Generative Models

Generative Adversarial Nets

Implicit Generative Model

- **Goal:** a sampler $g(\cdot)$ to generate images
- A simple generator $g(z;\theta)$:
  - $z \sim N(0,I)$
  - $x = g(z;\theta)$ deterministic transformation

- Likelihood-free training:
  - Given a dataset from some distribution p_{data}
  - Goal: $g(z;\theta)$ defines a distribution, we want this distribution $\approx p_{data}$
  - Training: minimize $D(g(z;\theta), p_{data})$
    - D is some distance metric (not likelihood)
  - Key idea: ***Learn* a differentiable** D

GAN (Goodfellow et al., '14)

- Parameterize the discriminator $D(\cdot\,;\phi)$ with parameter ϕ

- **Goal:** learn ϕ such that $D(x;\phi)$ measures how likely x is from p_{data}
    - $D(x,\phi) = 1$ if $x \sim p_{data}$
    - $D(x,\phi) = 0$ if $x! \sim p_{data}$
    - a.k.a., a binary classifier
- GAN: use a neural network for $D(\cdot\,;\phi)$

- **Training:** need both negative and positive samples
    - Positive samples: just the training data
    - Negative samples: use our sampler $g(\cdot\,;z)$ (can provide infinite samples).

- **Overall objectives:**
    - Generator: $\theta^* = \max_\theta D(g(z;\theta);\phi)$
    - Discriminator uses MLE Training:
      $\phi^* = \max_\phi \mathbb{E}_{x\sim p_{data}}[\log D(x;\phi)] + \mathbb{E}_{\hat{x}\sim g(\cdot)}[\log(1 - D(\hat{x};\phi))]$

GAN (Goodfellow et al., ‘14)

- Generator $G(z;\theta)$ where $z \sim N(0,I)$
  - Generate realistic data
- Discriminator $D(x;\phi)$
  - Classify whether the data is real (from p_{data}) or fake (from G)
- Objective function:

$$L(\theta,\phi) = \min_{\theta} \max_{\phi} \mathbb{E}_{x\sim p_{data}}\left[\log D(x;\phi)\right] + \mathbb{E}_{\hat{x}\sim G}\left[\log(1 - D(\hat{x};\phi))\right]$$

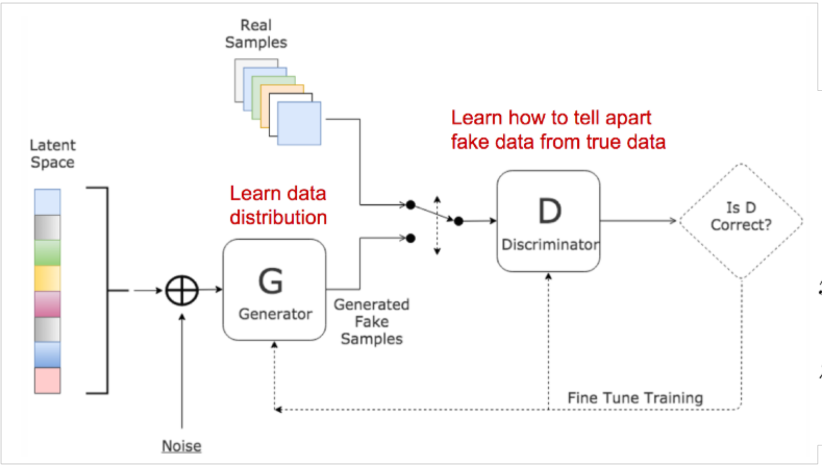
- Training procedure:
  - Collect dataset $\{(x,1)\,|\,x \sim p_{data}\} \cup \{(\hat{x},0) \sim g(z;\theta)\}$
  - Train discriminator

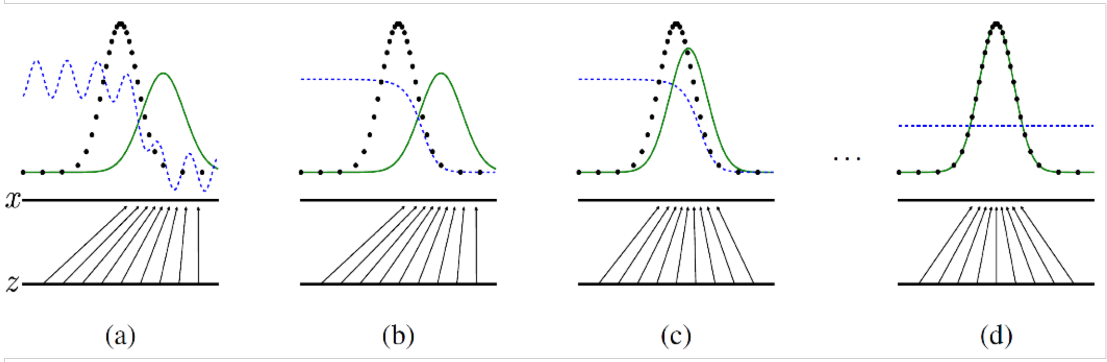
    $D : L(\phi) = \mathbb{E}_{x\sim p_{data}}\left[\log D(x;\phi)\right] + \mathbb{E}_{\hat{x}\sim G}\left[\log(1 - D(\hat{x};\phi))\right]$
  - Train generator $G : L(\theta) = \mathbb{E}_{z\sim N(0,I)}\left[\log D(G(z;\theta),\phi)\right]$
  - Repeat

GAN (Goodfellow et al., '14)

- Objective function:

$$L(\theta, \phi) = \min_{\theta} \max_{\phi} \mathbb{E}_{x \sim p_{data}} \left[\log D(x;\phi)\right] + \mathbb{E}_{\hat{x} \sim G} \left[\log(1 - D(\hat{x};\phi))\right]$$

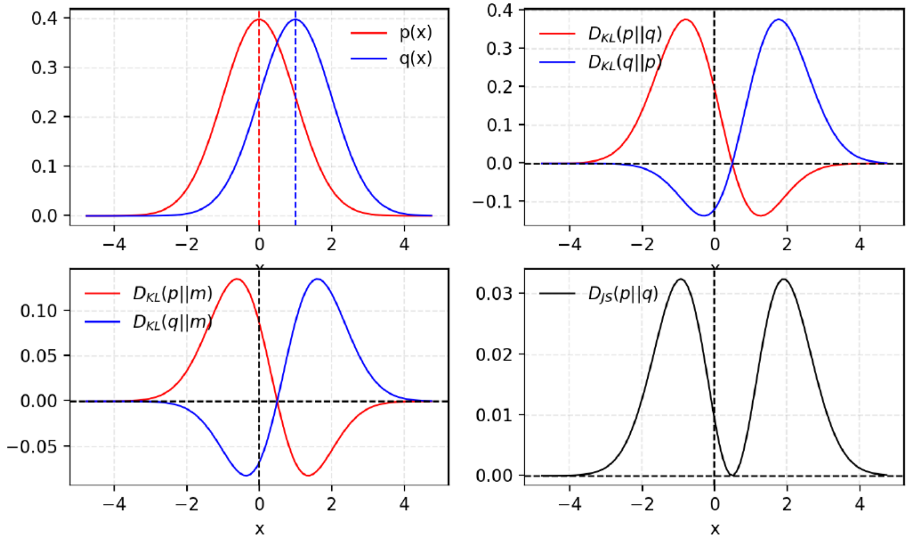




Math Behind GAN

Math Behind GAN

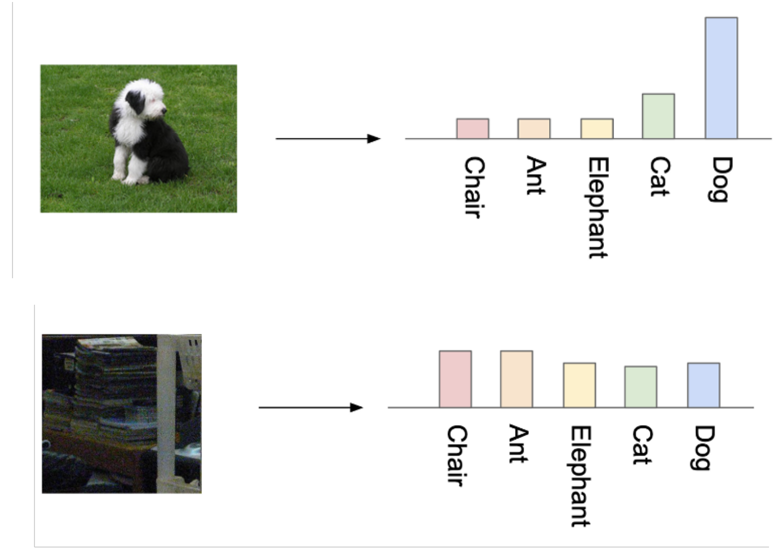
KL-Divergence and JS-Divergence

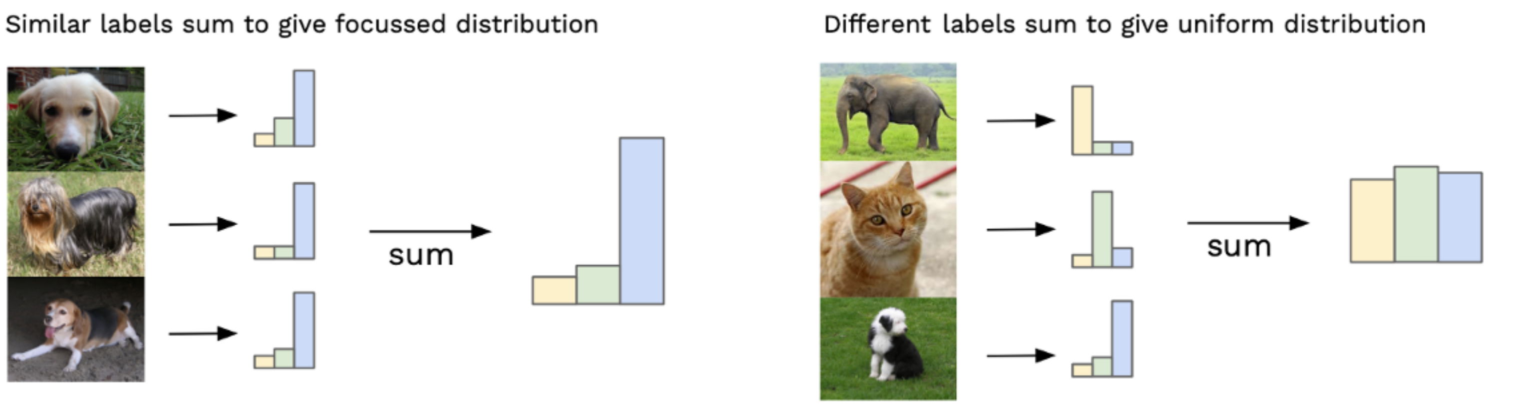


Math Behind GAN

Evaluation of GAN

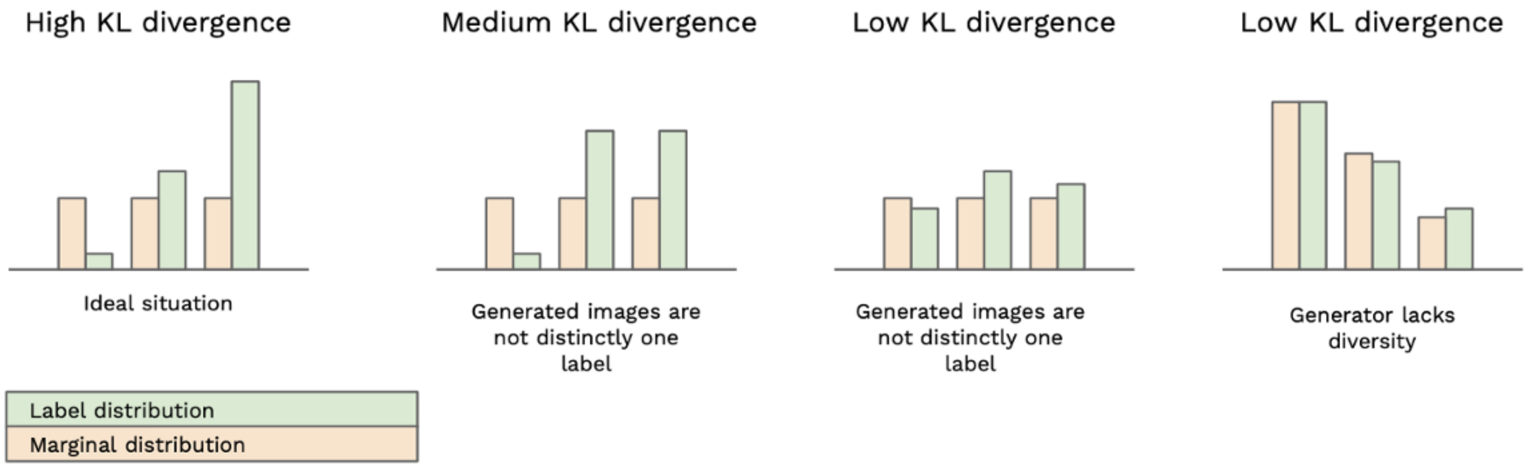
- No $p(x)$ in GAN.
- Idea: use a trained classifier $f(y \mid x)$:
- If $x \sim p_{data}$, $f(y \mid x)$ should have low entropy
  - Otherwise, $f(y \mid x)$ close to uniform.
- Samples from G should be diverse:
  - $p_f(y) = \mathbb{E}_{x \sim G}[f(y \mid x)]$ close to uniform.





Evaluation of GAN

- **Inception Score** (IS, Salimans et al. '16)
  - Use Inception V3 trained on ImageNet as $f(y \mid x)$
  - $IS = \exp\left(\mathbb{E}_{x \sim G}\left[KL(f(y \mid x) \,||\, p_f(y)))\right]\right)$
  - Higher the better



Comments on GAN

- Other evaluation metrics:
  - Fréchet Inception Distance (FID): Wasserstein distance between Gaussians

- Mode collapse:
  - The generator only generate a few type of samples.
  - Or keep oscillating over a few modes.

- Training instability:
  - Discriminator and generator may keep oscillating
  - Example: $-xy$, generator x, discriminatory y. NE: $x = y = 0$ but GD oscillates.
  - No stopping criteria.
  - Use Wsserstein GAN (Arjovsky et al. '17):
    $$\min_{G} \max_{f:\text{Lip}(f)\leq 1} \mathbb{E}_{x\sim p_{data}}\left[f(x)\right] - \mathbb{E}_{\hat{x}\sim p_G}[f(\hat{x})]$$
  - And need many other tricks…

Energy-Based Models

Energy-based Models

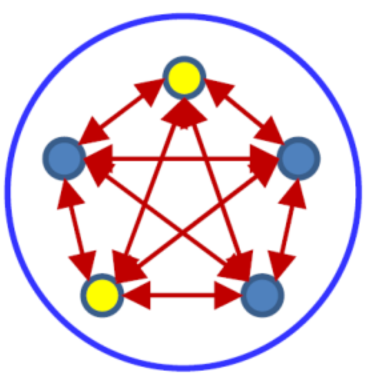
- Goal of generative models:
  - a probability distribution of data: $P(x)$

- Requirements
  - $P(x) \geq 0$ (non-negative)
  - $\int_x P(x)dx = 1$

- Energy-based model:
  - Energy function: $E(x;\theta)$, parameterized by θ
  - $P(x) = \frac{1}{z}\exp(-E(x;\theta))$ (why exp?)
  - $z = \int_z \exp(-E(x;\theta))dx$

Boltzmann Machine

- Generative model
    - $E(y) = -\frac{1}{2} y^\top W y$
    - $P(y) = \frac{1}{z} \exp(-\frac{E(y)}{T})$, T: temperature hyper-parameter
    - W: parameter to learn
- When y_i is binary, patterns are affecting each other through W



$$z_i = \frac{1}{T} \sum_j w_{ji} s_j$$

$$\boxed{P(s_i = 1 | s_{j \neq i}) = \frac{1}{1 + e^{-z_i}}}$$

Boltzmann Machine: Training

- Objective: maximum likelihood learning (assume T =1):
  - Probability of one sample:

$$P(y) = \frac{\exp(\frac{1}{2}y^\top y)}{\sum_{y'} \exp(y'^\top W y')}$$

  - Maximum log-likelihood:

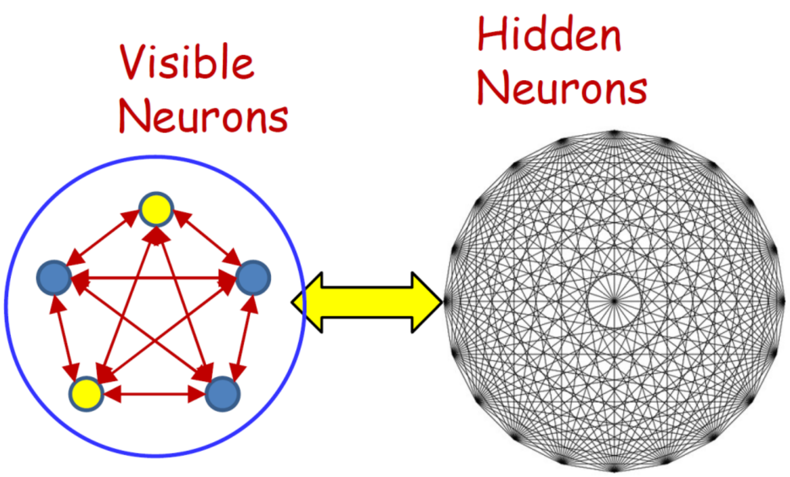
$$L(W) = \frac{1}{N}\sum_{y\in D}\frac{1}{2}y^\top W y - \log\sum_{y'}\exp(\frac{1}{2}y'^\top W y')$$

Boltzmann Machine: Training

Boltzmann Machine: Training

Boltzmann Machine with Hidden Neurons

- Visible and hidden neurons:
  - y: visible, h: hidden
- $P(y) = \sum_{h} P(y, v)$

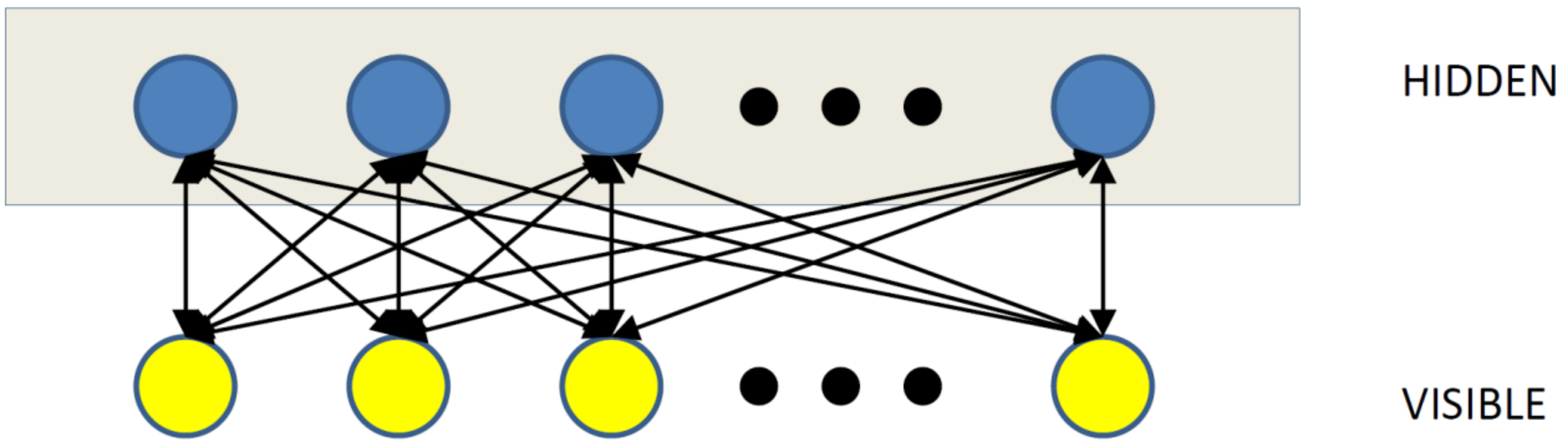


Boltzmann Machine with Hidden Neurons: Training

Boltzmann Machine with Hidden Neurons: Training

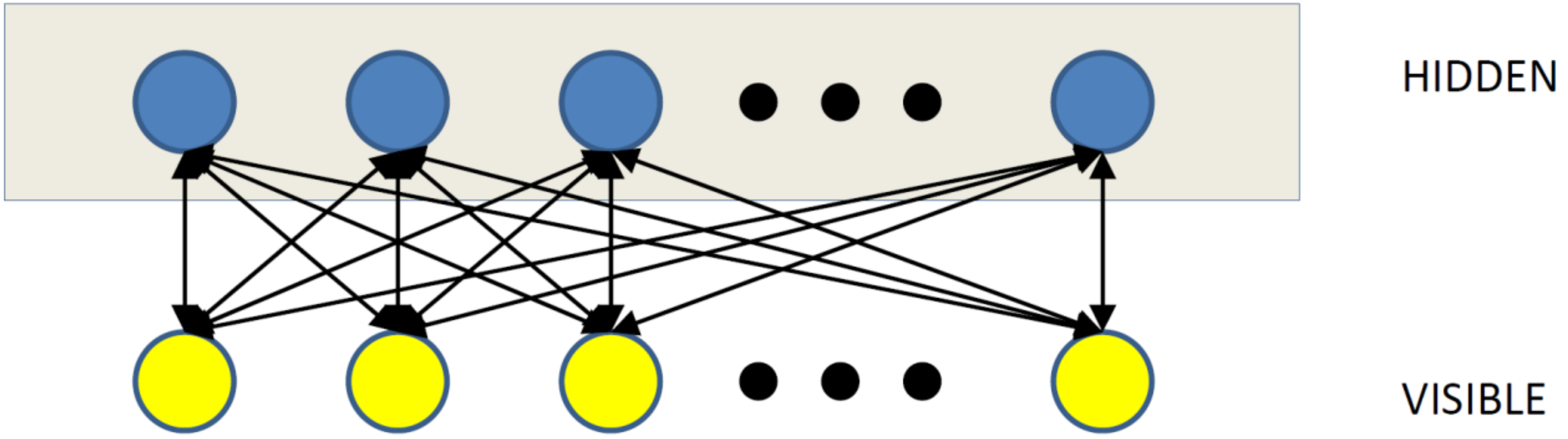
Restricted Bolzmann Machine

- A structured Boltzmann Machine
  - Hidden neurons are only connected to visible neurons
  - No intra-layer connections
  - Invented by Paul Smolensky in ’89
  - Became more practical after Hinton invested fast learning algorithms in mid 2000



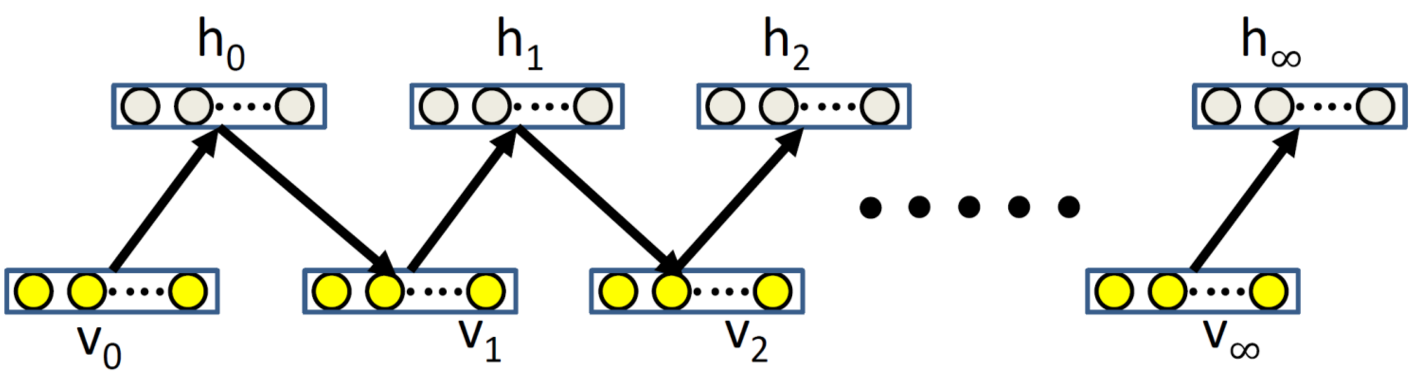
Restricted Bolzmann Machine

- Computation Rules
  - Iterative sampling
  - Hidden neurons h_i: $z_i = \sum_j w_{ij} v_j$, $P(h_i \mid v) = \dfrac{1}{1 + \exp(-z_i)}$
  - Visible neurons v_j: $z_j = \sum_i w_{ij} h_i$, $P(v_j \mid h) = \dfrac{1}{1 + \exp(-z_j)}$



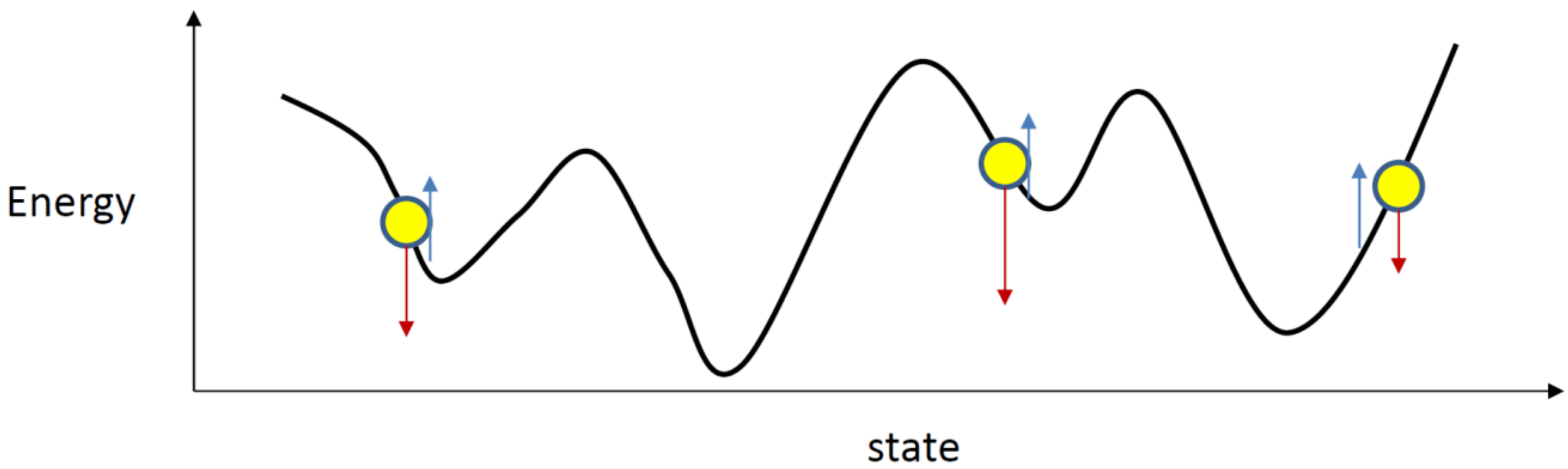
Restricted Bolzmann Machine

- Sampling:
  - Randomly initialize visible neurons v_0
  - Iterative sampling between hidden neurons and visible neurons
  - Get final sample (v_∞, h_∞)



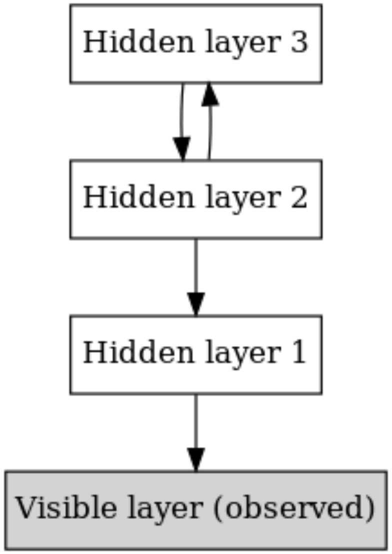
Restricted Bolzmann Machine

- Maximum likelihood estimated:
- $\nabla_{w_{ij}} L(W) = \frac{1}{N_P K} \sum_{v \in P} v_{0i} h_{0j} - \frac{1}{M} \sum v_{\infty i} h_{\infty j}$
- No need to lift up the entire energy landscape!
    - Raising the neighborhood of desired patterns is sufficient

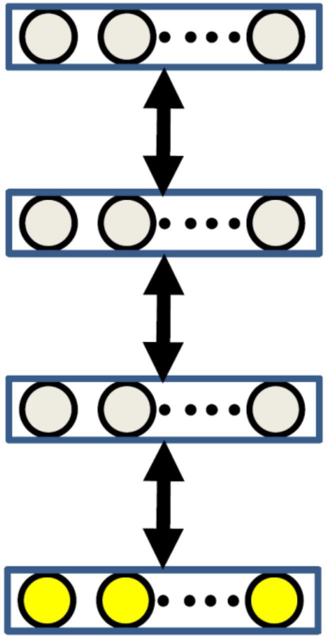


Deep Bolzmann Machine

- Can we have a **deep** version of RBM?
  - Deep Belief Net ('06)
  - Deep Boltzmann Machine ('09)
- Sampling?
  - Forward pass: bottom-up
  - Backward pass: top-down
- Deep Bolzmann Machine
  - The very first deep generative model
  - Salakhudinov & Hinton

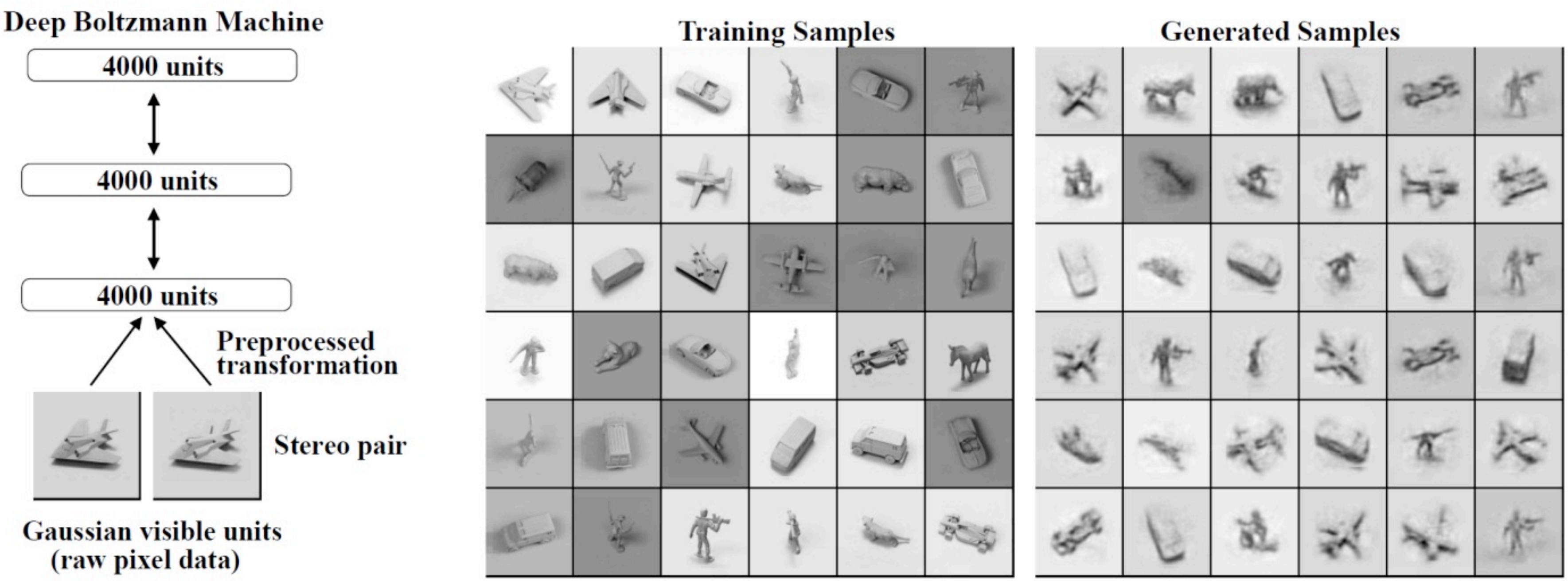


deep belief net



Deep Boltzmann Machine

Deep Bolzmann Machine



Summary

- Pros: powerful and flexible
  - An arbitrarily complex density function $p(x) = \frac{1}{z} \exp(-E(x))$
- Cons: hard to sample / train
  - Hard to sample:
    - MCMC sampling
  - Partition function
    - No closed-form calculation for likelihood
    - Cannot optimize MLE loss exactly
    - MCMC sampling