Journal: Cross Validation

Zane Billings

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Breakdown of Stein Method

1. Generate data (or obtain real data in correct format).
2. Partition the data into thirds (i.e. we are setting up for 3-fold cross validation).
3. Use two of the parts to build a model with a given smoothing parameter λ.
4. Use the third part to test the model, and compute the sum of square errors (SSE) for the model.
5. Repeat steps 4 and 5 for each possible testing dataset.
6. Compute the arithmetic mean of the three SSEs. This value is called the cross-validation error (CVE).
7. Repeat steps 2-6 for several values of λ.

Questions to ask before writing code

1. Is this procedure correct or am I missing something?

   This procedure is correct according to Stein's method. Dr. Wagaman also confirmed this is standard practice.

2. Why is $k = 3$ ok here? Every resource I have seen suggests $k = 5$ or $k = 10$ (or "leave-one-out" cross-validation for large datasets).

   This probably has to do with the trade-off between computational power and parameter fitting. If $k = 3$ recovers the parameters, there is not a compelling reason to do more computations.

3. Do I randomly sample the dataset each time I choose a new λ value, or do I only do a random partition at the beginning of the CV process?

   No, the data should only be partitioned at the beginning of the cross-validation process.

To-Do List:

1. Write a function to randomly partition the data.
2. Make sure the function to fit a model with a given *lambda* works as intended (I think it does but I'm going to give it a quick lookover).
3. Write a SSE function (might already be in the old stuff).
4. Write a CVE function.
5. Write a function that takes in a dataset and a value of lambda and does cross-validation.
6. Modify this function or write a wrapper to accept a list of lambdas and output a data frame of lambdas and CVEs.

Part 1: Randomly Partitioning the Data

The first thing I wanted to do was randomly generate a really simple dataframe to test how to randomly partition the data.

```
df <- data.frame(x = seq(1,100,1), y = seq(2,200,2))
```

Now, I have an idea for how to do this manually, so I will write it out for the case $k = 3$.

```
num_obs <- nrow(df)
k <- 3
num_each <- floor(num_obs/k)
# Set a random seed to ensure I can replicate results.
set.seed(100)
# Create a list of all remaining row indices.
rem <- seq(1,num_obs,1)
# Randomly sample 33 row indices.
choices <- sample(rem, 33, replace = F)
# Create the first partition, and remove all chosen indices from the list.
part1 <- df[choices, ]
rem <- setdiff(rem, choices)
# Repeat as above.
choices <- sample(rem, 33, replace = F)
part2 <- df[choices, ]
rem <- setdiff(rem, choices)
# Now set all remaining indices to the final partition.
part3 <- df[rem, ]
# Create a list of partitions so I can check for equality.
parts1 <- list(part1, part2, part3)
```

Now that I know how to do what I want, it's time to automate this process with a function.

```
random_partition <- function(data, k) {
  # data is a data frame of observations
  # k is the number of partitions to form
  # Returns a list of k random partitions of the data
  num_obs <- nrow(data)
  part_size <- floor(num_obs/k)
  rem <- seq(1, num_obs, 1)
  parts <- list()
  for (i in 1:(k - 1)) {
    choices <- sample(rem, part_size, replace = F)
    parts[[i]] <- data[choices, ]
    rem <- setdiff(rem, choices)
  }
  parts[[k]] <- data[rem, ]
  return(parts)
}
```

Here, I am testing to see if the functional output is identical to the manual result.

```
set.seed(100)
parts2 <- random_partition(df, 3)
identical(parts1,parts2)
```

```
## [1] TRUE
```

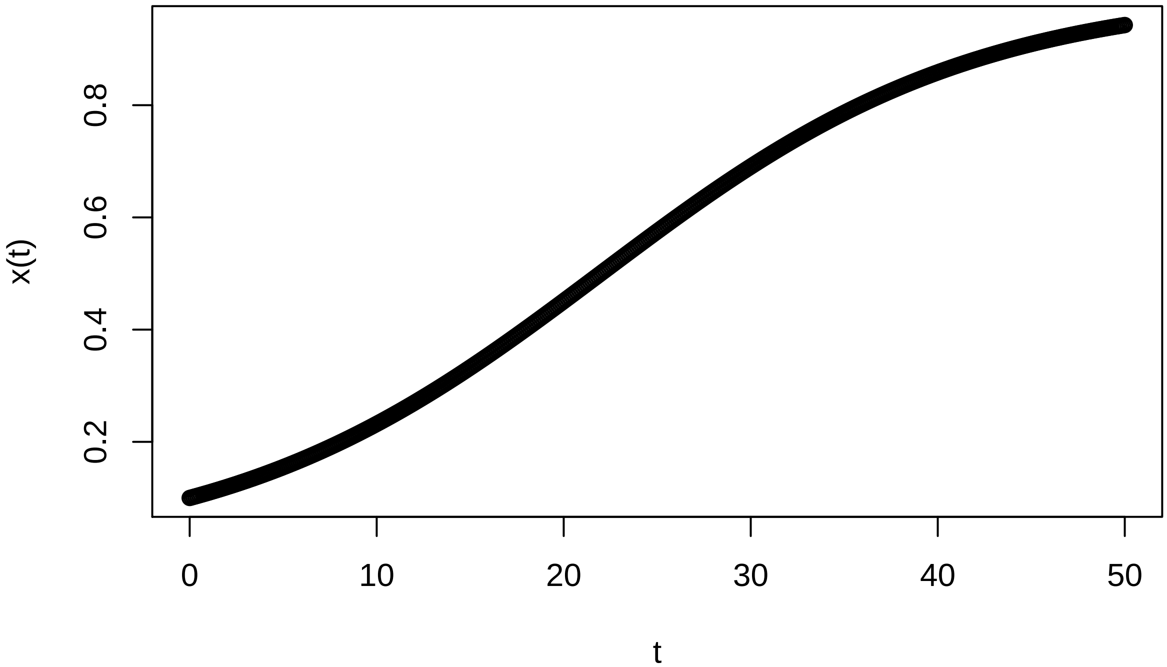
Part 2: Generating fake data and doing the thing

```r
source(here::here("Scripts","Dimensionless_exploration.R"))
```

```
## Loading required package: MASS
```

```r
source(here::here("Scripts", "Helpers.R"))

df <- generate_dimensionless_logistic_data(.1, 0.1, 50, 0.1, TRUE)
```



Now the data is generated with parameter $r = 0.1$.

```r
calculate_SSE <- function(true, fits) {
  # Calculate the sum of squared errors for a model.
  SSE <- sum((true - fits)^2)
  return(SSE)
}

lambdas <- c(0.001, 0.01, 0.1, 0.5, 1, 2, 5, 10, 20, 50, 100, 200, 500, 1000, 2000, 5000, 10000)
k <- 3
parts <- random_partition(df, k)
combos <- combn(1:k, k-1, simplify = F)
```

Now let's run do a test with one parameter value to see if I can do this right.

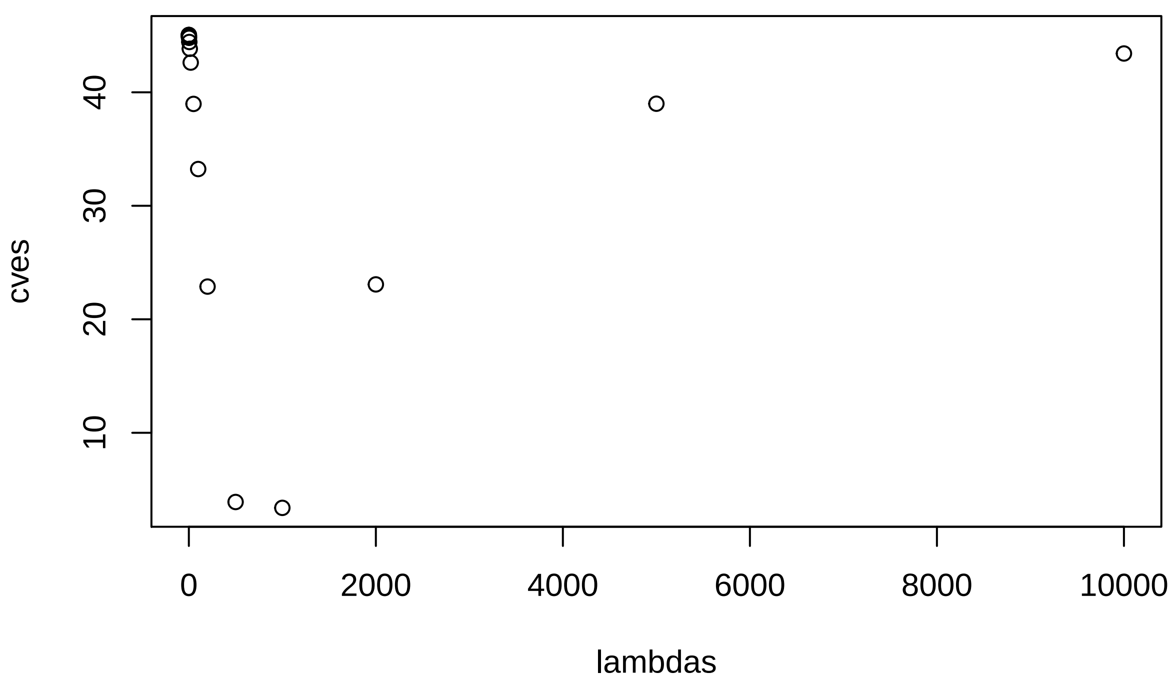
```r
source(here::here("Scripts", "Least_squares_methods.R"))
# Holder for calculated CVEs
cves <- numeric(length(lambdas))
for (a in 1:length(lambdas)) {
l = lambdas[[a]] # Grab the value of lambda
errors <- numeric(length(parts)) # Holder for SSEs
# Need to do this k number of times (# of parts)
for (i in 1:k) {
  # Grab the first combo of indices to use
```

```r
  to_use <- combos[[i]]
  # Make a blank dataframe
  train <- data.frame()
    # This part has to be done k-1 times to build training data.
  for (j in to_use) {
    # Get the next data frame.
    new_dat <- parts[[j]]
    # Add this data frame to the bottom of the rest.
    train <- rbind(train, new_dat)
  }
  # Now train has k-1 of the parts in it.
  # Set test to be the part that wasn't selected.
  not_used <- (1:k)[!(1:k %in% to_use)]
  test <- parts[[not_used]]
  # Prep and model the data, specify time step manually.
  prepped <- prep_data(train, 0.1)
  mod <- model_logistic_data_dimensionless_smoothing(prepped, l)
  # Next need to calculate predicted values using the estimated growth rate from the model.
  #P = (P0e^(rt))/(1+P0(1-e^(rt)))
  t <- test$t
  pred <- (0.1*exp(mod*t))/(1+0.1*(exp(mod*t)-1))
  errors[i] <- calculate_SSE(test$P,pred)
}

cves[a] <- mean(errors)}

this <- data.frame(lambdas,cves)
```

```r
plot(this)
```



To-Do 2020-03-24:

1. Write a line of code to grab the lambda value with the lowest CVE
2. Write a function to automate this whole process.
3. Make the results function stop automatically printing to console.
4. Run this for a bunch of different values of r and see what happens–plot r vs. min CVE lambda to see if there is a pattern.
5. Check that as lambda goes to infty, estimate of r goes to zero.
6. WOrk on 2 species.
7. Work on code organization (e.g. package?) and update manuscript.