On Autoencoders and Score Matching for Energy Based Models

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Goal: Unsupervised Feature Learning

- Automatically learn features from data
- Useful for modeling images, speech, text, etc. without requiring lots of prior knowledge
- Many models and algorithms, we will focus on two commonly used ones

Motivation

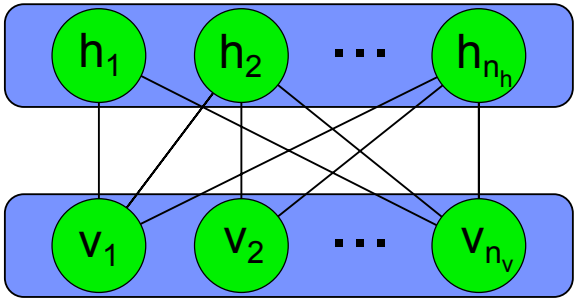
- Autoencoders and energy based models represent the state-of-the-art for feature learning in several domains
- We provide some unifying theory for these model families
- This will allow us to derive new autoencoder architectures from energy based models
- It will also give us an interesting way to regularize these autoencoders

Latent Energy Based Models

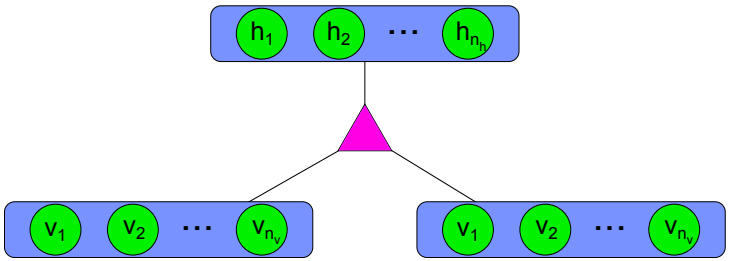
- A probability distribution over data vectors v, with latent variables h and parameters θ
- Defined using an *energy function* $E_\theta(v, h)$ as:

$$P_\theta(v) = \frac{\exp(-E_\theta(v,h))}{Z(\theta)}$$

- Normalized by the *partition function* $Z(\theta) = \int_v \int_h \exp(-E_\theta(v,h)) dh\, dv$
- $Z(\theta)$ is usually not analytical
- Features given by h



Restricted Boltzmann Machine



Factored EBM (e.g. mPoT)

Example: Gaussian-Bernoulli RBM

An Gaussian-Bernoulli restricted Boltzmann machine is an energy based model with visible (observed) variables $v \in \mathbb{R}^D$, hidden (latent) variables $h \in \{0,1\}^K$, and parameters $\theta = \{W\}$. The energy is given by:

$$E_\theta(v,h) = \frac{1}{2} v^T v - v^T W h$$

The free-energy is obtained by marginalizing over the hidden variables:

$$F_\theta(v) = \frac{1}{2} v^T v - \sum_{j=1}^{K} \log\left(1 + \exp\left(v^T W_j\right)\right)$$

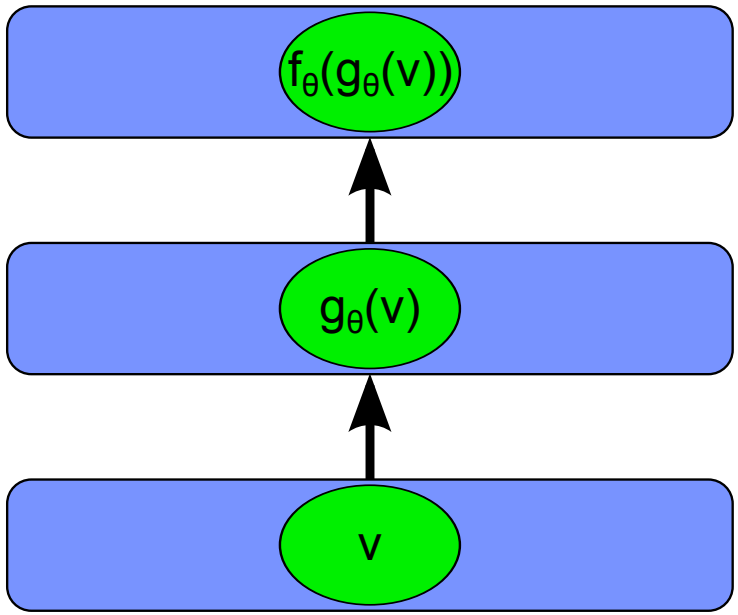
Where W_j represents the j^{th} column of W.

Autoencoders

- A feed-forward neural network designed to reconstruct its input
- Encoding function: $g_\theta(v)$
- Reconstruction function: $f_\theta(g_\theta(v))$
- Minimizes reconstruction error:

$$\hat{\theta} = \arg\min_\theta ||f_\theta(g_\theta(v)) - v||^2$$

- Features given by $g_\theta(v)$



Example: One-Layer Autoencoder

A commonly used autoencoder architecture maps inputs $v \in \mathbb{R}^D$ to outputs $\hat{v} \in \mathbb{R}^D$ through a deterministic hidden layer $\hat{h} \in [0,1]^K$ using parameters $\theta = \{W\}$ by the following system:

$$\hat{v} = f_\theta(g_\theta(v)) = W\hat{h}$$
$$\hat{h} = g_\theta(v) = \sigma(W^T v)$$

Where $\sigma(x) = \frac{1}{1+\exp(-x)}$.
We train this by minimizing the reconstruction error:

$$\ell(\theta) = \sum_{i=1}^{D} \frac{1}{2}(v_i - \hat{v}_i)^2$$

Comparison

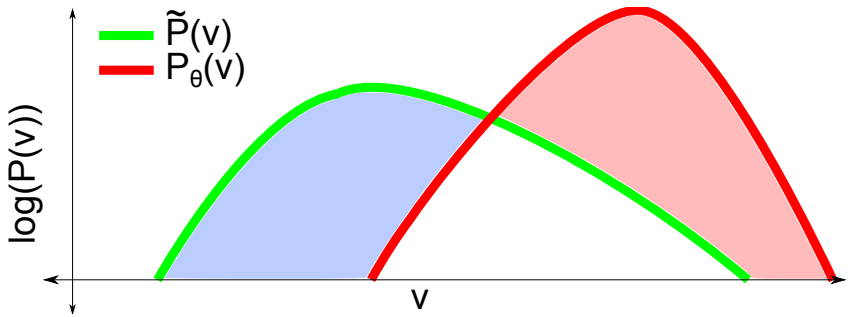
Energy based models	Autoencoders
• Undirected • Probabilistic • Slow inference • Intractable objective function	• Directed • Deterministic • Fast inference • Tractable objective function

- Unifying these model families lets us leverage the advantages of each

Maximum Likelihood for EBMs

- Minimize KL divergence between empirical data distribution $\widetilde{P}(v)$ and model distribution $P_\theta(v)$:

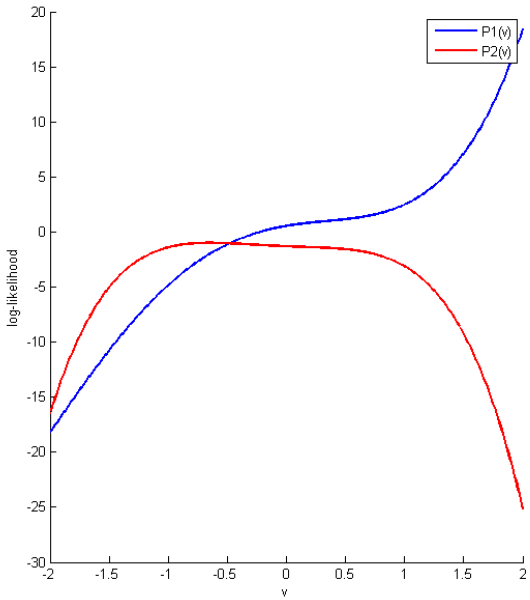
$$\hat{\theta} = \arg\min_\theta \mathbb{E}_{\widetilde{p}(v)} \left[\log(\widetilde{P}(v)) - \log(P_\theta(v)) \right]$$

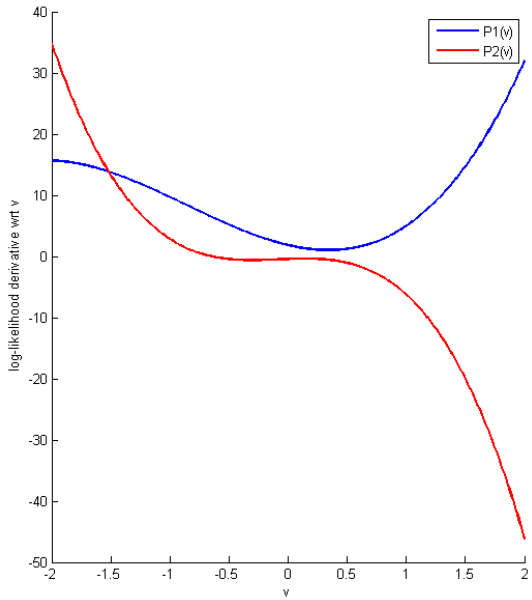


- Requires that we know $Z(\theta)$
- Idea: Approximate $Z(\theta)$ with samples from $P_\theta(v)$
  - Uses MCMC
  - Contrastive divergence (CD), persistent contrastive divergence (PCD), fast PCD (FPCD)

Score Matching (Hyvarinen, 2006)

- Intuition: If two functions have the same derivatives everywhere, then they are the same functions up to a constant
- We match $\frac{\partial}{\partial v_i} \log\left(\widetilde{P}(v)\right)$ and $\frac{\partial}{\partial v_i} \log\left(P_\theta(v)\right)$
- The constraint $\int_v P(v)dv = 1$ means that the distributions must be equal if their derivatives are perfectly matched





Score Matching (2)

- Minimize distance between the *score functions* $\nabla_v \log(\widetilde{P}(v))$ and $\nabla_v \log(P_\theta(v))$:

$$\hat{\theta} = \arg\min_\theta J(\theta) = \mathbb{E}_{\widetilde{p}(v)} \left[||\nabla_v \log(\widetilde{P}(v)) - \nabla_v \log(P_\theta(v))||^2 \right]$$

- Equivalent to (Hyvarinen, 2006):

$$J(\theta) = \mathbb{E}_{\widetilde{p}(v)} \left[\sum_{i=1}^{D} \frac{1}{2} \left(\frac{\partial \log(P_\theta(v))}{\partial v_i} \right)^2 + \frac{\partial^2 \log(P_\theta(v))}{\partial v_i^2} \right] + const$$

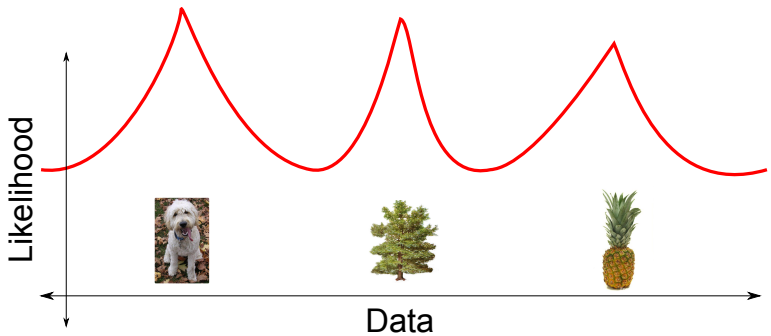
- Does not depend on $Z(\theta)$ since $\nabla_v Z(\theta) = 0$

Score Matching (3)

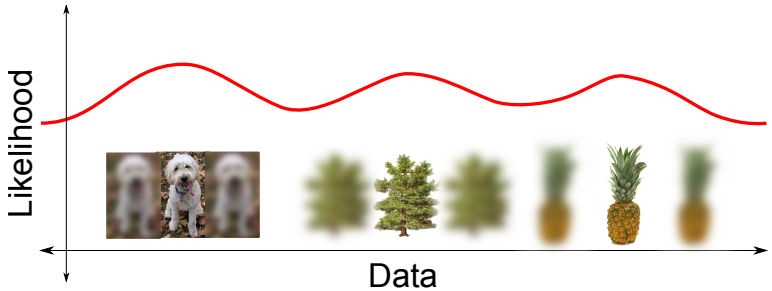
- Score matching is not as statistically efficient as maximum likelihood
  - It is in fact an approximation to pseudolikelihood (Hyvarinen, 2006)
- Statistical efficiency is only beneficial if you can actually find good parameters
- We trade efficiency for the ability to find better parameters with more powerful optimization

Denoising Score Matching (Vincent, 2011)

- Rough idea:
  1. Apply a kernel $q_\beta(v|v')$ to $\widetilde{P}(v)$ get a smoothed distribution $q_\beta(v) = \int q_\beta(v|v')\widetilde{P}(v')dv'$
  2. Apply score matching to $q_\beta(v)$
- Faster than ordinary score matching (no 2nd derivatives)
- Includes denoising autoencoders (for continuous data) as a special case



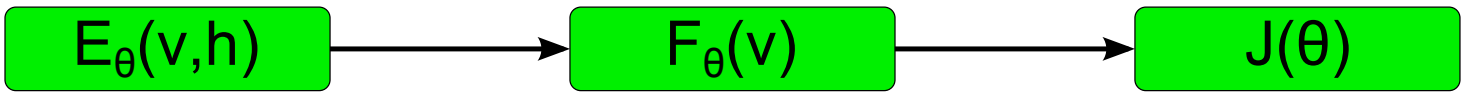
$\widetilde{P}_\theta(v)$



$q_\beta(v)$

Score Matching Recipe

1. Write down energy function $E_\theta(v, h)$
2. Marginalize over latent variables to form $F_\theta(v)$
3. Derive score matching objective $J(\theta)$
   - In practice, use Theano to do this step!



Example: RBM with All Gaussian Units

- If both v and h are Gaussian-distributed, we have the following energy and free-energy:

$$E_\theta(v,h) = \frac{1}{2}v^T v + \frac{1}{2}h^T h - v^T W h$$

$$F_\theta(v) = \frac{1}{2}v^T \left(\mathrm{I} - WW^T\right) v$$

$$J(\theta) = \sum_{i=1}^{D}\left[\frac{1}{2}\left(v_i - \sum_{j=1}^{K} W_{ij}\left(W_j^T v\right)\right)^2 + \sum_{j=1}^{K} W_{ij}^2\right]$$

- This is a linear autoencoder with weight-decay regularization

Example: RBM with All Gaussian Units (2)

- With denoising score matching:

$$J(\theta) = \sum_{i=1}^{D} \frac{1}{2} \left(v_i - \sum_{j=1}^{K} W_{ij} \left(W_j^T x \right) \right)^2$$

$$x \sim N(v, \sigma^2 \mathrm{I})$$

- Adding noise to the input is roughly equivalent to weight-decay (Bishop, 1994)

Example: Gaussian-Bernoulli RBMs

- We apply score matching to the GBRBM model:

$$J(\theta) = const + \sum_{i=1}^{D} \left[\frac{1}{2} (v_i - \hat{v}_i)^2 + \sum_{j=1}^{K} W_{ij}^2 \hat{h}_j \left(1 - \hat{h}_j\right) \right]$$

- This is also a regularized autoencoder
- The regularizer is a sum of weighted variances of the Bernoulli random variables h conditioned on v

Example: mPoT (Warning: lots of equations!)

- The GBRBM is bad at modelling heavy-tailed distributions, and capturing covariance structure in v
- We can use more sophisticated energy-based models to overcome these limitations

The mPoT is an energy based model with Gaussian-distributed visible units, Gamma-distributed hidden units $h^c \in \mathbb{R}^{+K}$, and Bernoulli-distributed hidden units $h^m \in \{0,1\}^M$ with parameters $\theta = \{C, W\}$.

$$E_\theta(v, h^m, h^c) = \sum_{k=1}^{K} \left[h_k^c (1 + \frac{1}{2}(C_k^T v)^2) + (1-\gamma)\log(h_k^c) \right] + \frac{1}{2} v^T v - v^T W h^m$$

$$F_\theta(v) = \sum_{k=1}^{K} \gamma \log(1 + \frac{1}{2}(\phi_k^c)^2) - \sum_{j=1}^{M} \log(1 + e^{\phi_j^m}) + \frac{1}{2} v^T v$$

$$\phi_k^c = C_k^T v$$

$$\phi_j^m = W_j^T v$$

Example: mPoT (2) (Warning: lots of equations!)

$$J(\theta) = \sum_{i=1}^{D} \frac{1}{2} \psi_i(p_\theta(v))^2 + \sum_{k=1}^{K} \left(\rho(\hat{h}_k^c) D_{ik}^2 + \hat{h}_k^c K_{ik} \right) + \sum_{j=1}^{M} \left(\hat{h}_j^m (1 - \hat{h}_j^m) W_{ij}^2 \right) - 1$$

$$\psi_i(p_\theta(v)) = \sum_{k=1}^{K} \hat{h}_k^c D_{ik} + \sum_{j=1}^{M} \hat{h}_j^m W_{ij} - v_i$$

$$K_{ik} = \sum_{k=1}^{K} -C_{ik}^2$$

$$D_{ik} = \sum_{k=1}^{K} \left(- \left(C_k^T v \right) C_{ik} \right)$$

$$\hat{h}_k^c = \frac{\gamma}{1 + \frac{1}{2}(\phi_k^c)^2}$$

$$\hat{h}_j^m = \text{sigm}(\phi_j^m)$$

$$\rho(x) = x^2$$

Score Matching for General Latent EBMs

- Score matching can produce complicated and difficult to interpret objective functions
- Our solution is to apply score matching to latent EBMs without directly specifying $E_\theta(v, h)$

Score Matching for General Latent EBMs (2)

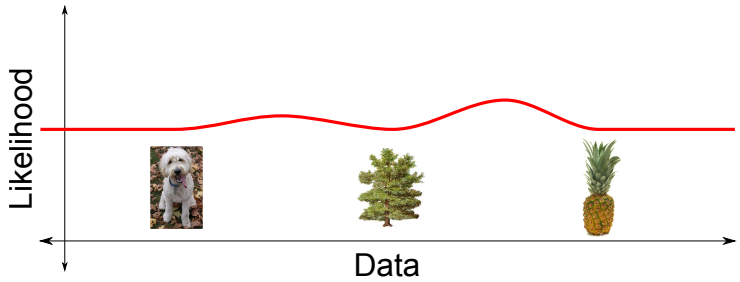
Theorem

The score matching objective for a latent EBM can be expressed succinctly in terms of expectations of the energy with respect to the conditional distribution $P_\theta(h|v)$.

$$J(\theta) = \mathbb{E}_{\tilde{p}(v)} \left[\sum_{i=1}^{n_v} \frac{1}{2} \left(\mathbb{E}_{p_\theta(h|v)} \left[\frac{\partial E_\theta(v,h)}{\partial v_i} \right] \right)^2 + var_{p_\theta(h|v)} \left[\frac{\partial E_\theta(v,h)}{\partial v_i} \right] - \mathbb{E}_{p_\theta(h|v)} \left[\frac{\partial^2 E_\theta(v,h)}{\partial v_i^2} \right] \right].$$

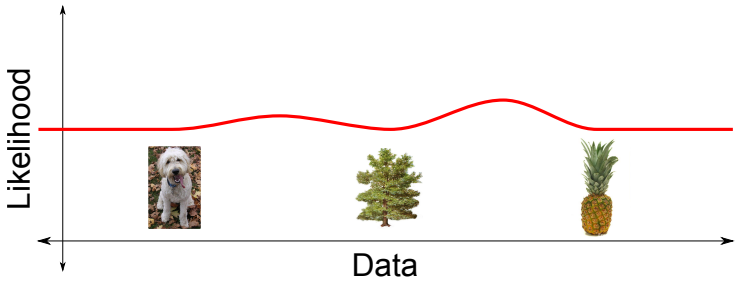
- The score matching objective for a latent EBM always consists of 3 terms:
  1. Squared error
  2. Variance of error
  3. Curvature
- Variance and curvature can be seen as regularizers

Visualization

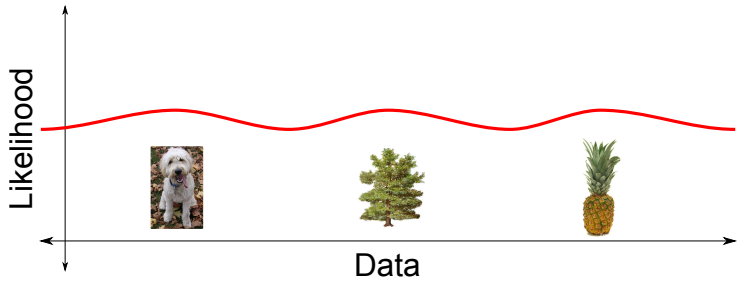


Model probability before learning

Visualization

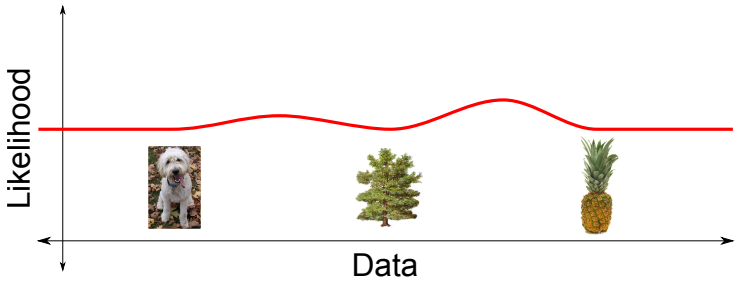


Model probability before learning



Squared error centers mass on data

Visualization



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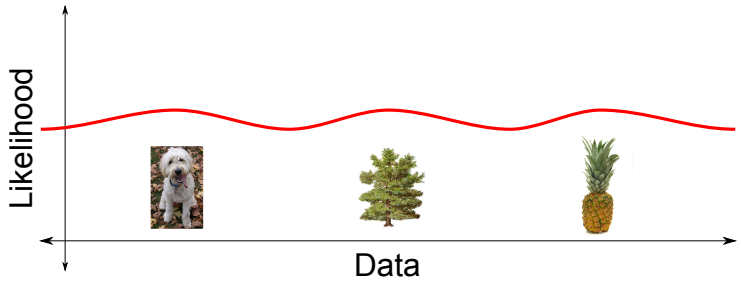
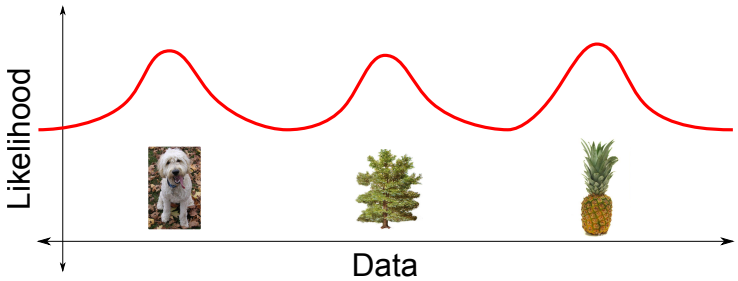


Squared error centers mass on data



Variance and Curvature shape the distribution

Gradient Steps on the Free Energy

- Consider taking a gradient step along the free-energy with step size ε:

$$v_i^{(t+1)} = v_i^{(t)} - \varepsilon \frac{\partial F_\theta(v)}{\partial v_i}$$

- When $F_\theta(v) = \tilde{F}_\theta(v) + \frac{1}{2} v^T v$ term, we get:

$$v_i^{(t+1)} = v_i^{(t)} - \varepsilon \left(v_i^{(t)} + \frac{\partial \tilde{F}\theta(v)}{\partial v_i} \right)$$

- Setting ε to 1:

$$v_i^{(t+1)} = \frac{\partial \tilde{F}\theta(v)}{\partial v_i}$$

- An autoencoder can be thought of as performing a reconstruction by taking a gradient step along its free energy with a step-size of 1

Gaussian Energy Functions

- If the energy function forms a Gaussian distribution in v:

$$E_\theta(v,h) = \tfrac{1}{2}(v-\mu_h)^T \Omega_h (v-\mu_h) + \text{const}$$

- Then the squared error will take the form:

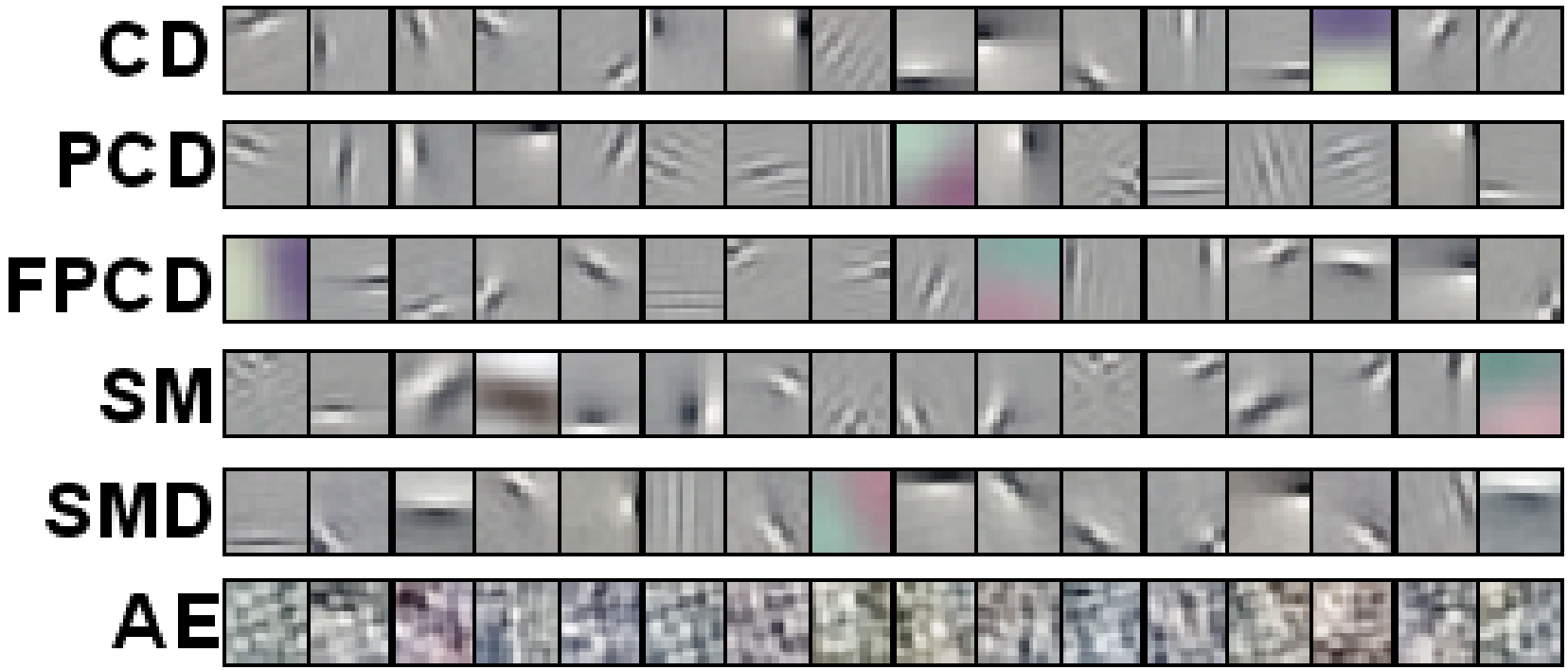
$$\tfrac{1}{2}\left(\mathbb{E}_{p_\theta(h|v)}\left[\Omega_h(v-\mu_h)\right]\right)^2$$

- This corresponds to a more general autoencoder reconstruction error
- For a GBRBM: $\Omega_h = \mathrm{I}$
- If $\Omega_h \neq \mathrm{I}$ then the autoencoder will also model covariance in v

Objectives

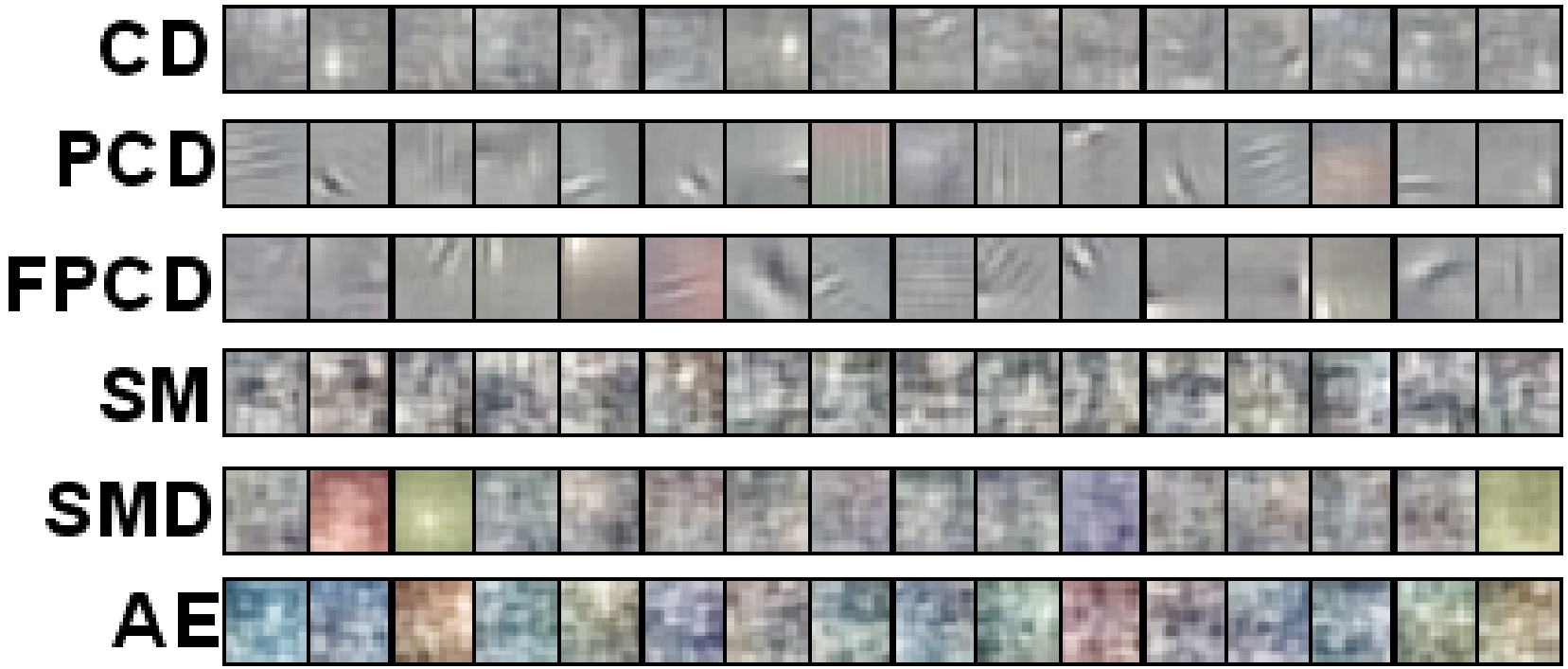
- Can we learn good features with richer autoencoder models?
- How do score matching estimators compare to maximum likelihood estimators?
- What are the effects of regularization in a score matching-based autoencoder?

Learned Features



Covariance filters

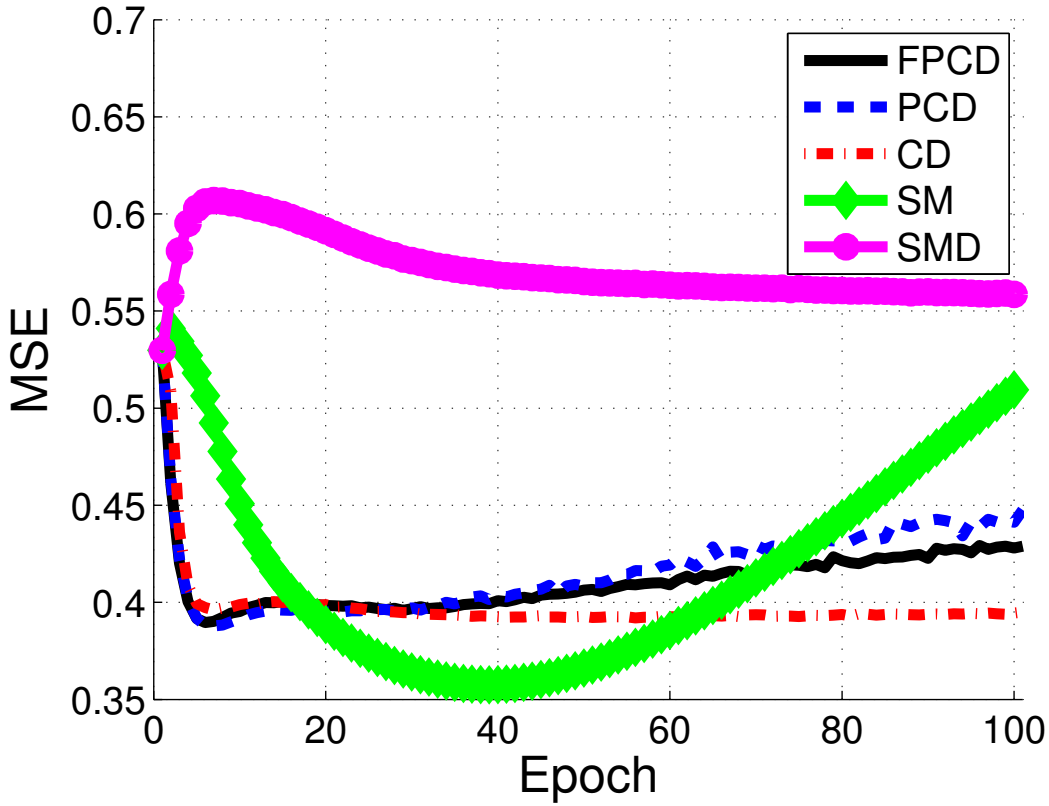
Learned Features (2)



Mean filters

Denoising

- Reconstruct an image from a blurry version
  - Finds a nearby image that has a high likelihood

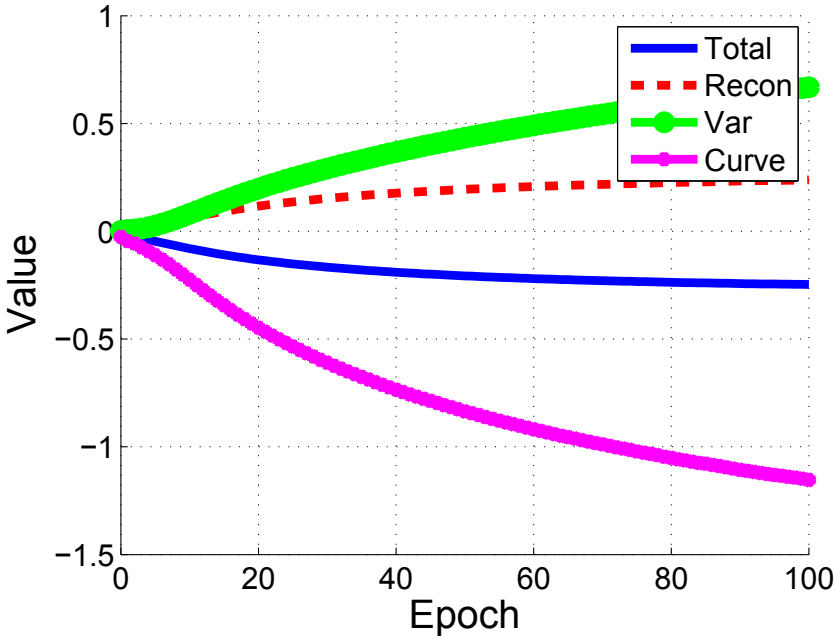


Classification on CIFAR-10

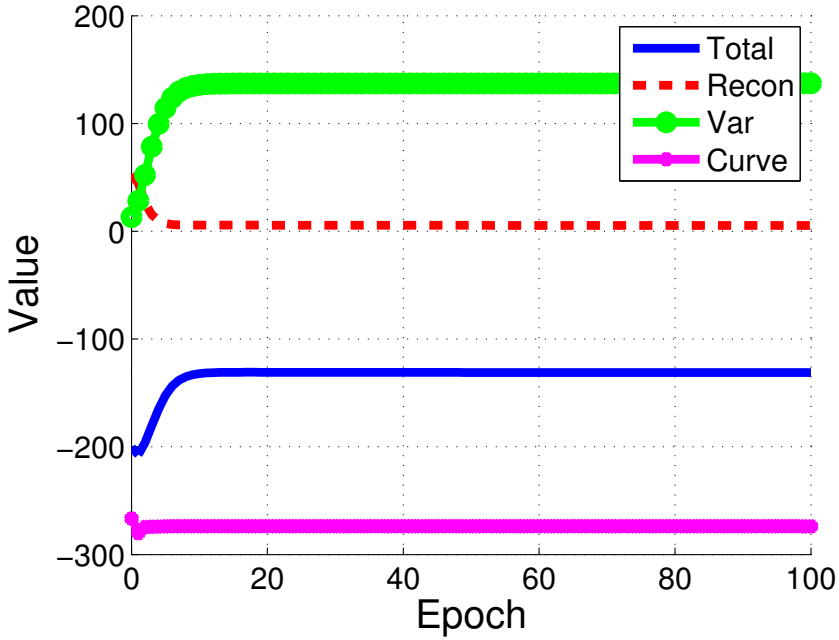
CD	PCD	FPCD	SM	SMD	AE
64.6%	64.7%	65.5%	65.0%	64.7%	57.6%

- Most methods are comparable
- mPoT autoencoder without regularization does significantly worse

Effect of Regularizers on mPoT Autoencoder



Score matching mPoT autoencoder ($\times 10^4$)



Autoencoder with no regularization

- Total (blue curve) is the sum of the other curves
- Other curves represent the 3 score matching terms

Quick Mention: Memisevic, 2011

- Roland Memisevic, a recent U of T grad published a paper in this year's ICCV
- He derived the same models through the idea of relating two different inputs using an autoencoder

Conclusion

- Score matching provides a unifying theory for autoencoders and latent energy based models
- It reveals novel regularizers for some models
- We can derive novel autoencoders that model richer structure
- We provide an interpretation of the score matching objective for all latent EBMs
- Properly shaping the implied energy of an autoencoder is one key to learning good features
  - This is done implicitly when noise is added to the input
  - Perhaps also done implicity with sparsity penalties, etc.

Future Work

- We can model other kinds of data with higher-order features by simply changing the loss function
- Extend higher-order models to deeper layers
- Apply Hessian-free optimization to EBMs and related autoencoders