

Instructions for EES 3310/5310 Lab #3

Exercises with the MODTRAN Model

Jonathan Gilligan

Lab: Mon. Jan. 10. Due: Mon. Feb. 3

Contents

Instructions	1
Using MODTRAN with RMarkdown.	1
Examples:	6
A few new R functions that we will use in this lab:	9
Iterating over a series	9
Combining character variables	11
Calculating with leads and lags	12
Modifying x and y axes in <code>ggplot</code>	13
Exercises for Lab #3	14
Chapter 4 Exercises	14
Chapter 5 Exercise	17

Instructions

It would be good to print these instructions and bring them to lab on Monday, or else to have the PDF with the instructions handy during lab.

For these exercises, I recommend that you work on them with the interactive web-based MODTRAN models to get a feel for how the models apply to the exercise.

Once you are clear what you are doing, you can use the R scripts and RMarkdown to turn those insights into reproducible research.

Using MODTRAN with RMarkdown.

This RMarkdown document includes the line `source("scripts/modtran.R")`, which loads a script with the following functions:

- `run_modtran()` allows you to automatically download a file with the data from a MODTRAN run. You call it with the following arguments:
 - `filename` is the name of the file to save the data to. I recommend giving it a meaningful name: for instance, a run with 550 ppm CO₂ and 3.4 ppm methane might be called “`modtran_440_34.txt`”. Make up your own file names, but think about how you will tell which is which.
 - `co2_ppm` is the amount of CO₂ in parts per million. The default is 400.
 - `ch4_ppm` is the amount of methane in parts per million. The default is 1.7.
 - `trop_o3_ppb` is the amount of ozone in the troposphere, in parts per billion. The default is 28. You probably won’t change this unless you’re setting all greenhouse gases to zero.
 - `strat_o3_scale` is the amount of stratospheric ozone, relative to the naturally occurring levels in the ozone layer. You probably won’t change this unless you’re setting all greenhouse gases to zero.
 - `h2o_scale` is the amount of water vapor, relative to the naturally occurring levels in the atmosphere. You probably won’t change this unless you’re setting all greenhouse gases to zero.
 - `freon_scale` is the amount of freon chemicals (used for refrigerators and air conditioners), relative to the current amounts. You probably won’t change this unless you’re setting all greenhouse gases to zero.
 - `delta_t` is the temperature offset, in degrees C. You adjust this to restore radiative equilibrium after you change the amount of CO₂ or other greenhouse gases.
 - `h2o_fixed` is what quantity to hold fixed for water vapor. Possible values are “vapor pressure” (the default), and “relative humidity”
 - `atmosphere` is the locality in the MODTRAN model. Possible values are:
 - * “tropical” (the default),
 - * “midlatitude summer”,
 - * “midlatitude winter”,
 - * “subarctic summer”,
 - * “subarctic winter”,
 - * and “standard” for the 1976 U.S. standard atmosphere.
 - `clouds` is the specification of clouds and rain. Possible values are
 - * “none” (the default),
 - * “cumulus”,
 - * “altostratus”,
 - * “stratus”,
 - * “stratocumulus”,
 - * “nimbostratus”,
 - * “drizzle”,

- * "light rain",
- * "medium rain",
- * "heavy rain",
- * "extreme rain",
- * "standard cirrus",
- * "subvisual cirrus",
- * and "NOAA cirrus".

Stratus clouds are flat, opaque, and low-altitude. **Altostratus clouds** are flat and medium altitude. **Cirrus clouds** are thin and high-altitude. They are hard to model, so there are three different varieties. **Cumulus clouds** are thick and stretch from low altitudes to medium altitudes. **Stratocumulus clouds** are like thunder clouds. They are very tall and reach from low altitudes to the top of the troposphere. **Nimbostratus clouds** are low and thick, like stratus, but produce rain.

- altitude_km is the altitude, in kilometers above sea level, that you put your virtual sensor in the model. The default is 70 km, which is above almost all of the atmosphere.

For some exercises, you may experiment with putting the sensor somewhere around 8 to 12 km, which is the top of the troposphere, below the stratospheric ozone layer.

For other exercises, you might want to put it at 0 km (ground level), and set it to look up instead of down, so you can see the IR radiation coming down to the ground from the atmosphere instead of looking at the IR radiation going out to space.

- looking is the direction the sensor is looking. The options are “down” (the default) or “up”.

Any arguments you don’t specify explicitly take on their default value. Thus, `run_modtran(file.path(data_dir, "modtran_experiment_1.txt"), co2_ppm = 800, delta_t = 1.0, h2o_fixed = "relative humidity")` would run with all the default values, except for 800 ppm CO₂, a temperature offset of 1°C, and holding relative humidity fixed.

You can assign the output of `run_modtran()` to a variable like this: `mod_data <- run_modtran("my_modtran_file.txt", co2_ppm = 400)` and then you can pass the value of `mod_data` to the `plot_modtran()` function, as described below.

- `plot_modtran` reads a MODTRAN output file and generates a plot. There are many arguments, and I won’t explain them all here, but the important ones are:

- filename is the MODTRAN output file with the data to use for the plot.

You can also provide data directly to `plot_modtran` instead of reading in a file: Instead of writing `plot_modtran("my_modtran_file.txt", ...)`, you could write, `plot_modtran(modtran_data = mod_data, ...)`, where `mod_data` is the output of `run_modtran()` or `read_modtran()`.

- descr is an optional string to use for the title of the plot. If you don’t specify anything, the function will make a title that indicates the CO₂ concentration and the altitude of

the virtual sensor.

- `i_out_ref` is a reference value for the outgoing infrared. If you don't specify it, it's ignored, but if you specify it, then the plotting function adds an annotation to indicate the difference in outgoing IR between the current run being plotted and the reference value. Typically, you'd run a baseline run of MODTRAN with default parameters and then use the upward IR flux from that run as `i_out_ref` when you change the CO₂ concentration or other model parameters.
- `delta_t` is the temperature offset for this model run. If you specify it, the plotting function adds an annotation to indicate it.
- `text_size` allows you to adjust the size of the text used for axis labels and the plot title.
- `read_modtran(filename)` allows you to read in a MODTRAN output file and examine the data. This function returns a list with 7 elements:
 - `spectrum` is a data tibble with the spectral information (wavelength `lambda`, wavenumber `k`, outgoing IR intensity `tk`, and a number of other variables.)
 - `profile` is the profile of the atmosphere: a tibble with seven columns:
 - * `Z` is the altitude in km,
 - * `P` is the atmospheric pressure, in millibars, and
 - * `T` is the temperature in Kelvin.
 - * `H2O` is the concentration of water vapor, in parts per million at each altitude.
 - * `O3` is the concentration of ozone, in parts per million at each altitude.
 - * `CO2` is the concentration of carbon dioxide, in parts per million at each altitude.
 - * `CH4` is the concentration of methane, in parts per million at each altitude.
 - `co2` is the atmospheric CO₂ concentration
 - `ch4` is the atmospheric methane concentration
 - `i_out` is the intensity of the outgoing IR radiation flux.
 - `t_ground` is the ground temperature (in Kelvin) used in the model run. (Remember that this is something you set when you run the model. MODTRAN cannot calculate the way ground temperature changes when you change greenhouse gases, clouds, or other characteristics of the atmosphere.)
 - `t_tropo` is the temperature at the tropopause (in Kelvin).
 - `h_tropo` is the height of the tropopause (in km).
 - `alt` is the altitude of the virtual sensor.
 - `sensor_direction` is the direction of the virtual sensor (“up” or “down”).

Converting temperature units

- Some handy functions for converting temperature measurements from one unit of measurement to another are:
 - `ktof(T)` converts T from Kelvin to Fahrenheit.
 - `ktoc(T)` converts T from Kelvin to Celsius.
 - `ftok(T)` converts T from Fahrenheit to Kelvin.
 - `ctok(T)` converts T from Celsius to Kelvin.
 - `ctof(T)` converts T from Celsius to Fahrenheit.
 - `ftoc(T)` converts T from Fahrenheit to Celsius.

But be aware that if you want to convert the *difference between two temperatures*, you need to convert the temperatures and then take the difference:

```
t1_k = 254 # Kelvin temperature
t2_k = 288 # Kelvin temperature
delta_t_k = t2_k - t1_k # Difference in temperature, in Kelvin

delta_t_k
```

```
## [1] 34
```

```
t1_f = ktof(t1_k) # Fahrenheit temperatures
t2_f = ktof(t2_k)
```

```
t1_f
```

```
## [1] -2.47
```

```
t2_f
```

```
## [1] 58.73
```

```
delta_t_f = t2_f - t1_f # Difference in temperature, in Fahrenheit
```

```
delta_t_f
```

```
## [1] 61.2
```

```
# This will give the wrong answer for the
# temperature difference in Fahrenheit!
ktof(delta_t_k)
```

```
## [1] -398.47
```

You see that 58.73 minus -2.47 is not -398.47.

- Some variables that I have defined for you are:

- `sigma_sb` is the Stefan-Boltzmann constant.
- `solar_constant` is the Solar Constant (the intensity of sunlight at the top of the atmosphere).

Examples:

```
run_modtran(filename = file.path(data_dir, "modtran_baseline.txt"))
modtran_baseline = read_modtran(file.path(data_dir, "modtran_baseline.txt"))
```

You could also write this as

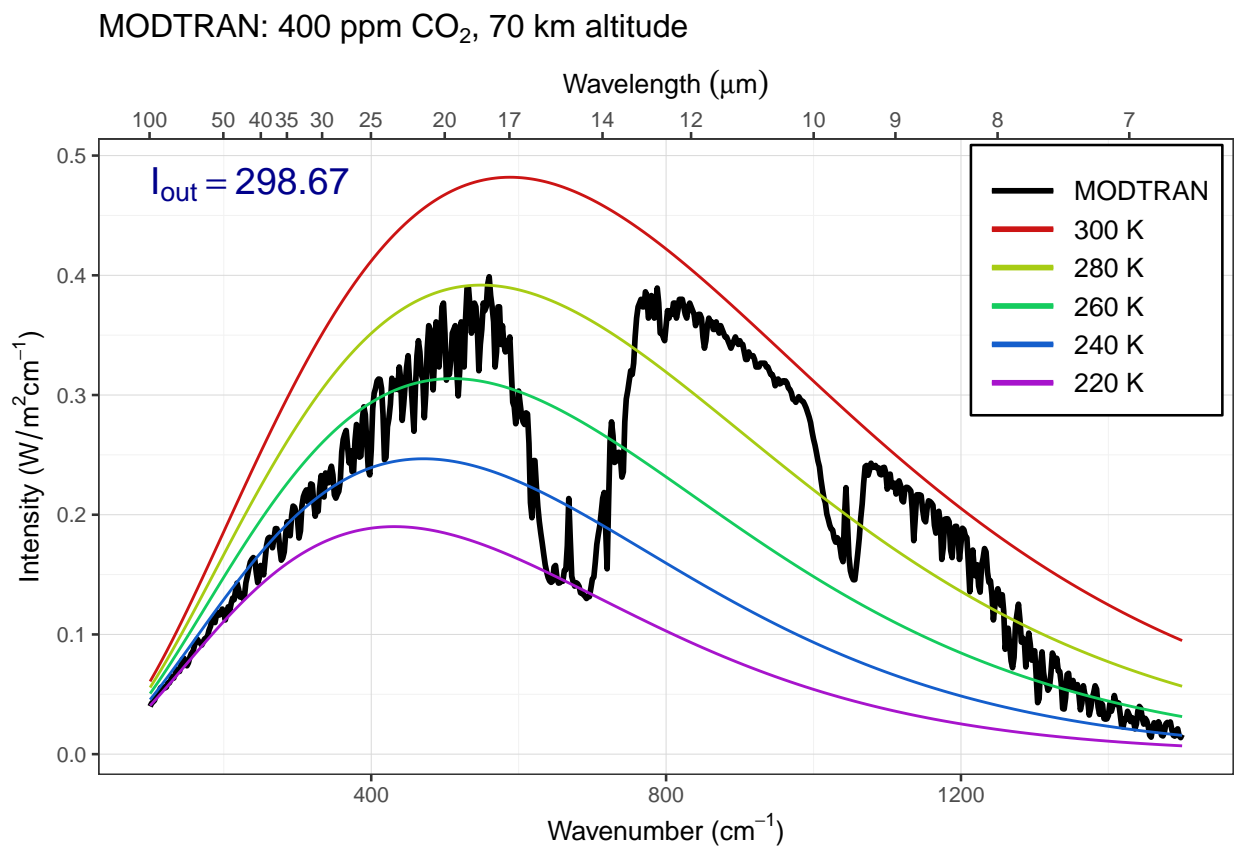
```
modtran_baseline = run_modtran(filename = file.path(data_dir, "modtran_baseline.txt"))
```

Now you can extract the various values from `modtran_baseline`:

```
baseline_i_out <- modtran_baseline$i_out
baseline_t_trop <- modtran_baseline$t_trop
```

The baseline MODTRAN run has $I_{\text{out}} = 299.$ and $T_{\text{tropopause}} = 190.$.

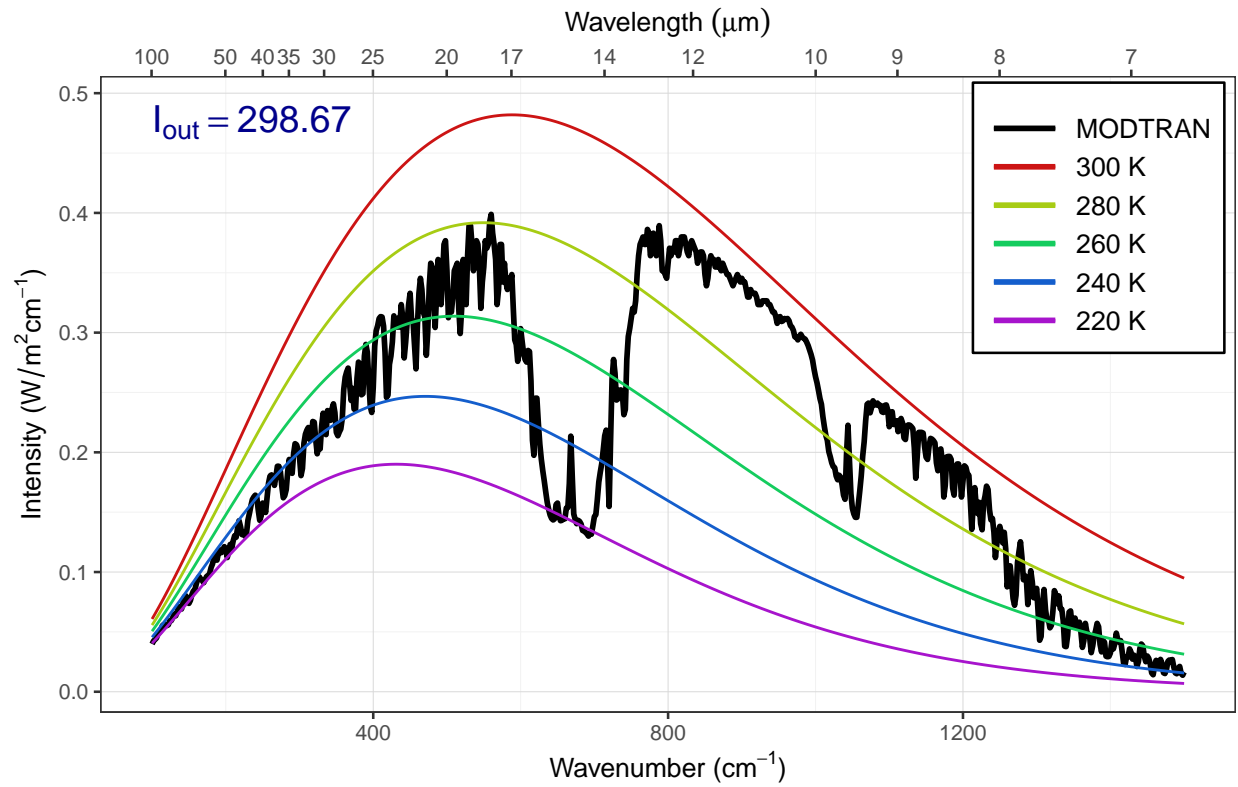
```
plot_modtran(file.path(data_dir, "modtran_baseline.txt"))
```



Or you could write

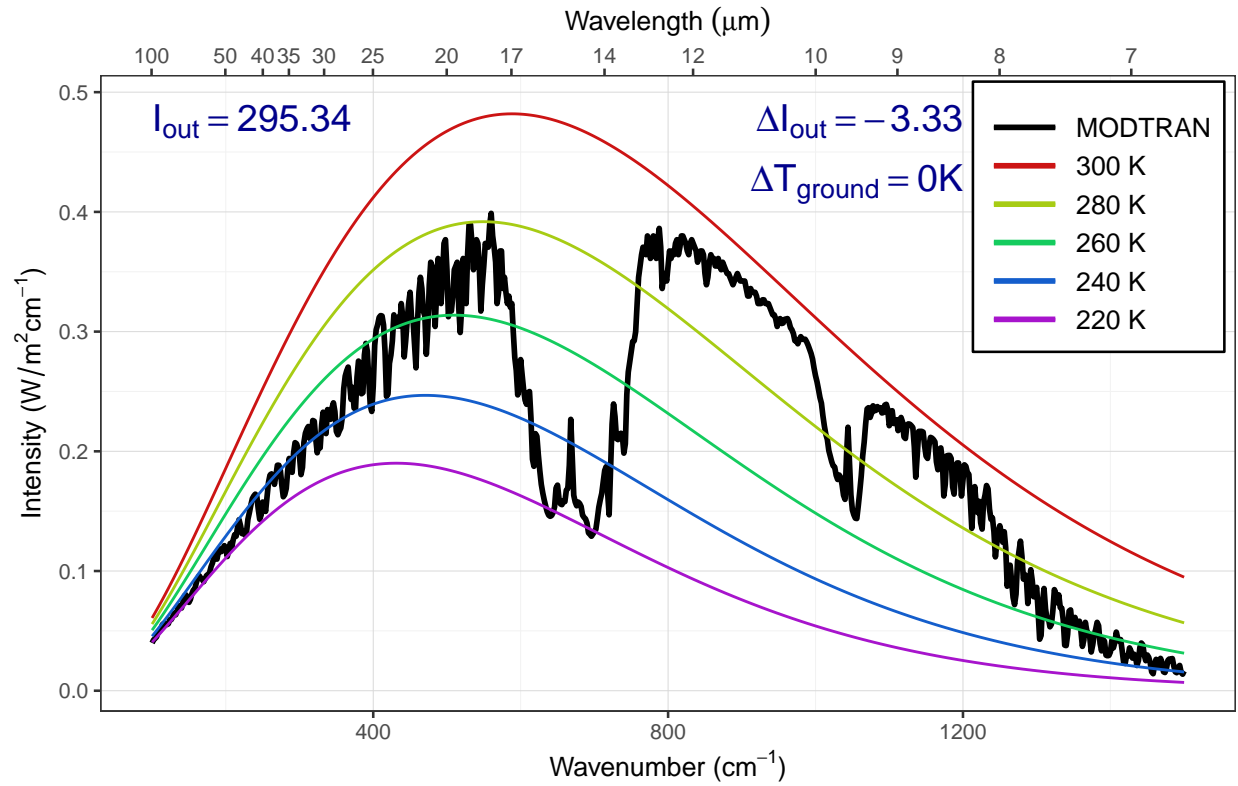
```
plot_modtran(modtran_data = modtran_baseline)
```

MODTRAN: 400 ppm CO₂, 70 km altitude



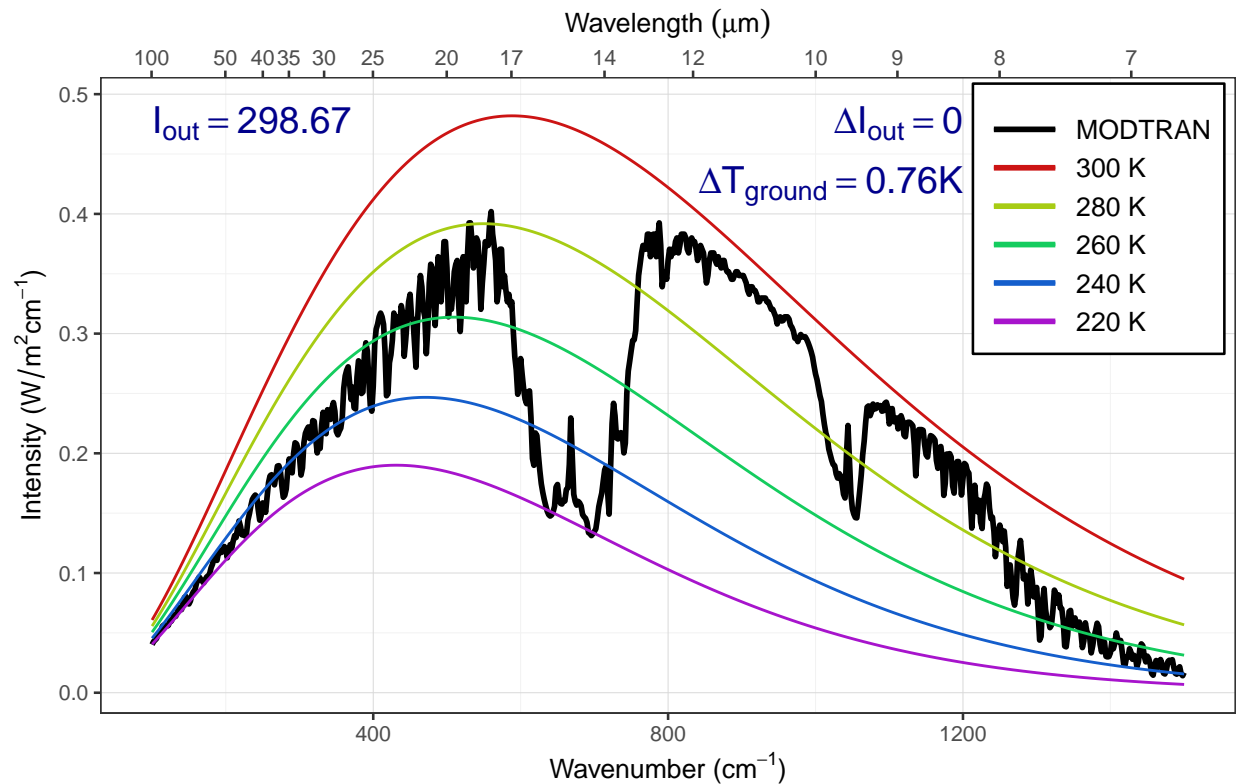
```
double_co2 = run_modtran(filename = file.path(data_dir, "modtran_double_co2.txt"),
                          co2_ppm = 800)
plot_modtran(double_co2, i_out_ref = baseline_i_out, delta_t = 0)
```

MODTRAN: 800 ppm CO₂, 70 km altitude



```
mod_file = file.path(data_dir, "modtran_double_co2_warming.txt")
double_co2_warming = run_modtran(filename = mod_file,
                                co2_ppm = 800, delta_t = 0.76)
plot_modtran(double_co2_warming, i_out_ref = baseline_i_out, delta_t = 0.76)
```


MODTRAN: 800 ppm CO₂, 70 km altitude



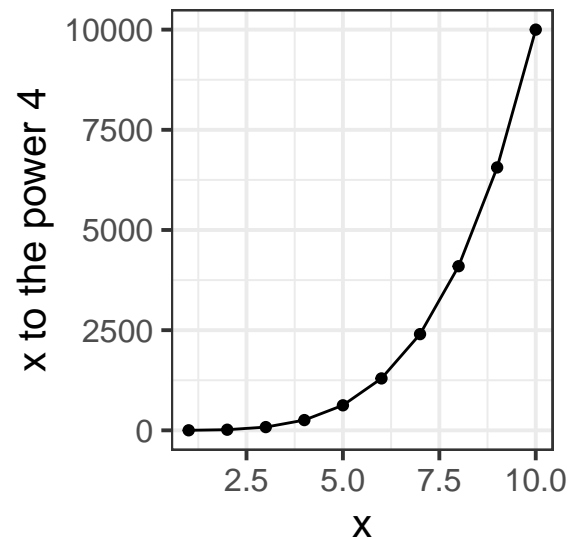
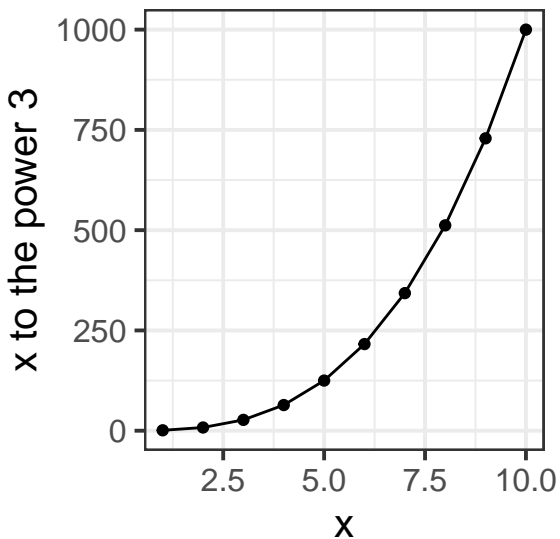
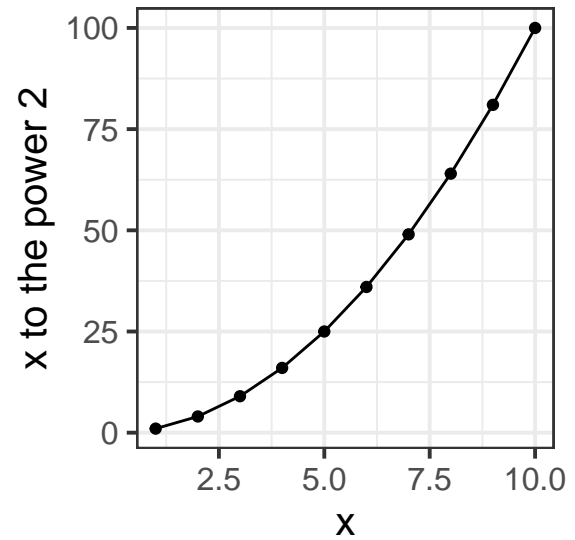
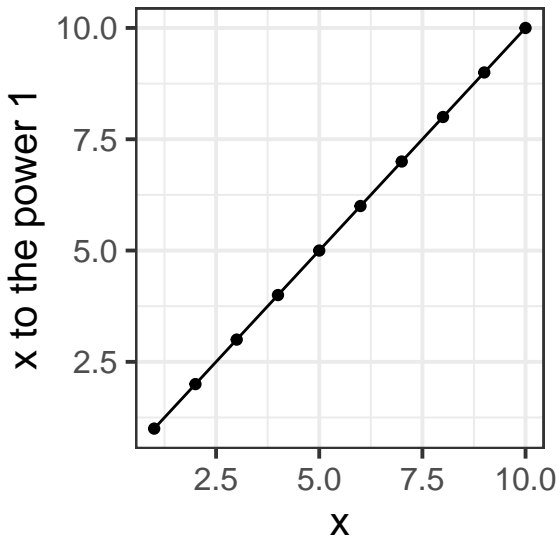
A few new R functions that we will use in this lab:

Iterating over a series

Sometimes you want to repeat something in R, executing the same commands for many different values of a variable. We can do this with the `for` command:

```
df = tibble(x = 1:10)

for (i in 1:4) {
  p = ggplot(df, aes(x = x, y = x^i)) +
    geom_point() + geom_line() +
    labs(x = "x", y = str_c("x to the power ", i))
  plot(p)
}
```



This gives us a nice way to run MODTRAN over and over, with many different values for the CO₂ concentration:

```
co2_values = c(0, 200, 400, 600, 800, 1000, 1200)
for (co2 in co2_values) {
  filename = str_c("modtran_", co2, ".txt")
  run_modtran(filename, co2_ppm = co2, atmosphere = "standard",
    altitude_km = 70)
}
```

This code runs `run_modtran` for each value of CO₂ in `co2_values` and saves the result to a file `modtran_0.txt`, `modtran_200.txt`, and so forth. I make the filenames from the values of `co2` using the `str_c` function, which I explain below.

Combining character variables

R has many functions for manipulating text. When R stores text, it stores it in character variables (these are also sometimes called “strings” because text is like a string of characters). For instance, we might want to make a label or a filename by combining several variables. Three functions that we can use are `str_c`, from the `stringr` package and `paste` and `paste0`, from basic R. All of these work pretty much the same way:

```
print(paste("mail", "box"))

## [1] "mail box"

print(paste("mail", "box", sep = ""))

## [1] "mailbox"

print(paste0("infra", "red"))

## [1] "infrared"

print(str_c("infra", "red"))

## [1] "infrared"

print(str_c("infra", "red", sep = "-"))

## [1] "infra-red"

print(str_c("one", "two", "three", "four", sep = ", "))

## [1] "one, two, three, four"

print(str_c(10, " km"))

## [1] "10 km"

x = 50

print(str_c(x, " Watts"))

## [1] "50 Watts"

print(str_c(x, "Watts", sep = " "))

## [1] "50 Watts"
```

Notice how `paste` puts spaces between the strings when it combines them unless you specify that `sep` (the separator) should be something different. `paste0` works just like `paste`, except that it doesn't have a separator, so the variables are combined without an extra space. `str_c` is like `paste0`, except that you can specify a separator if you do want something in between the different variables.

Calculating with leads and lags

Sometimes, when we are using `mutate` with a data tibble, we might want to look at differences between a row and the row before or after it in the tibble. We can do this with the `lead` and `lag` functions:

In the example below, the column `u` gets the value of the current row of `y` minus the previous row of `y`, and the column `v` gets the value of the next row of `y` minus the current row of `y`. Note that where there isn't a previous row, `lag` returns `NA` (missing value), and similarly for `lead` when there isn't a next row.

```
tbl = tibble(x = 0:5, y = x^2)

tbl = tbl %>% mutate(u = y - lag(y), v = lead(y) - y)
tbl
```

```
## # A tibble: 6 x 4
##       x     y     u     v
##   <int> <dbl> <dbl> <dbl>
## 1     0     0    NA     1
## 2     1     1     1     3
## 3     2     4     3     5
## 4     3     9     5     7
## 5     4    16     7     9
## 6     5    25     9    NA
```

If you want to lead or lag by more than one row, you can just say, `lag(y, 5)` to get the value of `y` 5 rows before the current one.

```
tbl = tibble(x = 1:10)

tbl = tbl %>% mutate(before = lag(x), after = lead(x),
                     before.2 = lag(x, 2), after.3 = lead(x, 3))
tbl
```

```
## # A tibble: 10 x 5
##       x before after before.2 after.3
##   <int> <int> <int>     <int>     <int>
## 1     1    NA     2         NA         4
## 2     2     1     3         NA         5
## 3     3     2     4           1         6
## 4     4     3     5           2         7
## 5     5     4     6           3         8
## 6     6     5     7           4         9
## 7     7     6     8           5        10
## 8     8     7     9           6        NA
## 9     9     8    10           7        NA
```

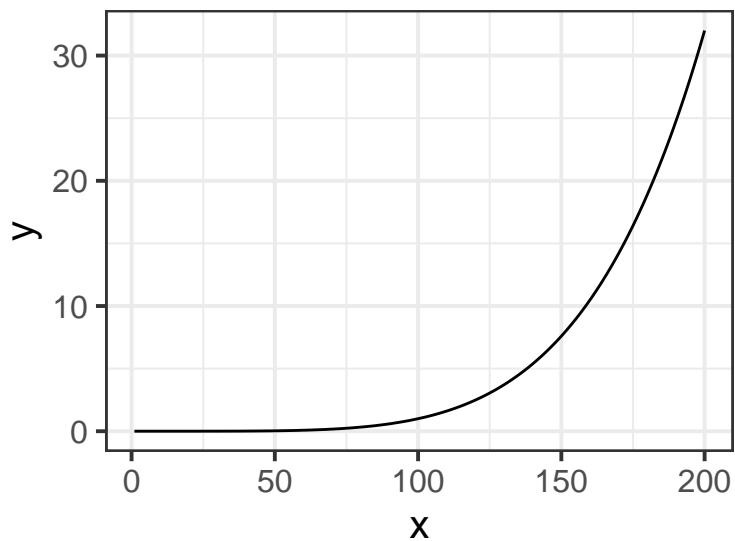
```
## 10    10    9    NA    8    NA
```

Modifying x and y axes in ggplot

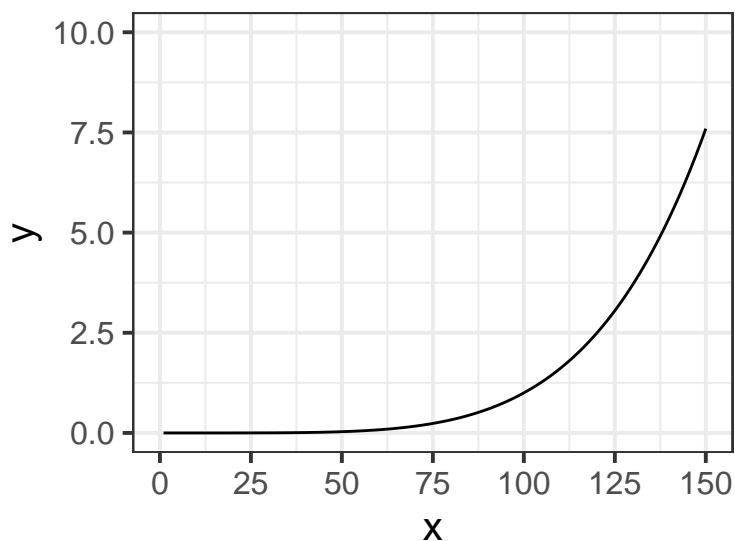
It is easy to modify the x or y axis in ggplot. For instance, if you want to put specific limits on the axis, or change where the labels go, you can use `scale_x_continuous` or `scale_y_continuous`:

```
tbl = tibble(x = 1:200, y = (x / 100)^5)

ggplot(tbl, aes(x = x, y = y)) + geom_line()
```



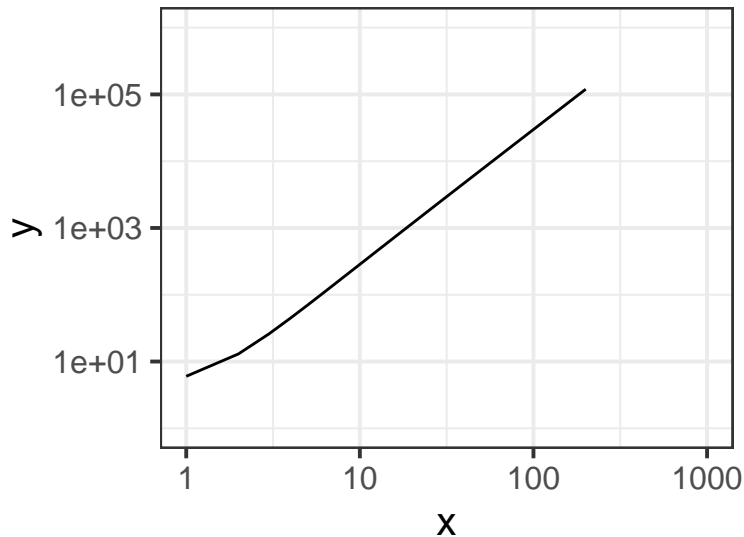
```
ggplot(tbl, aes(x = x, y = y)) + geom_line() +
  scale_x_continuous(limits = c(0,150), breaks = seq(0, 150, 25)) +
  scale_y_continuous(limits = c(0,10))
```



```
tbl = tibble(x = 1:200, y = 5 - 2 * x + 3 * x^2)

# Note that in R when we are typing numbers, we can express scientific notation
# as 1E6 for 1,000,000 2.67E-3 for 0.00267

ggplot(tbl, aes(x = x, y = y)) + geom_line() +
  scale_x_log10(limits = c(1,1000)) +
  scale_y_log10(limits = c(1,1E6))
```



Exercises for Lab #3

Chapter 4 Exercises

Exercise 4.1: Methane

Methane has a current concentration of 1.7 ppm in the atmosphere and is doubling at a faster rate than CO₂.

- Would an additional 10 ppm of methane in the atmosphere have a larger or smaller impact on the outgoing IR flux than an additional 10 ppm of CO₂ at current concentrations?
- Where in the spectrum does methane absorb? What concentration does it take to begin to saturate the absorption in this band? Explain what you are looking at to judge when the gas is saturated.

Suggestion:

- Run MODTRAN with no greenhouse gases, except 0.4 ppm of methane.
- Run MODTRAN several times, successively doubling the amount of methane: 0.4 ppm, 0.8 ppm, 1.6 ppm, ... 102.4 ppm.

Hint: You can use the following R commands to do this:

```
methane_data = tibble() # create a blank data tibble

for (x in 0:11) {
  # Repeat everything between the braces "{}" for x taking on
  # each value in 0, 1, 2, ..., 11.

  p_methane = 0.4 * (2^x) # methane concentration is 0.4 times 2 to the
                           # power of x.

  # Create a character variable that will be a file name of the form
  # file.path(data_dir, "methane_xx_x.txt"), where xx_x is the methane
  # concentration, with an underscore for the decimal point.
  methane_txt = formatC(p_methane, digits = 1, decimal.mark = "_",
                        format = "f")
  file_name = str_c('methane_', methane_txt, ".txt")
  file_name = file.path(data_dir, filename)

  # Now run MODTRAN
  results = run_modtran(file_name, co2_ppm = 0, ch4_ppm = p_methane,
                        trop_o3_ppb = 0, strat_o3_scale = 0, h2o_scale = 0,
                        freon_scale = 0,
                        delta_t = 0, h2o_fixed = "vapor pressure",
                        atmosphere = "tropical", clouds = "none",
                        altitude_km = 70, looking = "down")

  # Create a data tibble with columns for the methane concentration
  # and I out, and append it to the end of the tibble methane_data
  df = tibble(methane = results$ch4, i_out = results$i_out)
  methane_data = bind_rows(methane_data, df)
}
```

This will run MODTRAN for the different values of methane concentration and save them in the "_data" folder as "methane_0_4.txt", "methane_0_8.txt", "methane_1_6.txt", and so forth, up to "methane_819_2.txt", and also create a data tibble methane_data with a list of methane concentrations and the corresponding I_{out} .

- Use mutate to add a new column change, which contains the change in I_{out} between the previous row and this one. You can use the lag command to calculate this, as described above in the “new R functions” section.

```
methane_data = methane_data %>% mutate(change = i_out - lag(i_out))
```

- Now plot i_out versus the methane concentration several ways:
 - First, just plot i_out versus methane:

```
ggplot(methane_data, aes(x = methane, y = i_out)) +
  geom_point(size = 2) +
  geom_line(size = 1) +
  labs() # add parameters to labs to label your axes.
```

- Next, plot the same data, but with a logarithmic x -axis (use `scale_x_log10`, as described above in the “New R Functions” section)
 - Next, plot `methane_concentration`, but assign the column change to the y axis, instead of the column `i_out`.
 - Think back to the slides I showed in class #6 about identifying band saturation. Do you see a place where the successive changes in `i_out` flatten out? Estimate the concentration of methane where absorption saturates.
- c) Would a doubling of methane have as great an impact on the heat balance as a doubling of CO_2 ?

Suggestion:

- Run MODTRAN in its default configuration (400 ppm CO_2 and 1.7 ppm methane)
 - Run it again with 10 ppm of extra methane
 - Run it again with the default methane (1.7 ppm) but 10 ppm extra CO_2 .
 - Compare I_{out} for the three runs.
- d) What is the “equivalent CO_2 ” of doubling atmospheric methane? That is to say, how many ppm of CO_2 would lead to the same change in outgoing IR radiation energy flux as doubling methane? What is the ratio of ppm CO_2 change to ppm methane change?

Suggestion: This is easier to do interactively with the web-based interface to MODTRAN than by running it in R.

- Run MODTRAN in its default configuration (400 ppm CO_2 and 1.7 ppm methane)
- Run MODTRAN again with the methane doubled. Note I_{out} .
- Return methane to the default value (1.7 ppm), and adjust CO_2 until I_{out} is the same as it was for the doubled methane. Note what concentration of CO_2 does this.
- Now you can use R to run MODTRAN with doubled methane and with the equivalent concentration of CO_2 , and save these runs to the disk.

Exercise 4.2: CO_2 (Graduate students only)

- a) Is the direct effect of increasing CO_2 on the energy output at the top of the atmosphere larger in high latitudes or in the tropics? Compare the change in I_{out} from doubling CO_2 with the atmosphere set to `tropical`, `midlatitude` `summer`, and `subarctic` `summer`.

For each atmosphere, first record I_{out} with CO_2 at 400 ppm and then record the change when you increase CO_2 to 800 ppm.

- b) Set $p\text{CO}_2$ to an absurdly high value of 10,000 ppm. You will see a spike in the CO_2 absorption band. What temperature is this light coming from? Where in the atmosphere do you think

this comes from?

Now turn on clouds and run the model again. Explain what you see. Why are night-time temperatures warmer when there are clouds?

Exercise 4.3: Water vapor

Our theory of climate presumes that an increase in the temperature at ground level will lead to an increase in the outgoing IR energy flux at the top of the atmosphere.

- a) How much extra outgoing IR would you get by raising the temperature of the ground by 5°C? What effect does the ground temperature have on the shape of the outgoing IR spectrum and why?
 - Note the I_{out} for the default conditions. Then set `delta_t` to 5 and run MODTRAN again, and note the new value of I_{out} .
 - Plot the spectrum for both runs and compare.
- b) More water can evaporate into warm air than into cool air. Change the model settings to hold the water vapor at constant relative humidity rather than constant vapor pressure (the default), calculate the change in outgoing IR energy flux for a 5°C temperature increase. Is it higher or lower? Does water vapor make the Earth more sensitive to CO₂ increases or less sensitive?
- c) Now see this effect in another way.
 - Starting from the default base case, record the total outgoing IR flux.
 - Now double pCO₂. The temperature in the model stays the same (that's how the model is written), but the outgoing IR flux goes down.
 - Using constant water vapor pressure, adjust the temperature offset until you get the original IR flux back again. Record the change in temperature
 - Now repeat the exercise, but holding the relative humidity fixed instead of the water vapor pressure.
 - The ratio of the warming when you hold relative humidity fixed to the warming when you hold water vapor pressure fixed is the feedback factor for water vapor. What is it?

Chapter 5 Exercise

Exercise 5.2: Skin Height

- a) Run the MODTRAN model in using the “Tropical” atmosphere, without clouds, and with present-day pCO₂ (400 ppm). Use the ground temperature reported by the model to calculate $\epsilon \sigma T_{\text{ground}}^4$, the heat flux emitted by the ground.

Assume $\epsilon = 1$, and I have already provided the value of the Stefan-Boltzmann constant σ , as the R variable `sigma_sb`, which equals 5.670×10^{-8} . (I defined it in the script “utils.R”, which I loaded in the “setup” chunk in the RMarkdown document).

Next, look at the outgoing heat flux at the top of the atmosphere (70 km) reported by the MODTRAN model. Is it greater or less than the heat flux that you calculated was emitted by the ground?

- b) Use the outgoing heat flux at the top of the atmosphere to calculate the skin temperature (use the equation $I_{\text{out}} = \epsilon \sigma T_{\text{skin}}^4$). What is the skin temperature, and how does it compare to the ground temperature and the temperature at the tropopause, as reported by the MODTRAN model?

Assuming an environmental lapse rate of 6K/km, and using the skin temperature that you calculated above, and the ground temperature from the model, what altitude would you expect the skin height to be?

- c) Double the CO₂ concentration and run MODTRAN again. Do not adjust the ground temperature. Repeat the calculations from (b) of the skin temperature and the estimated skin height.

What is the new skin temperature? What is the new skin height?

- d) Put the CO₂ back to today's value, but add cirrus clouds, using the "standard cirrus" value for the clouds. Repeat the calculations from (b) of the skin temperature and the skin height.

What is the new skin temperature? What is the new skin height? Did the clouds or the doubled CO₂ have a greater effect on the skin height?