Deep learning summer camp
5 Unsupervised learning

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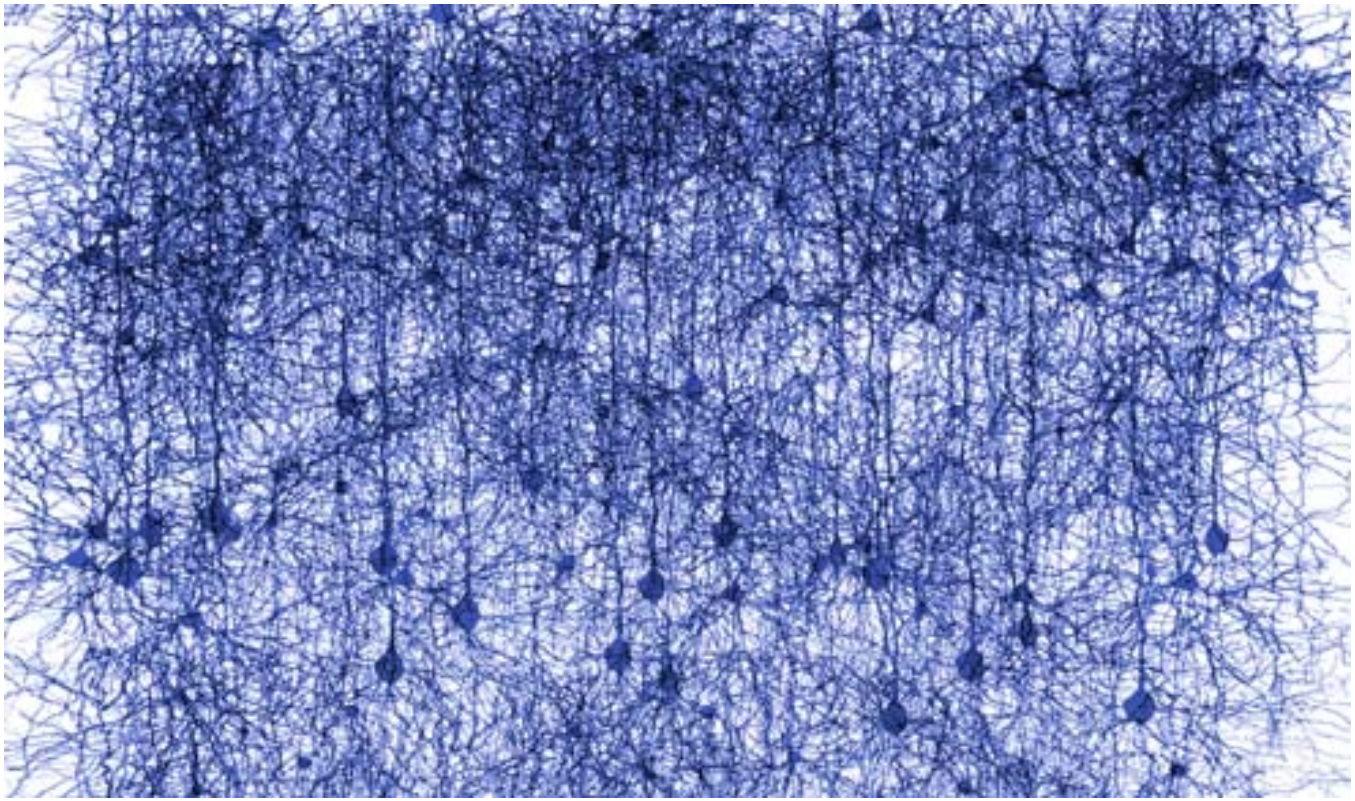
Objectives of talk

- What is unsupervised learning and
- why is it actually much more important than supervised learning.

Part 1:
Unsupervised learning

Neural networks (NNs)

- Feedforward neural networks (FFNNs)
- Convolutional neural networks (CNNs)
- Recurrent Neural Networks (RNNs)
- Auto-encoders (AE)



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

Generative models for complex data

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.

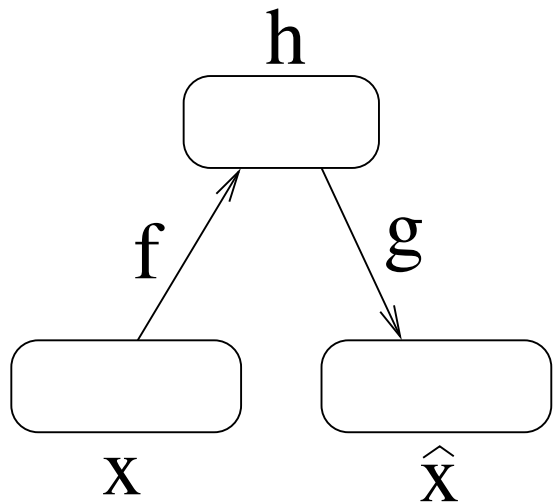
Approaches to unsupervised learning (1/2)

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 $\hat{\mathbf{x}}$



Approaches to unsupervised learning (2/2)

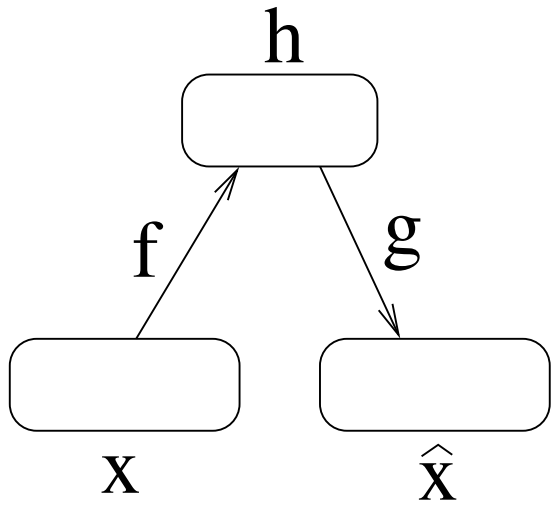
Often the encoder function $f : \mathbf{x} \to \mathbf{h}$ is implicit:

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

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!

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 $\mathbf{W}^{(2)} = \mathbf{W}^{(1)\top}$.

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?

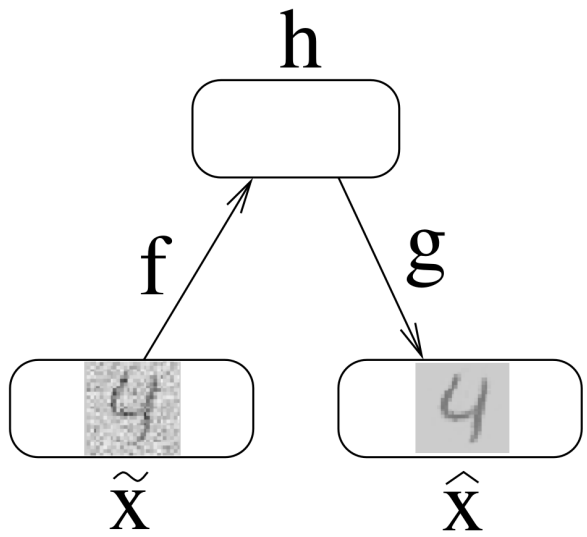
Part 2:
Autoencoders

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 autoencoders (probabilistic)
- Sometimes also weight sharing $\mathbf{W}^{(2)} = \mathbf{W}^{(1)\top}$.

Denoising autoencoder (Vincent et al., 2008)

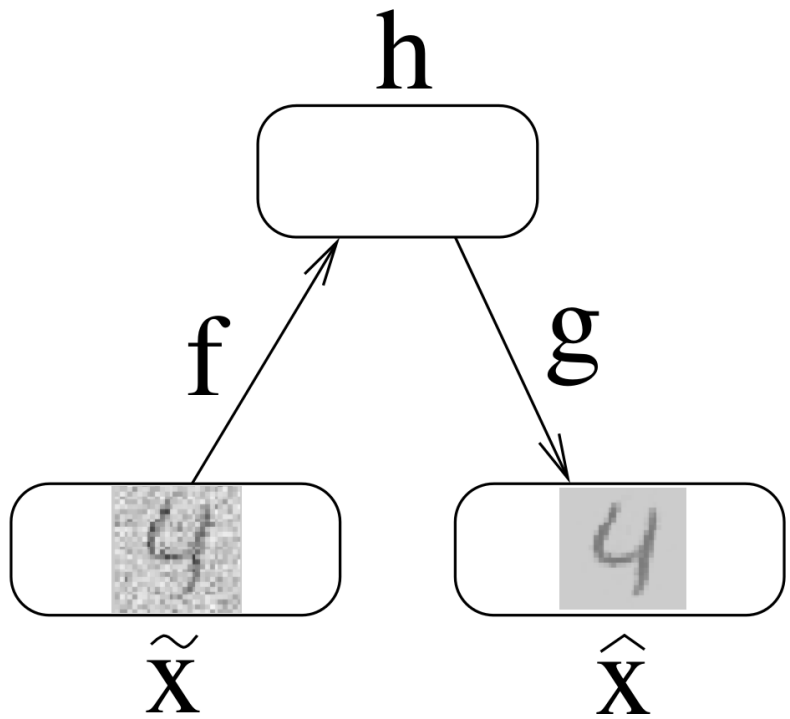


Feed corrupted inputs $\tilde{\mathbf{x}} \sim c(\tilde{\mathbf{x}}|\mathbf{x})$

- Additive noise $\tilde{\mathbf{x}} = \mathbf{x} + \epsilon$ 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 $m_i \sim$ Bernoulli(p)
- Masking noise $\tilde{\mathbf{x}} = [\mathbf{m} \odot \mathbf{x}; \mathbf{m}]$

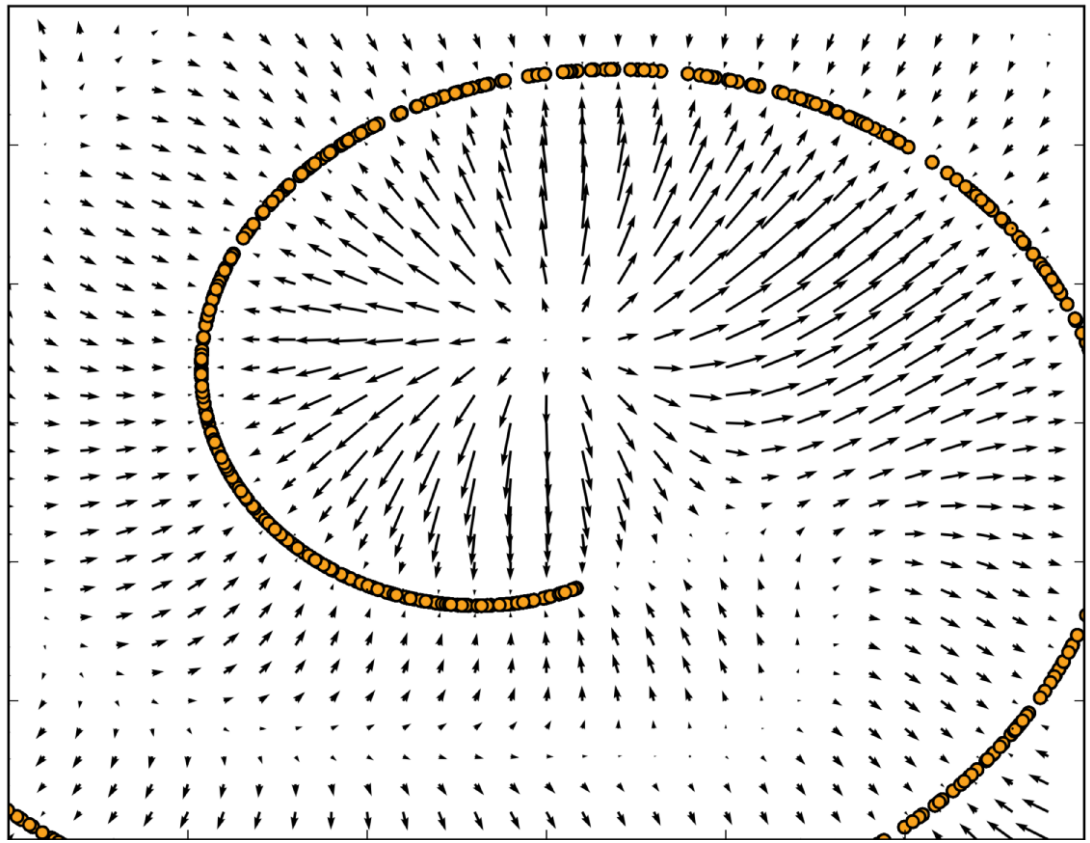
Train $\hat{\mathbf{x}} = g(f(\tilde{\mathbf{x}}))$ to minimize reconstruction error,
e.g. $C = \mathbb{E}\left[\|\hat{\mathbf{x}} - \mathbf{x}\|^2\right]$.

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.

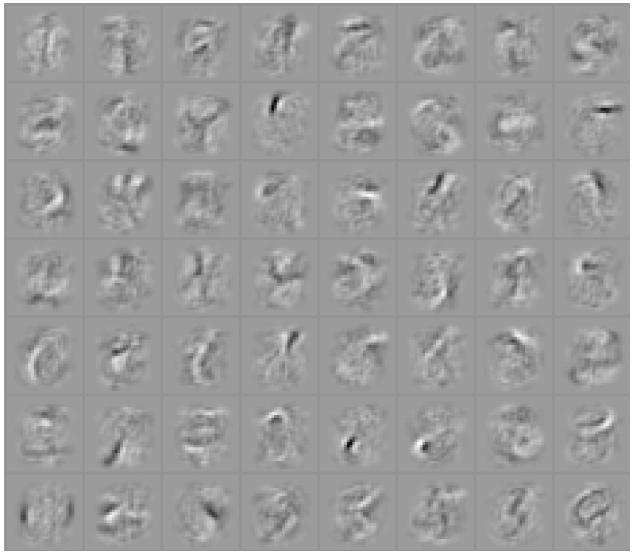
What does denoising autoencoder learn?

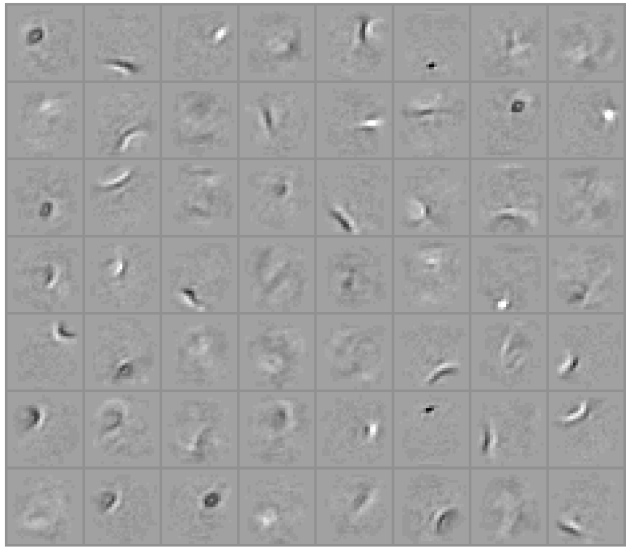


To point $g(f(\cdot))$ towards higher probability.

Image from (Alain and Bengio, 2014)

Comparison to training a classifier



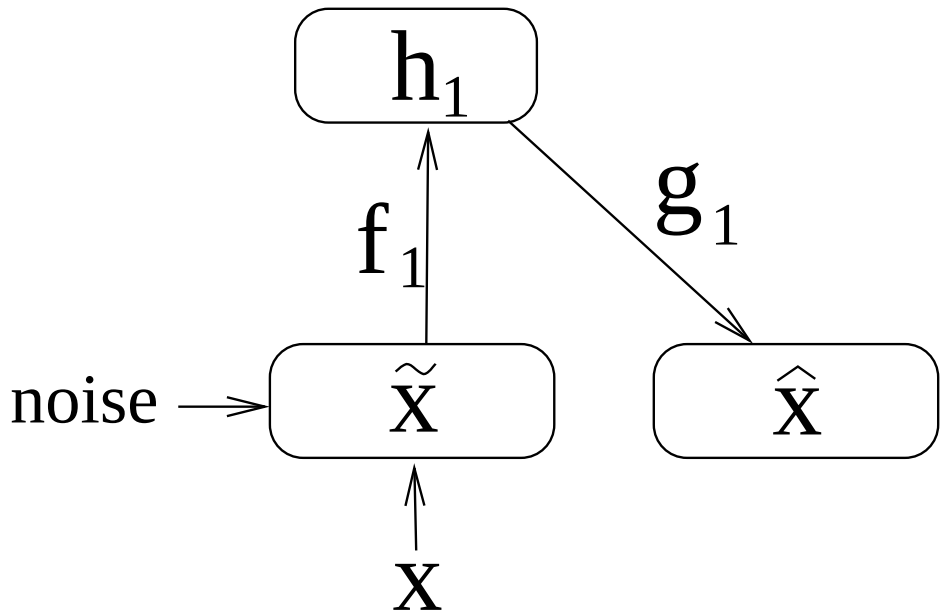


- Training a classifier (left), when you get the labels right, learning stops. $\Rightarrow$ Learned parameters are based on the information in labels:
  Less than #examples$\times$#classes bits.
- Training a denoising autoencoder (right), outputs are richer: #examples$\times$#dimensions.

Layerwise pretraining

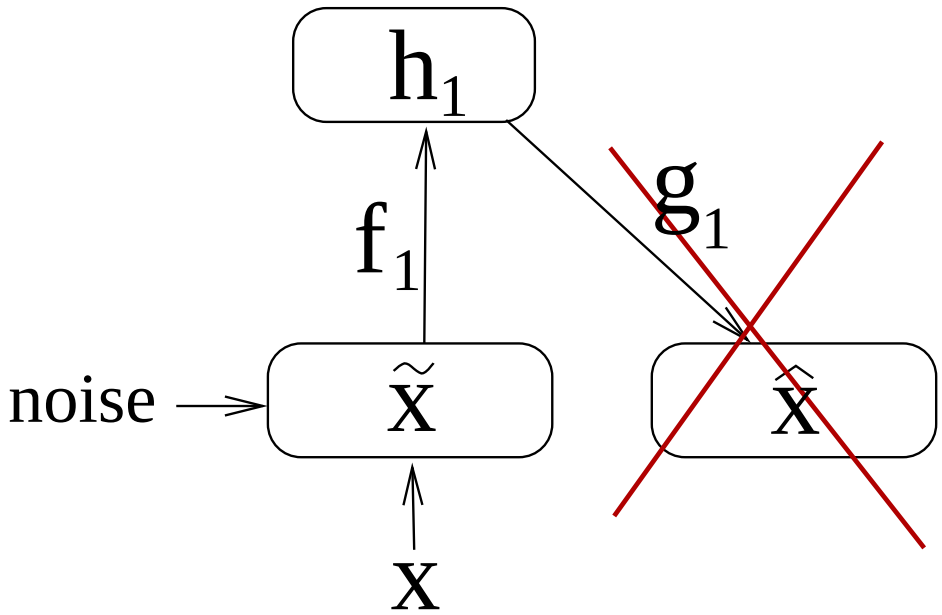
- Use unsupervised learning to construct representations layer by layer (Ballard, 1987).
- Breakthrough with Boltzmann machines (Hinton and Salakhutdinov 2006), starting deep learning boom.
- Presented here: Stacked denoising autoencoders

Layerwise pretraining



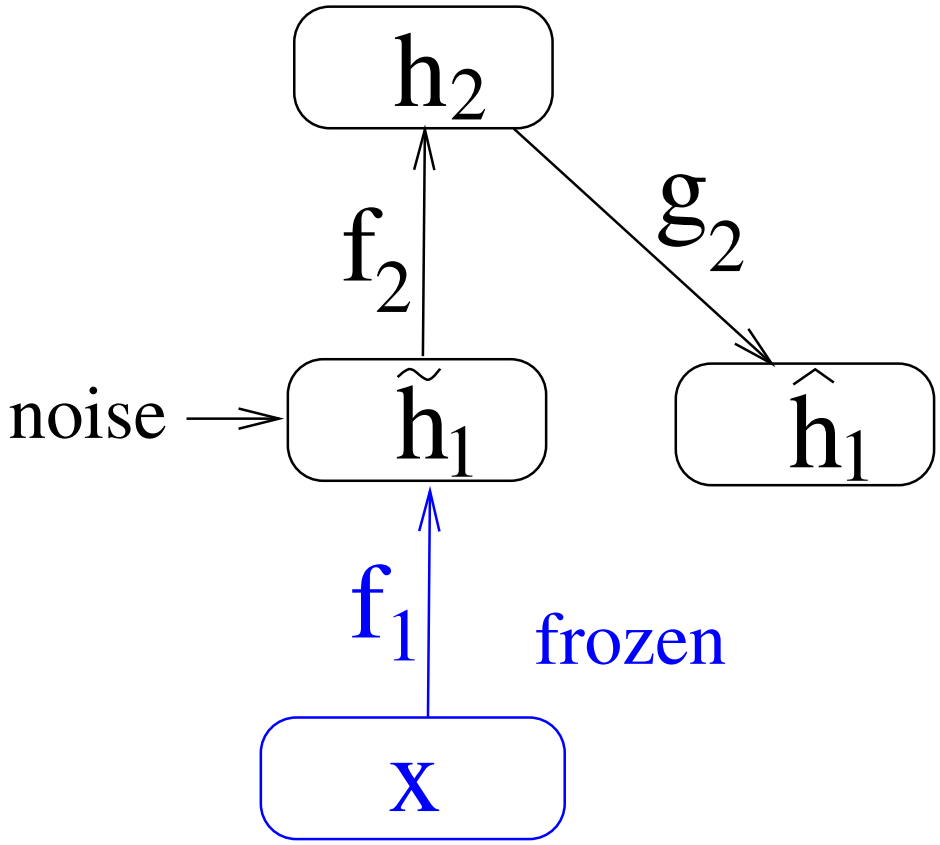
Phase 1: Denoising autoencoder.

Layerwise pretraining



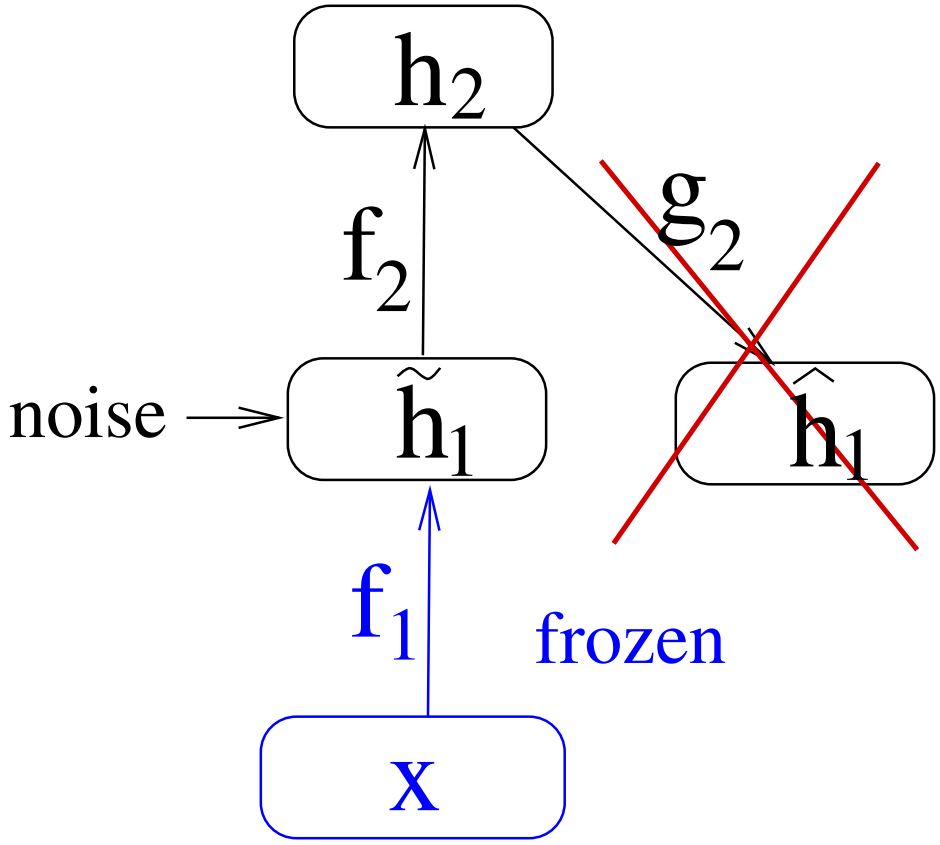
Toss away the decoder $g(\cdot)$.

Layerwise pretraining



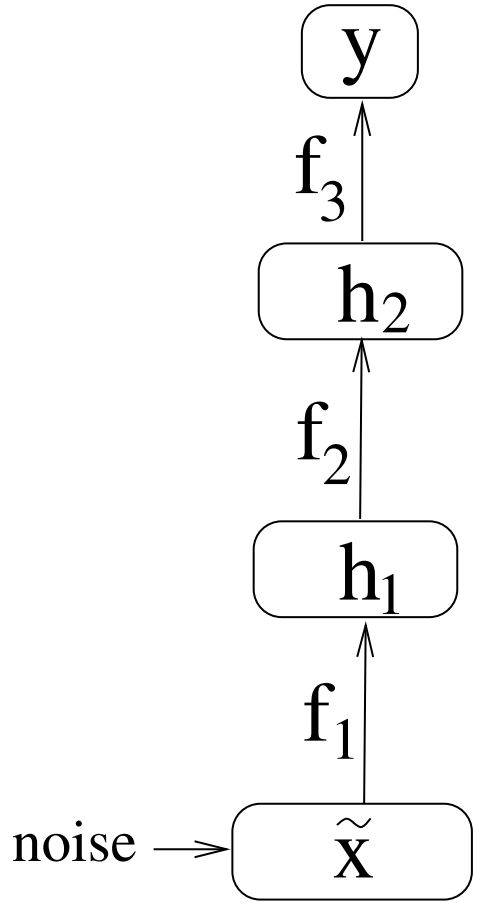
Phase 2: Stack another layer, keep the bottom fixed.

Layerwise pretraining



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

Supervised finetuning

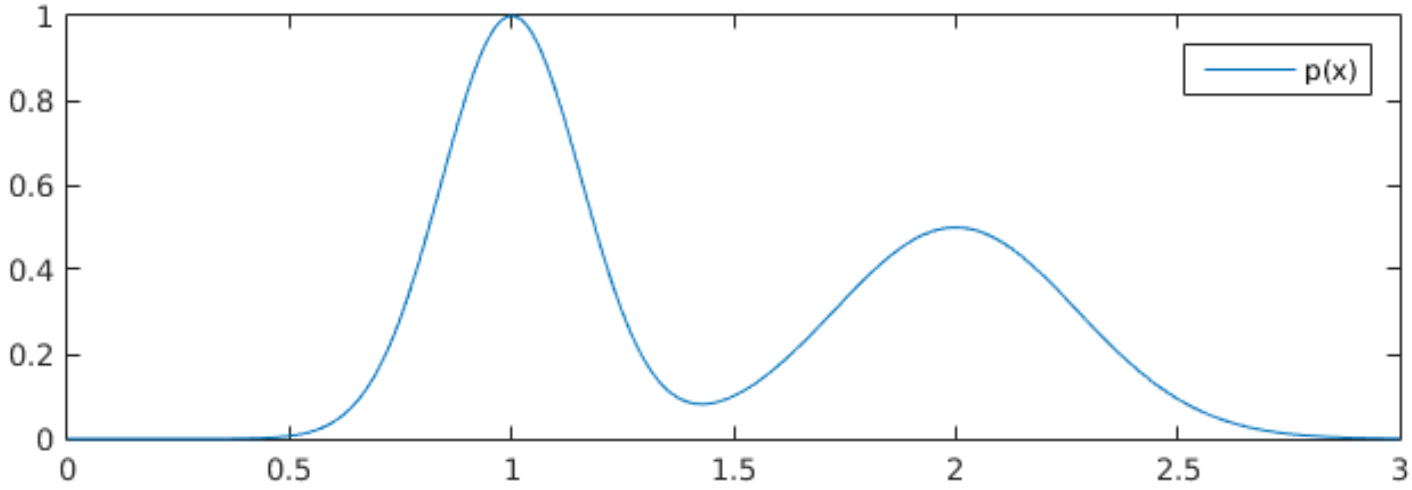


Phase 3: Supervised finetuning with labels y.
Note: Encoder f of an autoencoder is the same mapping as used in supervised learning.

Denoising versus probabilistic modelling

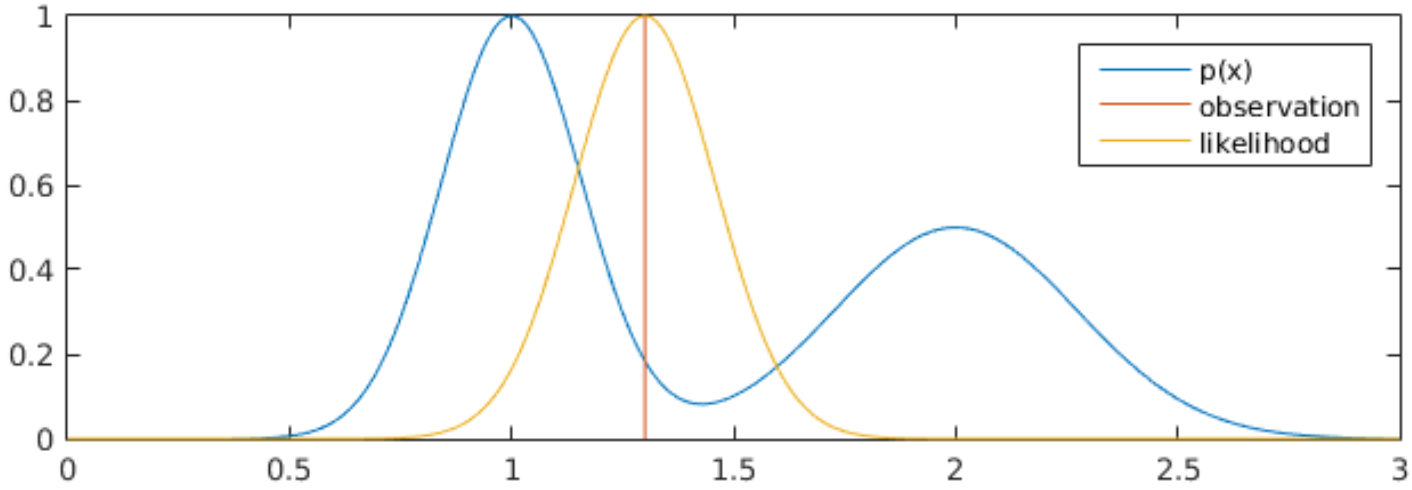
- We noted that denoising models are much easier to train than probabilistic models.
  Trainable by basic back-propagation.
- There is a strong connection between the two:
  Models can be converted into each other.

Probability to denoising



Given: Model $P(x)$ and observation $\tilde{x} = x + \text{noise}$.
Noise distribution known.
Task: Find $\hat{x} = \operatorname{argmin} \mathbb{E}_x \left[(x - \hat{x})^2\right]$.
Solution: Compute the posterior $P(x \mid \tilde{x})$,
use its center of gravity as reconstruction $\hat{x}$.

Probability to denoising



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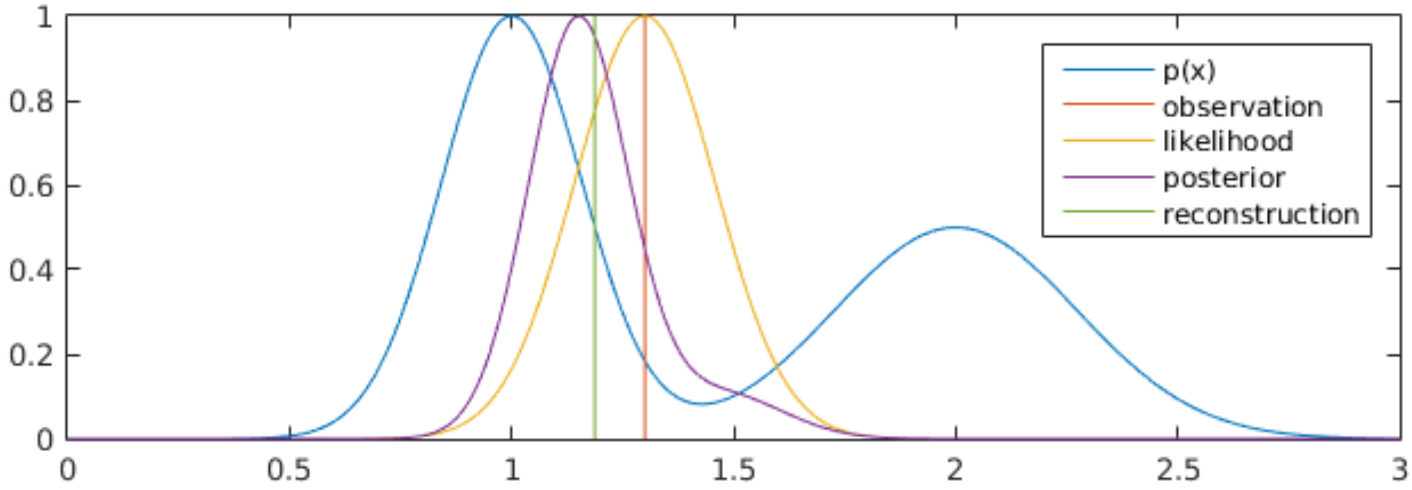

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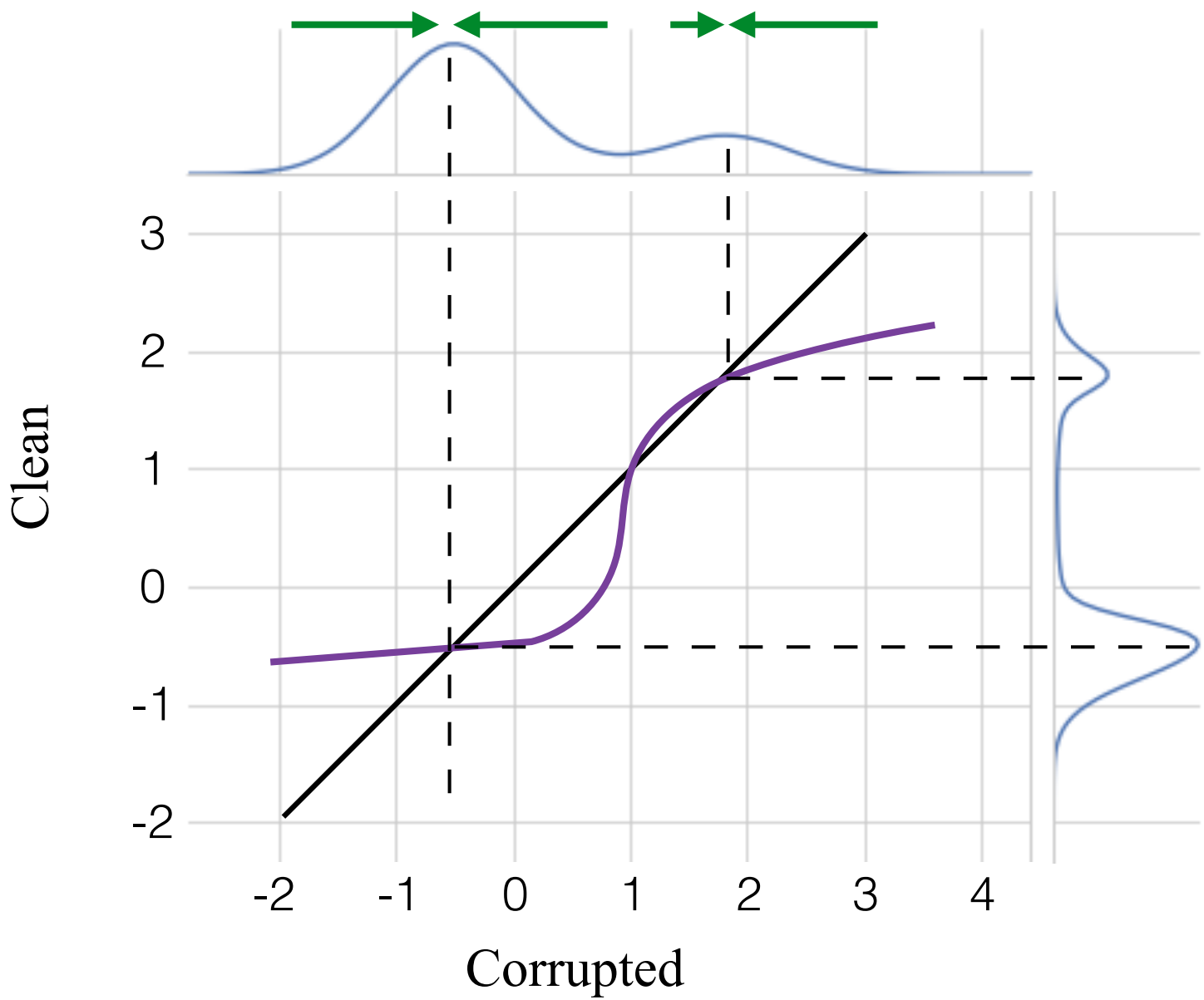
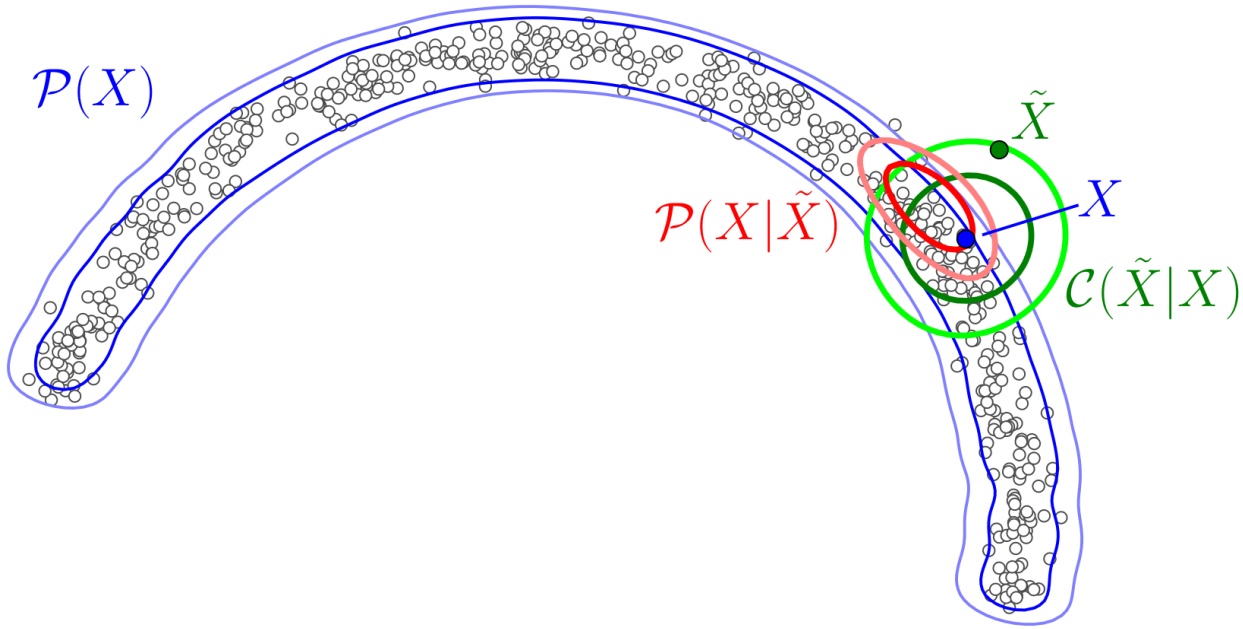
Probability to denoising



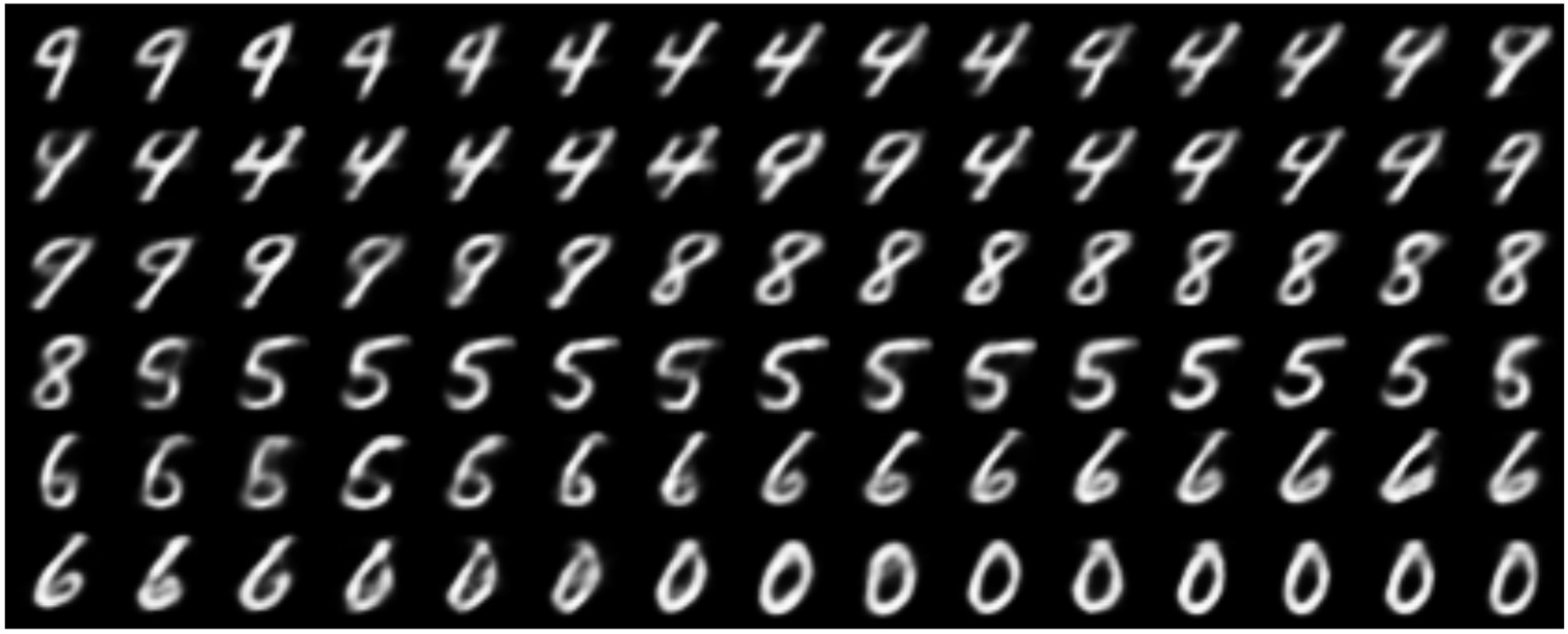
Denoising to probability

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



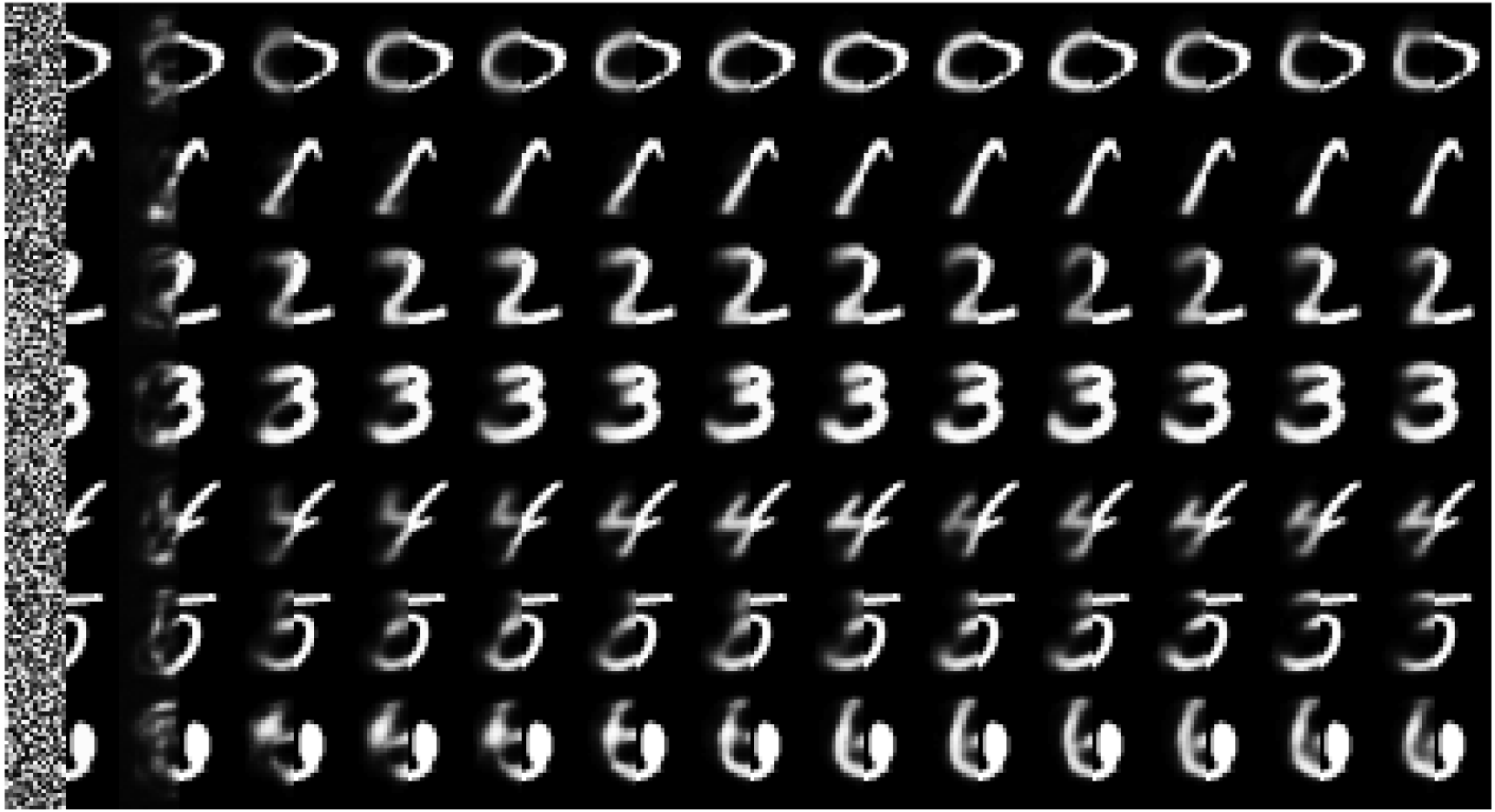
Markov chain alternating between corruption $C(\tilde{X}|X)$ and denoising $P(X|\tilde{X})$.
Theoretical result: Stationary distribution is $P(X)$.

Denoising to probability (Bengio et al., 2014)



Generating samples from the Markov chain.

Denoising to probability (Bengio et al., 2014)



Reconstructing the left half.

On details and invariance

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

On details and invariance

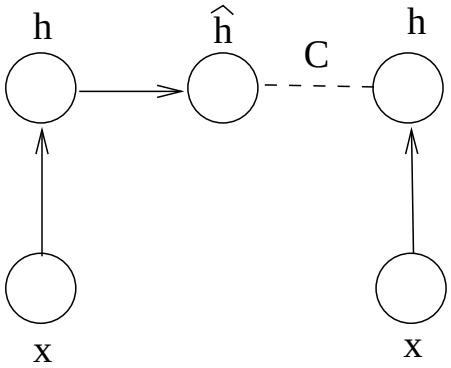
Answer: both are just blurry blobs.
Autoencoder tries to learn a representation from which it can reconstruct the observations.
It cannot discard details: position, pose, lighting...
$\Rightarrow$ Not well compatible with supervised learning.

Ladder network, main ideas

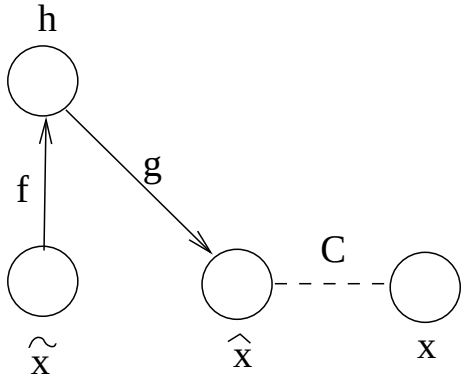
(Valpola, 2014, Rasmus et al., 2015)

- 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

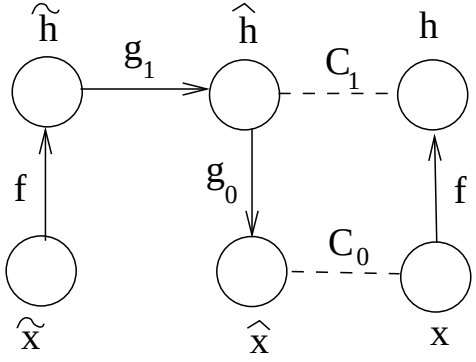
Combining DSS+DAE



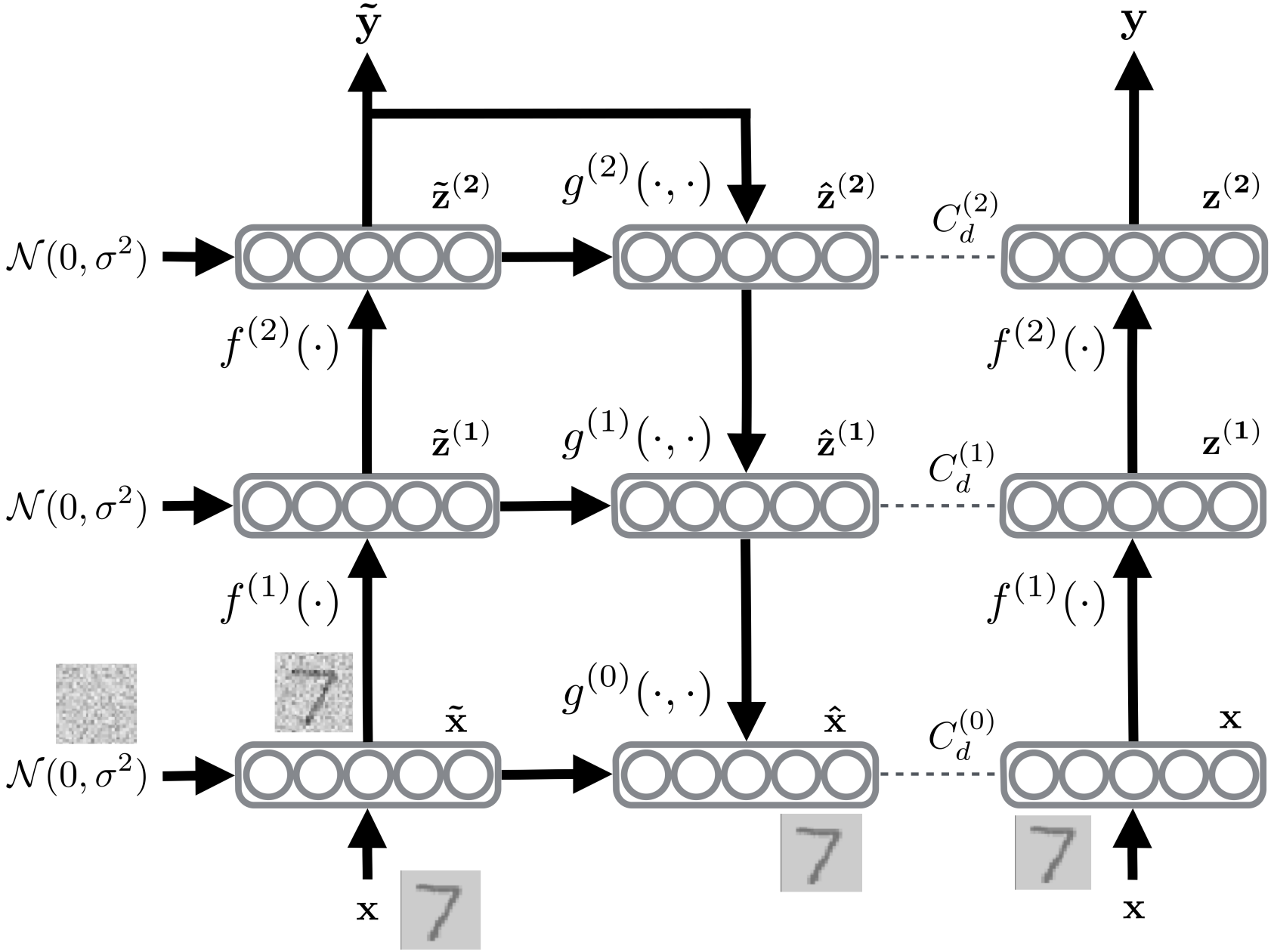
Denoising Source Separation
(Särelä and Valpola, 2005)



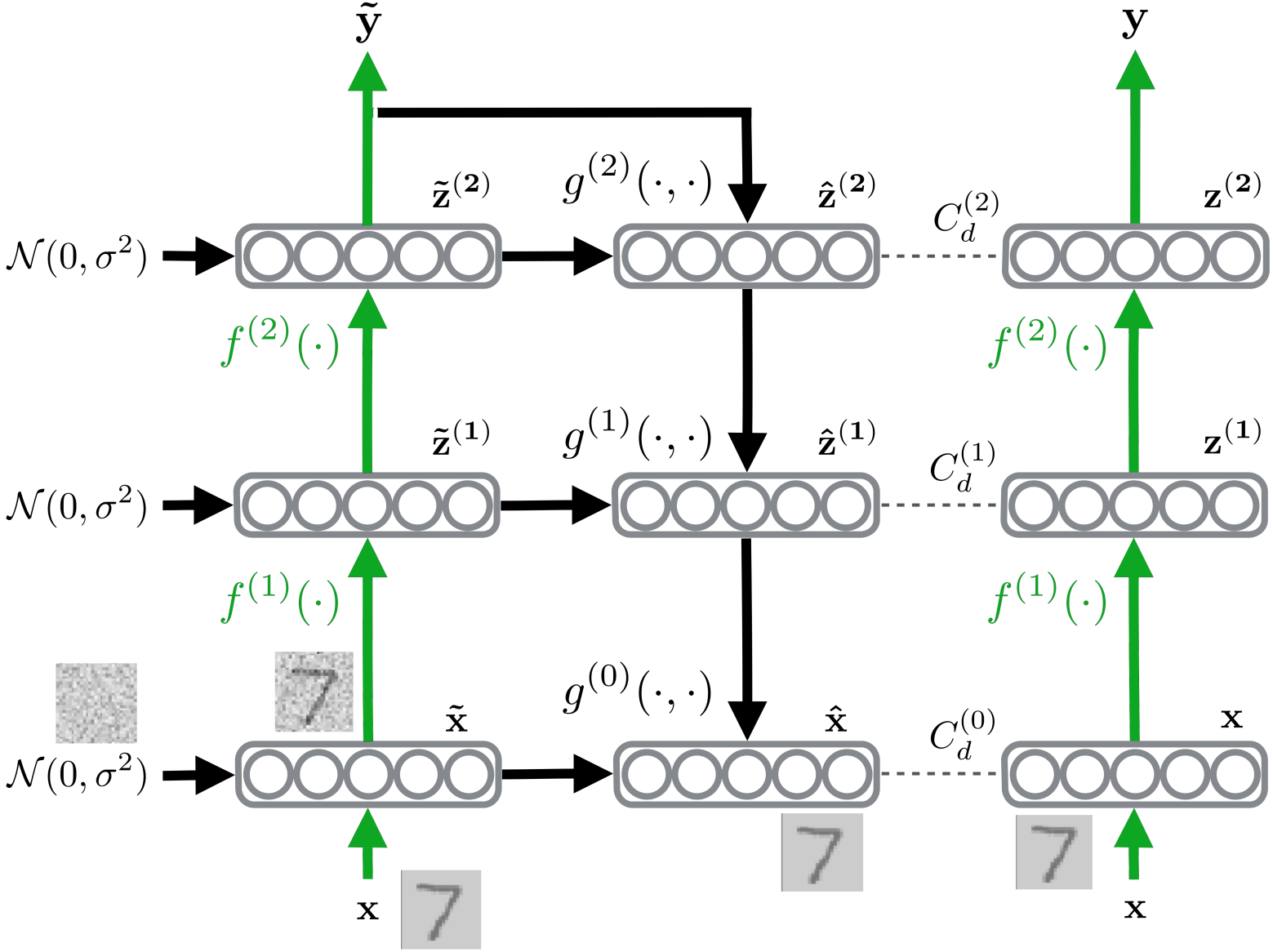
Denoising Autoencoder
(Vincent et al., 2008)



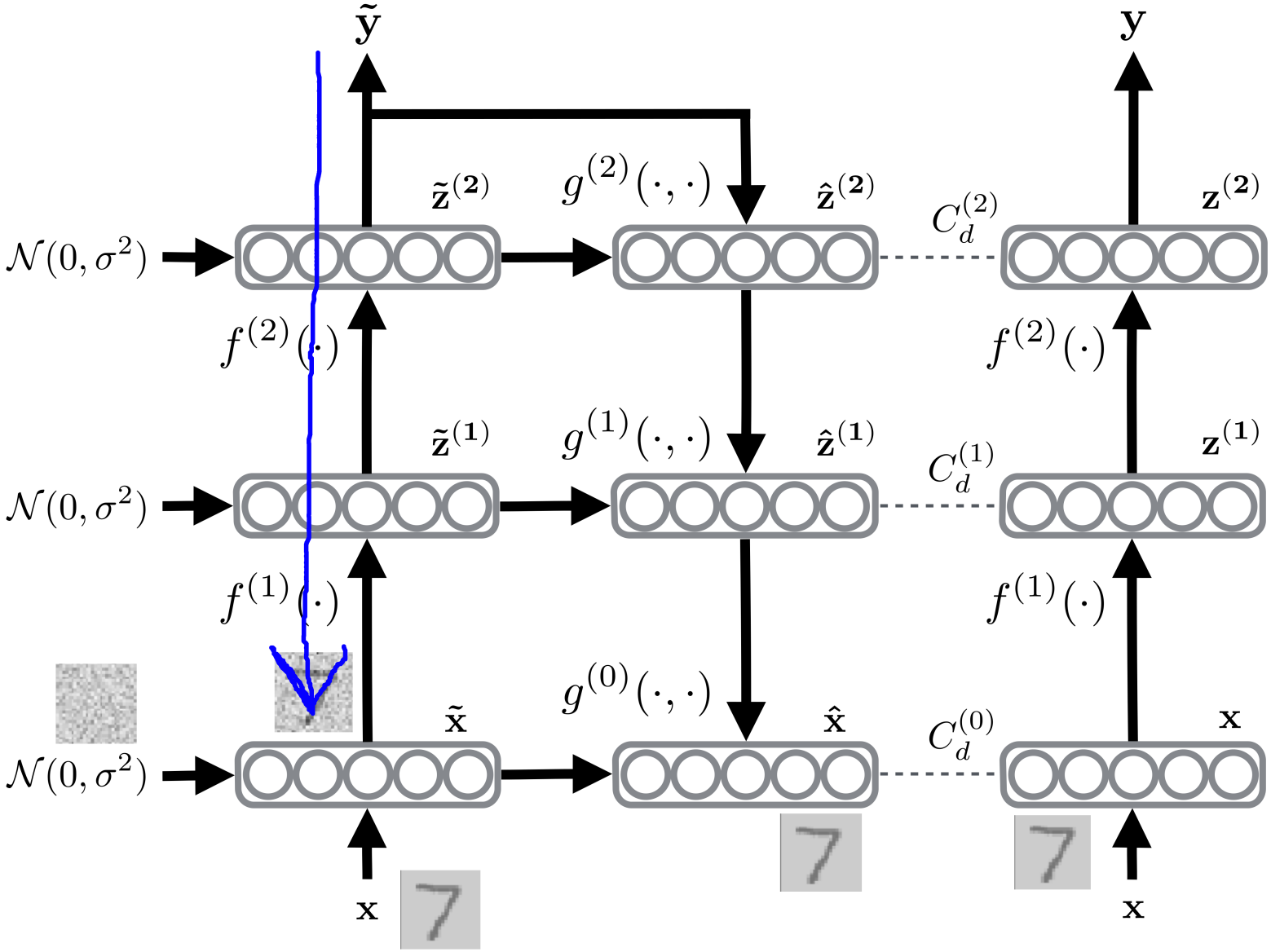
Ladder Networks
(Valpola, 2014, Rasmus et al., 2015)


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

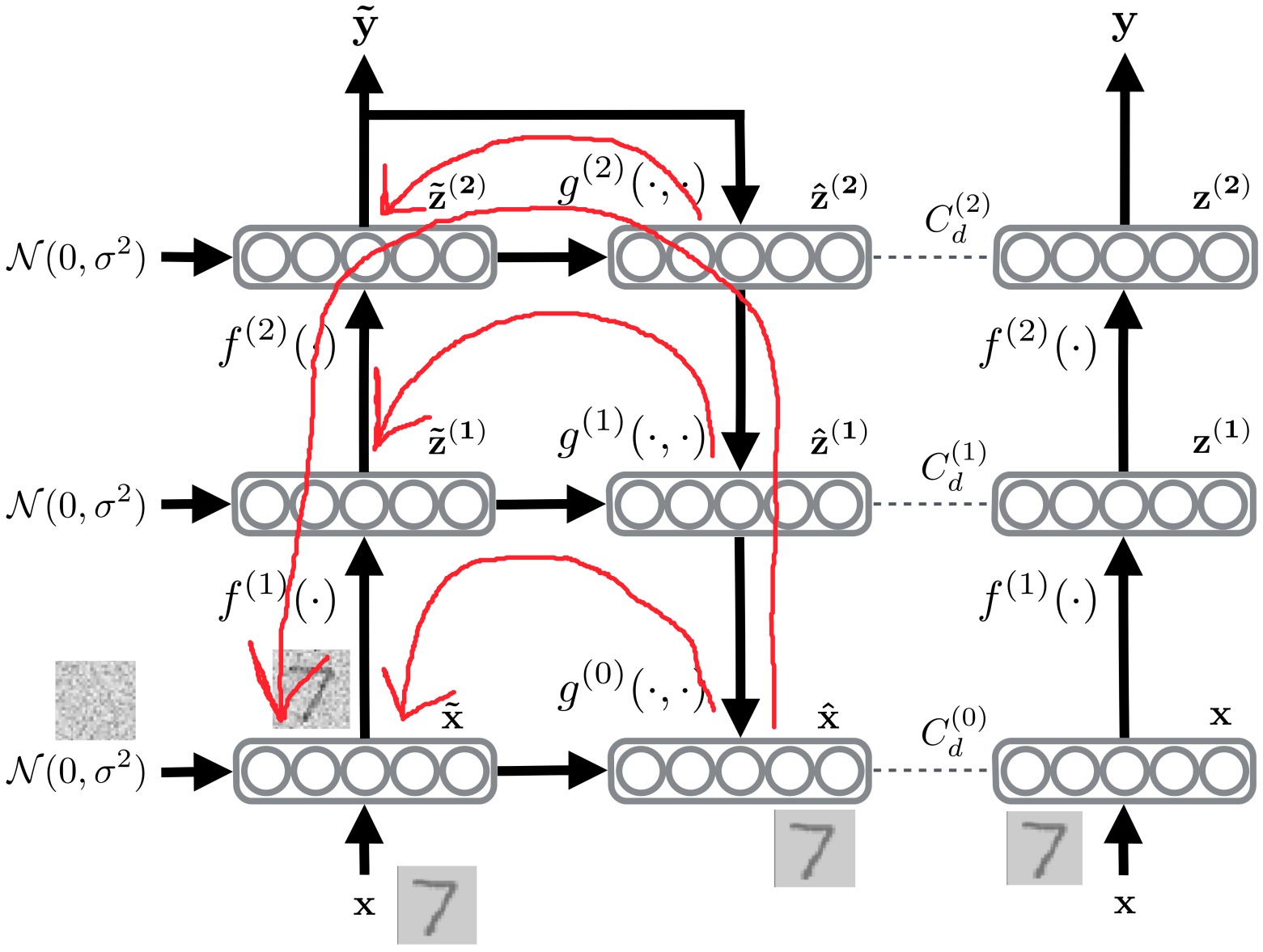
Same encoder $f(\cdot)$ used for corrupted and clean paths.



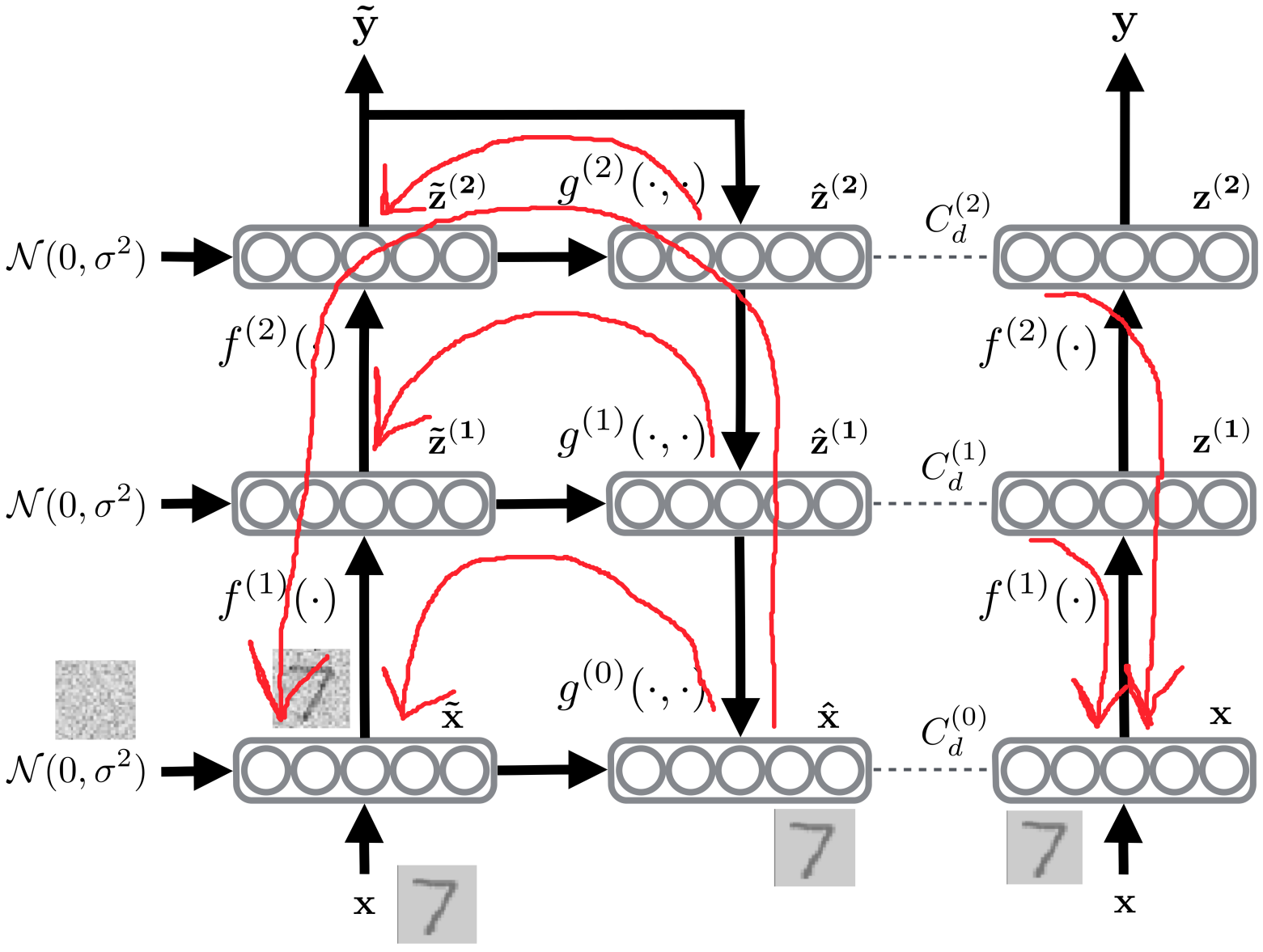
Supervised learning: Backprop from output $\tilde{\mathbf{y}}$.



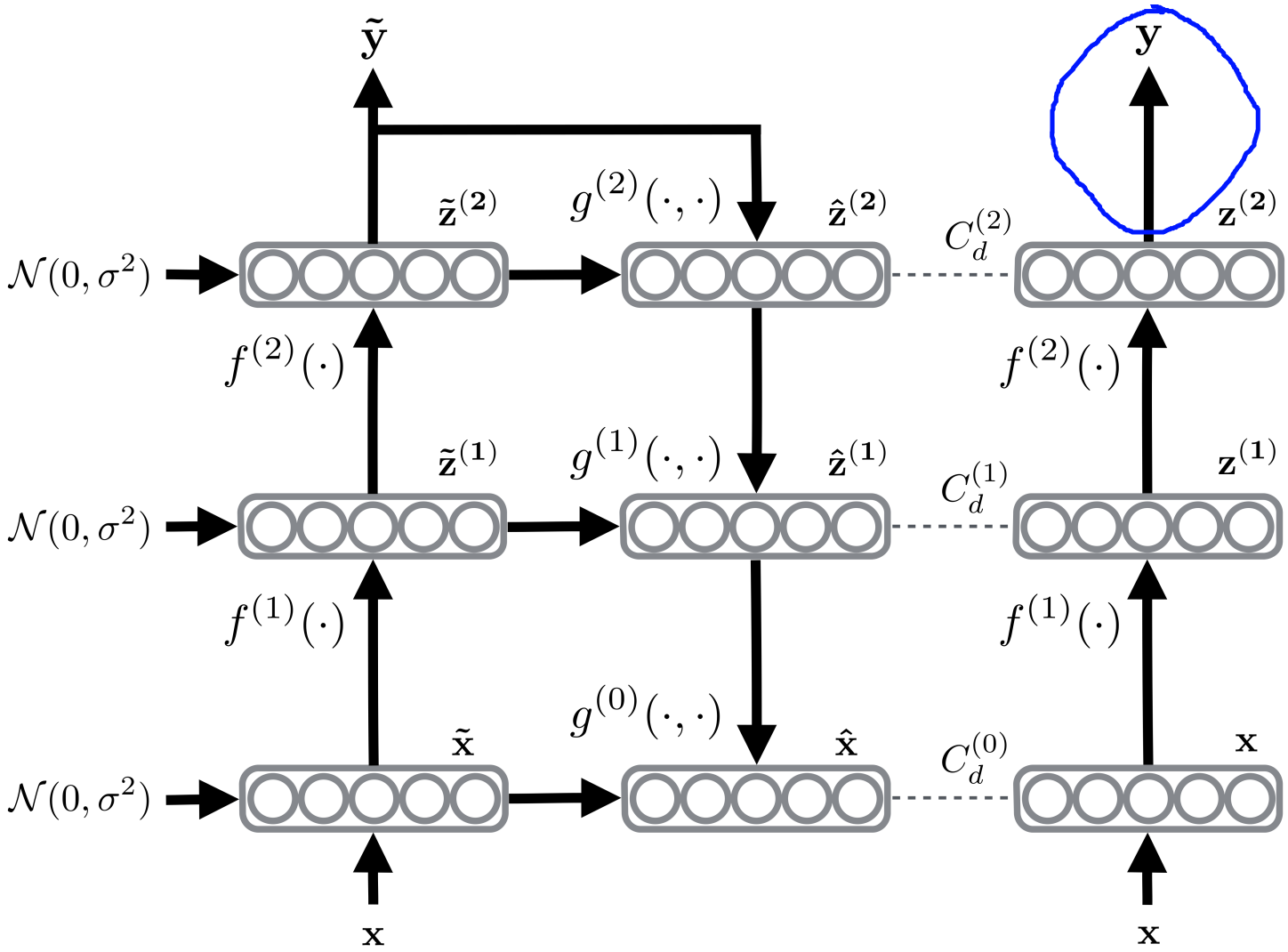
Unsupervised learning:
Several denoising autoencoders simultaneously.



Unsupervised learning:
Produce robust representations (DSS aspect).



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

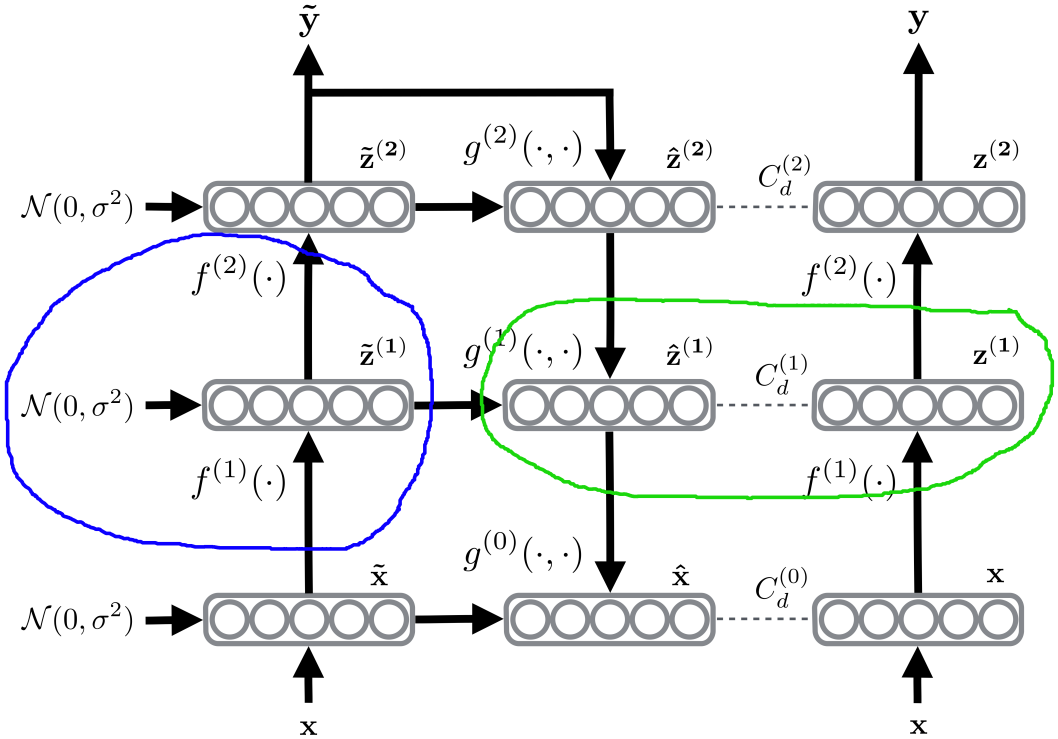


Training criterion

Only one phase of training: Minimize criterion C.

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

Scaling issues

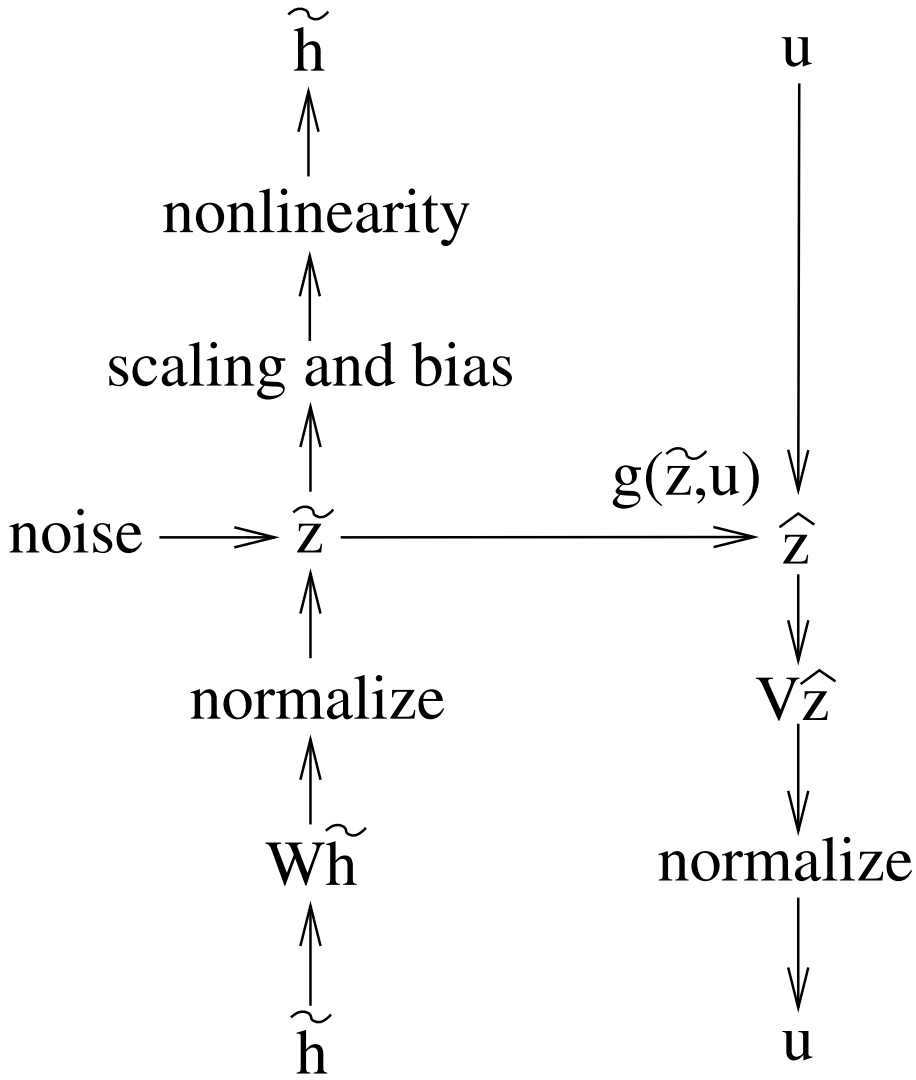


Issue 1: Doubling $\mathbf{W}^{(1)}$ and halving $\mathbf{W}^{(2)}$ decreases noise.

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

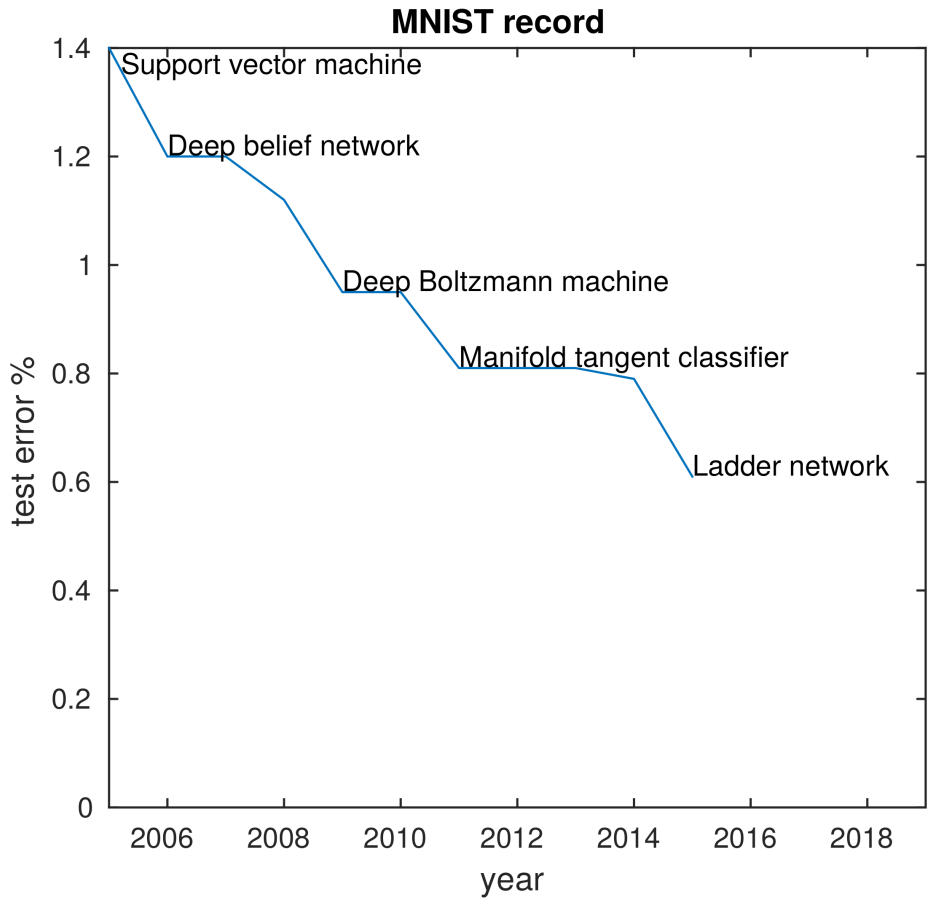
Solution: Batch normalization (Ioffe and Szegedy, 2015)

Some model details



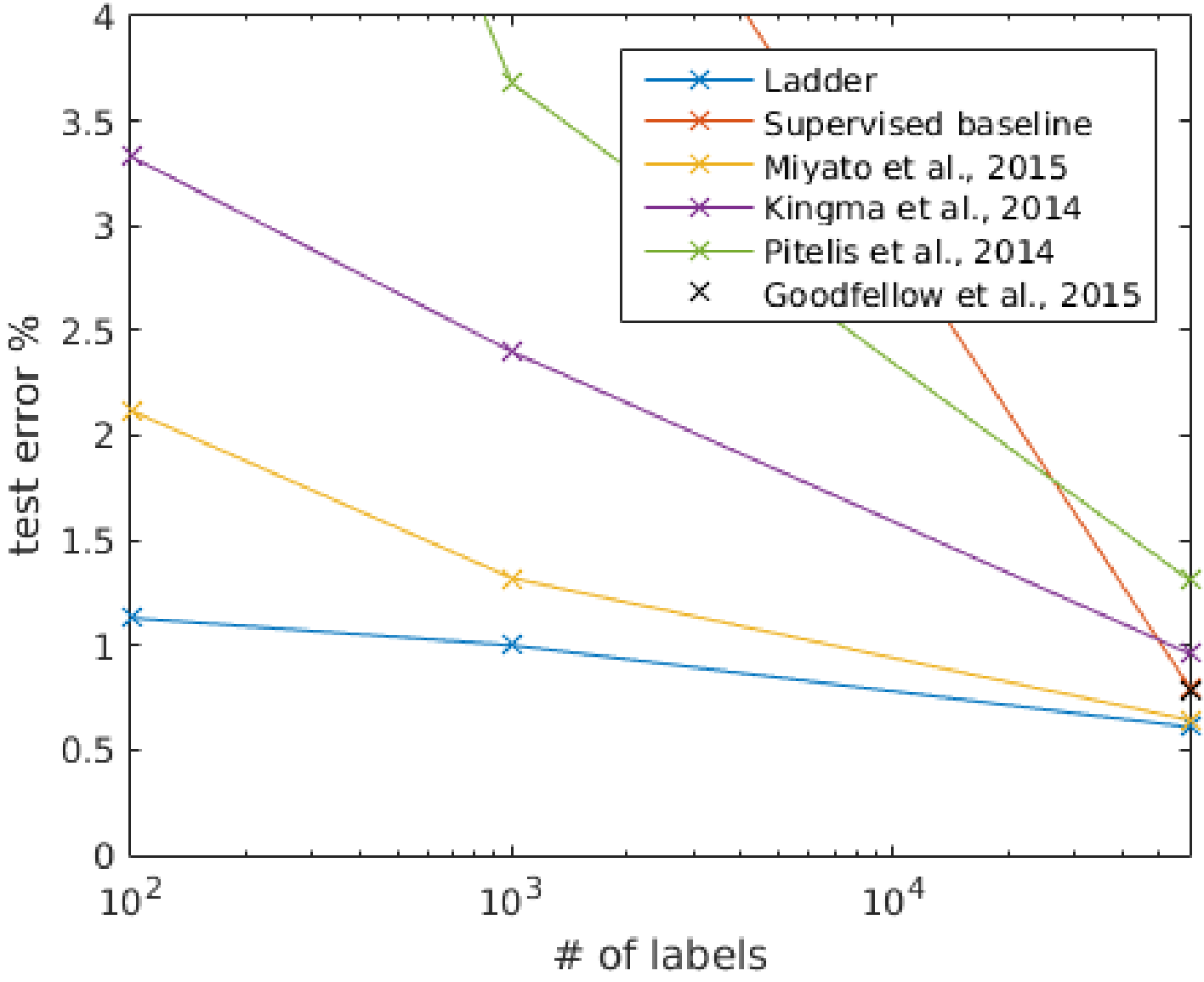
$g(\tilde{\mathbf{z}}, \mathbf{u})$ done componentwise: $g_i(\tilde{z}_i, u_i)$.

Supervised MNIST results



Yearly progress in permutation-invariant MNIST.

Semi-supervised MNIST results



Part 4:

Deep generative models for un- and semi-supervised learning

Generative models for complex data

Latent variable model

- Latent variable model:

$$p_\theta(x, z) = \underbrace{p_\theta(x|z)}_{\text{FFNN}} \underbrace{p(z)}_{\mathcal{N}(z|0,I)}$$

Latent variable model

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$$p_\theta(x, z) = \underbrace{p_\theta(x|z)}_{\text{FFNN}} \underbrace{p(z)}_{\mathcal{N}(z|0,I)}$$

- Inference

$$z \sim p(z|x) = \frac{p(x|z)p(z)}{p(x)}$$

- Likelihood

$$p(x) = \int p(x|z)p(z)dz$$

- Learning

$$\theta_{\text{ML}} = \underset{\theta}{\text{argmax}} \sum_{i=1}^{n} \log p_\theta(x_i)$$

- Difficult computations!

Deep variational auto-encoders

- Kingma+Welling 2013, Rezende et al 2013:
- Decoder: (example continuous observations)

$$p_\theta(x|z) = \mathcal{N}(x|\underbrace{\mu_\theta(z)}_{\text{FFNN}}, \underbrace{\text{diag}(\sigma^2_\theta(z))}_{\text{FFNN}})$$

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- Variational objective - optimize $\sum_i \mathcal{L}_{\theta,\phi}(x_i)$ wrt θ, ϕ:

$$\log p_\theta(x) \geq \mathcal{L}_{\theta,\phi}(x) = \int q_\phi(z|x) \log \frac{p_\theta(x|z)p(z)}{q_\phi(z|x)} dz$$

$$= \underbrace{\mathbb{E}_{q_\phi(z|x)}[\log p_\theta(x|z)]}_{\mathbb{E}_q[\log \text{likelihood}]} + \underbrace{\mathbb{E}_{q_\phi(z|x)}\left[\log \frac{p(z)}{q_\phi(z|x)}\right]}_{\text{regularization}}$$

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- Handle integration by sampling

$$\mathcal{L}_{\theta,\phi}(x) \approx \frac{1}{R} \sum_{r=1}^{R} \log \frac{p_\theta(x|z^r)p(z^r)}{q_\phi(z^r|x)},$$

$$z^r = \mu_\phi(x) + \sigma_\phi(x) \otimes \epsilon^r$$

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$$z^r = \mu_\phi(x) + \sigma_\phi(x) \otimes \epsilon^r$$

- Auto-encoder: map "$x \to z \to x$"
- This is a variational auto-encoder (VAE):

$$\text{Encoder} \quad z = \mu_\phi(x) + \sigma_\phi(x) \otimes \epsilon$$
$$\text{Decoder} \quad p_\theta(x|z) = \mathcal{N}(x|\mu_\theta(z), \text{diag}(\sigma^2_\theta(z)))$$

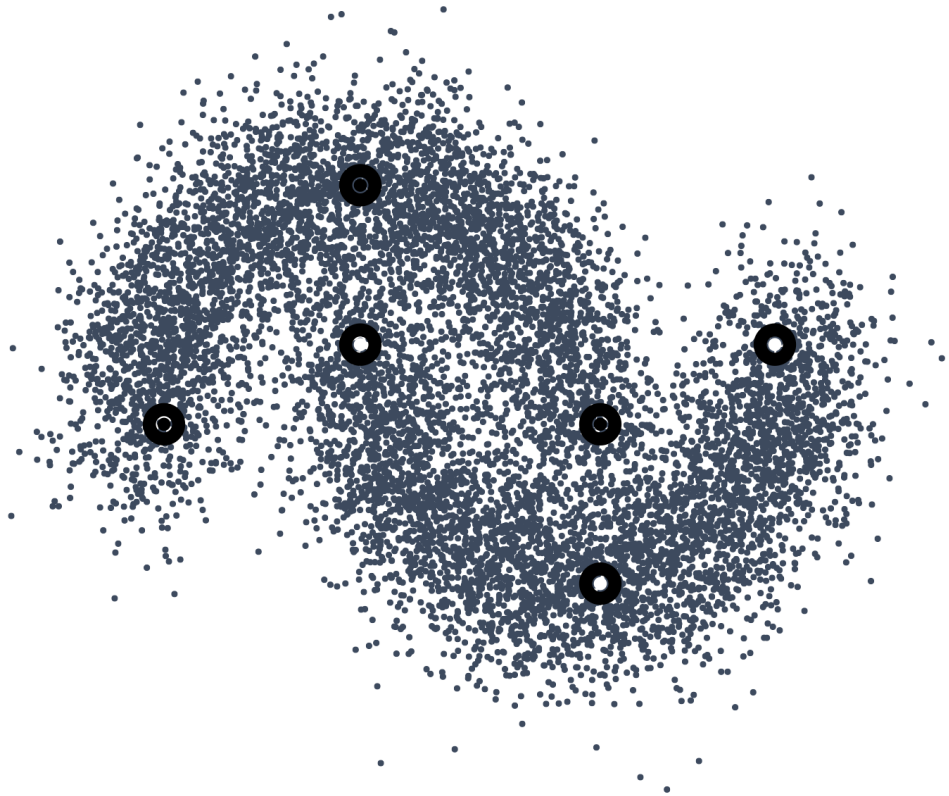
Generative models for complex data

- Once model is trained we can make it dream up new digits by:

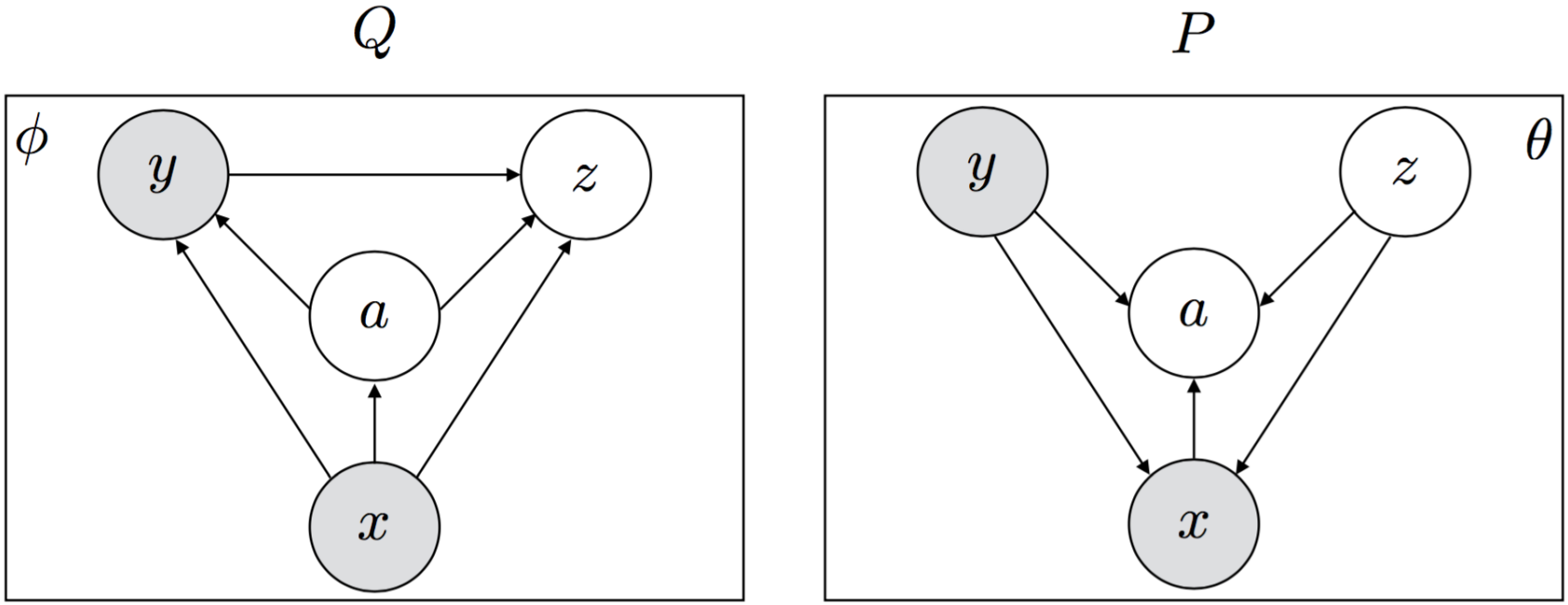
$$z \sim \mathcal{N}(z|0,1)$$

$$x \sim \mathcal{N}(x|\underbrace{\mu_\theta(z)}_{\text{FFNN}},\underbrace{\text{diag}(\sigma^2_\theta(z))}_{\text{FFNN}})$$

Semi-supervised learning

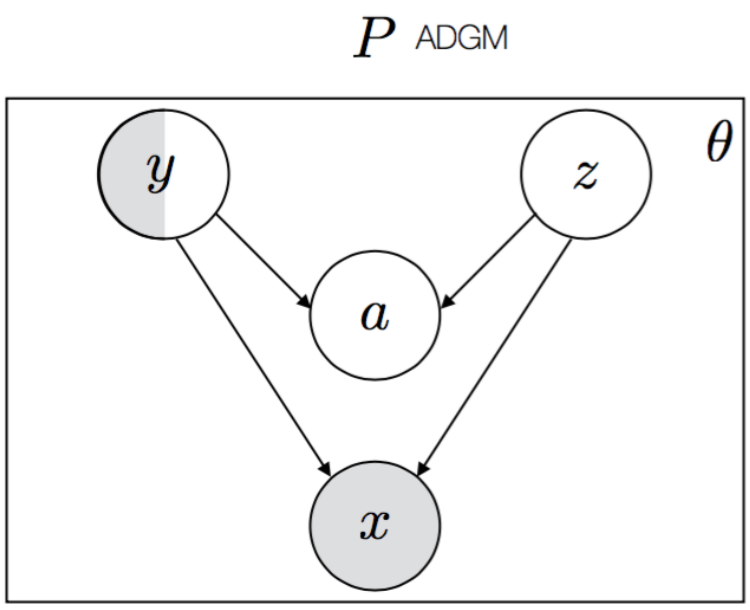


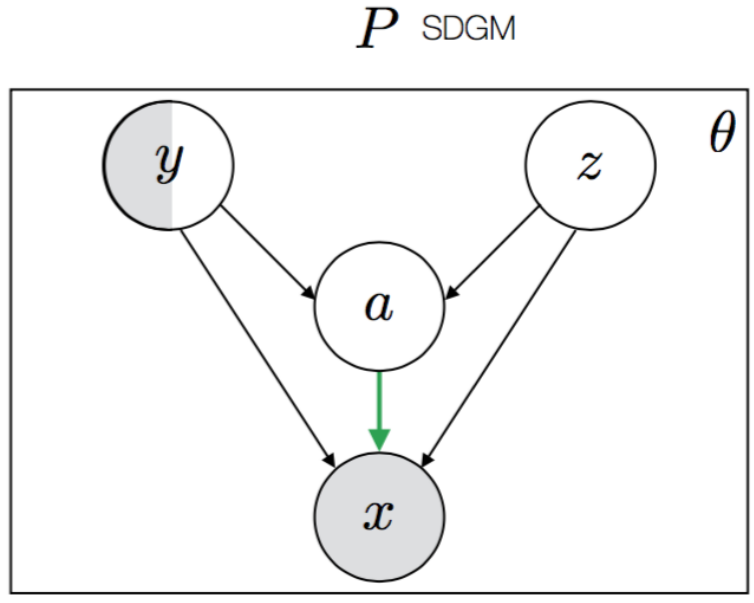
Auxiliary variable model for labeled data



L Maaloe et al, ICML, 2016.

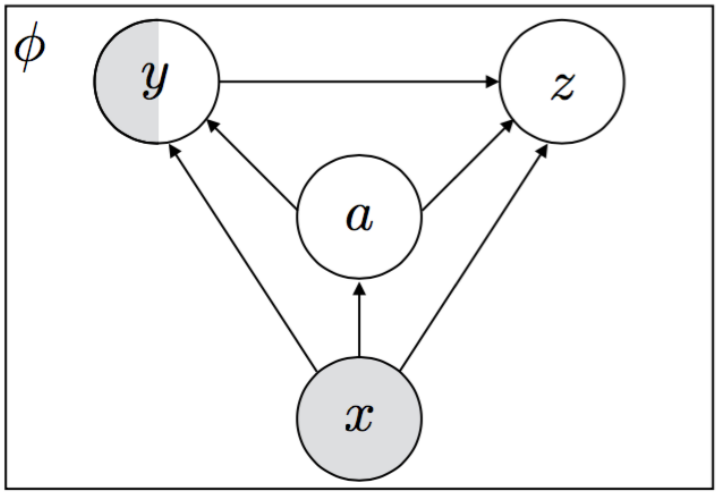
Skip deep generative model



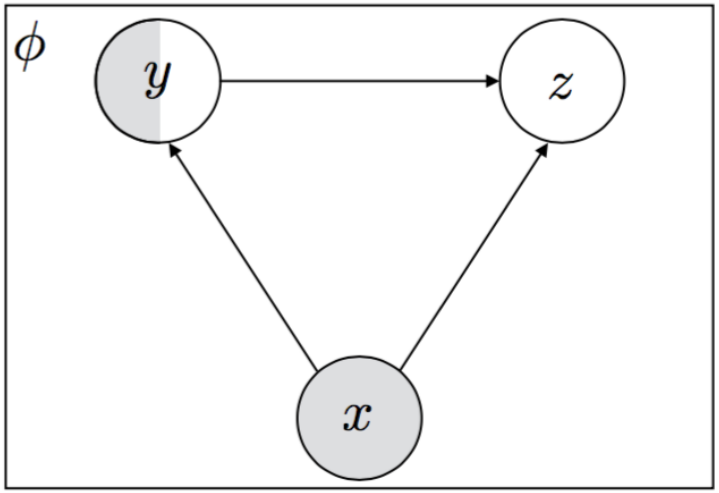


Kingma et al M1 and M2

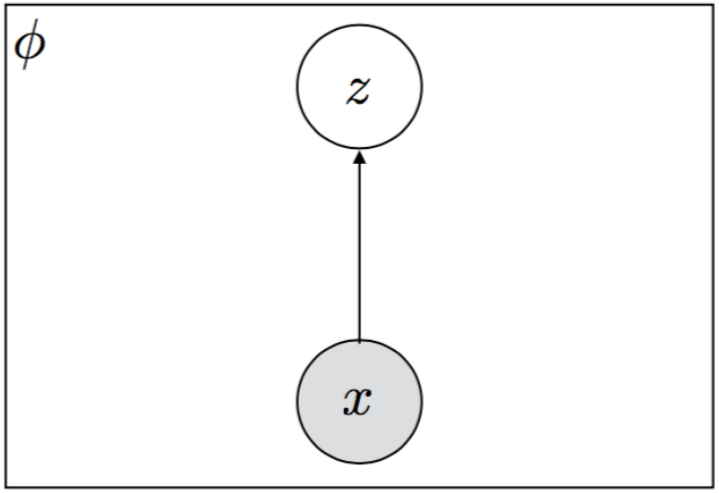
Q ADGM/SDGM



Q M2 (Kingma et al., 2014)



Q M1 (Kingma et al., 2014)



Semi-supervised benchmarks

	MNIST 100 labels	SVHN 1000 labels	NORB 1000 labels
M1+TSVM (Kingma et al., 2014)	11.82% (±0.25)	55.33% (±0.11)	18.79% (±0.05)
M1+M2 (Kingma et al., 2014)	3.33% (±0.14)	36.02% (±0.10)	
VAT (Miyato, 2015)	2.12 %	24.63 %	9.88 %
Ladder Network (Rasmus et al., 2015)	1.06% (±0.37)		
Auxiliary Deep Generative Model	**0.96% (±0.02)**	22.86 %	10.06% (±0.05)
Skip Deep Generative Model	1.32% (±0.07)	**16.61% (±0.24)**	**9.40% (±0.04)**

- Potential extensions: warm-up, batch normalisation, convolutional layers, combining with other improvements.
- The saga continues Salisman et al, Improved Techniques for Training GANs, 2016.

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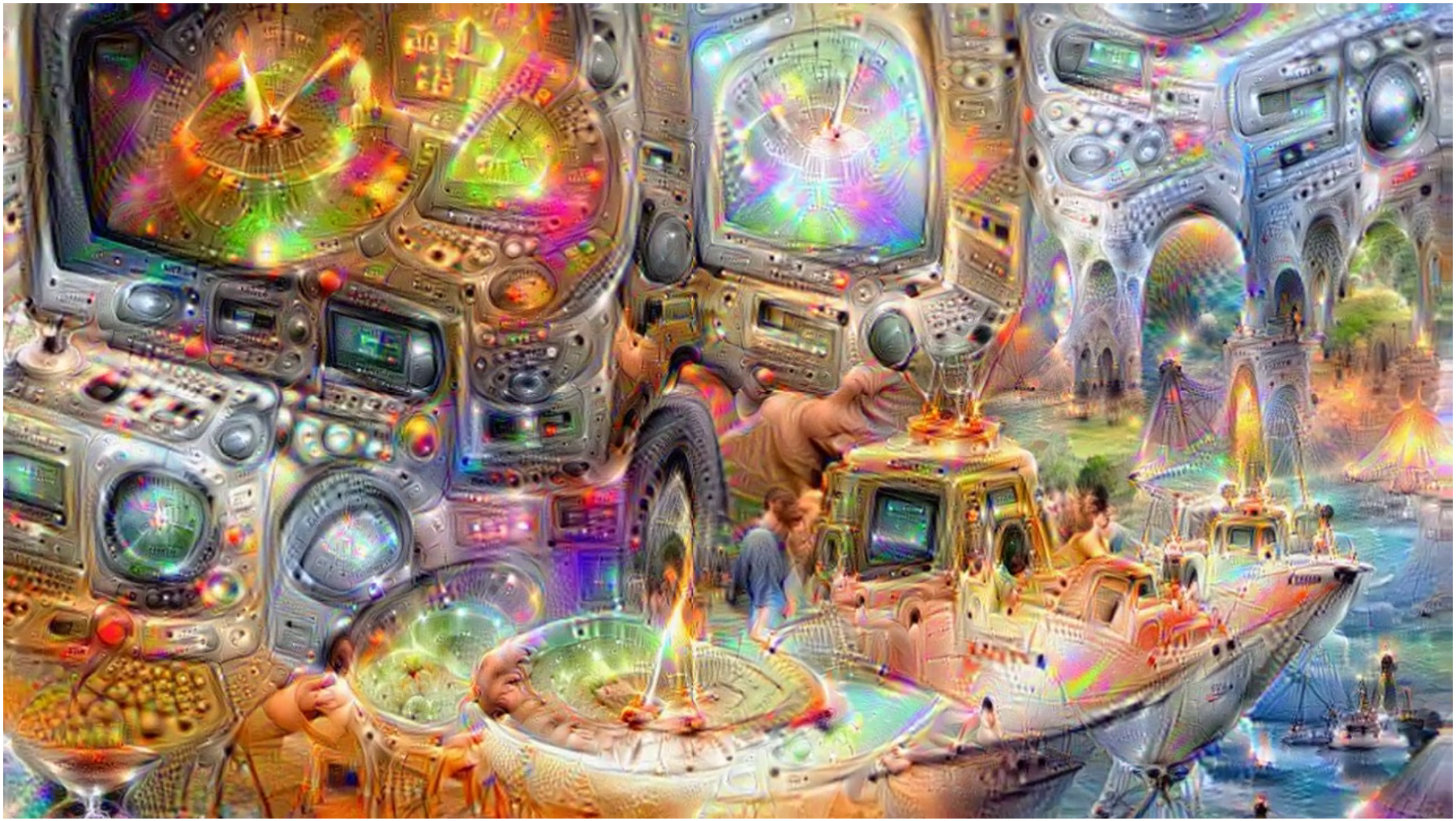

Thanks!
Ole Winther