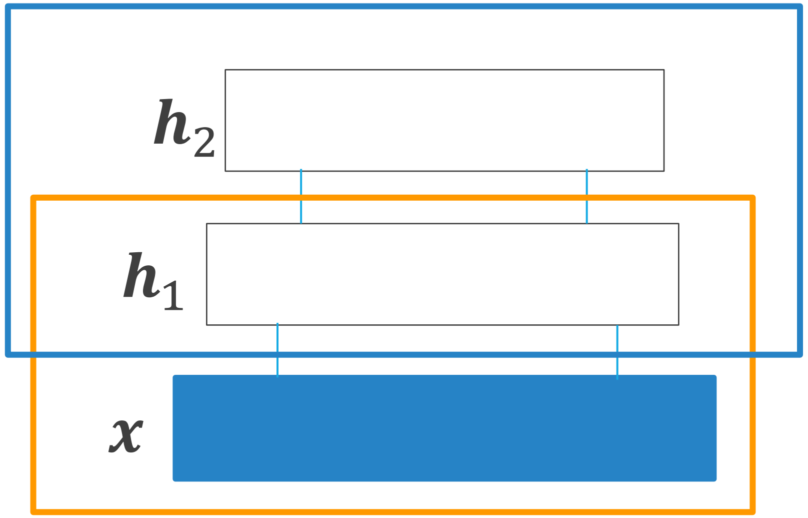
Training requires some attention because of the recurrent interactions from higher layers to the bottom

$$P(h_j^1 | \boldsymbol{x}, \boldsymbol{h}^2) = \sigma\left(\sum_i W_{ij}^1 x_i + \sum_m W_{jm}^2 h_m^2\right)$$

$$P(x_i | \boldsymbol{h}^1) = \sigma\left(\sum_j W_{ij}^1 h_j^1\right)$$

Pretraining DBM

How do we get this?



2) (Pre)training the second layer changes $\boldsymbol{h}^1$ prior by

$$P(\boldsymbol{h}^1|\boldsymbol{W}^2) = \sum_{\boldsymbol{h}^2} P(\boldsymbol{h}^1, \boldsymbol{h}^2|\boldsymbol{W}^2)$$

When putting things together, we need to average between the two

$$P(\boldsymbol{h}^1|\boldsymbol{W}^1) = \sum_{\boldsymbol{x}} P(\boldsymbol{h}^1, \boldsymbol{x}|\boldsymbol{W}^1)$$

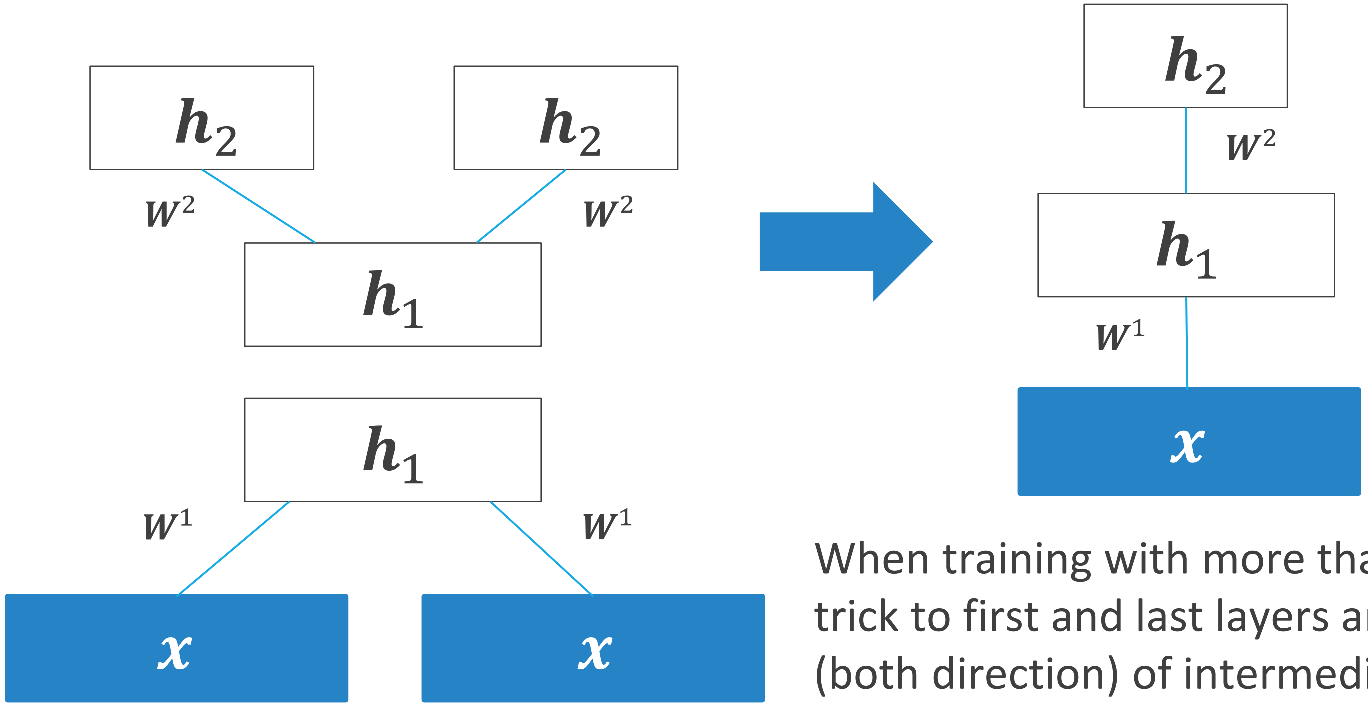
1) (Pre)training the first layer entails fitting this model

$$P(\boldsymbol{x}|\theta) = \sum_{\boldsymbol{h}^1} P(\boldsymbol{h}^1|\boldsymbol{W}^1) P(\boldsymbol{x}|\boldsymbol{h}^1, \boldsymbol{W}^1)$$

Pretraining DBM - Trick

Averaging the two models of $\boldsymbol{h}^1$ can be approximated by taking half contribution from $\boldsymbol{W}^1$ and half from $\boldsymbol{W}^2$

- Using full $\boldsymbol{W}^1$ and $\boldsymbol{W}^2$ would double count $\boldsymbol{x}$ contribution as $\boldsymbol{h}^2$ depends on $\boldsymbol{x}$



When training with more than two RBMs apply trick to first and last layers and halve weights (both direction) of intermediate RBM

Software - Deep Neural Autoencoders

- All deep learning frameworks offer facilities to build (deep) AEs
- Check out classic Theano-based tutorials for denoising autoencoders and their stacked version
- A variety of deep AE in Keras and their counterpart in Torch (plus a selection in Pytorch)
- Stacked autoencoders built with official Matlab toolbox functions

Matlab - Deep Boltzmann Models

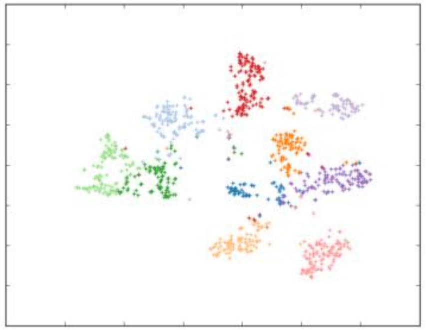
- Matlab code for the DBN paper with a demo on MNIST data
- Matlab code for Deep Boltzmann Machines with a demo on MNIST data
- Deepmat – Matlab library for deep generative models
- DeeBNet – Matlab/Octave toolbox for deep generative models with GPU support

Python - Deep Boltzmann Models

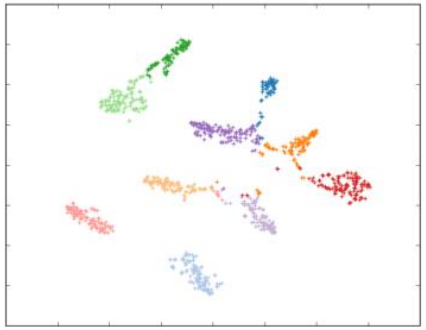
- DBN and DBM implementations exist for all major deep learning libraries
- Deep Boltzmann machine implementation (Tensorflow-based) with image processing application, pre-trained networks and notebooks
- Deepnet – A Toronto based implementation of deep autoencoders (neural and generative)
- Check out classic Theano-based tutorials for deep belief networks and RBM

AE Applications - Visualization

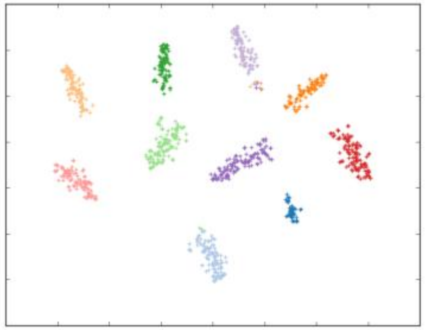
Visualizing complex data in learned latent space



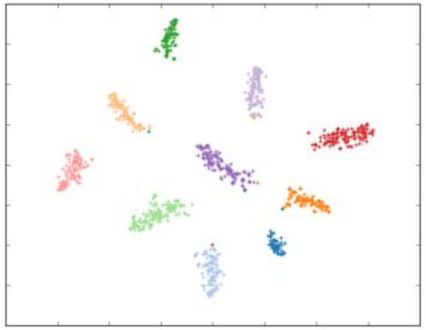
(a) Epoch 0



(b) Epoch 3

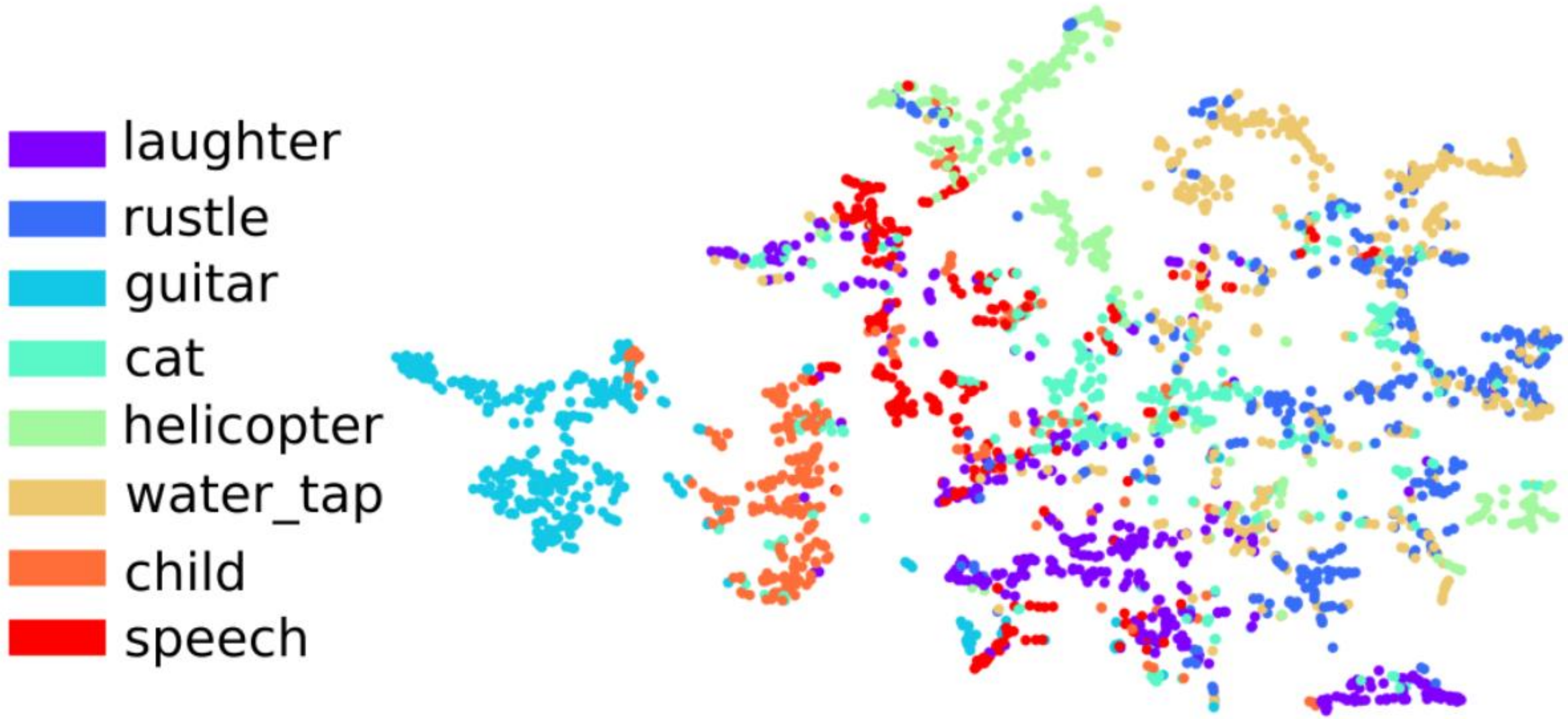


(d) Epoch 9

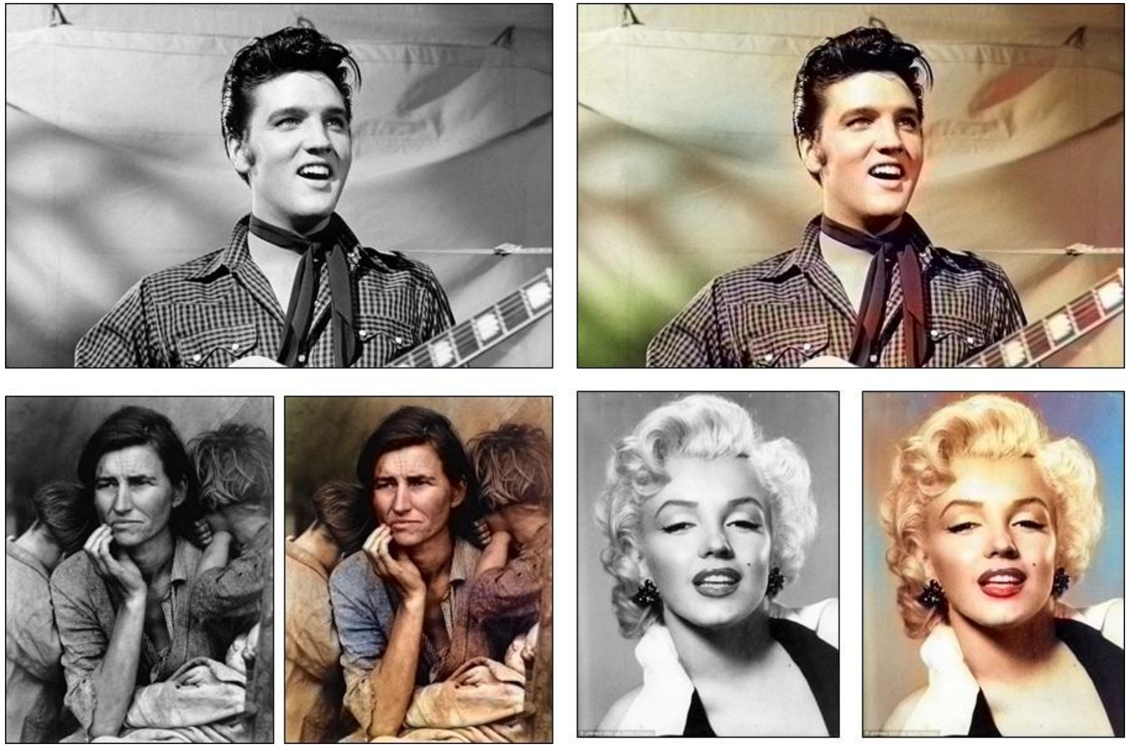


(e) Epoch 12

Visualizing Sound

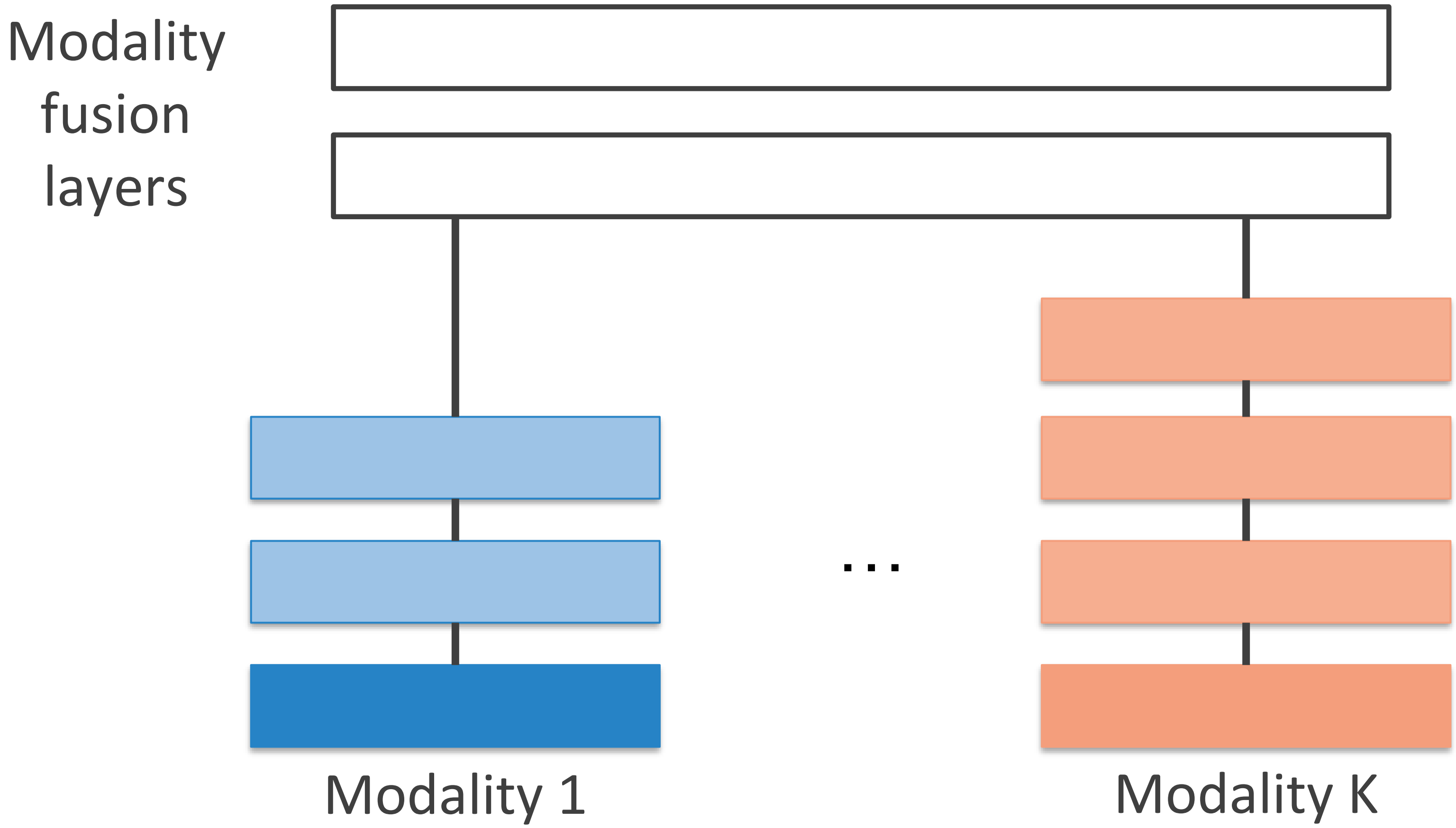


AE Applications – Image Restoration/Colorization



Apply autoencoder construction with advanced building blocks (e.g. CNN layers)

Multimodal DBM



N. Srivastava, R. Salakhutdinov, Multimodal Learning with Deep Boltzmann Machines, JMLR 2014

Multimodal DBM – Image and Text

$P(txt|img)$

Image	Given Tags	Generated Tags	Input Tags	Nearest neighbors to generated image features	
	pentax, k10d, kangarooisland, southaustralia, sa, 300mm, australia, australiansealion	beach, sea, surf, strand, shore, wave, seascape, sand, ocean, waves	nature, hill, scenery, green, clouds		
	< no text >	night, lights, christmas, nightshot, nacht, nuit, notte, longexposure, noche, nocturna	flower, nature, green, flowers, petal, petals, bud		
	aheram, 0505, sarahc, moo	portrait, bw, balckandwhite, people, faces, girl, blackwhite, person, man	blue, red, art, artwork, painted, paint, artistic, surreal, gallery, bleu		
	unseulpixel, naturey crap	fall, autumn, trees, leaves, foliage, forest, woods, branches, path	bw, blackandwhite, noiretblanc, bianconero, blancoynegro		

$P(img|txt)$

N. Srivastava, R. Salakhutdinov, Multimodal Learning with Deep Boltzmann Machines, JMLR 2014

Multimodal DBM – Sampling

Step 50	Step 100	Step 150	Step 200	Step 250
travel	beach	sea	water	italy
trip	ocean	beach	canada	water
vacation	waves	island	bc	sea
africa	sea	vacation	britishcolumbia	boat
earthasia	sand	travel	reflection	italia
asia	nikon	ocean	alberta	mare
men	surf	caribbean	lake	venizia
2007	rocks	tropical	quebec	acqua
india	coast	resort	ontario	ocean
tourism	shore	trip	ice	venice

Input tags	Step 50	Step 100	Step 150	Step 200	Step 250
purple, flowers					
car, automobile					

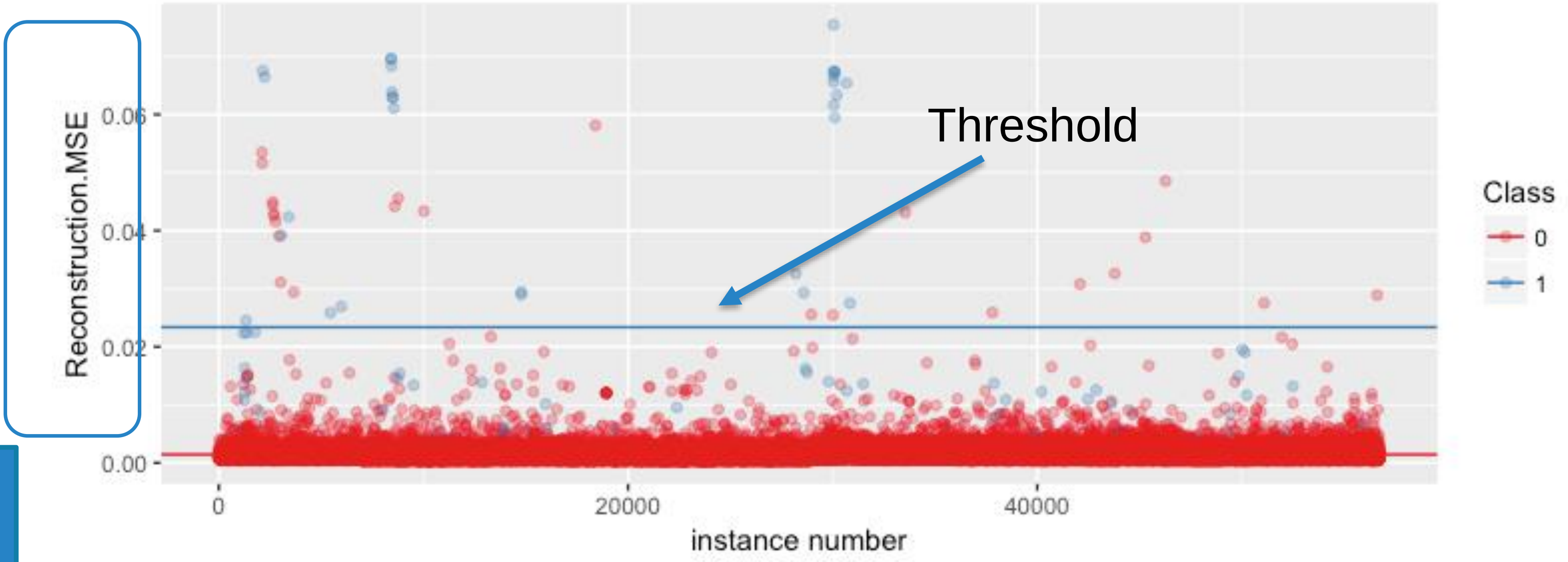
N. Srivastava, R. Salakhutdinov, Multimodal Learning with Deep Boltzmann Machines, JMLR 2014

Multimodal DBM – Multimodal Quering

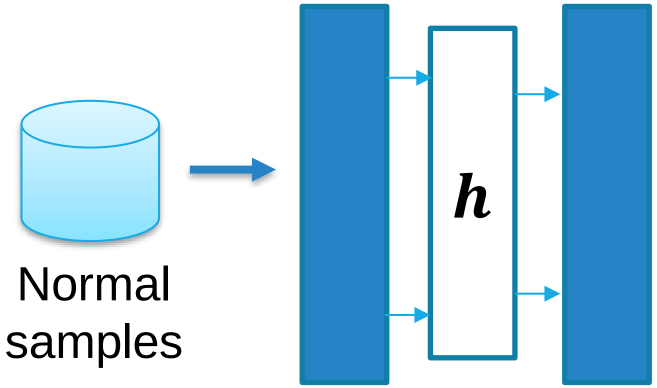
Multimodal Query	Top 4 retrieved results			
 hongkong, causewaybay, shoppingcentre, building, mall	 howell, bridge, genesee, river, rochester, downtown, building	 london, uk, night, skyline, river, thames, lights, bridge	 edinburgh, scotland, dusk, bank	 arcoiris, fincadehierro, lluvia, sannicolas, valencia
 me, myself, eyes, blue, hair	 urban, me, abigfave, fiveflickrfavs,	 trisha, mynewcamera, lake, field, girl	 me, ofme, self, selfportrait	 pink, prettyinpink, explored

N. Srivastava, R. Salakhutdinov, Multimodal Learning with Deep Boltzmann Machines, JMLR 2014

Anomaly Detection



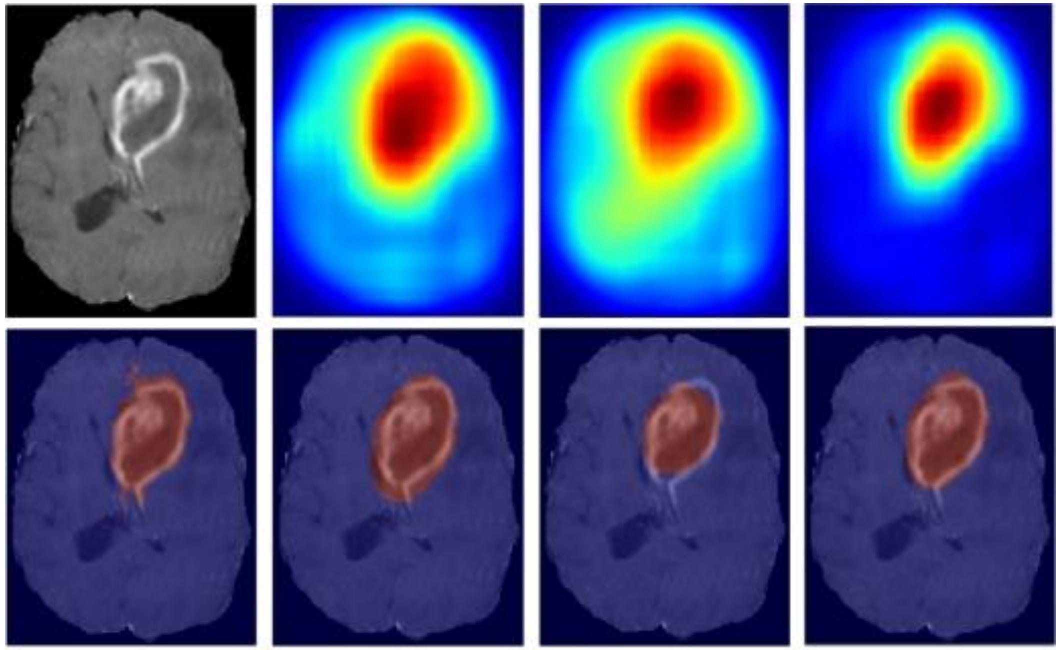
Reconstruction



Statistics on the «normal» differences between $\boldsymbol{x}$ and $\tilde{\boldsymbol{x}}$

Unsupervised pathology detection in biomedical images

Unsupervised pathology detection of a brain tumor image and resulting anomaly scores (growing values: blue → red)



(a) Test image (b) z-Space (c) Reconstruction (d) Combined

https://www.sciencedirect.com/science/article/pii/B9780128243497000153

Take Home Messages

- Regularized autoencoder
  - Optimize reconstruction quality
  - Constrain stored information
- Autoencoder training is manifold learning
  - Learn a latent space manifold where input data resides
  - Store only variations that are useful to represent training data
- Autoencoders learn a (conditional) distribution of input data $P(\hat{\boldsymbol{x}}| \dots)$
- Deep AE: pretraining, fine tuning, supervised optimization
- Use AE for finding new/useful data representations
  - Or to learn its distribution

Next Two Lectures

Convolutional Neural Networks

- Introduction to the Deep Learning module
- Basic components of a convolutional neural network
  - Convolutions, striding, pooling, ReLu, batchnorm layers
- Notable architectures
  - From AlexNet to ResNets and MobileNets
- CNN besides simple object recognition
  - Semantic segmentation, sequence processing, dilated convolutions