Bayesian inference in generative models

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BCS Computational Tutorial

2018-11-13

Overview

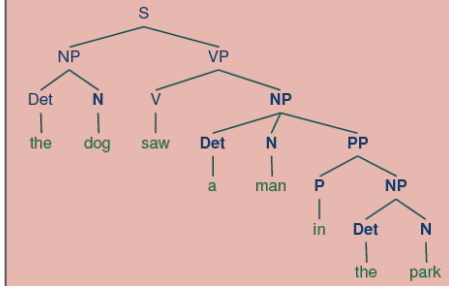
1. Intro to generative models (5 min)
2. Exact inference (10 min)
3. Sampling-based methods (25 min)
4. Variational inference (20 min)
5. Probabilistic programming languages (5 min)
6. Exercises (Last hour)

What is a generative model?

A probability distribution over observable variables

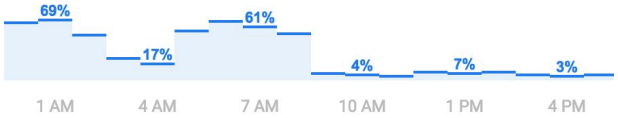
P(sentence)

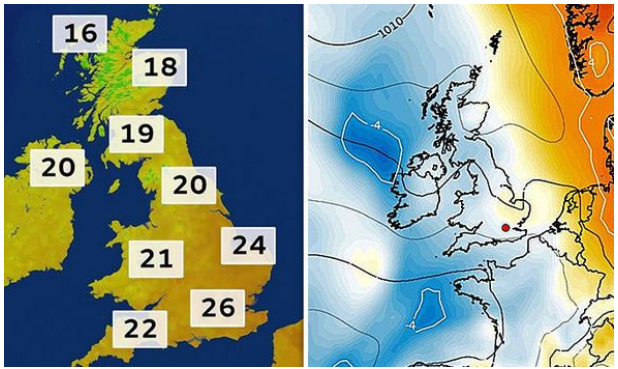
P(S → NP VP) = 1.0
P(VP → V NP) = 0.7
P(VP → VP PP) = 0.3
...
P(N → dog) = 0.02
P(N → fish) = 0.01
P(N → man) = 0.01



The dog saw a man in the park

P(rain)





P(face)

e.g. P(pixel1)
x P(pixel2|pixel1)
x ...

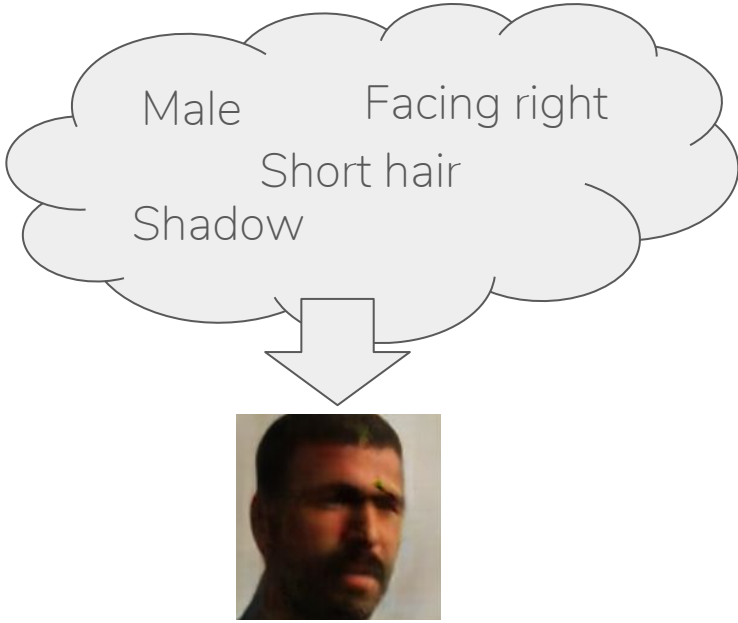
What is a generative model?

Common to describe distribution through unobservable **latent variables**

e.g. *directed causal model*:

Prior distribution of latent variables

Likelihood of observations given latent variables



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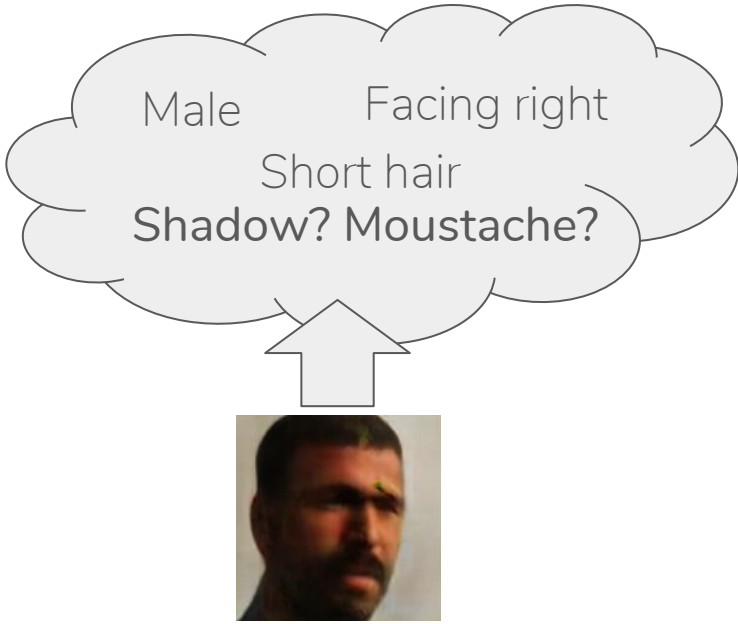


Bayes rule:

Given observations, infer latent variables

$$p(\text{shadow} \mid \text{img}) \propto \underbrace{p(\text{shadow})}_{\text{prior}} \underbrace{p(\text{img} \mid \text{shadow})}_{\text{likelihood}}$$

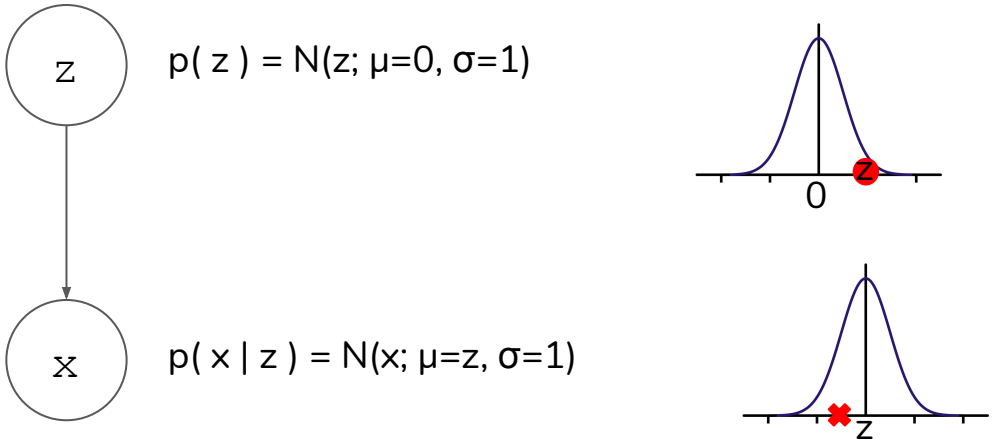
More generally: $p(\text{shadow} \mid \text{img}) \propto p(\text{shadow}, \text{img})$

(e.g. undirected models)

Graphical models

Generative model for which the conditional dependence structure between random variables is expressed as a graph

Simplest directed causal model: p(z, x) = p(z) p(x | z)



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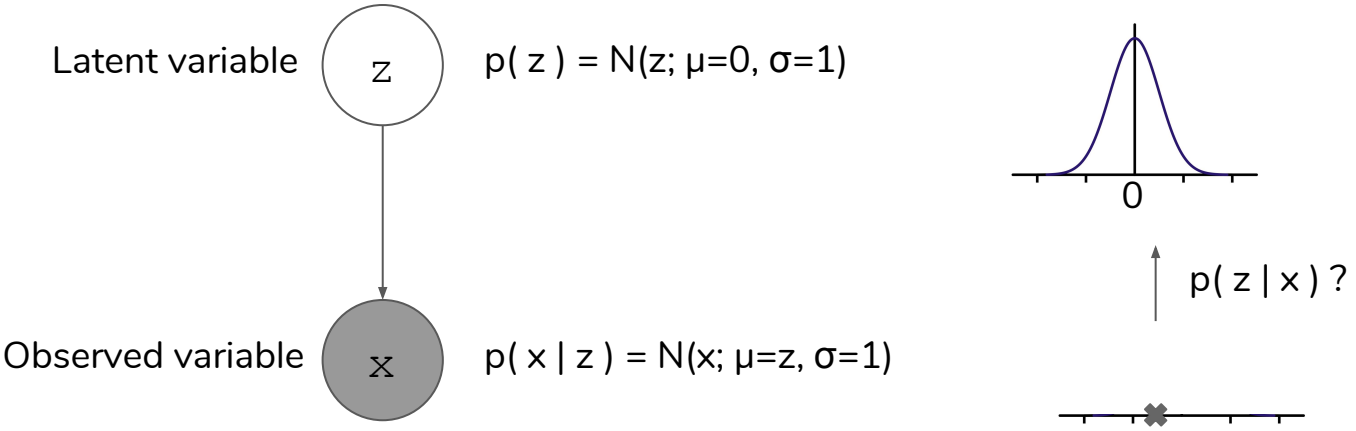
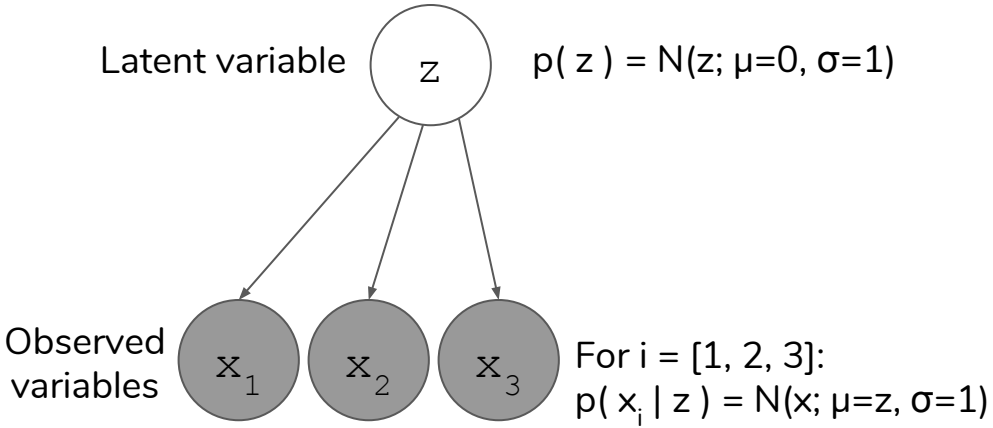
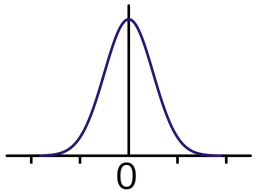


Graphical models

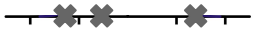
Generative model for which the conditional dependence structure between random variables is expressed as a graph

Directed causal model: $p(z, x_1, x_2, x_3) = p(z)\, p(x_1 \mid z) p(x_2 \mid z)\, p(x_3 \mid z)$





$p(z \mid x_1, x_2, x_3)$?



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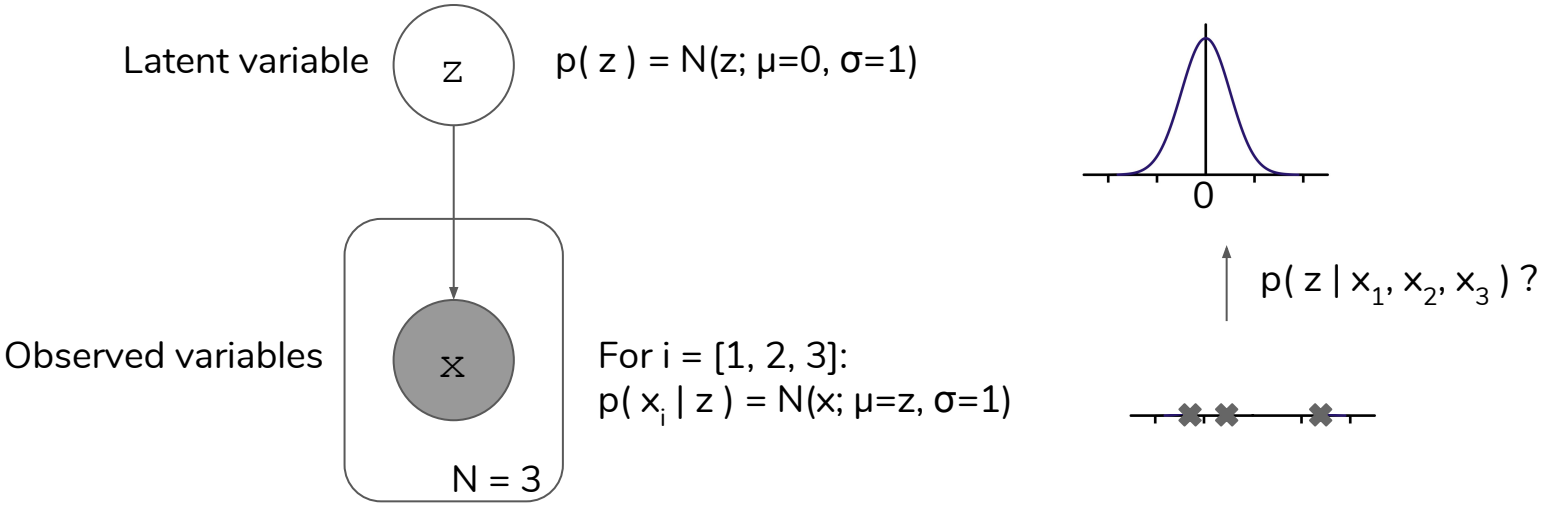

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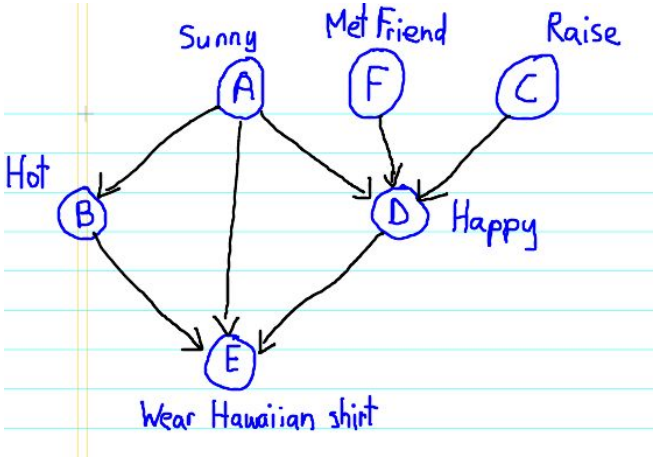
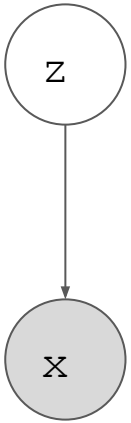


p(sun, friend, raise, hot, happy, shirt)
= p(sun)p(friend)p(raise)
*p(happy | sun, friend, raise)
*p(hot | sun) p(shirt | hot, happy)

Probabilistic programs: an extension of graphical models that express uncertainty over the structure of the graph itself

Exact Inference

Exact Inference



- When latent variable is **discrete** with finite support,
  - Can enumerate all possibilities

    $p(z|x) = p(z, x) / \sum_z p(z, x)$

- When latent variable is **continuous**:
  - Some likelihood functions $p(x \mid z)$ have ***conjugate priors***, which allow the posterior to be computed analytically
  - If a conjugate prior is used, $p(z \mid x)$ and $p(z)$ will be the same type of probability distribution: simply update the prior parameters

For a list of conjugate pairs: https://en.wikipedia.org/wiki/Conjugate_prior

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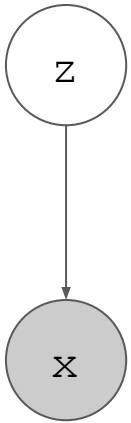
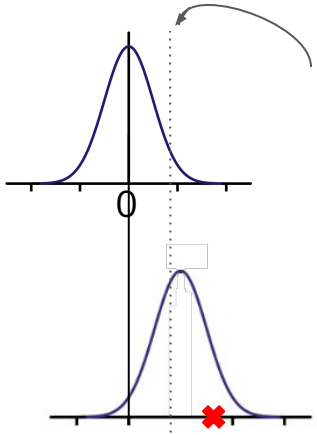


$p(z) = N(z; \mu=0, \sigma^2=1)$
Gaussian conjugate prior on μ

$p(x \mid z) = N(x; \mu=z, \sigma^2=1)$
Gaussian likelihood



Posterior is also Gaussian!
$N(z; \mu=\frac{1}{2}(x + 0), \sigma^2=\frac{1}{2})$

For a list of conjugate pairs: https://en.wikipedia.org/wiki/Conjugate_prior

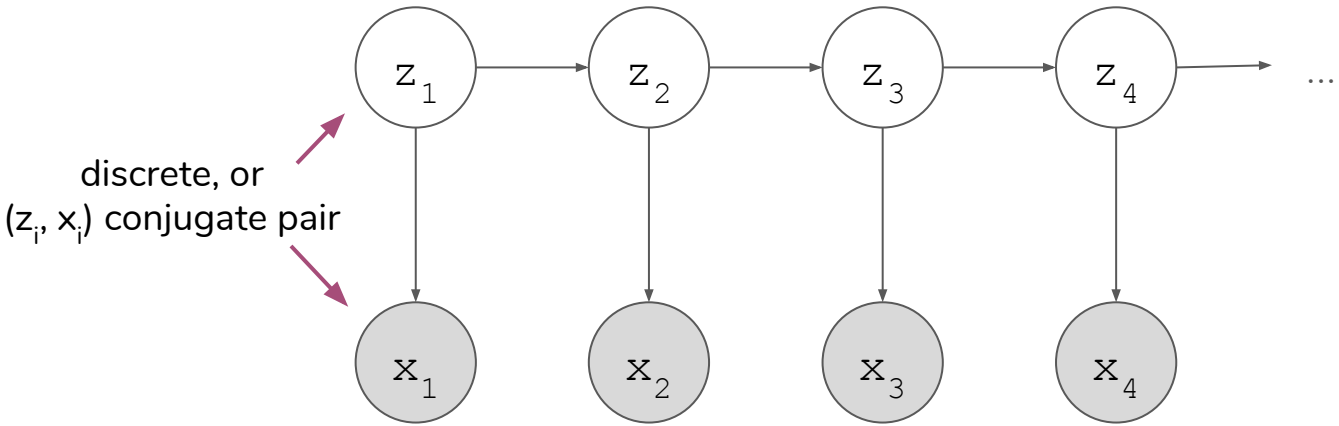
Conjugate priors

Likelihood	Conjugate prior	Posterior update
$x \sim \text{Normal}(\mu=z, 1)$	$z \sim \text{Normal}(\mu_0, \sigma_0^2)$	$z \mid x \sim \text{Normal}\left(\frac{x + \mu_0/\sigma_0^2}{1 + \sigma_0^2}, \frac{1}{1 + \sigma_0^2} \right)$
$x \sim \text{Normal}(\mu=0, \sigma^2=z)$	$z \sim \text{InvGamma}(\alpha, \beta)$	$z \mid x \sim \text{InvGamma}(\alpha + ½, \beta + ½ x^2)$
$x \sim \text{Bernoulli}(p=z)$	$z \sim \text{Beta}(\alpha, \beta)$	$z \mid x \sim \text{Beta}(\alpha + x, \beta + 1 - x)$

For a list of conjugate pairs: https://en.wikipedia.org/wiki/Conjugate_prior

Belief propagation ('Sum-product algorithm')

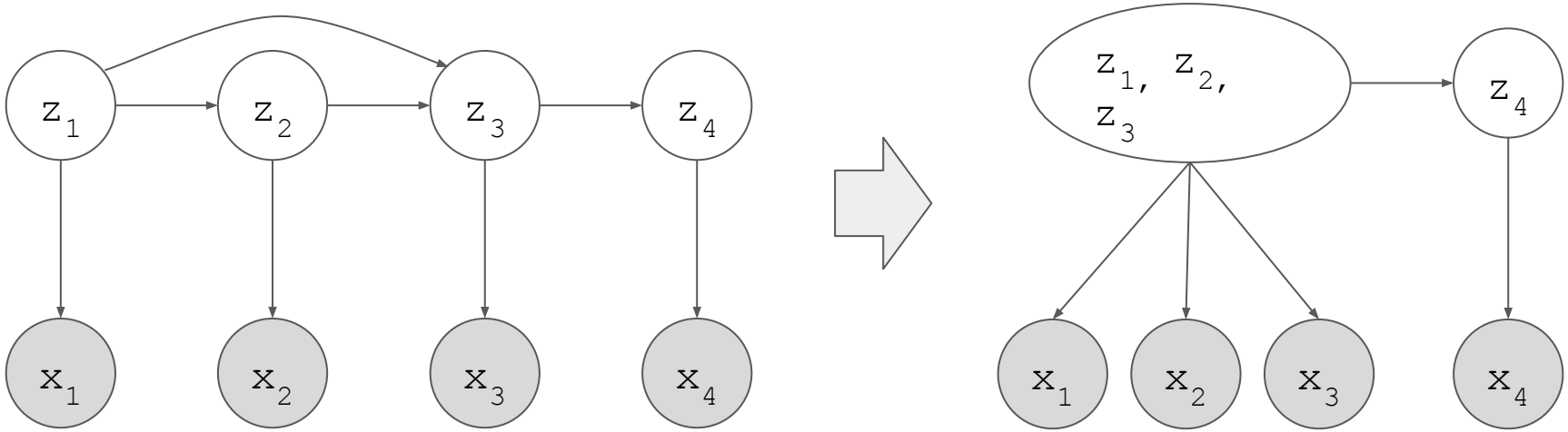
If latent variables form a sequence (or a tree) can find marginals $p(z_i)$ exactly
(Also 'max-product' for finding MAP)



e.g. Hidden Markov Models, Linear Gaussian State Space Models

Junction Tree Algorithm

If cyclic, must first group latent variables together.
(Still exact, but exponentially expensive…)



Exact Inference

Only possible…

1. For simple distributions which are either **finite** or **conjugate**
2. In small models, where you can enumerate all possible latent variables
3. In large models, if latent variables are not cyclic
   (see also, Junction Tree Algorithm)

Not very often…, BUT exact inference is often used as part of an approximate algorithm

Approximate Inference

Approximate Inference

To approximate the posterior, two main ideas (both from physicists):

- Monte Carlo (1946, 1953, 1970, …)
  Represent posterior as collection of (weighted) samples, $\{z_1, z_2, \ldots\}$
- Variational Inference (~1990s+)
  Represent posterior as a parametric distribution, Q(z) (e.g. gaussian)

To supplement these ideas (2000s):

- **Amortized Inference:** Learn to do inference quickly.
  (*'bottom-up', 'data driven', 'pattern-recognition'*)

Monte Carlo Methods

Stanisław Ulam

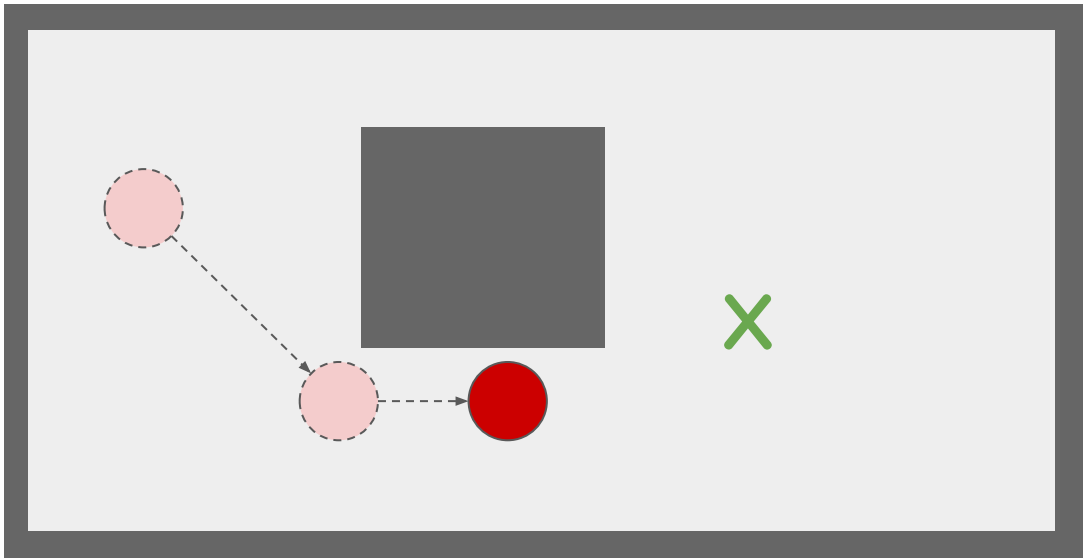
Monte Carlo inference

- We want to sample from some distribution
  - In this case, a posterior p(z|x)
- We can't sample from p directly, but maybe we can evaluate it
  - Or maybe we can only evaluate an unnormalised version of it, e.g. p(z, x)

Take samples from some other distribution (e.g. prior) and transform/reweight/etc. them so that they become samples from the posterior

Likelihood Weighting

- Basic example: Sample from prior and weight by likelihood



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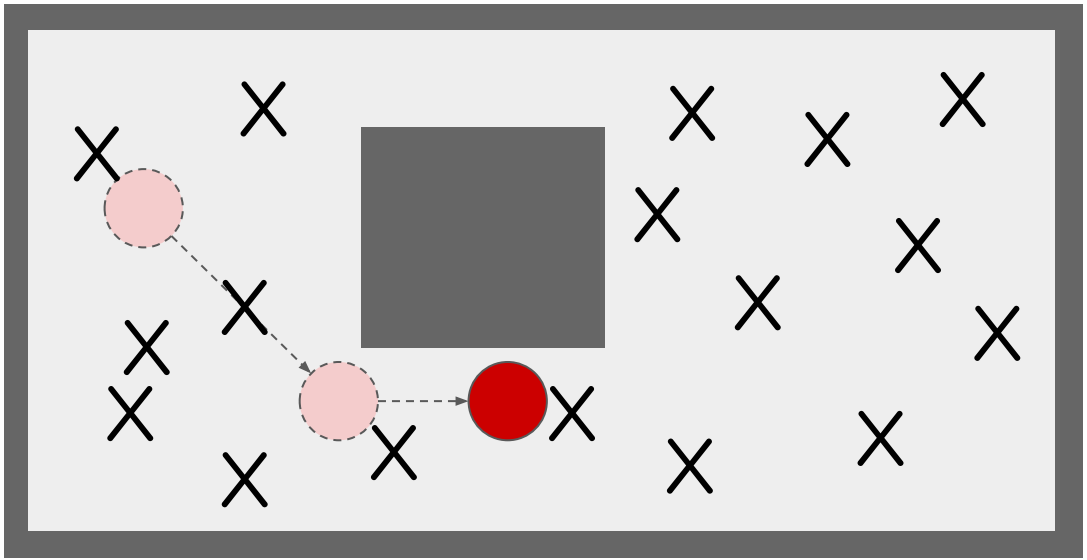

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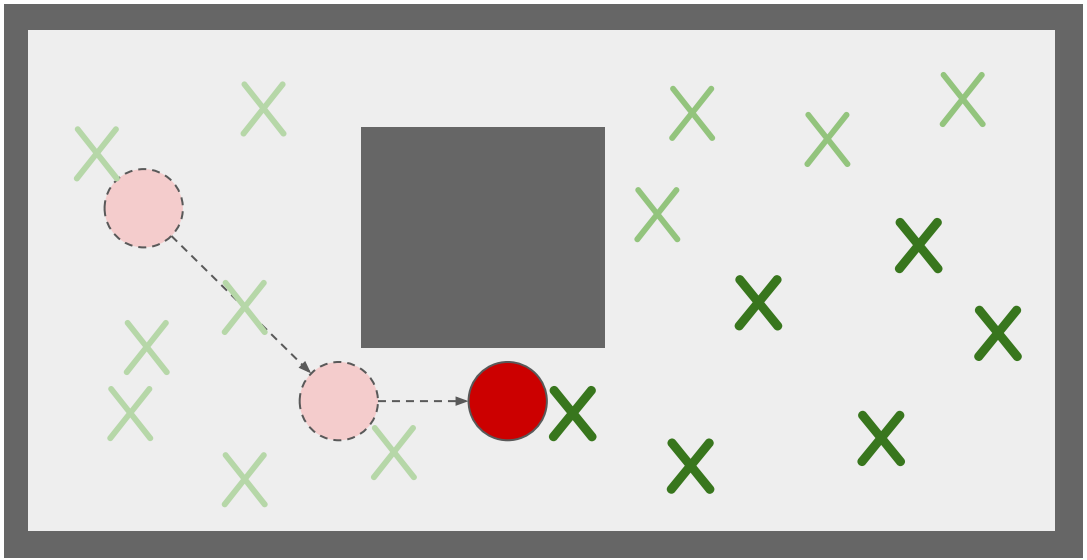

Importance Sampling

- Sample from guide $q(z)$, weight by $w = \mathbf{p(z,x)}/q(z)$

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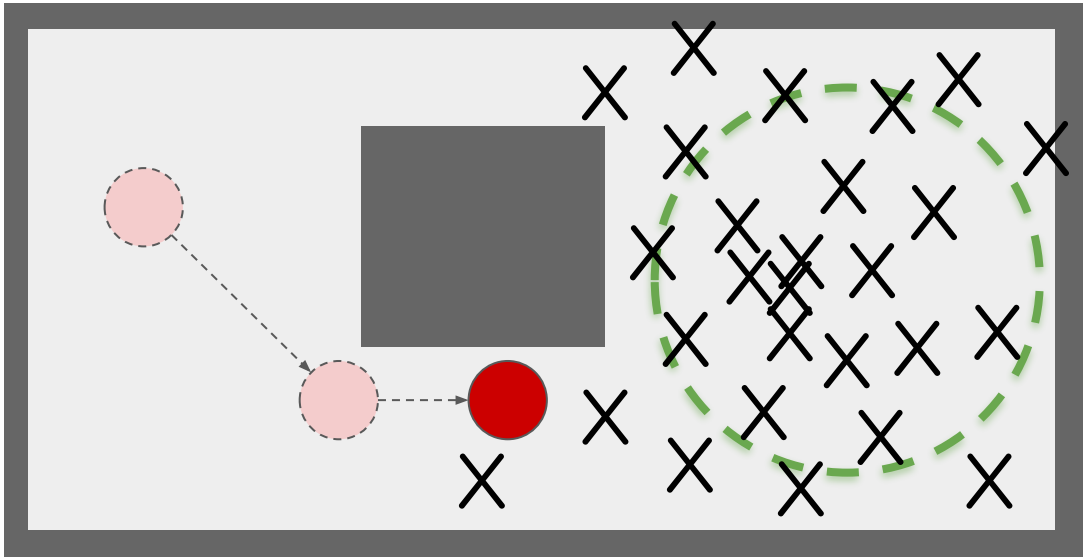

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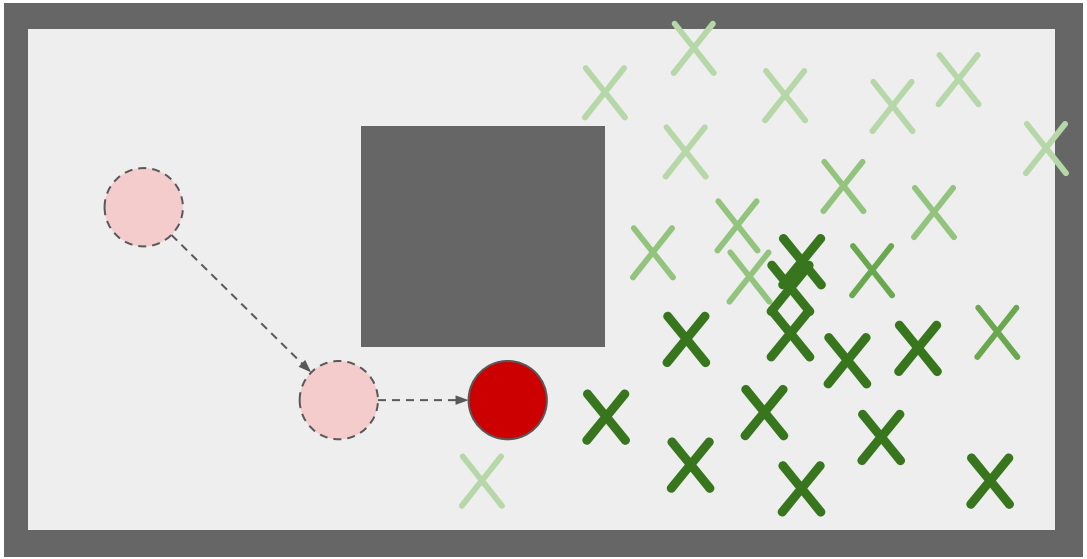

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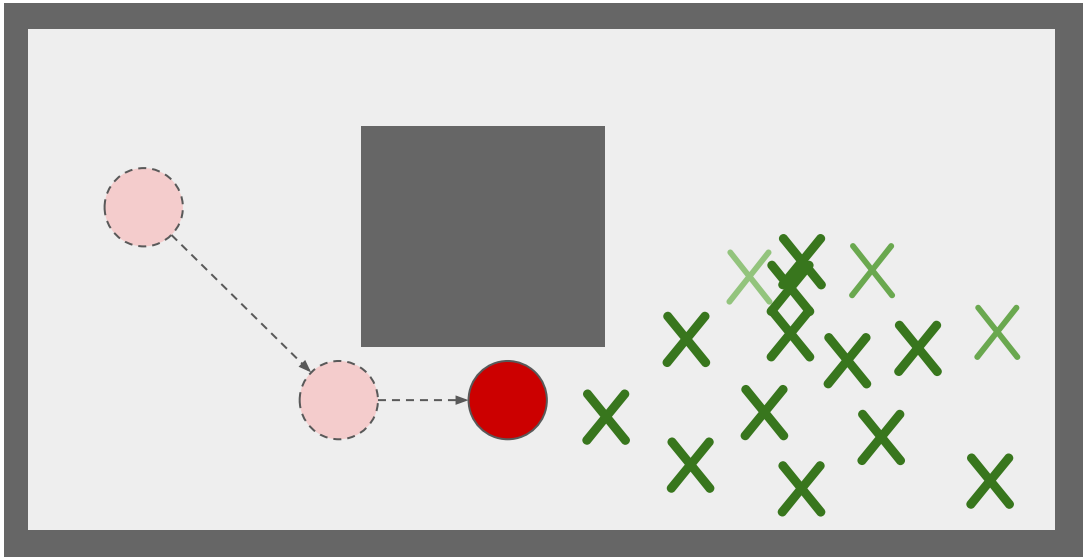
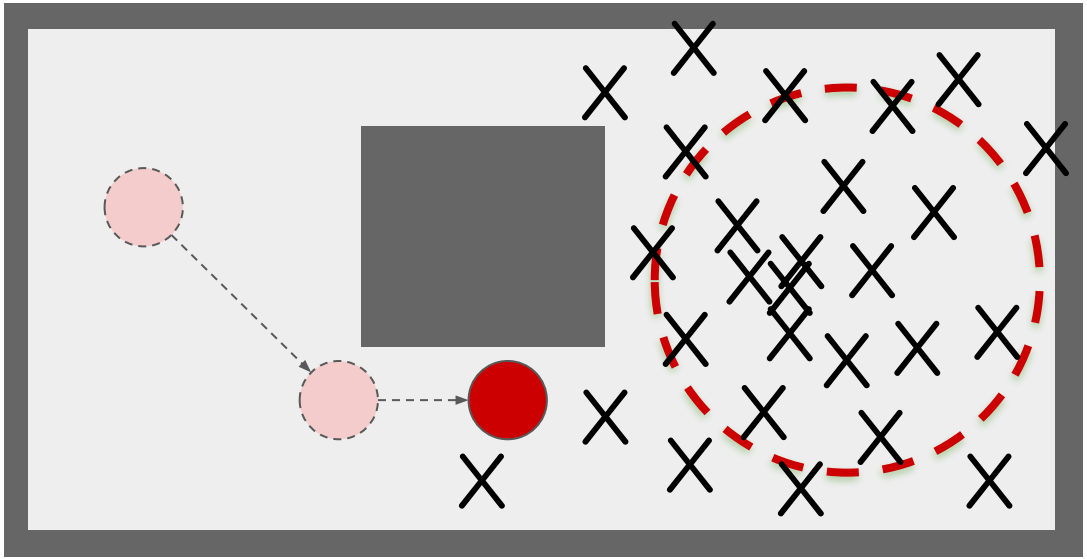


Importance Sampling

- Sample from guide q(z), weight by w = **p(z,x)**/q(z)
  Learn q with a neural network



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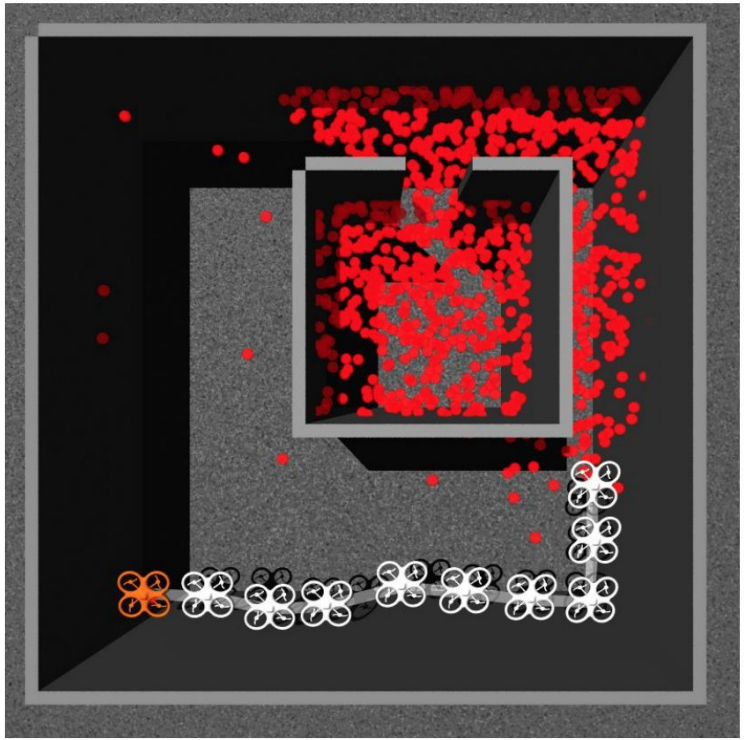


Cusumano-Towner et al. (2017)

Importance Sampling

- Works well if you can design, or learn, a guide distribution close to the true posterior
    - Should put a reasonable amount of probability mass on the true posterior
    - Much better to overshoot than undershoot!
- Usually **terrible** in high dimensional spaces

Markov Chain Monte Carlo (MCMC)

Rather than independent samples from a pre-determined guide distribution, take correlated samples that form a Markov Chain

New sample based on feedback from previous sample

Those samples are based on a random walk over Z, such that the proportion of samples equal to z* is proportional to p(z* | x)

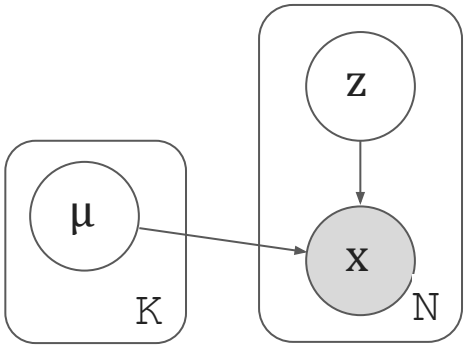
Neet to meet conditions:

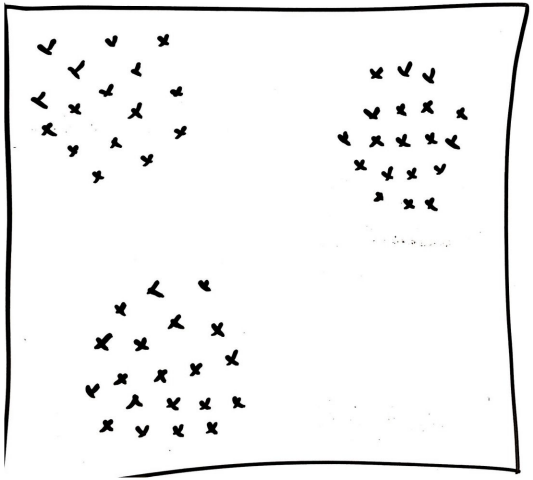
1. Markov chain is **ergodic** (eventually get to any possible z)
2. Posterior distribution is **stationary**

Markov Chain Monte Carlo (MCMC)

E.g. Mixture of Gaussians

$z_i \sim \text{Categorical}(\ldots)$
$\mu_j \sim \text{Normal}(\ldots)$
$x_i \sim \text{Normal}(\mu_{z_i})$





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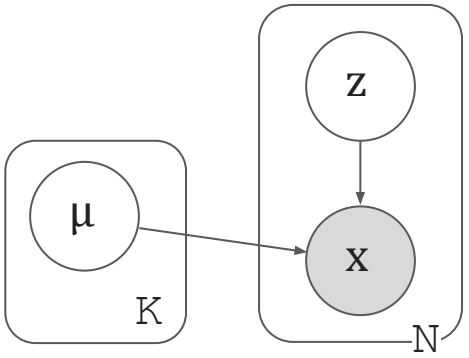
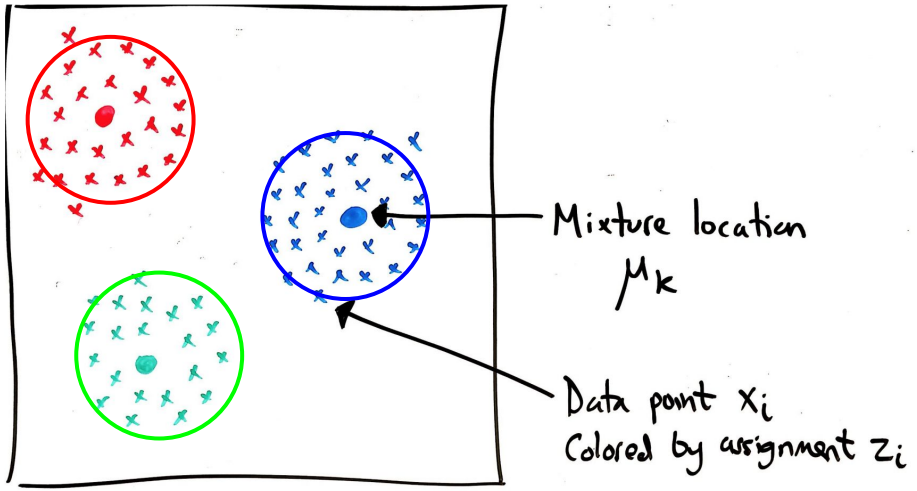




"If we knew the zs, we could just sample mu" (because mu has a *conjugate prior*)
"If we knew the μs, we could just sample z" (because z has a *finite* prior)

Gibbs Sampling

- If we can't sample from p(A,B) but we can sample from p(A|B) and p(B|A)
- Algorithm:
  1. Initialise A and B
  2. **Repeat**

     Sample A ~ p(A|B)

     Sample B ~ p(B|A)

Collapsed Gibbs Sampling

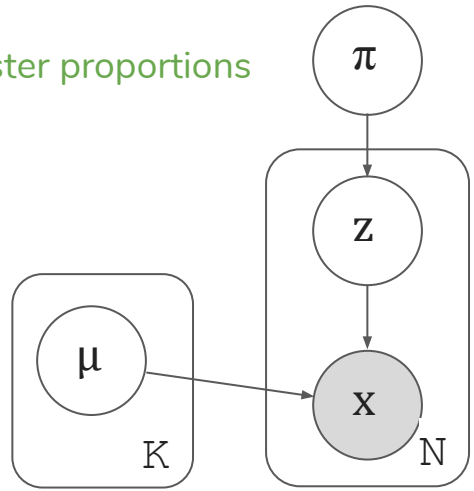
E.g. Mixture of Gaussians

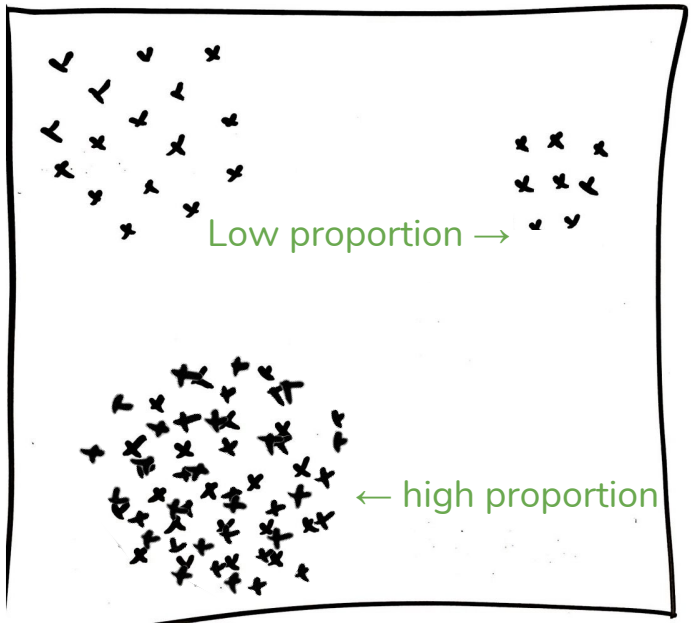
$\pi \sim \text{Dirichlet}(\ldots)$ ← cluster proportions

$z_i \sim \text{Categorical}(\pi)$

$\mu_j \sim \text{Normal}(\ldots)$

$x_i \sim \text{Normal}(\mu_{z_i})$





Dirichlet is **conjugate prior** for Categorical.

So: don't sample π, but marginalise

we can evaluate p(z|μ) exactly!

Markov Chain Monte Carlo (MCMC)

What if we don't know the conditional distributions exactly?

Similar idea to importance sampling:

1. Propose from a 'guide' distribution, and
2. Accept/reject proposal using feedback from model

Metropolis-Hastings (MH)

General algorithm for obtaining MH samples to approximate $p(z \mid x)$. [animation]

1 Initialize z^0
2 for s = 0, 1, 2, ... do
3 Define $z = z^s$
4 Sample $z' \sim q(z' \mid z)$ ← Proposal distribution (may be a mixture distribution)
5 Compute acceptance ratio:

$$r = \frac{\hat{p}(z', x)\, q(z \mid z')}{\hat{p}(z, x)\, q(z' \mid z)}$$

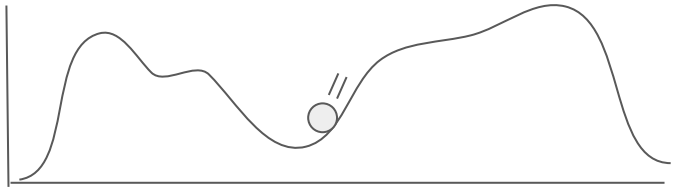
← Only an unnormalized posterior $\hat{p}$ is necessary
6 Compute $a = \min(1, r)$ ← Satisfies "detailed-balance"
7 Sample $u \sim U(0, 1)$
8 Set new sample to:

$$z^{s+1} = \begin{cases} z' \text{ if } u < a & \leftarrow \text{Accept} \\ z^s \text{ if } u \geq a & \leftarrow \text{Reject} \end{cases}$$

Some other MCMC ideas (mix ‘n match)

Data-driven proposals e.g. Tu & Zhu (2002), Kulkarni et al. (2015)
Sample (z, x) pairs from generative model, train neural network q(z|x). Proposal distribution can be a mixture of ‘global’ network proposals and ‘local’ (e.g. gaussian) proposals

Hamilton Monte Carlo animation
Use gradient information, follow the energy landscape



Annealing
e.g. start with a ‘smoothed’ likelihood (“high temperature”) and “cool” to true likelihood

Parallel tempering
Use multiple chains at different temperatures. Proposals jump between chains.

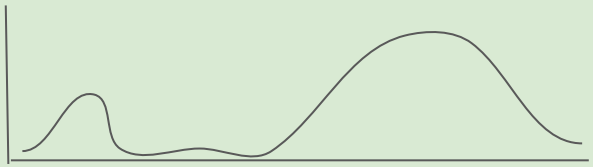
MCMC

Benefits

- Can be applied to any probability distributions including:
  - High dimensionality
  - Discrete variables / unknown dimensionality (probabilistic programs)
- Can use unnormalized posterior

Difficulties

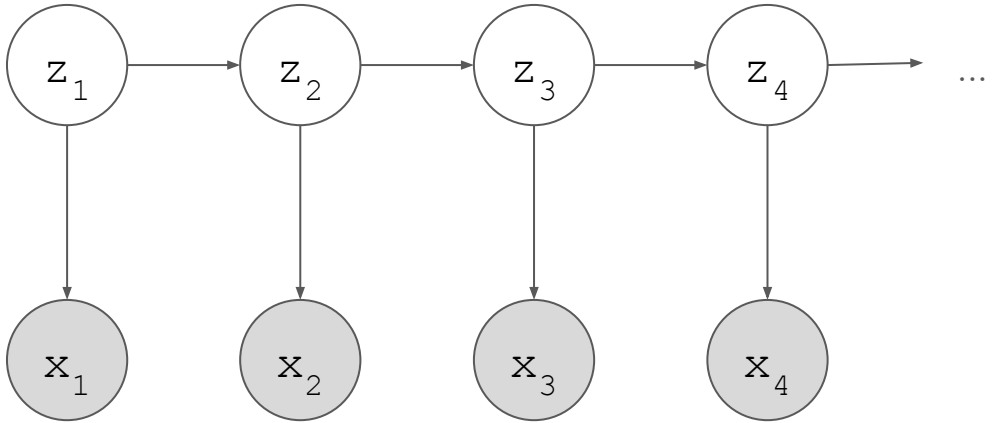
- '*Burn in*' - Find region of high probability, with only local information
- '*Mixing*' - How to move between modes?
- Difficult to assess convergence



Particle Filtering / Sequential Monte Carlo (SMC)

When your latent variables and observations form a sequence (so you get feedback over time)

Like importance sampling but reweight and resample **at each timestep**



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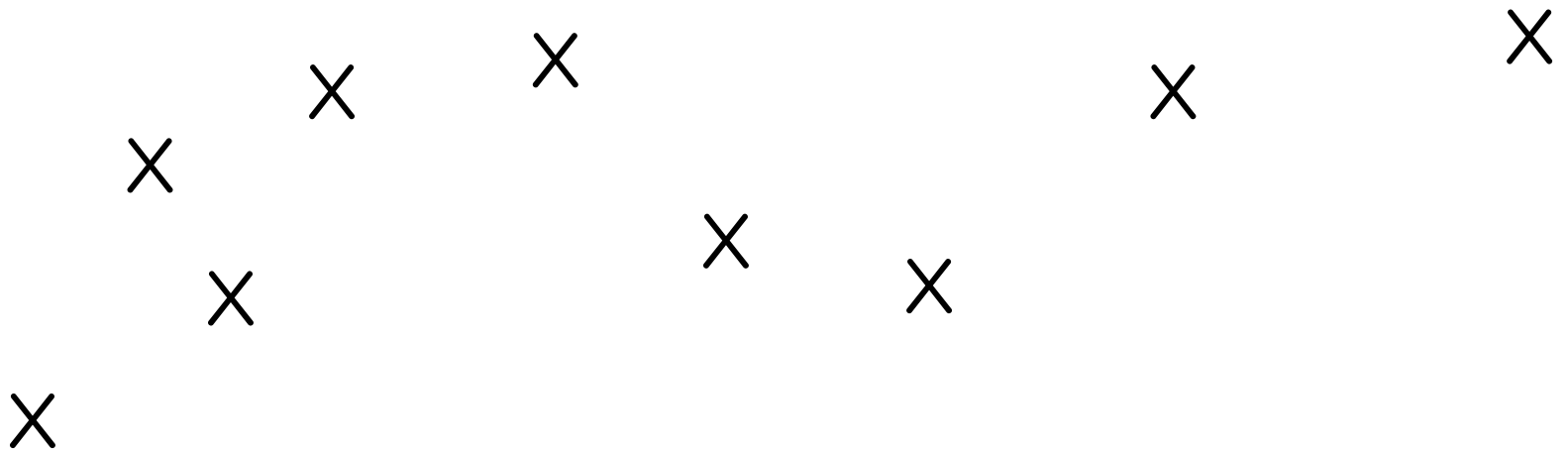

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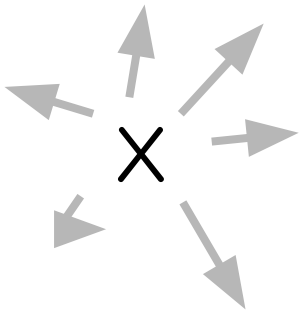

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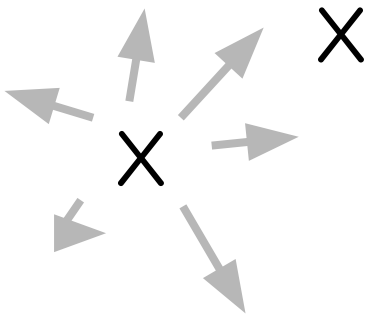

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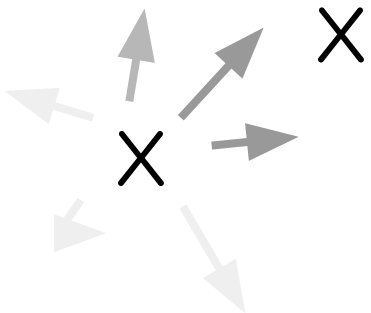

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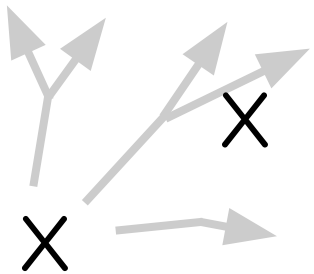

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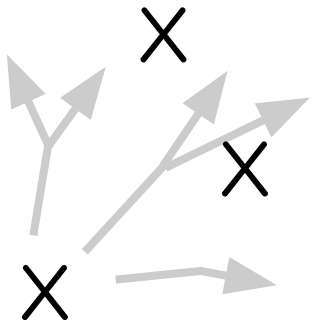

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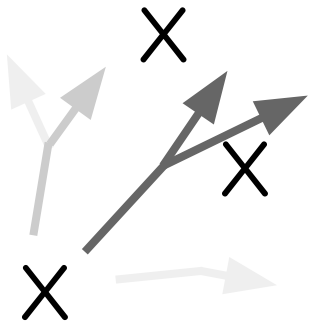

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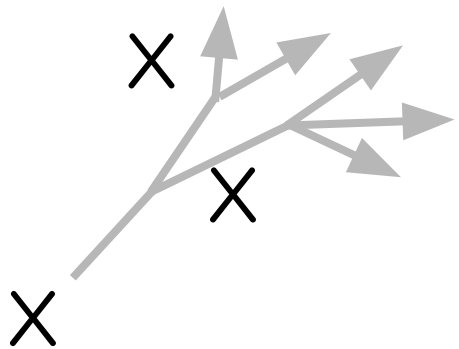

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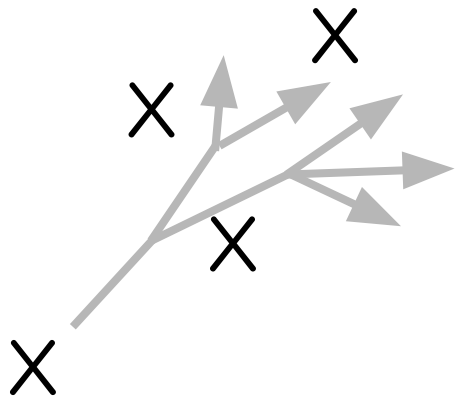

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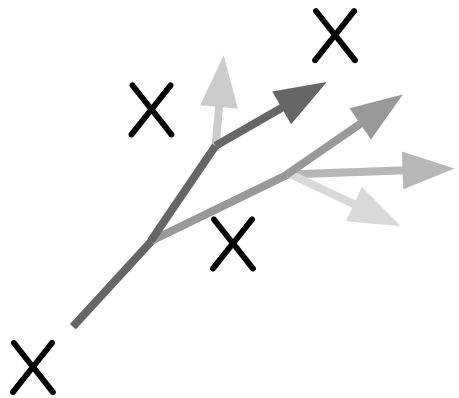

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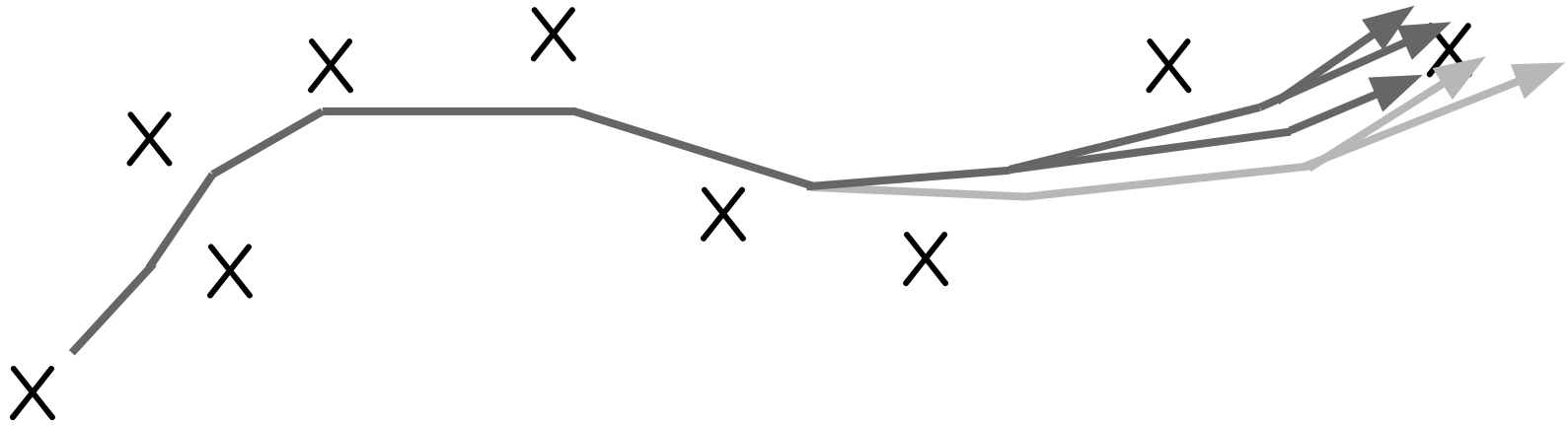

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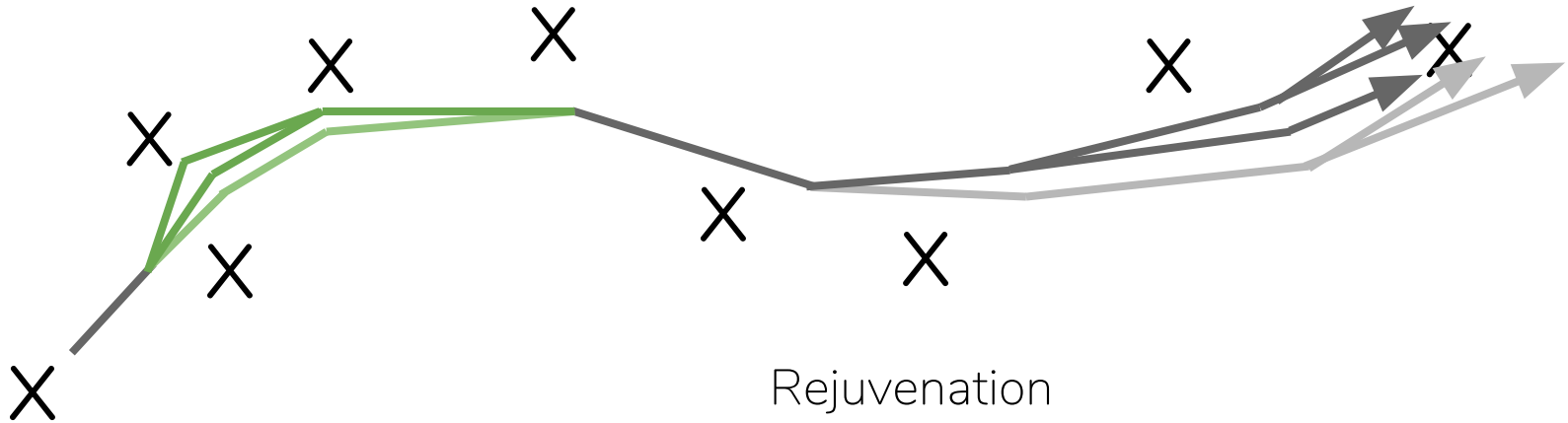
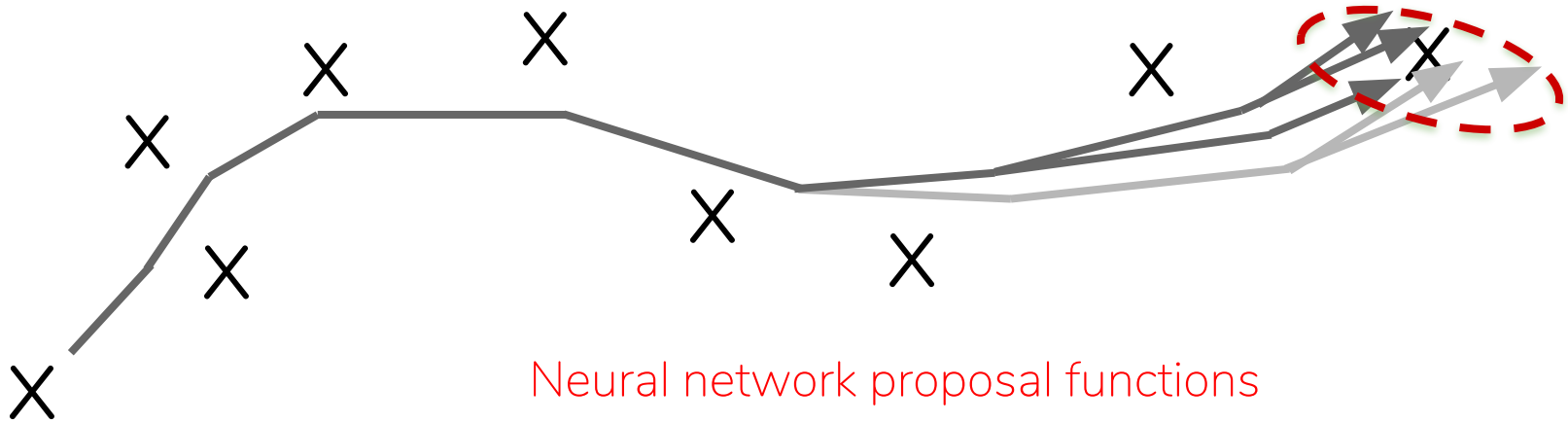


Rejuvenation

MCMC steps to update the whole state sequence

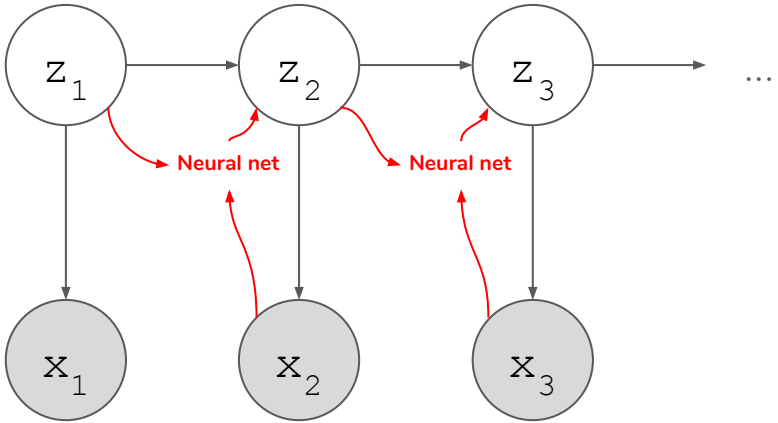
Particle Filtering / Sequential Monte Carlo (SMC)

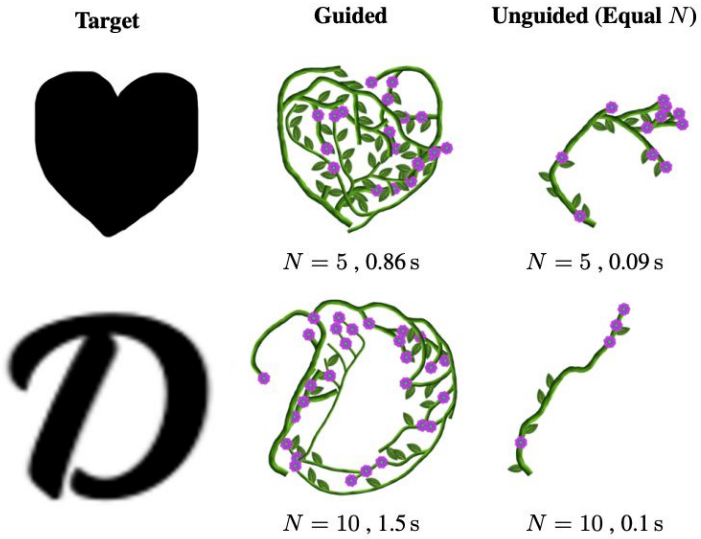


Neural network proposal functions

- Neural Adaptive Sequential Monte Carlo (Gu et al. 2015)
- Neurally Guided Procedural Models (Ritchie et al. 2016)

Particle Filtering / Sequential Monte Carlo (SMC)





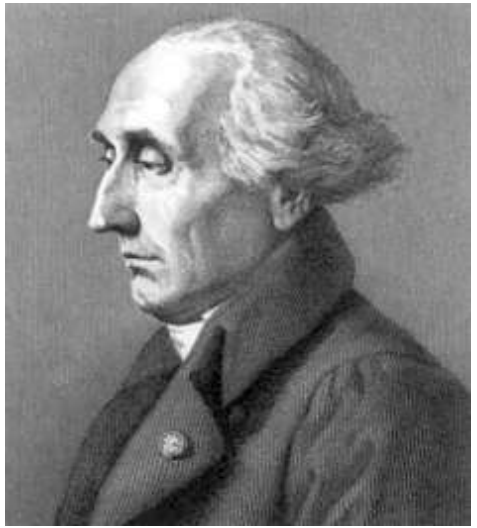
Neurally Guided Procedural Models (Ritchie et al. 2016)

Monte Carlo inference: summary

- Basic idea illustrated with importance sampling
- MCMC algorithms:
  - **MH**: General purpose
  - **Gibbs sampling**: when you have exact conditional distributions
  - **HMC**: when you have the gradients of the (unnormalised) posterior
  - **SMC**: when you have sequential observations
  - Many, many others!
- Use neural networks to learn proposal distributions

Variational Inference

Leonard Euler



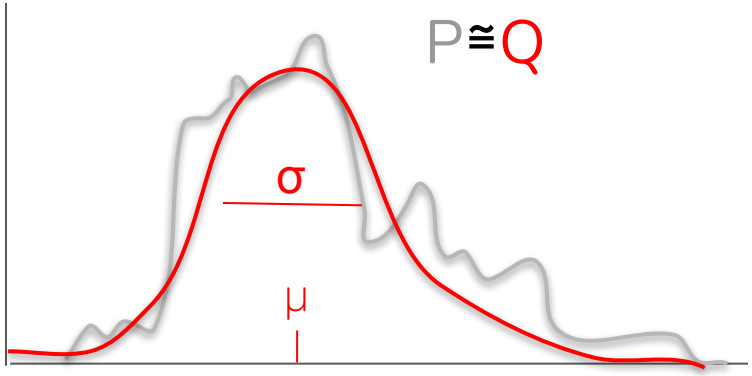
Joseph-Louis Lagrange

Variational Inference (Inference as optimisation)

Monte-Carlo: Obtain samples from posterior

Variational: Approximate posterior with a parametric distribution (e.g. Gaussian)

- Optimise parameters to most closely match posterior: minimise $D_{KL}(Q||P)$
- Trade off between ease of optimisation and accuracy of approximation



Matching the true posterior

Kullback-Leibler divergence KL(Q||P) = measure of distance* between Q and P

- Non-negative; zero only when P and Q are equal

$$D_{KL}\left[\, \mathbf{Q(z)} \,||\, \mathbf{p(z|x)} \,\right] = -E_{z\sim\mathbf{Q}}\left[\, \log \frac{\mathbf{p(z|x)}}{\mathbf{Q(z)}} \,\right]$$

$$= -E_{z\sim\mathbf{Q}}\left[\, \log \mathbf{p(z,x)} - \log \mathbf{Q(z)} \,\right] + \text{const.}$$

ELBO (evidence lower bound)
Lower bound on log p(x)

Matching the true posterior

ELBO

$$E_{z\sim Q}\left[\ \log \mathbf{p(z,x)} - \log \mathbf{Q(z)}\ \right]$$

How to choose and optimise the variational distribution, Q?

- *'Classical'* variational inference (1990s, 2000s)
  Find a variational family that you can optimise analytically (with the calculus of variations)

- *Stochastic gradient variational Bayes* (2014)
  Find a variational family that you can optimise with gradient descent

‘Classical’ variational inference

1. Choose **conjugate** prior distributions in **P** and choose **Q** from the same family, so that we will be able to derive analytical solutions

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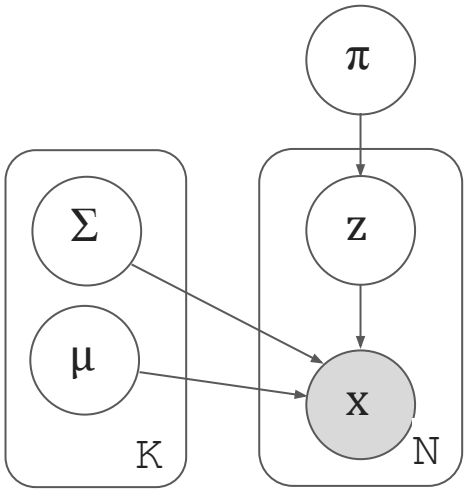
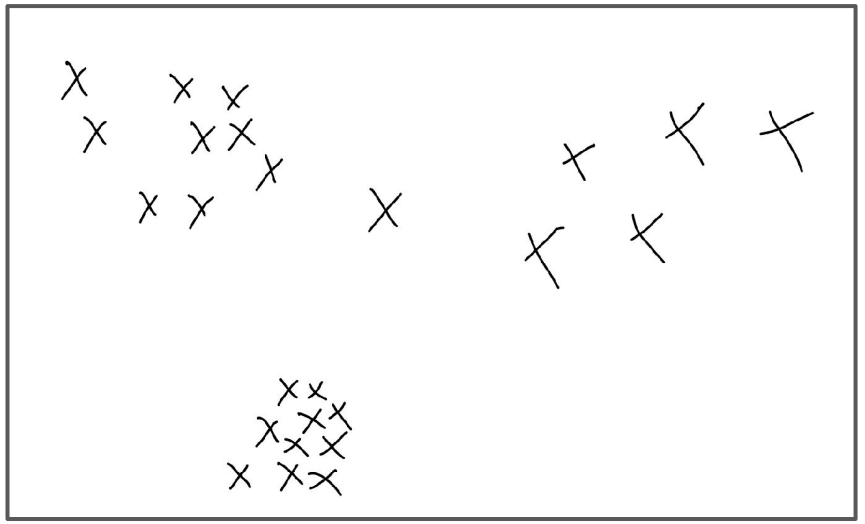
P: Gaussian mixture model

$\pi \sim \text{Dirichlet}(\ldots)$
$z_i \sim \text{Categorical}(\pi)$
$\mu_j \sim \text{Normal}(\ldots)$
$\sum_j \sim \text{InvWishart}(\ldots)$
$x_i \sim \text{Normal}(\mu_{zi}, \sum_{zi})$





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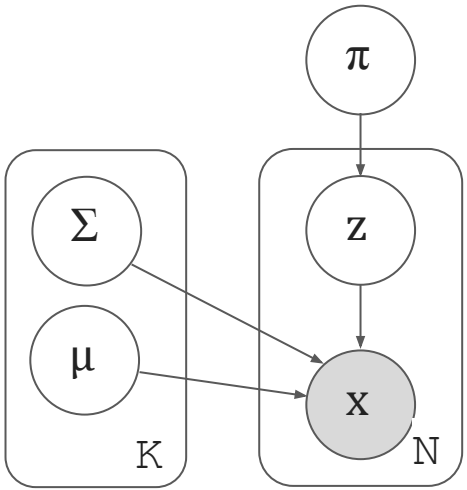

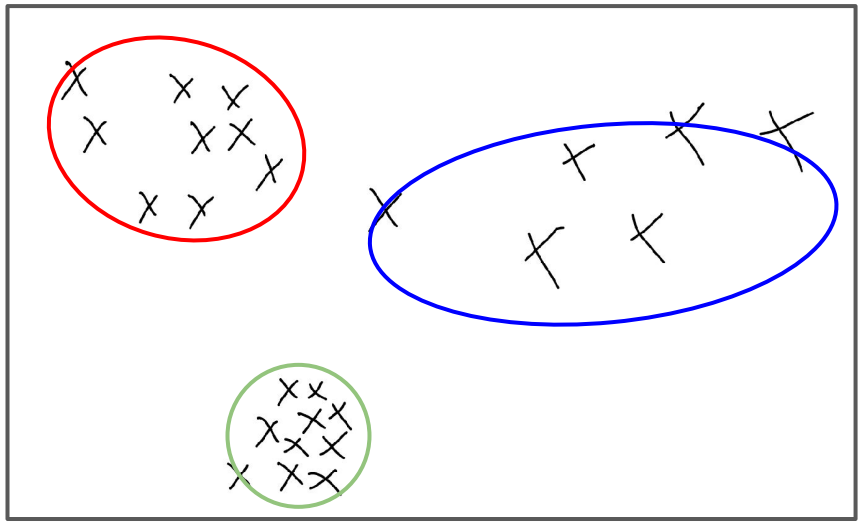

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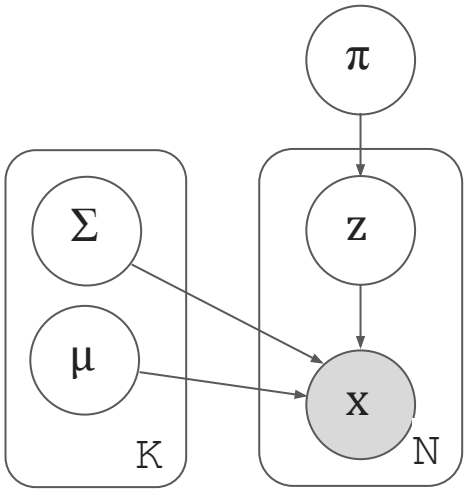

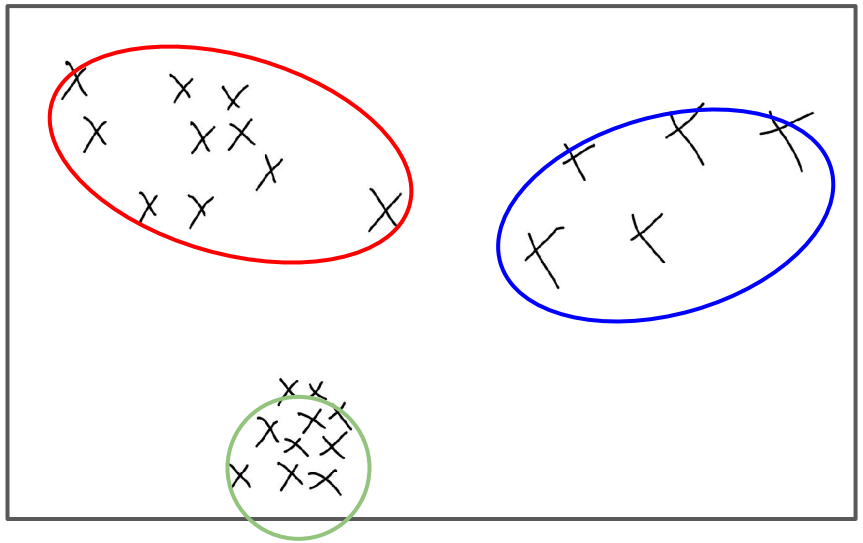

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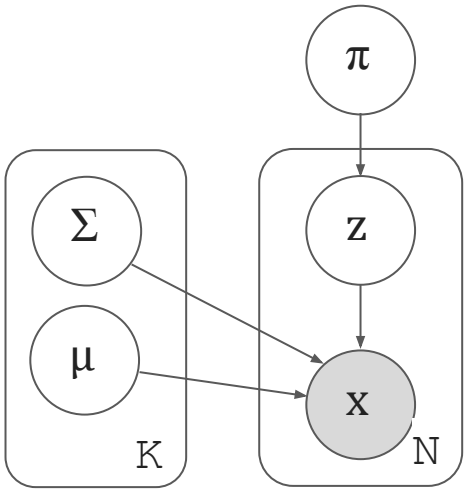
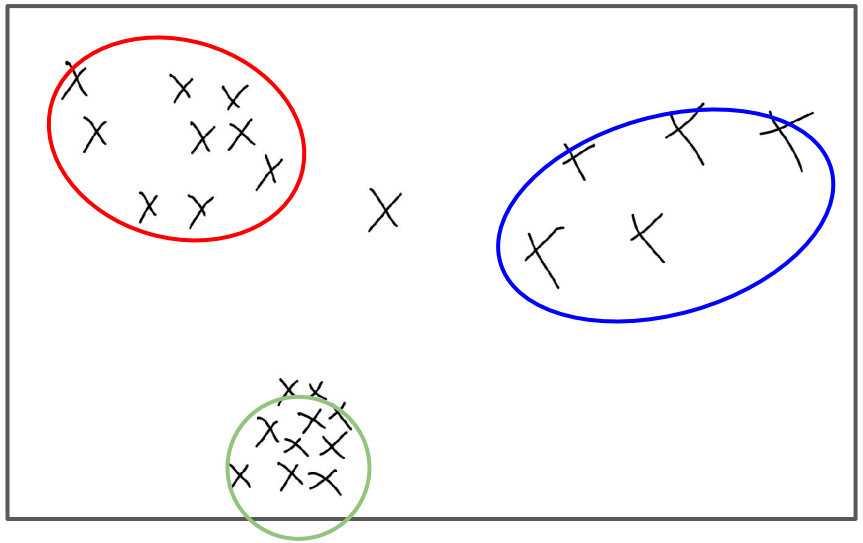


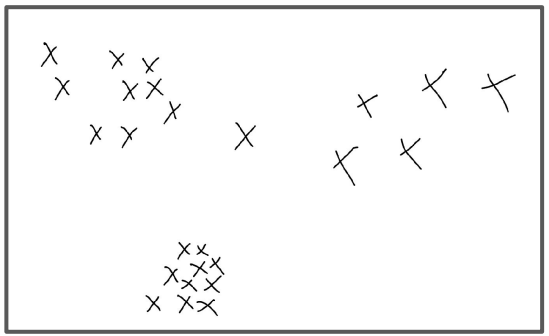


‘Classical’ variational inference

1. Choose **conjugate** prior distributions in **P** and choose **Q** from the same family, so that we will be able to derive analytical solutions
2. **Mean-field approximation**: make all latent variables independent in **Q**

$$Q(z_1, \ldots, z_n) = \prod_{i=1}^{n} q(z_i)$$

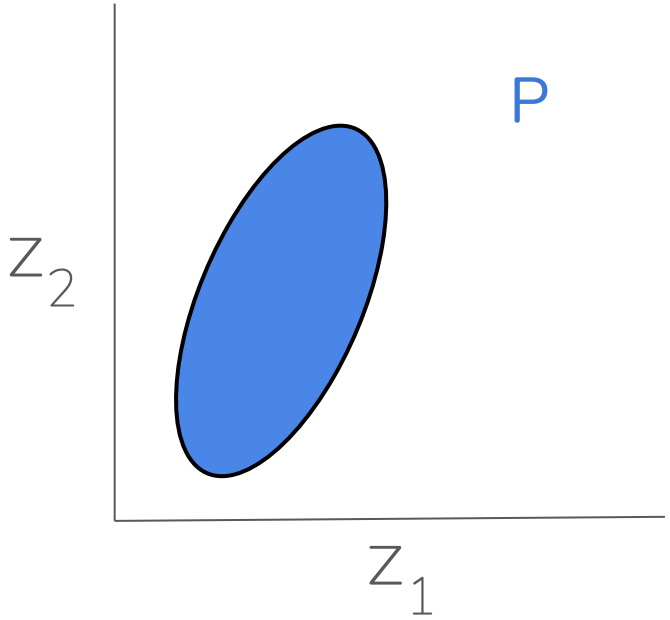
$$Q(\pi,\mu,\sum,z) = q(\pi) \prod q(\mu_k) q(\sum_k) \prod q(z_i)$$



‘Classical’ variational inference

Mean-field variational inference:

“Find the closest match to the posterior without allowing any correlations”



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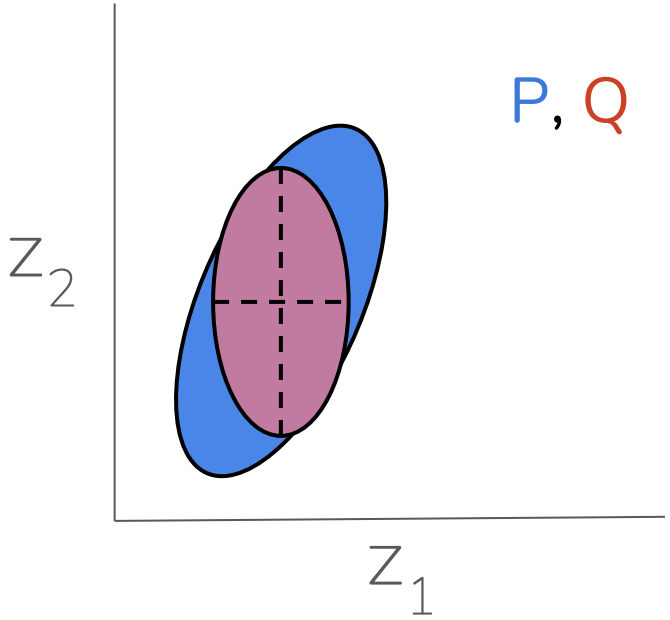

‘Classical’ variational inference

ELBO

$$E_{z\sim Q}\left[\ \log \mathbf{p(z,x)} - \log \mathbf{Q(z)}\ \right]$$

Gaussian mixture model

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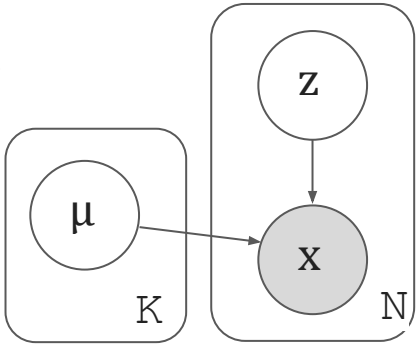

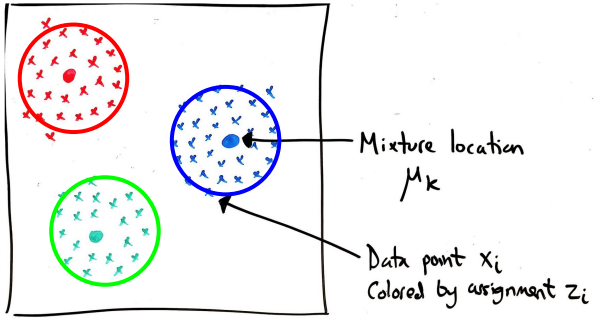

Mean field approximation: $Q(z, \mu) = q(z)q(\mu)$

$$\underset{q(z),\ q(\mu)}{\text{Argmax}}\ \underset{\substack{z\sim q(z)\\ \mu\sim q(\mu)}}{E}\left[\ \log \mathbf{p(z,\mu,x)} - \log q(z)q(\mu)\ \right]$$

‘Classical’ variational inference

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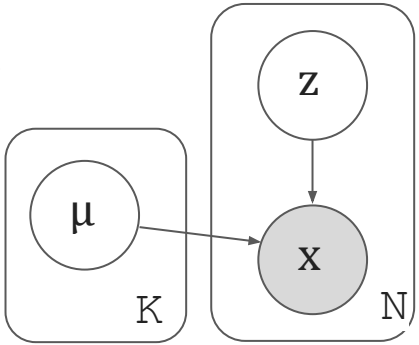

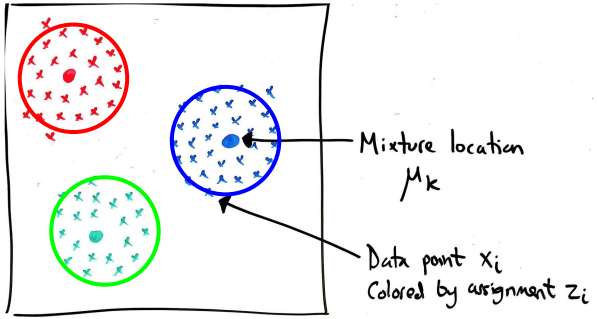

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“If we knew $q(z)$ we could find the best $q(\mu)$”

$$\mathbf{q^*(\mu)} \propto \exp\left[\ E_{q(z)} \log \mathbf{p(z,\mu,x)}\ \right]$$

“If we knew $q(\mu)$ we could find the best $q(z)$”

$$\mathbf{q^*(z)} \propto \exp\left[\ E_{q(\mu)} \log \mathbf{p(z,\mu,x)}\ \right]$$

So: Alternate updates to $q(z)$ and $q(\mu)$

‘Classical’ variational inference

- Algorithm:
  1. Initialise q(A) and q(B)
  2. **Repeat**

     Update q(A) to minimise $D_{KL}[\, q(A)q(B) \,||\, P(A,B) \,]$

     Update q(B) to minimise $D_{KL}[\, q(A)q(B) \,||\, P(A,B) \,]$

     Until convergence

Stochastic Gradient Variational Bayes

"But can't we just do

$$\text{Argmax}_Q \; E_{z\sim Q}[\, \log \mathbf{p(z,x)} - \log \mathbf{Q(z)} \,]$$

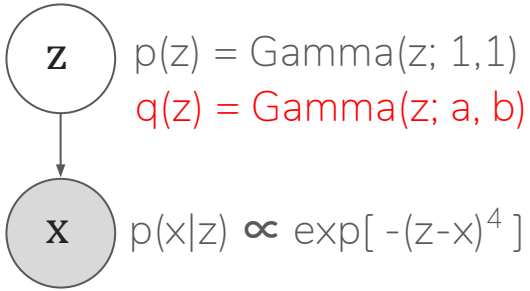
with gradient descent?"

- Kingma et al. (2014), Rezende et al. (2014)

- Answer: Yes, if we use *samples* to approximate the expectation (SGD)!
  But only if:
  - Unnormalized posterior p(z,x) is differentiable in z (no discrete random variables, unless you can marginalise them out)
  - Q(z) is 'reparametrisable' (e.g. multivariate Normal)

- No need for conjugate priors!
- No need for mean-field approximation!

Stochastic Gradient Variational Bayes



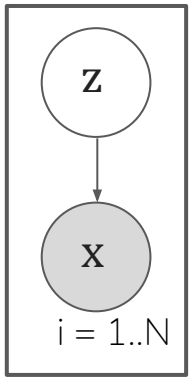

```python
import torch
theta = torch.nn.Parameter(torch.zeros(2))
optimizer = torch.optim.Adam([theta], lr=1e-3)

for i in range(100000):
    # Model
    log_prior = torch.distributions.gamma.Gamma(1,1).log_prob
    log_likelihood = lambda z, x: -(z-x)**4

    # Variational Distribution
    a, b = torch.exp(theta)
    Q = torch.distributions.gamma.Gamma(a, b)

    # Optimise ELBO
    z = Q.rsample()
    elbo = log_prior(z) + log_likelihood(z, 10) - Q.log_prob(z)
    (-elbo).backward(); optimizer.step(); optimizer.zero_grad()

print(Q.mean, Q.variance) #Returns (9.73, 1.18)

```

More stochastic variational inference

1. Normalizing flows (Rezende and Mohamed, 2016)
   - To make an expressive variational distribution Q, start with a simple distribution (e.g. Normal) and then run it through a bunch of invertible transformations.

$$q(z_i) = \text{Normal}(z_i; f_\theta(x_i))$$

2. **Amortized variational distribution**
   - Use a neural network f_θ to parametrize Q(z)
     Variational Autoencoders (Kingma et al, 2014)
   - **Afterwards, you not only solve your inference problem, but you also have a recognition model for future observations**



Variational inference: summary

Can mix methods: some latents stochastic, others analytical (e.g. Belief Propagation)

Benefits

- Fast and easy to assess convergence
- Provides model evidence log P(X)
- Normalising flows: Can handle multimodality

Limitations

- Unlike MH, restrictions on model:
  - Classical VI: Mean-field approximation and conjugate priors
    Often can't express multimodal posteriors
  - SGVB: everything has to be differentiable/enumerable
- Unlike MCMC, not exact in the limit, convergence =/= exact posterior

Probabilistic Programming Languages

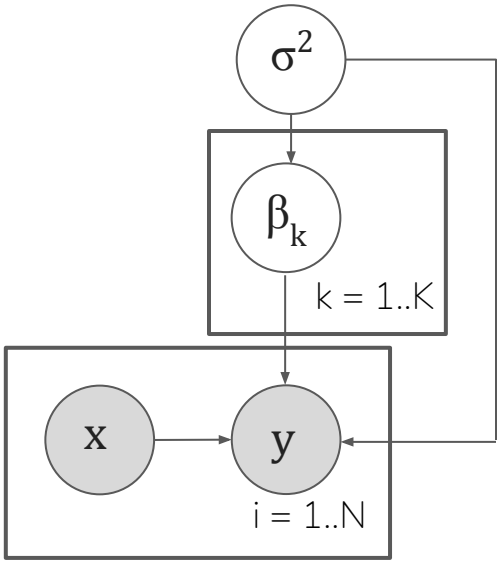
Programming languages which contain useful abstractions and functions for defining generative models and performing inference in them

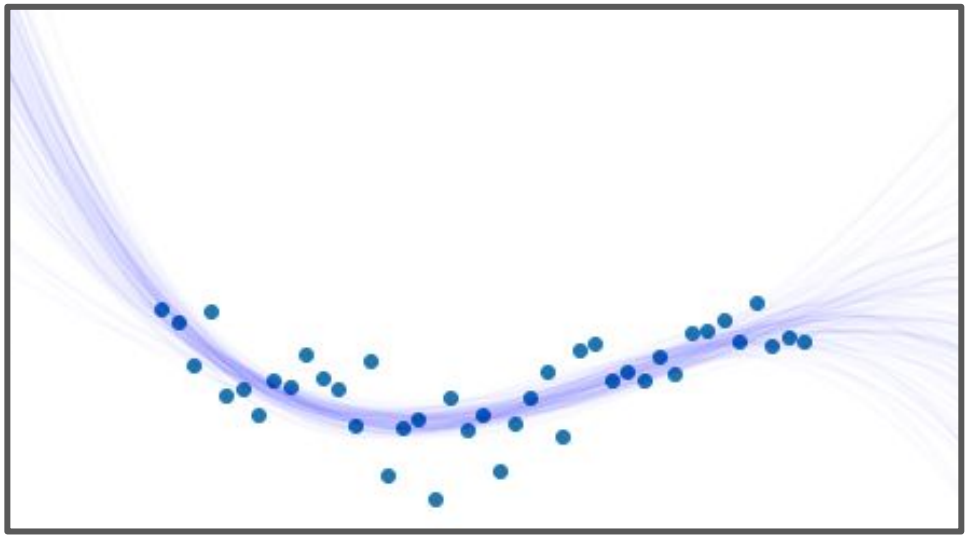
PPL	Strengths
Stan (Carpenter, Gelman et al.)	Optimised for graphical models
+ Edward (Tran, Blei et al.)	+ Deep generative models, SVI
WebPPL (Goodman & Stuhlmüller)	Universal (dynamic computation graph)
+ Pyro (Bingham, Goodman et al.)	+ Deep generative models, SVI
Gen (Cusumano-Towner & Mansinghka)	Programmable Inference

Learn ourselves Pyro - This Thursday @ 2:30pm, 46-5165

Exercises: Bayesian polynomial regression

$y \sim \text{Normal}(\beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3, \ \sigma^2)$

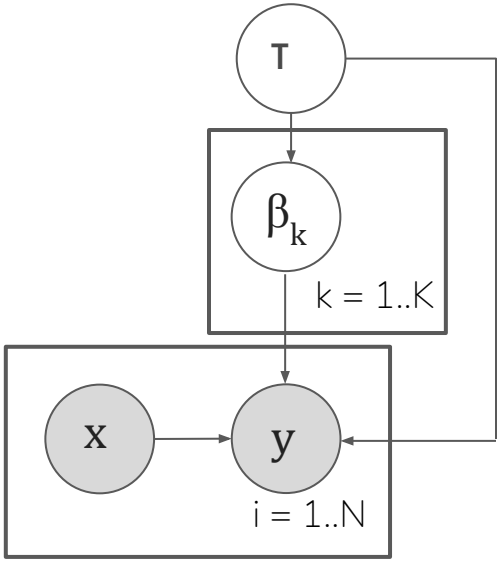




Inference exercises

1. Metropolis Hasting sampler
2. ‘Classical’ Variational Inference
3. Stochastic Gradient Variational Bayes

Defining the model

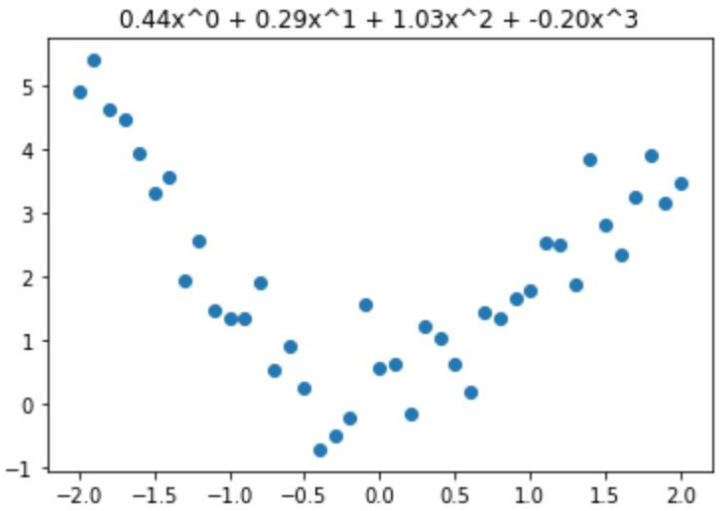


Fix prior parameters a_0, b_0, μ_0.

$\tau \sim \text{Gamma}(a_0, b_0) \quad \rightarrow \sigma^2 = 1/\tau$

$\beta_k \sim \text{Normal}(\mu_0, 1/\tau)$

$y \sim \text{Normal}(\beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3, \quad 1/\tau)$



Exact inference

For details see: https://en.wikipedia.org/wiki/Bayesian_linear_regression

Metropolis-Hastings (MH)

1 Initialize z^0
2 for s = 0, 1, 2, ... do
3 Define $z = z^s$
4 Sample $z' \sim q(z'|z)$
5 Compute acceptance ratio:

$$r = \frac{\hat{p}(z', x)q(z|z')}{\hat{p}(z, x)q(z'|z)}$$

6 Compute a = min(1, r)
7 Sample u ~ U(0, 1)
8 Set new sample to:

$$z^{s+1} = \begin{cases} z' \text{ if } u < a & \leftarrow \text{Accept} \\ z^s \text{ if } u >= a & \leftarrow \text{Reject} \end{cases}$$

1. `propose` samples z' and computes these probabilities:
   a. q(z' | z) and q(z | z')
   b. p(z') and p(z)

2. `propose` requires `transition_dist` q(z' | z)
   a. p(z) is already defined for you

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6 Compute $a = \min(1, r)$
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8 Set new sample to:

$$z^{s+1} = \begin{cases} z' \text{ if } u < a & \leftarrow \text{Accept} \\ z^s \text{ if } u >= a & \leftarrow \text{Reject} \end{cases}$$

3. `p(z', x)` needs to be calculated
   a. p(z', x) = p(z')p(x | z)
   b. E.g., p(z, x)
4. Combine outputs of `propose` and unnormalized posteriors to calculate acceptance ratio
5. Apply Metropolis-Hastings to accept or reject the sample

6. Do inference!

Classic Variational Inference

1. Write out the mean-field approximation
2. Derive the evidence lower bound (ELBO)
3. Derive analytical latent variable updates by either:
    a. Directly optimizing the ELBO
    b. Through the calculus of variations
4. Iterate updating each latent variable

Classic Variational Inference

1. Write out the mean-field approximation

Model P

$\tau \sim \text{Gamma}(a_0, b_0) \quad \rightarrow \sigma^2 = 1/\tau$

$\beta_k \sim \text{Normal}(\mu_0, 1/\tau)$

$y \sim \text{Normal}(\beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3, \quad 1/\tau)$

Variational Posterior Q

$Q(\tau, \beta) = Q(\tau) \prod^K Q(\beta_k)$

$\tau \sim \text{Gamma}(a, b)$

$\beta_k \sim \text{Normal}(\nu_k, 1/\omega_k)$

Classic Variational Inference

2. Derive the evidence lower bound (ELBO)

$$\log P(x) \geq \mathop{\mathbb{E}}_{\tau \sim Q} \left[\log P(\tau) - \log Q(\tau) \right] + \sum_{k=1}^{K} \mathop{\mathbb{E}}_{\tau, \beta_k \sim Q} \left[\log P(\beta_k | \tau) - \log Q(\beta_k | \tau) \right] + \sum_{i=1}^{N} \mathop{\mathbb{E}}_{\tau, \beta \sim Q} \left[\log P(y_i | \beta, x_i, \tau) \right]$$

Classic Variational Inference

2. Derive the evidence lower bound (ELBO)

To compute the first term:

$$\mathop{\mathbb{E}}_{\tau \sim Q}\left[\log P(\tau) - \log Q(\tau)\right] = -D_{KL}(Q_\tau || P_\tau)$$

Gamma distribution

Classic Variational Inference

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$$\mathop{\mathbb{E}}_{\tau \sim Q}\left[\log P(\tau) - \log Q(\tau)\right] = -D_{KL}(Q_\tau || P_\tau)$$

Gamma distribution

$$= (a_0 - a)\Psi(a) + \log\Gamma(a) - \log\Gamma(a_0)$$

$$- a_0(\log(b) - \log(b_0) - a(\frac{b_0 - b}{b})$$

Classic Variational Inference

2. Derive the evidence lower bound (ELBO)

To compute the second term:

$$\mathop{\mathbb{E}}_{\beta,\tau\sim Q}\left[\log P(\beta_k) - \log Q(\beta_k)\right] = \mathop{\mathbb{E}}_{\tau\sim Q}\left[-D_{KL}(Q_{\beta_k|\tau}||P_{\beta_k|\tau})\right]$$

Gamma distribution

Normal distribution

Classic Variational Inference

2. Derive the evidence lower bound (ELBO)

To compute the second term:

$$\mathop{\mathbb{E}}_{\beta,\tau\sim Q}\left[\log P(\beta_k) - \log Q(\beta_k)\right] = \mathop{\mathbb{E}}_{\tau\sim Q}\left[-D_{KL}(Q_{\beta_k|\tau}||P_{\beta_k|\tau})\right]$$

$$= -\frac{1}{2}\Big[\frac{a(\nu_k-\mu_0)^2}{b} + (\frac{a}{\omega_k b} - 1 - \Psi(a) + \log(b) + \log(\omega_k))\Big]$$

Gamma distribution

Normal distribution

Classic Variational Inference

2. Derive the evidence lower bound (ELBO)

We won't compute the third term today, it has long (but manageable) integrals.

$$
\begin{aligned}
\mathop{\mathbb{E}}_{\tau,\beta\sim Q}\left[\log P(y_i|\beta,x_i,\tau)\right] &= \mathop{\mathbb{E}}_{\tau\sim Q}\left[\mathop{\mathbb{E}}_{\beta\sim Q}\left(\log P(y_i|\beta,x_i,\tau)\right)\right] \\
&= \mathop{\mathbb{E}}_{\tau\sim Q}\Bigg[\frac{1}{2}(\log(\tau)-\log(2\pi)) - \frac{y_i^2\tau}{2} + y_i\tau\sum_{k=0}^{K}x_{ik}\nu_k \\
&\quad - \frac{\tau}{2}\Big[\sum_{k=0}^{K}x_{ik}^2\Big(\frac{1}{\omega_k}+\nu_k^2\Big) + 2\sum_{k=0}^{K}\sum_{j=0}^{k-1}x_{ik}x_{ij}\nu_k\nu_j\Big]\Bigg] \\
&= \frac{1}{2}(\Psi(a)-\log(b)-\log(2\pi)) - \frac{y_i^2 a}{2b} + \frac{y_i a}{b}\sum_{k=0}^{K}x_{ik}\nu_k \\
&\quad - \frac{a}{2b}\Big[\sum_{k=0}^{K}x_{ik}^2\Big(\frac{1}{\omega_k}+\nu_k^2\Big) + 2\sum_{k=0}^{K}\sum_{j=0}^{k-1}x_{ik}x_{ij}\nu_k\nu_j\Big]
\end{aligned}
$$

Classic Variational inference

3. Derive analytical latent variable updates by:
    a. Directly optimizing the ELBO

Take the partial derivatives of the ELBO with respect to $\boldsymbol{\nu}_k$ and $\boldsymbol{\omega}_k$ to derive each of their updates. (Remember to sum over N and K in deriving the entire ELBO!)

This will not lead to closed form solutions for a and b, though.

Classic Variational inference

3. Derive analytical latent variable updates by:
    b. Through the calculus of variations (we won't do this today)

$$Q(\tau) \propto \exp\left(\mathop{\mathbb{E}}_{\beta \sim Q} \left[\log P(\tau, \beta, y, x) \right] \right)$$

$$\log Q(\tau) = \mathop{\mathbb{E}}_{\beta \sim Q} \left[\log(P(\tau)) + \log(P(\beta|\tau)) \log(P(y|\beta, \tau, x)) \right] + Const.$$

Doing these expectations and folding anything constant with respect to τ into Const. eventually gets you to an expression with the form:

$$\log Q(\tau) = f_1(\nu, \omega, y, x) \log(\tau) - f_2(\nu, \omega, y, x)\tau + Const.$$

This is log of a Gamma distribution with a = f_1 & b = f_2, which are the updates.

Classic Variational inference

4. Enter your iterative updates and do inference!

Stochastic Gradient Variational Bayes

The ELBO is: $\underset{\substack{z\sim q(z)\\ \mu\sim q(\mu)}}{E}\left[\log \mathbf{p(\tau, \beta, y \mid x)} - \log q(\tau)q(\beta)\right]$

For each SGD iteration, we need a unbiased (monte-carlo) estimate of the ELBO, so:

1. Sample (τ, β) from q
   - Note: use *dist.rsample()* for a 'reparametrized' (differentiable) sample
2. Evaluate the term inside the expectation
3. Repeat until convergence!