Rejection Sampling

Goal: Generate samples uniformly from some complicated distrib

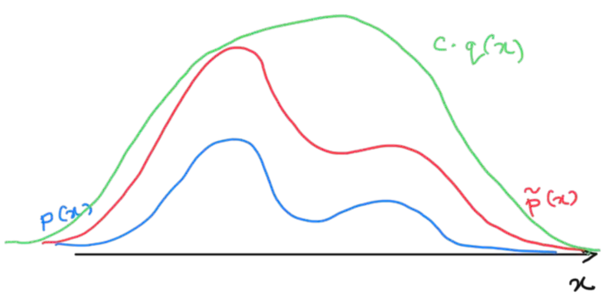
We assume that we can evaluate : $\mathbb{1}_{\{x \in A\}} = \begin{cases} 1, & \text{if} \\ 0, & \text{if } x \end{cases}$

Basic Idea: Draw samples from a simpler "proposal" distribution. Then evaluate some acceptance / rejection criterion to choose whether the sample should be kept or not.

In a more general setting our goal is to :

Sample $x_i \in \mathbb{R}^d$ from some pdf $p(x)$.

Assume we are given $\tilde{p}(x)$, $p(x) = \dfrac{\tilde{p}(x)}{Z_p}$, $Z_p := \int \tilde{p}(x)\,dx >$



Rejection sampling:

1. Choose a proposal dist. $q(x)$,

i.) $\exists c > 0$: $c \cdot q(x) \geq \tilde{p}(x) \;\forall x$

ii.) $q(x)$ is easy to sample from.

2. Sample $x \sim q(x)$, sample $u \sim U[0, c \cdot q(x)]$.

3.) If $u \leq \tilde{p}(x)$ then accept this sample x. Otherwise, reject

4.) Go back to step #2 and repea

Output: A collection of accepted samples :

$x_1, x_2, \dots, x_m \sim p(x)$

Questions: 1. How to choose the constant c ? ... $c = \max\left(\dfrac{\tilde{p}(x)}{q(x)}\right.$

Remark: Our intuition on choosing an appropriate proposal $q(x$ breaks down in high-dimension !

Markov Chain Monte Carlo (one of the top algorithms of the 20th century)

A powerful tool for approximating expectations and sampling from complex high-dimensional distributions.

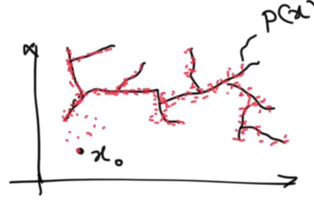
Goal: i) Sample $x \sim p(x)$, $x \in \mathbb{R}^d$.

ii) Compute / approximate , $\mathbb{E}_{x\sim p(x)}[f(x)] = \int f(x)p(x)\,dx$

Recall in M.C. $\mathbb{E}_{x\sim p(x)}[f(x)] \approx \frac{1}{n}\sum_{i=1}^{n} f(x_i)$, $x_i \overset{i.i.d.}{\sim} p(x)$

- $p(x)$ may be way too complicated to sample from.
- IS / R.S. face difficulties in high-dimensions.

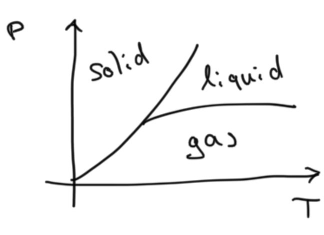
Intuition :



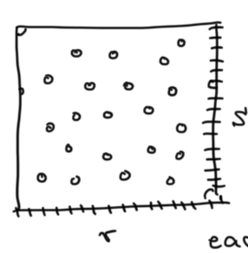
notional "high-dimensional space"

Idea : Start at some random location x and navigate/explore the space by moving randomly, staying close to regions of high probability.

Example of the Metropolis algorithm (1953, "Hard-disks in a box" model)



A box of non-overlapping rigid particles :



- N particles
- periodic B.C.s
- theoretical model for phase transition.

each particle coords : (r, s)

The goal is to find the equation of state :

e.g. ideal gas : $pV = nRT$

Setup: Observe a system configuration : $x = (r_1, s_1, r_2, s_2, \dots, r_N, s_N) \in \mathbb{R}$
↳ particle positions.

The Boltzmann distribution characterizes all possible states of this system :

$$p(x) = \frac{1}{Z_p} e^{-\frac{\mathcal{E}(x)}{kT}} \mathbb{1}_{\{x\}}$$

↳ Boltzmann dist.

$\mathcal{E}(x)$: energy of the system.

T : temperature

k : Boltzmann constant.

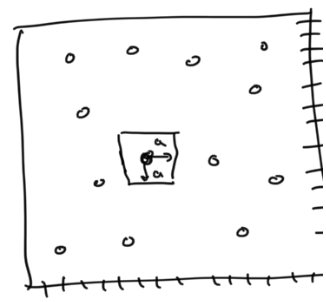
Z_p : Normalizing constant (part fun

↳ $Z_p = \int e^{-\frac{\mathcal{E}(x)}{kT}} p(x)\, dx$

Goal: Compute expectations:

$$\mathbb{E}_{x \sim p(x)} [f(x)]$$

Metropolis algorithm :



1.) Choose a symmetric proposal distribution $q(x)$:

Uniformely choose a particle :

$$Q(x, x') = q(x' | x) = \frac{1}{N} \mathbb{1}_{\{x'\}}$$

2.) Sample x' from $q(x'|x)$, sample $u \sim \mathcal{U}(0,1)$

3.) Evaluate : $\tilde{p}(x') = e^{-\frac{\mathcal{E}(x')}{kT}} \mathbb{1}_{\{x' \text{is valid}\}}$ and check if

$$u < \frac{\tilde{p}(x')}{\tilde{p}(x)} \begin{cases} \text{True, accept } x' \text{ (i.e. set } x = x') \\ \text{False, reject.} \end{cases}$$

4.) Go back to step # and repeat.

Output: Sequence of accepted states $x_1, x_2, \dots, x_n$

$$\Longrightarrow \mathbb{E}_{x \sim p(x)} [f(x)] \approx \frac{1}{n} \sum_{i=1}^{n} f(x_i), \quad x_i \sim \text{M.C.}$$