Introduction to unsupervised learning and generative models

From restricted Boltzmann machines to more advanced models

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Overview

Supervized learning

given: data $\mathbf{x}$ and labels y
common task:

predict labels for unknown data
$\Rightarrow$ estimate $p(y|\,\mathbf{x})$

Unsupervized learning

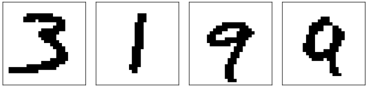
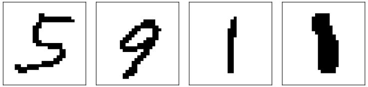
given: *unlabeled*, often high-dimensional data $\mathbf{x}$
possible tasks:

- Dimension reduction
- Clustering
- Sample generation $\Rightarrow$ estimate $p(\mathbf{x})$
  - (Restricted/ Deep) Boltzmann machines
  - Variational autoencoders
  - Generative adversarial networks

Outline

Energy-based models

- task: generate new samples similar to training data
  $\Rightarrow$ estimate $p(\mathbf{x})$ explicitly and draw samples from it

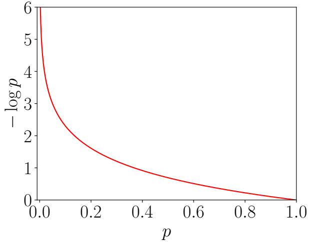
  e.g.  learn $\Rightarrow$ 

- parameterize probability distribution $p(\mathbf{x}; \boldsymbol{\theta})$ with parameters $\boldsymbol{\theta}$
  $\Rightarrow$ learn parameters $\boldsymbol{\theta}$
- parameterization of energy-based models:

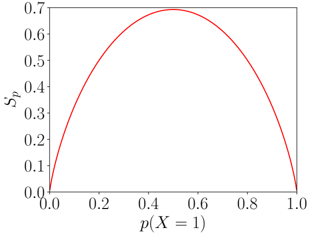
$$p(\mathbf{x}; \boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})} e^{-E(\mathbf{x}; \boldsymbol{\theta})} \qquad Z(\boldsymbol{\theta}) = \int d\,\mathbf{x}\, e^{-E(\mathbf{x}; \boldsymbol{\theta})}$$

Energy-based models: The principle of maximum entropy

- quantification of uncertainty of an event: $-\log p$
- Shannon entropy: $S_p = -\operatorname{Tr} p(\mathbf{x}) \log p(\mathbf{x})$



- example coin toss:
  $S_p = -p \log p - (1-p) \log(1-p)$



- Principle of maximum entropy: Best choice of probability distribution is the one, that maximizes the entropy given the current knowledge

Energy-based models: The principle of maximum entropy

- keep averages of functions $f_i(\mathbf{x})$ fixed (e.g. averages $\langle x_i \rangle$, correlations $\langle x_i x_j \rangle$)):

$$\langle f_i \rangle_{\text{model}} = \int d\,\mathbf{x}\, f_i(\mathbf{x}) p(\mathbf{x}) = \langle f_i \rangle_{\text{data}}$$

- impose constraints on the entropy using Langrange multipliers:

$$\mathcal{L}[p] = -S_p + \sum_i \lambda_i \left(\langle f_i \rangle - \int dx\, f_i(\mathbf{x}) p(\mathbf{x}) \right) + \gamma \left(1 - \int d\,\mathbf{x}\, p(\mathbf{x}) \right)$$

$$0 = \frac{\delta \mathcal{L}}{\delta p} = (\log p(\mathbf{x}) + 1) - \sum_i f_i(\mathbf{x}) - \gamma \quad \Leftrightarrow \quad p(\mathbf{x}) = e^{\Sigma_i \lambda_i f_i(\mathbf{x}) + (\gamma - 1)}$$

Energy-based models

- the definition of the energy $E(\mathbf{x};\lambda)$ and partition function $Z(\lambda)$

$$E(\mathbf{x};\lambda) = -\sum_i \lambda_i f_i(\mathbf{x}) \qquad Z(\lambda) = \int d\,\mathbf{x}\, e^{-E(\mathbf{x};\lambda)}$$

leads to

$$p(\mathbf{x};\lambda) = e^{\gamma-1} e^{\Sigma_i \lambda_i f_i(\mathbf{x})} = \frac{1}{Z(\lambda)} e^{-E(\mathbf{x};\lambda)}$$

- comparison to statistical physics:
  - canonical ensemble:

$$p(\mathbf{x}) = \frac{1}{Z} e^{-\beta E_{\mathsf{stat}}(\mathbf{x})}, \quad \beta = \frac{1}{k_B T}$$

  - grand canonical ensemble:

$$p(\mathbf{x}) = \frac{1}{Z} e^{-\beta(E_{\mathsf{stat}}(\mathbf{x}) - \mu N_{\mathsf{stat}}(\mathbf{x}))}$$

Energy-based models: loss function

- maximum likelihood loss

$$\mathcal{L}(\boldsymbol{\theta}) = \langle \log(p_{\boldsymbol{\theta}}(\mathbf{x})) \rangle_{\text{data}} = -\langle E(\mathbf{x}; \boldsymbol{\theta}) \rangle_{\text{data}} - \log Z(\boldsymbol{\theta})$$

- overfitting: learning training set specific details, that are not present in the *true* distribution (e.g. noise)
- usually a regularization term is added to prevent overfitting

$$E_{\text{reg}}(\boldsymbol{\theta}) = \Lambda \sum_i |\theta_i|^\alpha, \quad \alpha = 1, 2$$

Energy-based models: training procedure

$$-\mathcal{L}(\boldsymbol{\theta}) = -\langle \log(p_{\boldsymbol{\theta}}(\mathbf{x}))\rangle_{\mathsf{data}} = \langle E(\mathbf{x};\boldsymbol{\theta})\rangle_{\mathsf{data}} + \log Z(\boldsymbol{\theta})$$

$$Z(\boldsymbol{\theta}) = \int d\,\mathbf{x}\, e^{-E(\mathbf{x};\boldsymbol{\theta})}$$

- use a gradient descent-based method, e.g. stochastic gradient descent (SGD)

$\Rightarrow$ have to compute gradient:

$$\begin{aligned}
-\frac{\partial \mathcal{L}(\boldsymbol{\theta})}{\partial \theta_i} &= \left\langle \frac{\partial E(\mathbf{x};\boldsymbol{\theta})}{\partial \theta_i} \right\rangle_{\mathsf{data}} + \frac{\partial \log Z(\boldsymbol{\theta})}{\partial \theta_i} \\
&= \left\langle \frac{\partial E(\mathbf{x};\boldsymbol{\theta})}{\partial \theta_i} \right\rangle_{\mathsf{data}} + \frac{1}{Z(\boldsymbol{\theta})} \int d\,\mathbf{x}\, \frac{\partial}{\partial \theta_i} e^{-E(\mathbf{x};\boldsymbol{\theta})} \\
&= \left\langle \frac{\partial E(\mathbf{x};\boldsymbol{\theta})}{\partial \theta_i} \right\rangle_{\mathsf{data}} - \left\langle \frac{\partial E(\mathbf{x};\boldsymbol{\theta})}{\partial \theta_i} \right\rangle_{\mathsf{model}}
\end{aligned}$$

Energy-based models: sample generation

- drawing samples from model (fantasy particles) is necessary to compute gradients

$$p(\mathbf{x}; \boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})} e^{-E(\mathbf{x};\boldsymbol{\theta})}$$

- computation of partition function is often intractable
- only have a function proportional to the probability: $p(\mathbf{x}; \boldsymbol{\theta}) \propto e^{-E(\mathbf{x};\boldsymbol{\theta})}$

$\Rightarrow$ use Markov chain Monte Carlo algorithms, e.g. Metropolis-Hastings algorithm

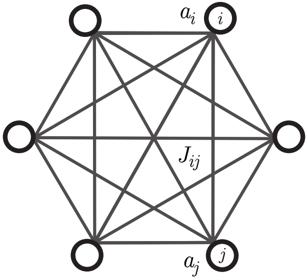
Energy-based models: sample generation

- Markov Chain of random variables: $X = \{X^{(k)} \mid k \in \mathbb{N}_0\}$, transition probability:

$$p_{ij}^{(k)} = \mathrm{Pr}(X^{(k+1)} = j \mid X^{(k)} = i)$$

- one can construct an update operator, such that for $k \to \infty$ the chain contains samples from the desired distribution
- cannot run the chain for an infinite amount of time $\Rightarrow$ approximation

Boltzmann machines



- Energy function:

$$E(x) = -\sum_i a_i x_i - \sum_{i,j} J_{ij} x_i x_j$$

$\Rightarrow$ fixes first and second order moment

- Type of variables: discrete or continuous?
  - discrete states:
    - often two state units (e.g. $\{0, 1\}$, Bernoulli units)

    $\Rightarrow$ Boltzmann machine
  - continuous states:
    - probability distribution is multi-dimensional Gaussian

    $\Rightarrow$ can solve partition function analytically

Boltzmann machines: hidden units

- energy function for Bernoulli units:

$$E(\mathbf{v},\mathbf{h}) = -\sum_i a_i v_i - \sum_\mu b_\mu h_\mu - \sum_{i,j} J_{ij} v_i v_j - \sum_{\mu,\nu} K_{\mu\nu} h_\mu h_\nu - \sum_{i,\mu} W_{i\mu} v_i h_\mu$$

- marginalized distribution:

$$p(\mathbf{v}) = \int d\,\mathbf{h}\, p(\mathbf{v},\mathbf{h}) = \int d\,\mathbf{h}\, \frac{e^{-E(\mathbf{v},\mathbf{h})}}{Z}$$

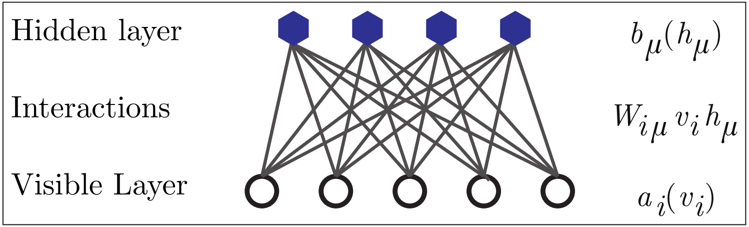
$\Rightarrow$ higher order interactions between visible units in the marginalized distribution

- problem: Boltzmann machines scale poorly with dimension of system

Restricted Boltzmann machines

- for Bernoulli units :

$$E(\mathbf{v},\mathbf{h}) = -\sum_i a_i v_i - \sum_\mu b_\mu h_\mu - \sum_{i\mu} W_{i\mu} v_i h_\mu$$



- general form:

$$E(\mathbf{v},\mathbf{h}) = -\sum_i a_i(v_i) - \sum_\mu b_\mu(h_\mu) - \sum_{i\mu} W_{i\mu} v_i h_\mu$$

Restricted Boltzmann machines

- can capture high order interactions between visible units
- variable number of hidden units
- sufficiently large RBM can take on any probability distribution
- bipartite structure leads to efficient training algorithm

Restricted Boltzmann machines: sample generation and training

- interactions: visible $\leftrightarrow$ hidden

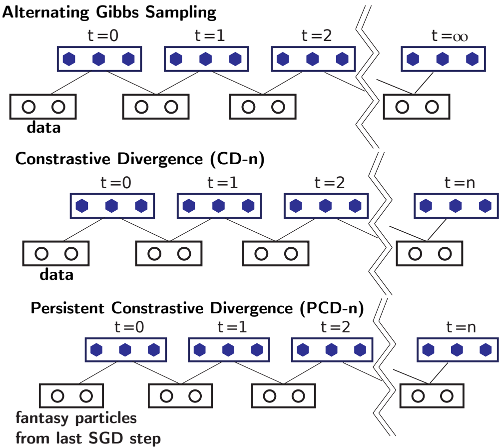
$$p(\mathbf{v}\,|\,\mathbf{h}) = \prod_i p(v_i|\,\mathbf{h})$$

$$p(\mathbf{h}\,|\,\mathbf{v}) = \prod_i p(h_i|\,\mathbf{v})$$

- probability for a single unit:

$$p(v_i = 1|\,\mathbf{h}) = \sigma(a_i + \sum_\mu W_{i\mu} h_\mu)$$

$$p(h_\mu = 1|\,\mathbf{v}) = \sigma(b_\mu + \sum_i W_{i\mu} v_i)$$

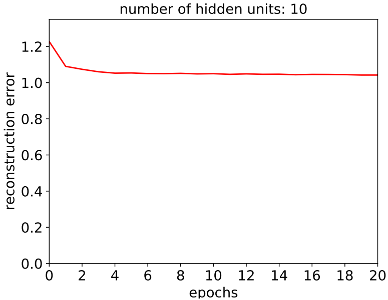


Restricted Boltzmann machines: MNIST with the Paysage package

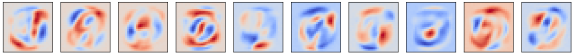
- MNIST dataset: 70000 handwritten digits (28px $\times$ 28px, black and white)
- Paysage package: built to train unsupervized generative models
- SGD with ADAM optimizer and minibatches of size 100
- L^2 regularization with $\Lambda = 10^{-3}$
- Persistent Constrastive Divergence with 1 Gibbs step per SGD step
- sample generation after training with 100000 Gibbs steps

$\Rightarrow$ vary number of hidden units and epochs

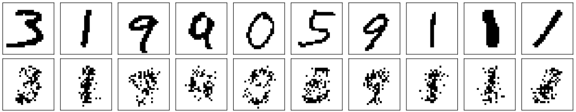
Restricted Boltzmann machines: MNIST with 10 hidden units



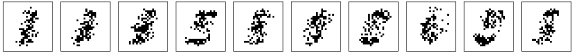
Weights of the hidden units:



Reconstructed samples:

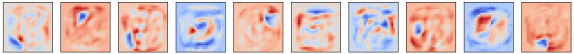


Fantasy particles:

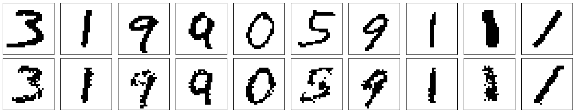


Restricted Boltzmann machines: MNIST with 100 hidden units

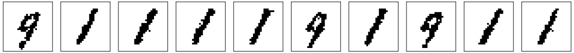
Weights of the hidden units:



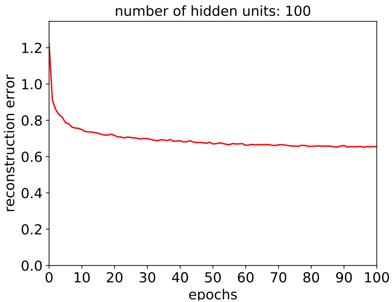
Reconstructed samples:



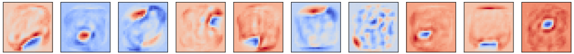
Fantasy particles:



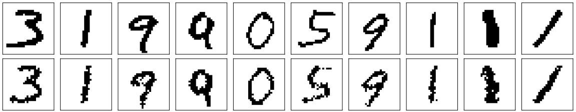
Restricted Boltzmann machines: MNIST with 100 hidden units



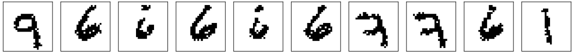
Weights of the hidden units:



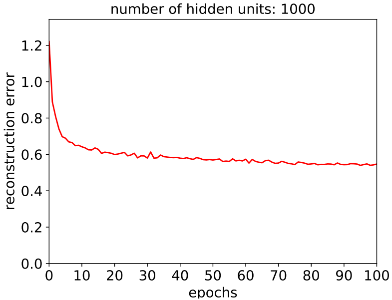
Reconstructed samples:



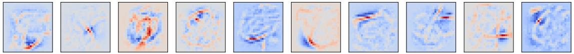
Fantasy particles:



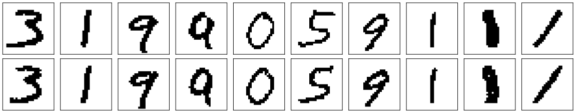
Restricted Boltzmann machines: MNIST with 1000 hidden units



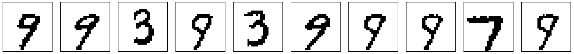
Weights of the hidden units:



Reconstructed samples:

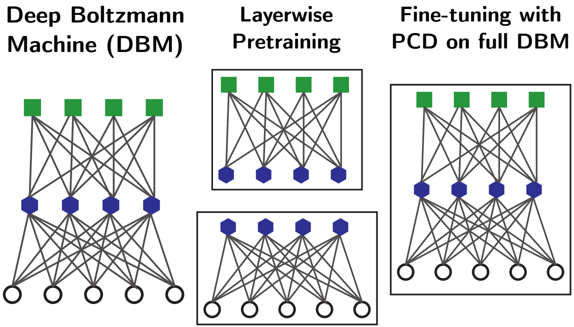


Fantasy particles:

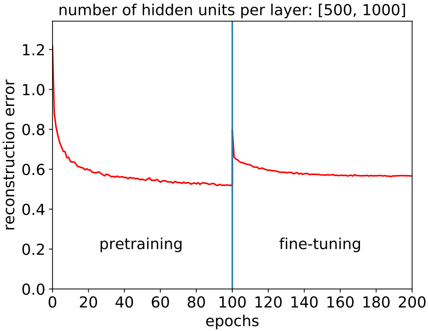


Deep Boltzmann machines

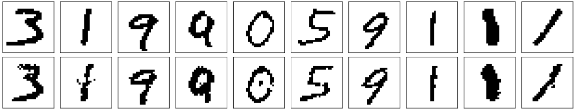
- capture complex interaction between hidden units
- not to be confused with deep belief networks



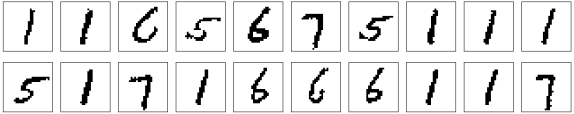
Deep Boltzmann machines: attempt on MNIST with two layers



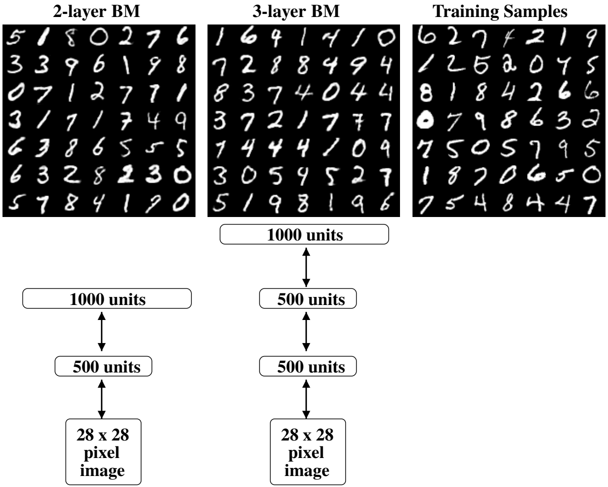
Reconstructed samples:



Fantasy particles:

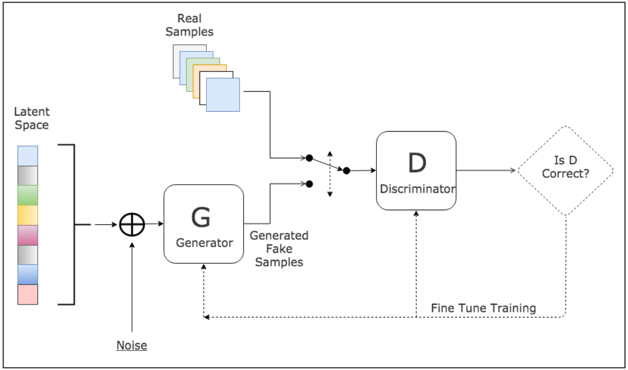


Deep Boltzmann machines: MNIST



Salakhutdinov, Hinton: Deep Boltzmann Machines

Generative adversarial networks



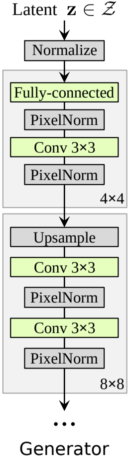


image sources: GAN, Generator: [arXiv:1812.04948]

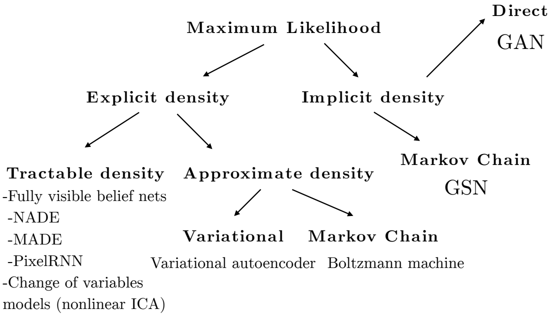
Generative adversarial networks: Style-based GANs

thispersondoesnotexist.com

[arXiv:1812.04948] A Style-based Generator Architecture for Generative Adversarial Networks

Summary

- Energy-based models
- Boltzmann machines
- Restricted Boltzmann machines
- Deep Boltzmann machines
- Generative adversarial networks



[arXiv:1701.00160] NIPS 2016 Tutorial: Generative Adversarial Networks