Lesson 5: Linear regression with real data

1 Earth temperature over time

In this lesson, we will apply all that we've learned (and more) to analyze real data of Earth temperature over time.

Is global temperature rising? How much? This is a question of burning importance in today's world!

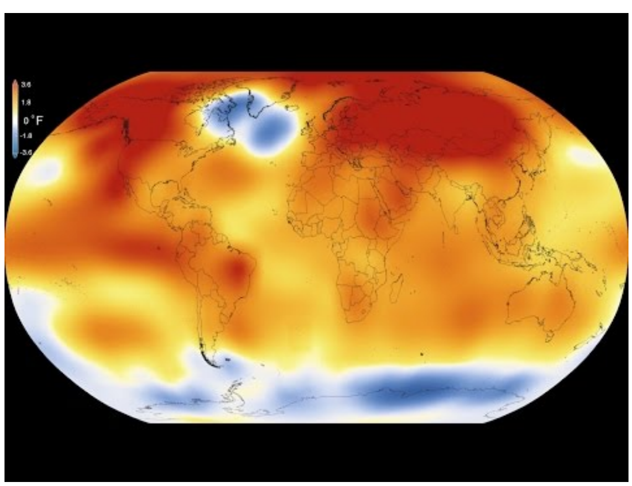
Data about global temperatures are available from several sources: NASA, the National Climatic Data Center (NCDC) and the University of East Anglia in the UK. Check out the University Corporation for Atmospheric Research (UCAR) for an in-depth discussion.

The NASA Goddard Space Flight Center is one of our sources of global climate data. They produced the video below showing a color map of the changing global surface **temperature anomalies** from 1880 to 2015.

The term global temperature anomaly means the difference in temperature with respect to a reference value or a long-term average. It is a very useful way of looking at the problem and in many ways better than absolute temperature. For example, a winter month may be colder than average in Washington DC, and also in Miami, but the absolute temperatures will be different in both places.

In [1]:
```
from IPython.display import YouTubeVideo
YouTubeVideo('gGOzHVUQCw0')
```

Out[1]:



How would we go about understanding the *trends* from the data on global temperature?

The first step in analyzing unknown data is to generate some simple plots using **Matplotlib**. We are going to look at the temperature-anomaly history, contained in a file, and make our first plot to explore this data.

We are going to smooth the data and then we'll fit a line to it to find a trend, plotting along the way to see how it all looks.

Let's get started!

2 Step 1: Read a data file

We took the data from the NOAA (National Oceanic and Atmospheric Administration) webpage. Feel free to play around with the webpage and analyze data on your own, but for now, let's make sure we're working with the same dataset.

We have a file named `land_global_temperature_anomaly-1880-2016.csv` in our `data` folder. This file contains the year on the first column, and averages of land temperature anomaly listed sequentially on the second column, from the year 1880 to 2016. We will load the file, then make an initial plot to see what it looks like.

Note: If you downloaded this notebook alone, rather than the full collection for this course, you may not have the data file on the location we assume below. In that case, you can download the data if you add a code cell, and execute the following code in it:

```
from urllib.request import urlretrieve
URL = 'http://go.gwu.edu/engcomp1data5?accessType=DOWNLOAD'
urlretrieve(URL, 'land_global_temperature_anomaly-1880-2016.csv')
```

The data file will be downloaded to your working directory, and you will then need to remove the path information, i.e., the string `'../../data/'`, from the definition of the variable `fname` below.

Let's start by importing NumPy.

```
In [2]: import numpy
```

To load our data from the file, we'll use the function `numpy.loadtxt()`, which lets us immediately save the data into NumPy arrays. (We encourage you to read the documentation for details on how the function works.) Here, we'll save the data into the arrays `year` and `temp_anomaly`.

```
In [3]: fname = '../../data/land_global_temperature_anomaly-1880-2016.csv'

        year, temp_anomaly = numpy.loadtxt(fname, delimiter=',', skiprows=5, unpack=True)
```

Exercise Inspect the data by printing `year` and `temp_anomaly`.

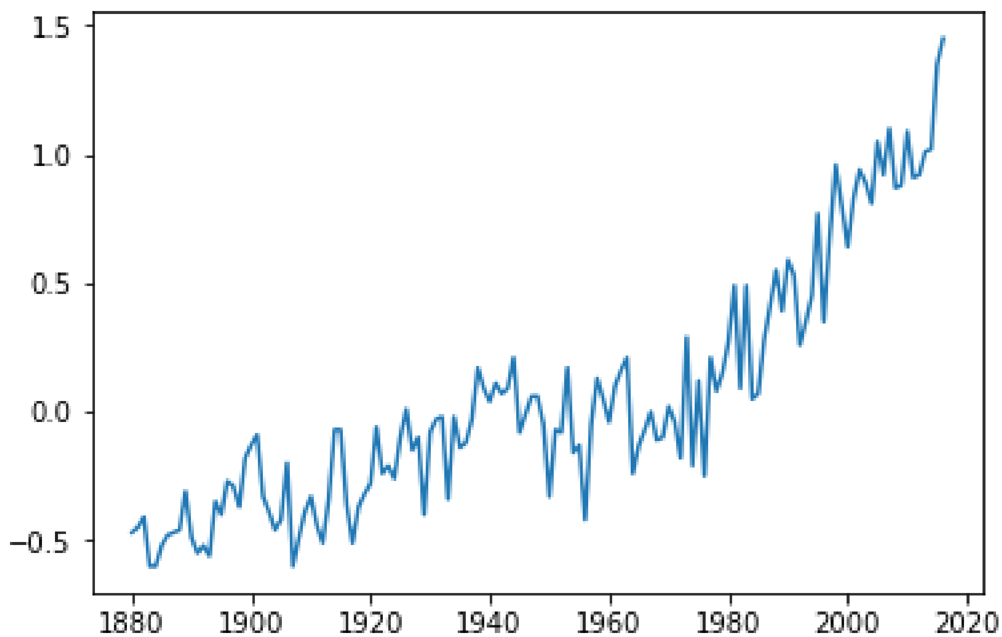
3 Step 2: Plot the data

Let's first load the **Matplotlib** module called `pyplot`, for making 2D plots. Remember that to get the plots inside the notebook, we use a special "magic" command, `%matplotlib inline`:

```
In [4]: from matplotlib import pyplot
        %matplotlib inline
```

The `plot()` function of the `pyplot` module makes simple line plots. We avoid that stuff that appeared on top of the figure, that `Out[x]: [< ...>]` ugliness, by adding a semicolon at the end of the plotting command.

```
In [5]: pyplot.plot(year, temp_anomaly);
```



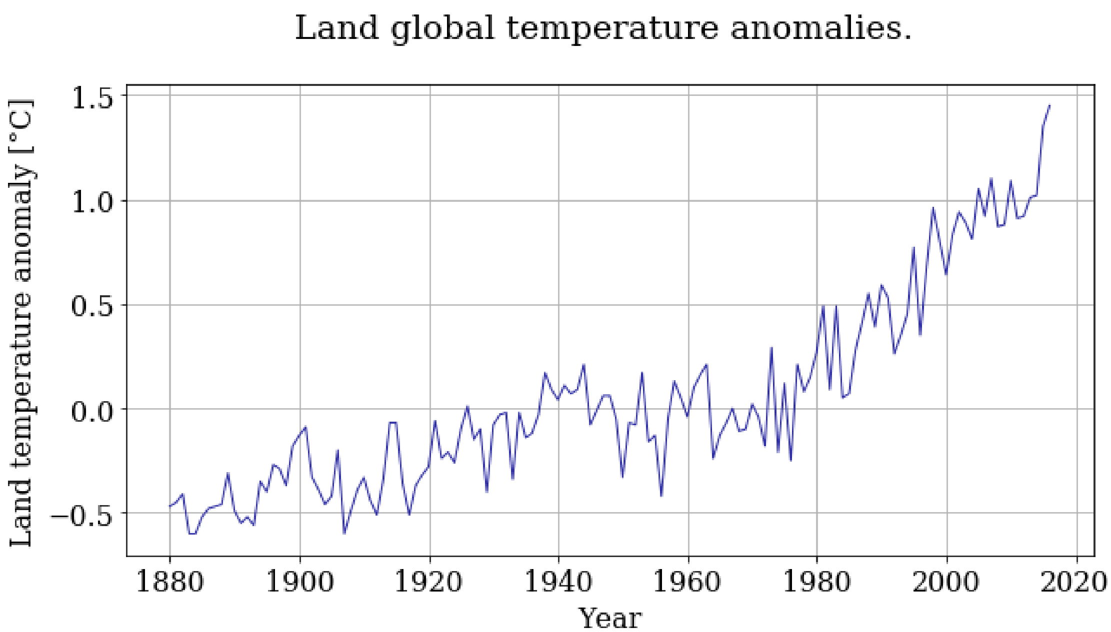
Now we have a line plot, but if you see this plot without any information you would not be able to figure out what kind of data it is! We need labels on the axes, a title and why not a better color, font and size of the ticks. **Publication quality** plots should always be your standard for plotting. How you present your data will allow others (and probably you in the future) to better understand your work.

We can customize the style of our plots using **Matplotlib**'s `rcParams`. It lets us set some style options that apply for all the plots we create in the current session. Here, we'll make the font of a specific size and type. You can also customize other parameters like line width, color, and so on (check out the documentation).

```
In [6]: from matplotlib import rcParams
        rcParams['font.family'] = 'serif'
        rcParams['font.size'] = 16
```

We'll redo the same plot, but now we'll add a few things to make it prettier and **publication quality**. We'll add a title, label the axes and, show a background grid. Study the commands below and looks at the result!

```
In [7]: #You can set the size of the figure by doing:
        pyplot.figure(figsize=(10,5))

        #Plotting
        pyplot.plot(year, temp_anomaly, color='#2929a3', linestyle='-', linewidth=1)
        pyplot.title('Land global temperature anomalies. \n')
        pyplot.xlabel('Year')
        pyplot.ylabel('Land temperature anomaly [°C]')
        pyplot.grid();
```



Better, no? Feel free to play around with the parameters and see how the plot changes. There's nothing like trial and error to get the hang of it.

4 Step 3: Least-squares linear regression

In order to have an idea of the general behavior of our data, we can find a smooth curve that (approximately) fits the points. We generally look for a curve that's simple (e.g., a polynomial), and does not reproduce the noise that's always present in experimental data.

Let $f(x)$ be the function that we'll fit to the $n+1$ data points: (x_i, y_i), $i = 0, 1, ..., n$:

$$f(x) = f(x; a_0, a_1, ..., a_m)$$

The notation above means that f is a function of x, with $m+1$ variable parameters $a_0, a_1, ..., a_m$, where $m < n$. We need to choose the form of $f(x)$ a priori, by inspecting the experimental data and knowing something about the phenomenon we've measured. Thus, curve fitting consists of two steps:

1. Choosing the form of $f(x)$.
2. Computing the parameters that will give us the "best fit" to the data.

5 What is the "best" fit?

When the noise in the data is limited to the y-coordinate, it's common to use a **least-squares fit**, which minimizes the function

$$S(a_0, a_1, ..., a_m) = \sum_{i=0}^{n} [y_i - f(x_i)]^2 \tag{1}$$

with respect to each a_j. We find the values of the parameters for the best fit by solving the following equations:

$$\frac{\partial S}{\partial a_k} = 0, \quad k = 0, 1, ..., m. \tag{2}$$

Here, the terms $r_i = y_i - f(x_i)$ are called residuals: they tell us the discrepancy between the data and the fitting function at x_i.

Take a look at the function S: what we want to minimize is the sum of the squares of the residuals. The equations (2) are generally nonlinear in a_j and might be difficult to solve. Therefore, the fitting function is commonly chosen as a linear combination of specified functions $f_j(x)$,

$$f(x) = a_0 f_0(x) + a_1 f_1(x) + ... + a_m f_m(x)$$

which results in equations (2) being linear. In the case that the fitting function is polynomial, we have have $f_0(x) = 1,\ f_1(x) = x,\ f_2(x) = x^2$, and so on.

6 Linear regression

When we talk about linear regression we mean "fitting a straight line to the data." Thus,

$$f(x) = a_0 + a_1 x \tag{3}$$

In this case, the function that we'll minimize is:

$$S(a_0, a_1) = \sum_{i=0}^{n} [y_i - f(x_i)]^2 = \sum_{i=0}^{n} (y_i - a_0 - a_1 x_i)^2 \tag{4}$$

Equations (2) become:

$$\frac{\partial S}{\partial a_0} = \sum_{i=0}^{n} -2(y_i - a_0 - a_1 x_i) = 2\left[a_0(n+1) + a_1 \sum_{i=0}^{n} x_i - \sum_{i=0}^{n} y_i\right] = 0 \tag{5}$$

$$\frac{\partial S}{\partial a_1} = \sum_{i=0}^{n} -2(y_i - a_0 - a_1 x_i)x_i = 2\left[a_0 \sum_{i=0}^{n} x_i + a_1 \sum_{i=0}^{n} x_i^2 - \sum_{i=0}^{n} x_i y_i\right] = 0 \tag{6}$$

Let's divide both equations by $2(n+1)$ and rearrange terms.

Rearranging (6) and (7):

$$2\left[a_0(n+1) + a_1 \sum_{i=0}^{n} x_i - \sum_{i=0}^{n} y_i\right] = 0$$

$$\frac{a_0(n+1)}{n+1} + a_1 \frac{\sum_{i=0}^{n} x_i}{n+1} - \frac{\sum_{i=0}^{n} y_i}{n+1} = 0 \tag{7}$$

$$\tag{8}$$

$$a_0 = \bar{y} - a_1 \bar{x} \tag{9}$$

where $\bar{x} = \frac{\sum_{i=0}^{n} x_i}{n+1}$ and $\bar{y} = \frac{\sum_{i=0}^{n} y_i}{n+1}$.

Rearranging (7):

$$2\left[a_0 \sum_{i=0}^{n} x_i + a_1 \sum_{i=0}^{n} x_i^2 - \sum_{i=0}^{n} x_i y_i\right] = 0 \tag{10}$$

$$a_0 \sum_{i=0}^{n} x_i + a_1 \sum_{i=0}^{n} x_i^2 - \sum_{i=0}^{n} x_i y_i = 0 \tag{11}$$

$$\tag{12}$$

Now, if we replace a_0 from equation (8) into (9) and rearrange terms:

$$(\bar{y} - a_1 \bar{x}) \sum_{i=0}^{n} x_i + a_1 \sum_{i=0}^{n} x_i^2 - \sum_{i=0}^{n} x_i y_i = 0$$

Replacing the definitions of the mean values into the equation,

$$\left[\frac{1}{n+1}\sum_{i=0}^{n} y_i - \frac{a_1}{n+1}\sum_{i=0}^{n} x_i\right]\sum_{i=0}^{n} x_i + a_1\sum_{i=0}^{n} x_i^2 - \sum_{i=0}^{n} x_i y_i = 0$$
$$\frac{1}{n+1}\sum_{i=0}^{n} y_i \sum_{i=0}^{n} x_i - \frac{a_1}{n+1}\sum_{i=0}^{n} x_i \sum_{i=0}^{n} x_i + a_1\sum_{i=0}^{n} x_i^2 - \sum_{i=0}^{n} x_i y_i = 0$$

Leaving everything in terms of $\bar{x}$,

$$\sum_{i=0}^{n} y_i\bar{x} - a_1\sum_{i=0}^{n} x_i\bar{x} + a_1\sum_{i=0}^{n} x_i^2 - \sum_{i=0}^{n} x_i y_i = 0$$

Grouping the terms that have a_1 on the left-hand side and the rest on the right-hand side:

$$a_1\left[\sum_{i=0}^{n} x_i^2 - \sum_{i=0}^{n} x_i\bar{x}\right] = \sum_{i=0}^{n} x_i y_i - \sum_{i=0}^{n} y_i\bar{x}$$
$$a_1\sum_{i=0}^{n}(x_i^2 - x_i\bar{x}) = \sum_{i=0}^{n}(x_i y_i - y_i\bar{x})$$
$$a_1\sum_{i=0}^{n} x_i(x_i - \bar{x}) = \sum_{i=0}^{n} y_i(x_i - \bar{x})$$

Finally, we get that:

$$a_1 = \frac{\sum_{i=0}^{n} y_i(x_i - \bar{x})}{\sum_{i=0}^{n} x_i(x_i - \bar{x})} \tag{13}$$

Then our coefficients are:

$$a_1 = \frac{\sum_{i=0}^{n} y_i(x_i - \bar{x})}{\sum_{i=0}^{n} x_i(x_i - \bar{x})} \quad , \quad a_0 = \bar{y} - a_1\bar{x} \tag{14}$$

7 Let's fit!

Let's now fit a straight line through the temperature-anomaly data, to see the trend over time. We'll use least-squares linear regression to find the slope and intercept of a line

$$y = a_1 x + a_0$$

that fits our data.

In our case, the x-data corresponds to `year`, and the y-data is `temp_anomaly`. To calculate our coefficients with the formula above, we need the mean values of our data. Sine we'll need to compute the mean for both `x` and `y`, it could be useful to write a custom Python *function* that computes the mean for any array, and we can then reuse it.

It is good coding practice to *avoid repeating* ourselves: we want to write code that is reusable, not only because it leads to less typing but also because it reduces errors. If you find yourself doing the same calculation multiple times, it's better to encapsulate it into a *function*.

Remember the *key concept* from Lesson 1: A function is a compact collection of code that executes some action on its arguments.

Once *defined*, you can *call* a function as many times as you want. When we *call* a function, we execute all the code inside the function. The result of the execution depends on the *definition* of the function and on the values that are *passed* into it as *arguments*. Functions might or might not *return* values in their last operation.

The syntax for defining custom Python functions is:

```
def function_name(arg_1, arg_2, ...):
    '''
    docstring: description of the function
    '''
    <body of the function>
```

The **docstring** of a function is a message from the programmer documenting what he or she built. Docstrings should be descriptive and concise. They are important because they explain (or remind) the intended use of the function to the users. You can later access the docstring of a function using the function `help()` and passing the name of the function. If you are in a notebook, you can also prepend a question mark `'?'` before the name of the function and run the cell to display the information of a function.

Try it!

```
In [8]: ?print
```

Using the `help` function instead:

```
In [9]: help(print)
```

```
Help on built-in function print in module builtins:

print(...)
    print(value, ..., sep=' ', end='\n', file=sys.stdout, flush=False)

    Prints the values to a stream, or to sys.stdout by default.
    Optional keyword arguments:
    file:  a file-like object (stream); defaults to the current sys.stdout.
    sep:   string inserted between values, default a space.
    end:   string appended after the last value, default a newline.
    flush: whether to forcibly flush the stream.
```

Let's define a custom function that calculates the mean value of any array. Study the code below carefully.

```
In [10]: def mean_value(array):
             """ Calculate the mean value of an array

             Arguments
             ---------
             array: Numpy array

             Returns
             -------
             mean: mean value of the array
             """
             sum_elem = 0
             for element in array:
                     sum_elem += element # this is the same as sum_elem = sum_elem + element

             mean = sum_elem / len(array)

             return mean
```

Once you execute the cell above, the functionmean_value() becomes available to use on any argument of the correct type. This function works on arrays of any length. We can try it now with our data.

```
In [11]: year_mean = mean_value(year)
         print(year_mean)
```

```
1948.0
```

```
In [12]: temp_anomaly_mean = mean_value(temp_anomaly)
         print(temp_anomaly_mean)
```

```
0.0526277372263
```

Neat! You learned how to write a Python function, and we wrote one for computing the mean value of an array of numbers. We didn't have to, though, because NumPy has a built-in function to do just what we needed: `numpy.mean()`.

Exercise Calculate the mean of the `year` and `temp_anomaly` arrays using the NumPy built-in function, and compare the results with the ones obtained using our custom `mean_value` function.

```
In [ ]:
```

Now that we have mean values, we can compute our coefficients by following equations (12). We first calculate a_1 and then use that value to calculate a_0.

Our coefficients are:

$$a_1 = \frac{\sum_{i=0}^{n} y_i(x_i - \bar{x})}{\sum_{i=0}^{n} x_i(x_i - \bar{x})} \quad , \quad a_0 = \bar{y} - a_1\bar{x}$$

We already calculated the mean values of the data arrays, but the formula requires two sums over new derived arrays. Guess what, NumPy has a built-in function for that: `numpy.sum()`. Study the code below.

```
In [13]: a_1 = numpy.sum(temp_anomaly*(year - year_mean)) / numpy.sum(year*(year - year_mean))
```

```
In [14]: print(a_1)
```

```
0.0103702839435
```

```
In [15]: a_0 = temp_anomaly_mean - a_1*year_mean
```

```
In [16]: print(a_0)
```

```
-20.1486853847
```

Exercise Write a function that computes the coefficients, call the function to compute them and compare the result with the values we obtained before. As a hint, we give you the structure that you should follow:

```
def coefficients(x, y, x_mean, y_mean):
    """
    Write docstrings here
    """

    a_1 =
    a_0 =

    return a_1, a_0
```

We now have the coefficients of a linear function that best fits our data. With them, we can compute the predicted values of temperature anomaly, according to our fit. Check again the equations above: the values we are going to compute are $f(x_i)$.

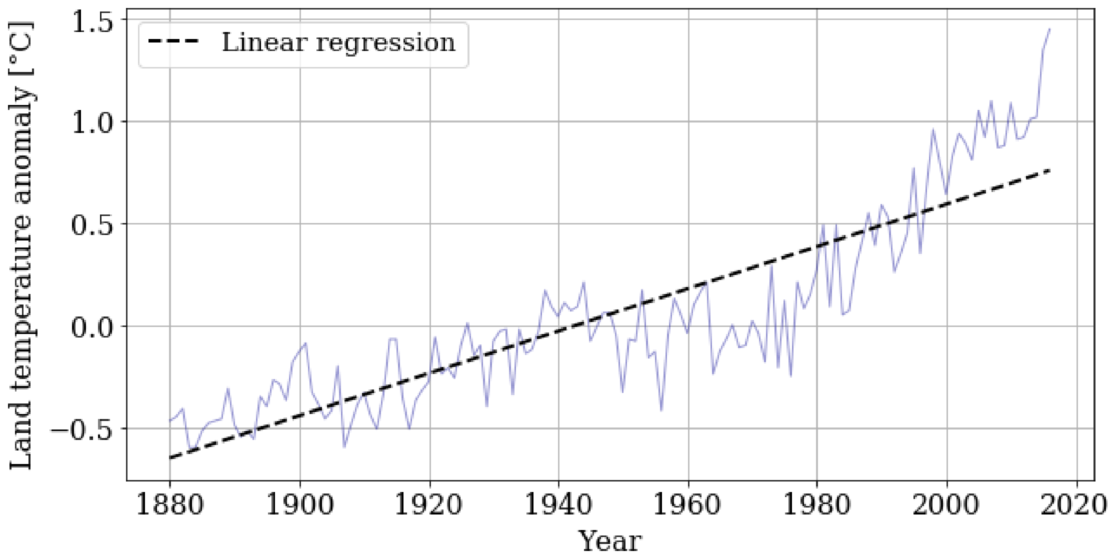
Let's call `reg` the array obtined from evaluating $f(x_i)$ for all years.

```
In [17]: reg = a_0 + a_1 * year
```

With the values of our linear regression, we can plot it on top of the original data to see how they look together. Study the code below.

```
In [18]: pyplot.figure(figsize=(10, 5))
```

```
pyplot.plot(year, temp_anomaly, color='#2929a3', linestyle='-', linewidth=1,
alpha=0.5)
pyplot.plot(year, reg, 'k--', linewidth=2, label='Linear regression')
pyplot.xlabel('Year')
pyplot.ylabel('Land temperature anomaly [°C]')
pyplot.legend(loc='best', fontsize=15)
pyplot.grid();
```



8 Step 4: Apply regression using NumPy

Above, we coded linear regression from scratch. But, guess what: we didn't have to because NumPy has built-in functions that do what we need!

Yes! Python and NumPy are here to help! With `polyfit()`, we get the slope and y-intercept of the line that best fits the data. With `poly1d()`, we can build the linear function from its slope and y-intercept.

Check it out:

```
In [19]: # First fit with NumPy, then name the coefficients obtained a_1n, a_0n:
         a_1n, a_0n = numpy.polyfit(year, temp_anomaly, 1)

         f_linear = numpy.poly1d((a_1n, a_0n))
```

```
In [20]: print(a_1n)
```

```
0.0103702839435
```

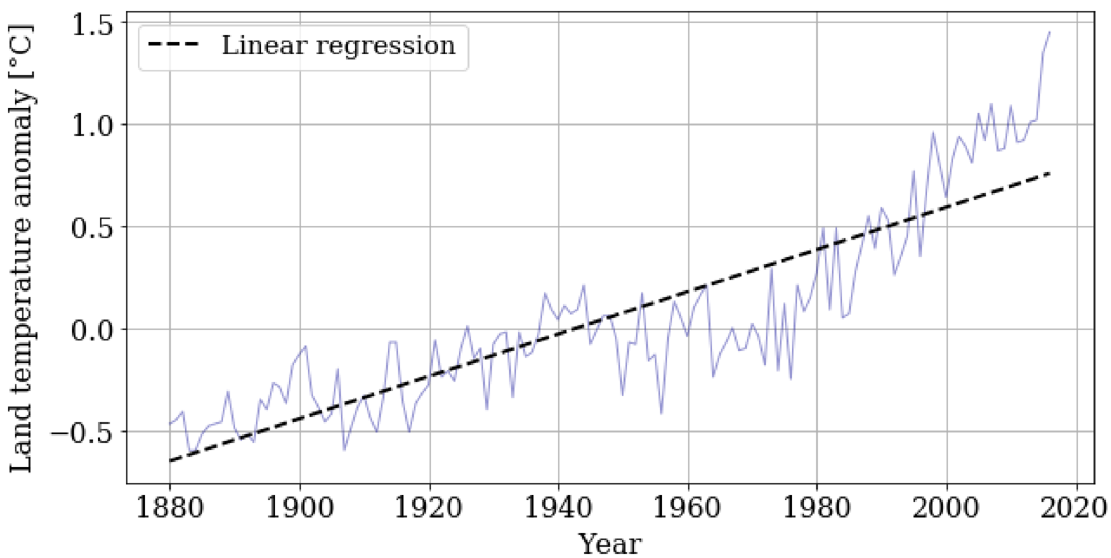
```
In [21]: print(a_0n)
```

```
-20.1486853847
```

```
In [22]: print(f_linear)
```

```
0.01037 x - 20.15
```

```
In [23]: pyplot.figure(figsize=(10, 5))

         pyplot.plot(year, temp_anomaly, color='#2929a3', linestyle='-', linewidth=1,
          alpha=0.5)
         pyplot.plot(year, f_linear(year), 'k--', linewidth=2, label='Linear regression')
         pyplot.xlabel('Year')
         pyplot.ylabel('Land temperature anomaly [°C]')
         pyplot.legend(loc='best', fontsize=15)
         pyplot.grid();
```



9 "Split regression"

If you look at the plot above, you might notice that around 1970 the temperature starts increasing faster that the previous trend. So maybe one single straight line does not give us a good-enough fit.

What if we break the data in two (before and after 1970) and do a linear regression in each segment?

To do that, we first need to find the position in our `year` array where the year 1970 is located.

Thankfully, NumPy has a function called `numpy.where()` that can help us. We pass a condition and `numpy.where()` tells us where in the array the condition is `True`.

```
In [24]: numpy.where(year==1970)
```

```
Out[24]: (array([90]),)
```

To split the data, we use the powerful instrument of *slicing* with the colon notation. Remember that a colon between two indices indicates a range of values from a `start` to an `end`. The rule is that `[start:end]` includes the element at index `start` but excludes the one at index `end`. For example, to grab the first 3 years in our `year` array, we do:

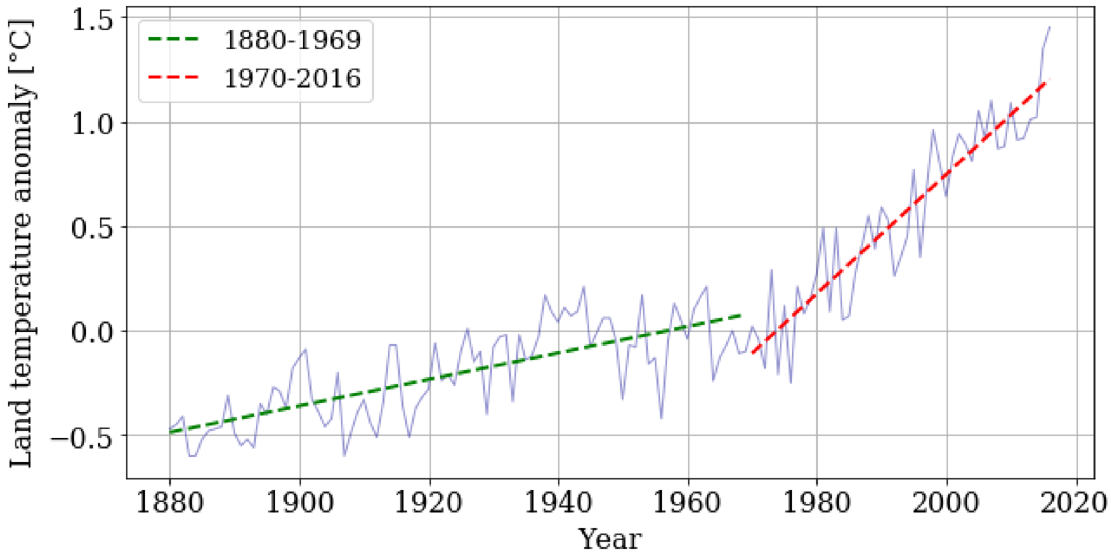
```
In [25]: year[0:3]
```

```
Out[25]: array([ 1880.,  1881.,  1882.])
```

Now we know how to split our data in two sets, to get two regression lines. We need two slices of the arrays `year` and `temp_anomaly`, which we'll save in new variable names below. After that, we complete two linear fits using the helpful NumPy functions we learned above.

```
In [26]: year_1 , temp_anomaly_1 = year[0:90], temp_anomaly[0:90]
         year_2 , temp_anomaly_2 = year[90:], temp_anomaly[90:]

         m1, b1 = numpy.polyfit(year_1, temp_anomaly_1, 1)
         m2, b2 = numpy.polyfit(year_2, temp_anomaly_2, 1)

         f_linear_1 = numpy.poly1d((m1, b1))
         f_linear_2 = numpy.poly1d((m2, b2))
```

```
In [27]: pyplot.figure(figsize=(10, 5))

         pyplot.plot(year, temp_anomaly, color='#2929a3', linestyle='-', linewidth=1,
         alpha=0.5)
         pyplot.plot(year_1, f_linear_1(year_1), 'g--', linewidth=2, label='1880-1969')
         pyplot.plot(year_2, f_linear_2(year_2), 'r--', linewidth=2, label='1970-2016')

         pyplot.xlabel('Year')
         pyplot.ylabel('Land temperature anomaly [°C]')
         pyplot.legend(loc='best', fontsize=15)
         pyplot.grid();
```



We have two different curves for two different parts of our data set. A little problem with this and is that the end point of our first regression doesn't match the starting point of the second regression. We did this for the purpose of learning, but it is not rigorously correct. We'll fix in in the next course module when we learn more about different types of regression.

10 We learned:

- Making our plots more beautiful
- Defining and calling custom Python functions
- Applying linear regression to data
- NumPy built-ins for linear regression
- The Earth is warming up!!!

11 References

1. *Essential skills for reproducible research computing* (2017). Lorena A. Barba, Natalia C. Clementi, Gilbert Forsyth.
2. *Numerical Methods in Engineering with Python 3* (2013). Jaan Kiusalaas. Cambridge University Press.
3. *Effective Computation in Physics: Field Guide to Research with Python* (2015). Anthony Scopatz & Kathryn D. Huff. O'Reilly Media, Inc.