EECE 571F: Deep Learning with Structures

Lecture 9: Energy-based Models (EBMs)

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Outline

- Classic EBMs
  - EBMs with Discrete Observable Variables and Discrete Latent Variables: RBMs
  - Inference: Gibbs Sampling
  - Learning: Contrastive Divergence
  - EBMs with Continuous Observable Variables and Discrete Latent Variables : GRBMs
- Modern EBMs
  - EBMs with Learnable Energy Functions
  - Inference: Langevin Monte Carlo (LMC)
  - Learning: Contrastive Divergence

Energy-based Models (EBMs)

EBMs are a class of generative models, originated from statistical physics (e.g., statistical mechanics and thermodynamics).

Image Credit: [1]

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It originates from Ludwig Boltzmann and his famous distribution (a.k.a., Boltzmann distribution):

$$p(X) \propto \exp\left(-\frac{E(X)}{kT}\right)$$

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Energy of the system

$$p(X) \propto \exp\left(-\frac{E(X)}{kT}\right)$$

Boltzmann Constant

Temperature

Image Credit: [1]

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Discrete Observable and Latent Variables

EBMs with both discrete observable and latent variables are extensively studied in the literature, e.g., Boltzmann Machines (BMs) [2,3] and Restricted Boltzmann Machines (RBMs) [4,5].

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Therefore, let us start with RBMs!

Restricted Boltzmann Machines

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- Energy function $E_\theta(x, h) = -a^\top x - b^\top h - x^\top W h$

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Partition function / Normalization constant

Restricted Boltzmann Machines

Binary visible units (observable variables) x, binary hidden units (latent variables) h

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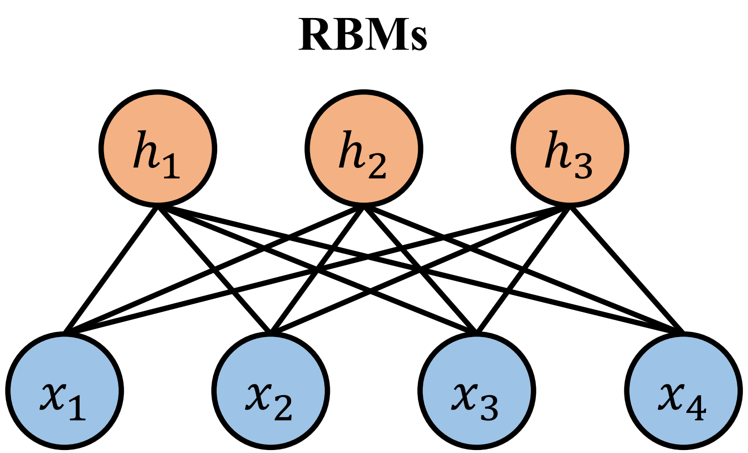
Bipartite Graphical Model



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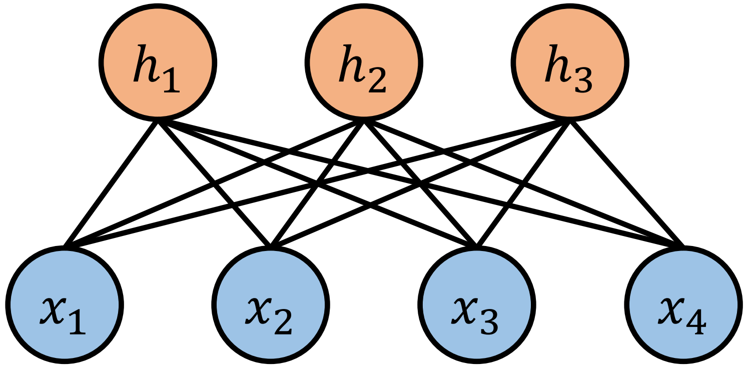
Bipartite Graphical Model

RBMs



- Probability distribution

$$p_\theta(x, h) = \frac{1}{Z} \exp\left(-E_\theta(x, h)\right)$$

- Bipartite graph structure implies conditional independence

$$p(h|x) = \prod\nolimits_j p(h_j|x)$$

$$p(x|h) = \prod\nolimits_i p(x_i|h)$$

Independent
Bernoulli distributions

Restricted Boltzmann Machines

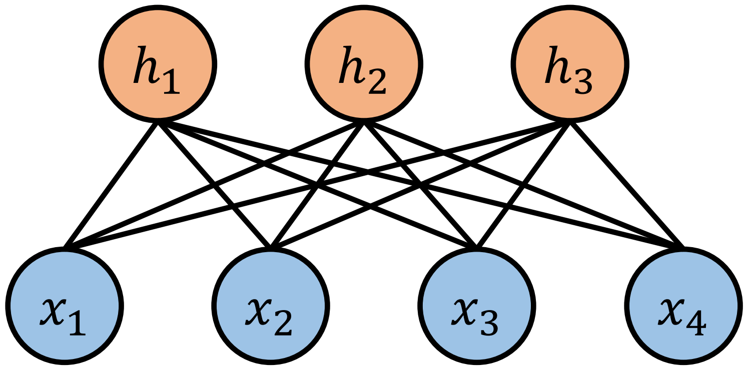
- Bipartite graph structure implies conditional independence

Why?

$$p(h|x) = \prod_j p(h_j|x)$$

$$p(x|h) = \prod_i p(x_i|h)$$

RBMs



Restricted Boltzmann Machines

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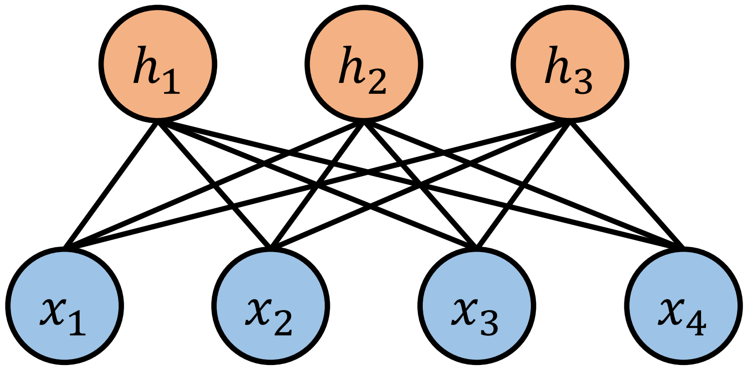
Intuition:

- Observed visible units block the paths among hidden units
- Change of one hidden unit would not affect others

RBMs



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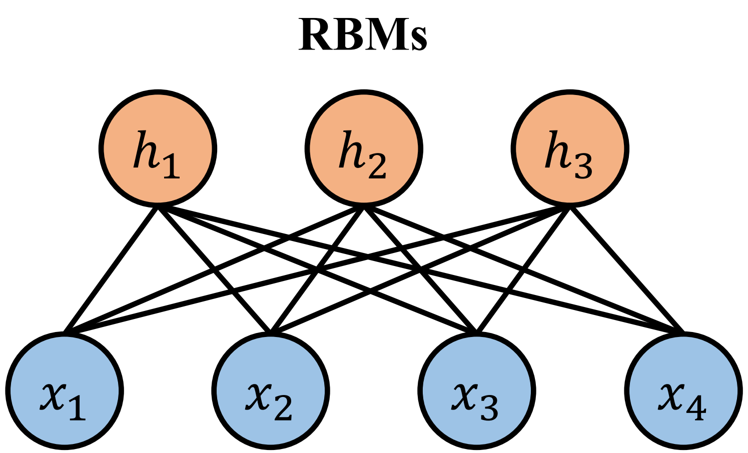

Formally:

$$E_\theta(x, h) = -a^\top x - b^\top h - x^\top W h$$

$$p(x|h = \tilde{h}) \propto \exp\left(-E_\theta(x, h = \tilde{h})\right) \propto \exp\left(-\tilde{a}^\top x\right) = \prod_i \exp\left(-\tilde{a}_i x_i\right)$$

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Restricted Boltzmann Machines

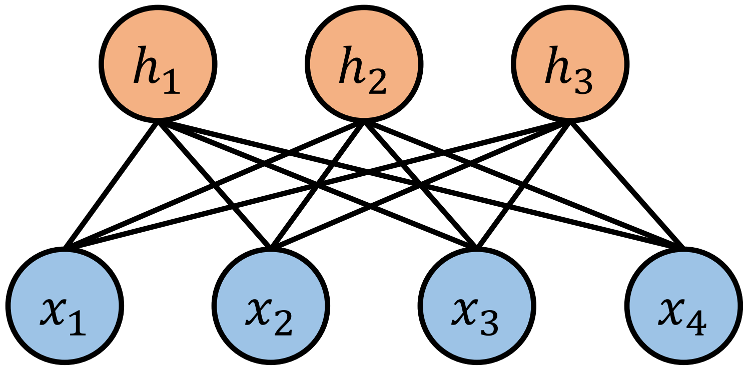
Inference: Computing Marginals $p(x)$ & Maximum A Posterior (MAP) $\arg\max_h p(h|x)$

- MAP is simple for RBMs due to the conditional independence.
- For computing marginals,

$$p(x) = \int \frac{1}{Z} \exp\left(-E(x,h)\right) dh$$

Intractable!

RBMs



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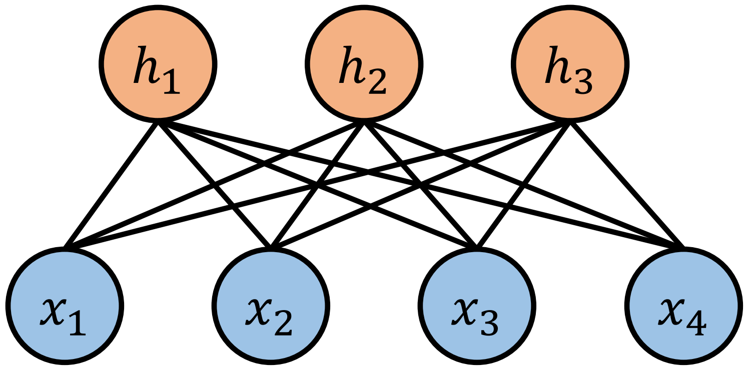

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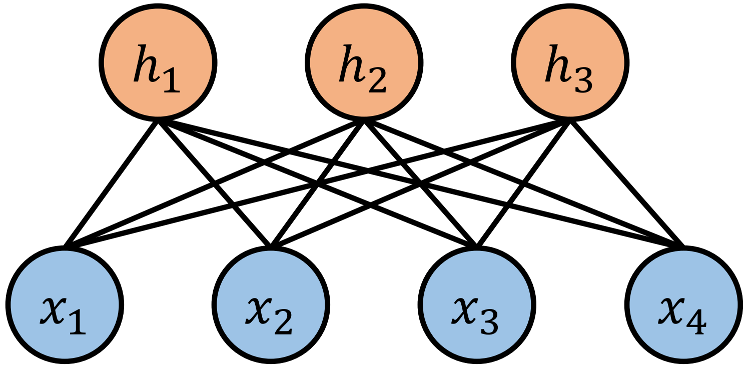
In general, Gibbs sampler draw samples from $p(x_1, x_2, \ldots, x_n)$ by iteratively sampling from the conditional distributions.

Given initial sample $(x_1^{(0)}, x_2^{(0)}, \ldots, x_n^{(0)})$
for $t = 1, \ldots, T$ **do**
  for $i = 1, \ldots, n$ **do**
    $x_i^{(t)} \sim p\left(x_i | x_1 = x_1^{(t)}, \ldots, x_{i-1} = x_{i-1}^{(t)}, x_{i+1} = x_{i+1}^{(t-1)}, \ldots, x_n = x_n^{(t-1)}\right)$
  end
end
Return $(x_1^{(T)}, x_2^{(T)}, \ldots, x_n^{(T)})$

RBMs



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In RBMs, we do not iterative over individual variables. Instead, we do block-Gibbs sampling, i.e., sampling a block of variables conditioned on the other block.

Given initial sample $(x^{(0)}, h^{(0)})$
for $t = 1, \ldots, T$ **do**
  $h^{(t)} \sim p\left(h|x = x^{(t-1)}\right)$
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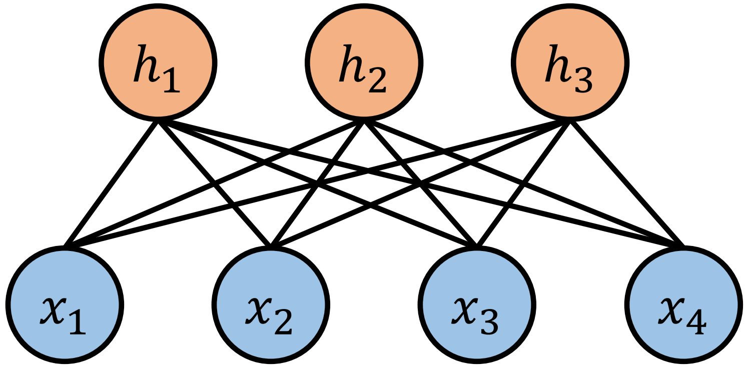
RBMs



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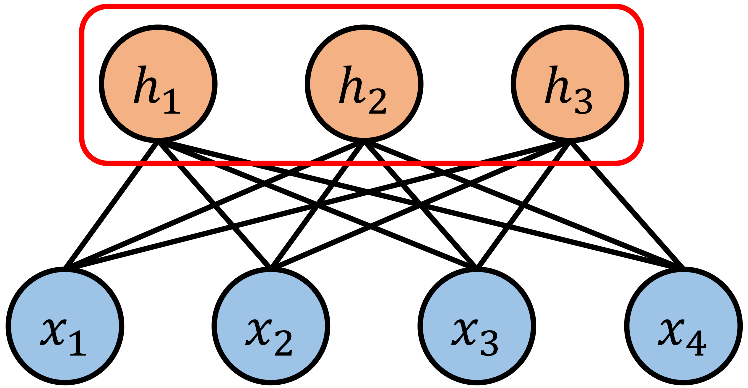

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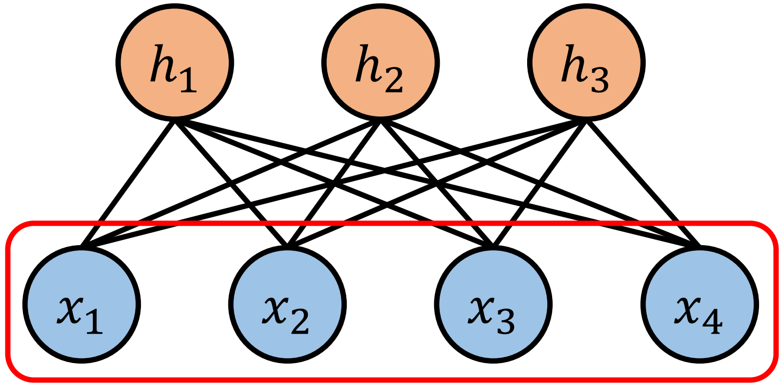

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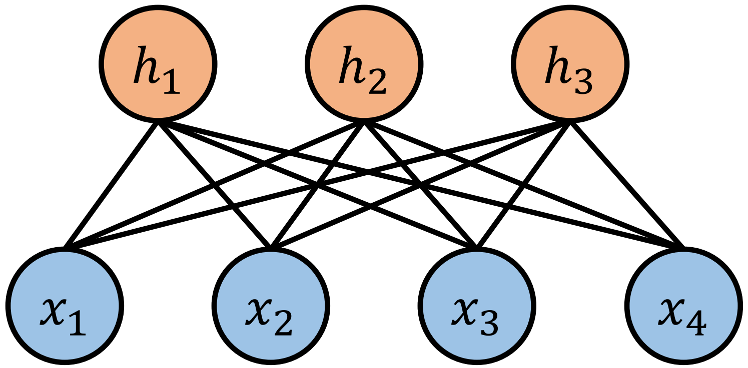

The block-Gibbs shares the same convergence guarantee as Gibbs (due to conditional independence) but is more efficient due to parallel sampling!

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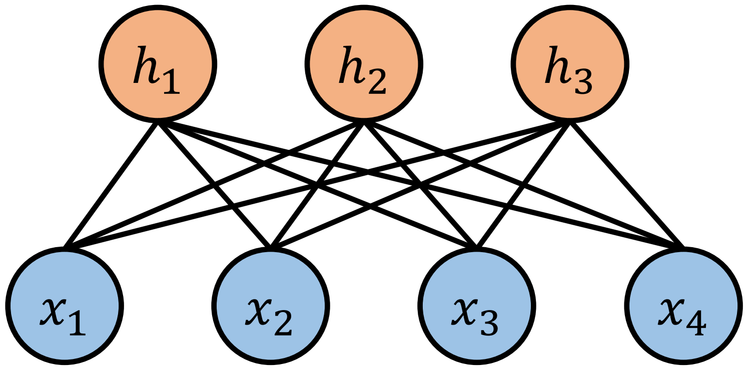
Learning RBMs

Learning: Maximum Likelihood

$$\max_{\theta} \quad \log p_{\theta}(x)$$

RBMs



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$$\max_{\theta} \quad \log p_\theta(x) = \log \int p_\theta(x,h)dh$$
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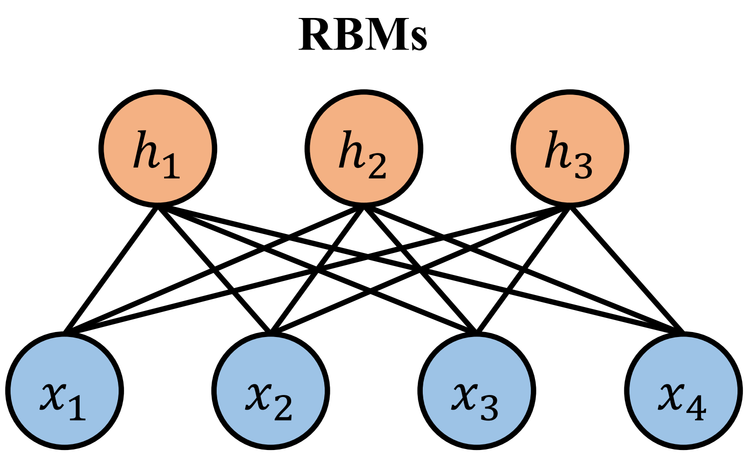
$$= \log \int \exp\left(-E_\theta(x,h) - \log Z\right) dh$$



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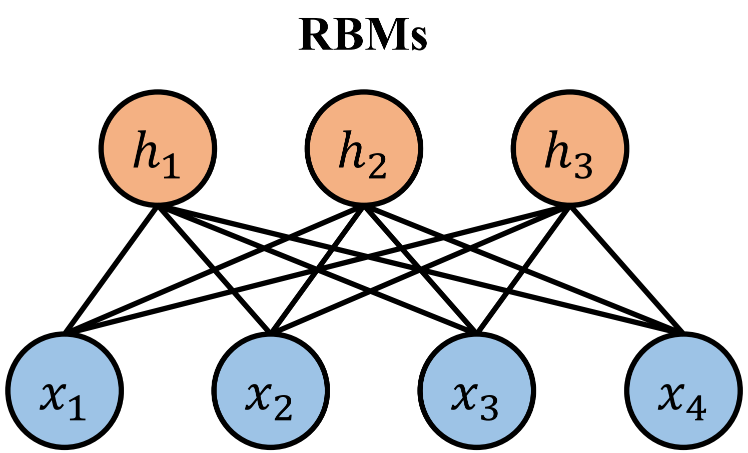
$$= \log \int \exp \log p_\theta(x,h)dh$$

$$= \log \int \exp\left(-E_\theta(x,h) - \log \boxed{Z}\right) dh$$

Intractable!

$$Z = \int \int \exp\left(-E_\theta(x,h)\right) dx dh$$



Stochastic Approximated Gradient

Learning: Maximum Likelihood

$$
\begin{aligned}
\frac{\partial \log p_\theta(x)}{\partial \theta} &= \frac{1}{p_\theta(x)} \frac{\partial p_\theta(x)}{\partial \theta} \\
&= \frac{1}{p_\theta(x)} \frac{\partial \int p_\theta(x,h) dh}{\partial \theta} \\
&= \frac{1}{p_\theta(x)} \int \frac{\partial p_\theta(x,h)}{\partial \theta} dh \\
&= \frac{1}{p_\theta(x)} \int \frac{\partial \frac{1}{Z} \exp\left(-E_\theta(x,h)\right)}{\partial \theta} dh \\
&= \frac{1}{p_\theta(x)} \int \frac{\left(-\frac{\partial E_\theta(x,h)}{\partial \theta}\right) \exp\left(-E_\theta(x,h)\right) Z - \frac{\partial Z}{\partial \theta} \exp\left(-E_\theta(x,h)\right)}{Z^2} dh
\end{aligned}
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Learning: Maximum Likelihood

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&= \frac{1}{p_\theta(x)} \int \left(-\frac{\partial E_\theta(x,h)}{\partial \theta}\right) p_\theta(x,h) dh - \frac{1}{p_\theta(x)} \int \frac{1}{Z} \frac{\partial Z}{\partial \theta} p_\theta(x,h) dh \\
&= \int \left(-\frac{\partial E_\theta(x,h)}{\partial \theta}\right) p_\theta(h|x) dh - \int \frac{1}{Z} \frac{\partial Z}{\partial \theta} p_\theta(h|x) dh \\
&= \int \left(-\frac{\partial E_\theta(x,h)}{\partial \theta}\right) p_\theta(h|x) dh - \frac{1}{Z} \frac{\partial Z}{\partial \theta} \\
&= \int \left(-\frac{\partial E_\theta(x,h)}{\partial \theta}\right) p_\theta(h|x) dh - \frac{1}{Z} \frac{\partial \int \int \exp\left(-E_\theta(x,h)\right) dx dh}{\partial \theta} \\
&= \int \left(-\frac{\partial E_\theta(x,h)}{\partial \theta}\right) p_\theta(h|x) dh - \int \int \left(-\frac{\partial E_\theta(x,h)}{\partial \theta}\right) p_\theta(x,h) dx dh
\end{aligned}
$$

Stochastic Approximated Gradient

Learning: Maximum Likelihood

$$\begin{aligned}\frac{\partial \log p_\theta(x)}{\partial \theta} &= \int \left(-\frac{\partial E_\theta(x,h)}{\partial \theta}\right) p_\theta(h|x)dh - \int\int \left(-\frac{\partial E_\theta(x,h)}{\partial \theta}\right) p_\theta(x,h)dxdh \\ &= \mathbb{E}_{p_\theta(h|x)}\left[-\frac{\partial E_\theta(x,h)}{\partial \theta}\right] - \mathbb{E}_{p_\theta(h,x)}\left[-\frac{\partial E_\theta(x,h)}{\partial \theta}\right]\end{aligned}$$

Stochastic Approximated Gradient

Learning: Maximum Likelihood

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Recall we sample multiple training data and maximize the summed log likelihood of them, which in expectation amounts to:

Stochastic Approximated Gradient

Learning: Maximum Likelihood

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$$\min_\theta \quad \mathrm{KL}\left(p_{\text{data}}(x) \| p_\theta(x)\right) = \int p_{\text{data}}(x)\log p_{\text{data}}(x)dx - \int p_{\text{data}}(x)\log p_\theta(x)dx$$
$$= -\mathcal{H}_{p_{\text{data}}(x)} + \mathrm{CrossEntropy}(p_{\text{data}}(x), p_\theta(x))$$

Stochastic Approximated Gradient

Learning: Maximum Likelihood

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$$= -\mathcal{H}_{p_{\text{data}}(x)} + \mathrm{CrossEntropy}(p_{\text{data}}(x), p_\theta(x))$$

$$\min_\theta \quad \mathrm{CrossEntropy}(p_{\text{data}}(x), p_\theta(x)) \quad \Leftrightarrow \quad \max_\theta \int p_{\text{data}}(x) \log p_\theta(x)dx$$

Maximum Likelihood

Stochastic Approximated Gradient

Learning: Maximum Likelihood

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\begin{aligned}
\frac{\partial \log p_\theta(x)}{\partial \theta} &= \int \left(-\frac{\partial E_\theta(x,h)}{\partial \theta}\right) p_\theta(h|x) dh - \int\int \left(-\frac{\partial E_\theta(x,h)}{\partial \theta}\right) p_\theta(x,h) dx dh \\
&= \mathbb{E}_{p_\theta(h|x)}\left[-\frac{\partial E_\theta(x,h)}{\partial \theta}\right] - \mathbb{E}_{p_\theta(h,x)}\left[-\frac{\partial E_\theta(x,h)}{\partial \theta}\right]
\end{aligned}
$$

Since we care about $\max_\theta \int p_{\text{data}}(x) \log p_\theta(x) dx$

Stochastic Approximated Gradient

Learning: Maximum Likelihood

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Since we care about $\max_\theta \int p_{\text{data}}(x) \log p_\theta(x) dx$

we have the gradient

$$\int p_{\text{data}}(x) \frac{\partial \log p_\theta(x)}{\partial \theta} dx = \mathbb{E}_{p_\theta(h|x)p_{\text{data}}(x)}\left[-\frac{\partial E_\theta(x,h)}{\partial \theta}\right] - \mathbb{E}_{p_\theta(h,x)}\left[-\frac{\partial E_\theta(x,h)}{\partial \theta}\right]$$

Stochastic Approximated Gradient

Learning: Maximum Likelihood

Stochastic Approximated Gradient

$$\int p_{\mathrm{data}}(x)\frac{\partial \log p_\theta(x)}{\partial \theta}dx = \mathbb{E}_{p_\theta(h|x)p_{\mathrm{data}}(x)}\left[-\frac{\partial E_\theta(x,h)}{\partial \theta}\right] - \mathbb{E}_{p_\theta(h,x)}\left[-\frac{\partial E_\theta(x,h)}{\partial \theta}\right]$$

Monte Carlo Estimation!

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Positive Gradient: sample from the data distribution $p_\theta(h|x) p_{\text{data}}(x)$

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If we use finite-step Gibbs sampler, this method is called *Contrastive Divergence* (CD) [6]!

Outline

- Classic EBMs
  - EBMs with Discrete Observable Variables and Discrete Latent Variables: RBMs
  - Inference: Gibbs Sampling
  - Learning: Contrastive Divergence
  - **EBMs with Continuous Observable Variables and Discrete Latent Variables : GRBMs**
- Modern EBMs
  - EBMs with Learnable Energy Functions
  - Inference: Langevin Monte Carlo (LMC)
  - Learning: Contrastive Divergence

Continuous Observable and Discrete Latent Variables

GRBMs: Gaussian-Bernoulli (a.k.a. Gaussian-Binary) Restricted Boltzmann Machines [7]

Continuous visible units (observable variables) $\mathbf{v}$, binary hidden units (latent variables) $\mathbf{h}$

Energy function: $E_\theta(\mathbf{v}, \mathbf{h}) = \frac{1}{2}\left(\frac{\mathbf{v}-\boldsymbol{\mu}}{\boldsymbol{\sigma}}\right)^\top \left(\frac{\mathbf{v}-\boldsymbol{\mu}}{\boldsymbol{\sigma}}\right) - \left(\frac{\mathbf{v}}{\boldsymbol{\sigma}^2}\right)^\top W\mathbf{h} - \mathbf{b}^\top\mathbf{h}$

Gaussian-Bernoulli Restricted Boltzmann Machines

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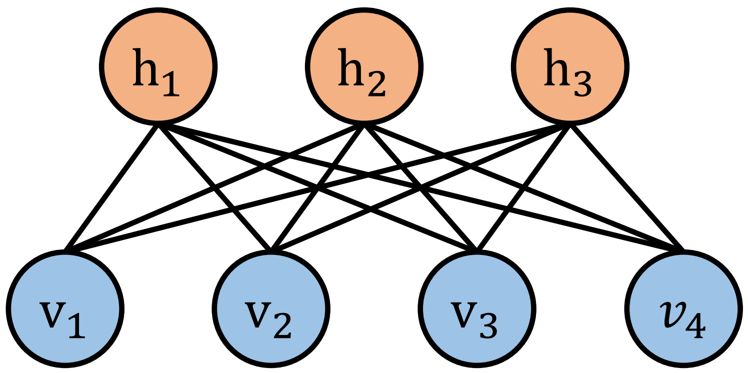
Conditional distributions (conditional independence holds again):

$$p(\mathbf{v}|\mathbf{h}) = \mathcal{N}\left(\mathbf{v}|W\mathbf{h}+\boldsymbol{\mu}, \mathrm{diag}(\boldsymbol{\sigma}^2)\right)$$
$$p(\mathbf{h}_j = 1|\mathbf{v}) = \left[\mathrm{Sigmoid}\left(W^\top \frac{\mathbf{v}}{\boldsymbol{\sigma}^2} + \mathbf{b}\right)\right]_j$$

GRBMs



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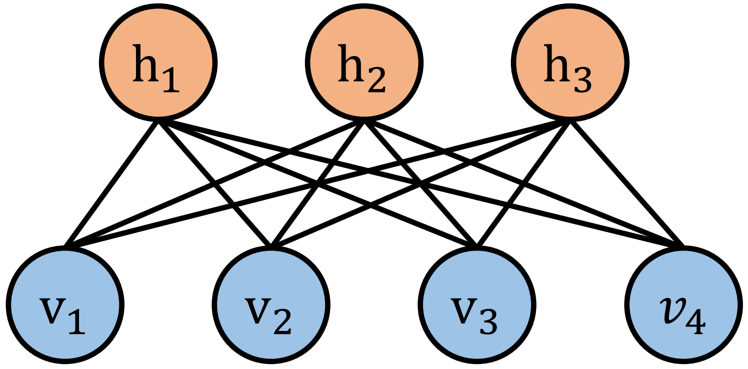
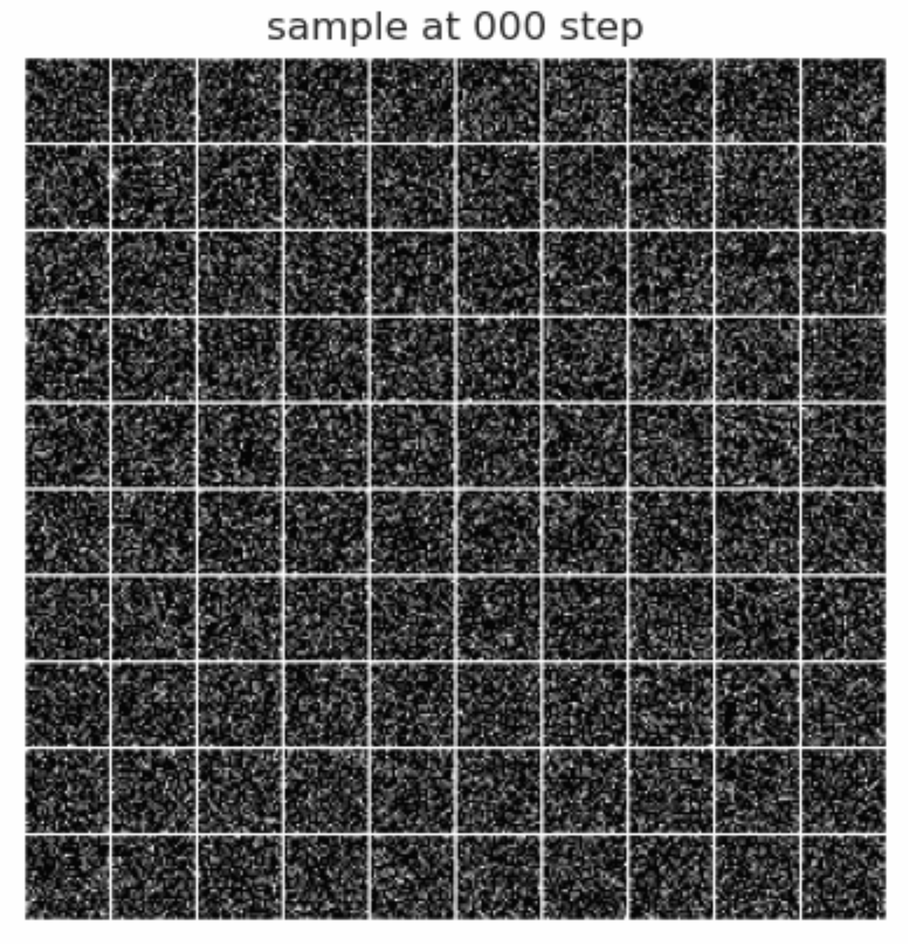


Recent work [8] introduces Gibbs-Langevin sampling, which makes CD-based learning work much better than before!

Gaussian-Bernoulli Restricted Boltzmann Machines

Results of training GRBMs for modelling MNIST Images [8]



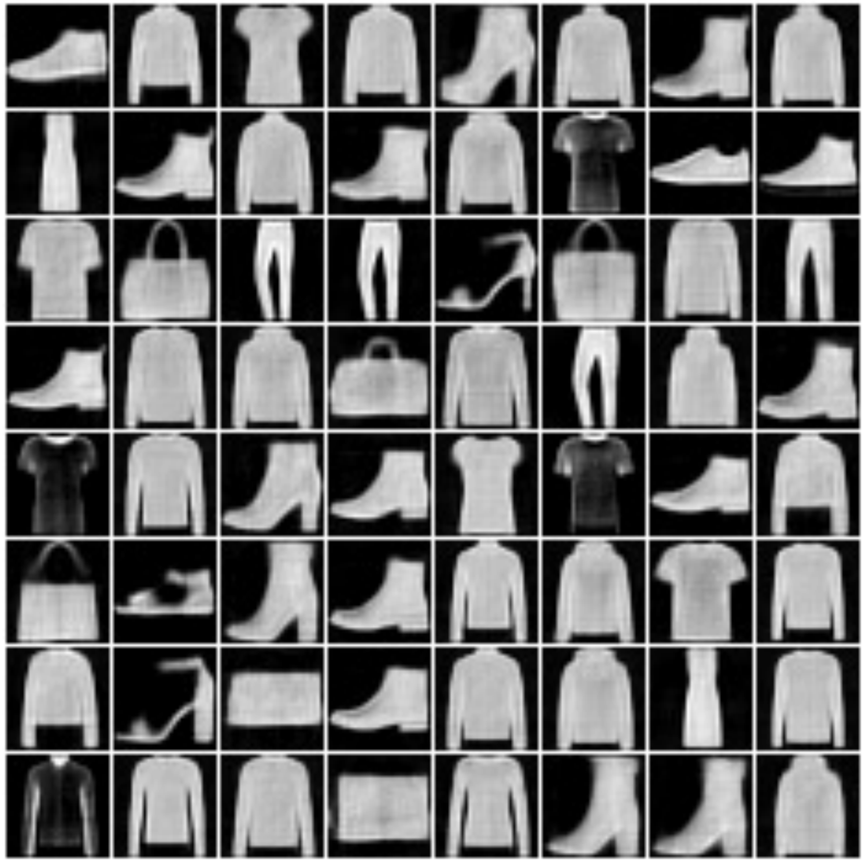
Methods	FID
VAE	16.13
2sVAE (Dai & Wipf, 2019)	12.60
PixelCNN++ (Salimans et al.)	11.38
WGAN (Arjovsky et al., 2017)	10.28
NVAE (Vahdat & Kautz, 2020)	7.93
GRBMs	
Gibbs	47.53
Langevin wo. Adjust	43.80
Langevin w. Adjust	41.24
Gibbs-Langevin wo. Adjust	17.49
Gibbs-Langevin w. Adjust	19.27

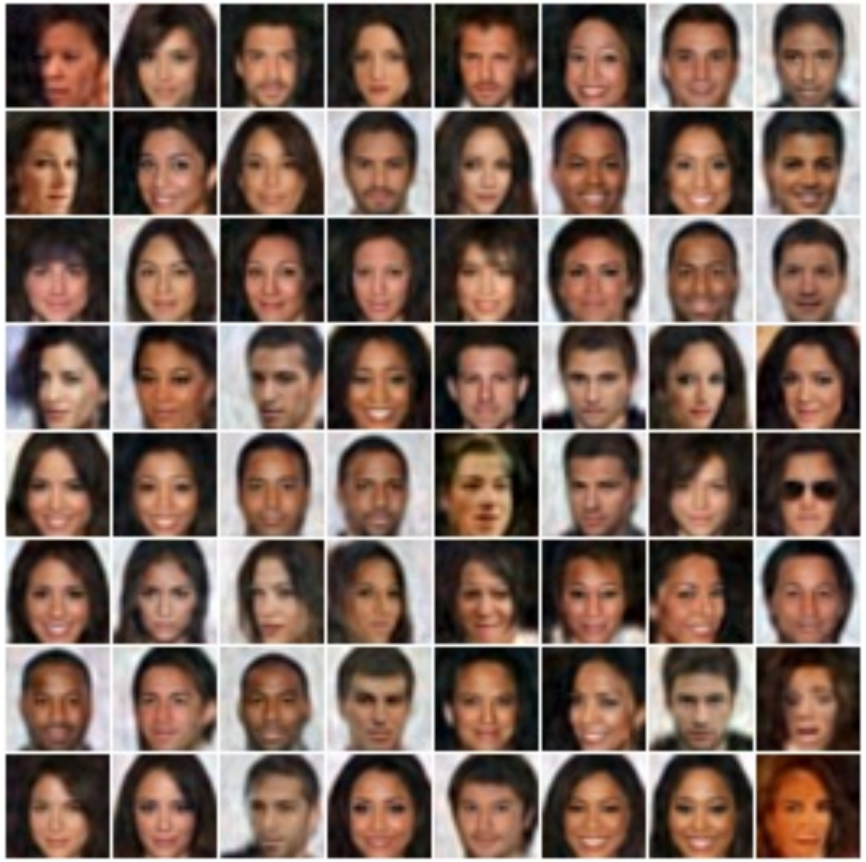
Table 1: Results on MNIST dataset.

Image Credit: [8]

Gaussian-Bernoulli Restricted Boltzmann Machines

Results of training GRBMs for modelling Fashion-MNIST and CelebA-32 Images [8]





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Recall EBMs without latent variables are: $$p_\theta(\mathbf{x}) = \frac{1}{Z} \exp\left(-E_\theta(\mathbf{x})\right)$$

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- It should be expressive enough to capture the complicated unnormalized probability density of data.
- It should be differentiable to enable CD-based learning.

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- It should be expressive enough to capture the complicated unnormalized probability density of data.
- It should be differentiable to enable CD-based learning.

We already have the answer, i.e., deep neural networks!

Deep EBMs

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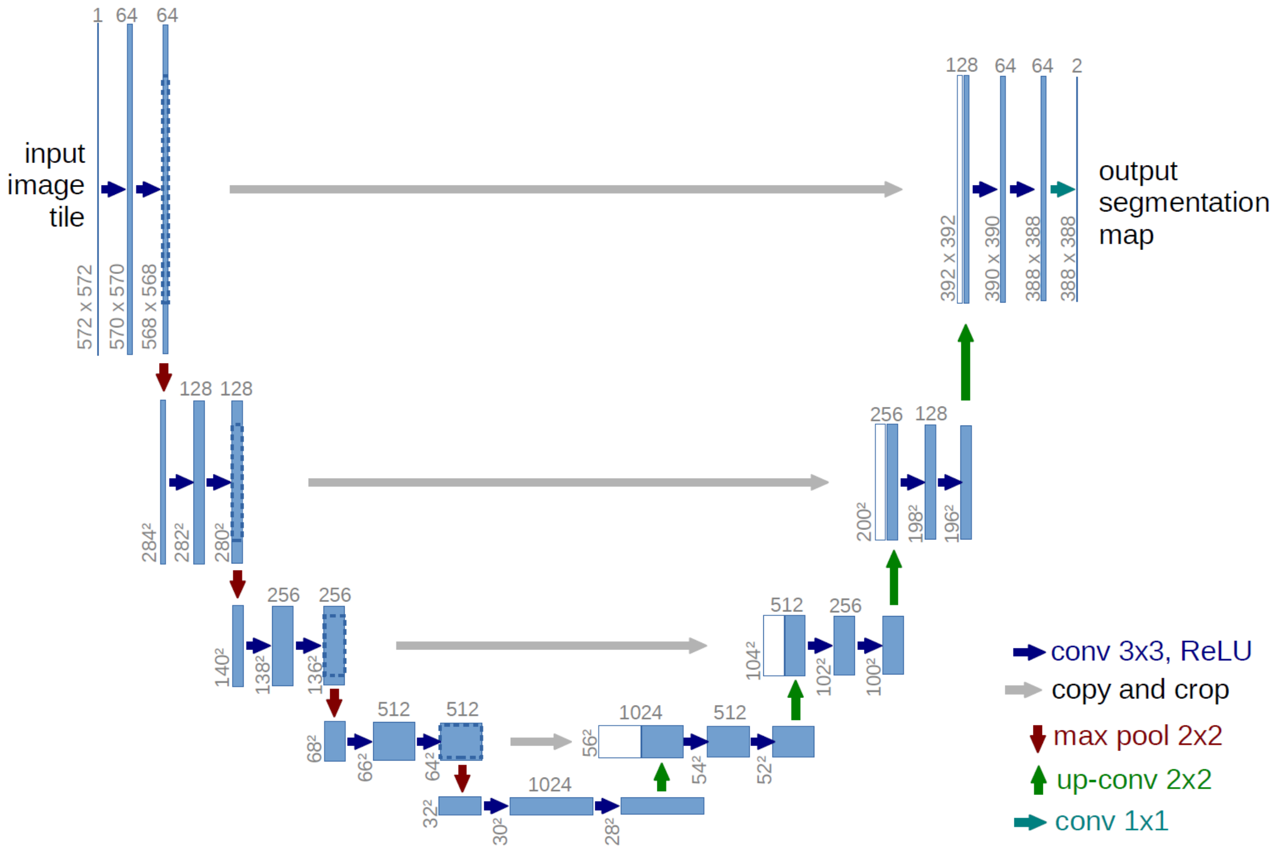
For image generation, U-Net architecture is crucial [9, 10].



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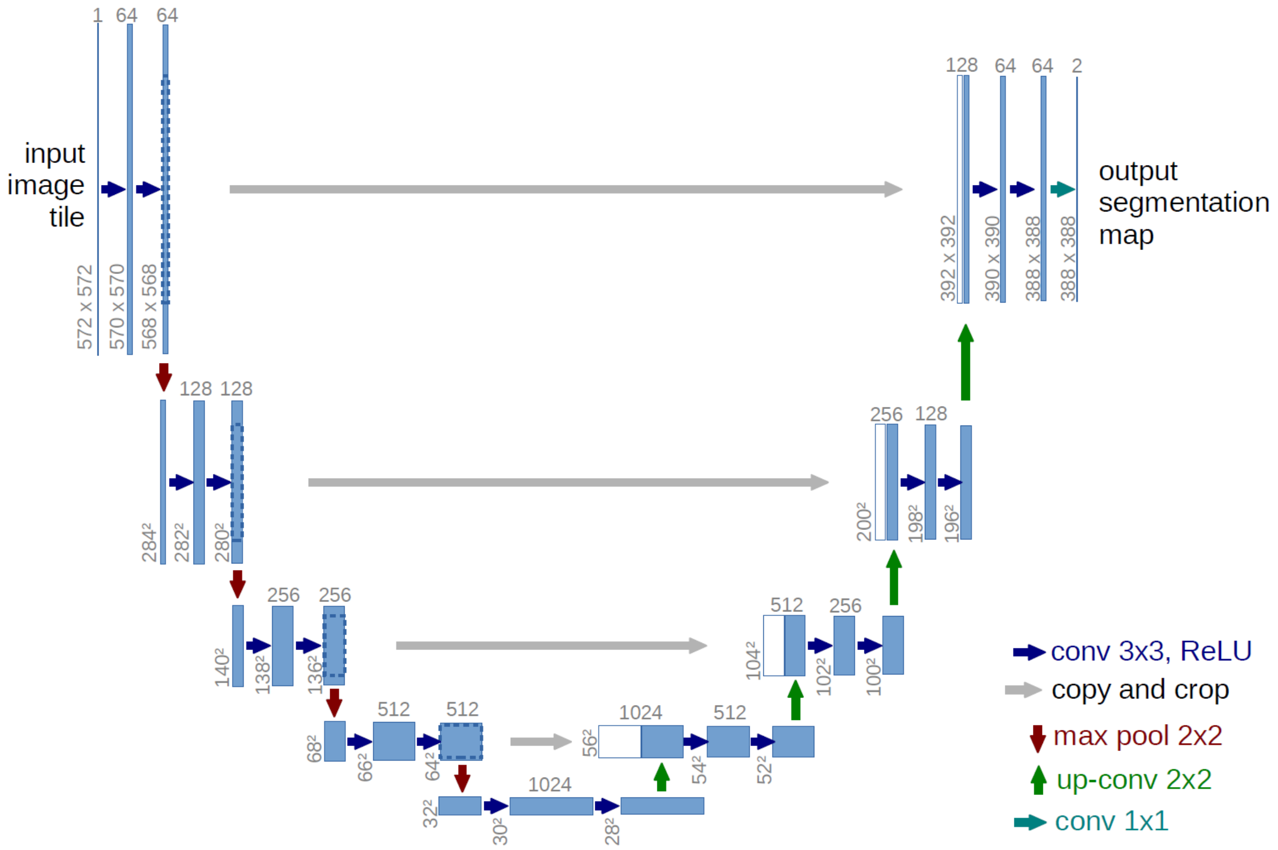

Recall energy is a scalar, we have several design choices:

$$E_\theta(\mathbf{x}) = \mathbf{x}^T f_\theta(\mathbf{x})$$

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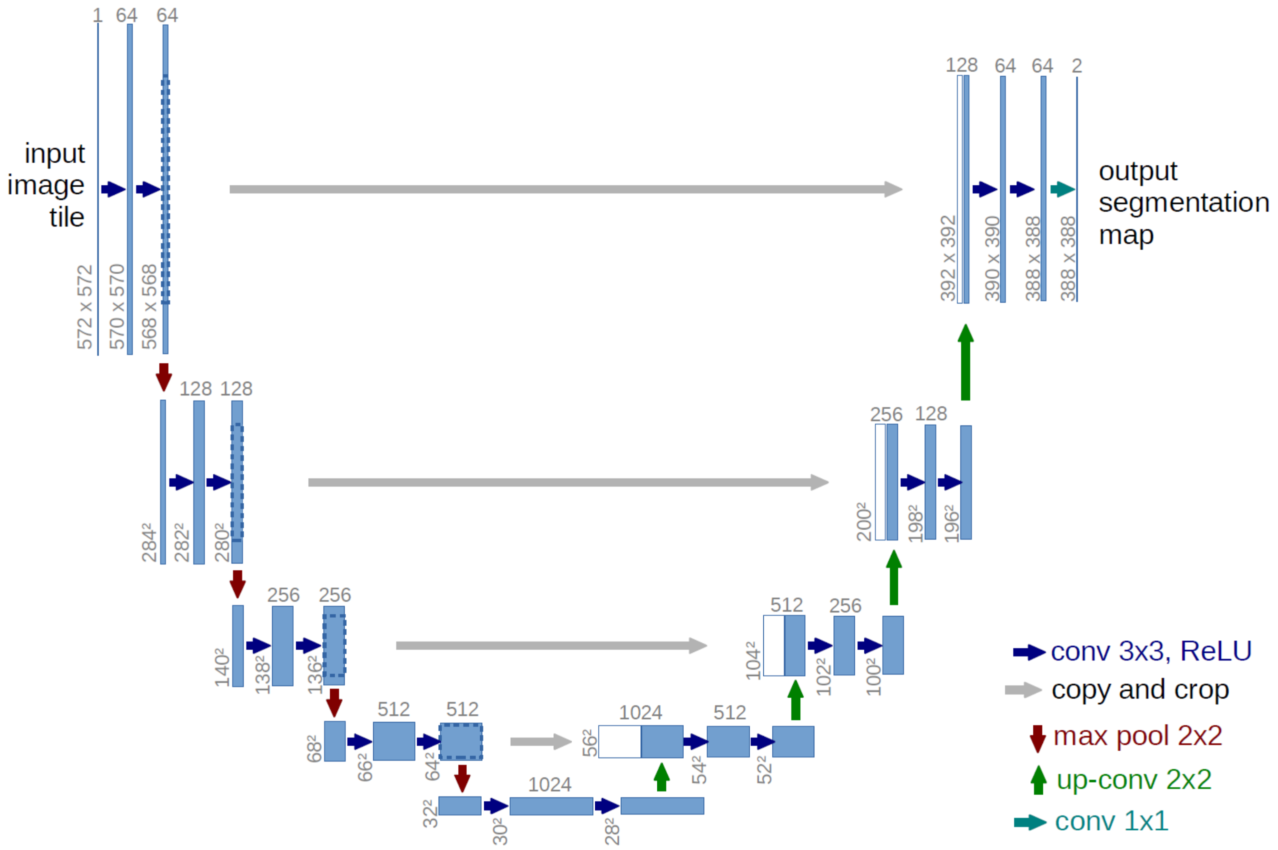

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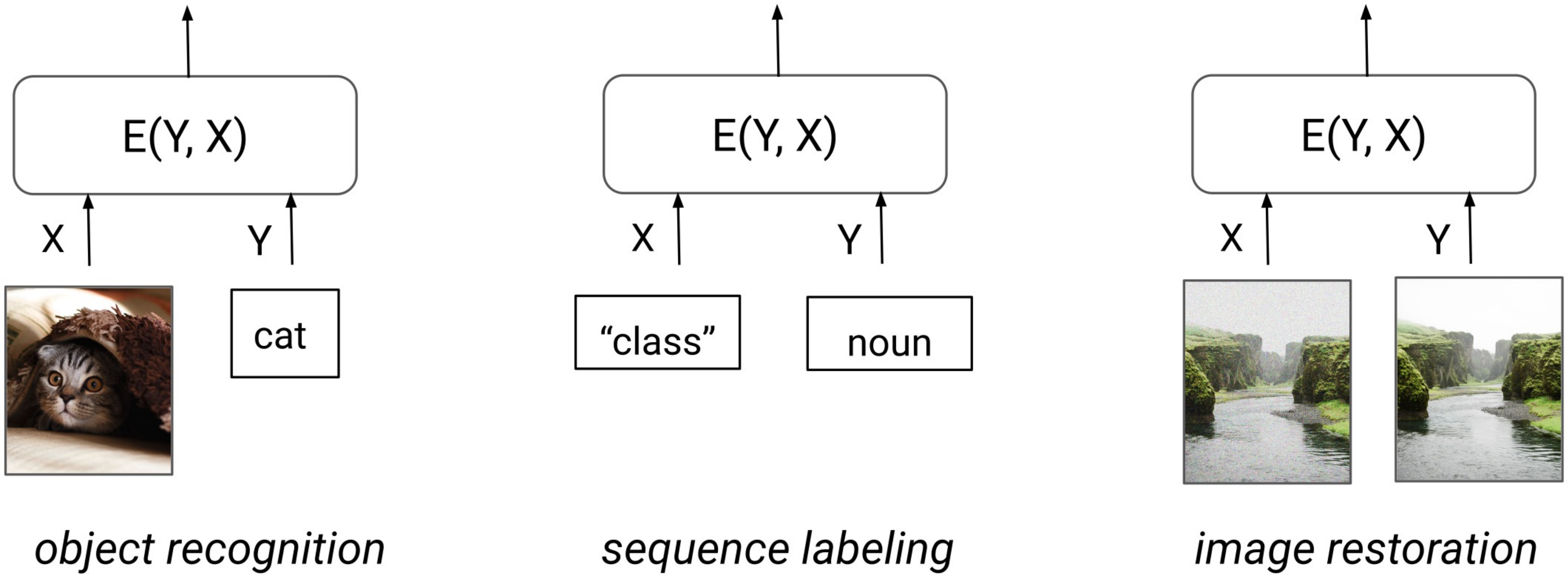
The inner-product version works the best empirically [10]!

Image Credit: [11]

Deep EBMs

We can also use deep EBMs for supervised learning tasks like classification [13,14].

$$p_\theta(\mathbf{x}, \mathbf{y}) = \frac{1}{Z} \exp\left(-E_\theta(\mathbf{x}, \mathbf{y})\right)$$



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Sampling from Deep EBMs

Suppose we have a deep EBM over continuous random variables, how can we draw samples from it?

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Langevin Monte Carlo

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One popular approach is Langevin Monte Carlo [15,16] originated from Langevin Diffusion [17].

$$\mathrm{d}\mathbf{x} = \underbrace{\nabla \log p_\theta(\mathbf{x})\mathrm{d}t}_{\text{drift term}} + \underbrace{\sqrt{2}\mathrm{d}B_t}_{\text{diffusion term}}$$

This is a stochastic differential equation (SDE), known as *Itô diffusion*.

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One can prove Langevin Diffusion is *irreducible*, *strong Feller*, and *aperiodic* [18].

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In other words, $p_\theta(\mathbf{x})$ is the stationary distribution of Langevin Diffusion. Therefore, we can use it as a Markov chain Monte Carlo sampling method.

Langevin Monte Carlo

To turn the Langevin Diffusion into a sampling algorithm, we need to discretize (Euler-Maruyama method) it:

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$$\Downarrow$$

$$\mathbf{x}_{t+\eta} - \mathbf{x}_t = \nabla \log p_\theta(\mathbf{x}_t)(t+\eta-t) + \sqrt{2}(B_{t+\eta} - B_t)$$

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⬇

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$$\mathbf{x}_{t+\eta} = \mathbf{x}_t + \eta \nabla \log p_\theta(\mathbf{x}_t) + \sqrt{2}\tilde{\epsilon}$$

Increments of Brownian motion satisfy:

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We can construct the *Unadjusted Langevin Algorithm (ULA)* based on the Euler-Maruyama discretization:

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for $t = 0, \ldots, T-1$ **do**
  $\epsilon_t \sim \mathcal{N}(0, I)$
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One can also perform Metropolis-Hasting to ensure *detailed balance*, which implies stationary distribution, leading to *Metropolis-adjusted Langevin Algorithm (MALA)*.

But the acceptance probability decreases as the dimension increases, making it impractical in deep learning.

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Learning Deep EBMs

To learn deep EBMs, we still resort to maximum likelihood and contrastive divergence:

$$
\begin{aligned}
\frac{\partial \log p_\theta(x)}{\partial \theta} &= \frac{1}{p_\theta(x)} \frac{\partial p_\theta(x)}{\partial \theta} \\
&= \frac{1}{p_\theta(x)} \frac{\partial \frac{1}{Z} \exp\left(-E_\theta(x)\right)}{\partial \theta} \\
&= \frac{1}{p_\theta(x)} \frac{\left(-\frac{\partial E_\theta(x)}{\partial \theta}\right) \exp\left(-E_\theta(x)\right) Z - \frac{\partial Z}{\partial \theta} \exp\left(-E_\theta(x)\right)}{Z^2} \\
&= \frac{1}{p_\theta(x)} \left(-\frac{\partial E_\theta(x)}{\partial \theta}\right) p_\theta(x) - \frac{1}{p_\theta(x)} \frac{1}{Z} \frac{\partial Z}{\partial \theta} p_\theta(x) \\
&= -\frac{\partial E_\theta(x)}{\partial \theta} - \frac{1}{Z} \frac{\partial Z}{\partial \theta} \\
&= -\frac{\partial E_\theta(x)}{\partial \theta} - \frac{1}{Z} \frac{\partial \int \exp\left(-E_\theta(x)\right) dx}{\partial \theta} \\
&= -\frac{\partial E_\theta(x)}{\partial \theta} - \frac{1}{Z} \int \left(-\frac{\partial E_\theta(x)}{\partial \theta}\right) \exp\left(-E_\theta(x)\right) dx \\
&= -\frac{\partial E_\theta(x)}{\partial \theta} - \int \left(-\frac{\partial E_\theta(x)}{\partial \theta}\right) p_\theta(x) dx
\end{aligned}
$$

Learning Deep EBMs

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We have the gradient:

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\int p_{\text{data}}(x) \frac{\partial \log p_\theta(x)}{\partial \theta} dx &= \int p_{\text{data}}(x) \left(-\frac{\partial E_\theta(x)}{\partial \theta} - \int \left(-\frac{\partial E_\theta(x)}{\partial \theta} \right) p_\theta(x) dx \right) dx \\
&= \mathbb{E}_{p_{\text{data}}(x)} \left[-\frac{\partial E_\theta(x)}{\partial \theta} \right] - \mathbb{E}_{p_\theta(x)} \left[-\frac{\partial E_\theta(x)}{\partial \theta} \right]
\end{aligned}$$

Learning Deep EBMs

Since we care about $$\max_{\theta} \int p_{\text{data}}(x) \log p_\theta(x) dx$$

We have the gradient:

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$$= \mathbb{E}_{p_{\text{data}}(x)} \left[-\frac{\partial E_\theta(x)}{\partial \theta} \right] - \mathbb{E}_{p_\theta(x)} \left[-\frac{\partial E_\theta(x)}{\partial \theta} \right]$$

Positive Gradient: sample from the data distribution

Negative Gradient: sample from the model distribution

We can still use *Contrastive Divergence* (CD) [6], with Langevin Monte Carlo sampling.

Inference & Learning Deep EBMs

In summary, we need score function (derivatives of energy w.r.t. data) in sampling:

$$\mathbf{x}_{t+1} = \mathbf{x}_t + \eta \left(-\frac{\partial E_\theta(\mathbf{x})}{\partial \mathbf{x}} \right)_{\mathbf{x}_t} + \sqrt{2\eta}\epsilon$$

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We need score function and derivatives of energy w.r.t. parameters in learning:

$$\theta_{t+1} = \theta_t + \beta \left(\mathbb{E}_{p_{\text{data}}(\mathbf{x})} \left[-\frac{\partial E_\theta(\mathbf{x})}{\partial \theta} \right]_{\theta_t} - \mathbb{E}_{p_\theta(\mathbf{x})} \left[-\frac{\partial E_\theta(\mathbf{x})}{\partial \theta} \right]_{\theta_t} \right)$$

Inference & Learning Deep EBMs

In summary, we need score function (derivatives of energy w.r.t. data) in sampling:

$$\mathbf{x}_{t+1} = \mathbf{x}_t + \eta \left(-\frac{\partial E_\theta(\mathbf{x})}{\partial \mathbf{x}} \right)_{\mathbf{x}_t} + \sqrt{2\eta}\epsilon$$

We need score function and derivatives of energy w.r.t. parameters in learning:

$$\theta_{t+1} = \theta_t + \beta \left(\mathbb{E}_{p_{\text{data}}(\mathbf{x})} \left[-\frac{\partial E_\theta(\mathbf{x})}{\partial \theta} \right]_{\theta_t} - \mathbb{E}_{p_\theta(\mathbf{x})} \left[-\frac{\partial E_\theta(\mathbf{x})}{\partial \theta} \right]_{\theta_t} \right)$$

Inference & Learning Deep EBMs

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They are available as long as the energy function is differentiable!

Image Generation of Deep EBMs

Results on CIFAR10 and LSUN datasets [19]

Image Completion of Deep EBMs

Results on LSUN and CelebA [19]:

References

[1] https://en.wikipedia.org/wiki/Ludwig_Boltzmann

[2] Hinton, G.E. and Sejnowski, T.J., 1983, May. Analyzing cooperative computation. In Proceedings of the fifth annual conference of the cognitive science society (pp. 2554-2558).

[3] Hinton, G.E. and Sejnowski, T.J., 1983, June. Optimal perceptual inference. In Proceedings of the IEEE conference on Computer Vision and Pattern Recognition (Vol. 448, pp. 448-453).

[4] Smolensky, P., 1986. Information processing in dynamical systems: Foundations of harmony theory. Colorado Univ at Boulder Dept of Computer Science.

[5] Hinton, G.E. and Salakhutdinov, R.R., 2006. Reducing the dimensionality of data with neural networks. science, 313(5786), pp.504-507.

[6] Hinton, G.E., 2002. Training products of experts by minimizing contrastive divergence. Neural computation, 14(8), pp.1771-1800.

[7] Welling, M., Rosen-Zvi, M. and Hinton, G.E., 2004. Exponential family harmoniums with an application to information retrieval. Advances in neural information processing systems, 17.

[8] Liao, R., Kornblith, S., Ren, M., Fleet, D.J. and Hinton, G., 2022. Gaussian-bernoulli rbms without tears. arXiv preprint arXiv:2210.10318.

[9] Salimans, T. and Ho, J., 2021, April. Should EBMs model the energy or the score?. In Energy Based Models Workshop-ICLR 2021.

[10] Liang, Z.Y, Vicol, P. and Liao, R., 2023. Training Energy-Based Models with Denoising Diffusion Herding. Under Review.

[11] https://lmb.informatik.uni-freiburg.de/people/ronneber/u-net/

References

[12] https://uvadlc-notebooks.readthedocs.io/en/latest/tutorial_notebooks/tutorial8/Deep_Energy_Models.html

[13] Du, Y. and Mordatch, I., 2019. Implicit generation and generalization in energy-based models. arXiv preprint arXiv:1903.08689.

[14] Grathwohl, W., Wang, K.C., Jacobsen, J.H., Duvenaud, D., Norouzi, M. and Swersky, K., 2019. Your classifier is secretly an energy based model and you should treat it like one. arXiv preprint arXiv:1912.03263.

[15] Roberts, G.O. and Tweedie, R.L., 1996. Exponential convergence of Langevin distributions and their discrete approximations. Bernoulli, pp.341-363.

[16] Karagulyan, A., 2021. Sampling with the Langevin Monte-Carlo (Doctoral dissertation, Institut polytechnique de Paris).

[17] Langevin, P. (1908). "Sur la théorie du mouvement brownien [On the Theory of Brownian Motion]". C. R. Acad. Sci. Paris. 146: 530–533.

[18] Bhattacharya, R.N., 1978. Criteria for recurrence and existence of invariant measures for multidimensional diffusions. The Annals of Probability, pp.541-553.

[19] Gao, R., Song, Y., Poole, B., Wu, Y.N. and Kingma, D.P., 2020. Learning energy-based models by diffusion recovery likelihood. arXiv preprint arXiv:2012.08125.

Questions?