

Scientific Computing Classes in Python 3

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Introduction to Classes in Python 3

Numerical software often takes the form of a “package”. You “tell your problem” to the package and the package applies the solution algorithm. The problem can be communicated to the package in the form of a class *instance*. That instance *object* contains the code and the data defining the problem. The package accesses this information by calling a class *attribute* that evaluates the function or functions defining the problem.

Programming languages define data *types*, such as *integer* or *string*. In Python, each *object* has a type, which can be *built in* (defined by the Python language), defined by a package (such as an `ndarray` in the *numpy* class), or defined by you, the programmer. A *class* is a defined datatype (or data type?). An *instance* of that class is an object whose datatype is that class. Creating a new object from a class is *instantiating* a class object. It can be complicated, for sophisticated classes, but it can be simple too.

The best introduction to Python classes (my opinion, others disagree!) is in the Python 3 documentation itself. This is not a “for dummies” collection of recipes, but an explanation of principles. It explains not only classes, but other basic principles of Python. Click on the link and see.

[Python 3 classes documentation](#)

An example

The sample code `ClassDemo.py` illustrates the class mechanism. It shows how simple classes are in Python. To run it, you also need the files (modules) `BlankSlate.py`, `GraySlate.py`, and `Helpers.py`. Copy all of these into a directory and then type `python ClassDemo.py`. The output should be identical to the screenshot `ClassDemoOutput.png`. Open the Python modules in editor windows that show line numbers. Lines 9 to 11 of `ClassDemo.py` illustrate that a class is defined in a module, such as `BlankSlate.py` that you import if you want to instantiate (create) an object of that class. Line 17 creates an object, `BlankInstance` (more correctly, a *name*, “`BlankInstance`”, that is bound to an object of that class). The `bs...` on right side of `=` says that you are looking for a name in the *namespace* “`bs`”. Line 9 of `BlankSlate.py` says that “`BlankSlate`” is a class. Line 17 of `ClassDemo.py` has `...BlankSlate()`, which uses the *constructor* of the `BlankSlate` class to create (instantiate) an object of that class.

Every class has a constructor, which is a function with the same name as the class, `BlankSlate` in this case. But the class definition in `BlankSlate.py` does not include any constructor code, so Python uses the *default constructor*. The constructor, possibly among other things, creates a namespace for the class instance.

As the documentation explains, a *namespace* is a *dictionary* of names and objects. The command `dir` returns a list of all the names of this dictionary. You can see in the output that there are quite a few, and that all of them have the format `__SomeName__`. The underscore characters “`__`” give the message: “you are allowed to access these, but please don’t unless you really know what you’re doing.” For example, if your code has `BlankInstance.__hash__`, it is a mistake in your judgement, but not a Python error. The module `Helpptes.py` returns only names without the underscore warning. Lines 23 to 26 show that there aren’t any. The `BlankSlate` class has nothing in it.

Line 28 creates a new name in the `BlankInstance` namespace, which is a function in the `h` namespace defined by importing the `Helpers` module. Lines 30 to 34 illustrate that this name was added to the namespace of `BlankInstance`. This name was not added to the `BlankSlate` class, only to the instance of that class `BlankInstance`. Line 37 shows that you can access that name. A numerical software package accesses its “problem” function in this way. In C++ or Java, you cannot insert a new member to a class instance as line 28 does. The simplicity of Python, which is a major strength of the language, allows this. A class instance is not much more than a namespace dictionary.

The `GraySlate.py` module defines a `GraySlate` class that has an `__init__()` function. This function is called whenever a new class instance is created. Line 43 of `ClassDemo.py` creates a `GraySlate` instance with `input=3`. Note that the name “`GraySlate`” (the name of the class) is in the `gs` namespace that is created by line 10. Using namespaces allows the same name to have different meanings in different places. In line 10, `GraySlate` refers to the module (file) `GraySlate.py`. A class instance has a personal namespace traditionally called `self` that is created by the constructor. Line 15 of `GraySlate.py` “remembers” the input `n` by copying its value into the instance namespace. The `self` namespace holds data associated to a class instance. Lines 17 and 18 define a *class function* `add_n` that is a member of any class instance. Lines 48 to 50 of `ClassDemo.py` show that the names were added to the instance `GS3` when that object was built. Lines 52 to 54 show that the class instance `GS3` remembered the input value 3 that was supplied in line 43. The name `n` in the instance namespace (accessed by `GS3.n` in line 53) is bound to that value.

The code in the class definition module `GraySlate.py` (the code defining the `GraySlate` class starts at line 10) needs a way to access the namespace associated to a class instance. That namespace is the first argument to any function defined within the class (i.e., after line 10). A good Python programmer will call that `self`, as the `__init__()` function does. A bad programmer can call it whatever he/she/they wants, as line 17 shows.

Lines 17 and 18 of `GraySlate.py` show how data “known” by a class instance `myself.n` can be combined with input data `x` to define a function. A function

that defines a numerical problem to a numerical software package can do it this way. This makes Python classes a convenient way to define computational problems to packages.

Lines 61 to 63 of `ClassDemo.py` illustrate the difference between *names* and *objects* in Python. Line 61 creates a new name, `newGI` (for “new Gray Instance”) but does not create a new object. Instead, the new name is bound to the same object that `GI3` was bound to. The names `newGI.n` and `GI3.n` point to the same object and therefore have the same value.

A package and a function for it

The module `IntegrationDemo.py` shows how a class can hold data that defines a function. This demo concerns

$$\int_{-1}^1 (1 + 2x + 3x^2) dx = 4 .$$

The integrand $f(x) = 1 + 2x + 3x^2$ is represent by an instance of the `Integrand` class defined in the module `IntegrandClass.py`. The integration “package” is in the module `IntegrationPackage.py`. Line 19 of `IntegrationPackage.py` has the integration package accessing the function, as the `f` attribute of the `f` object. You can recognize lines 18 and 19 as the rectangle rule, which is not very accurate (to see this, type: `python IntegrationDemo.py`).

Lines 13 to 17 of `IntegrationDemo.py` create the information that defines the integrand, which is a polynomial of degree 2 with coefficients $c + 0 = 1$, $c_1 = 2$ and $c_2 = 3$. Line 19 creates a class instance object which holds this information. Lines 21 to 29 show that the `f` attribute of the `poly` object, which is accessed in `poly.f(x)` in lines 23 and 28, evaluates the polynomial correctly, at least for $x = 0$ and $x = 2$. Line 38 demonstrates calling the integration package. It needs an object, `poly` in this case, that has a `f` attribute. This object contains the data and the code that defines $f(x)$.

The integrand class module `IntegrandClass.py` has an `__init__` that is slightly fancier than `GraySlate.py`. This one does error checking. It also makes a local copy of the data, done in line 21. That way, the integrand doesn’t change if some code elsewhere changes the array `coeffs`. Lines 30 and 31 illustrate the instance object accessing data that the integration package doesn’t know or want to know.