Combining Supervised and Unsupervised Learning (and the Ladder Network)

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About me (Tapani Raiko)

- MSc 2001 Helsinki University of Technology
  Deep learning (Hierarchical Nonlinear Factor Analysis)
  Erkki Oja, Juha Karhunen, Harri Valpola
- DSc 2006, Same group
  Variational Bayesian modelling, relational models
- ZenRobotics Ltd 2009-2014 (primary job 2013)
- Assistant prof 2014- Aalto University
- Research visits:
  - Luc De Raedt, Freiburg, 2001-2002
  - Yann Lecun, New York, 2010
  - Geoffrey Hinton, Toronto, 2012
  - Yoshua Bengio, Montreal, 2014

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Motivation

Deep learning today:

- Mostly about pure supervised learning
- Requires a lot of labeled data: expensive to collect

Deep learning in the future:

- Unsupervised, more human-like

"We expect unsupervised learning to become far more important in the longer term. Human and animal learning is largely unsupervised: we discover the structure of the world by observing it, not by being told the name of every object."
–LeCun, Bengio, Hinton, Nature 2015

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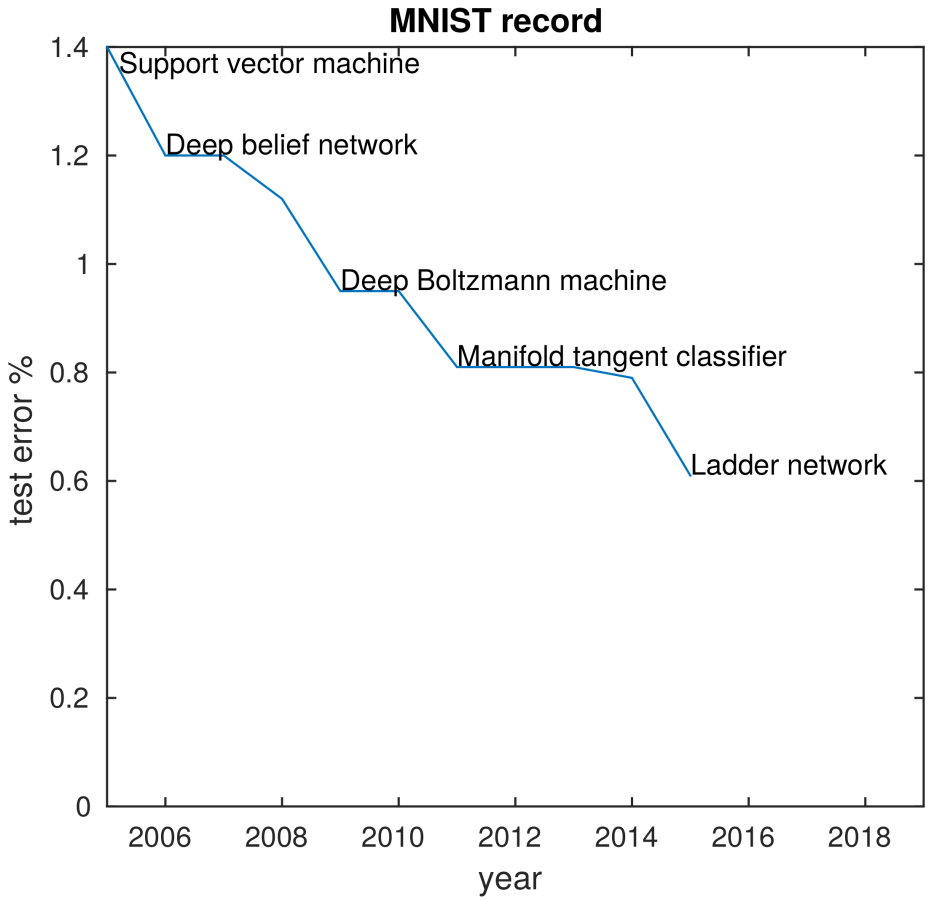
Motivation: Ladder network



Yearly progress in permutation-invariant MNIST.

A. Rasmus, H. Valpola, M. Honkala, M. Berglund, and T. Raiko. Semi-Supervised Learning with Ladder Network. ArXiv, July 2015.

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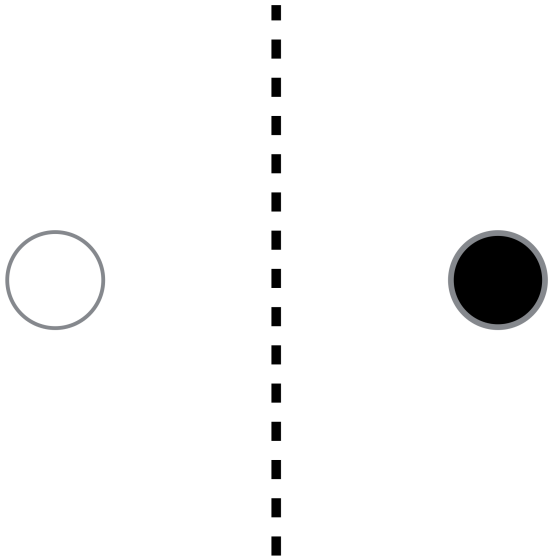
Semisupervised learning



How can unlabeled data help in classification?
Example: Only two data points with labels.

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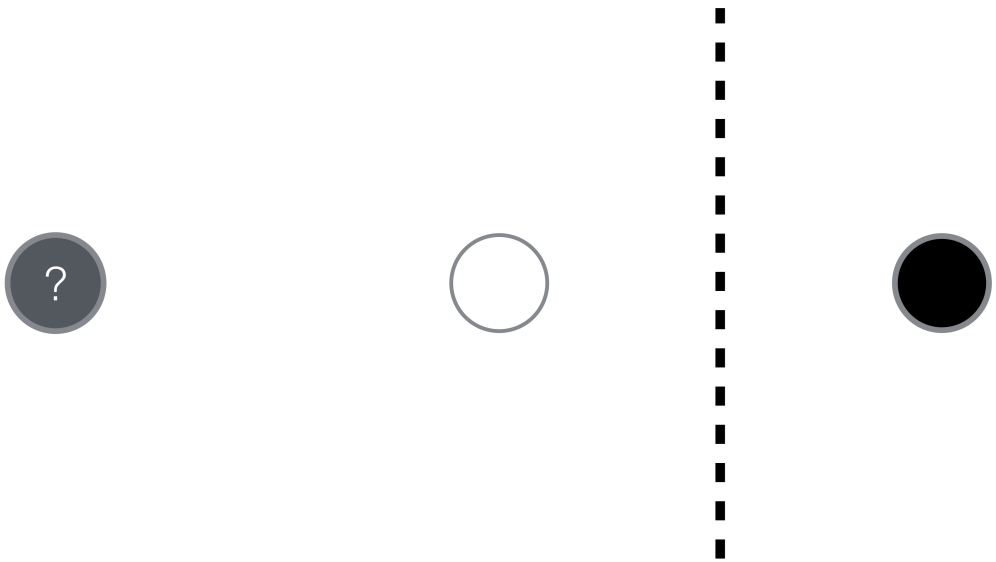
Semisupervised learning



How would you label this point?

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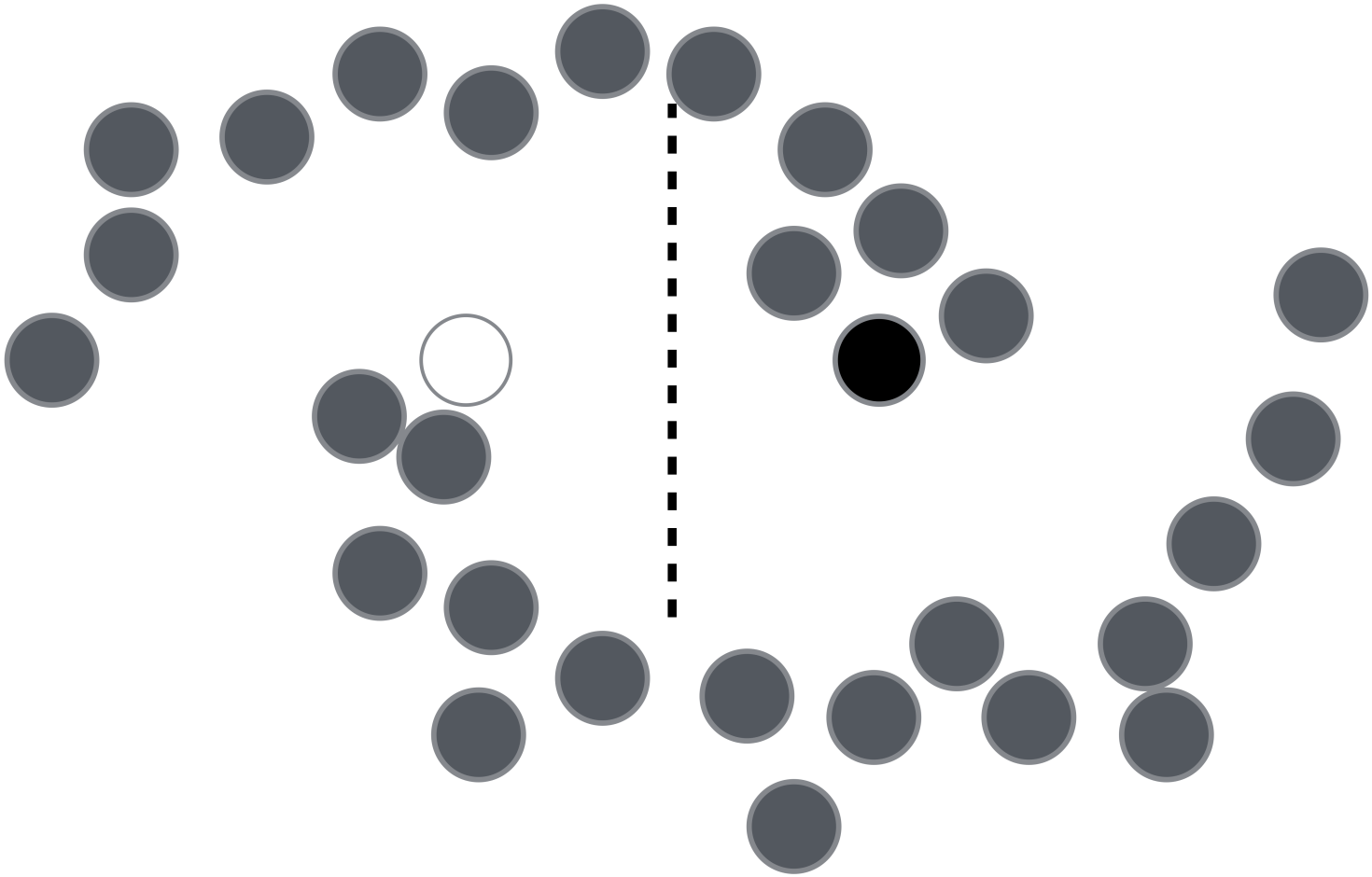
Semisupervised learning



What if you see all the unlabeled data?

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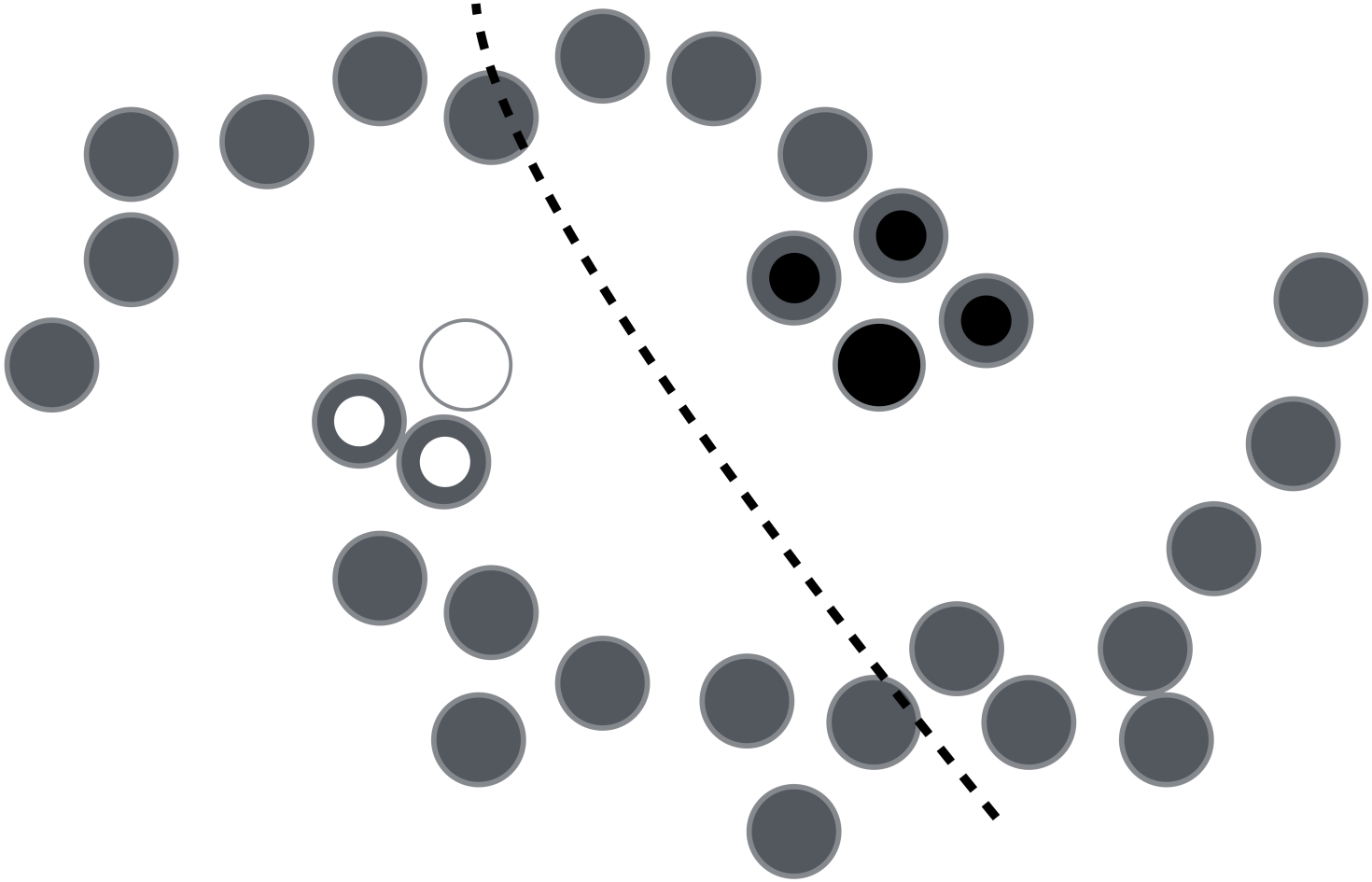
Semisupervised learning



Labels are homogenous in densely populated space.

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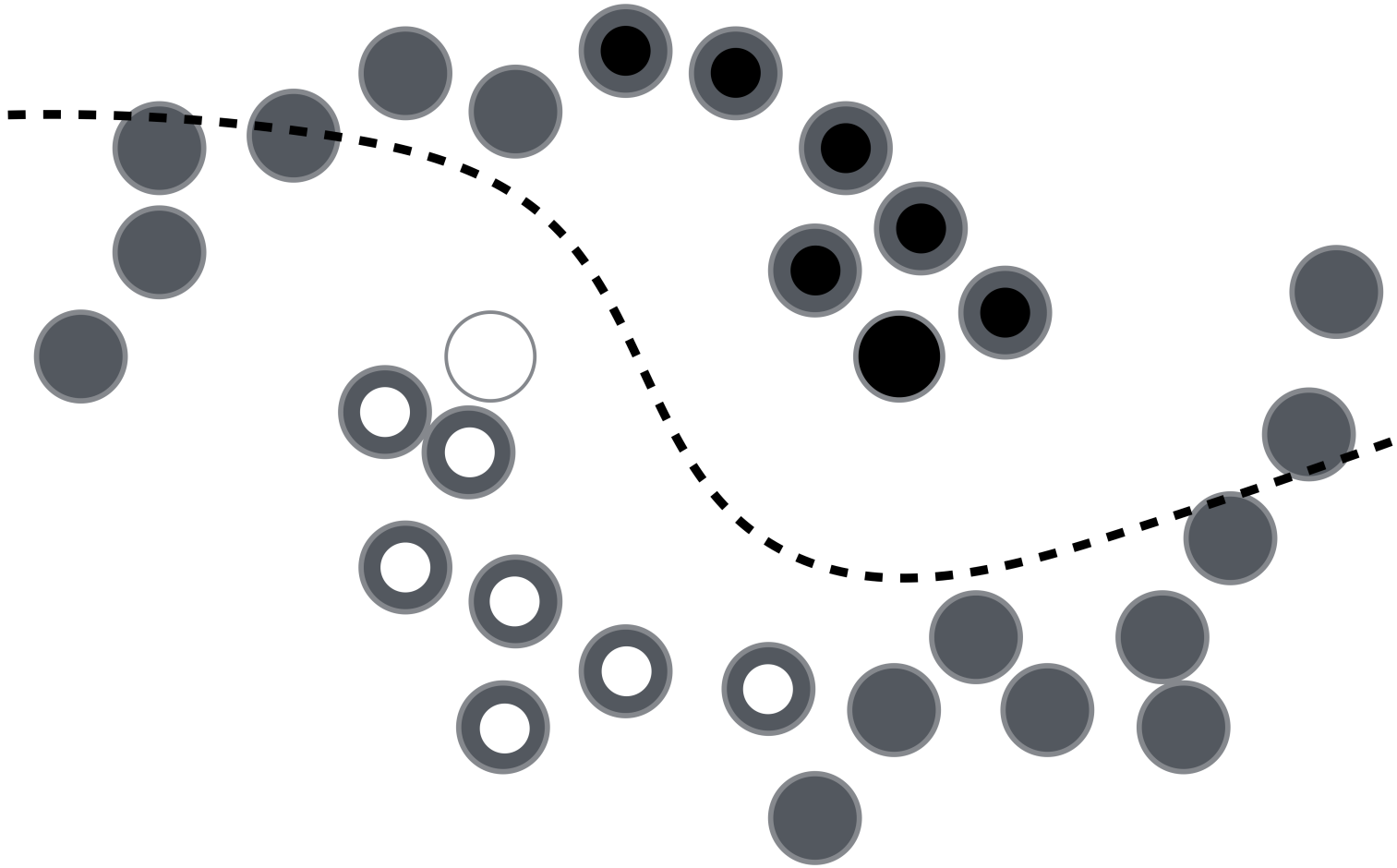
Semisupervised learning



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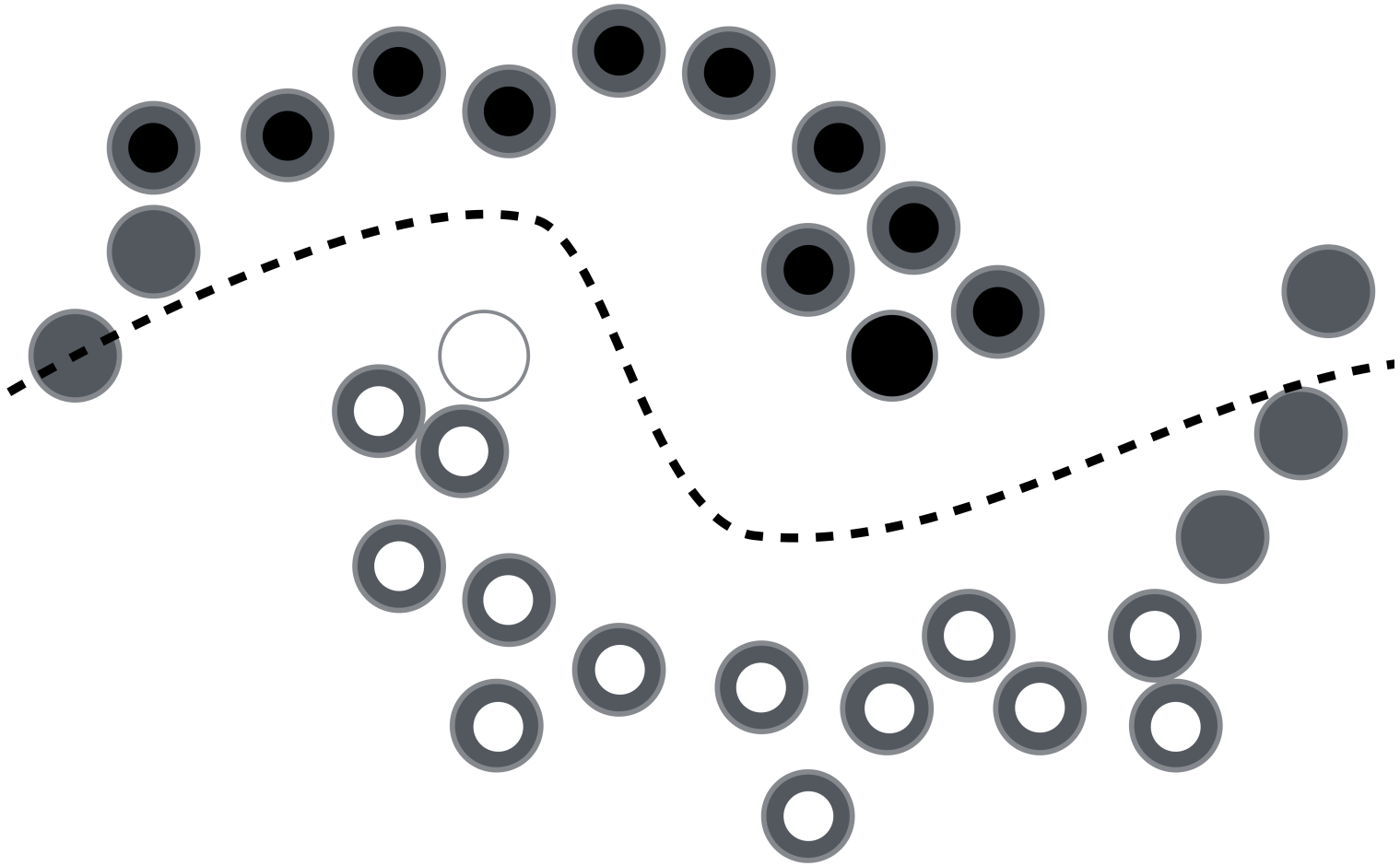
Semisupervised learning



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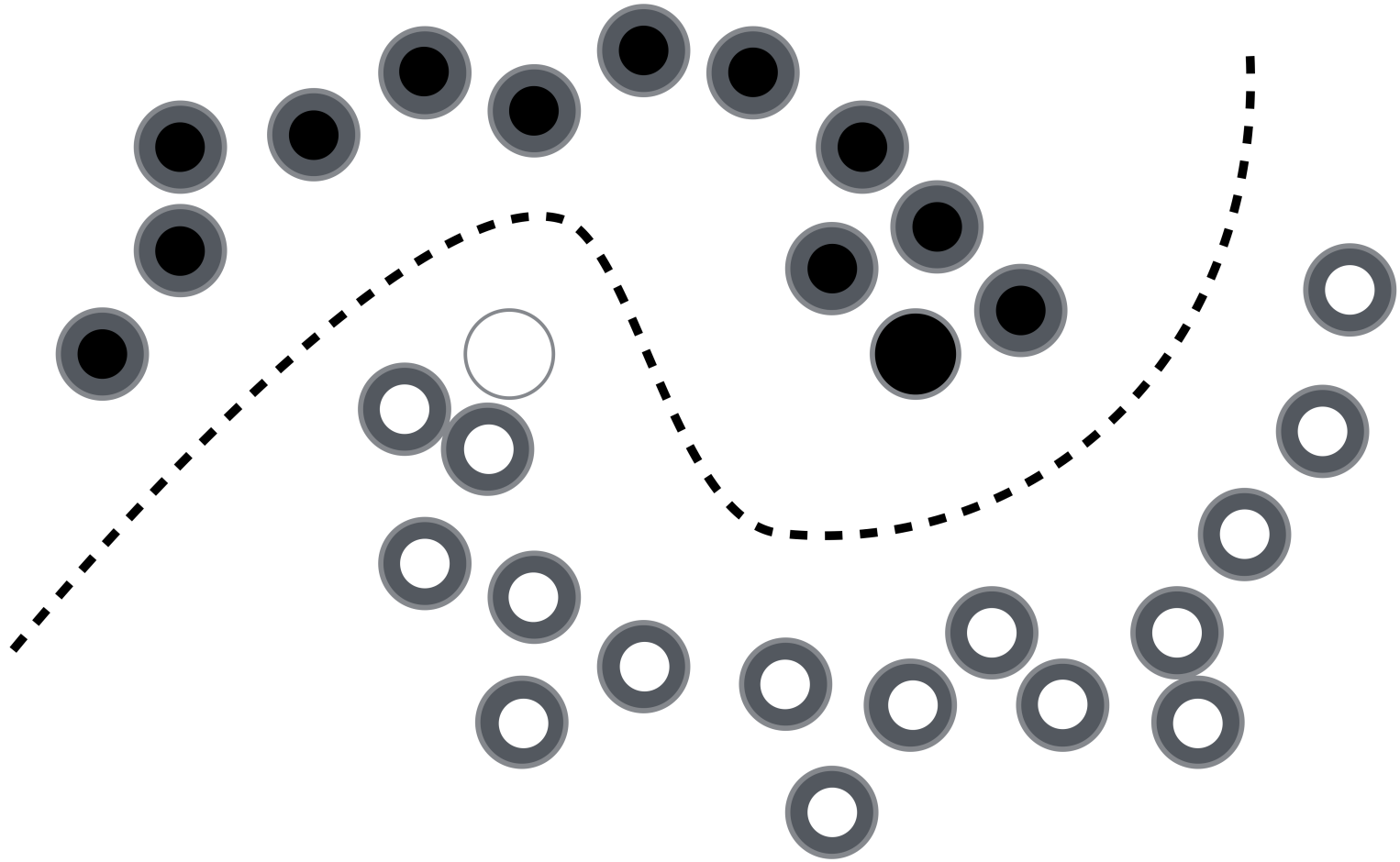
Semisupervised learning



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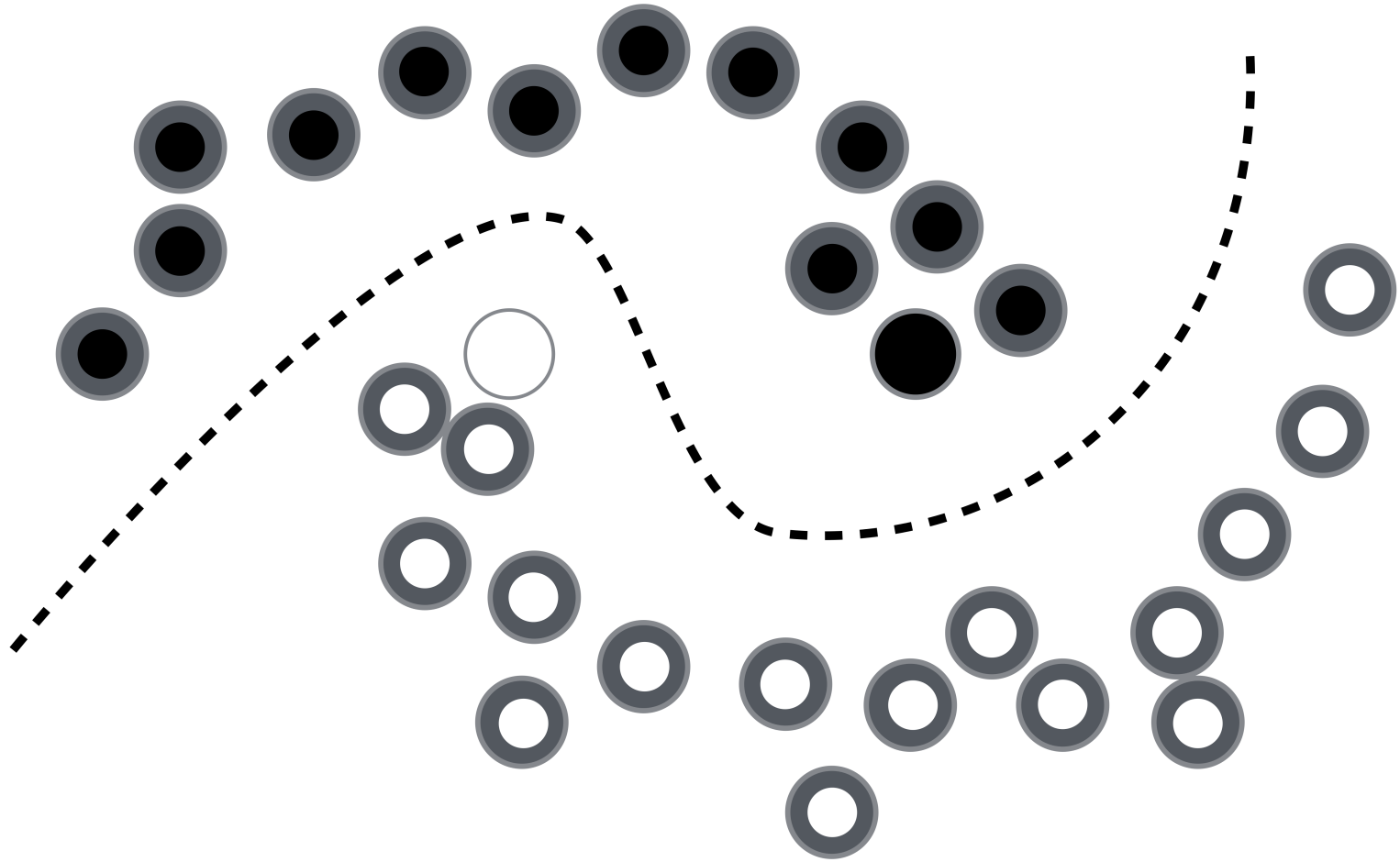
Semisupervised learning



Labels are homogenous in densely populated space.

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Semisupervised learning

Labeled data: $\{\mathbf{x}_t, y_t\}_{1 \leq t \leq N}$.
Unlabeled data: $\{\mathbf{x}_t\}_{N+1 \leq t \leq M}$.
Often labeled data is scarce, unlabeled data is plentiful: $N \ll M$.

Early works (McLachlan, 1975; Titterington et al., 1985)
modelled $P(\mathbf{x}|y)$ as clusters.
Unlabeled data affects the shape and size of clusters.
Use Bayes theorem $P(y|\mathbf{x}) \propto P(\mathbf{x}|y)P(y)$ to classify.

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How about $P(y|\mathbf{x})$ directly?

Modelling $P(\mathbf{x}|y)$ is inefficient when real task is $P(y|\mathbf{x})$.

Idea? Assign probabilistic labels $q(y_t) = P(y_t|\mathbf{x}_t)$ to unlabeled inputs $\mathbf{x}_t$, and train $P(y|\mathbf{x})$ with them. However, there is no effect as the gradient vanishes:

$$\mathbb{E}_{q(y)}\left[\frac{\partial}{\partial \boldsymbol{\theta}} \log P(y \mid \mathbf{x})\right] = \int q(y) \frac{\frac{\partial}{\partial \boldsymbol{\theta}} P(y \mid \mathbf{x})}{P(y \mid \mathbf{x})} \mathrm{d}y$$
$$= \frac{\partial}{\partial \boldsymbol{\theta}} \int P(y \mid \mathbf{x}) \mathrm{d}y = \frac{\partial}{\partial \boldsymbol{\theta}} 1 = 0.$$

There are ways to adjust the assigned labels $q(y_t)$ to make them count.

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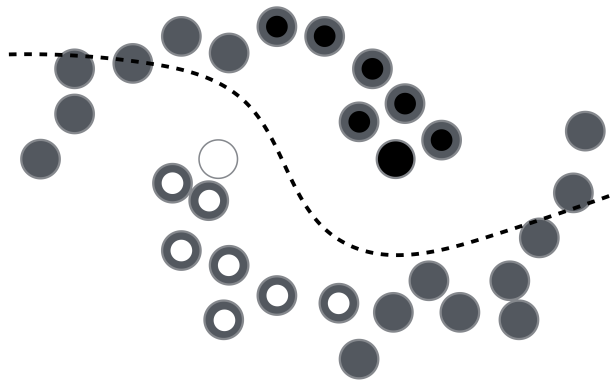
Adjusting assigned labels $q(y_t)$ (1/2)



Label propagation (Szummer and Jaakkola, 2003)

- Nearest neighbours tend to have the same label.
- Propagate labels to their neighbours and iterate.

Pseudo-labels (Lee, 2013)

- Round probabilistic labels $q(y_t)$ towards 0/1 gradually during training.

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Adjusting assigned labels $q(y_t)$ (2/2)

Co-training (Blum and Mitchell, 1998)

- Assumes multiple views on $\mathbf{x}$, say $\mathbf{x} = (\mathbf{x}^{(1)}, \mathbf{x}^{(2)})$.
- Train a separate classifier $P(y \mid \mathbf{x}^{(j)})$ for each view.
- For unlabeled data, the true label is the same for each view.
- Combine individual $q^{(j)}(y_t)$ into a joint $q(y_t)$ and feed it as target to each classifier.

Part of **Ladder network** (Rasmus et al., 2015)

- Corrupt input $\mathbf{x}_t$ with noise to get $\tilde{\mathbf{x}}_t$.
- Train $P(y|\tilde{\mathbf{x}})$ with a target from clean $q(y_t) = P(y_t|\mathbf{x}_t)$.

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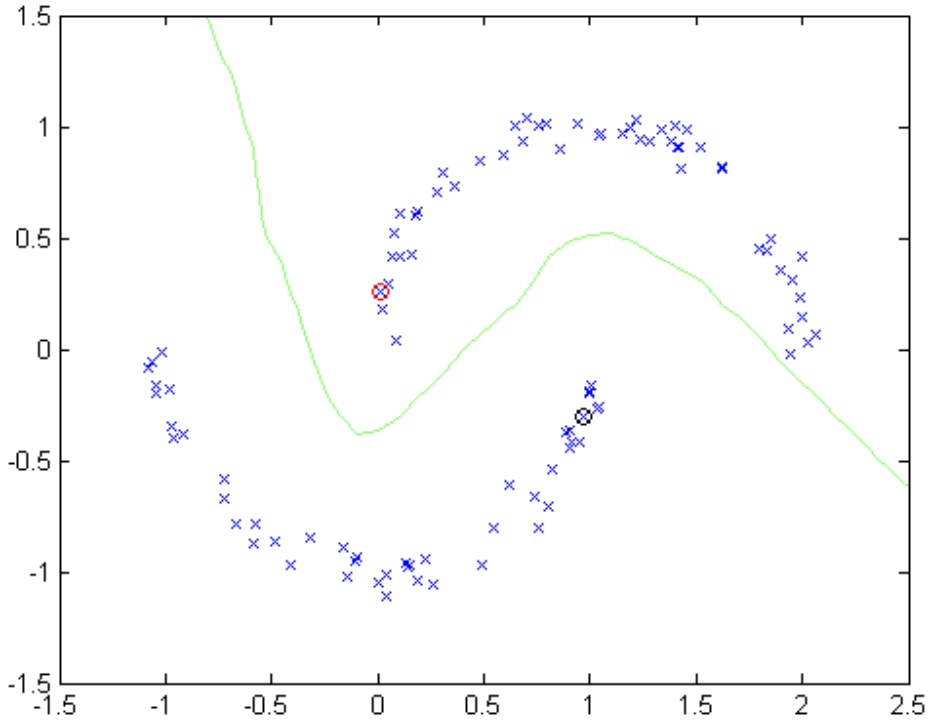
Code available



You can play with this as the last (third) exercise.
In low dimensions, bad local minima are an issue.

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Unsupervised learning

Data is just $\mathbf{x}'$, not input-output pairs $\mathbf{x}, \mathbf{y}$.
Possible goals:

- Model $P(\mathbf{x}')$, or
- Representation $f : \mathbf{x}' \rightarrow \mathbf{h}$.

Comparisons to supervised learning $P(\mathbf{y}|\mathbf{x})$:

- See data as $\mathbf{x}' = \mathbf{y}$, model $P(\mathbf{y}|\mathbf{x} = \varnothing)$
- No right output $\mathbf{y}$ given, invent your own output $\mathbf{h}$
- Concatenate inputs and outputs to $\mathbf{x}' = [\mathbf{x}; \mathbf{y}]$, prepare to answer any query, including $P(\mathbf{y}|\mathbf{x})$.

From here on, data is just $\mathbf{x}$. Notation $\mathbf{x}'$ was used to avoid confusion.

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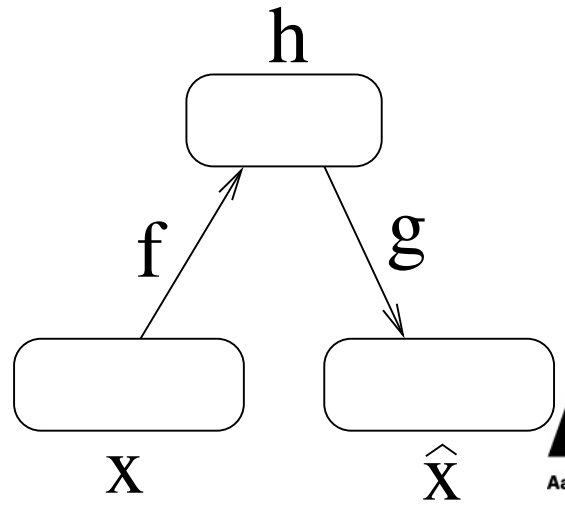
Approaches to unsupervised learning (1/2)

Besides kernel density estimation, virtually all unsupervised learning approaches use variables **h**.

- Discrete h (cluster index, hidden state of HMM, map unit of SOM)
- Binary vector **h** (most Boltzmann machines)
- Continuous vector **h** (PCA, ICA, NMF, sparse coding, autoencoders, state-space models, . . .)

Vocabulary:

- Encoder function $f : \mathbf{x} \rightarrow \mathbf{h}$
- Decoder function $g : \mathbf{h} \rightarrow \hat{\mathbf{x}}$
- Reconstruction $\hat{\mathbf{x}}$



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Approaches to unsupervised learning (2/2)

Often the encoder function $f : \mathbf{x} \to \mathbf{h}$ is implicit:

- Nearest cluster center $f(\mathbf{x}) = \arg\min_h \mathrm{D}(\mathbf{x}, \mathbf{c}_h)$
- Bayesian inference in a generative model, e.g. maximum a posteriori $f(\mathbf{x}) = \arg\max_{\mathbf{h}} P(\mathbf{x}|\mathbf{h})P(\mathbf{h})$

In complex models, exact inference is often impossible.
Approximate inference might hurt learning.

Autoencoders have an explicit encoder function $f(\cdot)$, which makes learning complex models easier:
Just backpropagation!

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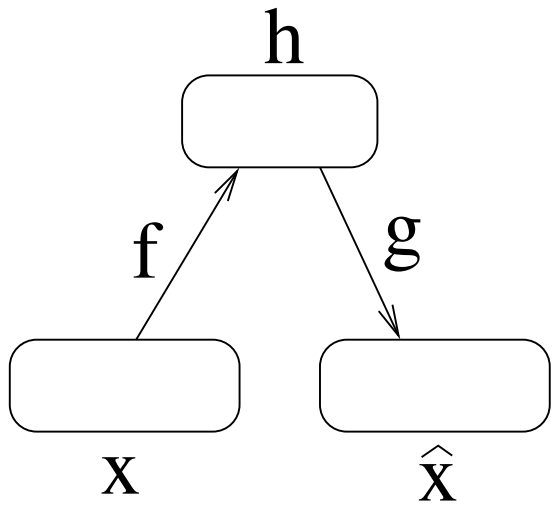
PCA as an autoencoder (1/2)



Assume linear encoder and decoder:

$f(\mathbf{x}) = \mathbf{W}^{(1)}\mathbf{x} + \mathbf{b}^{(1)}$

$g(\mathbf{h}) = \mathbf{W}^{(2)}\mathbf{h} + \mathbf{b}^{(2)}$

PCA solution minimizes criterion $C = \mathbb{E}\left[\|\mathbf{x} - \hat{\mathbf{x}}\|^2\right]$.

Note: Solution is not unique, even if restricting $\mathbf{W}^{(2)} = \mathbf{W}^{(1)\top}$.

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PCA as an autoencoder (2/2)

Just learning the identity mapping $g(f(\cdot)) = I(\cdot)$?
$\hat{\mathbf{x}} = g(f(\mathbf{x})) = \left(\mathbf{W}^{(2)}\mathbf{W}^{(1)}\right)\mathbf{x} + \left(\mathbf{W}^{(2)}\mathbf{b}^{(1)} + \mathbf{b}^{(2)}\right)$
We get $\hat{\mathbf{x}} = \mathbf{x}$ when $\mathbf{W}^{(2)} = (\mathbf{W}^{(1)})^{-1}$ and
$\mathbf{b}^{(2)} = -\mathbf{W}^{(2)}\mathbf{b}^{(1)}$.
So any encoder with an invertible $\mathbf{W}^{(1)}$ is optimal.

How to make the autoencoding problem harder?

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Regularized autoencoders

Regularization avoids learning the identity function:

- Bottleneck autoencoder (limit dimensionality of $\mathbf{h}$)
  (Bourlard and Kamp, 1988, Oja, 1991)
- Sparse autoencoder (penalize activations of $\mathbf{h}$)
  (Ranzato et al., 2006, Le et al., 2011)
- **Denoising autoencoder** (inject noise to input $\mathbf{x}$)
  (Vincent et al., 2008)
- Contractive autoencoder (penalize Jacobian of $f(\cdot)$)
  (Rifai et al., 2011)
- Variational autoencoder (probabilistic)
- Sometimes also weight sharing $\mathbf{W}^{(2)} = \mathbf{W}^{(1)\top}$.

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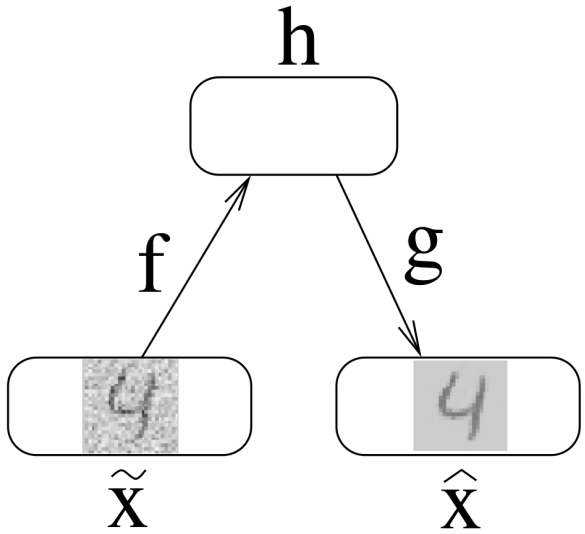
Denoising autoencoder (Vincent et al., 2008)



Feed corrupted inputs $\tilde{\mathbf{x}} \sim c(\tilde{\mathbf{x}}|\mathbf{x})$

- Additive noise $\tilde{\mathbf{x}} = \mathbf{x} + \boldsymbol{\epsilon}$ where e.g. $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$
- Salt noise $\tilde{\mathbf{x}} = \mathbf{m} \odot \mathbf{x}$ or $\tilde{x}_i = m_i x_i$
  where binary $m_i \sim \text{Bernoulli}(p)$
- Masking noise $\tilde{\mathbf{x}} = [\mathbf{m} \odot \mathbf{x}; \mathbf{m}]$

Train $\hat{\mathbf{x}} = g(f(\tilde{\mathbf{x}}))$ to minimize reconstruction error,
e.g. $C = \mathbb{E}\left[\|\hat{\mathbf{x}} - \mathbf{x}\|^2\right]$.

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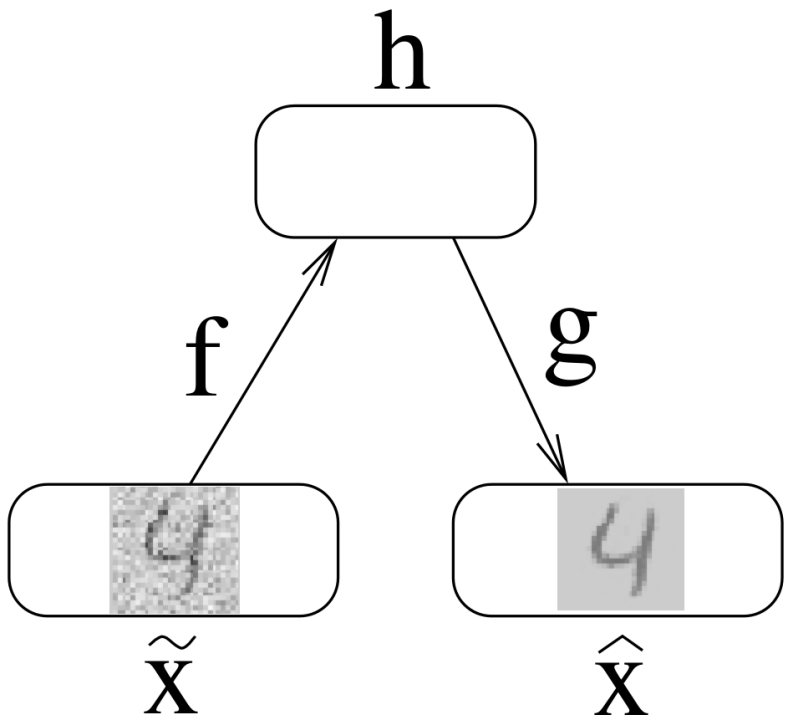
Denoising autoencoder



Basic encoder $\mathbf{h} = f(\tilde{\mathbf{x}}) = \Phi\left(\mathbf{W}^{(1)}\tilde{\mathbf{x}} + \mathbf{b}^{(1)}\right)$
and decoder $\hat{\mathbf{x}} = g(\mathbf{h}) = \mathbf{W}^{(2)}\mathbf{h} + \mathbf{b}^{(2)}$.
Deep autoencoder: both f and g multi-layered.

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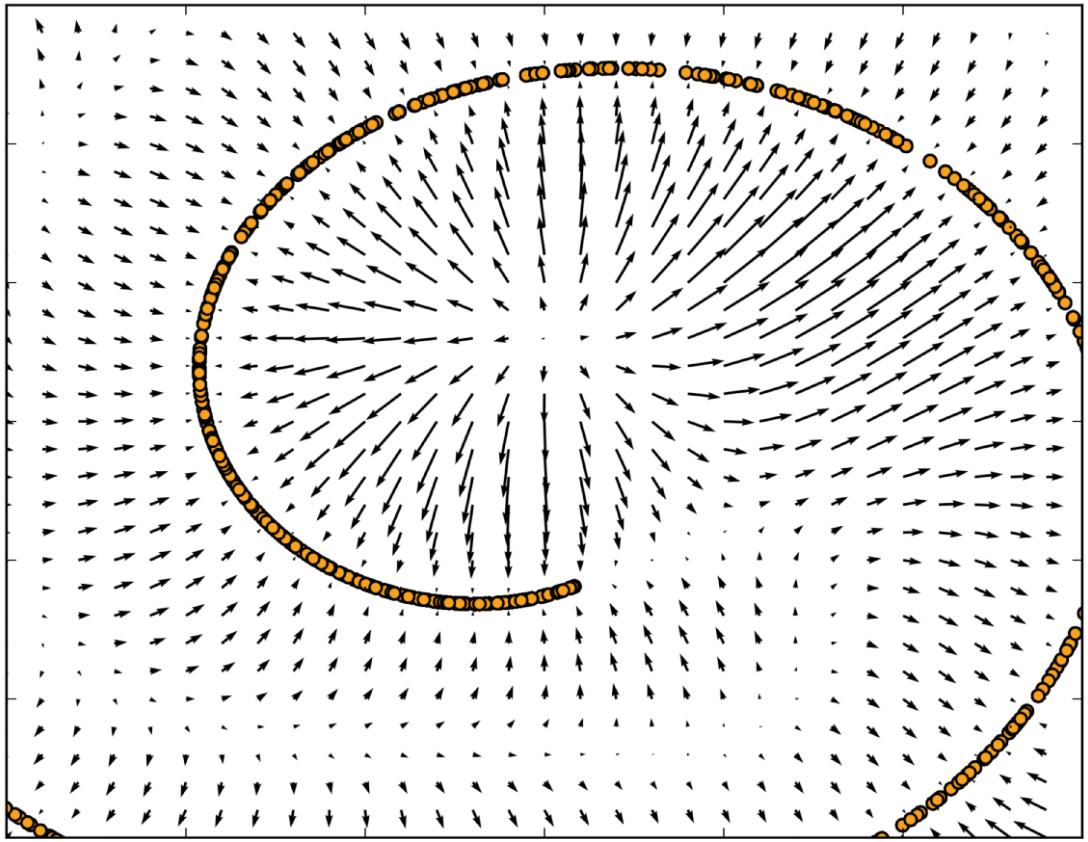
What does denoising autoencoder learn?



To point $g(f(\cdot))$ towards higher probability.

Image from (Alain and Bengio, 2014)

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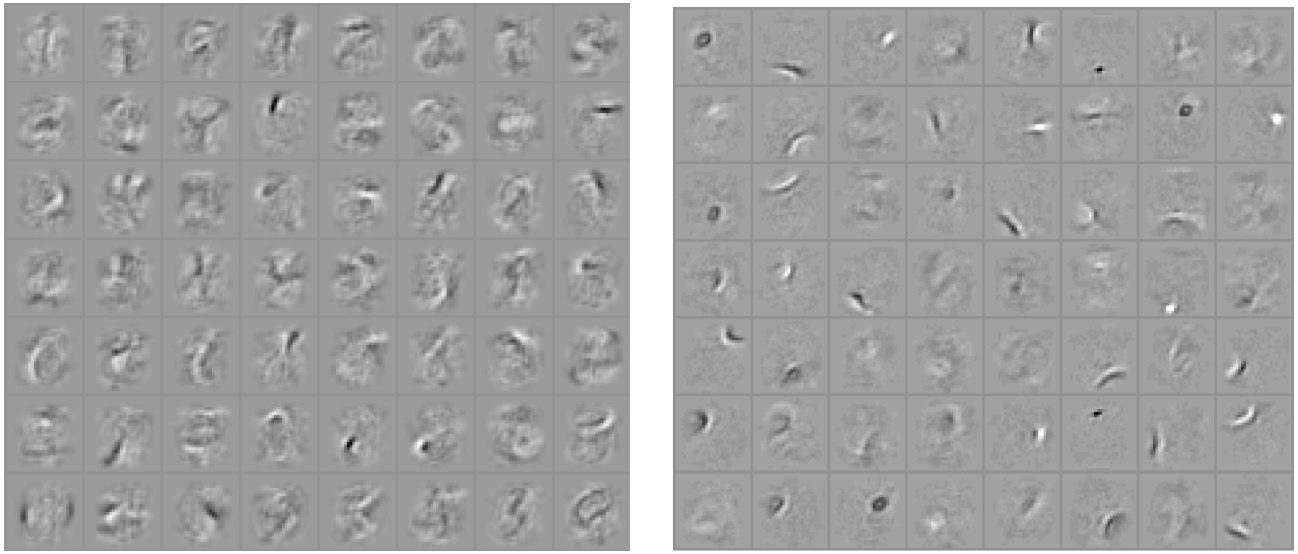
Comparison to training a classifier



- Training a classifier (left), when you get the labels right, learning stops. $\Rightarrow$ Learned parameters are based on the information in labels:
  Less than #examples$\times$#classes bits.
- Training a denoising autoencoder (right), outputs are richer: #examples$\times$#dimensions.

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Layerwise pretraining

- Use unsupervised learning to construct representations layer by layer (Ballard, 1987).
- Breakthrough with Boltzmann machines (Hinton and Salakhutdinov 2006), starting deep learning boom.
- Presented here: Stacked denoising autoencoders

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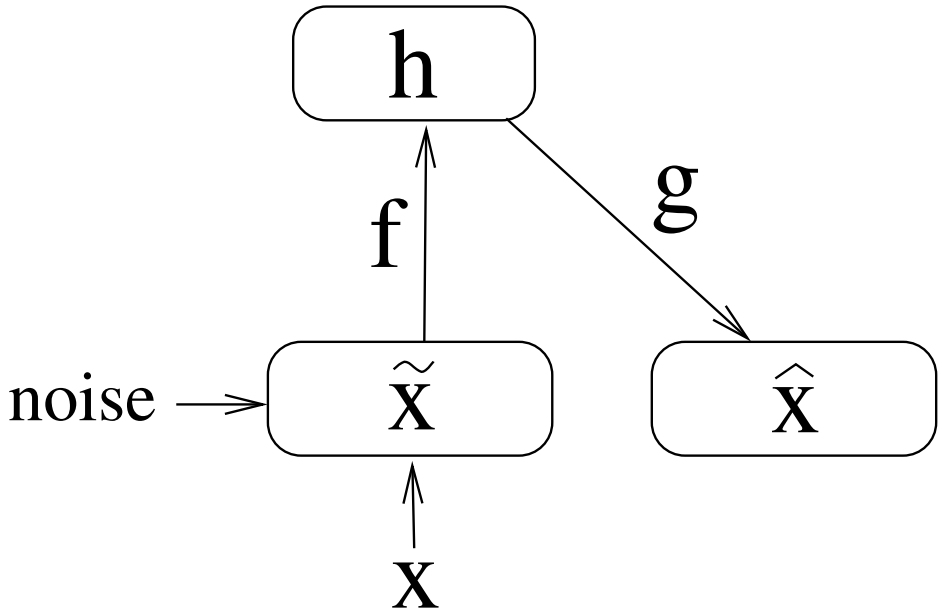
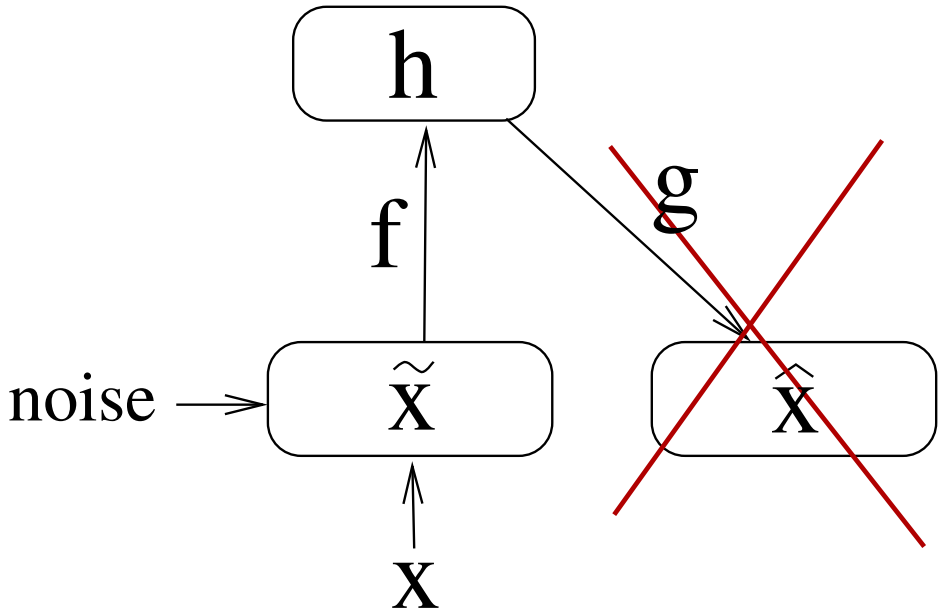
Layerwise pretraining



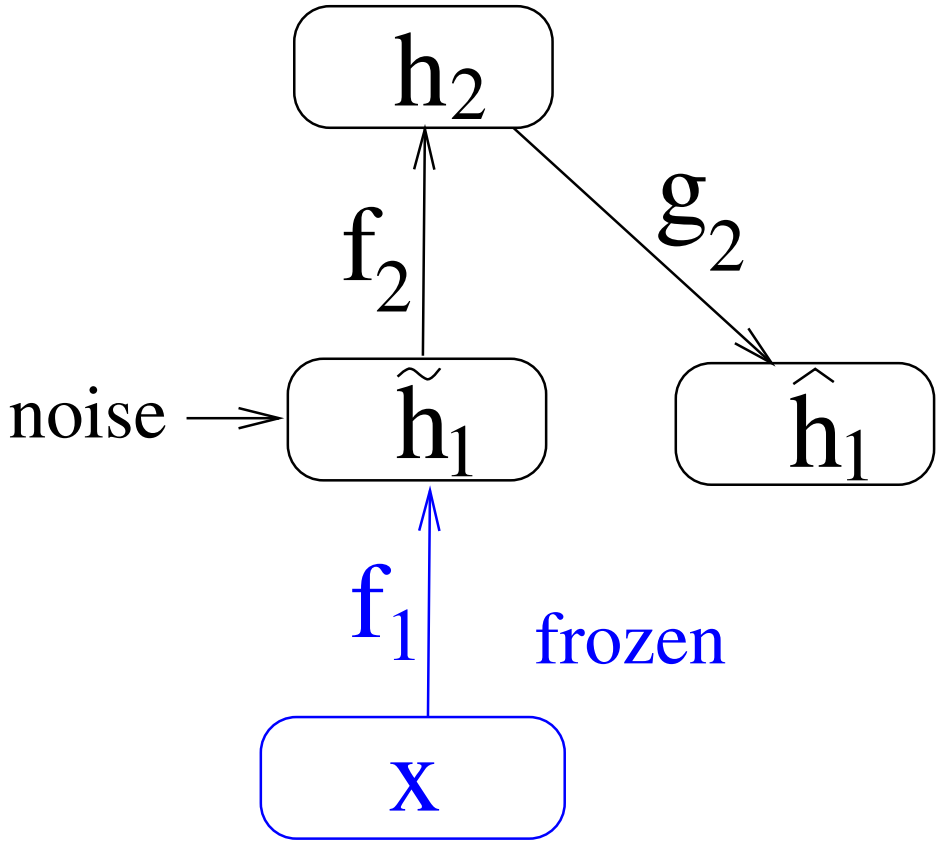
Phase 1: Denoising autoencoder.

Layerwise pretraining



Toss away the decoder $g(\cdot)$.

Layerwise pretraining



Phase 2: Stack another layer, keep the bottom fixed.

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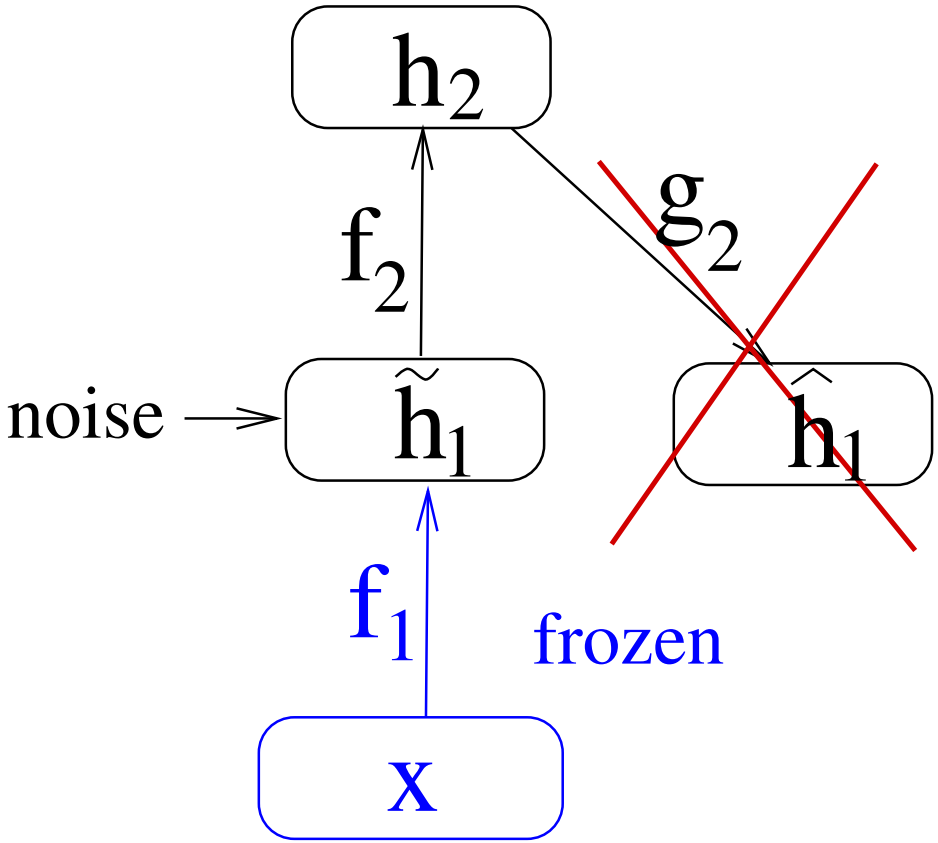
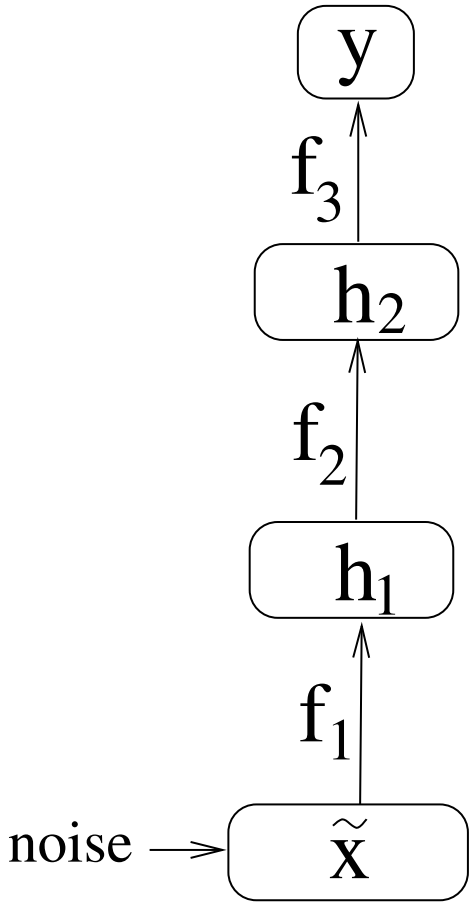
Layerwise pretraining



Toss away the second decoder $g_2(\cdot)$.

Supervised finetuning



Phase 3: Supervised finetuning with labels y.
Note: Encoder f of an autoencoder is the same mapping as used in supervised learning.

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On details and invariance

What is average of images in the category Cat?
What is the average of Dog?

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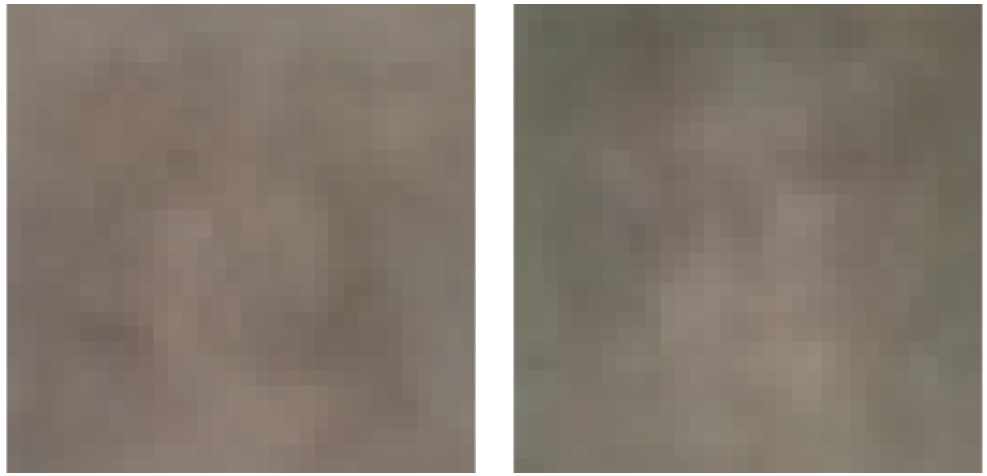
On details and invariance



Answer: both are just blurry blobs.
Autoencoder tries to learn a representation from which it can reconstruct the observations.
It cannot discard details: position, pose, lighting...
$\Rightarrow$ Not well compatible with supervised learning.

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Denoising versus probabilistic modelling

- We noted that denoising models are much easier to train than probabilistic models.
  Trainable by basic back-propagation.
- There is a strong connection between the two:
  Models can be converted into each other.

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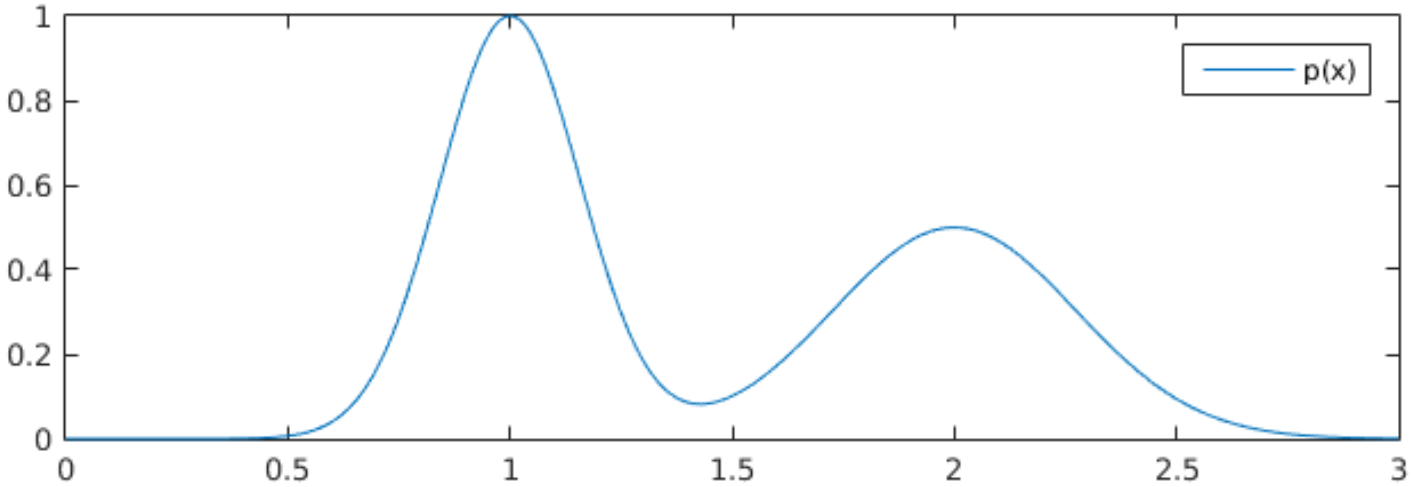
Probability to denoising



Given: Model $P(x)$ and observation $\tilde{x} = x + \text{noise}$.

Noise distribution known.

Task: Find $\hat{x} = \arg\min \mathbb{E}_x \left[(x - \hat{x})^2\right]$.

Solution: Compute the posterior $P(x \mid \tilde{x})$,
use its center of gravity as reconstruction $\hat{x}$.

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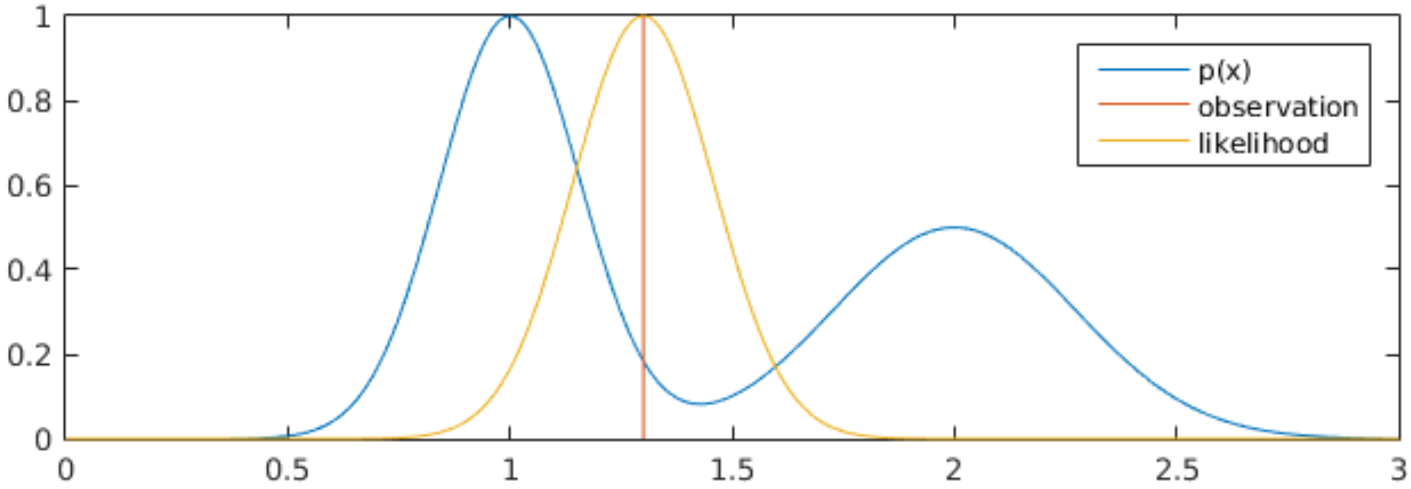
Probability to denoising



Given: Model $P(x)$ and observation $\tilde{x} = x + \text{noise}$.

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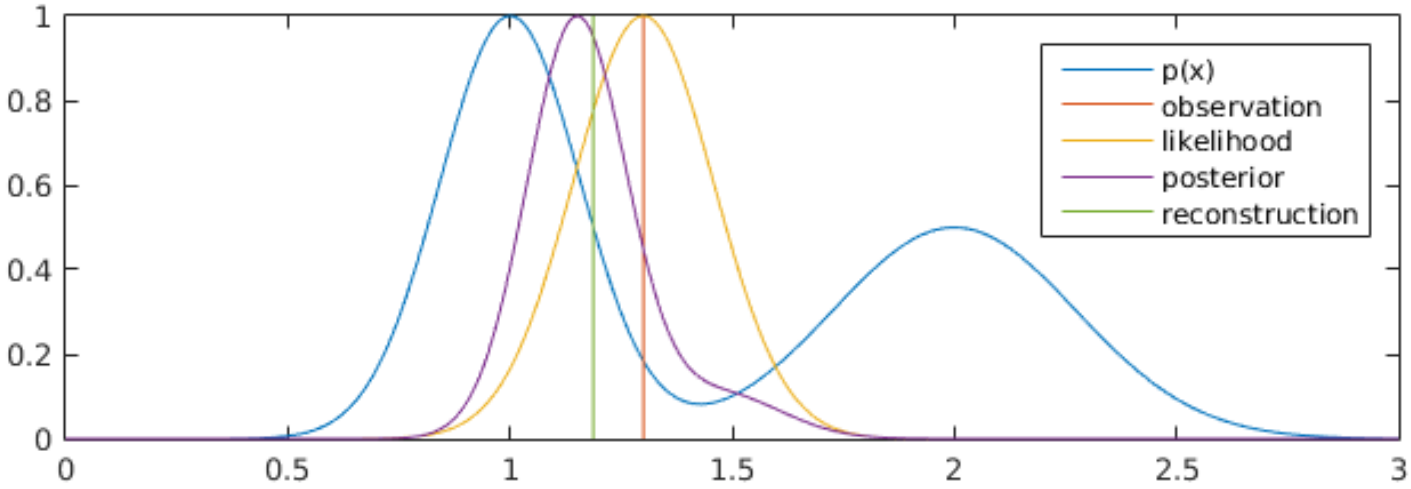
Probability to denoising



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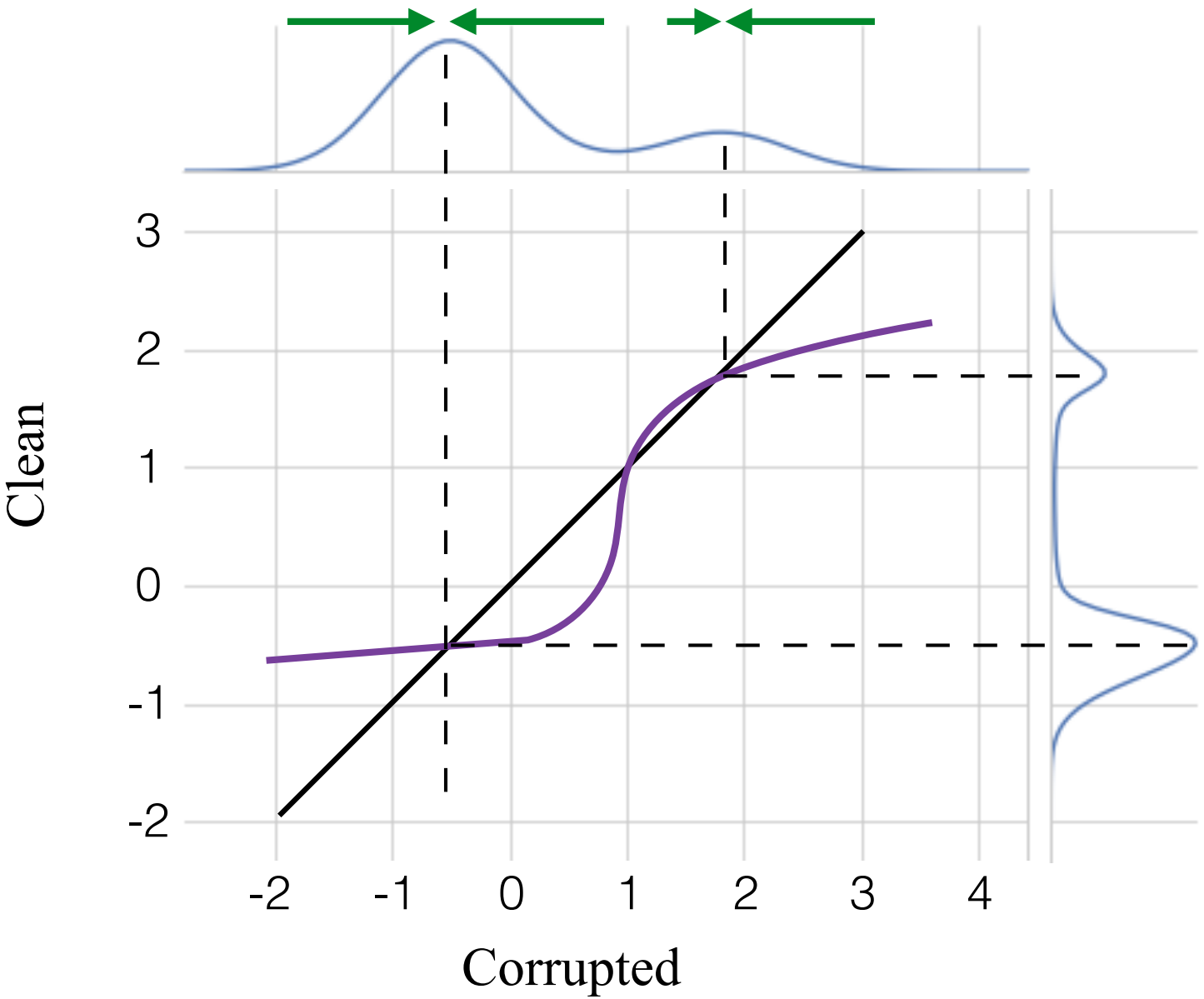
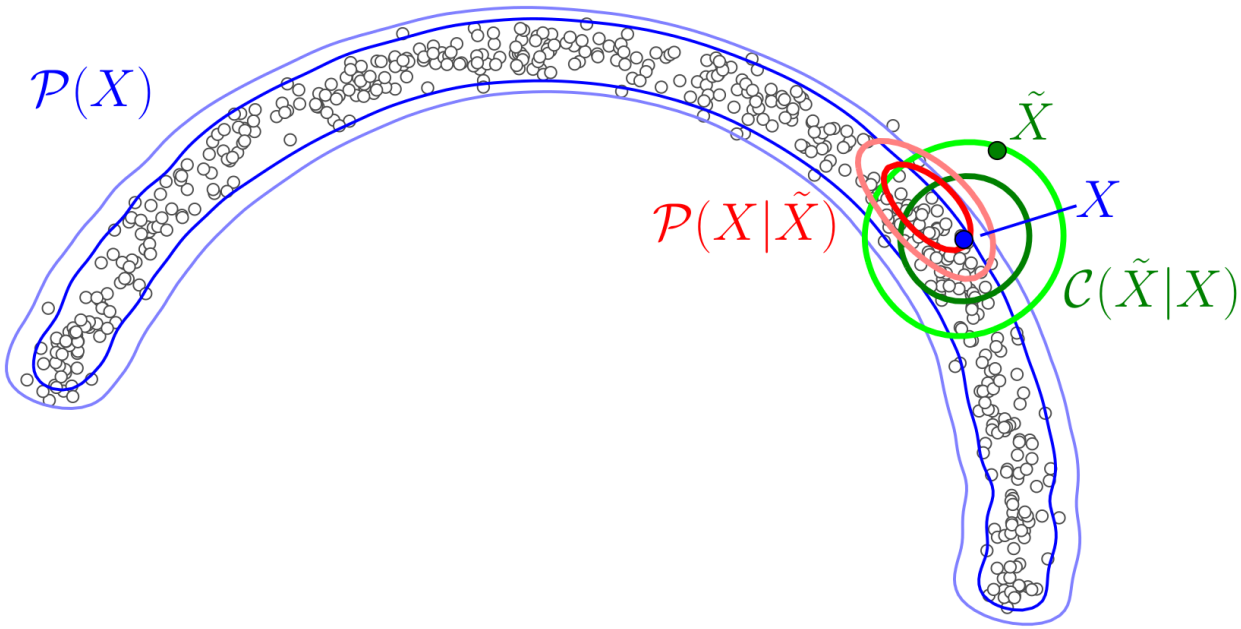
Probability to denoising



Denoising to probability

(Generative Stochastic Networks, Bengio et al., 2014)



Markov chain alternating between corruption $C(\tilde{X}|X)$ and denoising $P(X|\tilde{X})$.
Theoretical result: Stationary distribution is $P(X)$.

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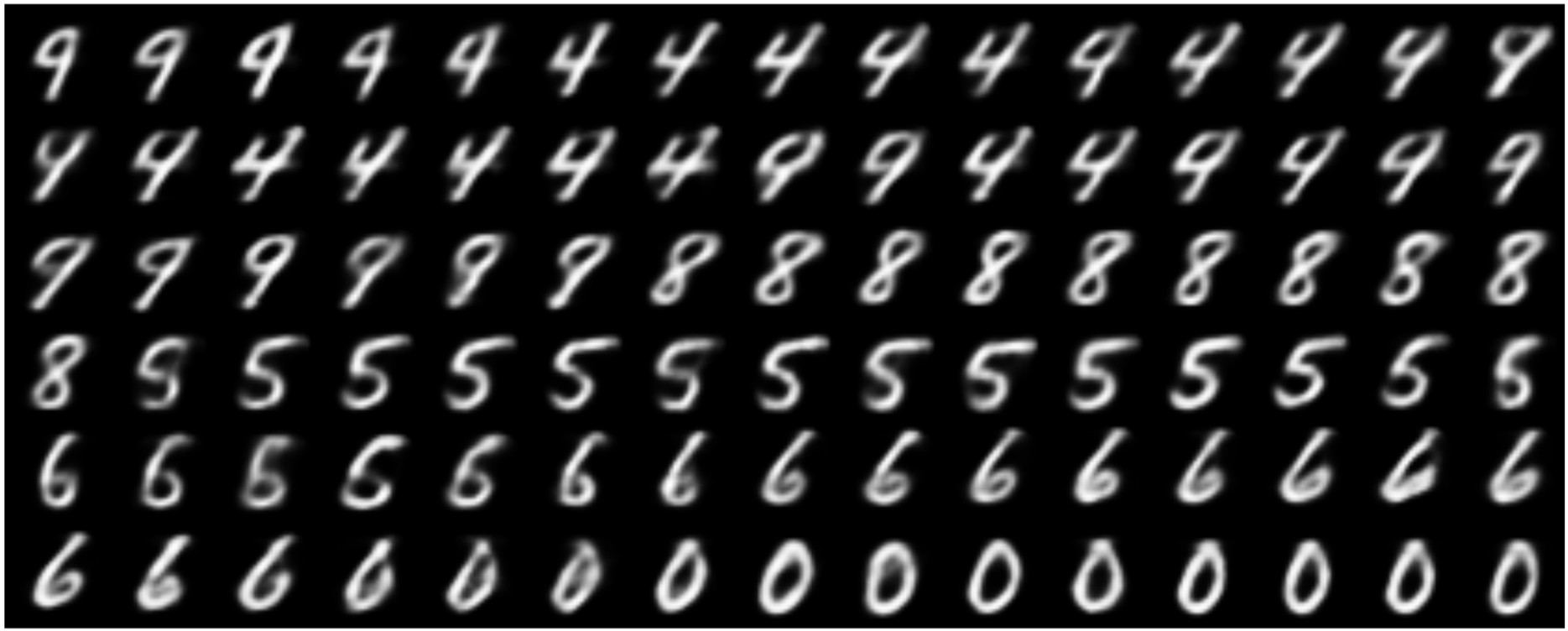
Denoising to probability (Bengio et al., 2014)



Generating samples from the Markov chain.

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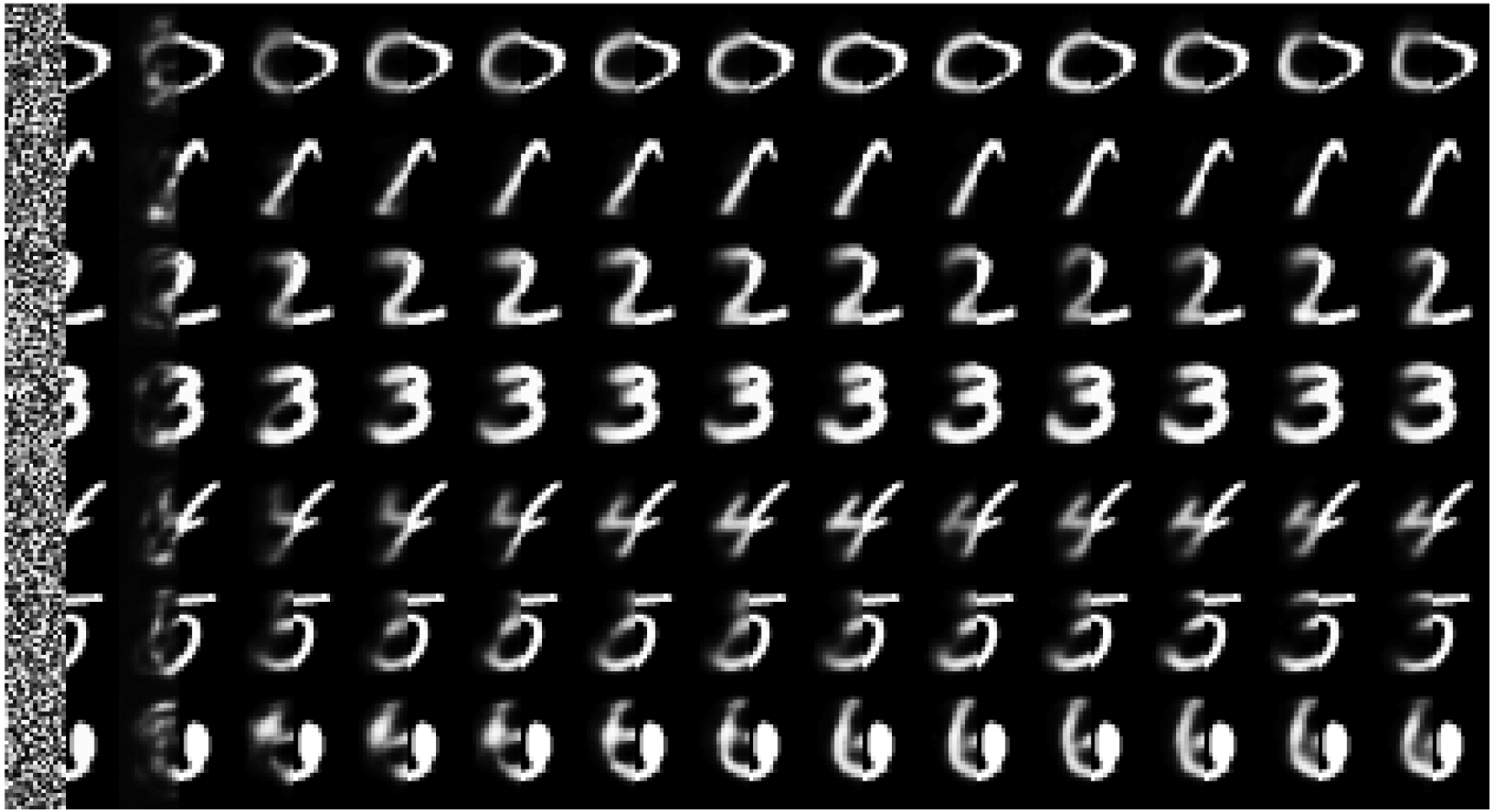
Denoising to probability (Bengio et al., 2014)



Reconstructing the left half.

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Ladder network, main ideas

- Shortcut connections in an autoencoder network allow it to discard details.
- Learning in deep networks can be made efficient by spreading unsupervised learning targets all over the network.

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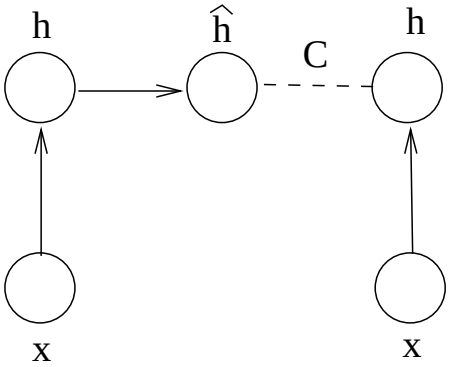
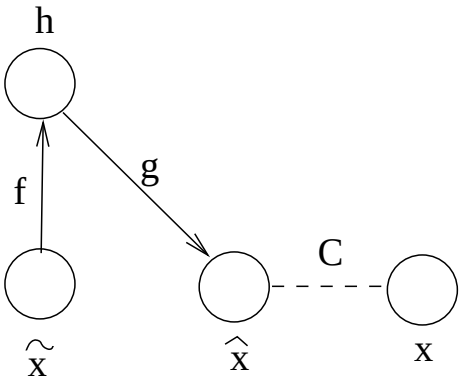
Combining DSS+DAE



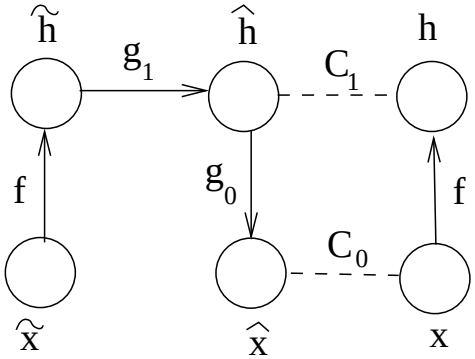
Denoising Source Separation

(Särelä and Valpola, 2005)



Denoising Autoencoder

(Vincent et al., 2008)



Ladder Network

(Valpola, 2015, Rasmus et al., 2015)

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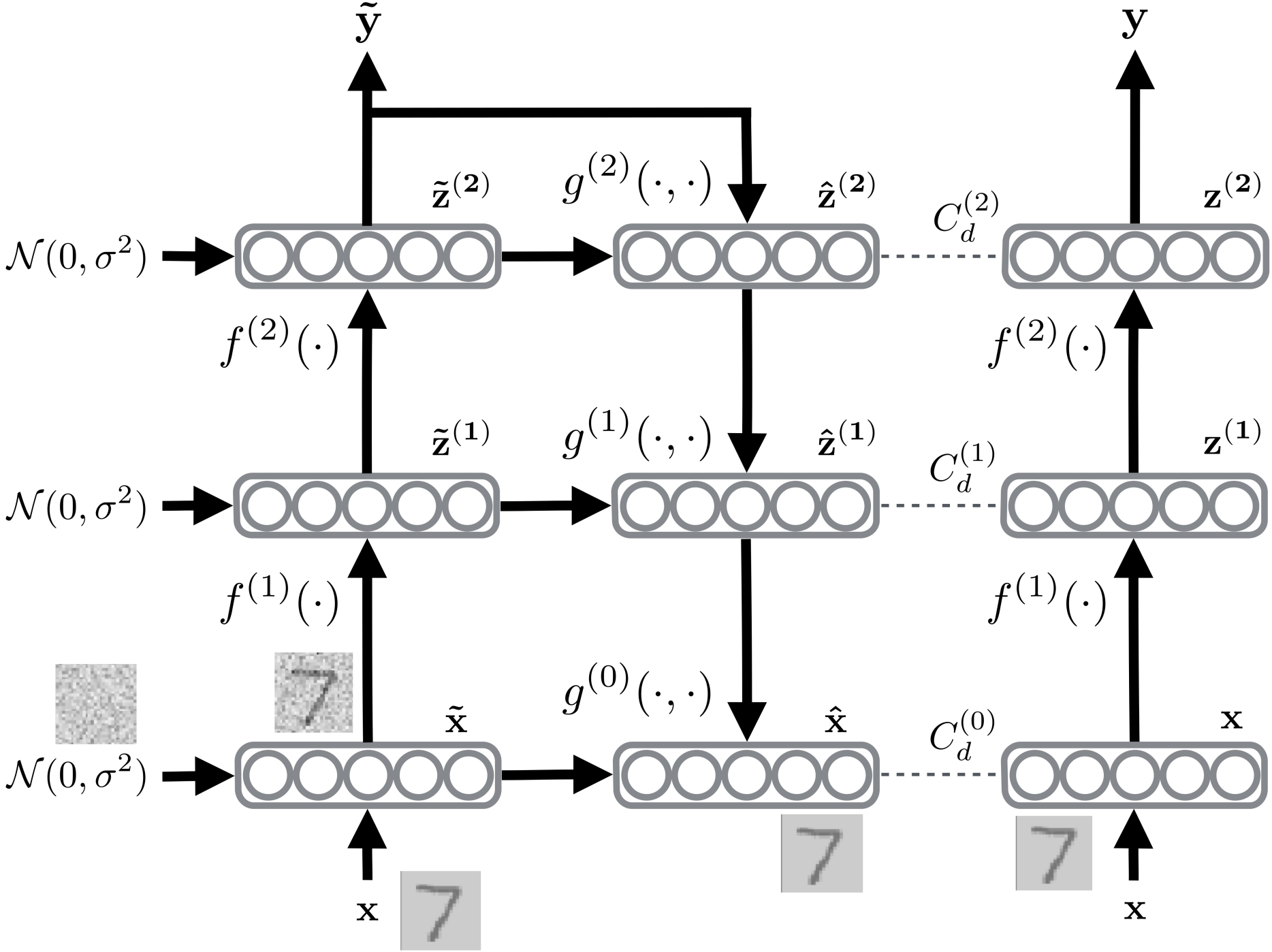
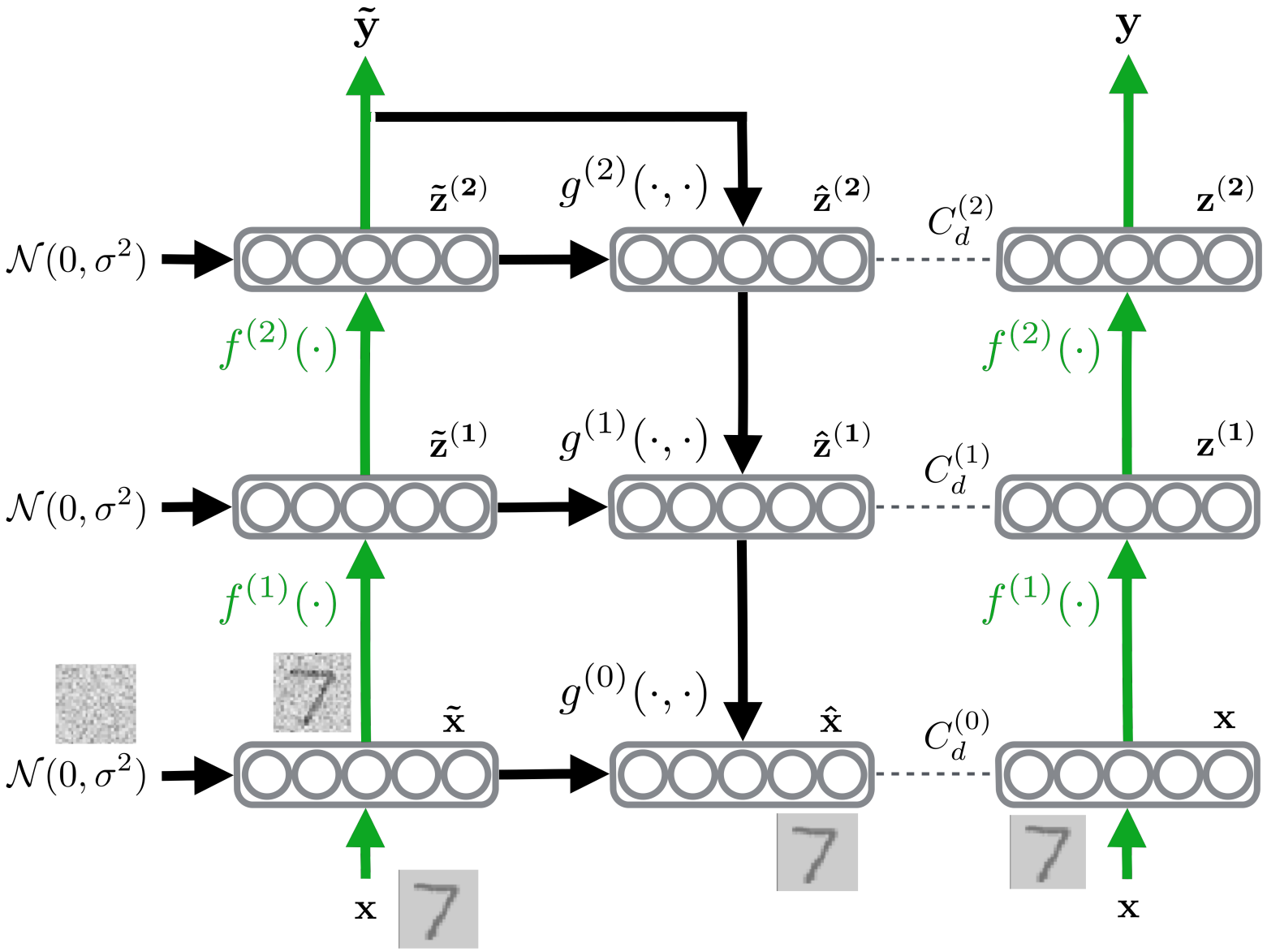

$\tilde{\mathbf{y}}$
$\mathbf{y}$
$\tilde{\mathbf{z}}^{(2)}$
$g^{(2)}(\cdot,\cdot)$
$\hat{\mathbf{z}}^{(2)}$
$C_d^{(2)}$
$\mathbf{z}^{(2)}$
$\mathcal{N}(0,\sigma^2)$
$f^{(2)}(\cdot)$
$f^{(2)}(\cdot)$
$\tilde{\mathbf{z}}^{(1)}$
$g^{(1)}(\cdot,\cdot)$
$\hat{\mathbf{z}}^{(1)}$
$C_d^{(1)}$
$\mathbf{z}^{(1)}$
$\mathcal{N}(0,\sigma^2)$
$f^{(1)}(\cdot)$
$f^{(1)}(\cdot)$
$g^{(0)}(\cdot,\cdot)$
$\tilde{\mathbf{x}}$
$\hat{\mathbf{x}}$
$C_d^{(0)}$
$\mathbf{x}$
$\mathcal{N}(0,\sigma^2)$
$\mathbf{x}$
$\mathbf{x}$

Same encoder $f(\cdot)$ used for corrupted and clean paths.



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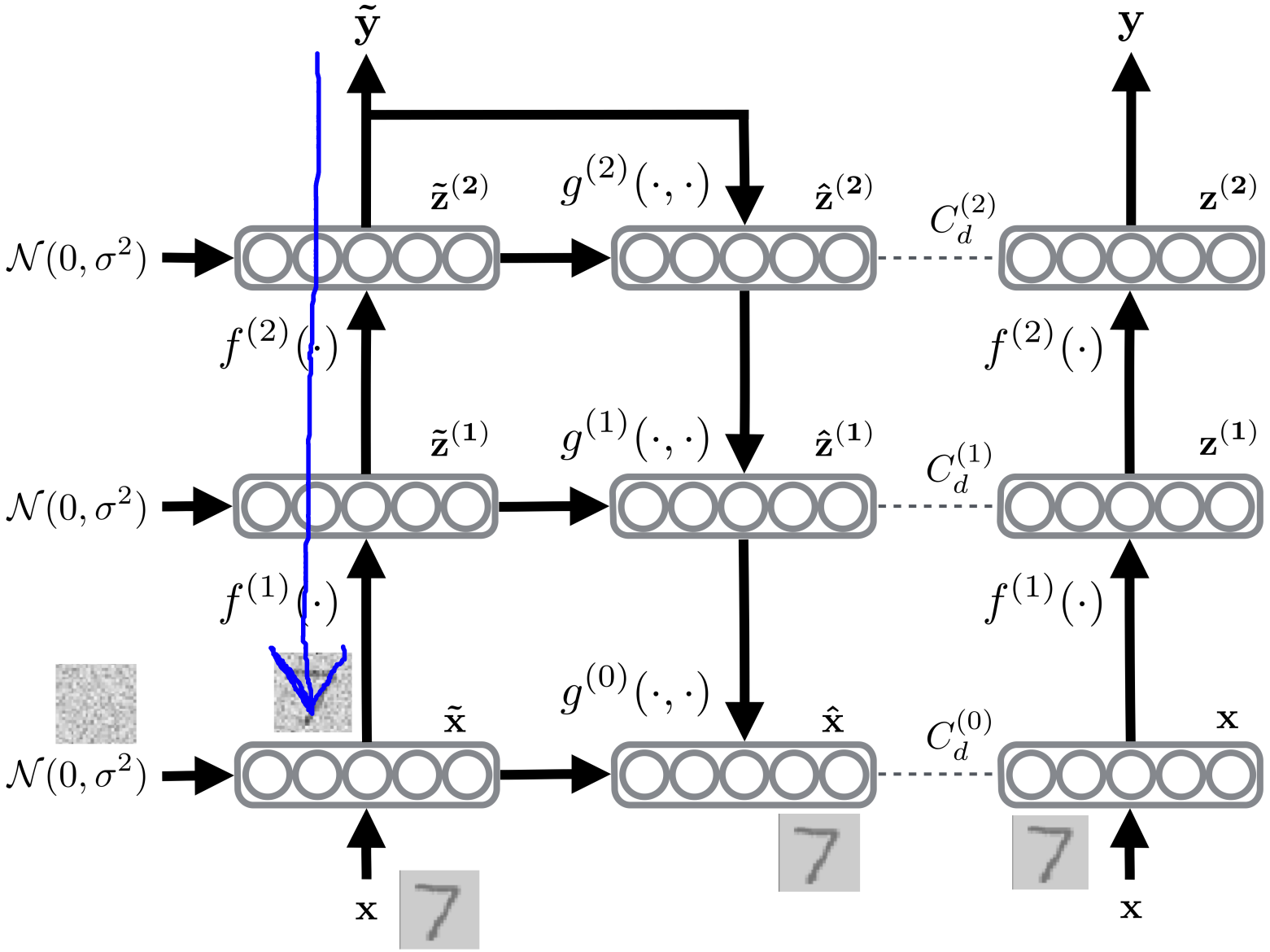
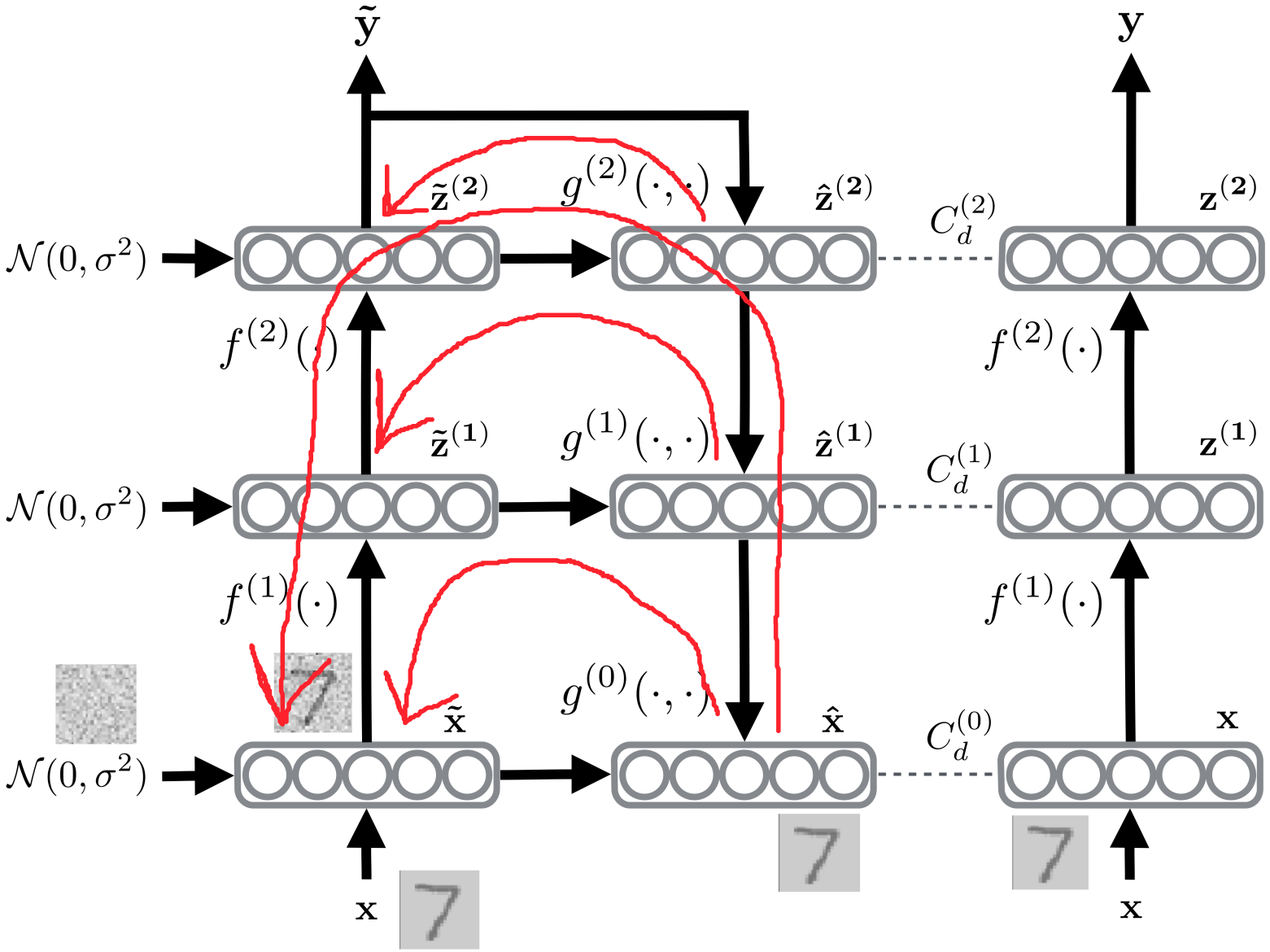
Supervised learning: Backprop from output $\tilde{\mathbf{y}}$.



Unsupervised learning:
Several denoising autoencoders simultaneously.



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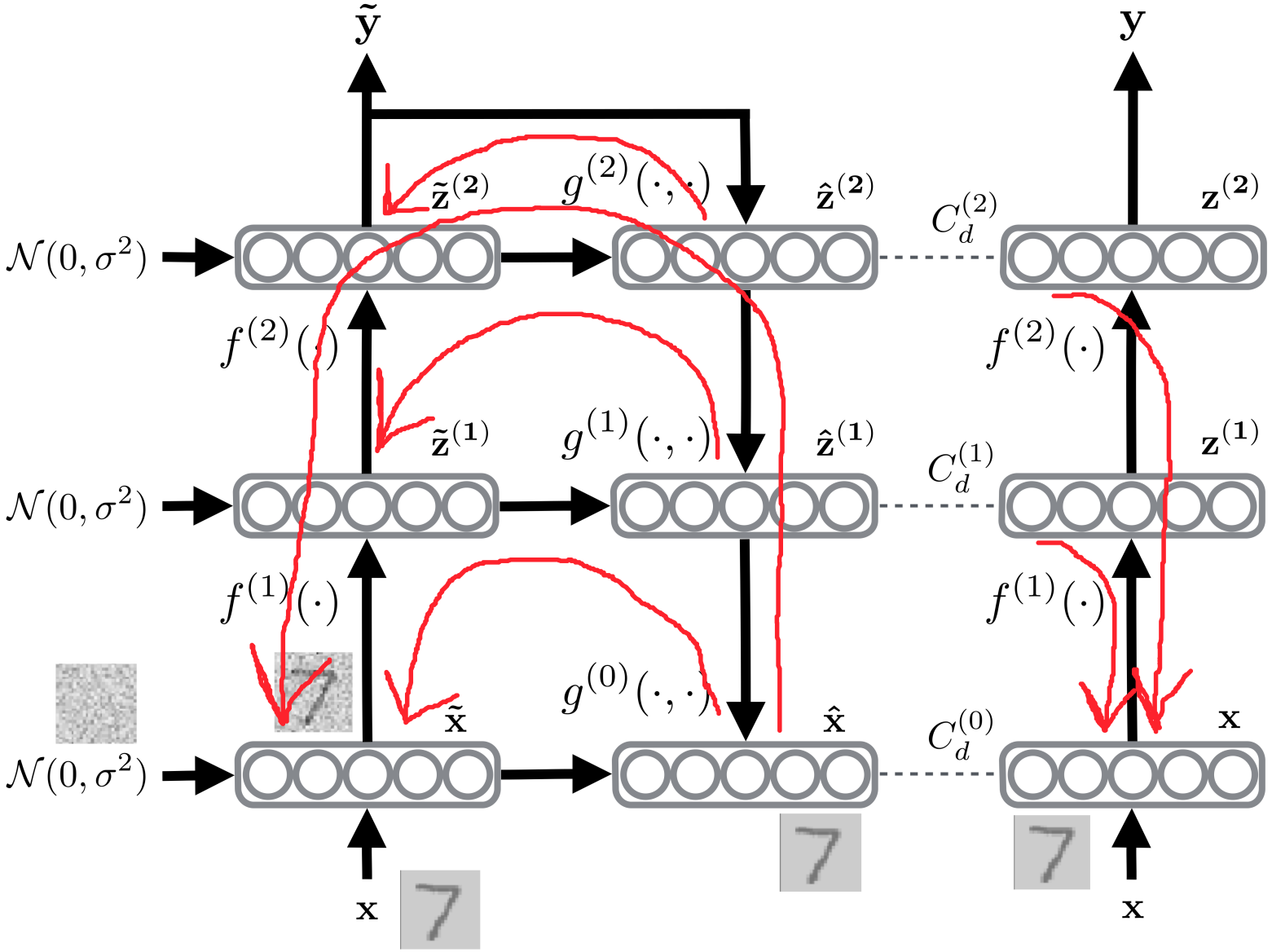
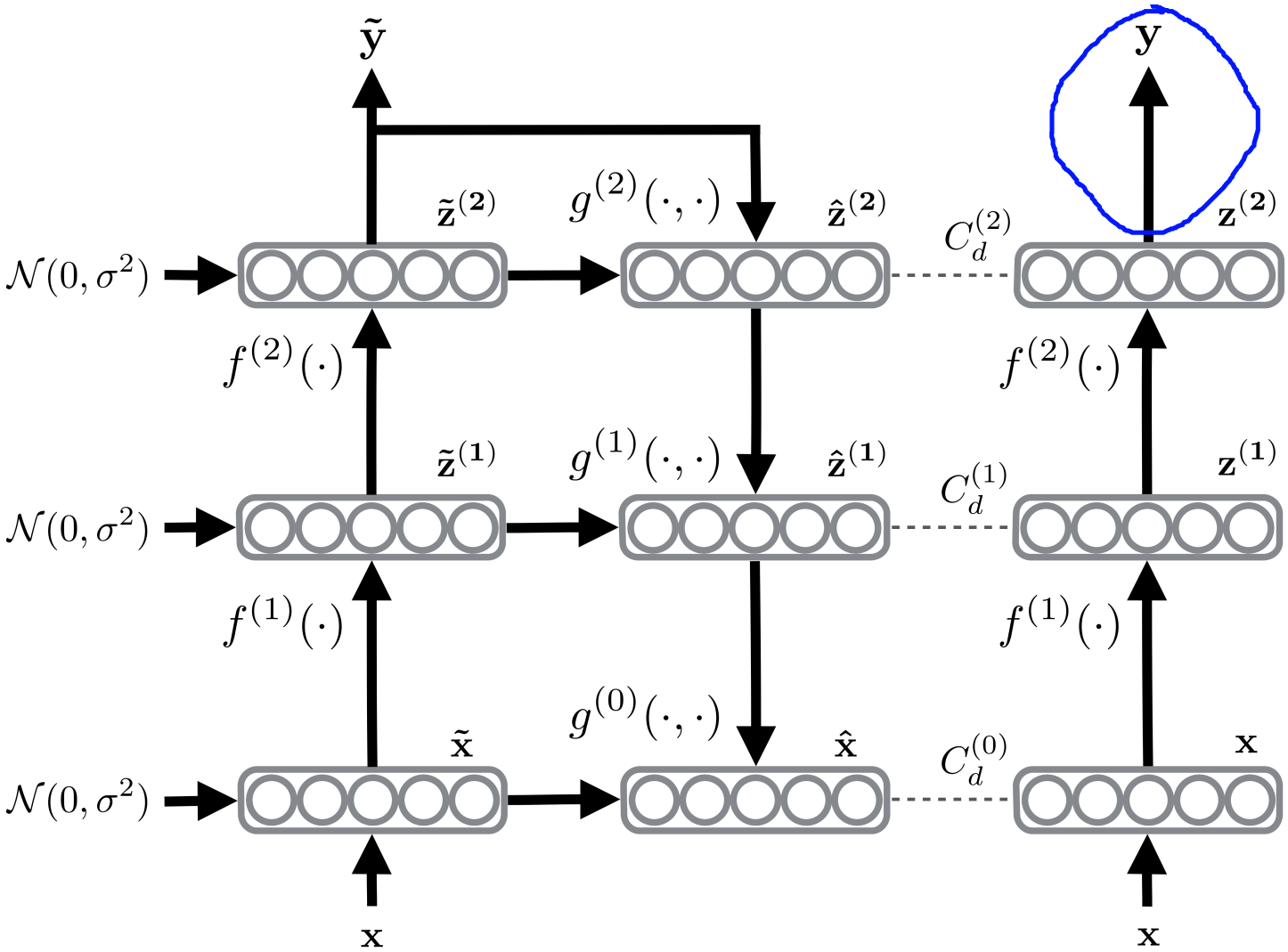
Unsupervised learning:
Produce robust representations (DSS aspect).



Read test output from the clean path. (Not used in training.)



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Training criterion

Only one phase of training: Minimize criterion C.

$$\mathrm{C} = -\log P(\tilde{\mathbf{y}} = \mathbf{y}_t | \mathbf{x}_t) + \sum_{l=0}^{L} \lambda_l \left\| \mathbf{z}^{(l)} - \hat{\mathbf{z}}_{\mathrm{BN}}^{(l)} \right\|^2$$

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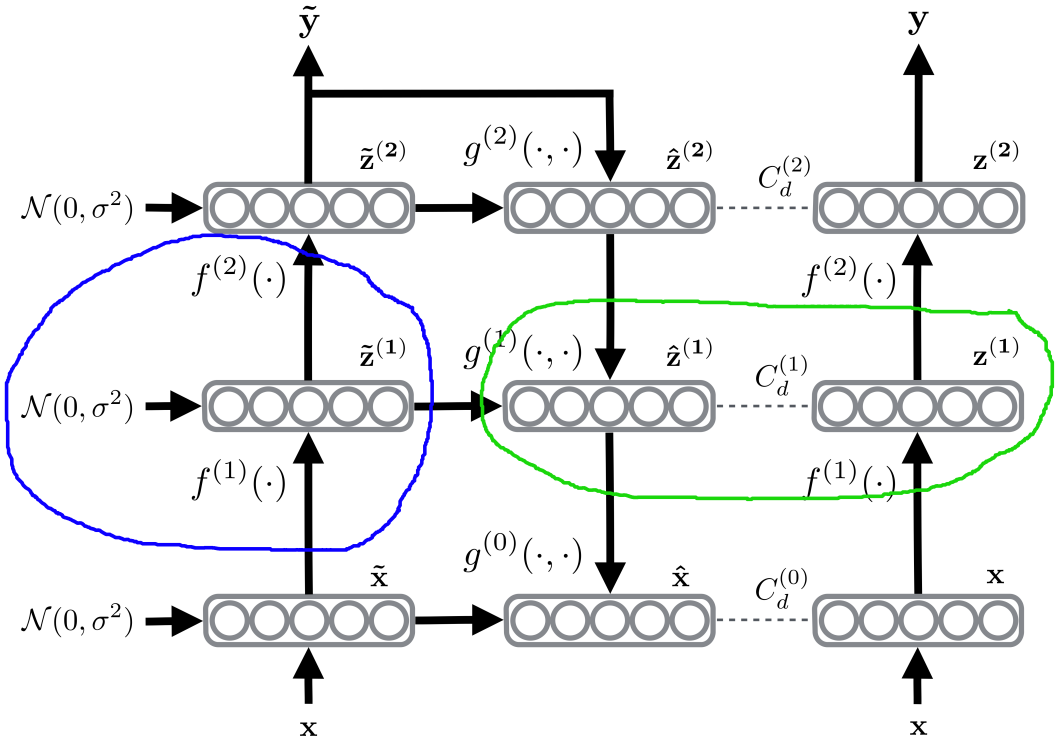
Scaling issues



Issue 1: Doubling $\mathbf{W}^{(1)}$ and halving $\mathbf{W}^{(2)}$ decreases noise.

Issue 2: Collapsing $\mathbf{z}^{(1)} = \hat{\mathbf{z}}^{(1)} = 0$ eliminates cost $C^{(1)}$.

Solution: Batch normalization (Ioffe and Szegedy, 2015)

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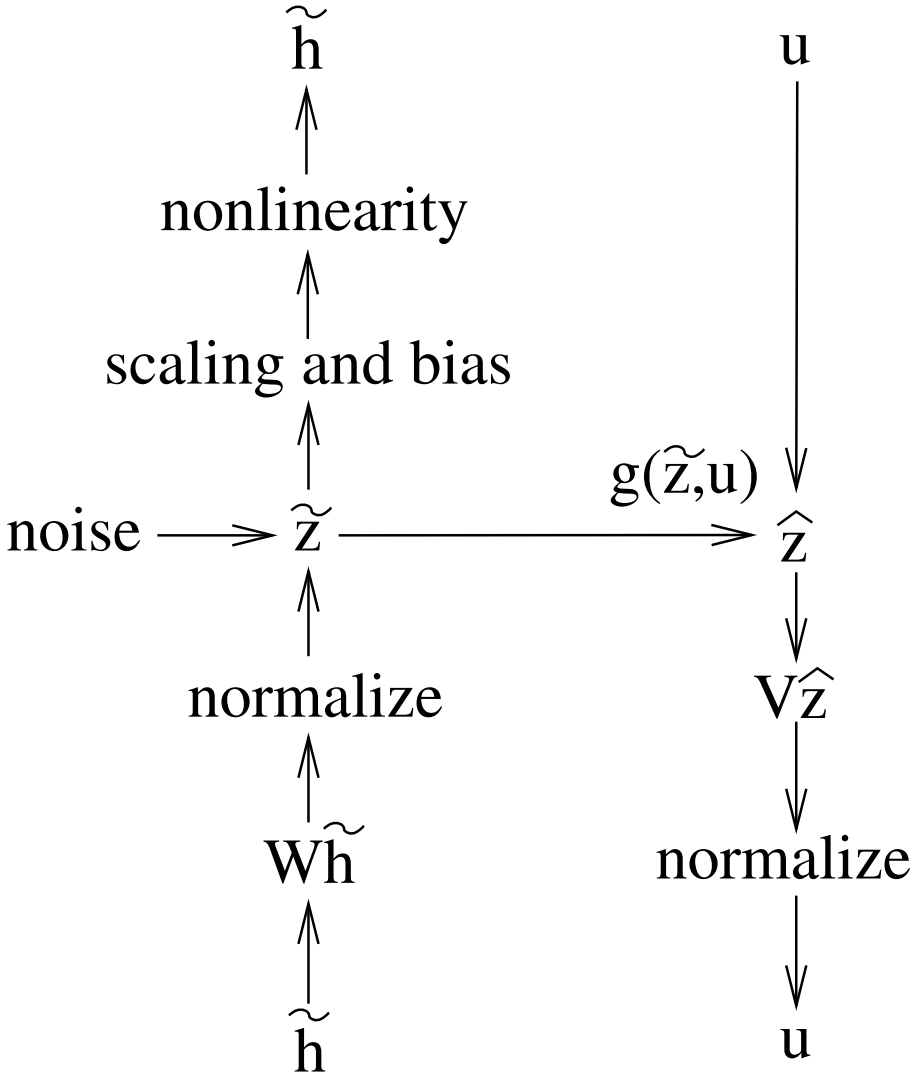
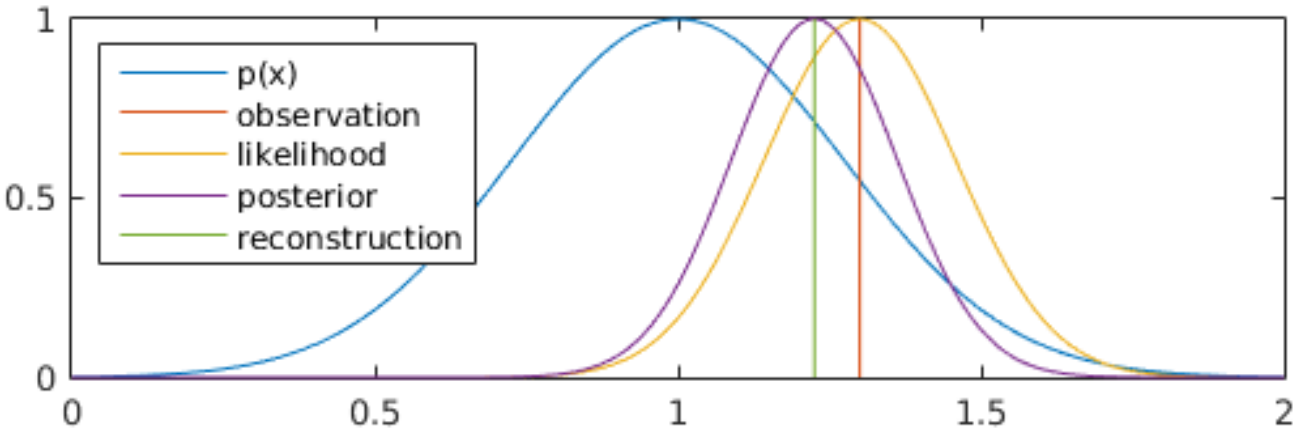
Some model details



$g(\tilde{\mathbf{z}}, \mathbf{u})$ done componentwise: $g_i(\tilde{z}_i, u_i)$.

Functional form of lateral connections?



Gaussian model: $P(z) = \mathcal{N}(\mu, \sigma_p^2)$

Gaussian noise: $P(\tilde{z}|z) = \mathcal{N}(z, \sigma_n^2)$

Optimal denoising: $\hat{z} = \frac{\sigma_n^2}{\sigma_p^2+\sigma_n^2}\mu + \frac{\sigma_p^2}{\sigma_p^2+\sigma_n^2}\tilde{z}$

Top-down signal u corresponds to $P(z)$.

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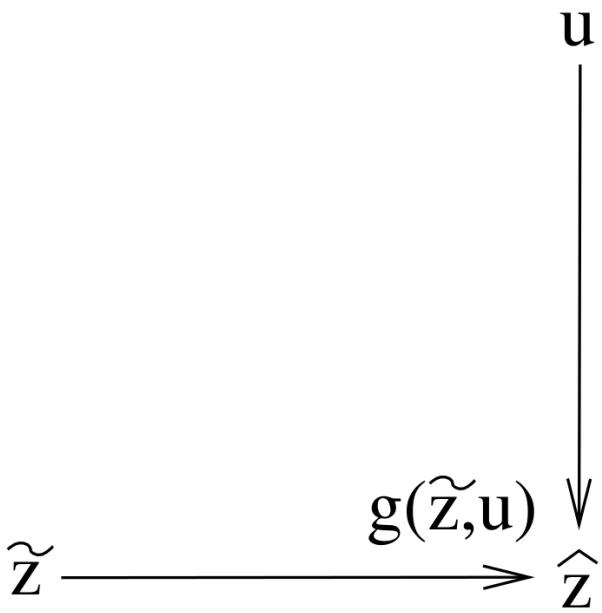
Functional form of lateral connections?



Recall $\hat{z} = \frac{\sigma_n^2}{\sigma_p^2+\sigma_n^2}\mu + \frac{\sigma_p^2}{\sigma_p^2+\sigma_n^2}\tilde{z}$ from previous slide.

Additive: $\hat{z}_{\text{add}} = g_1(\tilde{z}) + g_2(u)$
corresponds to modelling the mean μ with u.

Modulated: $\hat{z}_{\text{mod}} = g_3(\tilde{z}, u)(\tilde{z} + \text{bias})$
corresponds to modelling variance σ_p^2 with u.

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Functional form of lateral connections?

How to interpret top-down signal u modulating:
Does this detail in $\tilde{z}$ fit in the big picture?
If yes, trust it at let it through to reconstruction $\hat{z}$.
If not, filter it away as noise.

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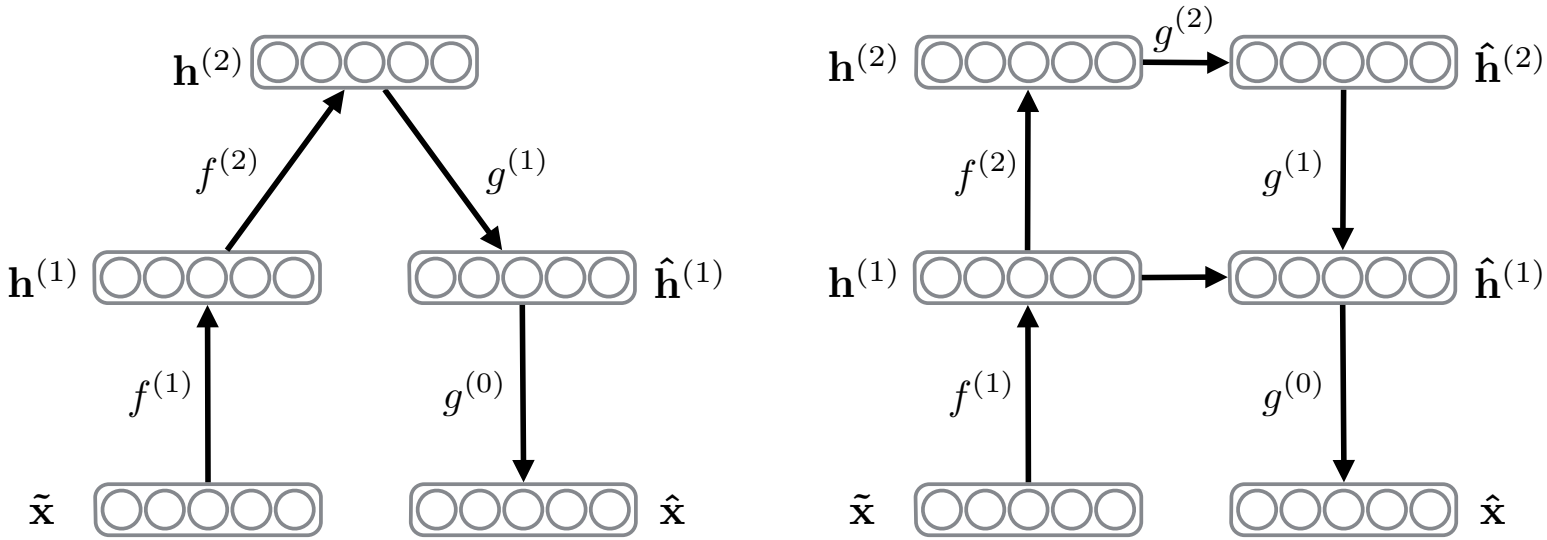
Analysis: Unsupervised learning



We compare deep denoising autoencoder and Ladder with additive or modulated lateral connections.
Data is small natural image patches.

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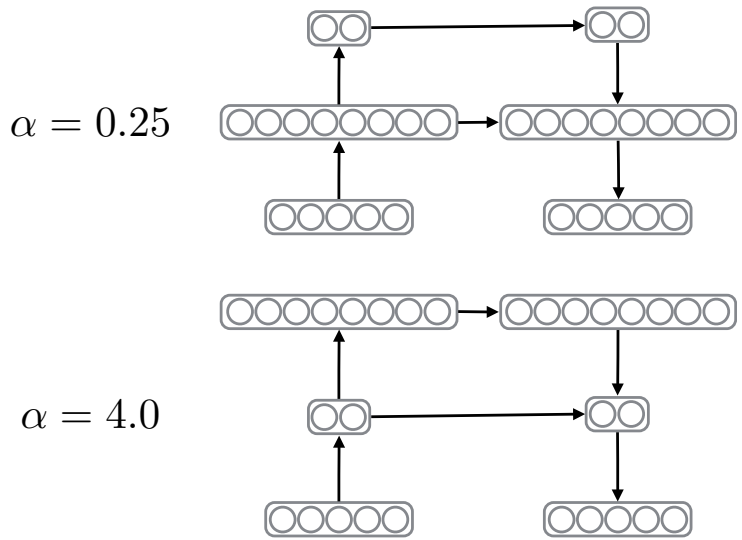
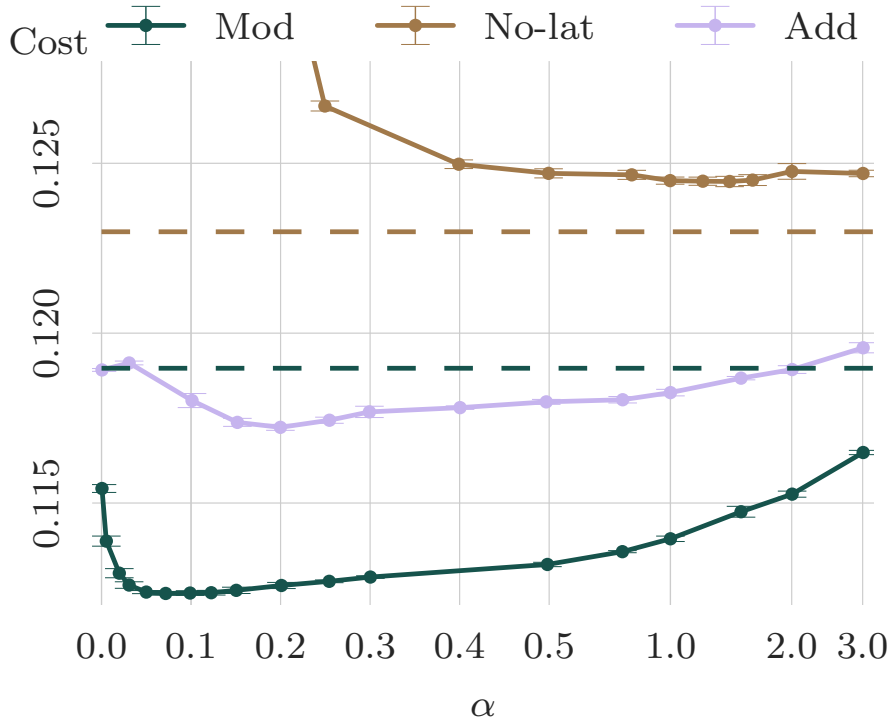
Analysis: Unsupervised learning

Denoising performance





1 million parameters, vary sizes of layers.
Result: Modulated connections best.
Ladder needs fewer units on $\mathbf{h}^{(2)}$.

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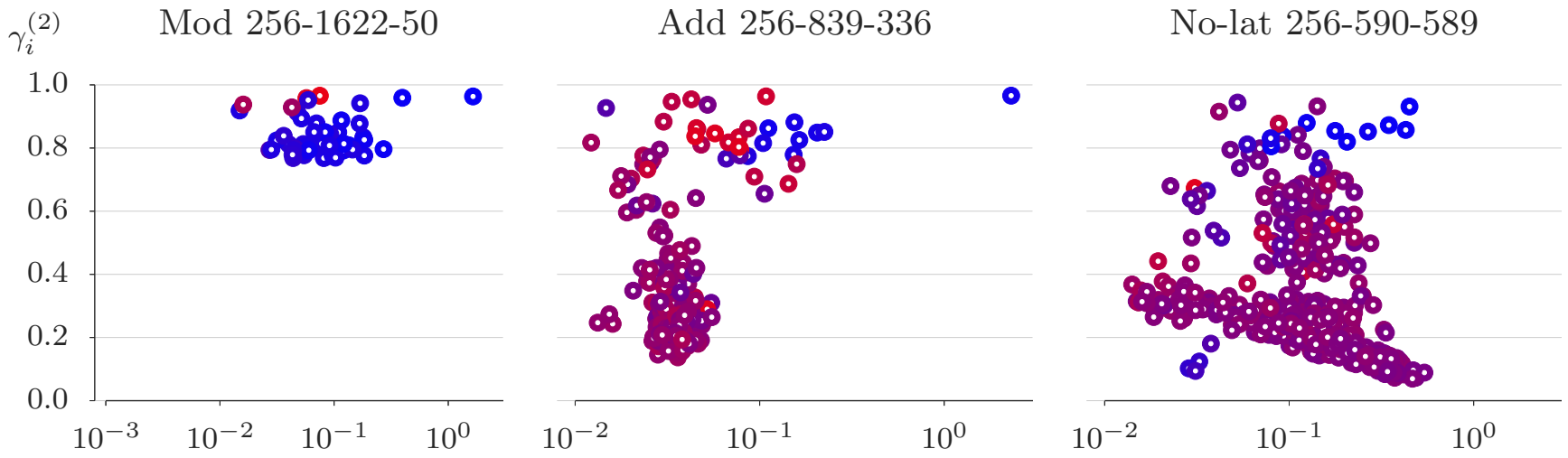
Analysis: Unsupervised learning

Translation invariance measure of units $\mathbf{h}^{(2)}$ as a function of unit significance.



With modulated connections, all units become invariant.

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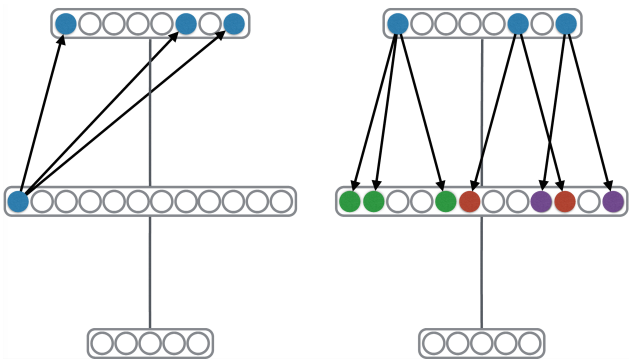
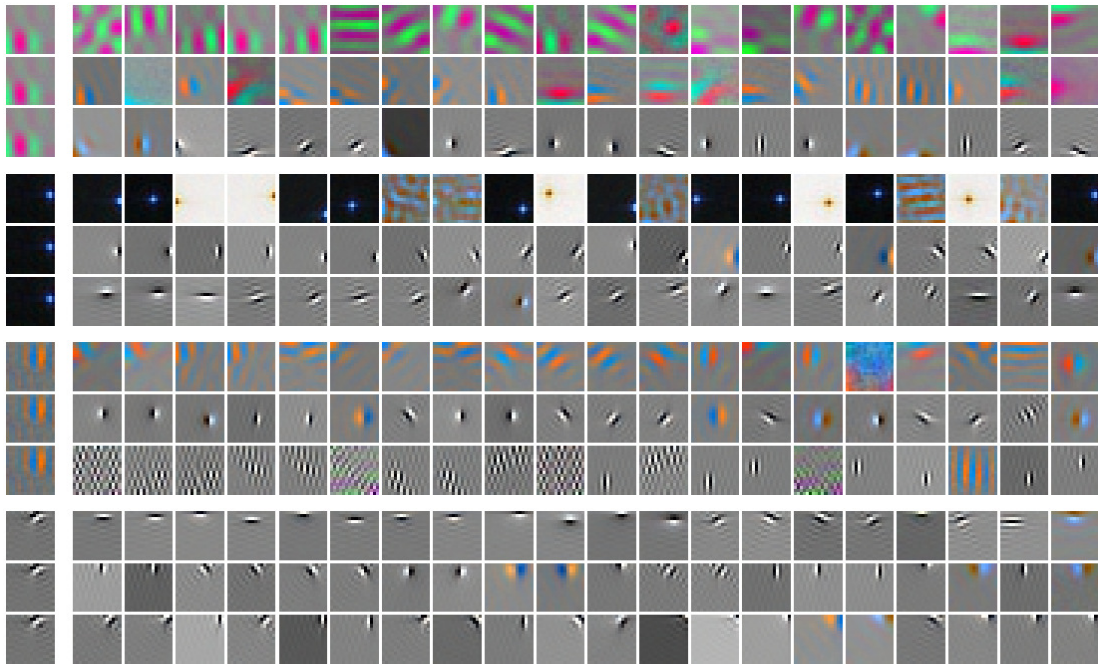
Analysis: Unsupervised learning

Learned pooling functions





Each $\mathbf{h}^{(1)}$ unit belongs to several pooling groups.
Units $\mathbf{h}^{(2)}$ specialize to colour, orientation, location, ...

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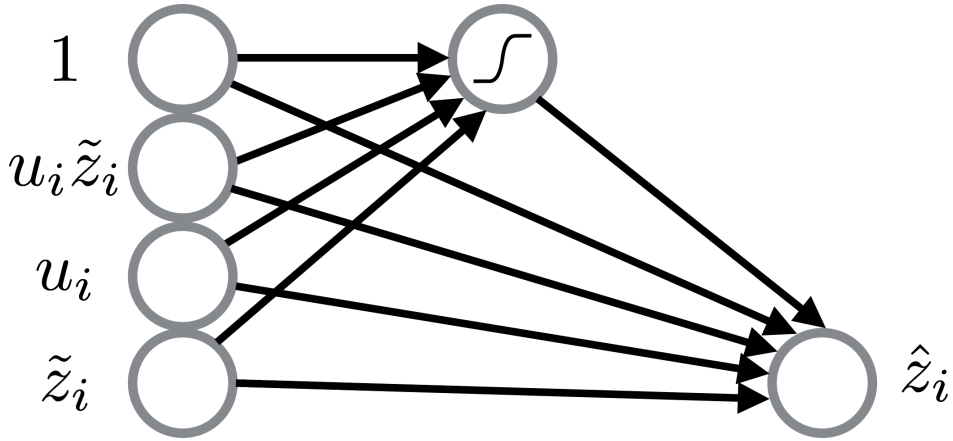
Small network for $\hat{z}_i = g(\tilde{z}_i, u_i)$



Each unit i has its own mini network with 9 parameters.
Few parameters compared to weight matrices.
Product $u_i\tilde{z}_i$ for modulating (variance modelling).
Nonlinearity for multimodal distributions.

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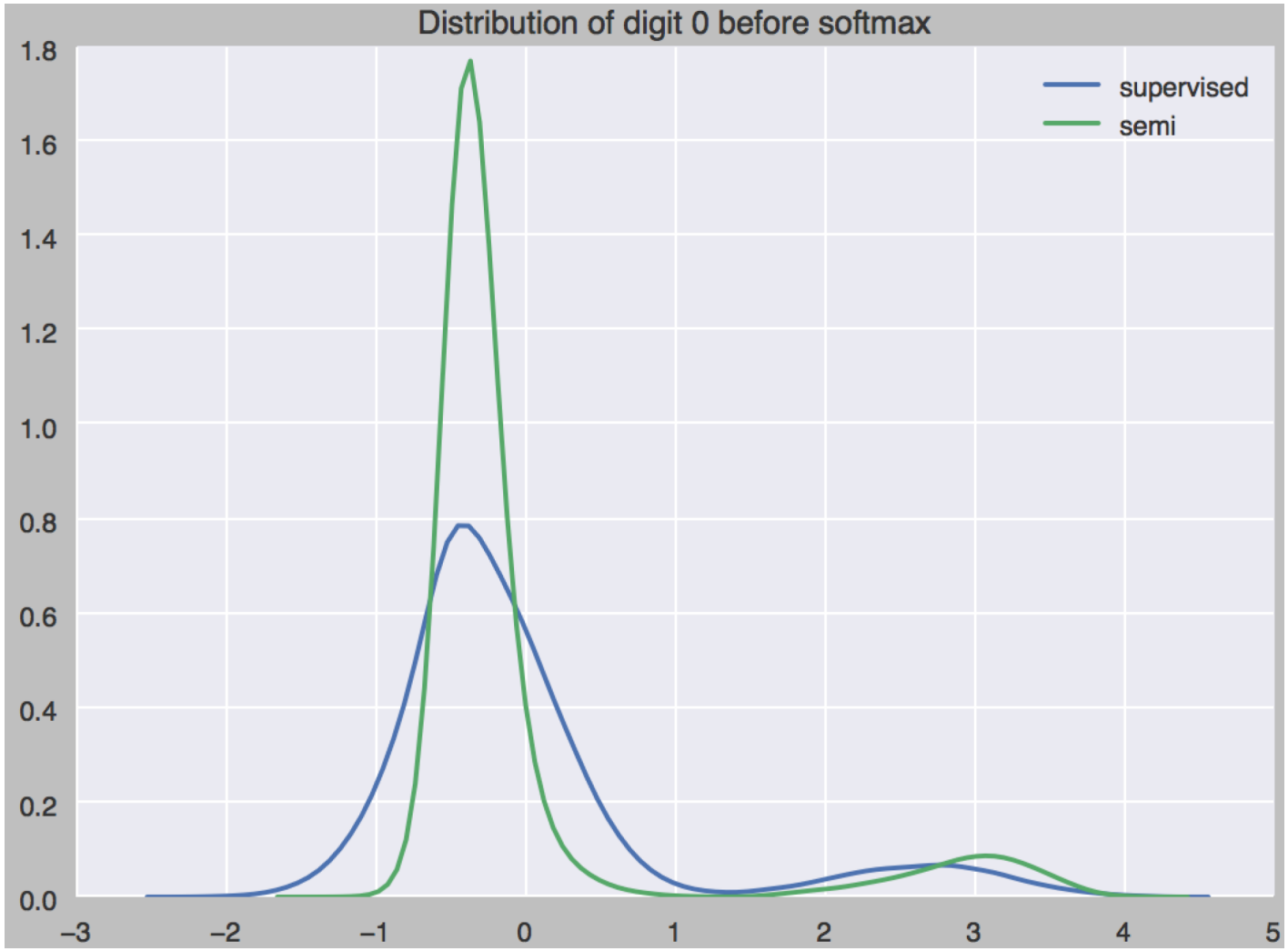
Example of a multimodal distribution



Signal $z_0^{(L)}$ for digit 0 just before softmax.

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Algorithm 1 Calculation of the output and cost function of the Ladder network

Require: $\mathbf{x}(n)$

Corrupted encoder and classifier

$\tilde{\mathbf{h}}^{(0)} \leftarrow \tilde{\mathbf{z}}^{(0)} \leftarrow \mathbf{x}(n) + \texttt{noise}$

for l = 1 **to** L **do**

$\tilde{\mathbf{z}}^{(l)}_{\text{pre}} \leftarrow \mathbf{W}^{(l)} \tilde{\mathbf{h}}^{(l-1)}$

$\tilde{\boldsymbol{\mu}}^{(l)} \leftarrow \texttt{batchmean}(\tilde{\mathbf{z}}^{(l)}_{\text{pre}})$

$\tilde{\boldsymbol{\sigma}}^{(l)} \leftarrow \texttt{batchstd}(\tilde{\mathbf{z}}^{(l)}_{\text{pre}})$

$\tilde{\mathbf{z}}^{(l)} \leftarrow \texttt{batchnorm}(\tilde{\mathbf{z}}^{(l)}_{\text{pre}}) + \texttt{noise}$

$\tilde{\mathbf{h}}^{(l)} \leftarrow \texttt{activation}(\boldsymbol{\gamma}^{(l)} \odot (\tilde{\mathbf{z}}^{(l)} + \boldsymbol{\beta}^{(l)}))$

end for

$P(\tilde{\mathbf{y}} \mid \mathbf{x}) \leftarrow \tilde{\mathbf{h}}^{(L)}$

Clean encoder (for denoising targets)

$\mathbf{h}^{(0)} \leftarrow \mathbf{z}^{(0)} \leftarrow \mathbf{x}(n)$

for l = 1 **to** L **do**

$\mathbf{z}^{(l)} \leftarrow \texttt{batchnorm}(\mathbf{W}^{(l)} \mathbf{h}^{(l-1)})$

$\mathbf{h}^{(l)} \leftarrow \texttt{activation}(\boldsymbol{\gamma}^{(l)} \odot (\mathbf{z}^{(l)} + \boldsymbol{\beta}^{(l)}))$

end for

Final classification:

$P(\mathbf{y} \mid \mathbf{x}) \leftarrow \mathbf{h}^{(L)}$

Decoder and denoising

for l = L **to** 0 **do**

if l = L **then**

$\mathbf{u}^{(L)} \leftarrow \texttt{batchnorm}(\tilde{\mathbf{h}}^{(L)})$

else

$\mathbf{u}^{(l)} \leftarrow \texttt{batchnorm}(\mathbf{V}^{(l)} \hat{\mathbf{z}}^{(l+1)})$

end if

$\forall i : \hat{z}^{(l)}_i \leftarrow g(\tilde{z}^{(l)}_i, u^{(l)}_i)$ # Eq. (1)

$\forall i : \hat{z}^{(l)}_{i,\text{BN}} \leftarrow \frac{\hat{z}^{(l)}_i - \tilde{\mu}^{(l)}_i}{\tilde{\sigma}^{(l)}_i}$

end for

Cost function C for training:

$\text{C} \leftarrow 0$

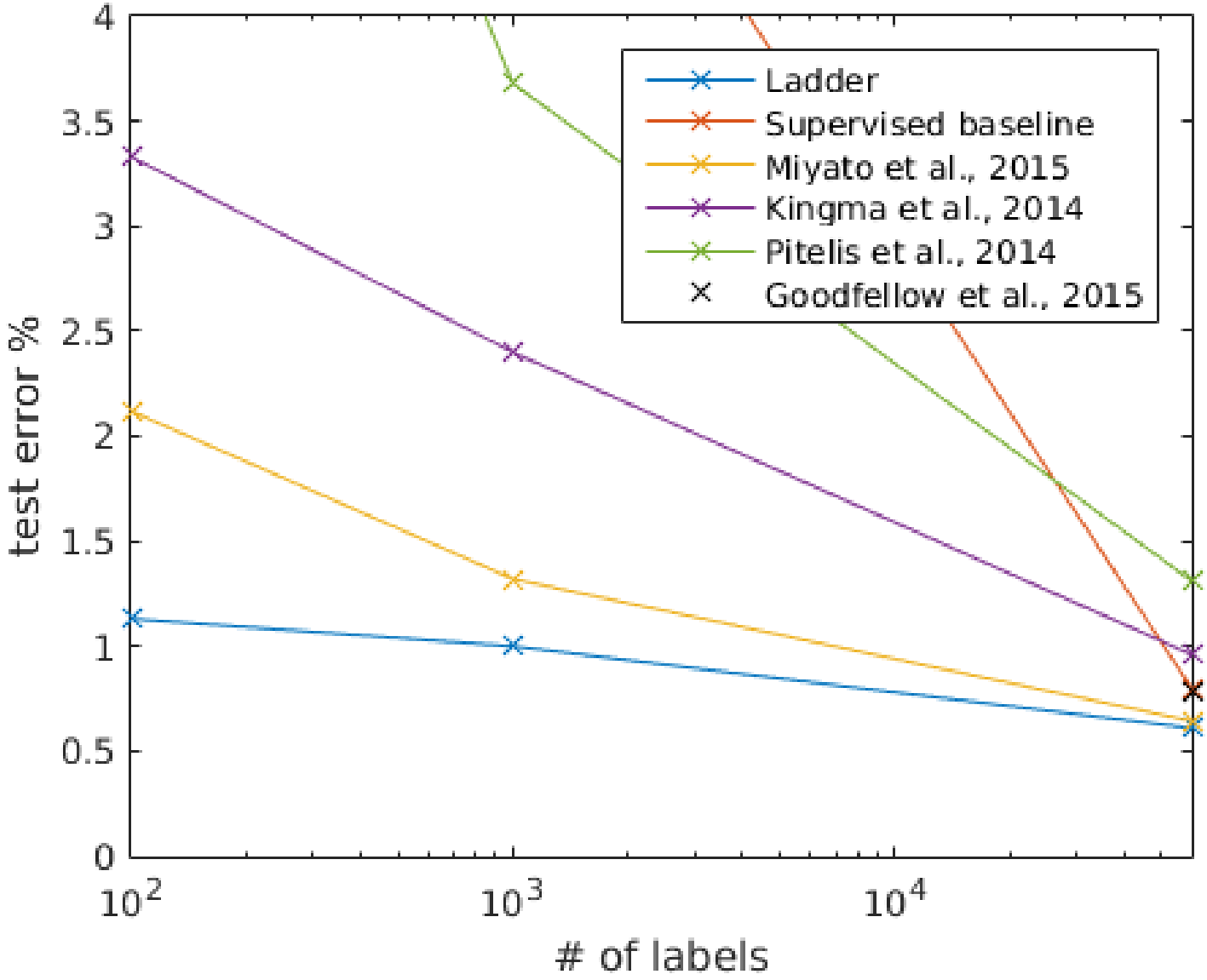
if $t(n)$ **then**

$\text{C} \leftarrow -\log P(\tilde{\mathbf{y}} = t(n) \mid \mathbf{x})$

end if

$\text{C} \leftarrow \text{C} + \sum_{l=0}^{L} \lambda_l \left\| \mathbf{z}^{(l)} - \hat{\mathbf{z}}^{(l)}_{\text{BN}} \right\|^2$

MNIST results



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Thanks for listening!

Deep Learning and Bayesian Modelling group

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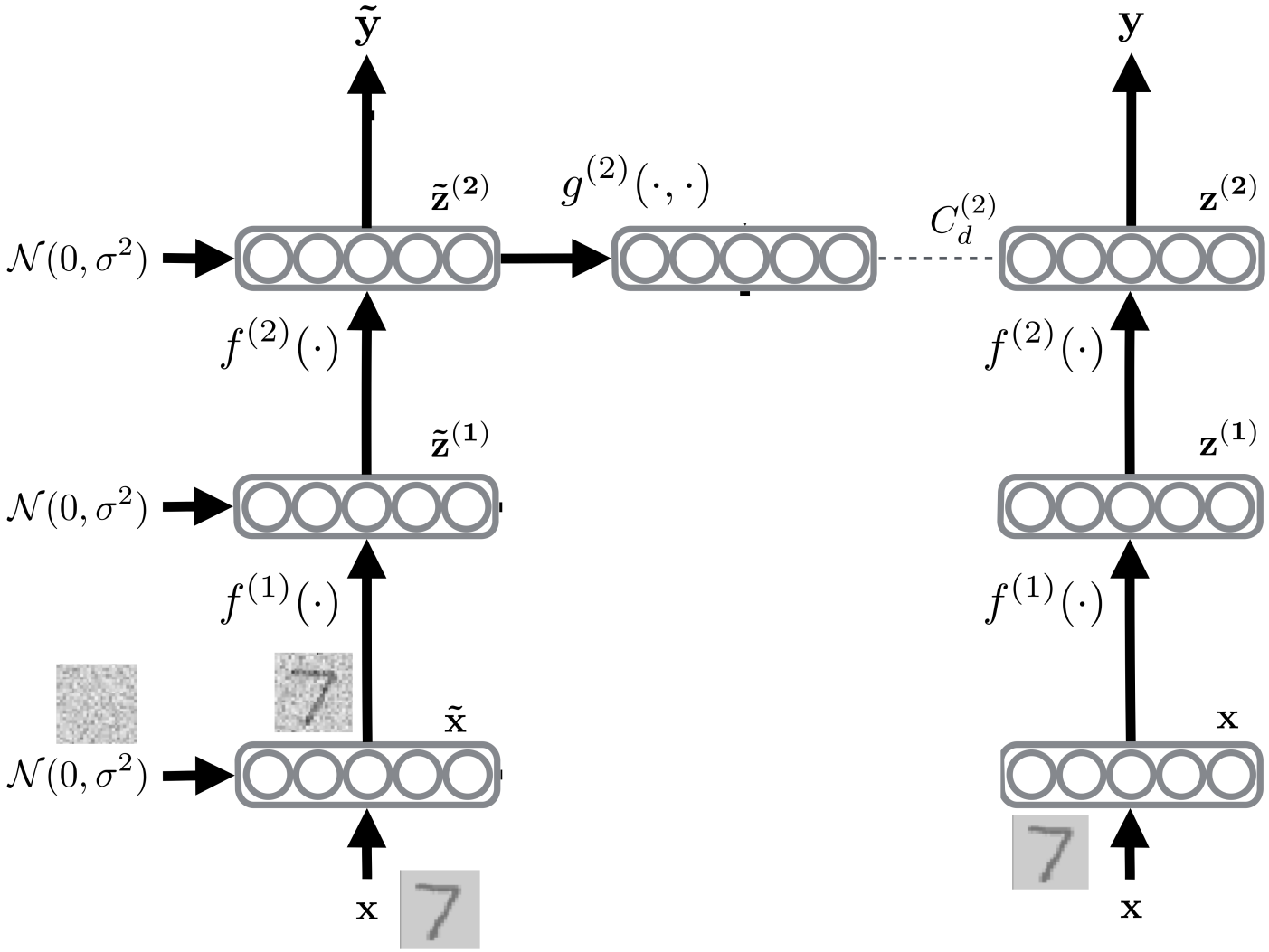
Gamma (Γ) model



Simplified model: Only auxiliary cost just before softmax.