Learning Goals for Computing Competence

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Abstract

This note lists a set of learning goals for mastering computer-based problem solving in mathematical subjects. A case study describes and discusses the learning goals in depth.

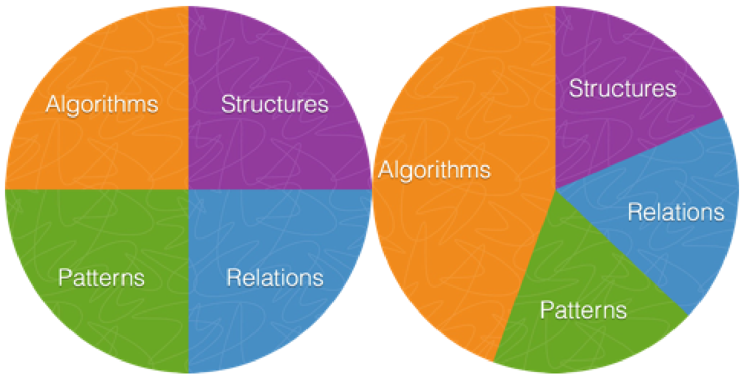
Why is computing competence important?

First of all, we need to define the term *computing* and what it contains.

Definition of computing.

Computing means in this document *mathematical problem solving using computers*. It covers numerical as well as symbolic computing. Computing is also about developing an understanding of the scientific process by enhancing the algorithmic thinking when solving problems.

Mathematics has traditionally been about identifying and verifying structures, patterns, relations, and algorithms. Mathematical recipes in the form of algorithms have always been in focus, but with modern computers that can perform 10^{17} arithmetic operations per second, the enormous computing power have led to an even stronger focus on algorithms and what we here call *computing competence*.



The computing competence is about

- derivation, verification, and implementation of algorithms
- understanding what can go wrong with algorithms
- overview of important, known algorithms
- understanding how algorithm are used to solve mathematical problems
- algorithmic thinking for gaining deeper insights about scientific problems

In the past, computing competence was about algorithms involving pen and paper and what is often referred to as *continuous models*. Application of computers calls for approximate *discrete models*. Much of the development of methods for continuous models are now being replaced by methods for discrete models in science and industry, simply because much larger problem classes can be addressed with discrete models, often also by simple and generic methodologies. However, verification of algorithms and understanding their limitations requires much of the classical knowledge on continuous models.

So, why should basic university education undergo a shift from classical mathematics to modern computing?

1. The impact of the computer on mathematics is tremendous: science and industry now rely on solving mathematical problems through computing.
2. Computing increases the relevance in education by solving more realistic problems earlier.
3. Computing through programming is excellent training of creativity.
4. Computing enhances the understanding of abstractions and generalization.

5. Computing decreases the need for special tricks and tedious algebra, and shifts the focus to problem definition, visualization, and "what if" discussions.

The result is a deeper understanding of mathematical modeling. We believe in the famous quote by Kristen Nygaard: "Programming is understanding".

For the mathematical training, there is one major new component among the arguments above: *understanding abstractions and generalization*. While many of the classical methods developed for continuous models are specialized for a particular problem or a narrow class of problems, computing-based algorithms are often developed for problems in a generic form and hence applicable to a large problem class.

Key principle in scientific modeling.

The power of the scientific method lies in identifying a given problem as a special case of an abstract class of problems, identifying general solution methods for this class of problems, and applying a general method to the specific problem (applying means, in the case of computing, calculations by pen and paper, symbolic computing, or numerical computing by ready-made and/or self-written software). This generic view on problems and methods is particularly important for understanding how to apply available, generic software to solve a particular problem.

Computing competence represents a central element in solving scientific problems, from basic education and research to essentially almost all advanced problems in modern societies. Computing competence is simply central to further progress. It enlarges the body of tools available to students and scientists beyond classical tools and allows for a more generic handling of problems. Focusing on algorithmic aspects results in deeper insights about scientific problems.

General goals for computing competence

Learning goals for *numerical algorithms*:

- Deep knowledge of the most fundamental algorithms for linear algebra, ordinary and partial differential equations, optimization, and statistical uncertainty quantification.
- Overview of advanced algorithms and how they can be accessed in available software.
- Application of fundamental and advanced algorithms to classial model problems as well as real-world problems with assessment of the uncertainty in the answer.

Learning goals for *symbolic computing*:

- Knowledge of at least one computer algebra system and how it is applied to perform classical mathematics (calculus, linear algebra, differential equations - with verification).

Learning goals for *programming*:

- Extensive experience with programming in a high-level language (MATLAB, Python, R). Experience with programming in a compiled language (Fortran, C, C++).
- Knowledge of basic software engineering elements: functions, classes, modules/libraries, testing procedures and frameworks, documentation tools, and version control systems.
- Extensive experience with implementing and applying numerical algorithms in reusable software that acknowledges the generic nature of the mathematical algorithms.
- Extensive experience with debugging software, e.g., as part of implementing comprehensive tests.

Learning goals for *verification*:

- Extensive experience with programming of testing procedures.
- Deep knowledge of testing/verification methods:
  - Exact solution of numerical models
  - Method of manufactured solutions (chose solution and fit a problem)
  - Classical analytical solutions (incl. asymptotic solutions)
  - Asymptotic results for approximation errors
  - Computing of asymptotic approximation errors (convergence rates)
- Step-wise construction of tests to aid debugging.

Learning goals for *mathematical modeling*:

- Experience with deriving computational models from basic principles in applied sciences (physics, geology, biology, etc.).
- Experinece with bringing models on dimensionless form to reduce and simpilify input data and increase the understanding of the model by interpreting its dimensionless parameters.
- Experience with solving real problems from applied sciences.

Learning goals for *presentation of results*:

- Experience with different visualization techniques for different types of computed data.
- Extensive experience with presenting computed results in scientific reports and oral presentations.

What is *deep knowledge*?

By deep knowledge we here mean the understanding of the underlying fundamental ideas and concepts from which a plethora of seemingly different methods and technologies can be derived. In other words, the deep knowledge brings structure to all the technical details.

Obtaining this type knowledge requires time in class and a lot of exercises. In addition, the students need to *reflect* about theory and practice. The reflection process is often difficult to implement. Below are some suggestions.

A useful concept is *simplify, understand, and then generalize.* Giving a superficial overview of a bunch of unrelated methods and their applications to unrelated scientific problems equips the students with a wide toolbox, but fails to enhance a fundamental understanding of how multidisciplinary topics play together. Instead, we believe in the following list.

1. Pick a few selected classes of problems,
2. start out with simplified models,
3. apply general, fundamental ideas to construct algorithms,
4. understand all details to correctly implement the algorithms,
5. understand how to judge the numerical quality of the algorithms,
6. understand how to verify that the computations are mathematically correct.

The verification process forces the student to reflect on all the points: What type of problem is actually solved? How can I test that the solution is right?

After obtaining an understanding of the simplified problem, one can generalize the models to real applications, but illustrate how the insight from the simplified models and methods gives very valueable knowledge when attacking the generalizations. The focus on simplified models help to detach the mathematics from a lot of discipline-dependent application details and cultivate the common mathematical and implementational ideas.

This philosophy is closely related to the *Key principle* stated eariler:

1. solving a complicated problem first starts with the purpose of breaking up the problem into subtasks that belong to general classes of well-studied problems in mathematics,

2. each subproblem is understood with great help simplified models in that class,

3. and finally a synthesis of the subproblems can solve the original problem.

hpl 1: Need to highlight educational methods: instruction based teaching, project work, ...

Case study

The series of goals above are briefly stated, but illustrated here in detail for a special, simple case study: numerical integration by the Trapezoidal rule.

Many science courses now have examples and exercises involving implementation and application of numerical methods. How to structure and verify such numerical programs has, unfortunately, received little attention in university education and the literature. Students and teachers occasionally write programs that are too tailored to the problem at hand instead of being a good starting point for future extensions, and testing is often limited to running a case where the answer seems reasonable. The standards of computing need to be raised to the levels found in experimental physics, chemistry, and biology.

Observation: poor versus good design of programs depends on the programming language (!).

A common conception is that simple scientific computing scripts implemented in Matlab and Python are very similiar - almost identical. However, practice observed by this author shows that students and teachers tend to make software with bad design in Matlab, while the design improves significantly when they use Python. Bad design means specializing a generic algorithm to a specific problem and making "flat" programs without functions. Good design means reusable implementations of generic algorithms and proper use of functions (or classes). The coming text demonstrates the assertions.

Exercise for the case study

Integrate the function $g(t) = \exp(-t^4)$ from -2 to 2 using the Trapezoidal rule, defined by

$$\int_a^b f(x)dx \approx h\left(\frac{1}{2}(f(a) + f(b)) + \sum_{i=1}^{n-1} f(a+ih)\right), \quad h = (b-a)/n \qquad (1)$$

Solution 1: Minimalistic Matlab

The simplest possible program may look as follows in Matlab:

```
a = -2; b = 2;
n = 1000;
h = (b-a)/n;
s = 0.5*(exp(-a^4) + exp(-b^4));
for i = 1:n-1
    s = s + exp(-(a+i*h)^4);
end
r = h*s;
r
```

The solution is minimalistic and correct. Nevertheless, this solution has a pedagogical and software engineering flaw: a special function $\exp(-t^4)$ is merged into a general algorithm (1) for integrating an arbitrary function $f(x)$.

The writer of the program runs it and reports the result: 1.81280494737. How can one assess that this result is correct? There is no analytical result to compare with. Even if it were, the comparison is not much worth. Say we try to integrate $h(t) = \cos t$ instead and report 1.81859242886 to be compared to the exact value 1.81859485365. The error $2.42 \cdot 10^{-6}$ is “small”, but we have no idea if this error is just the approximation error in the numerical method or if the program has a bug too. What if the error were $1.67 \cdot 10^{-3}$? It is impossible to say whether this answer is the correct numerical result or not. Actually, this error contains both the approximation error and a bug where the loop is `for i = 0:n-1`.

Also, the program above is not well suited for switching to an integrand where we can compare with an exact answer, because several lines need modification.

Solution 2: Matlab with functions

A successful software engineering practice is to use functions for splitting a program into natural pieces, and if possible, make these functions sufficiently general to be reused in other problems. In the present problem we should strive for the following principles:

1. Since the formula for the Trapezoidal rule works for “any” function, the implementation of the formula should be in terms of a *function* taking $f(x)$, a, b, and n as arguments.

2. The special $g(t)$ formula is implemented as a separate function.

3. A main program solves the *specific problem in question* by calling the *general algorithm* from point 1 with the special data of the given problem ($g(t)$, $a = -2$, $b = 2$, $n = 1000$).

Let us apply these desirable principles in a Matlab context. User-defined Matlab functions must be placed in separate files. This is sometimes found annoying, and therefore many students and teachers tend to avoid functions. In the present case, we should implement the Trapezoidal method in a file `Trapezoidal.m` containing

```
function r = Trapezoidal(f, a, b, n)
% TRAPEZOIDAL Numerical integration from a to b
% with n intervals by the Trapezoidal rule
f = fcnchk(f);
h = (b-a)/n;
s = 0.5*(f(a) + f(b));
for i = 1:n-1
    s = s + f(a+i*h);
end
r = h*s;
```

The special $g(t)$ function can be implemented in a separate file `g.m` or put in the main program. The function becomes

```
function v = g(t)
v = exp(-t^4)
end
```

Finally, a specialized main program (`main.m`) solves the problem at hand:

```
a = -2; b = 2;
n = 1000;
result = Trapezoidal(@g, a, b, n);
disp(result);
exit
```

The important feature of this solution is that `Trapezoidal.m` can be reused for "any" integral. In particular, it is straightforward to also integrate an integrand where we know the exact result.

An advantage of having the $g(t)$ as a separate function is that we can easily send this function to a different integration method, e.g., Simpson's rule.

Solution 3: Standard Python

Both Solution 1 and Solution 2 are readily implemented in Python. However, functions in Python do *not* need to be located in separate files to be reusable, and therefore there is no psychological barrier to put a piece of code inside a function. The consequence is that a Python programmer is more likely to go for Solution 2. (This may be the reason why the author has observed scientific Python codes to have better design than Matlab codes - modularization comes more natural.) The relevant code can be placed in a single file, say `main.py`, looking as follows:

```
def Trapezoidal(f, a, b, n):
    h = (b-a)/float(n)
    s = 0.5*(f(a) + f(b))
    for i in range(0,n,1):
        s = s + f(a + i*h)
    return h*s

from math import exp  # or from math import *
def g(t):
    return exp(-t**4)

a = -2;  b = 2
n = 1000
result = Trapezoidal(g, a, b, n)
print result
```

This solution acknowledges the fact that the implementation is a generally applicable function, just as the Trapezoidal formula.

However, a small adjustment of this implementation will make it much better. If somebody wants to reuse the `Trapezoidal` function for another integral, they can import `Trapezoidal` from the `main.py` file, but the special problem will be executed as part of the import. This is not desired behavior when solving another problem. Instead, our special exercise problem should be isoloated in its own function and called from a test block in the file (to avoid being executed as part of an import). This is the general software design of *modules* in Python.

We therefore rewrite the code in a new file `Trapezoidal.py`:

```
def Trapezoidal(f, a, b, n):
    h = (b-a)/float(n)
    s = 0.5*(f(a) + f(b))
    for i in range(1,n,1):
        s = s + f(a + i*h)
    return h*s

def _my_special_problem():
    from math import exp
    def g(t):
        return exp(-t**4)

    a = -2;  b = 2
    n = 1000
    result = Trapezoidal(g, a, b, n)
    print result

if __name__ == '__main__':
    _my_special_problem()
```

Now we have obtained the following important features:

- The file `Trapezoidal.py` is a module offering the widely applicable function `Trapezoidal` for integrating “any” function.
- If `Trapezoidal.py` is run as a program, the if test is true and the special integral of g is computed.
- In an import like `from Trapezoidal import Trapezoidal`, the if test is false and nothing gets computed.

Vectorization

This author has seen a lot of programs used for teaching which apply vectorization without explicit notice. Vectorization is a technique in high-level languages like IDL, MATLAB, Python, and R for removing loops and speed up computations. Unfortunately, the "distance" from the mathematical algorithm to vectorized code is larger than to a plain loop as we used above. Vectorization therefore tends to confuse students who are not well educated in the techniques. For example, the Trapezoidal rule can be vectorized as

```
import numpy as np

def Trapezoidal(f, a, b, n):
    x = np.linspace(a, b, n+1)
    return (b-a)/float(n)*(np.sum(f(x) - 0.5*(f(a) + f(b))))
```

The code is correct, but it takes some thinking to realize why these lines compute the formula (1). Because of the `sum` function, we need to adjust the summation result such that the weight of the end points becomes correct.

Tip: Implement scalar code first - then vectorize.

It is much easier to get a scalar code, with explicit loops that mimic the mathematical formula(s) as closely as possible, to work first. Then remove loops by vectorized expressions and test the code against the scalar version.

Verification and testing frameworks

An integral part of any implemention is verification, i.e., to bring evidence that the program works correctly. As we have seen, comparison of a numerical approximation with an exact answer does not say much unless the error is "huge" and therefore clearly points to fundamental bugs in the code.

For most numerical methods there are only two good verification methods:

1. Computation of a problem where the approximation error vanishes.
2. Empirical measurement of the convergence rate.

A simple test function. The Trapezoidal rule is obviously exact for linear integrands. Therefore, we should test an "arbitrary" linear function and check that the error is close to machine precision. This is done in a separate function in a separate file `test_Trapezoidal.py`:

```
from Trapezoidal import Trapezoidal

def linear():
    """Test linear integrand: exact result for any n."""
    def f(x):
        return 8*x + 6

    def F(x):
        """Anti-derivative of f(x)."""
        return 4*x**2 + 6*x

    a = 2
    b = 6
    exact = F(b) - F(a)
    numerical = Trapezoidal(f, a, b, n=4)
    error = exact - numerical
    print '%.16f' % error
```

The output of calling `linear()` is in this case zero exactly, but in general one must expect some small round-off errors in the numerical (and exact) result.

A proper test function for the nose or pytest test framework. The function `linear` performs the test, but it would be better to integrate the test into a *testing framework* such that we with one command can execute a comprehensive set of tests. This makes it easy to run all tests after every small change of the software. Students should adopt such compulsory habits from the software industry.

The dominating type of test frameworks today is based on what is called *unit testing* in software engineering. It means that we pick a unit in the software and write a function (or class) that runs the test after certain specifications:

- The test function must start with `test_`.
- The test function cannot have any arguments.
- If the test fails, an `AssertionError` exception (in Python) is raised, otherwise the function runs silently.

There are two very popular test frameworks in the Python world now: pytest and nose. There are similar frameworks developed for Matlab too, see a video, but they are not as user friendly since they require the programmer to embed tests in classes (this is still the dominating method in most programming languages). Using test functions instead of test classes requires writing less code and is easier to learn.

In our case, a proper test function means the following rewrite of the function `linear`:

```
def test_linear():
    """Test linear integrand: exact result for any n."""

    def f(x):
        return 8*x + 6

    def F(x):
        """Anti-derivative of f(x)."""
        return 4*x**2 + 6*x
    a = 2
    b = 6
    expected = F(b) - F(a)
    computed = Trapezoidal(f, a, b, n=4)
    error = abs(expected - computed)
    tol = 1E-14
    msg = 'expected=%g, computed=%g, error=%g' % \
          (expected, computed, error)
    assert error < tol, msg
```

The code is basically the same, but we comply to the rules above. The **assert** statement has the test as error < tol, with msg as an optional message that is printed only if the test fails (error < tol is False). The msg string can be left out and it suffices to do **assert** error < tol.

The reason why we comply to testing frameworks is that we can use software like nose or pytest to automatically find all our tests and execute them. We put tests in files or directories starting with test and run one of the commands

```
Terminal> nosetests -s -v .
Terminal> py.test -s -v .
```

All functions with names test_*() in all files test*.py in all subdirectories with names test* will be run, and statistics about how many tests that failed will be printed. The tests should be run after every modification of the software.

Use of symbolic computing for exact results. We integrated by hand the linear function. In more complicated cases it would be safer to use symbolic computing software to carry out the mathematics. Here we demonstrate how to use the Python package SymPy to do the integration:

```
def test_linear_symbolic():
    """Test linear integrand: exact result for any n."""
    import sympy as sym
    # Define a linear expression and integrate it
    x = sym.symbols('x')
    f = 8*x + 6
    F = sym.integrate(f, x)
    # Verify symbolic computation: F'(x) == f(x)
    assert sym.diff(F, x) == f
    # Transform expressions f and F to Python functions of x
    f = sym.lambdify([x], f)
    F = sym.lambdify([x], F)

    # Run one test with fixed a, b, n.
    a = 2
    b = 6
    expected = F(b) - F(a)
    computed = Trapezoidal(f, a, b, n=4)
    error = abs(expected - computed)
    tol = 1E-14
    msg = 'expected=%g, computed=%g, error=%g' % \
          (expected, computed, error)
    assert error < tol, msg
```

Test function for the convergence rate. Let us extend the verification with a case where we know the exact answer of the integral, but we do not know the approximation error. The only knowledge we usually have about the approximation error is of asymptotic type. For example, for the Trapezoidal rule we have an expression for the error from numerical analysis:

$$E = -\frac{(b-a)^3}{12n^2} f''(\xi), \quad \xi \in [a,b].$$

Since we do not know ξ, we cannot compute E. However, we realize that the error has an asymptotic behavior as n^{-2}:

$$E = Cn^{-2},$$

for some unknown constant C. In general, when verifying the implementation of a numerical method with discretization parameter n, we write $E = Cn^r$, estimate r, and compare with the exact result (here $n = -2$).

More precisely, we perform a set of experiments for $n = n_0, n_1, \ldots, n_m$, where we emprically estimate r from two consecutive experiments:

$$E_i = Cn_i^r,$$
$$E_{i+1} = Cn_{i+1}^r.$$

Dividing the equations and solving with respect to r gives

$$r = \frac{\ln(E_i/E_{i+1})}{\ln(r_i/r_{i+1})}$$

As $i = 0, \ldots, m-1$, the r values should approach the value -2.

It is easy to use the *method of manufactured solutions* to construct a test problem. That is, we first choose the solution, say the integral is given by $F(b) - F(a)$, where

$$F(x) = e^{-x} \sin(2x).$$

Then we fit the problem to accept this solution. In the present case it means that the integrand must be $f(x) = F'(x)$. We use for safety symbolic software to calculate $f(x)$. Thereafter, we run a series of experiments where n is varied, we compute the corresponding convergence rates r from two consecutive experiments and test if the final r, corresponding to the two largest n values, is sufficiently close to the expected convergence rate -2:

```python
def test_convergence_rate():
    import sympy as sym
    # Construct test problem
    x = sym.symbols('x')
    F = sym.exp(-x)*sym.sin(2*x)  # Anti-derivative
    f = sym.diff(F, x)
    f = sym.lambdify([x], f)      # Turn to Python function
    F = sym.lambdify([x], F)      # Turn to Python function
```

```
a = 0.1
b = 0.9
expected = F(b) - F(a)
# Run experiments (double n in each experiment)
n = 1
errors = []
for k in range(8):
    n *= 2
    computed = Trapezoidal(f, a, b, n)
    error = abs(expected - computed)
    errors.append((n, error))
# Compute empirical convergence rates
from math import log as ln
estimator = lambda E1, E2, n1, n2: ln(E1/E2)/ln(float(n1)/n2)
r = []
for i in range(len(errors)-1):
    n1, E1 = errors[i]
    n2, E2 = errors[i+1]
    r.append(estimator(E1, E2, n1, n2))
expected = -2
computed = r[-1]  # The "most" asymptotic value
error = abs(expected - computed)
tol = 1E-3
msg = 'Convergence rates: %s' % r
assert error < tol, msg
```

The emprical convergence rates are in this example

```
-2.022, -2.0056, -2.0014, -2.00035, -2.000086, -2.000022,
-2.0000054, -2.0000013, -2.00000033
```

Although the rates are known to approach -2 as $n \to \infty$, the rates are close to -2 even for large n (such as $n = 4$). A rough tolerance is often used for convergence rates, for instance 0.1, but here we may use a smaller one if desired.

Summary.

Knowing an exact solution to a mathematical problem and comparing the program output with such a solution, gives only an indication that the program may be correct, but it is only a rough indication. Any real test must use what we know about the approximation error, and that is usually only an asymptotic behavior as function of discretization parameters. The test needs to vary the discretization parameter(s) to estimate convergence rates for comparison with known asymptotic results.

Known analytical solutions are of value in convergence rate tests, but if they are not available, or restricted to very simplified cases, the method of manufactured solutions, where we solve a perturbed problem fitted to a constructed exact solution, is also a very useful technique.

Tests in Matlab. In Matlab, one must decide whether to use a class-based system for unit testing or just write test functions that mimic the behavior of the

Python test functions for the nose and pytest frameworks. Here is an example on doing the `test_linear()` function in Matlab:

```
function test_trapezoidal_linear
 %% Check that linear functions are integrated exactly
  f = @(x) 8*x + 6;
  F = @(x) 4*x**2 + 6*x;  %% Anti-derivative
  a = 2;
  b = 6;
  expected = F(b) - F(a);
  tol = 1E-14;
  computed = trapezoidal(f, a, b, 4);
  error = abs(expected - computed);
  assert(error < tol, 'n=%d, error=%g', n, error);
  end
end

test_trapezoidal_linear()
```

There is, unfortunately, no software available to run all tests in all files in all subdirectories and report on the success/failure statistics, but it is quite straightforward to write such software.

Extended Exercise

Compute the following integrals with the Midpoint rule, the Trapezoidal rule, and Simpson's rule:

$$\begin{aligned}
\int_0^\pi \sin x\,dx &= 2,\\
\int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-x^2}\,dx &= 1,\\
\int_0^1 3x^2 dx &= 1,\\
\int_0^{\ln 11} e^x dx &= 10,\\
\int_0^1 \frac{3}{2}\sqrt{x} dx &= 1.
\end{aligned}$$

For each integral, write out a table of the numerical error for the three methods using a n function evaluations, where n varies as $n = 2^k + 1$, $k = 1, 2, ..., 12$.

A Python solution

In the extended problem, Solution 1 is obviously inferior because we need to apply, e.g., the Trapezoidal rule to five different integrand functions for 12 different n values. Then it only makes sense to implement the rule in a separate function that can be called 60 times.

Similarly, a mathematical function to be integrated is needed in three different rules, so it makes sense to isolate the mathematical formula for the integrand in a function in the language we are using.

We can briefly sketch a compact and smart Python code, in a single file, that solves the extended problem:

```
def f1(x):
    return sin(x)

def f2(x):
    return 1/sqrt(2)*exp(-x**2)

...

def f5(x):
    return 3/2.0*sqrt(x)

def Midpoint(f, a, b, n):
    ...

def Trapezoidal(f, a, b, n):
    ...

def Simpson(f, a, b, n):
    ...

problems = [(f1, 0, pi),  # list of (function, a, b)
            (f2, -5, 5),
            ...
            (f3, 0, 1)]

methods = (Midpoint, Trapezoidal, Simpson)
result = []
for method in methods:
    for func, a, b in problems:
        for k in range(1,13):
            n = 2**k + 1
            I = method(func, a, b, n)
            result.append((I, method.__name__, func.__name__, n))

# write out results, nicely formatted:
for I, method, integrand, n in result:
    print '%-20s, %-3s, n=%5d, I=%g' % (I, method, integrand, n)
```

Note that since everything in Python is an object that can be referred to by a variable, it is easy to make a list `methods` (list of Python functions), and a list `problems` where each element is a list of a function and its two integration limits. A nice feature is that the name of a function can be extracted as a string in the function object (`name` with double leading and trailing underscores).

To summarize, Solution 2 or 3 can readily be used to solve the extended problem, while Solution 1 is not worth much. In courses with many very simple exercises, solutions of type 1 will appear naturally. However, published solutions should employ approach 2 or 3 of the mentioned reasons, just to train students to think that *this is a general mathematical method that I should make reusable through a function.*

Along with the code above there should be a file `test_integration_methods.py` containing test functions for the various rules. The error formula for Simpson's rule contains f'''', so one can integrate a third-degree polynomial in a test and expect an error about the machine precision. The Midpoint rule integrates linear functions exactly. For testing of convergence rates, the Trapezoidal and Midpoint rules have errors behaving as n^{-2}, while the error in Simpson's rule goes like n^{-4}.

Solution 4: a Java OO program

Introductory courses in computer programming, given by a computer science department, often employ the Java language and emphasize object-oriented programming. Many computer scientists argue that it is better to start with Java than Python or (especially) Matlab. But how well is Java suited for introductory numerical programming?

Let us look at our first integration example, now to be solved in Java. Solution 1 is implemented as a simple `main` method in a class, with a code that follows closely the displayed Matlab code. However, students are in a Java course trained in splitting the code between classes and methods. Therefore, Solution 2 should be an obvious choice for a Java programmer. However, it is not possible to have stand-alone functions in Java, functions must be methods belonging to a class. This implies that one cannot transfer a function to another function as an argument. Instead one must apply the principles of object-oriented programming and implement the function argument as a reference to a superclass. To call the "function argument", one calls a method via the superclass reference. The code below provides the details of the implementation:

```java
import java.lang.*;

interface Func {  // superclass for functions f(x)
    public double f (double x);  // default empty implementation
}

class f1 implements Func {
    public double f (double t)
    { return Math.exp(-Math.pow(t, 4)); }
}

class Trapezoidal {
    public static double integrate
           (Func f, double a, double b, int n)
    {
        double h = (b-a)/((double)n);
        double s = 0.5*(f.f(a) + f.f(b));
        int i;
        for (i = 1; i <= n-1; i++) {
            s = s + f.f(a+i*h);
        }
        return h*s;
    }
}

class MainProgram {
    public static void main (String argv[])
    {
        double a = -2;
        double b = 2;
        int n = 1000;
        double result = Trapezoidal.integrate(f, a, b, n);
        System.out.println(result);
    }
}
```

From a computer science point of view, this is a quite advanced solution since it relies on inheritance and true object-oriented programming. From a mathematical point of view, at least when compared to the Matlab and Python versions, the code looks unnecessarily complicated. Many introductory Java courses do not cover inheritance and true object-oriented programming, and without mastering these concepts, the students end up with Solution 1. On this background, one may argue that Java is not very suitable for implementing this type of numerical algorithms.

Conclusions

Simple exercises have pedagogical advantages, but some disadvantages with respect to programming, because the programs may easily become too specialized. In such cases, the exercise may explicitly ask the student to divide the program into functions and make general mathematical methods available as general, reusable functions for a set of problems. This requirement can be motivated by an extended exercise where a piece of code are needed many times, typically that several methods are applied to several problems.

Especially when using Matlab, students may be too lazy to use functions when this is not explicitly required.