Deep Generative Models

back-propagation through stochastic computation graphs

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May 24, 2018

Outline

Problems

Supervised problems

"learn a distribution over observed data"

- sentences in natural language
- images, . . .

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Supervised problems

"learn a distribution over observed data"

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- images, . . .

Unsupervised problems

"learn a distribution over observed and unobserved data"

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

Supervised problems

We have data $x^{(1)}, \dots, x^{(N)}$ e.g.

- sentences, images, ...

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$$\underbrace{X \sim \mathrm{Cat}(\pi_1, \ldots, \pi_K)}_{\text{e.g. nationality}} \qquad \text{or} \qquad \underbrace{X \sim \mathcal{N}(\mu, \sigma^2)}_{\text{e.g. height}}$$

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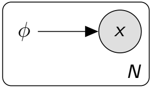
estimate parameters that assign maximum likelihood to observations

Multiple problems, same language



(Conditional) Density estimation

	Side information (ϕ)	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 θ of the NNs

NN as efficient parametrisation

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- they parametrise distributions
  which *by assumption* govern data
- map complex side information to parameter space

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Prediction is done by a decision rule outside the statistical model

- e.g. beam search

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Likelihood function quantifies the **fitness** of our model to data

$$\mathcal{L}(\theta|x^{(1:N)}) = \log \prod_{s=1}^{N} p(x^{(s)}|\theta)$$

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MLE via gradient-based optimisation

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

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and we can update θ in the direction

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

to attain a local optimum of the likelihood function

Big Data

For large N, computing the gradient is inconvenient

$$\nabla_\theta \mathcal{L}(\theta | x^{(1:N)}) = \underbrace{\sum_{s=1}^{N} \nabla_\theta \log p(x^{(s)} | \theta)}_{\text{too many terms}}$$

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$$= \sum_{s=1}^{N} \mathcal{U}(s|{}^1\!/\!_N) N \nabla_\theta \log p(x^{(s)}|\theta)$$

$$= \mathbb{E}_{S \sim \mathcal{U}({}^1\!/\!_N)} \left[N \nabla_\theta \log p(x^{(S)}|\theta) \right]$$

Stochastic optimisation

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$$\overset{\text{MC}}{\approx} \frac{1}{M}\sum_{m=1}^{M} N\nabla_\theta \log p(x^{(s_i)}|\theta)$$

$$S_i \sim \mathcal{U}(1/N)$$

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$$S_i \sim \mathcal{U}(1/N)$$

and take a step in the direction

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

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

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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

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

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

thus assessing the marginal likelihood requires marginalisation of latent variables

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

Examples of latent variable models

Discrete latent variable, continuous observation

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

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Continuous latent variable, discrete observation

$$p_\theta(x) = \underbrace{\int \mathcal{N}(z|0, I) \underbrace{\mathrm{Cat}(x|\pi_\theta(z))}_{\text{forward pass}} \mathrm{d}z}_{\textbf{infinitely many forward passes}}$$

But why latent variable modelling?

Some reasons

- organise a massive collection of data
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Some reasons

- organise a massive collection of data
  e.g. LDA
- learn from unlabelled data
  e.g. semi-supervised learning
- learn from little data
  e.g. Bayesian NNs
- induce discrete representations
  e.g. parse trees, dependency graphs, permutations, alignments

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 θ

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Marginal likelihood

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

intractable in general

Gradient

Exact gradient is intractable

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&= \underbrace{\mathbb{E}_{p_\theta(z|x)}\left[\nabla_\theta \log p_\theta(x,Z)\right]}_{\text{expected gradient :)}}
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MC estimate of gradient requires sampling from posterior

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

unavailable due to the intractability of the marginal

Summary

- We want richer probabilistic models

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We need approximate inference techniques!

Outline

The Basic Problem

The marginal likelihood

$$p(x) = \int p(x, z)\mathrm{d}z$$

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

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

Evidence lowerbound

$$\log p(x) = \log \int p(x, z)\mathrm{d}z$$

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Evidence lowerbound

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\log p(x) &= \log \int p(x, z)\mathrm{d}z \\
&= \log \int {\color{red}q(z|x)} \frac{p(x, z)}{{\color{red}q(z|x)}}\mathrm{d}z \\
&= \log \left(\mathbb{E}_{q(z|x)} \left[\frac{p(x, Z)}{q(Z|x)} \right] \right)
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&= \mathbb{E}_{q(z|x)} [\log p(x, Z)] - \mathbb{E}_{q(z|x)} [\log q(Z|x)] \\
&= \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]}_{\color{red}{\mathrm{KL}(q(z|x)||p(z|x))}} + \log p(x)
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$$= -\underbrace{\mathbb{E}_{q(z|x)}\left[\log \frac{q(Z|x)}{p(Z|x)}\right]}_{\color{red}{\mathrm{KL}(q(z|x)||p(z|x))}} + \log p(x)$$

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

Variational Inference

Objective

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

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

Blei et al. (2016)

Example Model

Let us consider a latent factor model for topic modelling:

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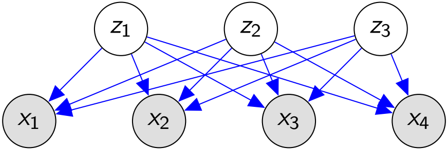
- a document $x = (x_1, \ldots, x_n)$ consists of n i.i.d. categorical draws from that model
- the categorical distribution in turn depends on Gaussian latent factors $z = (z_1, \ldots, z_k)$ which are also i.i.d.

$$
\begin{aligned}
z_j &\sim \mathcal{N}(0, 1) && (1 \leq j \leq k) \\
x_i &\sim \operatorname{Categorical}(f_\theta(z)) && (1 \leq i \leq n)
\end{aligned}
$$

$f_\theta(\cdot)$ is computed by a NN with softmax output.

Example Model

Forward pass: tractable by design



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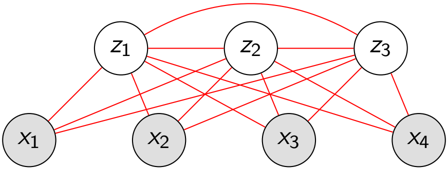


Backward pass: requires posterior
where latent variables are marginally dependent

Mean field assumption

We have k latent variables

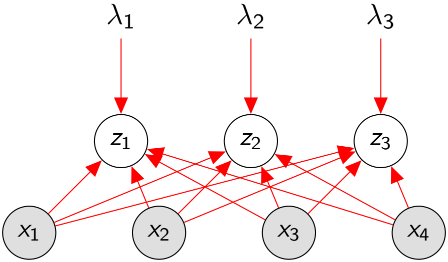
- assume the posterior factorises as k independent terms

$$q(z_1, \ldots, z_k) = \underbrace{\prod_{j=1}^{k} q_{\lambda_j}(z_j)}_{\text{mean field}}$$

with independent sets of parameters

$$Z_j \sim \mathcal{N}(u_j, s_j^2)$$

Mean field: example



Amortised variational inference

Amortise the cost of inference using NNs

$$q(z_1, \ldots, z_k|x) = \prod_{j=1}^{k} q_\lambda(z_j|x)$$

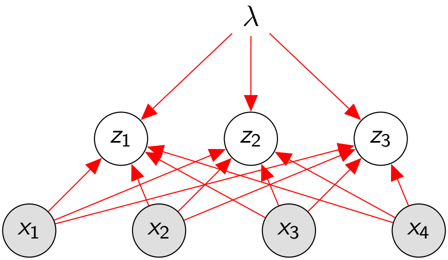
still mean field

$$Z_j|x_1^n \sim \mathcal{N}(u_j, s_j^2)$$

but with a shared set of parameters

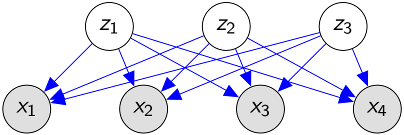
- where $u_1^k = \mu_\lambda(x_1^n)$
- and $s_1^k = \sigma_\lambda(x_1^n)$

Amortised VI: example

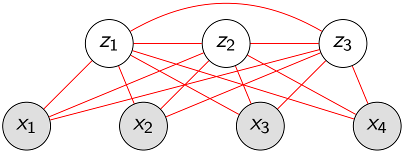


Summary

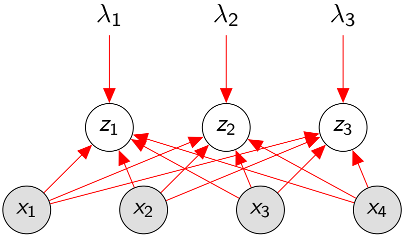
Joint distribution



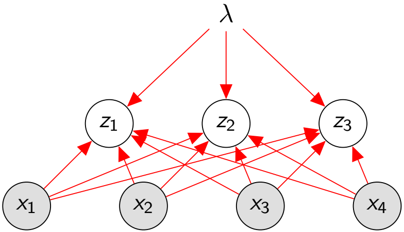
Posterior



Mean field



Amortised VI

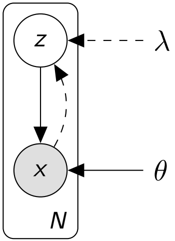


Outline

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

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)

Kingma and Welling (2013)

Objective

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

Objective

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

Parameter estimation

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

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\arg\max_{\theta,\lambda}\; \mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x|Z)\right] - \mathrm{KL}\left(q_\lambda(z|x) \mid\mid p(z)\right)
$$

- assume $\mathrm{KL}\left(q_\lambda(z|x) \mid\mid p(z)\right)$ analytical
  true for exponential families

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Parameter estimation

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

Generative Network Gradient

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

Generative Network Gradient

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

$$= \underbrace{\mathbb{E}_{q_\lambda(z|x)}\left[\frac{\partial}{\partial\theta}\log p_\theta(x|z)\right]}_{\text{expected gradient :)}}$$

Generative Network Gradient

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$$\overset{\text{MC}}{\approx} \frac{1}{K}\sum_{k=1}^{K}\frac{\partial}{\partial\theta}\log p_\theta(x|z^{(k)})$$

$$z^{(k)} \sim q_\lambda(Z|x)$$

Generative Network Gradient

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

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$$z^{(k)} \sim q_\lambda(Z|x)$$

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

Inference Network Gradient

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

Inference Network Gradient

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

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

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

Inference Network Gradient

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

Inference Network Gradient

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

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$$
\begin{aligned}
&\frac{\partial}{\partial\lambda}\mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x|z)\right] \\
&= \frac{\partial}{\partial\lambda}\int q_\lambda(z|x)\log p_\theta(x|z)\mathrm{d}z \\
&= \underbrace{\int \frac{\partial}{\partial\lambda}(q_\lambda(z|x))\log p_\theta(x|z)\,\mathrm{d}z}_{\text{not an expectation}}
\end{aligned}
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- MC estimator is non-differentiable: cannot sample first

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\end{aligned}
$$

- 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

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

Score function estimator: high variance

We can now build an MC estimator

$$
\begin{aligned}
&\frac{\partial}{\partial \lambda} \mathbb{E}_{q_\lambda(z|x)} \left[\log p_\theta(x|z)\right] \\
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&\overset{\text{MC}}{\approx} \frac{1}{K}\sum_{k=1}^{K} {\color{red}\log p_\theta(x|z^{(k)})}\frac{\partial}{\partial \lambda}\log q_\lambda(z^{(k)}|x) \\
&z^{(k)} \sim q_\lambda(Z|x)
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but

- magnitude of $\log p_\theta(x|z)$ varies widely

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but

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- model likelihood does not contribute to direction of gradient

Score function estimator: high variance

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&z^{(k)} \sim q_\lambda(Z|x)
\end{aligned}$$

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

- sample more

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When variance is high we can

- sample more
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- use variance reduction techniques (e.g. baselines and control variates)
  excellent idea, but not just yet
- stare at this $\frac{\partial}{\partial\lambda}\mathbb{E}_{q_\lambda(z|x)}\left[\log p_\theta(x|z)\right]$
  until we find a way to rewrite the expectation in terms of a density that **does not depend on** λ

Reparametrisation

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

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

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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

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

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

Inference Network – Reparametrised Gradient

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

Inference Network – Reparametrised Gradient

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Inference Network – Reparametrised Gradient

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

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$$= \int q(\epsilon) \frac{\partial}{\partial \lambda} \left[\log p_\theta(x| \overbrace{h^{-1}(\epsilon, \lambda)}^{=z}) \right] \mathrm{d}\epsilon$$

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

Reparametrised gradient estimate

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

Reparametrised gradient estimate

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Reparametrised gradient estimate

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$$\stackrel{\text{MC}}{\approx} \frac{1}{K} \sum_{k=1}^{K} \underbrace{\frac{\partial}{\partial z} \log p_\theta(x|\overbrace{h^{-1}(\epsilon^{(k)}, \lambda)}^{=z}) \times \frac{\partial}{\partial \lambda} h^{-1}(\epsilon^{(k)}, \lambda)}_{\text{backprop's job}}$$

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

Reparametrised gradient estimate

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

Both models contribute with gradients!

Gaussian KL

ELBO

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

Gaussian KL

ELBO

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

Analytical computation of $-\mathrm{KL}\left(q_\lambda(z|x) \mid\mid p(z)\right)$:

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

Gaussian KL

ELBO

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

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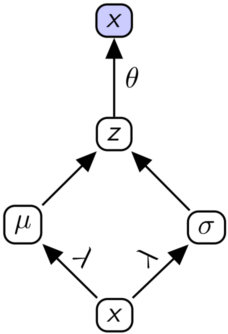
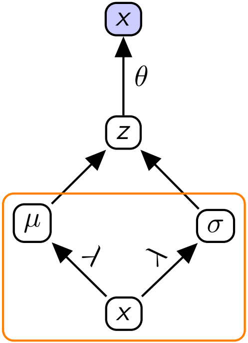
Thus backprop will compute $-\frac{\partial}{\partial\lambda}\mathrm{KL}\left(q_\lambda(z|x) \mid\mid p(z)\right)$ for us

Computation Graph



Computation Graph

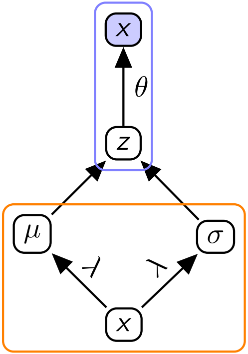
inference model



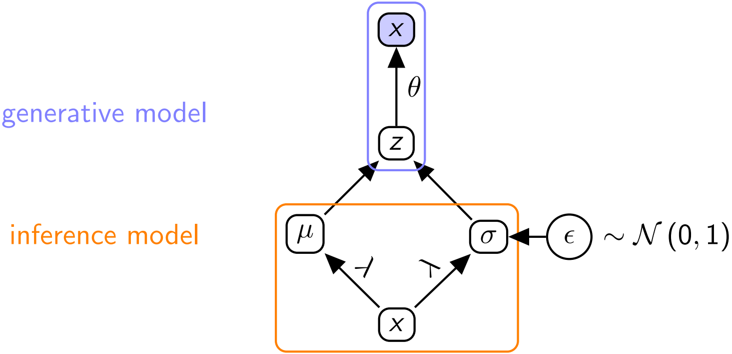
Computation Graph

generative model

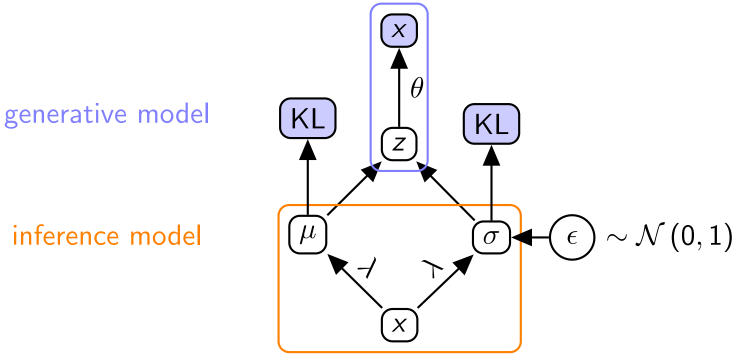
inference model



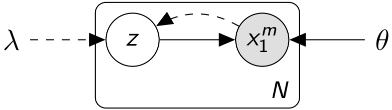
Computation Graph



Computation Graph



Example



Generative model

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

Inference model

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

Bowman et al. (2016)

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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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

- explicit (and hopefully more realistic) statistical assumptions
- compact models
- semi-supervised learning

Literature I

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