Foundations of Machine Learning
African Masters in Machine Intelligence

Variational Inference

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Learning Material

- Pattern Recognition and Machine Learning, Chapter 10 (Bishop, 2006)
- Machine Learning: A Probabilistic Perspective, Chapter 21 (Murphy, 2012)
- Variational Inference: A Review for Statisticians (Blei et al., 2017)
- NIPS-2016 Tutorial by Blei, Ranganath, Mohamed
  https://nips.cc/Conferences/2016/Schedule?showEvent=6199
- Tutorials by S. Mohamed
  http://shakirm.com/papers/VITutorial.pdf
  http://shakirm.com/slides/MLSS2018-Madrid-ProbThinking.pdf

Overview

Introduction and Background

Key Idea

Optimization Objective

Conditionally Conjugate Models

Mean-Field Variational Inference

Stochastic Variational Inference

Limits of Classical Variational Inference

Black-Box Variational Inference

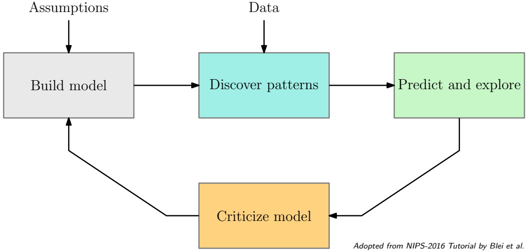
Computing Gradients of Expectations

- Score Function Gradients
- Pathwise Gradients

Amortized Inference

Richer Posterior Approximations

Probabilistic Pipeline



Adopted from NIPS-2016 Tutorial by Blei et al.

- Use knowledge and assumptions about the data to build a model
- Use model and data to discover patterns
- Predict and explore
- Criticize/revise the model

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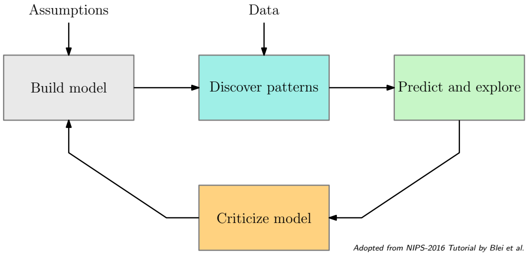

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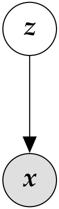
▶▶ **Inference is the key algorithmic problem**: What does the model say about the data?

▶▶ **Goal: general and scalable approaches to inference**

Probabilistic Machine Learning

- **Probabilistic model:** Joint distribution of latent variables $\boldsymbol{z}$ and observed variables $\boldsymbol{x}$ (data):

$$p(\boldsymbol{x}, \boldsymbol{z})$$



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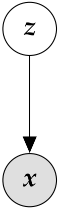

- **Inference**: Learning about the unknowns $\boldsymbol{z}$ through the posterior distribution

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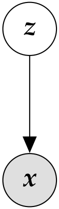

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- Normally: Denominator (marginal likelihood/evidence) intractable (i.e., we cannot compute the integral)
  ▶▶ Approximate inference to get the posterior

Some Options for Posterior Inference

- Markov Chain Monte Carlo (to sample from the posterior)
- Laplace approximation
- Expectation propagation (Minka, 2001)
- **Variational inference** (Jordan et al., 1999)

Variational Inference

- Variational inference is the most scalable inference method available (at the moment)
- Can handle (arbitrarily) large datasets

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- Applications include:
  - Topic modeling (Hoffman et al., 2013)
  - Community detection (Gopalan & Blei, 2013)
  - Genetic analysis (Gopalan et al., 2016)
  - Reinforcement learning (e.g., Eslami et al., 2016)
  - Neuroscience analysis (Manning et al., 2014)
  - Compression and content generation (Gregor et al., 2016)
  - Traffic analysis (Kucukelbir et al., 2016; Salimbeni & Deisenroth, 2017)

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Key Idea: Approximation by Optimization

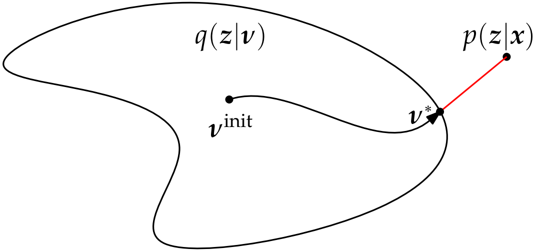
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Figure adopted from Blei et al.'s NIPS-2016 tutorial

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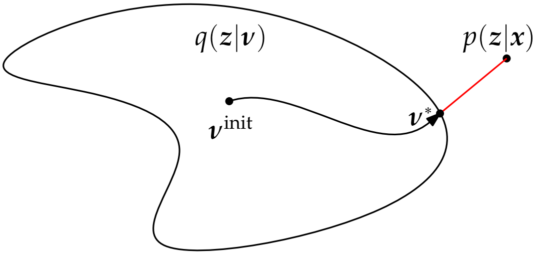
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- Find approximation of a probability distribution (e.g., posterior) by optimization:
  1. Define an objective function
  2. Define a (parametrized) family of approximating distributions $q_{\boldsymbol{\nu}}$
  3. Optimize objective function w.r.t. variational parameters $\boldsymbol{\nu}$
- Inference ⏩ Optimization

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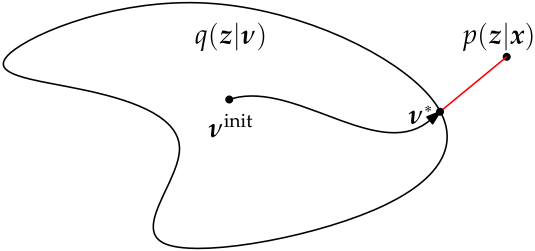
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Some Useful Quantities

- Kullback-Leibler divergence

$$\begin{aligned}\mathrm{KL}(q(\boldsymbol{x})\|p(\boldsymbol{x})) &= \int q(\boldsymbol{x})\log\frac{q(\boldsymbol{x})}{p(\boldsymbol{x})}d\boldsymbol{x}\\ &= \mathbb{E}_q\left[\log\frac{q(\boldsymbol{x})}{p(\boldsymbol{x})}\right] = \mathbb{E}_q[\log q(\boldsymbol{x})] - \mathbb{E}_q[\log p(\boldsymbol{x})]\end{aligned}$$

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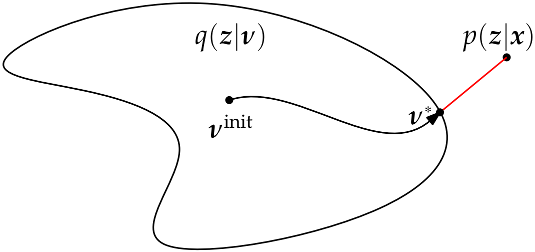
- Differential entropy

$$\mathrm{H}[q(\boldsymbol{x})] = -\mathbb{E}_q[\log q(\boldsymbol{x})] = -\int q(\boldsymbol{x}) \log q(\boldsymbol{x}) d\boldsymbol{x}$$

Optimization Objective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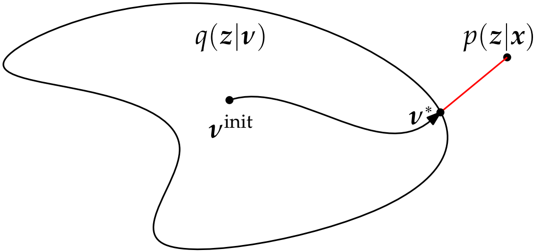
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- Need to compare distributions (variational approximation q, true posterior p)

  ⏩ Kullback-Leibler divergence

- Find variational parameters $\boldsymbol{\nu}$ by minimizing the KL divergence $\mathrm{KL}(q(\boldsymbol{z}|\boldsymbol{\nu})\|p(\boldsymbol{z}|\boldsymbol{x}))$ between the variational approximation q and the true posterior.

Optimization Objective (2)

- Minimize the KL divergence $\mathrm{KL}(q(\boldsymbol{z}|\boldsymbol{\nu})\|p(\boldsymbol{z}|\boldsymbol{x}))$ between the variational approximation q and the true posterior.

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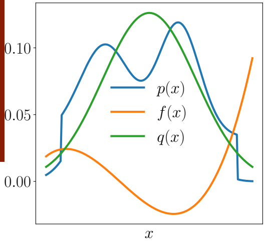
- Not required to know the unknown posterior $p(\boldsymbol{z}|\boldsymbol{x})$
- Minimizing $\mathrm{KL}(q(\boldsymbol{z})\|p(\boldsymbol{z}|\boldsymbol{x}))$ is equivalent to maximizing a lower bound on the marginal likelihood (ELBO)

Evidence Lower Bound

Importance Sampling

Key idea: Transform an intractable integral into an expectation under a simpler distribution q (proposal distribution):



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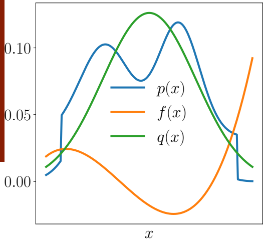

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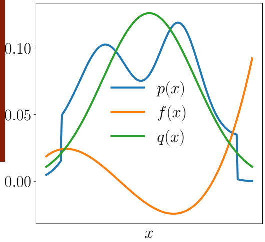

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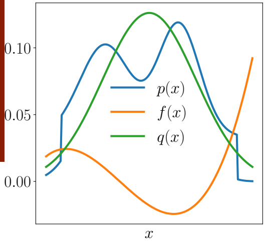

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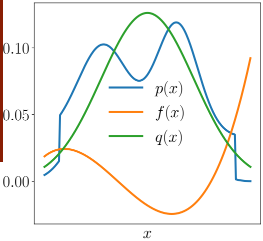

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If we choose q in a way that we can easily sample from it, we can approximate this last expectation by Monte Carlo:

$$
\mathbb{E}_q\left[f(\boldsymbol{x})\frac{p(\boldsymbol{x})}{q(\boldsymbol{x})}\right] \approx \frac{1}{S}\sum_{s=1}^{S} f(\boldsymbol{x}^{(s)})\frac{p(\boldsymbol{x}^{(s)})}{q(\boldsymbol{x}^{(s)})} \qquad , \quad \boldsymbol{x}^{(s)} \sim q(\boldsymbol{x})
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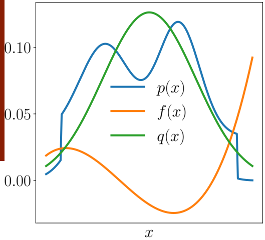

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Importance Sampling: Properties

- Unbiased estimate of the expectation
- Many draws from posterior needed, especially in high dimensions
- Good for evaluating integrals, but we don't know much about the posterior distribution
- Degeneracy

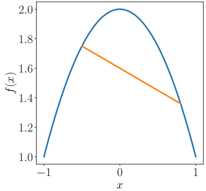
Jensen's Inequality

An important result from convex analysis:

Jensen's Inequality

For concave functions f:

$$f(\mathbb{E}[\boldsymbol{z}]) \geqslant \mathbb{E}[f(\boldsymbol{z})]$$



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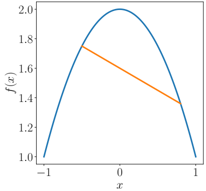

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For concave functions f:

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Logarithms are concave. Therefore:

$$\log \mathbb{E}[f(z)] = \log \int f(z)p(z)dz \geqslant \int p(z) \log f(z)dz = \mathbb{E}[\log f(z)]$$

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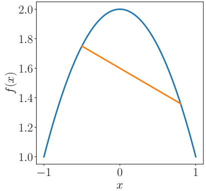

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Idea: For computing the marginal likelihood, use Jensen's inequality instead of MCMC

From Importance Sampling to Variational Inference

Look at log-marginal likelihood (log-evidence):

$$\log p(\boldsymbol{x}) = \log \int p(\boldsymbol{x}|\boldsymbol{z})p(\boldsymbol{z})d\boldsymbol{z}$$

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&= \mathbb{E}_q[\log p(\boldsymbol{x}|\boldsymbol{z})] - \mathbb{E}_q\left[\log\left(\frac{q(\boldsymbol{z})}{p(\boldsymbol{z})}\right)\right]
\end{aligned}
$$

From Importance Sampling to Variational Inference

Look at log-marginal likelihood (log-evidence):

$$
\begin{aligned}
\log p(\boldsymbol{x}) &= \log \int p(\boldsymbol{x}|z)p(z)dz \\
&= \log \int p(\boldsymbol{x}|z)p(z)\frac{q(z)}{q(z)}dz \\
&= \log \int p(\boldsymbol{x}|z)\frac{p(z)}{q(z)}q(z)dz \\
&= \log \mathbb{E}_q\left[p(\boldsymbol{x}|z)\frac{p(z)}{q(z)}\right] \\
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&= \mathbb{E}_q[\log p(\boldsymbol{x}|z)] - \mathbb{E}_q\left[\log\left(\frac{q(z)}{p(z)}\right)\right] \\
&= \mathbb{E}_q[\log p(\boldsymbol{x}|z)] - \mathrm{KL}(q(z)\|p(z))
\end{aligned}
$$

Evidence Lower Bound (ELBO)

- We just lower-bounded the evidence (marginal likelihood):

$$\log p(\boldsymbol{x}) \geqslant \mathbb{E}_q[\log p(\boldsymbol{x}|\boldsymbol{z})] - \mathrm{KL}(q(\boldsymbol{z})\|p(\boldsymbol{z})) =: \mathrm{ELBO}$$

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- Data-fit term (expected log-likelihood): Measures how well samples from $q(\boldsymbol{z})$ explain the data ("reconstruction cost").
  ▶▶ Place q's mass on the MAP estimate.
- Regularizer: Variational posterior $q(\boldsymbol{z})$ should not differ much from the prior $p(\boldsymbol{z})$

ELBO and KL Divergence

- Maximizing the ELBO w.r.t. the variational parameters $\boldsymbol{\nu}$ is equivalent to minimizing $\mathrm{KL}(q(\boldsymbol{z})\|p(\boldsymbol{z}|\boldsymbol{x}))$, where $p(\boldsymbol{z}|\boldsymbol{x})$ is the true posterior

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$$\begin{aligned}\mathrm{KL}(q(\boldsymbol{z})\|p(\boldsymbol{z}|\boldsymbol{x})) &= \mathrm{KL}(q(\boldsymbol{z})\|p(\boldsymbol{z})) - \mathbb{E}_q[\log p(\boldsymbol{x}|\boldsymbol{z})] + \mathrm{const}\\ &= -\mathrm{ELBO} + \mathrm{const}\end{aligned}$$

Optimizing the ELBO

$$\begin{aligned}\mathcal{F}(\boldsymbol{\nu}) &= \underbrace{\mathbb{E}_q[\log p(\boldsymbol{x}|\boldsymbol{z})]}_{\text{data-fit}} - \underbrace{\mathrm{KL}(q(\boldsymbol{z}|\boldsymbol{\nu})\|p(\boldsymbol{z}))}_{\text{regularizer}}\\ &= \mathbb{E}_q[\log p(\boldsymbol{x},\boldsymbol{z})] + \mathrm{H}[q(\boldsymbol{z}|\boldsymbol{\nu})]\end{aligned}$$

- Choice of the variational distribution $q(\boldsymbol{z}|\boldsymbol{\nu})$ ⏩ Parametrization

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- Choice of the variational distribution $q(\boldsymbol{z}|\boldsymbol{\nu})$ ⏩ Parametrization
- Computational challenges:
  - Compute expectation
  - Compute gradients $d\mathcal{F}/d\boldsymbol{\nu}$ for variational learning
  - ELBO is non-convex ⏩ Local optima

Overview

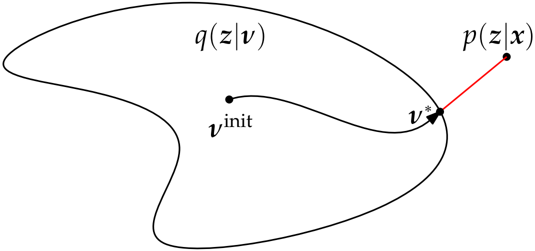
$q(\boldsymbol{z}|\boldsymbol{\nu})$
$p(\boldsymbol{z}|\boldsymbol{x})$
$\boldsymbol{\nu}^{\text{init}}$
$\boldsymbol{\nu}^*$

Figure adopted from Blei et al.'s NIPS-2016 tutorial

- Find approximation of a probability distribution (e.g., posterior) by optimization:
  1. Define an objective function
  2. **Define a (parametrized) family of approximating distributions** q_ν
  3. Optimize objective function w.r.t. variational parameters $\boldsymbol{\nu}$
- Inference ⏩ Optimization

Roadmap I

1. Define a generic class of conditionally conjugate models
2. Classical mean-field variational inference
3. Stochastic variational inference ⏩ Scales to massive data

Overview

Introduction and Background

Key Idea

Optimization Objective

Conditionally Conjugate Models

Mean-Field Variational Inference

Stochastic Variational Inference

Limits of Classical Variational Inference

Black-Box Variational Inference

Computing Gradients of Expectations

- Score Function Gradients
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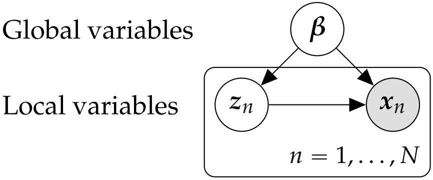
Richer Posterior Approximations

Model Class

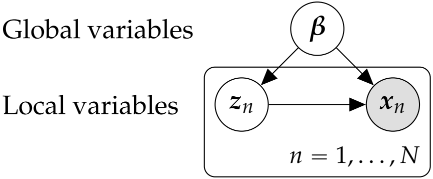


Global variables

Local variables

- All unknown parameters are described by random variables
  - Global random variables $\boldsymbol{\beta}$, which control all the data
  - Local random variables $\boldsymbol{z}_n$, which are local to individual data points $\boldsymbol{x}_n$

Model Class



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- Example: Gaussian mixture model

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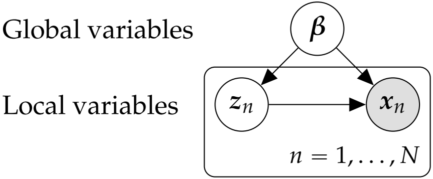

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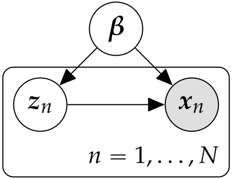
  - Local random variables $\boldsymbol{z}_n$, which are local to individual data points $\boldsymbol{x}_n$
- Example: Gaussian mixture model
  - Global: means, covariances, weights $\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k, \pi_k$
  - Local: binary assignments $\boldsymbol{z}_n$

Probabilistic Model

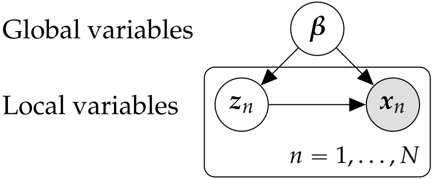
Global variables

Local variables



- Observations/data $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$
- nth data point depends only on local $\boldsymbol{z}_n$ and global $\boldsymbol{\beta}$
- Joint distribution:

Probabilistic Model



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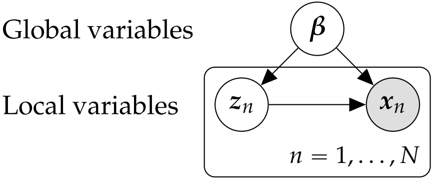
Probabilistic Model



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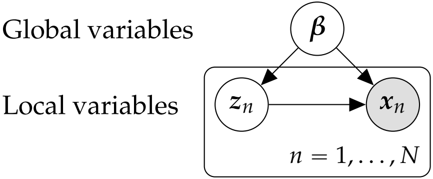
Objective

Compute posterior distribution of all unknowns: $p(\boldsymbol{\beta}, \boldsymbol{z}_{1:N} | \boldsymbol{x}_{1:N})$.

Complete Conditional

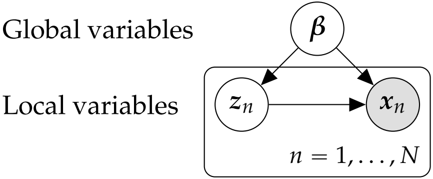


- **Complete conditional:** Conditional of a single latent variable given the observations and all other latent variables

$$p(\boldsymbol{z}_n | \boldsymbol{\beta}, \boldsymbol{x}_n)$$

$$p(\boldsymbol{\beta} | \boldsymbol{z}_{1:N}, \boldsymbol{x}_{1:N})$$

Complete Conditional



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- Assume that each complete conditional is a member of the exponential family (Bernoulli, Beta, Gamma, Gaussian, ...)
  ⏩ Conditionally conjugate models

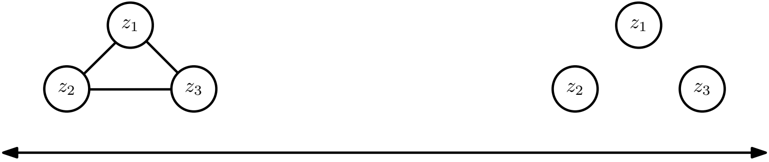
Generic Class of Models: Examples

- Bayesian mixture models
- Hidden Markov models
- Factor analysis
- Principal component analysis
- Linear regression

Approximating Distributions

True posterior

Fully factorized



Most expressive

$q(z|x) = p(z|x)$

Least expressive

$q(z|x) = \prod_i q_i(z_i)$

Approximating Distributions

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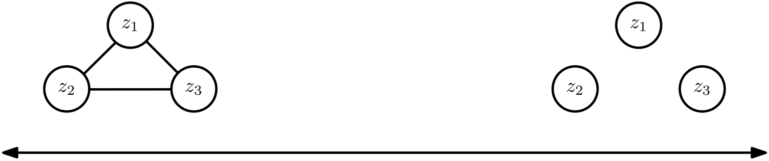

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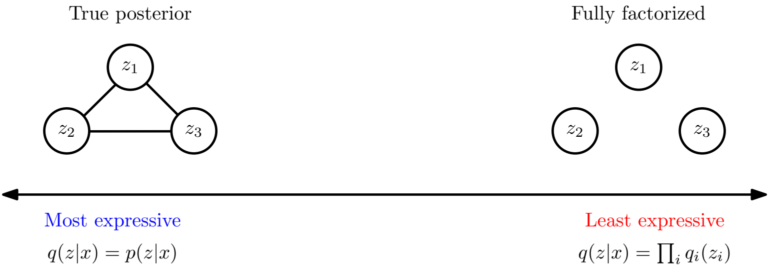
Approximating Distributions



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  ⏩ We have a lot of flexibility
- Generally:
  - Build expressive class of posteriors (no overfitting problems)
  - Maintain computational efficiency ⏩ Scalability

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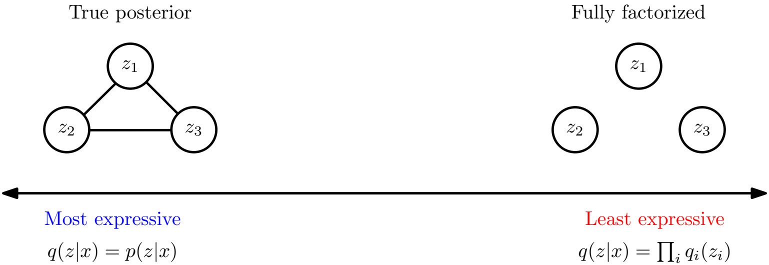

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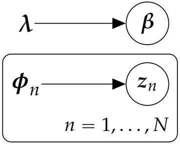
- Assume conditionally conjugate model
- Fully factorized (mean field) approximation:

$$q(\boldsymbol{\beta}, \boldsymbol{z}|\boldsymbol{\nu}) = q(\boldsymbol{\beta}|\boldsymbol{\lambda}) \prod_{n=1}^{N} q(\boldsymbol{z}_n|\boldsymbol{\phi}_n)$$



Fully Factorized Distribution

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- Maximize the ELBO w.r.t. variational parameters $\boldsymbol{\nu}$

Optimizing in Turn

- Independent latent variables: $q(\boldsymbol{z}) = \prod_n q(\boldsymbol{z}_n|\boldsymbol{\phi}_n) = \prod_n q_n(\boldsymbol{z}_n)$

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$$\text{ELBO}(q_n) = \mathbb{E}_{q_n}[\hat{p}(\boldsymbol{x},\boldsymbol{z}_n)] - \mathbb{E}_{q_n}[\log q_n(\boldsymbol{z}_n)] + \text{const}$$

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&= \mathbb{E}_{q_n}\left[\log\frac{\exp(\hat{p}(\boldsymbol{x},\boldsymbol{z}_n))}{q_n(\boldsymbol{z}_n)}\right] = -\text{KL}(q_n(\boldsymbol{z}_n)\|\exp(\hat{p}(\boldsymbol{x},\boldsymbol{z}_n)))
\end{aligned}$$

Optimal Factors

$$\mathrm{ELBO}(q_n) = -\mathrm{KL}(q_n(\boldsymbol{z}_n) \| \exp(\hat{p}(\boldsymbol{x}, \boldsymbol{z}_n)))$$

- Maximizing the ELBO w.r.t. q_n is equivalent to minimizing $\mathrm{KL}(q_n(\boldsymbol{z}_n) \| \exp(\hat{p}(\boldsymbol{x}, \boldsymbol{z}_n)))$

⏩ $\log q_n^*(\boldsymbol{z}_n) = \hat{p}(\boldsymbol{x}, \boldsymbol{z}_n) = \mathbb{E}_{q_{i \neq n}}[\log p(\boldsymbol{x}, \boldsymbol{z})] + \mathrm{const}$

Optimal Factors

$$\text{ELBO}(q_n) = -\text{KL}(q_n(\boldsymbol{z}_n) \| \exp(\hat{p}(\boldsymbol{x}, \boldsymbol{z}_n)))$$

- Maximizing the ELBO w.r.t. q_n is equivalent to minimizing $\text{KL}(q_n(\boldsymbol{z}_n) \| \exp(\hat{p}(\boldsymbol{x}, \boldsymbol{z}_n)))$

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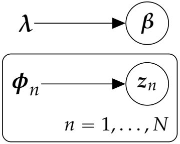
- Get the optimal factor q_n^* by
  1. Writing down the log-joint distribution of all latent and observed variables $\log p(\boldsymbol{x}, \boldsymbol{z})$
  2. Computing the expectation w.r.t. all other random variables

Mean-Field Approximation for Conditionally Conjugate Models



- Optimal factors (see Bishop (2006) or Ghahramani & Beal (2001)):

$$q^*(\boldsymbol{\beta}|\boldsymbol{\lambda}) \propto \exp\left(\mathbb{E}_{\boldsymbol{z}}[\log p(\boldsymbol{x}, \boldsymbol{z}, \boldsymbol{\beta})]\right)$$

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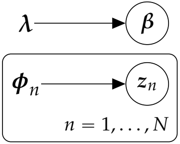

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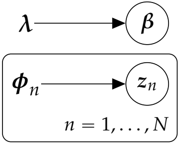
- Update one term at a time ⏩ Coordinate ascent

Mean-Field Approximation for Conditionally Conjugate Models



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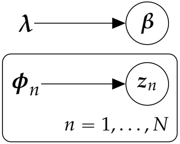

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- Update one term at a time ⏩ Coordinate ascent
- No closed-form solution (see EM algorithm)
- Iteratively optimize each parameter until we reach a local optimum (convergence guaranteed)

Mean-Field Approximation: Algorithm

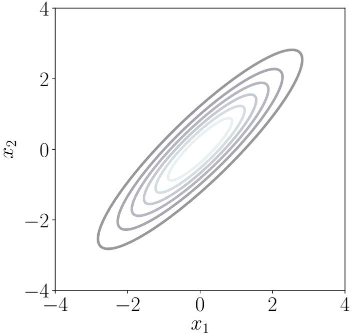
1. Input: data $\boldsymbol{x}$, model $p(\boldsymbol{\beta}, \boldsymbol{z}, \boldsymbol{x})$
2. Initialize global variational parameters $\boldsymbol{\lambda}$ randomly
3. While ELBO has not converged, repeat:

    3.1 For each data point $\boldsymbol{x}_n$

        3.1.1 Update local variational parameters $\boldsymbol{\phi}_n$

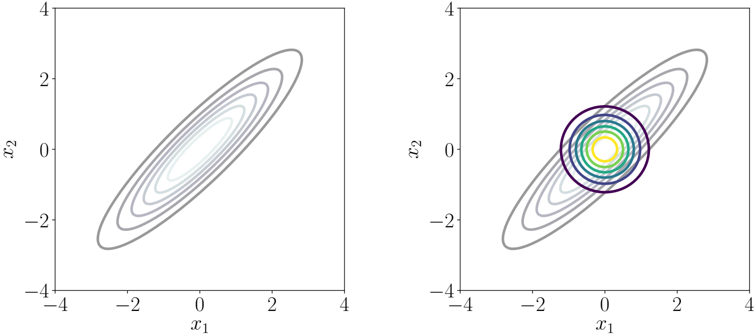
    3.2 Update global variational parameters $\boldsymbol{\lambda}$

Mean-Field Approximation: Limitation



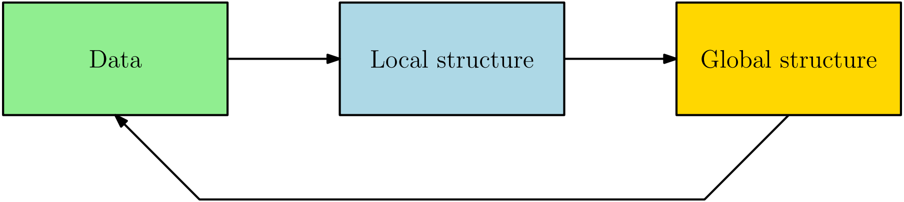
- Mean-field VI to approximate a correlated Gaussian with a factorized Gaussian

Mean-Field Approximation: Limitation



- Mean-field VI to approximate a correlated Gaussian with a factorized Gaussian
- Generally, mean-field VI tends to yield an approximation that is too compact ⏩ Need better classes of posterior approximations

Classical Variational Inference: Limitation



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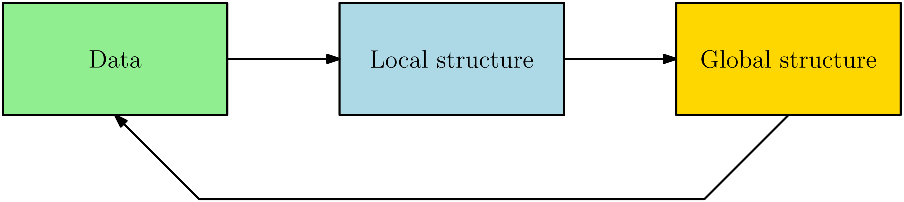

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  Can't handle massive data

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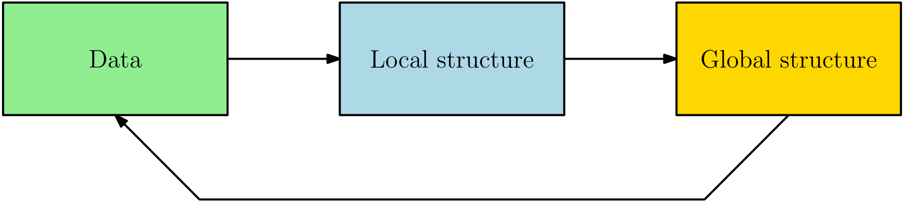

- Classical VI is inefficient: Need to crunch through the full dataset to update variational parameters

  Can't handle massive data

- **Stochastic variational inference** updates the global hidden structure once we have any update of the local structure

  ⏩ Stochastic optimization

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Mean-Field Variational Inference

Stochastic Variational Inference

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Computing Gradients of Expectations

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- Pathwise Gradients

Amortized Inference

Richer Posterior Approximations

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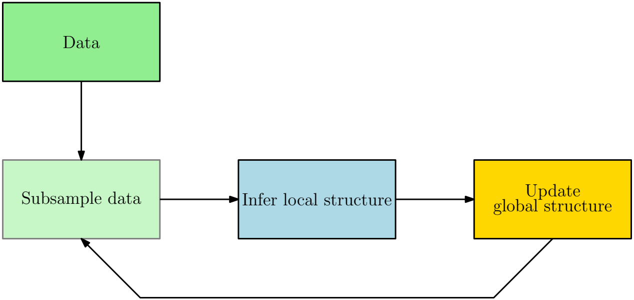

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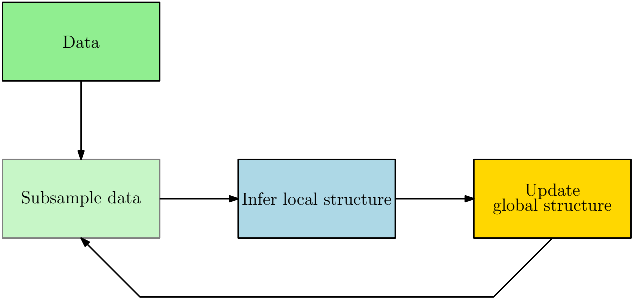
Stochastic Variational Inference



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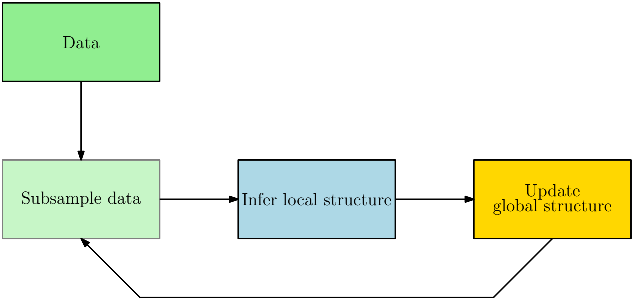

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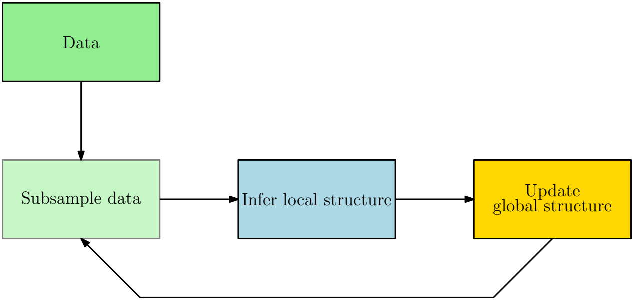

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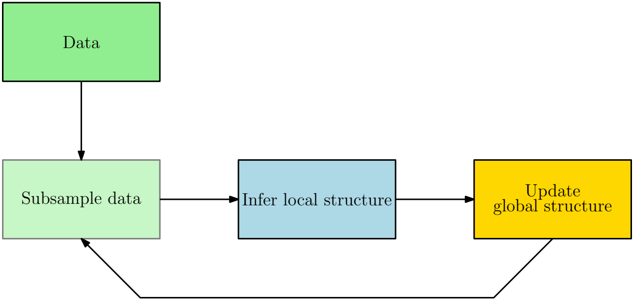

- Coordinate-ascent VI is inefficient: Need to look at the full dataset to update variational parameters
- Idea:
  - Do some local computations for each data point
  - Subsample data, infer local structure, update global structure
- Key: Stochastic optimization

Stochastic Optimization: Key Idea

- Replace exact gradient with cheaper (noisy) estimates (Robbins & Monro, 1951)
- This estimate could be based on a subset of the data (mini-batches)
- Guaranteed to converge to a local optimum
- Key driver of modern machine learning

Noisy Updates of Variational Parameters

- With noisy gradients, update the variational parameters:

$$\boldsymbol{\nu}_{t+1} = \boldsymbol{\nu}_t + \rho_t \hat{\nabla}_{\boldsymbol{\nu}} \mathcal{F}(\boldsymbol{\nu})$$

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- Some requirements on the step size parameter ρ_t
  ⏩ Convergence to local optimum

Natural Gradient

$$\tilde{\nabla}_{\boldsymbol{\nu}}\mathcal{F}(\boldsymbol{\nu}) = \boldsymbol{F}^{-1}\nabla_{\boldsymbol{\nu}}\mathcal{F}(\boldsymbol{\nu}) \qquad \boldsymbol{F}: \text{ Fisher information matrix}$$

- Points in the direction of maximum change in distribution space, not in parameter space ⏩ We maximize the ELBO/minimize KL
- Invariant to parametrization of distribution (e.g., variance vs precision of a Gaussian)
- Scales each parameter individually

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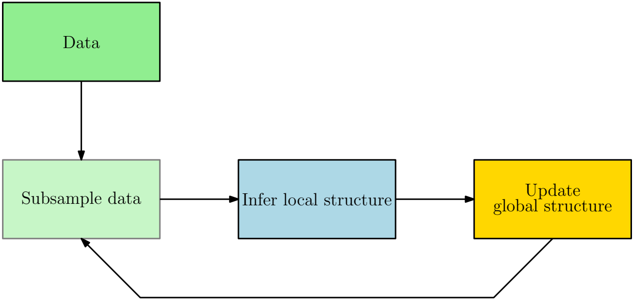
- Points in the direction of maximum change in distribution space, not in parameter space ⏩ We maximize the ELBO/minimize KL
- Invariant to parametrization of distribution (e.g., variance vs precision of a Gaussian)
- Scales each parameter individually
- Natural gradient for conditionally conjugate models easy to compute (Hoffman et al., 2013)
- Noisy natural gradient (one estimate per data point)
- Unbiased
- Only depends on optimized parameters of a single data point ⏩ cheap to compute

Algorithm

1. Input: data $\boldsymbol{x}$, model $p(\boldsymbol{\beta}, \boldsymbol{z}, \boldsymbol{x})$
2. Initialize global variational parameters $\boldsymbol{\lambda}$ randomly
3. Repeat
   - 3.1 Sample data point $\boldsymbol{x}_n$ uniformly at random
   - 3.2 Update local parameter $\boldsymbol{\phi}_n$
   - 3.3 Compute intermediate global parameter $\hat{\boldsymbol{\lambda}}$ based on noisy natural gradient
   - 3.4 Set global parameter

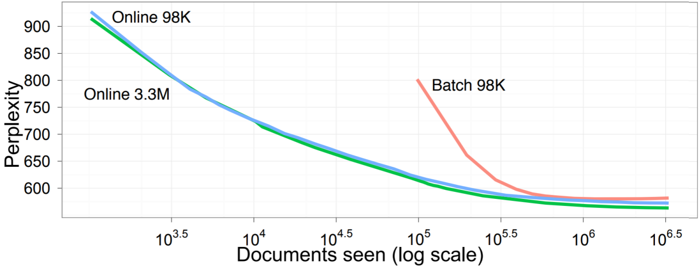
$$\boldsymbol{\lambda} \leftarrow (1 - \rho_t)\boldsymbol{\lambda} + \rho_t \hat{\boldsymbol{\lambda}}$$



- Look at a single data point in your dataset
- Infer local variational parameters
- Update global variational parameters using noisy natural gradient
- Repeat

➤➤ Simple way to scale variational inference to massive datasets

Example: Online LDA (Hoffman et al., 2010)



Documents analyzed	**2048**	**4096**	**8192**	**12288**	**16384**	**32768**	**49152**	**65536**
Top eight words	systems	systems	service	service	service	business	business	business
	road	health	systems	systems	companies	service	service	industry
	made	communication	health	companies	systems	companies	companies	service
	service	service	companies	business	business	industry	industry	companies
	announced	billion	market	company	company	company	services	services
	national	language	communication	billion	industry	management	company	company
	west	care	company	health	market	systems	management	management
	language	road	billion	industry	billion	services	public	public

From Hoffman et al. (2010)

Overview

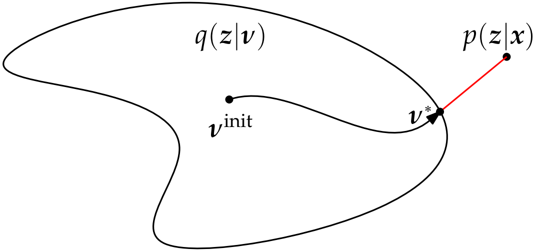

$q(\boldsymbol{z}|\boldsymbol{\nu})$
$p(\boldsymbol{z}|\boldsymbol{x})$
$\boldsymbol{\nu}^{\text{init}}$
$\boldsymbol{\nu}^*$

Figure adopted from Blei et al.'s NIPS-2016 tutorial

- Find approximation of a probability distribution (e.g., posterior) by optimization:
  1. Define an objective function
  2. Define a (parametrized) family of approximating distributions $q_{\boldsymbol{\nu}}$
  3. Optimize objective function w.r.t. variational parameters $\boldsymbol{\nu}$
- Inference ⏩ Optimization

Roadmap II

1. Limits of Classical Variational Inference
2. Black-Box Variational Inference
3. Computing Gradients of Expectations

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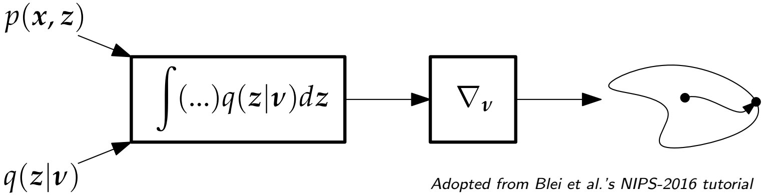
Variational Inference: General Recipe



$p(\boldsymbol{x}, \boldsymbol{z})$
$\int (\ldots) q(\boldsymbol{z}|\boldsymbol{\nu}) d\boldsymbol{z}$
$\nabla_{\boldsymbol{\nu}}$
$q(\boldsymbol{z}|\boldsymbol{\nu})$

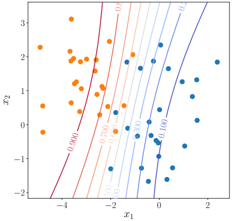
Adopted from Blei et al.'s NIPS-2016 tutorial

- Specify model $p(\boldsymbol{x}, \boldsymbol{z})$ and approximation $q(\boldsymbol{z}|\boldsymbol{\nu})$
- Objective $\mathcal{F}(\boldsymbol{\nu}) = \mathbb{E}_q[\log p(\boldsymbol{x}, \boldsymbol{z}) - \log q(\boldsymbol{z}|\boldsymbol{\nu})]$
- Compute expectation
- Compute gradient
- Optimize with gradient descent

This recipe is fairly generic.

Example: Bayesian Logistic Regression

- Binary classification
- Inputs $x \in \mathbb{R}$, labels $y \in \{0, 1\}$
- Model parameter z (normally denoted by θ)



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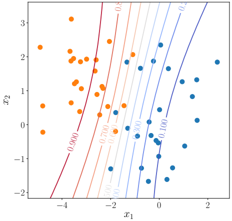

$$\text{Prior on model parameter: } p(z) = \mathcal{N}\big(0,\, 1\big)$$
$$\text{Likelihood: } p(y_n|x_n, z) = \mathrm{Ber}(\sigma(zx_n))$$

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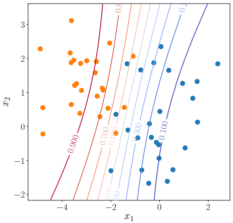

Prior on model parameter: $p(z) = \mathcal{N}(0, 1)$

Likelihood: $p(y_n | x_n, z) = \mathrm{Ber}(\sigma(z x_n))$

- Assume we have a single data point (x, y)
- Goal: Approximate the intractable posterior distribution $p(z|x, y)$ using variational inference

Example: Bayesian Logistic Regression (2)

- Choose Gaussian variational approximation:
  $q(z|\boldsymbol{\nu}) = \mathcal{N}\big(\mu, \sigma^2\big)$ ⏩ $\boldsymbol{\nu} =$

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- Objective function: ELBO $\mathcal{F}(\boldsymbol{\nu})$

$$\mathcal{F}(m, \sigma^2) = \mathbb{E}_q[\log p(z) - \log q(z) + \log p(y|x, z)]$$

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$$\begin{aligned}\mathcal{F}(m, \sigma^2) &= \mathbb{E}_q[\log p(z) - \log q(z) + \log p(y|x, z)] \\ &= -\tfrac{1}{2}(\mu^2 + \sigma^2) + \tfrac{1}{2}\log \sigma^2 + \mathbb{E}_q[\log p(y|x, z)] + \mathrm{c}\end{aligned}$$

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$$
\mathbb{E}_q[\log p(y|x, z)] =
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\mathbb{E}_q[\log p(y|x, z)] &= \mathbb{E}_q[y \log \sigma(xz) + (1 - y)\log(1 - \sigma(xz))]
\end{aligned}$$

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\mathbb{E}_q[\log p(y|x, z)] &= \mathbb{E}_q[y \log \sigma(xz) + (1-y) \log(1 - \sigma(xz))] \\
&= \mathbb{E}_q[yxz] - \mathbb{E}_q[y \log(1 + \exp(xz))] \\
&\quad + \mathbb{E}_q\left[(1-y) \log\left(1 - \frac{\exp(xz)}{1 + \exp(xz)}\right)\right]
\end{aligned}
$$

with

$$
\sigma(xz) = \frac{\exp(xz)}{1 + \exp(xz)}
$$

Computing the Expected Log-Likelihood

$$
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\mathbb{E}_q[\log p(y|x,z)] &= \mathbb{E}_q[yxz] - \mathbb{E}_q[y \log(1+\exp(xz))] \\
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&\quad + \mathbb{E}_q[(1-y)\log\left(\frac{1}{1+\exp(xz)}\right)] \\
&= yx\mu - \mathbb{E}_q[y\log(1+\exp(xz))] \\
&\quad - \mathbb{E}_q[\log(1+\exp(xz))] + \mathbb{E}_q[y\log(1+\exp(xz))]
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&= yx\mu - \mathbb{E}_q[y\log(1+\exp(xz))] \\
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&= yx\mu - \mathbb{E}_q[\log(1+\exp(xz))]
\end{aligned}
$$

Example: Bayesian Logistic Regression (ctd.)

- Choose Gaussian variational approximation:
  $q(z|\boldsymbol{\nu}) = \mathcal{N}\left(\mu,\, \sigma^2\right)$ ⏩ $\boldsymbol{\nu} = \{\mu, \sigma^2\}$
- Objective function: ELBO $\mathcal{F}(\boldsymbol{\nu})$

$$\begin{aligned}\mathcal{F}(\mu, \sigma^2) &= \mathbb{E}_q[\log p(z) + \log p(y|x, z) - \log q(z)] \\ &= -\tfrac{1}{2}(\mu^2 + \sigma^2) + \tfrac{1}{2}\log \sigma^2 + \mathbb{E}_q[\log p(y|x, z)] + \mathrm{c} \\ &= -\tfrac{1}{2}(\mu^2 + \sigma^2) + \tfrac{1}{2}\log \sigma^2 + yx\mu - \mathbb{E}_q[\log(1 + \exp(xz))]\end{aligned}$$

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- **Expectation cannot be computed in closed form**
- Pushing gradients through Monte Carlo estimates is very hard.

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$$

- **Expectation cannot be computed in closed form**
- Pushing gradients through Monte Carlo estimates is very hard.
- Option: Lower-bound this expectation; but this is model specific.

Non-Conjugate Models

- Nonlinear time series models
- Deep latent Gaussian models
- Attention models (e.g., DRAW)
- Generalized linear models (e.g., logistic regression)
- Bayesian neural networks
- ...

Non-Conjugate Models

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- Deep latent Gaussian models
- Attention models (e.g., DRAW)
- Generalized linear models (e.g., logistic regression)
- Bayesian neural networks
- ...

There are many interesting non-conjugate models
⏩ Look for a solution that is not model specific
⏩ **Black-Box Variational Inference**

Overview

Introduction and Background

Key Idea

Optimization Objective

Conditionally Conjugate Models

Mean-Field Variational Inference

Stochastic Variational Inference

Limits of Classical Variational Inference

Black-Box Variational Inference

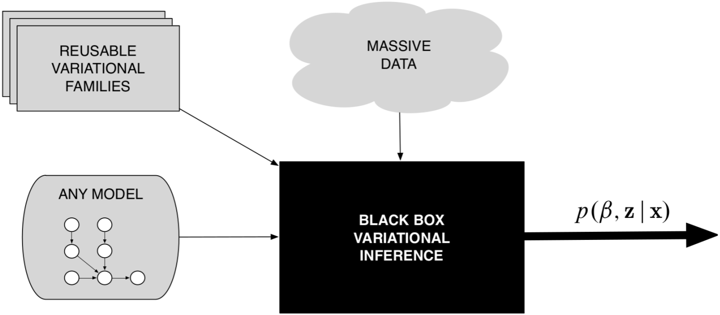
Computing Gradients of Expectations

- Score Function Gradients
- Pathwise Gradients

Amortized Inference

Richer Posterior Approximations

Black-Box Variational Inference

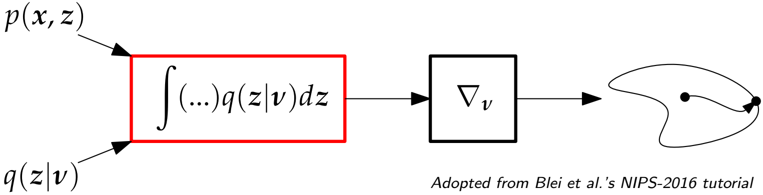


REUSABLE VARIATIONAL FAMILIES
MASSIVE DATA
ANY MODEL
BLACK BOX VARIATIONAL INFERENCE
$p(\beta, \mathbf{z} \mid \mathbf{x})$

From Blei et al.'s NIPS-2016 tutorial

- Any model
- Massive data
- Some general assumptions on the approximating family

Computational Challenge of Classical VI

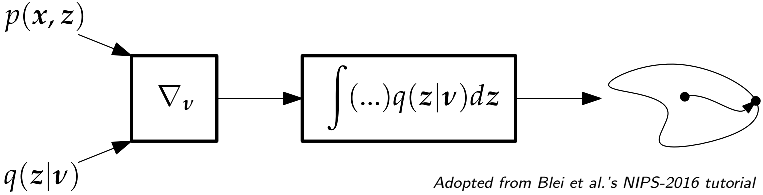

$p(\boldsymbol{x},\boldsymbol{z})$
$q(\boldsymbol{z}|\boldsymbol{\nu})$
$\int(\ldots)q(\boldsymbol{z}|\boldsymbol{\nu})d\boldsymbol{z}$
$\nabla_{\boldsymbol{\nu}}$

Adopted from Blei et al.'s NIPS-2016 tutorial

- Integral computation, which makes the ELBO explicitly a function of the variational parameters
- Integral cannot be computed for non-conjugate models

  ⏩ Gradient computation difficult

Approach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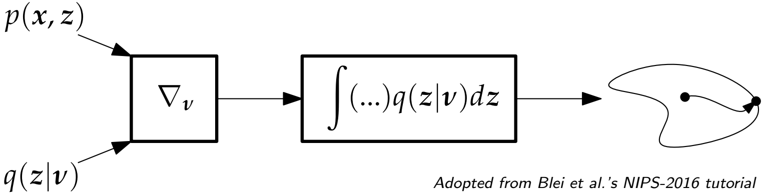
- Switch order of integration (compute expectations) and differentiation

Approach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- Approximate the expectation after having taken the gradient
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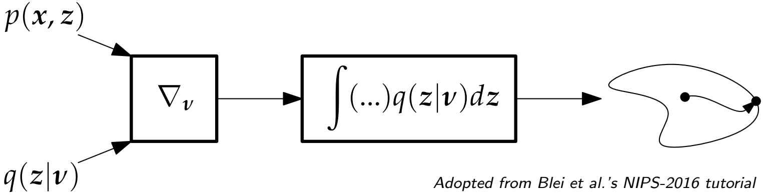
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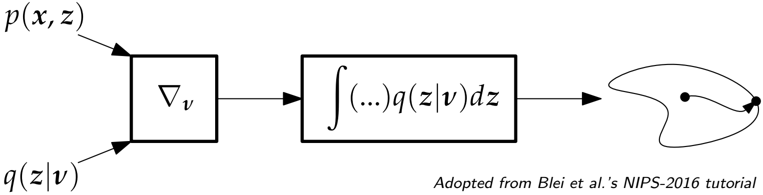
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⏩ Require a general way to compute gradients of expectations

Re-Writing the ELBO

$$\text{ELBO} = \mathbb{E}_q[\log p(\boldsymbol{x}|\boldsymbol{z})] - \text{KL}(q(\boldsymbol{z}|\boldsymbol{\nu})\|p(\boldsymbol{z}))$$

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Evidence Lower Bound

$$\text{ELBO} = \mathbb{E}_q[g(\boldsymbol{z},\boldsymbol{\nu})] = \int g(\boldsymbol{z},\boldsymbol{\nu})q(\boldsymbol{z}|\boldsymbol{\nu})d\boldsymbol{z}$$

$$g(\boldsymbol{z},\boldsymbol{\nu}) := \log p(\boldsymbol{x},\boldsymbol{z}) - \log q(\boldsymbol{z}|\boldsymbol{\nu})$$

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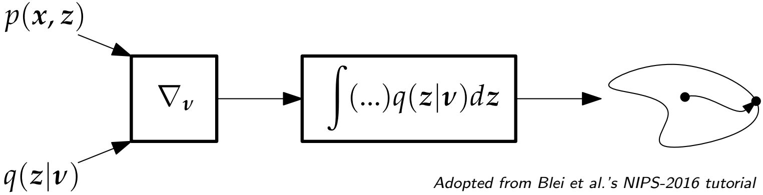

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- **Switch order of integration (compute expectations) and differentiation**
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Log-Derivative Trick

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$$\nabla_{\boldsymbol{\nu}} \log q(\boldsymbol{z}|\boldsymbol{\nu}) =$$

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$$\nabla_{\boldsymbol{\nu}} \log q(\boldsymbol{z}|\boldsymbol{\nu}) = \frac{\nabla_{\boldsymbol{\nu}} q(\boldsymbol{z}|\boldsymbol{\nu})}{q(\boldsymbol{z}|\boldsymbol{\nu})}$$

$$\iff \nabla_{\boldsymbol{\nu}} q(\boldsymbol{z}|\boldsymbol{\nu}) = q(\boldsymbol{z}|\boldsymbol{\nu}) \nabla_{\boldsymbol{\nu}} \log q(\boldsymbol{z}|\boldsymbol{\nu})$$

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- Therefore:

$$\begin{aligned}\int \nabla_\nu q(\boldsymbol{z}|\boldsymbol{\nu}) f(\boldsymbol{z}) d\boldsymbol{z} &= \int q(\boldsymbol{z}|\boldsymbol{\nu}) \nabla_\nu \log q(\boldsymbol{z}|\boldsymbol{\nu}) f(\boldsymbol{z}) d\boldsymbol{z} \\ &= \mathbb{E}_q[\nabla_\nu \log q(\boldsymbol{z}|\boldsymbol{\nu}) f(\boldsymbol{z})]\end{aligned}$$

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- If we can sample from q, this expectation can be evaluated easily (Monte Carlo estimation)

Gradients of Expectations: Approach 1

$$\text{ELBO} = \mathcal{F}(\boldsymbol{\nu}) = \mathbb{E}_q[g(\boldsymbol{z}, \boldsymbol{\nu})], \quad g(\boldsymbol{z}, \boldsymbol{\nu}) = \log p(\boldsymbol{x}, \boldsymbol{z}) - \log q(\boldsymbol{z}|\boldsymbol{\nu})$$

- Need gradient of ELBO w.r.t. variational parameters $\boldsymbol{\nu}$

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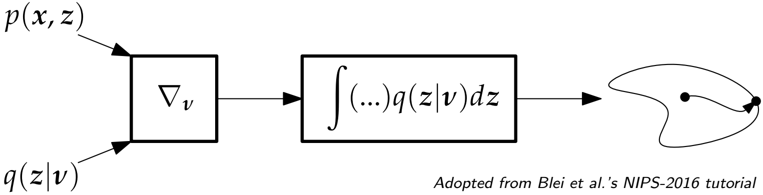
- We successfully swapped gradient and expectation
- q known
  - ▶▶ Sample from q and use Monte Carlo estimation

Approach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Adopted from Blei et al.'s NIPS-2016 tutorial

- Swap order of integration (compute expectations) and differentiation
- **Simplify the expectation after having taken the gradient**

Score Function Gradient Estimator of the ELBO

Simplifying the Gradient

$$\nabla_{\boldsymbol{\nu}}\text{ELBO} = \mathbb{E}_q[\nabla_{\boldsymbol{\nu}} \log q(\boldsymbol{z}|\boldsymbol{\nu})g(\boldsymbol{z},\boldsymbol{\nu}) + \nabla_{\boldsymbol{\nu}}g(\boldsymbol{z},\boldsymbol{\nu})]$$

- Let's simplify this gradient ⏩ Score function

Score Function

- Score function: Derivative of a log-likelihood with respect to the parameter vector $\boldsymbol{\nu}$:

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$$\text{score} = \nabla_{\boldsymbol{\nu}} \log q(\boldsymbol{z}|\boldsymbol{\nu}) = \frac{1}{q(\boldsymbol{z}|\boldsymbol{\nu})} \nabla_{\boldsymbol{\nu}} q(\boldsymbol{z}|\boldsymbol{\nu})$$

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- Measures the sensitivity of the log-likelihood w.r.t. $\boldsymbol{\nu}$

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- Measures the sensitivity of the log-likelihood w.r.t. $\boldsymbol{\nu}$
- Central to maximum likelihood estimation

Score Function (2)

$$\text{score} = \nabla_{\boldsymbol{\nu}} \log q(\boldsymbol{z}|\boldsymbol{\nu}) = \frac{1}{q(\boldsymbol{z}|\boldsymbol{\nu})} \nabla_{\boldsymbol{\nu}} q(\boldsymbol{z}|\boldsymbol{\nu})$$

- Important property:

$$\mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{\nu})}[\text{score}] =$$

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&= \int \frac{1}{q(\boldsymbol{z}|\boldsymbol{\nu})} q(\boldsymbol{z}|\boldsymbol{\nu}) \nabla_{\boldsymbol{\nu}} q(\boldsymbol{z}|\boldsymbol{\nu}) d\boldsymbol{z} \\
&= \int \nabla_{\boldsymbol{\nu}} q(\boldsymbol{z}|\boldsymbol{\nu}) d\boldsymbol{z} = \nabla_{\boldsymbol{\nu}} \int q(\boldsymbol{z}|\boldsymbol{\nu}) d\boldsymbol{z} = \nabla_{\boldsymbol{\nu}} 1 = 0
\end{aligned}$$

▸▸ Mean of the score function is 0

- Variance of the score: Fisher information ▸▸ Natural gradients

Score Function Gradient Estimator

$$\text{ELBO} = \mathbb{E}_q[g(\boldsymbol{z}, \boldsymbol{\nu})] = \mathbb{E}_q[\log p(\boldsymbol{x}, \boldsymbol{z}) - \log q(\boldsymbol{z}|\boldsymbol{\nu})]$$

- Gradient of ELBO:

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$$\text{ELBO} = \mathbb{E}_q[g(\boldsymbol{z}, \boldsymbol{v})] = \mathbb{E}_q[\log p(\boldsymbol{x}, \boldsymbol{z}) - \log q(\boldsymbol{z}|\boldsymbol{v})]$$

- Gradient of ELBO:

$$\begin{aligned}\nabla_{\boldsymbol{v}}\text{ELBO} &= \mathbb{E}_q[\nabla_{\boldsymbol{v}} \log q(\boldsymbol{z}|\boldsymbol{v}) g(\boldsymbol{z}, \boldsymbol{v})] + \mathbb{E}_q[\nabla_{\boldsymbol{v}} g(\boldsymbol{z}, \boldsymbol{v})] \\ &= \mathbb{E}_q[\nabla_{\boldsymbol{v}} \log q(\boldsymbol{z}|\boldsymbol{v}) g(\boldsymbol{z}, \boldsymbol{v})] \\ &\quad + \mathbb{E}_q[\underbrace{\nabla_{\boldsymbol{v}} \log p(\boldsymbol{x}, \boldsymbol{z})}_{=0} - \underbrace{\nabla_{\boldsymbol{v}} \log q(\boldsymbol{z}|\boldsymbol{v})}_{\text{score}}]\end{aligned}$$

- Exploit that the mean of the score function is 0. Then:

$$\begin{aligned}\nabla_{\boldsymbol{v}}\text{ELBO} &= \mathbb{E}_q[\nabla_{\boldsymbol{v}} \log q(\boldsymbol{z}|\boldsymbol{v}) g(\boldsymbol{z}, \boldsymbol{v})] \\ &= \mathbb{E}_q[\nabla_{\boldsymbol{v}} \log q(\boldsymbol{z}|\boldsymbol{v})(\log p(\boldsymbol{x}, \boldsymbol{z}) - \log q(\boldsymbol{z}|\boldsymbol{v}))]\end{aligned}$$

Score Function Gradient Estimator

$$\text{ELBO} = \mathbb{E}_q[g(\boldsymbol{z}, \boldsymbol{\nu})] = \mathbb{E}_q[\log p(\boldsymbol{x}, \boldsymbol{z}) - \log q(\boldsymbol{z}|\boldsymbol{\nu})]$$

- Gradient of ELBO:

$$\begin{aligned}\nabla_{\boldsymbol{\nu}}\text{ELBO} &= \mathbb{E}_q[\nabla_{\boldsymbol{\nu}} \log q(\boldsymbol{z}|\boldsymbol{\nu}) g(\boldsymbol{z}, \boldsymbol{\nu})] + \mathbb{E}_q[\nabla_{\boldsymbol{\nu}} g(\boldsymbol{z}, \boldsymbol{\nu})] \\ &= \mathbb{E}_q[\nabla_{\boldsymbol{\nu}} \log q(\boldsymbol{z}|\boldsymbol{\nu}) g(\boldsymbol{z}, \boldsymbol{\nu})] \\ &\quad + \mathbb{E}_q[\underbrace{\nabla_{\boldsymbol{\nu}} \log p(\boldsymbol{x}, \boldsymbol{z})}_{=0} - \underbrace{\nabla_{\boldsymbol{\nu}} \log q(\boldsymbol{z}|\boldsymbol{\nu})}_{\text{score}}]\end{aligned}$$

- Exploit that the mean of the score function is 0. Then:

$$\begin{aligned}\nabla_{\boldsymbol{\nu}}\text{ELBO} &= \mathbb{E}_q[\nabla_{\boldsymbol{\nu}} \log q(\boldsymbol{z}|\boldsymbol{\nu}) g(\boldsymbol{z}, \boldsymbol{\nu})] \\ &= \mathbb{E}_q[\nabla_{\boldsymbol{\nu}} \log q(\boldsymbol{z}|\boldsymbol{\nu}) (\log p(\boldsymbol{x}, \boldsymbol{z}) - \log q(\boldsymbol{z}|\boldsymbol{\nu}))]\end{aligned}$$

- Likelihood ratio gradient (Glynn, 1990)
- REINFORCE gradient (Williams, 1992)

Using Noisy Stochastic Gradients

- Gradient of the ELBO

$$\nabla_{\boldsymbol{\nu}}\text{ELBO} = \mathbb{E}_q[\nabla_{\boldsymbol{\nu}} \log q(\boldsymbol{z}|\boldsymbol{\nu})(\log p(\boldsymbol{x}, \boldsymbol{z}) - \log q(\boldsymbol{z}|\boldsymbol{\nu}))]$$

  is an expectation

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- Require that $q(\boldsymbol{z}|\boldsymbol{\nu})$ is differentiable w.r.t. $\boldsymbol{\nu}$

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  is an expectation
- Require that $q(\boldsymbol{z}|\boldsymbol{\nu})$ is differentiable w.r.t. $\boldsymbol{\nu}$
- Get noisy unbiased gradients using Monte Carlo by sampling from q:

  $$\frac{1}{S}\sum_{s=1}^{S} \nabla_{\boldsymbol{\nu}} \log q(\boldsymbol{z}^{(s)}|\boldsymbol{\nu})(\log p(\boldsymbol{x}, \boldsymbol{z}^{(s)}) - \log q(\boldsymbol{z}^{(s)}|\boldsymbol{\nu}))\,, \quad \boldsymbol{z}^{(s)} \sim q(\boldsymbol{z}|\boldsymbol{\nu})$$

Using Noisy Stochastic Gradients

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- Sampling from q is easy (we choose q)
- Use this within SVI to converge to a local optimum

BBVI: Algorithm

1. Input: model $p(\boldsymbol{x}, \boldsymbol{z})$, variational approximation $q(\boldsymbol{z}|\boldsymbol{\nu})$
2. Repeat
   2.1 Draw S samples $\boldsymbol{z}^{(s)} \sim q(\boldsymbol{z}|\boldsymbol{\nu})$
   2.2 Update variational parameters

$$\boldsymbol{\nu}_{t+1} = \boldsymbol{\nu}_t + \rho_t \underbrace{\frac{1}{S}\sum_{s=1}^{S} \nabla_{\nu} \log q(\boldsymbol{z}^{(s)}|\boldsymbol{\nu})(\log p(\boldsymbol{x}, \boldsymbol{z}^{(s)}) - \log q(\boldsymbol{z}^{(s)}|\boldsymbol{\nu}))}_{\text{MC estimate of the score-function gradient of the ELBO}}$$

   2.3 $t = t + 1$

Requirements for Inference

- Computing the noisy gradient of the ELBO requires:
  - Sampling from q. We choose q so that this is possible.
  - Evaluate the score function $\nabla_{\boldsymbol{\nu}} \log q(\boldsymbol{z}|\boldsymbol{\nu})$
  - Evaluate $\log q(\boldsymbol{z}|\boldsymbol{\nu})$ and $\log p(\boldsymbol{x}, \boldsymbol{z}) = \log p(\boldsymbol{z}) + \log p(\boldsymbol{x}|\boldsymbol{z})$

⏩ No model-specific computations for optimization

(computations are only specific to the choice of the variational approximation)

Issue: Variance of the Gradients

- Stochastic optimization ⏩ **Gradients are noisy (high variance)**
- The noisier the gradients, the slower the convergence
- Possible solutions:
  - Control variates (with the score function as control variate)
  - Rao-Blackwellization
  - Importance sampling

Non-Conjugate Models

- Nonlinear time series models
- Deep latent Gaussian models
- Attention models (e.g., DRAW)
- Generalized linear models (e.g., logistic regression)
- Bayesian neural networks
- ...

BBVI allows us to design models $p(\boldsymbol{x}, \boldsymbol{z})$ based on the data, and not on the inference we can do

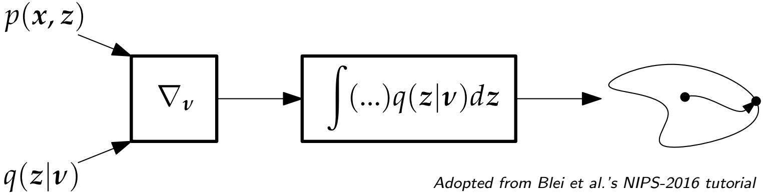
Assumptions

- Score-function gradient estimator only requires general assumptions
- Noisy gradients are a problem
- Address this issue by making some additional assumptions (not too strict)

  ▶▶ Pathwise gradient estimators

Pathwise Gradient Estimators of the ELBO

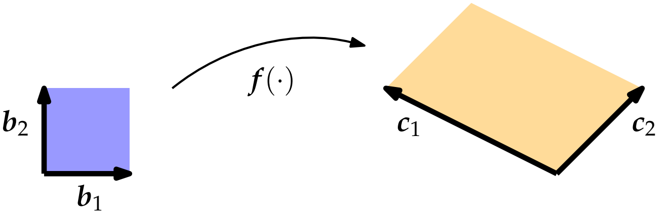
Approach


$p(\boldsymbol{x},\boldsymbol{z})$
$q(\boldsymbol{z}|\boldsymbol{\nu})$
$\nabla_{\boldsymbol{\nu}}$
$\int(\ldots)q(\boldsymbol{z}|\boldsymbol{\nu})d\boldsymbol{z}$

Adopted from Blei et al.'s NIPS-2016 tutorial

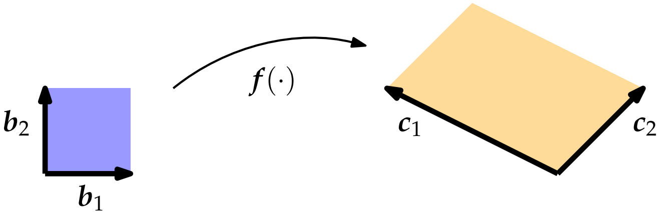
- **Switch order of integration (compute expectations) and differentiation**
- Approximate the expectation after having taken the gradient

Change of Variables



- Use function $\boldsymbol{f} : \mathcal{X} \to \mathcal{Y}, \quad \boldsymbol{x} \mapsto \boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{y}$
- Change of area/volume:

Change of Variables



- Use function $f:\mathcal{X}\to\mathcal{Y}, \quad x\mapsto f(x)=y$
- Change of area/volume:

$$\left|\int_{\mathcal{Y}} y d y\right| = \left|\frac{\mathrm{d}f}{\mathrm{d}x}\right|\left|\int_{\mathcal{X}} x d x\right|$$

Reparametrization Trick

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Base distribution $p(\boldsymbol{\epsilon})$ and a deterministic transformation $\boldsymbol{z} = t(\boldsymbol{\epsilon}, \boldsymbol{\nu})$ so that $\boldsymbol{z} \sim q(\boldsymbol{z}|\boldsymbol{\nu})$. Then:

$$\nabla_{\boldsymbol{\nu}} \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{\nu})}[f(\boldsymbol{z})] = \mathbb{E}_{p(\boldsymbol{\epsilon})}[\nabla_{\boldsymbol{\nu}} f(t(\boldsymbol{\epsilon}, \boldsymbol{\nu}))]$$

⏩ Expectation taken w.r.t. base distribution

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⏩ Expectation taken w.r.t. base distribution

- Key idea: change of variables using a deterministic transformation

Reparametrization Trick (2)

$$\nabla_{\boldsymbol{\nu}} \mathbb{E}_{q(\boldsymbol{z}|\boldsymbol{\nu})}[f(\boldsymbol{z})] = \mathbb{E}_{p(\boldsymbol{\epsilon})}[\nabla_{\boldsymbol{\nu}} f(t(\boldsymbol{\epsilon}, \boldsymbol{\nu}))]$$

Reparametrization Trick (2)

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- Change of variables ⏩ Probability mass contained in a differential area must be invariant under change of variables:

$$|q(\boldsymbol{z}|\boldsymbol{\nu}) d\boldsymbol{z}| = |p(\boldsymbol{\epsilon}) d\boldsymbol{\epsilon}|$$

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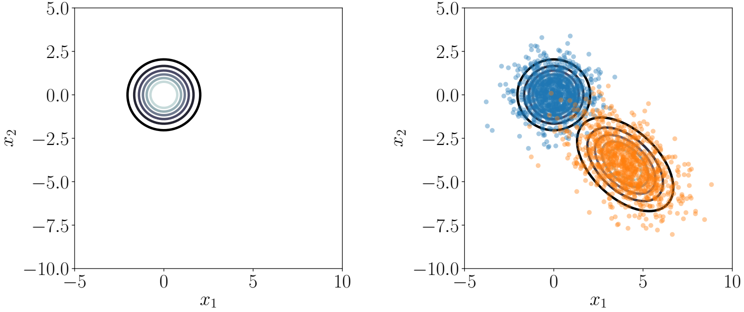
Example



$$\boldsymbol{\nu} := \{\boldsymbol{\mu}, \boldsymbol{R}\}\,, \quad \boldsymbol{R}\boldsymbol{R}^\top = \boldsymbol{\Sigma}$$

$$p(\boldsymbol{\epsilon}) = \mathcal{N}\big(\boldsymbol{0},\, \boldsymbol{I}\big)$$

$$t(\boldsymbol{\epsilon}, \boldsymbol{\nu}) = \boldsymbol{\mu} + \boldsymbol{R}\boldsymbol{\epsilon}$$

$$\implies p(\boldsymbol{z}) = \mathcal{N}\big(\boldsymbol{z}\,|\,\boldsymbol{\mu},\, \boldsymbol{\Sigma}\big)$$

Reparametrization as a System of Pipes

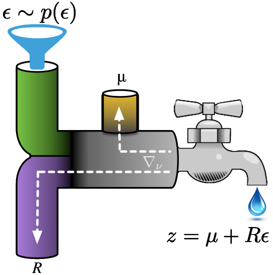
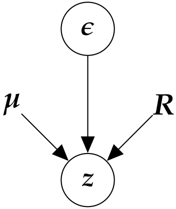


Figure provided by S. Mohamed



- Path: Follow the input noise through the pipes[2]

[2] https://tinyurl.com/hyakoj2

Reparametrization as a System of Pipes

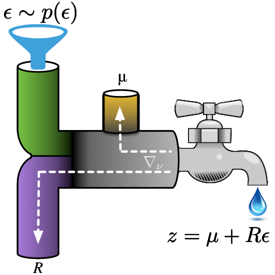
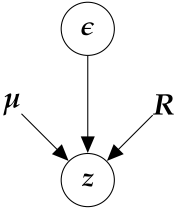


Figure provided by S. Mohamed



- Path: Follow the input noise through the pipes[2]
- Construction of pipes known (deterministic transformations)
  - Go back and push gradients through it

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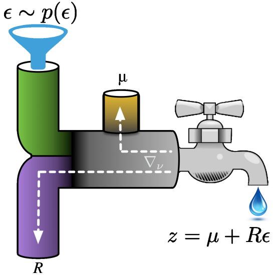
Reparametrization as a System of Pipes



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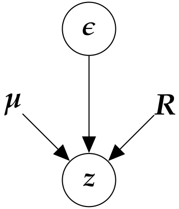

- Path: Follow the input noise through the pipes[2]
- Construction of pipes known (deterministic transformations)
  - ⏩ Go back and push gradients through it
- Also called "push-in method": Push the parameters of the z distribution into the deterministic transformations

[2] `https://tinyurl.com/hyakoj2`

Gradients of Expectations: Approach 2

$$\nabla_{\boldsymbol{\nu}}\text{ELBO} = \nabla_{\boldsymbol{\nu}}\mathbb{E}_q[g(\boldsymbol{z},\boldsymbol{\nu})]$$

Gradients of Expectations: Approach 2

$$\begin{aligned}\nabla_{\boldsymbol{\nu}}\text{ELBO} &= \nabla_{\boldsymbol{\nu}}\mathbb{E}_q[g(\boldsymbol{z},\boldsymbol{\nu})]\\ &= \nabla_{\boldsymbol{\nu}}\int g(\boldsymbol{z},\boldsymbol{\nu})q(\boldsymbol{z}|\boldsymbol{\nu})d\boldsymbol{z}\end{aligned}$$

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$$\boxed{q(\boldsymbol{z})d\boldsymbol{z} = p(\boldsymbol{\epsilon})d\boldsymbol{\epsilon}}$$

Gradients of Expectations: Approach 2

$$
\begin{aligned}
\nabla_{\boldsymbol{\nu}}\mathrm{ELBO} &= \nabla_{\boldsymbol{\nu}}\mathbb{E}_q[g(\boldsymbol{z},\boldsymbol{\nu})] \\
&= \nabla_{\boldsymbol{\nu}}\int g(\boldsymbol{z},\boldsymbol{\nu})q(\boldsymbol{z}|\boldsymbol{\nu})d\boldsymbol{z} \\
&= \nabla_{\boldsymbol{\nu}}\int g(\boldsymbol{z}|\boldsymbol{\nu})p(\boldsymbol{\epsilon})d\boldsymbol{\epsilon} && \boxed{q(\boldsymbol{z})d\boldsymbol{z} = p(\boldsymbol{\epsilon})d\boldsymbol{\epsilon}} \\
&= \nabla_{\boldsymbol{\nu}}\int g(t(\boldsymbol{\epsilon},\boldsymbol{\nu}),\boldsymbol{\nu})p(\boldsymbol{\epsilon})d\boldsymbol{\epsilon} && \boxed{\boldsymbol{z} = t(\boldsymbol{\epsilon},\boldsymbol{\nu})}
\end{aligned}
$$

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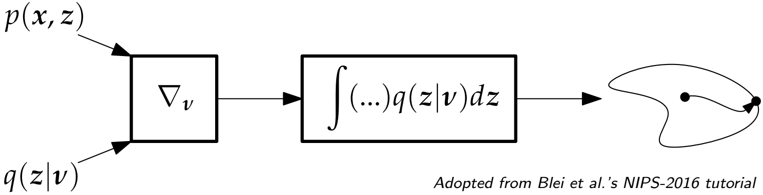
&= \mathbb{E}_{p(\boldsymbol{\epsilon})}[\nabla_{\boldsymbol{\nu}}g(t(\boldsymbol{\epsilon},\boldsymbol{\nu}),\boldsymbol{\nu})]
\end{aligned}$$

⏩ Turned gradient of an expectation into expectation of a gradient (and sampling from $p(\boldsymbol{\epsilon})$ is very easy).

Approach


$p(\boldsymbol{x}, \boldsymbol{z})$
$q(\boldsymbol{z}|\boldsymbol{\nu})$
$\nabla_{\boldsymbol{\nu}}$
$\int (\ldots) q(\boldsymbol{z}|\boldsymbol{\nu}) d\boldsymbol{z}$

Adopted from Blei et al.'s NIPS-2016 tutorial

- Swap order of integration (compute expectations) and differentiation
- **Approximate the expectation after having taken the gradient**

Pathwise Gradients

$$
\begin{aligned}
g(\boldsymbol{z}, \boldsymbol{\nu}) &= \log p(\boldsymbol{x}, \boldsymbol{z}) - \log q(\boldsymbol{z}|\boldsymbol{\nu}) \\
\boldsymbol{z} &= t(\boldsymbol{\epsilon}, \boldsymbol{\nu})
\end{aligned}
$$

Simplify gradient of the ELBO:

Pathwise Gradients

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Simplify gradient of the ELBO:

$$
\begin{aligned}
\nabla_{\boldsymbol{\nu}} \text{ELBO} &= \mathbb{E}_{p(\boldsymbol{\epsilon})}[\nabla_{\boldsymbol{\nu}} g(t(\boldsymbol{\epsilon}, \boldsymbol{\nu}), \boldsymbol{\nu})] \\
&= \mathbb{E}_{p(\boldsymbol{\epsilon})}[\nabla_{\boldsymbol{\nu}} \log p(\boldsymbol{x}, t(\boldsymbol{\epsilon}, \boldsymbol{\nu})) - \nabla_{\boldsymbol{\nu}} \log q(t(\boldsymbol{\epsilon}, \boldsymbol{\nu})|\boldsymbol{\nu})] \qquad \boxed{\text{Def. of } g} \\
&= \mathbb{E}_{p(\boldsymbol{\epsilon})}[\nabla_{\boldsymbol{z}} \log p(\boldsymbol{x}, \boldsymbol{z}) \nabla_{\boldsymbol{\nu}} t(\boldsymbol{\epsilon}, \boldsymbol{\nu}) \\
&\quad - \nabla_{\boldsymbol{z}} \log q(\boldsymbol{z}|\boldsymbol{\nu}) \nabla_{\boldsymbol{\nu}} t(\boldsymbol{\epsilon}, \boldsymbol{\nu}) - \underbrace{\nabla_{\boldsymbol{\nu}} \log q(t(\boldsymbol{\epsilon}, \boldsymbol{\nu})|\boldsymbol{\nu})}_{\text{score}}] \qquad \boxed{\text{Chain rule}} \\
&= \mathbb{E}_{p(\boldsymbol{\epsilon})}[\nabla_{\boldsymbol{z}} \big(\log p(\boldsymbol{x}, \boldsymbol{z}) - \log q(\boldsymbol{z}|\boldsymbol{\nu})\big) \nabla_{\boldsymbol{\nu}} t(\boldsymbol{\epsilon}, \boldsymbol{\nu})] \qquad \boxed{\text{Score property}}
\end{aligned}
$$

- Pathwise gradient
- Reparametrization gradient

Variance Comparison

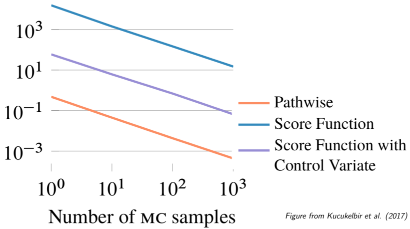


Figure from Kucukelbir et al. (2017)

- Drastically reduced variance compared to score-function gradient estimation

Variance Comparison

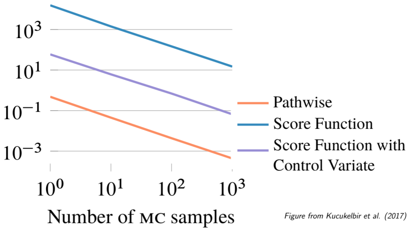


Figure from Kucukelbir et al. (2017)

- Drastically reduced variance compared to score-function gradient estimation
- Restricted class of models (compared with score function estimator)

Score Function vs Pathwise Gradients

$$\text{ELBO} = \int g(\boldsymbol{z}, \boldsymbol{\nu}) q(\boldsymbol{z}|\boldsymbol{\nu}) d\boldsymbol{z}$$

$$g(\boldsymbol{z}, \boldsymbol{\nu}) = \log p(\boldsymbol{x}, \boldsymbol{z}) - \log q(\boldsymbol{z}|\boldsymbol{\mu})$$

- Score function gradient:

$$\nabla_{\boldsymbol{\nu}} \text{ELBO} = \mathbb{E}_q\big[\big(\nabla_{\boldsymbol{\nu}} \log q(\boldsymbol{z}|\boldsymbol{\nu})\big) g(\boldsymbol{z}, \boldsymbol{\nu})\big]$$

  ⏩ Gradient of the variational distribution

- Reparametrization gradient:

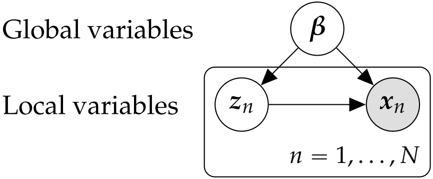
$$\nabla_{\boldsymbol{\nu}} \text{ELBO} = \mathbb{E}_{p(\boldsymbol{\epsilon})}\big[\big(\nabla_{\boldsymbol{z}} g(\boldsymbol{z}, \boldsymbol{\nu})\big) \nabla_{\boldsymbol{\nu}} t(\boldsymbol{\epsilon}, \boldsymbol{\nu})\big]$$

  ⏩ Gradient of the model and the variational distribution

Score Function vs Pathwise Gradients (2)

- Score function
  - Works for all models (continuous and discrete)
  - Works for a large class of variational approximations
  - Variance can be high ⏩ Slow convergence
- Pathwise gradient estimator
  - Requires differentiable models
  - Requires the variational approximation to be expressed as a deterministic transformation $\boldsymbol{z} = t(\boldsymbol{\epsilon}, \boldsymbol{\nu})$
  - Generally lower variance

Re-cap: Hierarchical Bayesian Models



- Joint distribution:

$$p(\boldsymbol{\beta}, \boldsymbol{z}, \boldsymbol{x}) = p(\boldsymbol{\beta}) \prod_{n=1}^{N} p(\boldsymbol{z}_n, \boldsymbol{x}_n | \boldsymbol{\beta})$$

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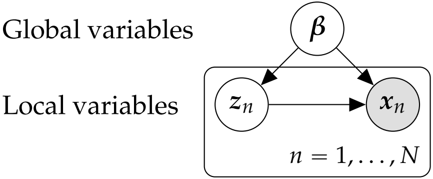

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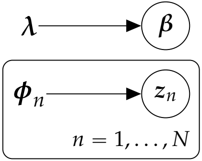
$$p(\boldsymbol{\beta}, \boldsymbol{z}, \boldsymbol{x}) = p(\boldsymbol{\beta}) \prod_{n=1}^{N} p(\boldsymbol{z}_n, \boldsymbol{x}_n | \boldsymbol{\beta})$$

- Mean-field variational approximation:



Re-cap: Mean-Field Stochastic Variational Inference

1. Input: data $\boldsymbol{x}$, model $p(\boldsymbol{\beta}, \boldsymbol{z}, \boldsymbol{x})$
2. Initialize global variational parameters $\boldsymbol{\lambda}$ randomly
3. Repeat
   - 3.1 Sample data point $\boldsymbol{x}_n$ uniformly at random
   - 3.2 Update local parameter $\boldsymbol{\phi}_n = \mathbb{E}_{\boldsymbol{\lambda}}[...]$
   - 3.3 Compute intermediate global parameter $\hat{\boldsymbol{\lambda}} = N\mathbb{E}_{\boldsymbol{\phi}_{1:N}}[...] + ...$
   - 3.4 Set global parameter $\boldsymbol{\lambda} \leftarrow (1 - \rho_t)\boldsymbol{\lambda} + \rho_t\hat{\boldsymbol{\lambda}}$

BBVI Stochastic Variational Inference

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    3.4 Set global parameter $\boldsymbol{\lambda} \leftarrow (1 - \rho_t)\boldsymbol{\lambda} + \rho_t\hat{\boldsymbol{\lambda}}$

Issue:

- Expectations we require to update the local and global parameters are no longer tractable

  ▶▶ No closed-form updating of variational factors

Addressing the Challenge

- Same problem we had with the ELBO: Integral intractable
  ⏩ Gradient descent for variational updates

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  ⏩ **SVI gets really slow**

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  ⏩ Need to run an optimization algorithm per data point
  ⏩ **SVI gets really slow**

⏩ **Amortized Inference**

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Mean-Field Variational Inference

Stochastic Variational Inference

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- Score Function Gradients
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Amortized Inference

Richer Posterior Approximations

Amortized (=shared) Inference

- **Key idea:** Learn a mapping (with global variational parameters) from data points $\boldsymbol{x}_n$ to local variational parameters $\boldsymbol{\phi}_n$:

$$f(\boldsymbol{x}_n, \boldsymbol{\theta}) = \boldsymbol{\phi}_n$$

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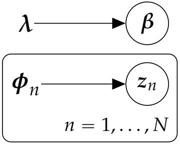
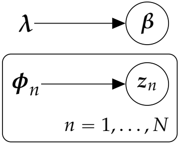
- Can we overfit? Discuss!

Amortized VI in Hierarchical Bayesian Models



$$\text{ELBO} = \mathbb{E}_q[\log p(\boldsymbol{x}, \boldsymbol{\beta}, \boldsymbol{z}_{1:N}) - \log q(\boldsymbol{\beta}, \boldsymbol{z}_{1:N} | \boldsymbol{\lambda}, \boldsymbol{\phi}_{1:N})] \qquad \boxed{\boldsymbol{\nu} = \{\boldsymbol{\beta}, \boldsymbol{\phi}_{1:N}\}}$$

Amortized VI in Hierarchical Bayesian Models

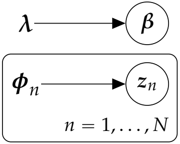


$$\begin{aligned}\text{ELBO} &= \mathbb{E}_q[\log p(\boldsymbol{x}, \boldsymbol{\beta}, \boldsymbol{z}_{1:N}) - \log q(\boldsymbol{\beta}, \boldsymbol{z}_{1:N} | \boldsymbol{\lambda}, \boldsymbol{\phi}_{1:N})] \\ &= \mathbb{E}_q[\log p(\boldsymbol{x}, \boldsymbol{\beta}, \boldsymbol{z}_{1:N})] \\ &\quad - \mathbb{E}_q[\log q(\boldsymbol{\beta} | \boldsymbol{\lambda}) + \sum_{n=1}^{N} \log q(z_n | \boldsymbol{\phi}_n)]\end{aligned}$$

$$\boxed{\boldsymbol{\nu} = \{\boldsymbol{\beta}, \boldsymbol{\phi}_{1:N}\}}$$

$$\boxed{\text{mean-field}}$$

Amortized VI in Hierarchical Bayesian Models



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$$= \mathbb{E}_q[\log p(\boldsymbol{x}, \boldsymbol{\beta}, \boldsymbol{z}_{1:N})]$$

$$- \mathbb{E}_q[\log q(\boldsymbol{\beta}|\boldsymbol{\lambda}) + \sum_{n=1}^{N} \log q(\boldsymbol{z}_n | \boldsymbol{\phi}_n)]$$

$$\boxed{\text{mean-field}}$$

$$= \mathbb{E}_q[\log p(\boldsymbol{x}, \boldsymbol{\beta}, \boldsymbol{z}_{1:N})]$$

$$- \mathbb{E}_q[\log q(\boldsymbol{\beta}|\boldsymbol{\lambda}) + \sum_{n=1}^{N} \log q(\boldsymbol{z}_n | f(\boldsymbol{x}_n, \boldsymbol{\theta}))]$$

$$\boxed{\boldsymbol{\phi}_n = f(\boldsymbol{x}_n, \boldsymbol{\theta})}$$

Stochastic Gradients

$$\nabla_{\boldsymbol{\theta}}\text{ELBO} = \frac{\mathrm{d}\text{ELBO}}{\mathrm{d}\boldsymbol{\phi}_n}\frac{\mathrm{d}\boldsymbol{\phi}_n}{\mathrm{d}\boldsymbol{\theta}}$$

- ELBO gradient w.r.t. local variational parameters is difficult
  ⏩ Stochastic gradient estimators (score function, reparametrization)
- Gradient of variational parameters w.r.t. parameters $\boldsymbol{\theta}$ of inference network are easy

Amortized SVI

1. Input: data $\boldsymbol{x}$, model $p(\boldsymbol{\beta}, \boldsymbol{z}, \boldsymbol{x})$
2. Initialize global variational parameters $\boldsymbol{\lambda}$ randomly
3. Repeat

   3.1 Sample $\boldsymbol{\beta} \sim q(\boldsymbol{\beta}|\boldsymbol{\lambda})$

   3.2 Sample data point $\boldsymbol{x}_n$ uniformly at random

   3.3 Compute stochastic natural gradients

$$\tilde{\nabla}_{\boldsymbol{\lambda}} \text{ELBO}$$

$$\tilde{\nabla}_{\boldsymbol{\theta}} \text{ELBO}$$

   3.4 Update global parameters

$$\boldsymbol{\lambda} \leftarrow \boldsymbol{\lambda} + \rho_t \tilde{\nabla}_{\boldsymbol{\lambda}} \text{ELBO}$$

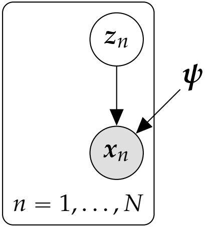
global variational parameters

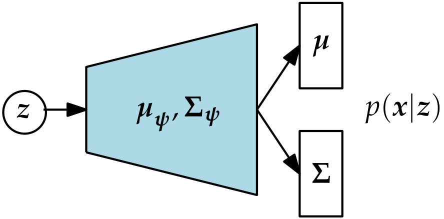
$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \rho_t \tilde{\nabla}_{\boldsymbol{\theta}} \text{ELBO}$$

inference network parameters

Example: Variational Auto-Encoder

Variational Auto-Encoder: Model



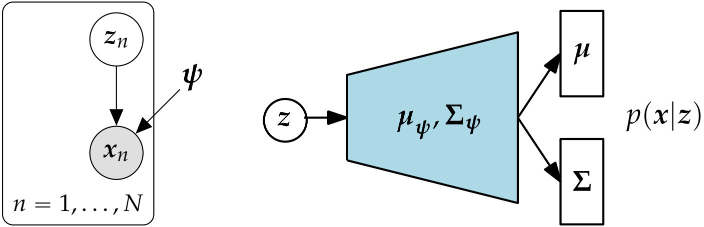


- Model (Rezende et al., 2014; Kinga & Welling, 2014):

$$p(\boldsymbol{z}) = \mathcal{N}\big(\boldsymbol{0},\, \boldsymbol{I}\big)$$

$$p(\boldsymbol{x}|\boldsymbol{z}) = \mathcal{N}\big(\boldsymbol{\mu}_{\psi}(\boldsymbol{z}),\, \boldsymbol{\Sigma}_{\psi}(\boldsymbol{z})\big)$$

Variational Auto-Encoder: Model

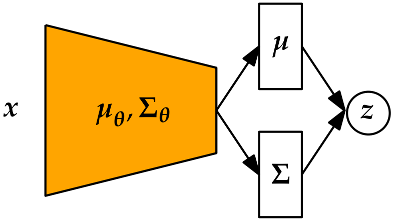


- Model (Rezende et al., 2014; Kinga & Welling, 2014):

$$p(z) = \mathcal{N}\big(\mathbf{0},\, \mathbf{I}\big)$$
$$p(x|z) = \mathcal{N}\big(\mu_\psi(z),\, \Sigma_\psi(z)\big)$$

- μ_ψ and Σ_ψ are deep networks with model parameters ψ

Variational Auto-Encoder: Inference

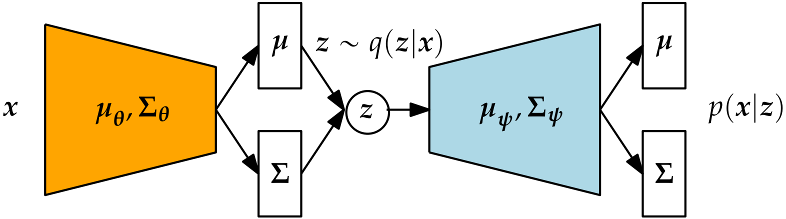


- Inference:

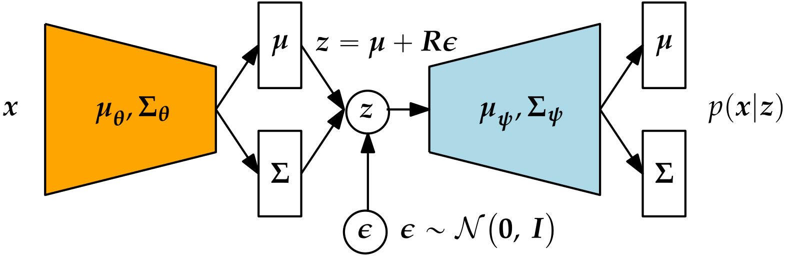
$$q(z|x) = \mathcal{N}\big(\mu_\theta(x), \Sigma_\theta(x)\big)$$

- μ_θ and Σ_θ are deep networks that map data onto (local) variational parameters ⏩ Inference network

Variational Auto-Encoder


$\boldsymbol{x}$
$\boldsymbol{\mu}_{\theta}, \boldsymbol{\Sigma}_{\theta}$
$\boldsymbol{\mu}$
$\boldsymbol{\Sigma}$
$\boldsymbol{z} \sim q(\boldsymbol{z}|\boldsymbol{x})$
$\boldsymbol{z}$
$\boldsymbol{\mu}_{\psi}, \boldsymbol{\Sigma}_{\psi}$
$\boldsymbol{\mu}$
$\boldsymbol{\Sigma}$
$p(\boldsymbol{x}|\boldsymbol{z})$

Variational Auto-Encoder


$\boldsymbol{x}$
$\boldsymbol{\mu}_\theta, \boldsymbol{\Sigma}_\theta$
$\boldsymbol{\mu}$
$\boldsymbol{\Sigma}$
$\boldsymbol{z} = \boldsymbol{\mu} + \boldsymbol{R}\boldsymbol{\epsilon}$
$\boldsymbol{z}$
$\boldsymbol{\epsilon}$
$\boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$
$\boldsymbol{\mu}_\psi, \boldsymbol{\Sigma}_\psi$
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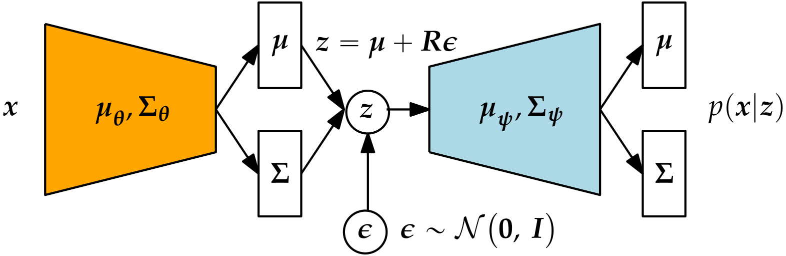
Variational Auto-Encoder



$\boldsymbol{x}$
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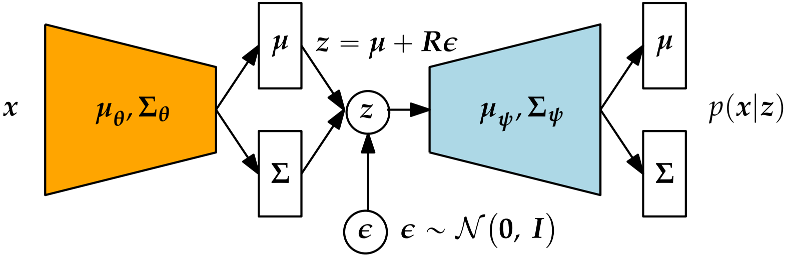
$p(\boldsymbol{x}|\boldsymbol{z})$

- Reparametrization trick introduces random noise $\boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$, but everything else are deterministic transformations

  ⏩ No need to push gradients through samples

Variational Auto-Encoder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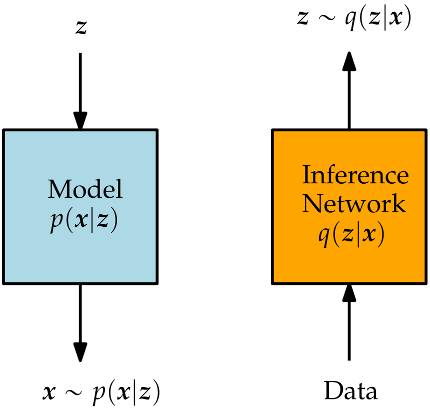
- Reparametrization trick introduces random noise $\boldsymbol{\epsilon} \sim \mathcal{N}(\boldsymbol{0}, \boldsymbol{I})$, but everything else are deterministic transformations

  ▶▶ No need to push gradients through samples
- Significance of the VAE:
  - Propagation of gradients through probability distributions (stochastic backpropagation)
  - Joint learning of model parameters and variational parameters

Variational Auto-Encoder: A Different Schematic


$\boldsymbol{z}$
Model
$p(\boldsymbol{x}|\boldsymbol{z})$
$\boldsymbol{x} \sim p(\boldsymbol{x}|\boldsymbol{z})$
$\boldsymbol{z} \sim q(\boldsymbol{z}|\boldsymbol{x})$
Inference Network
$q(\boldsymbol{z}|\boldsymbol{x})$
Data

- Generative process (left) (generator)
- Inference process (right) (recognition/inference network)

Applications

- Data compression/dimensionality reduction (similar to PCA)
- Data visualization
- Generation of new (realistic) data
- Denoising
- Probabilistic data imputation (fill gaps in data)

VAE: Data Visualization

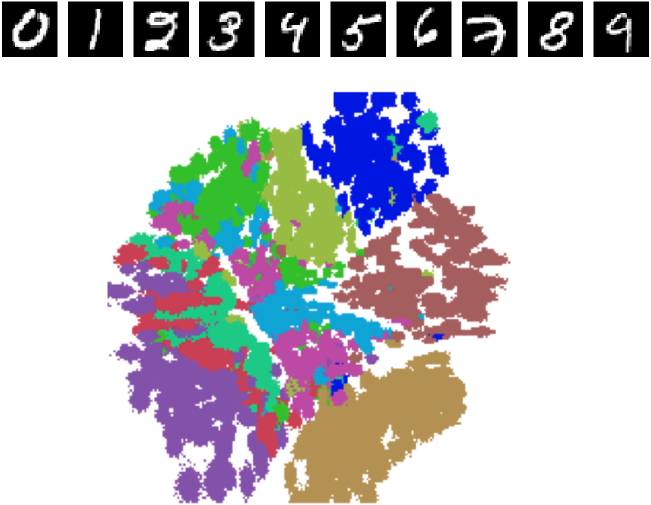


Figure from Rezende et al. (2014)

VAE: Generation of Realistic Images

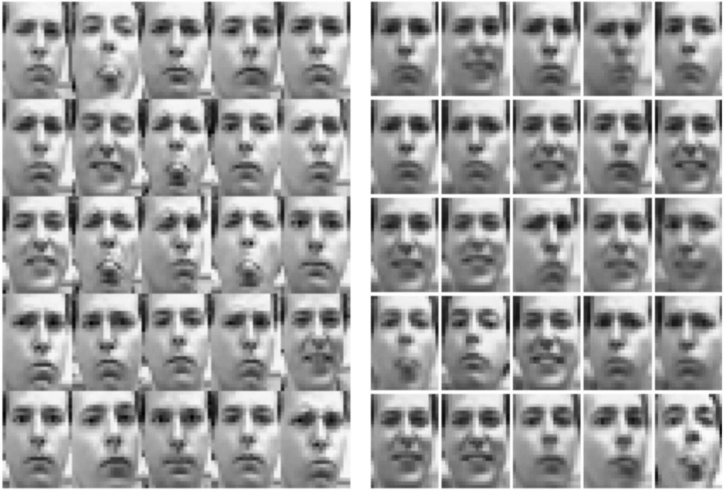


Figure from Rezende et al. (2014)

VAE: Probabilistic Data Imputation

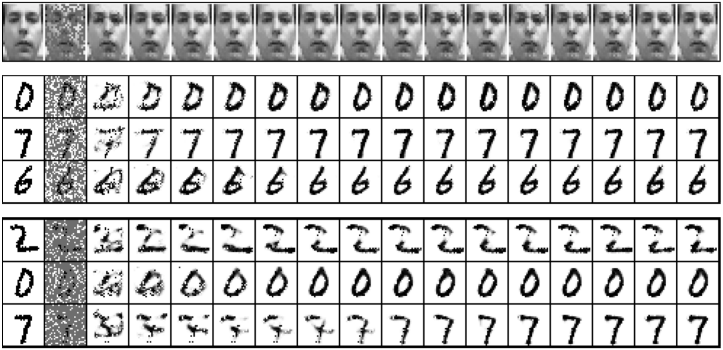


Figure from Rezende et al. (2014)

Overview

		Variational approximation of posterior	
		mean-field	more general
Model	conditionally conjugate	analytic solution	
	hierarchical Bayesian	stochastic gradient estimators; Example: VAE	dense Gaussian, mixture models, normalizing flows, auxiliary-variable models

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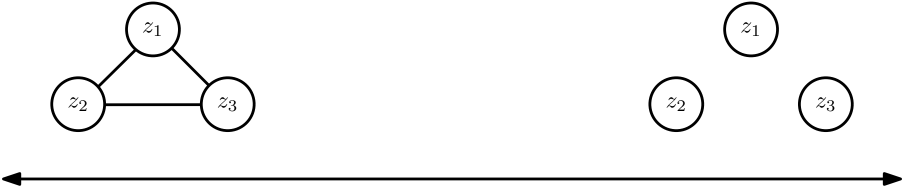
Amortized Inference

Richer Posterior Approximations

Richer Posterior Approximations

True posterior

Fully factorized



Most expressive

$q(z|x) = p(z|x)$

Least expressive

$q(z|x) = \prod_i q_i(z_i)$

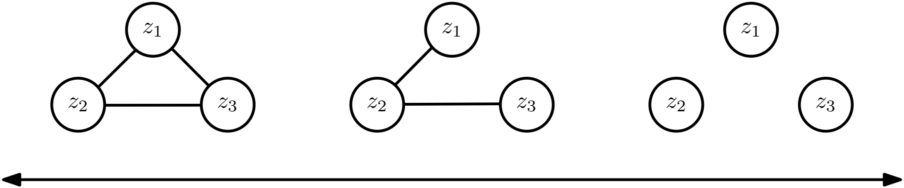
- Build richer posteriors
- Maintain computational efficiency and scalability
- Use all the things we know for specifying models of the data (but now for posterior approximations)

Structured Mean Field

True posterior

Structured approximation

Fully factorized



Most expressive

Least expressive

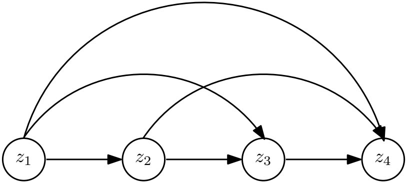
$q(z|x) = p(z|x)$

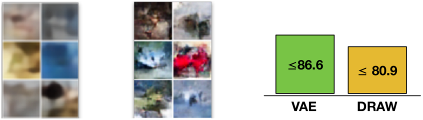
$q(z) = \prod_k q_k(z_k|z_{j\neq k})$

$q(z|x) = \prod_i q_i(z_i)$

- Introduce dependencies between latent variables
  - ⏩ Richer posterior than fully factorized

Autoregressive Distributions





[Gregor et al., 2015]

- Autoregressive structure:

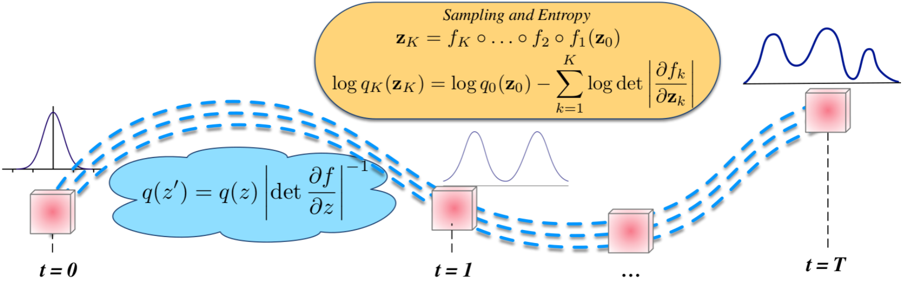
$$q(\boldsymbol{z}_{1:K}|\boldsymbol{\nu}) = \prod_{k=1}^{K} q(\boldsymbol{z}_k|\boldsymbol{z}_{1:k-1}, \boldsymbol{\nu}_k)$$

- Ordering of latent variables and nonlinear dependencies
- VAE (Rezende et al., 2014): mean-field Gaussian; DRAW (Gregor et al., 2015): autoregressive

Other Posteriors

- Mixture models (Saul & Jordan, 1996): $q(\boldsymbol{z}) = \sum_k \pi_k q_k(\boldsymbol{z}_k|\boldsymbol{\nu}_k)$
- Linking functions (Ranganath et al., 2016): $q(\boldsymbol{z}) = \left(\prod_{k=1}^{K} q(\boldsymbol{z}_k|\boldsymbol{\nu}_k)\right) L(\boldsymbol{z}_{1:K}|\boldsymbol{\nu}_{K+1})$

Normalizing Flows (1)



Sampling and Entropy

$$\mathbf{z}_K = f_K \circ \ldots \circ f_2 \circ f_1(\mathbf{z}_0)$$

$$\log q_K(\mathbf{z}_K) = \log q_0(\mathbf{z}_0) - \sum_{k=1}^{K} \log \det \left| \frac{\partial f_k}{\partial \mathbf{z}_k} \right|$$

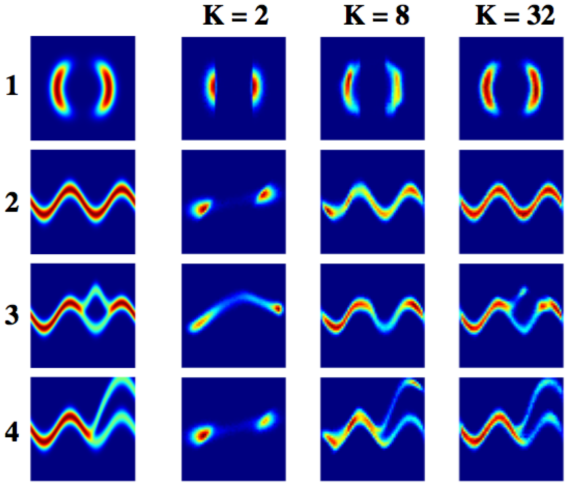
$$q(z') = q(z) \left| \det \frac{\partial f}{\partial z} \right|^{-1}$$

Distribution flows through a sequence of invertible transforms

[Rezende and Mohamed, 2015]

- Apply sequence of K invertible transformations to an initial distribution q_0 ⏩ Change-of-variables rule

Normalizing Flows (2)



Rezende & Mohamed (2015)

Summary

- Variational inference finds an approximate posterior by optimization
- Minimizing the KL divergence is equivalent to maximizing a lower bound on the marginal likelihood
- Mean-field VI: analytic updates in conditionally conjugate models
- Stochastic VI: Stochastic optimization for scalability
- General models require us to compute gradients of expectations
  - Score-function gradients
  - Pathwise gradients
- Amortized inference
- Modern VI allows us to specify rich classes of posterior approximations

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