Advanced Machine Learning
Summer 2019

Part 12 – Approximate Inference I
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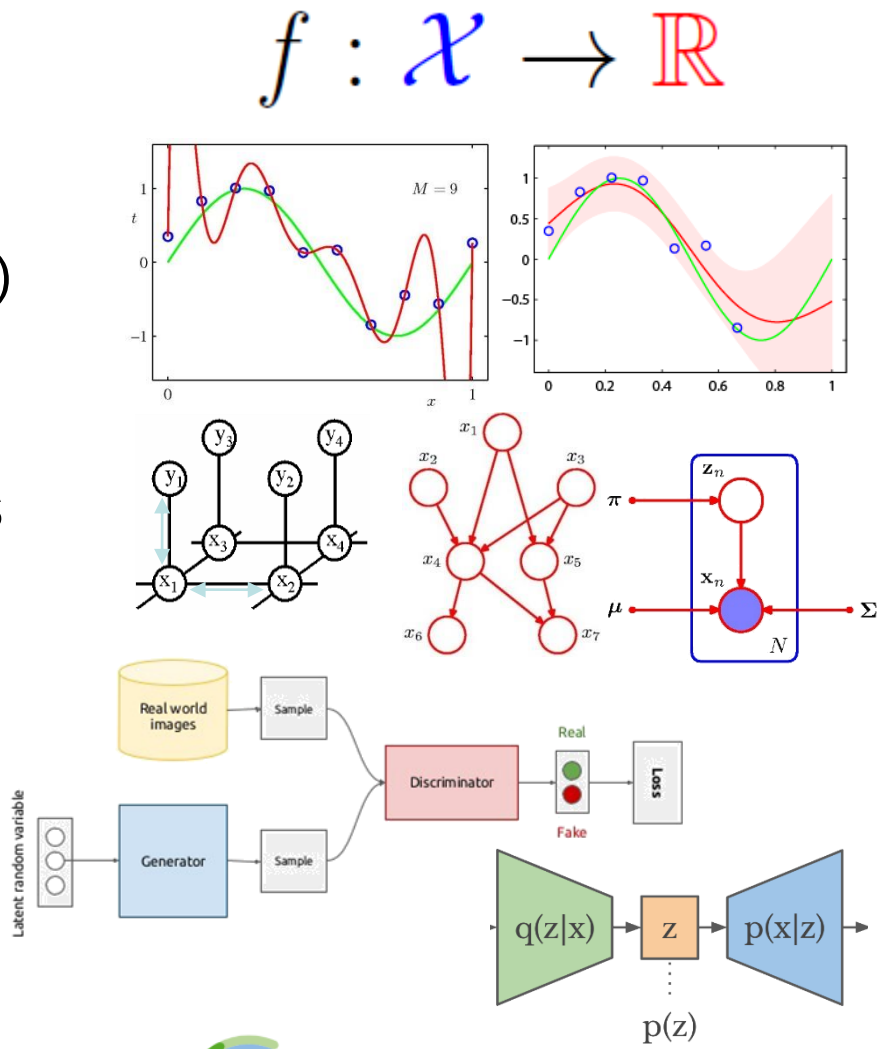
Prof. Dr. Bastian Leibe

RWTH Aachen University, Computer Vision Group
http://www.vision.rwth-aachen.de

Visual Computing Institute | RWTH AACHEN UNIVERSITY

Course Outline

- Regression Techniques
  - Linear Regression
  - Regularization (Ridge, Lasso)
  - Kernels (Kernel Ridge Regression)
- Deep Reinforcement Learning
- Probabilistic Graphical Models
  - Bayesian Networks
  - Markov Random Fields
  - Inference (exact & approximate)
- Deep Generative Models
  - Generative Adversarial Networks
  - Variational Autoencoders



Topics of This Lecture

- Approximate Inference
  - Variational methods
  - Sampling approaches
- Sampling approaches
  - Sampling from a distribution
  - Ancestral Sampling
  - Rejection Sampling
  - Importance Sampling
- Markov Chain Monte Carlo
  - Markov Chains
  - Metropolis Algorithm
  - Metropolis-Hastings Algorithm
  - Gibbs Sampling

Approximate Inference

- Exact Bayesian inference is often intractable.
  - Often infeasible to evaluate the posterior distribution or to compute expectations w.r.t. the distribution.
    - E.g. because the dimensionality of the latent space is too high.
    - Or because the posterior distribution has a too complex form.
  - Problems with continuous variables
    - Required integrations may not have closed-form solutions.
  - Problems with discrete variables
    - Marginalization involves summing over all possible configurations of the hidden variables.
    - There may be exponentially many such states.

$\Rightarrow$ We need to resort to approximation schemes.

Two Classes of Approximation Schemes

- Deterministic approximations (Variational methods)
  - Based on analytical approximations to the posterior distribution
    - E.g. by assuming that it factorizes in a certain form
    - Or that it has a certain parametric form (e.g., a Gaussian).

  $\Rightarrow$ Can never generate exact results, but are often scalable to large applications.

- Stochastic approximations (Sampling methods)
  - Given infinite computationally resources, they can generate exact results.
  - Approximation arises from the use of a finite amount of processor time.

  $\Rightarrow$ Enable the use of Bayesian techniques across many domains.

  $\Rightarrow$ But: computationally demanding, often limited to small-scale problems.

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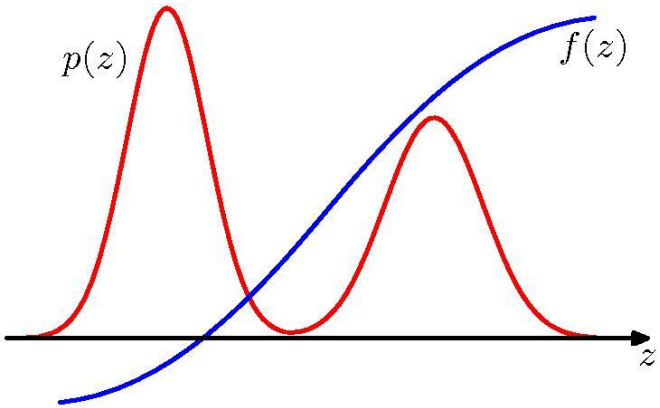
Sampling Idea

- Objective:
  - Evaluate expectation of a function $f(\mathbf{z})$ w.r.t. a probability distribution $p(\mathbf{z})$.

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



- Sampling idea
  - Draw L independent samples $\mathbf{z}^{(l)}$ with l = 1,…,L from $p(\mathbf{z})$.
  - This allows the expectation to be approximated by a finite sum

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

  - As long as the samples $\mathbf{z}^{(l)}$ are drawn independently from $p(\mathbf{z})$, then

$\Rightarrow$ Unbiased estimate, independent of the dimension of $\mathbf{z}$!

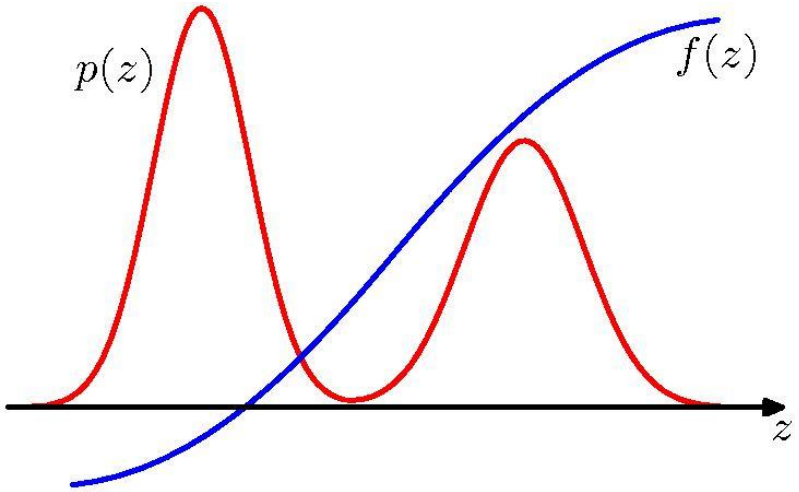
$$\mathbb{E}[\hat{f}] = \mathbb{E}[f]$$

Image source: C.M. Bishop, 2006

Sampling – Challenges

- Problem 1: Samples might not be independent

  ⇒ Effective sample size might be much smaller than apparent sample size.



- Problem 2:
  - If f(z) is small in regions where p(z) is large and vice versa, the expectation may be dominated by regions of small probability.

  ⇒ Large sample sizes necessary to achieve sufficient accuracy.

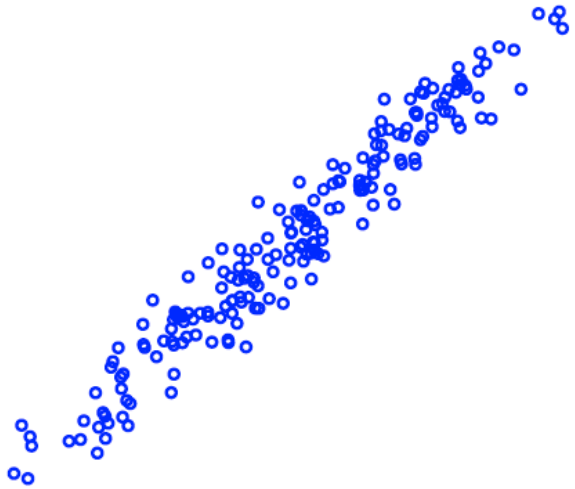
Image source: C.M. Bishop, 2006

Parametric Density Model

- Example:
  - A simple multivariate (d-dimensional) Gaussian model

$$p(\mathbf{x}|\boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{D/2}|\boldsymbol{\Sigma}|^{1/2}} \exp\left\{-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu})^{\mathrm{T}}\boldsymbol{\Sigma}^{-1}(\mathbf{x}-\boldsymbol{\mu})\right\}$$

  - This is a “generative” model in the sense that we can generate samples $\mathbf{x}$ according to the distribution.



Sampling from a Gaussian

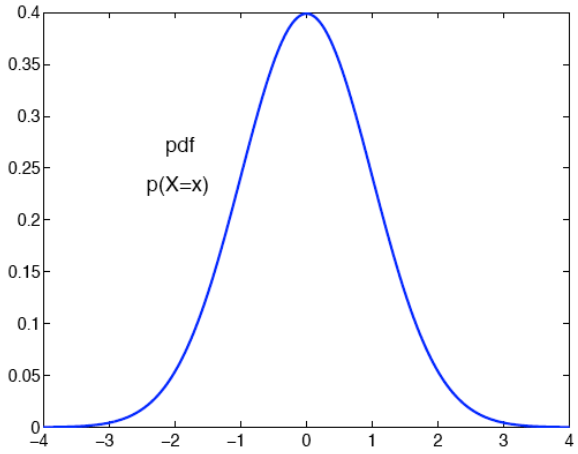
- Given:
  - 1-dim. Gaussian pdf $p(\mathbf{x}|\mu,\sigma^2)$ and the corresponding cumulative distribution:

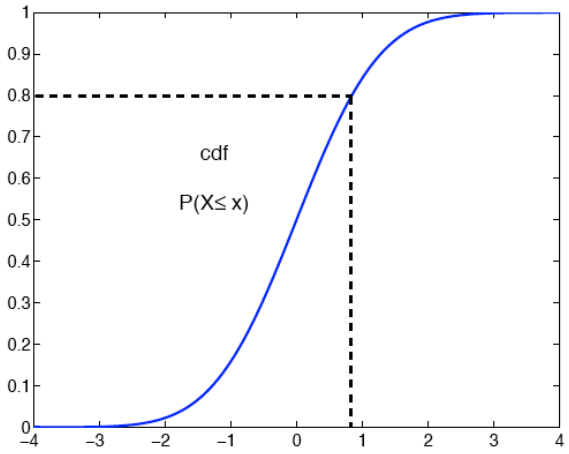
$$F_{\mu,\sigma^2}(x) = \int_{-\infty}^{x} p(x|\mu,\sigma^2)dx$$

  - To draw samples from a Gaussian, we can invert the cumulative distribution function:

$$u \sim Uniform(0,1) \Rightarrow F^{-1}_{\mu,\sigma^2}(u) \sim p(x|\mu,\sigma^2)$$

$p(x|\mu,\sigma^2)$





$F_{\mu,\sigma^2}(x)$

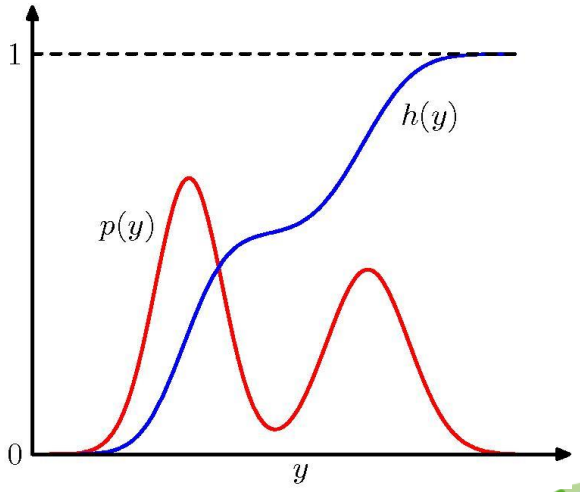
Sampling from a pdf (Transformation method)

- In general, assume we are given the pdf $p(\mathbf{x})$ and the corresponding cumulative distribution:

$$F(x) = \int_{-\infty}^{x} p(z)dz$$

  - To draw samples from this pdf, we can invert the cumulative distribution function:

$$u \sim Uniform(0,1) \Rightarrow F^{-1}(u) \sim p(x)$$

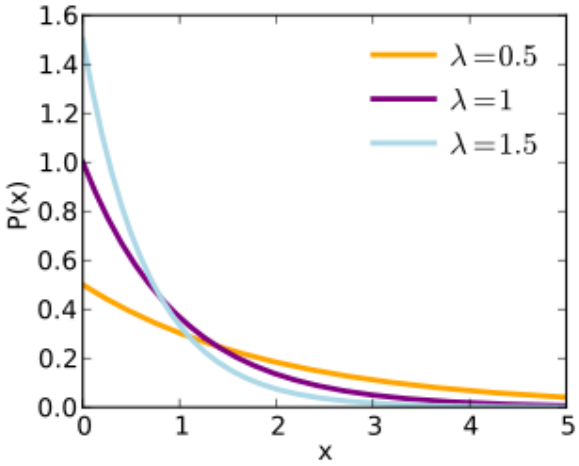


Example 1: Sampling from Exponential Distrib.

- Exponential Distribution

$$p(y) = \lambda \exp(-\lambda y)$$

where $0 \leq y < \infty$.



- Transformation sampling
  - Indefinite Integral $h(y) = 1 - \exp(-\lambda y)$
  - Inverse function

$$y = h(y)^{-1} = -\lambda^{-1} \ln(1 - z)$$

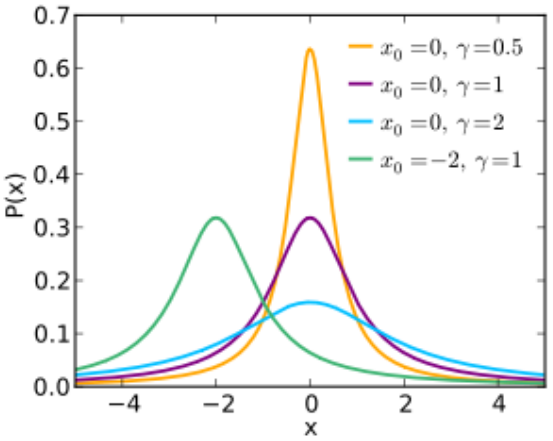
for a uniformly distributed input variable z.

Image source: Wikipedia

Example 2: Sampling from Cauchy Distrib.

- Cauchy Distribution

$$p(y) = \frac{1}{\pi}\frac{1}{1+y^2}$$



- Transformation sampling
  - Inverse of integral can be expressed as a $\tan$ function.

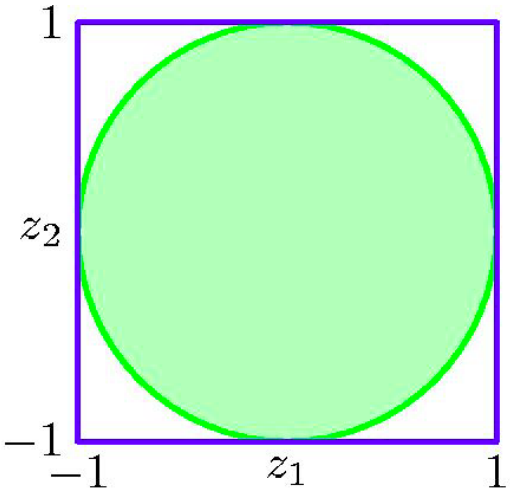
$$y = h(y)^{-1} = \tan(z)$$

for a uniformly distributed input variable z.

Image source: Wikipedia

Note: Efficient Sampling from a Gaussian

- Problem with transformation method
  - Integral over Gaussian cannot be expressed in analytical form.
  - Standard transformation approach is very inefficient.



- More efficient: Box-Muller Algorithm
  - Generate pairs of uniformly distributed random numbers $z_1, z_2 \in$ (-1,1).
  - Discard each pair unless it satisfies $r^2 = z_1^2 + z_2^2 \leq 1$
  - This leads to a uniform distribution of points inside the unit circle with $p(z_1, z_2) = 1/\pi$.

Image source: C.M. Bishop, 2006

Box-Muller Algorithm (cont'd)

- Box-Muller Algorithm (cont'd)

$$r^2 = z_1^2 + z_2^2$$

  - For each pair z_1, z_2 evaluate

$$y_1 = z_1 \left(\frac{-2 \ln r^2}{r^2} \right)^{1/2} \qquad y_2 = z_2 \left(\frac{-2 \ln r^2}{r^2} \right)^{1/2}$$

  - Then the joint distribution of y_1 and y_2 is given by

$$p(y_1, y_2) = p(z_1, z_2) \left| \frac{\partial(z_1, z_2)}{\partial(y_1, y_2)} \right|$$

$$= \left[\frac{1}{\sqrt{2\pi}} \exp(-y_1^2/2) \right] \left[\frac{1}{\sqrt{2\pi}} \exp(-y_2^2/2) \right]$$

  $\Rightarrow$ y_1 and y_2 are independent and each has a Gaussian distribution with mean μ and variance σ^2.

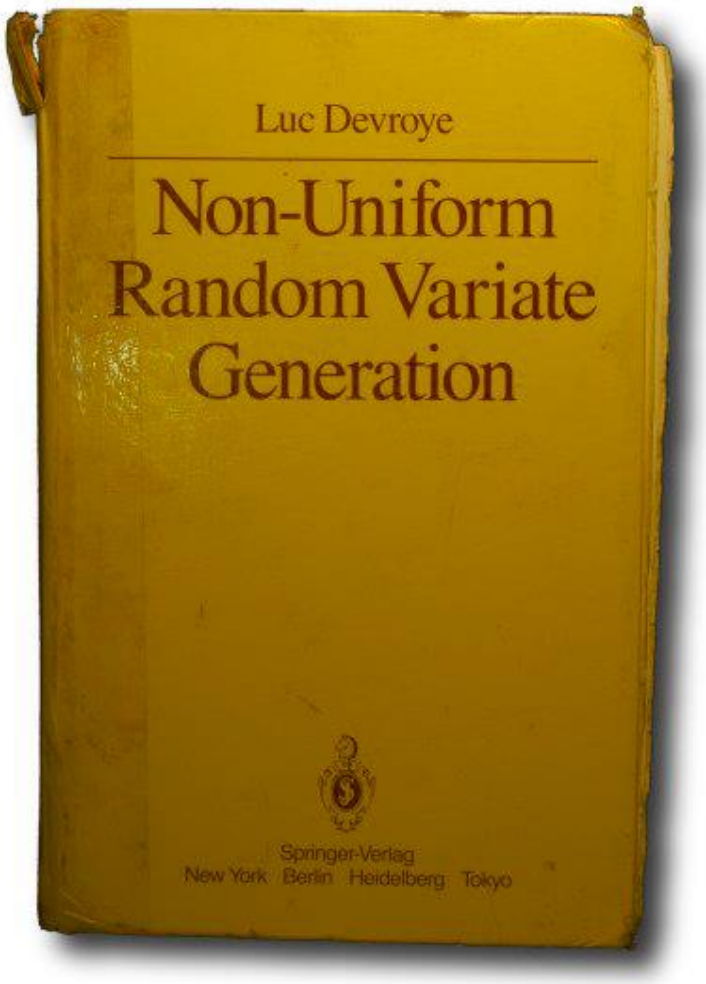
  - If $y \sim \mathcal{N}(0,1)$, then $\sigma y + \mu \sim \mathcal{N}(\mu, \sigma^2)$.

Box-Muller Algorithm (cont'd)

- Multivariate extension
  - If $\mathbf{z}$ is a vector valued random variable whose components are independent and Gaussian distributed with $\mathcal{N}(0,1)$,
  - Then $\mathbf{y} = \mu + \mathbf{L}\mathbf{z}$ will have mean μ and covariance $\mathbf{\Sigma}$.
  - Where $\mathbf{\Sigma} = \mathbf{L}\mathbf{L}^{\mathsf{T}}$ is the Cholesky decomposition of $\mathbf{\Sigma}$.

General Advice

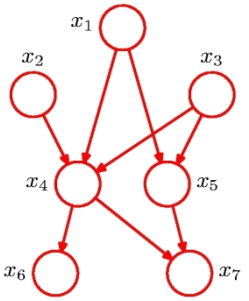
- Use library functions whenever possible
  - Many efficient algorithms available for known univariate distributions (and some other special cases)
  - This book (free online) explains how some of them work
  - http://www.nrbook.com/devroye/



Ancestral Sampling

- Generalization of this idea to directed graphical models.
  - Joint probability factorizes into conditional probabilities:

$$p(\mathbf{x}) = \prod_{k=1}^{K} p(x_k|\mathrm{pa}_k)$$



- Ancestral sampling
  - Assume the variables are ordered such that there are no links from any node to a lower-numbered node.
  - Start with lowest-numbered node and draw a sample from its distribution.

$$\hat{x}_1 \sim p(x_1)$$

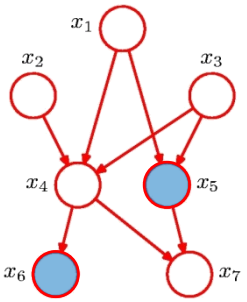
  - Cycle through each of the nodes in order and draw samples from the conditional distribution (where the parent variable is set to its sampled value).

$$\hat{x}_n \sim p(x_n|\mathrm{pa}_n)$$

Image source: C.M. Bishop, 2006

Logic Sampling

- Extension of Ancestral sampling
  - Directed graph where some nodes are instantiated with observed values.



- Use ancestral sampling, except
  - When sample is obtained for an observed variable, if they agree then sample value is retained and proceed to next variable.
  - If they don't agree, whole sample is discarded.

- Result
  - Approach samples correctly from the posterior distribution.
  - However, probability of accepting a sample decreases rapidly as the number of observed variables increases.

  $\Rightarrow$ Approach is rarely used in practice.

Discussion

- Transformation method
  - Limited applicability, as we need to invert the indefinite integral of the required distribution $p(\mathbf{z})$.
  - This will only be feasible for a limited number of simple distributions.

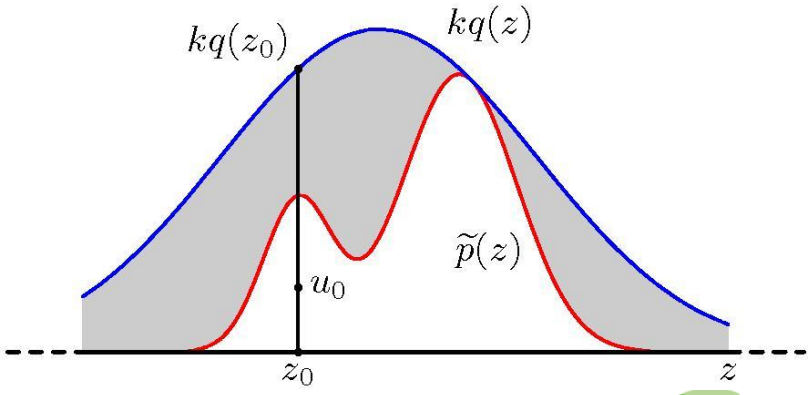
- More general
  - Rejection Sampling
  - Importance Sampling

Rejection Sampling

- Assumptions
  - Sampling directly from $p(\mathbf{z})$ is difficult.
  - But we can easily evaluate $p(\mathbf{z})$ (up to some normalization factor Z_p):

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

- Idea
  - We need some simpler distribution $q(\mathbf{z})$ (called proposal distribution) from which we can draw samples.
  - Choose a constant k such that: $\forall z : kq(z) \geq \tilde{p}(z)$

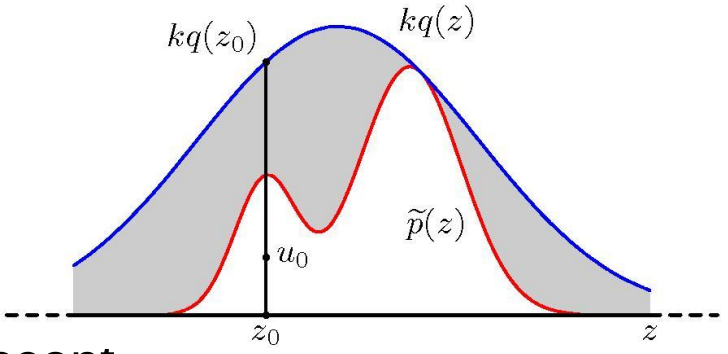


Slide credit: Bernt Schiele

Image source: C.M. Bishop, 2006

Rejection Sampling

- Sampling procedure
  - Generate a number z_0 from $q(z)$.
  - Generate a number u_0 from the uniform distribution over $[0, kq(z_0)]$.
  - If $u_0 > \tilde{p}(z_0)$ reject sample, otherwise accept.
    - Sample is rejected if it lies in the grey shaded area.
    - The remaining pairs (u_0, z_0) have uniform distribution under the curve $\tilde{p}(z)$.



- Discussion
  - Original values of $\mathbf{z}$ are generated from the distribution $q(\mathbf{z})$.
  - Samples are accepted with probability $\tilde{p}(z)/kq(z)$

$$p(accept) = \int \frac{\tilde{p}(z)}{kq(z)} q(z) dz = \frac{1}{k} \int \tilde{p}(z) dz$$

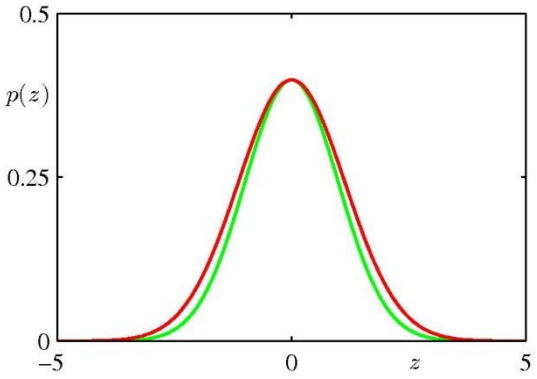
$\Rightarrow k$ should be as small as possible!

Slide credit: Bernt Schiele

Image source: C.M. Bishop, 2006

Rejection Sampling – Discussion

- Limitation: high-dimensional spaces
  - For rejection sampling to be of practical value, we require that $kq(z)$ be close to the required distribution, so that the rate of rejection is minimal.
- Artificial example
  - Assume that $p(\mathbf{z})$ is Gaussian with covariance matrix $\sigma_p^2 I$
  - Assume that $q(\mathbf{z})$ is Gaussian with covariance matrix $\sigma_q^2 I$
  - Obviously: $\sigma_q^2 \geq \sigma_p^2$
  - In D dimensions: $k = (\sigma_q/\sigma_p)^D$.
    - Assume σ_q is just 1% larger than σ_p.
    - $D = 1000 \Rightarrow k = 1.01^{1000} \geq 20{,}000$
    - And $p(accept) < \frac{1}{20000}$



$\Rightarrow$ Impractical to find good proposal distributions for high dimensions!

Slide credit: Bernt Schiele

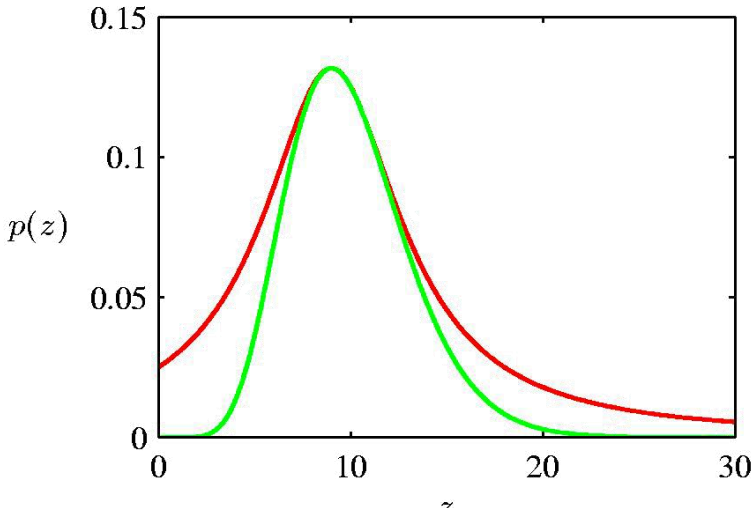
Image source: C.M. Bishop, 2006

Example: Sampling from a Gamma Distrib.

- Gamma distribution

$$\mathrm{Gam}(z|a,b) = \frac{1}{\Gamma(a)} b^a z^{a-1} \exp(-bz) \qquad a > 1$$

- Rejection sampling approach
  - For a>1, Gamma distribution has a bell-shaped form.
  - Suitable proposal distribution is Cauchy (for which we can use the transformation method).
  - Generalize Cauchy slightly to ensure it is nowhere smaller than Gamma: $y = b \tan y + c$ for uniform y.
  - This gives random numbers distributed according to



$$q(z) = \frac{k}{1 + (z-c)^2/b^2}$$

with optimal rejection rate for

$$c = a - 1$$
$$b^2 = 2a - 1$$

Image source: C.M. Bishop, 2006

Evaluating Expectations

- Motivation
  - Often, our goal is not sampling from $p(\mathbf{z})$ by itself, but to evaluate expectations of the form

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

- Simplistic strategy: Grid sampling
  - Discretize $\mathbf{z}$-space into a uniform grid.
  - Evaluate the integrand as a sum of the form

$$\mathbb{E}[f] \simeq \sum_{l=1}^{L} f(\mathbf{z}^{(l)})p(\mathbf{z}^{(l)})d\mathbf{z}$$

  - Problem: number of terms grows exponentially with number of dimensions!

Importance Sampling

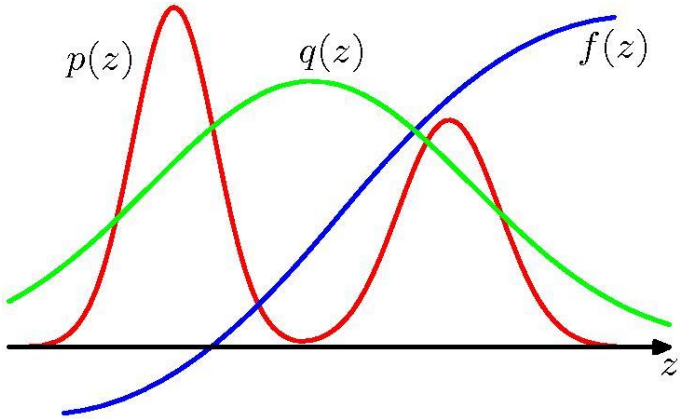
- Idea
  - Use a proposal distribution $q(\mathbf{z})$ from which it is easy to draw samples.
  - Express expectations in the form of a finite sum over samples $\{\mathbf{z}^{(l)}\}$ drawn from $q(\mathbf{z})$.

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

$$\simeq \frac{1}{L}\sum_{l=1}^{L}\frac{p(\mathbf{z}^{(l)})}{q(\mathbf{z}^{(l)})}f(\mathbf{z}^{(l)})$$

  - with importance weights

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



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Importance Sampling

- Typical setting:
  - $p(\mathbf{z})$ can only be evaluated up to an unknown normalization constant $$p(\mathbf{z}) = \tilde{p}(\mathbf{z})/Z_p$$
  - $q(\mathbf{z})$ can also be treated in a similar fashion. $$q(\mathbf{z}) = \tilde{q}(\mathbf{z})/Z_q$$
  - Then $$\mathbb{E}[f] = \int f(\mathbf{z})p(\mathbf{z})d\mathbf{z} = \frac{Z_q}{Z_p}\int f(\mathbf{z})\frac{\tilde{p}(\mathbf{z})}{\tilde{q}(\mathbf{z})}q(\mathbf{z})d\mathbf{z}$$ $$\simeq \frac{Z_q}{Z_p}\frac{1}{L}\sum_{l=1}^{L}\tilde{r}_l f(\mathbf{z}^{(l)})$$
  - with: $$\tilde{r}_l = \frac{\tilde{p}(\mathbf{z}^{(l)})}{\tilde{q}(\mathbf{z}^{(l)})}$$

Importance Sampling

- Removing the unknown normalization constants
  - We can use the sample set to evaluate the ratio of normalization constants

$$\frac{Z_p}{Z_q} = \frac{1}{Z_q}\int \tilde{p}(\mathbf{z})d\mathbf{z} = \int \frac{\tilde{p}(\mathbf{z}^{(l)})}{\tilde{q}(\mathbf{z}^{(l)})}q(\mathbf{z})d\mathbf{z} \simeq \frac{1}{L}\sum_{l=1}^{L}\tilde{r}_l$$

  - and therefore

$$\mathbb{E}[f] \simeq \sum_{l=1}^{L} w_l f(\mathbf{z}^{(l)})$$

with

$$w_l = \frac{\tilde{r}_l}{\sum_m \tilde{r}_m} = \frac{\frac{\tilde{p}(\mathbf{z}^{(l)})}{\tilde{q}(\mathbf{z}^{(l)})}}{\sum_m \frac{\tilde{p}(\mathbf{z}^{(m)})}{\tilde{q}(\mathbf{z}^{(m)})}}$$

⇒ In contrast to Rejection Sampling, all generated samples are retained (but they may get a small weight).

Importance Sampling – Discussion

- Observations
  - Success of importance sampling depends crucially on how well the sampling distribution $q(\mathbf{z})$ matches the desired distribution $p(\mathbf{z})$.
  - Often, $p(\mathbf{z})f(\mathbf{z})$ is strongly varying and has a significant propor-tion of its mass concentrated over small regions of $\mathbf{z}$-space.

  $\Rightarrow$ Weights r_l may be dominated by a few weights having large values.

  - Practical issue: if none of the samples falls in the regions where $p(\mathbf{z})f(\mathbf{z})$ is large…
    - The results may be arbitrary in error.
    - And there will be no diagnostic indication (no large variance in r_l) !
  - Key requirement for sampling distribution $q(\mathbf{z})$:
    - Should not be small or zero in regions where $p(\mathbf{z})$ is significant!

Sampling-Importance-Resampling

- Two stages
  - Draw L samples $\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(L)}$ from $q(\mathbf{z})$.
  - Construct weights using importance weighting

$$w_l = \frac{\tilde{r}_l}{\sum_m \tilde{r}_m} = \frac{\frac{\tilde{p}(\mathbf{z}^{(l)})}{\tilde{q}(\mathbf{z}^{(l)})}}{\sum_m \frac{\tilde{p}(\mathbf{z}^{(m)})}{\tilde{q}(\mathbf{z}^{(m)})}}$$

    and draw a second set of samples $\mathbf{z}^{(1)}, \ldots, \mathbf{z}^{(L)}$ with probabilities given by the weights $w^{(1)}, \ldots, w^{(L)}$.

- Result
  - The resulting L samples are only approximately distributed according to $p(\mathbf{z})$, but the distribution becomes correct in the limit $L \to \infty$.

Curse of Dimensionality

- Problem
  - Rejection & Importance Sampling both scale badly with high dimensionality.
  - Example:

$$p(\mathbf{z}) \sim \mathcal{N}(0, I), \qquad q(\mathbf{z}) \sim \mathcal{N}(0, \sigma^2 I)$$

- Rejection Sampling
  - Requires $\sigma \geq 1$. Fraction of proposals accepted: σ^{-D}.

- Importance Sampling
  - Variance of importance weights: $\left(\frac{\sigma^2}{2 - 1/\sigma^2} \right)^{D/2} - 1$
  - Infinite / undefined variance if $\sigma \leq 1/\sqrt{2}$

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  - Rejection Sampling
  - Importance Sampling
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  - Gibbs Sampling

Independent Sampling vs. Markov Chains

- So far
  - We've considered two methods, Rejection Sampling and Importance Sampling, which were both based on independent samples from $q(\mathbf{z})$.
  - However, for many problems of practical interest, it is difficult or impossible to find $q(\mathbf{z})$ with the necessary properties.

- Different approach
  - We abandon the idea of independent sampling.
  - Instead, rely on a Markov Chain to generate dependent samples from the target distribution.
  - Independence would be a nice thing, but it is not necessary for the Monte Carlo estimate to be valid.

MCMC – Markov Chain Monte Carlo

- Overview
  - Allows to sample from a large class of distributions.
  - Scales well with the dimensionality of the sample space.
- Idea
  - We maintain a record of the current state $\mathbf{z}^{(\tau)}$
  - The proposal distribution depends on the current state: $q(\mathbf{z}|\mathbf{z}^{(\tau)})$
  - The sequence of samples forms a Markov chain $\mathbf{z}^{(1)}$, $\mathbf{z}^{(2)}$,…
- Setting
  - We can evaluate $p(\mathbf{z})$ (up to some normalizing factor Z_p):

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

  - At each time step, we generate a candidate sample from the proposal distribution and accept the sample according to a criterion.

MCMC – Metropolis Algorithm

- Metropolis algorithm [Metropolis et al., 1953]
  - Proposal distribution is symmetric: $q(\mathbf{z}_A|\mathbf{z}_B) = q(\mathbf{z}_B|\mathbf{z}_A)$
  - The new candidate sample $\mathbf{z}^*$ is accepted with probability

$$A(\mathbf{z}^\star, \mathbf{z}^{(\tau)}) = \min\left(1, \frac{\tilde{p}(\mathbf{z}^\star)}{\tilde{p}(\mathbf{z}^{(\tau)})}\right)$$

- Implementation
  - Choose random number u uniformly from unit interval (0,1).
  - Accept sample if $A(\mathbf{z}^\star, \mathbf{z}^{(\tau)}) > u$
- Note
  - New candidate samples always accepted if $\tilde{p}(\mathbf{z}^\star) \geq \tilde{p}(\mathbf{z}^{(\tau)})$.
    - I.e. when new sample has higher probability than the previous one.
  - The algorithm sometimes accepts a state with lower probability.

MCMC – Metropolis Algorithm

- Two cases
  - If new sample is accepted: $\mathbf{z}^{(\tau+1)} = \mathbf{z}^{\star}$
  - Otherwise: $\mathbf{z}^{(\tau+1)} = \mathbf{z}^{(\tau)}$
  - This is in contrast to rejection sampling, where rejected samples are simply discarded.

$\Rightarrow$ Leads to multiple copies of the same sample!

MCMC – Metropolis Algorithm

- Property
  - When $q(\mathbf{z}_A|\mathbf{z}_B) > 0$ for all $\mathbf{z}$, the distribution of $\mathbf{z}^\tau$ tends to $p(\mathbf{z})$ as $\tau \rightarrow \infty$.
- Note
  - Sequence $\mathbf{z}^{(1)}$, $\mathbf{z}^{(2)}$,… is not a set of independent samples from $p(\mathbf{z})$, as successive samples are highly correlated.
  - We can obtain (largely) independent samples by just retaining every Mth sample.
- Example: Sampling from a Gaussian
  - Proposal: Gaussian with $\sigma = 0.2$.
  - Green: accepted samples
  - Red: rejected samples

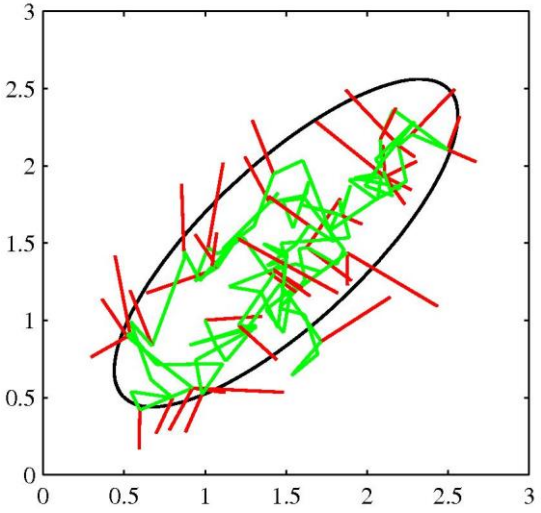
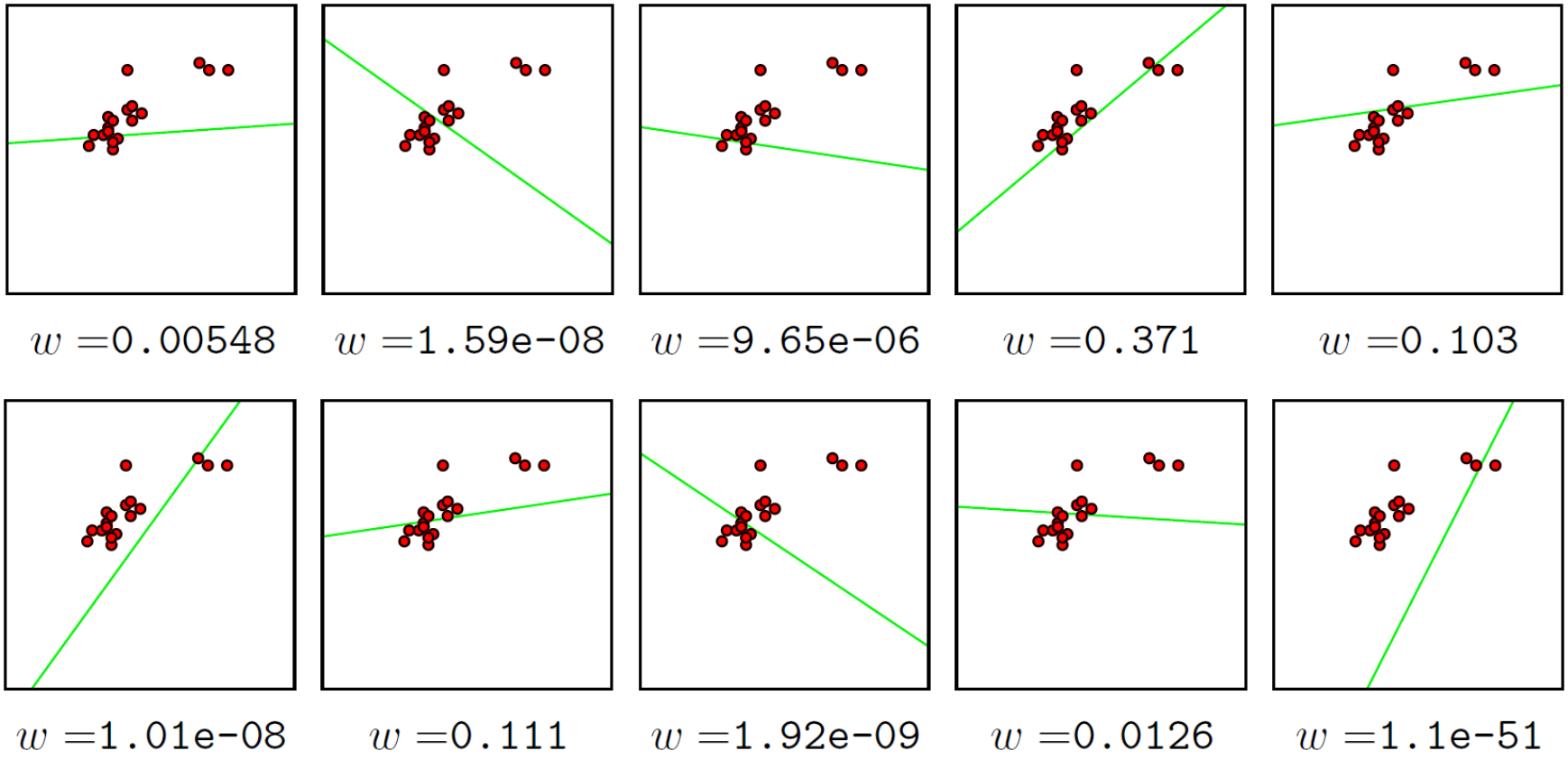


Image source: C.M. Bishop, 2006

Slide credit: Bernt Schiele

Line Fitting Example

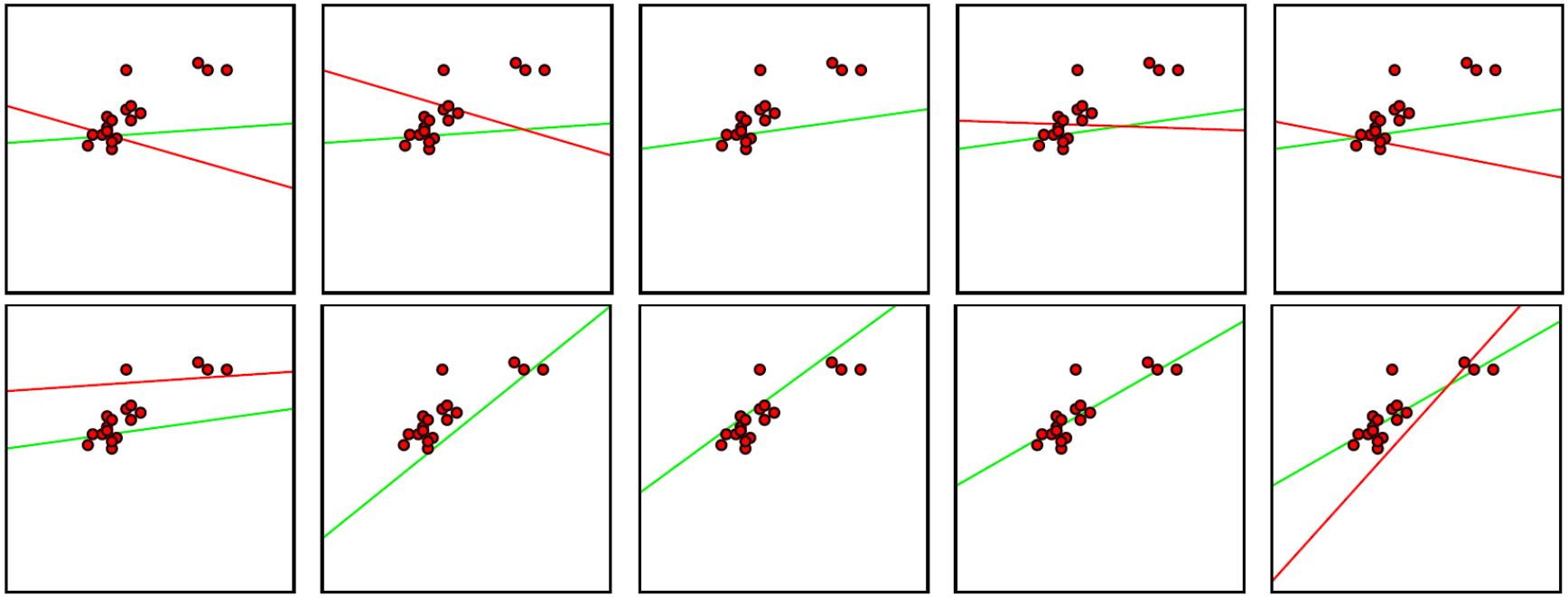
- Importance Sampling weights



$\Rightarrow$ Many samples with very low weights…

Line Fitting Example (cont'd)

- Metropolis algorithm



  - Perturb parameters: $Q(\mathbf{z}'; \mathbf{z})$, e.g. $\mathcal{N}(\mathbf{z}, \sigma^2)$
  - Accept with probability $\min\left(1, \frac{p(\mathbf{z}'|\mathcal{D})}{p(\mathbf{z}|\mathcal{D})}\right)$
  - Otherwise, keep old parameters.

Markov Chains

- Question
  - How can we show that $\mathbf{z}^{\tau}$ tends to $p(\mathbf{z})$ as $\tau \rightarrow \infty$?

- Markov chains
  - First-order Markov chain:

$$p\left(\mathbf{z}^{(m+1)}|\mathbf{z}^{(1)},\ldots,\mathbf{z}^{(m)}\right) = p\left(\mathbf{z}^{(m+1)}|\mathbf{z}^{(m)}\right)$$

  - Marginal probability

$$p\left(\mathbf{z}^{(m+1)}\right) = \sum_{\mathbf{z}^{(m)}} p\left(\mathbf{z}^{(m+1)}|\mathbf{z}^{(m)}\right) p\left(\mathbf{z}^{(m)}\right)$$

  - A Markov chain is called homogeneous if the transition probabilities $p(\mathbf{z}^{(m+1)} \mid \mathbf{z}^{(m)})$ are the same for all m.

Markov Chains – Properties

- Invariant distribution
  - A distribution is said to be invariant (or stationary) w.r.t. a Markov chain if each step in the chain leaves that distribution invariant.
  - Transition probabilities:
$$T\left(\mathbf{z}^{(m)}, \mathbf{z}^{(m+1)}\right) = p\left(\mathbf{z}^{(m+1)} | \mathbf{z}^{(m)}\right)$$
  - Distribution $p^{\star}(\mathbf{z})$ is invariant if:
$$p^{\star}(\mathbf{z}) = \sum_{\mathbf{z}'} T\left(\mathbf{z}', \mathbf{z}\right) p^{\star}(\mathbf{z}')$$
- Detailed balance
  - Sufficient (but not necessary) condition to ensure that a distribution is invariant:
$$p^{\star}(\mathbf{z}) T\left(\mathbf{z}, \mathbf{z}'\right) = p^{\star}(\mathbf{z}') T\left(\mathbf{z}', \mathbf{z}\right)$$
  - A Markov chain which respects *detailed balance* is reversible.

Detailed Balance

- Detailed balance means
  - If we pick a state from the target distribution $p(\mathbf{z})$ and make a transition under T to another state, it is just as likely that we will pick $\mathbf{z}_A$ and go from $\mathbf{z}_A$ to $\mathbf{z}_B$ than that we will pick $\mathbf{z}_B$ and go from $\mathbf{z}_B$ to $\mathbf{z}_A$.

  - It can easily be seen that a transition probability that satisfies detailed balance w.r.t. a particular distribution will leave that distribution invariant, because

$$\begin{aligned}\sum_{\mathbf{z}'} p^\star(\mathbf{z}')T(\mathbf{z}',\mathbf{z}) &= \sum_{\mathbf{z}'} p^\star(\mathbf{z})T(\mathbf{z},\mathbf{z}') \\ &= p^\star(\mathbf{z})\sum_{\mathbf{z}'} p(\mathbf{z}'|\mathbf{z}) = p^\star(\mathbf{z})\end{aligned}$$

Ergodicity in Markov Chains

- Remark
  - Our goal is to use Markov chains to sample from a given distribution.
  - We can achieve this if we set up a Markov chain such that the desired distribution is invariant.
  - However, must also require that for $m \to \infty$, the distribution $p(\mathbf{z}^{(m)})$ converges to the required invariant distribution $p^*(\mathbf{z})$ irrespective of the choice of initial distribution $p(\mathbf{z}^{(0)})$.
  - This property is called ergodicity and the invariant distribution is called the equilibrium distribution.
  - It can be shown that this is the case for a homogeneous Markov chain, subject only to weak restrictions on the invariant distribution and the transition probabilities.

Mixture Transition Distributions

- Mixture distributions
  - In practice, we often construct the transition probabilities from a set of 'base' transitions $B_1,\ldots,B_K$.
  - This can be achieved through a mixture distribution

$$T(\mathbf{z}', \mathbf{z}) = \sum_{k=1}^{K} \alpha_k B_k(\mathbf{z}', \mathbf{z})$$

with mixing coefficients $\alpha_k \geq 0$ and $\sum_k \alpha_k = 1$.

- Properties
  - If the distribution is invariant w.r.t. each of the base transitions, then it will also be invariant w.r.t. T(z',z).
  - If each of the base transitions satisfies detailed balance, then the mixture transition T will also satisfy detailed balance.
  - Common example: each base transition changes only a subset of variables.

MCMC – Metropolis-Hastings Algorithm

- Metropolis-Hastings Algorithm
  - Generalization: Proposal distribution not required to be symmetric.
  - The new candidate sample $\mathbf{z}^*$ is accepted with probability

$$A(\mathbf{z}^\star, \mathbf{z}^{(\tau)}) = \min\left(1, \frac{\tilde{p}(\mathbf{z}^\star) q_k(\mathbf{z}^{(\tau)} | \mathbf{z}^\star)}{\tilde{p}(\mathbf{z}^{(\tau)}) q_k(\mathbf{z}^\star | \mathbf{z}^{(\tau)})}\right)$$

  - where k labels the members of the set of possible transitions considered.

- Note
  - Evaluation of acceptance criterion does not require normalizing constant Z_p.
  - When the proposal distributions are symmetric, Metropolis-Hastings reduces to the standard Metropolis algorithm.

MCMC – Metropolis-Hastings Algorithm

- Properties
  - We can show that $p(\mathbf{z})$ is an invariant distribution of the Markov chain defined by the Metropolis-Hastings algorithm.
  - We show detailed balance:

$$A(\mathbf{z}', \mathbf{z}) = \min\left\{1, \frac{\tilde{p}(\mathbf{z}')q_k(\mathbf{z}|\mathbf{z}')}{\tilde{p}(\mathbf{z})q_k(\mathbf{z}'|\mathbf{z})}\right\}$$

$$\begin{aligned}
\tilde{p}(\mathbf{z})q_k(\mathbf{z}'|\mathbf{z})A_k(\mathbf{z}', \mathbf{z}) &= \min\{\tilde{p}(\mathbf{z})q_k(\mathbf{z}'|\mathbf{z}), \tilde{p}(\mathbf{z}')q_k(\mathbf{z}|\mathbf{z}')\} \\
&= \min\{\tilde{p}(\mathbf{z}')q_k(\mathbf{z}|\mathbf{z}'), \tilde{p}(\mathbf{z})q_k(\mathbf{z}'|\mathbf{z})\} \\
\tilde{p}(\mathbf{z})q_k(\mathbf{z}'|\mathbf{z})A_k(\mathbf{z}', \mathbf{z}) &= \tilde{p}(\mathbf{z}')q_k(\mathbf{z}|\mathbf{z}')A_k(\mathbf{z}, \mathbf{z}') \\
\tilde{p}(\mathbf{z})T(\mathbf{z}', \mathbf{z}) &= \tilde{p}(\mathbf{z}')T(\mathbf{z}, \mathbf{z}')
\end{aligned}$$

Note: This is wrong in the Bishop book!

Random Walks

- Example: Random Walk behavior
  - Consider a state space consisting of the integers $z \in \mathbb{Z}$ with initial state $z(1) = 0$ and transition probabilities

$$\begin{aligned} p(z^{(\tau+1)} = z^{(\tau)}) &= 0.5 \\ p(z^{(\tau+1)} = z^{(\tau)} + 1) &= 0.25 \\ p(z^{(\tau+1)} = z^{(\tau)} - 1) &= 0.25 \end{aligned}$$

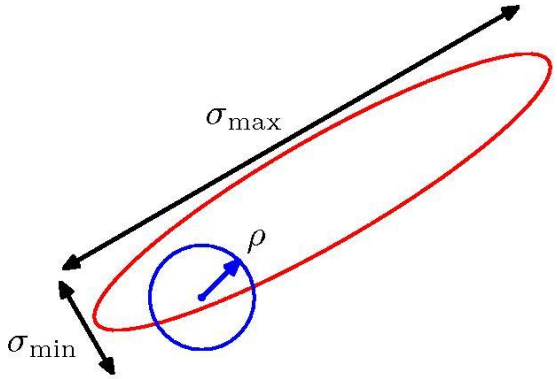
- Analysis
  - Expected state at time τ : $\mathbb{E}[z^{(\tau)}] = 0$
  - Variance: $\mathbb{E}[(z^{(\tau)})^2] = \tau/2$
  - After τ steps, the random walk has only traversed a distance that is on average proportional to $\sqrt{\tau}$.

    $\Rightarrow$ Central goal in MCMC is to avoid random walk behavior!

MCMC – Metropolis-Hastings Algorithm

- Schematic illustration
  - For continuous state spaces, a common choice of proposal distribution is a Gaussian centered on the current state.

  ⇒ What should be the variance of the proposal distribution?



    - Large variance: rejection rate will be high for complex problems.
    - The scale ρ of the proposal distribution should be as large as possible without incurring high rejection rates.

    ⇒ ρ should be of the same order as the smallest length scale $\sigma_{\min}$.

  - This causes the system to explore the distribution by means of a random walk.
    - Undesired behavior: number of steps to arrive at state that is independent of original state is of order $(\sigma_{\max}/\sigma_{\min})^2$.
    - Strong correlations can slow down the Metropolis algorithm!

Image source: C.M. Bishop, 2006

Gibbs Sampling

- Approach
  - MCMC-algorithm that is simple and widely applicable.
  - May be seen as a special case of Metropolis-Hastings.
- Idea
  - Sample variable-wise: replace $\mathbf{z}_i$ by a value drawn from the distribution $p(z_i|\mathbf{z}_{\setminus i})$.
    - This means we update one coordinate at a time.
  - Repeat procedure either by cycling through all variables or by choosing the next variable.

Gibbs Sampling

- Example
  - Assume distribution $p(z_1, z_2, z_3)$.
  - Replace $z_1^{(\tau)}$ with new value drawn from $z_1^{(\tau+1)} \sim p(z_1 | z_2^{(\tau)}, z_3^{(\tau)})$
  - Replace $z_2^{(\tau)}$ with new value drawn from $z_2^{(\tau+1)} \sim p(z_2 | z_1^{(\tau+1)}, z_3^{(\tau)})$
  - Replace $z_3^{(\tau)}$ with new value drawn from $z_3^{(\tau+1)} \sim p(z_3 | z_1^{(\tau+1)}, z_2^{(\tau+1)})$
  - And so on…

Gibbs Sampling

- Properties
  - The factor that determines the acceptance probability in the Metropolis-Hastings is determined by

$$A(\mathbf{z}^\star, \mathbf{z}) = \frac{p(\mathbf{z}^\star) q_k(\mathbf{z}|\mathbf{z}^\star)}{p(\mathbf{z}) q_k(\mathbf{z}^\star|\mathbf{z})} = \frac{p(z_k^\star|\mathbf{z}_{\setminus k}^\star) p(\mathbf{z}_{\setminus k}^\star) p(z_k^\star|\mathbf{z}_{\setminus k}^\star)}{p(z_k|\mathbf{z}_{\setminus k}) p(\mathbf{z}_{\setminus k}) p(z_k|\mathbf{z}_{\setminus k})} = 1$$

  - (we have used $q_k(\mathbf{z}^*|\mathbf{z}) = p(z^*_k|\mathbf{z}_{\setminus k})$ and $p(\mathbf{z}) = p(z_k|\mathbf{z}_{\setminus k})\, p(\mathbf{z}_{\setminus k})$).
  - I.e. we get an algorithm which always accepts!

$\Rightarrow$ If you can compute (and sample from) the conditionals, you can apply Gibbs sampling.

$\Rightarrow$ The algorithm is completely parameter free.

$\Rightarrow$ Can also be applied to subsets of variables.

Discussion

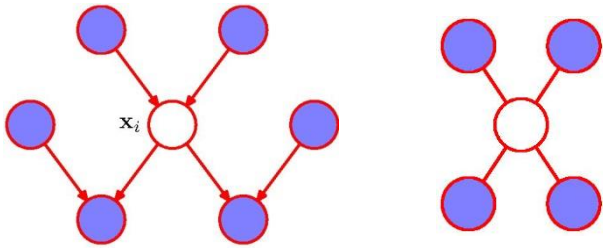
- Gibbs sampling benefits from few free choices and convenient features of conditional distributions:
  - Conditionals with a few discrete settings can be explicitly normalized:

$$p(x_i|\mathbf{x}_{j\neq i}) = \frac{p(x_i, \mathbf{x}_{j\neq i})}{\sum_{x_i'} p(x_i', \mathbf{x}_{j\neq i})}$$

This sum is small and easy.

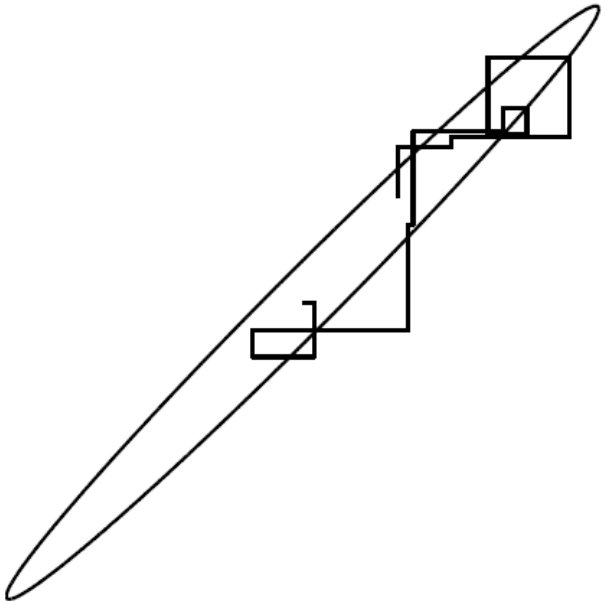
  - Continuous conditionals are often only univariate.
    $\Rightarrow$ amenable to standard sampling methods.

  - In case of graphical models, the conditional distributions depend only on the variables in the corresponding Markov blankets.



Gibbs Sampling

- Example
  - 20 iterations of Gibbs sampling on a bivariate Gaussian.



  - Note: strong correlations can slow down Gibbs sampling.

How Should We Run MCMC?

- Arbitrary initialization means starting iterations are bad
  - Discard a "burn-in" period.
- How do we know if we have run for long enough?
  - You don't. That's the problem.
- The samples are not independent
  - Solution 1: Keep only every Mth sample ("thinning").
  - Solution 2: Keep all samples and use the simple Monte Carlo estimator on MCMC samples
    - It is consistent and unbiased if the chain has "burned in".

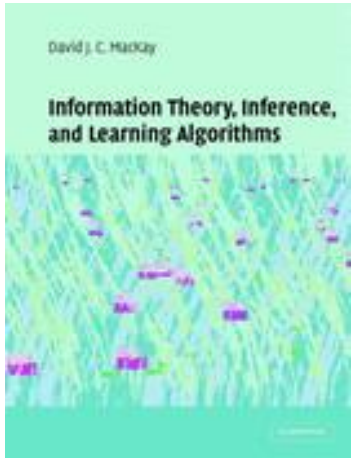
    $\Rightarrow$ Use thinning only if computing $f(\mathbf{x}^{(s)})$ is expensive.
- For opinion on thinning, multiple runs, burn in, etc.
  - Charles J. Geyer, Practical Markov chain Monte Carlo, Statistical Science. 7(4):473{483, 1992. (http://www.jstor.org/stable/2246094)

Summary: Approximate Inference

- Exact Bayesian Inference often intractable.
- Rejection and Importance Sampling
  - Generate independent samples.
  - Impractical in high-dimensional state spaces.
- Markov Chain Monte Carlo (MCMC)
  - Simple & effective (even though typically computationally expensive).
  - Scales well with the dimensionality of the state space.
  - Issues of convergence have to be considered carefully.
- Gibbs Sampling
  - Used extensively in practice.
  - Parameter free
  - Requires sampling conditional distributions.

References and Further Reading

- Sampling methods for approximate inference are described in detail in Chapter 11 of Bishop's book.



Christopher M. Bishop
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David MacKay
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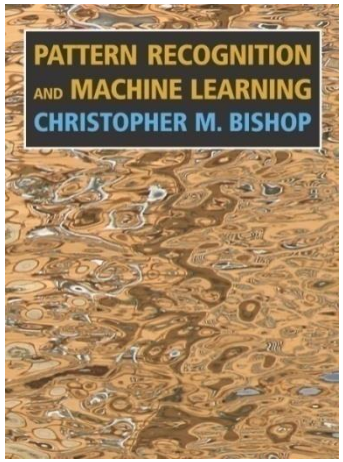
Cambridge University Press, 2003



- Another good introduction to Monte Carlo methods can be found in Chapter 29 of MacKay's book (also available online: http://www.inference.phy.cam.ac.uk/mackay/itprnn/book.html)