Instructions for EES 3310/5310 Lab #3

Exercises with the MODTRAN Model

Lab: Wed. Jan. 24.,2024, Due: Wed. Jan. 31,2024

Contents

Instructions

It would be good 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. http://modtran.spectral.com/modtran_home

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 an optional name for a file to save the data to. If you don't specify the `filename`, then `run_modtran` will not save the model output to the disk. I recommend giving it a meaningful name: for instance, a run with 440 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. I also recommend that you save the files in the `_data` subdirectory to keep your project nicely organized.
  - `co2_ppm` is the amount of CO_2 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 CO_2 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 CO_2, a temperature offset of 1°C, and holding relative humidity fixed.

The 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 CO_2 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”).

  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.

- `read_modtran(filename)` allows you to read in a MODTRAN output file (saved to the disk by `run_modtran()`. It returns a list with the same elements as `run_modtran()`.

- `plot_modtran` generates a plot of the radiative spectrum. There are many arguments, and I won’t explain them all here, but the important ones are:

  - `modtran_data` is the data that would be returned by the `run_modtran()` function. If you want to plot
  - `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 CO_2 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.

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 temeprature, 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
```

```r
# 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, 1350.).

Examples:

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

You could also write this as

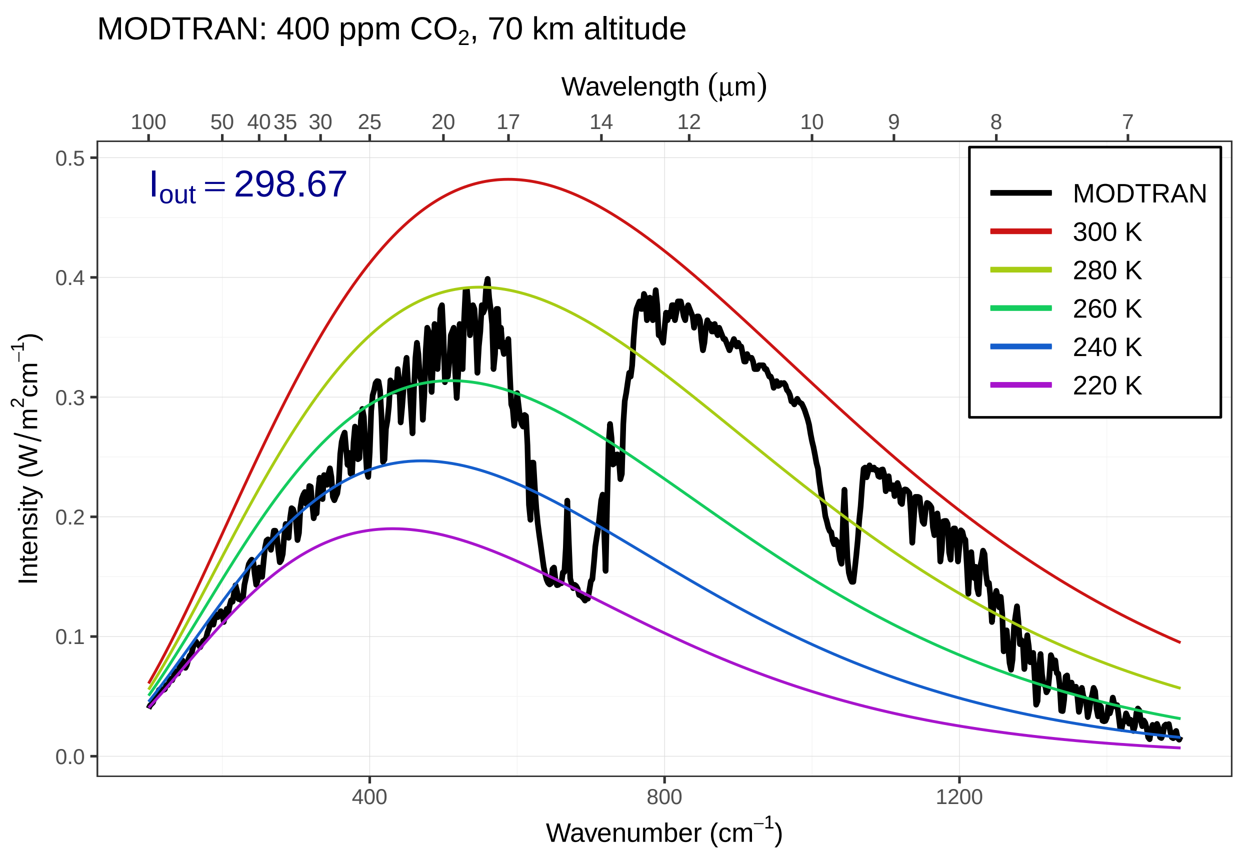
```r
run_modtran(filename = file.path(data_dir, "modtran_baseline.txt"))
modtran_baseline = read_modtran(file.path(data_dir, "modtran_baseline.txt"))
```

Now you can extract the various values from modtran_baseline:

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

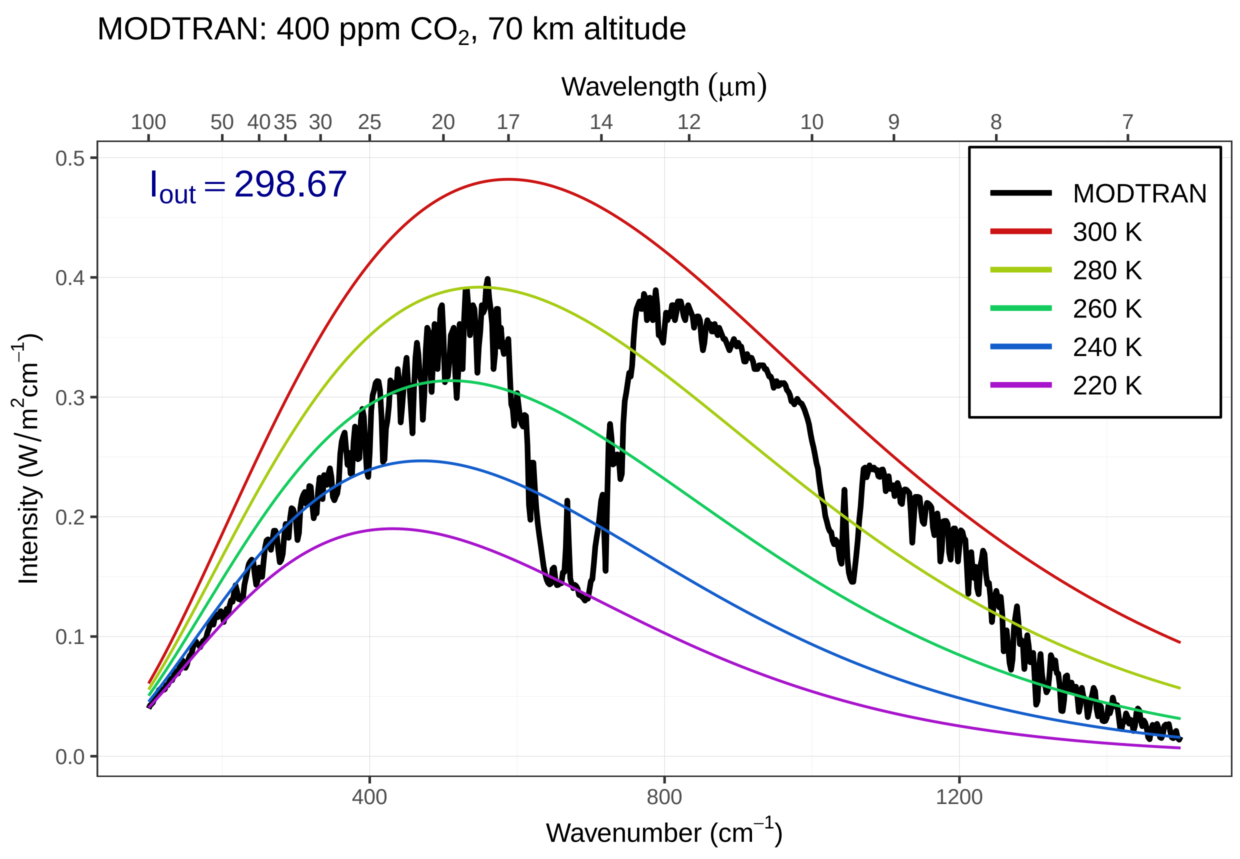
The baseline MODTRAN run has $I_{\text{out}} = 299.$ and $T_{\text{tropopause}} = 190.$.

```r
plot_modtran(modtran_baseline)
```

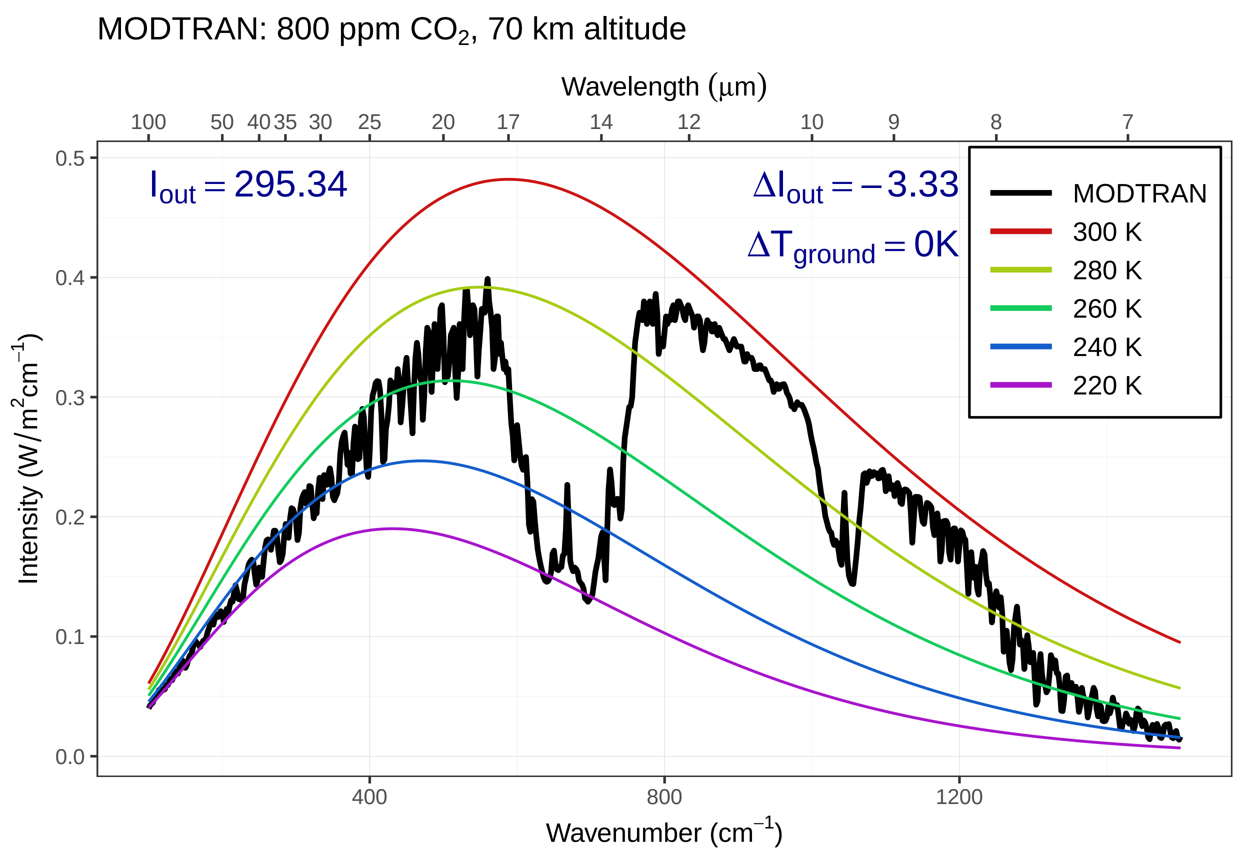


Or you could write

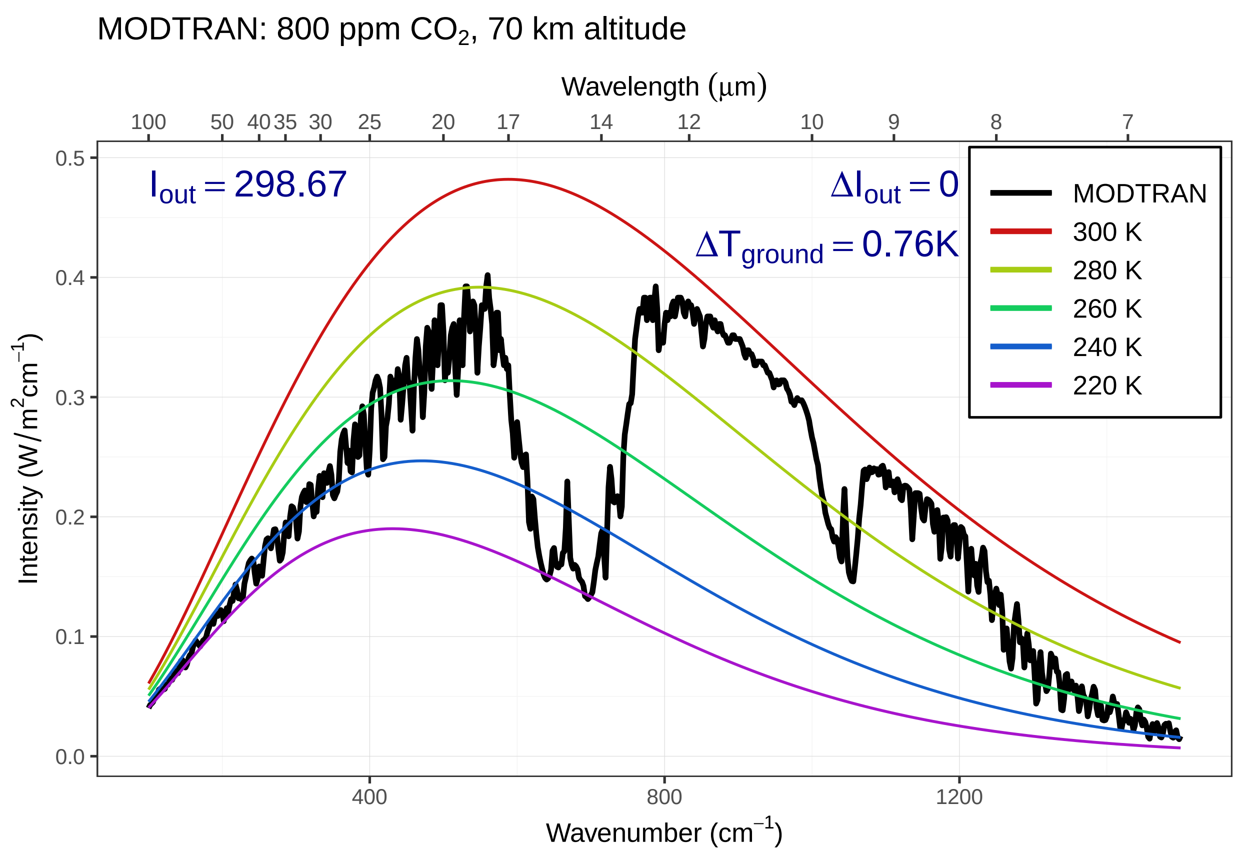
```r
plot_modtran(filename = file.path(data_dir, "modtran_baseline.txt"))
```



```
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)
```



```
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)
```



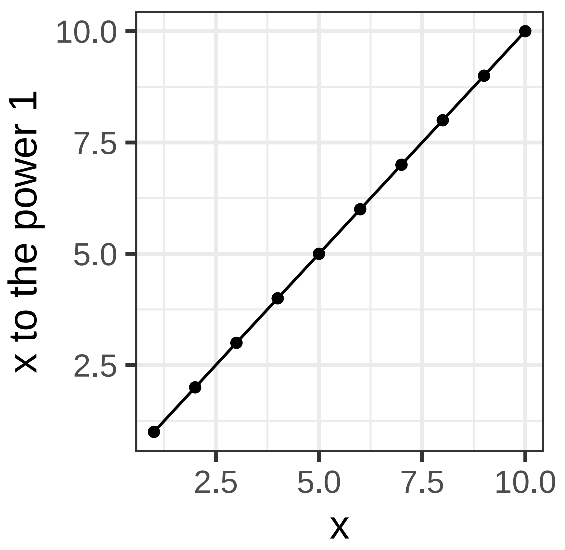
A few new R functions that we will use in this lab:

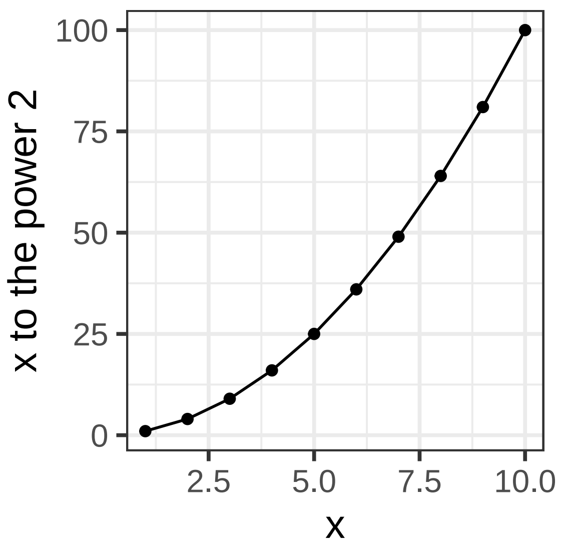
Iterating over a series

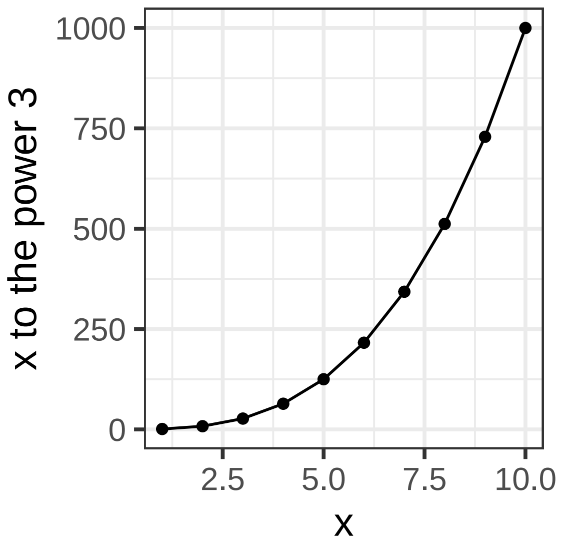
Sometimes you want to repeat something in R, executing the same commands for many different values of a variable. We can do this with the `for` command:

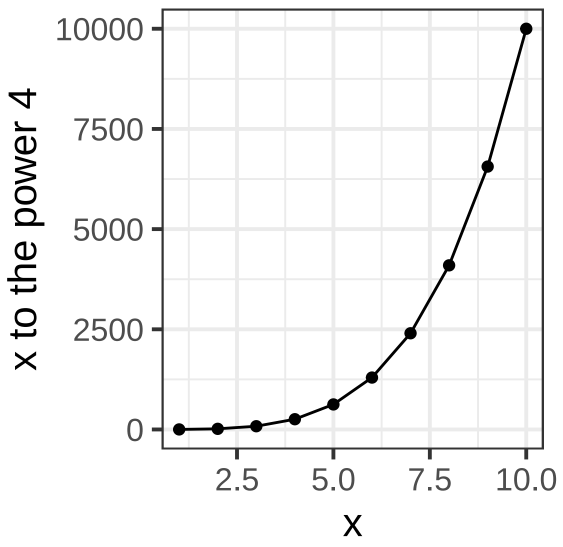
```
df = tibble(x = 1:10)

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)
}
```


x to the power 1
10.0
7.5
5.0
2.5
2.5
5.0
7.5
10.0
x


x to the power 2
100
75
50
25
0
2.5
5.0
7.5
10.0
x





This gives us a nice way to run MODTRAN over and over, with many different values for the CO_2 concentration and recording the value of I_{out} for each concentration.

In the loop below, we set all the greenhouse gases to zero and then vary CO2~. We use a trick in R by making an empty tibble before we start the loop and then for each iteration of the loop, we use `bind_rows` to append a row with the data from that loop iteration.

```
co2_values = c(0, 200, 400, 600, 800, 1000, 1200)
tbl = tibble()
for (co2 in co2_values) {
  filename = str_c("modtran_co2_", co2, ".txt")
  mod_data = run_modtran(filename, co2_ppm = co2, ch4_ppm = 0, trop_o3_ppb = 0,
                         strat_o3_scale = 0, h2o_scale = 0, freon_scale = 0,
                         atmosphere = "standard", altitude_km = 70)
  tbl = bind_rows(tbl, tibble(co2_ppm = co2, i_out = mod_data$i_out))
}

# The digits argument below sets the number of decimal places
# for each column in the table.
kable(tbl, digits = c(co2_ppm = 0, i_out = 1))
```

This code runs `run_modtran` for each value of CO_2 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.

Manipulating text in R

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. We can use the function `str_c`, from the `tidyverse`:

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

```
## [1] "infrared"
```

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

```
## [1] "infra-red"
```

```
print(str_c(10, "km", sep = " "))
```

```
## [1] "10 km"
```

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

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

```
x = 50

print(str_c(x, "Watts"))
```

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

```r
print(str_c(x, " Watts"))
```

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

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

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

Notice how `str_c` pastes the text together without any spaces between the parts unless you tell it to use a separator (`sep`) between them.

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.

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

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

x	y	lag y	lead y	u	v
0	0	NA	1	NA	1
1	1	0	4	1	3
2	4	1	9	3	5
3	9	4	16	5	7
4	16	9	25	7	9
5	25	16	NA	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))
kable(tbl)
```

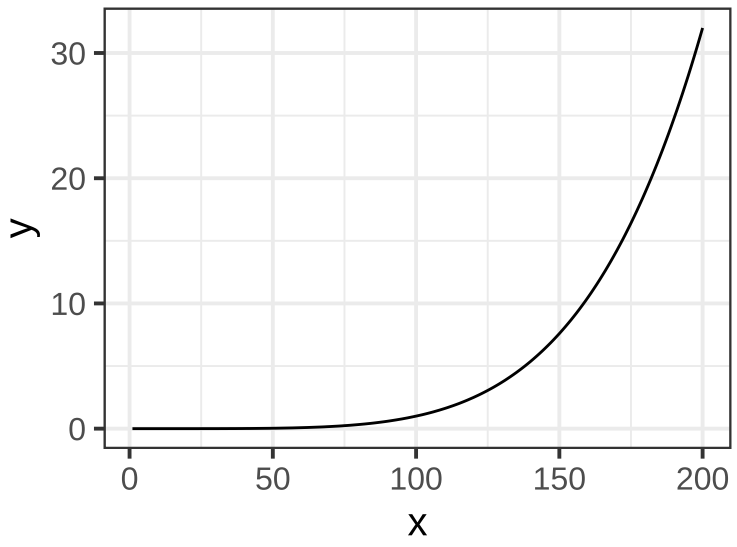
x	before	after	before.2	after.3
1	NA	2	NA	4
2	1	3	NA	5
3	2	4	1	6
4	3	5	2	7
5	4	6	3	8
6	5	7	4	9
7	6	8	5	10
8	7	9	6	NA
9	8	10	7	NA
10	9	NA	8	NA

Modifying *x* and *y* axes in `ggplot`

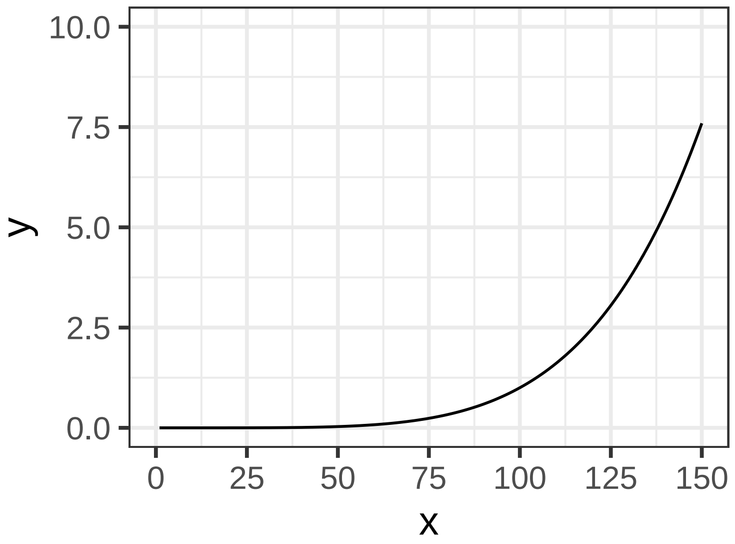
It is easy to modify the *x* or *y* axis in `ggplot`. For instance, if you want to put specific limits on the axis, or change where the labels go, you can use `scale_x_continuous` or `scale_y_continuous`:

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

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



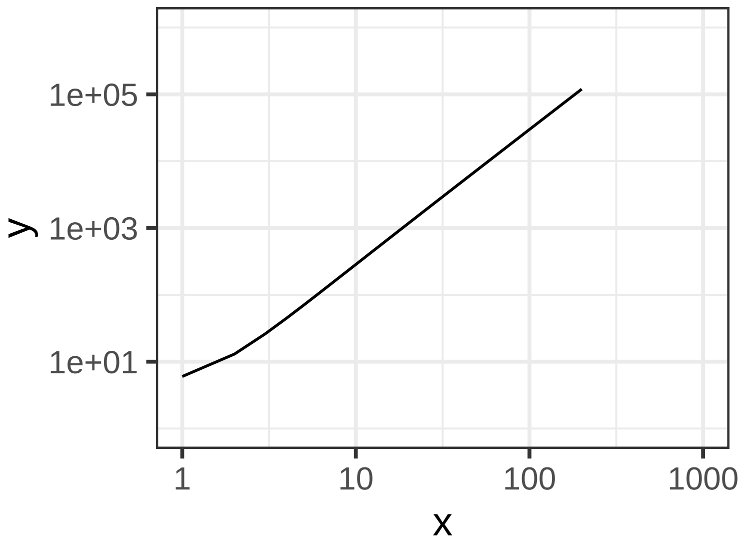
```r
ggplot(tbl, aes(x = x, y = y)) + geom_line() +
  scale_x_continuous(limits = c(0,150), breaks = seq(0, 150, 25)) +
  scale_y_continuous(limits = c(0,10))
```



```r
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

You should open the file `lab-03-report.Rmd` to do these 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 CO_2.

a) **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 CO_2 at current concentrations?**

   Suggestion:

   - Run MODTRAN in the default configuration (400 ppm CO_2 and 1.7 ppm methane)
   - Run MODTRAN with an extra 10 ppm of CO_2 and the normal amount of methane.
   - Run MODTRAN with the normal amount of CO_2 and an extra 10 ppm of methane.

   What would you look at from the three runs to figure out whether 10 ppm of methane or 10 ppm of CO_2 had the greater effect?

b) **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.**

   Hints:
   I recommend setting all the greenhouse gases to zero, and run MODTRAN. Then run MODTRAN for several values of methane, starting at 1 ppm and doubling the concentration until you get to around 128 ppm. You can do this using a `for` loop, following the examples from the lab instructions.

   To set all the greenhouse gases to zero, you would call `run_modtran(co2_ppm = 0, ch4_ppm = 0, trop_o3_ppb = 0, strat_o3_scale = 0, h2o_scale = 0, freon_scale = 0)`

   The spectrum of methane is complicated so it doesn't saturate all at once. Use `plot_modtran` to plot the spectrum for each concentration and describe what you see and where you think methane begins to saturate and why.

   By default, `plot_modtran` gives a plot a title that indicates the CO_2 concentration. Here, CO_2 doesn't change and we're interested in the CH_4 concentration, so you can use the `descr` argument to `plot_modtran` to give the plots different titles. See the example below.

   Remember that if you want to make several plots using a `for` loop, you need to assign the result from `plot_modtran` or `ggplot` to a variable and then use the `plot` or `print` function.

```r
for (ch4 in ch4_list) {
  mod_data = run_modtran(co2_ppm = 0, ch4_ppm = ch4, trop_o3_ppb = 0,
  strat_o3_scale = 0, h2o_scale = 0, freon_scale = 0)
  p = plot_modtran(mod_data)
  plot(p) # you could also say print(p) here.
}
```

This will take some time to run because it needs to run MODTRAN for each different value of `ch4`, so you might want to tell R to save the output from the model in a file, and tell R to check whether that file exists and if it does, read from the file instead of running the model again:

```r
for (ch4 in ch4_list) {
  # make a name for the model-output file: "_data/modtran_ch4_0_ppm.txt",
  # "_data/modtran_ch4_1.7_ppm.txt", etc.
  mod_file = str_c("_data/modtran_ch4_", ch4, "_ppm.txt")
  if (! file.exists(mod_file)) {
    mod_data = run_modtran(filename = mod_file, co2_ppm = 0, ch4_ppm = ch4,
                           trop_o3_ppb = 0, strat_o3_scale = 0,
                           h2o_scale = 0, freon_scale = 0)
  } else {
    mod_data = read_modtran(mod_file)
  }
  p = plot_modtran(mod_data)
  plot(p) # you could also say print(p) here.
}
```

But if you do this, then if you change the way you run the model (e.g., change some of the parameters to `run_modtran`, such as the altitude or the atmosphere), you will need to manually delete the files in the `_data` directory to make R run the model with the new parameters.

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 double the methane concentration.
- Run it again with the default methane (1.7 ppm) but double the CO_2 concentration.
- 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?**

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?**

   Hint: Run MODTRAN with the atmosphere set to `tropical`, `midlatitude summer`, and `subarctic summer`, and for each atmosphere, at 400 ppm and 800 ppm CO_2. For each atmosphere, calculate the difference between I_{out} at 400 and 800 ppm CO_2 and determine how the effect of doubling CO_2 varies as you go from tropical latitudes to subarctic ones.

b) **Set pCO_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?

   Hint: MODTRAN simulates the upward directed, outgoing longwave radiation as seen by a sensor looking down from some height. For the first part of this exercise, start with the sensor at its default altitude of 70 km (you set this with the `altitude_km` argument to `run_modtran`), and successively lower it by 10 km at a time until you get to 10 km. What happens to the spike as you lower the sensor? What does this say about what part of the atmosphere is responsible for the spike in the middle of the CO_2 absorption at very high values of CO_2?

   For the second part of this exercise, try using "altostratus" 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?**

   HINT: You can raise the temperature of the ground with the `delta_t` artument to MODTRAN.

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 CO_2 increases or less sensitive?**

   Note: By default, the MODTRAM model holds water vapor pressure constant, but you can set it to hold relative humidity constant instead with the option `h2o_fixed = "relative humidity"`, like this: `run_modtran(file_name, delta_t = 5, h2o_fixed = "relative humidity")`.

c) **Now see this effect in another way.**

- **Starting from the default base case, record the total outgoing IR flux.**
- **Now double CO_2. 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?**