Tutorial:

Deep Latent NLP (bit.do/lvnlp)

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Deep Latent-Variable Models of Natural Language

Yoon Kim, Sam Wiseman, Alexander Rush



Tutorial 2018

https://github.com/harvardnlp/DeepLatentNLP

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Goal of Latent-Variable Modeling

Probabilistic models provide a declarative language for specifying prior knowledge and structural relationships in the context of unknown variables.

Makes it easy to specify:

- Known interactions in the data
- Uncertainty about unknown factors
- Constraints on model properties

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Latent-Variable Modeling in NLP

Long and rich history of latent-variable models of natural language.

Major successes include, among many others:

- Statistical alignment for translation
- Document clustering and topic modeling
- Unsupervised part-of-speech tagging and parsing

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Goals of Deep Learning

Toolbox of methods for learning rich, non-linear data representations through numerical optimization.

Makes it easy to fit:

- Highly-flexible predictive models
- Transferable feature representations
- Structurally-aligned network architectures

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Deep Learning in NLP

Current dominant paradigm for NLP.

Major successes include, among many others:

- Text classification
- Neural machine translation
- NLU Tasks (QA, NLI, etc)

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Tutorial: Deep Latent-Variable Models for NLP

- How should a contemporary ML/NLP researcher reason about latent-variables?
- What unique challenges come from modeling text with latent variables?
- What techniques have been explored and shown to be effective in recent papers?

We explore these through the lens of variational inference.

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Tutorial Take-Aways

- 1 A collection of deep latent-variable models for NLP
- 2 An understanding of a variational objective
- **3** A toolkit of algorithms for optimization
- 4 A formal guide to advanced techniques
- **5** A survey of example applications
- 6 Code samples and techniques for practical use

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Tutorial Non-Objectives

Not covered (for time, not relevance):

- Many classical latent-variable approaches.
- Undirected graphical models such as MRFs
- Non-likelihood based models such as GANs
- Sampling-based inference such as MCMC.
- Details of deep learning architectures.

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What are deep networks?

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Deep networks are parameterized non-linear functions; They transform input z into features h using parameters π .

Important examples: The multilayer perceptron,

$$h = MLP(\mathbf{z}; \pi) = V\sigma(W\mathbf{z} + b) + a \quad \pi = \{V, W, a, b\},$$

The recurrent neural network, which maps a sequence of inputs $\mathbf{z}_{1:T}$ into a sequence of features $h_{1:T}$,

$$h_t = \text{RNN}(h_{t-1}, \mathbf{z}_t; \pi) = \sigma(U\mathbf{z}_t + Vh_{t-1} + b) \qquad \pi = \{V, U, b\}$$

What are deep networks?

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Deep Latent NLP (bit.do/lvnlp)	What are latent variable models?
Introduction	Latent variable models give us a joint distribution
Goals Background	p(x,z; heta).
Models	
Variational Objective	ullet x is our observed data
	ullet z is a collection of latent variables
Inference	

 θ are the deterministic parameters of the model, such as the neural network

• Data consists of N i.i.d samples,

 $p(x^{(1:N)}, z^{(1:N)}; \theta) = \prod^{N} p(x^{(n)} | z^{(n)}; \theta) p(z^{(n)}; \theta).$

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What are latent variable models?

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Latent variable models give us a joint distribution

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What are latent variable models?

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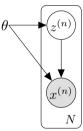
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Probabilistic Graphical Models

- A directed PGM shows the conditional independence structure.
- By chain rule, latent variable model over observations can be represented as,



$$p(x^{(1:N)}, z^{(1:N)}; \theta) = \prod_{n=1}^{N} p(x^{(n)} | z^{(n)}; \theta) p(z^{(n)}; \theta)$$

• Specific models may factor further.

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Tutorial: NLP

For models $p(x, z; \theta)$, we'll be interested in the posterior over latent variables z:

hy?
$$z \mbox{ will often represent interesting information about our data (e.g., the) }$$

$$\theta(\theta) = \frac{p(x,z,\theta)}{p(x;\theta)}.$$

• Learning the parameters θ of the model often requires calculating posteriors

Posterior Inference

$$=\frac{p(x,z;\theta)}{p(x;\theta)}.$$

$$p(x \mid z; \theta) = \frac{p(x, z; \theta)}{p(x; \theta)}.$$

$$=rac{p(x,z;\, heta)}{p(x;\, heta)}.$$

$$p(x,z;\theta)$$

$$\frac{(x,z;\, heta)}{\phi(x;\, heta)}$$
.

$$\frac{\partial f}{\partial f}$$
.

Deep Latent NLP (bit.do/lynlp)

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Posterior Inference

For models $p(x, z; \theta)$, we'll be interested in the *posterior* over latent variables z:

 $p(x \mid z; \theta) = \frac{p(x, z; \theta)}{p(x; \theta)}.$

Whv?

ullet z will often represent interesting information about our data (e.g., the cluster $x^{(n)}$ lives in, how similar $x^{(n)}$ and $x^{(n+1)}$ are).

• Learning the parameters θ of the model often requires calculating posteriors

as a subroutine. Intuition: if I know likely $z^{(n)}$ for $x^{(n)}$, I can learn by

maximizing $p(x^{(n)} | z^{(n)}; \theta)$.

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Problem Statement: Two Views

Deep Models & LV Models are naturally complementary:

- Rich function approximators with modular parts.
- Declarative methods for specifying model constraints.

Deep Models & LV Models are frustratingly incompatible:

- Deep networks make posterior inference intractable.
- Latent variable objectives complicate backpropagation.

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Our goal is to model a sentence, $x_1 \dots x_T$.

Context: RNN language models are remarkable at this task,

$$x_{1:T} \sim \text{RNNLM}(x_{1:T}; \theta).$$

Defined as,

$$p(x_{1:T}) = \prod_{t=1}^{T} p(x_t \mid x_{< t}) = \prod_{t=1}^{T} \operatorname{softmax}(\boldsymbol{W} \boldsymbol{h}_t)_{x_t}$$

where
$$\boldsymbol{h}_t = \text{RNN}(\boldsymbol{h}_{t-1}, \mathbf{x}_{t-1}; \theta)$$



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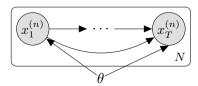
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A Collection of Model Archetypes

Focus: semi-supervised or unsupervised learning, i.e. don't just learn the probabilities, but the process. Range of choices in selecting z

- Discrete LVs z (Clustering)
- 2 Continuous LVs z (Dimensionality reduction)
- 3 Structured LVs z (Structured learning)

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A Collection of Model Archetypes

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Model 1: Discrete Clustering

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Inference Process:

In an old house in Paris that was covered with vines lived twelve little girls in two straight lines.

Discrete latent variable models induce a clustering over sentences $x^{(n)}$.

Example uses:

- Document/sentence clustering [Willett 1988; Aggarwal and Zhai 2012].
- Mixture of expert text generation models [Jacobs et al. 1991; Garmash and Monz 2016: Lee et al. 2016]

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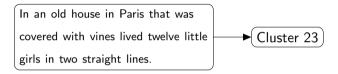
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Model 1: Discrete Clustering

Inference Process:



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Generative process:

- **1** Draw cluster $z \in \{1, \dots, K\}$ from a categorical with param μ .
- 2 Draw word T words x_t from a categorical with word distribution π_z .

Model 1: Discrete - Mixture of Categoricals

Parameters: $\theta = \{ \mu \in \Delta^{K-1}, K \times V \text{ stochastic matrix } \pi \}$

Gives rise to the "Naive Bayes" distribution:

$$p(x, z; \theta) = p(z; \mu) \times p(x \mid z; \pi) = \mu_z \times \prod_{t=1}^{T} \mathsf{Cat}(x_t; \pi)$$

$$= \mu_z \times \prod_{t=1}^{T} \pi_{z, x_t}$$

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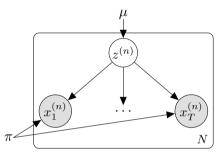
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Model 1: Graphical Model View



$$\begin{split} \prod_{n=1}^{N} p(x^{(n)}, z^{(n)}; \, \mu, \pi) &= \prod_{n=1}^{N} p(z^{(n)}; \, \mu) \times p(x^{(n)} \, | \, z^{(n)}; \, \pi) \\ &= \prod_{n=1}^{N} \mu_{z^{(n)}} \times \prod_{t=1}^{T} \pi_{z^{(n)}, x_{t}^{(n)}} \end{split}$$

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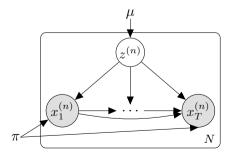
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Deep Model 1: Discrete - Mixture of RNNs

Generative process:

- **1** Draw cluster $z \in \{1, \dots, K\}$ from a categorical.
- 2 Draw words $x_{1:T}$ from RNNLM with parameters π_z .

$$p(x, z; \theta) = \mu_z \times \text{RNNLM}(x_{1:T}; \pi_z)$$



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Difference Between Models

- Dependence structure:
 - Mixture of Categoricals: x_t independent of other x_j given z.
 - Mixture of RNNs: x_t fully dependent.

Interesting question: how will this affect the learned latent space?

- Number of parameters:
 - Mixture of Categoricals: $K \times V$.
 - Mixture of RNNs: $K \times d^2 + V \times d$ with RNN with d hidden dims

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For both discrete models, can apply Bayes' rule:

$$p(z \mid x; \theta) = \frac{p(z) \times p(x \mid z)}{p(x)}$$

$$= \frac{p(z) \times p(x \mid z)}{\sum_{k=1}^{K} p(z=k) \times p(x \mid z=k)}$$

- For mixture of categoricals, posterior uses word counts under each π_k .
- For mixture of RNNs, posterior requires running RNN over x for each k.

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Model 2: Continuous / Dimensionality Reduction

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Inference Process:

In an old house in Paris that was covered with vines lived twelve little girls in two straight lines.

Find a lower-dimensional, well-behaved continuous representation of a sentence latent variables in \mathbb{R}^d make distance/similarity easy. Examples:

- Recent work in text generation assumes a latent vector per sentence [Bowman et al. 2016; Yang et al. 2017; Hu et al. 2017].
- Certain sentence embeddings (e.g., Skip-Thought vectors [Kiros et al. 2015]) can be interpreted in this way.

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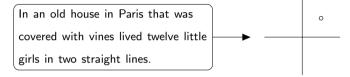
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Inference Process:



Model 2: Continuous / Dimensionality Reduction

Find a lower-dimensional, well-behaved continuous representation of a sentence. Latent variables in \mathbb{R}^d make distance/similarity easy. Examples:

- Recent work in text generation assumes a latent vector per sentence [Bowman et al. 2016; Yang et al. 2017; Hu et al. 2017].
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Model 2: Continuous "Mixture"

Generative Process:

- **1** Draw continuous latent variable z from Normal with param μ .
- **2** For each t, draw word x_t from categorical with param $\operatorname{softmax}(\boldsymbol{W}\mathbf{z})$.

Parameters: $\theta = \{\mu \in \mathbb{R}^d, \pi\}, \pi = \{\boldsymbol{W} \in \mathbb{R}^{V \times d}\}$

Intuition: μ is a global distribution, ${\bf z}$ captures local word distribution of the sentence.

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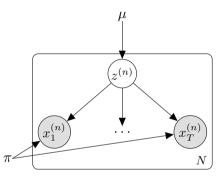
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Graphical Model View



Gives rise to the joint distribution:

$$\prod_{n=1}^{N} p(x^{(n)}, z^{(n)}; \theta) = \prod_{n=1}^{N} p(z^{(n)}; \mu) \times p(x^{(n)} | z^{(n)}; \pi)$$

Deep Model 2: Continuous "Mixture" of RNNs

Generative Process:

- **1** Draw latent variable $\mathbf{z} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{I})$.
- 2 Draw each token x_t from a conditional RNNLM.

$$p(x, \mathbf{z}; \pi, \boldsymbol{\mu}, \boldsymbol{I}) = p(\mathbf{z}; \boldsymbol{\mu}, \boldsymbol{I}) \times p(x \mid \mathbf{z}; \pi)$$
$$= \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}, \boldsymbol{I}) \times \text{CRNNLM}(x_{1:T}; \pi, \mathbf{z})$$

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CRNNLM
$$(x_{1:T}; \pi, \mathbf{z}) = \prod_{t=1}^{T} \operatorname{softmax}(\boldsymbol{W}\boldsymbol{h}_t)_{x_t}$$

Deep Model 2: Continuous "Mixture" of RNNs

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Generative Process:

1 Draw latent variable $\mathbf{z} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{I})$.

2 Draw each token x_t from a conditional RNNLM.

RNN is also conditioned on latent z,

$$p(x, \mathbf{z}; \pi, \boldsymbol{\mu}, \boldsymbol{I}) = p(\mathbf{z}; \boldsymbol{\mu}, \boldsymbol{I}) \times p(x \mid \mathbf{z}; \pi)$$
$$= \mathcal{N}(\mathbf{z}; \boldsymbol{\mu}, \boldsymbol{I}) \times \text{CRNNLM}(x_{1:T}; \pi, \mathbf{z})$$

where

CRNNLM
$$(x_{1:T}; \pi, \mathbf{z}) = \prod_{t=1}^{T} \operatorname{softmax}(\boldsymbol{W}\boldsymbol{h}_t)_{x_t}$$

$$\boldsymbol{h}_t = \text{RNN}(\boldsymbol{h}_{t-1}, [\mathbf{x}_{t-1}; \mathbf{z}]; \pi)$$

Deep Model 2: Continuous "Mixture" of RNNs

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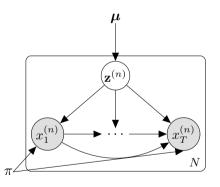
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Deep Latent NLP (bit.do/lvnlp)

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Posterior Inference

For continuous models, Bayes' rule is harder to compute,

$$p(z \mid x; \theta) = \frac{p(z; \mu) \times p(x \mid z; \pi)}{\int_{z} p(z; \mu) \times p(x \mid z; \pi) dz}$$

- Shallow and deep Model 2 variants mirror Model 1 variants exactly, but with continuous z.
- Integral intractable (in general) for both shallow and deep variants

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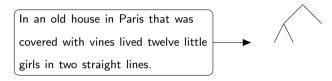
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Model 3: Structure Learning

Inference Process:



Structured latent variable models are used to infer unannotated structure:

- Unsupervised POS tagging [Brown et al. 1992; Merialdo 1994; Smith and Eisner 2005]
- Unsupervised dependency parsing [Klein and Manning 2004; Headden III et al. 2009]

Or when structure is useful for *interpreting* our data:

- Segmentation of documents into topical passages [Hearst 1997]
- Alignment [Vogel et al. 1996]

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Model 3: Structured - Hidden Markov Model

Generative Process:

- **1** For each t, draw $z_t \in \{1, \dots, K\}$ from a categorical with param $\mu_{z_{t-1}}$.
- 2 Draw observed token x_t from categorical with param π_{z_t} .

Parameters: $\theta = \{K \times K \text{ stochastic matrix } \mu, K \times V \text{ stochastic matrix } \pi\}$

Gives rise to the joint distribution

$$p(x, z; \theta) = \prod_{t=1}^{T} p(z_t | z_{t-1}; \mu_{z_{t-1}}) \times \prod_{t=1}^{T} p(x_t | z_t; \pi_{z_t})$$
$$= \prod_{t=1}^{T} \mu_{z_{t-1}, z_t} \times \prod_{t=1}^{T} \pi_{z_t, x_t}$$

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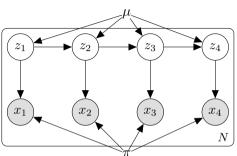
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$$p(x, z; \theta) = \prod_{t=1}^{T} p(z_t | z_{t-1}; \mu_{z_{t-1}}) \times \prod_{t=1}^{T} p(x_t | z_t; \pi_{z_t})$$
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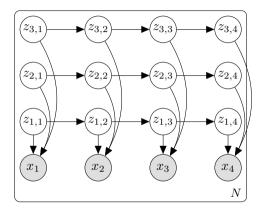
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Further Extension: Factorial HMM



$$p(x, z; \theta) = \prod_{l=1}^{L} \prod_{t=1}^{T} p(z_{l,t} | z_{l,t-1}) \times \prod_{t=1}^{T} p(x_t | z_{1:L,t})$$

Deep Model 3: Deep HMM

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Parameterize transition and emission distributions with neural networks (c.f., Tran et al. [2016])

Model transition distribution as

$$p(z_t \mid z_{t-1}) = \operatorname{softmax}(\operatorname{MLP}(z_{t-1}; \mu))$$

Model emission distribution as

$$p(x_t | z_t) = \operatorname{softmax}(MLP(z_t; \pi))$$

Note: $K \times K$ transition parameters for standard HMM vs. $O(K \times d + d^2)$ for deep version.

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Deep Model 3: Deep HMM

Parameterize transition and emission distributions with neural networks (c.f., Tran

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et al. [2016])

Model transition distribution as

 $p(z_t \mid z_{t-1}) = \operatorname{softmax}(\operatorname{MLP}(z_{t-1}; \mu))$

Model emission distribution as

 $p(x_t | z_t) = \operatorname{softmax}(\operatorname{MLP}(z_t; \pi))$

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Note: $K \times K$ transition parameters for standard HMM vs. $O(K \times d + d^2)$ for deep version.

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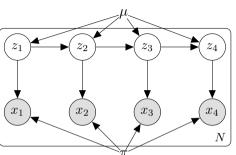
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Graphical Model View



$$p(x, z; \theta) = \prod_{t=1}^{T} p(z_t | z_{t-1}; \mu_{z_{t-1}}) \times \prod_{t=1}^{T} p(x_t | z_t; \pi_{z_t})$$
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For structured models, Bayes' rule may tractable,

$$p(z \mid x; \theta) = \frac{p(z; \mu) \times p(x \mid z; \pi)}{\sum_{z'} p(z'; \mu) \times p(x \mid z'; \pi)}$$

- Unlike previous models, z contains interdependent "parts."
- For both shallow and deep Model 3 variants, it's possible to calculate $p(x;\,\theta)$ exactly, with a dynamic program.
- For some structured models, like Factorial HMM, the dynamic program may still be intractable.

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Learning with Maximum Likelihood

Objective: Find model parameters $\boldsymbol{\theta}$ that maximize the likelihood of the data,

$$\theta^* = \underset{\theta}{\operatorname{arg max}} \sum_{n=1}^{N} \log p(x^{(n)}; \theta)$$

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Learning Deep Models

$$L(\theta) = \sum_{n=1}^{N} \log p(x^{(n)}; \theta)$$



• Dominant framework is gradient-based optimization:

$$\theta^{(i)} = \theta^{(i-1)} + \eta \nabla_{\theta} L(\theta)$$

- $\nabla_{\theta} L(\theta)$ calculated with backpropagation.
- Tactics: mini-batch based training, adaptive learning rates [Duchi et al. 2011;
 Kingma and Ba 2015].

Deep Latent NLP (bit.do/lynln)

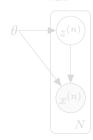
Maximum Likelihood

Learning Deep Latent-Variable Models: Marginalization

Likelihood requires summing out the latent variables.

$$p(x; \theta) = \sum_{z \in \mathcal{Z}} p(x, z; \theta)$$
 (= $\int p(x, z; \theta) dz$ if continuous z)

$$L(\theta) = \sum_{n=1}^{N} \log \sum_{z \in \mathcal{Z}} p(x^{(n)}, z; \theta)$$



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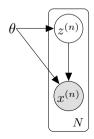
Learning Deep Latent-Variable Models: Marginalization

Likelihood requires summing out the latent variables,

$$p(x; \theta) = \sum_{z \in \mathcal{Z}} p(x, z; \theta)$$
 (= $\int p(x, z; \theta) dz$ if continuous z)

In general, hard to optimize log-likelihood for the training set,

$$L(\theta) = \sum_{n=1}^{N} \log \sum_{z \in \mathcal{Z}} p(x^{(n)}, z; \theta)$$



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Variational Inference

High-level: decompose objective into lower-bound and gap.

$$L(heta) \left\{ egin{array}{c} \mathsf{GAP}(heta,\lambda) \ & \mathsf{LB}(heta,\lambda) \end{array}
ight.$$

$$L(\theta) = \mathsf{LB}(\theta, \lambda) + \mathsf{GAP}(\theta, \lambda)$$
 for some λ

Provides framework for deriving a rich set of optimization algorithms.

Marginal Likelihood: Variational Decomposition

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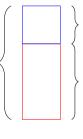
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For any 1 distribution $q(z \mid x; \lambda)$ over z,

$$L(\theta) = \mathbb{E}_q \left[\log \frac{p(x, z; \theta)}{q(z \mid x; \lambda)} \right] + \text{KL}[q(z \mid x; \lambda) \parallel p(z \mid x; \theta)]$$



posterior gap

ELBO (evidence lower bound)

Since KL is always non-negative, $L(\theta) \geq \text{ELBO}(\theta, \lambda)$.

¹Technical condition: $supp(q(z)) \subset supp(p(z \mid x; \theta))$

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Evidence Lower Bound: Proof

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$$\begin{split} \log p(x;\,\theta) &= \mathbb{E}_q \log p(x) \quad \textit{(Expectation over z)} \\ &= \mathbb{E}_q \log \frac{p(x,z)}{p(z\,|\,x)} \quad \textit{(Mult/div by } p(z|x) \textit{, combine numerator)} \\ &= \mathbb{E}_q \log \left(\frac{p(x,z)}{q(z\,|\,x)} \frac{q(z\,|\,x)}{p(z\,|\,x)} \right) \quad \textit{(Mult/div by } q(z|x) \textit{)} \\ &= \mathbb{E}_q \log \frac{p(x,z)}{q(z\,|\,x)} + \mathbb{E}_q \log \frac{q(z\,|\,x)}{p(z\,|\,x)} \quad \textit{(Split Log)} \\ &= \mathbb{E}_q \log \frac{p(x,z;\,\theta)}{q(z\,|\,x;\,\lambda)} + \mathrm{KL}[q(z\,|\,x;\,\lambda) \, \| \, p(z\,|\,x;\,\theta)] \end{split}$$

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Evidence Lower Bound over Observations

ELBO
$$(\theta, \lambda; x) = \mathbb{E}_{q(z)} \Big[\log \frac{p(x, z; \theta)}{q(z \mid x; \lambda)} \Big]$$

• ELBO is a function of the generative model parameters, θ , and the variational parameters, λ .

$$\begin{split} \sum_{n=1}^{N} \log p(x^{(n)}; \, \theta) &\geq \sum_{n=1}^{N} \mathrm{ELBO}(\theta, \lambda; \, x^{(n)}) \\ &= \sum_{n=1}^{N} \mathbb{E}_{q(z \, | \, x^{(n)}; \, \lambda)} \Big[\log \frac{p(x^{(n)}, z; \, \theta)}{q(z \, | \, x^{(n)}; \, \lambda)} \Big] \\ &= \mathrm{ELBO}(\theta, \lambda; \, x^{(1:N)}) = \mathrm{ELBO}(\theta, \lambda) \end{split}$$

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Setup: Selecting Variational Family

- Just as with p and θ , we can select any form of q and λ that satisfies ELBO conditions.
- ullet Different choices of q will lead to different algorithms.
- We will explore several forms of *q*:
 - Posterior
 - Point Estimate / MAP
 - Amortized
 - Mean Field (later)

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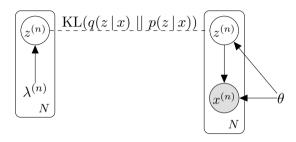
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Example Family: Full Posterior Form



$$\lambda = [\lambda^{(1)}, \dots, \lambda^{(N)}]$$
 is a concatenation of local variational parameters $\lambda^{(n)}$, e.g.

$$q(z^{(n)} | x^{(n)}; \lambda) = q(z^{(n)} | x^{(n)}; \lambda^{(n)}) = \mathcal{N}(\lambda^{(n)}, 1)$$

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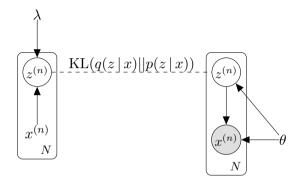
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Example Family: Amortized Parameterization [Kingma and Welling 2014]



 λ parameterizes a global network (encoder/inference network) that is run over $x^{(n)}$ to produce the local variational distribution, e.g.

$$q(z^{(n)} | x^{(n)}; \lambda) = \mathcal{N}(\mu^{(n)}, 1), \qquad \mu^{(n)} = \text{enc}(x^{(n)}; \lambda)$$

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Maximizing the Evidence Lower Bound

Central quantity of interest: almost all methods are maximizing the ELBO

$$\operatorname*{arg\,max}_{\theta,\lambda}\operatorname{ELBO}(\theta,\lambda)$$

Aggregate ELBO objective,

$$\underset{\theta,\lambda}{\operatorname{arg\,max}} \operatorname{ELBO}(\theta,\lambda) = \underset{\theta,\lambda}{\operatorname{arg\,max}} \sum_{n=1}^{N} \operatorname{ELBO}(\theta,\lambda; \, x^{(n)})$$
$$= \underset{\theta,\lambda}{\operatorname{arg\,max}} \sum_{n=1}^{N} \mathbb{E}_{q} \Big[\log \frac{p(x^{(n)}, z^{(n)}; \, \theta)}{q(z^{(n)} \mid x^{(n)}; \, \lambda)} \Big]$$

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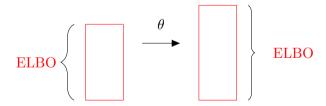
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Maximizing ELBO: Model Parameters

$$\arg\max_{\theta} \mathbb{E}_{q} \left[\log \frac{p(x, z; \theta)}{q(z \mid x; \lambda)} \right] = \arg\max_{\theta} \mathbb{E}_{q} [\log p(x, z; \theta)]$$



Intuition: Maximum likelihood problem under variables drawn from $q(z \mid x; \lambda)$.

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Model Estimation: Gradient Ascent on Model Parameters

Easy: Gradient respect to θ

$$\nabla_{\theta} \operatorname{ELBO}(\theta, \lambda; x) = \nabla_{\theta} \mathbb{E}_{q} \Big[\log p(x, z; \theta) \Big]$$
$$= \mathbb{E}_{q} \Big[\nabla_{\theta} \log p(x, z; \theta) \Big]$$

- Since q not dependent on θ , ∇ moves inside expectation.
- Estimate with samples from q. Term $\log p(x,z;\theta)$ is easy to evaluate. (In practice single sample is often sufficient).
- In special cases, can exactly evaluate expectation.

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Model Estimation: Gradient Ascent on Model Parameters

Easy: Gradient respect to θ

$$\nabla_{\theta} \operatorname{ELBO}(\theta, \lambda; x) = \nabla_{\theta} \mathbb{E}_{q} \Big[\log p(x, z; \theta) \Big]$$
$$= \mathbb{E}_{q} \Big[\nabla_{\theta} \log p(x, z; \theta) \Big]$$

- Since q not dependent on θ . ∇ moves inside expectation.
- Estimate with samples from q. Term $\log p(x, z; \theta)$ is easy to evaluate. (In practice single sample is often sufficient).
- In special cases, can exactly evaluate expectation.

 $\arg \max ELBO(\theta, \lambda)$

Maximizing ELBO: Variational Distribution

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 $= \arg \max \log p(x; \theta) - \mathrm{KL}[q(z \mid x; \lambda) \parallel p(z \mid x; \theta)]$ $= \arg\min \mathrm{KL}[q(z \mid x; \lambda) \parallel p(z \mid x; \theta)]$ posterior gap FI BO

Intuition: q should approximate the posterior p(z|x). However, may be difficult if q or p is a deep model. 59/153

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Model Inference: Gradient Ascent on λ ?

Hard: Gradient respect to λ

$$\nabla_{\lambda} \operatorname{ELBO}(\theta, \lambda; x) = \nabla_{\lambda} \mathbb{E}_{q} \Big[\log p(x, z; \theta) \Big]$$

$$\neq \mathbb{E}_{q} \Big[\nabla_{\lambda} \log p(x, z; \theta) \Big]$$

- Cannot naively move ∇ inside the expectation, since q depends on λ .
- This section: Inference in practice
 - Exact gradient
 - 2 Sampling: score function, reparameterization
 - Conjugacy: closed-form, coordinate ascent

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Model Inference: Gradient Ascent on λ ?

Hard: Gradient respect to λ

$$\nabla_{\lambda} \operatorname{ELBO}(\theta, \lambda; x) = \nabla_{\lambda} \mathbb{E}_{q} \Big[\log p(x, z; \theta) \Big]$$

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- This section: Inference in practice:
 - Exact gradient
 - 2 Sampling: score function, reparameterization
 - 3 Conjugacy: closed-form, coordinate ascent

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Strategy 1: Exact Gradient

$$\nabla_{\lambda} \operatorname{ELBO}(\theta, \lambda; x) = \nabla_{\lambda} \mathbb{E}_{q(z \mid x; \lambda)} \left[\log \frac{p(x, z; \theta)}{q(z \mid x; \lambda)} \right]$$
$$= \nabla_{\lambda} \left(\sum_{z \in \mathcal{Z}} q(z \mid x; \lambda) \log \frac{p(x, z; \theta)}{q(z \mid x; \lambda)} \right)$$

- Naive enumeration: Linear in $|\mathcal{Z}|$.
- Depending on structure of q and p, potentially faster with dynamic programming.
- Applicable mainly to Model 1 and 3 (Discrete and Structured), or Model 2 with point estimate.

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Strategy 1: Exact Gradient

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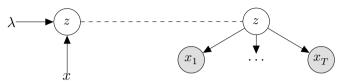
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Example: Model 1 - Naive Bayes



Let
$$q(z \,|\, x;\, \lambda) = \mathsf{Cat}(\nu)$$
 where $\nu = \mathrm{enc}(x;\lambda)$

$$\nabla_{\lambda} \operatorname{ELBO}(\theta, \lambda; x) = \nabla_{\lambda} \mathbb{E}_{q(z \mid x; \lambda)} \left[\log \frac{p(x, z; \theta)}{q(z \mid x; \lambda)} \right]$$
$$= \nabla_{\lambda} \left(\sum_{z \in \mathcal{Z}} q(z \mid x; \lambda) \log \frac{p(x, z; \theta)}{q(z \mid x; \lambda)} \right)$$
$$= \nabla_{\lambda} \left(\sum_{z \in \mathcal{Z}} \nu_{z} \log \frac{p(x, z; \theta)}{\nu_{z}} \right)$$

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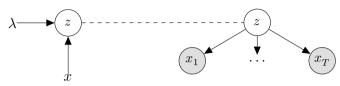
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Example: Model 1 - Naive Bayes



Let
$$q(z\,|\,x;\,\lambda) = \mathsf{Cat}(\nu)$$
 where $\nu = \mathrm{enc}(x;\lambda)$

$$\nabla_{\lambda} \operatorname{ELBO}(\theta, \lambda; x) = \nabla_{\lambda} \mathbb{E}_{q(z \mid x; \lambda)} \left[\log \frac{p(x, z; \theta)}{q(z \mid x; \lambda)} \right]$$
$$= \nabla_{\lambda} \left(\sum_{z \in \mathcal{Z}} q(z \mid x; \lambda) \log \frac{p(x, z; \theta)}{q(z \mid x; \lambda)} \right)$$
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Strategy 2: Sampling

 $\nabla_{\lambda} \operatorname{ELBO}(\theta, \lambda; x) = \nabla_{\lambda} \mathbb{E}_{q} \left[\log \frac{\log p(x, z; \theta)}{\log q(z \mid x; \lambda)} \right]$

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 $= \nabla_{\lambda} \mathbb{E}_{q} \Big[\log p(x, z; \theta) \Big] - \nabla_{\lambda} \mathbb{E}_{q} \Big[\log q(z \mid x; \theta) \Big]$

How can we approximate this gradient with sampling? Naive algorithm fails

 $\nabla_{\lambda} \frac{1}{J} \sum_{j=1}^{J} \left[\log p(x, z^{(j)}; \theta) \right] = 0$

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$$\nabla_{\lambda} \operatorname{ELBO}(\theta, \lambda; x) = \nabla_{\lambda} \mathbb{E}_{q} \Big[\log \frac{\log p(x, z; \theta)}{\log q(z \mid x; \lambda)} \Big]$$
$$= \nabla_{\lambda} \mathbb{E}_{q} \Big[\log p(x, z; \theta) \Big] - \nabla_{\lambda} \mathbb{E}_{q} \Big[\log q(z \mid x; \theta) \Big]$$

 How can we approximate this gradient with sampling? Naive algorithm fails to provide non-zero gradient.

$$z^{(1)}, \dots, z^{(J)} \sim q(z \mid x; \lambda)$$

$$\nabla_{\lambda} \frac{1}{J} \sum_{i=1}^{J} \left[\log p(x, z^{(j)}; \theta) \right] = 0$$

• Manipulate expression so we can move ∇_{λ} inside \mathbb{E}_q before sampling.

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Strategy 2a: Sampling — Score Function Gradient Estimator

First term. Use basic identity:

$$\nabla \log q = \frac{\nabla q}{q} \Rightarrow \nabla q = q \nabla \log q$$

$$\nabla_{\lambda} \mathbb{E}_{q} \Big[\log p(x, z; \theta) \Big] = \sum_{z} \nabla_{\lambda} q(z \mid x; \lambda) \log p(x, z; \theta)$$

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Strategy 2a: Sampling — Score Function Gradient Estimator

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$$\nabla_{\lambda} \mathbb{E}_{q} \left[\log p(x, z; \theta) \right] = \sum_{z} \underbrace{\nabla_{\lambda} q(z \mid x; \lambda)}_{q \nabla \log q} \log p(x, z; \theta)$$

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Strategy 2a: Sampling — Score Function Gradient Estimator

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$$= \sum_{z} q(z \mid x; \lambda) \nabla_{\lambda} \log q(z \mid x; \lambda) \log p(x, z; \theta)$$

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Strategy 2a: Sampling — Score Function Gradient Estimator

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$$\nabla_{\lambda} \mathbb{E}_{q} \Big[\log p(x, z; \theta) \Big] = \sum_{z} \nabla_{\lambda} q(z \mid x; \lambda) \log p(x, z; \theta)$$

$$= \sum_{z} q(z \mid x; \lambda) \nabla_{\lambda} \log q(z \mid x; \lambda) \log p(x, z; \theta)$$

$$= \mathbb{E}_{q} \Big[\log p(x, z; \theta) \nabla_{\lambda} \log q(z \mid x; \lambda) \Big]$$

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Strategy 2a: Sampling — Score Function Gradient Estimator

$$\sum \nabla q = \nabla \sum q = \nabla 1 = 0$$

$$\nabla_{\lambda} \mathbb{E}_{q} \Big[\log q(z \mid x; \lambda) \Big] = \sum_{z} \nabla_{\lambda} \Big(q(z \mid x; \lambda) \log q(z \mid x; \lambda) \Big)$$

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Strategy 2a: Sampling — Score Function Gradient Estimator

$$\sum \nabla q = \nabla \sum q = \nabla 1 = 0$$

$$\begin{split} & \nabla_{\lambda} \mathbb{E}_{q} \Big[\log q(z \mid x; \lambda) \Big] = \sum_{z} \nabla_{\lambda} \Big(q(z \mid x; \lambda) \log q(z \mid x; \lambda) \\ & = \sum_{z} \Big(\underbrace{\nabla_{\lambda} q(z \mid x; \lambda)}_{q \nabla \log q} \Big) \log q(z \mid x; \lambda) + q(z \mid x; \lambda) \Big(\underbrace{\nabla_{\lambda} \log q(z \mid x; \lambda)}_{\nabla q} \Big) \end{split}$$

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Strategy 2a: Sampling — Score Function Gradient Estimator

$$\sum \nabla q = \nabla \sum q = \nabla 1 = 0$$

$$\nabla_{\lambda} \mathbb{E}_{q} \Big[\log q(z \mid x; \lambda) \Big] = \sum_{z} \nabla_{\lambda} \Big(q(z \mid x; \lambda) \log q(z \mid x; \lambda) \Big)$$

$$= \sum_{z} \log q(z \,|\, x;\, \lambda) \nabla_{\lambda} \log q(z \,|\, x;\, \lambda) + \sum_{z} \nabla_{\lambda} q(z \,|\, x;\, \lambda)$$

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Strategy 2a: Sampling — Score Function Gradient Estimator

$$\sum \nabla q = \nabla \sum q = \nabla 1 = 0$$

$$\nabla_{\lambda} \mathbb{E}_{q} \Big[\log q(z \mid x; \lambda) \Big] = \sum_{z} \nabla_{\lambda} \Big(q(z \mid x; \lambda) \log q(z \mid x; \lambda) \Big)$$

$$= \sum_{z} \log q(z \mid x; \lambda) \nabla_{\lambda} \log q(z \mid x; \lambda) + \underbrace{\sum_{z} \nabla_{\lambda} q(z \mid x; \lambda)}_{\text{2.5}}$$

$$=\nabla \sum q = \nabla 1 = 0$$

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Strategy 2a: Sampling — Score Function Gradient Estimator

$$\sum \nabla q = \nabla \sum q = \nabla 1 = 0$$

$$\nabla_{\lambda} \mathbb{E}_{q} \Big[\log q(z \mid x; \lambda) \Big] = \sum_{z} \nabla_{\lambda} \Big(q(z \mid x; \lambda) \log q(z \mid x; \lambda) \Big)$$

$$= \sum_{z} \log q(z \mid x; \lambda) \nabla_{\lambda} \log q(z \mid x; \lambda) + \sum_{z} \nabla_{\lambda} q(z \mid x; \lambda)$$

$$= \mathbb{E}_q[\log q(z \mid x; \lambda) \nabla_{\lambda} q(z \mid x; \lambda)]$$

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Strategy 2a: Sampling — Score Function Gradient Estimator

Putting these together,

$$\nabla_{\lambda} \operatorname{ELBO}(\theta, \lambda; x) = \nabla_{\lambda} \mathbb{E}_{q} \left[\log \frac{p(x, z; \theta)}{q(z \mid x; \lambda)} \right]$$

$$= \mathbb{E}_{q} \left[\log \frac{p(x, z; \theta)}{q(z \mid x; \lambda)} \nabla_{\lambda} \log q(z \mid x; \lambda) \right]$$

$$= \mathbb{E}_{q} \left[R_{\theta, \lambda}(z) \nabla_{\lambda} \log q(z \mid x; \lambda) \right]$$

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Strategy 2a: Sampling — Score Function Gradient Estimator

Estimate with samples,

$$z^{(1)}, \dots, z^{(J)} \sim q(z \mid x; \lambda)$$

$$\mathbb{E}_{q} \left[R_{\theta,\lambda}(z) \nabla_{\lambda} \log q(z \mid x; \lambda) \right]$$

$$\approx \frac{1}{J} \sum_{j=1}^{J} R_{\theta,\lambda}(z^{(j)}) \nabla_{\lambda} \log q(z^{(j)} \mid x; \lambda)$$

Intuition: if a sample $z^{(j)}$ is has high reward $R_{\theta,\lambda}(z^{(j)})$, increase the probability of $z^{(j)}$ by moving along the gradient $\nabla_{\lambda} \log q(z^{(j)} \,|\, x;\, \lambda)$.

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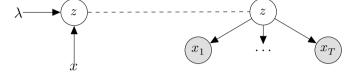
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Strategy 2a: Sampling — Score Function Gradient Estimator

- Essentially reinforcement learning with reward $R_{\theta,\lambda}(z)$
- Score function gradient is generally applicable regardless of what distribution q takes (only need to evaluate $\nabla_{\lambda} \log q$).
- This generality comes at a cost, since the reward is "black-box": unbiased estimator, but high variance.
- In practice, need variance-reducing **control variate** B. (More on this later).

Exact Gradient Sampling Conjugacy

Example: Model 1 - Naive Bayes

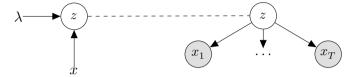


Let $q(z \mid x; \lambda) = \mathsf{Cat}(\nu)$ where $\nu = \mathrm{enc}(x; \lambda)$

$$\nabla_{\lambda} \operatorname{ELBO}(\theta, \lambda; x) = \mathbb{E}_q \Big[\log x \Big]$$

$$\approx \frac{1}{J} \sum_{j=1}^{J} \nu_{z^{(j)}} \log \frac{p(x, z^{(j)}; \theta)}{\nu_{z^{(j)}}} \nabla_{\lambda} \log \nu_{z^{(j)}}$$

Example: Model 1 - Naive Bayes



Exact Gradient Sampling

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Computational complexity: O(J) vs $O(|\mathcal{Z}|)$

Let $q(z \mid x; \lambda) = \mathsf{Cat}(\nu)$ where $\nu = \mathsf{enc}(x; \lambda)$

Sample $z^{(1)}, \ldots, z^{(J)} \sim q(z \mid x; \lambda)$

 $\nabla_{\lambda} \operatorname{ELBO}(\theta, \lambda; x) = \mathbb{E}_q \left[\log \frac{p(x, z; \theta)}{q(z \mid x; \lambda)} \nabla_{\lambda} \log q(z \mid x; \lambda) \right]$

 $\approx \frac{1}{J} \sum_{i=1}^{J} \nu_{z^{(j)}} \log \frac{p(x, z^{(j)}; \theta)}{\nu_{z^{(j)}}} \nabla_{\lambda} \log \nu_{z^{(j)}}$

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Strategy 2b: Sampling — Reparameterization

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Suppose we can sample from q by applying a deterministic, differentiable transformation g to a base noise density,

$$\epsilon \sim \mathcal{U}$$
 $z = g(\epsilon, \lambda)$

Gradient calculation (first term):

$$\nabla_{\lambda} \mathbb{E}_{z \sim q(z \mid x; \lambda)} \Big[\log p(x, z; \theta) \Big] = \nabla_{\lambda} \mathbb{E}_{\epsilon \sim \mathcal{U}} \Big[\log p(x, g(\epsilon, \lambda); \theta) \Big]$$
$$= \mathbb{E}_{\epsilon \sim \mathcal{U}} \Big[\nabla_{\lambda} \log p(x, g(\epsilon, \lambda); \theta) \Big]$$
$$\approx \frac{1}{J} \sum_{i=1}^{J} \nabla_{\lambda} \log p(x, g(\epsilon^{(j)}, \lambda); \theta)$$

where

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Strategy 2b: Sampling — Reparameterization

Suppose we can sample from q by applying a deterministic, differentiable transformation g to a base noise density,

$$\epsilon \sim \mathcal{U}$$
 $z = g(\epsilon, \lambda)$

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Gradient calculation (first term):

$$\nabla_{\lambda} \mathbb{E}_{z \sim q(z \mid x; \lambda)} \Big[\log p(x, z; \theta) \Big] = \nabla_{\lambda} \mathbb{E}_{\epsilon \sim \mathcal{U}} \Big[\log p(x, g(\epsilon, \lambda); \theta) \Big]$$
$$= \mathbb{E}_{\epsilon \sim \mathcal{U}} \Big[\nabla_{\lambda} \log p(x, g(\epsilon, \lambda); \theta) \Big]$$
$$\approx \frac{1}{J} \sum_{j=1}^{J} \nabla_{\lambda} \log p(x, g(\epsilon^{(j)}, \lambda); \theta)$$

where

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Strategy 2b: Sampling — Reparameterization

- Unbiased-like score function gradient estimator, but empirically lower variance.
- In practice, single sample is often sufficient.
- Cannot be used out-of-the-box for discrete z.

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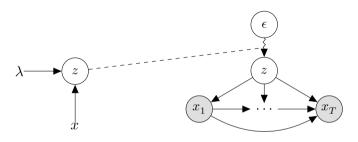
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Strategy 2: Continuous Latent Variable RNN



Choose variational family to be an amortized diagonal Gaussian

$$q(z \mid x; \lambda) = \mathcal{N}(\mu, \sigma^2)$$

$$\mu, \sigma^2 = \mathrm{enc}(x; \lambda)$$

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Strategy 2b: Sampling — Reparameterization

(Recall
$$R_{\theta,\lambda}(z) = \log \frac{p(x,z;\theta)}{q(z|x;\lambda)}$$
)

Score function:

$$\nabla_{\lambda} \text{ELBO}(\theta, \lambda; x) = \mathbb{E}_{z \sim q}[R_{\theta, \lambda}(z) \nabla_{\lambda} \log q(z \mid x; \lambda)]$$

Reparameterization:

$$\nabla_{\lambda} \operatorname{ELBO}(\theta, \lambda; x) = \mathbb{E}_{\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} [\nabla_{\lambda} R_{\theta, \lambda}(g(\epsilon, \lambda; x))]$$

where $g(\epsilon, \lambda; x) = \mu + \sigma \epsilon$.

Informally, reparameterization gradients differentiate through $R_{\theta,\lambda}(\cdot)$ and thus has "more knowledge" about the structure of the objective function.

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Strategy 3: Conjugacy

For certain choices for p and q, we can compute parts of

$$\underset{\lambda}{\operatorname{arg\,max}} \operatorname{ELBO}(\theta, \lambda; x)$$

exactly in closed-form.

Recall that

$$\underset{\lambda}{\operatorname{arg\,max}} \operatorname{ELBO}(\theta, \lambda; x) = \underset{\lambda}{\operatorname{arg\,min}} \operatorname{KL}[q(z \mid x; \lambda) || p(z \mid x; \theta)]$$

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Strategy 3: Conjugacy

For certain choices for p and q, we can compute parts of

$$\underset{\lambda}{\operatorname{arg\,max}} \operatorname{ELBO}(\theta, \lambda; x)$$

exactly in closed-form.

Recall that

$$\mathop{\arg\max}_{\lambda} \mathrm{ELBO}(\theta, \lambda; x) = \mathop{\arg\min}_{\lambda} \mathrm{KL}[q(z \,|\, x; \, \lambda) \| p(z \,|\, x; \, \theta)]$$

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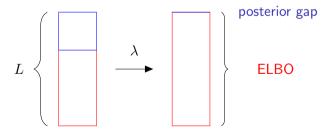
References

Strategy 3a: Conjugacy — Tractable Posterior Inference

Suppose we can tractably calculate $p(z \mid x; \theta)/$. Then $\mathrm{KL}[q(z \mid x; \lambda) || p(z \mid x; \theta)]$ is minimized when.

$$q(z \mid x; \lambda) = p(z \mid x; \theta)$$

• The E-step in Expectation Maximization algorithm [Dempster et al. 1977]



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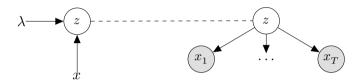
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Example: Model 1 - Naive Bayes



$$p(z \mid x; \theta) = \frac{p(x, z; \theta)}{\sum_{z'=1}^{K} p(x, z'; \theta)}$$

So λ is given by the parameters of the categorical distribution, i.e.

$$\lambda = [p(z = 1 \mid x; \theta), \dots, p(z = K \mid x; \theta)]$$

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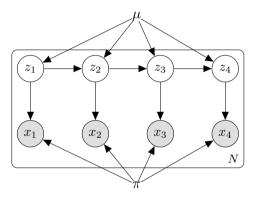
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Reminder: Model 3 — HMM



$$p(x, z; \theta) = p(z_0) \prod_{t=1}^{I} p(z_t | z_{t-1}; \mu) p(x_t | z_t; \pi)$$

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Example: Model 3 — HMM

Run forward/backward dynamic programming to calculate posterior marginals,

$$p(z_t, z_{t+1} \mid x; \theta)$$

variational parameters $\lambda \in \mathbb{R}^{TK^2}$ store edge marginals. These are enough to calculate

$$q(z; \lambda) = p(z \mid x; \theta)$$

(i.e. the exact posterior) over any sequence a

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Example: Model 3 — HMM

Run forward/backward dynamic programming to calculate posterior marginals,

$$p(z_t, z_{t+1} \mid x; \theta)$$

variational parameters $\lambda \in \mathbb{R}^{TK^2}$ store edge marginals. These are enough to calculate

$$q(z; \lambda) = p(z \mid x; \theta)$$

(i.e. the exact posterior) over any sequence z.

Connection: Gradient Ascent on Log Marginal Likelihood

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Why not perform gradient ascent directly on log marginal likelihood?

$$\log p(x; \theta) = \log \sum_{z} p(x, z; \theta)$$

Same as optimizing ELBO with posterior inference (i.e EM). Gradients of model parameters given by (where $q(z \mid x; \lambda) = p(z \mid x; \theta)$):

$$\nabla_{\theta} \log p(x; \theta) = \mathbb{E}_{q(z \mid x; \lambda)} [\nabla_{\theta} \log p(x, z; \theta)]$$



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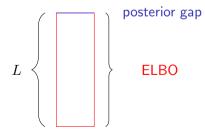
Connection: Gradient Ascent on Log Marginal Likelihood

Why not perform gradient ascent directly on log marginal likelihood?

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Connection: Gradient Ascent on Log Marginal Likelihood

- Practically, this means we don't have to manually perform posterior inference in the E-step. Can just calculate $\log p(x; \theta)$ and call backpropagation.
- Example: in deep HMM, just implement forward algorithm to calculate $\log p(x;\,\theta)$ and backpropagate using autodiff. No need to implement backward algorithm. (Or vice versa).

(See Eisner [2016]: "Inside-Outside and Forward-Backward Algorithms Are Just Backprop")

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Strategy 3b: Conditional Conjugacy

- Let $p(z \mid x; \theta)$ be intractable, but suppose $p(x, z; \theta)$ is conditionally conjugate, meaning $p(z_t \mid x, z_{-t}; \theta)$ is exponential family.
- Restrict the family of distributions q so that it factorizes over z_t , i.e.

$$q(z; \lambda) = \prod_{t=1}^{T} q(z_t; \lambda_t)$$

(mean field family)

• Further choose $q(z_t;\, x\lambda_t)$ so that it is in the same family as $p(z_t\,|\, x,z_{-t};\, \theta)$.

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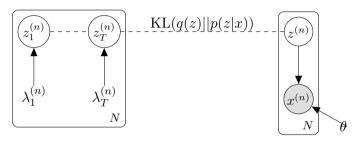
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Strategy 3b: Conditional Conjugacy



$$q(z; \lambda) = \prod_{t=1}^{T} q(z_t; \lambda_t)$$

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ullet Optimize ELBO via coordinate ascent, i.e. iterate for $\lambda_1,\dots,\lambda_T$

$$\underset{\lambda_t}{\operatorname{arg\,max}} \operatorname{KL}\left[\prod_{t=1}^{T} q(z_t; \, \lambda_t) \| p(z \, | \, x; \, \theta)\right]$$

Coordinate ascent updates will take the form

$$q(z_t; \lambda_t) \propto \exp\left(\mathbb{E}_{q(z_{-t}; \lambda_{-t})}[\log p(x, z; \theta)]\right)$$

where

$$\mathbb{E}_{q(z_{-t}; \lambda_{-t})}[\log p(x, z; \theta)] = \sum_{j \neq t} \prod_{j \neq t} q(z_j; \lambda_j) \log p(x, z; \theta)$$

• Since $p(z_t | x, z_{-t})$ was assumed to be in the exponential family, above updates can be derived in closed form.

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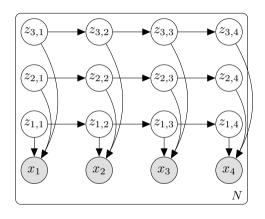
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Example: Model 3 — Factorial HMM



$$p(x, z; \theta) = \prod_{l=1}^{L} \prod_{t=1}^{L} p(z_{l,t} | z_{l,t-1}; \theta) p(x_t | z_{l,t}; \theta)$$

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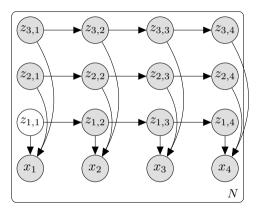
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Example: Model 3 — Factorial HMM



$$q(z_{1,1}; \lambda_{1,1}) \propto \exp\left(\mathbb{E}_{q(z_{-(1,1)}; \lambda_{-(1,1)})}[\log p(x, z; \theta)]\right)$$

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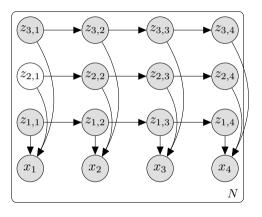
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Example: Model 3 — Factorial HMM



$$q(z_{2,1}; \lambda_{2,1}) \propto \exp\left(\mathbb{E}_{q(z_{-(2,1)}; \lambda_{-(2,1)})}[\log p(x, z; \theta)]\right)$$

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Example: Model 3 — Factorial HMM

Exact Inference:

ullet Naive: K states, L levels \Longrightarrow HMM with K^L states \Longrightarrow $O(TK^{2L})$

• Smarter: $O(TLK^{L+1})$

Mean Field

ullet Gaussian emissions: $O(TLK^2)$ [Ghahramani and Jordan 1996].

 • Categorical emission: need more variational approximations, but ultimately O(LKVT) [Nepal and Yates 2013].

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- Gumbel-Softmax: Extend reparameterization to discrete variables.
- f 2 Flows: Optimize a tighter bound by making the variational family q more flexible.
- **3** Importance Weighting: Optimize a tighter bound through importance sampling.

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Challenges of Discrete Variables

Review: we can always use score function estimator

$$\nabla_{\lambda} \operatorname{ELBO}(x, \theta, \lambda) = \mathbb{E}_{q} \Big[\log \frac{p(x, z; \theta)}{q(z \mid x; \lambda)} \nabla_{\lambda} \log q(z \mid x; \lambda) \Big]$$
$$= \mathbb{E}_{q} \Big[\Big(\log \frac{p(x, z; \theta)}{q(z \mid x; \lambda)} - B \Big) \nabla_{\lambda} \log q(z \mid x; \lambda) \Big]$$

- $\mathbb{E}_q[B\nabla_\lambda \log q(z \mid x; \lambda)] = 0$
- Control variate B (not dependendent on z, but can depend on x).
- Estimate this quantity with another neural net [Mnih and Gregor 2014]

$$\left(B(x; \psi) - \log \frac{p(x, z; \theta)}{q(z \mid x; \lambda)}\right)^{\dagger}$$

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$$\left(B(x; \psi) - \log \frac{p(x, z; \theta)}{q(z \mid x; \lambda)}\right)^{2}$$

Deep Latent NLP (bit.do/lvnlp)

Gumbel-Softmax: Discrete Reparameterization [Jang et al. 2017; Maddison et al. 2017]

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The "Gumbel-Max" trick [Papandreou and Yuille 2011]

$$p(z_k = 1; \alpha) = \frac{\alpha_k}{\sum_{j=1}^K \alpha_j}$$

where $z = [0, 0, \dots, 1, \dots, 0]$ is a one-hot vector.

Can sample from $p(z; \alpha)$ by

① Drawing independent Gumbel noise $\epsilon = \epsilon_1, \ldots, \epsilon_K$

$$\epsilon_k = -\log(-\log u_k)$$
 $u_k \sim \mathcal{U}(0,1)$

2 Adding ϵ_k to $\log \alpha_k$, finding argmax, i.e.

$$i = \underset{k}{\operatorname{arg\,max}} [\log \alpha_k + \epsilon_k]$$
 $z_i = 1$

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The "Gumbel-Max" trick [Papandreou and Yuille 2011]

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Gumbel-Softmax: Discrete Reparameterization [Jang et al. 2017; Maddison et al. 2017]

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Gumbel-Softmax: Discrete Reparameterization [Jang et al. 2017; Maddison et al. 2017]

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Reparameterization:

$$z = \underset{s \in \Delta^{K-1}}{\operatorname{arg max}} (\log \alpha + \epsilon)^{\top} s = g(\epsilon, \alpha)$$

 $z=g(\epsilon,\alpha)$ is a deterministic function applied to stochastic noise. Let's try applying this:

$$q(z_k = 1 \mid x; \lambda) = \frac{\alpha_k}{\sum_{j=1}^K \alpha_j} \quad \alpha = \text{enc}(x; \lambda)$$

(Recalling
$$R_{\theta,\lambda}(z) = \log \frac{p(x,z;\theta)}{q(z|x;\lambda)}$$
)

$$\nabla_{\lambda} \mathbb{E}_{q(z \mid x; \lambda)}[R_{\theta, \lambda}(z)] = \nabla_{\lambda} \mathbb{E}_{\epsilon \sim \mathsf{Gumbel}}[R_{\theta, \lambda}(g(\epsilon, \alpha))]$$
$$= \mathbb{E}_{\epsilon \sim \mathsf{Gumbel}}[\nabla_{\lambda} R_{\theta, \lambda}(z)]$$

Gumbel-Softmax: Discrete Reparameterization [Jang et al. 2017; Maddison et al. 2017]

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(Recalling $R_{\theta,\lambda}(z) = \log \frac{p(x,z;\theta)}{q(z|x;\lambda)}$),

$$\nabla_{\lambda} \mathbb{E}_{q(z \mid x; \lambda)}[R_{\theta, \lambda}(z)] = \nabla_{\lambda} \mathbb{E}_{\epsilon \sim \mathsf{Gumbel}}[R_{\theta, \lambda}(g(\epsilon, \alpha))]$$
$$= \mathbb{E}_{\epsilon \sim \mathsf{Gumbel}}[\nabla_{\lambda} R_{\theta, \lambda}(z)]$$

But this won't work, because zero gradients (almost everywhere)

Gumbel-Softmax: Discrete Reparameterization [Jang et al. 2017; Maddison et al. 2017]

 $z = g(\epsilon, \alpha) = \arg\max(\log \alpha + \epsilon)^{\top} s \implies \nabla_{\lambda} R_{\theta, \lambda}(z) = 0$

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Gumbel-Softmax: Discrete Reparameterization [Jang et al. 2017; Maddison et al. 2017]

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Gumbel-Softmax trick: replace $rg \max$ with $\operatorname{softmax}$

$$z = \operatorname{softmax}\left(\frac{\log \alpha + \epsilon}{\tau}\right)$$
 $z_k = \frac{\exp((\log \alpha_k + \epsilon_k)/\tau)}{\sum_{j=1}^K \exp((\log \alpha_j + \epsilon_j)/\tau)}$

$$\nabla_{\lambda} \mathbb{E}_{q(z \mid x; \lambda)}[R_{\theta, \lambda}(z)] \approx \mathbb{E}_{\epsilon \sim \mathsf{Gumbel}} \left[\nabla_{\lambda} R_{\theta, \lambda} \left(\operatorname{softmax} \left(\frac{\log \alpha + \epsilon}{\tau} \right) \right) \right]$$

where au is a temperature term.

But this won't work, because zero gradients (almost everywhere)

Gumbel-Softmax: Discrete Reparameterization [Jang et al. 2017; Maddison et al. 2017]

 $z = q(\epsilon, \alpha) = \arg\max(\log \alpha + \epsilon)^{\top} s \implies \nabla_{\lambda} R_{\theta, \lambda}(z) = 0$

 $z = \operatorname{softmax}\left(\frac{\log \alpha + \epsilon}{\tau}\right)$ $z_k = \frac{\exp((\log \alpha_k + \epsilon_k)/\tau)}{\sum_{k=1}^K \exp((\log \alpha_k + \epsilon_k)/\tau)}$

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Gumbel-Softmax trick: replace arg max with softmax

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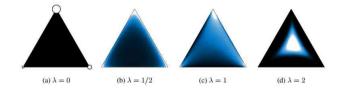
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Gumbel-Softmax: Discrete Reparameterization [Jang et al. 2017; Maddison et al. 2017]

- Approaches a discrete distributution as $\tau \to 0$ (anneal τ during training).
- Reparameterizable by construction
- Differentiable and has non-zero gradients



(from Maddison et al. [2017])

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Reference:

Gumbel-Softmax: Discrete Reparameterization [Jang et al. 2017; Maddison et al. 2017]

- See Maddison et al. [2017] on whether we can use the original categorical densities p(z), q(z), or need to use relaxed densities $p_{\mathsf{GS}}(z), q_{\mathsf{GS}}(z)$.
- Requires that $p(x \mid z; \theta)$ "makes sense" for non-discrete z (e.g. attention).
- Lower-variance, but biased gradient estimator. Variance $\to \infty$ as $\tau \to 0$.

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Flows [Rezende and Mohamed 2015; Kingma et al. 2016]

Recall

$$\log p(x; \theta) = \text{ELBO}(\theta, \lambda; x) - \text{KL}[q(z \mid x; \lambda) || p(z \mid x; \theta)]$$

Bound is tight when variational posterior equals true posterior

$$q(z \mid x; \lambda) = p(z \mid x; \theta) \implies \log p(x; \theta) = \text{ELBO}(\theta, \lambda; x)$$

We want to make $q(z \mid x; \lambda)$ as flexible as possible: can we do better than just Gaussian?

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Flows [Rezende and Mohamed 2015; Kingma et al. 2016]

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Flows [Rezende and Mohamed 2015; Kingma et al. 2016]

Idea: transform a sample from a simple initial variational distribution,

$$z_0 \sim q(z \mid x; \lambda) = \mathcal{N}(\mu, \sigma^2)$$
 $\mu, \sigma^2 = \text{enc}(x; \lambda)$

into a more complex one

$$z_K = f_K \circ \cdots \circ f_2 \circ f_1(z_0; \lambda)$$

where $f_i(z_{i-1}; \lambda)$'s are **invertible** transformations (whose parameters are absorbed by λ).

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Flows [Rezende and Mohamed 2015; Kingma et al. 2016]

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Flows [Rezende and Mohamed 2015; Kingma et al. 2016]

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Sample from final variational posterior is given by z_K . Density is given by the change of variables formula:

$$\begin{split} \log q_K(z_K \,|\, x;\, \lambda) &= \log q(z_0 \,|\, x;\, \lambda) + \sum_{k=1}^K \log \left| \frac{\partial f_k^{-1}}{\partial z_k} \right| \\ &= \underbrace{\log q(z_0 \,|\, x;\, \lambda)}_{\text{log density of Gaussian}} - \sum_{k=1}^K \underbrace{\log \left| \frac{\partial f_k}{\partial z_{k-1}} \right|}_{\text{log determinant of Jacobian}} \end{split}$$

Determinant calculation is $O(N^3)$ in general, but can be made faster depending on parameterization of f_k

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Flows [Rezende and Mohamed 2015; Kingma et al. 2016]

Can still use reparameterization to obtain gradients. Letting

$$F(z) = f_K \circ \cdots \circ f_1(z),$$

ELBO(
$$\theta, \lambda; x$$
) = $\nabla_{\lambda} \mathbb{E}_{q_{K}(z_{K} \mid x; \lambda)} \Big[\log \frac{p(x, z; \theta)}{q_{K}(z_{K} \mid x; \lambda)} \Big]$
= $\nabla_{\lambda} \mathbb{E}_{q(z_{0} \mid x; \lambda)} \Big[\log \frac{p(x, F(z_{0}); \theta)}{q(z_{0} \mid x; \lambda)} - \log \Big| \frac{\partial F}{\partial z_{0}} \Big| \Big]$
= $\mathbb{E}_{\epsilon \sim \mathcal{N}(\mathbf{0}, \mathbf{I})} \Big[\nabla_{\lambda} \Big(\log \frac{p(x, F(z_{0}); \theta)}{q(z_{0} \mid x; \lambda)} - \log \Big| \frac{\partial F}{\partial z_{0}} \Big| \Big) \Big]$

Flows [Rezende and Mohamed 2015; Kingma et al. 2016]

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Examples of $f_k(z_{k-1}; \lambda)$

Normalizing Flows [Rezende and Mohamed 2015]

$$f_k(z_{k-1}) = z_{k-1} + u_k h(w_k^{\top} z_{k-1} + b_k)$$

Inverse Autoregressive Flows [Kingma et al. 2016]

$$f_k(z_{k-1}) = z_{k-1} \odot \sigma_k + \mu_k$$

$$\sigma_{k,d} = \operatorname{sigmoid}(\operatorname{NN}(z_{k-1,< d})) \qquad \mu_{k,d} = \operatorname{NN}(z_{k-1,< d})$$

(In this case the Jacobian is upper triangular, so determinant is just the product of diagonals)

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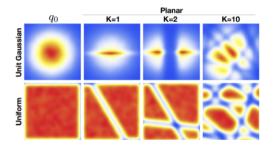
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Flows [Rezende and Mohamed 2015; Kingma et al. 2016]



(from Rezende and Mohamed [2015])

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Importance Weighted Autoencoder (IWAE) [Burda et al. 2015]

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 Flows are a way of tightening the ELBO by making the variational family more flexible.

• Not the only way: can obtain a tighter lower bound on $\log p(x;\,\theta)$ by using multiple importance samples.

Consider

$$I_K = \frac{1}{K} \sum_{k=1}^{K} \frac{p(x, z^{(k)}; \theta)}{q(z^{(k)} | x; \lambda)},$$

where each $z^{(k)} \sim q(z \mid x; \lambda)$.

Note that I_K is an unbiased estimator of $p(x; \theta)$

$$\Xi_{q(z^{(1:K)}|x;\lambda)}[I_K] = p(x;\theta).$$

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Gumbel-Softmax Flows

Importance Weighted Autoencoder (IWAE) [Burda et al. 2015]

 Flows are a way of tightening the ELBO by making the variational family more flexible.

• Not the only way: can obtain a tighter lower bound on $\log p(x;\,\theta)$ by using multiple importance samples.

Consider:

$$I_K = \frac{1}{K} \sum_{k=1}^K \frac{p(x, z^{(k)}; \theta)}{q(z^{(k)} | x; \lambda)},$$

where each $z^{(k)} \sim q(z \mid x; \lambda)$.

where each $z \mapsto q(z \mid x, x)$

Note that I_K is an unbiased estimator of $p(x; \theta)$:

Note that I_K is an unbiased estimator of $p(x;\theta)$: $\mathbb{E}_{q(z^{(1:K)}\mid x:\lambda)}\left[I_K\right] = p(x;\theta).$

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Importance Weighted Autoencoder (IWAE) [Burda et al. 2015]

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Any unbiased estimator of $p(x;\,\theta)$ can be used to obtain a lower bound, using Jensen's inequality:

$$p(x; \theta) = \mathbb{E}_{q(z^{(1:K)} \mid x; \lambda)} [I_K]$$

$$\implies \log p(x; \theta) \ge \mathbb{E}_{q(z^{(1:K)} \mid x; \lambda)} [\log I_K]$$

$$= \mathbb{E}_{q(z^{(1:K)} \mid x; \lambda)} \left[\log \frac{1}{K} \sum_{k=1}^K \frac{p(x, z^{(k)}; \theta)}{q(z^{(k)} \mid x; \lambda)} \right]$$

However, can also show [Burda et al. 2015]:

- $\log p(x; \theta) \ge \mathbb{E} [\log I_K] \ge \mathbb{E} [\log I_{K-1}]$
- $\lim_{K\to\infty} \mathbb{E}\left[\log I_K\right] = \log p(x; \theta)$ under mild conditions

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Importance Weighted Autoencoder (IWAE) [Burda et al. 2015]

$$\mathbb{E}_{q(z^{(1:K)} \mid x; \lambda)} \left[\log \frac{1}{K} \sum_{k=1}^{K} \frac{p(x, z^{(k)}; \theta)}{q(z^{(k)} \mid x; \lambda)} \right]$$

- Note that with K=1, we recover the ELBO.
- Can interpret $\frac{p(x,z^{(k)};\theta)}{q(z^{(k)}\,|\,x;\lambda)}$ as importance weights.
- If $q(z \mid x; \lambda)$ is reparameterizable, we can use the reparameterization trick to optimize $\mathbb{E}\left[\log I_K\right]$ directly.
- Otherwise, need score function gradient estimators [Mnih and Rezende 2016].

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Sentence VAE Example [Bowman et al. 2016]

Generative Model (Model 2):

- Draw $\mathbf{z} \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$
- Draw $x_t \mid \mathbf{z} \sim \text{CRNNLM}(\theta, \mathbf{z})$

Variational Model (Amortized): Deep Diagonal Gaussians,

$$q(\mathbf{z} \mid x; \lambda) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\sigma^2})$$

$$\tilde{\boldsymbol{h}}_T = \text{RNN}(x; \psi)$$

$$\mu = \mathbf{W}_1 \tilde{h}_T$$
 $\sigma^2 = \exp(\mathbf{W}_2 \tilde{h}_T)$ $\lambda = {\mathbf{W}_1, \mathbf{W}_2, \psi}$

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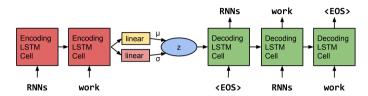
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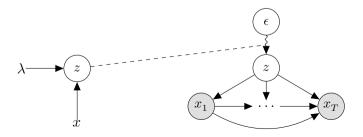
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Sentence VAE Example [Bowman et al. 2016]



(from Bowman et al. [2016])



Issue 1: Posterior Collapse

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ELBO
$$(\theta, \lambda)$$
 = $\mathbb{E}_{q(z \mid x; \lambda)}[\log \frac{p(x, z; \theta)}{q(z \mid x; \lambda)}]$

$$= \underbrace{\mathbb{E}_{q(z \,|\, x;\, \lambda)}[\log p(x \,|\, z;\, \theta)]}_{\text{Reconstruction likelihood}} - \underbrace{\text{KL}[q(z \,|\, x;\, \lambda) \| p(z)]}_{\text{Regularizer}}$$

Model	L/ELBO	Reconstruction	KL
RNN LM	-329.10	-	-
RNN VAE	-330.20	-330.19	0.01

(On Yahoo Corpus from Yang et al. [2017])

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Issue 1: Posterior Collapse

- x and z become independent, and $p(x,z;\,\theta)$ reduces to a non-LV language model.
- Chen et al. [2017]: If it's possible to model $p_{\star}(x)$ without making use of z, then ELBO optimum is at:

$$p_{\star}(x) = p(x \mid z; \theta) = p(x; \theta) \quad q(z \mid x; \lambda) = p(z)$$

$$\mathrm{KL}[q(z \mid x; \, \lambda) || p(z)] = 0$$

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Mitigating Posterior Collapse

Use less powerful likelihood models [Miao et al. 2016; Yang et al. 2017], or "word dropout" [Bowman et al. 2016].

Model	LL/ELBO	Reconstruction	KL
RNN LM	-329.1	-	-
RNN VAE	-330.2	-330.2	0.01
+ Word Drop	-334.2	-332.8	1.44
CNN VAE	-332.1	-322.1	10.0

(On Yahoo Corpus from Yang et al. [2017])

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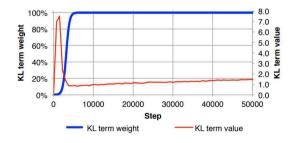
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Gradually anneal multiplier on KL term, i.e.

$$\mathbb{E}_{q(z \mid x; \lambda)}[\log p(x \mid z; \theta)] - \beta \operatorname{KL}[q(z \mid x; \lambda) || p(z)]$$

eta goes from 0 to 1 as training progresses



(from Bowman et al. [2016])

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Mitigating Posterior Collapse

Other approaches:

- Use auxiliary losses (e.g. train z as part of a topic model) [Dieng et al. 2017; Wang et al. 2018]
- Use von Mises-Fisher distribution with a fixed concentration parameter [Guu et al. 2017; Xu and Durrett 2018]
- Combine stochastic/amortized variational inference [Kim et al. 2018]
- Add skip connections [Dieng et al. 2018]

In practice, often necessary to combine various methods.

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Issue 2: Evaluation

- ELBO always lower bounds $\log p(x; \theta)$, so can calculate an upper bound on PPL efficiently.
- When reporting ELBO, should also separately report,

$$\mathrm{KL}[q(z \mid x; \lambda) || p(z)]$$

to give an indication of how much the latent variable is being "used".

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Issue 2: Evaluation

Also can evaluate $\log p(x; \theta)$ with importance sampling

$$p(x; \theta) = \mathbb{E}_{q(z \mid x; \lambda)} \left[\frac{p(x \mid z; \theta)p(z)}{q(z \mid x; \lambda)} \right]$$
$$\approx \frac{1}{K} \sum_{k=1}^{K} \frac{p(x \mid z^{(k)}; \theta)p(z^{(k)})}{q(z^{(k)} \mid x; \lambda)}$$

So

$$\implies \log p(x; \theta) \approx \log \frac{1}{K} \sum_{k=1}^{K} \frac{p(x|z^{(k)}; \theta)p(z^{(k)})}{q(z^{(k)}|x; \lambda)}$$

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Qualitative evaluation

- Evaluate samples from prior/variational posterior.
- Interpolation in latent space.

i went to the store to buy some groceries .
i store to buy some groceries .
i were to buy any groceries .
horses are to buy any groceries .
horses are to buy any animal .
horses the favorite any animal .
horses the favorite favorite animal .
horses are my favorite animal .

(from Bowman et al. [2016])

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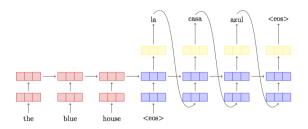
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Encoder | Sutskever et al. 2014; Cho et al. 2014]



Given: Source information $s = s_1, \ldots, s_M$.

Generative process:

• Draw $x_{1:T} \mid s \sim \text{CRNNLM}(\theta, \mathbf{enc}(s))$.

Latent, Per-token Experts [Yang et al. 2018]

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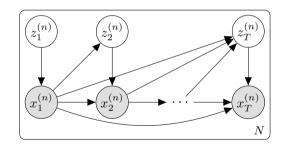
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Generative process: For t = 1, ..., T,

- Draw $z_t \mid x_{< t}, s \sim \operatorname{softmax}(\boldsymbol{U}\boldsymbol{h}_t)$.
- Draw $x_t \mid z_t, x_{< t}, s \sim \operatorname{softmax}(\boldsymbol{W} \tanh(\boldsymbol{Q}_{z_t} \boldsymbol{h}_t); \theta)$



If $m{U} \in \mathbb{R}^{K imes d}$, used K experts; increases the flexibility of per-token distribution $_{32/153}$

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Case-Study: Latent Per-token Experts [Yang et al. 2018]

Learning: z_t are independent given $x_{< t}$, so we can marginalize at each time-step (Method 3: Conjugacy).

$$\underset{\theta}{\operatorname{arg \, max} \log p(x \mid s; \, \theta)} = \underset{\theta}{\operatorname{arg \, max} \log \prod_{t=1}^{T} \sum_{k=1}^{K} p(z_{t}=k \mid s, x_{< t}; \, \theta) \, p(x_{t} \mid z_{t}=k, x_{< t}, s; \, \theta)}.$$

Test-time:

$$\underset{x_{1:T}}{\operatorname{arg \, max}} \prod_{t=1}^{T} \sum_{k=1}^{K} p(z_{t} = k \mid s, x_{< t}; \, \theta) \, p(x_{t} \mid z_{t} = k, x_{< t}, s; \, \theta).$$

Case-Study: Latent, Per-token Experts [Yang et al. 2018]

PTB language modeling results (s is constant):

Model **PPL** 57.30 Merity et al. [2018] Softmax-mixture [Yang et al. 2018] 54.44

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Dialogue generation results (s is context):

Model	BLEU	
	Prec	Rec
No mixture	14.1	11.1
Softmax-mixture [Yang et al. 2018]	15.7	12.3

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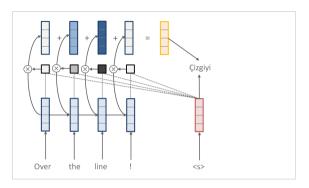
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Attention [Bahdanau et al. 2015]



Decoding with an attention mechanism:

$$x_t \mid x_{< t}, s \sim \operatorname{softmax}(\boldsymbol{W}[\boldsymbol{h}_t, \sum_{m=1}^{M} \alpha_{t,m} \operatorname{enc}(s)_m]).$$

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Copy Attention [Gu et al. 2016; Gulcehre et al. 2016]

Copy attention models copying words directly from s.

Generative process: For t = 1, ..., T,

- Set α_t to be attention weights.
- Draw $z_t \mid x_{< t}, s \sim \text{Bern}(\text{MLP}([\boldsymbol{h}_t, \mathbf{enc}(s)])).$
- If $z_t = 0$
 - Draw $x_t | z_t, x_{\leq t}, s \sim \operatorname{softmax}(\boldsymbol{W}\boldsymbol{h}_t)$.
- Else
 - Draw $x_t \in \{s_1, \ldots, s_M\} \mid z_t, x_{< t}, s \sim \operatorname{Cat}(\boldsymbol{\alpha}_t)$.

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Copy Attention

Learning: Can maximize the log per-token marginal [Gu et al. 2016], as with per-token experts:

$$\max_{\theta} \log p(x_1, \dots, x_T \mid s; \theta)$$

$$= \max_{\theta} \log \prod_{t=1}^{T} \sum_{z' \in \{0,1\}} p(z_t = z' \mid s, x_{< t}; \theta) p(x_t \mid z', x_{< t}, x; \theta).$$

Test-time:

$$\underset{x_{1:T}}{\operatorname{arg \, max}} \prod_{t=1}^{T} \sum_{z' \in \{0,1\}} p(z_t = z' \mid s, x_{< t}; \, \theta) \, p(x_t \mid z', x_{< t}, s; \, \theta).$$

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Attention as a Latent Variable [Deng et al. 2018]

Generative process: For t = 1, ..., T,

- Set α_t to be attention weights.
- Draw $z_t \mid x_{\leq t}, s \sim \operatorname{Cat}(\boldsymbol{\alpha}_t)$.
- Draw $x_t | z_t, x_{< t}, s \sim \operatorname{softmax}(\boldsymbol{W}[\boldsymbol{h}_t, \mathbf{enc}(s_{z_t})]; \theta).$

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Attention as a Latent Variable [Deng et al. 2018]

Marginal likelihood under latent attention model:

$$p(x_{1:T} \mid s; \theta) = \prod_{t=1}^{T} \sum_{m=1}^{M} \alpha_{t,m} \operatorname{softmax}(\boldsymbol{W}[\boldsymbol{h}_{t}, \mathbf{enc}(s_{m})]; \theta)_{x_{t}}.$$

Standard attention likelihood:

$$p(x_{1:T} \mid s; \theta) = \prod_{t=1}^{T} \operatorname{softmax}(\boldsymbol{W}[\boldsymbol{h}_t, \sum_{m=1}^{M} \alpha_{t,m} \operatorname{enc}(s_m)]; \theta)_{x_t}.$$

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Attention as a Latent Variable [Deng et al. 2018]

Learning Strategy #1: Maximize the log marginal via enumeration as above.

Learning Strategy #2: Maximize the ELBO with AVI:

$$\max_{\lambda, \theta} \mathbb{E}_{q(z_t; \lambda)} \left[\log p(x_t \, | \, x_{< t}, z_t, s) \right] - \text{KL}[q(z_t; \, \lambda) \| p(z_t \, | \, x_{< t}, s)].$$

- $q(z_t \mid x; \lambda)$ approximates $p(z_t \mid x_{1:T}, s; \theta)$; implemented with a BLSTM.
- ullet q isn't reparameterizable, so gradients obtained using REINFORCE + baseline.

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Attention as a Latent Variable [Deng et al. 2018]

Test-time: Calculate $p(x_t | x_{< t}, s; \theta)$ by summing out z_t .

MT Results on IWSLT-2014:

Model	PPL	BLEU
Standard Attn	7.03	32.31
Latent Attn (marginal)	6.33	33.08
Latent Attn (ELBO)	6.13	33.09

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Encoder/Decoder with Structured Latent Variables

At least two EMNLP 2018 papers augment encoder/decoder text generation models with *structured* latent variables:

- 1 Lee et al. [2018] generate $x_{1:T}$ by iteratively refining sequences of words $z_{1:T}$.
- 2 Wiseman et al. [2018] generate $x_{1:T}$ conditioned on a latent template or plan $z_{1:S}$.

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Summary as a Latent Variable [Miao and Blunsom 2016]

Generative process for a document $x = x_1, \dots, x_T$:

- Draw a latent summary $z_1, \dots, z_M \sim \mathrm{RNNLM}(\theta)$
- Draw $x_1, \ldots, x_T \mid z_{1:M} \sim \text{CRNNLM}(\theta, z)$

Posterior Inference

 $p(z_{1:M} \mid x_{1:T}; \theta) = p(\mathsf{summary} \mid \mathsf{document}; \theta).$

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Summary as a Latent Variable [Miao and Blunsom 2016]

Generative process for a document $x = x_1, \dots, x_T$:

- Draw a latent summary $z_1, \ldots, z_M \sim \mathrm{RNNLM}(\theta)$
- Draw $x_1, \ldots, x_T \mid z_{1:M} \sim \text{CRNNLM}(\theta, z)$

Posterior Inference:

$$p(z_{1:M} \mid x_{1:T}; \theta) = p(\text{summary} \mid \text{document}; \theta).$$

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Summary as a Latent Variable [Miao and Blunsom 2016]

Learning: Maximize the ELBO with amortized family:

$$\max_{\lambda,\theta} \mathbb{E}_{q(z_{1:M};\,\lambda)} \left[\log p(x_{1:T} \,|\, z_{1:M};\,\theta) \right] - \text{KL}[q(z_{1:M};\,\lambda) \| p(z_{1:M};\,\theta) \right]$$

- $q(z_{1:M}; \lambda)$ approximates $p(z_{1:M} | x_{1:T}; \theta)$; also implemented with encoder/decoder RNNs.
- $q(z_{1:M}; \lambda)$ not reparameterizable, so gradients use REINFORCE + baselines.

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Summary as a Latent Variable [Miao and Blunsom 2016]

Semi-supervised Training: Can also use documents *without* corresponding summaries in training.

- Train $q(z_{1:M}; \lambda) \approx p(z_{1:M} | x_{1:T}; \theta)$ with labeled examples.
- Infer summary z for an unlabeled document with q.
- Use inferred z to improve model $p(x_{1:T} | z_{1:M}; \theta)$.
- Allows for outperforming strictly supervised models!

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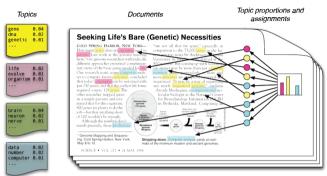
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Topic Models [Blei et al. 2003]



Generative process: for each document $x^{(n)} = x_1^{(n)}, \dots, x_T^{(n)}$,

- Draw topic distribution $\mathbf{z}_{top}^{(n)} \sim Dir(oldsymbol{lpha})$
- For t = 1, ..., T:
 - Draw topic $z_t^{(n)} \sim Cat(\mathbf{z}_{top}^{(n)})$
 - Draw $x_t \sim Cat(\pmb{\beta}_{z_t^{(n)}})$

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Simple, Deep Topic Models [Miao et al. 2017]

Motivation: easy to learn deep topic models with VI if $q(\mathbf{z}_{top}^{(n)}; \lambda)$ is reparameterizable.

Idea: draw $\mathbf{z}_{top}^{(n)}$ from a transformation of a Gaussian.

- ullet Draw $\mathbf{z}_0^{(n)} \sim \mathcal{N}(oldsymbol{\mu}_0, oldsymbol{\sigma}_0^2)$
- Set $\mathbf{z}_{top}^{(n)} = \operatorname{softmax}(\boldsymbol{W}\mathbf{z}_0^{(n)}).$
- Use analogous transformation when drawing from $q(\mathbf{z}_{top}^{(n)}; \lambda)$.

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Simple, Deep Topic Models [Miao et al. 2017]

Learning Step #1: Marginalize out per-word latents $z_t^{(n)}$.

$$p(\{x^{(n)}\}_{n=1}^{N}, \{\mathbf{z}_{top}^{(n)}\}_{n=1}^{N}; \theta) = \prod_{n=1}^{N} p(\mathbf{z}_{top}^{(n)} | \theta) \prod_{t=1}^{T} \sum_{k=1}^{K} z_{top,k}^{(n)} \beta_{k,x_{t}^{(n)}}$$

Learning Step #2: Use AVI to optimize resulting ELBO.

$$\max_{\lambda,\theta} \mathbb{E}_{q(\mathbf{z}_{top}^{(n)};\lambda)} \left[\log p(x^{(n)} \mid \mathbf{z}_{top}^{(n)};\theta) \right] - \text{KL}[\mathcal{N}(\mathbf{z}_0^{(n)};\lambda) || \mathcal{N}(\mathbf{z}_0^{(n)};\boldsymbol{\mu}_0,\boldsymbol{\sigma}_0^2)]$$

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Perplexities on held-out documents, for three datasets:

Model	MXM	20News	RCV1
OnlineLDA [Hoffman et al. 2010]	342	1015	1058
AVI-LDA [Miao et al. 2017]	272	830	602

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Deep Latent-Variable NLP: Two Views

Deep Models & LV Models are naturally complementary:

- Rich set of model choices: discrete, continuous, and structured.
- Real applications across NLP including some state-of-the-art models.

Deep Models & LV Models are frustratingly incompatible:

- Many interesting approaches to the problem: reparameterization, score-function, and more.
- Lots of area for research into improved approaches.

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- Modern toolkits make it easy to implement these models.
- Combine the flexibility of auto-differentiation for optimization (PyTorch) with distribution and VI libraries (Pyro).

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