



# Python intro notes (hopefully helpful for people coming from R)

Notes from [openHPI pythonjunior2020](#), [Python for Digital Health](#) and personal learning.

RefCards [search](#)

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RefCard [example](#)

!!! means this will fry your brain if you're used to R. Especially subsetting with positions will be horrible. Most python interpreters don't print unless explicitly stated. `print()` is mostly left away here for brevity.

[Download & install](#), hints for [Windows users](#). [tutorial](#), standard [libraries](#), language [reference](#), [documentation](#).

## IDEs

<a href="#">PyCharm</a>	Good for scientific development, but slow in startup
<a href="#">VScode</a>	(Visual studio code) increasingly popular, supports multiple languages, e.g. R
IDLE	Installed by default, not suitable for large projects
More:	<a href="http://www.programiz.com/python-programming/ide">www.programiz.com/python-programming/ide</a> , <a href="https://colab.research.google.com">colab.research.google.com</a> , <a href="#">Jupyter Manual</a>

## Syntax

```
function(arg, "txt", 'single quotes', 77.86) # comment
""" multi-line comment
with line breaks """
7*6 ; 21+21 # semicolon possible, but not good practice. here for effective space use
9 // 2 ; 20 % 7 ; 3 ** 2 # ≈ 9 %/% 2 ; 20 %% 7 ; 3^2 in R (int.div, modulo)
a = 5 ; a += 1 # short for a = a + 1 ; a *= a+2 # short for a = a * (a+2)
```

`variable_name = "value"` # naming convention: lowercase, underscore

**NameError**: non-existing objects - [List of errors](#)

Variable names cannot start with numbers, Python is case sensitive

Reserved statements ([keywords](#)) like `else` cannot be used as variable name

**SyntaxError**: often forgotten brackets or colons (e.g. in loops)

**Method** = function for an object class, e.g. `listobject.append`

**Linter**: program to analyze code style and determine structural problems (pointless lines of code, potentially overwriting variable names, etc)

## Collections (Arrays)

type	example	changeable	ordered	indexed	notes
list	[1,3]	yes	yes	yes	-
tuple	(1,2)	no	yes	yes	-
set	{1,4}	no, but add	no	no	no duplicates
dictionary	{"a":7, "b":3}	yes	no*	by key	no duplicates

## Data types

integer, float, string, boolean (`True/False`), complex (`2+1j`) !!!

```
isinstance(7.5, int) # check for class
```

```
isinstance("Hello", (float, int, str, list, dict, tuple)) # one of types
```

```
value = input("Enter number: ") # interactive input ≈ readline("Enter num: ")
```

```
print("Type is: ", type(value)) ; type(int(value)) ; type(float(value))
```

```
value + 7 # ValueError if keyboard input was charstring
```

```
value = float(input("Give a number: ")) # read keyboard input and convert
```

## Lists

```
list = [7, -4, 9, 1, 2, 3, 9] ; len(list)
```

```
list[0] # first element !!! ; list[1] # second element !!!
```

```
list[-1] # last element
```

```
list[-2] # second-to-last element list[5:-2] # range from left + right
```

```
list[2] = "newvalue" # overwrite third element, mixed data types possible !!!
```

```
list[2:5] # elements 3,4,5 exclusive at the right end !!!
```

```
list[4:] ; list[:6] # slicing: fifth till last element ; first till sixth
```

```
: is not an operator outside subsetting !!! list = [] # empty list
```

```
bar = list
```

```
list.append(66) # mutable object: changed even without re-assigning !!!
```

```
id(list) == id(bar) # both with 7, -4, "new value", 1, 2, 3, 9, 66 !!!
```

```
list.pop() # remove last element (+ return it invisibly)
list.pop(index) # remove (+ return) selected element
del(list[index]) # only remove element at given index
list.insert(5, "new_val") # insert at given position
list.index(9) # location of 9 ; list.remove(9) # remove first instance of 9
9 not in list # check for non-presence, returns a boolean ≈ ! 9 %in% vec in R
list.reverse() ; list.sort() ; list.sort(reverse=True)

list = [1,2,3,[31,32,33],4] # Nesting possible
list_with_charstrings[3][7] # eighth letter in fourth element

one_list.extend(another_list) # ≈ one_list <- c(one_list, another_list) in R
one_list + another_list # ≈ c(one_list, another_list) in R
one_list * 2 # ≈ rep(one_list, 2) in R
```

## Dictionaries

```
*: since python version 3.6/3.7, dictionaries are ordered
dict = {'name': "Berry", 'age': 31} # keys (name, age) must be unique
len(dict)
dict ['name'] = "new_value" # key + value = 'pair' dict['new_key'] = 42
f"Hi, {dict['name']}" # fstring double and single quotes cannot be mixed
print("Hello, {name}" .format(name=dict['name']))
dict.get('NAME', "value_if_key_not_present")
del(dict['age']) # delete pair (entire entry). del d['k'] brackets optional!!
dict.keys() ; dict.values() ; dict.items()
list(dict.items()) # -> list with tuples -> very high memory usage!
the_age = dict.pop('age') # KeyError: key no longer in dict
other_dict = dict.copy() ; dict.clear() ; dict.update(another_dictionary)
```

## Sets

```
s1 = {1,2,3,4,5} ; s2 = {3,4,5,6,7,8} ; {} empty dict ; set() empty set
s1 | s2 ; s1 & s2 ; s1 - s2 # union ; intersection ; difference
```

## Charstrings

```
"Hey" + "You there" # + operator to concatenate (chain) strings
3*"Hi" # -> "HiHiHi" # * operator to repeat strings
len("char string") # ≈ nchar in R. Not the same as len(some_list) !!!
print("Hey", "You there", sep=" ", end="--\n")
charstring = "Hi this is a text. with words"
"this" in charstring # ≈ grepl("this", charstring) in R
charstring[0] # ≈ substr(cs, 1,1) in R. Not the same as some_list[0] !!!
charstring[1] = "b" # not possible: unlike lists, strings are immutable
charstring[5:-2] # subset region
charstring[300] # IndexError: subsetting outside of existing range
charstring.split() # split at spaces. immutable - does not change object !!!
charstring.split(".") # split at periods. The default includes \n as space.
"_.join(["list", "of", "words"]) # ≈ paste(wordvec, collapse=" ") in R
"char string ".strip() # strip white space (or given symbols) on both sides
"CharString".lower() # ≈ tolower("CharString") in R
"CharString".startswith("Ch") # ≈ startsWith("CharString", "Ch") in R
"CharString".count("r") ; max("CharString")
"CharString".find("tri") # grexexpr("tri", "CharString") in R

"Chars".replace("Ch", "K") # ≈ gsub("Ch", "K", "Chars", fixed=TRUE) in R
re module for regular expressions aka. wildcards (see section Packages):
import re ; re.sub('[xyz]', 'K', "abycd") # ≈ gsub("[xyz]", "K", "abycd")

F-string placeholder (since Python 3.6). Inline arithmetics possible:
person="Berry" ; f"{person} is a nice guy with {5+5} fingers"

print("%d %s cost $%.2f" % (6, "bananas", 1.74)) # -> 6 bananas cost $1.74
print("{0} {1} cost ${2}" .format(6, "bananas", 1.74))
```

## Packages

[pip](#) to install packages e.g from [pypi.org](#) (PYthon Package Index) ≈ CRAN for R. [pip install pandas](#)  
[Anaconda](#) to install binary packages (also R) from their [cloud](#). Anaconda Prompt: [conda install pandas](#) ; [conda list](#)  
**Popular packages:** Data science: [pandas](#), [numpy](#), Machine learning: [tensorflow](#), [pytorch](#), Statistical analysis: [scipy](#),  
 Web application: [django](#), Plotting: [matplotlib](#), [seaborn](#), package version management: [virtualenv](#)  
**ImportError:** wrong library/module/script name, non-existing objects

```
from library import * # all functions -> bad practice: object origin unclear
from library import function1, function2 # specific function(s)
import library then you can use library.function(...)
import library as lib then you can use lib.function(...)

from random import random, randint # random, math, etc come with python
random() # float between 0 (inclusive) and 1 (exclusive!!!), ≈ runif() in R
randint(1, 6) # int between start and end, including these
import os # os is a module in the standard library, no installation needed
print(os.getcwd()) # ≈ getwd() in base R ; os.chdir() # ≈ setwd()
from math import pi
```

## Read files

If at `os.getcwd()`, there is `mydataset.py` with `age = 45`, we can use:

```
from mydataset import age # to then use age + 2
from mydataset import * # to import all ≈ source("mydataset.py") in R
import mydataset # to then use mydataset.age + 2
print(dir(mydataset)) # list the objects in the module
```

```
import os, sys ; fname = os.path.join(sys.path[0], "file.txt") # for wd
with open(fname) as f: # with closes the connection (even in case of error)
    content = f.read().splitlines() # ≈ readLines("file.txt") in R
```

## Logicals

```
< ; <= ; > ; >= ; == ; != ; and ; or ; not # comparison / logical operators
7 < 8 ; "9" < "A" ; "A" < "B" ; "A" < "a" ; "a" < "b" !!order in R: "a" < "A"
7>1 & 6>1 in R, Python needs: (7>1) & (6>1), Py reads 7 > 1&6 > 1 and 1&6=0
```

## Conditional code execution

```
IndentationError: wrong number of spaces at the beginning of a line
if cond:
    do (1)
    do (2)
else:
    do (3)

if cond1:
    do (1)
elif cond2:
    do (2)
else:
    do (3)

if cond1 and (cond2 or cond3):
    print("stuff")
```

## Loops

```
for number in (0,1,2,3): # or in range(4)
    print(number) # range(8, 0, -2)
# range stop exclusive!!!
# convention for unused index variable:
for _ in range(8): # or _var
    print("stuff")

for a,b in ( (1,4), (5,7), (6,9) ):
    print(f"a={a}, b={b}, a+b={a+b}")

while cond:
    run_things()
    if(cond2):
        break
# continue ≈ next in R

enumerate("hello") ; iter # iterators
```

```
result = []
for item in item_list:
    new_item = do_something_with(item)
    result.append(new_item)
```

```
result = [do_something_with(item) for item in item_list] # list comprehension
```

```
out = [] for word in charstring_list if word[0] == "B": out.append(word)
```

```
out = [x for x in charstring_list if x[0] == "B"]
```

```
≈ char_vec[substr(char_vec, 1, 1) == "B"] in R # not vectorizable in Python !!!
```

**Write custom functions**

```
def greet(name, time="morning"): # name+time are parameters
    return f"Hello {name}! Good {time}." # return exits function execution
# explicit return is needed !!! else a function returns None (~ NULL in R)

greet("Berry") # Berry+evening are arguments
greet("Berry", "evening") # parameter=argument ~ argument=value in R

def change_object():
    global ab
    ab = 2
ab = 1 ; ab ; change_object() ; ab # is now 2

multiply = lambda x,y: x*y # single expression function on one line of code
multiply(7, 3)
```

**Multiple assignment**

```
def myfun(x, y): # related: swap two variables: a, b = b, a
    return x*2, y*2
a, b = myfun(3, 4) # two int objects, each with a single value
c = myfun(3, 4) # tuple object with (6, 8)

list(map(len, ["abcdef", "ab", "abc"])) # apply(c("abcdef", "ab", "abc"), nchar)
```

**Error management**

```
import traceback
try:
    7 + "2" # code that might fail. int("seven") would give ValueError
except TypeError: # TypeError: wrong data type for operator or function
    print("That mixed charstrings and numbers")
except Exception: # print instead of error
    print("another error occured: ", traceback.format_exc() )
else:
    do("stuff")
```

**Write custom class**

```
class Person:
    pass # Placeholder for future code. A class body may not be empty.

p1 = Person() # create object instance
p1.name = "Berry" ; p1.age = 31 # add attributes

class Person: # class attributes, generate w/ constructor
    def __init__(self, name, age): # initialize (assign values) to data members
        self.name = name # of the object when Person() is called
        self.age = age
        if name=="forbidden":
            raise Exception("Name cannot be 'forbidden'") # ~ stop("msg") in R
    def can_watch_movie(self): # class methods
        if self.age >= 18:
            return "Sure, watch it" # self represents object of class Person,
        else: # always first arg to __init__
            return "Too young, sorry"

p2 = Person("John", 25) ; p2.name ; p2.can_watch_movie() # instantiation
p2.__dict__ # dictionary of all given parameters and arguments
p2 = Person("forbidden", 25) ;
```

**turtle**

```
package to draw figures on plot range -200:200
forward(nsteps), right(degrees), goto(x,y), penup(), pendown(),
shape("turtle"), register_shape(), pencolor("yellow"), bgcolor(),
fillcolor(), begin_fill(), end_fill()
```

**Count table**

```
colors = ['red', 'blue', 'blue', 'yellow', 'blue', 'red', 'green']
import collections
collections.Counter(colors).most_common(6) ≈ sort(table(colors))[1:6] in R
```

**Numpy**: computationally efficient numerical arrays. `pip install numpy`

```
import numpy as np ;
np.array([1,2,3,4,5,6]) # 1D array. type: numpy.ndarray
ar = np.array([[1,2,3,4], [5,6,7,8]]) # 2D array from list of lists
np.random.randint(10, size=(3,4)) # random integers 0-9, 3 rows, 4 columns
Attributes: accessed without brackets (methods with brackets):
ar.ndim ; ar.shape ; ar.size # ≈ length(dim(ar)); dim(ar); length(ar) in R
ar.dtype # numpy-internal data type ar.itemsize ; ar.nbytes # in bytes
```

```
ar1 = np.arange(10) # sequential 1D array
ar1[4] ; ar1[-1] # fifth and last element of 1D array
ar1[start:stop:step] # general subsetting of 1D arrays
ar1[:5] ; ar1[4:] ; ar1[4:7] ; ar1[::2] / ar1[1::3] # every other element
ar1[::-1] # all elements, reversed. Works for lists & charstrings as well
```

```
ar[:2, :3] ; ar[:, 5] # 2 rows, 3 columns. all values in sixth column
ar[0] # first row, not first column !!!# as in R, not recommended!
ar[2,0] = 3.1415 # change single element at row three, column 1 of 2D array
# If array is integer, float is silently truncated to 3: Downcasting !!!
```

```
ar_sub = ar[:2, :2] ; ar_sub[0,0] = 99 # changes both ar_sub and ar !!!
ar_sub = ar[:2, :2].copy() ; ar_sub[0,0] = 42 # does not change ar
```

```
ar = np.arange(1,10) ; grid = ar.reshape((3,3)) # 1D array to 2D array
ar[np.newaxis, :] # 2D, 1 row. Both do not change ar.
```

```
np.concatenate((ar1, [67,68,69]))
np.concatenate([grid, grid]) # ≈ rbind(grid, grid) in R
np.concatenate([grid, grid], axis=1) # ≈ cbind(grid, grid) in R
np.vstack(); np.hstack(); np.dstack() # the same, d for depth (3rd dimension)
s1,s2,s3 = np.split([1,2,3,4,5,6,7,8,9], [3,5]) ; np.hsplit; np.vsplit for 2D
```

**Ufunc** (Universal functions operating on full array)

```
%timeit compute_long_thing(big_array). # %timeit by Ipython
Numpy enables very fast vectorized operations: 1.0/ar ; ar1/ar2 ; ar>=3.
```

```
ar + 5 # element-wise operation: broadcasting (≈ recycling in R)
np.ones((3,4)); np.zeros() # arrays full of 1 (or 0)
ar3x3 + ar3 -> ar3x3 # ar3 (1D)repeated for each row of ar3x3 (2D).
ar3 + ar3x1 -> ar3x3.
```

```
angles = np.linspace(0, np.pi, 3) # ≈ seq(0, pi, len=3) in R
np.sin(); np.exp(); np.log10(); np.power()
```

```
np.count_nonzero(ar<6) or np.sum(ar<6) # ≈ sum(ar<6) in R
np.sum(ar<6, axis=1) # ≈ rowSums(ar<6) or apply(ar, 1, sum) in R
np.any() ; np.all() # can be called without np. as well
np.any(ar<6, axis=0) # columns ≈ apply(ar, 2, any) in R -> axis != MARGIN !!!
np.any(ar<6, axis=1) # rows ≈ apply(ar, 1, any) in R
ar[ar < 6] # reduces dimension (e.g. 2D to 1D)
```

```
ar.mean(); ar.mean(axis=0);ar.mean(axis=1) #≈ mean(ar); colMeans(ar);rowMeans
```

```
np.corrcoef(ar1, ar2) ; np.isfinite() ; np.isnan() ; np.asarray() ;
np.nanstd(ar) # ≈ sd(ar, na.rm=TRUE) in R ; np.nanmean(ar) ; np.nanmedian(ar)
np.sort(ar)
np.random.poisson(5, 100) # 100 random numbes from poisson distribution
np.random.normal(mu, sigma, 100)
```

**Pandas**: panel data analysis, builds on numpy. [API docs](#). `pip install pandas`  
 Series (column) with axis labels and DataFrame of Series

```
import pandas as pd ;
pd.Series(data=list_of_vals, index=list_of_strings) # data can be numpy array
s1 = pd.Series(dictionary) ; s1.to_list() ; s1.to_dict() ; s1.size ;
s1 = pd.Series([1,2,3,4], index=["A","C","D","E"])
s2 = pd.Series([1,2,5,4], index=["A","B","C","E"]) ; s1["A"] # subset by name
s1 + s2 # returns: A:2, B:NaN, C:7, D:NaN, E:8 # Operations per index
```

```
df = pd.DataFrame(randn(5,4), index='A B C D E'.split(), # ~ rownames in R
                  columns='W X Y Z'.split()) # ~ colnames in R
df.shape ; df.index ; df.columns ; df.values ; df.index.values ;
df.info() ~ str(df) in R ; df.dtypes
df.select_dtypes(include='number') # see dtypes # does not change df
```

Select columns	Select rows	Select elements
df["colname"]	df.loc["rowname"]	df.iloc[2, 5]
df.colname	df.iloc[2]	df.loc["rname", "cname"]
df[["col1", "col2"]]	df.iloc[0:3] # first 3 r	df.colname[3:5]
df.iloc[:, -1] # last C	df.iloc[-1] # last row	
df.iloc[:, 1:3] # C 2+3	df[ df.colname < 15 ]	iloc for index location

### Missing values

```
df1 = pd.DataFrame({'A':[1,2,np.nan],
                   'B':[5,None,np.nan],
                   'C':[1,2,3]})
df1.isna() # ~ is.na(df) in R
df1.isna().sum() # ~ apply(df, 2, is.na) in R # number of NAs per column
df1.isna().sum(axis=1) # number of NAs per row
df1[df1["B"].notna()] # ~ df[!is.na(df$B), ] in R
df1.dropna() # ~ na.omit(df) in R # see also df1.dropna(axis=1)
df1.dropna(thresh=2) # at least 2 finite numbers needed to be kept
df1.fillna(value='missing') # replace NA with "missing" # value=0 possible
df1.A.fillna(value=df1.A.mean()) # Replace with mean value of column
df1[df1.A.isna()].index.tolist() # ~ rownames(df)[is.na(df$A)] in R
rows_with_nan = [index for index,row in df1.iterrows() if row.isna().any()]
df1.index[df1.isna().sum(axis=1) > 0].tolist() # the same, more readable
```

### Combining dataframes

```
df.groupby('Age_group').mean() # .min() ; .count() # mean only for numerics
pd.merge(df1, df2, on='key_column', how="outer") # on=['key1','key2']
how: outer, inner, left, right # ~ merge(all=T) all=F, all.x=T, all.y=T in R
df1.join(df2, how="outer") # cbind by rownames
pd.concat([df1, df2], axis=0) # outer by default. ~ rbind in R, but expands
pd.concat([df1, df2], axis=1) # inner by default. ~ cbind in R, but expands
```

### Pandas misc

```
df.col.unique() # .nunique() ; df.col.value_counts() # ~ table(df$col) in R
df = df.assign(new_col = lambda x: (x.col*1000)) # df["new_col"] = df.col*1000
df.apply(lambda x : x/100, axis=1) ~ apply(df, 1, function(x) x/100) in R
(df.colA > 6) & df.colB # &, |, !=, ==, ~ (not), >, <, >=, <=
df = df.sort_values(by='colname') # ~ df = df[order(df$colname)] in R
df.sort_values(by='colname', inplace=True) # modify df directly
dfcp = df ; dfcp[5,2] = 42 # changes df as well, dfcp is only a pointer to df
dfcp = df.copy() # as usual :)
df.pivot_table(index=['c1','c2'], columns=['c3'])
pd.crosstab(df.c1, df.c2); pd.crosstab(index=x, columns="Count") # ~ table(x)
pd.read_csv ; pd.read_excel ; pd.read_html ; df.to_csv() ; pd.to_excel()
df.describe() ~ summary(df) in R ; df.head() ; df.tail()
```

**Statistics**

```
import pandas as pd ; import numpy as np ; import scipy ; import statistics

statistics.mean(x)
df.mean() # pandas.mean excludes nan by default ; df.median()
np.nanmedian() safer than statistics.median() with nans

statistics.quantiles(x, n=4) # in Python >3.8
df.quantile([0, 0.05, .25, .5, .75, .95, 1]) ; scipy.stats.iqr(x)

statistics.stdev(x) ; df.std() ; np.var(x, ddof=1) ; df.var()
statistics.mode(x) ; statistics.multimode(x) # Py>3.8 ; scipy.stats.mode(x)
scipy.stats.skew(x) ; df.skew(axis=0, skipna=True)

scipy.stats.kstest(x, 'norm') # Kolmogorov-Smirnov test for normality
scipy.stats.shapiro(x)[1] # Shapiro-Wilk test for normality
corcoef,pvalue = scipy.stats.pearsonr(x, y) ; df.corr(method="pearson")
scipy.stats.ttest_1samp(x, popmean=182) # "is mean of x = 182?"
scipy.stats.ks_2samp(x,y).pvalue # to answer "is x different from y?"
scipy.stats.ttest_ind(x,y) # independent T-test "is x diff from y?"
scipy.stats.ttest_rel(x,y) # paired T-test, when x and y related
scipy.stats.mannwhitneyu(x,y, alternative="greater") # one-sided Mann-Whitney-U Wilcoxon Rank test (~ T-test for non-normal distribution shape)
scipy.stats.chi2_contingency([x,y]) # categories. can take pd.crosstab output
scipy.stats.chisquare(f_obs=observed, f_exp=expected) # Goodness of fit test
scipy.stats.f_oneway(x,y,z) # ANOVA "are x, y and z the same?"
mod=statsmodels.formula.api.ols('y ~ C(x1)+C(x2)+C(x1):C(x2)', data=df).fit()
statsmodels.api.stats.anova_lm(mod, typ=2) # kind of ~ lm\(y~x1+x2+x1:x2\) in R
```

**Data visualisation with matplotlib**

```
import matplotlib.pyplot as plt
%matplotlib inline # in notebook ; plt.show() in last line in other editors
plt.scatter(x,y) ; plt.hist(x) ; plt.boxplot(data, vert=True)
plt.plot(x, y, 'r--') # 'r--': red dashed line ; 'g*-' : green stars + line
plt.xlabel('X axis title') ; plt.title('Plot title') ;
plt.savefig("filename.png", dpi=200) # save to disc as png, pdf, svg, etc

fig = plt.figure() ; ax = fig.add_subplot(1,1,1) # object-oriented API
ax.plot(x, x**3, label="x**3", linewidth=3, color="blue", alpha=0.5)
ax.plot(x, x**2, label="x**2", linestyle="-.", marker="s")
ax.legend(loc='lower right') (ax is an axes, i.e. a figure window)
```

**Multipanel plots**

```
plt.subplot(1,2,1) # 1 is figure number. ~ par\(mfrow=c\(1,2\)\) in R
plt.plot(x, y) ; plt.subplot(1,2,2) ; plt.plot(y, x)

fig = plt.figure(figsize=(8,4), dpi=100) # nested plots
window = fig.add_axes([0.1,0.1, 0.8,0.8]) # bottomleft + proportion of canvas
window.plot(x, y) ; window.set_ylabel("ylab") ; window.set_xlim([0,20])

fig,ax = plt.subplots(1,2) # ~ par\(mfrow=1:2, mar=c\(3,2,1,0.5\)\) in R
ax[0].plot(x,y) ; ax[1].plot(x,y);ax[1].set_ylabel('y') ; plt.tight_layout()
```

**Data visualisation with seaborn**

```
(builds on matplotlib, nice with pandas df)
import seaborn as sns # histogram with kernel density estimate:
sns.displot(data=df, x='column', kde=True, bins=30) # distributional summary

sns.catplot(data=df, kind="swarm", x="catcol", y="numcol", hue="catcolumn")
kind="box"; kind="bar" # categorical data; swarmplot, boxplot, barplot
sns.catplot(..., palette="Set2") # mypal={cat1:"g", cat2:"b"} color palettes
sns.pairplot(data=df, kind="kde", diag_kind="hist", hue="category",
             corner=True, diag_kws=dict(fill=False), ...)

sns.set_theme() # ~ par\(...\) in R
sns.relplot() # relationship scatterplots
```

**Machine learning** - classification, regression, clustering, dimensionality reduction, model selection

```
pip install scikit-learn ; import sklearn # note different names for install / import
```

### Data prep

```
y = df.target ; x = df.drop('target', axis=1)
x_train, x_test, y_train, y_test = sklearn.model_selection.train_test_split(
    x, y, test_size=0.3, random_state=12) # 70% for training, seed for shuffle
scaler = sklearn.preprocessing.StandardScaler() # see also: minmax_scale
x_train_norm = scaler.fit_transform(x_train.values)
x_test_norm = scaler.transform(x_test.values)
```

### Multivariate linear regression

```
logreg = sklearn.linear_model.LogisticRegression(max_iter=1000)
logreg.fit(x_train, y_train) ; logreg_pred = logreg.predict(x_test)
pd.crosstab(y_test, logreg_pred) ; logreg.score(x_test, y_test) # accuracy
logreg.predict_proba(x_test) ; logreg.coef_ ;
```

**k-Nearest-Neighbors Classification:** predict outcome by majority at k most similar data points

```
knn_5 = sklearn.neighbors.KNeighborsClassifier(n_neighbors=5) # set the model
knn_5.fit(x_train_norm, y_train) # train the model
knn_5.predict(x_test_norm) ; knn_5.score(x_test_norm, y_test)
```

### Decision trees & Random forests

Hyperparameter: how high can tree depth be? (too high -> overfitting)

```
dt = sklearn.tree.DecisionTreeClassifier(random_state=2, max_depth=3)
dt.fit(x_train, y_train) ; dt.score(x_test, y_test)
sklearn.tree.plot_tree(dt, feature_names=x_train.columns, filled=True)
```

```
rf = sklearn.ensemble.RandomForestClassifier(random_state=2)
rf.fit(x_train, y_train) ; rf.score(x_test, y_test)
```

### Evaluation

```
y_pred = rf.predict(x_test)
sklearn.metrics.confusion_matrix(y_test, y_pred) ;
sklearn.metrics.plot_confusion_matrix(rf, x_test, y_test) # normalize='true'

sklearn.metrics.recall_score(y_test, y_pred) # TP/(TP+FN)
sklearn.metrics.precision_score(y_test, y_pred) # TP/(TP+FP), WikiLink
sklearn.metrics.plot_precision_recall_curve(rf, x_test, y_test) # doc

rf.score(x_test, y_test) # 'regular' accuracy, good when labels are balanced
sklearn.metrics.balanced_accuracy_score(y_test, y_pred)
```

**Unsupervised learning:** cluster analysis & PCA - No target variable, goal is not to predict something

```
kmeans = sklearn.cluster.KMeans(n_clusters=2, init='random', random_state=3)
kmeans.fit(x_train_norm) ; kmeans.cluster_centers_ # n dimensions = n columns
pred_k_means_test = kmeans.predict(x_test_norm)
sklearn.metrics.accuracy_score(y_test, pred_k_means_test)
```

```
pca = sklearn.decomposition.PCA(n_components=2) # number of target dimensions
pd.DataFrame(np.vstack([x_train.columns, # component contributions
    pca.components_.round(2)]).transpose()) # (feature effects)
pc = pca.fit_transform(x_test_norm)
sns.scatterplot(x=pc[:,0], y=pc[:,1], hue=pred_k_means_test, palette="Blues")
```

```
hierarc_clust = sklearn.cluster.hierarchy.linkage(x_test_norm, method='ward')
sklearn.cluster.hierarchy.dendrogram(hierarc_clust)
```

```
agg_clustering = sklearn.cluster.AgglomerativeClustering(n_clusters=2,
    affinity='euclidean', linkage='ward')
pred_agg_test = agg_clustering.fit_predict(x_test_norm)
sklearn.metrics.accuracy_score(y_test, pred_agg_test) # and sns pred_agg_test
X_agg_values = scaler.inverse_transform(x_test_norm)
X_agg = pd.DataFrame(X_agg_values, index=x_test.index,
    columns=x_test.columns) ; X_agg['clust'] = pred_agg_test
sns.pairplot(X_agg, hue='clust', palette='Blues')
```