Phys 512 Lecture 2+3 Polynomial Interpolation/ Integration

Admin

- Tutorials/debugs Fridays 9-11 AM
- Lecturer office hours Thursdays 2:30 PM ERP 333
- Problem sets due 11:59 PM on Mondays
- Github TA's setting up an organization please send invitations to follow your repos to the organization.
- Slack: https://phys512fall2024.slack.com/join/shared_invite/
 zt-2pzfaz8g1-z6mRfRqicfYfqYz7pbOCKg#/shared-invite/email

Note - info now on the syllabus

Interpolation

- Let's say we have a function y_i tabulated at some values x_i
 but we want to know it at arbitrary x.
- If the new values are between current values, we call this interpolation. If outside, extrapolation. Extrapolation decidedly dodgier.
- How should we do this?

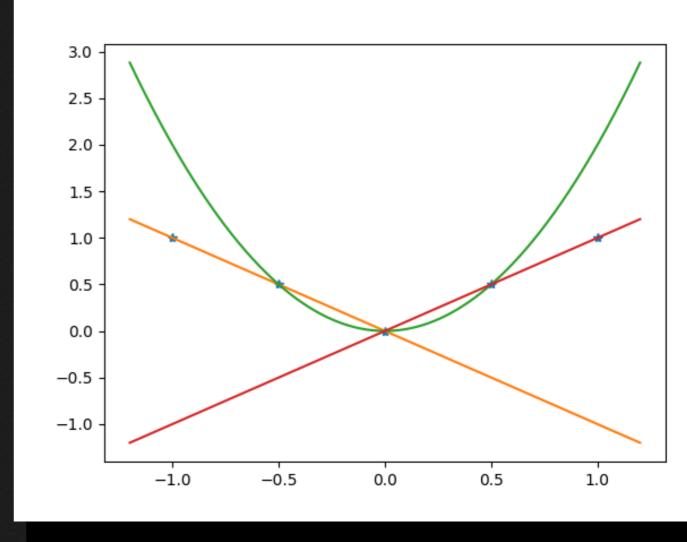
Simple Solutions

- Dumbest thing we can do is find the x_i nearest our target x, and take y_i. This is nearest neighbor. Is this going to be accurate? Is it ever going to go crazy?
- Next dumbest thing is find the interval x_i , x_{i+1} that x sits in. Then draw a line between (x_i, y_i) and (x_{i+1}, y_{i+1}) and evaluate it at x. This is linear interpolation. Will this be accurate? Is it every going to go crazy?
- NB by "crazy" we usually mean that the interpolated y is far from the spread covered by y_i and its neighbors.
- For linear, y will be between y_i and y_{i+1} , so it can't go crazy.

Higher Order

- If we want more accuracy AND our function is "smooth", we can win by Taylor expanding.
- Next order is quadratic. We could take y_{i-1},y_i,y_{i+1} and draw a parabola.
- This is almost certainly a bad idea! Why?

```
import numpy as np
from matplotlib import pyplot as plt
x=np.linspace(-1,1,5)
y=np.sqrt(np.abs(x))
y=np.abs(x)
xx = np.linspace(-1.2, 1.2, 1000)
plt.clf()
plt.plot(x,y,'*')
for i in range(len(x)-2):
    pp=np.polyfit(x[i:i+3],y[i:i+3],2)
    yy=np.polyval(pp,xx)
    plt.plot(xx,yy)
plt.savefig('parabolas.png')
```

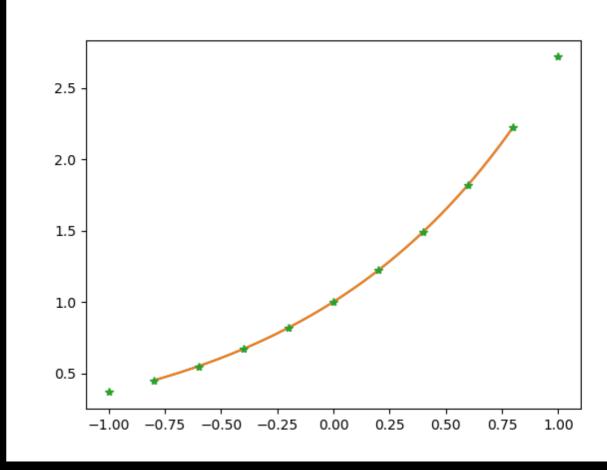


How would I decide on x_i ? Natural thing is to take nearest neighbor.

However, that changes halfway between points. I then move to a different parabola. In general, interpolation will be discontinuous. This is (almost certainly) bad!

NB - no guarantee anymore that y is bracketed by function values.

```
fun=np.exp
xmin=-1
xmax=1
x=np.linspace(xmin,xmax,11)
dx=np.median(np.diff(x))
y=fun(x)
xx=np.linspace(x[1],x[-2]-1e-13,1001) #skip the first/last region
                                #since we aren't double-bracketed
yy_true=fun(xx)
yy=0*yy_true
for i,myx in enumerate(xx):
    j=np.int((myx-xmin)/dx)
    pp=np.polyfit(x[j-1:j+3],y[j-1:j+3],3)
    yy[i]=np.polyval(pp,myx)
plt.clf();
plt.plot(xx,yy_true);
plt.plot(xx,yy);
plt.savefig('cubic_interp.png')
print('mean error is ' + repr(np.mean(np.abs(yy-yy_true))))
```



- Cubic polynomials don't suffer from discontinuity since interval is well defined.
- Mean error has done pretty well! ~1e-5
- However we are doing a polynomial fit for every point.
 This can be quite slow.

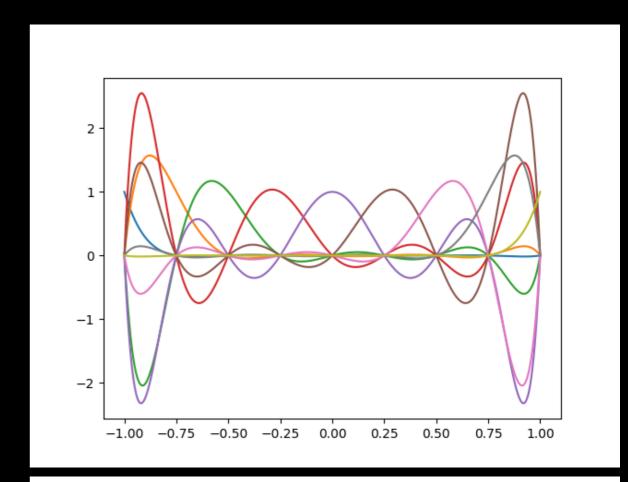
Simple Polynomial Construction

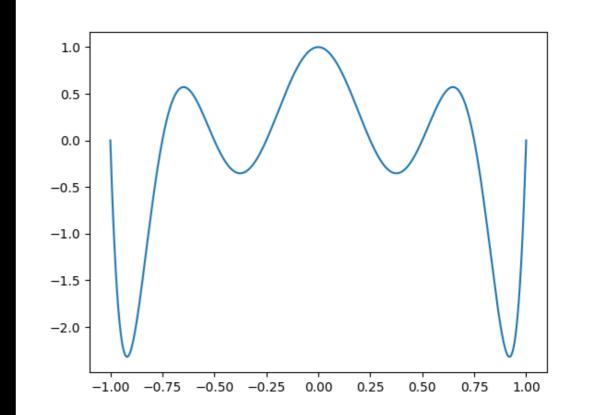
- How can I construct a polynomial that goes through n points?
- Well, I can construct a polynomial that is zero at n-1 points, say x_1 through x_{n-1} . NB n-1 is because we zero index.
- $(x-x_1)(x-x_2)(x-x_3)..(x-x_{n-1})$ by construction is zero.
- What is it at x_0 ? well, $(x_0-x_1)(x_0-x_2)...(x_0-x_{n-1})$.
- If I take the ratio, I have a polynomial P_0 that is 1 at x_0 and zero at all other x_i .
- I can now take $\sum P_i y_i$ to have a polynomial that goes exactly through all y_i .

What Those Look Like

```
ord=8
x=np.linspace(-1,1,ord+1)
xx=np.linspace(x[0],x[-1],1001)
plt.clf()
for i in range(len(x)):
    x_use=np.append(x[:i],x[i+1:])
    x0=x[i]
    mynorm=np.prod(x0-x_use)
    p0=1.0
    for xi in x_use:
        p0=p0*(xi-xx)
    p0=p0/mynorm
    plt.plot(xx,p0)
    if i==4:
        bad_p0=p0.copy()
plt.savefig('delta_polys_out.png')
plt.clf()
plt.plot(xx,bad_p0)
plt.savefig('delta_polys_one.png')
```

- This should make you nervous. At high order, polys could jiggle quite a bit between points. OK iff your function is smooth, in the sense that $(ord^*dx)^n f^{(n)}/n!$ is converging.
- What happens if your values have errors/noise?





Poly Interpolation ctd.

- Cubic interpolation from earlier look OK. At least was continuous.
- I didn't need to do the polynomial fit for each interpolated value. Rather, I could fit every interval and store coefficients.
- Then, when interpolating, look up the segment, take the relevant coefficients, and evaluate.
- Note that nowhere have we assumed the x_i are equally spaced. The lookup is faster when they are, but still only $\log_2(n)$ when they aren't.

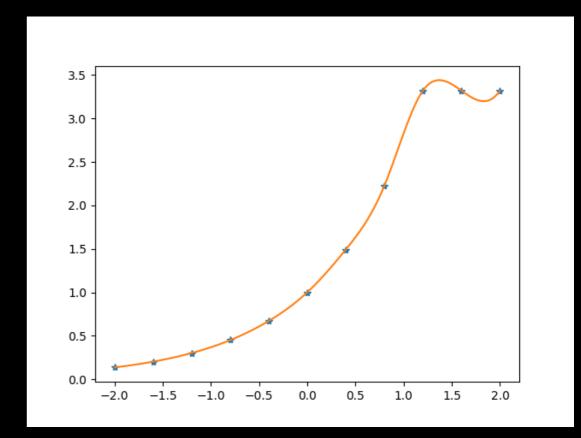
Cubic Splines

- My old cubic interpolation was continuous. Were its derivatives?
- An important class of interpolation forces the function and the first *n* derivatives to be continuous. These are called splines.
- By far most common is requirement that second derivate is continuous (so first deriv is guaranteed smooth). Specifying function values and derivatives at edges is 2+2=4 values, so we will need a cubic to fit them.
- Cubic splines are so common, we usually drop the cubic, just call them splines.
- My 2nd deriv has to match left and right neighbors. But what about at ends? You need to specify. Most common is set f" to zero on edges, but can also set f to specific values, or require periodic boundary conditions (right edge has to match left).

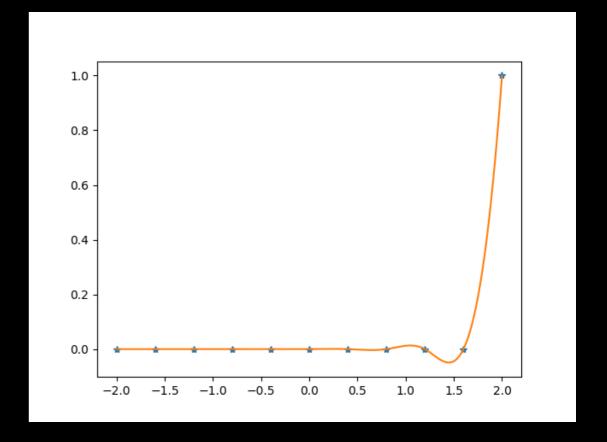
```
import numpy as np
from matplotlib import pyplot as plt
from scipy.interpolate import CubicSpline
from scipy import interpolate
plt.ion()
x=np.linspace(-2,2,11)
y=np.exp(x)
xx=np.linspace(x[0],x[-1],2001)
spln=CubicSpline(x,y)
yy = spln(xx)
plt.clf();
plt.plot(x,y,'*')
plt.plot(xx,yy)
                                                                       1.0
```

- Spline in use. Lives in scipy.interpolate
- First, set up the spline fit with splrep.
- Then evaluate with splev.
- Broader range of options in BSpline class (also in scipy.interpolate).

```
x=np.linspace(-2,2,11)
y=np.exp(x)
y[-2:]=y[-3]
xx=np.linspace(x[0],x[-1],2001)
spln=CubicSpline(x,y)
yy=spln(xx)
```



- Be aware splines can ring near jumps/kinks. This might be OK, this might not be. But you should not be caught by surprise.
- Another option is cubic Hermite polynomials similar to spline, but y(x∈(x1,x2))∈(y1,y2) (scipy.interpolate.PchipInterpolator)



Rational Functions

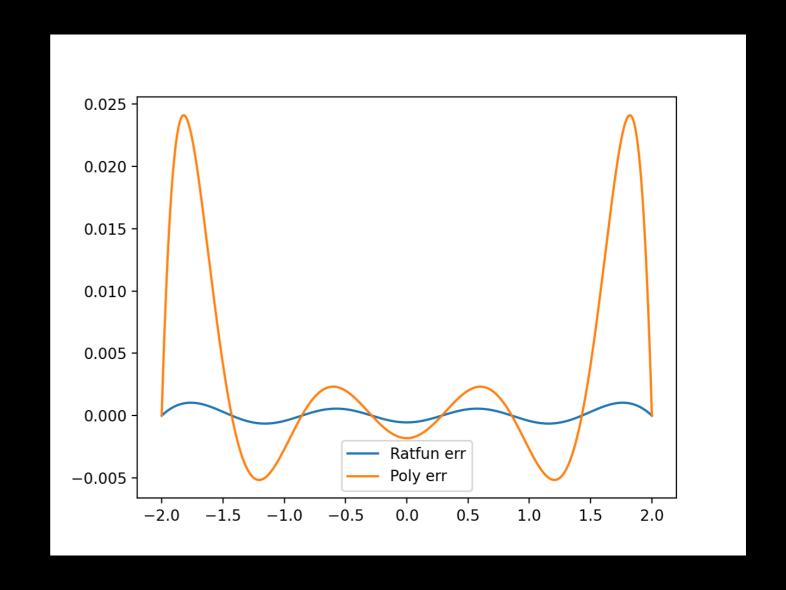
- Another useful class is rational functions, ratios of two polynomials.
- Can be especially useful when your function has poles.
- Nominally non-linear: p(x)/q(x)=y(x). Without loss, set $q(x)=1+ax+bx^2+...=1+qq(x)$
- For simple case of number of degrees matches number of points can get around: p(x)=q(x)y(x) = y(x)+qq(x)y(x)
- Matrix: [1 x x² x³... -yx -yx² -yx³...][p;q]=y

```
def rat_eval(p,q,x):
    top=0
    for i in range(len(p)):
        top=top+p[i]*x**i
    bot=1
    for i in range(len(q)):
        bot=bot+q[i]*x**(i+1)
    return top/bot
def rat_fit(x,y,n,m):
    assert(len(x)==n+m-1)
    assert(len(y)==len(x))
    mat=np.zeros([n+m-1,n+m-1])
    for i in range(n):
        mat[:,i]=x**i
    for i in range(1,m):
        mat[:,i-1+n]=-y*x**i
    pars=np.dot(np.linalg.inv(mat),y)
    p=pars[:n]
    q=pars[n:]
    return p,q
```

```
n=4
m=5
x=np.linspace(-2,2,n+m-1)
y=np.exp(-0.5*x**2)
p,q=rat_fit(x,y,n,m)
pred=rat_eval(p,q,x)

xx=np.linspace(-2,2,1001)
yy=np.exp(-0.5*xx**2)
yy_interp=rat_eval(p,q,xx)
plt.ion()
plt.clf()
plt.plot(xx,yy_interp-yy)
```

```
#we can use numpy's polynomial fitter to see how that does
pp=np.polyfit(x,y,n+m) #use same number of terms
yy_poly=np.polyval(pp,xx)
plt.plot(xx,yy_poly-yy)
plt.savefig('ratfit_vs_poly.png')
```



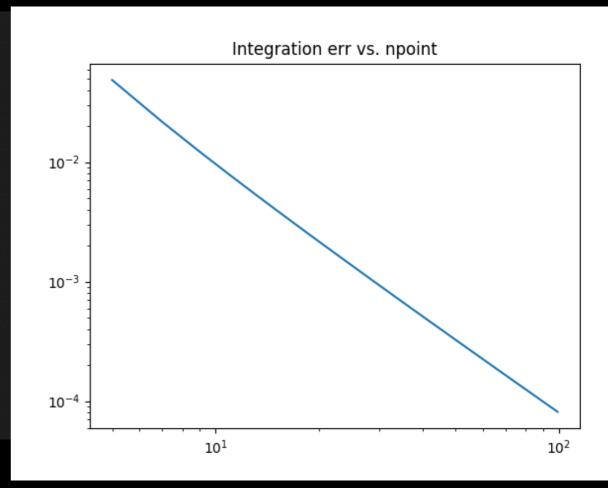
Integration

- Interpolation & numerical integration are closely coupled
- Interpolation schemes are often easy to integrate analytically.
- Usually end up as a set of coefficients times function values, where coefficients are set by scheme.
- Can think of this as finding the "average" value in a region, based on some interpolation scheme.

Integration with Linear

- Break function into series of regions, draw a line between points.
- What is the average value of y if it is based on a line between y_i and y_{i+1} ? just $0.5(y_{i+1}y_{i+1})$.
- If points are dx apart, then area/dx=0.5(y_0+y_1)+0.5(y_1+y_2)... +0.5($y_{n-2}+y_{n-1}$)=0.5(y_0+y_{n-1})+ $\sum y_i$, i=1..n-2.
- How should error scale with # of points?

```
x0=-1
x1=1
nn=np.arange(5,101,2)
errs=np.zeros(nn.size)
for i,npt in enumerate(nn):
    x=np.linspace(x0,x1,npt)
    y=np.exp(x)
    dx=np.median(np.diff(x))
    myint=0.5*(y[0]+y[-1])+np.sum(y[1:-1])
    myint=myint*dx
    targ=np.exp(x1)-np.exp(x0)
    errs[i]=np.abs(myint-targ)
plt.loglog(nn,errs)
plt.title('Integration err vs. npoint')
plt.savefig('linear_integral_errs.png')
pp=np.polyfit(np.log10(nn),np.log10(errs),1)
print('error is scaling as step size to the power ' + repr(pp[0]))
```



Scaling is going as step size squared, as expected.

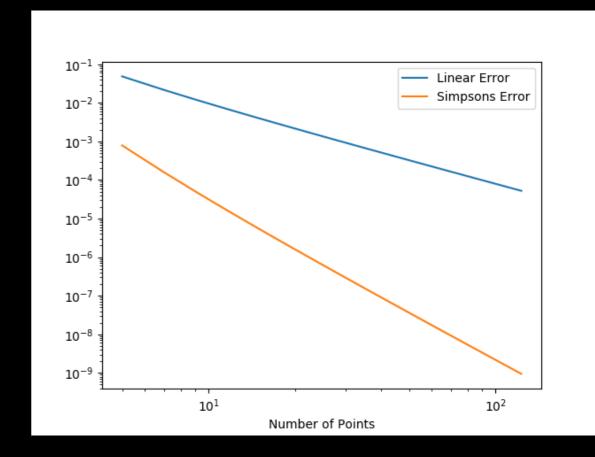
But Wait!

- If error is going like dx^2 , can I use that for fun and profit?
- $f(dx)=f_{true}+adx^2+...$ $f(2dx)=f_{true}+a(2dx)^2+...$
- $4f(dx)-f(2dx)=4f_{true}-f_{true}+...=3f_{true}+...$ or $f_{true}=(4f(dx)-f(2dx))/3$
- 3 points:f(dx)=(y₀+2y₁+y₂)dx/2. f(2dx)=(y₀+y₂)dx (NB dx went to 2 dx, cancelling usual factor of 2)
- $4f(dx)-f(2dx)=(2y_0+4y_1+2y_2-y_0-y_2)dx/3=(y_0+4y_1+y_2)dx/3$
- We have cancelled 2nd order error term. Should be more accurate.

Equivalent

- We could also fit a parabola to 3 points. For simplicity take x=-1,0,1. There's a trapezoid going through y₀ and y₂, with a parabola that goes through y₁ minus (y₀+y₂)/2.
- Parabola is $(y_1-(y_0+y_2)/2)(1-x^2)$. Integral is $(x-x^3/3)$, evaluates to 4/3 over 2dx, so average is 2/3. Leaves $(y_0+y_2)/2*(2dx)+2/3(y_1-(y_0+y_2)/2)(2dx=dx(y_0+4y_1+y_2)/3$.
- This is exactly what we had before! Cancelling 2nd order error term is identical to fitting quadratic & integrating.
- This second-order scheme is called Simpson's rule.
- How should error scale? Hint what is the average value of x³?

```
nn=np.arange(5,125,2)
x0 = -1
x1=1
ints_lin=np.zeros(len(nn))
ints_quad=np.zeros(len(nn))
for i,npt in enumerate(nn):
    x=np.linspace(x0,x1,npt)
    y=np.exp(x)
    dx=np.median(np.diff(x))
    ints_lin[i]=dx*(0.5*y[0]+0.5*y[-1]+np.sum(y[1:-1]))
    ints_quad[i]=dx/3.0*(y[0]+y[-1]+4*np.sum(y[1::2])+2*np.sum(y[2:-1:2]))
targ=np.exp(x1)-np.exp(x0)
plt.clf();
errs lin=np.abs(ints lin-targ)
errs_quad=np.abs(ints_quad-targ)
pp=np.polyfit(np.log(nn),np.log(errs_quad),1)
print('Simpsons scaling is ' + repr(pp[0]))
plt.loglog(nn,errs_lin)
plt.loglog(nn,errs_quad)
plt.xlabel('Number of Points')
plt.legend(['Linear Error', 'Simpsons Error'])
plt.savefig('simpson_errs.png')
```

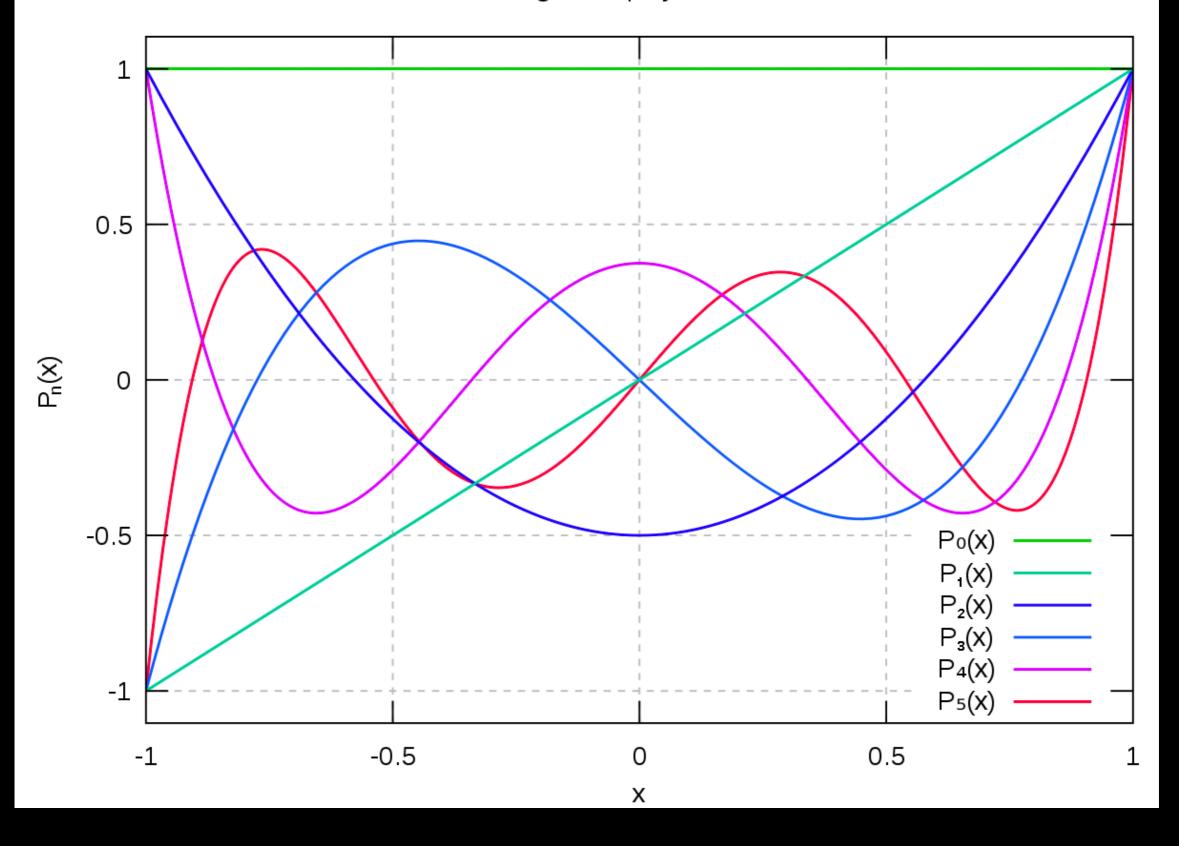


- Simpsons is far more accurate than trapezoid.
- Error goes like dx⁴, since x³ term integrates to zero.
- I didn't have to make any more function calls, just used the ones I had more cleverly.
- NB would this work with an even number of y_i?

Can We Turn it up to 11?

- Yes! Regular polynomials (x,x²,x³...) are not what we want, though.
- Legendre polynomials are an important class. They arise in separation of variables in spherical coordinates.
- We could think of regular polynomials as defined by a recurrence relation. $F_{n+1}=xF_n$.
- Legendre polynomials best generated with a different recurrence relation. $(n+1)P_{n+1}=(2n+1)xP_n-nP_{n-1}$. $P_0=1$, $P_1=x$.

legendre polynomials



Legendre ctd.

- They have the important property that they are orthogonal on the interval (-1,1). $\int P_n P_m \propto \delta_{nm}$
- Given this, what is ∫Pndx from -1 to 1?
- 2 for P₀, and zero for everything else.
- I can fit Legendre polynomials to a set of data, and integral will just be P₀ coefficient(!).
- How do I get this?

Legendre Fitting

- $y_i = \sum c_j P_j(x_i)$. If I can figure out the c_j then I'm in business.
- But this is just a matrix equation! y=Pc. If we have as many polynomials as we have points, then the matrix P is square, and we can just get c=P⁻¹y. Pull c₀, and then we're done.
- But, c_0 is just $\sum P^{-1}_{0,k}y_k$, so I can just take the first column of P^{-1} . This gives me my weights.
- Now I can integrate to whatever order I want (making sure I have a suitable number of y_i for my chosen order).

Code to Make Coeffs

```
def legendre_mat(npt):
    #Make a square legendre polynomial matrix of desired dimension
    x=np.linspace(-1,1,npt)
    mat=np.zeros([npt,npt])
   mat[:,0]=1.0
   mat[:,1]=x
    if npt>2:
        for i in range(1,npt-1):
            mat[:,i+1]=((2.0*i+1)*x*mat[:,i]-i*mat[:,i-1])/(i+1.0)
    return mat
def integration_coeffs_legendre(npt):
    #Find integration coefficients using
    #square legendre polynomial matrix
    mat=legendre_mat(npt)
    mat_inv=np.linalg.inv(mat)
    coeffs=mat_inv[0,:]
    coeffs=coeffs/coeffs.sum()*(npt-1.0)
    return coeffs
```

Code to Integrate Stuff

```
def integrate(fun,xmin,xmax,dx_targ,ord=2,verbose=False):
   coeffs=legendre.integration_coeffs_legendre(ord+1)
    if verbose: #should be zero
        print("fractional difference between first/last coefficients is "+repr(coeffs[0]/coeffs[-1]-1))
    npt=np.int((xmax-xmin)/dx_targ)+1
   nn=(npt-1)%(ord)
   if nn>0:
        npt=npt+(ord-nn)
    assert(npt%(ord)==1)
    x=np.linspace(xmin,xmax,npt)
    dx=np.median(np.diff(x))
    dat=fun(x)
    #we could have a loop here, but note that we can also reshape our data, then som along columns, and only then
    #apply coefficients. Some care is required with the first and last points because they only show up once.
   mat=np.reshape(dat[:-1],[(npt-1)/(ord),ord]).copy()
   mat[0,0]=mat[0,0]+dat[-1] #as a hack, we can add the last point to the first
   mat[1:,0]=2*mat[1:,0] #double everythin in the first column, since each element appears as the last element in the previous row
    vec=np.sum(mat,axis=0)
    tot=np.sum(vec*coeffs[:-1])*dx
    return tot
```

Code to Call it +Output

```
if True:
                                          def lorentz(x):
    print("Integrating sin")
    fun=np.sin
                                                return 1.0/(1.0+x**2)
    xmin=0
    xmax=np.pi
    targ=2.0
    dx_targ=0.1
else:
    print("Integrating Lorentzian")
    fun=lorentz
    xmin=-5
    xmax=5
    targ=np.arctan(xmax)-np.arctan(xmin)
    dx targ=0.5
for ord in range(2,16,2):
    val=integrate(fun,xmin,xmax,dx_targ,ord)
    print('For order ' + repr(ord) + ' error is ' + repr(np.abs(val-targ)))
```

```
Integrating sin
For order 2 error is 1.0333694131503535e-06
For order 4 error is 3.809155213474469e-09
For order 6 error is 7.276845792603126e-12
For order 8 error is 1.0769163338864018e-13
For order 10 error is 0.0
For order 12 error is 1.9984014443252818e-15
For order 14 error is 2.6645352591003757e-15
```

```
Integrating Lorentzian
For order 2 error is 0.0038935163714279852
For order 4 error is 0.01097767769723701
For order 6 error is 0.002621273236311783
For order 8 error is 0.01837703807845159
For order 10 error is 0.005032084054994446
For order 12 error is 0.001118349714313016
For order 14 error is 0.0003964865376655524
```

What Happened?

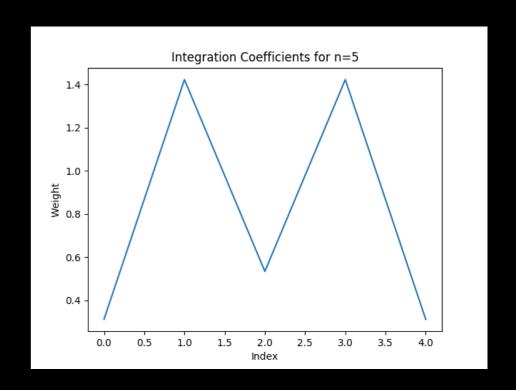
- In all cases, we used roughly the same number of function evaluations.
- Sin is a smooth function. Its error rapidly went to zero as we increased the order. If you know you're integrating a sin, crank away!
- Lorentzian is not a smooth function since it has poles at +/-i. Its power series expanded at zero does not converge for |x| >1. Integral is less accurate, and does not improve very rapidly as we increase order.
- Lorentzian sometimes gets worse at higher order!

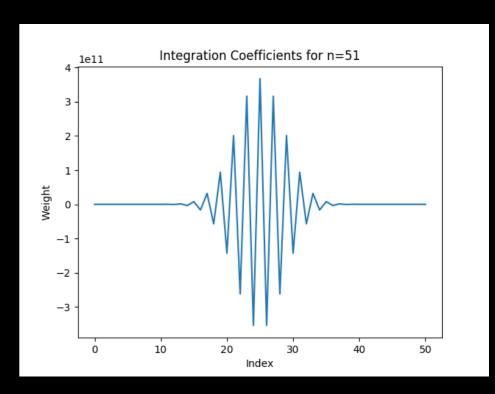
Error Estimate

- Usual scheme is to pick an order, then vary step size until accuracy is good.
- How do I know accuracy? If I'm in happy Taylor regime, errors predictable. Compare f(4dx) & f(2dx) against f(2dx) & f(dx). Did differences shrink as expected? If not, try smaller step size.
- If you beat hard enough, eventually Taylor wins out.

Interpolation Coefficients to High Order

- Top: 5th order polynomial integration weights.
- Bottom: 51st order polynomial integration weights.
- Do you want to go to (very) high order this way?





Romberg Integration

- Another way to get to high order.
- If I integrate from -a to a, only even terms survive in integral.
- If I have n estimates of area with varying dx, I could kill off n terms in even error series, giving accuracy of dx²ⁿ.
- More stable than high order polynomial weights.

Scipy Romberg

In scipy.integrate have 2 options:
 scipy.integrate.romb = integral from pre-evaluated points
 scipy.integrate.romberg = integral from function

for k=1 and 3 function calls, error is 0.011651369255893052 for k=2 and 5 function calls, error is 6.851628176995916e-05 for k=3 and 9 function calls, error is 1.0674648986963575e-07 for k=4 and 17 function calls, error is 4.2089887131169235e-11 for k=5 and 33 function calls, error is 4.440892098500626e-15

```
for k=6 and 65 function calls, error is 8.881784197001252e-16
                                        for k=7 and 129 function calls, error is 4.440892098500626e-16
                                        for k=8 and 257 function calls, error is 0.0
                                        for k=9 and 513 function calls, error is 0.0
import numpy as np
                                        Romberg integration of <function vfunc at 0x11b243140> from [-1, 1]
from scipy import integrate
                                         Steps StepSize
                                                        Results
                                             1 2.000000 3.086161
a = -1
                                             2 1.000000 2.543081 2.362054
b=1
                                             4 0.500000 2.399166 2.351195 2.350471
for k in range(1,10):
                                             8 0.250000 2.362631 2.350453 2.350404 2.350402
                                            16 0.125000 2.353462 2.350406 2.350402 2.350402 2.350402
    n=1+2**k
                                            32 0.062500 2.351167 2.350403 2.350402 2.350402 2.350402 2.350402
    dx=(b-a)/(n-1.0)
    x=np.linspace(a,b,n)
                                        The final result is 2.350402387287607 after 33 function evaluations.
    y=np.exp(x)
    pred=np.exp(b)-np.exp(a)
    f=dx*integrate.romb(y)
    print('for k=' + repr(k) + ' and ' + repr(n) + ' function calls, error is ' + repr(np.abs(f-pred)
f=integrate.romberg(np.exp,a,b,show=True)
```

Indefinite Integrals

- Handy trick: $\int_{a^b} f(x) dx = \int_{1/b^{1/a}} f(1/t) t^{-2} dt$ for t = 1/x
- Can now set e.g. b to ∞, and take integral happily since 1/ b=0.
- Happily, as long as function falls off quickly enough.

scipy quad

- Quad is the general purpose routine for integrating.
- Supports indefinite integrals, integrals against integrable singularities:

Variable Step Size

- For Lorentzian, areas well away from poles should integrate nicely. Only around |x| < 1 is problematic.
- If I keep track, I will be able to see that away from the origin I converge, but less well at origin.
- I can find regions that behave, and not shrink dx when their errors are small.
- Regions that do not behave: shrink dx by a factor of 2, and try again.
- Life experience: Bad functions are usually bad in a small piece.
- Variable step size integration can easily save factors of ~hundred.

Side Note: Recursion

- A recursive function calls itself.
- In this case, we'll evaluate function across interval. If error small enough, we're done.
- Otherwise integral is integral of left half + integral of right half. Just call ourselves twice.
- If you don't have good stopping point, recursion can run away on you, easily crash computer.
- Good practice to think how stopping might go wrong.

Let's play with our integrator

- Throw out some functions where you know the analytic integral. How do we do?
- If we shrink the input tolerance, does our error get more accurate?
- What's a (finite, integrable function) with a spike? Does our integrator do lots of work around the spike and little elsewhere?

Cautionary Tale

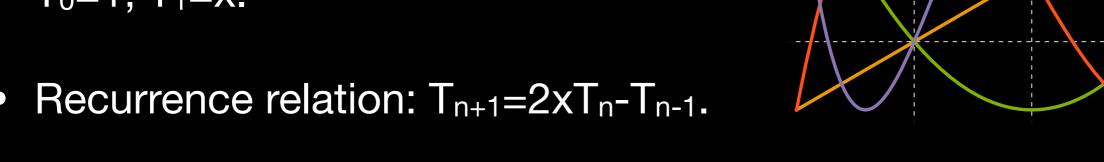
- Let's integrate f(x)=1+exp(-0.5*(x/0.1)²) from a (<<0) to b (>>0).
- What should the answer be?
- What do we get from (-20,20)?
- Does using scipy's quad help us here?
- How can we fix things?

Gaussian Quadrature

- We did well with high order and orthogonal polynomials. We might be able to do even better.
- Problem: polynomials not quite orthogonal on evenly spaced points.
- Gaussian quadrature: if we can pick x positions (instead of evenly spaced), we can make points orthogonal to odd polynomials. By only fitting even, can go to twice the order. Weights depend on positions.
- Unexpected bonus this works well for integrating w(x)f(x) for fixed w. One way to integrate over singularities.
- Example: integrate f(x)/sqrt(x) we calculate quadrature positions, weights for w=1/sqrt(x), then use that to integrate f(x).
- Many weight function have already been generated if you need this, have a look.

Chebyshev Polynomials

- T_n=cos(nacos(x)), -1≤x≤1
- $T_0=1, T_1=x$.



- Bounded by +/-1
- Orthogonal under weight: $\int T_n T_m / (1-x^2)^{1/2} dx = 0$ (i \neq j), π (i=j=0) or $\pi/2$ (i=j>0).
- Make a natural way of doing Gaussian quadrature (Gauss-Chebyshev quadrature) of $f(x)/(1-x^2)^{1/2}$.

Chebyshev Series

- Let's say we want to make a polynomial expansion for some function with the smallest maximum errors.
- Common case when, say, trying to write code for evaluating functions.
- For smooth functions, Chebyshev coefficients tend to drop smoothly.
- Because T_n are bounded, max error is \sum of cut coefficients.
- If you want to have fast functions at possibly relaxed precision over possibly restricted range, T_n are very useful.

How This Looks

- Look at cheb_expand.py
- Fits chebyshev and least-squares to same order.

