Lecture 8

Higher-order integration methods

trapezoidal rule based on straight line segments

Simpson rule based on quadratics

can use higher-order rules, fitting $f(x)$ w/ cubics, quartics, etc.

General form of trap. rule & Simpson rule is

$$\int_a^b f(x)\,dx \simeq \sum_{k=1}^{N} w_k f(x_k)$$

x_k are positions of sample points & w_k are weights.

For trap. rule, x_k are uniformly spaced, 1st & last weights are 1/2 in between are 1

Simpson rule has
weights 1/3 for 1st & last
& weights in between alternate
between 4/3 & 2/3

Higher-order rules have same idea:
fit to some polynomial &
integrate to get weights w_k
that multiply samples $f(x_k)$

Weights up to quartic order

Degree	polynomial	coefficients
1 (trap.)	line	$1/2, 1, 1, \ldots, 1, 1/2$
2 (Simpson)	quadratic	$\frac{1}{3}, \frac{4}{3}, \frac{2}{3}, \frac{4}{3}, \ldots, \frac{1}{3}$
3	cubic	$3/8, 9/8, 9/8, 3/4, 9/8, 9/8, 3/4 \ldots$
4	quartic	$\frac{14}{45}, \frac{64}{45}, \frac{8}{15}, \frac{64}{45}$

Higher-order integration rules
are called Newton-Cotes formulas

Can do better...

trap. rule is exact for straight lines

Simpson rule is exact for quadratics

If we have N sample points, then
we can just fit an N-1 degree
polynomial to the whole interval
⇒ resulting method will be exact
for N-1 degree or lower polynomials.

Can do even better:

been using uniformly spaced sample
points. Advantages are that
1) simple to program
2) increase # of points by picking in between
ones

can use non-uniformly spaced sample points. Main advantage is that they can give very accurate answers w/ small # of sample points.

So let's allow for the possibility to vary not only weights but also sample points.
This is now 2N degrees of freedom & suggests that we could have an integration rule exact for polynomials of order 2N-1

Method to do this is called Gaussian quadratures

Approach: 1) derive integration rules w/ non-uniform sample points

2) Then choose an optimal set of non-uniform sample points.

1) Suppose non-uniform sample points are $\{x_k\}_{k=1}^{N}$

we want an integration rule of the form

$$\int_a^b f(x)\,dx \simeq \sum_k w_k f(x_k)$$

need to choose weights w_k for general $f(x)$

Use method of interpolating polynomials (Lagrange polynomials)

$$\phi_k(x) = \prod_{\substack{m=1,\dots,N \\ m\neq k}} \frac{x - x_m}{x_k - x_m}$$

$$= \frac{(x-x_1)}{(x_k-x_1)} \times \cdots \times \frac{(x-x_{k-1})}{(x_k-x_{k-1})} \times \frac{(x-x_{k+1})}{(x_k-x_{k+1})} \times \cdots \times \frac{(x-x_N)}{(x_k-x_N)}$$

So one factor for each sample point except x_k

So $\phi_k(x)$ is poly in x w/ degree $N-1$

+ there are N different $\phi_k(x)$ for N different sample points

evaluate $\phi_k(x)$ at sample point $x=x_m$

+ get $\phi_k(x_m) = \begin{cases} 1 & m=k \\ 0 & m\neq k \end{cases}$

$= \delta_{m,k}$

Now consider function

$$\Phi(x) = \sum_{k=1}^{N} f(x_k)\, \phi_k(x)$$

This is poly. of degree $N-1$

evaluating at any sample point gives

$$\Phi(x_m) = \sum_{k=1}^{N} f(x_k)\, \phi_k(x_m) = \sum_{k=1}^{N} f(x_k)\, \delta_{km} = f(x_m)$$

So $\Phi(x)$ fits $f(x)$ at all sample points. It is also the *unique* polynomial which does so.

There are N coefficients & N constraints, so this is ~~the~~ one

To get an approximation, just integrate $\Phi(x)$ from a to b

$$\int f(x)\,dx \simeq \int_a^b \Phi(x)\,dx$$

$$= \int_a^b \left[\sum_{k=1}^{N} f(x_k)\,\phi_k(x) \right] dx$$

$$= \sum_{k=1}^{N} f(x_k) \int_a^b \phi_k(x)\,dx$$

So weights are given by

$$w_k = \int_a^b \phi_k(x)\,dx$$

Unfortunately,
No closed-form formula
for $w_k = \int_a^b \phi_k(x)\,dx$

so we need to approximate them
w/ Romberg integration
or Simpson rule.

Point is that we calculate weights
w_k once & then use them to integrate
very many functions.

Another point: you can calculate
weights for a particular set
of sample points & domain of
integration & then map to others

Standard interval for this is
$[-1, 1]$.

So give a set of sample points $x_k \in [-1,1]$
& weights $w_k = \int_{-1}^{1} \phi_k(x)\,dx$

then translate $[-1, 1]$ to $[a, b]$
+ stretch

rule for mapping $x_k \in [-1, 1]$ to $[a, b]$

is $x_k' = \frac{1}{2}(b-a)x_k + \frac{1}{2}(b+a)$

interpretation: translate to midpoint of $[a, b]$ + then stretch out to size of $[a, b]$

if width of interval changes, then rescale by

$$w_k' \equiv \frac{1}{2}(b-a)\,w_k$$

After doing so integral approx. is

$$\int_a^b f(x)\,dx \simeq \sum_{k=1}^{n} w_k' \, f(x_k')$$

We're only solved half the problem.

Now figure out where to place sample points

Figuring this out is based on mathematics of Legendre polynomials.

Recall that our goal is to pick sample points such that integration is exact for polynomials of degree $2N-1$ or less

Legendre polynomial $P_N(x)$ is an Nth order polynomial in x w/ property that

$$\int_{-1}^{1} x^k P_N(x)\, dx = 0 \quad \forall \quad k \in \{0, \dots, N-1\}$$

so orthogonal to all polynomials w/ degree $N-1$ or less

& satisfies normalization $\int_{-1}^{1} [P_N(x)]^2 dx = \frac{2}{2N+1}$

How to find them?

$P_0(x) =$ constant

& normalization imply that

$P_0(x) = 1$

$P_1(x)$ is 1^{st} order poly. $ax+b$

satisfying

$$\int_{-1}^{1} x^0 (ax+b)\, dx = 0$$

Computing integral gives

$$\left. \frac{ax^2}{2} + bx \right|_{-1}^{1} = 2b \Rightarrow b = 0$$

normalization gives $a = 1$

So $P_1(x) = x$

can then use recurrence (non-obvious)

$$(N+1) P_{N+1}(x) = (2N+1)\, x P_N(x) - N P_{N-1}(x)$$

to get higher orders

can find them online...

Suppose $q(x)$ is a polynomial of degree less than N, so that

$$q(x) = \sum_{k=0}^{N-1} c_k x^k$$

Then $\int_{-1}^{1} q(x) P_N(x)\, dx =$

$$\sum_{k=0}^{N-1} c_k \int_{-1}^{1} x_k P_N(x)\, dx = 0$$

Another property: For all N, $P_N(x)$ has N real roots that all lie in $[-1, 1]$

so N values of x in $[-1, 1]$ such that $P_N(x) = 0$

Suppose that $f(x)$ is a polynomial in x of degree $2N-1$ or less

Can divide $f(x)$ by $P_N(x)$
(remember poly. division from high school?)

to get $f(x) = q(x)\, P_N(x) + r(x)$
where $q(x)$ & $r(x)$ are poly's of degree $N-1$ or less

So we can write integral as

$$\int_{-1}^{1} f(x)\,dx = \int_{-1}^{1} q(x)\,P_N(x)\,dx + \int_{-1}^{1} r(x)\,dx$$

$$= \int_{-1}^{1} r(x)\,dx$$

so we only need to find integral of polynomial of degree $N-1$ or less

But we've already done this

For any choice of sample points x_k, a polynomial of degree $N-1$ ~~or~~ or less can be fitted using interpolating polynomials $\phi_k(x)$ & so we have

$$\int_{-1}^{1} f(x)\,dx = \int_{-1}^{1} r(x)\,dx$$

$$= \sum_{k=1}^{N} w_k \, r(x_k)$$

where $w_k = \int_{-1}^{1} \phi_k(x)\,dx$

this equality is exact.

So the method for any poly of degree $2N-1$ or less over $[-1,1]$ is as follows:

1) divide by the Legendre polynomial $P_N(x)$ to get $r(x)$ (remainder poly)
2) Then integrate $r(x)$ using any N sample along w/ corresponding weights

We can be slightly more clever:

We can pick sample points to be any that we wish.

Consider that

$$\sum_{k=1}^{N} w_k f(x_k) = \sum_{k=1}^{N} w_k q(x_k) P_N(x_k) + \sum_{k=1}^{N} w_k r(x_k)$$

recall that $P_N(x)$ has N zeros between -1 $+1$ so choose N sample points to be positions of these zeros.

$$\Rightarrow \sum_{k=1}^{N} w_k f(x_k) = \sum_{k=1}^{N} w_k r(x_k)$$

Since $\int_{-1}^{1} f(x)\,dx = \int_{-1}^{1} r(x)\,dx = \sum_{k=1}^{N} w_k r(x_k)$

$$\Rightarrow \int_{-1}^{1} f(x)\,dx = \sum_{k=1}^{N} w_k f(x_k)$$

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→ we have an integration rule that allows for integrating any poly. $f(x)$ w/ order $2N-1$ or less from $[-1,1]$ + we get an exact answer (up to rounding error).

This is done by using only N sample points.

So choose sample points to coincide w/ zeros of $P_N(x)$ + can show that weights are given by

$$w_k = \left[\frac{2}{1-x^2}\left[\frac{dP_N}{dx}\right]^{-1}\right]_{x=x_k}$$

This method reduces error by $\frac{c}{N^2}$ by including just one extra sample point.
Means we need just about 10-100 sample points to ...