# Data Wrangling and M
# Regressio

## JSC 370: Data Sc

February 5, 20

# Today's goals

We will learn how to wrangle and manipulate large data with `dtplyr` - i

- Selecting variables.
- Filtering data.
- Creating variables.
- Summarize data.

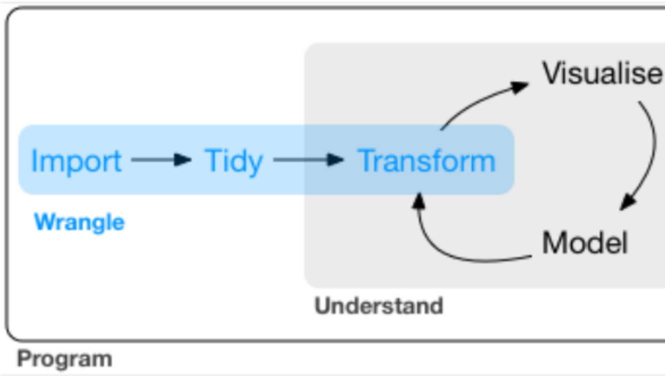
Throughout the session we will see examples using:

- **data.table** in R,
- **dtplyr** in R, and
- **pydatatable**

All with the MET dataset.

We will also take a look at advanced regression, for which you will need

# Data wrangling in R




Data wrangling describes the processes designed to import, clean up, a
complex "raw" forms into high-quality data. You can use your wrangled

# Data wrangling in R

Overall, you will find the following approaches:

- **base R**: Use only base R functions.
- **dplyr**: Using "verbs".
- **data.table**: High-performing (ideal for large data)
- **dplyr + data.table = dtplyr**: High-performing + dplyr verbs.

Other methods involve, for example, using external tools such as Spark,

We will be focusing on data.table because of this

Take a look at this very neat cheat sheet by Erik Petrovski here.

# Selecting variables: Load the p

```r
library(data.table)
library(dtplyr)
library(dplyr)
library(ggplot2)
library(mgcv)
library(lubridate)
```

The `dtplyr` R package translates `dplyr` (`tidyverse`) syntax to `data`
**verbs** while at the same time leveraging the performance of `data.tab`

The `mgcv` package enables advanced regression models with basis spli

# Loading the data

We will use the MET dataset, which we can download (and load) directl

```
# Where are we getting the data from
met_url <- "https://raw.githubusercontent.com/JSC370/JSC3

# Downloading the data to a tempfile (so it is destroyed
# you can replace this with, for example, your own data:
# tmp <- tempfile(fileext = ".gz")
tmp <- "met.gz"

# We sould be downloading this, ONLY IF this was not down
# otherwise is just a waste of time.
if (!file.exists(tmp)) {
  download.file(
    url      = met_url,
    destfile = tmp,
    # method   = "libcurl", timeout = 1000 (you may need
  )
}
```

Now we can load the data using the `fread()` function.

# Reading in the data

In R, fread, do a quick wrangle to remove outliers (discovered earlier), ar

```
met_dt <- fread(tmp)
met_dt <- met_dt[temp > -10][order(temp)]
head(met_dt)
```

In Python, import with `datatable`, read, and print first 5 rows

```
import datatable as dt
met_dt_py = dt.fread("met.gz")
met_dt_py.head(5)
```

Before we continue, let's learn a bit more on `data.table` and `dtplyr`

# `data.table` and `dtplyr`: Dat

- As you have seen in previous lectures, in `data.table` all happens with
imagine DT:

**DT[i , j, b**

Rows or logical rule
to subset the rows

Some function
of the data

Take **DT**
Subset rows using
then calculate **j**
grouped by **by**

- Any time that you see **:=** in **j** that is "Assignment by reference." Using **=**

# `data.table` and `dtplyr`: Dat

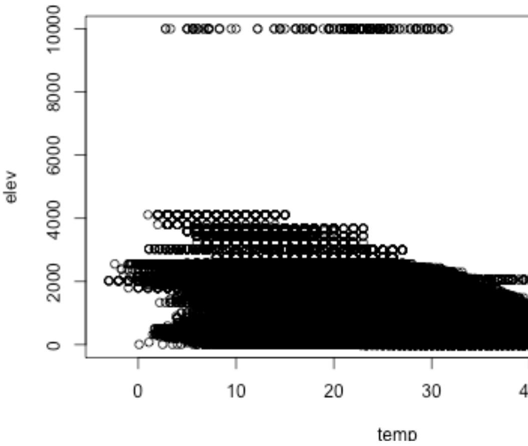
Operations applied in **j** are evaluated *within* the data, meaning that nam

```
# This returns an error (met is not referencing the data.
met[, elev]

# This works fine
met_dt[, elev]
```

# data.table and dtplyr: Dat

Furthermore, we can do things like this:

```
met_dt[, plot(temp, elev)]
```



```
## NULL
```

# Lazy loading, queries

- From Wikipedia "Lazy Loading" (also known as asynchronous loadi computer programming and mostly in web design and developmen at which it is needed. It can contribute to efficiency in the program'
- Lazy loading means that the code for a particular function doesn't a minute – when it's actually being used.
- When you create a "lazy" query, you're creating a pointer to a set o actually run and the data isn't actually loaded until you call "next" o and load it into an object.

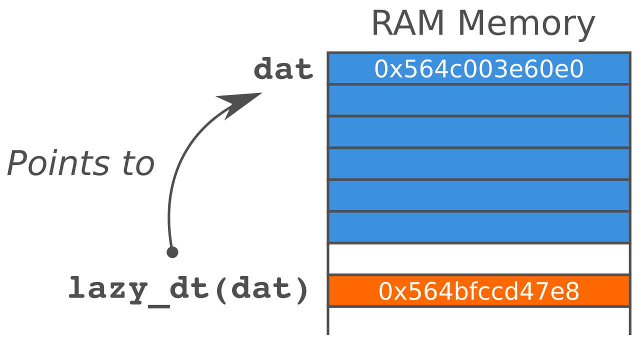
## `data.table` and `dtplyr`: Laz

- The `dtplyr` package provides a way to translate `dplyr` verbs to d
- The key lies on the function `lazy_dt` from `dtplyr` (see `?dtplyr`
- This function creates a wrapper that "points" to a `data.table` obj

# data.table and dtplyr: Laz

```r
# Creating a lazy table object
met_ldt <- lazy_dt(met_dt, immutable = FALSE)

# We can use the address() function from data.table
address(met_ldt)
address(met_ldt$parent)
```

```
## [1] "0x7fcbff8c9788"
## [1] "0x7fcbe5255c00"
```



s
c

# data.table selecting columr

How can we select the columns USAFID, lat, and lon, using data.ta
names:

```
met_dt[, list(USAFID, lat, lon, temp, elev)]
# met_dt[, .(USAFID, lat, lon, temp, elev)]  # Alternativ
# met_dt[, c("USAFID", "lat", "lon", "temp", "elev")] # A
```

```
##           USAFID    lat      lon temp elev
##       1: 726764 44.683 -111.116 -3.0 2025
##       2: 726764 44.683 -111.116 -3.0 2025
##       3: 726764 44.683 -111.116 -3.0 2025
##       4: 726764 44.683 -111.116 -3.0 2025
##       5: 720411 36.422 -105.290 -2.4 2554
##      ---
## 2317200: 690150 34.300 -116.166 52.8  696
## 2317201: 690150 34.296 -116.162 52.8  625
## 2317202: 690150 34.300 -116.166 53.9  696
## 2317203: 690150 34.300 -116.166 54.4  696
## 2317204: 720267 38.955 -121.081 56.0  467
```

What happens if instead of `list()` you used `c()`?

# Selecting columns (cont. 1)

Using the **dplyr::select** verb:

```
met_dt |>
  select(USAFID, lat, lon, temp, elev)
```

```
##           USAFID    lat      lon temp elev
##       1: 726764 44.683 -111.116 -3.0 2025
##       2: 726764 44.683 -111.116 -3.0 2025
##       3: 726764 44.683 -111.116 -3.0 2025
##       4: 726764 44.683 -111.116 -3.0 2025
##       5: 720411 36.422 -105.290 -2.4 2554
##      ---
## 2317200: 690150 34.300 -116.166 52.8  696
## 2317201: 690150 34.296 -116.162 52.8  625
## 2317202: 690150 34.300 -116.166 53.9  696
## 2317203: 690150 34.300 -116.166 54.4  696
## 2317204: 720267 38.955 -121.081 56.0  467
```

# Selecting columns (cont. 2)

In the case of `pydatatable`

```
met_dt_py[:,["USAFID", "lat", "lon", "temp","elev"]]
```

What happens if instead of `["USAFID", "lat", "lon", "temp",` `"lon", "temp", "elev"}` (vector vs set).

# Selecting columns (cont. 3)

For the rest of the session we will be using these variables: USAFID, WB
wind.sp, temp, and atm.press.

```
# Data.table
met_dt <- met_dt[,
  .(USAFID, WBAN, year, month, day,
    hour, min, lat, lon, elev,
    wind.sp, temp, atm.press)
  ]

# Need to redo the lazy table
met_ldt <- lazy_dt(met_dt)
```

# Data filtering: Logical conditio

- Based on logical operations, e.g. `condition 1 [and|or condi`
- Need to be aware of ordering and grouping of `and` and `or` operato
- Fundamental **logical** operators:

| x | y | Negate !x | And x & y | Or x \| y | Xor xor(x, y) |
|---|---|---|---|---|---|
| true | true | false | true | true | false |
| false | true | true | false | true | true |
| true | false | false | false | true | true |
| false | false | true | false | false | false |

- Fundamental **relational** operators, in R: `<`, `>`, `<=`, `>=`, `==`, `!=`.

# XOR operations

- The XOR logical operation, exclusive or, takes two Boolean operand
are different. Conversely, it returns false if the two operands have th

- So, for example, the XOR operator can be used when we have to ch
same time.

# How many ways can you write

Write a function that takes two arguments `(x,y)` and applies the XOR
template:

```
myxor <- function(x, y) {
  res <- logical(length(x))
  for (i in 1:length(x)) {
    res[i] <- # do something with x[i] and y[i]
  }
  return(res)
}
```

Or if vectorized (this would be better)

```
myxor <- function(x, y) {
  # INSERT YOUR CODE HERE
}
```

Hint 1: Remember that negating `(x & y)` equals `(!x | !y)`.

Hint 2: Logical operators are a distributive, meaning a `* (b + c) =` `|`.

In R

```r
myxor1 <- function(x,y) {(x & !y) | (!x & y)}
myxor2 <- function(x,y) {!((!x | y) & (x | !y))}
myxor3 <- function(x,y) {(x | y) & (!x | !y)}
myxor4 <- function(x,y) {!((!x & !y) | (x & y))}
cbind(
  ifelse(xor(test[,1], test[,2]), "true", "false"),
  ifelse(myxor1(test[,1], test[,2]), "true", "false"),
  ifelse(myxor2(test[,1], test[,2]), "true", "false"),
  ifelse(myxor3(test[,1], test[,2]), "true", "false"),
  ifelse(myxor4(test[,1], test[,2]), "true", "false")
)
```

```
##      [,1]    [,2]    [,3]    [,4]    [,5]
## [1,] "false" "false" "false" "false" "false"
## [2,] "true"  "true"  "true"  "true"  "true"
## [3,] "true"  "true"  "true"  "true"  "true"
## [4,] "false" "false" "false" "false" "false"
```

Or in Python

```python
# Loading the libraries
import numpy as np
import pandas as pa

# Defining the data
x = [True, True, False, False]
y = [False, True, True, False]
ans = {
    'x'   : x,
    'y'   : y,
    'and' : np.logical_and(x, y),
    'or'  : np.logical_or(x, y),
    'xor' : np.logical_xor(x, y)
    }
pa.DataFrame(ans)
```

Or in Python (bis)

```python
def myxor(x,y):
    return np.logical_or(
        np.logical_and(x, np.logical_not(y)),
        np.logical_and(np.logical_not(x), y)
    )

ans['myxor'] = myxor(x,y)
pa.DataFrame(ans)
```

We will now see applications using the `met` dataset

# Filtering (subsetting) the data

Need to select records according to some criteria. For example:

- First day of the month, and
- Above latitude 40, and
- Elevation outside the range 500 and 1,000.

The logical expressions would be

- `(day == 1)`
- `(lat > 40)`
- `((elev < 500) | (elev > 1000))`

Respectively.

In R with `data.table`:

```
met_dt[(day == 1) & (lat > 40) & ((elev < 500) | (elev >
  nrow()
```

```
## [1] 27049
```

In R with **dplyr::filter()**:

```
met_ldt |>
  filter(day == 1, lat > 40, (elev < 500) | (elev > 1000)
  collect() |> # Notice this line!
  nrow()
```

```
## [1] 27049
```

With lazy tables, R delays doing any work until the last possible moment
and then sends it to the database in one step.

In Python

```
met_dt_py[(dt.f.day == 1) & (dt.f.lat > 40) & ((dt.f.elev
# met_dt_py[dt.f.day == 1,:][dt.f.lat > 40,:][(dt.f.elev
```

In the case of pydatatable we use `dt.f.` to refer to a column. `df.` is wh

The [`f.` is a symbol](#) that allows accessing column names in a datatable's

# More wrangling questions

1. How many records have a temperature within 18 and 25 C?
2. Some records have missings. Count how many records have `temp`
3. Following the previous question, plot a sample of 1,000 of `(lat,` with data.

# Solutions

```
# Question 1
message("Question 1: ", nrow(met_dt[(temp < 25) & (temp >
```

```
## Question 1: 908047
```

```
# met_dt[temp %between% c(18, 25), .N]

# met_ldt |>
#   filter(between(temp, 18, 25)) |>
#   collect() |>
#   nrow()

# Question 2
message("Question 2: ", met_dt[is.na(temp), .N])
```

```
## Question 2: 60089
```

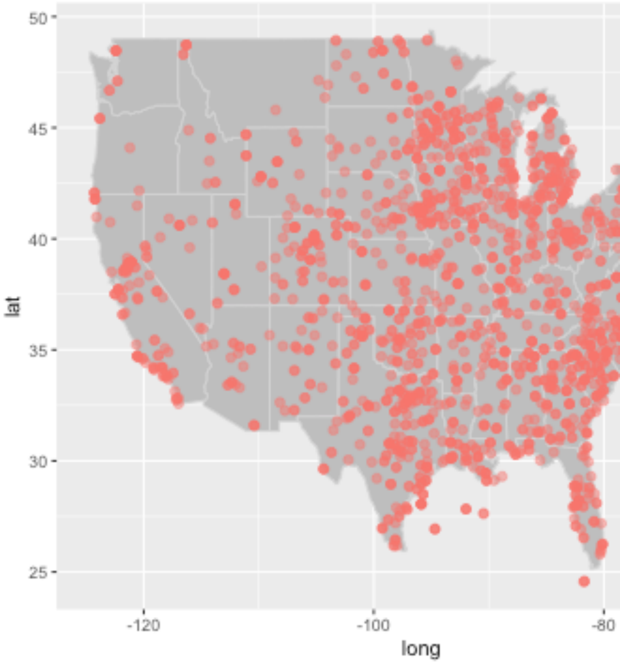
- Note the special symbol `.N` in j

- `.N` can be used in `j`, which is particularly useful to get the number

# Solutions (con't)

```
# Question 3
set.seed(123)
message("Question 3")

# Drawing a sample
idx <- met_dt[, list(x = sample.int(.N, 2000, replace = F

# Visualizing the data
ggplot(map_data("state"), aes(x = long, y = lat)) +
  geom_map(aes(map_id = region), map = map_data("state"),
  geom_jitter(
    data    = met_dt[idx],
    mapping = aes(x = lon, y = lat, col = is.na(temp)),
    inherit.aes = FALSE, alpha = .5, cex = 2
    )
```

# Solutions (con't)



# Creating variables: Data types

- **logical**: Bool true/false type, e.g. dead/alive, sick/healthy, good/bad
- **strings**: string of characters (letters/symbols), e.g. names, text, etc
- **integer**: Numeric variable with no decimal (discrete), e.g. age, days
- **double**: Numeric variable with decimals (continuous), e.g. distance

In C (and other languages), strings, integers, and doubles may be speci
9, 16, and 32 bits. This is relevant when managing large datasets, where

# Creating variables: Special dat

Most programming languages have special types which are built using b

- **time**: Could be date, date + time, or a combination of both. Usually
  R, the `Date` class has as reference 1970-01-01, in other words, "da

- **categorical**: Commonly used to represent strata/levels of variables
  as a factor, where the data is stored as numbers but has a label.

- **ordinal**: Similar to factor, but it has ordering, e.g. "satisfaction level

Other special data types could be ways to represent missings (usually d
e.g. `+–Inf` and Undefined (`NaN`).

When storing/sharing datasets, it is a good practice to do it along a dict

# Questions 3: What's the best w following

- 0, 1, 1, 0, 0, 1
- Diabetes type 1, Diabetes type 2, Diabetes type 1, Diabetes type 2
- on, off, off, on, on, on
- 5, 10, 1, 15, 0, 0, 1
- 1.0, 2.0, 10.0, 6.0
- high, low, medium, medium, high
- -1, 1, -1, -1, 1,
- .2, 1.5, .8, $\pi$
- $\pi$, $\exp 1$, $\pi$, $\pi$

# Variable creation

If we wanted to create two variables, `elev^2` and the scaled version of
do the following

With `data.table`

```
met_dt[, elev2          := elev^2]
met_dt[, windsp_scaled := wind.sp/sd(wind.sp, na.rm = TRU

# Alternatively:
# met_dt[, c("elev2", "windsp_scaled") := .(elev^2, wind.
```

# Variable creation (cont. 1)

With the verb **dplyr::mutate()**:

```
met_dt[, c("elev2", "windsp_scaled") := NULL] # This to d
met_ldt |>
  mutate(
    elev2         = elev ^ 2,
    windsp_scaled = wind.sp/sd(wind.sp,na.rm=TRUE)
  ) |>
  collect()
```

```
## # A tibble: 2,317,204 × 15
##    USAFID  WBAN  year month   day  hour   min   lat    l
##     <int> <int> <int> <int> <int> <int> <int> <dbl> <db
##  1 726764 94163  2019     8    27    11    50  44.7 -11
##  2 726764 94163  2019     8    27    12    10  44.7 -11
##  3 726764 94163  2019     8    27    12    30  44.7 -11
##  4 726764 94163  2019     8    27    12    50  44.7 -11
##  5 720411   137  2019     8    18    12    35  36.4 -10
##  6 726764 94163  2019     8    26    12    30  44.7 -11
```

```
##  7 726764 94163  2019     8    26    12    50  44.7 -11
##  8 726764 94163  2019     8    26    13    10  44.7 -11
##  9 726764 94163  2019     8    27    10    30  44.7 -11
## 10 726764 94163  2019     8    27    10    50  44.7 -11
```

# Variable creation (cont. 2)

Imagine that we needed to generate all those calculations (scale by sd)
**.SD** symbol:

```
# Listing the names
in_names  <- c("wind.sp", "temp", "atm.press")
out_names <- paste0(in_names, "_scaled")
met_dt[,
    c(out_names) := lapply(.SD, function(x) x/sd(x, na.rm
    .SDcols = in_names
    ]

# Looking at the first 4
head(met_dt[, .SD, .SDcols = out_names], n = 4)
```

```
##    wind.sp_scaled temp_scaled atm.press_scaled
## 1:              0  -0.4955951               NA
## 2:              0  -0.4955951               NA
## 3:              0  -0.4955951               NA
## 4:              0  -0.4955951               NA
```

- Key things to notice here: **c(out_names)**, **.SD**, and **.SDCols**.
- More on `.SD`

# Variable creation (cont. 3)

In the case of dplyr, we could use the following

```
as_tibble(met_ldt) |>
  mutate(
    across(
      all_of(in_names),
      function(x) x/sd(x, na.rm = TRUE),
      .names = "{col}_scaled2"
      )
  ) |>
  # Just to print the last columns
  select(ends_with("_scaled2")) |>
  head(n = 4)
```

```
## # A tibble: 4 × 3
##   wind.sp_scaled2 temp_scaled2 atm.press_scaled2
##             <dbl>        <dbl>             <dbl>
## 1               0       -0.496                NA
## 2               0       -0.496                NA
```

```
## 3                0       -0.496                NA
## 4                0       -0.496                NA
```

Key thing here: This approach has no direct translation to `data.table`

# Merging data

- While building the MET dataset, we dropped the State data.
- We can use the original Stations dataset and *merge* it to the MET d
- But we cannot do it right away. We need to process the data somew

# Merging data (cont. 1)

```
stations <- fread("ftp://ftp.ncdc.noaa.gov/pub/data/noaa/
stations[, USAF := as.integer(USAF)]

# Dealing with NAs and 999999
stations[, USAF   := fifelse(USAF == 999999, NA_integer_,
stations[, CTRY   := fifelse(CTRY == "", NA_character_, C
stations[, STATE  := fifelse(STATE == "", NA_character_,

# Selecting the three relevant columns, and keeping uniqu
stations <- unique(stations[, list(USAF, CTRY, STATE)])

# Dropping NAs
stations <- stations[!is.na(USAF)]

head(stations, n = 4)
```

```
##    USAF CTRY STATE
## 1: 7018 <NA>  <NA>
## 2: 7026   AF  <NA>
## 3: 7070   AF  <NA>
```

```
## 4: 8260 <NA>  <NA>
```

Notice the function `fifelse()`. Now, let's try to merge the data!

# Merging data (cont. 2)

```
merge(
  # Data
  x     = met_dt,
  y     = stations,
  # List of variables to match
  by.x  = "USAFID",
  by.y  = "USAF",
  # Which obs to keep?
  all.x = TRUE,
  all.y = FALSE
  ) |> nrow()
```

```
## [1] 2385443
```

This is more rows! The original dataset, `met_dt`, has 2317204. This me
IDs. We can fix this:

```r
stations[, n := 1:.N, by = .(USAF)]
stations <- stations[n == 1,][, n := NULL]
```

# Merging data (cont. 3)

We now can use the function `merge()` to add the extra data

```r
met_dt <- merge(
  # Data
  x     = met_dt,
  y     = stations,
  # List of variables to match
  by.x  = "USAFID",
  by.y  = "USAF",
  # Which obs to keep?
  all.x = TRUE,
  all.y = FALSE
  )

head(met_dt[, list(USAFID, WBAN, STATE)], n = 4)
```

```
##    USAFID  WBAN STATE
## 1: 690150 93121    CA
## 2: 690150 93121    CA
```

```
## 3: 690150 93121    CA
## 4: 690150 93121    CA
```

What happens when you change the options `all.x` and `all.y`?

# Aggregating data: Adding grou

- Many times we need to either impute some data, or generate variab
- If we, for example, wanted to impute missing temperature with the with the **data.table::fcoalesce()** function:

```
met_dt[, temp_imp := fcoalesce(temp, mean(temp, na.rm =
  by = .(STATE, year, month, day)]
```

- In the case of dplyr, we can do the following using **dplyr::group_by** toge

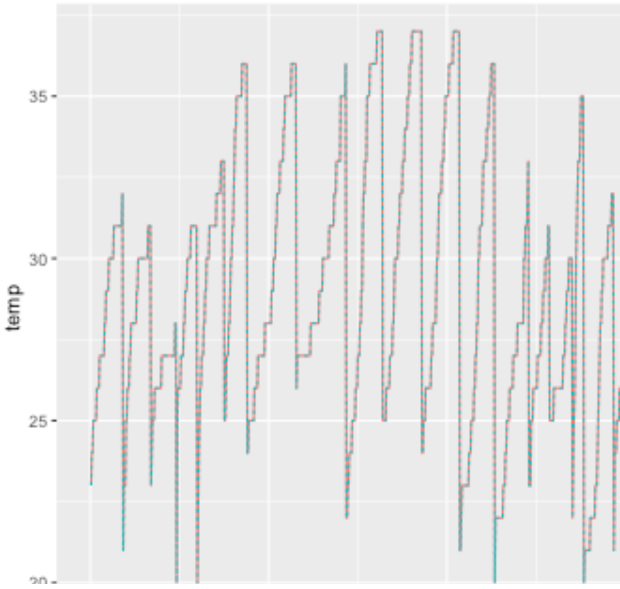
```
# We need to create the lazy table again, since we repl
met_ldt <- lazy_dt(met_dt, immutable = FALSE)

met_ldt |>
  group_by(STATE, year, month, day) |>
  mutate(
    temp_imp2 = coalesce(temp, mean(temp, na.rm = TRUE)
    ) |> collect()
```

# Aggregating data: Adding grou
(cont.)

Let's see how it looks like

```
# Preparing for ggplot2
plotdata <-met_dt[USAFID == 720172][order(year, month, da
plotdata <- rbind(
  plotdata[, .(temp = temp, type = "raw")],
  plotdata[USAFID == 720172][, .(temp = temp_imp, type =
)

# Generating an 'x' variable for time
plotdata[, id := 1:.N, by = type]

plotdata |>
  ggplot(aes(x = id, y = temp, col = type, lty = type)) +
  geom_line()
```

# Aggregating data: Adding grou
(cont.)




# Aggregating data: Summary ta

- Using by also allow us creating summaries of our data.
- For example, if we wanted to compute the average temperature, wi
  we could do the following

```
met_dt[, .(
  temp_avg      = mean(temp, na.rm=TRUE),
  wind.sp_avg   = mean(wind.sp, na.rm=TRUE),
  atm.press_avg = mean(atm.press, na.rm = TRUE)
  ),
  by = STATE
  ][order(STATE)] |> head(n = 4)
```

```
##    STATE temp_avg wind.sp_avg atm.press_avg
## 1:    AL 26.19799    1.563645      1016.148
## 2:    AR 26.20697    1.872876      1014.551
## 3:    AZ 28.80596    2.983999      1010.771
## 4:    CA 22.36199    2.614711      1012.637
```

# Aggregating data: Summary ta

When dealing with too many variables, we can use the `.SD` special sym

```
# Listing the names
in_names  <- c("wind.sp", "temp", "atm.press")
out_names <- paste0(in_names, "_avg")

met_dt[,
  setNames(lapply(.SD, mean, na.rm = TRUE), out_names),
  .SDcols = in_names, keyby   = STATE
  ] |> head(n = 4)
```

```
##    STATE wind.sp_avg temp_avg atm.press_avg
## 1:    AL    1.563645 26.19799      1016.148
## 2:    AR    1.872876 26.20697      1014.551
## 3:    AZ    2.983999 28.80596      1010.771
## 4:    CA    2.614711 22.36199      1012.637
```

Notice the **keyby** option here: "Group by STATE and order by STATE".

# Aggregating data: Summary ta

- Using **dplyr** verbs

```
met_ldt |>
  group_by(STATE) |>
  summarise(
    temp_avg      = mean(temp, na.rm=TRUE),
    wind.sp_avg   = mean(wind.sp, na.rm=TRUE),
    atm.press_avg = mean(atm.press, na.rm = TRUE)
  ) |> arrange(STATE) |> head(n = 4)
```

```
## Source: local data table [4 x 4]
## Call:   head(setorder(`_DT3`[, .(temp_avg = mean(temp,
##     wind.sp_avg = mean(wind.sp, na.rm = TRUE), atm.pres
##         na.rm = TRUE)), keyby = .(STATE)], STATE, na.la
##     n = 4)
##
##   STATE temp_avg wind.sp_avg atm.press_avg
##   <chr>    <dbl>       <dbl>         <dbl>
## 1 AL        26.2        1.56         1016.
```

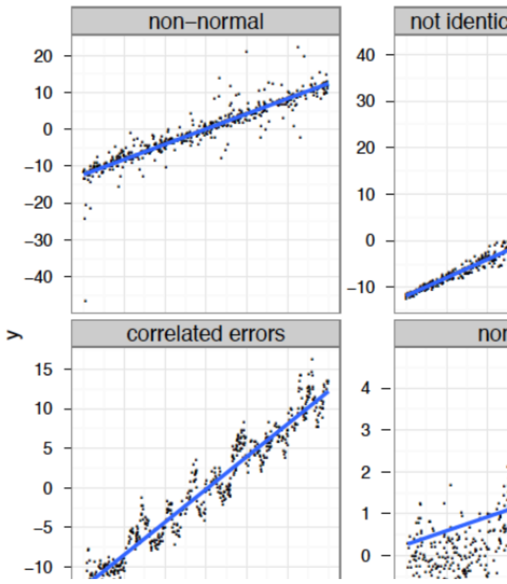
```
## 2 AR        26.2        1.87         1015.
## 3 AZ        28.8        2.98         1011.
## 4 CA        22.4        2.61         1013.
##
```

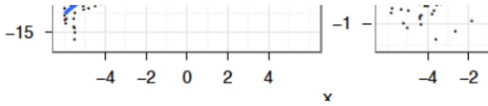
# Other data.table goodies

- `shift()` Fast lead/lag for vectors and lists.
- `fifelse()` Fast if-else, similar to base R's `ifelse()`.
- `fcoalesce()` Fast coalescing of missing values.
- `%between%` A short form of `(x < lb) & (x > up)`
- `%inrange%` A short form of `x %in% lb:up`
- `%chin%` Fast match of character vectors, equivalent to `x %in% X`,
- `nafill()` Fill missing values using a constant, last observed value

# Machine Learning 1: Advanced

- Linear regression is useful, but there are so many ways in which it can fai






# Machine Learning 1: Advanced

- A linear model tries to fit the best straight line that passes through t
- In general, $Y(s) = f(s) + \epsilon$ where in regular linear regression $f(s$
- If we want to represent the regression more generally, we can defin basis function consisting of 'non-linear' terms.

# Basis Function

Basics of Basis Functions

- We will start with a 1-dimensional, univariate case. For example this coul
time (x) with basis functions.
- Polynomial bases are a good way to illustrate what is going on. Consider

$$y_i = f(x_i) + \epsilon_i$$

and let's expand it out by a polynomial

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3 x_i^3 +$$

# Basis Function

Here

$$f(x_i) = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \beta_3$$

is a 4th order polynomial. So, $f(x)$ is a function represented by **five** bas

$$f(x_i) = \sum_{j=1}^{5} x^j \beta_j = \sum_{j=1}^{5} b_j$$

that are defined by:

$$b_1(x) = 1, b_2(x) = x, b_3(x) = x^2, b_4(x)$$

# Basis Functions

- In general, a basis is a set of functions that can be added together
  complicated function
- Here our weights are the regression coefficients $\beta_j$
- In general, a basis function is represented by

$$f_i = \sum b_j(x_i)\beta_j$$

$$\begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ f_4 \\ f_5 \end{pmatrix} = \begin{bmatrix} 1 & b_1(x_1) & b_2(x_1) & b_3(x_1) & b_4(x_1) & b_5(x_1 \\ 1 & b_1(x_2) & b_2(x_2) & b_3(x_2) & b_4(x_2) & b_5(x_2 \\ 1 & b_1(x_3) & b_2(x_3) & b_3(x_3) & b_4(x_3) & b_5(x_3 \\ 1 & b_1(x_4) & b_2(x_4) & b_3(x_4) & b_4(x_4) & b_5(x_4 \\ 1 & b_1(x_5) & b_2(x_5) & b_3(x_5) & b_4(x_5) & b_5(x_5 \end{bmatrix}$$

# Polynomial Basis

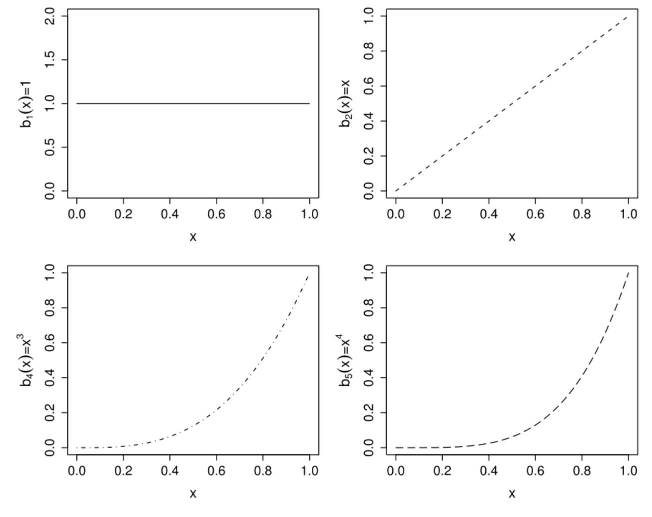
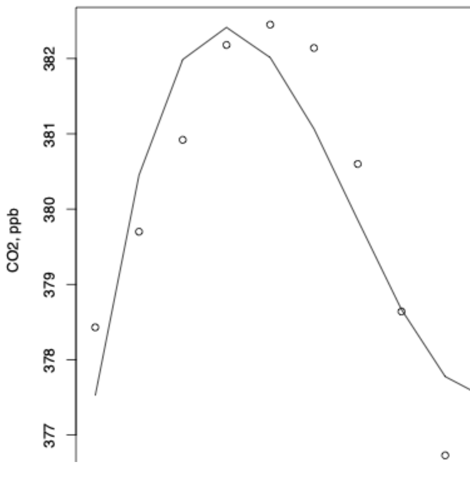


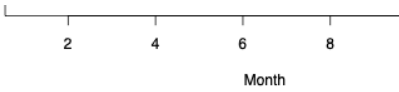

Figure 3.1 *Illustration of the idea of representing a function in*
*a polynomial basis. The first 5 panels (starting from top left),*
*$b_i(x)$, for a 4th order polynomial basis. The basis functions*

$b_j(x)$, for a 4th order polynomial basis. The basis functions
valued parameter, $\beta_j$, and are then summed to give the final c
is shown in the bottom right panel. By varying the $\beta_j$, we can v
any polynomial function of order 4 or lower. See also figure 3.

# Polynomial Basis

- The basis functions are each multiplied by $\beta_j$ and then summed to give th
  shown in the bottom left figure.
- Below, we show this concept in terms of an example of $CO_2$ concentratio





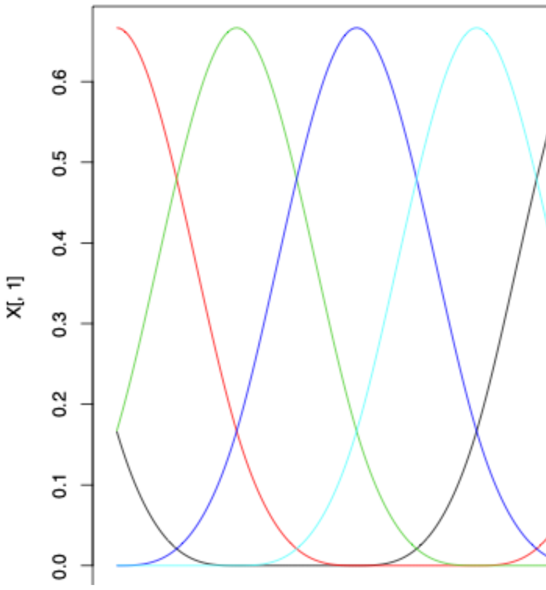

# Splines

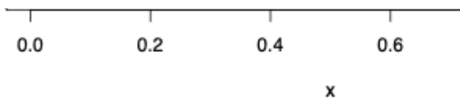
- In general, splines are curves that are formed by combining pieces
- There are several types of splines including natural, cubic, and b-sp

$$f(t_i) = \sum_{j=1}^{4} t^j \beta_j$$

- B-spline curves are made up of polynomial pieces and are defined
- Choosing the number of knots defines how smooth (few) or wiggly

# Splines






# Splines

- Smoothing splines with penalty allows us to estimate where to put the kn
- Minimize the function

$$\sum_i (y_i - f(t_i))^2 + \lambda \int f''$$

.

- Here, $\lambda$ is a penalty parameter that controls how much to penalize wiggly
- Trade-off between the goodness of fit (the sum of squares) and the wiggli
- Start by putting a knot at every data point, then penalize.
- It is an optimization problem m where we minimize:

$$\sum_i (y_i - B_i^T \beta)^2 + \lambda \beta^T$$

- the matrix S is constructed by using the spline basis we chose, B is the ba

# Splines

- This function

$$\sum_i (y_i - f(t_i))^2 + \lambda \int f''$$

  represents the loss + penalty.
- We see similar functions in lasso and ridge regression.
- The second derivative $f''(t)^2$ corresponds to how much the slope is chang slope of the function at $t$).
- The integral $\int f''(t)^2 \mathrm{d}t$ is a measure of the total change in the function $f$ $f'(t)$ will be close to constant and the integral will take on a small value.
- A large $\lambda$ will will make the function $f$ smoother, but $\lambda = 0$ means the pe wiggly.
- As $\lambda \to \infty$, $f$ will be perfectly smooth, a straight line that passes through

# 1-D Splines

Types of 1-D splines include:

- cubic splines (basically piecewise cubic polynomials)
- cyclic splines (cubic splines with connected ends)
- basis splines (B-spline) with other polynomial orders
- cardinal splines (where knot placement is always a certain distance)
- wavelets (often cardinal wavelet splines)

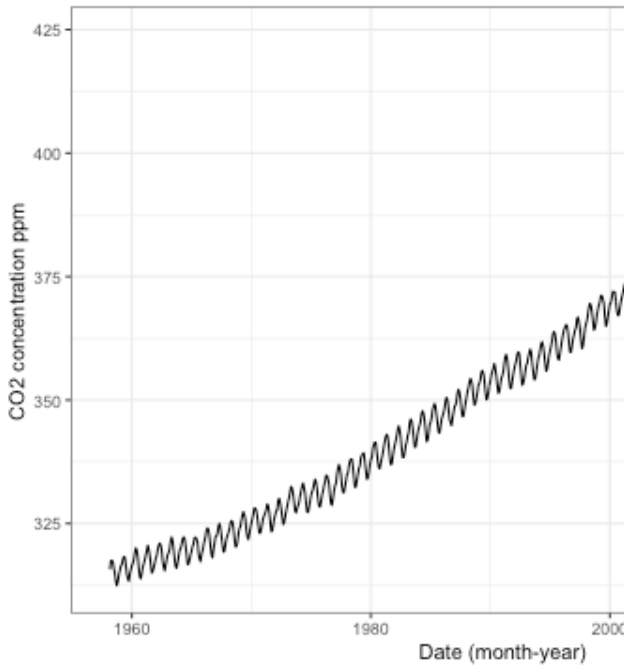
# Fitting Spline Regression Mode

We will use CO$_2$ data from the Mauna Loa observatory in Hawaii: ht

- important variables are: average (monthly CO$_2$ concentrations)
- we will make a month-year variable

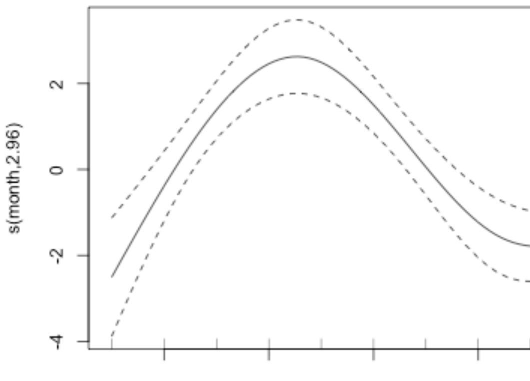
```
co2 <- read.csv("co2_mm_mlo.csv", skip=40)

co2 <- co2 |>
  mutate(month_year = make_date(co2$year, co2$month)) |>
  rename(co2 = average)

co2 |>
  ggplot(aes(y=co2,x=month_year)) +
  geom_line() +
  labs(x='Date (month-year)', y='CO2 concentration ppm')+
  theme_bw()
```

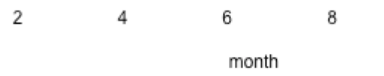
# Fitting Spline Regression Mode



# Fitting Spline Regression Mode

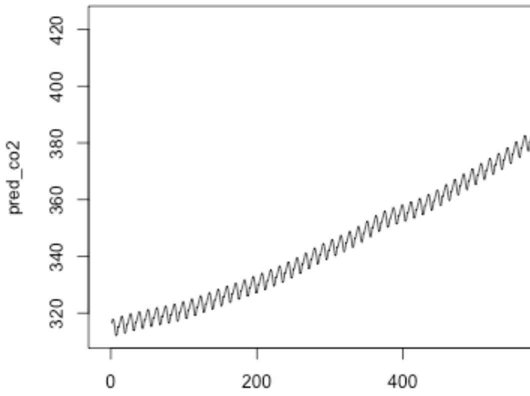
```
library(mgcv)
# Using cubic regression spline bases with 4 knots to sho
co2_2023 <- co2[co2$year==2023,]
gam_co2 <- gam(co2~s(month,bs="cr", k=4),data=co2_2023)
plot(gam_co2)
```






# Fitting Spline Regression Models

```
# try fitting to all data and smoothing date (overall tre
gam_co2_all <- gam(co2~s(decimal.date,bs="cr",k=20)+s(mon
# predict on data
pred_co2 <- predict.gam(gam_co2_all,co2)
plot(pred_co2,type='l')
```



# 2-D Splines

- Thin plate splines are smoothing splines in 2-d
- Extend the 1-d case to:

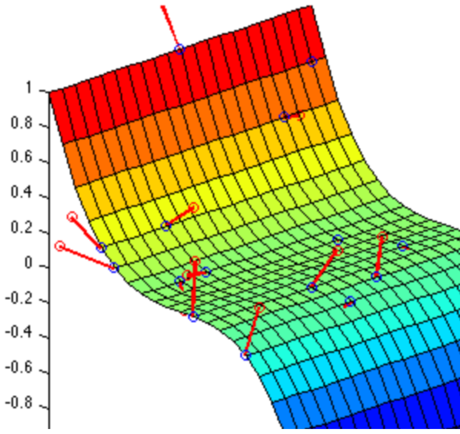
$$\sum_i (z_i - g(s_1, s_2))^2 + \lambda \iint g''(s$$

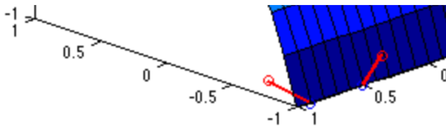
- where the penalty breaks down to the sum of the partial second derivative
- $\lambda$ controls the "wiggliness" as in the 1-D spline (roughness penalty)

# Thin Plate Splines

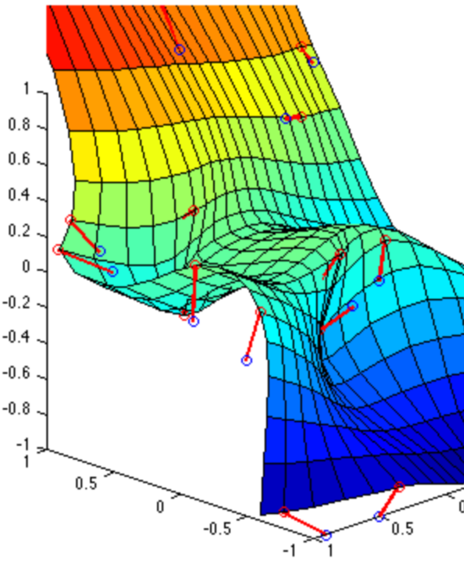
The idea behind a thin plate spline is:

- Basically we put a bendable plane through over the space and the points i
- Where there are more points grouped, we expect the plane to be pulled m
- If there is a very bumpy surface, there will be more knots used and a mor



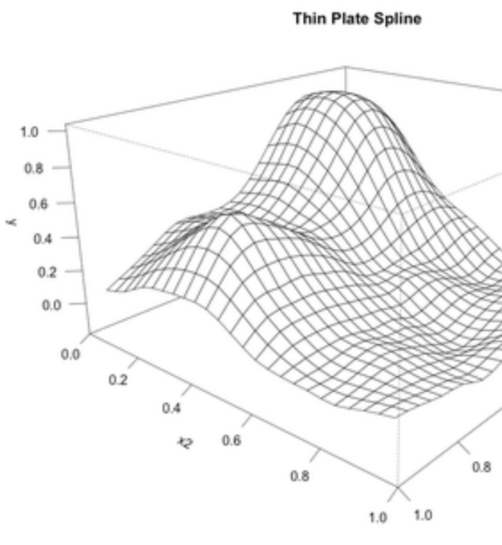


# Thin Plate Splines

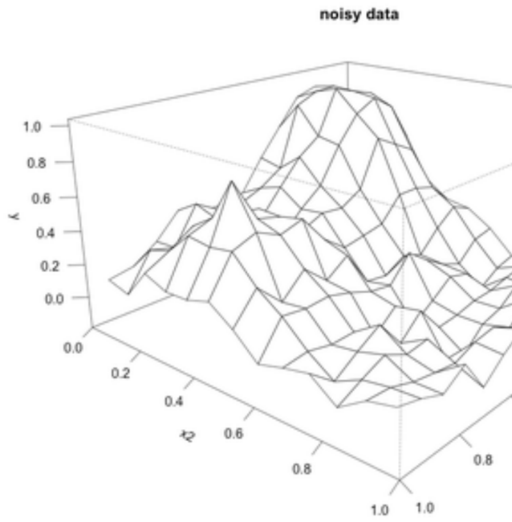


# Thin Plate Spline Regression

The height of where the surface is pulled is going to depend on the mag

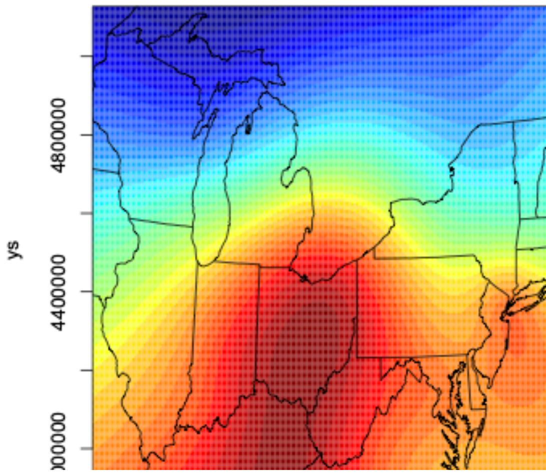


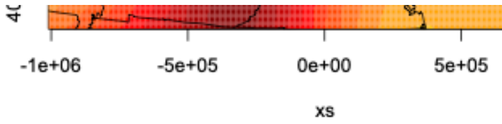
# Thin Plate Spline Regression



## Fitting Spline Regression Models

```
gam_temp <- gam(temp~s(x,y,bs="ts",k=60, fx=TRUE),data=id
plot(gam_temp)
summary(gam_temp)
```






# More on Advanced Regression

For more information and examples about regression that includes basis
[Statistical Learning with applications in R]