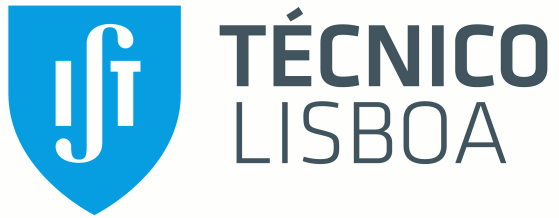
Lecture 13: Deep Generative Models

André Martins, Francisco Melo, Mário Figueiredo



Deep Learning Course, Winter 2021-2022

Announcements

- This Friday, 15:00–17:00, Centro de Congressos (Pav. Civil, Alameda): guest lecture by Prof. Chrysoula Zerva!

Today's Roadmap

Most of the course was about supervised learning.

Today we'll talk about deep generative models and unsupervised learning.

- Deep auto-regressive models
- Boltzmann machines
- Evidence lower bound (ELBO) and variational inference
- Variational auto-encoders
- Generative adversarial networks

Which of these people is real?

(http://www.whichfaceisreal.com)

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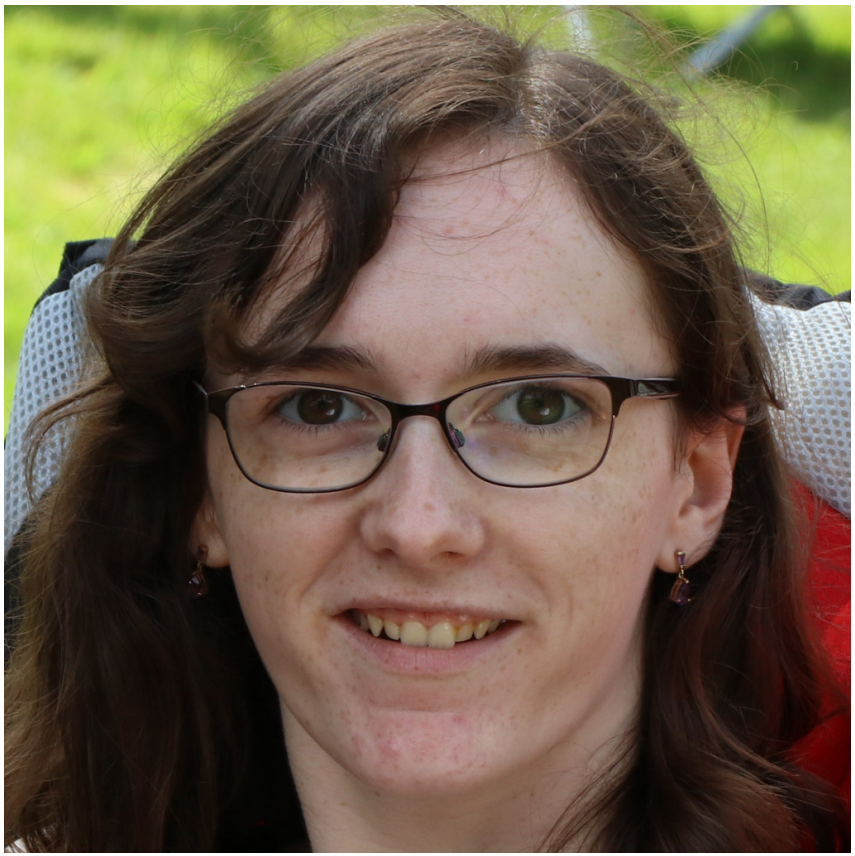

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Generative Modeling

- Modelling complex high-dimensional data is a hard, open problem
- Deep generative models are currently making progress on this.
- **Goal:** model $\mathbb{P}(\boldsymbol{x})$ (unsupervised learning) or $\mathbb{P}(\boldsymbol{x}, \boldsymbol{y})$ (supervised learning)
- Often, deep generative models also use latent variables $\boldsymbol{h}$, in which case they may model $\mathbb{P}(\boldsymbol{x}, \boldsymbol{h})$ or $\mathbb{P}(\boldsymbol{x}, \boldsymbol{h}, \boldsymbol{y})$, such that

$$\mathbb{P}(\boldsymbol{x}) = \sum_{\boldsymbol{h}} \mathbb{P}(\boldsymbol{x}, \boldsymbol{h}) \quad \text{or} \quad \mathbb{P}(\boldsymbol{x}, \boldsymbol{y}) = \sum_{\boldsymbol{h}} \mathbb{P}(\boldsymbol{x}, \boldsymbol{h}, \boldsymbol{y})$$

Examples of Deep Generative Models

- Auto-Regressive Networks
- Restricted Boltzmann Machines
- Deep Belief Networks
- Deep Boltzmann Machines
- Gaussian-Bernoulli RBMs
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1. Deep Auto-Regressive Models
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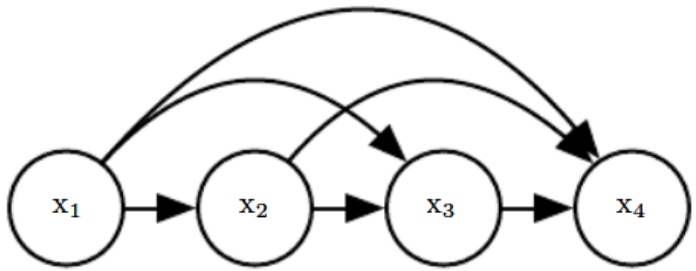
Deep Auto-Regressive Models

- Deep auto-regressive (AR) models have no latent variables.
- Use the chain rule of probabilities to decompose:

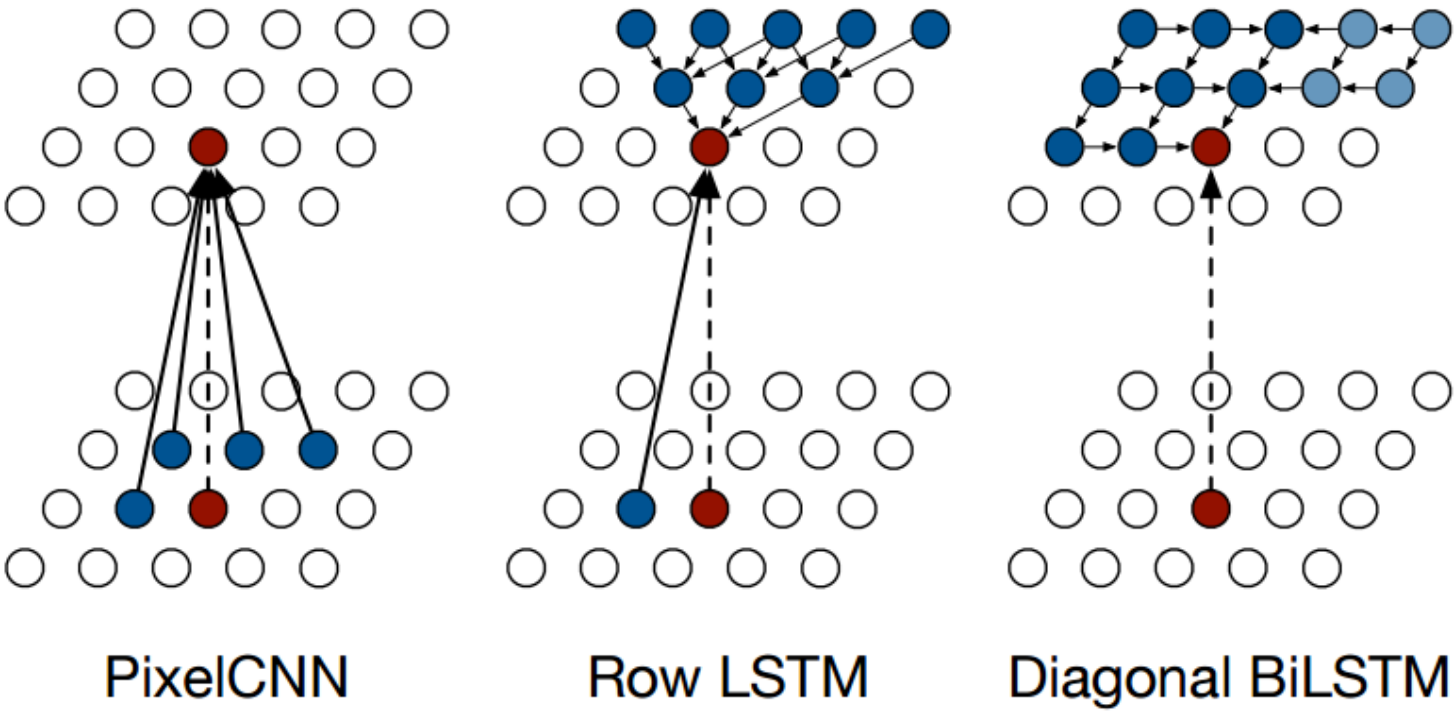
$$\mathbb{P}(\boldsymbol{x}) = \mathbb{P}(x_1)\,\mathbb{P}(x_2 \mid x_1) \cdots \mathbb{P}(x_D \mid x_1, \ldots, x_{D-1})$$



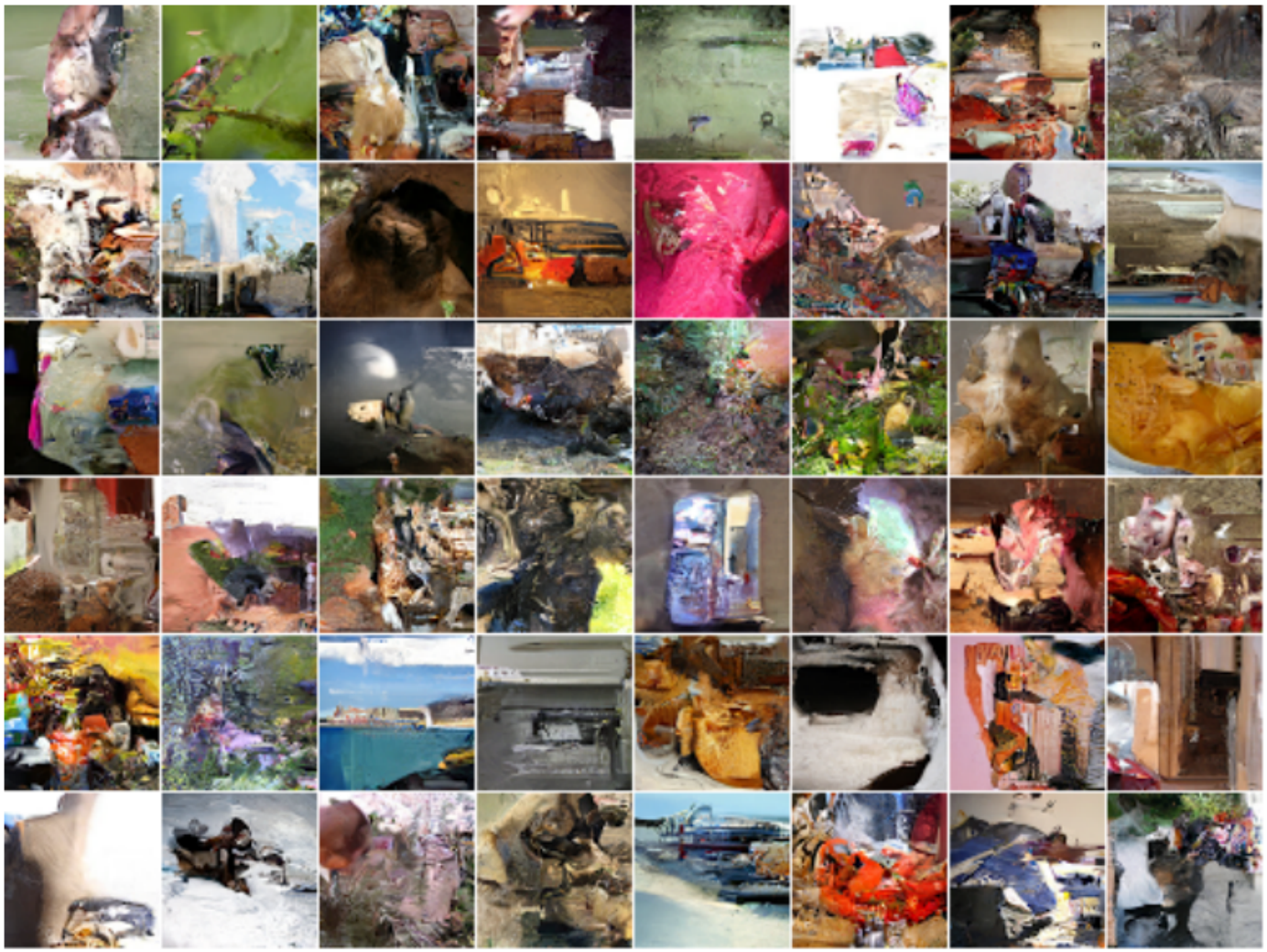
- Also called fully-visible Bayes networks.
- We saw examples already: RNNs, Pixel RNNs, Pixel CNNs, ...

Examples: PixelCNNs and PixelRNNs

- Input-to-state and state-to-state mappings for PixelCNN and two PixelRNN models (Oord et al., 2016):



RNNs for Generating Images



(Oord et al., 2016)

Summary

- Despite their simplicity, deep AR models can be very powerful.
- However, they may require too many parameters/complex functions due to the assumption all variables are observed.
- Models with latent variables are an appealing alternative: they can represent "clusters", yielding simpler representations.

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Energy Based Models

- A probability distribution (mixing observed and latent variables) via an energy function $E(\boldsymbol{x}, \boldsymbol{h}; \boldsymbol{\theta})$:

$$\mathbb{P}(\boldsymbol{x}, \boldsymbol{h}) = \frac{\exp(-E(\boldsymbol{x}, \boldsymbol{h}; \boldsymbol{\theta}))}{Z(\boldsymbol{\theta})}$$

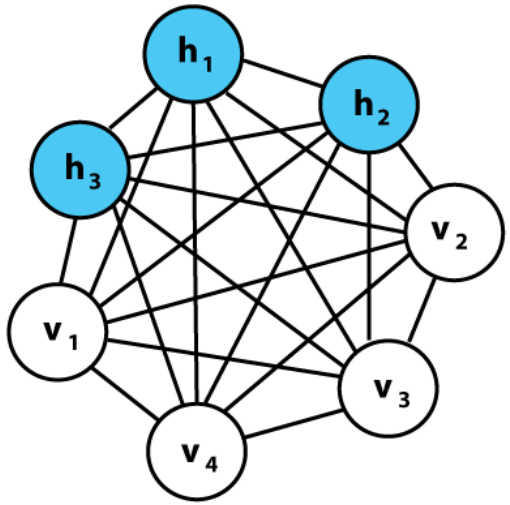
- Maximizing probability corresponds to minimizing the energy.

- Challenges:
  - Computing the partition function $Z(\boldsymbol{\theta})$
  - Computing the evidence $\mathbb{P}(\boldsymbol{x})$
  - Computing the posterior $\mathbb{P}(\boldsymbol{h} \mid \boldsymbol{x})$
  - Sampling from $\mathbb{P}(\boldsymbol{x}, \boldsymbol{h})$ or from $\mathbb{P}(\boldsymbol{x})$

Boltzmann Machine (Ackley et al., 1985)

- Energy-based model over binary vectors

- Some variables are observed ($\boldsymbol{v}$), others are latent/hidden ($\boldsymbol{h}$)



- Probability distribution over $(\boldsymbol{v}, \boldsymbol{h}) \in \{0,1\}^{N+M}$:

$$\mathbb{P}(\boldsymbol{v}, \boldsymbol{h}) = \frac{\exp(-E(\boldsymbol{v}, \boldsymbol{h}; \boldsymbol{\theta}))}{Z(\boldsymbol{\theta})}$$

- Energy function, with $\boldsymbol{\theta} = (\boldsymbol{R}, \boldsymbol{W}, \boldsymbol{S}, \boldsymbol{b}, \boldsymbol{c})$,

$$\begin{aligned} E(\boldsymbol{v}, \boldsymbol{h}; \boldsymbol{\theta}) &= -\begin{bmatrix} \boldsymbol{v}^\top & \boldsymbol{h}^\top \end{bmatrix} \begin{bmatrix} \boldsymbol{R} & \boldsymbol{W}/2 \\ \boldsymbol{W}^\top/2 & \boldsymbol{S} \end{bmatrix} \begin{bmatrix} \boldsymbol{v} \\ \boldsymbol{h} \end{bmatrix} - \begin{bmatrix} \boldsymbol{b}^\top & \boldsymbol{c}^\top \end{bmatrix} \begin{bmatrix} \boldsymbol{v} \\ \boldsymbol{h} \end{bmatrix} \\ &= -\boldsymbol{v}^\top \boldsymbol{R} \boldsymbol{v} - \boldsymbol{v}^\top \boldsymbol{W} \boldsymbol{h} - \boldsymbol{h}^\top \boldsymbol{S} \boldsymbol{h} - \boldsymbol{b}^\top \boldsymbol{v} - \boldsymbol{c}^\top \boldsymbol{h} \end{aligned}$$

Boltzmann Machine

- The Boltzmann machine (BM) is a universal approximator of probability mass functions over discrete variables (Le Roux and Bengio, 2008)

- Emulates the idea in Hebbian learning: "neurons that fire together wire together."

- However, in general,
  - Sampling is hard,
  - Inference is hard,
  - Learning is hard.

How to Learn a Boltzmann Machine?

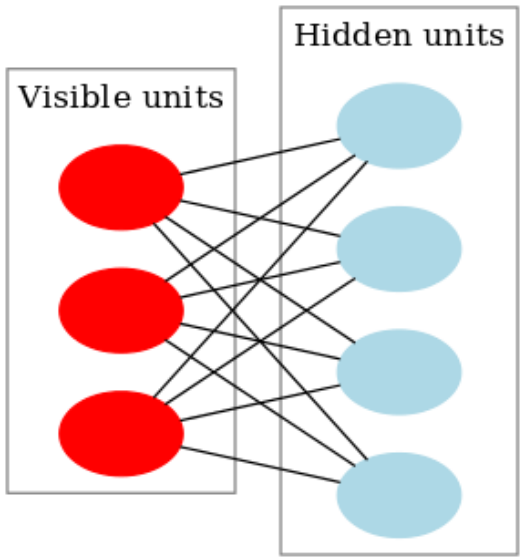
- Learning is usually based on maximum likelihood.
- The partition function $Z(\boldsymbol{\theta})$ is intractable: for learning, the gradient must be approximated:
  - contrastive divergence
  - pseudo-likelihood
  - noise-contrastive estimation
  - annealed importance sampling
- Not covered here, but check Goodfellow et al. (2016, Chapter 18).
- In a nutshell, learning a fully general BM is usually very challenging, so we typically use a particular version.

Some Particular Cases

- Restricted Boltzmann machines
- Deep belief networks
- Deep Boltzmann machines
- ...

Restricted Boltzmann Machines

- Also called harmonium (Smolensky, 1986)
- A layer of observable variables
- A single layer of latent variables.



- Bipartite graph, no intra-layer connections: $\boldsymbol{R} = 0$; $\boldsymbol{S} = 0$.
- The energy function becomes:

$$E(\boldsymbol{v}, \boldsymbol{h}; \boldsymbol{\theta}) = -\boldsymbol{v}^\top \boldsymbol{W}\boldsymbol{h} - \boldsymbol{b}^\top \boldsymbol{v} - \boldsymbol{c}^\top \boldsymbol{h}$$

- What is the advantage?

Restricted Boltzmann Machines

- Unfortunately, the partition function $Z(\boldsymbol{\theta})$ is still intractable
- ... but the conditionals $\mathbb{P}(\boldsymbol{h} \mid \boldsymbol{v})$ and $\mathbb{P}(\boldsymbol{v} \mid \boldsymbol{h})$ are now tractable!
  - easy to compute!
  - easy to sample!
  - using Markov-Chain Monte Carlo (MCMC) with Gibbs sampling.
- Why are these easy? Conditional independence (next slide)

Restricted Boltzmann Machines

- Why are the conditionals tractable?
- Because, without intra-layer connections, $h_1, \ldots, h_N$ are conditionally independent given $\boldsymbol{v}$:

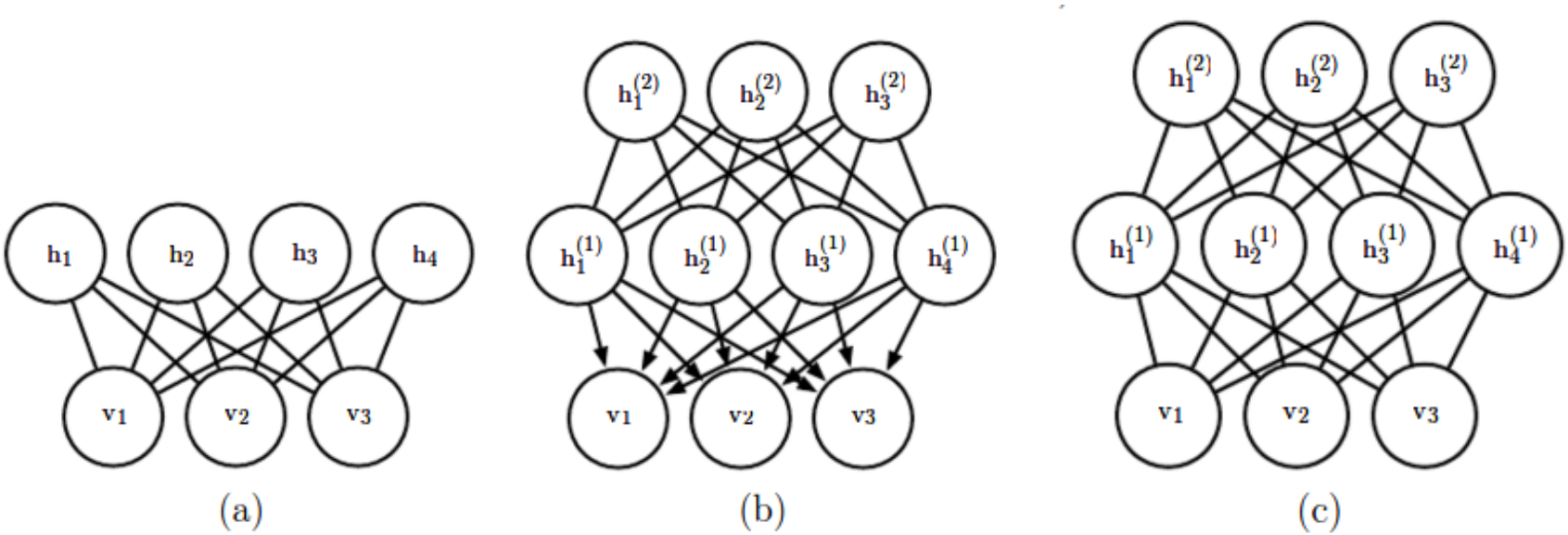
$$\mathbb{P}(\boldsymbol{h} \mid \boldsymbol{v}) = \prod_{j=1}^{M} \mathbb{P}(h_j \mid \boldsymbol{v})$$

where

$$\mathbb{P}(h_j = 1 \mid \boldsymbol{v}) \quad = \quad \sigma\big(c_j + (\boldsymbol{W}\boldsymbol{v})_j\big), \quad \forall j = 1, \ldots, M.$$

- Reciprocally for $\mathbb{P}(\boldsymbol{v} \mid \boldsymbol{h})$.
- RBMs are relatively easy to train by approximating $Z(\boldsymbol{\theta})$ (see Goodfellow et al. (2016, Chapter 18)).
- RBMs may be stacked to form deeper models.

Some RBM's Friends



(Image from Goodfellow et al. (2016))

(a) Restricted Boltzmann machine (RBM)

(b) Deep belief network (DBN): hybrid directed/undirected GM with multiple latent layers

(c) Deep Boltzmann machine (DBM): undirected GM with several layers of latent variables.

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Next: Differentiable Generator Networks

- Several recent models are based on differentiable generator networks.
- This is a differentiable function $G(\boldsymbol{h}; \boldsymbol{\theta})$ that maps latent variables $\boldsymbol{h}$ into sample reconstructions $\boldsymbol{x}$ (or distributions $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{h})$).
- This idea underlies
  - Variational auto-encoders (VAE)
  - Generative adversarial networks (GAN)
- We'll cover those next.

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Variational Auto-Encoders

- Many latent variable models have:
  - intractable evidence $\mathbb{P}(\boldsymbol{x})$
  - intractable posterior $\mathbb{P}(\boldsymbol{h} \mid \boldsymbol{x})$.
- Variational inference (e.g. mean field approximation) is a technique used to approximate these quantities.
- Widely used in Bayesian inference, topic models, etc...
- Auto-encoders: effective to learn data representations or codes (i.e. $\boldsymbol{x} \longrightarrow \boldsymbol{h} \longrightarrow \hat{\boldsymbol{x}}$)
- Key idea: combine auto-encoders with variational inference.

Assumptions

- Henceforth, we assume that:
  - the prior $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{h})$ is tractable (e.g.. zero-mean, unit-variance Gaussian)
  - the conditional $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{h})$ is tractable (e.g. a feed-forward neural network or an RNN).
- However,
  - he evidence $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x})$ (i.e. marginalizing out $\boldsymbol{h}$) is still intractable
  - computing the posterior $\mathbb{P}(\boldsymbol{h} \mid \boldsymbol{x})$ is still intractable.
- Next: using variational inference to approximate these computations

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Recap: Shannon's Entropy

- Let $\mathbb{P}$ be a distribution over $\mathcal{X}$. The entropy of $\mathbb{P}$ is

$$H(\mathbb{P}) = -\sum_{\boldsymbol{x} \in \mathcal{X}} \mathbb{P}(\boldsymbol{x}) \log \mathbb{P}(\boldsymbol{x})$$

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- Always non-negative: $H(\mathbb{P}) \geq 0$
- $H(\mathbb{P}) = 0$ iff $\mathbb{P}(\boldsymbol{x}) = 1$, for some $\boldsymbol{x}$ and $\mathbb{P}(\boldsymbol{x}') = 0$, for any $\boldsymbol{x}' \neq \boldsymbol{x}$.

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- Coding perspective: expected number of bits (using $\log_2$) to optimally encode $\boldsymbol{x} \sim \mathbb{P}(\boldsymbol{x})$

Recap: Kullback-Leibler (KL) Divergence

- Let $\mathbb{P}$ and $\mathbb{Q}$ be two distributions over $\mathcal{X}$.

$$KL(\mathbb{P}\|\mathbb{Q}) = \sum_{\boldsymbol{x}} \mathbb{P}(\boldsymbol{x}) \log \frac{\mathbb{P}(\boldsymbol{x})}{\mathbb{Q}(\boldsymbol{x})}$$

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- Let $\mathbb{P}$ be a probability density over $\mathcal{X}$. The differential entropy of $\mathbb{P}$ is

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- Let $\mathbb{P}$ and $\mathbb{Q}$ be two probability densities over $\mathcal{X}$.

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- Intuition: $KL(\mathbb{P}\|\mathbb{Q})$ measure how different $\mathbb{Q}$ is from $\mathbb{P}$

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- Old roots in calculus of variations (Newton, Bernoulli, Euler, Lagrange, ...)

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- The ELBO can be written in different ways:

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- The ELBO mirrors the usual trade-off between **likelihood** and **prior**.

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  i.e., model the h_i are independent.

- More sophisticated: structured mean field imposes a graphical model on $\mathbb{Q}$ capturing (some) interactions among the h_i, but still tractable. (see the book by Wainwright and Jordan (2008) for details).

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- Alternative: use amortized variational inference!

- Key idea: instead of optimizing $\mathbb{Q}(\boldsymbol{h})$ for every example, use an encoder with shared parameters $\boldsymbol{\phi}$ and define $\mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x})$.

  For each example:

  - make a forward pass on the encoder to obtain $\mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x})$
  - backpropagate through the encoder to update $\boldsymbol{\phi}$.

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- Approximate the posterior with a variational distribution

$$\mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) = \mathcal{N}(\boldsymbol{h}; \boldsymbol{\mu}(\boldsymbol{x}; \boldsymbol{\phi}), \boldsymbol{\sigma}^2(\boldsymbol{x}; \boldsymbol{\phi}))$$

  where $\boldsymbol{\mu}(\boldsymbol{x}; \boldsymbol{\phi}$ and $\boldsymbol{\sigma}^2(\boldsymbol{x}; \boldsymbol{\phi})$ are MLPs

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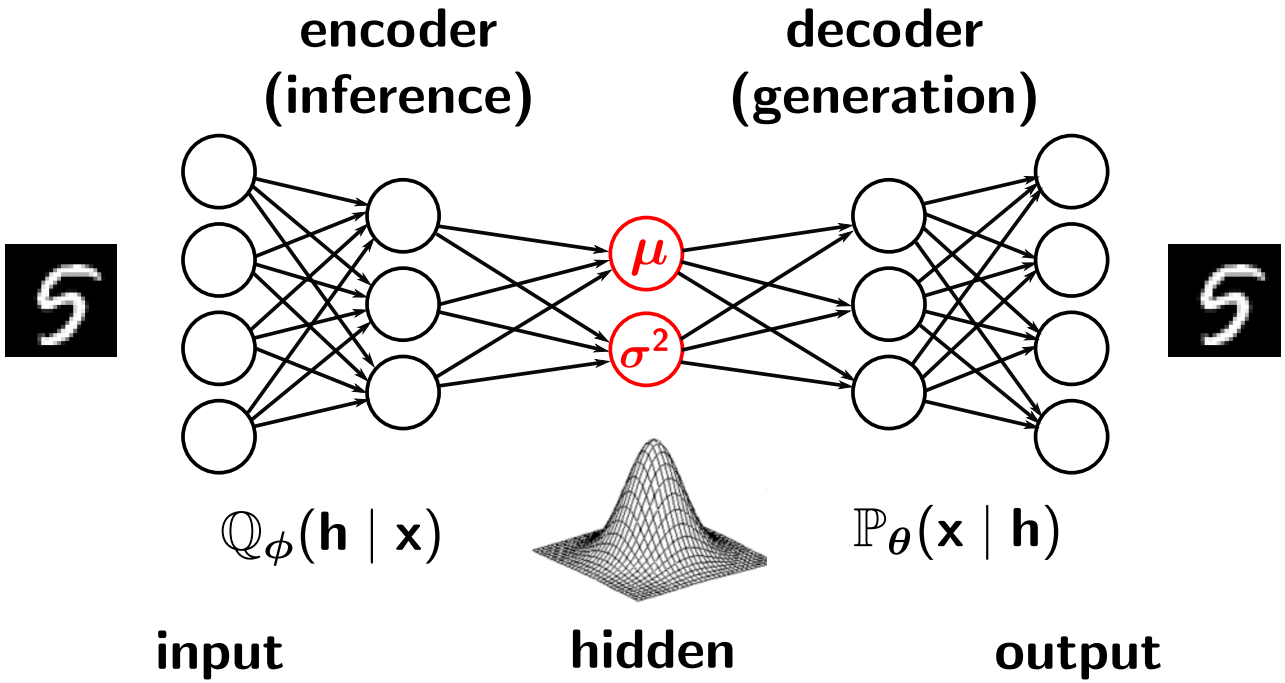
- This leads to variational auto-encoders:



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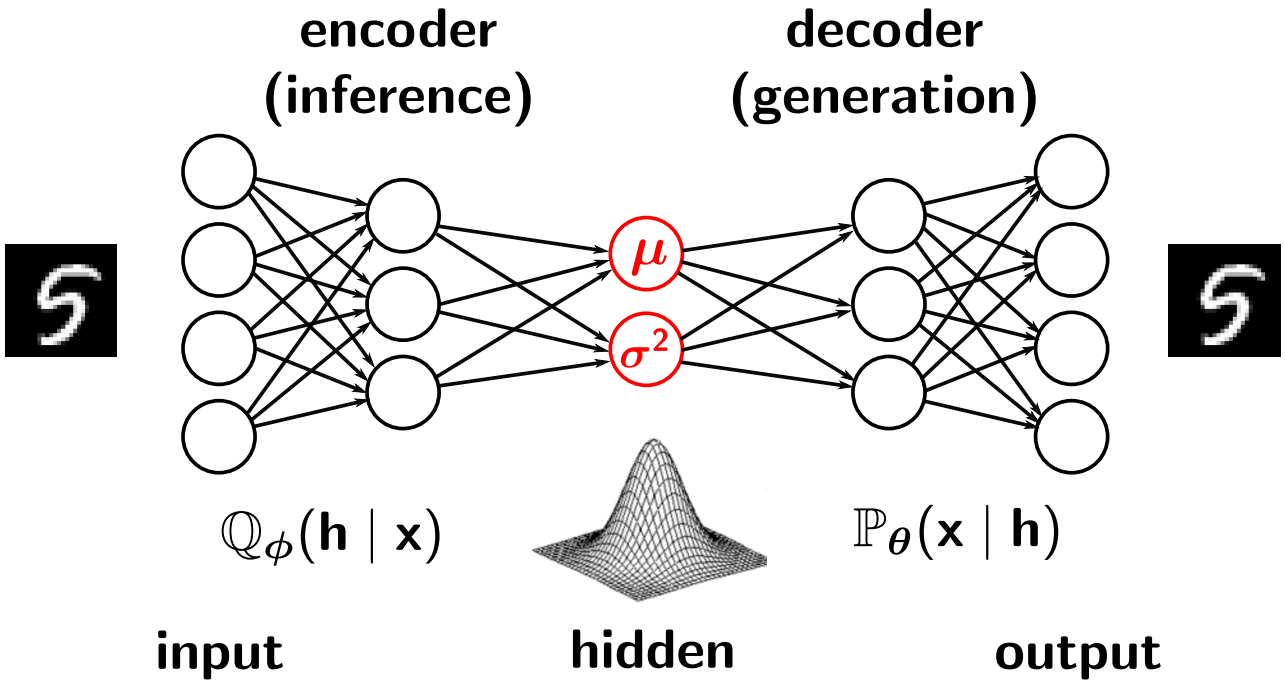

- ... we'll come back to this!

Outline

1. Deep Auto-Regressive Models
2. Boltzmann Machines
3. Variational Auto-Encoders
   - Variational Inference and ELBO
   - Gradients and Reparameterization Trick
4. Generative Adversarial Networks
5. Conclusions

Parameter Gradients

- Recall that:

$$\text{ELBO}(\boldsymbol{\phi}; \boldsymbol{\theta}) = \mathbb{E}_{\mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h}|\boldsymbol{x})}[\log \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{h}) - \log \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x})].$$

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- Gradient w.r.t. $\boldsymbol{\theta}$, parameters of the generation network:

$$\nabla_{\boldsymbol{\theta}} \text{ELBO}(\boldsymbol{\phi}; \boldsymbol{\theta}) = \mathbb{E}_{\mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h}|\boldsymbol{x})}[\nabla_{\boldsymbol{\theta}} \log \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{h})]$$

  - Follows from linearity of the expectation.

  - This is simple and can be well approximated with Monte Carlo samples.

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(derivation in the next slide)

  - Problem: Monte Carlo estimators have high variance due to the left part!
  - Requires variance reduction techniques.
  - Resembles REINFORCE (Williams, 1992) (a reinforcement learning algorithm)

Derivation of the Inference Network Gradient

$$
\begin{aligned}
&\nabla_{\boldsymbol{\phi}} \text{ELBO}(\boldsymbol{\phi}; \boldsymbol{\theta}) \\
&= \nabla_{\boldsymbol{\phi}} \mathbb{E}_{\mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h}|\boldsymbol{x})}[\log \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{h}) - \log \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x})] \\
&= \nabla_{\boldsymbol{\phi}} \sum_{\boldsymbol{h}} \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) \log \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{h}) - \nabla_{\boldsymbol{\phi}} \sum_{\boldsymbol{h}} \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) \log \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) \\
&= \sum_{\boldsymbol{h}} \log \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{h}) \nabla_{\boldsymbol{\phi}} \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) - \sum_{\boldsymbol{h}} (1 + \log \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x})) \nabla_{\boldsymbol{\phi}} \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) \\
&= \sum_{\boldsymbol{h}} (\log \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{h}) - \log \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x})) \nabla_{\boldsymbol{\phi}} \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) \\
&= \mathbb{E}_{\mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h}|\boldsymbol{x})}[(\log \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}, \boldsymbol{h}) - \log \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x})) \nabla_{\boldsymbol{\phi}} \log \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x})],
\end{aligned}
$$

where we used the facts:

$$
\sum_{\boldsymbol{h}} \nabla_{\boldsymbol{\phi}} \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) = \nabla_{\boldsymbol{\phi}} \sum_{\boldsymbol{h}} \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) = \nabla_{\boldsymbol{\phi}} 1 = 0.
$$

$$
\nabla_{\boldsymbol{\phi}} \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) = \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) \nabla_{\boldsymbol{\phi}} \log \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}).
$$

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- Is there a better strategy?
- Yes: the reparameterization trick.

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- Consequently, for any function f,

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- Gradients w.r.t. $\boldsymbol{\phi}$ can be estimated with regular backpropagation over $\boldsymbol{g}_{\boldsymbol{\phi}}$.

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- This construction is possible in many cases for continuous latent variables:
  - exponential
  - Gaussian
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  - log-normal
  - etc...

Reparameterization Trick

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  - exponential
  - Gaussian
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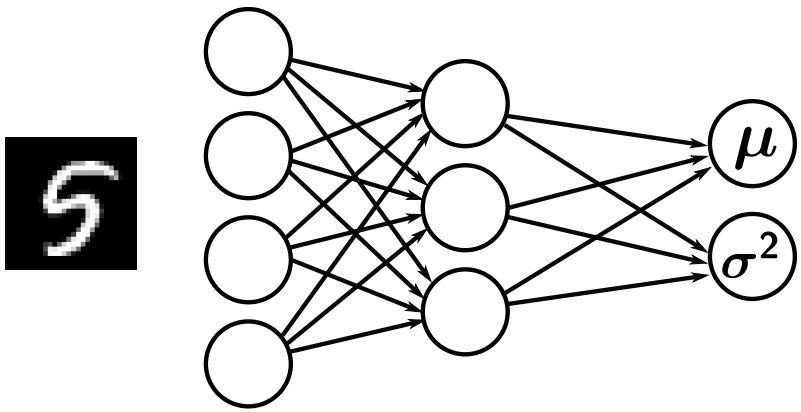
  - etc...
- For discrete latent variables, it is still possible via the Gumbel-softmax trick (not covered in the course).

Example: Gaussian

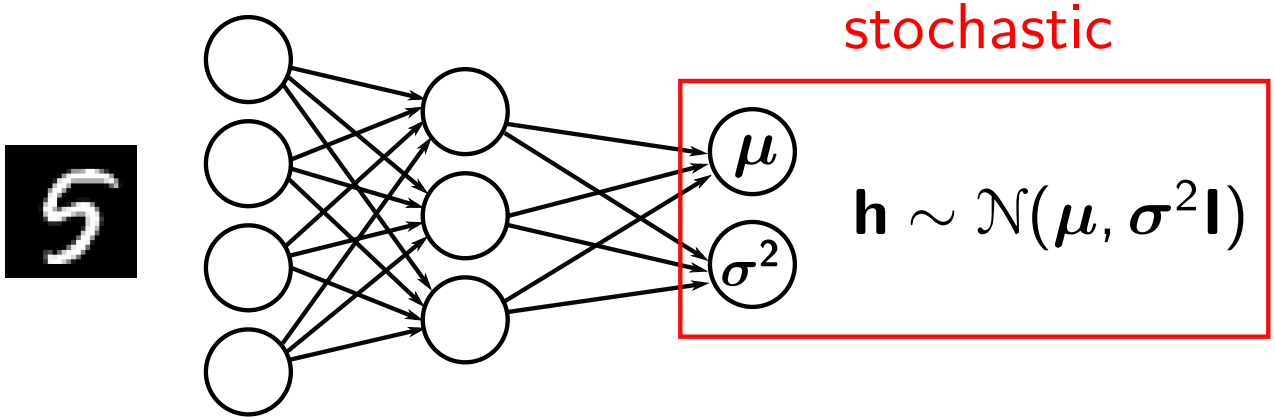
1. Sample $\boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{\epsilon}; 0, \boldsymbol{I})$
2. Use inference network $\boldsymbol{g}_{\phi}$ with input $\boldsymbol{x}$ to output mean $\boldsymbol{\mu}(\boldsymbol{x})$ and variance $\boldsymbol{\sigma}^2(\boldsymbol{x})$
3. Set $\boldsymbol{h} = \boldsymbol{\mu}(\boldsymbol{x}) + \boldsymbol{\epsilon}\, \boldsymbol{\sigma}(\boldsymbol{x})$.
4. Thus, $\boldsymbol{h} \mid \boldsymbol{x} \sim \mathcal{N}\big(\boldsymbol{\mu}(\boldsymbol{x}), (\boldsymbol{\sigma}(\boldsymbol{x}))^2\big)$

Reparameterization Trick



$$\mathbf{h} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\sigma}^2 \mathbf{I})$$

Reparameterization Trick



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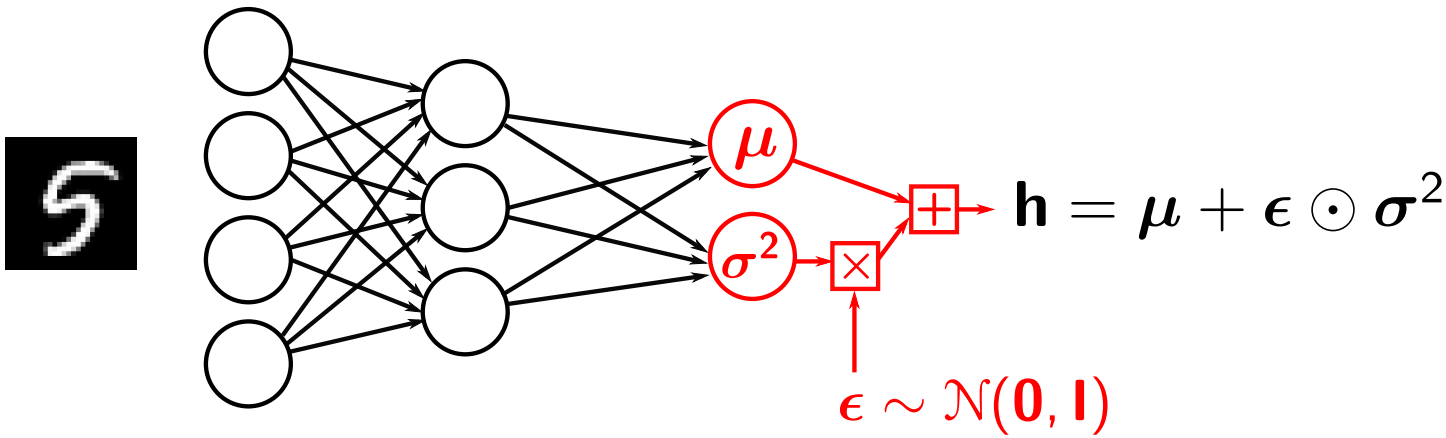

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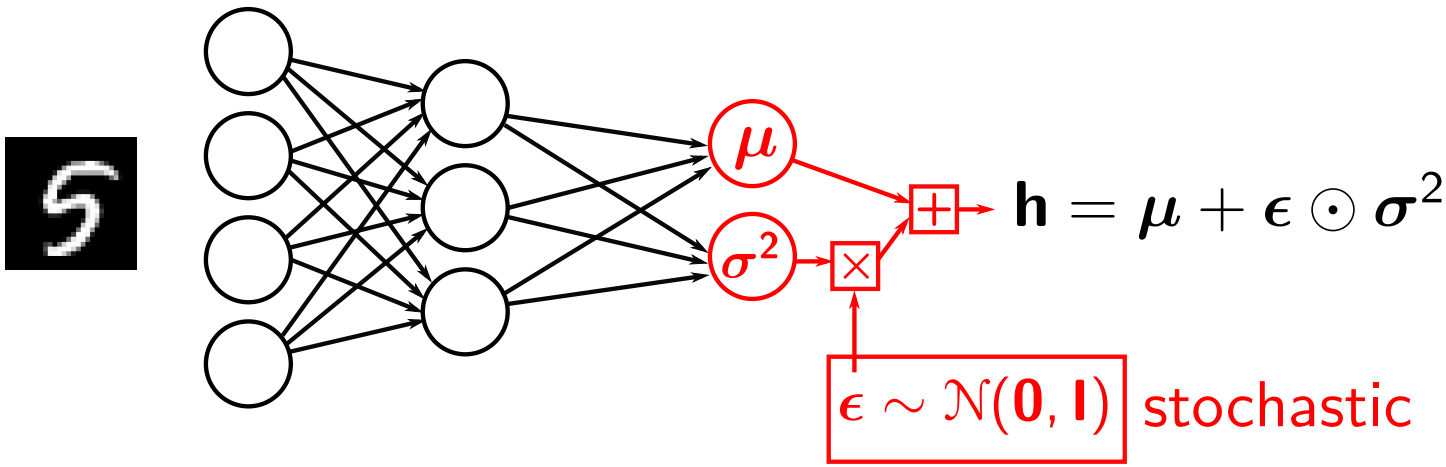

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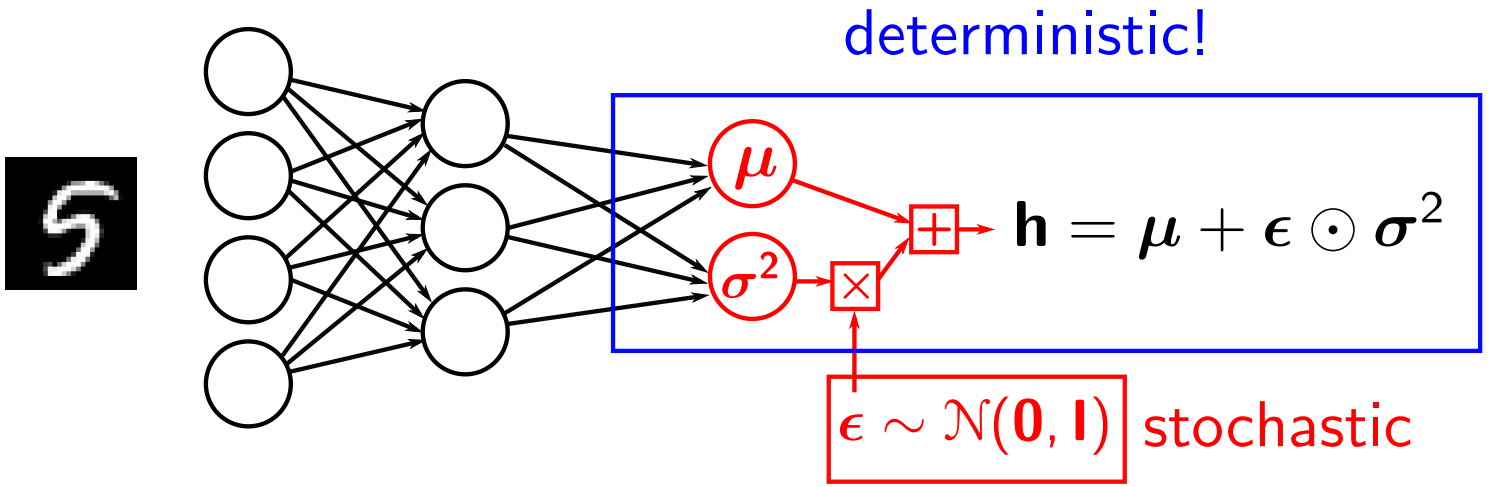
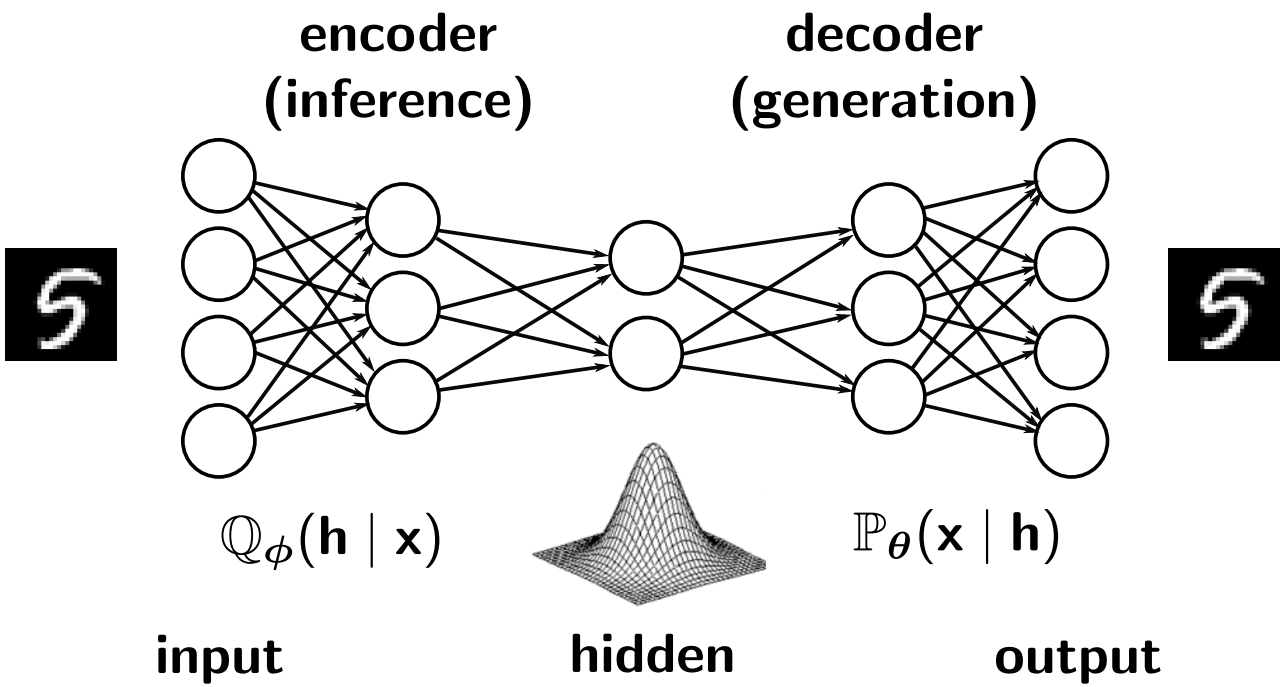


Variational Auto-Encoders (Kingma and Welling, 2013)



- Decoder computes $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{h})$ and $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{h})$
- Encoder computes $\mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) = \mathcal{N}(\boldsymbol{h}; \boldsymbol{\mu}_{\boldsymbol{\phi}}(\boldsymbol{x}), \boldsymbol{\sigma}^2_{\boldsymbol{\phi}}(\boldsymbol{x}))$
- Loss function: ELBO.

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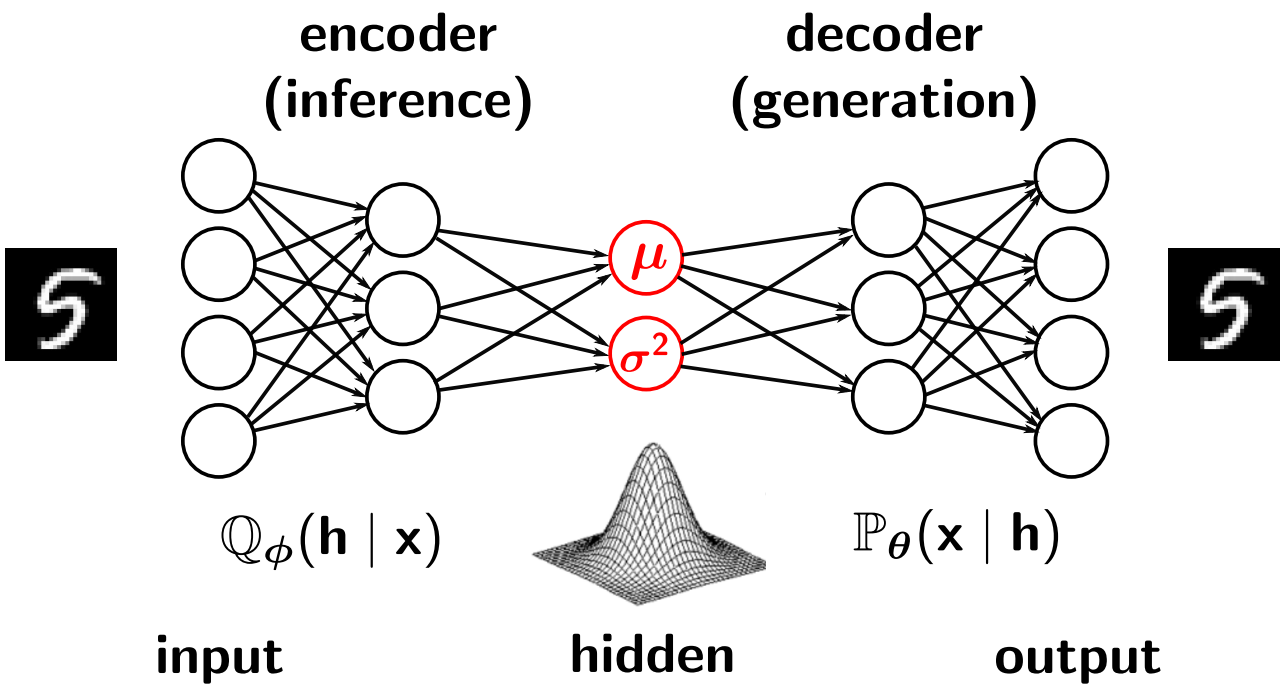

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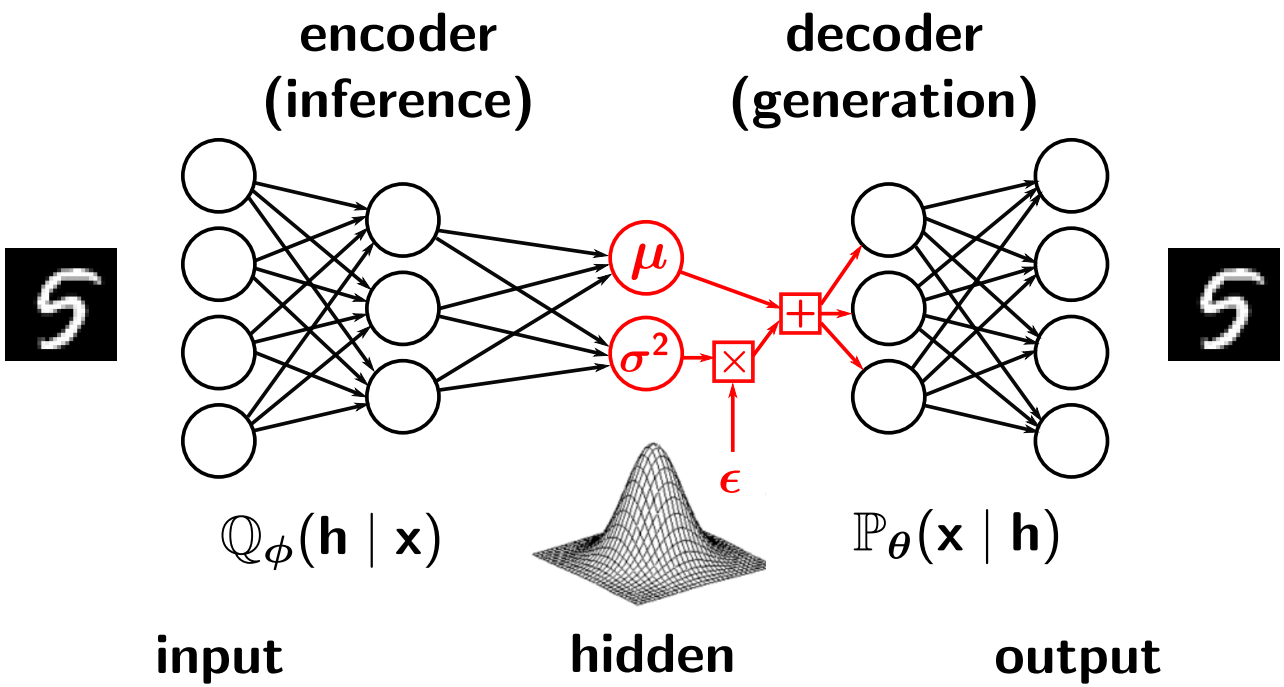

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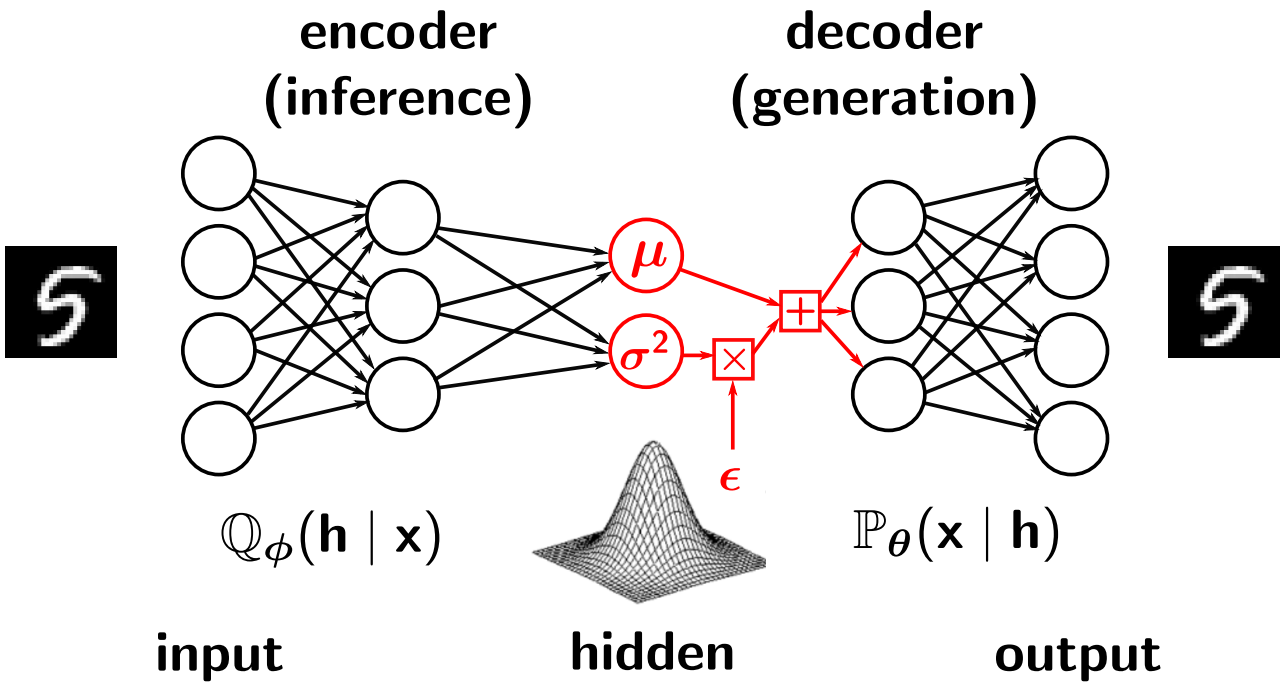
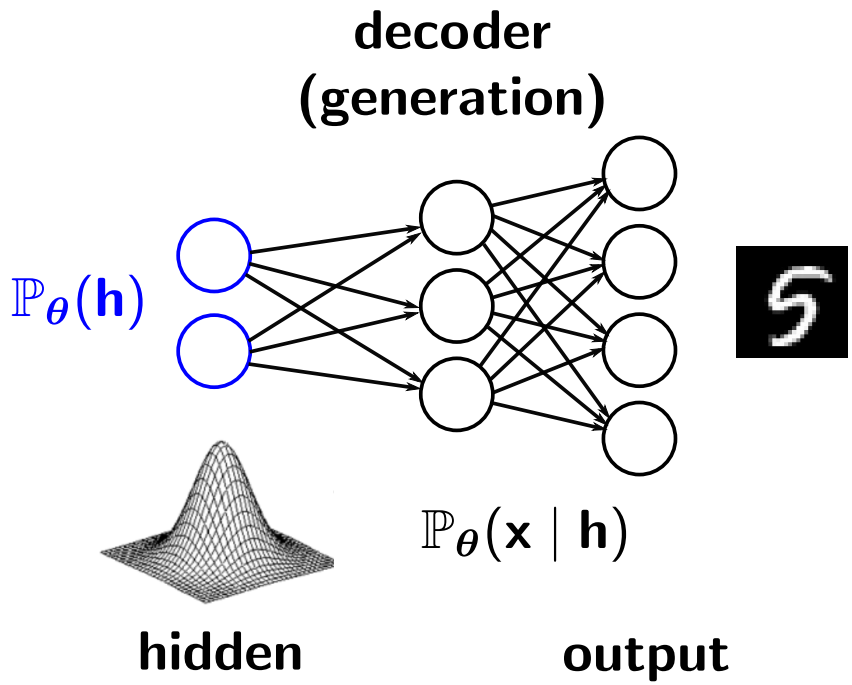
Summing Up: VAEs at Training Time



Summing Up: VAEs at Test Time



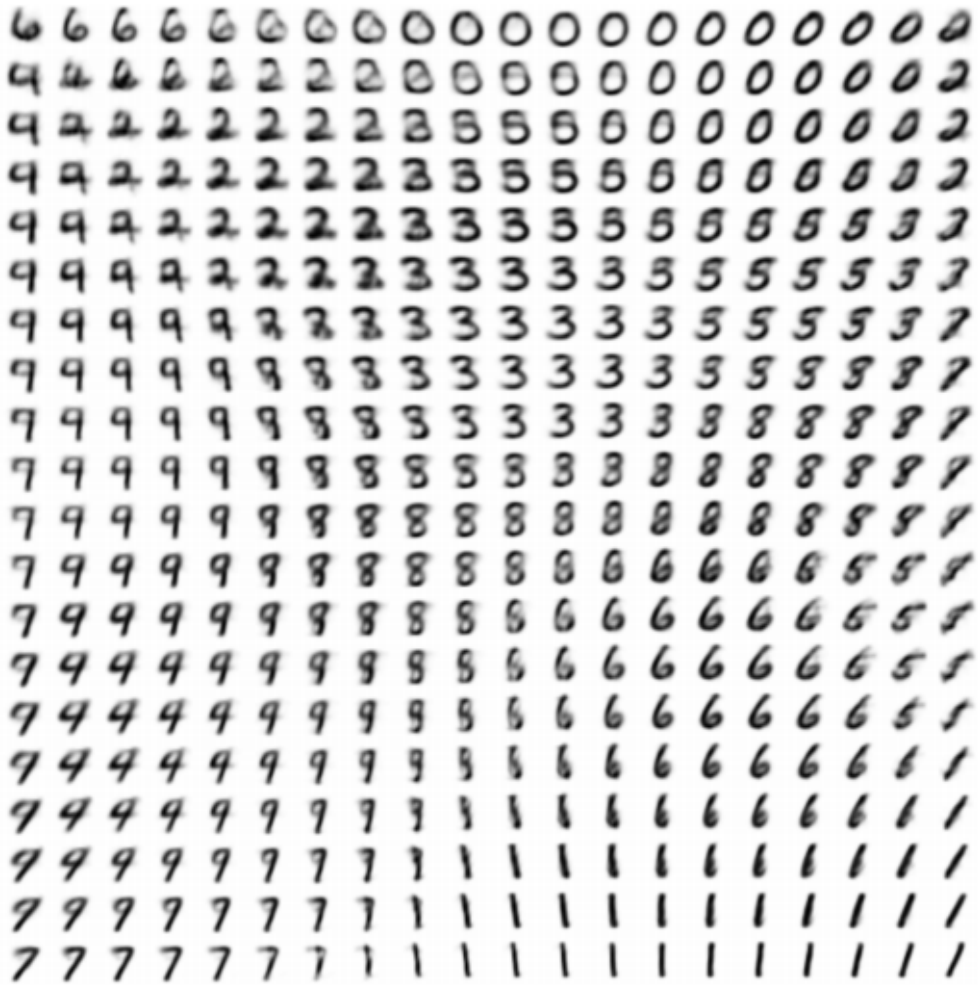
What is the Latent Variable Representing?

- Nice property of VAE: simultaneously training a parametric encoder in combination with a generator network forces the model to learn a predictable coordinate system that the encoder can capture.
- This makes it an excellent manifold learning algorithm.
- Example: the algorithm discovered two independent factors of variation present in images of faces: angle of rotation and emotional expression.

What is the Latent Variable Representing?

From Kingma and Welling (2013).

What is the Latent Variable Representing?



(b) Learned MNIST manifold

From Kingma and Welling (2013).

Issues with VAEs

- Posterior collapse: if the generative part is strong, the model may learn to ignore the latent variables:

$$\begin{aligned} \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{h}) &\approx \mathbb{P}(\boldsymbol{x}) \\ \mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) &\approx \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{h}). \end{aligned}$$

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- Can be mitigated with a few tricks:
  - Decrease/anneal the weight of $KL(\mathbb{Q}_{\boldsymbol{\phi}}(\boldsymbol{h} \mid \boldsymbol{x}) \| \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{h}))$ in the ELBO objective
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  - Combine stochastic and amortized inference.
- In general, reporting both reconstruction loss and the KL term is needed to be able to tell if the model makes use of the latent variables.

Examples of Deep Generative Models

- Auto-Regressive Networks ✓
- Restricted Boltzmann Machines ✓
- Deep Belief Networks
- Deep Boltzmann Machines
- Gaussian-Bernoulli RBMs
- Convolutional Boltzmann Machines
- Sigmoid Belief Nets
- Variational Auto-Encoders ✓
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Why Maximum Likelihood?

- All models discussed aim to maximize the likelihood (evidence) $\mathbb{P}(\boldsymbol{x})$
- In fact, since this is intractable, they maximize a lower bound (ELBO)
- But if we want to build a generator, is this really the best criterion?
- Maximum likelihood tends to produce blurry images

Generative Adversarial Networks (GANs) (Goodfellow et al., 2014)

- **Key idea:**
  - keep the generation network $G = \{\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{h}), \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x} \mid \boldsymbol{h})\}$
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- This is like a Turing test: distinguish artificial from real.

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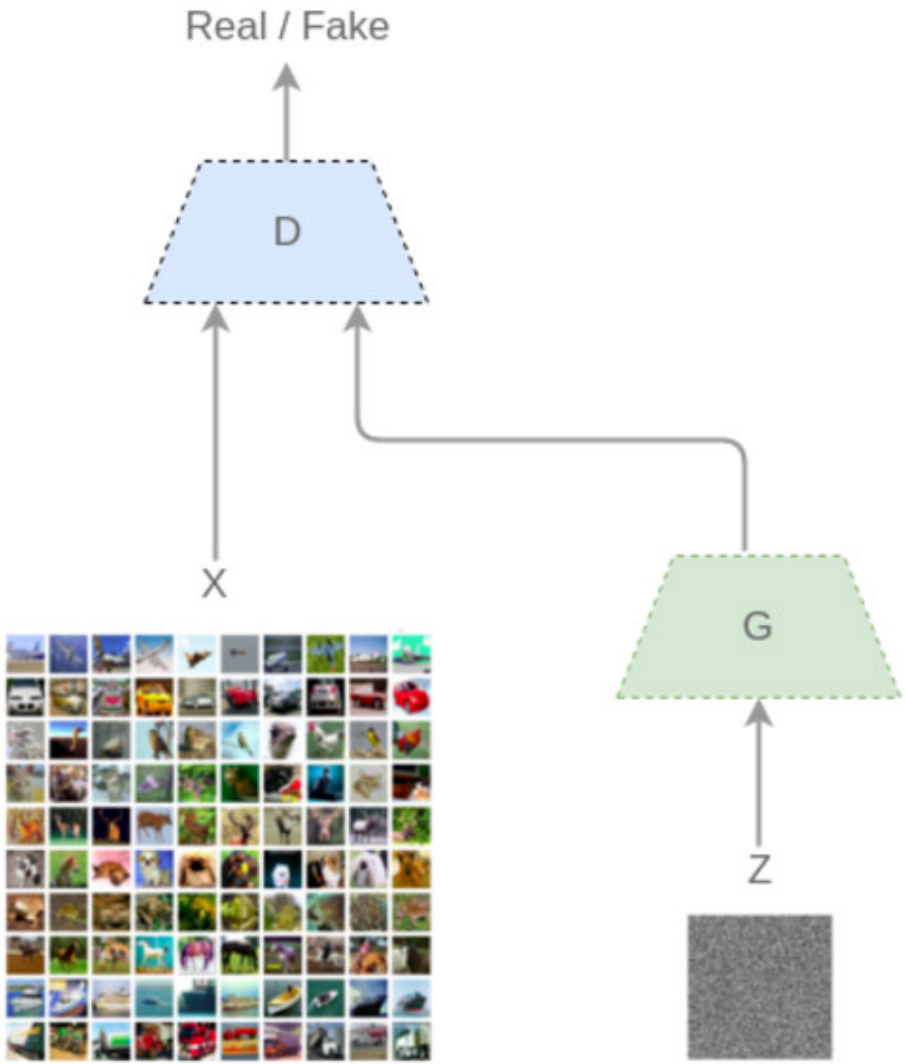

Minimax Game

- Saddle point problem:

$$\min_G \max_D V(D, G) = \mathbb{E}_{\mathbb{P}_{\text{data}}(\boldsymbol{x})}[\log D(\boldsymbol{x})] + \mathbb{E}_{\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{h})}[\log(1 - D(G(\boldsymbol{h})))].$$

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- The optimal discriminator (intractable to compute) is:

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- Given $D^\star(\boldsymbol{x})$, the optimal generator $G^\star(\boldsymbol{x})$ minimizes the Jensen-Shannon divergence between $\mathbb{P}_{\text{data}}(\boldsymbol{x})$ and $\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x})$:

$$JS(\mathbb{P}_{\text{data}}(\boldsymbol{x}), \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x})) = \frac{1}{2} KL\left(\mathbb{P}_{\text{data}}(\boldsymbol{x}) \| \bar{\mathbb{P}}(\boldsymbol{x})\right) + \frac{1}{2} KL\left(\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x}) \| \bar{\mathbb{P}}(\boldsymbol{x})\right),$$

where $\bar{\mathbb{P}}(\boldsymbol{x}) = \frac{\mathbb{P}_{\text{data}}(\boldsymbol{x}) + \mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{x})}{2}$.

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- Several variants and schedules have been proposed.
- Caveats:
  - no convergence guarantees
  - optimization in GANs is often difficult

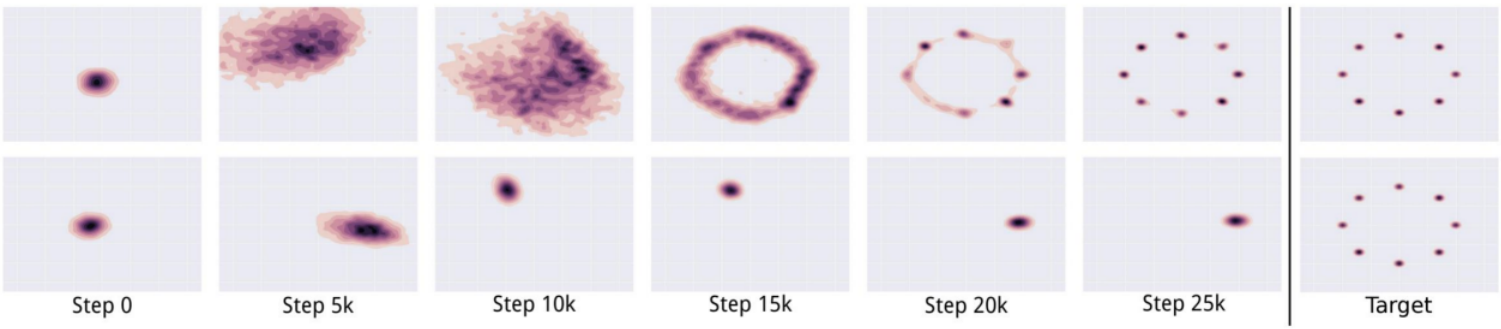
Images Generated by GANs

(https://tryolabs.com/blog/2016/12/06/major-advancements-deep-learning-2016/)

Mode Collapse

$$\min_G \max_D V(D, G) \neq \max_D \min_G V(D, G).$$

- G in inner loop: place all mass on most likely point



(From Metz et al. (2016))

- What prevents the generator from always picking the same example?
- The top row finds all the modes, the bottom finds just one mode.

Mode Collapse

- GANs often seem to collapse to far fewer modes than the model can represent
- This causes low output diversity.
- How to mitigate mode collapse?
- One strategy: minibatch (Salimans et al., 2016)
  - Let the discriminator make a decision by comparing an example to a whole minibatch of fake/real examples
  - Discriminator can now consider diversity.

Wasserstein GANs (WGANs)

- Instead of optimizing the Jensen-Shannon divergence, optimize instead:

$$\min_G \max_D V(D,G) \quad = \quad \mathbb{E}_{\boldsymbol{x}\sim\mathbb{P}_{\text{data}}(\boldsymbol{x})}[D(\boldsymbol{x})] - \mathbb{E}_{\boldsymbol{h}\sim\mathbb{P}_{\boldsymbol{\theta}}(\boldsymbol{h})}[D(G(\boldsymbol{h}))].$$

- This is related to the Wasserstein distance (also called Earth mover's distance).

- A technical condition is that ∇D is bounded; in practice this is ensured with gradient clipping.

- This improves stability and mitigates the mode collapse problem.

Pros and Cons of GANs

Advantages:

- They currently generate the sharpest images
- They are cheap to train (since no statistical inference is required), and only back-propogation is needed to obtain gradients

Disadvantages:

- GANs are difficult to optimize due to unstable training dynamics.
- No statistical inference can be done with them.

Still Improving...

Ian Goodfellow
@goodfellow_ian

Follow

4 years of GAN progress (source: eff.org/files/2018/02/ …)

2014

2015

2016

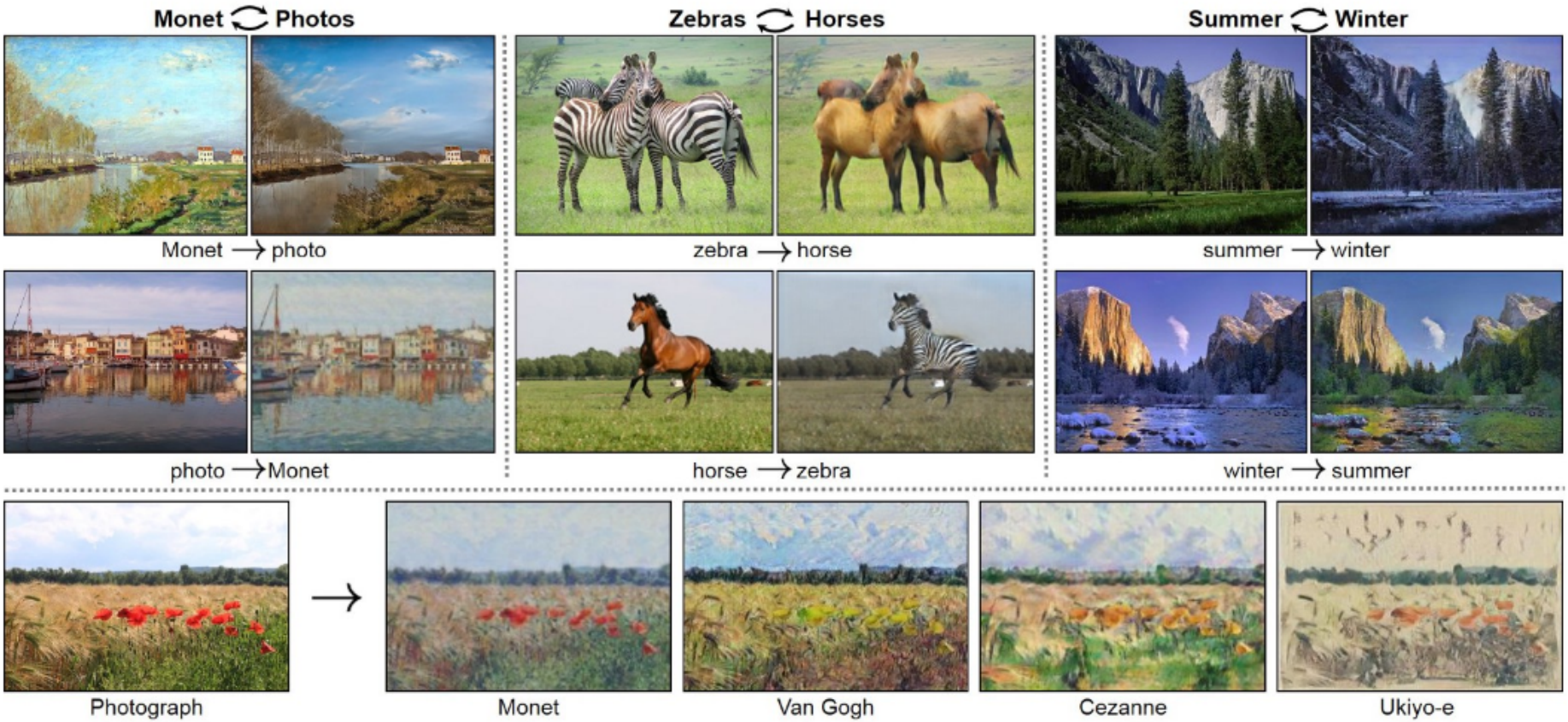
2017

7:26 PM - 2 Mar 2018

Some Extensions of GANs

- Augmenting GANs with an inference network (Dumoulin et al., 2016; Donahue et al., 2016)
- Domain adversarial training for domain adaptation (Ganin et al., 2016)
- Conditional GANs and semi-supervised GANs (Salimans et al., 2016)
- CycleGAN (Zhu et al., 2017): "translate" images from a source domain $\mathcal{X}$ to a target domain $\mathcal{Y}$ without paired examples. Use two generators $G : \mathcal{Y} \to \mathcal{X}$ and $F : \mathcal{X} \to \mathcal{Y}$ and introduce a **cycle consistency loss** to push $F(G(\boldsymbol{y})) \approx \boldsymbol{y}$ and $G(F(\boldsymbol{x})) \approx \boldsymbol{x}$.

Image-to-Image Translation w/ CycleGAN (Zhu et al., 2017)



(https://junyanz.github.io/CycleGAN)

Failure Cases

(https://junyanz.github.io/CycleGAN)

Evaluation

There is no single compelling way to evaluate a generative model.

- Models with good likelihood can produce bad samples
- Models with good samples can have bad likelihood
- There is no standard way to quantify how good samples are
- For GANs, it is also hard to even estimate the likelihood
- See "A note on the evaluation of generative models," Theis et al. (2015), for a good overview.

Discrete Outputs

To train a GAN, G must be differentiable

But G cannot be differentiable if the output is discrete.

Possible workarounds:

- REINFORCE (Williams, 1992)
- Concrete/Gumbel-softmax distribution (Maddison et al., 2016; Jang et al., 2016)
- Learn distribution over continuous embeddings, decode to discrete

How does this compare with VAEs?

- VAEs have trouble with discrete latent variables (cannot differentiate through the inference network)
- GANs have trouble with discrete output variables (cannot differentiate through the generator network).

Connections to Reinforcement Learning

We can regard the discriminator loss as a reward signal for the generator.

- GANs interpreted as actor-critic (Pfau and Vinyals, 2016)
- GANs as inverse reinforcement learning (Finn et al., 2016)

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Conclusions

- Generative models are useful to model high-dimensional data
- Latent-variable generative models are appealing since they are more compact ("minimum description length" principle)
- Often, computing evidence and posterior distributions is intractable (e.g. Boltzmann machines)
- A common surrogate for maximum likelihood is the evidence lower bound (ELBO)
- Variational auto-encoders optimize the ELBO with amortized VI
- Their main drawback is posterior collapse
- Generative adversarial networks (GANs) are formulated as a game between a generator and a discriminator
- They manage to generate sharp outputs, but suffer from mode collapse and do not return a likelihood score
- Open problem (both VAEs/GANs): how to deal with discrete data?

Thank you!

Questions?

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