# 10: Introduction to Bayesian Computation

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# Introduction

This chapter gives an overview for how to approximate intractable quantities such as posterior expectations and predictions.

# Definitions

**Numerical integration** methods approximate integrals.

These methods can be loosely categorized as either **stochastic** or **deterministic** (e.g. quadrature methods).

# Deterministic Methods

**Deterministic methods** don't draw samples, and instead approximate the integral by summing up approximate volumes:

$$E[h(\theta) \mid y] = \int h(\theta)p(\theta \mid y)\mathrm{d}\theta \approx \frac{1}{S}\sum_{s=1}^{S} w_s h(\theta^s)p(\theta^s \mid y)$$

# Approximating the posterior on a grid

We used this method earlier for the rat tumor example!

Given that we can evaluate the unnormalized target $p(\theta, y) = p(y \mid \theta)p(\theta)$, we choose a nonrandom grid of points (think `seq`) $\theta_1, \ldots, \theta_S$, and then we approximate the the continuous posterior with a discrete random variable with pmf equal to

$$\tilde{p}(\theta_j \mid y) = \frac{p(y \mid \theta_j)p(\theta_j)}{\sum_{s=1}^{S} p(y \mid \theta_s)p(\theta_s)}$$

for any $\theta_j \in \{\theta_1, \ldots, \theta_S\}$. Then

$$E[h(\theta) \mid y] \approx \sum_{j=1}^{S} h(\theta_j)\tilde{p}(\theta_j \mid y).$$

# Stochastic Methods

**Stochastic methods** involve sample averages of simulated draws from some distribution. There are **many** ways to do this, but here are a couple examples that we've seen:

$$E[h(\theta) \mid y] = \int h(\theta)p(\theta \mid y)\mathrm{d}\theta \approx \frac{1}{S}\sum_{s=1}^{S} h(\theta^s)$$

with $\theta^s \sim p(\theta \mid y)$, or

$$E[h(\tilde{y}) \mid y] = \int h(\tilde{y})p(\tilde{y} \mid y)\mathrm{d}\tilde{y} \approx \frac{1}{S}\sum_{s=1}^{S} h(\tilde{y}^s)$$

with $\tilde{y} \sim p(\tilde{y} \mid y)$

# Stochastic Methods

Drawing $\tilde{y}$ samples can be done in a two-stage way:

1. draw $\theta^s \sim p(\theta \mid y)$
2. draw $\tilde{y}^s \sim p(\tilde{y} \mid \theta^s)$

# Stochastic Methods





Drawing $\tilde{y}$ samples can be done in a two-stage way:

1. draw $\theta^s \sim p(\theta \mid y)$
2. draw $\tilde{y}^s \sim p(\tilde{y} \mid \theta^s)$

If you can derive $E\left(h(\tilde{y}) \mid \theta\right)$, you should probably use a Rao-Blackwellized procedure:

$$E[h(\tilde{y}) \mid y] = E[E\left(h(\tilde{y}) \mid \theta\right) \mid y] \approx \frac{1}{S}\sum_{s=1}^{S} E\left(h(\tilde{y}) \mid \theta^s\right)$$

with $\theta^s \sim p(\theta \mid y)$

# The general setup





From now on we will write the posterior in terms of an unnormalized density $q(\theta \mid y)$. In other words:

$$p(\theta \mid y) = \frac{q(\theta \mid y)}{\int q(\theta \mid y) \mathrm{d}\theta}$$

Most (maybe all) of the sampling techniques will assume that we can't evaluate $p(\theta \mid y)$, but that we can evaluate $q(\theta \mid y)$

# Rejection Sampling aka Accept-Reject sampling

Setup

1. $p(\theta \mid y)$ the target, posterior
2. $q(\theta \mid y) = p(y \mid \theta)p(\theta)$ the unnormalized target
3. $g(\theta)$ the "instrumental" or "proposal" distribution
4. need $q(\theta \mid y)/g(\theta) \leq M$ uniformly
5. need $g \gg q$ i.e. the proposal "dominates" your target (won't divide by 0)

We are free to choose our own $g(\theta)$. For the time being, we assume that $\int g(\theta) \mathrm{d}\theta = 1$.

# Rejection Sampling aka Accept-Reject sampling

To (potentially) produce one draw:

1. propose the draw $\theta^s \sim g(\theta)$
2. accept $\theta^s$ with probability $\frac{q(\theta^s|y)}{g(\theta^s)M}$

# Rejection Sampling aka Accept-Reject sampling



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1. propose the draw $\theta^s \sim g(\theta)$
2. accept $\theta^s$ with probability $\frac{q(\theta^s|y)}{g(\theta^s)M}$

Note this is the same as

1. propose the draw $\theta^s \sim g(\theta)$
2. draw $U \sim \text{Uniform}(0, 1]$
3. accept $\theta^s$ if $U < q(\theta^s \mid y)/\{g(\theta^s)M\}$

# Proof

$$P\left(\theta \le t \middle| U \le \frac{q(\theta \mid y)}{Mg(\theta)}\right) = \frac{P\left(\theta \le t, U \le \frac{q(\theta|y)}{Mg(\theta)}\right)}{P\left(U \le \frac{q(\theta|y)}{Mg(\theta)}\right)}$$

$$= \frac{\int_{-\infty}^{t} \int_{0}^{\frac{q(\theta|y)}{Mg(\theta)}} g(\theta) 1 \mathrm{d}u \mathrm{d}\theta}{\int_{-\infty}^{\infty} \int_{0}^{\frac{q(\theta|y)}{Mg(\theta)}} g(\theta) 1 \mathrm{d}u \mathrm{d}\theta}$$

$$= \frac{\int_{-\infty}^{t} g(\theta) \frac{q(\theta|y)}{Mg(\theta)} \mathrm{d}\theta}{\int_{-\infty}^{\infty} g(\theta) \frac{q(\theta|y)}{Mg(\theta)} \mathrm{d}\theta}$$

$$= \frac{\int_{-\infty}^{t} q(\theta \mid y) \mathrm{d}\theta}{\int_{-\infty}^{\infty} q(\theta \mid y) \mathrm{d}\theta}$$

$$= P(\theta \le t \mid y).$$

# Example 1

Assume $y \sim \text{Normal}(\theta, 1)$, and $p(\theta) = \frac{1}{\pi(1+\theta^2)}$. Our goal is to draw from

$$\begin{aligned} p(\theta \mid y) &\propto q(\theta \mid y) \\ &= p(y \mid \theta) p(\theta) \\ &= \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}(y-\theta)^2\right] \frac{1}{\pi(1+\theta^2)} \\ &\propto \exp\left[-\frac{(\theta-y)^2}{2} - \log(1+\theta^2)\right], \end{aligned}$$

# Example 1

Let's assume that we want to use our prior distribution as a proposal: $g(\theta) = p(\theta)$. Then we have to find $M$:

$$
\begin{aligned}
\frac{q(\theta \mid y)}{g(\theta)} &= \frac{p(y \mid \theta)p(\theta)}{p(\theta)} \\
&= p(y \mid \theta) \\
&= \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}(y-\theta)^2\right] \\
&\leq \frac{1}{\sqrt{2\pi}} \stackrel{\text{def}}{=} M
\end{aligned}
$$

Our acceptance probability for draw $\theta^s$ is then

$$q(\theta^s \mid y)/\{g(\theta^s)M\} = p(y \mid \theta^s)/M = \exp\left[-\frac{1}{2}(y-\theta^s)^2\right]$$

# Rejection Sampling aka Accept-Reject sampling



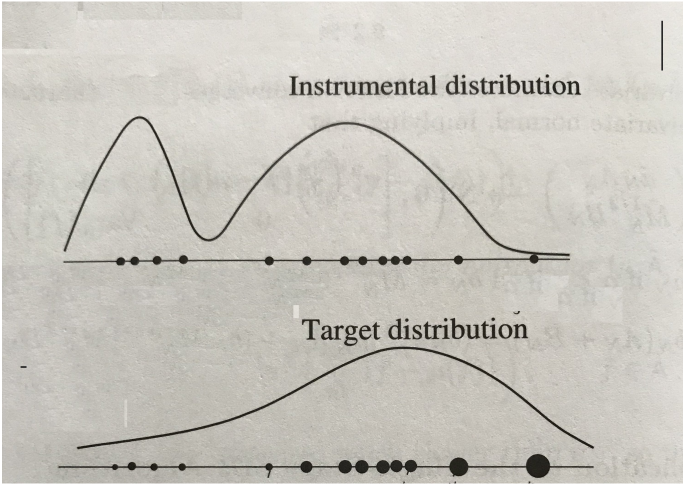
Generally a good strategy is work with logarithms, and then exponentiate as late as possible.

```
y <- 2 # fake data
num_trials <- 1000
theta_proposals <- rt(num_trials, 1)
us <- runif(num_trials, min = 0, max = 1)
log_accept_prob <- function(theta){
  -.5*(y - theta)^2
}
probs <- exp(log_accept_prob(theta_proposals))
accepts <- ifelse(us < probs, TRUE, FALSE)
hist(theta_proposals[accepts]) # only the accepted draws
#hist(theta_proposals) # all draws!
```

# Importance Sampling

**importance sampling** also involves ratios like the previous algorithm. However, instead of using those ratios to either accept or discard samples, it uses the ratios to weight samples.

# Importance Sampling

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# Importance Sampling





Setup

1. $p(\theta \mid y)$ the target, posterior
2. $q(\theta \mid y) = p(y \mid \theta)p(\theta)$ the unnormalized target
3. $g(\theta)$ the "instrumental" or "proposal" distribution
4. $g \gg q$ i.e. the proposal dominates your target

We are free to choose our own $g(\theta)$. For the time being, we assume that $\int g(\theta)\mathrm{d}\theta = 1$.

# Importance Sampling

Algorithm: for each iteration $s$

1. draw $\theta^s \sim g(\theta)$
2. calculate unnormalized weight $\tilde{w}(\theta^s) = \frac{q(\theta^s|y)}{g(\theta^s)}$
3. calculate normalized weights $w(\theta^s) = \tilde{w}(\theta^s)/\sum_r \tilde{w}(\theta^r)$

Final calculation:

$$E_q[h(\theta) \mid y] \approx \sum_s w(\theta^s)h(\theta^s)$$

# Importance Sampling

Motivation:

$$
\begin{aligned}
E_q[h(\theta) \mid y] &= \int h(\theta)p(\theta \mid y)\mathrm{d}\theta \\
&= \frac{\int h(\theta)q(\theta \mid y)\mathrm{d}\theta}{\int q(\theta \mid y)\mathrm{d}\theta} \\
&= \frac{\int h(\theta)\frac{q(\theta|y)}{g(\theta)}g(\theta)\mathrm{d}\theta}{\int \frac{q(\theta|y)}{g(\theta)}g(\theta)\mathrm{d}\theta}
\end{aligned}
$$

# Importance Sampling





Motivation:

$$
\begin{aligned}
E_q[h(\theta) \mid y] &= \int h(\theta) p(\theta \mid y) \mathrm{d}\theta \\
&= \frac{\int h(\theta) q(\theta \mid y) \mathrm{d}\theta}{\int q(\theta \mid y) \mathrm{d}\theta} \\
&= \frac{\int h(\theta) \frac{q(\theta|y)}{g(\theta)} g(\theta) \mathrm{d}\theta}{\int \frac{q(\theta|y)}{g(\theta)} g(\theta) \mathrm{d}\theta}
\end{aligned}
$$

So first:

$$
\frac{1}{S} \sum_{s=1}^{S} \frac{q(\theta^s \mid y)}{g(\theta^s)} \rightarrow E_g\left[\frac{q(\theta \mid y)}{g(\theta)}\right] = \int \frac{q(\theta \mid y)}{g(\theta)} g(\theta) \mathrm{d}\theta = \int q(\theta \mid y) \mathrm{d}\theta
$$

# Importance Sampling





1. $E_q[h(\theta) \mid y] = \frac{\int h(\theta)q(\theta|y)\mathrm{d}\theta}{\int q(\theta|y)\mathrm{d}\theta}$
2. $\frac{1}{S}\sum_{s=1}^{S} \frac{q(\theta^s|y)}{g(\theta^s)} \to \int q(\theta \mid y)\mathrm{d}\theta$ ( for the denominator)

And second:

$$\frac{1}{S}\sum_{s=1}^{S} h(\theta^s)\frac{q(\theta^s \mid y)}{g(\theta^s)} \to E_g\left[h(\theta)\frac{q(\theta \mid y)}{g(\theta)}\right] = \int h(\theta)q(\theta \mid y)\mathrm{d}\theta$$

which converges to the numerator

# Importance Sampling





1. $E_q[h(\theta) \mid y] = \frac{\int h(\theta)q(\theta|y)\mathrm{d}\theta}{\int q(\theta|y)\mathrm{d}\theta}$
2. $\frac{1}{S}\sum_{s=1}^{S} \frac{q(\theta^s|y)}{g(\theta^s)} \to \int q(\theta \mid y)\mathrm{d}\theta$
3. $\frac{1}{S}\sum_{s=1}^{S} h(\theta^s)\frac{q(\theta^s|y)}{g(\theta^s)} \to \int h(\theta)q(\theta \mid y)\mathrm{d}\theta$

So finally

$$\sum_{i=1}^{S} w(\theta^s)h(\theta^s) = \frac{\sum_{s=1}^{S} h(\theta^s)\frac{q(\theta^s|y)}{g(\theta^s)}}{\sum_{r=1}^{S} \frac{q(\theta^r|y)}{g(\theta^r)}} = \frac{\frac{1}{S}\sum_{s=1}^{S} h(\theta^s)\frac{q(\theta^s|y)}{g(\theta^s)}}{\frac{1}{S}\sum_{r=1}^{S} \frac{q(\theta^r|y)}{g(\theta^r)}} \to E[h(\theta) \mid y]$$

where $w(\theta^s) = \frac{q(\theta^s|y)}{g(\theta^s)} \Big/ \sum_{r=1}^{S} \frac{q(\theta^r|y)}{g(\theta^r)}$ are the self-normalized weights

# Example 2

Assume $y \sim \text{Normal}(\theta, 1)$, and $p(\theta) = \frac{1}{\pi(1+\theta^2)}$. Approximate $E_q[\theta \mid y]$ using proposal $g(\theta) = p(\theta)$.

# Example 2

Assume $y \sim \text{Normal}(\theta, 1)$, and $p(\theta) = \frac{1}{\pi(1+\theta^2)}$. Approximate $E_q[\theta \mid y]$ using proposal $g(\theta) = p(\theta)$.

If we sample from $g(\theta) = p(\theta) = \frac{1}{\pi(1+\theta^2)}$ then the unnormalized weights are

$$\begin{aligned}
\tilde{w}(\theta^s) &= \frac{q(\theta^s \mid y)}{g(\theta^s)} \\
&= p(y \mid \theta^s) \\
&= \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}(y - \theta^s)^2\right]
\end{aligned}$$

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&= p(y \mid \theta^s) \\
&= \frac{1}{\sqrt{2\pi}} \exp\left[-\frac{1}{2}(y - \theta^s)^2\right]
\end{aligned}$$

then normalize these...

# Example 2

```
y <- 2 # fake data
num_samples <- 1000000
theta_draws <- rt(num_samples , 1)
log_unnorm_weight <- function(theta){
  # sqrt(2pi) because it will cancel out
  -.5*(y - theta)^2
}
lunws <- log_unnorm_weight(theta_draws)
norm_weights <- exp(lunws)/sum(exp(lunws))
sum(norm_weights * theta_draws)
hist(norm_weights)
```

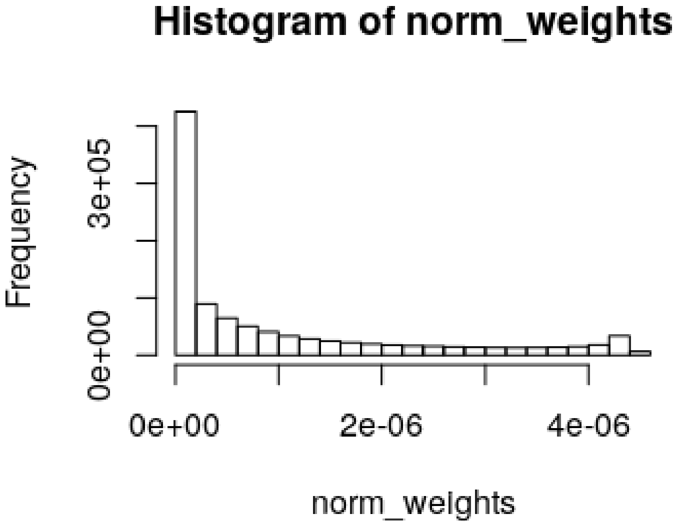
# Example 2

The choice of proposal is very important:

Using the Delta method:

$$\mathrm{Var}_g\left(\sum_{s=1}^{S} w(\theta^s)h(\theta^s)\right) \approx \frac{1}{S}E_g\left[\underbrace{\left(\frac{\tilde{w}(\theta)}{E_g[\tilde{w}(\theta)]}\right)^2}_{!}(h(\theta) - E_q[h(\theta)])^2\right]$$

# Example 2



Histogram of norm_weights
Frequency
0e+00
3e+05
0e+00
2e-06
4e-06
norm_weights

# Example 2

Beware of bad proposal distributions!

A sample estimator of this approximate variance is

$$\sum_{s=1}^{S} w(\theta^s) \left( h(\theta^s) - \hat{E}[h(\theta)] \right)^2$$

where $\hat{E}[h(\theta)] = \sum_s w(\theta^s) h(\theta^s)$.

Note the weights aren't the same for each sample, like a "standard" estimation of the sample variance.

# Example 2

```
y <- 2 # fake data
log_unnorm_weight <- function(theta){
  # sqrt(2pi) because it will cancel out
  -.5*(y - theta)^2 }
getISEstimator <- function(num_samples){
  theta_draws <- rt(num_samples , 1)
  lunws <- log_unnorm_weight(theta_draws)
  norm_weights <- exp(lunws)/sum(exp(lunws))
  estimator <- sum(norm_weights * theta_draws)
  list("estimate" = estimator,
       "approx_var" =
       sum( norm_weights*(theta_draws - estimator)^2) ) }
# two ways to calculate standard errors
num_samps_per_estimate <- 10
sqrt(getISEstimator(num_samps_per_estimate)$approx_var)
sd(replicate(1000,
    getISEstimator(num_samps_per_estimate)$estimate))
```

# Effective Sample Size





Effective sample size calculations use the delta method, too.

One form is

$$\mathrm{ESS} = \frac{S}{1 + \mathrm{Var}_g(W)}.$$

and the other form is

$$\mathrm{ESS} = \frac{1}{\sum_{i=1}^{S} w_i^2}.$$

You will derive these in a homework problem using the multivariate delta method.

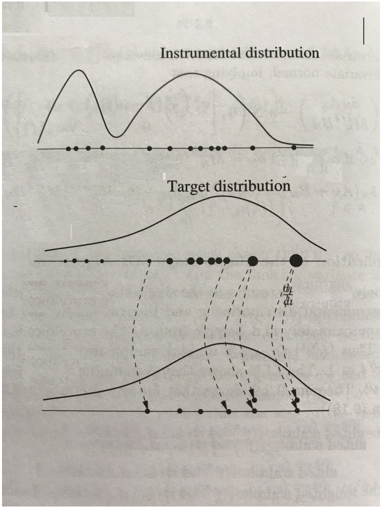
# Adding Resampling

Importance Sampling gives you weighted draws $(\theta^1, w(\theta^1)), (\theta^2, w(\theta^2)), \ldots$

You can draw from these, with replacement. At the expense of more variance, it will give you unweighted draws from your target distribution: $\tilde{\theta}^1, \tilde{\theta}^2, \ldots$

This is known as **factored sampling** or **importance sampling with resampling** or **sampling importance resampling** (SIR).

# Adding Resampling

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# SIR

Stage 1: do importance sampling to get $\{\theta^i, w(\theta^i)\}_{i=1}^S$.

Stage 2: for $i = 1, \ldots, S$, select

$$P[\tilde{\theta}^i = \theta^j \mid \theta^1, w(\theta^1), \ldots, \theta^S, w(\theta^S)] = \frac{w(\theta^j)}{\sum_k w(\theta^k)}.$$

# SIR

Another way to write it:

Stage 1: do importance sampling to get $\{\theta^i, w(\theta^i)\}_{i=1}^S$.

Stage 2: for $i = 1, \ldots, S$, select indexes

$$P[I^i = j \mid \theta^1, w(\theta^1), \ldots, \theta^S, w(\theta^S)] = \frac{w(\theta^j)}{\sum_k w(\theta^k)}$$

and then set

$$\tilde{\theta}^i = \theta^{I^i}.$$

# Example 2 revisited

```
y <- 2 # fake data
log_unnorm_weight <- function(theta){
  # sqrt(2pi) because it will cancel out
  -.5*(y - theta)^2 }
num_samples <- 10000
theta_draws <- rt(num_samples , 1)
lunws <- log_unnorm_weight(theta_draws)
# note: prob arg automatically normalizes
random_indexes <- sample(x = num_samples,
                         size = num_samples,
                         replace = T,
                         prob = exp(lunws))
sort(random_indexes) # repeats!
resampled_draws <- theta_draws[random_indexes]
hist(resampled_draws) # can't do this unless we resample
```

# Going sequential

Resampling adds variance, so why do it?

It throws away bad samples, and duplicates promising ones. When you're looking at a sequence of distribution targets, this can have a good effect on future samples.

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It throws away bad samples, and duplicates promising ones. When you're looking at a sequence of distribution targets, this can have a good effect on future samples.

**sequential monte carlo** or **particle filtering** methods are basically doing SIR over and over again.

# Examples of sequences of distributions

**Data annealing**[1]

$$p(\theta), p(\theta \mid y_1), p(\theta \mid y_{1:2}), \ldots, p(\theta \mid y_{1:n}),$$

**Temperature annealing**[2]

$$p(y \mid \theta)^{a_0} p(\theta), p(y \mid \theta)^{a_1} p(\theta), \ldots p(y \mid \theta)^{a_n} p(\theta)$$

with $0 = a_0 < a_1 < \cdots < a_n = 1$.

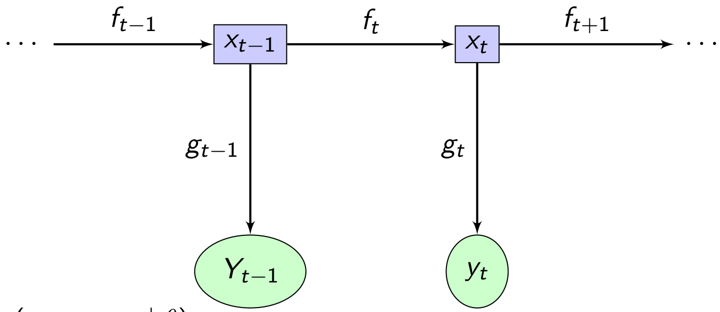
**filtering and smoothing** in state space models

$$p(x_1 \mid y_1, \theta), \ldots, p(x_n \mid y_{1:n}, \theta)$$

[1] Chopin, *A Sequential Particle Filter Method for Static Models*.

[2] Neal, "Annealed Importance Sampling".

## state space models




$$
\begin{aligned}
&p(x_{1:T}, y_{1:T} \mid \theta) \\
&= g(y_1 \mid x_1, \theta) f(x_1 \mid \theta) \prod_{t=2}^{T} g(y_t \mid x_t, \theta) f(x_t \mid x_{t-1}, \theta)
\end{aligned}
$$

# Example: filtering in state space models

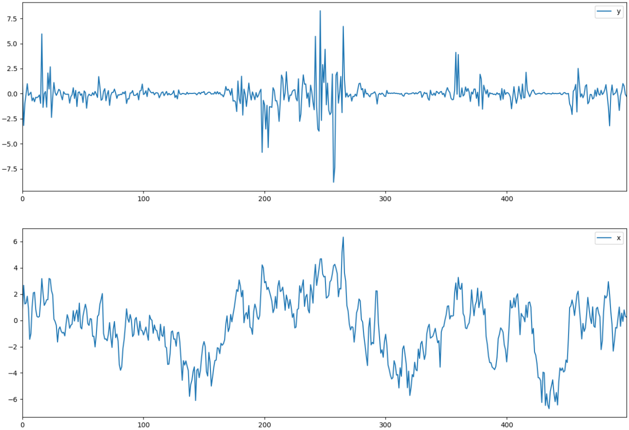
Here's an example of a state space model. $y_t$ is a univariate time series, and $x_t$ is a hidden/unobserved/latent time series.

$$y_t = \exp(x_t/2)\epsilon_t \tag{1}$$
$$x_t = c + \phi x_{t-1} + v_t \tag{2}$$

We sometimes refer to (1) as $g(y_t \mid x_t, \theta)$ or the observation equation, and (2) as the state transition equation or $f(x_t \mid x_{t-1}, \theta)$.

# Example: filtering in state space models

$y_{1:t}$ observed, $x_{1:t}$ hidden. Goal: $p(x_t \mid y_{1:t})$ in real-time.



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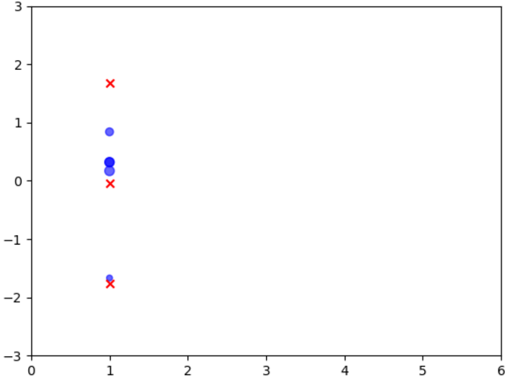
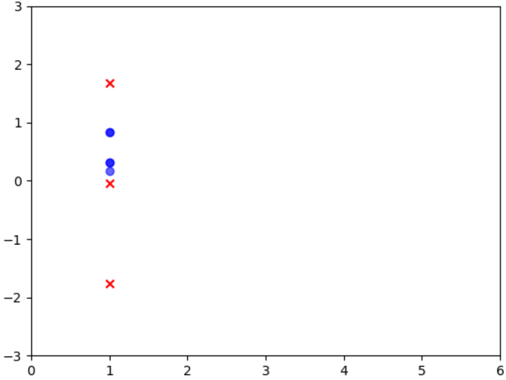


# Going sequential



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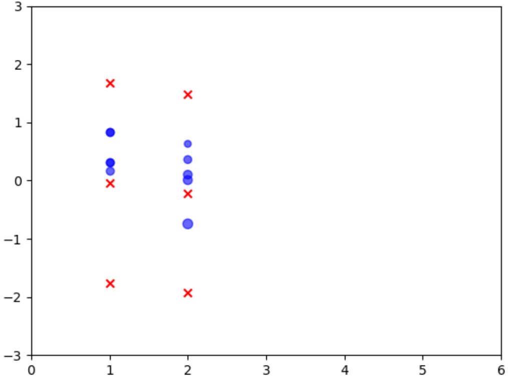

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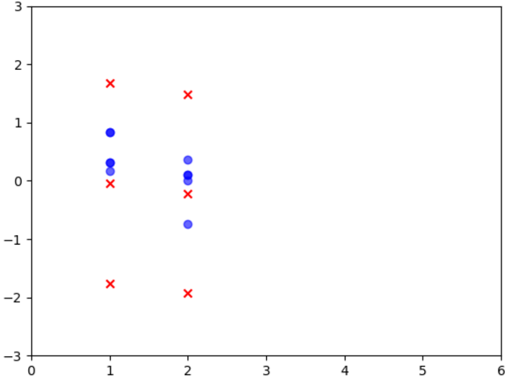

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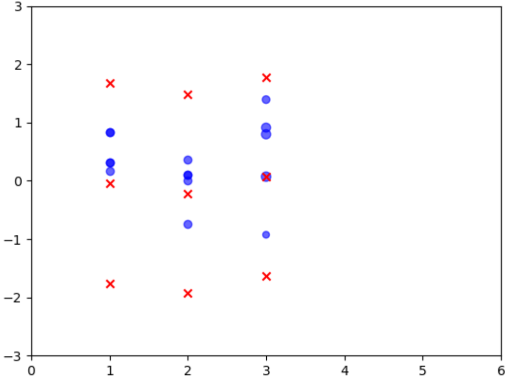

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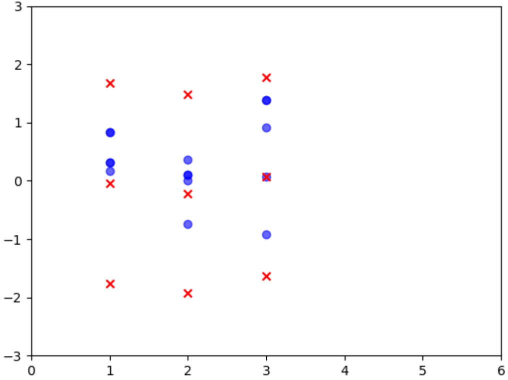

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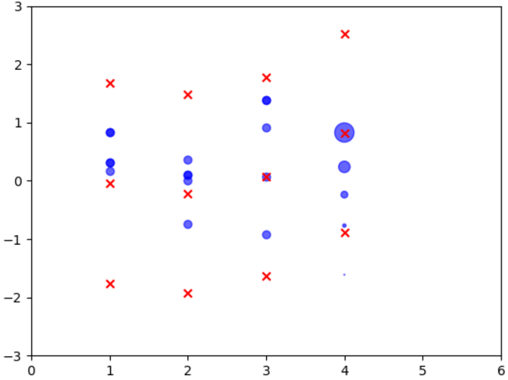

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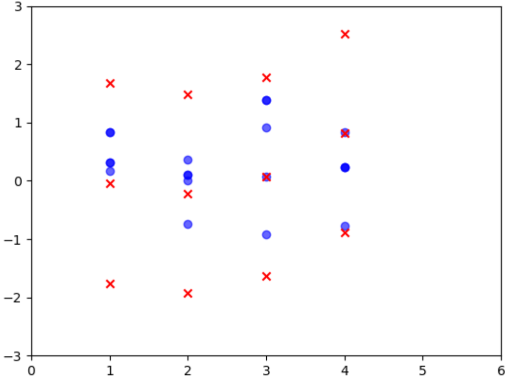

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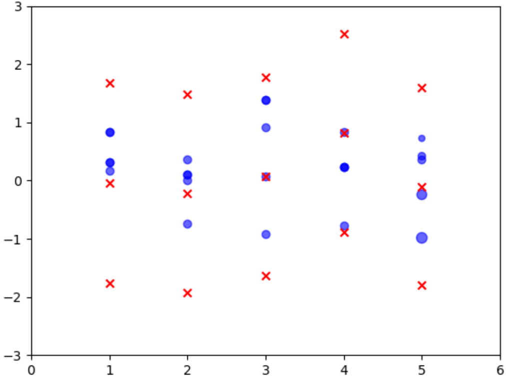

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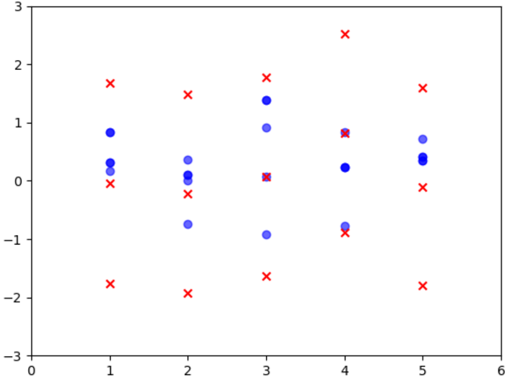

# Filtering recursions

Drop dependence on $\theta$ from the notation...

$$
\begin{aligned}
p(x_{1:t}|y_{1:t}) &= C_t^{-1} p(x_t, y_t \mid x_{t-1}) p(x_{1:t-1} \mid y_{1:t-1}) \\
&= C_t^{-1} \frac{p(x_t, y_t \mid x_{t-1})}{q_t(x_t \mid y_t, x_{t-1})} \times \\
&\qquad\qquad q_t(x_t \mid y_t, x_{t-1}) p(x_{1:t-1} \mid y_{1:t-1}) \\
&= C_t^{-1} \frac{g(y_t|x_t) f(x_t|x_{t-1})}{q_t(x_t|x_{t-1}, y_t)} \times \\
&\qquad\qquad q_t(x_t \mid x_{t-1}, y_t) p(x_{1:t-1} \mid y_{1:t-1})
\end{aligned}
$$

Repeat through time:

1. start with samples from $p(x_{1:t-1} \mid y_{1:t-1})$
2. mutate/propogate/extend using $q_t(x_t \mid x_{t-1}, y_t)$
3. adjust weights by multiplying by $\frac{g(y_t|x_t) f(x_t|x_{t-1})}{q_t(x_t|x_{t-1}, y_t)}$
4. resample, giving you particles distributed as $p(x_{1:t} \mid y_{1:t})$

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