ME140A: Numerical Analysis in Engineering

Lecture Notes

Alexander Meiburg

9/22/22 - 11/6/22

Course Organization

- Goal: **Numerical solution of integrals and differential equations**
- Homework will rely significantly on you programming these methods you learn. MATLAB recommended, alternatives welcome
- Collaborate on the homework! You learn more that way. Just make sure that you are, in fact, learning. ☺
- HW: 10% of grade. Exams: 30%/30%/30%.
- Submit homework via email
- Office hours by appointment or Zoom, but my schedule is very open!
- Full syllabus available here
- These notes will be continually updated here

Numerical Integration

Recall: **Differentiation** systematically lets you take a function $F(x)$ and find its derivative $f(x) = F'(x)$.

$$\frac{d}{dx}\left(e^{\sin(x+\log x)}\right) = e^{\sin(x+\log x)}\cos(x+\log x)\,(1+1/x)$$

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Integration asks for the opposite. You have a handful of rules(!), but they can't cover every case. Often impossible, and we resort to defining new functions or using the computer

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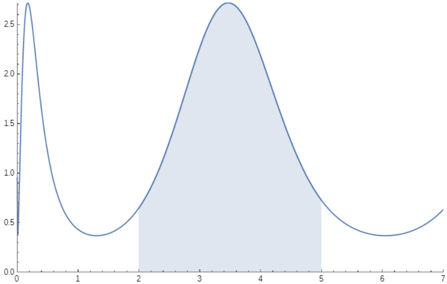

Numerical Integration

Example: Computing the position of an object after some movement.

$$y(t) = \text{Position as a function of time}$$

$$v(t) = \text{Velocity}$$

$$v = \frac{dy(t)}{dt}, \quad y(t) = \int_0^t v(t)\,dt$$

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This last one forms a differential equation, and will need different methods. But many ideas will transfer!
May also have y as an integral over *several* variables, not just one. *e.g.* Dust accumulating on a surface varies with x, y, and t. Can do three integrals in a row (analytically), or one 3D integral (numerically).

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But consider:

t	y(t)
0	5
1	6.1
2	7.3
3	8.4
4	9.8
7	15.3
8	17.4
9	59.8
10	138.7
11	138.8

Issues such as irregular data, or gaps in time too large to understand what happened. Big question in its own right, Week 2!

Newton-Cotes

Problem: given $f(t)$, find $F(t) = \int_0^t f(t)\,dt$. If $f(t)$ is too complicated, let's find something simpler we can integrate. What's simple? Polynomials!

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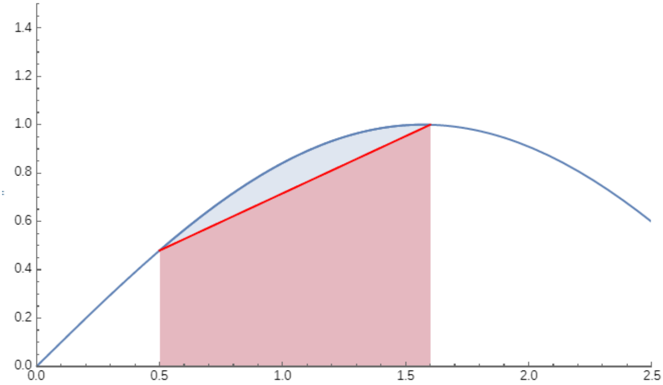
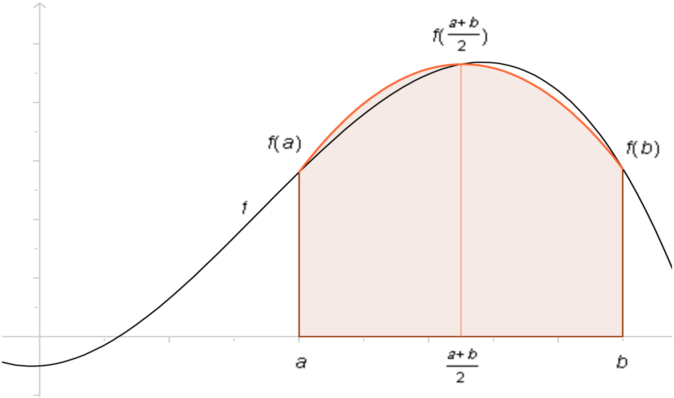
Simplest: Linear fit through two points. ("Trapezoidal rule")



Newton-Cotes

Fit quadratic (”Simpson’s rule”):



Credit: Wikimedia

Newton-Cotes

In general, find

$$f_n(x) = a_0 + a_1 x + a_2 x^2 + \ldots a_n x^n$$

and integrate

$$\int_a^b f_n(x)\, dx$$

Turns out: a_i depend linearly on the $f(x_i)$, so the result is some weighted sum of the $f(x_i)$.

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Trapezoidal:

$$\int_a^b f(x)\, dx \approx \frac{b-a}{2}(f(b) + f(a))$$

Simpson's:

$$\int_a^b f(x)\, dx \approx \frac{b-a}{6}\left(f(b) + 4f\left(\frac{a+b}{2}\right) + f(a)\right)$$

Newton-Cotes

If our function is too complicated over $[a, b]$, then subdivide and do each separately.

$$\int_{x=a}^{b} f(x) = \int_{x=a}^{(a+b)/2} f(x) \quad + \quad \int_{x=(a+b)/2}^{b} f(x)$$

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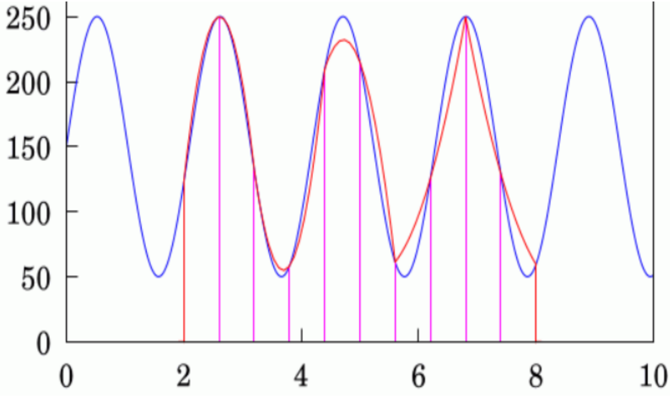

Credit: Wikimedia

Error Analysis

Write

$$f(x) = f(a) + f'(a)(x - a) + \frac{f''(a)}{2}(x - a)^2 + \dots$$

First and second terms accurate, third isn't. Fitting gives

$$E_{trap} \approx \frac{1}{12}|f''(\xi)|(b - a)^2$$

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Refine this with subintervals

Simple Integration Rules

- Left endpoint rule:

$$F = \int_a^b f(x) \approx \frac{(a-b)}{2} f(a)$$

$$\mathrm{Err} \leq |f'| \frac{(b-a)^2}{2}$$

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- Midpoint rule:

$$F = \int_a^b f(x) \approx \frac{(a-b)}{2} f\left(\frac{a+b}{2}\right)$$

$$\mathrm{Err} \leq |f''| \frac{(b-a)^3}{24}$$

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- Trapezoid rule:

$$F = \int_a^b f(x) \approx \frac{(a-b)}{2} \frac{f(a)+f(b)}{2}$$

$$\mathrm{Err} \leq |f''| \frac{(b-a)^3}{12}$$

Simple Integration Rules

- Simpson's "1/3" rule:

$$F = \int_a^b f(x) \approx \frac{(a-b)}{2} \frac{f(a) + 4f((a+b)/2) + f(b)}{3}$$

$$\text{Err} \leq |f^4| \frac{(b-a)^5}{180}$$

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- Simpson's "3/8" rule:

$$F = \int_a^b f(x) \approx \frac{(a-b)}{2} \frac{f(a) + 3f((2a+b)/3) + 3f((a+2b)/3) + f(b)}{8}$$

$$\mathrm{Err} \leq |f^4| \frac{(b-a)^5}{6480}$$

Composite Integration Rules

Subdivide into intervals of size $h = (b - a)/n$.

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$$\int_a^b f(x)\,dx \approx \frac{h}{2}\sum_{j=2}^{n}\left[f(x_{j-1}) + f(x_j)\right] \tag{1}$$

$$= \frac{h}{2}\left[f(x_0) + 2\sum_{j=2}^{n-1} f(x_j) + f(x_n)\right] \tag{2}$$

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Error changes from

$$\mathrm{Err} \le |f''|\frac{(b-a)^3}{12}$$

into

$$\mathrm{Err} \le n \cdot |f''|\frac{((b-a)/n)^3}{12} = |f''|\frac{(b-a)^3}{12n^2}$$

Scaling like $1/n^2$, so this has a *second order* approximation error. (It is a *first order* rule, because it fits a first order polynomial – a line segment.)

Composite Integration Rules

Simpson's 1/3 Rule:

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\sum_{j=1}^{n/2}\left[f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})\right] \tag{3}$$

$$= \frac{h}{3}\left[f(x_0) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + 2\sum_{j=1}^{n/2-1} f(x_{2j}) + f(x_n)\right] \tag{4}$$

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Error changes from

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into

$$\mathrm{Err} \leq n\cdot|f^4|\frac{((b-a)/n)^5}{180} = |f^4|\frac{(b-a)^5}{180n^4}$$

Scaling like $1/n^4$, so this has a *fourth order* approximation error. (It is a *second order* rule, because it fits a second order polynomial.)

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...and beyond?

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...and beyond? These have been extended to use 4th, 5th, 6th... order polynomials, and get higher-order methods. In practice, the $1/n^k$ is not the limiting factor if $k > 4$, and the integral will only improve with smaller intervals.

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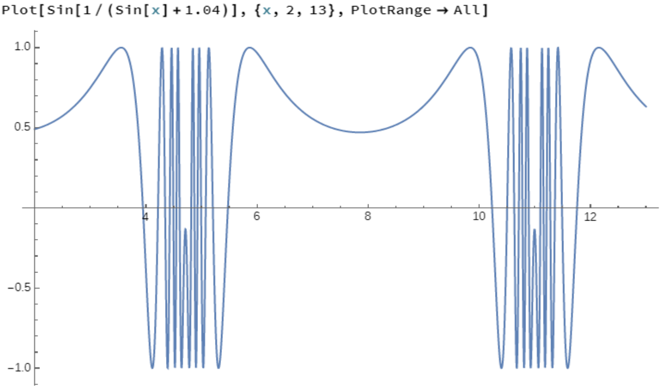
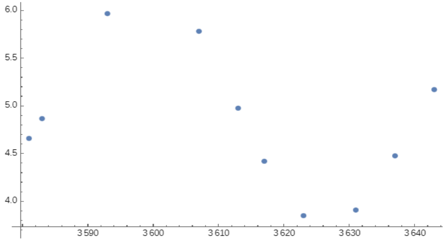


You just can't get this accurate, without having small intervals! And once you get small enough, the function will be roughly quadratic anyway.

Irregular Integration



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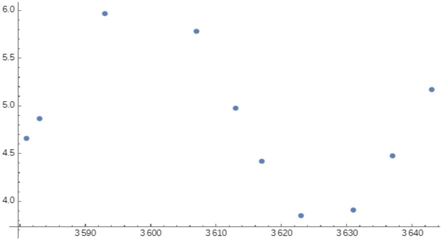
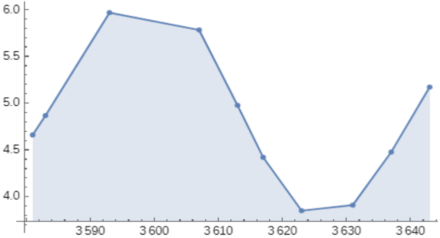
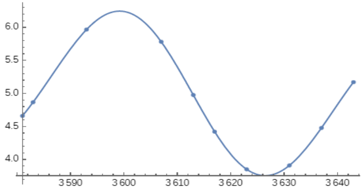


Trapezoidal integration on each part:



Irregular Integration

In principle, we can fit higher-order polynomials as well



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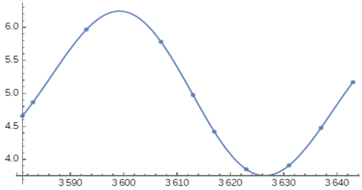
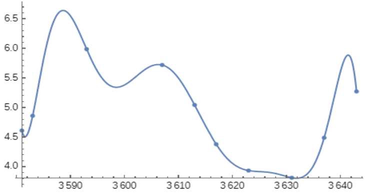


But this can again be very sensitive and unstable:



In practice, also expensive to compute. Need to recompute the "weights" each time, which requires solving a linear system.

Multidimensional Integration

Computing

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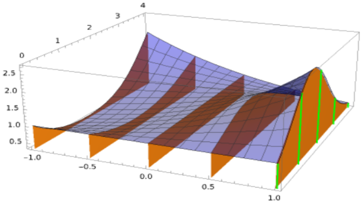
One option: do each integral with its own 1D algorithm.

$$F = \int_{x_1}^{x_2} G(x) \, dx$$

$$G(x) = \int_{y_1}^{y_2} e^{x \sin(y)} + \frac{\ln(y-x)}{\ln(y)} \, dy$$



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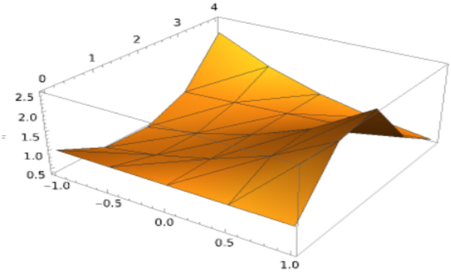
Or, custom multi-dimensional versions of integration rules. Simple functions integrated over squares, triangles, etc.



Richardson Extrapolation

Trapezoidal rule:

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As a function of n, can we study the behavior?

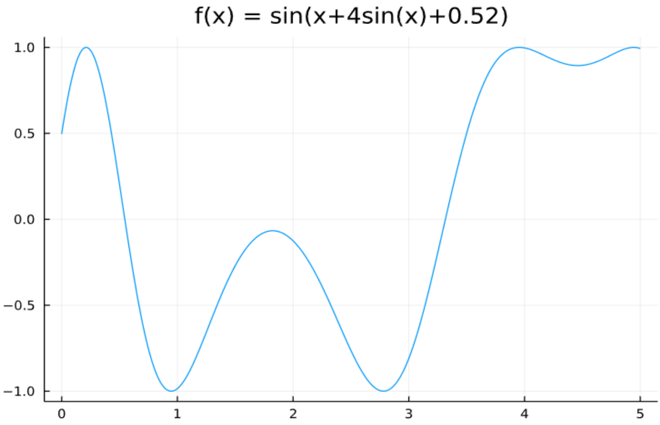
$$I_n \approx c_1 + \frac{c_2}{n^2}$$

Fit some data points, extract the true integral c_1?
With the higher terms,

$$I_n \approx c_1 + \frac{c_2}{n^2} + \frac{c_3}{n^3} + \ldots ?$$

(NB: Actually the next term is only $1/n^4$)

Richardson Extrapolation

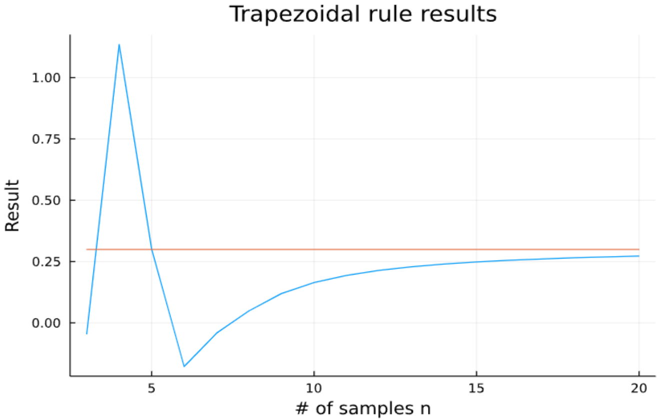


Inspect our function. What kind of accuracy do you think we need?

Richardson Extrapolation

Accuracy has initial "bad" period, then for $n \geq 6$ we see smooth $1/n^2$ decay in error. Estimate the asymptote

Richardson Extrapolation



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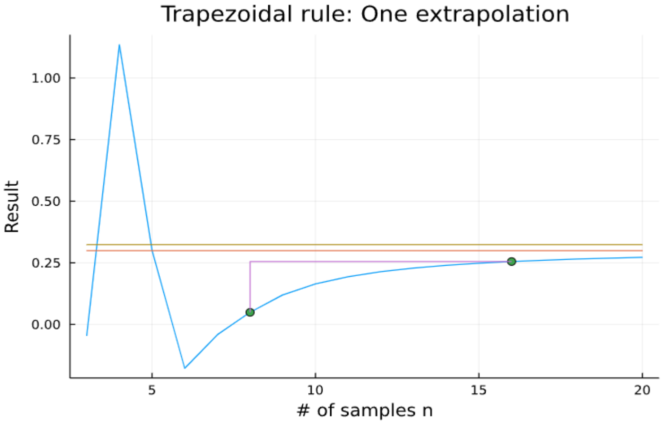

Two point estimate of asymptote: $\frac{4}{3}I_{16} - \frac{1}{3}I_8$

Richardson Extrapolation

This result is a *new* integration rule: take any previous rule with error $1/n^k$, and cancel out the errors. This gives you a new rule with error $1/n^{k+2}$.

If we one integral uses a subset of the other integral's points, we don't need any new samples.

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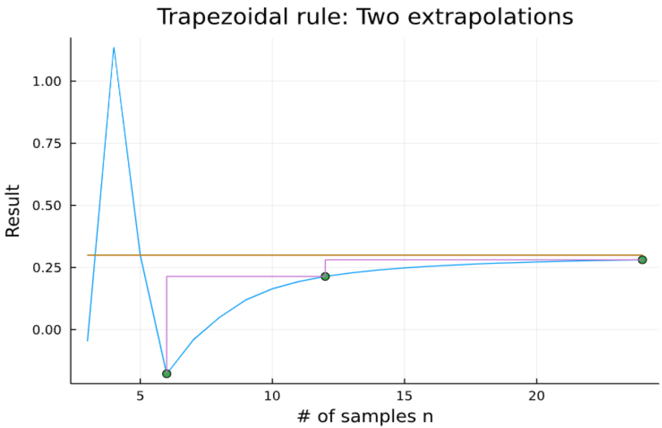
Richardson Extrapolation



Four point estimate of asymptote: $\frac{64}{45} I_{24} - \frac{20}{45} I_{12} + \frac{1}{45} I_6$

Richardson Extrapolation

$n = 24$ trapezoidal error: 0.0183
$n = 24$ one extrapolation: 0.00402
$n = 24$ two extrapolations: 0.00127
We got 10x the accuracy with no extra samples!

Romberg Algorithm

$$I_{j,k} = \frac{4^{k-1} I_{j+1,k-1} - I_{j,k-1}}{4^{k-1} - 1}$$

Here, j is doubling the number of samples: e.g. $j = 4$ has 1000 samples means $j = 5$ has 2000 samples. k is the order of the method: original trapezoid rule starts at $k = 1$.

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$$|\epsilon| \approx \left| \frac{I_{1,k} - I_{2,k-1}}{I_{1,k}} \right|$$

Gaussian Quadrature

Choosing our integration points wisely: reducing error.

$$x_0 = \frac{a+b}{2} - \frac{b-a}{\sqrt{3}}, \quad x_1 = \frac{a+b}{2} + \frac{b-a}{\sqrt{3}}$$

yields a *fourth* order method (depends on $|f^4|$) with only two samples.
[Picture]

1D Stability

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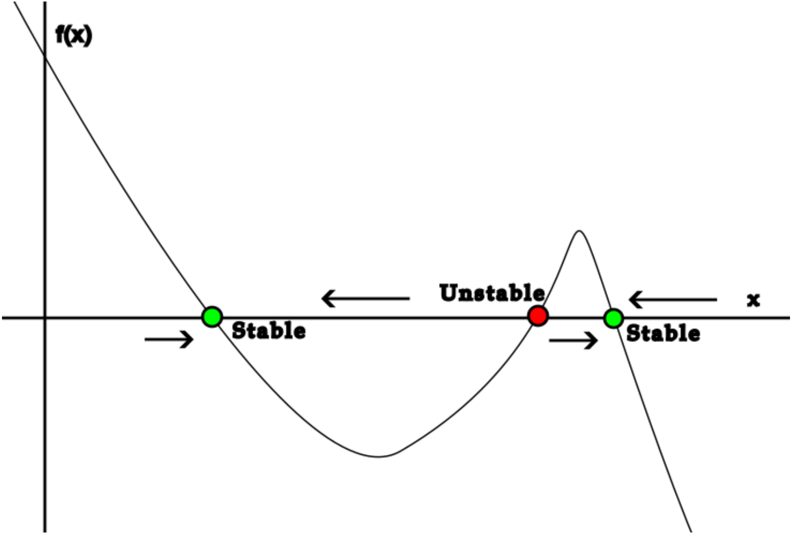
Can't have $x(t) = \sin(t)$, because at the same value of $x = 0$ we have both $\frac{dx}{dt} = 1$ (when $t = 0$) and $\frac{dx}{dt} = -1$ (when $t = \pi$).

1D Stability



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If we're at $x(0) = x_0 - \epsilon$, opposite occurs. Can tell which will happen using the *derivative of* f.

1D Stability

The *fixed points* will occur where

$$\frac{dx}{dt} = 0 \implies f(x) = 0$$

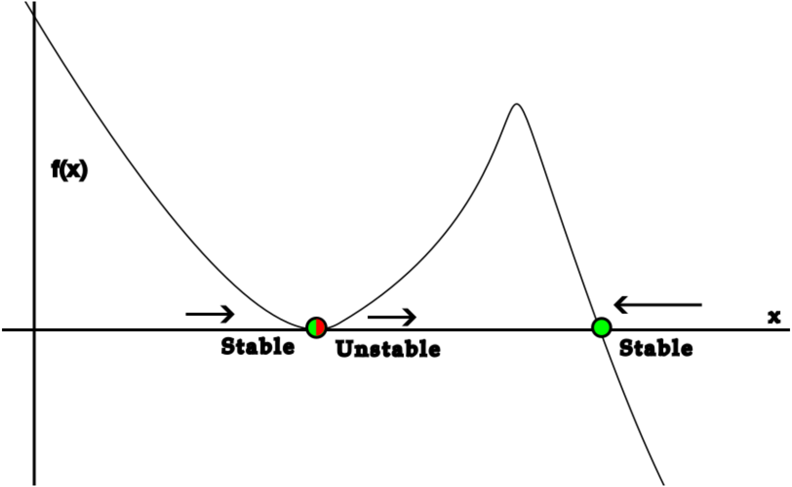
Suppose x_0 is a fixed point, and we're at $x(0) = x_0 + \epsilon$. What happens?

If $f(x)$ is positive, then we'll keep increasing, and move away from the fixed point, and ϵ grows. If $f(x)$ is negative, we'll decrease, and head back towards x_0.

If we're at $x(0) = x_0 - \epsilon$, opposite occurs. Can tell which will happen using the *derivative of f*.

$$\begin{aligned} f'(x_0) > 0 &\implies \epsilon \text{ grows} &\implies \text{Unstable} \\ f'(x_0) < 0 &\implies \epsilon \text{ shrinks} &\implies \text{Stable} \end{aligned}$$

1D Stability



1D Stability

When $f(x_0) = 0$ and $f'(x_0) = 0$, we can have *half stability*: stable from one side, not from the other. Which side is which depends on $f''(x_0)$. Not all such points are half-stable. For example, consider $f(x) = x^3$. Also keep in mind $f(x) = |x|$ or $f(x) = -\sqrt[3]{x}$. Now f isn't differentiable at zero, but we can still see that $|x|$ is half-stable and $-\sqrt[3]{x}$ is stable.

Multivariate Stability

What happens with the two-variable system

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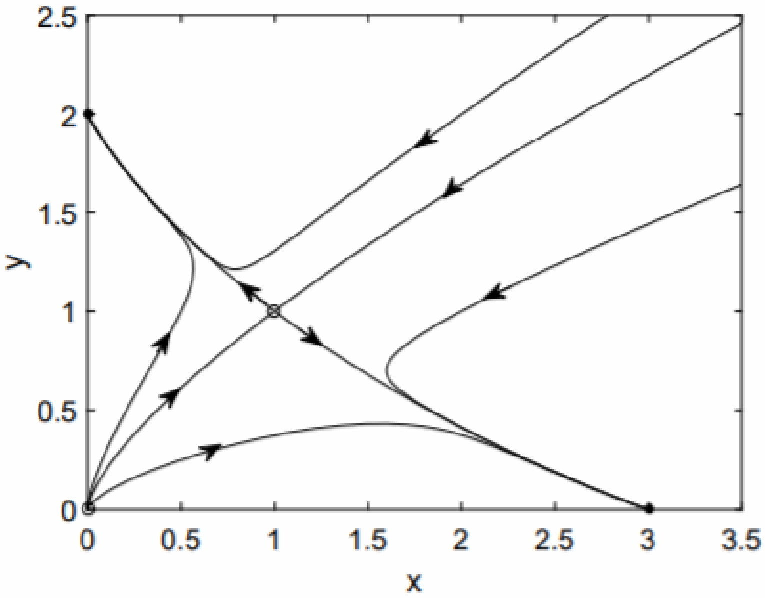
More than just unstable and stable! Can have indefinite oscillations.

Multivariate Stability



Can still discuss fixed points, at least. Points where

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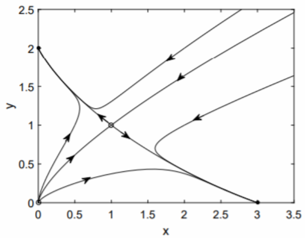
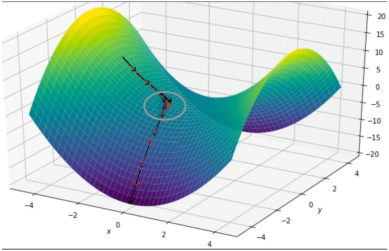
Fixed points can be:

- Stable: small perturbation shrinks in size
- Unstable: small perturbations grow without bound
- Saddle nodes / saddle points: approach from two directions, but ultimately unstable

Multivariate Stability





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Multivariate Stability

Cordura Trail

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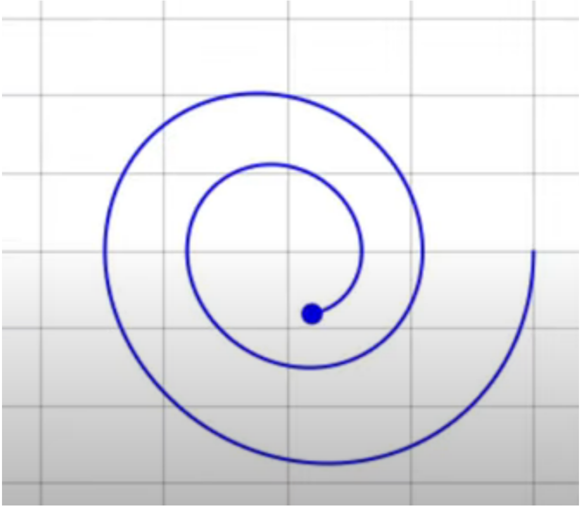
Cycles could:

- Gradually peter out – actually a stable fixed point! Damped harmonic oscillator.
- Conserve some quantity. Infinitely many cycles, coexisting. Undamped oscillator
- Have a natural radius – stable cycles! Driven, damped oscillator (e.g. vibrating, resonating machinery)

Multivariate Stability

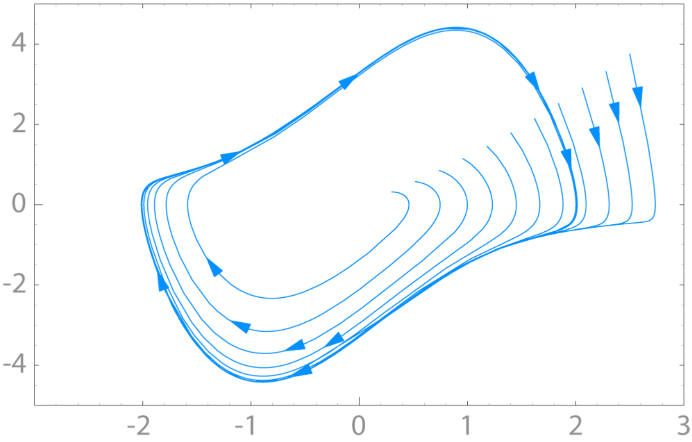
Damped harmonic oscillator:



Fixed point at $(0, 0)$. The derivatives there can tell us whether it falls "straight" in or spirals around.

Multivariate Stability

Stable, driven cycle – or *limit cycle*. e.g. Van der Pol equation:



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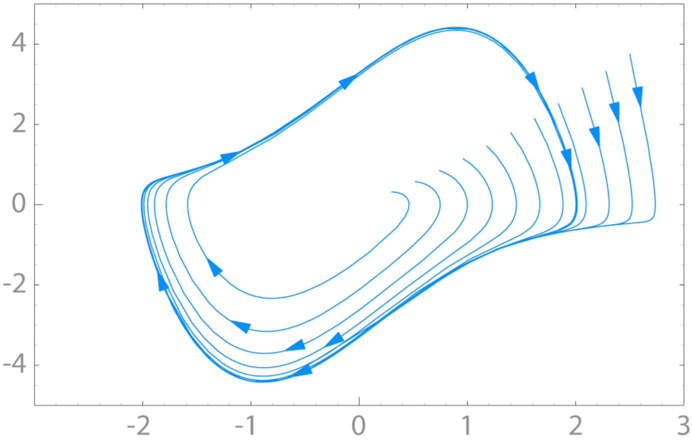

credit Run it backwards, and we have an *unstable limit cycle*.

Jacobian

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$$J = \begin{bmatrix} \frac{\partial f}{\partial x} & \frac{\partial f}{\partial y} \\ \frac{\partial g}{\partial x} & \frac{\partial g}{\partial y} \end{bmatrix}$$

Intuitively, J tells us how

$$x(0) = x_0 + \epsilon_x, \quad y(0) = y_0 + \epsilon_y$$

evolves. Approximately,

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This *linear* ODE has a simple solution in terms of the eigenvalues of J.

Jacobian

In terms of the eigenvalues of J:

- All eigenvalues of J have positive real part: unstable
- All negative: stable fixed point
- Mixture of positive and negative: saddle node
- Zero real part: like 1D, needs further analysis.
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This all holds in any number of variables. In 2D, easy tests:

$$J = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$$

$$\det(J) = ad - bc, \quad \mathrm{Tr}(J) = a + d$$

The $\det(J)$ is the product of the two eigenvalues, $\mathrm{Tr}(J)$ is the sum.

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$$\det(J) > \frac{(\mathrm{Tr}(J))^2}{4}$$

Jacobian: Damped Harmonic Oscillator

Example: a damped harmonic oscillator.

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If $\gamma = 0$, the eigenvalues are $\pm i\sqrt{k}$ – purely imaginary, and it's neither stable nor unstable (just oscillates forever).