

# Probabilistic modelling for NLP powered by deep learning

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April 3, 2018

# Outline

- 1 Deep generative models
- 2 Variational inference
- 3 Variational auto-encoder

# Problems

## Supervised problems

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- images, ...

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## Unsupervised problems

*“learn a distribution over **observed** and **unobserved** data”*

- sentences in natural language + parse trees
- images + bounding boxes, ...

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$$\underbrace{X \sim \text{Cat}(\pi_1, \dots, \pi_K)}_{\text{e.g. nationality}}$$

or

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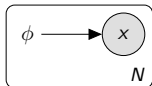
or

$$\underbrace{X \sim \mathcal{N}(\mu, \sigma^2)}_{\text{e.g. height}}$$

**estimate parameters** that assign maximum likelihood to observations



# Multiple problems, same language



(Conditional) Density estimation

	Side information ( $\phi$ )	Observation ( $x$ )
Parsing	a sentence	parse tree
Translation	a sentence in French	translation in English
Captioning	an image	caption in English
Entailment	a text and hypothesis	entailment relation

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and proceed to **estimate parameters**  $\theta$  of the NNs

# NN as efficient parametrisation

From the statistical point of view NNs do not generate data

- they parametrise distributions that *by assumption* govern data
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Prediction is done by a decision rule outside the statistical model

- e.g. beam search

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quantifies the fitness of our model to data

## MLE via gradient-based optimisation

If assessing the log-likelihood is **differentiable** and assessing it is **tractable**, then backpropagation can give us the gradient

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and we can update  $\theta$  in the direction

$$\gamma \nabla_{\theta} \mathcal{L}(\theta | x^{(1:N)})$$

to attain a local optimum of the likelihood function

# Stochastic optimisation

We can also use a gradient estimate

$$\nabla_{\theta} \mathcal{L}(\theta | x^{(1:N)}) = \nabla_{\theta} \underbrace{\mathbb{E}_{S \sim \mathcal{U}(1..N)} \left[ N \log p(x^{(S)} | \theta) \right]}_{\mathcal{L}(\theta | x^{(1:N)})}$$

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and take steps in the direction

$$\gamma \frac{N}{M} \nabla_{\theta} \mathcal{L}(\theta | x^{(s_1:s_M)})$$

where  $x^{(s_1)}, \dots, x^{(s_M)}$  is a random mini-batch of size  $M$

# DL in NLP recipe

## Maximum likelihood estimation

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## DL in NLP recipe

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### Automatic differentiation (*backprop*)

- chain rule of derivatives: “give me a tractable forward pass and I will give you **gradients**”

### Stochastic optimisation powered by backprop

- general purpose gradient-based optimisers

# Tractability is central

Likelihood gives us a differentiable objective to optimise for

- but we need to stick with **tractable** likelihood functions

# When do we have intractable likelihood?

**Unsupervised problems** contain unobserved random variables

$$p_{\theta}(x, z) = \overbrace{p(z)}^{\text{latent variable model}} \underbrace{p_{\theta}(x|z)}_{\text{observation model}}$$

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$$p_{\theta}(x, z) = \overbrace{p(z)}^{\text{latent variable model}} \underbrace{p_{\theta}(x|z)}_{\text{observation model}}$$

thus assessing the marginal likelihood requires **marginalisation of latent variables**

$$p_{\theta}(x) = \int p_{\theta}(x, z) dz = \int p(z)p_{\theta}(x|z) dz$$

# Examples of latent variable models

Discrete latent variable, continuous observation

- too many forward passes

$$p_{\theta}(x) = \sum_{c=1}^K \text{Cat}(c|\pi_1, \dots, \pi_K) \underbrace{\mathcal{N}(x|\mu_{\theta}(c), \sigma_{\theta}(c)^2)}_{\text{forward pass}}$$



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Continuous latent variable, discrete observation

- infinitely many forward passes

$$p_{\theta}(x) = \int \mathcal{N}(z|0, I) \underbrace{\text{Cat}(x|\pi_{\theta}(z))}_{\text{forward pass}} dz$$

# Deep generative models

Joint distribution with **deep observation model**

$$p_{\theta}(x, z) = \underbrace{p(z)}_{\text{prior}} \underbrace{p_{\theta}(x|z)}_{\text{likelihood}}$$

mapping from latent variable  $z$  to  $p(x|z)$  is a NN with parameters  $\theta$

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Marginal likelihood (or evidence)

$$p_{\theta}(x) = \int p_{\theta}(x, z) \, dz = \int p(z) p_{\theta}(x|z) \, dz$$

**intractable** in general

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MC estimate of gradient requires sampling from posterior

$$p_{\theta}(z|x) = \frac{p(z)p_{\theta}(x|z)}{p_{\theta}(x)}$$

unavailable due to the intractability of the marginal

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- But we cannot use backprop for parameter estimation

We need **approximate inference** techniques!

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# The Basic Problem

The marginal likelihood

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

is generally **intractable**, which prevents us from computing quantities that depend on the posterior  $p(z|x)$

- e.g. gradients in MLE
- e.g. predictive distribution in Bayesian modelling

# Strategy

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- approximate it by an auxiliary distribution  $q(z|x)$  that is computable
- choose  $q(z|x)$  as close as possible to  $p(z|x)$  to obtain a faithful approximation

## Evidence lowerbound

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 &= \mathbb{E}_{q(z|x)} [\log p(x, Z)] - \mathbb{E}_{q(z|x)} [\log q(Z)] \\
 &= \mathbb{E}_{q(z|x)} [\log p(x, Z)] + \mathbb{H}(q(z|x))
 \end{aligned}$$

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 &= - \underbrace{\mathbb{E}_{q(z|x)} \left[ \log \frac{q(Z|x)}{p(Z|x)} \right]}_{\text{KL}(q(z|x) || p(z|x))} + \log p(x)
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 \end{aligned}$$

We have derived a lower bound on the log-evidence whose gap is exactly  $\text{KL}(q(z|x) || p(z|x))$ .



# Variational Inference

## Objective

$$\max_{q(z|x)} \mathbb{E} [\log p(x, Z)] + \mathbb{H}(q(z|x))$$

- The ELBO is a lower bound on  $\log p(x)$

# Mean field assumption

Suppose we have  $N$  latent variables

- assume the posterior factorises as  $N$  independent terms
- each with an independent set of parameters

$$q(z_1, \dots, z_N) = \underbrace{\prod_{i=1}^N q_{\lambda_i}(z_i)}_{\text{mean field}}$$

# Amortised variational inference

Amortise the cost of inference using NNs

$$q(z_1, \dots, z_N | x_1, \dots, x_N) = \prod_{i=1}^N q_\lambda(z_i | x_i)$$

with a shared set of parameters

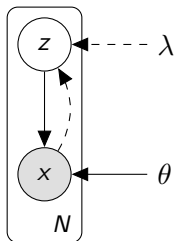
- e.g.  $Z|x \sim \mathcal{N}(\underbrace{\mu_\lambda(x), \sigma_\lambda(x)^2}_{\text{inference network}})$

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# Variational auto-encoder

## Generative model with NN likelihood



- complex (non-linear) observation model  $p_{\theta}(x|z)$
- complex (non-linear) mapping from data to latent variables  $q_{\lambda}(z|x)$

Jointly optimise generative model  $p_{\theta}(x|z)$  and inference model  $q_{\lambda}(z|x)$  under the same objective (ELBO)

$$\log p_{\theta}(x) \geq \overbrace{\mathbb{E}_{q_{\lambda}(z|x)} [\log p_{\theta}(x, Z)] + \mathbb{H}(q_{\lambda}(z|x))}^{\text{ELBO}}$$

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Parameter estimation

$$\arg \max_{\theta, \lambda} \mathbb{E}_{q_{\lambda}(z|x)} [\log p_{\theta}(x|Z)] - \text{KL}(q_{\lambda}(z|x) \parallel p(z))$$

$$\begin{aligned}\log p_{\theta}(x) &\geq \overbrace{\mathbb{E}_{q_{\lambda}(z|x)} [\log p_{\theta}(x, Z)] + \mathbb{H}(q_{\lambda}(z|x))}^{\text{ELBO}} \\ &= \mathbb{E}_{q_{\lambda}(z|x)} [\log p_{\theta}(x|Z) + \log p(Z)] + \mathbb{H}(q_{\lambda}(z|x)) \\ &= \mathbb{E}_{q_{\lambda}(z|x)} [\log p_{\theta}(x|Z)] - \text{KL}(q_{\lambda}(z|x) || p(z))\end{aligned}$$

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true for exponential families

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- assume  $\text{KL}(q_{\lambda}(z|x) || p(z))$  analytical  
true for exponential families
- approximate  $\mathbb{E}_{q_{\lambda}(z|x)} [\log p_{\theta}(x|z)]$  by sampling  
true because we design  $q_{\lambda}(z|x)$  to be simple

# Generative Network Gradient

$$\frac{\partial}{\partial \theta} \left( \mathbb{E}_{q_{\lambda}(z|x)} [\log p_{\theta}(x|z)] - \overbrace{\text{KL}(q_{\lambda}(z|x) || p(z))}^{\text{constant wrt } \theta} \right)$$

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Note:  $q_{\lambda}(z|x)$  does not depend on  $\theta$ .

# Inference Network Gradient

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The first term again requires approximation by sampling,  
but there is a problem

# Inference Network Gradient

$$\frac{\partial}{\partial \lambda} \mathbb{E}_{q_{\lambda}(z|x)} [\log p_{\theta}(x|z)]$$

## Inference Network Gradient

$$\begin{aligned} & \frac{\partial}{\partial \lambda} \mathbb{E}_{q_{\lambda}(z|x)} [\log p_{\theta}(x|z)] \\ &= \frac{\partial}{\partial \lambda} \int q_{\lambda}(z|x) \log p_{\theta}(x|z) dz \end{aligned}$$

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- MC estimator is non-differentiable: cannot sample first
- Differentiating the expression does not yield an expectation: cannot approximate via MC

## Score function estimator

We can again use the log identity for derivatives

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## Score function estimator: high variance

We can now build an MC estimator

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but

- magnitude of  $\log p_{\theta}(x|z)$  varies widely
- model likelihood does not contribute to direction of gradient
- too much variance to be useful

# When variance is high we can

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excellent idea, but not just yet
- stare at this  $\frac{\partial}{\partial \lambda} \mathbb{E}_{q_{\lambda}(z|x)} [\log p_{\theta}(x|z)]$   
until we find a way to rewrite the expectation in terms of a density that **does not depend on  $\lambda$**

# Reparametrisation

Find a transformation  $h : z \mapsto \epsilon$  that expresses  $z$  through a random variable  $\epsilon$  such that  $q(\epsilon)$  does not depend on  $\lambda$

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(Kingma and Welling, 2013; Rezende et al., 2014; Titsias and Lázaro-Gredilla, 2014)

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- $h(z, \lambda)$  needs to be differentiable

Invertibility implies

- $h(z, \lambda) = \epsilon$
- $h^{-1}(\epsilon, \lambda) = z$

---

(Kingma and Welling, 2013; Rezende et al., 2014; Titsias and Lázaro-Gredilla, 2014)

# Gaussian Transformation

If  $Z \sim \mathcal{N}(\mu_\lambda(x), \sigma_\lambda(x)^2)$  then

$$h(z, \lambda) = \frac{z - \mu_\lambda(x)}{\sigma_\lambda(x)} = \epsilon \sim \mathcal{N}(0, 1)$$

$$h^{-1}(\epsilon, \lambda) = \mu_\lambda(x) + \sigma_\lambda(x) \odot \epsilon \quad \epsilon \sim \mathcal{N}(0, 1)$$

$$= \frac{\partial}{\partial \lambda} \int q_{\lambda}(z|x) \log p_{\theta}(x|z) \, dz$$

$$\begin{aligned} &= \frac{\partial}{\partial \lambda} \int q_{\lambda}(z|x) \log p_{\theta}(x|z) \, dz \\ &= \frac{\partial}{\partial \lambda} \int \mathbf{q}(\epsilon) \log p_{\theta}(x | \overbrace{h^{-1}(\epsilon, \lambda)}^{=z}) \, d\epsilon \end{aligned}$$

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 &= \underbrace{\mathbb{E}_{q(\epsilon)} \left[ \frac{\partial}{\partial \lambda} \log p_{\theta}(x | h^{-1}(\epsilon, \lambda)) \right]}_{\text{expected gradient :D}} \, d\epsilon
 \end{aligned}$$

## Reparametrised gradient estimate

$$= \underbrace{\mathbb{E}_{q(\epsilon)} \left[ \frac{\partial}{\partial \lambda} \log p_{\theta}(x|h^{-1}(\epsilon, \lambda)) \right]}_{\text{expected gradient :D}} d\epsilon$$

# Reparametrised gradient estimate

$$\begin{aligned} &= \underbrace{\mathbb{E}_{q(\epsilon)} \left[ \frac{\partial}{\partial \lambda} \log p_{\theta}(x|h^{-1}(\epsilon, \lambda)) \right]}_{\text{expected gradient :D}} d\epsilon \\ &= \mathbb{E}_{q(\epsilon)} \left[ \underbrace{\frac{\partial}{\partial z} \log p_{\theta}(x|\overbrace{h^{-1}(\epsilon, \lambda)}^{=z})}_{\text{chain rule}} \times \frac{\partial}{\partial \lambda} h^{-1}(\epsilon, \lambda) \right] \end{aligned}$$



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$$\epsilon^{(k)} \sim q(\epsilon)$$

Note that both models contribute with gradients

# Gaussian KL

## ELBO

$$\mathbb{E}_{q_{\lambda}(z|x)} [\log p_{\theta}(x|z)] - \text{KL}(q_{\lambda}(z|x) || p(z))$$

# Gaussian KL

## ELBO

$$\mathbb{E}_{q_{\lambda}(z|x)} [\log p_{\theta}(x|z)] - \text{KL} (q_{\lambda}(z|x) || p(z))$$

Analytical computation of  $-\text{KL} (q_{\lambda}(z|x) || p(z))$ :

$$\frac{1}{2} \sum_{i=1}^d (1 + \log (\sigma_i^2) - \mu_i^2 - \sigma_i^2)$$

# Gaussian KL

## ELBO

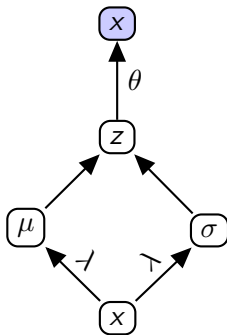
$$\mathbb{E}_{q_{\lambda}(z|x)} [\log p_{\theta}(x|z)] - \text{KL}(q_{\lambda}(z|x) || p(z))$$

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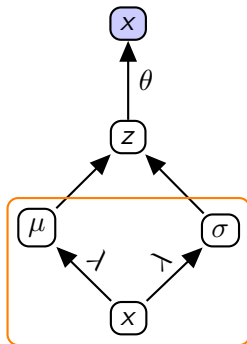
Thus backprop will compute  $-\frac{\partial}{\partial \lambda} \text{KL}(q_{\lambda}(z|x) || p(z))$  for us

# Computation Graph



# Computation Graph

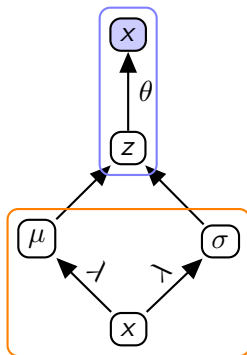
inference model



# Computation Graph

generative model

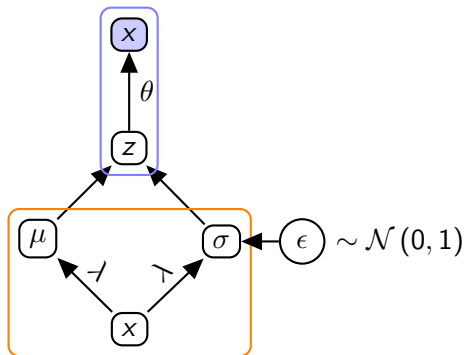
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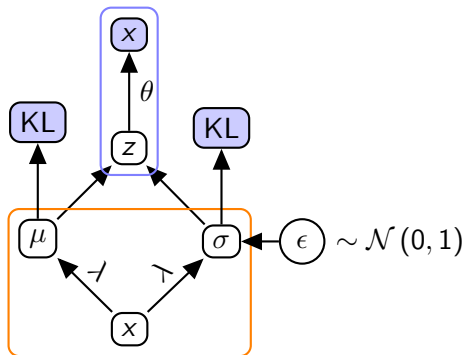




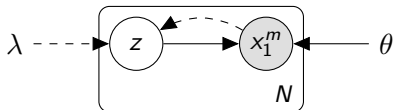
# Computation Graph

generative model

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# Example



Generative model

- $Z \sim \mathcal{N}(0, I)$
- $X_i | z, x_{<i} \sim \text{Cat}(f_\theta(z, x_{<i}))$

Inference model

- $Z \sim \mathcal{N}(\mu_\lambda(x_1^m), \sigma_\lambda(x_1^m)^2)$

# VAEs – Summary

## Advantages

- Backprop training
- Easy to implement
- Posterior inference possible
- One objective for both NNs

# VAEs – Summary

## Advantages

- Backprop training
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- Posterior inference possible
- One objective for both NNs

## Drawbacks

- Discrete latent variables are difficult
- Optimisation may be difficult with several latent variables
- Location-scale families only  
but see Ruiz et al. (2016) and Kucukelbir et al. (2017)

# Summary

## Deep learning in NLP

- task-driven feature extraction
- models with more realistic assumptions

## Probabilistic modelling

- better (or at least more explicit) statistical assumptions
- compact models
- semi-supervised learning

# Literature I

- Dzmitry Bahdanau, Kyunghyun Cho, and Yoshua Bengio. Neural machine translation by jointly learning to align and translate. 2014. URL <http://arxiv.org/abs/1409.0473>.
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## Literature II

- Alp Kucukelbir, Dustin Tran, Rajesh Ranganath, Andrew Gelman, and David M. Blei. Automatic differentiation variational inference. *Journal of Machine Learning Research*, 18(14):1–45, 2017. URL <http://jmlr.org/papers/v18/16-107.html>.
- Danilo J. Rezende, Shakir Mohamed, and Daan Wierstra. Stochastic backpropagation and approximate inference in deep generative models. In *ICML*, pages 1278–1286, 2014. URL <http://jmlr.org/proceedings/papers/v32/rezende14.pdf>.
- Francisco R Ruiz, Michalis Titsias RC AUEB, and David Blei. The generalized reparameterization gradient. In D. D. Lee, M. Sugiyama, U. V. Luxburg, I. Guyon, and R. Garnett, editors, *NIPS*, pages 460–468. 2016. URL <http://papers.nips.cc/paper/6328-the-generalized-reparameterization-gradient.pdf>.

## Literature III

Rico Sennrich, Barry Haddow, and Alexandra Birch. Improving neural machine translation models with monolingual data. In *Proceedings of the 54th Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pages 86–96, Berlin, Germany, August 2016. Association for Computational Linguistics. URL <http://www.aclweb.org/anthology/P16-1009>.

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