Introduction to Matlab

Lesson 03 — Basics of Root Finding, Numerical Differentiation, and Integration

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Basics of Root Finding

Root Finding — The Problem

Say we want to find all x such that $f(x) = 0$. If:

- $f(x) = ax^2 + bx + c \Rightarrow x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$ solves the problem for any $\{a, b, c\} \in \mathbb{R}$ (and $a \neq 0$).
- Sometimes, we cannot solve explicitly for x even in the realm of polynomials!
- If $f(x) = ax^5 + bx^4 + cx^3 + dx^2 + ex + f$ where $\{a, b, c, d, e, f\} \in \mathbb{R}$ we do not have an explicit formula to solve for $f(x) = 0$. Neither for polynomials of order ≥ 5. But we know **such roots do exist!** see Fundamental Theorem of Algebra
- Then... what should we do?

Root Finding — Intuition

Say we have a nonlinear $f(x)$ for which we know at least one root exists.

- Suppose we know the root is *somewhere around* x_0.
- Starting from x_0 construct a sequence of $\{x_k\}$ hoping it converges to a root x^* such that $f(x^*) = 0$.

This highlights two important features of root finding *algorithms*:

- **Convergence:** is the sequence $\{f(x_k)\}$ getting *closer* to $f(x^*) = 0$?
- **Stopping criteria:** how do we know we are *close enough*?

We can discuss convergence and stopping criteria in each method studied.

Bisection Method

Bisection Method — Intuition

- Say you have a phone book (old school, I know). You need to find García in there.
- What method do you use?

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  1. Turn page by page until you find it.

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  1. Turn page by page until you find it.

  2. Turn every two pages.

Bisection Method — Intuition

- Say you have a phone book (old school, I know). You need to find García in there.

- What method do you use?
  1. Turn page by page until you find it.
  2. Turn every two pages.
  3. Open by the middle, check if G is left or right. Discard one half. Repeat until you find it.

Bisection Method — Intuition

Consider $f : \mathbb{R} \mapsto \mathbb{R}$ where the problem is $f(x^*) = 0$. Suppose $f(x)$ is continuous in $[a, b]$ and we know $\exists x^* \in [a, b]$ (The ideas presented generalize to n dimensions)

- **Bisect** the interval $[a, b]$ and take the middle point $c = \frac{a+b}{2}$. If $f(c) = 0$ we are done. Otherwise, x^* must be in either $[a, c]$ or $[c, b]$.
- Find the one that contains x^* and bisect again. **How?!?**
- Continue until the interval is as small as the accuracy desired.

Bisection Method — Intuition

Theorem 1 (The Intermediate Value Theorem (IVT))
Suppose $f(x)$ is continuous on $[a,b] \subseteq \mathbb{R}$ and M in between $f(a)$ and $f(b)$. Then, there is at least one $c \in (a,b)$ such that $f(c) = M$. If $f(a) < 0 < f(b)$ then, there is a root $x = c$ such that $f(c) = 0$.

- If $f(c) < 0$, by the IVT, the root of $f(x)$ must be in $[c,b]$
- Otherwise, if $f(c) > 0$, by the IVT, the root must be in $[a,c]$
- Note that this algorithm finds **a zero, not all zeros** of $f(x)$

Bisection Method — the Algorithm

1. Initialize and bracket a zero. **(Initial guess)**
   - Find $x^L < x^R$ such that $f(x^L)f(x^R) < 0$
   - Choose stopping rule parameters
2. Compute $x^M = \frac{x^L + x^R}{2}$
3. Test if x^M is a root. If so, stop. **(Test if it is an acceptable solution)**
4. If x^M is not a root, refine interval. **(Iterate)**
   - If $f(x^M)f(x^L) < 0$ let $x^R = x^M$ and leave x^L unchanged.
   - Else, $x^L = x^M$ and leave x^R unchanged.
5. Repeat until the stopping rule tells us to stop.

Bisection Method — Remarks

- The algorithm **always converges** (we always find a solution).
- Convergence can be very slow but it is a very **reliable** method.
- We have not yet defined proper stopping criteria.

Stopping Criteria:

1. The value of the function is lower than or equal to the tolerance $|f(x^M)| \leq \delta$.
2. The length of the interval is very small. $(x^R - x^L)/(1 + |x^L| + |x^R|) \leq \varepsilon$.
3. The number of iterations is larger than a predetermined number N.

Bisection Method — Stopping Criteria

Criterion 1:

- Parameter δ controls the *"acceptable error"*.
- Sometimes, computing $f(x)$ involves other numerical operations that add errors to the computation of f.
- We should take that into account when choosing a value for δ

Bisection Method — Stopping Criteria

Criterion 2:

- The size of the interval is too small whenever

$$\frac{x^R - x^L}{(1 + |x^L| + |x^R|)} \leq \varepsilon$$

- No sense in choosing $\varepsilon = 0$, unachievable. Same for $\varepsilon = 10^{-130}$, computers store finite digits.

- Bear in mind the sizes of x^L and x^R. If x^L and x^R are of the order 10^{10}, convergence of $x^R - x^L < 10^{-5}$ is infeasible.

- Note that adding 1 avoids problems when $x^R \approx x^L \approx 0$

Bisection Method — Stopping Criteria

Criterion 3:

- We can compute the minimum number of iterations N to achieve accuracy δ

- We want the length of the interval after N iterations lower than δ

$$\frac{x^R - x^L}{2^N} \leq \delta \Rightarrow 2^N \geq \frac{x^R - x^L}{\delta}$$

taking logs on both sides and simplifying

$$N \geq \frac{\log(x^R - x^L) - \log(\delta)}{\log(2)}$$

which depends on the length of the interval $[x^L, x^R]$ and the value of δ

Bisection Method — Example

Compute the positive root of $f(x) = x^3 - 6x^2 + 11x - 6$

1. Find the interval $[x^L, x^R]$
2. The function has three positive roots, let's focus on the one on the interval $[2.5, 4]$
3. Note $f(2.5)f(4) = -2.25 < 0 \Rightarrow$ by IVT there is a root in $[2.5, 4]$
4. Choose $\delta = 10^{-4}$ and $\varepsilon = 10^{-8}$
5. The minimum number of iterations needed to achieve accuracy δ is $N^{min} = 13.8$, choose $N = N^{min} + 50$

Bisection Method — The Actual Code

- Initialize with a `while` loop with three conditionals

```
while (error_f > delta) && (error_i > epsil) && (it < maxit
    )
% Actual algorithm in here
end
```

- Middle steps

```
% Compute xm
xm = xl + (xr - xl) / 2; % Slightly improves performance

% Compute value of f at xm
fxm = myf(xm);

% Compute bounds values of f
fxl = myf(xl);
fxr = myf(xr);
```

Bisection Method — The Actual Code

- Compute errors

```
% Compute errors
error_f = abs(fxm);
error_i = (xr - xl)./(1 + abs(xl) + abs(xr));
```

- Update iteration counter and refine interval

```
% Update iteration counter
it = it + 1;

% Update if necessary
if fxm*fxl < 0
    xr = xm;
else
    xl = xm;
end
```

Newton-Raphson Method

Newton-Raphson Method — Intuition

- When using bisection, we have only assumed continuity of $f(x)$
- However, bisection can be slow. Newton-Raphson's method uses properties of **smooth** functions.
- This method is faster but may not always converge.
- **Key idea:** approximate $f(x)$ by a succession of linear functions. Approximate zeros with the zeros of the linear approximations.

Newton-Raphson — Preliminaries

Definition 2

A number c is a **fixed point** of $g(x)$ if $g(c) = c$.

- Note then that $f(x) = 0 \Rightarrow f(x) = x - g(x) = 0$ and any fixed point c of $g(x)$ is a root of $f(x)$ because

$$f(c) = c - g(c) = c - c = 0$$

- Finding a root of $f(x) \equiv$ find a fixed point of $x = g(x)$ such that $f(x) = 0$

- **Problem:** How to rewrite $f(x) = 0$ as $x = g(x)$?

Newton-Raphson — Existence, Uniqueness, and Convergence

Theorem 3 (Fixed-Point Iteration Theorem)

Let $f(x) = 0$ be written as $x = g(x)$. Let $g(x)$ satisfy:

1. $\forall x \in [a, b], g(x) \in [a, b]$

2. $g'(x) \in (a, b)$ *and, for* $q \in (0, 1)$, $g'(x)$ *satisfies* $|g'(x)| < q$ *for all* $x \in (a, b)$

then

1. $\exists! c \in (a, b) : g(c) = c$ ***(Existence of a unique solution)***

2. *For any* $x_0 \in [a, b]$, *the sequence* $\{x_k\}$ *defined by*

$$x_{k+1} = g(x_k)\ ,\ k = 0, 1, \ldots$$

converges to the fixed point $c = g(c)$, *that is to the root* c *of* $f(x) = 0$.

Newton-Raphson — Preliminaries

- In practice, verifying Assumption 1 in Theorem 3 is not easy.
- This method chooses $g(x)$ as $g(x) = x - \frac{f(x)}{f'(x)}$ and the iteration scheme is:

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)} \tag{1}$$

- For this choice, we can state sufficient conditions for convergence.

Theorem 4

Suppose $f(x)$ is $\mathcal{C}^2$ and that $f(x^*) = 0$. If x_0 is sufficiently close to x^*, $f'(x) \neq 0$, and $|f''(x)/f'(x)| < \infty$, the iteration scheme defined by (1) converges to x^*.

Newton-Raphson — Preliminaries

Where does the choice for $g(x)$ come from? Recall Taylor's Theorem and linearly approximate $f(x)$ around x_k:

$$p(x) = f(x_k) + (x - x_k)f'(x_k)$$

- $p(x)$ and $f(x)$ are tangent at x_k and close in the neighborhood of x_k
- Solving for a zero of $p(x) \Rightarrow x = x_k - \frac{f(x_k)}{f'(x_k)}$ which is the iteration scheme (1)
- Which yields our new guess for x_{k+1}

Newton-Raphson — The Algorithm

1. Choose stopping criterion parameters $\{\varepsilon, \delta, N\}$, and a starting point x_0. Set the iteration counter $k = 0$.

2. Compute next iteration using (1)

3. Test for convergence. If either one of the following:
   - $|x_k - x_{k+1}| \leq \varepsilon(1 + |x_{k+1}|)$
   - $|f(x_{k+1})| \leq \delta$
   - $k > N$

   Stop

4. Repeat until one of the convergence criteria is satisfied.

Newton-Raphson — Remarks

- The method is not guaranteed to converge. If after N iterations we have not found a root, the method failed.
- Note that we rely on our initial guess being **close** to the root. If we are far, we may very well fail.
- For some functions and starting points, we may enter an infinite loop. The sequence of iterations will oscillate without converging to any value.
- Even when passing both ε and δ tests, we may not have found a zero.

Newton-Raphson — Some Issues

- Consider $f(x) = x^6$
- $x_{k+1} = (5/6)x_k$
- Still far after 100 iterations!

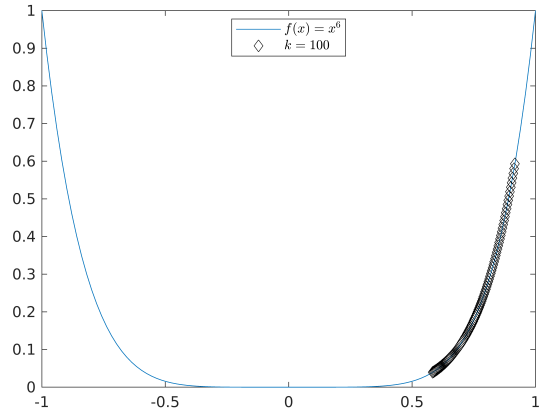

Figure 1: Convergence Issues with Newton-Raphson

Newton-Raphson Method — Example

As with the bisection method, let's compute the root of $f(x) = x^3 - 6x^2 + 11x - 6$ in the interval $[2.5, 4]$. Keep the same stopping criteria parameters.

1. Choose $N = 64, \delta = 10^{-4}$, and $\varepsilon = 10^{-8}$

2. Choose $x_0 = 2.65$.

Newton-Raphson Method — The Actual Code

- Initialize with a `while` loop with three conditionals as in bisection

```
while (error_f > delta) && (error_i > epsil) && (it < maxit
    )
% Actual algorithm in here
end
```

- Middle steps

```
% Compute next guess
xkp = xk - myf(xk) ./ fprime(xk);

% Compute the errors at current guess
error_f = abs(myf(xk));
error_i = abs(xk - xkp) ./ (1 + abs(xkp));

% Update iteration counter and guess
it = it+1;
xk = xkp;
```

Newton-Raphson vs Bisection

- In previous example, it took 14 iterations for the bisection method to find a solution.
- It took Newton-Raphson **half** of those. In 7 iterations it was done.
- Both achieved the same solution.
- Note that the first guess for bisection yields $x^M = 3.25$. If we start Newton-Raphson with that guess, only 4 iterations are needed.
- If we give Newton-Raphson $x_0 = 2.5$, we end up in the root $x^* = 1$.
- Both methods have pros and cons. It depends on the problem which one to choose.

Root Finding in Matlab

- We have learned two very powerful methods to find roots
- Matlab has implemented `fzero` for such problems.
- This function combines bisection with secant and inverse quadratic interpolation (we have not seen this but many ideas apply).
- Another function is `roots` which finds the roots of polynomials.
- Familiarize yourselves with these functions and compare them with the methods we have implemented.

Basics of Numerical Differentiation

Numerical Differentiation — Why?

- Numerical evaluation of the derivatives in economics is **crucial!**
  - Newton-Raphson, optimization, ODEs …

- Sometimes, it is difficult or cumbersome to compute derivatives analytically. In those cases, we turn to *numerical* evaluation of derivatives.

- Recall the definition of the derivative of a function

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$ (can recall why?)

  we can approximate $f'(x)$ by choosing a *step size* h.

- That is called, *finite differences*.

Numerical Differentiation — An Example

Take the function

$$f(x) = x^3 - 6x^2 + 11x - 6$$

- The analytical derivative is

$$f'(x) = 3x^2 - 12x + 11$$

- Let's approximate the derivative by using finite differences in Matlab with on $x \in [-5, 5]$

- Compute dy as $f(x+h) - f(x)$ for a fixed h and $dx = h$.

- The numerical derivative is given by $f'(x) = \frac{dy}{dx}$.

Numerical Differentiation — An Example

As $h \to 0$, the derivative converges.

```
N = 10;
x = linspace(-5,5,N);
h = 1;
% Numerical derivative
dy = myf(x+h) - myf(x);
dx = h.*ones(size(dy));
fp_num = dy./dx;
```

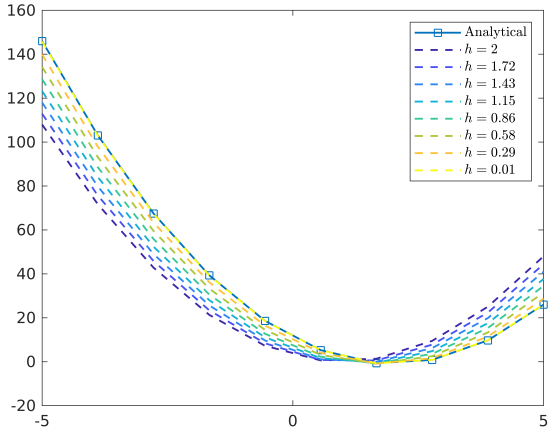

Figure 2: Accuracy of Finite Difference

Numerical Differentiation — An Application to ODEs

- The Solow-Swan growth model finds an equilibrium solution by solving the ODE

$$\dot{k} = \frac{dk}{dt} = sf(k) - \delta k \tag{2}$$

where k is physical capital, $f(k)$ is the production function, s is an exogenous savings rate, and δ is the depreciation rate of capital.

- Approximate $k(t)$ at N discrete points in the time dimension $t^n, n = 1, \ldots, N$ and denote the distance between the points by h.

- Approximate $\dot{k}$ using finite differences $\dot{k}(t^n) \approx \frac{k^{n+1} - k^n}{h}$

- We can compute $k(t^{n+1})$ recursively given h and $k(0) = k_0$

$$k(t^{n+1}) = k(t^n) + h\left(sf(k^n) - \delta k^n\right)$$

Numerical Differentiation — An Application to ODEs

- Horizon $T = 70$
- $N = 10$ points.
- Compare with `ode45` and analytical solution.

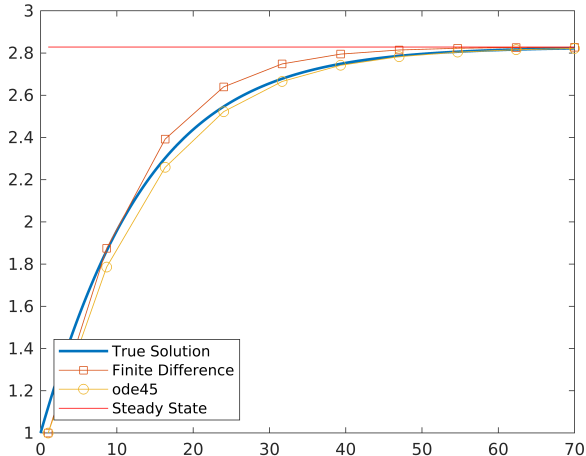

Figure 3: Trajectory for $k(t)$

Symbolic and Automatic Differentiation

- Symbolic differentiation applies the rules of derivatives to symbolic expressions. What we humans do.
- Automatic differentiation breaks codes into smaller sections and applies the chain rule [Kwon 2019, See Chapter 4].
- The advantage of automatic differentiation is that computes **analytical** derivatives at the same cost. No error!
- Automatic differentiation evaluates expressions numerically early, symbolic differentiation at the end.
- Thus, symbolic is more costly. Check Matlab's documentation

Basics of Numerical Integration

Numerical Integration — Why?

- Numerical evaluation of integrals in economics is ubiquitous.
  - Expectations, posteriors in Bayesian statistics, ODEs (again…)
- Again, sometimes it is computationally expensive to compute integrals.
- The definite integral of $f(x)$ is the area under its graph.
- Furthermore, the definition of the definite integral involves an infinte sum (Riemann Sum).
- We will approximate integrals by computing sums in particular ways.

Numerical Integration — Preliminaries

Definition 5

Let $f : [a,b] \mapsto \mathbb{R}$. Let $\mathcal{P}$ and $\mathcal{T}$ be a **partition pair** such that $\mathcal{P}, \mathcal{T} \subset [a,b]$ where $\mathcal{P} = \{x_0, \ldots, x_n\}$, $\mathcal{T} = \{t_1, \ldots, t_n\}$ and

$$a = x_0 \leq t_1 \leq x_1 \leq t_2 \leq x_2 \leq \cdots \leq t_n \leq x_n = b$$

where we assume the points $\{x_0, \ldots, x_n\}$ are distinct. The **Riemann sum** corresponding to $f, \mathcal{P}, \mathcal{T}$ is

$$\mathcal{R}(f, \mathcal{P}, \mathcal{T}) = \sum_{i=1}^{n} f(t_i)\Delta x_i = f(t_1)\Delta x_1 + f(t_2)\Delta x_2 + \ldots + f(t_n)\Delta x_n$$

and $\Delta x_i = x_i - x_{i-1}$.

Notice this is just the area of the rectangles of base Δx_i under the curve of f.

Numerical Integration — Preliminaries

Definition 6

The **mesh** of the partition $\mathcal{P}$ is the length of the largest subinterval $[x_{i-1}, x_i]$.

Definition 7

A real number I is the **Riemann Integral** of f over $[a, b]$ if it satisfies $\forall \epsilon > 0, \exists \delta > 0$ such that if $\mathcal{P}, \mathcal{T}$ is any partition pair, then

$$\text{mesh}(\mathcal{P}) < \delta \Rightarrow |\mathcal{R}(f, \mathcal{P}, \mathcal{T}) - I| < \epsilon$$

If such an I exists it is unique and we denote it by

$$\int_a^b f(x)dx = I = \lim_{\text{mesh}(\mathcal{P}) \to 0} \mathcal{R}(f, \mathcal{P}, \mathcal{T})$$

and we say that f is **Riemann integrable** with Riemann integral I.

Numerical Integration — Intuition

- Notice the definition of the **Riemann integral** is just a weighted sum of the values of f at certain points.

- If the subintervals $[x_{i-1}, x_i]$ are all the same length, the weights are all equal. But we do not need to choose equal weights.

- The problem of numerical integration is also called *cuadrature*.

- There are many cuadrature methods, we will only study a couple of Newton-Cotes formulas. But the general idea is to use a formula such as (3)

$$\int_a^b f(x)dx \approx \sum_{i=1}^{n} \omega_i f(x_i) \tag{3}$$

where ω_i are the weights, and x_i the points.

Numerical Integration — Newton-Cotes Quadratures

General Idea:

- Evaluate $f(x)$ at a finite number of points.
- Construct a piece-wise polynomial approximation of f based on those points.
- Integrate the approximation of f to approximate $\int_a^b f(x)dx$

Numerical Integration — Newton-Cotes Quadratures

- $aUQVb \Rightarrow$ *midpoint rule.*
- $aPRb \Rightarrow$ *trapezoid rule.*
- Parabola $PQSR$

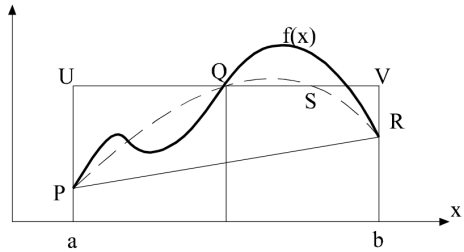

Figure 4: See Judd 1998

Numerical Integration — Newton Cotes Quadratures

Midpoint Rule:

- The simplest quadrature formula with one point given by

$$\int_a^b f(x)dx = \underbrace{(b-a)f\left(\frac{a+b}{2}\right)}_{Rule} + \underbrace{\frac{(b-a)^3}{24}f''(\xi)}_{Error}$$

  for some $\xi \in [a,b]$. Based on Taylor's theorem and the IVT.

- Let $n \geq 1$ be the number of subintervals, $h = (b-a)/n$, and $x_j = a + (j - \frac{1}{2})h$, $j = 1, 2, \ldots, n$. The **composite midpoint rule** (omitting the error) is given by

$$\int_a^b f(x)dx = h\sum_{j=1}^{n} f(x_j) \Rightarrow \textbf{Same as the Riemann Sum!!}$$

Numerical Integration — Newton-Cotes Quadratures

Example 8

Compute $\int_1^5 x^2 dx = \frac{124}{3} \approx 41.333$. Errors decline with the number of points n.

```
function [value] =
    midpoint_rule(a,b,n,myfunc)
  % Numerical integration with
      midpoint rule
  xpts = zeros(n,1);
  h = (b-a)/n;
  for jj=1:n
      xpts(jj,1) = a + (jj -
          1/2)*h;
  end
  value = h*sum(myfunc(xpts));
end
```

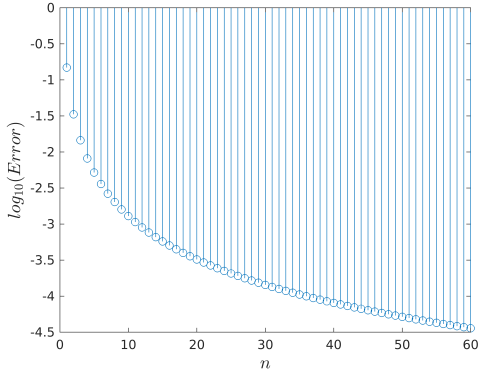

Figure 5: Relative errors in $\log_{10}$ units

Numerical Integration — Newton-Cotes Quadratures

Trapezoid Rule:

- Use linear approximations of f using the end-points of $[a, b]$.
- The rule is

$$\int_a^b f(x)dx = \frac{b-a}{2}(f(a)+f(b)) - \frac{(b-a)^3}{12}f''(\xi)$$

  for some $\xi \in [a, b]$.

- Composite trapezoid rule letting $h = (b-a)/n$ and $x_i = a + ih$

$$\int_a^b f(x)dx = \frac{h}{2}\left(f(x_0) + 2f(x_1) + \cdots + 2f(x_{n-1}) + f(x_n)\right)$$

Numerical Integration in Matlab

- As with root finding, Matlab has routines for numerical integration.
- The trapezoid rule is implemented in `trapz` (you'll work with this on the Problem Set).
- Another routine is `integral`.
- The latter uses adaptive quadratures. Basically, adapts the subintervals refining the process. But the quadrature rules can still be Newton-Cotes.
- For double and triple integrals, Matlab has `integral2` and `integral3` respectively.