

# Lecture 4: Rejection Sampling and Sampling from Compositions, Conditionals, Marginals

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# Rejection sampling

The algorithm

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▶  $X' \sim q(x),$

# Rejection sampling

## The algorithm

The rejection sampler:

- ▶  $X' \sim q(x)$ ,
- ▶ Accept the sample  $X'$  with probability

$$a(X') = \frac{p(X')}{Mq(X')}$$

We have

$$\begin{aligned}\hat{a} &= \mathbb{E}[a(X')] = \int a(x')q(x')dx' \\ &= \int \frac{p(x')}{Mq(x')}q(x')dx' \\ &= \frac{1}{M} \int p(x')dx' \\ &= \frac{1}{M}.\end{aligned}$$

For the unnormalised case:

$$\begin{aligned}\hat{a} &= \mathbb{E}[a(X')] = \int a(x')q(x')dx' \\ &= \int \frac{\bar{p}(x')}{Mq(x')}q(x')dx' \\ &= \int Z \frac{p(x')}{Mq(x')}q(x')dx' \\ &= \frac{Z}{M} \int p(x')dx' \\ &= \frac{Z}{M}.\end{aligned}$$

# Rejection sampling

Example: Optimising rejection sampling

Assume that we would like to sample from

$$X \sim \Gamma(\alpha, 1),$$

for  $\alpha > 1$ . The density is given by

$$p(x) = \frac{x^{\alpha-1} e^{-x}}{\Gamma(\alpha)}, \quad \text{for } x > 0,$$

where  $\Gamma(\alpha)$  is the Gamma function.  $\Gamma(n) = (n-1)!$

# Rejection sampling

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Choose as a *proposal*:

$$q_{\lambda}(x) = \text{Exp}(x; \lambda) = \lambda e^{-\lambda x}, \quad x > 0,$$

with  $0 < \lambda < 1$ .



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$$M_\lambda = \sup_x \frac{p(x)}{q_\lambda(x)}.$$

Find  $M_\lambda$  for fixed  $\lambda$  first:

$$\frac{p(x)}{q_\lambda(x)} = \frac{x^{\alpha-1} e^{(\lambda-1)x}}{\lambda \Gamma(\alpha)}.$$

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Find  $M_\lambda$  for fixed  $\lambda$  first:

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Maximise this w.r.t.  $x$ ?

# Rejection sampling

## Example: Optimising rejection sampling

How to compute a maximum? It is useful to take log:

$$\arg \max_x f(x) = \arg \max_x \log f(x).$$

Take the log of

$$\frac{p(x)}{q_\lambda(x)} = \frac{x^{\alpha-1} e^{(\lambda-1)x}}{\lambda \Gamma(\alpha)}.$$

So we want to optimise

$$G(x) = \log \frac{p(x)}{q_\lambda(x)} = (\alpha - 1) \log x + (\lambda - 1)x - \log \lambda \Gamma(\alpha).$$

Set  $\frac{dG(x)}{dx} = 0$ .

# Rejection sampling

Example: Optimising rejection sampling

The derivative

$$\frac{dG(x)}{dx} = \frac{\alpha - 1}{x} + (\lambda - 1) = 0$$

which implies

$$x^* = \frac{\alpha - 1}{1 - \lambda}.$$

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which implies

$$x^* = \frac{\alpha - 1}{1 - \lambda}.$$

How do we understand if this is a maximum? Compute

$$\frac{d^2G(x)}{dx^2} = -\frac{\alpha - 1}{x^2},$$

plug  $x^*$  into this

$$\frac{d^2G(x^*)}{dx^2} = -\frac{(\alpha - 1)(1 - \lambda)^2}{(\alpha - 1)^2} < 0,$$

as  $\alpha > 1$  and  $0 < \lambda < 1$ .

# Rejection sampling

Example: Optimising rejection sampling

Therefore,

$$\begin{aligned} M_\lambda &= \frac{p(x^\star)}{q_\lambda(x^\star)}, \\ &= \frac{x^{\star\alpha-1} e^{(\lambda-1)x^\star}}{\lambda\Gamma(\alpha)}, \\ &= \frac{\left(\frac{\alpha-1}{1-\lambda}\right)^{\alpha-1} e^{(\lambda-1)\frac{\alpha-1}{1-\lambda}}}{\lambda\Gamma(\alpha)} \\ &= \frac{\left(\frac{\alpha-1}{1-\lambda}\right)^{\alpha-1} e^{-(\alpha-1)}}{\lambda\Gamma(\alpha)}. \end{aligned}$$



# Rejection sampling

Example: Optimising rejection sampling

Recall that, we are interested in the acceptance probability (or maximising it)

$$\frac{p(x)}{M_\lambda q_\lambda(x)} = \left( \frac{x(1-\lambda)}{\alpha-1} \right)^{\alpha-1} e^{(\lambda-1)x+\alpha-1}.$$

Now, the task is to minimise  $M_\lambda$  w.r.t.  $\lambda$  so we get the *optimal* proposal ( $\hat{a} = 1/M_\lambda$  would be maximised).

# Rejection sampling

Example: Optimising rejection sampling

Recall

$$M_{\lambda} = \frac{\left(\frac{\alpha-1}{1-\lambda}\right)^{\alpha-1} e^{-(\alpha-1)}}{\lambda \Gamma(\alpha)}.$$

Compute log

$$\begin{aligned} \log M_{\lambda} &= (\alpha - 1) \log(\alpha - 1) - (\alpha - 1) \log(1 - \lambda) \\ &\quad - (\alpha - 1) - \log \lambda - \log \Gamma(\alpha). \end{aligned}$$

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Example: Optimising rejection sampling

Take the derivative

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therefore

$$\lambda^* = \frac{1}{\alpha}.$$

Finally we get the optimal  $M$  by computing

$$M_{\lambda^*} = \frac{\alpha^\alpha e^{-(\alpha-1)}}{\Gamma(\alpha)}.$$

# Rejection sampling

Example: Optimising rejection sampling

In order to sample from  $\Gamma(\alpha, 1)$ , we perform

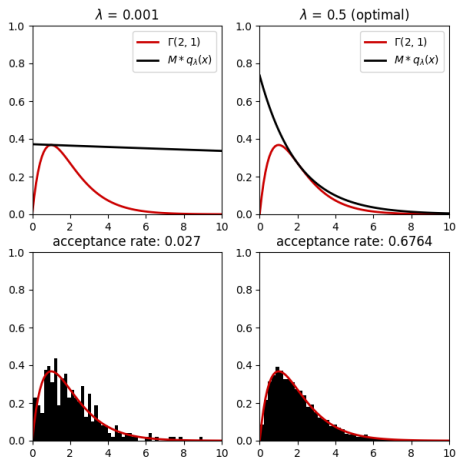
- ▶ Sample  $X' \sim \text{Exp}(1/\alpha)$  and  $U \sim \text{Unif}(0, 1)$
- ▶ If

$$U \leq (x/\alpha)^{\alpha-1} e^{(1/\alpha-1)x+\alpha-1},$$

*accept*  $X'$ , otherwise start again.

# Rejection sampling

## Example: Optimising rejection sampling





# Example: Rejection sampling

Sample Gaussian using Cauchy

Let

$$\begin{aligned}\bar{p}(x) &= e^{-x^2/2} \\ q(x) &= \frac{1}{\pi} \frac{1}{1+x^2}.\end{aligned}$$

Compute

$$M = \sup_x \frac{\bar{p}(x)}{q(x)}.$$

# Example: Rejection sampling

Sample Gaussian using Cauchy

Compute

$$\log \bar{p}(x)/q(x) = -\frac{x^2}{2} + \log(1 + x^2) + \log(1/\pi)$$

Find the roots.

# Example: Rejection sampling

Sample Gaussian using Cauchy

Compute

$$\log \bar{p}(x)/q(x) = -\frac{x^2}{2} + \log(1 + x^2) + \log(1/\pi)$$

Find the roots. Taking the derivative

$$\begin{aligned} \frac{d}{dx} \log \bar{p}(x)/q(x) &= -x + \frac{2x}{1 + x^2} = 0 \\ x &= 0, \pm 1. \end{aligned}$$

Which one is the maximum?

# Example: Rejection sampling

Sample Gaussian using Cauchy

Compute the second derivative

$$\frac{d^2}{dx^2} \log \bar{p}(x)/q(x) = -1 + \frac{2(1-x^2)}{(1+x^2)^2} = 0$$

- ▶ When  $x = 0$ , the second derivative is positive - which means  $x = 0$  is a minimum.
- ▶ When  $x = \pm 1$ , the second derivative is negative - which means  $x = \pm 1$  is a maximum.
- ▶  $x^* = \pm 1$ .

So we have

$$M = \frac{\bar{p}(1)}{q(1)} = 2\pi e^{-1/2}.$$

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- ▶ Given a  $p(x)$  (or unnormalised  $\bar{p}(x)$ ), how to draw independent samples
  - ▶ Inversion
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Let us look at how to *utilise* sampling methods.



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We say that  $X$  and  $Y$  are independent if  $p(x, y)$  satisfies

$$p(x, y) = p(x)p(y).$$

Similar property naturally follows for expectations.

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The Bayes' rule follows from this formula:

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

We will look at it in detail later.

Let us finally settle on some notions

Let us look into details the structure of joint distributions. Given  $p(x, y)$ , we have for continuous variables

$$p(y) = \int p(x, y) dx,$$

or for discrete variables

$$p(y) = \sum_{x \in X} p(x, y).$$

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The same is true for

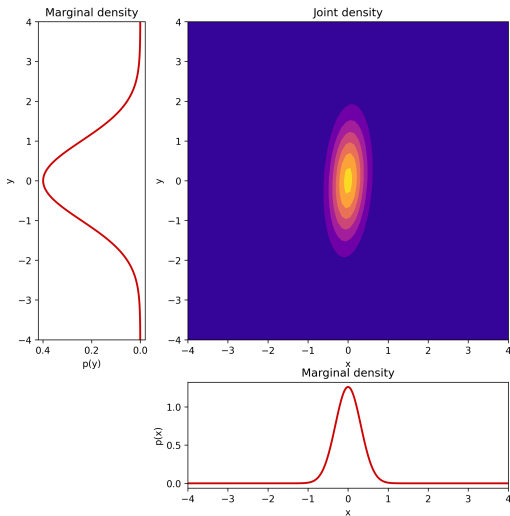
$$p(x) = \int p(x, y) dy,$$

for continuous variables and

$$p(x) = \sum_{y \in Y} p(x, y)$$



## Joint continuous distribution and marginals



An example table for a joint distribution  $p(x, y)$

$p(x, y)$	$X = 0$	$X = 1$	$X = 2$	$X = 3$	$p_Y(y)$
$Y = 0$	1/6	1/6	0	0	2/6
$Y = 1$	1/6	0	1/6	0	2/6
$Y = 2$	0	0	1/6	0	1/6
$Y = 3$	0	0	0	1/6	1/6
$p_X(x)$	2/6	1/6	2/6	1/6	1

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We can sample from this mixture by

- ▶ Sampling from the discrete distribution  $p(k)$  with  $p(k = 1) = w_1$  and  $p(k = 2) = w_2$ , i.e.,

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- ▶ Sampling from the distribution  $q_k(x)$ .

The resulting distribution is  $p(x) = w_1 q_1(x) + w_2 q_2(x)$ .

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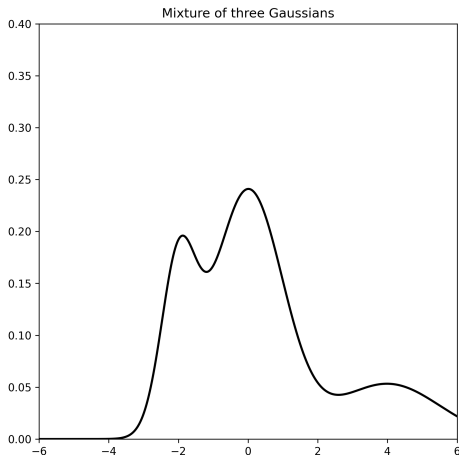
- ▶ Sampling from the distribution  $q_k(x)$ .

The resulting distribution is  $p(x) = \sum_{n=1}^K w_n q_n(x)$ .

Compose the discrete sampling with any other sampling method.



## Sampling from a discrete mixture: A Gaussian example



**Figure:** The density of a mixture of three Gaussians:  $p(x) = \sum_{k=1}^3 w_k \mathcal{N}(x; \mu_k, \sigma_k^2)$  with  $\mu_1 = -2, \mu_2 = 0, \mu_3 = 4, \sigma_1 = 0.5, \sigma_2 = 1, \sigma_3 = 0.5, w_1 = 0.2, w_2 = 0.6, w_3 = 0.2$ .

Let us consider a conditional distribution  $p(y|x)$ . This is a density for fixed  $x$ , i.e.,

$$\int p(y|x)dy = 1.$$

# Conditionals

## Sampling from conditional distributions

Let us consider a conditional distribution  $p(y|x)$ . This is a density for fixed  $x$ , i.e.,

$$\int p(y|x)dy = 1.$$

Sampling from this distribution is trivial given  $x$  with known techniques

- ▶ Inversion
- ▶ Transformation
- ▶ Rejection
- ▶ Thousand other methods

Simple example:

$$p(y|x) = \mathcal{N}(y; x, 1).$$

Just sample by fixing  $x$  from a Gaussian with mean  $x$ .

Recall that we have for any joint distribution  $p(x, y)$

$$p(x, y) = p(y|x)p(x).$$

This decomposition can be used for sampling  $(x, y) \sim p(x, y)$ . Indeed, we can sample from the joint by

- ▶ Sampling  $X \sim p(x)$
- ▶ Sampling  $Y|X = x \sim p(y|x)$

Surprisingly, we can use the samples from joint to compute  $p(y)$ :

$$p(y) = \int p(x, y) dx.$$

The above operation is called *marginalisation*<sup>1</sup>.

---

<sup>1</sup>Mathematically same as continuous mixtures, more on this later.

Suppose we have 2D samples  $(x_1, y_1), \dots, (x_n, y_n)$  from  $p(x, y)$ .  
How to sample from  $p(y)$ ?

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Do nothing! Just keep the  $y$ 's and discard the  $x$ 's. The resulting samples are from  $p(y)$ !



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This is a neat way to avoid computing an integral.

Example: Consider the following model:

$$p(x) = \mathcal{N}(x; \mu, \sigma_0^2)$$
$$p(y|x) = \mathcal{N}(y; x, \sigma^2).$$

The samples  $(x_i, y_i)_{i=1}^n$  can be drawn straightforwardly and  $y$ 's will be distributed w.r.t.  $p(y)$ .

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But what is  $p(y)$ ? We can compute it by marginalisation.

$$p(y) = \int p(y|x)p(x)dx$$
$$= \int \mathcal{N}(y; x, \sigma^2)\mathcal{N}(x; \mu, \sigma_0^2)dx.$$

This is given as

$$p(y) = \mathcal{N}(y; \mu, \sigma_0^2 + \sigma^2).$$

Two ways to sample  $p(y)$

# Marginalisation

## Sampling from marginals

Two ways to sample  $p(y)$

Sample from joint and keep  $y$ 's

- ▶  $X \sim p(x) = \mathcal{N}(x; \mu, \sigma_0^2)$
- ▶  $Y|X = x \sim p(y|x) = \mathcal{N}(y; x, \sigma^2)$

Sample  $n$  times and keep  $Y$ 's which will be  $Y \sim p(y)$ .

# Marginalisation

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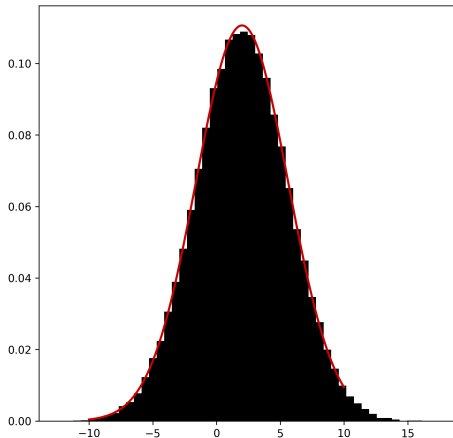
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- ▶ Derive  $p(y) = \mathcal{N}(y; \mu, \sigma_0^2 + \sigma^2)$
- ▶ Sample  $Y \sim p(y)$



# Marginalisation

## Sampling from marginals



**Figure:** The sampling from marginal  $p(y)$  with  $p(x) = \mathcal{N}(x; 2, 2)$  and  $p(y|x) = \mathcal{N}(y; x, 3)$ . The marginal  $p(y)$  is given by  $\mathcal{N}(y; 2, 5)$ . Samples drawn from  $p(x)$  and  $p(y|x)$  as described. Red line is true  $p(y)$  and the histogram is obtained by drawing  $(x, y)$  and keeping only  $y$ .

Define a multivariate Gaussian as

$$p(x) = \mathcal{N}(x; \mu, \Sigma) = \frac{1}{(2\pi)^{d/2} \sqrt{\det \Sigma}} \exp \left( -\frac{1}{2} (x - \mu)^T \Sigma^{-1} (x - \mu) \right).$$

Recall the univariate sampling, using  $X \sim \mathcal{N}(0, 1)$  and  $Y = \mu + \sigma X$ .

# Multivariate Gaussian

## Sampling from Multivariate Gaussian

Define a multivariate Gaussian as

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In the multivariate case, we first compute  $L$  such that  $\Sigma = LL^T$  and then sample  $X \sim \mathcal{N}(0, I)$  (i.e.,)

- ▶ Sample  $X_1, \dots, X_d$  from  $\mathcal{N}(0, 1)$
- ▶ Set  $Y = \mu + LX$

Cholesky decomposition can be computed using `np.linalg.cholesky` in `numpy`.

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- ▶ Sample from mixtures  $p(x) = \sum_{k=1}^M w_k q_k(x)$ 
  - ▶ Sample  $k$  from a discrete distribution  $p(k) = w_k$
  - ▶ Sample  $x \sim q_k(x)$  from the mixture component

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- ▶ Sample from joint  $p(x, y)$ 
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  - ▶  $Y|X = x \sim p(y|x)$
- ▶ Sample from marginal
  - ▶ Sample  $(X, Y) \sim p(x, y)$  as above
  - ▶ Keep only  $Y$  samples

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  - ▶ Sample  $(X, Y) \sim p(x, y)$  as above
  - ▶ Keep only  $Y$  samples
- ▶ Sample from multivariate Gaussian (using Cholesky decomposition)



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  - ▶  $Y|X = x \sim p(y|x)$
- ▶ Sample from marginal
  - ▶ Sample  $(X, Y) \sim p(x, y)$  as above
  - ▶ Keep only  $Y$  samples
- ▶ Sample from multivariate Gaussian (using Cholesky decomposition)

Let us see some examples.

Consider

$$p(x) = \mathcal{N}(x; \mu, \sigma_0^2)$$
$$p(y|x) = \mathcal{N}(y; x, \sigma^2).$$

Compute  $p(y)$ .

# Example 1: Marginalisation of Gaussians

## Solution

The direct computation of the integral

$$p(y) = \int p(y|x)p(x)dx = \int \mathcal{N}(y; x, \sigma^2)\mathcal{N}(x; \mu, \sigma_0^2)dx.$$

could be tedious. Note that

$$y = (y - x) + x$$

$$y - x \sim \mathcal{N}(y - x; 0, \sigma^2)$$

$$x \sim \mathcal{N}(x; \mu, \sigma_0^2).$$

This is a sum of Gaussians. Therefore,  $p(y)$  is also a Gaussian with means and variances summed.

$$p(y) = \mathcal{N}(y; \mu, \sigma_0^2 + \sigma^2).$$

Imagine we would like to simulate data from a linear model. The linear relationship we aim to simulate is

$$y = ax + b + \epsilon,$$

where  $\epsilon \sim \mathcal{N}(0, \sigma^2)$ . In order to simulate data, we could choose  $p(x)$  (modelling assumption). Assume

$$p(x) = \text{Unif}(x; -10, 10).$$

Next, we need to sample from  $p(y|x)$ :

$$p(y|x) = \mathcal{N}(y; ax + b, \sigma^2).$$

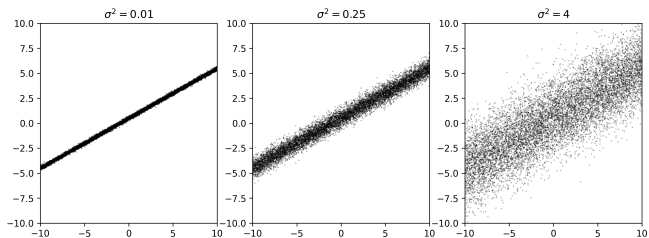
```
import numpy as np
import matplotlib.pyplot as plt

n = 10000
x = np.random.uniform(-10, 10, n)

a = 0.5
b = 0.5
sigma = 2

y = a * x + b + sigma * np.random.normal(0, 1, n)
```

## Example 2: Sample from a linear model



# Example 3: Conditionals

Sampling from joint distributions: The discrete case

Recall our example of a discrete joint distribution  $p(x, y)$

	$X = 0$	$X = 1$	$X = 2$	$X = 3$	$p_Y(y)$
$Y = 0$	1/6	1/6	0	0	2/6
$Y = 1$	1/6	0	1/6	0	2/6
$Y = 2$	0	0	1/6	0	1/6
$Y = 3$	0	0	0	1/6	1/6
$p_X(x)$	2/6	1/6	2/6	1/6	1

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$Y = 3$	0	0	0	1/6	1/6
$p_X(x)$	2/6	1/6	2/6	1/6	1

How to sample e.g.  $p(y|X = 2)$ ?



# Example 3: Conditionals

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$Y = 3$	0	0	0	1/6	1/6
$p_X(x)$	2/6	1/6	2/6	1/6	1

The joint  $p(Y = y, X = 2)$  for  $y = 0, 1, 2, 3$ . The conditional is given by

$$\begin{aligned}
 p(Y = y | X = 2) &= \frac{p(Y = y, X = 2)}{p(X = 2)} \\
 &= \frac{p(Y = y, X = 2)}{2/6}, \\
 &\rightarrow 3 \times [0, 1/6, 1/6, 0] = [0, 1/2, 1/2, 0].
 \end{aligned}$$

# Example 3: Conditionals

Sampling from joint distributions: The discrete case

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 &\rightarrow 3 \times [0, 1/6, 1/6, 0] = [0, 1/2, 1/2, 0].
 \end{aligned}$$

In order to sample, we can use good old inversion.

$p(x, y)$	$X = 0$	$X = 1$	$X = 2$	$X = 3$	$p_Y(y)$
$Y = 0$	1/6	1/6	0	0	2/6
$Y = 1$	1/6	0	1/6	0	2/6
$Y = 2$	0	0	1/6	0	1/6
$Y = 3$	0	0	0	1/6	1/6
$p_X(x)$	2/6	1/6	2/6	1/6	1

Compute and fill in

$p(y x)$	$X = 0$	$X = 1$	$X = 2$	$X = 3$
$Y = 0$				
$Y = 1$				
$Y = 2$				
$Y = 3$				

$p(x, y)$	$X = 0$	$X = 1$	$X = 2$	$X = 3$	$p_Y(y)$
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$Y = 1$	$1/6$	$0$	$1/6$	$0$	$2/6$
$Y = 2$	$0$	$0$	$1/6$	$0$	$1/6$
$Y = 3$	$0$	$0$	$0$	$1/6$	$1/6$
$p_X(x)$	$2/6$	$1/6$	$2/6$	$1/6$	$1$

Compute and fill in

$p(y x)$	$X = 0$	$X = 1$	$X = 2$	$X = 3$
$Y = 0$	$1/2$			
$Y = 1$	$1/2$			
$Y = 2$	$0$			
$Y = 3$	$0$			

$p(x, y)$	$X = 0$	$X = 1$	$X = 2$	$X = 3$	$p_Y(y)$
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$Y = 1$	1/6	0	1/6	0	2/6
$Y = 2$	0	0	1/6	0	1/6
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$Y = 1$	$1/6$	$0$	$1/6$	$0$	$2/6$
$Y = 2$	$0$	$0$	$1/6$	$0$	$1/6$
$Y = 3$	$0$	$0$	$0$	$1/6$	$1/6$
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$Y = 2$	$0$	$0$	$1/6$	$0$	$1/6$
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$p(x y)$	$X = 0$	$X = 1$	$X = 2$	$X = 3$
$Y = 0$	$1/2$	$1/2$	$0$	$0$
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$Y = 1$	$1/2$	$0$	$1/2$	$0$
$Y = 2$	$0$	$0$	$1$	$0$
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Prove the fundamental theorem of simulation.

Theorem 1 (Theorem 2.2, Martino et al., 2018)

*Drawing samples from one dimensional random variable  $X$  with a density  $p(x) \propto \bar{p}(x)$  is equivalent to sampling uniformly on the two dimensional region defined by*

$$A = \{(x, y) \in \mathbb{R}^2 : 0 \leq y \leq \bar{p}(x)\}. \quad (1)$$

*In other words, if  $(x', y')$  is uniformly distributed on  $A$ , then  $x'$  is a sample from  $p(x)$ .*

The proof idea: Start from a uniform distribution  $q(x, y)$  on  $A$  and show that the marginal in  $x$  is  $p(x)$ .

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*Proof.* Consider the pair  $(X, Y)$  uniformly distributed on the region  $A$ . We denote their joint density as  $q(x, y)$  as

$$q(x, y) = \frac{1}{|A|}, \quad \text{for } (x, y) \in A. \quad (2)$$

where  $|A|$  is the area of the set  $A$ .



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$$q(x, y) = \frac{1}{|A|}, \quad \text{for } (x, y) \in A. \quad (2)$$

where  $|A|$  is the area of the set  $A$ . We note that

$$p(x) = \frac{\bar{p}(x)}{|A|}.$$

We use the standard formula for the joint density  $q(x, y) = q(y|x)q(x)$ . Note that, since  $(X, Y)$  is uniform in  $A$ , for fixed  $x$ , we have

$$q(y|x) = \frac{1}{\bar{p}(x)} \quad \text{for } (x, y) \in A.$$

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We therefore write

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We therefore write

$$q(x, y) = q(y|x)q(x) = \frac{q(x)}{\bar{p}(x)} \quad \text{for } (x, y) \in A. \quad (3)$$

We consider now (2) and (3) which are both valid on  $(x, y) \in A$ . Combining them gives

$$q(x) = \frac{\bar{p}(x)}{|A|},$$

which means  $q(x) = p(x)$ . ■

See you next Monday!

- ① Martino, Luca, David Luengo, and Joaquín Míguez (2018). *Independent random sampling methods*. Springer.