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Python Fortran Rosetta Stone

Python with NumPy and Fortran are very similar in terms of expressiveness and features. This rosetta stone shows how to implement many common idioms in both languages side by side.

How to Execute Code Snippets

Consider for example the following code snippets:

```
NumPy
                                                       Fortran
from numpy import array, size, shape, min, max, sum
                                                       integer :: a(3)
a = arrav([1, 2, 3])
                                                       a = [1, 2, 3]
print shape(a)
                                                       print *, shape(a)
print size(a)
                                                       print *, size(a)
print max(a)
                                                       print *, maxval(a)
print min(a)
                                                       print *, minval(a)
print sum(a)
                                                       print *, sum(a)
```

In Python, just save the code to a file a.py and execute using python a.py. In Fortran, save it to a file a.f90 and append the line end at the end of the file (see the section *Modules* for more info how this works). Compile using gfortran a.f90 and execute using ./a.out (you can of course add compilation options to gfortran, for example to produce the executable with a different name).

Arrays

Arrays are builtin in Fortran, and available in the NumPy module in Python. The usage is identical, except for the following differences:

- Fortran counts (by default) from 1, NumPy always from 0
- Fortran array sections (slices) include both ends, in NumPy the initial point is included, the final is excluded
- In C the array is stored row wise in the memory (by default NumPy uses C storage), while in Fortran it is stored column wise (this only matters in the next two points)
- By default reshape uses Fortran ordering in Fortran, and C ordering in NumPy (in both cases an optional argument order allows to use the other ordering). This also matters when reshape is used implicitly in other operations like flattening.
- The first index is the fastest in Fortran, while in NumPy, the last index is the fastest
- By default NumPy prints the 2d array nicely, while in Fortran one has to specify a format to print it (also Fortran prints column wise, so one has to transpose the array for row wise printing)

Everything else is the same, in particular:

- There is one-to-one correspondence between NumPy and Fortran array operations and things can be expressed the same easily/naturally in both languages
- For 2D arrays, the first index is a row index, the second is the column index (just like in mathematics)

- NumPy and Fortran arrays are equivalent if they have the same shape and same elements corresponding to the same index (it doesn't matter what the internal memory storage is)
- Any array expression involving mathematical functions is allowed, for example a**2 + 2*a + exp(a), sin(a), a * b and a + b (it operates element wise)
- You need to use a function to multiply two matrices using matrix multiplication
- · Advanced indexing/slicing
- Arrays can be of any integer, real or complex type
- ...

```
NumPy
```

```
from numpy import array, size, shape, min, max, sum
a = array([1, 2, 3])
print shape(a)
print size(a)
print max(a)
print min(a)
print sum(a)
integer :: a(3)
a = [1, 2, 3]
print *, shape(a)
print *, size(a)
print *, maxval(a)
print *, minval(a)
print *, sum(a)
```

Fortran

```
from numpy import reshape
                                                      integer :: a(2, 3), b(2, 3)
a = reshape([1, 2, 3, 4, 5, 6], (2, 3))
                                                      a = reshape([1, 2, 3, 4, 5, 6], [2, 3], order=[2, 1])
b = reshape([1, 2, 3, 4, 5, 6], (2, 3), order="F")
                                                      b = reshape([1, 2, 3, 4, 5, 6], [2, 3])
print a[0, :]
                                                      print *, a(1, :)
                                                      print *, a(2, :)
print a[1, :]
                                                      print *
print
                                                      print *, b(1, :)
print b[0, :]
print b[1, :]
                                                      print *, b(2, :)
```

Output:

Output:

```
    [1 2 3]

    [4 5 6]

    1 2 3

    [4 5 6]

    2 3 6

    [1 3 5]

    [2 4 6]

    2 4 6
```

```
from numpy import array, size, shape, max, min
                                                      integer :: a(2, 3)
a = array([[1, 2, 3], [4, 5, 6]])
                                                      a = reshape([1, 2, 3, 4, 5, 6], [2, 3], order=[2, 1])
print shape(a)
                                                      print *, shape(a)
print size(a, 0)
                                                      print *, size(a, 1)
                                                      print *, size(a, 2)
print size(a, 1)
                                                      print *, maxval(a)
print max(a)
                                                      print *, minval(a)
print min(a)
print a[0, 0], a[0, 1], a[0, 2]
                                                      print *, a(1, 1), a(1, 2), a(1, 3)
                                                      print *, a(2, 1), a(2, 2), a(2, 3)
print a[1, 0], a[1, 1], a[1, 2]
                                                      print "(3i5)", transpose(a)
print a
```

Output:

Output (whitespace trimmed):

```
3
                                                       6
1
                                                      1
1 2 3
                                                      1 2 3
4 5 6
                                                      4 5 6
[[1 2 3]
                                                      1 2 3
 [4 5 6]]
                                                      4 5 6
from numpy import array, all, any
                                                       integer :: i(3)
i = array([1, 2, 3])
                                                      i = [1, 2, 3]
all(i == [1, 2, 3])
                                                       all(i == [1, 2, 3])
any(i == [2, 2, 3])
                                                       any(i == [2, 2, 3])
from numpy import array, empty
                                                       integer :: a(10), b(10)
a = array([1, 2, 3, 4, 5, 6, 7, 8, 9, 10])
                                                       a = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]
b = empty(10)
                                                       where (a > 5)
b[:] = 0
                                                           b = a - 3
b[a > 2] = 1
                                                       elsewhere (a > 2)
b[a > 5] = a[a > 5] - 3
                                                           b = 1
                                                       elsewhere
                                                           b = 0
                                                       end where
from numpy import array, empty
                                                       integer :: a(10), b(10)
a = array([1, 2, 3, 4, 5, 6, 7, 8, 9, 10])
                                                       a = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]
b = empty(10)
                                                       where (a > 5)
for i in range(len(a)):
                                                          b = a - 3
    if a[i] > 5:
                                                       elsewhere (a > 2)
        b[i] = a[i] - 3
                                                           b = 1
    elif a[i] > 2:
                                                       elsewhere
        b[i] = 1
                                                           b = 0
                                                       end where
    else:
        b[i] = 0
from numpy import array, sum, ones, size
                                                       integer :: a(10)
a = array([1, 2, 3, 4, 5, 6, 7, 8, 9, 10])
                                                       a = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]
print sum(a)
                                                       print *, sum(a)
print sum(a[(a > 2) & (a < 6)])</pre>
                                                       print *, sum(a, mask=a > 2 .and. a < 6)
o = ones(size(a), dtype="int")
                                                       print *, count(a > 2 .and. a < 6)
print sum(o[(a > 2) \& (a < 6)])
                                                       integer :: a(2, 2), b(2, 2)
from numpy import array, dot
                                                       a = reshape([1, 2, 3, 4], [2, 2], order=[2, 1])
a = array([[1, 2], [3, 4]])
b = array([[2, 3], [4, 5]])
                                                       b = reshape([2, 3, 4, 5], [2, 2], order=[2, 1])
print a * b
                                                       print *, a * b
print dot(a, b)
                                                       print *, matmul(a, b)
Output:
                                                      Output:
                                                       2
[[ 2 6]
                                                                   12
                                                                                6
                                                                                           20
[12 20]]
                                                      10
                                                                   22
                                                                               13
                                                                                           29
```

```
from numpy import array, pi
a = array([i for i in range(1, 7)])
b = array([(2*i*pi+1)/2 for i in range(1, 7)])
c = array([i for i in range(1, 7) \
    for j in range(1, 4)])

### use types, only: dp
use constants, only: pi
integer :: a(6), c(18)
real(dp) :: b(6)
integer :: i, j
a = [ (i, i = 1, 6) ]
b = [ ((2*i*pi+1)/2, i = 1, 6) ]
c = [ ((i, j = 1, 3), i = 1, 6) ]
```

Some indexing examples

```
NumPy
                             Fortran
 from numpy import array
                              integer :: a(3), b(-1:1)
 a = array([1, 2, 3])
                              a = [1, 2, 3]
                              b = a
 b = a
                             print *, a(:)
print *, b(:)
print *, a(:2)
 print a[:]
 print b[:]
 print a[:2]
 print b[:2]
                              print *, b(:0)
Output:
                             Output:
 [1 2 3]
                                                        3
 [1 2 3]
                                           2
 [1 2]
                                           2
 [1 2]
First n elements:
                                                    Fortran
NumPy
 a[:n]
                                                    a(:n)
                                                               ! assuming starting index 1 (default)
                                                    a(:n+m-1) ! assuming starting index m
Last n elements:
NumPy
                                          Fortran
 a[-n:] # equivalent to a[size(a)-n:]
                                          a(size(a)-n+1:)
Select elements between i and j (inclusive):
NumPy
            Fortran
```

```
a[i:j+1] a(i:j)
```

Select *n* elements starting with index *i*:

NumPy Fortran

a[i:i+n] a(i:i+n-1)

Select elements between -n, ..., n (inclusive):

NumPy

Fortran

```
# Not possible (arrays start at 0 index)
```

a(-n:n)

Loop over the whole array:

NumPy

Fortran

```
r = 1

for i in range(len(a)):

r *= a[i]

r = 1

do i = 1, size(a)

r = r*a(i)

end do
```

Loop between index 3 and 7 (inclusive):

NumPy

Fortran

$$r = 1$$

for i in range(3, 8):
 $r *= a[i]$
 $r = 1$
do i = 3, 7
 $r = r*a(i)$
end do

Loop between 3-th and 7-th elements (inclusive):

NumPy

Fortran

```
r = 1

for i in range(2, 7):

r *= a[i]

r = 1

do i = 3, 7

r = r*a(i)

end do
```

Split a string into three parts at indices *i* and *j*, the parts are:

NumPy Fortran

```
a[:i] a(:i-1)
a[i:j] a(i:j-1)
a[j:] a(j: )
```

Laplace update:

Modules

Comparison of Fortran and Python import statements:

```
Fortran

from A import foo from A import foo as Afoo from A import *

use A, only: foo use A, only: Afoo => foo use A
```

The following Python statements have no equivalent in Fortran:

```
Python Fortran

import A import ALongName as A
```

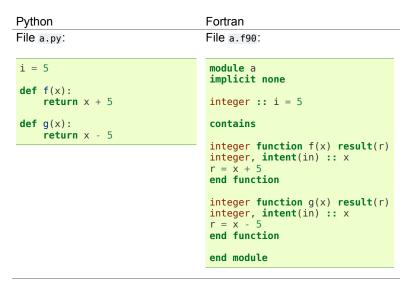
Fortran modules work just like Python modules. Differences:

- Fortran modules cannot be nested (i.e. they are all top level, while in Python one can nest the module arbitrarily using the __init__.py files)
- There is no Fortran equivalent of Python's import A
- One can specify private module symbols in Fortran

Identical features:

- A module contains variables, types and functions/subroutines
- By default all variables/types/functions can be accessed from other modules, but one can change this by explicitly specifying which symbols are private or public (in Python this only works for implicit imports)
- Symbols that are public don't pollute the global namespace, but need to be explicitly imported from the module in order to use them
- Importing a symbol into a module becomes part of that module and can then be imported from other modules
- One can use explicit or implicit imports (explicit imports are recommended)

One creates the module:



And uses it from the main program as follows:

Python	Fortran		
File main.py:	File main.f90:		
<pre>from a import f, i print f(3) print i Output:</pre>	<pre>program main use a, only: f, i implicit none print *, f(3) print *, i end program</pre>		
8	Output:		
5	8 5		

In Fortran, one can ommit the line program main, also one can just end the file with end instead of end program. That way one can test any code snippet just by appending end at the end.

In order to specify which symbols are public and private, one would use:

Python	Fortran
File a.py:	File a.f90:

```
all = ["i", "f"]
                                 module a
                                 implicit none
i = 5
                                 private
                                 public i, f
def f(x):
    return x + 5
                                 integer :: i = 5
def g(x):
                                 contains
    return x - 5
                                 integer function f(x) result(r)
                                 integer, intent(in) :: x
                                 r = x + 5
                                 end function
                                 integer function g(x) result(r)
                                 integer, intent(in) :: x
                                 r = x - 5
                                 end function
                                 end module
```

There is a difference though. In Fortran, the symbol g will be private (not possible to import from other modules no matter if we use explicit or implicit import), f and i public. In Python, when implicit import is used, the symbol g will not be imported, but when explicit import is used, the symbols g can still be imported.

Floating Point Numbers

Both NumPy and Fortran can work with any specified precision and if no precision is specified, then the default platform precision is used.

In Python, the default precision is typically double precision, while in Fortran it is single precision. See also the relevant Python and NumPy documentation.

```
Python 2.x
                                      Fortran
Single precision:
                                      Single precision:
from numpy import float32
                                       real :: f
f = float32(1.1)
                                       f = 1.1
Double precision:
                                      Double precision:
f = 1.1
                    # 1.1
                                      integer, parameter :: dp=kind(0.d0)
f = 1e8
                    # 100000000.0
                                       real(dp) :: f
f = float(1) / 2 # 0.5
                                       f = 1.1 dp
                                                               ! 1.1
f = float(1 / 2) # 0.0
                                       f = 1e8 dp
                                                               ! 100000000.0
                                                              ! 0.5
f = float(5)
                    # 5.0
                                       f = real(1, dp) / 2
                                       f = 1 / 2
                                                              ! 0.0
                                       f = 5
                                                               ! 5.0
```

In Fortran the habit is to always specify the precision using the _dp suffix, where dp is defined in the types.f90 module below as integer, parameter :: dp=kind(0.d0) (so that one can change the precision at one place if needed). If no precision is specified, then single precision is used (and as such, this leads to single/double corruption), so one always needs to specify the precision.

In all Fortran code snippets below, it is assumed, that you did use types, only: dp. The types.f90 module is:

Math and Complex Numbers

Fortran has builtin mathematical functions, in Python one has to import them from the math module or (for the more advanced functions) from the SciPy package. Fortran doesn't include constants, so one has to use the constants. f90 module (included below).

Otherwise the usage is identical.

```
Python Fortran
```

```
from math import cos, pi, e

I = 1j
print e**(I*pi) + 1
print cos(pi)
print 4 + 5j
print 4 + 5*I
use constants, only: pi, e
complex(dp) :: I = (0, 1)
print *, e**(I*pi) + 1
print *, cos(pi)
print *, cos(pi)
print *, (4, 5)
print *, 4 + 5*I
```

Output:

Output:

Fortran module constants.f90:

```
module constants
use types, only: dp
implicit none
private
public pi, e, I
! Constants contain more digits than double precision, so that
! they are rounded correctly:
real(dp), parameter :: pi = 3.1415926535897932384626433832795_dp
real(dp), parameter :: e = 2.7182818284590452353602874713527_dp
complex(dp), parameter :: I = (0, 1)
end module
```

Strings and Formatting

The functionality of both Python and Fortran is pretty much equivalent, only the syntax is a little different.

In both Python and Fortran, strings can be delimited by either " or ".

There are three general ways to print formatted strings:

Python

Fortran

Output:

```
print "Integer", 5, "and float", 5.5, "works fine." print "Integer " + str(5) + " and float " + str(5.5) + "." print "Integer %d and float %f." % (5, 5.5)
```

use utils, only: str print *, "Integer", 5, "and float", 5.5, "works fine." print *, "Integer " // str(5) // " and float " // str(5.5_dp) // "." print '("Integer ", i0, " and float ", f0.6, ".")', 5, 5.5

Output:

```
Integer 5 and float 5.5 works fine.
Integer 5 and float 5.5.
Integer 5 and float 5.500000.
```

```
Integer 5 and float 5.5000000 works fine.
Integer 5 and float 5.500000.
Integer 5 and float 5.500000.
```

And here are some of the frequently used formats:

Python

Fortran

```
print "%3d" % 5
print "%03d" % 5
print "%03d" % 5
print "%5" % "text"
print "%15.7f" % 5.5
print "%23.16e" % -5.5
print '(i3)', 5
print '(i3)', 5
print '(a)', "text"
print '(f15.7)', 5.5_dp
print '(es23.16)', -5.5_dp
```

Output:

Output:

```
5
005
text
5.5000000
-5.500000000000000E+00
```

Nested Functions

Both Python and Fortran allow nested functions that can access the outer function's namespace:

Python

Fortran

```
def foo(a, b, c):
    def f(x):
        return a*x**2 + b*x + c
    print f(1), f(2), f(3)
subroutine foo(a, b, c)
real(dp) :: a, b, c
print *, f(1._dp), f(2._dp), f(3._dp)
contains
```

```
real(dp) function f(x) result(y)
real(dp), intent(in) :: x
y = a*x**2 + b*x + c
end function f
end subroutine foo
```

Use it like:

Python Fortran

You can use the nested functions in callbacks to pass context:

Python Fortran

```
def simpson(f, a, b):
    return (b-a) / 6 * (f(a) + 4*f((a+b)/2) + f(b))

def foo(a, k):
    def f(x):
        return a*sin(k*x)
    print simpson(f, 0., pi)
    print simpson(f, 0., 2*pi)
```

```
real(dp) function simpson(f, a, b) result(s)
real(dp), intent(in) :: a, b
interface
    real(dp) function f(x)
    use types, only: dp
    implicit none
    real(dp), intent(in) :: x
    end function
end interface
s = (b-a) / 6 * (f(a) + 4*f((a+b)/2) + f(b))
end function
subroutine foo(a, k)
real(dp) :: a, k
print *, simpson(f, 0. dp, pi)
print *, simpson(f, 0. dp, 2*pi)
contains
real(dp) function f(x) result(y)
real(dp), intent(in) :: x
y = a*sin(k*x)
end function f
end subroutine foo
```

And use it like:

```
Python
                       Fortran
foo(0.5, 1.)
                        call foo(0.5 dp, 1. dp)
foo(0.5, 2.)
                        call foo(0.5 dp, 2. dp)
Output:
                       Output:
1.0471975512
                         1.0471975511965976
1.28244712915e-16
                        1.28244712914785977E-016
6.41223564574e-17
                        6.41223564573929883E-017
-7.69468277489e-16
                       -7.69468277488715811E-016
```

Control flow in loops

The common loop types in Python and Fortran are the for and do loops respectively. It is possible to skip a single loop or to stop the execution of a loop in both languages but the statements to do so differ.

break and exit statements

In Python, break is used to stop the execution of the innermost loop. In Fortran, this is accomplished by the exit statement. For named loops, it is possible to speficy which loop is affected by appending its name to the exit statement. Else, the innermost loop is interrupted.

Python's exit() interrupts the execution of program or of an interactive session.

```
NumPy Fortran

for i in range(1, 9):
    if i>2:
        break
    print i loop_name: do i = 1, 8
        if (i>2) exit loop_name
        print *, i
    end do loop_name
```

continue and cycle statements

Python's continue statement is used to skip the rest of a loop body. The loop then continues at its next iteration cycle. Fortran's continue statement does not do anything and one should use cycle instead. For named loops, it is possible to speficy which loop is affected by appending its name to the cycle statement.

```
NumPy

Fortran

for i in range(1, 9):
    if i%2 == 0:
        continue
    print i

Fortran

loop_name: do i = 1, 8
    if (modulo(i, 2) == 0) cycle loop_name
    print *, i
end do loop_name
```

Examples

Mandelbrot Set

Here is a real world program written in NumPy and translated to Fortran.

Python

```
import numpy as np
ITERATIONS = 100
DENSITY = 1000
x \min, x \max = -2.68, 1.32
y \min, y \max = -1.5, 1.5
x, y = np.meshgrid(np.linspace(x min, x max, DENSITY),
                   np.linspace(y min, y max, DENSITY))
c = x + 1j*y
z = c.copy()
fractal = np.zeros(z.shape, dtype=np.uint8) + 255
for n in range(ITERATIONS):
    print "Iteration %d" % n
    mask = abs(z) \ll 10
    z[mask] *= z[mask]
    z[mask] += c[mask]
    fractal[(fractal == 255) & (-mask)] = 254. * n / ITERATIONS
print "Saving..."
np.savetxt("fractal.dat", np.log(fractal))
np.savetxt("coord.dat", [x_min, x_max, y_min, y_max])
```

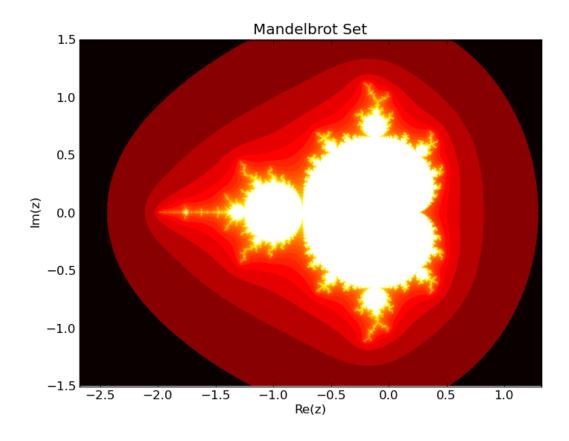
Fortran

```
program Mandelbrot
use types, only: dp
use constants, only: I
use utils, only: savetxt, linspace, meshgrid
implicit none
integer, parameter :: ITERATIONS = 100
integer, parameter :: DENSITY = 1000
real(dp) :: x_min, x_max, y_min, y_max
real(dp), dimension(DENSITY, DENSITY) :: x, y
complex(dp), dimension(DENSITY, DENSITY) :: c, z
integer, dimension(DENSITY, DENSITY) :: fractal
integer :: n
x \min = -2.68 dp
x max = 1.32 dp
y \min = -1.5 dp
y \text{ max} = 1.5 \text{ dp}
call meshgrid(linspace(x min, x max, DENSITY), &
   linspace(y min, y max, DENSITY), x, y)
c = x + I*y
z = c
fractal = 255
do n = 1, ITERATIONS
    print "('Iteration ', i0)", n
    where (abs(z) <= 10) z = z**2 + c
    where (fractal == 255 .and. abs(z) > 10) fractal = 254 * (n-1) / ITERATIONS
end do
print *, "Saving..."
call savetxt("fractal.dat", log(real(fractal, dp)))
call savetxt("coord.dat", reshape([x min, x max, y min, y max], [4, 1]))
end program
```

To run the Python version, you need Python and NumPy. To run the Fortran version, you need types.f90, constants.f90 and utils.f90 from the fortran-utils package. Both versions generate equivalent fractal.dat and coord.dat files.

The generated fractal can be viewed by (you need matplotlib):

```
from numpy import loadtxt
import matplotlib.pyplot as plt
fractal = loadtxt("fractal.dat")
x_min, x_max, y_min, y_max = loadtxt("coord.dat")
```



Timings on Acer 1830T with gfortran 4.6.1 are:

	Python	Fortran	Speedup
Calculation	12.749	00.784	16.3x
Saving	01.904	01.456	1.3x
Total	14.653	02.240	6.5x

Least Squares Fitting

In Python we use Minpack via SciPy, in Fortran we use Minpack directly. We first create a module find fit module with a function find fit:

Python

Fortran

```
from numpy import array
from scipy.optimize import leastsq

def find_fit(data_x, data_y, expr, pars):
    data_x = array(data_x)
    data_y = array(data_y)
    def fcn(x):
        return data_y - expr(data_x, x)
    x, ier = leastsq(fcn, pars)
    if (ier != 1):
        raise Exception("Failed to converge.")
    return x
```

```
module find fit module
use minpack, only: lmdif1
use types, only: dp
implicit none
private
public find fit
contains
subroutine find fit(data x, data_y, expr, pars)
real(dp), intent(in) :: data x(:), data y(:)
interface
    function expr(x, pars) result(y)
    use types, only: dp
    implicit none
    real(dp), intent(in) :: x(:), pars(:)
    real(dp) :: y(size(x))
    end function
end interface
real(dp), intent(inout) :: pars(:)
real(dp) :: tol, fvec(size(data x))
integer :: iwa(size(pars)), info, m, n
real(dp), allocatable :: wa(:)
tol = sqrt(epsilon(1. dp))
m = size(fvec)
n = size(pars)
allocate(wa(m*n + 5*n + m))
call lmdif1(fcn, m, n, pars, fvec, tol, info, iwa, wa, size(wa))
if (info /= 1) stop "failed to converge"
contains
subroutine fcn(m, n, x, fvec, iflag)
integer, intent(in) :: m, n, iflag
real(dp), intent(in) :: x(n)
real(dp), intent(out) :: fvec(m)
! Suppress compiler warning:
fvec(1) = iflag
fvec = data y - expr(data x, x)
end subroutine
end subroutine
end module
```

Then we use it to find a nonlinear fit of the form a*x*log(b + c*x) to a list of primes:

Python

Fortran

from numpy import size, log
from find_fit_module import find_fit

program example_primes
use find_fit_module, only: find_fit

```
def expression(x, pars):
    a, b, c = pars
    return a*x*log(b + c*x)

y = [2, 3, 5, 7, 11, 13, 17, 19, 23, 29, 31,
    37, 41, 43, 47, 53, 59, 61, 67, 71]
pars = [1., 1., 1.]
pars = find_fit(range(1, size(y)+1), y, expression, pars)
print pars
```

```
use types, only: dp
implicit none
real(dp) :: pars(3)
real(dp), parameter :: y(*) = [2, 3, 5, 7, 11, 13, 17, 19, 23, 29, 31, &
    37, 41, 43, 47, 53, 59, 61, 67, 71]
integer :: i
pars = [1._dp, 1._dp, 1._dp]
call find_fit([(real(i, dp), i=1,size(y))], y, expression, pars)
print *, pars
contains
function expression(x, pars) result(y)
real(dp), intent(in) :: x(:), pars(:)
real(dp) :: y(size(x))
real(dp) :: a, b, c
a = pars(1)
b = pars(2)
c = pars(3)
y = a*x*log(b + c*x)
end function
end program
```

This prints:

1.4207732655565537

1.6556111085593115

0.53462502018670921

Fortran90 1.0 documentation »

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