Machine Learning

Stochastic Approximative Inference

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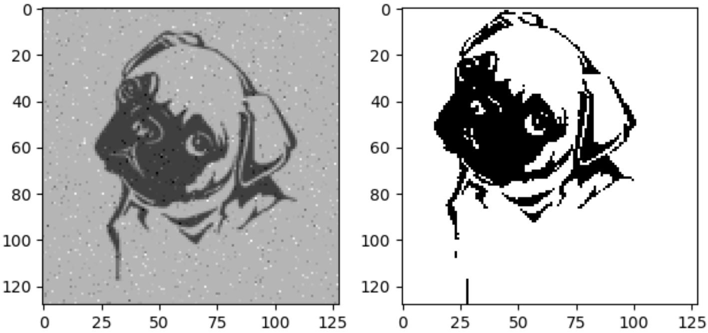
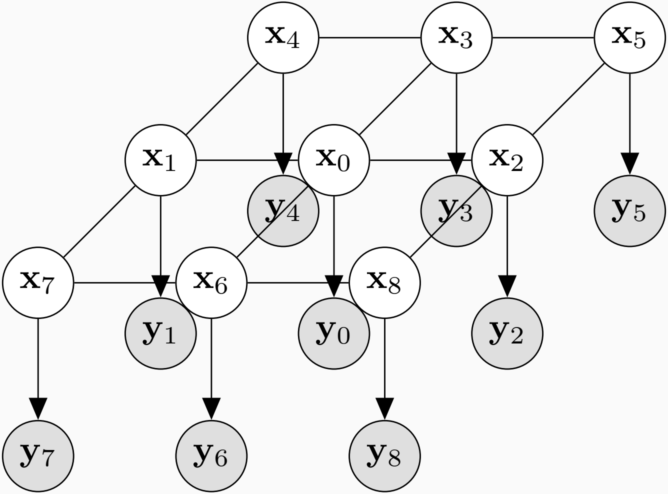
Introduction

Coursework II



Coursework II



Posterior: Markov Random Field

- Posterior

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- $\mathbf{x}_i$ is a specific binary image


3G
9:42 AM
SMS
Text
26
Calendar
Photos
Camera
YouTube
Stocks
Maps
Clock
Calculator
Weather
Notes
Settings
iTunes
App Store
Remote
Remote
Phone
Mail
Safari
iPod

Number of terms I

2290593203500326442498254071102
8779924646158308390547680551234
5054431338510774037915738775865
8057318635099533562444284837656
6408900340661545734126916095393
4651531316272895970961099648619
5486636741656944283948869330648
4701733713508133208092688099524
0707971539803921050200955733579
43662055566676730638553849508752
9677470990968153918788613785751
3890052212385415364000233552517

Number of terms II

9230941551480812783648467474496
15787812522261713953420063416790
7552057630497077601674681891226
1453204962575441115371836944715
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6507334054019330445298798029650
8746618030728963410359112463410
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7461331023628146001054998291892
8850448033966038407878196527044
7157474368533868315778800203562
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Number of terms III

8982409725023084881200238736500

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8476965948928382396693052519124

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2837023543516588536916371046489

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8926097153382729134531621865313

9786085815417055159827515344471

3326325034781836776513703100360

9793889758575377908303501066776

6548311999605347475370343426743

Number of terms IV

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8900202322285082544979530967870

6304437009833849217731493021674

2550624871750833859476679189509

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1524092173016464047938013691439

6671843203605981118777513627755

7250792266837423597968228683403

4089138475154767372727122932222

8878852083218796660305975797728

8778298768646815994259957325408

Number of terms V

8749600987758158350339985951647
5121708697580746029473842801833
8592485796034133919973077413533
6869491956368516611377674237208
1780419191068702807890339161440
9912666138730775266005780452422
5302437317858452782485229505751
3761093944464722805553911771716
4315059230286413698788578331540
1782239495790781650110059887274
5959467831004471989549305375741
9073809906471822251882514747849
0657161167548497523333968812279

Number of terms VI

4911475119965635459462447339289
7828672753085721621023943443062
0144907278084466853892944205719
8697060107876495003418069047901
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6461274039931292984401423199725
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3508530232037816302115328138866
8643014293963947674718567131663
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2361702749907044372801683830358
6991365299464326205642839343150

Number of terms VII

4053504888101754720253838078891

9253939272110382634932825138554

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3474751813846542682825520838131

0069117625217360239526199430454

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5778664863093617634553900426210

Number of terms VIII

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6543122517479114466613670208736
0842313671545657762822696089905
6802168279902278674508669673834
7816102210900054189076993778672
7705964820658607375143364171301
1744511704016132334906338900377
1777472580944833242545989973822

Number of terms IX

5646744609738390155521757096422

2619375692340966923479020630115

9076383049447801135255878205328

2752643299087648267991015324907

4963538068771014944040060242262

3804497742682401904233153226013

9373317250133351983527123955504

2292211010517136771541981666250

0131430427440349387764312765762

4870317305687566284108475166000

1324414350620739304183073837766

8972502903711649967733818943578

9237255328232566165426546313829 1135999395862937 6

Numbers

- Possible black and white 3 Megapixel images

$$2^{3145728}$$

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$$4.35 \cdot 10^{17} \approx 2^{59}$$

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$$4.35 \cdot 10^{17} \approx 2^{59}$$

- *Lets agree that this for loop is intractable*

$$\hat{\boldsymbol{\theta}} = \mathrm{argmax}_{\theta} p(\mathcal{D}|\boldsymbol{\theta})$$

MCMC Man

Bio

- Takes his time
- Works on his own and is hard to understand
- Will in the limit always catch the right guy
- Works a lot of cold cases

"To catch the right guy we need to consider every avenue, every possibility"

Variational Bayes Woman

Bio

- Gets the job done
- Reports to central command
- Believes smoke implies fire
- Sometimes catches the wrong guy

"Shoot first, ask questions later"

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    - Iterative Conditional Modes (ICM)
    - Markov Chain Monte Carlo, Gibbs Sampler

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        - derivation tomorrow lecture 2

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    - derivation tomorrow lecture 2
- Extra [Kingma and Welling, 2014]
  - Amortised Inference in tensorflow

Coursework

- Availible on GitHub
- 10 Questions
- Deadline Friday 7th of December 12:00
  - extended one week from previous date
- Groups of two submits report

Laplace Approximation

Analytical Intractability

$$\log\, p(\mathbf{w}|\mathbf{t}) = \log\left(\prod_i^N \sigma(\mathbf{w}^{\mathrm{T}}\mathbf{x}_i)^{t_i} \cdot (1-\sigma(\mathbf{w}^{\mathrm{T}}\mathbf{x}_i))^{1-t_i}\right) - \frac{1}{2}(\mathbf{w}-\mathbf{m}_0)^{\mathrm{T}}\mathbf{S}_0^{-1}(\mathbf{w}-\mathbf{m}_0) - \log(Z)$$

- Sometimes conjugacy does not make sense
- The prior and the likelihood makes sense by themselves
- Classification is the typical example

Laplace Approximation

$$p(z) = \frac{1}{Z} f(z) = \frac{f(z)}{\int f(z) dz}$$

- $p(z)$ is unknown as we cannot compute Z
- $f(z)$ is possible to compute if we have likelihood and prior

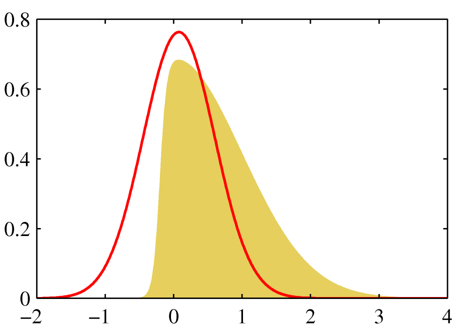
$$f(z) = p(x|z)p(z)$$

Laplace Approximation

$$\log\, p(z) = \log\, (\frac{1}{Z} f(z)) = \log(f(z)) + \text{const w.r.t. } z$$

- $p(z)$ and $f(z)$ will have the same modes
- Idea: we can approximate each mode with a distribution we can normalise

Laplace Approximation Ch. 4.4 [Bishop, 2006]



- Find the mode of the posterior
- Fit Gaussian to this mode

Taylor Expansion

$$f(x) = f(x_0) + \frac{\partial}{\partial x} f(x_0)(x - x_0) + \frac{1}{2}\frac{\partial^2}{\partial x^2} f(x_0)(x - x_0)^2 + \mathcal{O}((x - x0)^3)$$

- A Taylor expansion is an approximation of a function around a specific value
- If we expand around a maxima x_0

$$\frac{\partial}{\partial x} f(x_0) = 0$$

- This leads to

$$f(x) = f(x_0) - \frac{1}{2}\left|\frac{\partial^2}{\partial x^2} f(x_0)\right|(x - x_0)^2 + \mathcal{O}((x - x0)^3)$$

Laplace Approximation

1. Find mode of $p(z)$

$$\frac{\partial}{\partial z} p(z_0) = \frac{\partial}{\partial z} f(z_0) = 0$$

2. Make Taylor Expansion around mode

$$\log f(z) \approx \log f(z_0) - \frac{1}{2} \frac{\partial^2}{\partial^2} \log(f(z_0))(z - z_0)^2$$

3. Take exponential to get function

$$f(z) \approx f(z_0) e^{-\frac{1}{2} \underbrace{\frac{\partial^2}{\partial^2} \log(f(z_0))}_{A} (z-z_0)^2} = f(z_0) e^{-\frac{1}{2} A (z-z_0)^2}$$

Laplace Approximation

$$f(z) \approx f(z_0) e^{-\frac{1}{2}A(z-z_0)^2}$$

- we want to find an approximation, to $p(z)$ so we need to normalise to a distribution

$$p(z) = \frac{1}{Z} f(z) \approx q(z)$$

- assume that $q(z)$ is Gaussian, i.e. $f(z_0) = p(\text{mean})$

$$q(z) = \left(\frac{A}{2\pi}\right)^{\frac{1}{2}} e^{-\frac{A}{2}(z-z_0)^2}$$

Laplace Approximation

- Compute a mode of the posterior distribution, i.e MAP estimate

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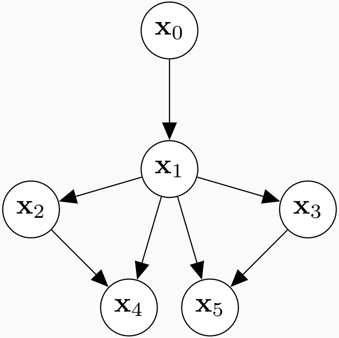
Laplace Approximation

- Compute a mode of the posterior distribution, i.e MAP estimate
- Perform Taylor expansion around mode to quadratic term
- Identify elements in expansion as parameters of a Gaussian
- Normalise to a distribution

Stochastic Approximative Inference

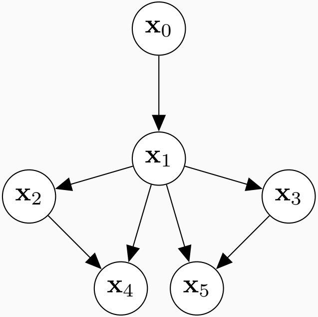
Cookbook

How to sample?



$$p(\mathbf{x}) = \prod_i p(x_i | \mathrm{pa}_i)$$

Ancestral Sampling

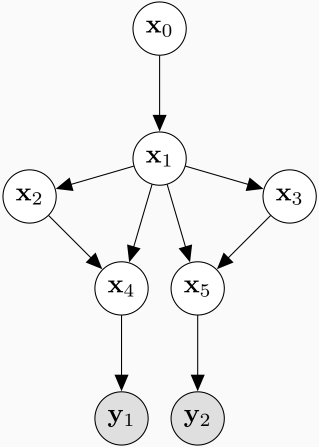


Sample from $p(\mathbf{x})$

1. pick top nodes and draw sample
2. fix the top nodes and sample from conditonals
3. arrive at sample from $\mathbf{x}$

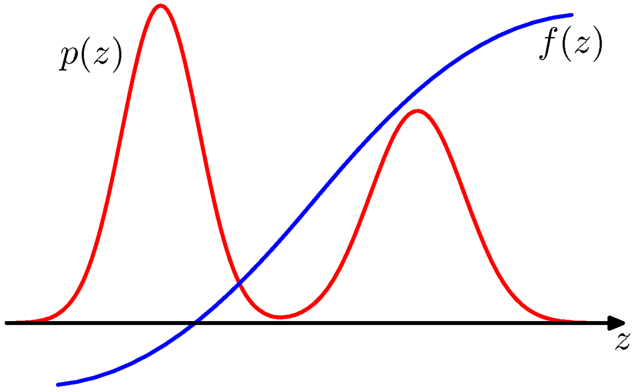
$$p(\mathbf{x}) = p(x_5|x_3, x_1)p(x_4|x_2, x_1)p(x_3|x_1)p(x_2|x_1)p(x_1|x_0)p(x_0)$$

Observed Data



Sample from $p(\mathbf{x}|\mathbf{y})$

1. Ancestral sampling for all latent variables
2. When latent variables child is observed
    - sample from conditional
    - if sample agrees with observation $\mathbf{x}$ comes from posterior
    - if not discard sample and restart



$$\mathbb{E}_{p(z)}[f] = \int f(z)p(z)\mathrm{d}z \approx \frac{1}{L}\sum_{l=1}^{L} f(z^{(l)})$$

$$\mathbf{z}^{(l)} \sim p(\mathbf{z})$$

Sampling

$$\hat{f} = \frac{1}{L}\sum_{l=1}^{L} f(z^{(l)})$$

$$z^{(l)} \sim p(z)$$

$$\mathbb{E}[\hat{f}] = \mathbb{E}[f]$$

$$\text{var}[\hat{f}] = \frac{1}{L}\mathbb{E}\left[(f(z) - \mathbb{E}[f])^2\right]$$

- Approximation not dependent on dimensionality of z
- Variance of estimator shrinks with number of samples

Basic Sampling Ch 11.1 [Bishop, 2006]

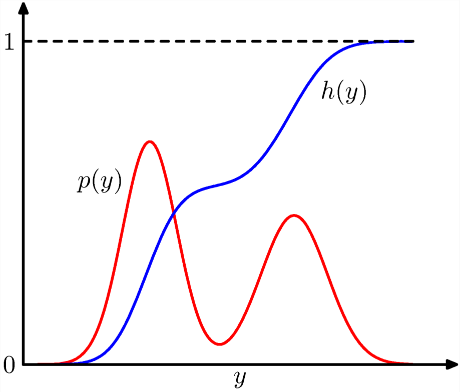
$$z^{(l)} \sim p(z)$$

- Lets assume that we can get uniformly random numbers $z \sim \text{Uniform}(0, 1)$
- A computer cannot, but lets assume it could
- Idea: can we transform this uniform distribution to something interesting
- If we could then we could use samples from z

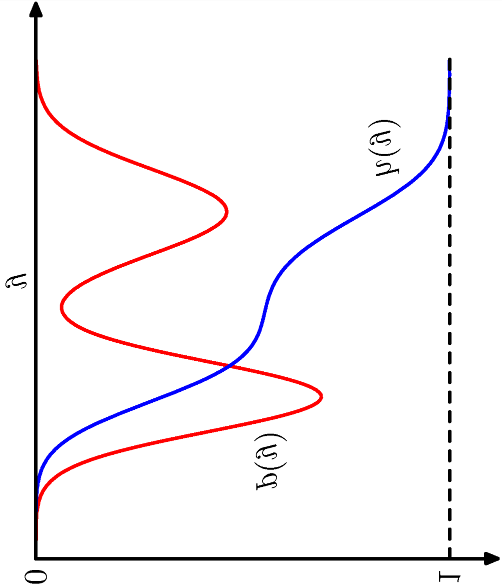
$$z \sim \text{Uniform}(0,1)$$

- We have access to a uniformly distributed variable z
- Change of variable
$$y = f(z)$$
- Idea: can we find $f(z)$ such that it induces $p(y)$ to be the distribution that we want?

Basic Probabilities

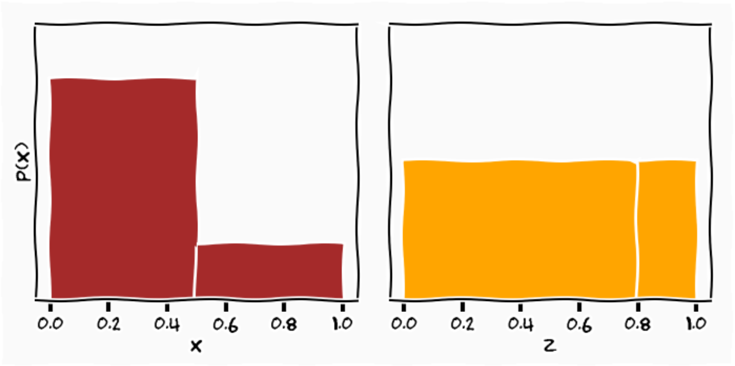


$$z = f^{-1}(y) = \int_{-\infty}^{y} p(y)\mathrm{d}y$$



y
$p(y)$
$h(y)$
0
1

Change of Variables



Sampling

- We know how to transform samples from uniform to any distribution we can formulate the cummulative distribution
- Can we sample from distrubitons we do not know the form of?

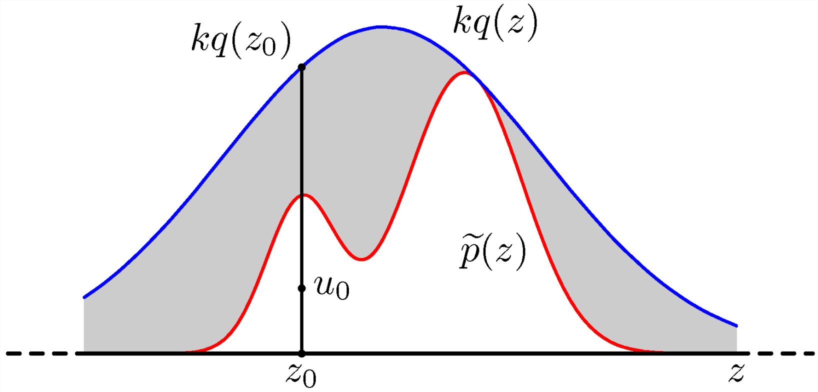
    1. Rejection Sampling
    2. Importance Sampling
    3. Markov Chain Monte Carlo

Rejection Sampling Ch 11.1.2 [Bishop, 2006]

$$p(\mathbf{z}) = \frac{1}{Z}\tilde{p}(\mathbf{z})$$

- $p(\mathbf{z})$ is a distribution of unknown form
- We can evaluate $\tilde{p}(\mathbf{z})$
- Can we draw samples from a simpler distribution and transform them?

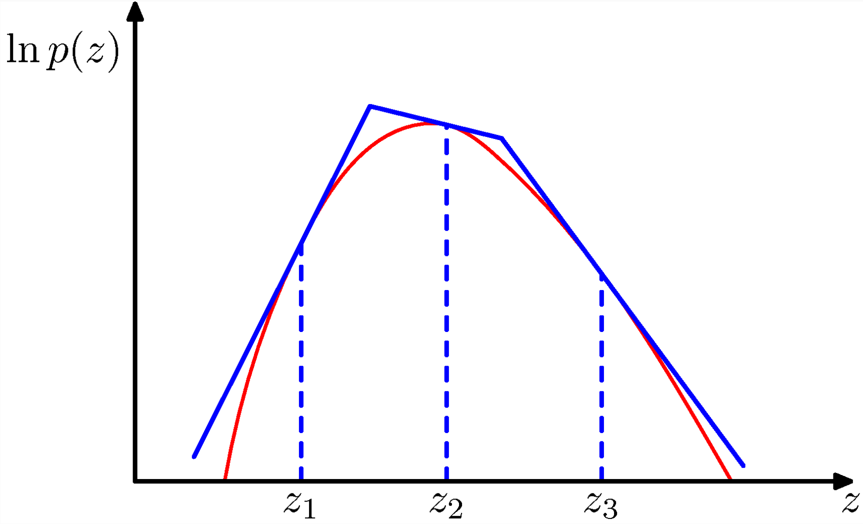
Rejection Sampling



Rejection Sampling

1. Pick approximate distribution $q(\mathbf{z})$
2. Pick constant k such that $k \cdot q(\mathbf{z}) \geq \tilde{p}(\mathbf{z})$
3. Pick random location $\mathbf{z}_0 \sim q(\mathbf{z})$
4. Pick random number $u_0 \sim \text{Uniform}(0, k \cdot q(\mathbf{z}_0))$
5. If $u_0 > \tilde{p}(\mathbf{z}_0)$ reject z_0 otherwise retain

Adaptive Rejection Sampling



Rejection Sampling

- Basic sampling allows us to draw samples from known distributions
- We can use these distributions as *proposal distributions*
- If bound is small we will get an efficient sampler
- Generally works well in few dimensions but do not scale
- We reject too many samples

Importance Sampling Ch 11.1.4 [Bishop, 2006]

$$\mathbb{E}_{p(\mathbf{z})}[f] = \int f(\mathbf{z})p(\mathbf{z})\mathrm{d}\mathbf{z}$$

Importance Sampling Ch 11.1.4 [Bishop, 2006]

$$\mathbb{E}_{p(\mathbf{z})}[f] = \int f(\mathbf{z})p(\mathbf{z})\mathrm{d}\mathbf{z} = \int f(\mathbf{z})p(\mathbf{z})\frac{q(\mathbf{z})}{q(\mathbf{z})}\mathrm{d}\mathbf{z}$$

Importance Sampling Ch 11.1.4 [Bishop, 2006]

$$
\begin{aligned}
\mathbb{E}_{p(\mathbf{z})}[f] &= \int f(\mathbf{z})p(\mathbf{z})\mathrm{d}\mathbf{z} = \int f(\mathbf{z})p(\mathbf{z})\frac{q(\mathbf{z})}{q(\mathbf{z})}\mathrm{d}\mathbf{z} \\
&= \int f(\mathbf{z})\frac{p(\mathbf{z})}{q(\mathbf{z})}q(\mathbf{z})\mathrm{d}\mathbf{z}
\end{aligned}
$$

Importance Sampling Ch 11.1.4 [Bishop, 2006]

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&= \int f(\mathbf{z})\frac{p(\mathbf{z})}{q(\mathbf{z})}q(\mathbf{z})\mathrm{d}\mathbf{z} = \mathbb{E}_{q(\mathbf{z})}\left[f(\mathbf{z})\frac{p(\mathbf{z})}{q(\mathbf{z})}\right]
\end{aligned}
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$$
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&\approx \frac{1}{L}\sum_{l=1}^{L} f(\mathbf{z}^{(l)})\frac{p(\mathbf{z}^{(l)})}{q(\mathbf{z}^{(l)})}
\end{aligned}
$$

Importance Sampling Ch 11.1.4 [Bishop, 2006]

$$
\begin{aligned}
\mathbb{E}_{p(\mathbf{z})}[f] &= \int f(\mathbf{z}) p(\mathbf{z}) \mathrm{d}\mathbf{z} = \int f(\mathbf{z}) p(\mathbf{z}) \frac{q(\mathbf{z})}{q(\mathbf{z})} \mathrm{d}\mathbf{z} \\
&= \int f(\mathbf{z}) \frac{p(\mathbf{z})}{q(\mathbf{z})} q(\mathbf{z}) \mathrm{d}\mathbf{z} = \mathbb{E}_{q(\mathbf{z})} \left[f(\mathbf{z}) \frac{p(\mathbf{z})}{q(\mathbf{z})} \right] \\
&\approx \frac{1}{L} \sum_{l=1}^{L} f(\mathbf{z}^{(l)}) \frac{p(\mathbf{z}^{(l)})}{q(\mathbf{z}^{(l)})} \\
&= \frac{1}{L} \sum_{l=1}^{L} r_l \cdot f(\mathbf{z}^{(l)})
\end{aligned}
$$

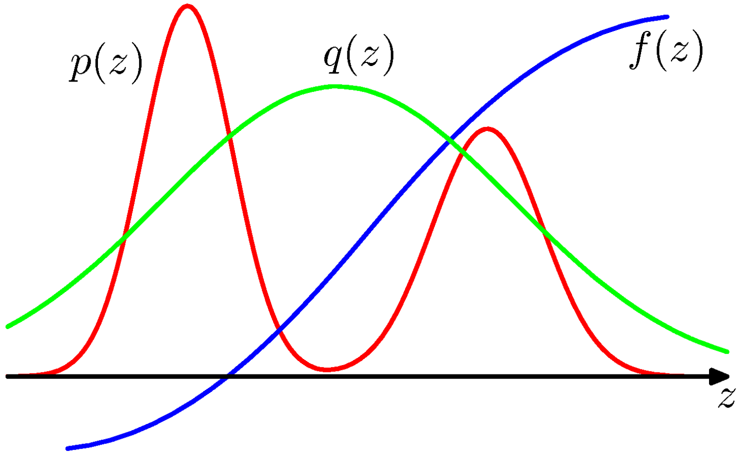
Importance Sampling

$$\mathbb{E}_{p(\mathbf{z})}[f] \approx \frac{1}{L}\sum_{l=1}^{L} r_l \cdot f(\mathbf{z}^{(l)})$$

$$\mathbf{z}^{(l)} \sim q(\mathbf{z}), \qquad r_l = \frac{p(\mathbf{z}^{(l)})}{q(\mathbf{z}^{(l)})}$$

- Directly approximate expectation
- Accepts all samples
- r_l corrects bias in sampling from wrong distribution

Importance Sampling



Importance Sampling

$$p(\mathbf{z}) = \frac{1}{Z_p}\tilde{p}(\mathbf{z}), \qquad\qquad q(\mathbf{z}) = \frac{1}{Z_q}\tilde{q}(\mathbf{z})$$

- Often it will not be possible to evaluate $p(\mathbf{z})$ and maybe not even $q(\mathbf{z})$

$$\mathbb{E}[f] = \frac{Z_q}{Z_p}\int f(\mathbf{z})\frac{\tilde{p}(\mathbf{z})}{\tilde{q}(\mathbf{z})}q(\mathbf{z})\mathrm{d}\mathbf{z} \approx \frac{Z_q}{Z_p}\frac{1}{L}\sum_{l=1}^{L}\tilde{r}_l \cdot f(\mathbf{z}^{(l)})$$

Importance Sampling

$$\frac{Z_p}{Z_q} = \frac{1}{Z_q} \int \tilde{p}(\mathbf{z}) \mathrm{d}\mathbf{z}$$

Importance Sampling

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Importance Sampling

$$
\begin{aligned}
\frac{Z_p}{Z_q} &= \frac{1}{Z_q}\int \tilde{p}(\mathbf{z})\mathrm{d}\mathbf{z} = \frac{1}{Z_q}\int \tilde{p}(\mathbf{z})\frac{q(\mathbf{z})}{q(\mathbf{z})}\mathrm{d}\mathbf{z} \\
&= \frac{1}{Z_q}\int \tilde{p}(\mathbf{z})\frac{q(\mathbf{z})}{\frac{1}{Z_q}\tilde{q}(\mathbf{z})}\mathrm{d}\mathbf{z}
\end{aligned}
$$

Importance Sampling

$$
\begin{aligned}
\frac{Z_p}{Z_q} &= \frac{1}{Z_q}\int \tilde{p}(\mathbf{z})\mathrm{d}\mathbf{z} = \frac{1}{Z_q}\int \tilde{p}(\mathbf{z})\frac{q(\mathbf{z})}{q(\mathbf{z})}\mathrm{d}\mathbf{z} \\
&= \frac{1}{Z_q}\int \tilde{p}(\mathbf{z})\frac{q(\mathbf{z})}{\frac{1}{Z_q}\tilde{q}(\mathbf{z})}\mathrm{d}\mathbf{z} = \int \frac{\tilde{p}(\mathbf{z})}{\tilde{q}(\mathbf{z})}q(\mathbf{z})\mathrm{d}\mathbf{z}
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&\approx \frac{1}{L}\sum_{l=1}^{L}\frac{\tilde{p}(\mathbf{z}^{(l)})}{\tilde{q}(\mathbf{z}^{(l)})} = \frac{1}{L}\sum_{l=1}^{L} r_l
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\end{aligned}
$$

- Not very surprising can we take the average ratio between the unormalised functions to get the normalisers
- We can use the same samples

Importance Sampling

$$\mathbb{E}[f] \approx \frac{Z_q}{Z_p} \frac{1}{L} \sum_{l=1}^{L} r_l f(\mathbf{z}^{(l)})$$

Importance Sampling

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$$= \sum_{l=1}^{L} \frac{r_l}{\sum_{k=1}^{L} r_k} f(\mathbf{z}^{(l)}) = \sum_{l=1}^{L} w_l f(\mathbf{z}^{(l)})$$

Importance Sampling

- More efficient compared to Rejection sampling as it uses all samples
- Hard to know how well you are doing
- We want to make sure that the importance weights are of small variance
  - $q(\mathbf{z})$ should not be small where $p(\mathbf{z})$ is large
- Will work wonders if $q(\mathbf{z})$ is good

Markov Chain Monte Carlo

Markov Chain Monte Carlo Ch 11.2 [Bishop, 2006]

- Sample from a proposal distribution
- Remembers the state and samples from a conditional
- Can lead to much better exploration of the space

Metropolis Sampling

1. start with state $\mathbf{z}^{(0)}$

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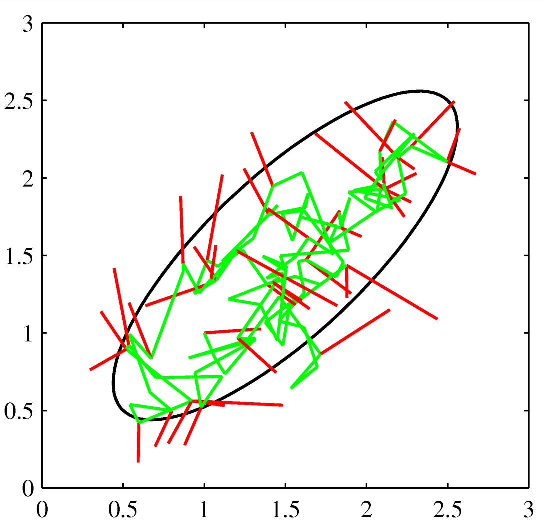
   - otherwise reject $\mathbf{z}^*$ and start over

Metropolis Gaussian



Gibbs Sampling Ch 11.3 [Bishop, 2006]

- Often 1D samples are easy to get
- Gibbs sampling exploits this to create a very simple Markov Chain
- Sample each variable in turn conditioned on the others and cycle through
- Each variable depends only on its Markov blanket so conditionals can be very simple

Gibbs Sampling

1. Initialise $\mathbf{z}^{(0)}$

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$$z_i^{(1)} \sim p(z_i|\mathbf{z}_{\neg i})$$

Gibbs Sampling

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3. Formulate posterior $p(z_i|\mathbf{z}_{\neg i})$
4. Sample from posterior

$$z_i^{(1)} \sim p(z_i|\mathbf{z}_{\neg i})$$

5. cycle through variables

Why is this easier?

Multivariate case

$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{y}, \mathbf{x})}{p(\mathbf{y})}$$
$$p(\mathbf{y}) = \sum_i p(\mathbf{y}|\mathbf{x}^{(i)})p(\mathbf{x}^{(i)})$$

Why is this easier?

Multivariate case

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1D case

$$p(x_i|\mathbf{x}_{\neg i},\mathbf{y}) = \frac{p(\mathbf{x},\mathbf{y})}{p(\mathbf{x}_{\neg i},\mathbf{y})}$$

Why is this easier?

Multivariate case

$$p(\mathbf{x}|\mathbf{y}) = \frac{p(\mathbf{y}, \mathbf{x})}{p(\mathbf{y})}$$

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1D case

$$p(x_i|\mathbf{x}_{\neg i}, \mathbf{y}) = \frac{p(\mathbf{x}, \mathbf{y})}{p(\mathbf{x}_{\neg i}, \mathbf{y})}$$

$$p(\mathbf{x}_{\neg i}, \mathbf{y}) = \int p(\mathbf{x}, \mathbf{y})\mathrm{d}x_i = \sum_{x_i \in [1, -1]} p(x_i, \mathbf{x}_{\neg i}, \mathbf{y})$$

$$= p(x_i = 1, \mathbf{x}_{\neg i}, \mathbf{y}) + p(x_i = -1, \mathbf{x}_{\neg i}, \mathbf{y})$$

Summary

Summary

- Using sampling we can approximate tricky integrals by computing samples from distributions we do not know
- Sampling is a bit of a black-art
- Often exact given infinite time
- Generally works but often time consuming

eof

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