Lecture 9

Choosing an integration method from

1) trapezoidal rule
2) Simpson rule
3) Romberg integration
4) Gaussian quadrature

general rule: higher order methods work better for smooth functions. If not, then just better to use simpler methods, because variation in data will not be reflected @ sample points.

Trap. rule good for integrating data from experiments @ uniformly spaced sample points. good for poorly behaved functions

Simpson's rule relies on a higher-order approx. of integrand in order to be accurate.

Gaussian quad. very accurate but not desirable if you require uniformly spaced sample points.

How to compute integrals over infinite ranges? e.g.,

$$\int_0^\infty f(x)\,dx$$

simple idea is to use change of variables.

For $\int_0^\infty$, the most common change is

$$z = \frac{x}{1+x} \qquad x = \frac{z}{1-z}$$

which changes interval to [0,1]

Then $\frac{dx}{dz} = \frac{1}{(1-z)^2} \Rightarrow dx = \frac{dz}{(1-z)^2}$

& $\int_0^\infty f(x)\,dx = \int_0^1 f\left(\frac{z}{1-z}\right)\frac{1}{(1-z)^2}\,dz$

Then just use standard techniques

This is the usual change of variables, but not the only one.

E.g., for gamma function

$$\Gamma(a) = \int_0^\infty x^{a-1} e^{-x}\,dx$$

this change is not so good

Most of area falls under maximum @ $a-1$, but the change puts the peak near the edge of [0,1] + uniformly spaced samples won't do well ...

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So we can use a different transformation

$$z = \frac{x}{c+x}$$

(~~can~~ pick $c = a-1$ for gamma function to place peak @ 1/2)

Other choices are

$$z = \frac{x^\gamma}{1+x^\gamma} \quad \text{for some } \gamma$$

To do integral from a to ∞, approach is similar. 1st translate, then scale.

i.e., $y = x - a$

& $z = \frac{y}{1+y}$ or just

$$z = \frac{x-a}{1+x-a} \quad \& \quad x = \frac{z}{1-z} + a$$

(5)

$$dx = \frac{dz}{(1-z)^2} \Rightarrow$$

$$\int_a^\infty f(x)\,dx = \int_0^1 \frac{1}{(1-z)^2} f\left(\frac{z}{1-z}+a\right)dz$$

going from $-\infty$ to a, just substitute $z = -z$

For integrals going from $-\infty$ to ∞, split into two parts.

could also use a single change of variables, such as

$$x = \frac{z}{1-z^2} \qquad dx = \frac{1+z^2}{(1-z^2)^2}dz$$

to get

$$\int_{-\infty}^\infty f(x)\,dx = \int_{-1}^1 \frac{1+z^2}{(1-z^2)^2} f\left(\frac{z}{1-z^2}\right)dz$$

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Another possibility:

$$x = \tan z \qquad dx = \frac{dz}{\cos^2 z}$$

$$\Rightarrow \int_{-\infty}^{\infty} f(x)\,dx = \int_{-\pi/2}^{\pi/2} \frac{f(\tan z)}{\cos^2 z}\,dz$$

<u>Example:</u> Calculate

$$I = \int_0^{\infty} e^{-t^2}\,dt$$

Make the variable change

$z = \frac{t}{1+t}$ & we get

$$I = \int_0^1 \frac{e^{-z^2/(1-z)^2}}{(1-z)^2}\,dz$$

Bring up 1-intinf.py

Value of integral is $\frac{1}{2}\sqrt{\pi}$

& Gaussian quadrature is accurate to machine precision

Multiple integrals

Suppose integral is

$$I = \int_0^1 \int_0^1 f(x,y)\, dx\, dy$$

Rewrite in terms of $F(y) = \int_0^1 f(x,y)\,dx$

as

$$I = \int_0^1 F(y)\, dy$$

Then the idea is to approximate $F(y)$ at some points y & then integrate.

Gaussian quadrature would suggest to do

$$I \simeq \sum_{j=1}^{N} w_j F(y_j)$$

for some weights w_j + sample points y_j

+ then

$$F(y) \simeq \sum_{i=1}^{N} w_i f(x_i, y)$$

can substitute in to find that approx. is

$$I \simeq \sum_{i=1}^{N} \sum_{j=1}^{N} w_i w_j f(x_i, y_j)$$

Bring up 2-two-D-int-samples.png

There's no reason that sample points need to be on a grid. We could attempt to find the "best fit" as with Gaussian quadratures

But there is no answer known here.

could also select sample points randomly (called Monte Carlo integration, which we will get to later)

What if integral is

$$I = \int_0^1 dy \int_0^y dx \, f(x,y)$$

then define $F(y) = \int_0^y f(x,y)\,dx$

$\quad$ & $I = \int_0^1 F(y)\,dy$

If we use same method as before, the sample points are crammed in near each other in certain regions

Bring up 3-int-domain.png

Derivatives

Recall definition of derivative as a slope:

$$\frac{df}{dx} = \lim_{h \downarrow 0} \frac{f(x+h) - f(x)}{h}$$

basic idea is to implement this formula, but we cannot pass to limit, so make h small & approximate as

$$\frac{df}{dx} \simeq \frac{f(x+h) - f(x)}{h}$$

called <u>forward difference</u>

backward difference is then

$$\frac{df}{dx} \simeq \frac{f(x) - f(x-h)}{h}$$

little reason to pick one over the other.

What are errors in approximating derivatives?

- rounding error (as discussed before)
- approx. error since we cannot do $h \downarrow 0$

to see errors, let's use Taylor expansions, assuming function is smooth

$$f(x+h) = f(x) + h f'(x) + \tfrac{1}{2}h^2 f''(x) + \ldots$$

Rearrange to get

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{1}{2} h f''(x) + \ldots$$

forward difference only gives 1st term

& to leading order, approx. error is $\frac{1}{2} h |f''(x)|$

But the problem now is that subtracting numbers can lead to large rounding errors if h is very small

(recall example of

$$x = 100 \cdots\cdots 0$$

$$y = 100 \cdots\cdots 01,2345678\ldots$$

& $x - y$ gives 1.2, truncating the rest)

So there is a trade-off between small h & rounding error.

Recall that computer can calculate $f(x)$ to accuracy $C f(x)$ where $C = 10^{-16}$.

Given that $f(x+h)$ is usually close to $f(x)$, the absolute value on rounding error in worst case will be of $f(x+h) - f(x)$ $2C|f(x)|$

so worst-case rounding error on

$$\frac{f(x+h)-f(x)}{h} \quad \text{is} \quad \frac{2C\,|f(x)|}{h}$$

Also, approx. error is

$\frac{1}{2}h\,|f''(x)|$ for a total error of

$$\varepsilon = \frac{2C\,|f(x)|}{h} + \frac{1}{2}h\,|f''(x)|$$

Find h that minimizes this error,

so take $\frac{d\varepsilon}{dh} = 0$, giving

$$0 = -\frac{2C\,|f(x)|}{h^2} + \frac{1}{2}\,|f''(x)|$$

$$\Rightarrow h = \sqrt{4C\left|\frac{f(x)}{f''(x)}\right|}$$

plugging back in for ε gives

$$\varepsilon = \sqrt{4C\,|f(x)f''(x)|}$$

So if $f(x)$ & $f''(x)$ are of order 1,
then pick h to be of order $\sqrt{c}$,
$\approx 10^{-8}$ & final error will be $\approx 10^{-8}$

Ideas for improvement?

Central difference

$$\frac{df}{dx} \simeq \frac{f(x+h/2) - f(x-h/2)}{h}$$

sample points are still h apart

What is approx. error?

$$f(x+h/2) = f(x) + \tfrac{1}{2} h f'(x) + \tfrac{1}{8} h^2 f''(x) + \frac{1}{48} h^3 f'''(x) + \ldots$$

$$f(x-h/2) = f(x) - \tfrac{1}{2} h f'(x) + \tfrac{1}{8} h^2 f''(x) - \frac{1}{48} h^3 f'''(x) + \ldots$$

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$$\Rightarrow f'(x) = \frac{f(x+h/2) - f(x-h/2)}{h}$$

$$-\frac{1}{24} h^2 f'''(x) + \ldots$$

So we canceled $f''(x)$ term &

approx. error to leading order is

$$\frac{1}{24} h^2 |f'''(x)|$$

Going through what we just did,
total error is

$$\varepsilon = \frac{2c|f(x)|}{h} + \frac{1}{24} h^2 |f'''(x)|$$

differentiating & ~~set~~ nulling gives

$$h = \left(24c\left|\frac{f(x)}{f'''(x)}\right|\right)^{1/3}$$

substituting back in gives error

$$\varepsilon = \left(9/8\, c^2 [f(x)]^2 \,|f'''(x)|\right)^{1/3}$$

So w/ $f(x)$ & $f'''(x)$ of order 1,

take h of order $\epsilon^{1/3}$

$\approx 10^{-5}$ but error is $\approx 10^{-10}$,

a bit better than before.

Taking derivative of a sampled function:

Suppose we have a sampled function @ evenly spaced intervals, a distance h apart.

If we use central differences, then we use points @ $x+h$ & $x-h$

& formula is

$$\frac{df}{dx} \simeq \frac{f(x+h) - f(x-h)}{2h}$$

Does central or forward difference give the more accurate answer?

depends...

total error for central difference w/ $h \to 2h$ is $h^2 |f'''(x)|$

while that for forward differences

$h\,|f''(x)|$, so we would need

$$h < \left| \frac{f''(x)}{f'''(x)} \right| .$$

However, we could calculate derivative @ points in between samples & get better answer, because we would have $x + h/2$ & $x - h/2$

calc derivative here.