Today

- Recap & questions from homework
- Functions
- Coding descent algorithm (training)
  - using optim()

Git skills

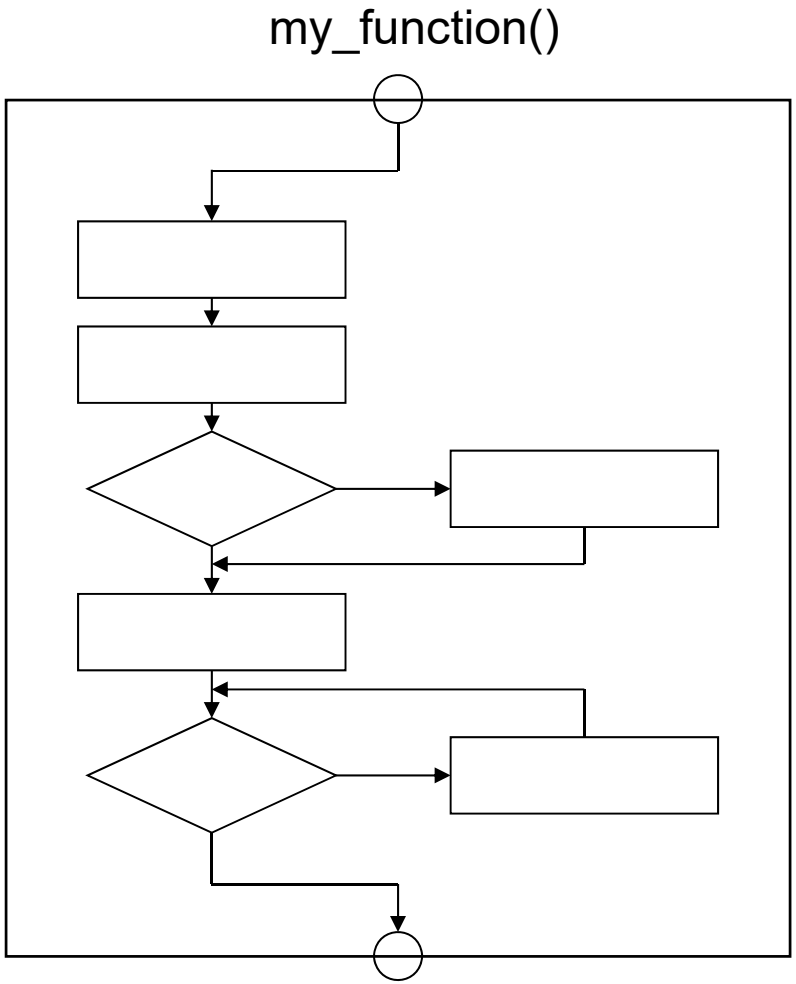
- git amend
- .gitignore
- gitgui
- gitk

Fit ecological model

- Natural process culture of data science
- Paramecium logistic growth
- Parameters: r, K, N(0)
- Grid search

Programming: functions

- A function encapsulates an algorithm
- Functions break a program down into modules
- Modularized programs are easier to write, debug, maintain, and modify
- Functions make algorithms easier to reuse



Making a function in R

- ?"function" – only the bare bones

```
function_name <- function(arguments) {
    expression
    return(object)
}
```

Class style

explicit return

indent (4 spaces)

closing brace aligns with first letter of function name

Making a function in R

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```
function_name <- function(arguments) {
    expression
    return(object)
}
```

```
diff_two_nums <- function(x, z) {
    y <- x - z
    return(y)
}
```

Making a function in R

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```

Objects listed in the arguments or defined in the function can only be seen inside the function. These are called local variables. Concept: scope.

Scope

- See examples in functions.R
- Good programming practice: avoid global variables
  - Define local variables by including in argument list or initializing within the function
  - Global variables make programs harder to maintain and debug

Make a function

```
function_name <- (arguments) {
    expression
    return(object)
}
```

Exercise:
Make a function to calculate the linear model given the model parameters and a vector of x data. In other words, turn the following into a function:

```
y <- b_0 + b_1 * x
```

Make a function

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Exercise:
Make a function to calculate the linear model given the model parameters and a vector of x data. In other words, turn the following into a function:

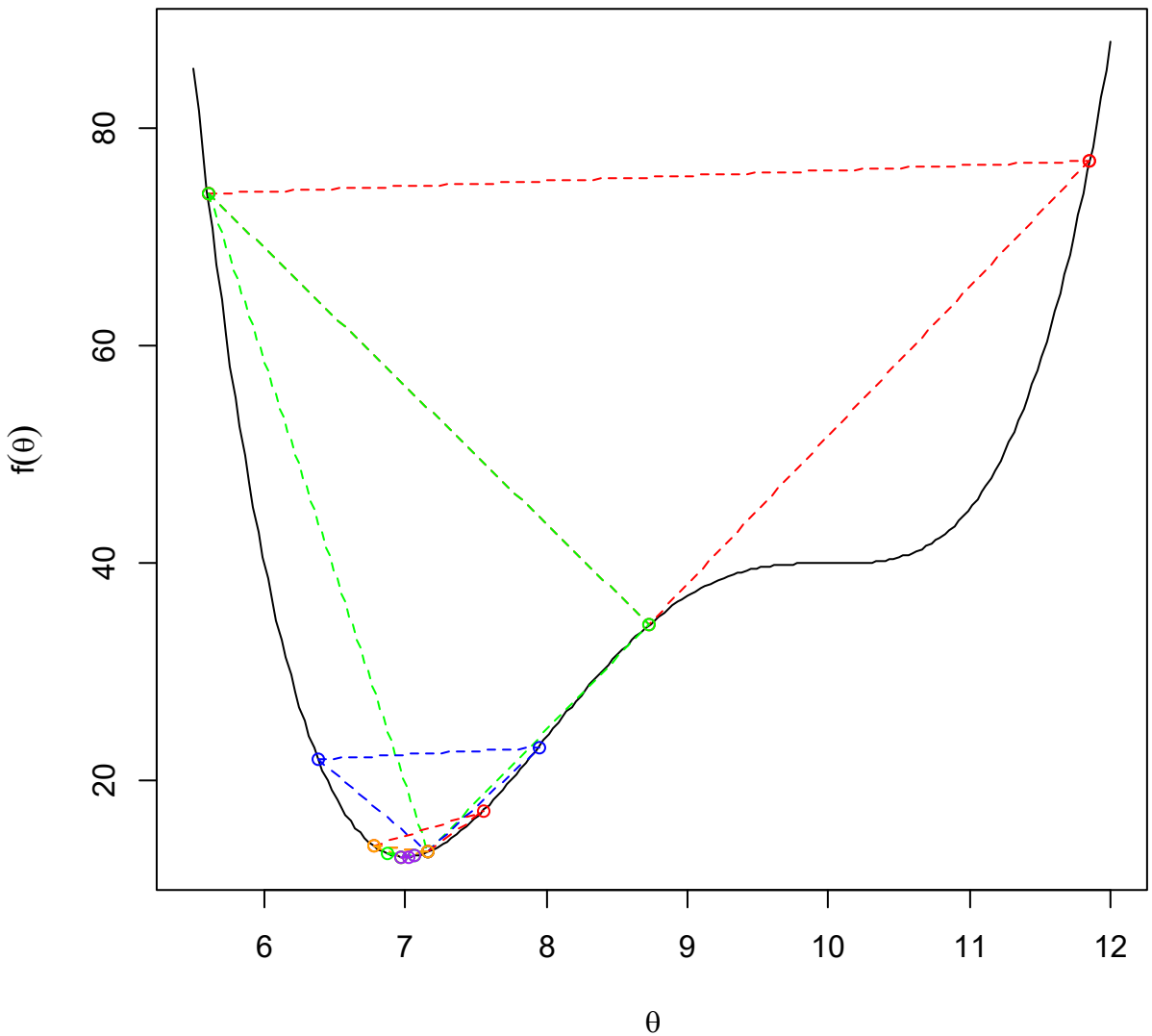
```
  y <- b_0 + b_1 * x
```

Solution:

```
linmod <- function(b_0, b_1, x) {
  y <- b_0 + b_1 * x
  return(y)
}
```

Descent algorithms

Optimize θ: find θ such that f(θ) is minimum



Narrowing in:

keep changing parameters in the direction that leads to lower SSQ

optim()

- Has various descent and Monte Carlo methods
- Nelder-Mead algorithm is default (`method="Nelder-Mead"`)

```
optim(par, fn, ...)
```

A vector of parameters to be estimated

The name of the function to be minimized

Other arguments to pass to the function. Usually the data plus any parameters not to be estimated.

Training models: general recipe

- 1) biology function
  - complex mechanistic to abstract pattern
- 2) error function
  - e.g. SSQ: distance of the model from the data

```
sum((observed - predicted) ^ 2)
```

- 3) optimize
  - find biology parameters that minimize the error
- This recipe is the same no matter how complicated the process model or error function

Code (train_ssq_optim.R)

Biology function (linear)

```
linmod <- function(b_0, b_1, x) {
    y <- b_0 + b_1 * x
    return(y)
}
```

Parameters are first argument

Response data

Auxiliary data

Error function (SSQ)

```
ssq_linmod <- function(p, y, x) {
    y_pred <- linmod(b_0=p[1], b_1=p[2], x)
    e <- y - y_pred
    ssq <- sum(e^2)
    return(ssq)
}
```

Call the biology function to get predicted values

Compare predicted to the data

"Unpack" the parameters (self documenting)

Call to optim

```
par <- c(b_0_start, b_1_start)
fit <- optim(par, ssq_linmod, y=data$y, x=data$x)
```

Starting values for parameters

Need = sign