Chapter 3: Approximation

Interpolation

- functions in chapter 1:
  - evaluation of function values $f(x)$ and Ax
  - approximation of real numbers and arithmetic expressions
- functions in chapter 2:
  - computing zeros x^* of functions, i.e., solution of equations $Ax = b$ and $f(x) = 0$
  - using functions $F(x)$ for iterative methods $x^{(k+1)} = F(x^{(k)})$
  - approximation of zeros x^*
- chapter 3:
  - approximation of functions $u(x)$ by simpler functions, in particular polynomials

Functions in scientific computing

- functions are not only arithmetic expressions
- they may solve complicated equations and usually are not known explicitely
  - they need to be approximated
  - these approximations are then used for predictions, diagnosis and decisions
- some functions are univariate, and for example depend on time
  - average temperature, blood pressure
- other functions vary spatially
  - hyper-spectrum of pasture or forest
  - flow speeds of water in ocean
- many functions also depend on various parameters
  - flow through soil and rocks depends on density and other paramters
- some functions are random

- fundamentally, a function is a mapping $u : X \to Y$ with domain X and range Y
- here we will mostly consider $X = \mathbb{R}^d$ and $Y = \mathbb{R}$
- there are now a variety of ways on how to determine a function.
  - they may be specified by a formula like $u(x) = \exp(-2x)$.
  - they may be defined implicitely, as the solution of some partial differential equation like $\Delta u = f$
  - one may only have partial and indirect information (measurements) of a function
- some functions satisfy equations with unknown parameters which may be determined from observations

Functions in Python

- one-liners using lambda

```
u = lambda x : x*x
```

- Python procedures

```
def u(x):
  y = x*x
  return y
```

- imported from Python modules

```
from math import exp
```

Polynomial evaluation

Polynomials, their representation and evaluation

- mathematical form of polynomial

$$p_n(x) = a_0 + a_1 x + \cdots + a_n x^n$$

- simple python code

```
def pn(x,a):
  y = 0.0
  n = a.shape[0]
  for k in range(n):
    y += a[k]*x**k
  return y
```

```
# timing polynomial evaluation
def pn(x,a):
    y = 0.0
    n = a.shape[0]
    for k in range(n):
        y  += a[k]*x**k
    return y
```

```
%%timeit
from numpy.random import random, seed;
n= 200; x = random();a = random(n)
y = pn(x,a) # timing polynomial
```

```
1000 loops, best of 3: 423 µs per loop
```

Using Cython to be faster

```
%%cython
import cython
cimport cython
# timing polynomial evaluation
def pc0(x,a):
    y = 0.0
    n = a.shape[0]
    for k in range(n):
        y  += a[k]*x**k
    return y
```

```
%%timeit
from numpy.random import random, seed;
n= 200; x = random();a = random(n)
y = pc0(x,a) # timing polynomial
```

```
1000 loops, best of 3: 336 µs per loop
```

Typing

- Python uses *dynamic typing*, where the type of each object is determined at run time
- C uses *static typing*, the type of each object needs to be specified explicitely
- Cython can do both but dynamic typing may prevent code optimisation
  - for efficient code, type all objects explicitely except where one actually requires dynamically typed objects

```
%%cython
cimport numpy as np
def pnc(np.float64_t x,\
        np.ndarray[np.float64_t, ndim=1] a):
    cdef int k
    cdef int n = a.shape[0]
    cdef np.float64_t y = 0
    for k in range(n):
        y  += a[k]*x**k
    return y
```

```
%%timeit
from numpy.random import random; n= 200;\
      x = random(); a = random(n)
y = pnc(x,a) # timing polynomial
```

```
10000 loops, best of 3: 62.8 µs per loop
```

how to get faster code

- computational hardware costs substantially reduced in recent years
- code transformations used by compilers to get faster code
- faster code often by exploiting the *distributive law*

$$(a + b)c = ac + bc$$

- application to polynomial evaluation: *Horner's rule*

$$p_n(x) = a_0 + x(a_1 + x(a_2 + x(a_3 + \cdots)))$$

```
# fast polynomial evaluation with Horner's method

def pnh(x,a):
    n = a.shape[0]
    y = 0.0
    for k in range(n):
        y  = x*y + a[n-k-1]
    return y

%%timeit
from numpy.random import random, seed;
n= 200; x = random(); a = random(n)
y = pnh(x,a)

1000 loops, best of 3: 184 µs per loop
```

```
%%cython
import numpy as np
cimport numpy as np

# two versions: pnc for scalar x and png for vector xg

def pnc(np.float64_t x, np.ndarray[np.float64_t, ndim=1] a
    cdef int k
    cdef int n = a.shape[0]
    cdef np.float64_t y = 0
    for k in range(n):
        y  = x*y + a[n-k-1]
    return y
```

```
%%cython
import numpy as np
cimport numpy as np

from __main__ import pnc

def png(np.ndarray[np.float64_t, ndim=1] xg, np.ndarray[np.
    cdef int k
    cdef int ng = xg.shape[0]
    cdef int n  = a.shape[0]
    cdef np.ndarray[np.float64_t, ndim=1] yg = np.zeros(ng)
    for i in range(ng):
        for k in range(n):
            yg[i] = xg[i]*yg[i] + a[n-k-1]
    return yg
```

```
# testing
from numpy.random import random
n=200; x = random(); a = random(n)
print(pnc(x,a)-pnh(x,a))
```

```
0.0
```

```
%%timeit
from numpy.random import random;
n= 200; x = random(); a = random(n)
y = pnc(x,a) # timing polynomial
```

```
10000 loops, best of 3: 32.3 µs per loop
```

Polynomial approximation and the Taylor polynomial

Weierstrass' theorem

Every continuous function over a finite interval can be approximated arbitrarily well by a polynomial of sufficiently high degree.

- we do not know in advance how high the degree has to be
- polynomial approximation works well for very smooth functions
- no quantitative error bound
- several proofs, including one using probability theory!

Taylor remainder theorem *If $u(x)$ is $n+1$ times continuously differentiable in $[a,b]$ then for all $x \in [a,b]$ there exists a $\xi \in [a,b]$ such that*

$$u(x) = u(a) + u'(a)(x-a) + \frac{u''(a)}{2}(x-a)^2 + \cdots + \frac{u^{(n)}(a)}{n!}(x-a)^n + \frac{u^{(n+1)}(\xi)}{(n+1)!}(x-a)^{n+1}$$

- if $|u^{(n+1)}(x)| \leq C$ for all $x \in [a, b]$ then error of Taylor polynomial is bounded by

$$C\frac{(b-a)^{n+1}}{(n+1)!}$$

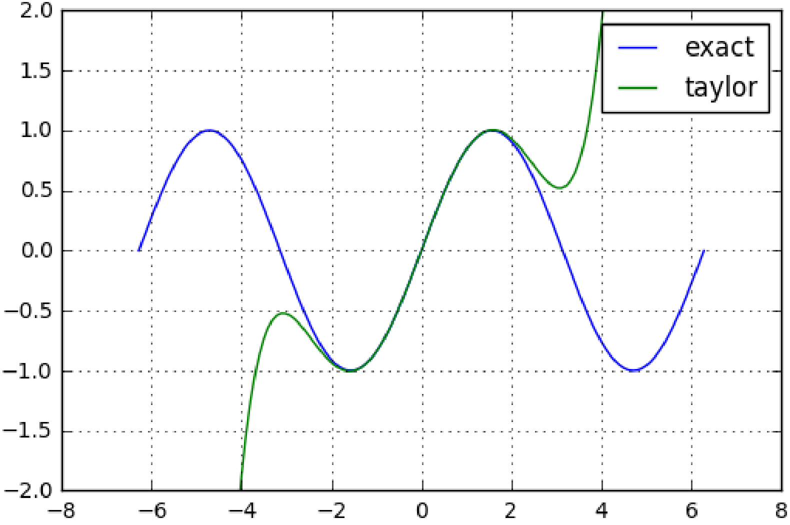
```
# Taylor series  y = sin(x) around x=0

from math import pi
n = 6
# compute taylor coefficients
taycoeff        = np.ones(n)
taycoeff[::2]   =  0
taycoeff[3::4] *= -1
taycoeff[1:]   /= np.cumprod(np.arange(1,n))
uex  = np.sin
ut = lambda x, a=taycoeff, p = png: p(x, a) # taylor appro

xg = np.linspace(-2*pi,2*pi,128)
yg = np.sin(xg)
print('time for evaluation:')
%timeit -r 1 ygt = ut(xg)
ygt = ut(xg)
```

```
time for evaluation:
The slowest run took 12.68 times longer than the fastest. T
```

```
plt.grid('on'); plt.axis(ymin = -2, ymax = 2)
plt.plot(xg,yg, label="exact"); plt.plot(xg, ygt, label="ta
```



Polynomial Interpolation

Collocation

Proposition
There is exactly one polynomial p_n of degree n which satisfies the interpolation conditions

$$p_n(x_k) = y_k, \quad k = 0, \ldots, n$$

if all x_k are distinct
Proof by construction, will give 3 different approaches below which choose three different sets of basis functions for the linear space of polynomials of degree n

Approach 1: power basis x^k

- if $p_n(x) = a_0 + a_1 x + \cdots + a_n x^n$, then the interpolation conditions lead to a linear system of equations for the a_k:

$$\begin{bmatrix} 1 & x_0 & x_0^2 & \cdots & x_0^n \\ 1 & x_1 & x_1^2 & \cdots & x_1^n \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^n \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} y_0 \\ y_1 \\ \vdots \\ y_n \end{bmatrix}$$

- the matrix X of this system is a *Vandermonde matrix*
- **Proposition:** if no two x_k are the same then X is invertible

Example: linear interpolation

Example

- $p_2(x) = a_0 + a_1 x + a_2 x^2$
- collocation points

i	0	1	2
x_i	0	0.5	2
y_i	0.2	0.6	-1.0

- system of equations for a_k:

$$\begin{bmatrix} 1 & 0 & 0 \\ 1 & 0.5 & 0.25 \\ 1 & 2 & 4 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} 0.2 \\ 0.6 \\ -1 \end{bmatrix}$$

- solution $a_0 = 1/5$, $a_1 = 19/15$ and $a_2 = -14/15$
- interpolating polynomial

$$p_2(x) = 1/5 + 19/15x + -14/15x^2$$

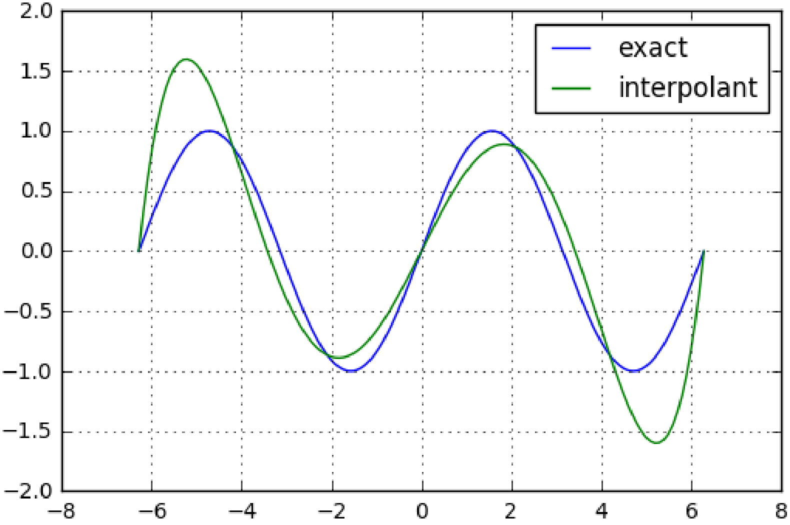
```python
# polynomial interpolant

n    = 6
xpts = np.linspace(-2*pi,2*pi,n+1)
ypts = uex(xpts)
# Collocation matrix
A = []
for i in range(n+1):
    A.append(xpts**i)
A = np.array(A).T
```

```
# solve problem
print('time for computing polynomial coefficients:')
%timeit -r 1 coeffs = nla.solve(A,ypts)
coeffs = nla.solve(A,ypts)
# interpolant: ui
ui = lambda x, a=coeffs, p = png, n=n : p(x, a, n)
xg = np.linspace(-2*pi,2*pi,128); yg = np.sin(xg);
print('time for evaluation:')
%timeit -r 1 ygi = ui(xg)
ygi = ui(xg)
```

```
time for computing polynomial coefficients:
The slowest run took 158.51 times longer than the fastest.
10000 loops, best of 1: 66.3 µs per loop
time for evaluation:
10000 loops, best of 1: 29.3 µs per loop
```

```
plt.grid('on'); plt.axis(ymin = -2, ymax = 2)
plt.plot(xg,yg, label="exact"); plt.plot(xg, ygi, label="in
plt.legend();
```



Approach 2: cardinal basis l_j

- basis functions
$$l_j(x) = \prod_{k \neq j} \frac{x - x_k}{x_j - x_k}$$
- this forms a basis of the linear space of polynomials of degree n if the x_k are all distinct
- collocation matrix is identity
- basis functions satisfy
$$l_j(x_k) = \delta_{j,k}$$
where $\delta_{j,k}$ is Kronecker delta
  - thus they are the solution of a special interpolation problem
- interpolation polynomial
$$p_n(x) = \sum_{j=0}^{n} y_j l_j(x)$$
- no need to solve any equations!
- also called the *Lagrange form* of the interpolation polynomial

Derivation of the Lagrangian (or cardinal) functions $l_j(x)$

- aim: compute $l_j(x)$, a polynomial of degree n which satisfies $l_j(x_k) = \delta_{j,k}$
- property: $l_j(x)$ is zero for all $x = x_k$ *except* $x = x_j$
- consequence:

$$l_j(x) = c_j \prod_{k \neq j} (x - x_k)$$

  where the product is to be taken over all $k = 0, \ldots, n$ *excluding* $k = j$
- property:

$$l_j(x_j) = c_j \prod_{k \neq j} (x_j - x_k) = 1$$

- consequence:

$$c_j = \left(\prod_{k \neq j} (x_j - x_k) \right)^{-1}$$

Example: linear interpolation

Example – cardinal functions

- for the data points

i	0	1	2
x_i	0	0.5	2
y_i	0.2	0.6	-1.0

the cardinal functions are

$$l_0(x) = \frac{(x-0.5)(x-2)}{(0-0.5)(0-2)} = (x-0.5)(x-2),$$

$$l_1(x) = \frac{(x-0)(x-2)}{(0.5-0)(0.5-2)} = -\frac{4}{3}x(x-2),$$

$$l_2(x) = \frac{(x-0)(x-0.5)}{(2-0)(2-0.5)} = \frac{1}{3}x(x-0.5).$$

Example – Lagrangian interpolant

$$p_2(x) = 0.2 * l_0(x) + 0.6 * l_1(x) - l_2(x)$$

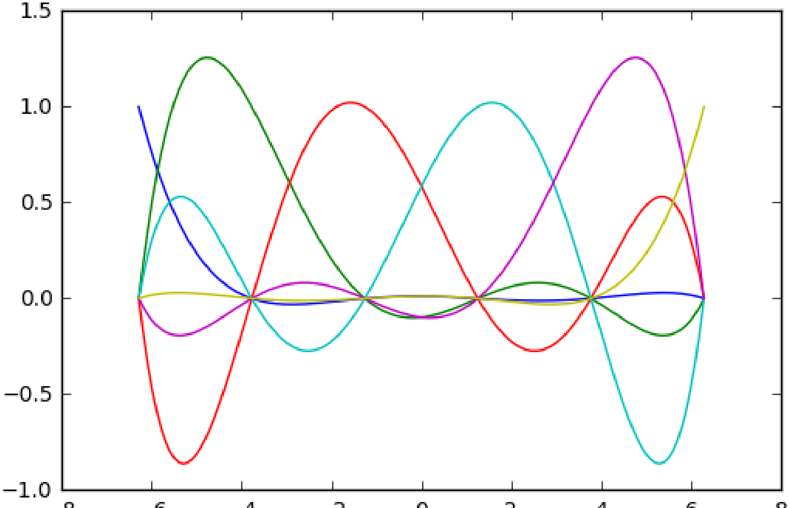
- verification:
  1. $p_2(x)$ has degree at most 2
  2. satisfies interpolation conditions

$$\begin{aligned} p_n(x_j) = & \quad y_0 l_0(x_j) + \cdots + y_j l_j(x_j) + \cdots + y_n l_n(x_j) \\ = & \quad y_0 \cdot 0 + \cdots + y_j \cdot 1 + \cdots + y_n \cdot 0 \\ = & \quad y_j \end{aligned}$$

- uniqueness of this interpolant:
  - suppose $p(x)$ and $q(x)$ both satisfy collocation equations
  - then $r(x) = p(x) - q(x)$ is a polynomial of degree at most n
  - and $r(x)$ has $n+1$ roots $x_0 \dots x_n$
  - thus $r(x)$ must be identically zero, and so $p = q$

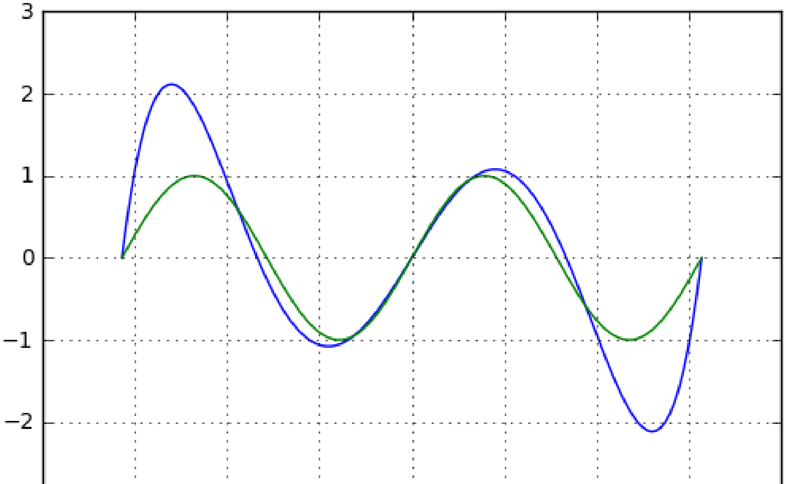
```
%%cython
import numpy as np
cimport numpy as np
def eval_lj(np.ndarray[np.float64_t,ndim=1] xpts, \
            np.ndarray[np.float64_t,ndim=1] xg):
    cdef int ng = xg.shape[0]
    cdef int npts = xpts.shape[0]
    cdef np.ndarray[np.float64_t,ndim=2] \
                    lj = np.ones((ng,npts))
    cdef int i
    cdef int j
    cdef int k
    for i in range(npts):
        for j in range(npts):
            if (i != j):
                for k in range(ng):
                    lj[k,i] *= (xg[k]-xpts[j])\
                              /(xpts[i]-xpts[j])
    return lj
```

```
# Lagrangian or cardinal polynomials lj(x)
npts = 6; xpts = np.linspace(-2*pi,2*pi,npts)
ypts = uex(xpts); ng = 128; xg = np.linspace(-2*pi,2*pi,ng)
ljg = eval_lj(xpts,xg);
for j in range(npts): plt.plot(xg,ljg[:,j])
```



```
print('time for polynomial evaluation:')
%timeit -r 1 yg = np.dot(eval_lj(xpts,xg),ypts.T)
plt.plot(xg, np.dot(eval_lj(xpts,xg),ypts.T),xg,uex(xg)); p
```

```
time for polynomial evaluation:
10000 loops, best of 1: 150 µs per loop
```



Approach 3: Newton's basis $n_j(x)$

- basis functions $n_0(x) = 1$ and
$$n_{j+1}(x) = \prod_{k=0}^{j} (x - x_k)$$
  - collocation matrix is triangular
- interpolant for points $(x_0, y_0), \ldots, (x_k, y_k)$:
$$p_k(x) = \sum_{j=0}^{k} c_j n_j(x)$$
NB: the c_j are independent of k!
- first polynomial $p_0(x) = y_0$
- recursion
$$p_{k+1}(x) = p_k(x) + c_{k+1} n_{k+1}(x)$$
  - substituting $x = x_{k+1}$ to get
$$c_{k+1} = \frac{y_{k+1} - p_k(x_{k+1})}{n_{k+1}(x_{k+1})}$$

Example: linear interpolant

Example Polynomial Interpolation

- same interpolation points

i	0	1	2
x_i	0	0.5	2
y_i	0.2	0.6	-1.0

- Newton's functions are

$$n_0(x) = 1,$$
$$n_1(x) = x,$$
$$n_2(x) = x(x - 0.5)$$

- and so

$$p_0(x) = 0.2,$$
$$p_1(x) = 0.2 + 0.8x,$$
$$p_2(x) = 0.2 + 0.8x - \frac{14}{15}x(x - 0.5)$$

Evaluation of Newton polynomial with Horner-like method

```
def pnh(x,a,xk,n):
    y = a[-1]
    for k in range(n-2,-1,-1):
        y  = (x-xk[k])*y + a[k]
    return y
```

```
%%timeit
from numpy.random import random; n= 200; x = random(); \
               a = random(n); xk = np.linspace(0,1,n)
y = pnh(x,a,xk, n) # timing polynomial
```

```
1000 loops, best of 3: 327 µs per loop
```

```
%%cython
# fast Newton polynomial evaluation with Horner's method
cimport numpy as np
import numpy as np

def pnhc(np.float64_t x,
         np.ndarray[np.float64_t, ndim=1] a,
         np.ndarray[np.float64_t, ndim=1] xk):

    cdef np.float64_t y = 0.0
    n = a.shape[0]
    for k in range(n-1,-1,-1):
        y  = (x-xk[k])*y + a[k]
    return y
```

```
%%cython
# fast Newton polynomial evaluation with Horner's method
cimport numpy as np
import numpy as np
def pnhg(np.ndarray[np.float64_t, ndim=1] xg, \
         np.ndarray[np.float64_t,ndim=1] a,
         np.ndarray[np.float64_t,ndim=1] xk):
    cdef int k
    cdef int ng = xg.shape[0]
    cdef int n  = a.shape[0]
    cdef np.ndarray[np.float64_t, ndim=1] \
                   yg = np.zeros(ng)
    for i in range(ng):
        for k in range(n-1,-1,-1):
            yg[i] = (xg[i]-xk[k])*yg[i] + a[k]
    return yg
```

```
%%timeit
from numpy.random import random; n= 200; x = random(); \
      a = random(n); xk = np.linspace(0,1,n)
y = pnhc(x,a,xk) # timing polynomial

1000 loops, best of 3: 398 µs per loop
```

```
%%cython
import numpy as np
cimport numpy as np

# compute the values of the Newton functions on some grid

def eval_nj(np.ndarray[np.float64_t,ndim=1] xpts, \
            np.ndarray[np.float64_t,ndim=1] xg):

    cdef int i, j, k
    cdef int ng = xg.shape[0]
    cdef int npts = xpts.shape[0]
    cdef np.ndarray[np.float64_t,ndim=2] \
                     nj = np.ones((ng,npts))
    for i in range(npts):
        for j in range(0,i):
            for k in range(ng):
                nj[k,i] *= (xg[k]-xpts[j])
    return nj
```

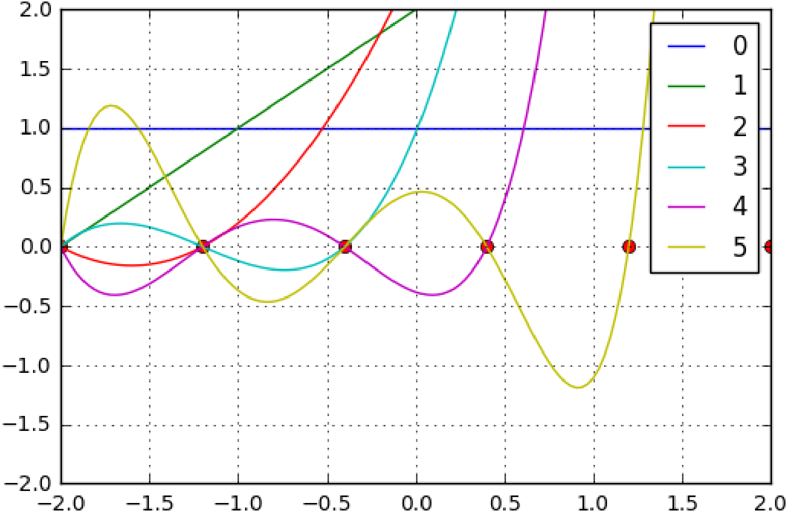
```python
# Newton polynomials lj(x)

s = 2
h = s

npts = 6
xpts = np.linspace(-s,s,npts)
ypts = uex(xpts)
ng = 129
xg = np.linspace(-s,s,ng)

njg = eval_nj(xpts,xg)
```

```python
plt.plot(xpts,np.zeros(npts),'ro')
for j in range(npts): plt.plot(xg,njg[:,j],label=j)
plt.legend();plt.grid('on');plt.axis(ymin=-h,ymax=h);
```



```
%%cython
import numpy as np
cimport numpy as np
from __main__ import pnhc

def ncoeffs(np.ndarray[np.float64_t,ndim=1] xpts, \
            np.ndarray[np.float64_t,ndim=1] ypts):
    cdef int n = xpts.shape[0]
    cdef np.ndarray[np.float64_t, ndim=1] c = np.zeros(n)
    cdef int k
    c[0] = ypts[0]
    for k in range(n):
        c[k] = (ypts[k] - pnhc(xpts[k],c[:k],xpts[:k]))  \
                         / np.prod(xpts[k]-xpts[:k])
    return c
```

```
%%timeit
from numpy.random import random; n= 200; \
    xpts = np.linspace(0,1,n); ypts = random(n)
c = ncoeffs(xpts, ypts)
```

```
10 loops, best of 3: 32.9 ms per loop
```

```
%%cython
import numpy as np
cimport numpy as np
def ncoeffs2(np.ndarray[np.float64_t,ndim=1] xpts, \
              np.ndarray[np.float64_t,ndim=1] ypts):
    cdef int k, i
    cdef np.float64_t qk, yi
    cdef int n = xpts.shape[0]
    cdef np.ndarray[np.float64_t,ndim=1] c = np.zeros(n)
    c[0] = ypts[0]
    for k in range(n):
        qk = 1.0
        for i in range(k):
            qk *= (xpts[k]-xpts[i])
        yi = 0.0
        for i in range(k-1,-1,-1):
            yi  = (xpts[k]-xpts[i])*yi + c[i]
        c[k] = (ypts[k] - yi)/qk
    return c
```

```
%%timeit
from numpy.random import random; n= 200; \
    xpts = np.linspace(0,1,n); ypts = random(n)
c = ncoeffs2(xpts, ypts)
```

```
The slowest run took 346.33 times longer than the fastest.
1000 loops, best of 3: 246 µs per loop
```

```
# computing the interpolant with Newton
# first we compute the coefficients
npts = 6
xpts = np.linspace(-2*pi,2*pi,npts)
ypts = uex(xpts)

ng = 127
xg = np.linspace(-2*pi,2*pi,ng)
yg = uex(xg)
#plt.plot(xg,yg)

%timeit c = ncoeffs2(xpts,ypts)
c = ncoeffs2(xpts,ypts)
%timeit yig = pnhg(xg, c, xpts)
yig = pnhg(xg, c, xpts)
# plt.plot(xg, yig);

100000 loops, best of 3: 12 µs per loop
```

Another example

- another illustration of how the same polynomial is represented in three different forms
- Consider the polynomial $p_3(x) = 4x^3 + 35x^2 - 84x - 954$
- Show that the four points with coordinates $(5, 1)$, $(-7, -23)$, $(-6, -54)$ and $(0, -954)$ are on the graph of p_3

Example - Newton's Form

- the Newton functions are then $n_0(x) = 1, \quad n_1(x) = x - 5, \quad n_2(x) = (x-5)(x+7), \quad n_3(x) = (x-5)(x+7)(x+6)$
- An application of Newton's interpolation method gives then

$$p_3(x) = n_0(x) + 2n_1(x) + 3n_2(x) + 4n_3(x)$$