Interpolation & ODEs

Scientific Computing Course, Jan 2013



- Questions about Make for targets
- Imagine we had the following very simple (Id) diffusion in diffuse.cxx:

```
void derivative(double *y, double *x, double *d2y, int n) {
  for (int i=1; i<n-1; i++) {
     double dxl = x[i+1] - x[i-1];
     double dxr = x[i] - x[i-1];
     double dx = 0.5*(dxl + dxr);
     d2y[i] = ((y[i+1] - y[i])/dxr - (y[i] - y[i-1])/dxl ) / dx;
  }
  return;
}
void diffuse(double *tin, double *tout, double *x, int n, double coeff) {
    double *deriv = new double[n];
    derivative(tin, x, deriv, n);
    for (int i=1; i<n-1; i++) {
        tout[i] = tin[i] - coeff*deriv[i];
    }
</pre>
```



 And a main program which drove it, main.cxx

```
double *old = tin;
double *cur = tout;
const int nsteps = 100;
for (int step=0; step < nsteps; step++) {
    diffuse(old, cur, x, npts, coeff);
    double *tmp = old;
    old = cur;
    cur = tmp;
}
out = fopen(outfilename,"w");
if (!out) {
    fprintf(stderr,"Could not open file \"%s\"; exiting\n", out
    return -1;
}
fprintf(out, "%d\n", npts);
```



 We might have a Makefile that looks like this:

```
CXXFLAGS = -02 - Wall - g
CXX = g++
LDLIBS = -lm
all: main
main: main.o diffuse.o
   $(CXX) -0 $@ $(LDLIBS) $^
main.o: main.cxx diffuse.h
   $(CXX) -c -o $@ $(CXXFLAGS) $<
diffuse.o: diffuse.cxx
   $(CXX) -c -o $@ $(CXXFLAGS) $<
clean:
    rm -f *.o output*.txt *~ main
```

 But we can add a different main() which does a couple simple tests on the diffusion routine (unit or integrated?)

```
int main(int argc, char **argv) {
```

```
int err;
int allerr=0;
int n=100;
```

```
printf("Performing Constant Test...\n");
err = doConstTest(n);
if (!err)
    printf("PASS\n");
else
    printf("FAIL\n");
allerr += err;
```

```
printf("Performing Linear Test...\n");
err = doLinearTest(n);
if (!err)
    printf("PASS\n");
else
    printf("FAIL\n");
allerr += err;
```

```
return allerr;
```

```
CXXFLAGS = -O2 -Wall -g
CXX = g++
LDLIBS = -lm
all: main tests
```

And create a makefile to automatically compile this and run it:
 Math tests
 main: main.o diffuse.o \$(CXX) -o \$@ \$(LDLIBS) \$^
 tests: tests.o diffuse.o \$(CXX) -o \$@ \$(LDLIBS) \$^

runtests: tests ./tests



Git Bisect

- Version Control (git) and automation (make) are tools to make your computing life better and more productive.
- Note that the tests had main return zero on success and non-zero on failure, by long convention.
- Now let's say I had been developing this program for a while without testing, and then...



Git Bisect

- Bah.
- We could use git diff to figure out what code change caused the bug..

gpc-f103n084-\$ make runtests g++ -c -o tests.o -02 -Wall -g tests.cxx g++ -c -o diffuse.o -02 -Wall -g diffuse.cxx g++ -o tests -lm tests.o diffuse.o ./tests Performing Constant Test... FAIL Performing Linear Test... FAIL make: *** [runtests] Error 2 gpc-f103n084-\$ ■



known bad

Git Bisect

- But we're not sure when the bug was introduced, so it's a little hard to figure out which commit caused it.
- Could checkout different versions and test...

gpc-f103n084-\$ git log commit a333719bb5c8bfb0a46211bd3914329a8d4383fe Author: Jonathan Dursi <ljdursi€scinet.utoronto.ca> Date: Wed Jan 30 16:16:32 2013 -0500

Allow user-specified output file name

commit 06dcde1bc7734f294161484bebe26da64f6aae02 Author: Jonathan Dursi <ljdursi@scinet.utoronto.ca> Date: Wed Jan 30 16:12:41 2013 -0500

Allow user-specified input filename

commit cd5c32f3307e5d11b170efa01e9c6428e84d73cd Author: Jonathan Dursi <ljdursi@scinet.utoronto.ca> Date: Wed Jan 30 16:03:51 2013 -0500

Have x read in from the input file

commit e641ddffd255ef4f495e81217cbf2fd7c634efae Author: Jonathan Dursi <ljdursi@scinet.utoronto.ca> Date: Wed Jan 30 16:01:32 2013 -0500

Add x for non-uniform grid

commit 2f367d4220393eb1e85aafec18487df40a8fb159 Author: Jonathan Dursi <ljdursi@scinet.utoronto.ca> Date: Wed Jan 30 15:55:52 2013 -0500

Better names for derivative arguments

commit ffd76e9e72b6e4746e8666e8e529f35ff38edb64 Author: Jonathan Dursi <ljdursi@scinet.utoronto.ca> Date: Wed Jan 30 15:53:37 2013 -0500

Get rid of extraneous files

commit 8be8a4e5e83ca89b5d67ca5df2cc1298a6987e31 Author: Jonathan Dursi <ljdursi@scinet.utoronto.ca> Date: Wed Jan 30 15:52:46 2013 -0500

Move diffusion into diffuse.cxx

commit afb7ad5fc0ec13c7fdc8ffb92318d3ffd7e95c02 Author: Jonathan Dursi <ljdursi@scinet.utoronto.ca> Date: Tue Jan 29 09:34:59 2013 -0500

Initial commit of 1d diffusion with tests



CANADA





Git Bisect

isecting: 0 revisions left to test after this (roughly 0 steps) e641ddffd255ef4f495e81217cbf2fd7c634efae] Add x for non-uniform grid unning make runtests	
/tests erforming Constant Test commit that brake the test	ı
	1
erforming Linear Test	
AIL	
ake: *** [runtests] Error 2	
641ddffd255ef4f495e81217cbf2fd7c634efae is the first bad commit	
ommit e641ddffd255ef4f495e81217cbf2fd7c634efae by this known	
uthor: Jonathan Dursi <ljdursi@scinet.utoronto.ca></ljdursi@scinet.utoronto.ca>	
ate: Wed Jan 30 16:01:32 2013 -0500	
Add x for non-uniform grid	
100644 100644 24dfc324a72163252edb63cb013606cacad72c61 bde5145d11d29c687ccf50a007ce547bf66ecacf M	(

:100644 100644 79e12641dbcc2e8776a7d45da99b6ca9e644ea7b 7984946e380d7ddd63318a59301f0ef91364

:100644 100644 7b8da7f207dc9ca8346d2108f2d4644d8062b17f fc5be55fed2e275ee73257b80f88973eb4

bisect run success

diffuse.cxx :100644 100644 c9ef874c3fb731454965f43087856dfd809de2e2 bfdebae4341e1dfde11fc0905ff0831da312120c M diffuse.h main.cxx 🚽 M

> tests.cxx м

> > compute • calcu

who changed these files

```
HEAD is now____
                                        gpc-f103n084-$ git show HEAD diffuse.cxx
                                        commit e641ddffd255ef4f495e81217cbf2fd7c634efae
                                        Author: Jonathan Dursi <ljdursi@scinet.utoronto.ca>
the first broken
                                               Wed Jan 30 16:01:32 2013 -0500
                                        Date:
                                            Add x for non-uniform grid
        commit
                                        diff --git a/diffuse.cxx b/diffuse.cxx
                                        index 24dfc32..bde5145 100644
                                        --- a/diffuse.cxx
                                        +++ b/diffuse.cxx
                                        @@ -1,18 +1,21 @@
                                        -// assumes regular spacing
                                        -void derivative(double *y, double *d2y, int n) {
       Ah ha! One
                                        +void derivative(double *y, double *x, double *d2y, int n) {
                                             for (int i=1; i<n-1; i++) {</pre>
          of my dx's
                                                d2y[i] = (y[i+1] - 2.*y[i] + y[i-1]);
                                                double dxl = x[i+1] - x[i-1];
                                                double dxr = x[i] - x[i-1];
           is wrong.
                                                double dx = 0.5*(dxl + dxr);
                                                d2y[i] = ((y[i+1] - y[i])/dxr - (y[i] - y[i-1])/dxl) / dx;
                                             }
                                             return;
                                         }
     git bisect reset
                                        -void diffuse(double *tin, double *tout, int n, double coeff) {
                                        +void diffuse(double *tin, double *tout, double *x, int n, double coeff) {
     to get back to
                                             double *deriv = new double[n];
                                             derivative(tin, deriv, n);
     the way things
                                             derivative(tin, x, deriv, n);
                                             for (int i=1; i<n-1; i++) {</pre>
                                                tout[i] = tin[i] - coeff*deriv[i];
              were.
                                        gpc-f103n084-$ git bisect reset
```



- Note that:
 - the more frequent the checkins, and
 - the more specific the unit tests,
- the more precisely this will hone in on the error.



Git Bisect

• If you

- commit regularly,
- have a good test suite,
- have build/test automation,
- Then those tools can help you automatically find where bugs were introduced.
- Even without automation (say bug introduced before the tests were), you can use git bisect
- \$ git help bisect



Final Testing Note

- You're not finished when you fix a bug.
- If it's the sort of bug that could conceivably crop up again, add a test for it, in your test suite or just in the code (eg, assert(n > 0).)
- Nothing is more frustrating than finding and fixing the same bug twice.



Interpolation & ODEs

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Interpolation

- We're often given, or compute, discrete data
- But to use our mathematical machinery on it we need continuous function
- Or need to know value between points, if even just to plot.





Interpolation

- Interpolation returns a function that passes through all input points,
- Or values of that function at intermediate points.
- Not what you want when you have noisy data: fitting or regression. Different topic.





Polynomial interpolation

- Common approach
- For n points, use n-lth order polynomial: n coefficients
- Solve a linear system (nonlinear in input data)

$$y_{1} = a_{0} + a_{1}x_{1}^{1} + \dots + a_{n-1}x_{1}^{n-1}$$

$$y_{2} = a_{0} + a_{1}x_{2}^{1} + \dots + a_{n-1}x_{2}^{n-1}$$

$$\dots$$

$$y_{n} = a_{0} + a_{1}x_{n}^{1} + \dots + a_{n-1}x_{n}^{n-1}$$

$$y_{1}^{1} = \begin{pmatrix} 1 & x_{1} & x_{1}^{2} & \dots & x_{1}^{n-1} \\ 1 & x_{2} & x_{2}^{2} & \dots & x_{2}^{n-1} \\ \dots & 1 & x_{n} & x_{n}^{2} & \dots & x_{n}^{n-1} \end{pmatrix} \begin{pmatrix} a_{0} \\ a_{1} \\ \dots \\ a_{n-1} \end{pmatrix}$$

 $\mathbf{y} = \mathbf{X}\mathbf{a}$



Polynomial Interpolation

- Common approach
- For n points, use n-lth order polynomial: n coefficients
- Solve a linear system (nonlinear in input data)



```
In [92]: x = arange(.1,.91,.2); y = rand(5);
...: xx = arange(0,1,.02)
...:
In [93]: plot(x,y,'ro')
Out[93]: [<matplotlib.lines.Line2D at 0x8933070>]
In [94]: polyInterpFun = scipy.interpolate.lagrange(x,y
In [95]: yy = polyInterpFun(xx)
In [96]: plot(xx,yy,'b-')
Out[96]: [<matplotlib.lines.Line2D at 0x8933470>]
```

Basis Functions

- Here we're solving for parameters which generate a linear combination of basis functions
- The basis functions here are I, x, x², x³, ...
- They can be any other functions that span the relevant function space.

$$y_1 = a_0 + a_1 x_1^1 + \dots + a_{n-1} x_1^{n-1}$$
$$y_2 = a_0 + a_1 x_2^1 + \dots + a_{n-1} x_2^{n-1}$$
$$\dots$$

$$y_n = a_0 + a_1 x_n^1 + \dots + a_{n-1} x_n^{n-1}$$

$$\begin{pmatrix} y_1 \\ y_2 \\ \dots \\ y_n \end{pmatrix} = \begin{pmatrix} 1 & x_1 & x_1^2 & \dots & x_1^{n-1} \\ 1 & x_2 & x_2^2 & \dots & x_2^{n-1} \\ \dots & & & & \\ 1 & x_n & x_n^2 & \dots & x_n^{n-1} \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \dots \\ a_{n-1} \end{pmatrix}$$

$$\mathbf{y} = \mathbf{X}\mathbf{a}$$



Orthogonal Basis Functions

- We have to solve a linear system, which is expensive
- Can't just write down form for (say) a1 without calculating all others; basis functions overlap.
- If the basis functions are orthogonal in some (any) sense, can skip this; can calculate individual coefficients explicitly
- Any set of basis functions can be orthogonalized

 $y = \sum_{i} a_{i} f_{i}(x)$ $\langle y, f_{j}(x) \rangle = \sum_{i} a_{i} \langle f_{i}(x), f_{j}(x) \rangle$ $\langle y, f_{j}(x) \rangle = \sum_{i} a_{i} \delta_{i,j}$ $a_{j} = \langle y, f_{j}(x) \rangle$



Orthogonal Basis Functions

- In polynomials, there are several ways of orthogonalization (depending on your inner product)
- Lagrange interpolating polynomials particularly straightforward
- Functions in a Fourier series are orthogonal

$$l_j = \frac{\prod_{m \neq j} (x - x_m)}{\prod_{m \neq j} (x_j - x_m)}$$



- Often don't want a single, global closed-form function to describe our data.
- (But note: spectral methods)
- Global function very dependent on every piece of data
- That high order polynomial - very wiggly





- In each between-points, perform an interpolant as before based on nearby points.
- Piecewise constant; pick value of closest point
- Linear: draw a straight line between neighbouring points, etc.



- In each between-points, perform an interpolant as before based on nearby points.
- Piecewise constant; pick value of closest point
- Linear: draw a straight line between neighbouring points, etc.

```
import scipy
import scipy.interpolate
x = sort(rand(11))
y = sin(x*2*pi)
xx = arange(0, .99, .005)
nearest = scipy.interpolate.interp1d(x,y,kind='nearest',bounds_error=False)
linear = scipy.interpolate.interp1d(x,y,kind='linear',bounds_error=False)
        = scipy.interpolate.interp1d(x,y,kind='cubic',bounds_error=False)
cubic
subplot(2,2,1)
plot(x,y,'ro')
xlim([0,1])
title("Data")
subplot(2,2,2)
plot(x,y,'ro')
plot(xx, nearest(xx),'b-')
xlim([0,1])
title("Piecewise Const")
subplot(2,2,3)
plot(x,y,'ro')
plot(xx, linear(xx), 'b-')
xlim([0,1])
title("Piecewise Linear")
subplot(2,2,4)
plot(x,y,'ro')
plot(xx, cubic(xx),'b-')
xlim([0,1])
title("Piecewise Cubic")
                                                            compute • calcu
```

Piecewise Polynomial

interpolant(x,y,newx,p) =

find $i : x_i < newx < x_{i+1}$

build lagrange polynomial from $(x_{i-p/2},...,x_{i+p/2+1})$, $(y_{i-p/2},...,y_{i+p/2+1})$

interpolate to newx



- There's obviously some sense in which higherorder local interpolants approximate the "true" function better.
- Can formalize this intuition with Taylor series analysis.
- Approximation error of a p^{th} order polynomial leaves error of only $O(\Delta x^{p+1})$



Danger! Danger! Danger!
 Thinking in terms of O(Δx^{p+1}) can be helpful; error converging faster rather than slower is good. But remember:

- Assumes smooth underlying function
- Higher order more sensitive to ringing
- Performs abysmally at extrapolation
- Needs more data more difficulty at ends of domain
- Statement of *asymptotics*. For a given Δx , a specific pth-order accurate approximation may or may not be more accurate than a specific (p-1)th order method.





- Desired properties of interpolant depends on what you're going to use them for
- Piecewise polynomials as above: good, and continuous: but derivatives aren't continuous.
- If needed, use same lower number of points but higher order interpolating polynomial.
- Use extra d.o.f.s to match derivatives at interpolated points.
- Impose some condition at ends of interpolated region.



Multidimensional piecewise interpolation

- Note that piecewise interpolation of irregular multidimensional data is harder
- Not trivial to figure out which region a given point is in
- On regular lattice, however, much simpler





Bilinear interpolation

- On 2d grids, simple approaches such as bilinear interpolants are sometimes used
- Product of two linear interpolations
- 4 values, 4 unknowns.
- Lends itself to an interesting geometric interpretation.

$$f(x,y) = (a_1 + a_2(x - x_0))(a_3 + a_4(y - y_0))$$

$$f(x, y) = b_1 + b_2(x - x_0) + b_3(y - y_0) + b_4(x - x_0)(y - y_0)$$



http://en.wikipedia.org/wiki/File:Bilinear_interpolation_visualisation.svg



Initial Value ODEs

- Given some initial conditions and a differential equation, evolve the differential equation.
- Eg, given:

$$\mathbf{y}' = \mathbf{f}(\mathbf{y}, t)$$
$$(\mathbf{y}_0, t_0)$$

• evolve relevant y(t)



Initial Value ODEs

- If our **f** is Lipshitz continuous (differentiable), ∃ unique solution given ICs.
- However, that doesn't necessarily mean we can calculate it well.
- Stability of equation; stability of method; accuracy.



 $\mathbf{y}' = \mathbf{f}(\mathbf{y}, t)$



Equation stability

- Some systems are inherently challenging to integrate
- Eigenvalues > I; small deviations pull you further away from solution
- Since small errors will always creep in (Part II), very challenging for correctness.





Equation stability

- Accuracy: how close to you stay to current solution?
- Stability: how do nearby solutions diverge from each other?





Method stability

- Even with perfectly wellbehaved functions, some methods can be unstable
- Errors grow without bound
- Often see oscilatory behaviour





Euler's Method

- Simplest possible integration method
- stepsize h
- Calculate local deriviative, and approximate (first term in Taylor's series):

$$\begin{aligned} \frac{d\mathbf{y}}{dt} \Big|_{(y_0, t_0)} &= \mathbf{f}(\mathbf{y}_0, t_0) \\ \mathbf{y}(t_0 + h) \approx \mathbf{y}_0 + h \left. \frac{d\mathbf{y}}{dt} \right|_{(y_0, t_0)} \\ &\approx \mathbf{y}_0 + h \mathbf{f}(\mathbf{y}_0, t_0) \end{aligned}$$



Accuracy

- Accuracy improves with smaller stepsize
- As with interpolation, error in a linear step from Taylor series is

 $\mathcal{O}(h^2)$

- "Too large" h unstable.
- Also as with interpolation, can improve accuracy with higher-order methods.



Backward Euler



- Solve for step implicitly
- Take slope approximation as slope at **new** point
- Same accuracy as forward Euler, better stability

$$\begin{aligned} \frac{d\mathbf{y}}{dt} \Big|_{(y_0 + \Delta y, t_0 + h)} &= \mathbf{f}(\mathbf{y}_0 + \Delta y, t_0 + h) \\ \mathbf{y}(t_0 + h) \approx \mathbf{y}_0 + h \left. \frac{d\mathbf{y}}{dt} \right|_{(y_0 + \Delta y, t_0 + h)} \\ \mathbf{y}_0 + \Delta \mathbf{y} \approx \mathbf{y}_0 + h \mathbf{f}(\mathbf{y}_0 + \Delta y, t_0 + h) \end{aligned}$$



Predictor-Corrector

- As with interpolation, can get higher accuracy by using more points
- Can evaluate **f** anywhere
- Predictor-corrector: take forward Euler step, use f value there to improve estimate.





Error estimation

- Note! With multiple function evaluations, one can use different combinations of them to derive different estimates.
- Can use higher- and lower- order methods, and use difference to infer error in estimate.
- This allows adaptive stepsizing to satisfy an error tolerance. Redo with smaller step if error too large.
- Without error estimate, all one can do is say whether solution "looks good" or not.





Multi-step methods

- More complex approaches are tradeoffs between stability, accuracy, and cost (function evaluation or nonlinear solves)
- Take multiple function evaluations between t and t+∆t, and use the combination of those to get next value
- Runge-Kutta methods are classics of these kinds.
- Again, can return error estimates.





Multi-stage methods

- Multiple function evaluations "for free"; use previous evaluations!
- Require something special to start.







- Very well established techniques, code, for doing this.
- Except for most trivial cases, do **not** code yourself. Libraries will do this for you.
- GSL (gnu scientific library) ubiquitious, has several methods for both.
- Allows you to easily experiment with different methods without rewriting code.



```
#include <stdlib.h>
#include <stdio.h>
#include <math.h>
#include <gsl/gsl errno.h>
#include <gsl/gsl spline.h>
int
main (void)
{
  int i;
  double xi, yi, x[10], y[10];
  printf ("#m=0,S=2\n");
  for (i = 0; i < 10; i++)
    {
      x[i] = i + 0.5 * sin (i);
      y[i] = i + cos (i * i);
      printf ("%g %g\n", x[i], y[i]);
    }
  printf ("#m=1,S=0\n");
  {
    gsl interp accel *acc
      = gsl interp accel alloc ();
    gsl spline *spline
      = gsl_spline_alloc (gsl_interp_cspline, 10);
    gsl_spline_init (spline, x, y, 10);
    for (xi = x[0]; xi < x[9]; xi += 0.01)
      {
        yi = gsl_spline_eval (spline, xi, acc);
        printf ("%g %g\n", xi, yi);
      3
    gsl_spline_free (spline);
    gsl interp accel free (acc);
  }
```

roturn 0.



Interpolation

```
int
func (double t, const double y[], double f[],
      void *params)
{
  double mu = *(double *)params;
  f[0] = y[1];
  f[1] = -y[0] - mu*y[1]*(y[0]*y[0] - 1);
  return GSL_SUCCESS;
}
int
jac (double t, const double y[], double *dfdy,
     double dfdt[], void *params)
{
  double mu = *(double *)params;
  gsl_matrix_view dfdy_mat
   = gsl_matrix_view_array (dfdy, 2, 2);
  gsl_matrix * m = &dfdy_mat.matrix;
  gsl_matrix_set (m, 0, 0, 0.0);
  gsl_matrix_set (m, 0, 1, 1.0);
  gsl_matrix_set (m, 1, 0, -2.0*mu*y[0]*y[1] - 1.0);
  gsl_matrix_set (m, 1, 1, -mu*(y[0]*y[0] - 1.0));
  dfdt[0] = 0.0;
  dfdt[1] = 0.0;
  return GSL SUCCESS;
}
int
main (void)
{
  double mu = 10;
  gsl_odeiv2_system sys = {func, jac, 2, &mu};
  gsl_odeiv2_driver * d =
    gsl_odeiv2_driver_alloc_y_new (&sys, gsl_odeiv2_step_rk8pd,
                             le-6, le-6, 0.0);
  int i;
  double t = 0.0, t1 = 100.0;
  double y[2] = \{ 1.0, 0.0 \};
  for (i = 1; i <= 100; i++)
    {
      double ti = i * t1 / 100.0;
      int status = gsl_odeiv2_driver_apply (d, &t, ti, y);
      if (status != GSL_SUCCESS)
   {
     printf ("error, return value=%d\n", status);
     break;
   }
      printf ("%.5e %.5e %.5e\n", t, y[0], y[1]);
    }
  gsl odeiv2 driver free (d);
 return 0;
```

}

ODE Integration

