Restricted Boltzmann Machine

Machine Learning and Data Mining

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Generative models

Generative models

- Informally, given samples we wish to learn generative procedure.
- Formally, given samples of a random variable X, we wish to find X', so that:

$$P(X) \approx P(X')$$

Sampling generative models

- direct sampling procedure, usually in form:

$$\begin{aligned} X &= f(Z); \\ \\ Z &\sim U^n[0, 1] \\ &\text{or} \\ Z &\sim \mathcal{N}^n[0, 1]; \end{aligned}$$

- density is usually unknown, since:

$$p(x) = \sum_{z \mid f(z) = x} p(z) \left| \frac{\partial}{\partial z} f(z) \right|^{-1}$$

Density generative models

- density function $P(x)$ or unnormalized density function:

$$P(x) = \frac{1}{C}\rho(x)$$

- sampling is usually done via some kind of Monte-Carlo Markov Chains (possible for unnormalized density).

Boltzmann machines

Energy models

$$P(x) = \frac{1}{Z} \exp(-E(x))$$

where:

- $E(x)$ - **energy function**;
- $Z = \sum_x \exp(-E(x))$ - normalization constant, **partition function**.

Latent variables

- one of the simplest way to model a complex distribution is via hidden or *latent* variables h:

$$
\begin{aligned}
P(x,h) &= \frac{1}{Z}\exp(-E(x,h));\\
P(x) &= \frac{1}{Z}\exp(-E(x));\\
E(x) &= \text{FreeEnergy}(x) = -\log\sum_h \exp(-E(x,h));\\
Z &= \sum_x \exp(-\text{FreeEnergy}(x)).
\end{aligned}
$$

Maximum Likelihood fit

$$\mathcal{L} = \sum_i \log P(x_i) \to \max;$$

$$\frac{\partial}{\partial\theta}\log P(x) =$$

$$\frac{\partial}{\partial\theta}\log\left[\frac{1}{Z}\exp(-\text{FreeEnergy}(x))\right] =$$

$$-\frac{\partial}{\partial\theta}\log Z - \frac{\partial}{\partial\theta}\text{FreeEnergy}(x) =$$

$$-\frac{1}{Z}\frac{\partial}{\partial\theta}Z - \frac{\partial}{\partial\theta}\text{FreeEnergy}(x) =$$

$$-\frac{1}{Z}\frac{\partial}{\partial\theta}\left[\sum_\chi \exp(-\text{FreeEnergy}(\chi))\right] - \frac{\partial}{\partial\theta}\text{FreeEnergy}(x)$$

Maximum Likelihood fit

$$\frac{\partial}{\partial\theta}\log P(x) =$$

$$-\frac{1}{Z}\frac{\partial}{\partial\theta}\left[\sum_{\chi}\exp(-\mathrm{FreeEnergy}(\chi))\right]-\frac{\partial}{\partial\theta}\mathrm{FreeEnergy}(x) =$$

$$\sum_{\chi}\frac{1}{Z}\exp(-\mathrm{FreeEnergy}(\chi))\frac{\partial}{\partial\theta}\mathrm{FreeEnergy}(\chi)-\frac{\partial}{\partial\theta}\mathrm{FreeEnergy}(x) =$$

$$\sum_{\chi}P(\chi)\frac{\partial}{\partial\theta}\mathrm{FreeEnergy}(\chi)-\frac{\partial}{\partial\theta}\mathrm{FreeEnergy}(x)$$

Maximum Likelihood fit

$$\frac{\partial}{\partial\theta}\log P(x) = \sum_{\chi} P(\chi)\frac{\partial}{\partial\theta}\mathrm{FreeEnergy}(\chi) - \frac{\partial}{\partial\theta}\mathrm{FreeEnergy}(x)$$

$$\mathbb{E}_x\left[\frac{\partial}{\partial\theta}\log P(x)\right] = \mathbb{E}_\chi\left[\frac{\partial}{\partial\theta}\mathrm{FreeEnergy}(\chi)\right] - \mathbb{E}_x\left[\frac{\partial}{\partial\theta}\mathrm{FreeEnergy}(x)\right]$$

where:

- x - sampled from ‘real’ data;
- χ - sampled from current model.

Maximum Likelihood fit

$$\Delta\theta \sim \frac{\partial}{\partial\theta}\mathrm{FreeEnergy}(\chi) - \frac{\partial}{\partial\theta}\mathrm{FreeEnergy}(x)$$

Energy model can be trained by:

- sampling x from given data;
- sampling χ from the current model;
- following difference between deriviatives of $\mathrm{FreeEnergy}$.

This is known as **contrastive divergence**.

Latent variables

$$
\begin{aligned}
&\frac{\partial}{\partial\theta}\mathrm{FreeEnergy}(x) = \\
&\qquad -\frac{\partial}{\partial\theta}\left[\log\sum_h \exp(-E(x,h))\right] = \\
&\qquad \frac{1}{\sum_h \exp(-E(x,h))}\left[\sum_h \exp(-E(x,h))\frac{\partial}{\partial\theta}E(x,h)\right] = \\
&\qquad \frac{1}{\frac{1}{Z}\sum_h \exp(-E(x,h))}\left[\frac{1}{Z}\sum_h \exp(-E(x,h))\frac{\partial}{\partial\theta}E(x,h)\right] = \\
&\qquad \frac{1}{\sum_h P(x,h)}\left[\sum_h P(x,h)\frac{\partial}{\partial\theta}E(x,h)\right] = \\
&\qquad \mathbb{E}_h\left[\frac{\partial}{\partial\theta}E(x,h)\,\middle|\, x\right]
\end{aligned}
$$

Maximum Likelihood fit

$$\Delta\theta \sim \frac{\partial}{\partial\theta}\mathrm{Energy}(\chi, h') - \frac{\partial}{\partial\theta}\mathrm{Energy}(x, h)$$

Energy model can be trained by:

- sampling x from given data and sampling h from $P(h \mid x)$;
- sampling χ from the current model and sampling h' from $P(h \mid \chi)$;
- following difference between deriviatives of Energy.

Gibbs sampling

Sampling $x = (x^1, x^2, \ldots, x^n) \in \mathbb{R}^n$ *from* $P(x)$.

Repeat until the end of the time:

- for i in $1, \ldots, n$:
  - $x^i := \text{sample from } P(X^i \mid X^{-i} = x^{-i})$

where:

- x^{-i} - all components of x except i-th.

Boltzmann machine

Model with energy function:

$$E(x,h) \quad = \quad -b^T x - c^T h - h^T W x - x^T U x - h^t V h;$$

is called **Boltzmann machine**.

If $\mathrm{diag}(U) = 0$ and $\mathrm{diag}(V) = 0$ then x and h are binomial: $x_i, h_j \in \{0, 1\}$.

Training Boltzmann machine

Let $s = (x, h)$, then:

$$E(s) = -d^T s - s^T A s$$

then for binomial units:

$$P\left(s^i = 1 \mid S^{-i} = s^{-i}\right) =$$

$$\frac{\exp\left(-E\left(s^i = 1, s^{-i}\right)\right)}{\exp\left(-E\left(s^i = 1, s^{-i}\right)\right) + \exp\left(-E\left(s^i = 0, s^{-i}\right)\right)} =$$

$$\sigma\left(d_i + 2a^{-i} s^{-i}\right)$$

where:

- a^{-i} - i-th row without i-th element;
- $\sigma(x)$ - sigmoid function.

Training Boltzmann machine

Positive phase:

- sample x from real data;
- perform Gibbs sampling of h under fixed x;

Negative phase:

- init Gibbs chain with x;
- sample both χ and h' from the model.

$$\Delta\theta = \frac{\partial}{\partial\theta}\mathrm{Energy}(x, h) - \frac{\partial}{\partial\theta}\mathrm{Energy}(\chi, h')$$

Boltzmann machine: discussion

- two MCMC chains (positive and negative) for each step of SGD;
- training is slow...

Restricted Boltzmann machine

Product of experts

Consider energy function in form of **product of experts**:

$$E(x,h) = -\beta(x) + \sum_i \gamma(x,h_i)$$

$$\begin{aligned}
P(X) = \frac{1}{Z}\sum_h \exp(-E(x,h)) = \\
\frac{1}{Z}\sum_h \exp(\beta(x))\exp(-\sum_i \gamma(x,h_i)) = \\
\frac{1}{Z}\exp(\beta(x))\sum_h \prod_i \exp(-\gamma(x,h_i)) = \\
\frac{1}{Z}\exp(\beta(x))\prod_i \sum_{h_i} \exp(-\gamma(x,h_i)).
\end{aligned}$$

Product of experts

Consider energy function in form of **product of experts**:

$$
\begin{aligned}
E(x,h) &= -\beta(x) + \sum_i \gamma(x,h_i); \\
\mathrm{FreeEnergy}(x) &= -\beta(x) - \sum_i \log \sum_{h_i} \exp(-\gamma(x,h_i)).
\end{aligned}
$$

Product of experts

Pros:

- efficient computing procedure for $\mathrm{FreeEnergy}(x)$;
- each component of h can be sampled independently.

Cons:

- a special case.

Restricted Boltzmann machine

Restricted Boltzmann machine forbids interactions:

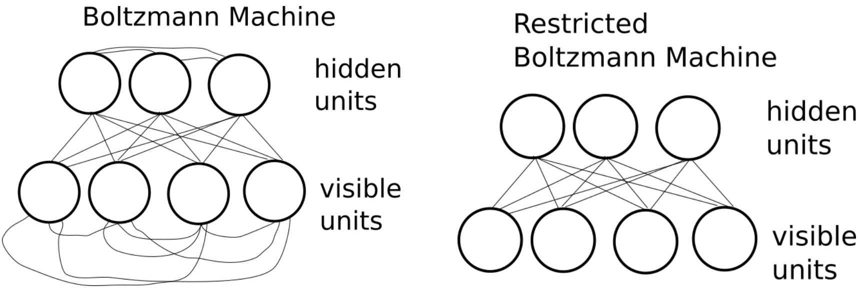
- within visible variables;
- within hidden variables.

$$E(x,h) = \sum_j \phi_j(x_j) + \sum_i \xi(h_i) + \sum_{i,j} \eta_{ij}(x_j, h_i)$$

which can be rewritten simply as:

$$E(x,h) = \sum_{i,j} \eta_{ij}(x_j, h_i)$$

RBM as NN


Boltzmann Machine
hidden units
visible units
Restricted Boltzmann Machine
hidden units
visible units

Gibbs sampling for RBM

- each component of h given x (and vice versa) can be sampled independently;
- whole vector of hidden or visible units can be sampled simultaneously;
- e.g. for binomial hidden variables:

$$P(h^k = 1 \mid X = x) = \frac{\exp\left[-\sum_j \eta_{kj}(x_j, 1)\right]}{\exp\left[-\sum_j \eta_{kj}(x_j, 0)\right] + \exp\left[-\sum_j \eta_{kj}(x_j, 1)\right]}$$

$$P(x^l = 1 \mid H = h) = \frac{\exp\left[-\sum_i \eta_{il}(1, h_i)\right]}{\exp\left[-\sum_i \eta_{il}(0, h_i)\right] + \exp\left[-\sum_i \eta_{il}(1, h_i)\right]}$$

Gibbs sampling for RBM

Gibbs sampling for RBM is especially simple:

$$
\begin{aligned}
h^0 &\sim P(H \mid X = x^0); \\
x^1 &\sim P(X \mid H = h^1); \\
h^1 &\sim P(H \mid X = x^1); \\
x^2 &\sim P(X \mid H = h^2); \\
\ldots & \\
h^{k-1} &\sim P(H \mid X = x^{k-1}); \\
x^k &\sim P(X \mid H = h^{k-1}); \\
h^k &\sim P(H \mid X = x^k);
\end{aligned}
$$

CD-k update

Free energy version:

- sample x^0 from real data;
- compute $\frac{\partial}{\partial\theta}\mathrm{FreeEnergy}(x^0)$;
- initialize Gibbs chain with x^0, perform k steps of Gibbs sampling to obtain x^k;
- compute $\frac{\partial}{\partial\theta}\mathrm{FreeEnergy}(x^k)$;
- update step:

$$\theta := \theta + \alpha\left[-\frac{\partial}{\partial\theta}\mathrm{FreeEnergy}(x^0) + \frac{\partial}{\partial\theta}\mathrm{FreeEnergy}(x^k)\right]$$

CD-k update

Energy version:

- sample x^0 from real data;
- initialize Gibbs chain with x^0, sample h^0;
- compute $\frac{\partial}{\partial\theta}\text{Energy}(x^0, h^0)$;
- perform further k steps of Gibbs sampling to obtain h^k, x^k;
- compute $\frac{\partial}{\partial\theta}\text{Energy}(x^k, h^k)$;
- update step:

$$\theta := \theta + \alpha\left[-\frac{\partial}{\partial\theta}\text{Energy}(x^0, h^0) + \frac{\partial}{\partial\theta}\text{Energy}(x^k, h^k)\right]$$

Justification of CD-k update

For Gibbs chain

$$x^0 \to h^0 \to x^1 \to h^1 \to \dots$$

$$\frac{\partial}{\partial\theta}\log P(x^0) = \\ -\frac{\partial}{\partial\theta}\mathrm{FreeEnergy}(x^0) + \mathbb{E}\left[\frac{\partial}{\partial\theta}\mathrm{FreeEnergy}(x^t)\right] + \\ \mathbb{E}\left[\frac{\partial}{\partial\theta}\log P(x^t)\right];$$

$$\mathbb{E}\left[\frac{\partial}{\partial\theta}P(x^t)\right] \to 0, \text{as } t \to \infty$$

CD-$1/2$

Consider truncated Gibbs chain $x^0 \to h^0$:

$$\frac{\partial}{\partial\theta} \log P\left(x^0\right) \quad = \quad \mathbb{E}\left[\frac{\partial}{\partial\theta} P\left(x^0 \mid h^1\right)\right] + \mathbb{E}\left[\frac{\partial}{\partial\theta} \log P\left(h^1\right)\right];$$

Using mean-field approximation:

$$\mathbb{E}\left[\frac{\partial}{\partial\theta} P\left(x^0 \mid h^1\right)\right] \approx \frac{\partial}{\partial\theta} P\left(x^0 \mid \mathbb{E}h^1\right)$$

and ignoring the second term we end up optimizing **reconstruction error**:

$$\mathcal{L} = -\log P\left(x^0 \mid \mathbb{E}h^0\right)$$

Bernulli-Bernulli RBM

$$
\begin{aligned}
E(x,h) &= -b^T x - c^T h - h^T W x; \\
P(h \mid x) &= \sigma\left(c + W x\right); \\
P(x \mid h) &= \sigma\left(b + W^T h\right);
\end{aligned}
$$

Types of units

- binomial unit u with total input x:

$$P(u = 1 \mid x) = \sigma(x);$$

- multinomial (softmax) unit:

$$P(u = k \mid x) = \frac{\exp(x_k)}{\sum_i \exp(x_i)};$$

- rectified linear unit: infinite series of binomial units with shared connection and different biases:

$$\begin{aligned} u(x) &\sim \sum_i \text{binomial}\left(x - \frac{1}{2} + i\right); \\ u(x) &\sim \max\left[0, x + \mathcal{N}(0, \sigma(x))\right]; \\ P(u = k \mid x) &\approx \log\left(1 + e^x\right). \end{aligned}$$

Types of units

- Gaussian visible units:

$$E(x,h) = \sum_i \frac{(x_i - b_i)^2}{2\sigma_i^2} - \sum_j c_j h_j - \sum_{ij} h_j W_{ij} \frac{x_i}{\sigma_i}$$

- Gaussian-Gaussian RBM:

$$E(x,h) = \sum_i \frac{(x_i - b_i)^2}{2\sigma_i^2} - \sum_j \frac{(h_j - c_j)^2}{2\sigma_j} - \sum_{ij} \frac{h_j}{\sigma_j} W_{ij} \frac{x_i}{\sigma_i}$$

- σ can be learned, but it makes optimization hard;
- usually each input feature is scaled to have zero mean and unit variance, σ is fixed to 1.

Weight decay

Introducing l_2 regularization on W leads to *weight decay*:

- faster mixing (convergence) of MCMC chain;
- thus, faster training.

Introducing l_1 on *activation* of hidden units leads to sparse RBM:

- presumably, easier interpretation;
- e.g. for visual data learns localized features.

RBM for discrimination

As a feature extractor

- train RBM on X to obtain hidden units h_i;
- train a discriminative model on $h_i \rightarrow \hat{y}_i$.

Possible applications:

- reducing dimensionality (somewhat equivalent to e.g. AE):
  - high-dimensional inputs;
  - small number of training samples;
- ...

Cons:

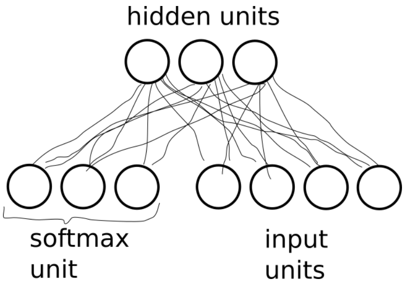
- there are a number of more fancier and simpler techniques.

Discriminative RBM

- train RBM to recover joint distribution $P(x, y)$;

$$f(x) = \frac{\exp\left[-\mathrm{FreeEnergy}(k, x)\right]}{\sum_i \exp\left[-\mathrm{FreeEnergy}(i, x)\right]}$$

- visible units can be divided into two groups:
  - it is possible to use different types of units for each group;
  - softmax unit, probably, the best choice for class unit.



Deep Belief Networks

Deep Belief Networks

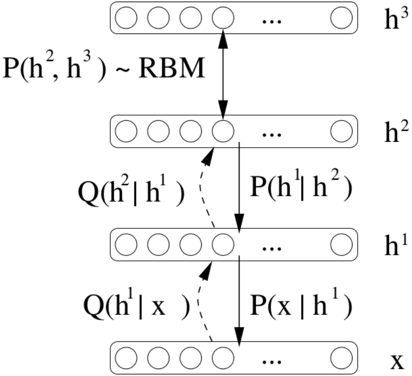


Figure 11: Deep Belief Network as a generative model (generative path with P distributions, full arcs) and a means to extract multiple levels of representation of the input (recognition path with Q distributions, dashed arcs). The top two layers $\mathbf{h}^2$ and $\mathbf{h}^3$ form an RBM (for their joint distribution). The lower layers form a directed graphical model (sigmoid belief net $\mathbf{h}^2 \Rightarrow \mathbf{h}^1 \Rightarrow \mathbf{x}$) and the prior for the penultimate layer $\mathbf{h}^2$ is provided by the top-level RBM. $Q(\mathbf{h}^{k+1}|\mathbf{h}^k)$ approximates $P(\mathbf{h}^{k+1}|\mathbf{h}^k)$ but can be computed easily.

Deep Belief Networks

- Greedy training:
  - usually, trained in a greedy manner: each pair of layers is trained as an RBM.
  - then, fine-tuned with back-propagation w.r.t to a supervised criteria.
- Sleep-Wake algorithm;
- transform DBN into Deep Boltzmann machine.

Summary

Summary

Restricted Boltzmann Machine:

- is an undirected two-layer energy-based generative model;
- can be trained by Contrastive Divergence;
- is a building block of Deep Belief Network.

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