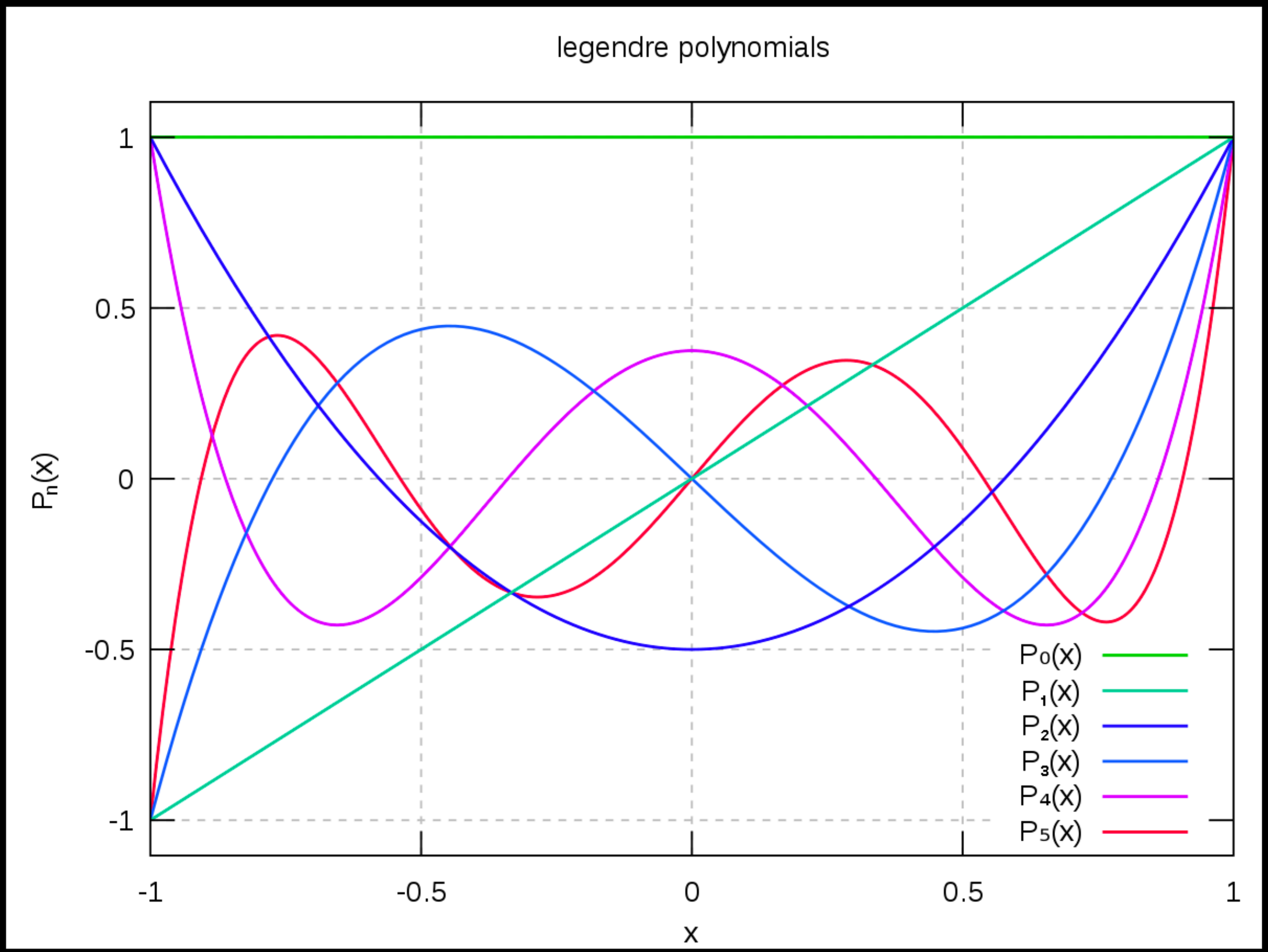
Phys 512 Lecture 5
Integration ctd./ODEs


legendre polynomials
1
0.5
0
-0.5
-1
$P_n(x)$
-1
-0.5
0
0.5
1
x
$P_0(x)$
$P_1(x)$
$P_2(x)$
$P_3(x)$
$P_4(x)$
$P_5(x)$

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:
    print("Integrating sin")
    fun=np.sin
    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)))
```

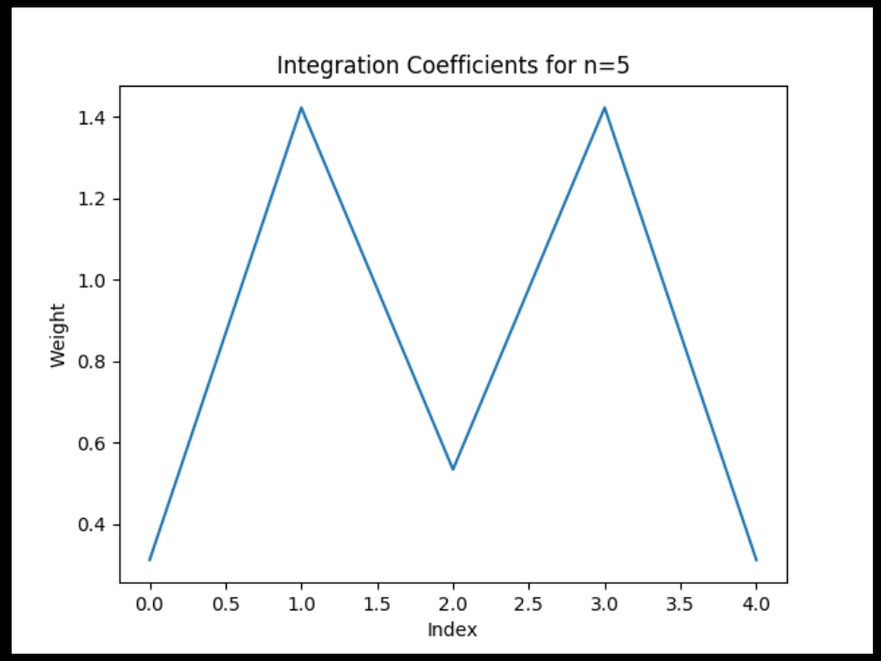
```
def lorentz(x):
    return 1.0/(1.0+x**2)
```

```
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 1.0769163388864018e-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 0.003893516371427985 2
For order 4 error is 0.010977677697237 01
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
```

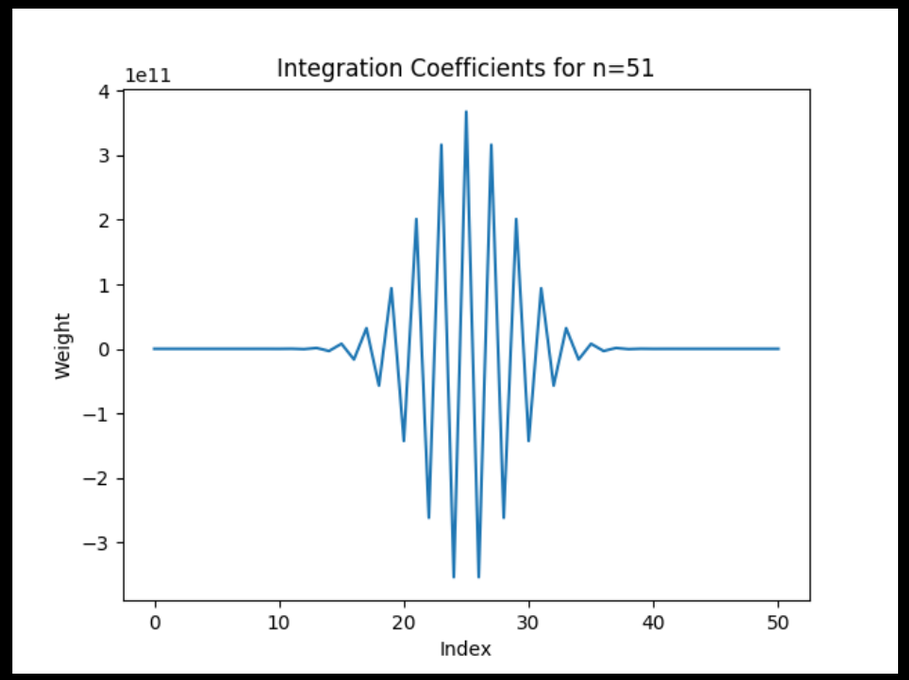
Interpolation Coefficients to High Order

- 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 d*x*, I could kill off n terms in *even* error series, giving accuracy of dx^{2n}.
- 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
Romberg integration of <function vfunc at 0x11b243140> from [-1, 1]

 Steps  StepSize   Results
     1  2.000000  3.086161
     2  1.000000  2.543081  2.362054
     4  0.500000  2.399166  2.351195  2.350471
     8  0.250000  2.362631  2.350453  2.350404  2.350402
    16  0.125000  2.353462  2.350406  2.350402  2.350402  2.350402
    32  0.062500  2.351167  2.350403  2.350402  2.350402  2.350402  2.350402

The final result is 2.350402387287607 after 33 function evaluations.
```

```python
import numpy as np
from scipy import integrate

a=-1
b=1
for k in range(1,10):
    n=1+2**k
    dx=(b-a)/(n-1.0)
    x=np.linspace(a,b,n)
    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)
```

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.

- Let’s write one.

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?

scipy quad

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

```
>>> ans=integrate.quad(np.exp,-np.inf,-1)
>>> print([ans[0]-np.exp(-1),ans[1]])
[-5.551115123125783e-17, 2.1493749551987453e-11]
>>>
```

```
>>> def fun(x):
...     return 1.0/np.sqrt(x)
...
>>> integrate.quad(fun,0.0,2)
(2.8284271247461907, 3.1401849173675 51e-15)
>>> print np.sqrt(8)
2.8284271247461903
>>>
```

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)? How about (-25,15)?
- Does using scipy's quad help us here?
- How can we fix things?

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.

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.

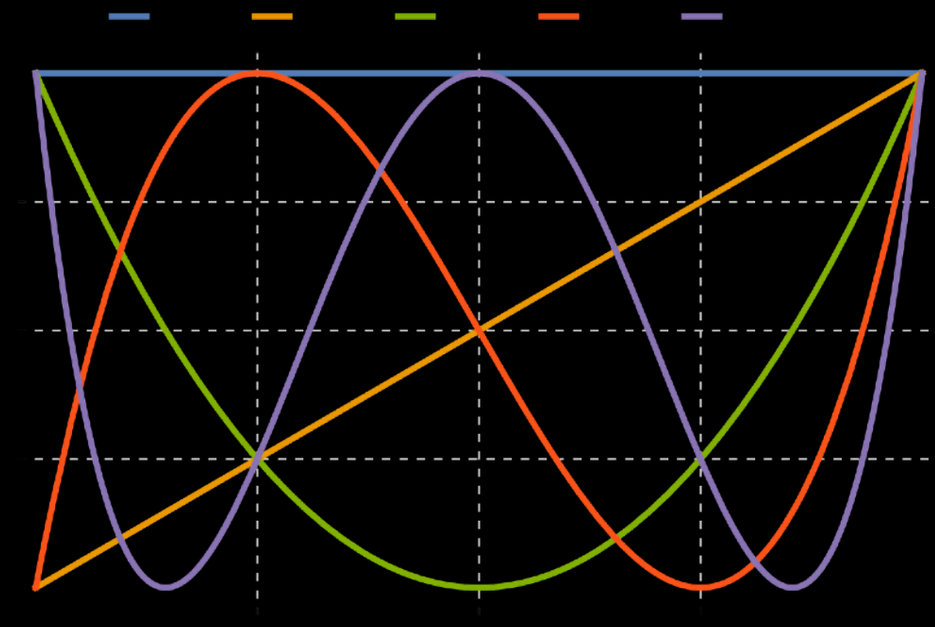
- Gaussian quadrature: if we can pick x positions (instead of evenly spaced), we can make points orthogonal to odd polynomials. By only fitting even, can go to twice the order. Weights depend on positions.

- 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



- $T_n=\cos(n\arccos(x))$, $-1\le x\le 1$
- $T_0=1$, $T_1=x$.
- Recurrence relation: $T_{n+1}=2xT_n-T_{n-1}$.
- 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.

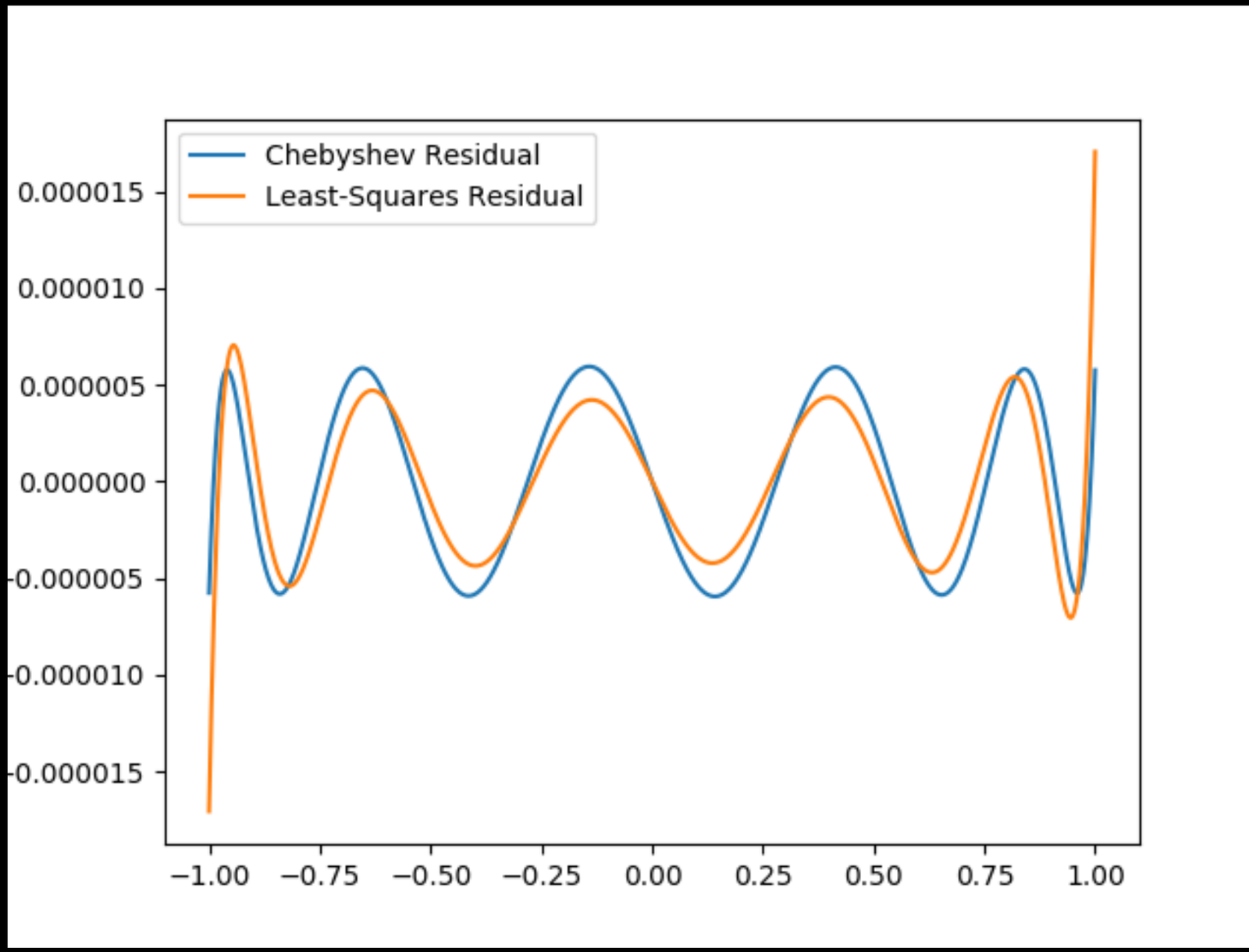
- For smooth functions, Chebyshev coefficients tend to drop smoothly.

- 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.




```
[Jonathans-MacBook-Pro:lecture_3 sievers$ python3 cheb_expand.py
 rms error for least-squares is  3.6653313842173857e-06  with max error  1.7044661309315215e-05
 rms error for chebyshev     is  4.155908892551404e-06  with max error  5.9427933866151 86e-06
```

ODEs

- usual case: we have $y(x_0)$, find $y(x_0+h)$ given $dy/dx=f(x,y)$
- Harder than integration, because we don't know how to evaluate dy/dx along the path - that depends on the (unknown) value of y.
- We can still apply many of the Taylor series tricks we've learned.
- NB - we could have a system of equations just as well as a single equation.
- NB 2 - we can also have higher order equations recast into a system. variables are then y,y',y"…

1st order

- We could just take y(x+h)=y(x)+h dy/dx = y(x)+hf
- How will error scale with size of h?
- This isn’t very good…
- Can we do better?

RK2

(see https://web.mit.edu/10.001/Web/Course_Notes/Differential_Equations_Notes/node5.html)

- I could take a trial step, then evaluate derivative. Maybe combine with first derivative to do better?

- Taylor expand y(x+h) to 2nd order.

- Take $k_1=hf(x,y)$, $k_2=hf(x+\alpha h,y+\beta k_1)=hf(x+\alpha h,y+\beta fh)$

- Let answer be $y(x+h)=ak_1+bk_2$.

- Solve for a,b,α,β to make agree with Taylor.

- Answer underconstrained - have freedom to pick. Usual is $\alpha=\beta=1$, $a=b=1/2$, or $\alpha=\beta=1/2$ and $a=0,b=1$.

RK4

- Can extend to 4^{th} order. Mathy, but not very illustrative.

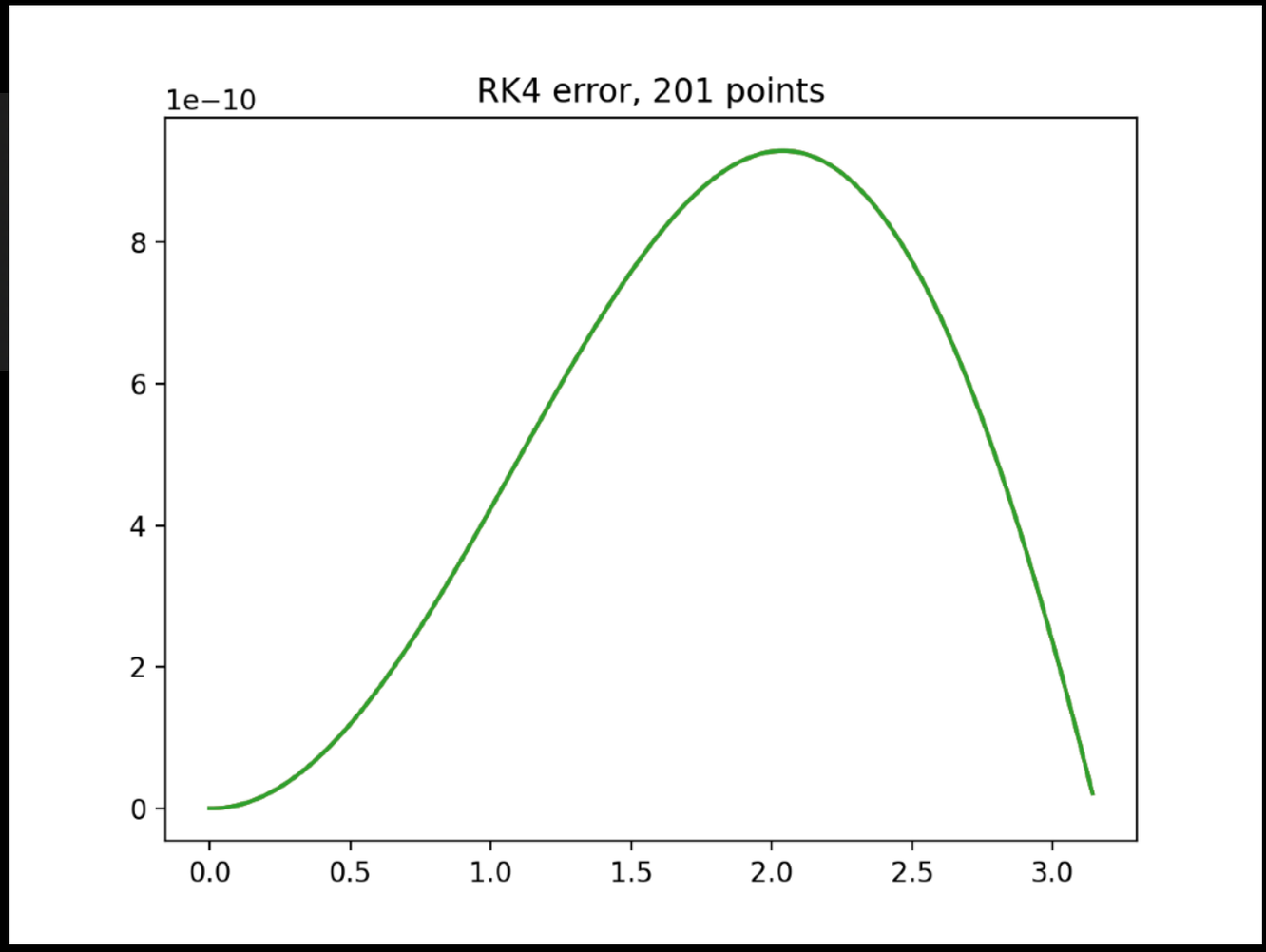
- $k_1=hf(x,y)$
  $k_2=hf(x+h/2,y+k_1/2)$
  $k_3=hf(x+h/2,y+k_2/2)$
  $k_4=hf(x+h,y+k_3)$
  $y(x+h)=y(x)+(k_1+2k_2+2k_3+k_4)/6$

- Accurate to 4th order - ODE equivalent of Simpson's rule.

- Adaptive stepsize *highly* recommended.

```python
def f(x,y):
    dydx=np.asarray([y[1],-y[0]])
    return dydx
```

```python
def rk4(fun,x,y,h):
    k1=fun(x,y)*h
    k2=h*fun(x+h/2,y+k1/2)
    k3=h*fun(x+h/2,y+k2/2)
    k4=h*fun(x+h,y+k3)
    dy=(k1+2*k2+2*k3+k4)/6
    return y+dy
```




```python
npt=201
x=np.linspace(0,np.pi,npt)
y=np.zeros([2,npt])
y[0,0]=1 #starting conditions
y[1,0]=0 #if I start at peak, then first derivative =0
for i in range(npt-1):
    h=x[i+1]-x[i]
    y[:,i+1]=rk4(f,x[i],y[:,i],h)
truth=np.cos(x)
print(np.std(truth-y[0,:]))
```

Systems of Equations

- RK4 etc. also work on systems of equations: $d(y_1,y_2\ldots)/dx=f(y1,y2\ldots,x)$

- Higher order systems can always be recast as a system

- example: y”(x)=f(x,y) turns into:
  dy/dx=z
  dz/dx=-f(x,y)

- once you have a first order system, solve as usual

Bulirsch-Stoer

- We saw we could take multiple not-very accurate integrals, and combine to get high accuracy by estimating error terms.
- Can do the same with ODEs - Romberg equivalent is called Bulirsch-Stoer.
- If you need high accuracy, have smooth function, try this!

Stability

- let y'=-cy. Answer should be exp(-cx)
- Solve the stupid way: y(x+h)=y(x)+hf(x,y)= y(x)-hcy(x)
- y(x+h)=y(x)(1-hc). $y(x+nh) = y(x)(1-hc)^n$.
- What happens if h is to large? For |1-hc|>1, this *grows* exponentially. Large steps have made our answer *unstable*.

Stiff Equations

- Very often in systems, one equation (or eigenmode) has a large c, other has a small c.

- Solution is large c converges very quickly, and stays at solution while we wait for small c to evolve.

- If we aren’t careful and take steps for small c, then large c becomes unstable, and solution blows up.

- Shrinking time step enough to track large c may be impracticle.

- Such systems are called *stiff*. Solutions presented here are simplistic, but knowing you have a stiff set is most of the battle.

U238 Decay

- Radioactive decay common situation.
- U238 takes 4 billion years to go to Th234. Po214 takes 160 microseconds to go to Pb210.
- To solve naively, takes (4 billion years/160 microsconds) $=10^{21}$ timesteps.

	Half-Life	Time unit	Emitter
Uranium-238	4,468	billion of years	alpha
Thorium-234	24,10	days	beta -
Protactinium-234	6,70	hours	beta -
Uranium-234	245 500	years	alpha
Thorium-230	75380	years	alpha
Radium-226	1 600	years	alpha
Radon-222	3,8235	days	alpha
Polonium-218	3,10	minutes	alpha
Plomb-214	26,8	minutes	beta -
Bismuth-214	19,9	minutes	beta -
Polonium-214	164,3	microseconds	alpha
Plomb-210	22,3	years	beta
Bismuth-210	5,015	years	beta
Polonium-210	138,376	days	alpha
Plomb-206	Stable		

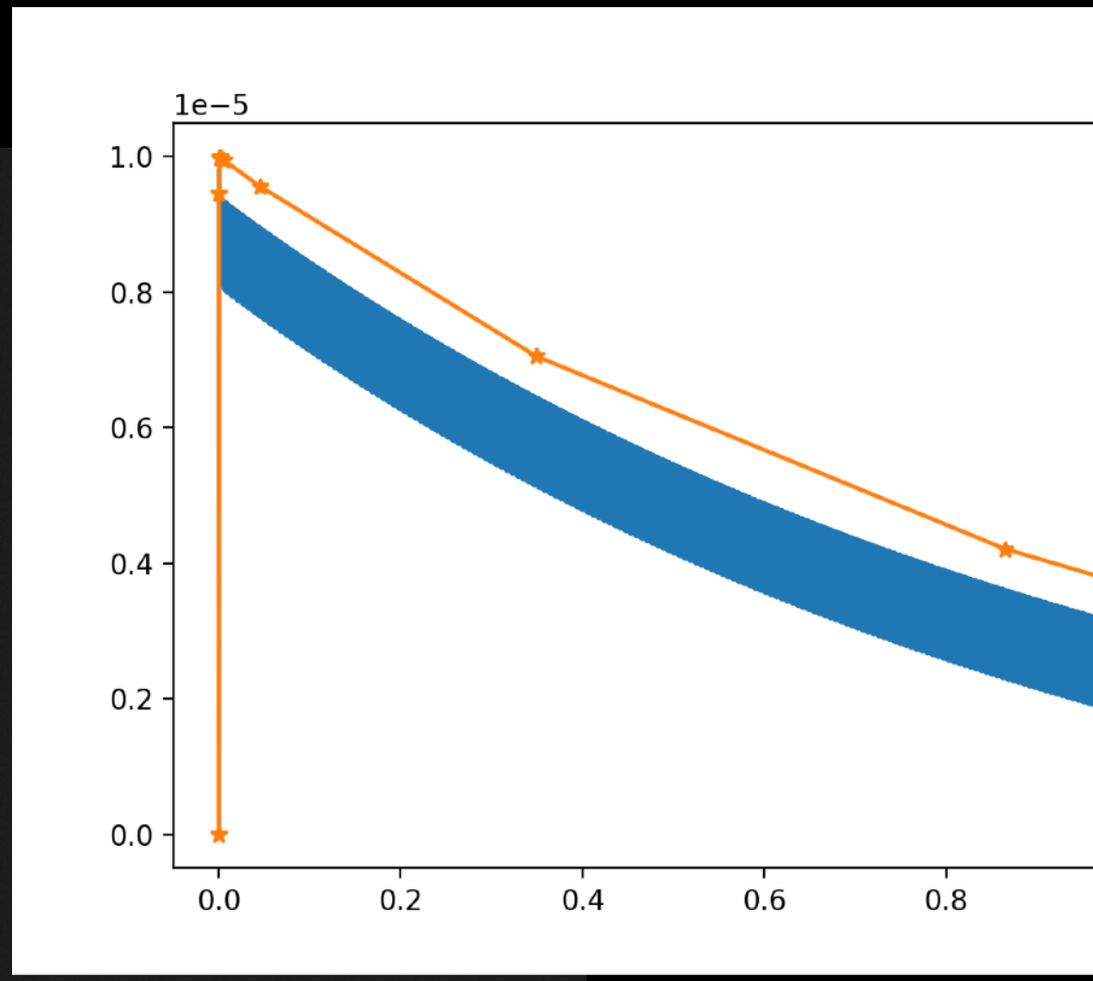
Implicit

- Common solution - use derivative at end of interval.
- In constant coefficient case $y_{n+1}=y_n-hcy_{n+1}$.
- Solve: $y_{n+1}(1+hc)=y_n$, $y_{n+1}=y_n/(1+hc)$. (reminder - old way was $y_{n+1}=y_n(1-hc)$. Agrees to 1st order but not 2nd.)
- I can now make h very large and remain stable. I may not be accurate, but I can crank up h.
- This is just an introduction, much better ways to handle stiff equations exist, but at least you know to look for them…

Scipy ODE Driver

```
import numpy as np
from scipy import integrate
def fun(x,y,half_life=[1,1e-5]):
    #let's do a 2-state radioactive decay
    dydx=np.zeros(len(half_life)+1)
    dydx[0]=-y[0]/half_life[0]
    dydx[1]=y[0]/half_life[0]-y[1]/half_life[1]
    dydx[2]=y[1]/half_life[1]
    return dydx


y0=np.asarray([1,0,0])
x0=0
x1=1
ans_rk4=integrate.solve_ivp(fun,[x0,x1],y0)
ans_stiff=integrate.solve_ivp(fun,[x0,x1],y0,method='Radau')
print('took ',ans_rk4.nfev,' evaluations to solve with RK4.')
print('took ',ans_stiff.nfev,' evaluationg to solve implicitly')
print('final values were ',ans_rk4.y[0,-1],' and ',ans_stiff.y[0,-1],'
```




```
>>> exec(open('stiff.py').read())
took  212618  evaluations and  3.1277468204498 29  seconds to solve with RK4.
took  72  evaluations and  0.0035657882690429688  seconds to solve implicitly
final values were  0.3678794411714445  and  0.3678803705878816  with truth  0.3678794411714423
>>> plt.clf();plt.plot(ans_rk4.t,ans_rk4.y[1,:]);plt.plot(ans_stiff.t,ans_stiff.y[1,:],'*-')
```