APSTA-GE 2352

Statistical Computing: Lecture 9

Klint Kanopka

New York University

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Announcements

- PS4 is now late
  - Very spooky
  - How’s it going?
- PS5 is up!
  - It’s long
  - The code you write will take time to run

Check-In

- PollEv.com/klintkanopka

A Very Important Problem

A Problem

Klint now finds that he can make even more money by selling both hot dogs and actual dogs. He finds that his daily revenue for selling x dozen hot dogs and y dozen actual dogs is:

$$R(x, y) = -5x^2 - 8y^2 - 2xy + 42x + 102y$$

If he can only obtain 10 dozen of either item in a day, what should he prepare to maximize revenue?

Four Potential Solutions:

1. Find an analytic solution (calculus)
2. Reframe as an optimization problem and find a numeric solution (`optim()`)
3. Guess random numbers until you find the right answer (terrible idea)
4. A secret fourth thing!

A Solution We Know!

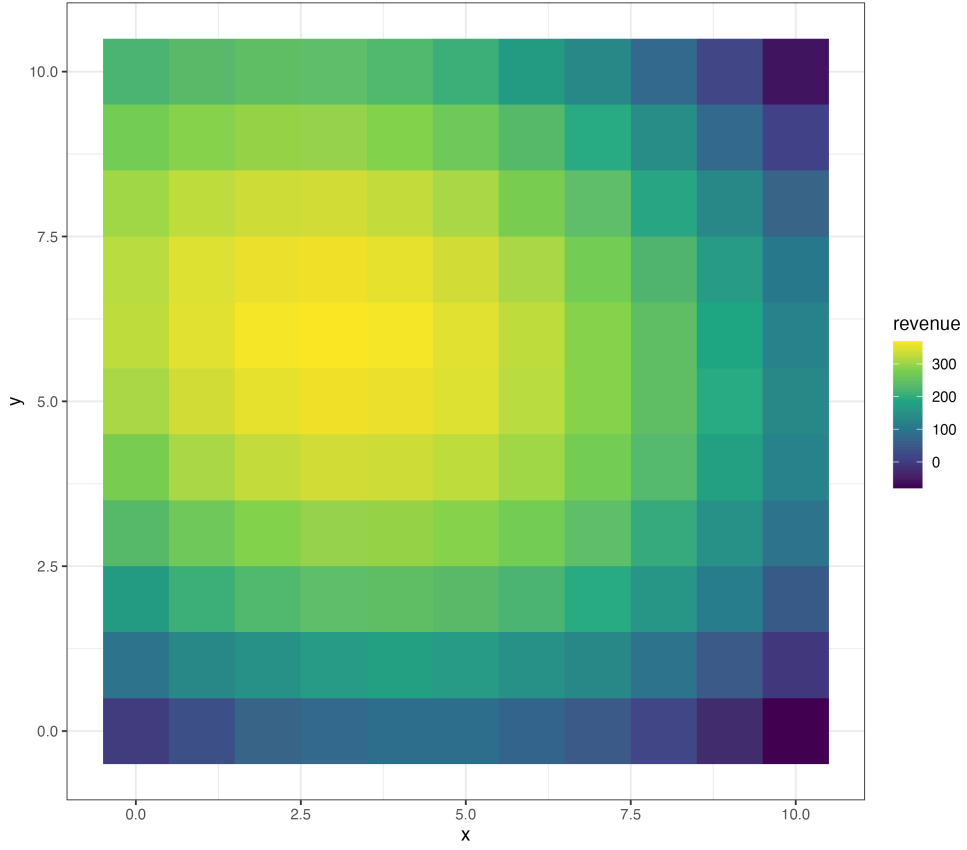
- We can write a function and maximize it to find the best values of x, y
- If you write this function carefully, you can just use `optim()` to spit out an answer

A variety of dogs with `optim()`

```r
HotDogsDogs <- function(par){
  x <- par[1]
  y <- par[2]
  R <- -5*x^2 -8*y^2 -2*x*y + 42*x + 102*y
  return(R)
}

hotdogs <- expand.grid(x=0:10, y=0:10, revenue=0)

for (i in 1:nrow(hotdogs)){
  hotdogs$revenue[i] <- HotDogsDogs(c(hotdogs$x[i], hotdogs$y[i]))
}
```

A variety of dogs with `optim()`

```r
ggplot(hotdogs,
       aes(x = x,
           y = y,
           fill = revenue)) +
  geom_tile() +
  scale_fill_viridis_c() +
  coord_equal() +
  theme_bw()

out <- optim(
  c(1, 1),
  HotDogsDogs,
  lower = c(0, 0),
  upper = c(10, 10),
  method = "L-BFGS-B",
  control = list(fnscale = -1)
)

out$par

# [1] 3 6
```



Markov Chain Monte Carlo

Markov Chain Monte Carlo (MCMC)

- A super clever algorithm that fits somewhere between direct numerical optimization and just guessing random answers
- Conceptually really kind of weird, but practically pretty straightforward
- **Core idea:** We define a random walk across our search space that places higher probability of landing on "good" answers than "bad" answers. Then we take the walk for a while and find our answer from the places we go

Random Walks

- A process that describes a succession of random steps on some mathematical space
- Imagine a new way to pick a restaurant:
  1. Stand outside your apartment and flip a coin twice
     - If you get H,H, you walk one block north
     - If you get H,T, you walk one block south
     - If you get T,H you walk one block east
     - If you get T,T you walk one block west
  2. Repeat this a whole bunch of times
  3. After some number of steps, eat at the first restaurant you pass
- Sometimes called a “drunkard’s walk”

Markov Chains

- A Markov process is defined by two parts:
  1. A set of states
  2. A transition function that dictates the probability of moving from one state to any other
- Markov processes are “memoryless”
  - Predicting the next state relies only on the current state, not anything before!
  - Called the “Markov Property”
  - Sampling from a Markov process is a sequential process
- A Markov chain is a type of Markov process
  - Nobody really agrees on the exact definition
  - This doesn’t really matter

The Stationary Distribution

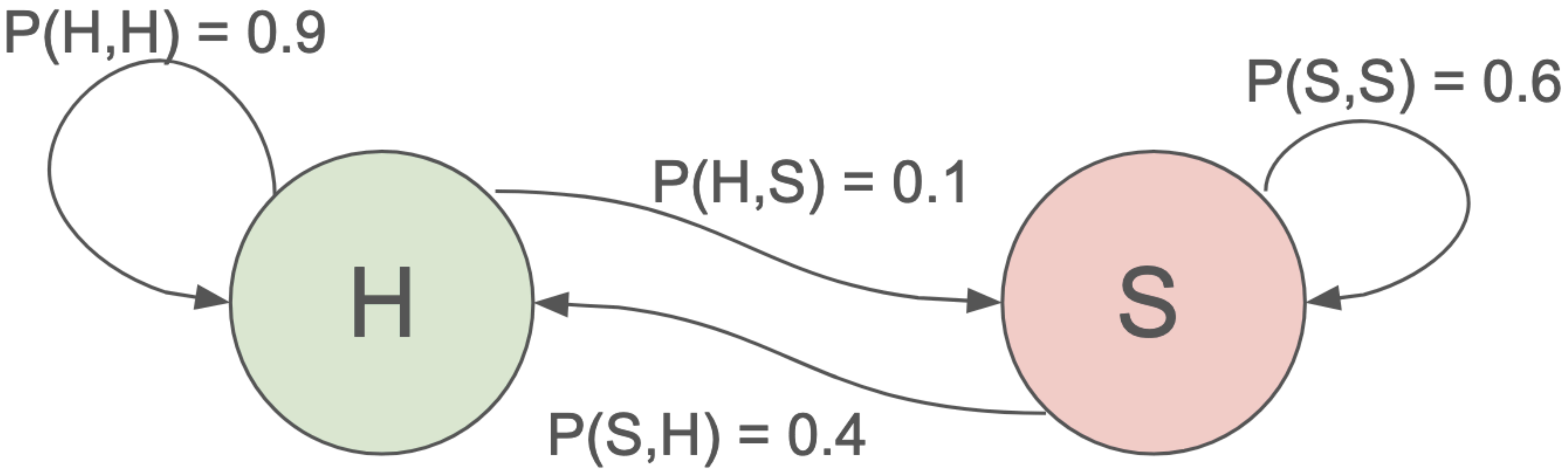
- **The Fundamental Theorem of Markov Chains**: Consider a Markov Chain that satisfies the following two conditions
  1. For all pairs of states s_i, s_j, it is possible to eventually get to state s_j if you start at s_i
  2. The chain is *aperiodic* (satisfied if there are no directed cycles and the states aren't bipartite)
- As the number of samples from the chain grows large, the probability of being in any particular state converges to a *stationary distribution* and this distribution is independent of time and starting state

Getting Sick as a Markov Chain

- Two states: Healthy (H) and Sick (S)
- Transition Probabilities:
  - $P(H, H) = 0.9$
  - $P(H, S) = 0.1$
  - $P(S, H) = 0.4$
  - $P(S, S) = 0.6$

$$T(S_1, S_2) = \begin{bmatrix} 0.9 & 0.1 \\ 0.4 & 0.6 \end{bmatrix}$$

Getting Sick as a Markov Chain



Taking the Walk

- If we want to know what percentage of the time we can expect to be sick, we just start somewhere and take the random walk
- If we sample from the Markov Chain for a while, eventually we converge to the stationary distribution
- The proportion of time we spend in each state is the proportion of time we expect to be in that state given the Markov Chain
- Also gives the probability a random observation is in that location
- Another approach is *power iteration*
  1. Pick some random state vector to start (doesn't matter where you start!)
  2. Multiply by the transition matrix a bunch of times
  3. The state vector converges to the stationary distribution

Google PageRank

- Google is Google because of PageRank
- **Core idea**: Important and relevant webpages have incoming links from important and relevant webpages
- **How to estimate**: Take a random walk through websites and see what sites are visited the most often
- **Core problem**: It's not possible to reach every possible website from every possible starting location—so it doesn't satisfy the fundamental theorem of Markov Chains!
- **Solution**: Teleportation! With some random chance, instead of clicking a link, teleport to a random website
- You'll implement this on a smallish graph in the homework

MCMC Problem Solving Process

1. Define your state space
2. Define the transition function

- Be sure it can (eventually) make it to every possible state
- Be sure it is aperiodic (no directed loops)

3. Start somewhere and sample from your Markov Chain a bunch of times
4. Throw away the samples in the beginning (burn-in)
5. Look at what's left

Today's approach will be a slightly simplified version of the Metropolis-Hastings algorithm, which will show up a lot in Bayesian inference, but it's not the only way to MCMC!

Back to Dogs

- We have a pretty easy to optimize function, so MCMC is way less efficient than solutions we already know
- Who cares, let’s do it anyway

Setting Up

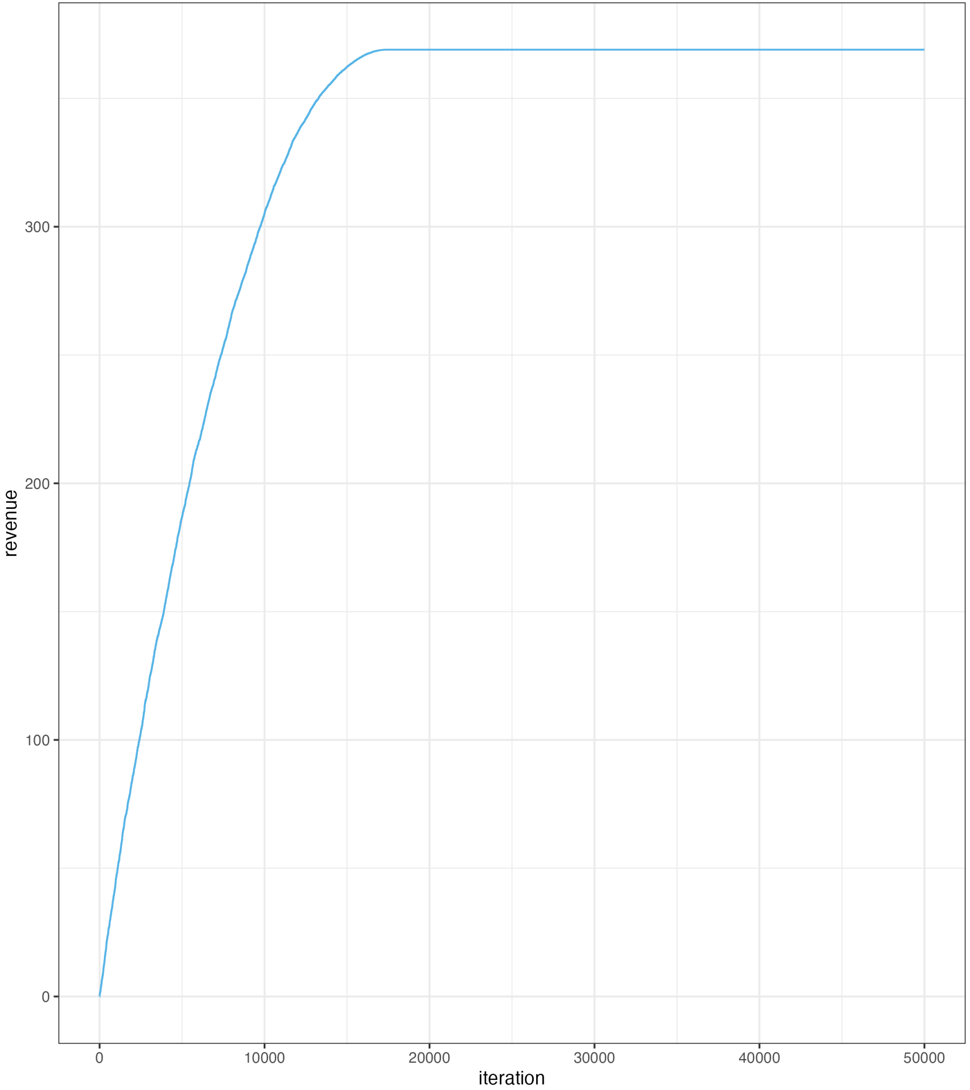
```r
# First, we optimize the same loss function:

HotDogsDogs <- function(par){
  x <- par[1]
  y <- par[2]
  R <- -5*x^2 -8*y^2 -2*x*y + 42*x + 102*y
  return(R)
}

# Next, we propose new parameters:

ProposeParams <- function(params, lambda){
  new_params <- params + rnorm(2, mean=0, sd=lambda)
  return(new_params)
}
```

Dogs with MCMC

```r
N_iter <- 5e4

revenue <- vector('numeric', length=N_iter)
params <- rep(0,2)
best <- params

param_history <- matrix(NA, nrow=N_iter, ncol=1+length(params))

lambda <- 1e-3
temp <- 0.025

for (i in 1:N_iter){
  new_params <- ProposeParams(params, lambda)
  if (HotDogsDogs(new_params) > HotDogsDogs(params) | runif(1) < temp){
    params <- new_params
  }
  if (HotDogsDogs(params) > HotDogsDogs(best)){
    best <- params
  }
  param_history[i,] <- c(i, params)
  revenue[i] <- HotDogsDogs(params)
}
```

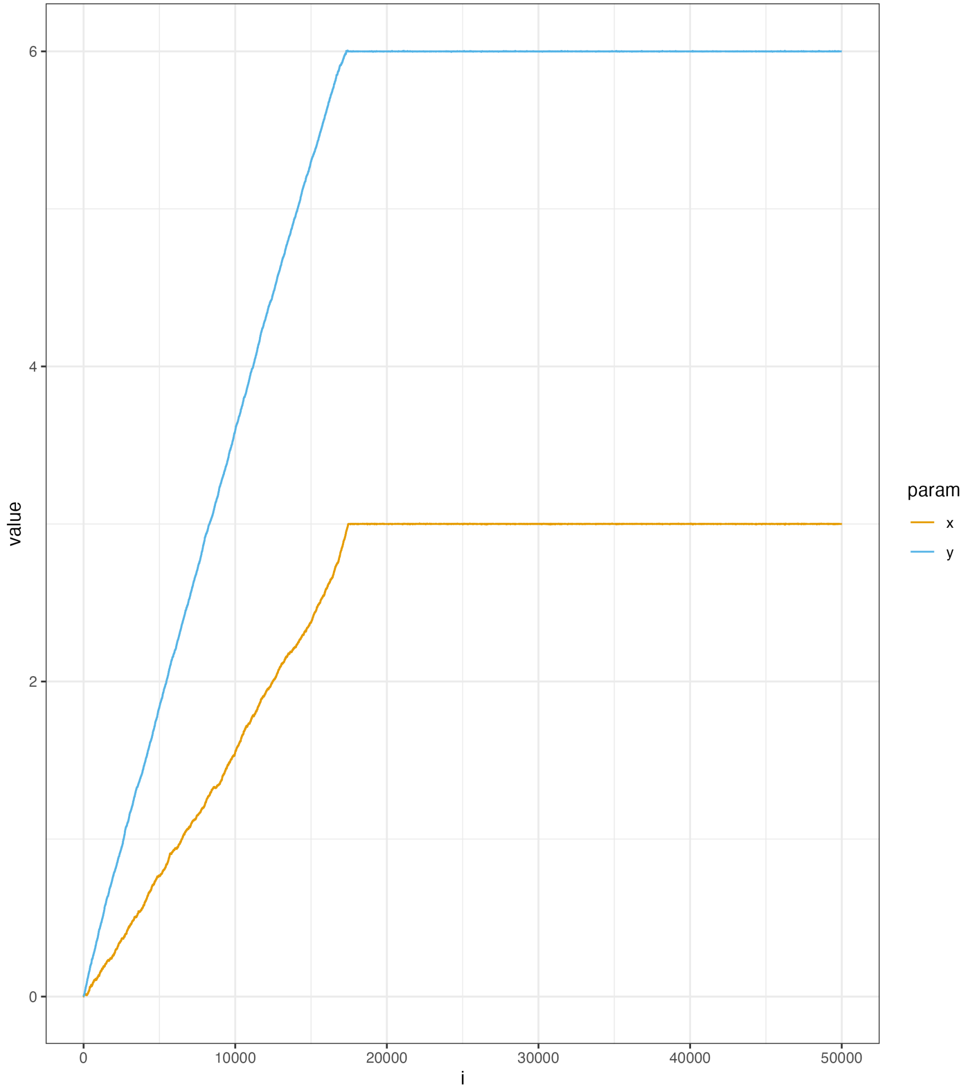
MCMC Results

```
conv <- data.frame(
  i = 1:N_iter,
  revenue=revenue
)

ggplot(conv, aes(x=i, y=revenue)) +
  geom_line(color=okabeito_colors(2)) +
  labs(x='iteration', y='revenue') +
  theme_bw()
```



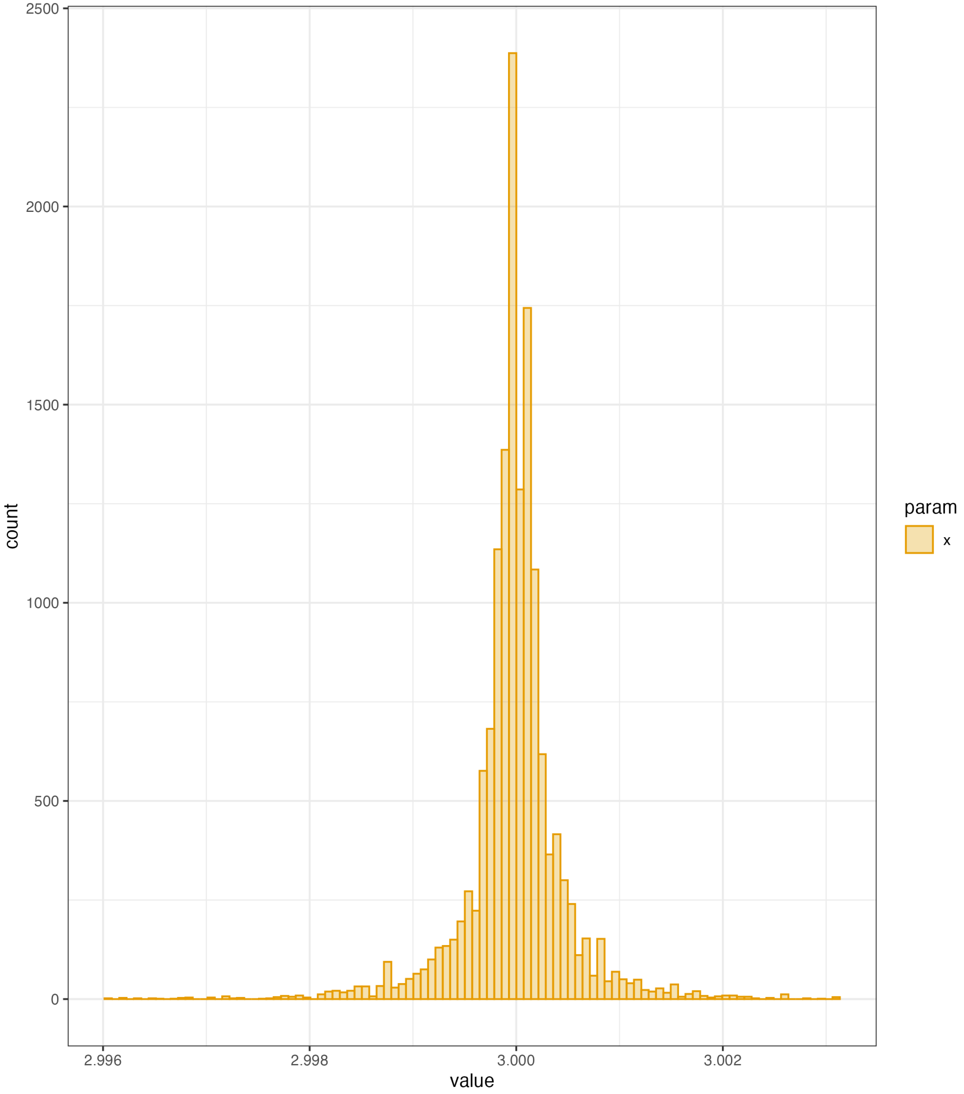
MCMC Results

```r
param_history <- data.frame(param_history)
names(param_history) <- c('i', 'x', 'y')

param_history |>
  pivot_longer(-i, names_to='param') |>
  ggplot(aes(x=i, y=value, color=param)) +
  geom_line() +
  scale_color_okabeito() +
  theme_bw()
```



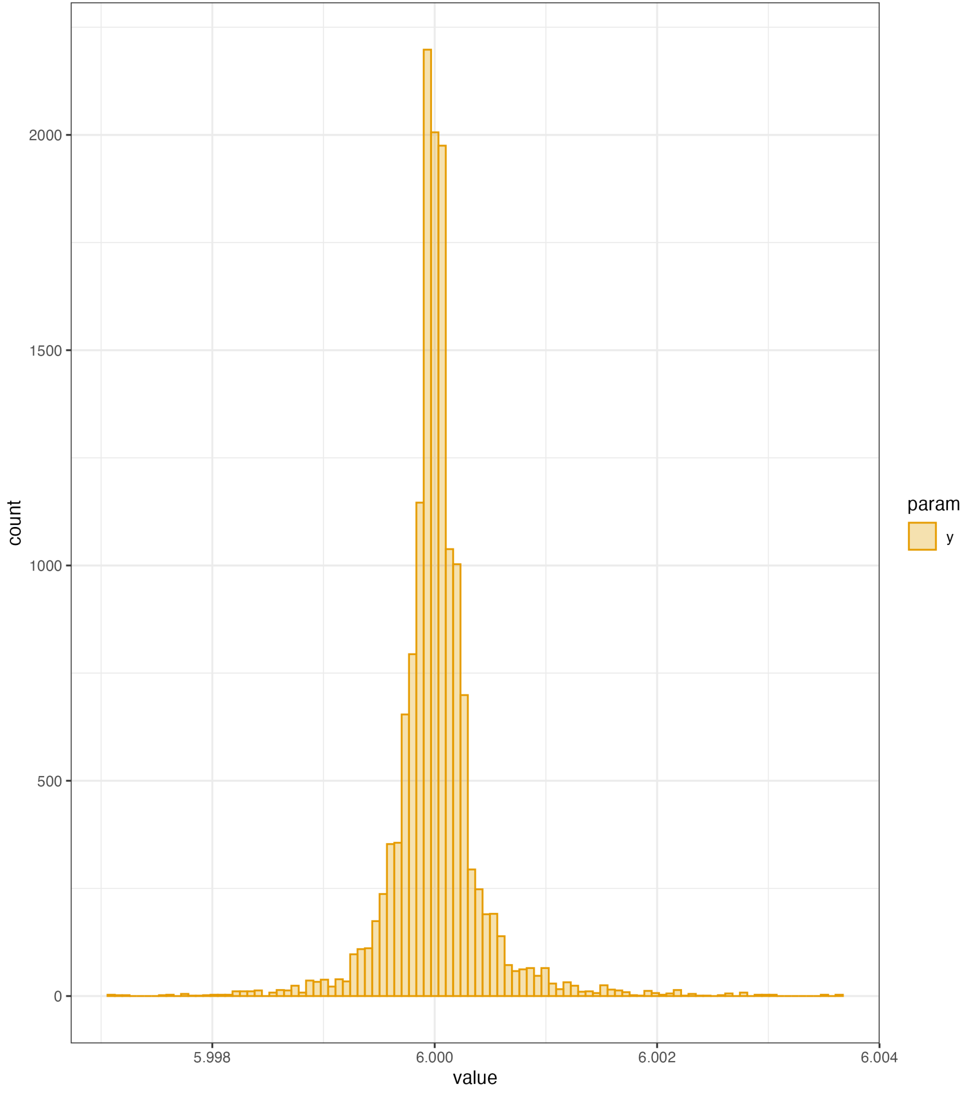
MCMC Results

```
param_history |>
  pivot_longer(-i, names_to='param') |>
  filter(i >= 35000) |>
  filter(param=='x') |>
  ggplot(aes(x=value,
             color=param,
            fill=param)) +
  geom_histogram(alpha=0.3, bins=100) +
  scale_color_okabeito() +
  scale_fill_okabeito() +
  theme_bw()
```



MCMC Results

```r
param_history |>
  pivot_longer(-i, names_to='param') |>
  filter(i >= 35000) |>
  filter(param=='y') |>
  ggplot(aes(x=value,
             color=param,
             fill=param)) +
  geom_histogram(alpha=0.3, bins=100) +
  scale_color_okabeito() +
  theme_bw()

colMeans(param_history[35000:N_iter, 2:3])

#        x        y
# 2.999987 6.000010

best

# [1] 3.000002 6.000000
```



What About Temperature?

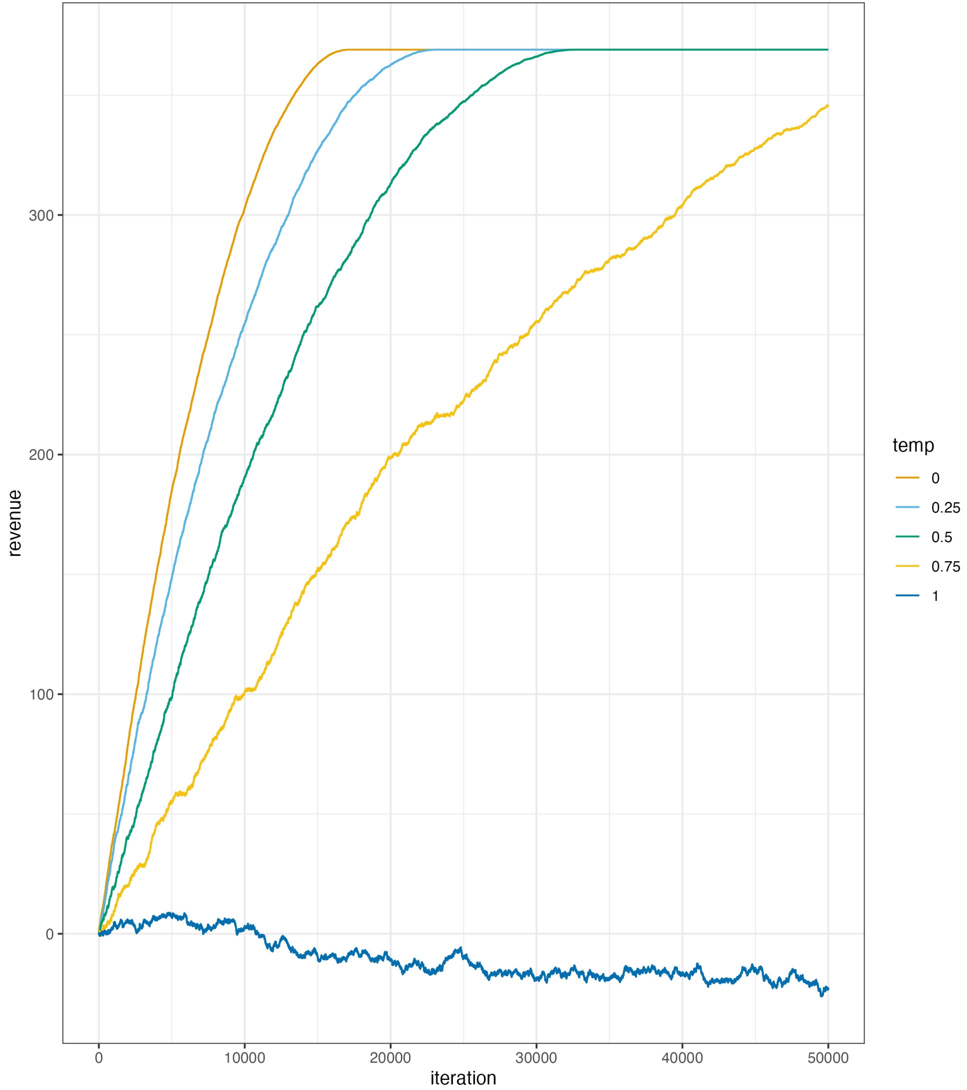
```r
N_iter <- 5e4
lambda <- 1e-3
Ts <- seq(from=0, to=1, by=0.25)
conv <- best <- T_param_history <- vector('list', length=length(Ts))

for (j in seq_along(Ts)){
  revenue <- vector('numeric', length=N_iter)
  params <- rep(0,2)
  best[[j]] <- params
  param_history_tmp <- matrix(NA, nrow=N_iter, ncol=2+length(params))
  for (i in 1:N_iter){
    new_params <- ProposeParams(params, lambda)
    if (HotDogsDogs(new_params) > HotDogsDogs(params) | runif(1) < Ts[j]){
      params <- new_params
    }
    if (HotDogsDogs(params) > HotDogsDogs(best[[j]])){
      best[[j]] <- params
    }
    param_history_tmp[i,] <- c(i, Ts[j], params)
    revenue[i] <- HotDogsDogs(params)
  }
  conv[[j]] <- data.frame(i = 1:N_iter, revenue=revenue, T=Ts[j])
  T_param_history[[j]] <- param_history_tmp
}
```

MCMC Results

```
conv <- do.call('rbind', conv)
T_param_history <- do.call('rbind', T_param_history)
T_param_history <- data.frame(T_param_history)
names(T_param_history) <- c('i', 'T', 'x', 'y')

best

# [[1]]
# [1] 3.000006 6.000006

# [[2]]
# [1] 2.999985 6.000006

# [[3]]
# [1] 3.000041 6.000000

# [[4]]
# [1] 1.870241 4.682416

# [[5]]
# [1] 0.16900318 0.01831097
```

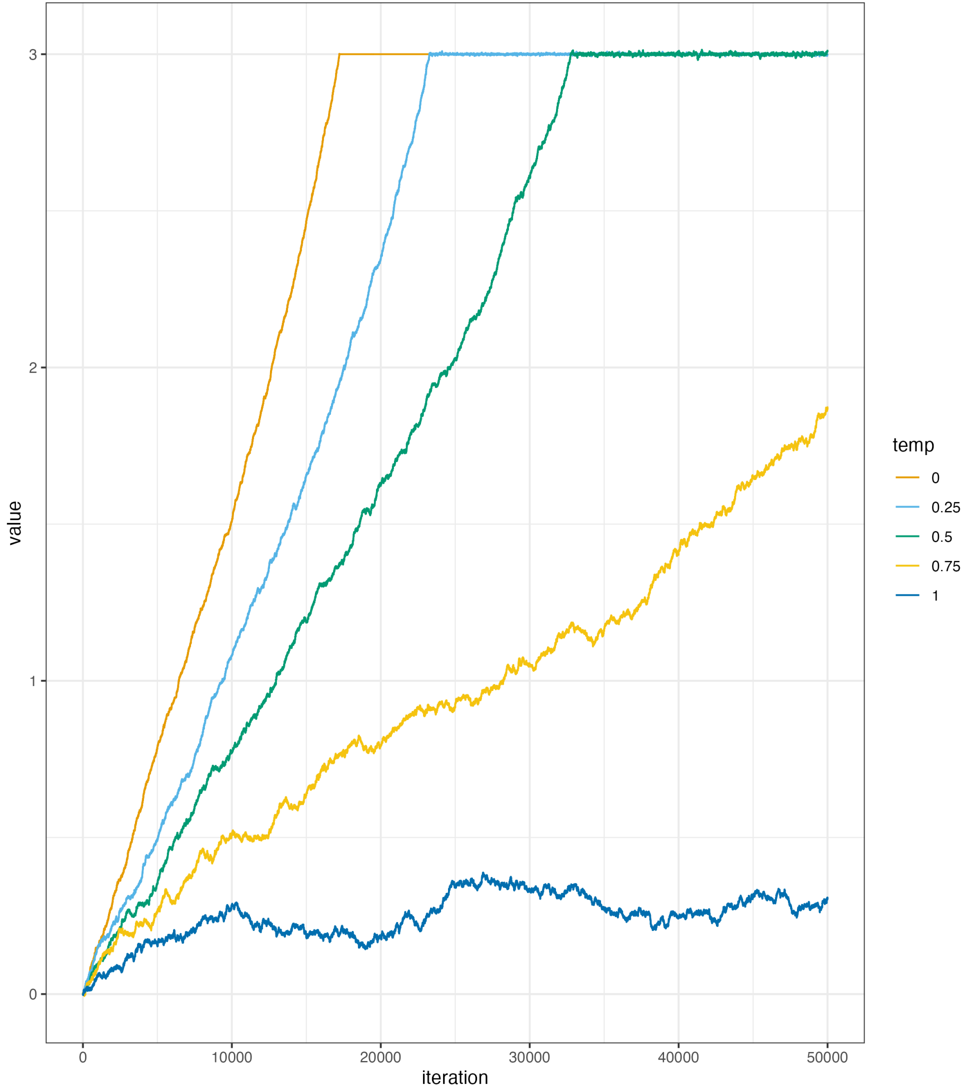
MCMC Results

```r
ggplot(conv,
       aes(x=i,
           y=revenue,
           color=as.character(T))) +
  geom_line() +
  labs(x='iteration',
       y='revenue',
       color='temp') +
  scale_color_okabeito() +
  theme_bw()
```



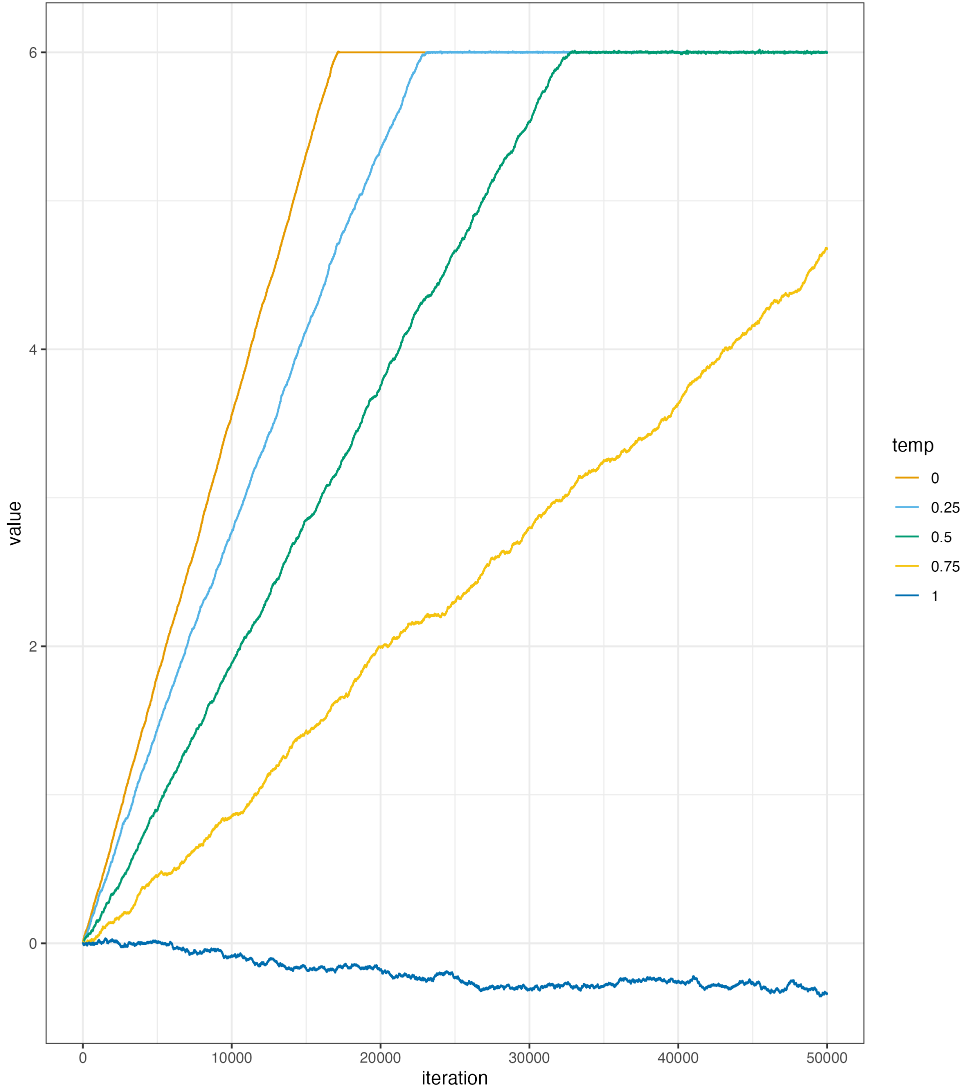
MCMC Results

```r
T_param_history |>
  pivot_longer(c(x,y),
               names_to='param',
               values_to='value') |>
  filter(param == 'x') |>
  ggplot(aes(x=i,
             y=value,
             color=as.character(T))) +
  geom_line() +
  labs(x='iteration', color='temp') +
  scale_color_okabeito() +
  theme_bw()
```



MCMC Results

```
T_param_history |>
  pivot_longer(c(x,y),
               names_to='param',
               values_to='value') |>
  filter(param == 'y') |>
  ggplot(aes(x=i,
             y=value,
             color=as.character(T))) +
  geom_line() +
  labs(x='iteration', color='temp') +
  scale_color_okabeito() +
  theme_bw()
```



A (Much) Harder Problem

Given a list of cities and the distances between each pair of cities, what is the shortest possible route that visits each city exactly once and returns to the origin city?

- Known as the "Traveling Salesman Problem" (TSP)
- NP-Hard Problem
- We think (but have not proven) that there are no polynomial-time algorithms to solve NP-Hard problems
- The issue is that this problem is non-convex, meaning that we're not trying to find the min/max on some smooth curve that's a function of some variables!
- This makes optimization potentially trickier than what we've dealt with so far!

Plan of Attack

- Write down a function to minimize
- Decide how to explore the solution space
- MCMC the hell out of it!

The Traveling Salesman with MCMC

First, we generate a matrix that holds distances between locations:

```
n_locations <- 10
dist_mat <- matrix(0, nrow=n_locations, ncol=n_locations)

for (i in 1:n_locations){
  for (j in 1:n_locations){
    if (i == j){
      dist_mat[i,j] <- 0
    } else if (j > i){
      dist_mat[i,j] <- runif(1, min=1, max=10)
    } else if (j < i) {
      dist_mat[i,j] <- dist_mat[j,i]
    }
  }
}

dist_mat[1:3, 1:3]

#            [,1]     [,2]     [,3]
#  [1,] 0.000000 4.388056 8.869981
#  [2,] 4.388056 0.000000 3.998735
#  [3,] 8.869981 3.998735 0.000000
```

The Traveling Salesman with MCMC

Next, we need a loss function to evaluate the total trip length of our proposed solution:

```r
TripDist <- function(path, dist_matrix){
  total_dist <- 0
  for (i in seq_along(path)){
    if (i == length(path)) {
      total_dist <- total_dist + dist_mat[path[i], path[1]]
    } else {
      total_dist <- total_dist + dist_mat[path[i], path[i+1]]
    }
  }
  return(total_dist)
}

TripDist(1:10, dist_mat)

# [1] 51.36853
```

The Traveling Salesman with MCMC

Finally, we need a "transition matrix"—something to draw our new proposal from:

```
PermutePath <- function(path){
  new_path <- path
  p <- sample(1:length(path), 1)
  if (p == length(path)){
    new_path[p] <- path[1]
    new_path[1] <- path[p]
  } else {
    new_path[p] <- path[p+1]
    new_path[p+1] <- path[p]
  }
  return(new_path)
}

PermutePath(1:10)

#  [1]  1  2  3  4  5  6  7  8 10  9
```

The Traveling Salesman with MCMC

Now we implement MCMC:

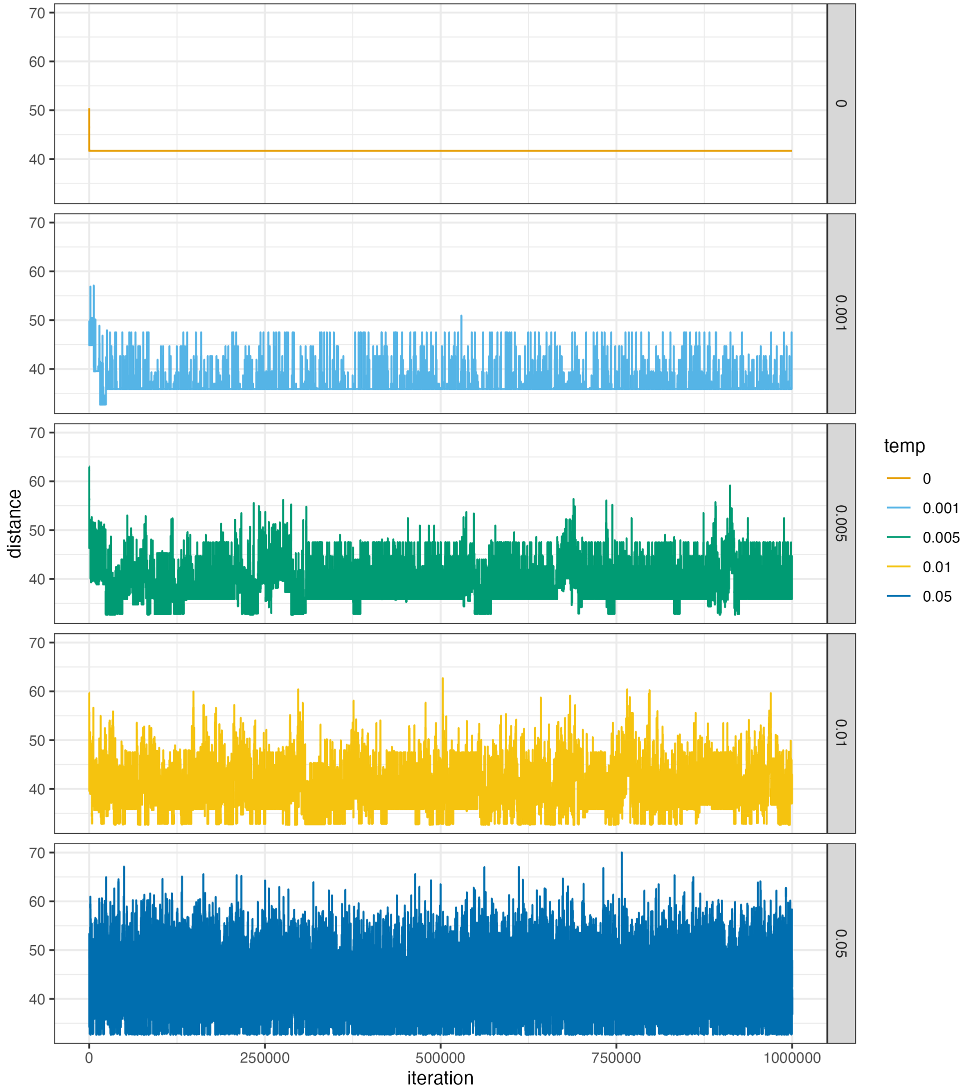
```r
points <- 1:n_locations
N_iter <- 1e6
Ts <- c(0, 0.001, 0.005, 0.01, 0.05)
conv <- best <- vector('list', length=length(Ts))
for (j in seq_along(Ts)){
  dist <- vector('numeric', length=N_iter)
  path <- sample(points)
  best[[j]] <- path
  for (i in 1:N_iter){
    new_path <- PermutePath(path)
    if (TripDist(new_path, dist_mat)<TripDist(path, dist_mat) | runif(1)<Ts[j]){
      path <- new_path
    }
    if (TripDist(path, dist_matrix) < TripDist(best[[j]], dist_mat)){
      best[[j]] <- path
    }
    dist[i] <- TripDist(path, dist_mat)
  }
  conv[[j]] <- data.frame(i = 1:N_iter, dist=dist, T=Ts[j])
}
```

Traveling Salesman Results by Temperature

```r
for (j in 1:length(Ts)) {
  print(Ts[j])
  print(best[[j]])
  print(TripDist(best[[j]], dist_mat))
}

# [1] 0
# [1]  7  9  5  3 10  2  1  6  8  4
# [1] 35.75039
# [1] 0.001
# [1]  7  9  2 10  3  5  6  1  8  4
# [1] 32.90462
# [1] 0.005
# [1]  2 10  9  1  6  3  5  8  4  7
# [1] 32.65007
# [1] 0.01
# [1]  8  4  7  2 10  9  1  6  3  5
# [1] 32.65007
# [1] 0.05
# [1]  6  1  9 10  2  7  4  8  5  3
# [1] 32.65007
```

Traveling Salesman Results by Temperature

```r
conv <- do.call('rbind', conv)

ggplot(conv,
       aes(x=i,
           y=dist,
           color=as.character(T))) +
  geom_line() +
  facet_grid(T~.) +
  labs(x='iteration',
       y='distance',
       color='temp') +
  theme_bw()
```



Wrap Up

Recap

- Markov Chain Monte Carlo is an exceptionally powerful algorithm!
- It has way more applications than we talked about today
- Take a course in Bayesian inference if you want to do more MCMC
- There are also tons of great extensions to MCMC
  - Simulated annealing
  - Hamiltonian Monte Carlo
  - Gibbs Sampling
- This stuff is challenging, but you'll practice and implement it in your homework. Please ask questions!

Final Thoughts

- PollEv.com/klintkanopka