

Inference and Representation

Lecture 9

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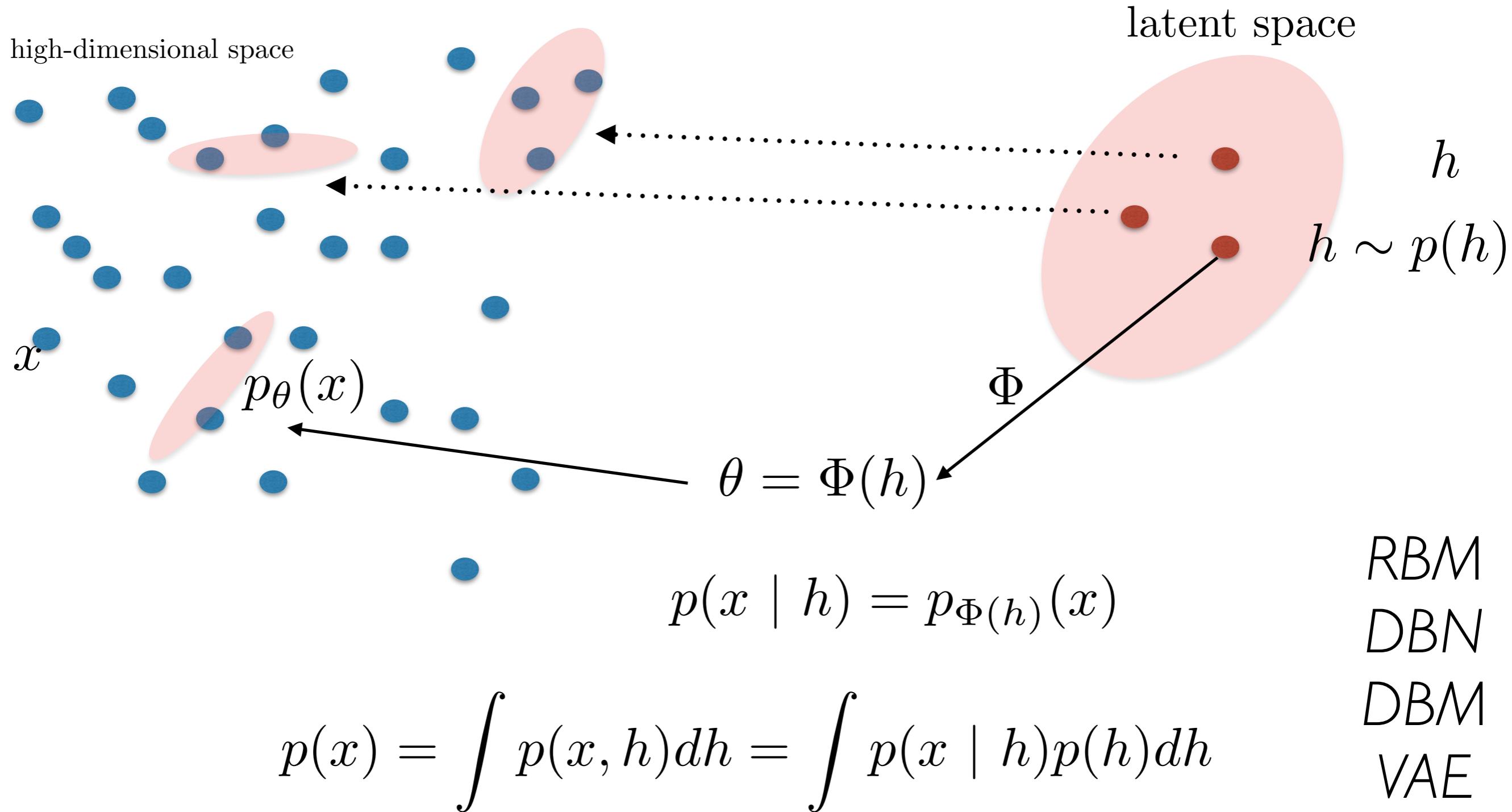


Lecture 9 Objectives

- Variational Autoencoders
- Structured Output Prediction
 - Conditional Markov Fields (CRFs)
 - Under the exponential family
 - Pseudo-likelihood methods

Latent Graphical Models

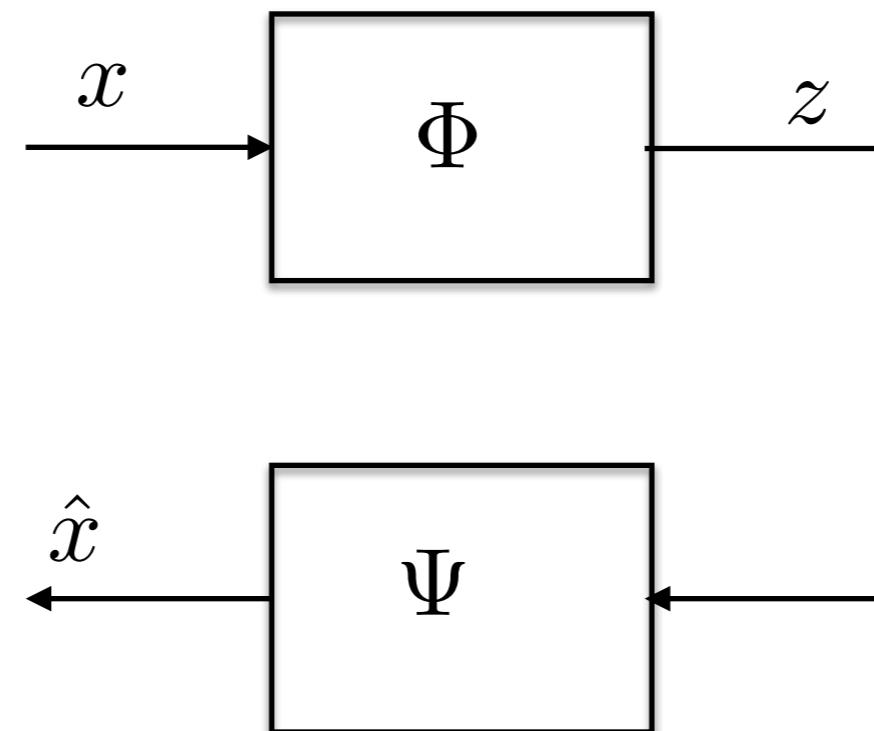
- Latent Graphical Models or *Mixtures*.



Model: additive combination of simple parametric models

Auto encoders

- Goal: given data $X = \{x_i\}$ learn a reparametrization $z_i = \Phi(x_i)$ that approximates X well with minimal capacity.



- The model contains an encoder Φ and a decoder Ψ .
- It introduces an *information bottleneck* to characterize input data from ambient space.

Auto encoders

- Motivations:
 - Dimensionality reduction:
$$x_i \in \mathbb{R}^d, \Phi : \mathbb{R}^d \rightarrow \mathbb{R}^{\tilde{d}}, \tilde{d} \ll d.$$
 - Metric learning (in sequential datasets):
$$z_t \approx \frac{1}{2}(z_{t-1} + z_{t+1})$$

*linearization in transformed domain
Slow Feature Analysis*
 - Unsupervised Pre-training (less popular nowadays): provide good initialization for supervised learning.
- Q: How to limit the reconstruction capacity?

Auto encoders

- Optimization set-up:

$$\min_{\Phi, \Psi} \frac{1}{n} \sum_{i \leq n} \ell(x_i, \Psi(\Phi(x_i))) + \mathcal{R}(\Phi(X))$$

$\ell(x, x')$: Reconstruction loss

\mathcal{R} : Regularization term

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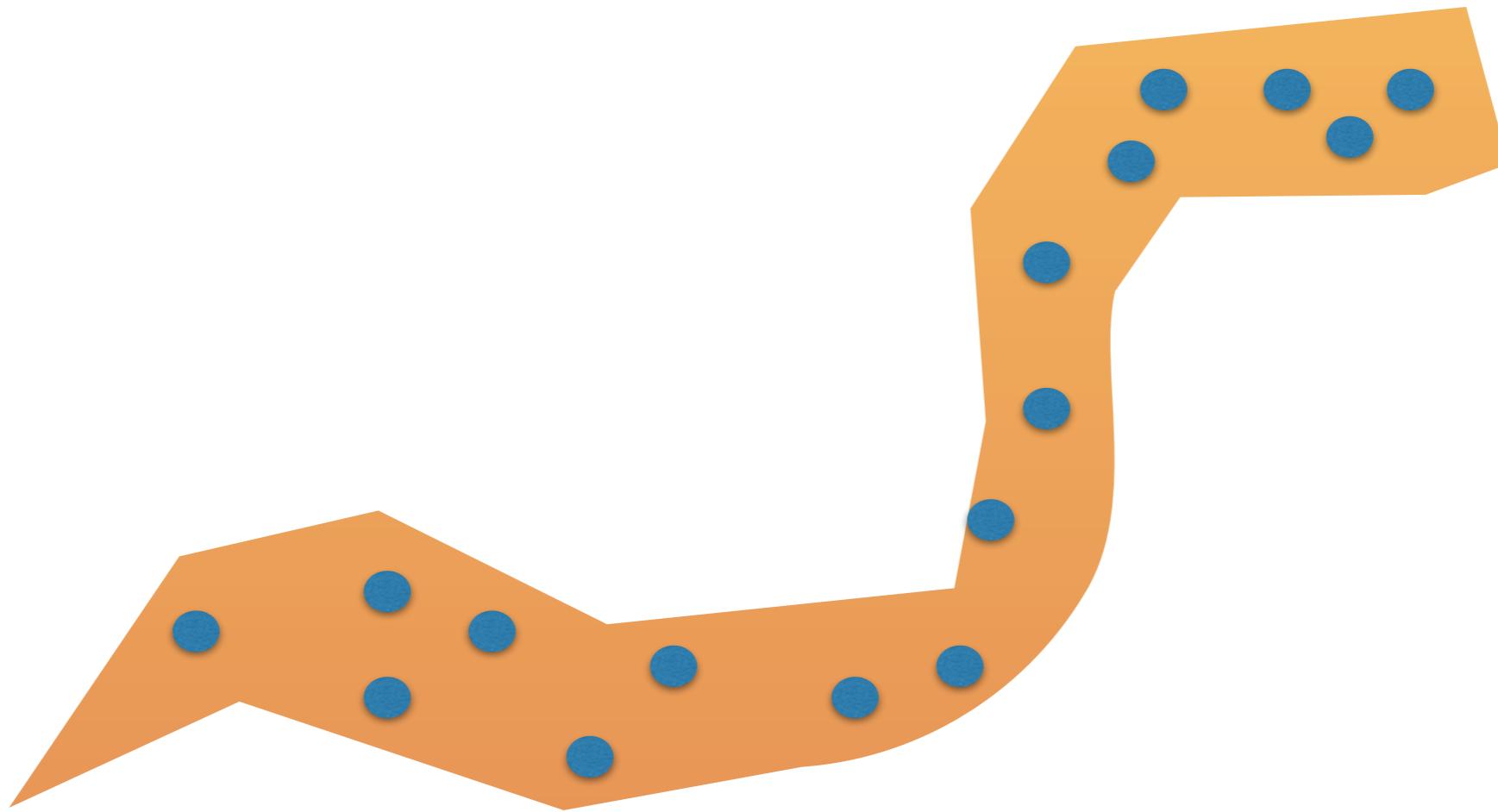
- Choice of models:
 - Ψ Linear / Non-linear.
 - $\mathcal{R}(Z) = \|Z\|_1$ (or $\|Z\|_0$) leads to sparse auto-encoders
(capacity can be measured by Gaussian Mean Width)
 - $\mathcal{R}(\Phi(x)) = \|\nabla \Phi(x)\|^2$ leads to contractive autoencoders.
 - Denoising autoencoders: limit the capacity of the channel by making it noisy.

More Examples

- Sparse Coding approximations
 - Predictive Sparse Decomposition (PSD) [Kavockoglu et al., '08] considers an Augmented Lagrangian of the Sparse Autoencoder:
$$\min_{D, Z, \Phi} \|X - DZ\|^2 + \lambda \|Z\|_1 + \alpha \|Z - \Phi(X)\|^2$$
$$\Phi(X) = \text{diag}(\beta) \tanh(WX + b)$$
 - LISTA [Gregor et al, '10]: Deeper Encoder using Recurrent weights.

Auto encoders: Geometric Interpretation

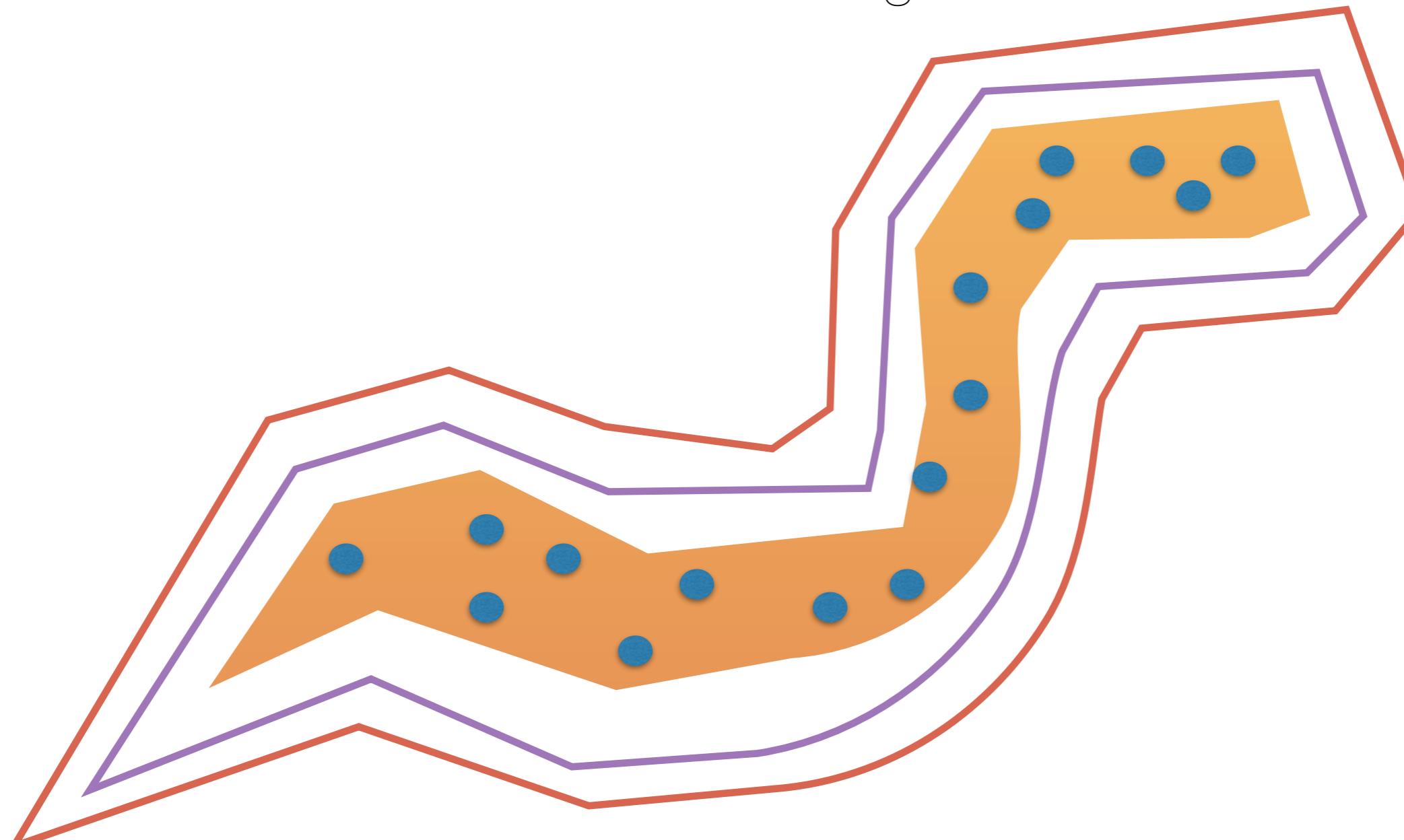
- The reconstruction error approximates a distance to a covering manifold of \mathcal{X}



$$\Omega(\epsilon) = \{x \text{ s.t. } \|\Psi(\Phi(x)) - x\| \leq \epsilon\}$$

Auto encoders: Geometric Interpretation

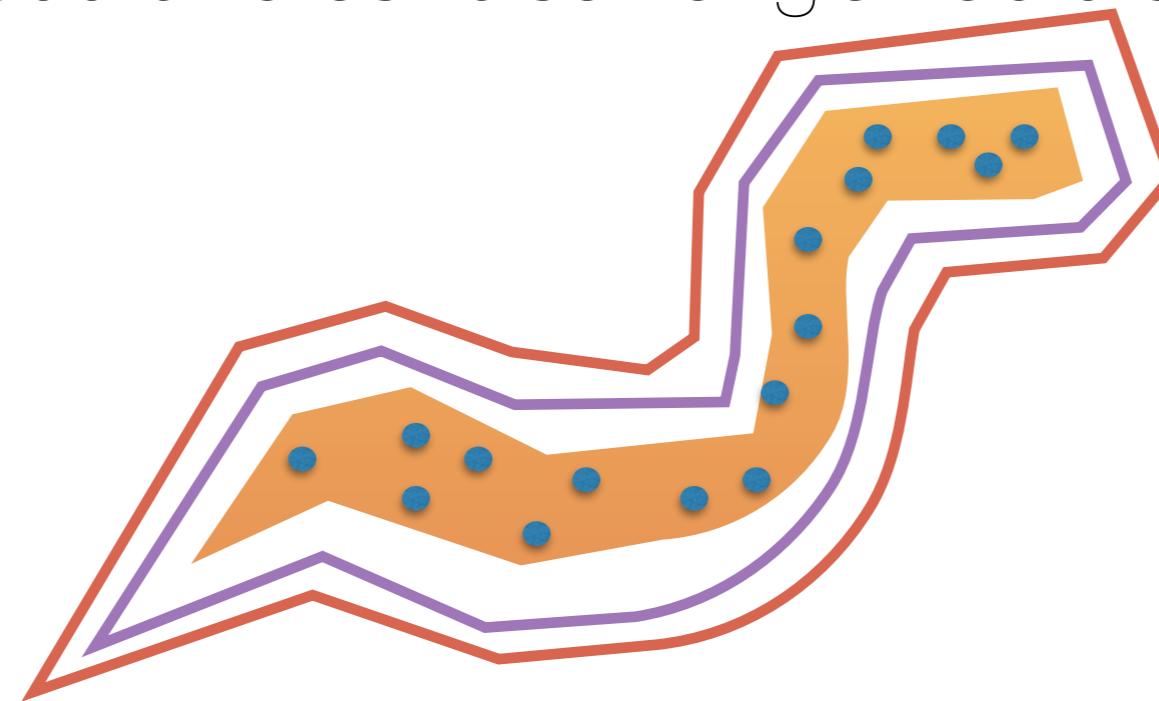
- The reconstruction error approximates a distance to a covering manifold of \mathcal{X} .
- Intrinsic manifold coordinates “disentangle” factors.



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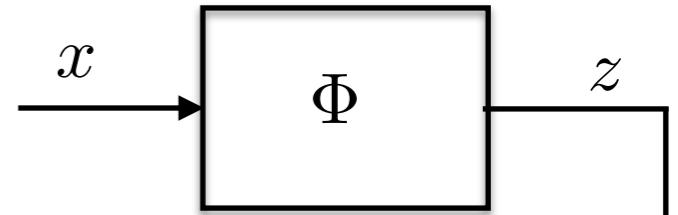


- We are thus building a representation $\Phi(\mathbf{x})$ with prescribed structure (metric, dimensionality, separation, etc.)
- Q: What is the link with inference and latent variables?

Auto encoders: Probabilistic Interpretation

- We can also interpret z as latent variables of an underlying generative model for X :

$$p(x) = \int p(z)p(x | z)dz$$



- Rather than evaluating the true posterior

$$p(z | x) = \frac{p(z)p(x|z)}{\int p(z')p(x|z')dz'}$$



we consider a point estimate $p(z | x) = \delta(z - \Phi(x))$

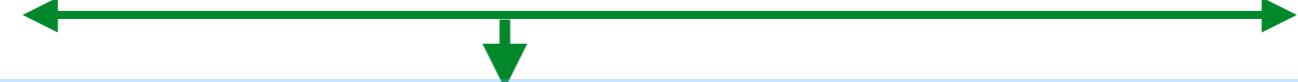
- It can model the mode (MAP) or the mean of the posterior.
- Q: How to perform "correct" posterior inference? or a better approximation?

Variational Autoencoders

[Kingma & Welling'14, Rezende et al.'14]

- Recall the variational lower bound:

$$\log p(X \mid \theta) = \mathbb{E}_{q(z|\beta)} \{ \log(p(X, Z \mid \theta)) \} + H(q(z \mid \beta)) + D_{KL}(q(z|\beta) \parallel p(z|x, \theta))$$



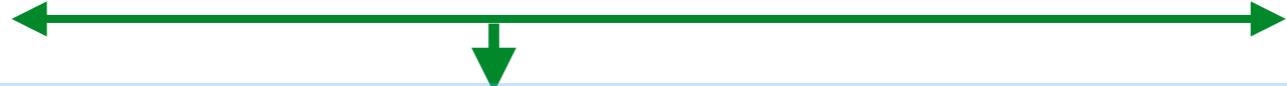
$$\log p(X \mid \theta) = \mathcal{L}(\theta, \beta, X) + D_{KL}(q(z|\beta) \parallel p(z|X, \theta))$$

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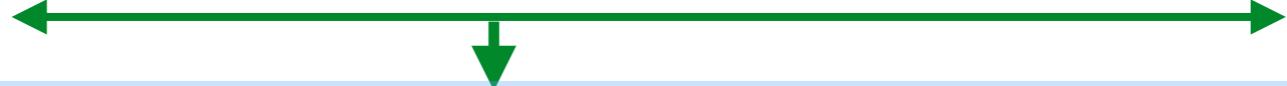
- Can we optimize jointly both generative and variational parameters efficiently?

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$$\log p(X \mid \theta) = \mathcal{L}(\theta, \beta, X) + D_{KL}(q(z|\beta) \parallel p(z|X, \theta))$$

- Can we optimize jointly both generative and variational parameters efficiently?
- For appropriate posterior approximations, we can reparametrize samples as

$$Z \sim q(z|x, \beta) \Rightarrow Z \stackrel{d}{=} g_\beta(\epsilon, x) , \quad \epsilon \sim p_0$$

$$\left(\text{e.g. } q(z|x, \beta) = \mathcal{N}(z; \mu(x), \Sigma(x)) \leftrightarrow z = \mu(x) + \Sigma(x)^{1/2}\epsilon , \quad \epsilon \sim \mathcal{N}(0, 1) \right)$$

Variational Autoencoders

- It follows that

$$\mathcal{L}(\theta, \beta, X) = -D_{KL}(q_\beta(z|X)||p_\theta(z)) + \mathbb{E}_{q_\beta(z|X)}\{\log p(X|z, \theta)\}$$

can be estimated via Monte-Carlo by

$$\widehat{\mathcal{L}(\theta, \beta, X)} = -D_{KL}(q_\beta(z|X)||p_\theta(z)) + \frac{1}{S} \sum_{s \leq S} \log p(X|z^{(s)}, \theta)$$

$$z^{(s)} = g_\beta(X, \epsilon^{(s)}) \text{ and } \epsilon^{(s)} \sim p_0 .$$

Variational Autoencoders

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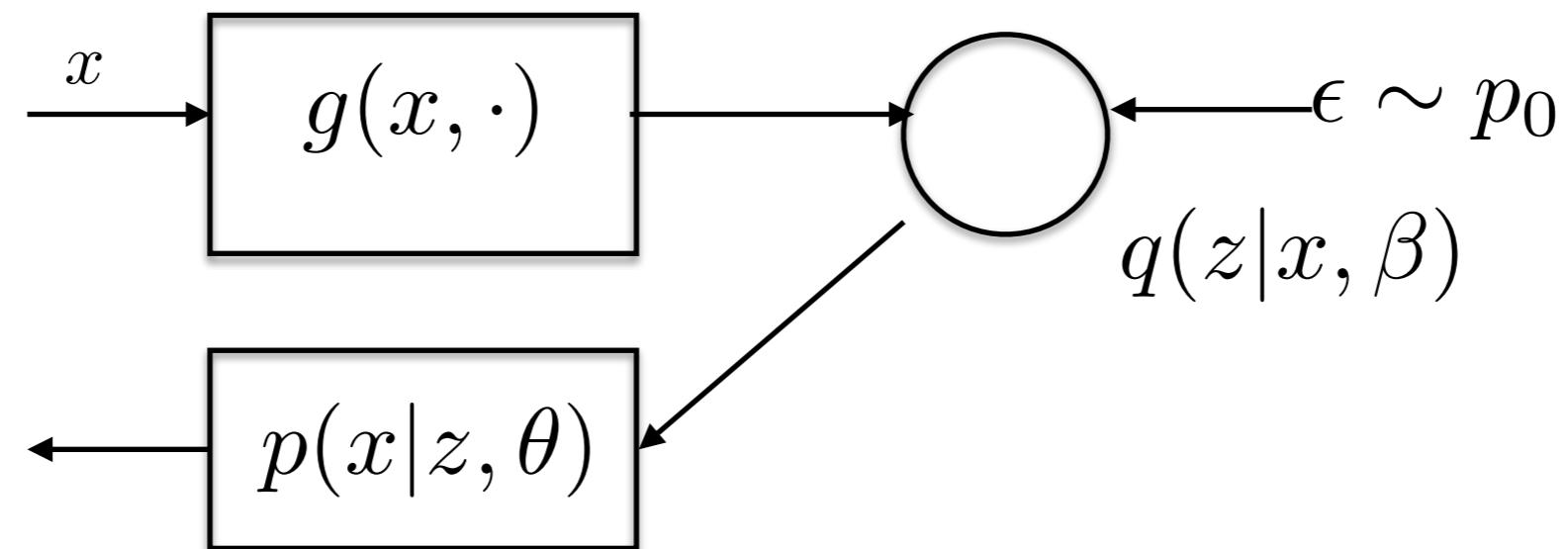
- First term acts as a regularizer: limits the capacity of the encoder
- Second term is a reconstruction error.

Variational Autoencoders

- How to model $x \mapsto g_\beta(x, \cdot)$ and $z \mapsto p_\theta(\cdot, z)$?

Variational Autoencoders

- How to model $x \mapsto g_\beta(x, \cdot)$ and $z \mapsto p_\theta(\cdot, z)$?
- VAE idea: use neural networks to approximate variational and generative parameters.



Variational Autoencoder

- Example: Let the prior over latent variables be Gaussian isotropic:

$$p(z) = \mathcal{N}(z; 0, \mathbf{I})$$

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- Let the conditional likelihood be also Gaussian:

$$p(x|z) = (x; \mu(z), \Sigma(z)) \quad \mu(z), \Sigma(z) : \text{Neural networks}$$

Variational Autoencoder

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- Let the conditional likelihood be also Gaussian:

$$p(x|z) = (x; \mu(z), \Sigma(z)) \quad \mu(z), \Sigma(z) : \text{Neural networks}$$

- Variational approximate posterior also Gaussian:

$$q_\beta(z|x) = \mathcal{N}(z; \bar{\mu}(x), \bar{\Sigma}(x))$$

$$\bar{\mu}(z), \bar{\Sigma}(z) : \text{Neural networks}, (\bar{\Sigma} \text{ diagonal})$$

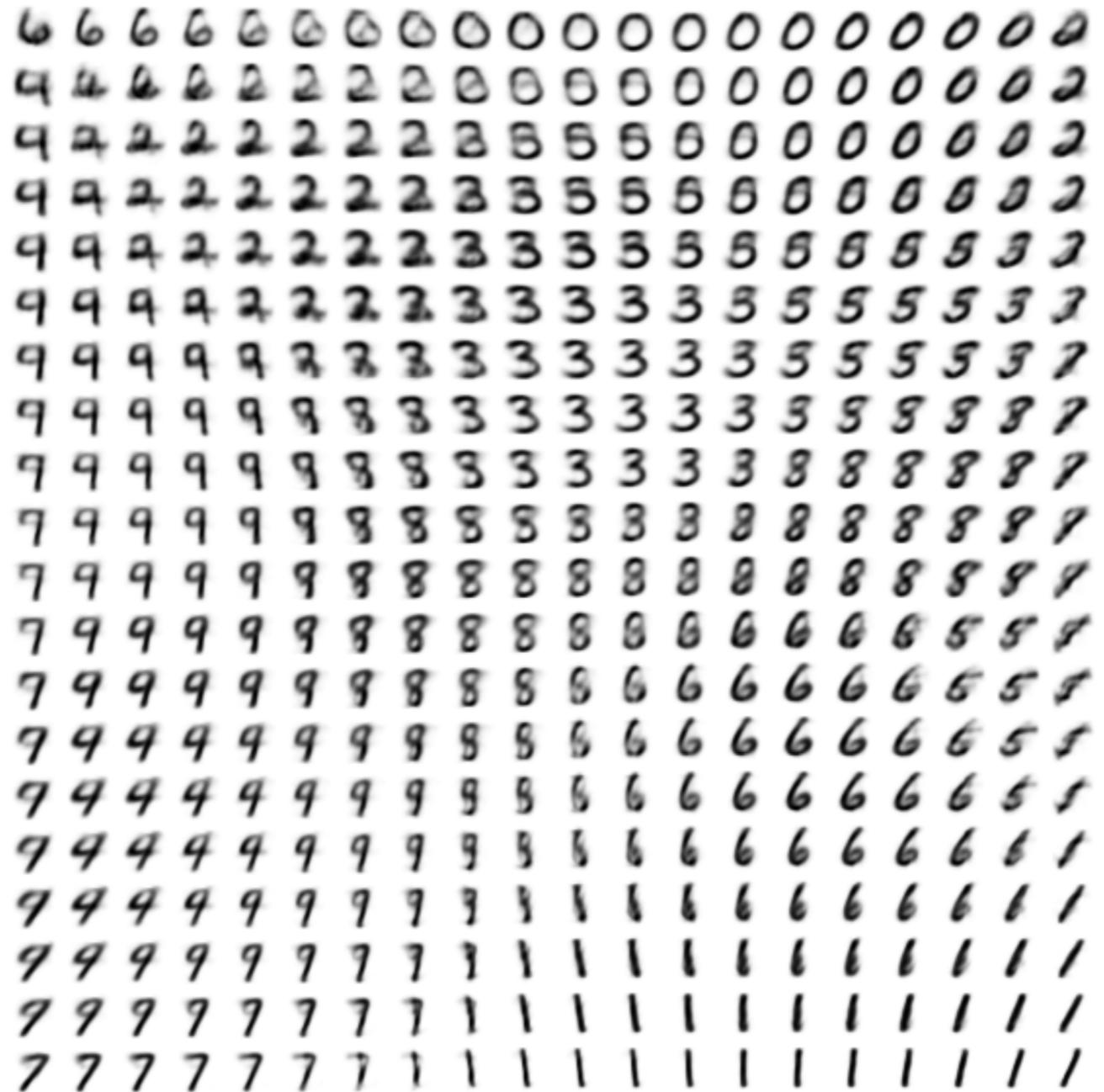
$$Z \sim q_\beta(z|x) \Leftrightarrow Z = \bar{\mu}(x) + \bar{\Sigma}(x)^{1/2}\epsilon, \quad \epsilon \sim \mathcal{N}(0, 1)$$

Variational Autoencoder

- Examples using a two-dimensional latent space:



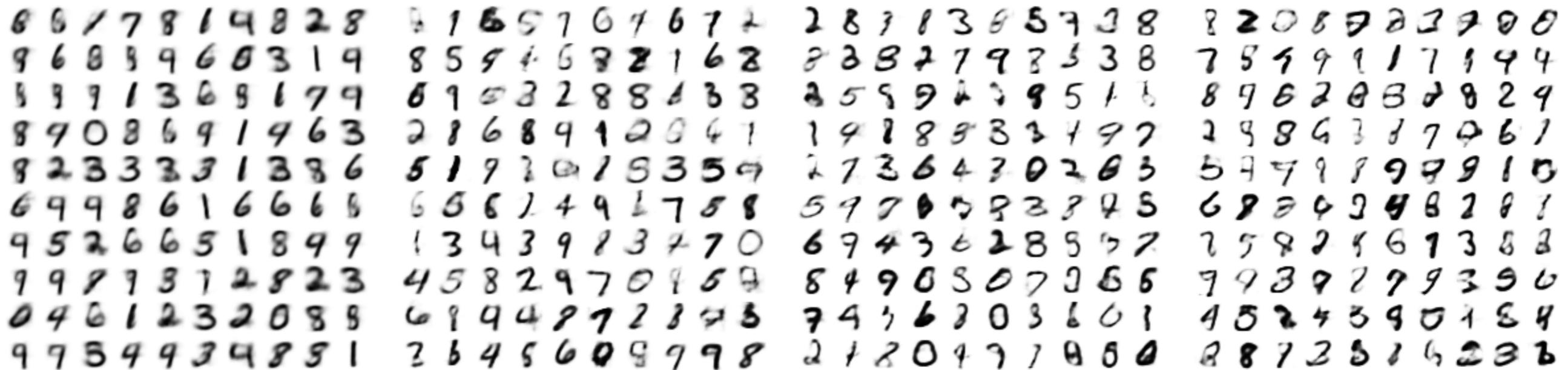
(a) Learned Frey Face manifold



(b) Learned MNIST manifold

Examples

- Increasing latent dimensionality:



(a) 2-D latent space

(b) 5-D latent space

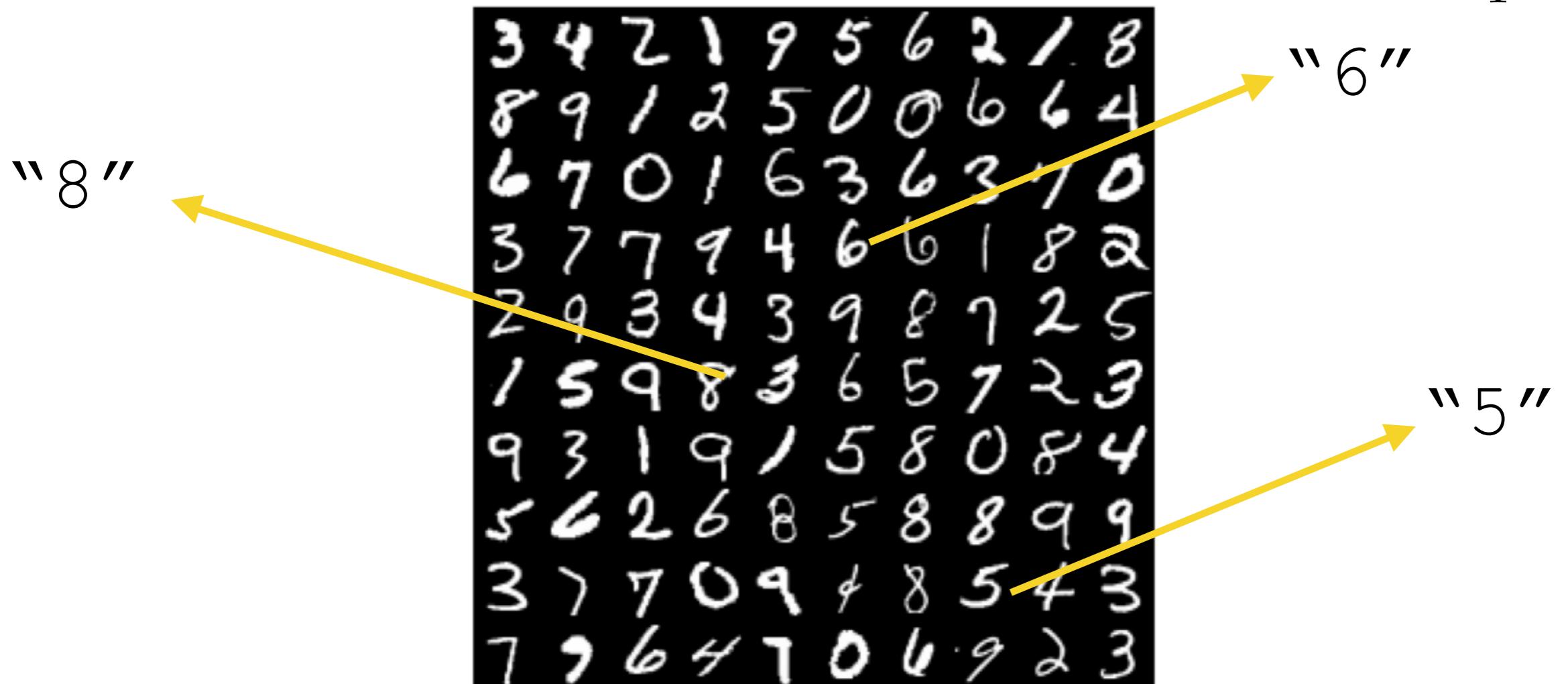
(c) 10-D latent space

(d) 20-D latent space

Extensions to semi-supervised learning

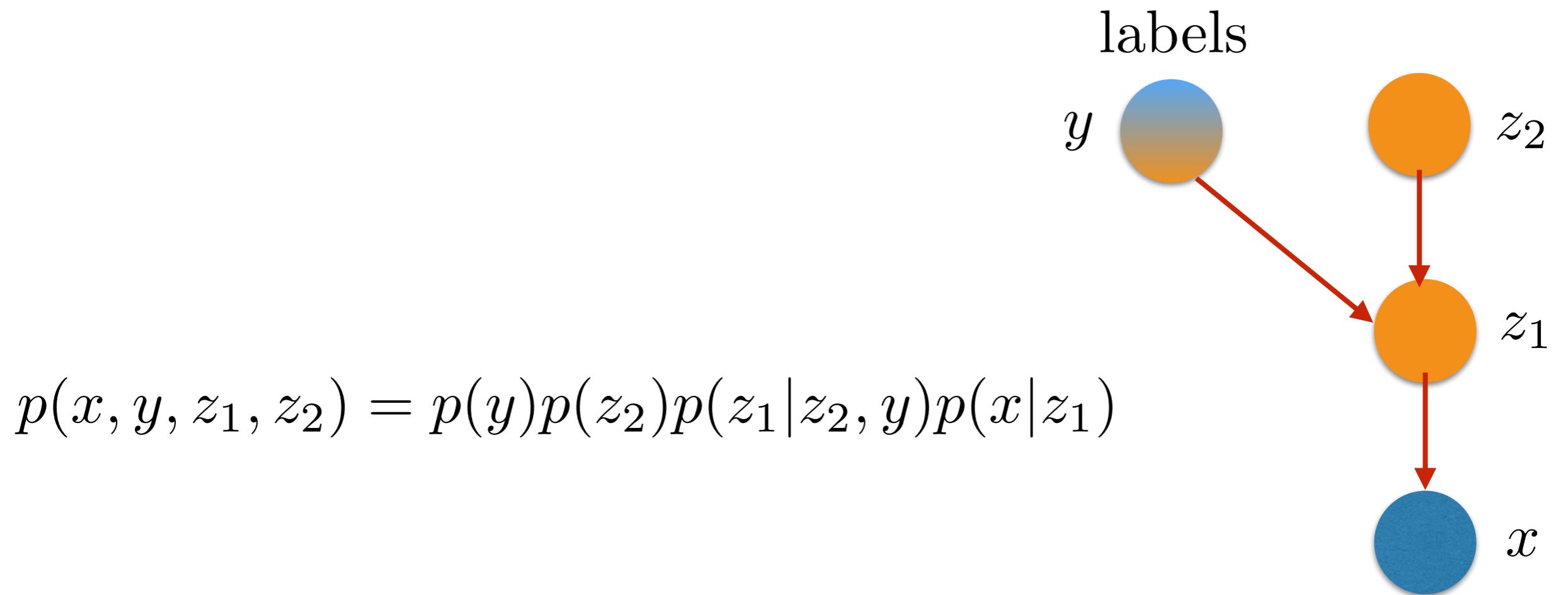
- Semi-supervised learning:

We observe $\{x_i\}_{i \leq L_1}$ and $\{x_j, y_j\}_{j \leq L_2}$, with $x_i \sim p(x)$, $x_j \sim p(x)$.
 $L_1 \gg L_2$



Extensions to semi-supervised learning

- "Semi-supervised Learning with Deep Generative Networks", Kingma et al,'14.
- Labels are treated as either observed or hidden.



Extension to Semi-Supervised Learning

- "Semi-supervised Learning with Deep Generative Networks", Kingma et al,'14.

- For datapoint with labels:

$$\log p_{\theta}(x, y) \geq \mathbb{E}_{q_{\beta}(z|x, y)} (\log p_{\theta}(x|y, z) + \log p_{\theta}(y) + \log p(z) - \log q_{\beta}(z|x, y))$$

- For datapoint with no labels:

$$\log p_{\theta}(x) \geq \mathbb{E}_{q_{\beta}(y, z|x)} (\log p_{\theta}(x|y, z) + \log p_{\theta}(y) + \log p(z) - \log q_{\beta}(z, y|x))$$

Extension to Semi-Supervised Learning

- “*Semi-supervised Learning with Deep Generative Networks*”, Kingma et al,’14.
- Classification results on MNIST:

Table 1: Benchmark results of semi-supervised classification on MNIST with few labels.

N	NN	CNN	TSVM	CAE	MTC	AtlasRBF	M1+TSVM	M2	M1+M2
100	25.81	22.98	16.81	13.47	12.03	8.10 (± 0.95)	11.82 (± 0.25)	11.97 (± 1.71)	3.33 (± 0.14)
600	11.44	7.68	6.16	6.3	5.13	–	5.72 (± 0.049)	4.94 (± 0.13)	2.59 (± 0.05)
1000	10.7	6.45	5.38	4.77	3.64	3.68 (± 0.12)	4.24 (± 0.07)	3.60 (± 0.56)	2.40 (± 0.02)
3000	6.04	3.35	3.45	3.22	2.57	–	3.49 (± 0.04)	3.92 (± 0.63)	2.18 (± 0.04)

- Now there are stronger models on that task.
 - Ladder-Networks [Rasmus et al'15]
 - GANs [Salimans et al'16]
 - Graph Neural Networks [Kipf & Welling, '17].

Extension to Semi-Supervised Learning

- “Semi-supervised Learning with Deep Generative Networks”, Kingma et al,’14.
- Disentangling label and “style”:

2 2 2 2 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3 4 4 4 4 4 4 4 4 4 4
2 2 2 2 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3 4 4 4 4 4 4 4 4 4 4
2 2 2 2 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3 4 4 4 4 4 4 4 4 4 4
2 2 2 2 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3 4 4 4 4 4 4 4 4 4 4
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2 2 2 2 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3 4 4 4 4 4 4 4 4 4 4

(a) Handwriting styles for MNIST obtained by fixing the class label and varying the 2D latent variable \mathbf{z}

4 0 1 2 3 4 5 6 7 8 9
9 0 1 2 3 4 5 6 7 8 9
5 0 1 2 3 4 5 6 7 8 9
4 0 1 2 3 4 5 6 7 8 9
2 0 1 2 3 4 5 6 7 8 9
7 0 1 2 3 4 5 6 7 8 9
5 0 1 2 3 4 5 6 7 8 9
1 0 1 2 3 4 5 6 7 8 9
7 0 1 2 3 4 5 6 7 8 9
1 0 1 2 3 4 5 6 7 8 9

(b) MNIST analogies



(c) SVHN analogies

Incorporate MCMC to posterior approx.

“*Markov Chain Monte Carlo and Variational Inference: Bridging the Gap*”, Salimans et al’15

- We saw in Lecture 7 how to use Markov Chains to approximate intractable posteriors.

$$p(z \mid x) \stackrel{d}{=} \lim_{T \rightarrow \infty} q_0(z_0 \mid x) \prod_{t \leq T} q(z_t \mid z_{t-1}, x) .$$

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- For fixed T , this can be seen as another variational approximation, by considering $y = z_1, \dots, z_{T-1}$ as extra hidden variables.

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- The resulting Variational Lower bound becomes

$$\begin{aligned}\mathcal{L}_{MCMC} &= \mathcal{L} - \mathbb{E}_{q(z_T \mid x)} \{ D_{KL}(r(y|z_T, x) \parallel q(y \mid z_T, x)) \} \\ &\leq \mathcal{L} \leq \log p(x) .\end{aligned}$$

$r(y|x, z_T)$: auxiliary variational approximation

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$$\begin{aligned}\mathcal{L}_{aux} &= \mathcal{L} - \mathbb{E}_{q(z_T|x)}\{D_{KL}[q(y|z_T, x) \parallel r(y|z_T, x)]\} \\ &\leq \mathcal{L} \leq \log p(x).\end{aligned}$$

$r(y|x, z_T)$: auxiliary variational approximation

- If we choose r to be an inverse Markov chain, we obtain

$$\mathcal{L}_{aux} = \mathbb{E}_q \{\log p(x, z_T) - \log q(z_0|x)\} + \sum_{t=1}^T (\log r_t(z_{t-1}|x, z_t) - \log q_t(z_t|x, z_{t-1}))$$

Incorporate MCMC to posterior approx.

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- The authors consider Hamilton Monte-Carlo as MCMC choice, resulting in Hamiltonian Variational Inference.
- It provides a flexible (albeit more computationally demanding) variational approximation that can be adjusted with the number T of MCMC steps.

Variational inference with Importance Sampling

“Importance Weighted Autoencoders”

Burda et al’16

- Another mechanism to improve the variational lower bound is to use importance sampling.

Variational inference with Importance Sampling

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- For each k , we define

$$\mathcal{L}_k(x) = \mathbb{E}_{z_1, \dots, z_k \sim q(z|x)} \left[\log \frac{1}{k} \sum_{i=1}^k \frac{p(x, z_i)}{q(z_i|x)} \right].$$

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- It follows that

$$\forall k , \log p(x) \geq \mathcal{L}_{k+1}(x) \geq \mathcal{L}_k(x) , \text{ and}$$

$$\lim_{k \rightarrow \infty} \mathcal{L}_k(x) = \log p(x) \text{ if } \frac{p(x, z)}{q(z|x)} \text{ is bounded .}$$

Structured Output Prediction

- Conditional Random Fields (CRF) [Lec 9]
- Parameter Learning in the Exponential Family
 - ML / Maximum Entropy
 - Monte-Carlo
- Pseudo-likelihood
- MAP Inference
 - Max-Product
- Sequence-to-Sequence Models
- Unrolling BP with Graph Neural Networks.

Conditional Random Fields (CRF)

- Goal: Model structured outputs Y from observations X

Computer vision
Image segmentation

input: image



output: segmentation



Stereopsis

input: two images

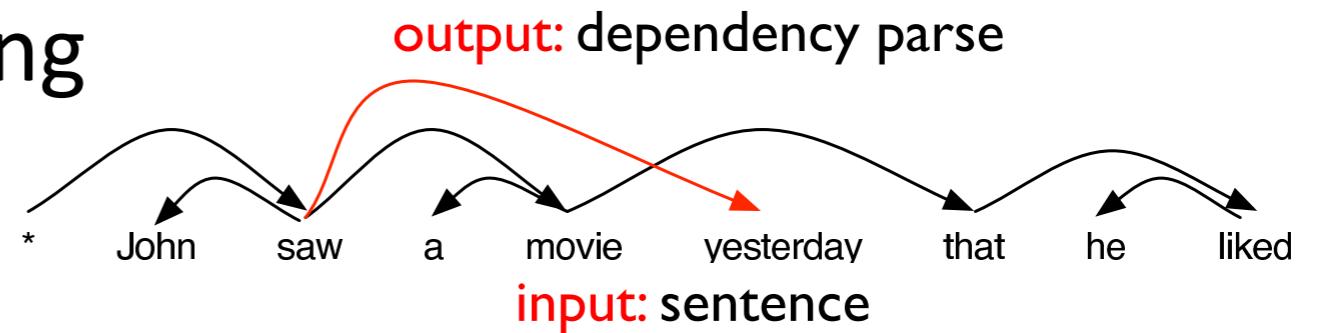


output: disparity



Natural language processing
Parsing

output: dependency parse



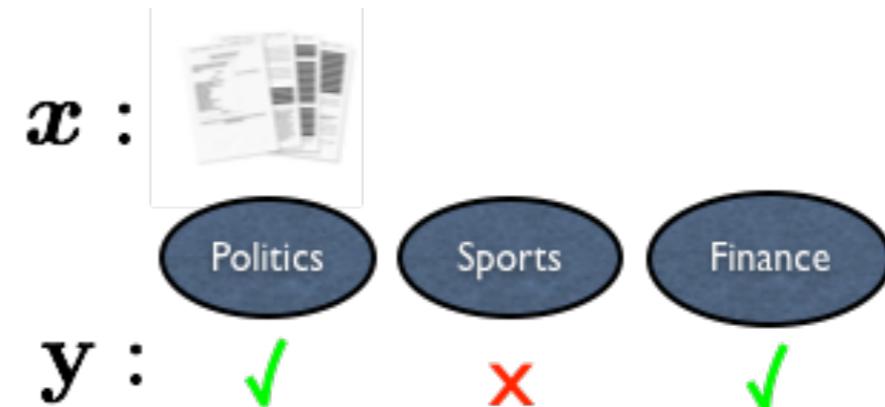
input: sentence

Conditional Random Fields (CRF)

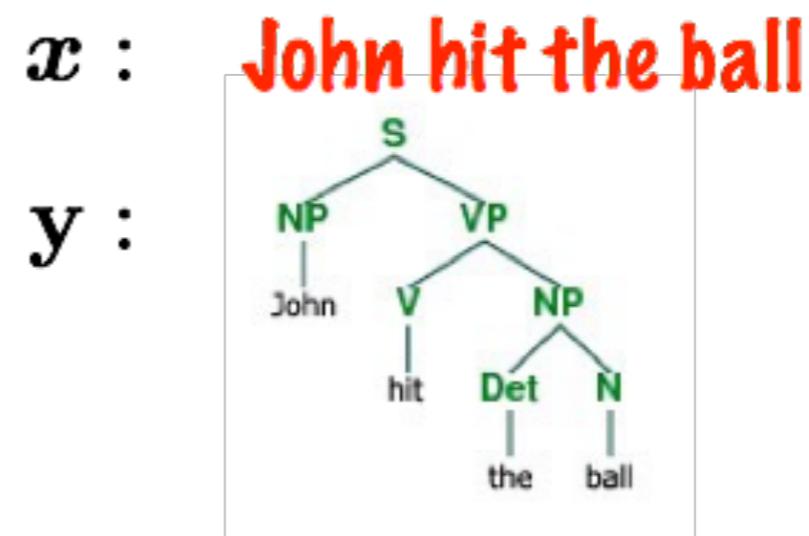
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- **Examples:**

- **Multi-label prediction:**



- **Natural language parsing:**

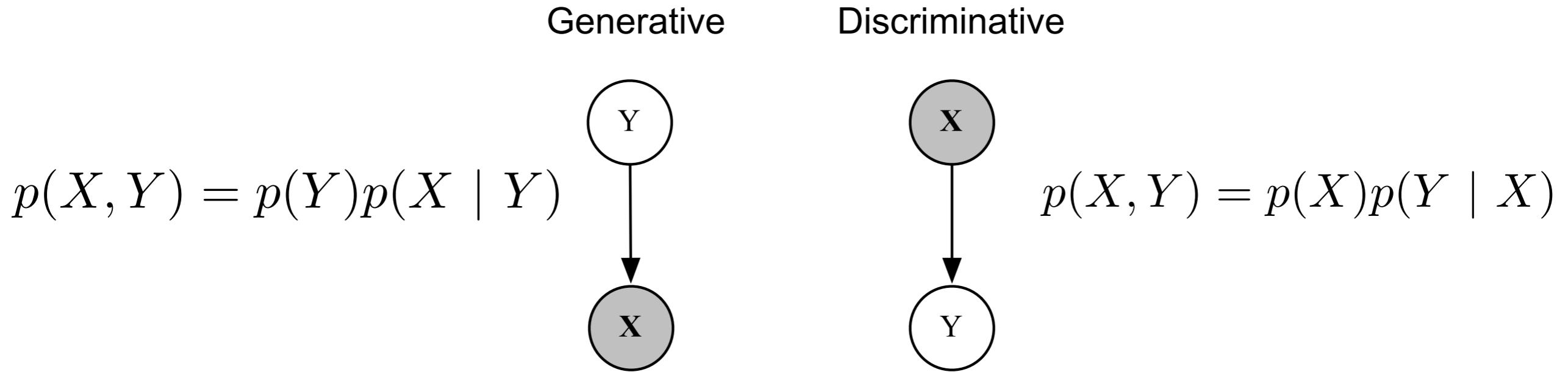


- **Protein side-chain placement:**



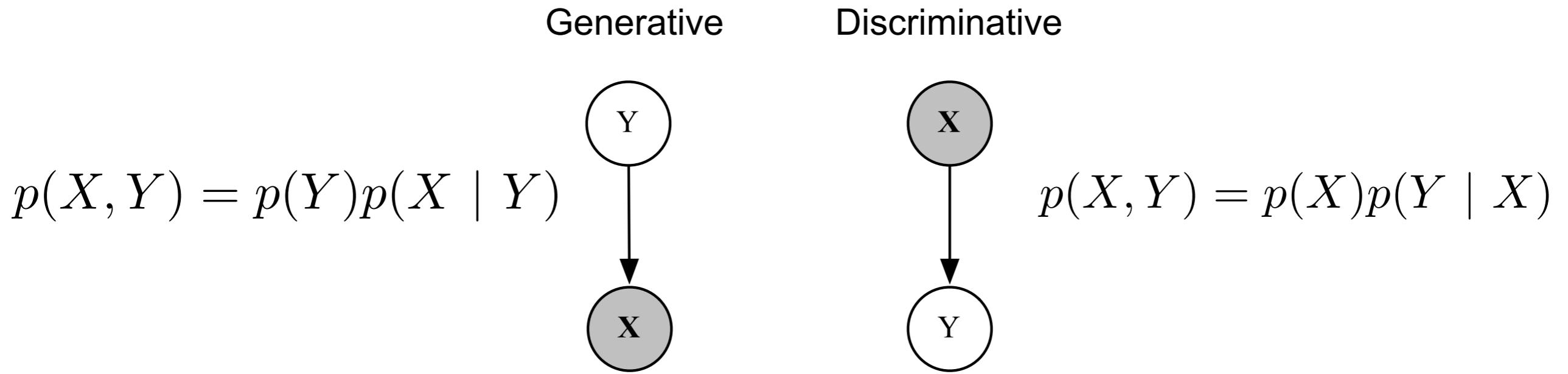
Discriminative vs Generative Models

- Two equivalent models for $p(X, Y)$:



Discriminative vs Generative Models

- Two equivalent models for $p(X, Y)$:



- However, in some setups, we only care about prediction $p(Y \mid X)$
- In the generative setup, we need to estimate both $p(Y)$ and $p(X|Y)$
 - If $\dim(X) \gg \dim(Y)$, this is exponentially harder than directly estimating $p(Y|X)$!!

Conditional Random Fields (CRF)

- CRFs are undirected graphical models for the conditional distribution $p(Y|X)$ (Y = target variables, X = observed variables).
- A particular case of what we have seen so far:

$$p(Y|X = x) = \frac{1}{Z(x)} \prod_{c \in \mathcal{C}} \phi_c(x_c, y_c) ,$$

$$Z(x) = \sum_y \prod_{c \in \mathcal{C}} \phi_c(x_c, y_c) .$$

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- The only difference with unconditional MRF is the normalization:
 - In a CRF, we marginalize only over Y .
 - In a MRF, we marginalize over both X, Y .

CRFs

- We will consider the exponential family parametrization:

$$\phi_c(x_c, y_c) = \exp(\langle w_c, f(x_c, y_c) \rangle)$$

- adjustable weights: w_c
- feature vector: $f(x_c, y_c)$
- Special, important case: $w_c = w \quad \forall c \in \mathcal{C}.$ (weight sharing).

CRFs

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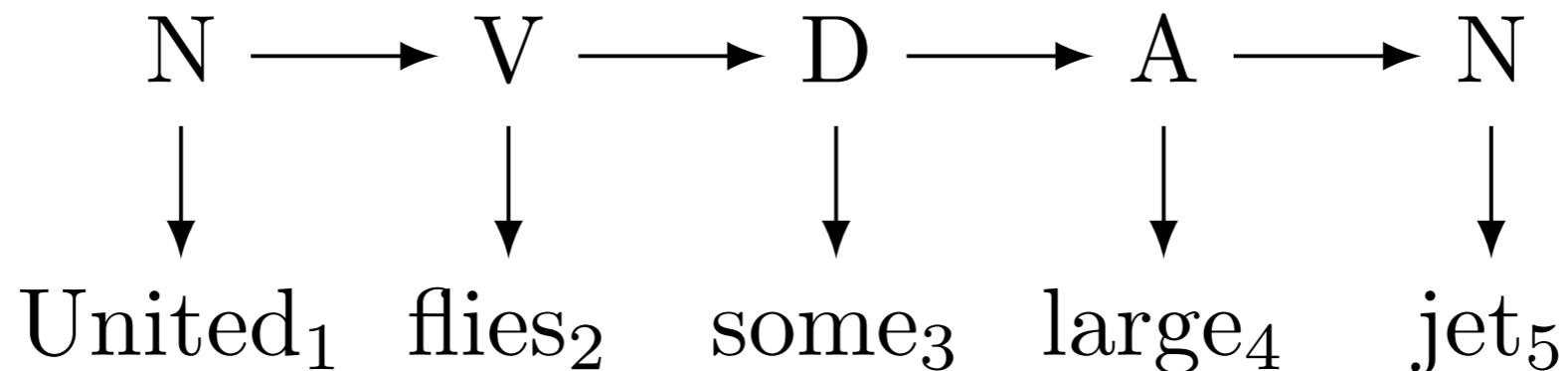
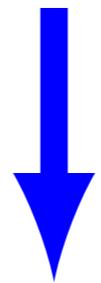
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- feature vector: $f(x_c, y_c)$
- Special, important case: $w_c = w \quad \forall c \in \mathcal{C}$. (weight sharing).
- We can always reduce to the weight sharing case by *lifting* the sufficient statistics (how?)

CRF Examples

- Part-of-Speech Tagging:

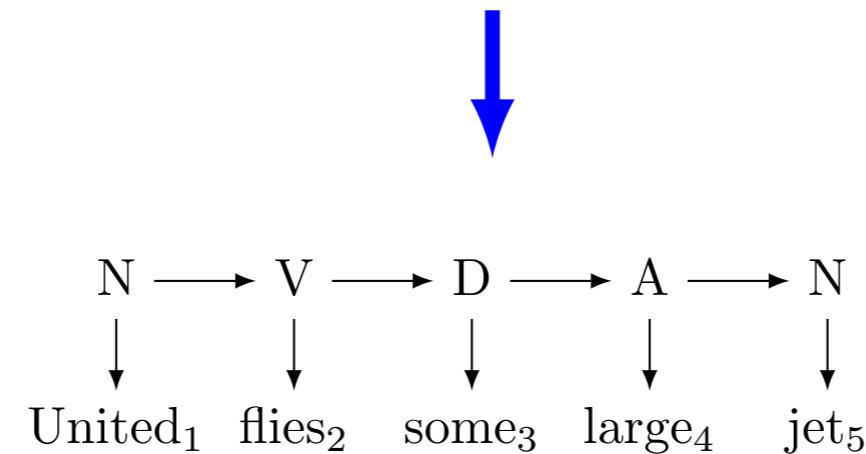
United flies some large jet



CRF Examples

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United flies some large jet



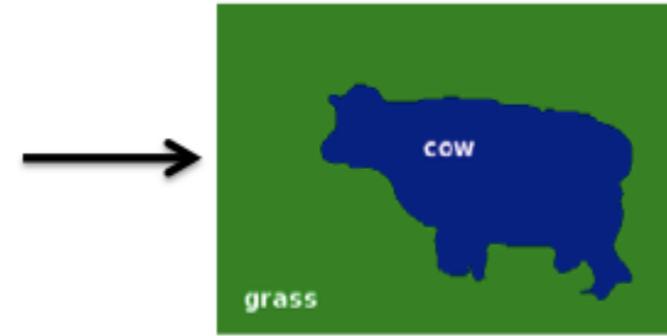
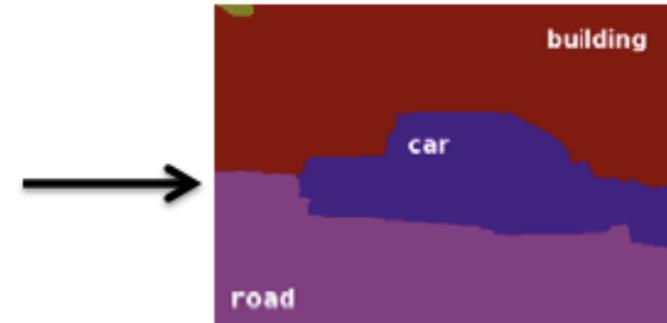
- Model:

- A sentence of length n and a tag set \mathcal{T} .
- One variable taking values in \mathcal{T} for each word.
- Edge potentials $\theta(i - 1, i, t', t)$, $i \in 2, n$, $t, t' \in \mathcal{T}$.
- Ex: $\mathcal{T} = \{A, D, N, V\}$.

CRF Examples

- Parametrization using exponential family:
 - Weights: $w \in \mathbb{R}^d$
 - Feature vectors $f_c(x, y_c) \in \mathbb{R}^d$.
 - ❖ presence or absence of certain attributes of each word (e.g. capitalization, "ing").
 - ❖ conditional on the whole input sequence x
- Unary potentials: $\phi_c(x, y_c; w) = \exp(\langle w, f_c(x, y_c) \rangle)$
- Edge potentials: Fully parametrized $\mathcal{T} \times \mathcal{T}$ and stationary, i.e.
$$\theta(i-1, i, t', t) = \bar{w}_{t', t}$$
- Weights are shared for all nodes/edges.

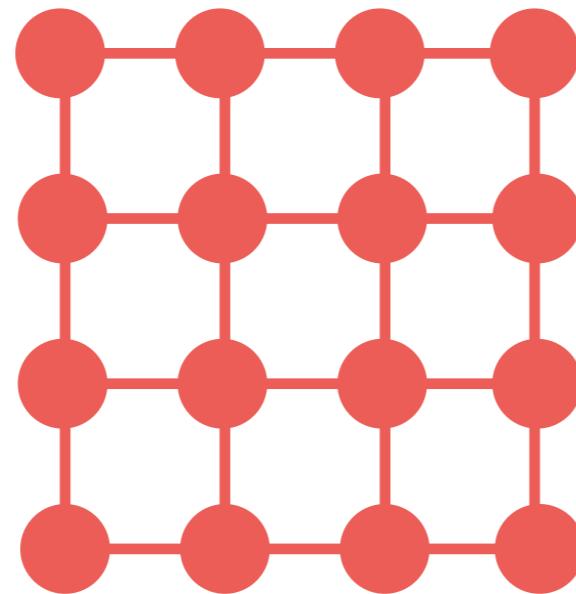
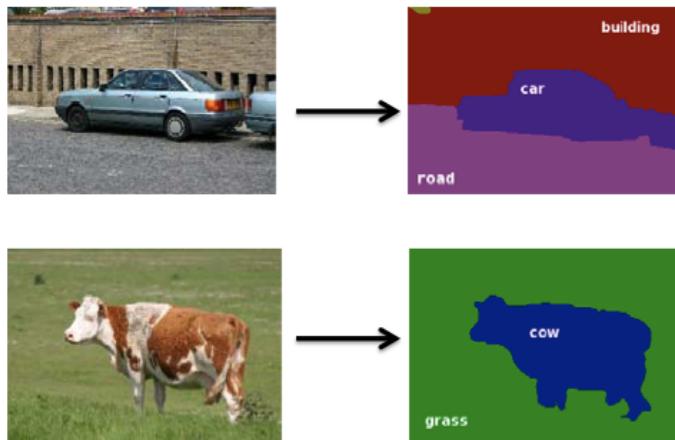
CRF Examples: Semantic Segmentation



- Given an image $I(u)$, $u \in \Omega \subset \mathbb{R}^2$, produce a label map

$$Y(u) \in \{1, K\}, u \in \Omega$$

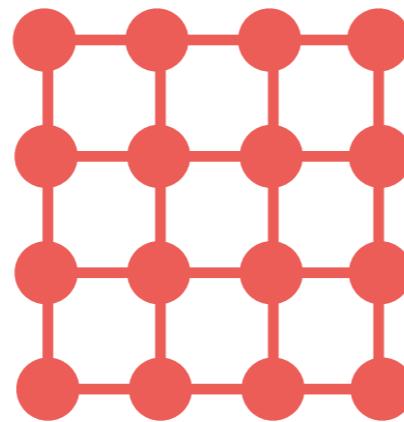
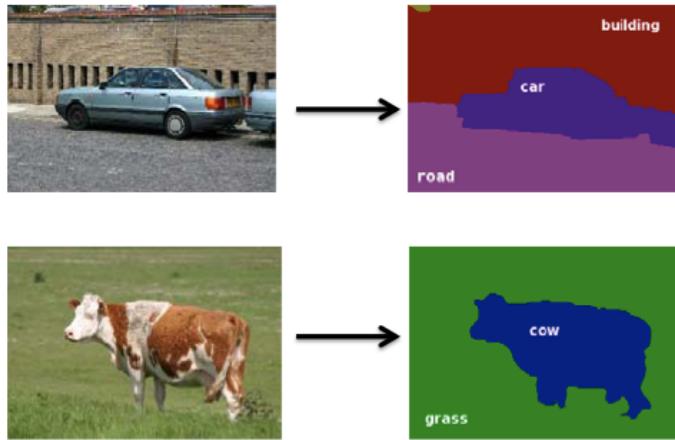
CRF Examples: Semantic Segmentation



- Define a CRF on the graph defined by the square grid.
 - Neighboring pixels with similar colors are likely to have the same label.
 - E.g.

$$\phi_{i,j} = \exp \{ (-\mathbf{1}(y_i = y_j) + \mathbf{1}(y_i \neq y_j)) |x_i - x_j| \}$$

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- Single node potentials over labels, e.g. a CNN which sees a local patch around the target pixel.
- MAP estimation over Y :

$$Y^* = \arg \max_Y \log P(Y \mid X) .$$

CRF Examples: Named-Entity Recognition

- Given a sentence, determine the people/entities involved and the relevant locations:

"Mrs Green spoke today in New York. Green chairs the finance committee"

- Entities sometimes span multiple words. Require the context to disambiguate.

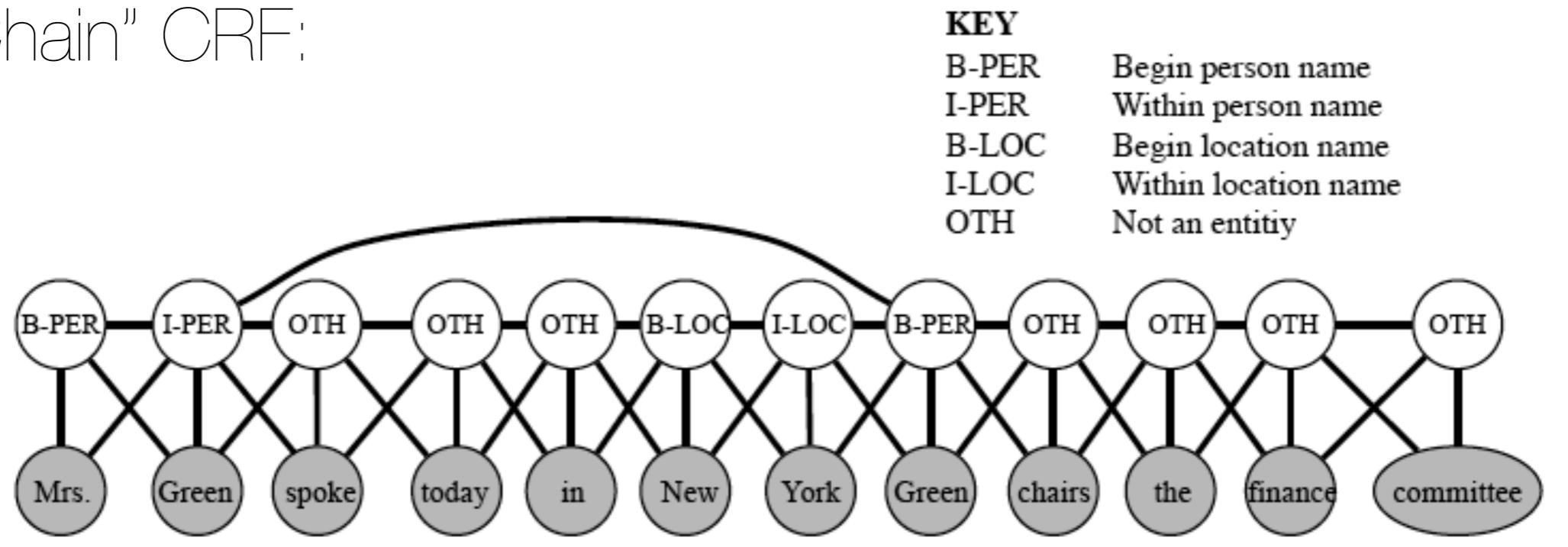
CRF Examples: Named-Entity Recognition

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"Mrs Green spoke today in New York. Green chairs the finance committee"
- Entities sometimes span multiple words. Require the context to disambiguate.
- CRF has a variable Y_i for each word, encoding the possible labels of that word.
 - E.g. "B-person, I-person, B-location, I-location, B-organization, I-organization"
 - ❖ Beginning (B) and within (I) allows the model to segment adjacent entities.

CRF Examples: named-entity recognition

- “Skip-Chain” CRF:



- Three types of potentials:

- $\phi^A(Y_i, Y_{i+1})$ models dependencies between neighboring target variables (such as in a HMM).
- $\phi^B(Y_i, Y_j)$ for all pairs (i, j) such that $x_i = x_j$, since it is likely the same word represents the same entity.
- $\phi^C(Y_i, X_1, \dots, X_T)$ for dependencies between entity and the word input sequence.

Reminder: Exponential Families

- The exponential family associated with ϕ is defined as the parametric family

$$p_\theta(x) = \exp\{\langle \theta, \phi(x) \rangle - A(\theta)\} , \text{ with}$$

$$A(\theta) = \log \int \exp\{\langle \theta, \phi(x) \rangle\} dx \quad \text{log-partition function}$$

- It is well defined for the family of parameters

$$\Omega = \{\theta ; A(\theta) < \infty\}$$

- Several well-known models belong to the exponential family:
 - Energy based models
 - Gaussian Mixtures
 - Latent Dirichlet Allocation

Reminder: Exponential Families

- **Proposition:** The log-partition function $A(\theta)$ satisfies

$$\frac{\partial A}{\partial \theta_k}(\theta) = \mathbb{E}_\theta\{\phi_k(X)\} = \int \phi_k(x)p_\theta(x)dx .$$

$A(\theta)$ is convex in its domain Ω .

$$\frac{\partial^2 A}{\partial \theta_k \partial \theta_l}(\theta) = \mathbb{E}_\theta\{[\phi_k(X) - \mathbb{E}(\phi_k(X))][\phi_l(X) - \mathbb{E}(\phi_l(X))]\} .$$

- Higher order derivatives always exist.

Learning under the Exponential Family

- Let us start with Maximum-Likelihood.

- On a MRF,

$$p(x; \theta) = \frac{1}{Z(\theta)} \exp \left(\sum_{c \in \mathcal{C}} \phi_c(x_c; \theta) \right)$$

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- The optimization is NOT separable into cliques.

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- Suppose $p(x)$ is in the exponential family with shared parameters across cliques, ie

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- Then

$$\log p(x^1, \dots, x^L; \theta) = \left\langle \theta, \sum_{c \in \mathcal{C}} L^{-1} \sum_{l \leq L} f(x_c^l) \right\rangle - A(\theta) .$$

- With

$$A(\theta) = \log \int \exp \left(\langle \theta, \sum_{c \in \mathcal{C}} f_c(x_c) \rangle \right) dx .$$

- No closed form solution for MLE!

Learning under the Exponential Family

$$\mathcal{L}(\theta) = \log p(x^1, \dots, x^L; \theta) = \left\langle \theta , \sum_{c \in \mathcal{C}} L^{-1} \sum_{l \leq L} f_c(x_c^l) \right\rangle - A(\theta).$$

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- MLE is a convex (concave) optimization problem (why?).

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- Thus

$$\frac{\partial \mathcal{L}(\theta)}{\partial \theta} = \bar{f} - \mathbb{E}_\theta\{f\}$$

Empirical average Population average

MLE under Exponential Family

$$\text{MLE: } \sup_{\theta} \langle \theta, f(x) \rangle - A(\theta)$$

- Q1: Have we seen this function before?

$$\frac{\partial \mathcal{L}(\theta)}{\partial \theta} = \bar{f} - \mathbb{E}_{\theta}\{f\}$$

- Q2: How to implement this ascent algorithm in practice?

MLE and Maximum Entropy

- Recall that

$$A^*(\mu) = \sup_{\theta} \langle \theta, f(x) \rangle - A(\theta)$$

is the convex conjugate of the log-partition function.

- $A^*(\mu)$ = (negative) maximum entropy of any distribution p such that $\mathbb{E}_{X \sim p} f(X) = \bar{f}$. ($\mu = \bar{f}$)

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- $A^*(\mu) =$ (negative) maximum entropy of any distribution p such that $\mathbb{E}_{X \sim p} f(X) = \bar{f}$. ($\mu = \bar{f}$)
- MLE solution satisfies $\mathbb{E}_{\theta} f = \bar{f}$. (why?)
 - This is denoted as *Moment Matching*: Empirical and model moments match at optimality.

MLE and Maximum Entropy

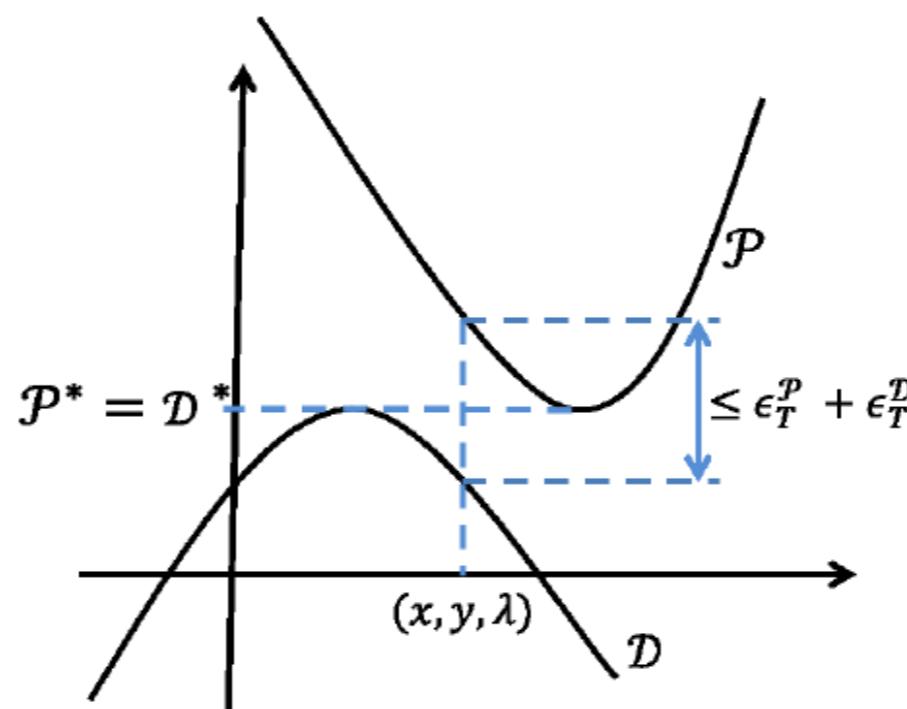
- This is an instance of convex duality:
 - On the one hand, we assume exponential family and have shown that MLE implies model moments = empirical moments.
 - On the other hand, we assume model moments match empirical moments and shown that Max Ent implies exponential family.

MLE and Maximum Entropy

- This is an instance of convex duality:
 - On the one hand, we assume exponential family and have shown that MLE implies model moments = empirical moments.
 - On the other hand, we assume model moments match empirical moments and shown that Max Ent implies exponential family.
- Moreover, both objectives reach the same value at optimality:

$$A^*(\mu) = \sup_{\theta} \langle \theta, \mu \rangle - A(\theta)$$

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Monte-Carlo

- Q2: How to efficiently implement such ascent method?

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Monte-Carlo

- Q2: How to efficiently implement such ascent method?

$$\frac{\partial \mathcal{L}(\theta)}{\partial \theta} = \bar{f} - \mathbb{E}_\theta\{f\}$$

- Use MCMC and estimate the gradient from

$$\widehat{\mathbb{E}_\theta f} = \frac{1}{S} \sum_{x^{(s)} \sim p_\theta} f(x^{(s)})$$

- We never need to estimate $A(\theta)$.

- Q: Other alternatives?

Approximating log-partition function

- The original learning objective function was

$$\mathcal{L}(\theta) = \log p(x^1, \dots, x^L; \theta) = \left\langle \theta, \sum_{c \in \mathcal{C}} L^{-1} \sum_{l \leq L} f_c(x_c^l) \right\rangle - A(\theta).$$

- We can consider a tractable approximation of the log-partition function

$$\tilde{\mathcal{L}}(\theta) = \left\langle \theta, \sum_{c \in \mathcal{C}} L^{-1} \sum_{l \leq L} f_c(x_c^l) \right\rangle - \tilde{A}(\theta).$$

- For instance using convex relaxations, ie variational methods.
 - tree-reweighted belief propagation [Wainwright, Willsky & Jakkola] (based on “convexifying” Bethe approximation).
 - log-determinant relaxation [Wainwright & Jordan].

Pseudo-Likelihood

- An alternative route is to replace the objective function $\mathcal{L}(\theta)$ by another one $\bar{\mathcal{L}}(\theta)$, such that they are asymptotically maximized at the same parameter value as $L \rightarrow \infty$

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- From Bayes rule, we have

$$p(x; \theta) = \prod_i p(x_i \mid x_1, \dots, x_{i-1}; \theta) .$$

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- From Bayes rule, we have

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- We consider the approximation

$$p(x; \theta) \approx \prod_i p(x_i \mid x_1, \dots, x_{i-1}, \textcolor{red}{x_{i+1}}, \dots, \textcolor{red}{x_n}; \theta) = \prod_i p(x_i \mid x_{-i}; \theta)$$

– conditioning over all the other variables (similarly as in Gibbs sampling).

Pseudo-Likelihood

- We replace the likelihood $\mathcal{L}(\theta)$ by the "pseudo-likelihood"

$$\mathcal{L}_P(\theta) = \frac{1}{L} \sum_{l \leq L} \sum_{i=1}^n \log p(x_i^l \mid x_{N(i)}^l; \theta) .$$

$N(i)$ = Markov Blanket of node i .

- Example: pair-wise MRF. Then

$$p(x_i \mid x_{N(i)}; \theta) = \frac{1}{Z(x_{N(i)}; \theta)} \exp \left(\sum_{j \in N(i)} \theta_{ij}(x_i, x_j) \right) ,$$

$$Z(x_{N(i)}; \theta) = \sum_{x_i} \exp \left(\sum_{j \in N(i)} \theta_{ij}(x_i, x_j) \right) .$$

Pseudo-Likelihood

- This approximation only involves “local” partition functions
 - We need to compute n univariate integrals instead of a single n -dimensional one.
- In the exponential family, the pseudo-likelihood is still concave.
- Although it is asymptotically consistent as $L \rightarrow \infty$, this does not mean it is optimal for a fixed L .
 - Again, we have a computational/statistical tradeoff.