Generative models, selected topics

Machine Learning and Data Mining

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RBM

Contrastive Divergence

Contrastive Divergence (CD-k) update:

- repeat:
  - sample X^+ from known points;
  - k-steps of Gibbs sampling initializing chain with X^+.
  - $\theta := \theta + \alpha \left[\nabla_\theta \mathrm{E}(X^-) - \nabla_\theta \mathrm{E}(X^+)\right]$

Properties:

- small k lead to correlated X^- and X^+, which negatively impacts quality;
  - nevetheless, CD-1 provides decent results;
- large k are expensive.

Persistent CD

Persistent Contrastive Divergence:

- initialize negative chain X^- (*virtual particles*) with known points;
- repeat:
    - sample X^+ from known points;
    - continue sampling from negative chain without resetting;
    - $\theta := \theta + \alpha \left[\nabla_\theta \mathrm{E}(X^-) - \nabla_\theta \mathrm{E}(X^+)\right]$

Properties:

- small k leads to correlated negative samples instead;
- better suited for small learning rates;
- seems to be superior to CD-k even for large k.

Persistent CD

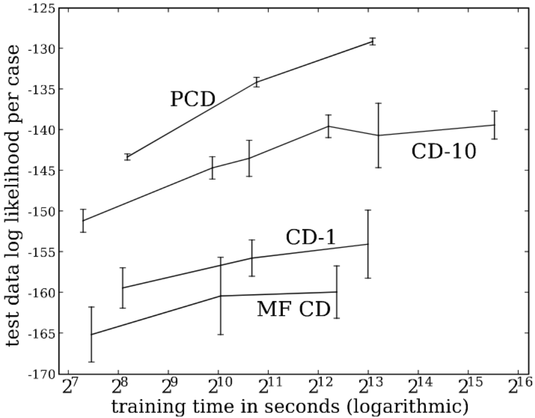


Figure 1. Modeling MNIST data with 25 hidden units (exact log likelihood)

Persistent CD

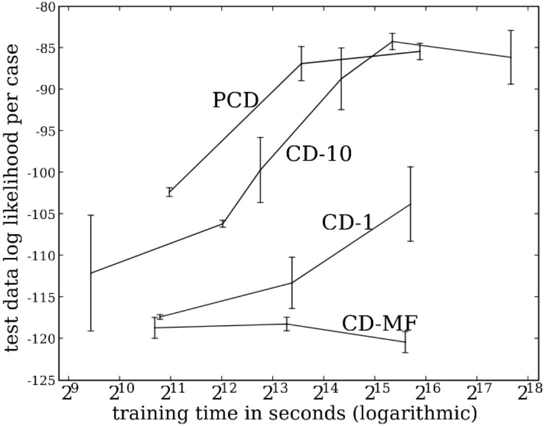


Figure 2. Modeling MNIST data with 500 hidden units (approximate log likelihood)

Persistent CD

Gibbs sampling corresponds to a slightly different distribution R than the one define by energy function Q_θ.
The actual loss:

$$C = \mathrm{KL}(P \mid Q_\theta) - \mathrm{KL}(R \mid Q_\theta) \to \min$$

- $\mathrm{KL}(R \mid Q_\theta)$ large: negative chain mixes fast (R gets closer to Q_θ);
- $\mathrm{KL}(R \mid Q_\theta)$ small: updates closely follow $\nabla\mathcal{L}$, but mixing slows.

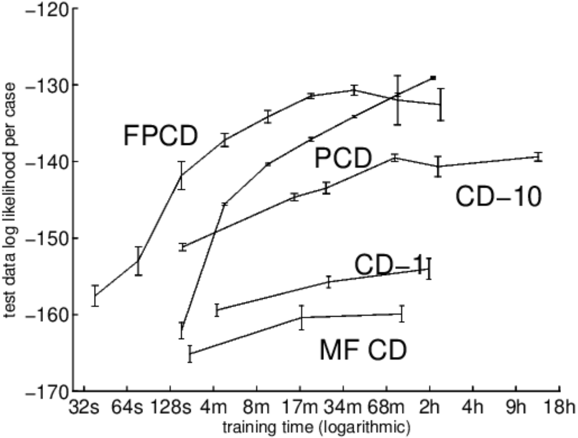
Fast weights PCD

- FPCD introduces two sets of weights:
  - θ - regular parameters;
  - θ_f - fast parameters for MCMC.
- fast parameters are used for negative sampling;
- fast parameters have higher learning rate $\beta > \alpha$ and strong decay ρ.
- virtual particles follow smoothed energy function, thus even faster mixing.

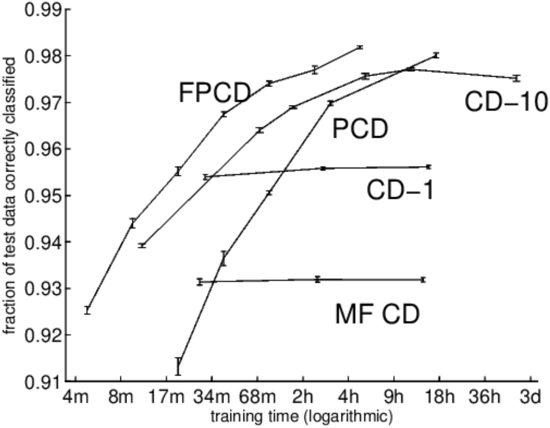
Fast weights PCD

- initialize virtual particles;
- repeat:
    - sample from known points, sample hidden units from Q_θ;
    - samples virtual particles from Gibbs chain over $Q_{\theta+\theta_f}$;
    - compute CD-update and gradient g.
    - $\theta := \theta + \alpha g$;
    - $\theta_f := \rho\theta_f + \beta g$.

Fast Persistent CD



Fast Persistent CD



From RBM to Deep Energy Models

Energy Models

$$
\begin{aligned}
\frac{\partial}{\partial\theta}\log P(x) = & \\
& \frac{\partial}{\partial\theta}\log\left[\frac{1}{Z}\exp(-\mathrm{E}(x))\right] = \\
& -\frac{\partial}{\partial\theta}\log Z - \frac{\partial}{\partial\theta}\mathrm{E}(x) = \\
& -\frac{1}{Z}\frac{\partial}{\partial\theta}Z - \frac{\partial}{\partial\theta}\mathrm{E}(x) = \\
& \underset{\chi\sim P_\theta}{\mathbb{E}}\frac{\partial}{\partial\theta}\mathrm{E}(\chi) - \frac{\partial}{\partial\theta}\mathrm{E}(x)
\end{aligned}
$$

Energy Models

$$\frac{\partial}{\partial \theta} \log P(x) = \mathop{\mathbb{E}}_{\chi \sim P_\theta} \frac{\partial}{\partial \theta} \mathrm{E}(\chi) - \frac{\partial}{\partial \theta} \mathrm{E}(x)$$

- nothing stops us from using an arbitrary energy function, e.g. defined by a deep network;
- except for $\chi \sim P_\theta$.

Instead of using $\chi \sim P_\theta$:

- introduce generator G;
- sample $\chi = G_\phi(z)$, $z \sim P_z = \mathcal{N}^k(0, 1)$;
- make generator G_ϕ to be close to P_θ:

$$\mathrm{KL}(P_\phi \mid P_\theta) = -\mathop{\mathbb{E}}_{z \sim P_z} \log P_\theta(G_\phi(z)) - H\left[P_\phi\right]$$

where $H(P)$ — entropy of P.

Deep Energy Models

$$\mathrm{KL}(P_\phi \mid P_\theta) = -\mathop{\mathbb{E}}_{z\sim P_z} \log P_\theta(G_\phi(z)) - H\left[P_\phi\right]$$

$$\begin{aligned}
\nabla_\phi \mathrm{KL}(P_\phi \mid P_\theta) &= -\mathop{\mathbb{E}}_{z\sim P_z} \nabla_\phi \log P_\theta(G_\phi(z)) - \nabla_\phi H\left[P_\phi\right]; \\
-\mathop{\mathbb{E}}_{z\sim P_z} \nabla_\phi \log P_\theta(G_\phi(z)) &= \mathop{\mathbb{E}}_{z\sim P_z} \nabla_\phi E_\theta(G_\phi(z)); \\
\nabla_\phi H\left[P_\phi\right] &= ???
\end{aligned}$$

Deep Energy Models

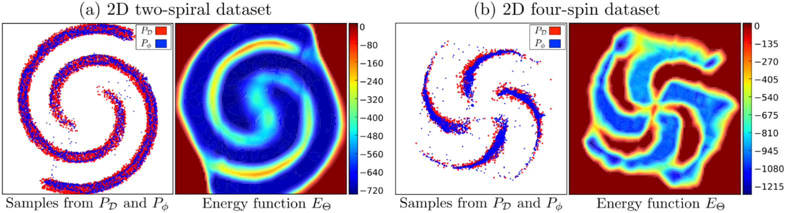
$$\nabla_\phi H\left[P_\phi\right] = ???$$

- entropy is to be maximized;
- entropy term prevents generator from collapsing into a single point $\arg\min_x E_\theta(x)$;
- instead of computing entropy directly, authors suggest:
  - replace $H\left[P_\phi\right]$ by entropy of activation;
  - use batch normalization;
  - assume all activation are independent and normally distributed.

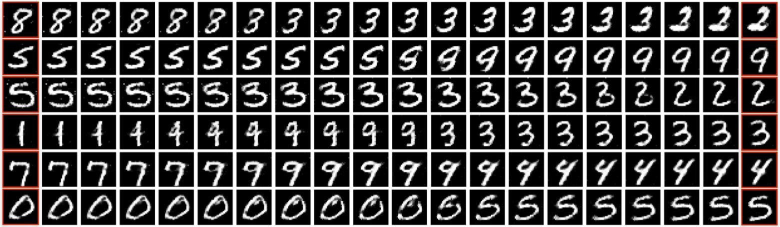
$$H\left[P_\phi\right] \to H\left[\mathcal{N}(\mu_i, \sigma_i)\right] = \frac{1}{2}\sum_i \log(2e\pi\sigma_i^2)$$

where μ_i and σ_i are mean and variance of activation of i-th hidden unit.

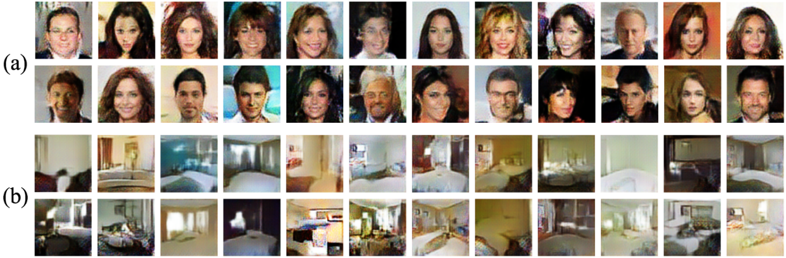
Deep Energy Models



Deep Energy Models



Deep Energy Models



Generative Moment Matching Network

Maximum Mean Discrepancy

$$\mathcal{L}_{MMD}(X,Y) = \left\| \frac{1}{N}\sum_i \varphi(x_i) - \frac{1}{M}\sum_i \varphi(y_i) \right\|^2 =$$

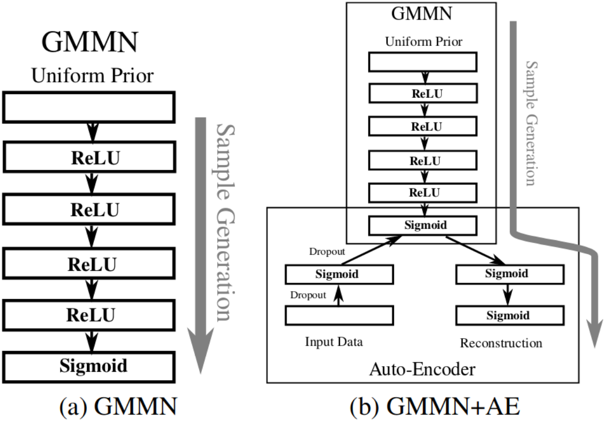
$$\frac{1}{N^2}\sum_{i,j}\varphi(x_i)^T\varphi(x_j) + \frac{2}{NM}\sum_{i,j}\varphi(x_i)^T\varphi(y_j) + \frac{1}{M^2}\sum_{i,j}\varphi(y_i)^T\varphi(y_j) =$$

$$\frac{1}{N^2}\sum_i\sum_j k(x_i,x_j) + \frac{2}{NM}\sum_i\sum_j k(x_i,y_j) + \frac{1}{M^2}\sum_i\sum_j k(y_i,y_j).$$

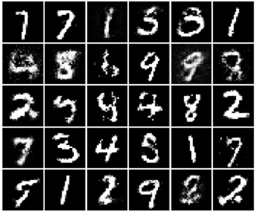
where:

- $\phi(x)$ - feature map;
- $k(x,y) = \varphi(x)^T\varphi(y)^T$, e.g. $k(x,y) = \exp(-\frac{1}{2\sigma}\|x-y\|^2)$.

Generative Moment Matching Network

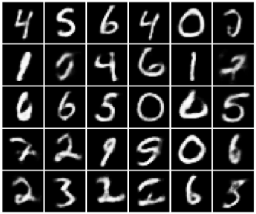


Generative Moment Matching Network



(a) GMMN MNIST samples

(b) GMMN TFD samples



(c) GMMN+AE MNIST samples

(d) GMMN+AE TFD samples

Denoising Auto-Encoder

Denoising Auto-Encoder

If:

- X - sample of real data;
- $\varepsilon \sim \mathcal{N}(0, \sigma^2)$;
- $X' = X + \varepsilon$;
- $g(x) = x + \alpha \nabla \log P_X(x)$

then:

$$g \approx \arg\min_f \mathop{\mathbb{E}}_{X,\varepsilon} \|X - f(X')\|^2$$

Denoising Auto-Encoder

- $C(X' \mid X)$ - corruption, e.g. adding Gaussian noise;
- $P_\theta(X \mid X')$ - reconstruction, e.g. by an Auto-Encoder.

If:

$$P_\theta(X \mid X') \sim P(X \mid X')$$

then Markov chain:

$$\begin{aligned} X_t &= P_\theta(X \mid X'_{t-1}); \\ X'_t &= C(X' \mid X_t) \end{aligned}$$

converges to $P(x)$.

Denoising Auto-Encoder

Simple training:

- sample X from real data;
- apply corruption $X' \sim C(X' \mid X)$;
- $\theta := \theta + \beta \nabla_\theta \log P_\theta(X \mid X')$;
- repeat.

Denoising Auto-Encoder

Walkback algorithm:

- sample X from real data;
- $X^* := X$, $\mathrm{batch} = []$
- until coin says so:
  - apply corruption $X' \sim C(X' \mid X^*)$;
  - extend batch with X';
  - reconstruct $X^* := P_\theta(X \mid X')$
- $\theta := \theta + \beta \nabla_\theta \frac{1}{n} \sum_i \log P_\theta(X \mid X'_i)$;

Denoising Auto-Encoder

Simple training:

Denoising Auto-Encoder

Walkback training:

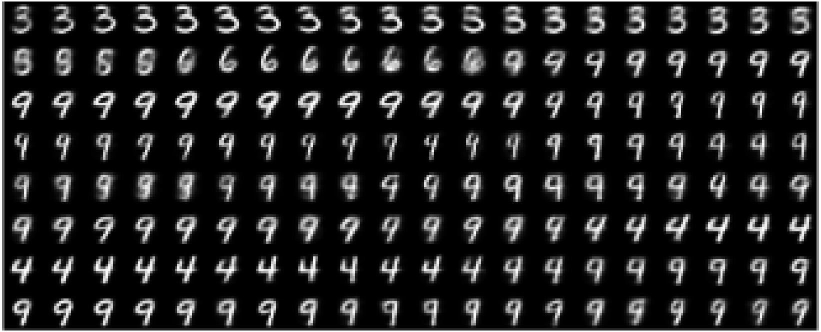
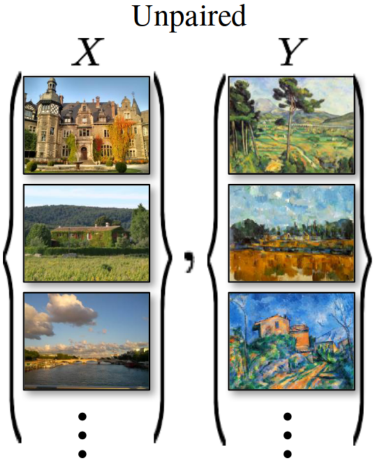


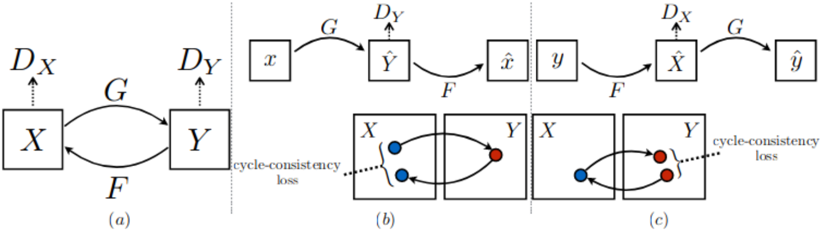
Image-to-Image

Cycle-GAN

Cycle-GAN considers **unpaired** image-to-image translation.



Cycle-GAN



D_X
D_Y
G
F
X
Y
(a)
x
$\hat{Y}$
$\hat{x}$
y
$\hat{X}$
$\hat{y}$
cycle-consistency loss
(b)
cycle-consistency loss
(c)

Cycle Loss

Adversarial loss:

$$\mathcal{L}_{\mathrm{GAN}}(G, D, X, Y) = \mathop{\mathbb{E}}_{x \sim X} \log(1 - D(G(x))) + \mathop{\mathbb{E}}_{y \sim Y} \log D(y)$$

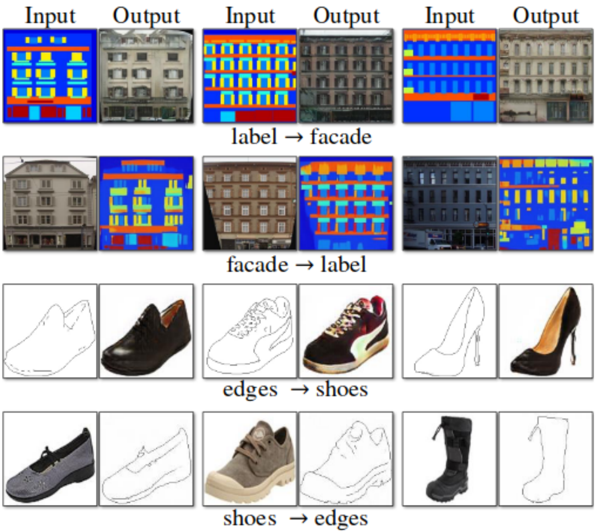
Self-consistency loss:

$$\mathcal{L}_{\mathrm{cycle}}(G, F, X) = \mathop{\mathbb{E}}_{x \sim X} \|F(G(x) - x\|_1$$

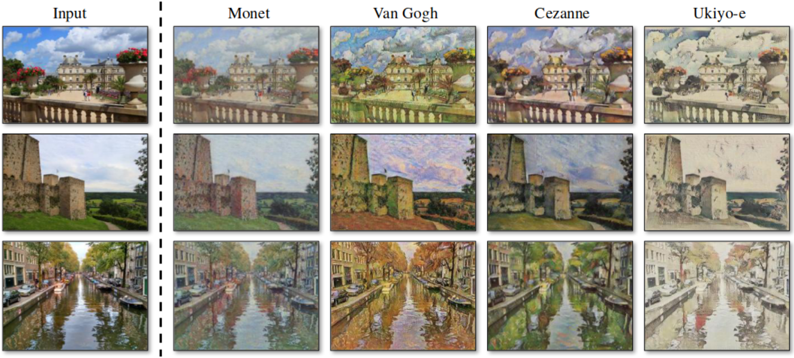
Full loss:

$$\begin{aligned}\mathcal{L} = \mathcal{L}_{\mathrm{GAN}}(G, D_Y, X, Y) + \mathcal{L}_{\mathrm{GAN}}(F, D_X, Y, X) + \\ \mathcal{L}_{\mathrm{cycle}}(G, F, X) + \mathcal{L}_{\mathrm{cycle}}(F, G, Y)\end{aligned}$$

Examples

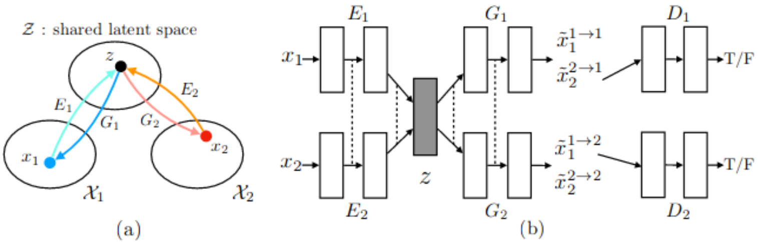

Input
Output
Input
Output
Input
Output
label → facade
facade → label
edges → shoes
shoes → edges

Examples



UNIT

UNIT



$$
\begin{aligned}
\mathcal{L} &= \mathcal{L}_{\mathrm{VAE}}(E_1, G_1) + \mathcal{L}_{\mathrm{GAN}}(E_1, G_1, D_1) + \mathcal{L}_{\mathrm{CC}}(E_1, G_1, E_2, G_2) \\
&+ \mathcal{L}_{\mathrm{VAE}}(E_2, G_2) + \mathcal{L}_{\mathrm{GAN}}(E_2, G_2, D_2) + \mathcal{L}_{\mathrm{CC}}(E_2, G_2, E_1, G_1)
\end{aligned}
$$

UNIT

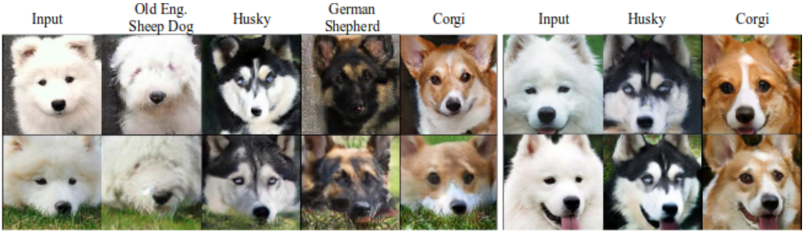
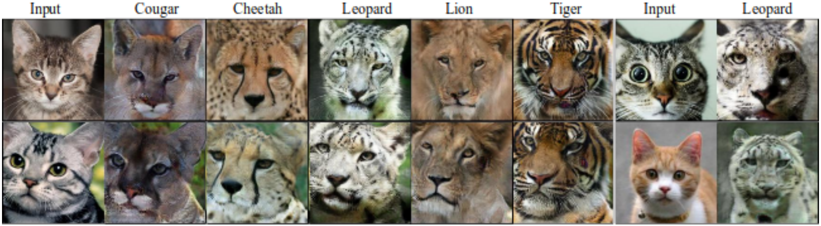


Figure 4: Dog breed translation results.



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