BIOQ 2011/12
A401N1 - Análise Matemática
Lecture notes

Salvatore Cosentino

Departamento de Matemática e Aplicações - Universidade do Minho

Campus de Gualtar, 4710 Braga - PORTUGAL

gab B.4023, tel 253 604086 (atendimento: 4ª-feira 11h-12h e 14h-16h)

e-mail scosentino@math.uminho.pt

url http://w3.math.uminho.pt/~scosentino

January 14, 2012

Abstract

This is not a book! These are personal notes written while preparing lectures on "Análise Matemática" for students of BIOQ in the a.y. 20011/12. They are rather informal and may even contain mistakes. I tried to be as synthetic as I could, without missing the observations that I consider important.

I probably will not lecture all I wrote, and did not write all I plan to lecture. So, I included empty or sketched paragraphs, about material that I think should/could be lectured within the same course.

References contain some introductory manuals that I like, some classics, and other books where I have learnt things in the past century. Besides, good material and further references can easily be found on the web, for example in Scholarpedia , in Wikipedia or in KhanAcademy. For a modern statement (and a good bibliography) about the interplay between Mathematics and Biology you may read the report in `http://www.bio.vu.nl/nvtb/Contents.html`

We will do simulations, using some of the software at our disposal in laboratories: this includes proprietary software like `Mathematica`®`8` , `Matlab` and Maple , or open software like `Maxima` and GeoGebra . Occasionally, we'll also use some `c++` code and `Java` applets. Some applets are in the bestiario in my web page, and everything about the course may be found in my page `http://w3.math.uminho.pt/~scosentino/teaching/am_BIOQ_2011-12.html`.

e.g. means EXEMPLI GRATIA, that is, "for example", and is used to introduce important or (I hope!) interesting examples.

ex: means "exercise", so that you are invited to solve it by yourself.

ref: means "references", places where you can find and study what follows inside each section.

Pictures were made with *Grapher* on my MacBook, or with `Mathematica`®`8` , or taken from the Wikipedia.

Contents

1 Crescimento e decaimento

ref: [Ap69] [EK05]

e.g. Fibonacci numbers. Considere o seguinte problema, posto por Leonardo Pisano (mais conhecido como Fibonacci, ou seja, "filius Bonacci") no seu *Liber Abaci*, 1202:

> *Quot paria cuniculorum in uno anno ex uno pario germinentur.*
> *Quidam posuit unum par cuniculorum in quodam loco, qui erat undique pariete circundatus, ut sciret, quot ex eo paria germinarentur in uno anno: cum natura eorum sit per singulum mensem aliud par germinare; et in secundo mense ab eorum nativitate germinant.*[1]

Seja f_n o número de pares de coelhos presentes no n-ésimo mês. O número $f_{n+1} - f_n$ de pares de recém-nascidos no $(n+1)$-ésimo mês é igual ao número de pares adultos presentes no n-ésimo mês, que é igual a f_{n-1}. Portanto, os f_n's satisfazem a lei recursiva

$$f_{n+1} = f_n + f_{n-1}\,, \tag{1.1}$$

que determina os valores de f_n dados os valores iniciais f_0 and f_1.

The sequence grows quite fast, as you can see,

$$1, 1, 2\ , 3, 5, 8, 13, 21, 34, 55, 89, 144, 233, 377, 610, 987, 1597, 2584\ , \dots$$

and the numbers soon become astronomically large. For example, after 10 years we get (assuming there is no death!)

$$f_{120} \simeq 8.67 \times 10^{24}\,,$$

larger than the Avogadro number!

help: An applet which computes the sequence is in my bestiario.

help: A `Java` or `c++` recursive definition could be

```
int Fib(int n)
  {
    if (n==0) return 1;
    else if (n==1) return 1;
    else return Fib(n-1) + Fib(n-2);
  }
```

help: With `Mathematica`®`8` , you may use the command

```
RecurrenceTable[{f[n + 1] == f[n] + f[n - 1], f[0] == 1,  f[1] == 1}, f, {n, 0, 12}]
```

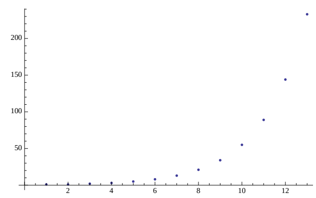
press `shift` + `return` and get the answer

```
{1, 1, 2, 3, 5, 8, 13, 21, 34, 55, 89, 144, 233}
```

Then, you may want to plot your sequence with the command

```
ListPlot[%, PlotRange -> All]
```

press `shift` + `return` and here is what you get:



[1] Quantos pares de coelhos podem ser gerados por um par em um ano.
Alguém tem um par de coelhos, em um lugar inteiramente fechado, para descobrir quantos pares de coelhos podem ser gerados deste par em um ano: por natureza, cada par de coelhos gera cada mês outro par, e começa a procrear a partir do segundo mês após o nascimento.

e.g. Duplicação de células. As experiências mostram que a população de uma colónia de bactérias, num período de tempo em que podemos considerar ilimitado o nutrimento e desprezáveis as toxinas produzidas, duplica-se em cada tempo característico $\tau > 0$. Assim, uma população inicial de N_0 células, dá origem a uma população de $N_1 = 2N_0$ células passado o tempo τ, $N_2 = 4N_0$ células passado o tempo 2τ, ..., de

$$N_n = 2^n N_0$$

células passado o tempo $n\tau$. A lei recursiva que produz esta sucessão é

$$N_{n+1} = 2N_n \, .$$

Por exemplo, uma única célula dá origem a 1024 células passado um tempo $n\tau$ dado por $2^n = 1024$, ou seja, $n\tau = (\log_2 1024)\tau = 10\tau$.

Sequences. A (real valued) *sequence* is a collection $(x_n)_{n\in\mathbb{N}_0}$ of (real) numbers $x_n \in \mathbb{R}$, indexed (hence ordered) by a non-negative integer $n \in \mathbb{N}_0 := \{0, 1, 2, 3, \dots\}$. We may think of the index n as "time", and therefore at the n-th term x_n as the value of some "observable" (something that we may observe, i.e. measure) x at time n. Clearly, we may as well define sequences with values in an arbitrary set X, for example in the Euclidean space $\mathbb{R}^d$.

Sequences may be defined as functions are. Indeed, a sequence with values in the set X is nothing but a function $x : \mathbb{N}_0 \to X$, disguised by the notation $x_n := x(n)$. A second possibility is some recursive law

$$x_{n+1} = f(x_0, x_1, \dots, x_n)$$

prescribing the value of x_{n+1} given the (past) values of x_0, x_1, ..., x_n. A third possibility, is using some property that the successive terms must have.

[Ap69]

e.g. Arithmetic progression. An *arithmetic progression*

$$x_n = a + nb$$

which may also be defined using the recursion $x_{n+1} = x_n + b$, with initial term $x_0 = a$. It represents the successive positions of a walk starting at a with step b.

e.g. The primes sequence. The sequence

$$2, \; 3, \; 5, \; 7, \; 11, \; 13, \; 17, \; 19, \; 23, \; \dots$$

whose generic term is the n-th prime number p_n. It is not clear what the recursive law could be.[2]

Limits. We say that the real sequence (x_n) *converges* to some *limit* $a \in \mathbb{R}$, and we write $\lim_{n\to\infty} x_n = a$ or simply $x_n \to a$ (as $n \to \infty$), if for any "precision" $\varepsilon > 0$ there exists a time $\overline{n}$ such that $|x_n - a| < \varepsilon$ for all times $n \geqslant \overline{n}$. This means that the values x_n are within an arbitrarily small neighborhood of a as long as the time n is sufficiently large.

The basic fact about limits in the real line $\mathbb{R}$ is that monotone (non-decreasing or non-increasing, i.e. satisfying $x_{n+1} \geqslant x_n$ or $x_{n+1} \leqslant x_n$, for any n, respectively) bounded (i.e. such that $|x_n| \leqslant M$ for some $M > 0$ and all n) sequences of real numbers do admit limit.

We also use the notation $x_n \to \pm\infty$ to say that given an arbitrarily large $K > 0$ we can find a time $\overline{n}$ such that $\pm x_n > K$ for all times $n \geqslant \overline{n}$.

Of course, there exist sequences which do not admit limits in either senses. These are, for example, oscillating sequences, as $x_n = (-1)^n$. We'll encounter sequences with much more wild behavior.

[Ap69]

[2] This is not the place to talk about it, but if you find it intriguing, you may take a look at the wonderful book by Marcus du Sautoy, *The music of primes*, Harper-Collins, 2003 [*A música dos números primos*, Zahar, 2008].

Geometric progression. The most important sequence is the *geometric progression*, defined starting from an initial term $x_0 = a$ using the recursion

$$x_{n+1} = \lambda x_n .$$

Thus, the sequence is

$$x_0 = a \qquad x_1 = a\lambda \qquad x_2 = a\lambda^2 \qquad \dots \qquad x_n = a\lambda^n \qquad \dots$$

The parameter λ (which may be real or complex) is called *ratio*, since it is the ratio x_{n+1}/x_n between successive terms of the sequence. The geometric sequence clearly converges to zero when $|\lambda| < 1$, and is constant, hence trivially convergent, when $\lambda = 1$. We may also observe that $|\lambda^n| \to \infty$ when $|\lambda| > 1$.

Computing limits. Observe that $x_n \to a$ is equivalent to $x_n - a \to 0$. Therefore, we only need to understand how to "prove" that some sequence converges to zero.

One possibility is to "compare" the sequence (x_n) under investigation with a sequence with known behavior, as for example the geometric progression. Indeed, if $|x_n| \leqslant y_n$ for all n sufficiently large, then $y_n \to 0$ implies $x_n \to 0$ too.

Limsup and liminf. Sometimes we are only interested in a rough estimate of the growth of a sequence (x_n). The "limsup" is the limit

$$\limsup_{n\to\infty} x_n := \lim_{n\to\infty} a_n \in \mathbb{R} \cup \{\infty\}$$

of the non-increasing sequence $a_n := \sup\{x_n, x_{n+1}, x_{n+2}, \dots\}$. The "liminf" is the limit

$$\liminf_{n\to\infty} x_n := \lim_{n\to\infty} b_n \in \mathbb{R} \cup \{-\infty\}$$

of the non-decreasing sequence $b_n := \inf\{x_n, x_{n+1}, x_{n+2}, \dots\}$.

e.g. Tempo de meia-vida. O decaimento de uma substância radioactiva pode ser caracterizado pelo "tempo de meia-vida" τ, passado o qual aproximadamente metade dos núcleos inicialmente presentes terá decaido (dentro de uma amostra suficientemente grande). Se q_n denota a quantidade de substância radioactiva presente no instante $n\tau$, com $n = 0, 1, 2, \dots$, então

$$q_{n+1} = \frac{1}{2} q_n .$$

Portanto a quantidade de substância radioactiva no instante $n\tau$ é $q_n = q_0 2^{-n}$, enquanto o produto do decaimento é $q_0 - q_n = q_0(1 - 2^{-n})$. Observe que $q_n \to 0$ quando $n \to \infty$.

Se os a radiação solar produz núcleos radioactivos a uma taxa constante $\alpha > 0$ (i.e. α núcleos cada tempo τ), a quantidade de núcleos radioactivos no instante $n\tau$ é dada pela lei recursiva

$$q_{n+1} = \frac{1}{2} q_n + \alpha . \tag{1.2}$$

Um equilíbrio é possível quando a quantidade inicial q_0 é igual a $\overline{q} := 2\alpha$, pois então $q_1 = \alpha + \alpha = q_0$, $q_2 = \alpha + \alpha = q_1 = q_0$, e assim a seguir, $q_n = \overline{q}$ para todos os $n \in \mathbb{N}$.

O que acontece se $q_0 \neq \overline{q}$? A equação recursiva diz que

$$\begin{aligned}
q_1 &= \frac{1}{2} q_0 + \alpha \\
q_2 &= \frac{1}{4} q_0 + \frac{1}{2}\alpha + \alpha \\
q_3 &= \frac{1}{8} q_0 + \frac{1}{4}\alpha + \frac{1}{2}\alpha + \alpha \\
&\vdots \\
q_n &= \frac{1}{2^n} q_0 + \left(\frac{1}{2^{n-1}} + \cdots + \frac{1}{8} + \frac{1}{4} + \frac{1}{2} + 1 \right) \alpha
\end{aligned}$$

A primeira parcela $q_0/2^{n+1} \to 0$ quando $n \to \infty$, ou seja, o futuro é independente da condição inicial q_0. A segunda parcela tem limite 2α quando $n \to \infty$ (uma prova está no parágrafo sobre a série geométrica!).

Uma fórmula (aparentemente) mais simples para os q_n pode ser obtida usando a substituição $x_n := q_n - \overline{q}$, onde $\overline{q} = 2\alpha$ é a solução estacionária. De facto,

$$\begin{aligned} x_{n+1} &= q_{n+1} - 2\alpha \\ &= \frac{1}{2} q_n + \alpha - 2\alpha \qquad \text{(usando a (1.2))} \\ &= \frac{1}{2} x_n \, , \end{aligned}$$

ou seja, a diferênça entre q_n e $\overline{q}$ é uma progressão geométrica de razão 1/2. Portanto $x_n = x_0 2^{-n}$, donde

$$q_n = 2\alpha + (q_0 - 2\alpha) \cdot 2^{-n} \, .$$

É interessante observar que $x_n \to 0$, e de consequência $q_n \to \overline{q}$, quando $n \to \infty$. Ou seja, a quantidade de substância radioactiva converge para o valor estacionário, independentemente do valor inicial.

ex: O tempo de meia-vida do radiocarbono ^{14}C é $\tau \simeq 5730$ anos. Mostre como datar um fóssil, sabendo que a proporção de ^{14}C num ser vivente é fixa e conhecida.[3]

e.g. Crescimento exponencial. O crescimento exponencial de uma população num meio ambiente ilimitado é modelado pela equação recursiva

$$p_{n+1} = \lambda p_n \, ,$$

onde p_n representa a população no tempo n, dada uma certa população inicial p_0. Um significado do parâmetro λ é o seguinte: em cada unidade de tempo o incremento $p_{n+1} - p_n$ da população é igual a soma de uma parcela αp_n, onde $\alpha > 0$ é um coeficiênte de fertilidade, e uma parcela $-\beta p_n$, onde $\beta > 0$ é um coeficiênte de mortalidade.

Se a uma população que cresce segundo o modelo exponencial, é adicionada ou retirada uma certa quantidade β em cada unidade de tempo, o modelo é

$$p_{n+1} = \lambda p_n + \beta \, ,$$

onde β é um parâmetro positivo ou negativo.

ex: Determine a solução estacionária de $p_{n+1} = \lambda p_n + \beta$, e a solução com condição inicial p_0 arbitrária (considere a substituição $x_n = p_n - \overline{p}$, onde $\overline{p}$ é a solução estacionária). Para quais valores dos parâmetros λ e β as soluções p_n convergem para a solução estacionária quando o tempo $n \to \infty$?

help: An applet with the simulations is in exponentialgrowth.

help: A `Java` or `c++` cycle could be

```
for (int i = 0, i < n, i++)
  {
    population = lambda * population + beta;
  }
```

[3] J.R. Arnold and W.F. Libby, Age determinations by Radiocarbon Content: Checks with Samples of Known Ages, *Sciences* **110** (1949), 1127-1151.

e.g. Growth of Fibonacci numbers. We want to understand how fast do Fibonacci numbers grow. We call $q_n := f_{n+1}/f_n$the quotients between successive Fibonacci numbers. They satisfy the recursive law

$$q_{n+1} = 1 + 1/q_n \tag{1.3}$$

which is an immediate consequence of (1.1). An applet with the sequence is in fibonacci. We compute:

$$1 \,, \quad 2 \,, \quad 3/2 = 1.5 \,, \quad 5/3 \simeq 1.66666 \,, \quad 8/5 = 1.6 \,, \quad 13/8 = 1.625 \,, \quad 21/13 \simeq 1.61538 \,, \quad \dots$$

It turns out that the sequence of the q_n converge, namely $q_n \to \phi$ as $n \to \infty$. Taking limits in the recursive equation $q_{n+1} = 1 + 1/q_n$ we see that $\phi = 1 + 1/\phi$, so that ϕ is a root (positive) of the polynomial $x^2 - x - 1$, i.e.

$$\phi = \frac{1+\sqrt{5}}{2} \simeq 1.6180339887498948482\dots$$

Hence, for large values of n we may approximate Fibonacci law as

$$f_{n+1} \approx \phi f_n \,,$$

an exponential growth with rate ϕ. In particular, we expect $f_n \sim \phi^n$.

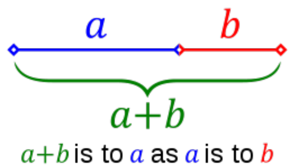
The limit ϕ is a famous irrational, the Greeks' *ratio/proportion*. As described by Euclid[4]:

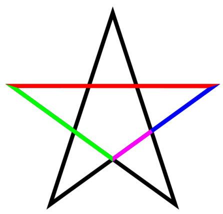
> *"A straight line is said to have been cut in extreme and mean ratio when, as the whole line is to the greater segment, so is the greater to the less."*

If a is the greater part and b the less of a line of lenght $a+b$, Euclid's requirement is

$$\frac{a+b}{a} = \frac{a}{b}$$

There follows that the ratio $\phi = a/b$ satisfies $1 + 1/\phi = \phi$. This division of an interval is used in Book IV of the *Elements* to construct a regular pentagon.





Extreme and mean ratio, and regular pentagon.
(from http://en.wikipedia.org/wiki/Golden_ratio)

e.g. Invenção do xadrez. Dizem que o sábio hindu Sissa inventou o jogo do xadrez e o ofreceu ao rei de Pérsia. Ao rei, que o convidou a escolher uma recompensa, pediu um grão de arroz (ou era trigo?) para o primeiro quadrado do tabuleiro, o dobro, ou seja, dois grãos, para o segundo quadrado, o dobro, ou seja, quatro grãos, pelo terceiro quadrado, e assim a seguir até o último dos quadrados do tabuleiro. O rei riu-se, num primeiro instante, mas ... a recompensa é

$$1 + 2 + 4 + 8 + \cdots + 2^{63} \simeq 1.84 \times 10^{19}$$

(see (1.4) below) grãos de arroz.

Se 1 Kg de arroz contém ≈ 30000 grãos, isto significa algo como 6.13×10^{11} toneladas de arroz (which you may want to compare with People's Republic of China's production in 2008, which has been, according to FAO, about 1.93×10^8 metric tons!).

[4]Euclid, *Elements*, Book VI, Definition 3.

Series. A *series* is a formal infinite sum

$$“\sum_{n=0}^{\infty} x_n = x_0 + x_1 + x_2 + x_3 + \dots” ,$$

where the $x_n \in \mathbb{R}$ are elements of some given real (or complex) sequence. If the sequence (s_n) of *partial sums*, defined as $s_n := \sum_{k=0}^{n} x_k$ (which are honest numbers) converges to some limit, say $\lim_{n\to\infty} s_n = s$, then we say the series is *convergent* (or *summable*), and that its *sum* is

$$\sum_{n=0}^{\infty} x_n := s .$$

A series $\sum_n x_n$ is *absolutely convergent* is the series $\sum_n |x_n|$, formed with the absolute values of its terms, is convergent. Of course, absolute convergence is stronger than mere convergence.

[Ap69]

Geometric series. A identidade $(1 + \lambda + \lambda^2 + \lambda^3 + ... + \lambda^n)(\lambda - 1) = \lambda^{n+1} - 1$ mostra que, se $\lambda \neq 1$, a soma dos primeiros $n + 1$ termos da progressão geométrica (com $a = 1$) é

$$1 + \lambda + \lambda^2 + \lambda^3 + ... + \lambda^n = \frac{\lambda^{n+1} - 1}{\lambda - 1} \tag{1.4}$$

Em particular, quando $|\lambda| < 1$, a *série geométrica* $\sum_{n=0}^{\infty} \lambda^n$ é (absolutamente) convergente, e a sua soma é

$$1 + \lambda + \lambda^2 + \lambda^3 + ... + \lambda^n + ... = \frac{1}{1 - \lambda} . \tag{1.5}$$

e.g. **Dichotomy paradox.** Using the above formula (1.5) for the sum of the geometric series, you may try to convince Zeno that

$$1/2 + 1/4 + 1/8 + 1/16 + 1/32 + ... = 1 .$$

e.g. **Decimal expansions.** Also, you may convince yourself that 0.99999 . . . , which by definition is the sum of the series

$$0.99999\ldots \quad = \quad \frac{9}{10} + \frac{9}{100} + \frac{9}{1000} + \frac{9}{10000} + \dots ,$$

is not “almost one” or “a bit less than one”, as somebody says, but actually equal to

$$\begin{aligned} 0.99999\ldots &= \frac{9}{10}\left(1 + \frac{1}{10} + \frac{1}{100} + \frac{1}{100} + \dots\right) \\ &= \frac{9}{10} \cdot \frac{1}{1 - \frac{1}{10}} \\ &= 1 . \end{aligned}$$

Moreover, you may learn how to recognize rational numbers as 0.33333 . . . or 1.285714285714 . . . from their (eventually) periodic expansion. Indeed, *a real number is rational if and only if its base 10 (or any other base $d \geqslant 2$) expansion is eventually periodic.*

ex: Diga se a seguintes séries são convergentes, e, se for o caso, calcule a soma.

$$1 + 1/2 + 1/4 + 1/8 + 1/16 + ... \qquad 1 + 10 + 100 + 1000 + ... \qquad 1 + 1/10 + 1/100 + 1/1000 + ...$$

$$\sum_{n=0}^{\infty} (4/5)^n \qquad 9/10 + 9/100 + 9/1000 + ... \qquad 0.3333... \qquad 0.\overline{123}$$

Convergence tests. Deciding convergence or divergence of a series is not easy. The only tool at our disposal is comparison with known series, and essentially the only known non-trivial series is the geometric one. Comparison means the obvious observation that $0 \leqslant x_n \leqslant y_n$ for any n sufficiently large implies the following two conclusions: $\sum_n y_n < \infty \Rightarrow \sum_n x_n < \infty$, and $\sum_n x_n = \infty \Rightarrow \sum_n y_n = \infty$.

Now, if $|x_n| \leqslant C\,\lambda^n$ for some constant $C > 0$ and any n sufficiently large, then the partial sums of the series $\sum_n x_n$ are bounded by a constant times the partial sums of the geometric series $\sum_n \lambda^n$, therefore the series $\sum_n x_n$ is absolutely convergent whenever $|\lambda| < 1$. This happens when

- $\limsup_{n\to\infty} |x_n|^{1/n} < 1$ (*root test*)
- or when $\limsup_{n\to\infty} |x_{n+1}/x_n| < 1$ (*ratio test*).

[Ap69]

e.g. The exponential. Take $x_n = t^n/n!$, where the "factorial" is $n! := 1 \cdot 2 \cdot 3 \cdot \dots \cdot (n-1) \cdot n$ (and $0! := 1$). The series

$$\exp(t) := \sum_{n \geqslant 0} \frac{t^n}{n!} = 1 + t + \frac{t^2}{2} + \frac{t^3}{6} + \frac{t^4}{24} + \dots$$

is absolutely convergent for any $t \in \mathbb{R}$ (for example, by the ratio test). Therefore, it defines a function $\exp : \mathbb{R} \to \mathbb{R}$, which we call *exponential*, and also denote by e^t.

Comparing the coefficients of the power series and using the binomial formula, one may show that the exponential "sends sums into products", namely

$$e^{t+s} = e^t e^s$$

for any $t, s \in \mathbb{R}$. Consequently, $e^{-t} = (e^t)^{-1}$, and in particular e^t is never zero.

2 Modelos discretos e iteração

ref: [EK05, HK03]

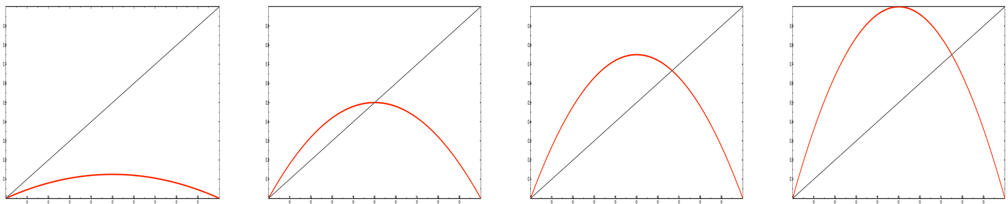
e.g. Transformação logística. Um modelo mais realista da dinâmica de uma população num meio ambiente limitado é

$$P_{n+1} = \lambda P_n \left(1 - P_n/M\right)$$

onde $P_n \geqslant 0$ é a população no tempo n, e a contante $M > 0$ é a maior população suportada pelo meio ambiente (observe que $P_{n+1} < 0$ quando $P_n > M$, o que pode ser interpretado como "extinção" no tempo $n+1$). A substituição $x_n = P_n/M$ transforma a lei acima na forma adimensional

$$x_{n+1} = \lambda x_n (1 - x_n)\,,$$

chamada *transformação logística*[5]. Se $0 \leqslant \lambda \leqslant 4$, a transformação logística $f_\lambda(x) := \lambda x(1-x)$ envia o intervalo unitário no intervalo unitário, i.e. $f_\lambda : [0,1] \to [0,1]$.



Gráficos da transformação logística $f_\lambda|_{[0,1]}$ quando $\lambda = 0.5$, $\lambda = 2$, $\lambda = 3$ e $\lambda = 4$.

Os ponto estacionários são o estado trivial 0 e

$$\overline{x} = \frac{\lambda - 1}{\lambda}$$

desde que $\lambda \geqslant 1$. Um applet `Java` com simulações do sistema está no meu bestiario.

ex: Discuta e interprete o comportamento das soluções para valores do parâmetro $0 < \lambda \leqslant 1$. Discuta e interprete o comportamento das soluções para valores do parâmetro $1 < \lambda \leqslant 3$. Observe os fenómenos que acontecem ao variar o parâmetro λ entre 3 e 4. O que acontece quando $\lambda > 4$?

Modelos discretos. Um sistema dinâmico com tempo discreto é definido por uma equação/lei recursiva

$$x_{n+1} = f(x_n)\,, \tag{2.1}$$

onde $x_n \in X$ denota o *estado* (posição, população, concentração, temperatura, ...) do sistema no *tempo* $n \in \mathbb{N}_0 := \{0,1,2,3,\dots\}$ (segundos, horas, meses, anos, ...). O *espaço dos estados* pode ser um intervalo $X \subset \mathbb{R}$ da recta real, um domínio $X \subset \mathbb{R}^d$ do espaço euclidiano de dimensão d, ou um conjunto mais exótico. A dinâmica é portanto determinada por uma *transformação* $f : X \to X$ do espaço dos estados em si mismo.

As *trajetórias* do sistema dinâmico são as sucessões $(x_n)_{n\in\mathbb{N}_0}$,

$$x_0 \quad\mapsto\quad x_1 := f(x_0) \quad\mapsto\quad x_2 := f(x_1) \quad\mapsto\quad \dots \quad\mapsto\quad x_{n+1} := f(x_n) \quad\mapsto\quad \dots\,,$$

definidas a partir de uma *condição/estado inicial* $x_0 \in X$ usando a recursão (2.1). A imagem de uma trajetória, o conjunto $\mathcal{O}(x_0) := \{x_0, x_1, x_2, \dots\} \subset X$, é dito *órbita* do estado inicial x_0.

Equilíbrios e soluções periódicas. As *soluções estacionárias*, ou *de equilíbrio*, são as trajetórias constantes $x_n = c$ para todos os tempos $n \in \mathbb{N}_0$, onde o *estado estacionário*, ou *de equilíbrio*, $c \in X$ é um "ponto fixo" da transformação $f : X \to X$, ou seja, um ponto tal que

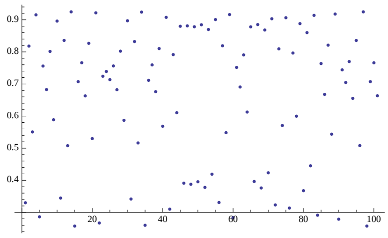
$$f(c) = c\,.$$

As *soluções periódicas* são as trajetórias (x_n) tais que $x_{n+p} = x_n$ para todos os tempos n e algum tempo minimal $p \geqslant 1$, dito *período*. Portanto, uma órbita periódica é um conjunto finito $\{x_0, x_1, \dots, x_{p-1}\} \subset X$ de pontos que são permutados pela transformação f.

[5] Robert M. May, Simple mathematical models with very complicated dynamics, *Nature* **261** (1976), 459-467.

help: As we already know, `Mathematica`®`8` may compute and plot trajectories of, for example, the logistic map $x_{n+1} = 3.7x_n(1 - x_n)$, with initial condition $x_0 = 0.33$, with the instructions

```
RecurrenceTable[{x[n + 1] == 3.7 x[n] (1- x[n]), x[0] == 0.33}, x, {n, 0, 100}]
ListPlot[%, PlotRange -> All]
```



help: Trajectories may be obtained with `Maxima` using the "evolution" command, as

```
(%i1) load("dynamics")$
(%i2) evolution(3.7*x*(1-x), 0, 100);
```

Trajetórias convergentes. Se uma trajectória (x_n) é convergente e se a transformação $f : X \to X$ é contínua, então o limite $x_\infty = \lim_{n\to\infty} x_n$ é um estado estacionário, pois

$$f(x_\infty) = f\left(\lim_{n\to\infty} x_n\right) = \lim_{n\to\infty} f(x_n) = \lim_{n\to\infty} x_{n+1} = x_\infty .$$

Solving a problem by recursion. The above is a most useful idea in mathematics. If we are looking for a solution of some "equation" $g(x) = y$, we may try to rewrite it in the form $f(x) = x$ (in a naive way summing $x - y$ to both sides, or in some other clever way as we will encounter later), so that we are really looking for a fixed point of a transformation $f : T \to X$. Then, we may try to decide if some trajectory of the recurrence $x_{n+1} = f(x_n)$ converges. If this happens, the limit x_∞ is one of the solutions we were after.

Limits and continuity in Euclidean spaces. Limits may be defined for sequences in any metric space (X, d), simply replacing $|x_n - a|$ with the distance $\text{dist}(x_n, a)$. A *metric space* is a set X equipped with a *metric*, a symmetric non-negative function $\text{dist} : X \times X \to [0, \infty)$ which is non-degenerate, i.e. $\text{dist}(x, y) = 0$ iff $x = y$, and which satisfies the "triangular inequality"

$$\text{dist}(x, y) \leqslant \text{dist}(x, z) + \text{dist}(z, y) \qquad \text{for any } x, y, z \in X .$$

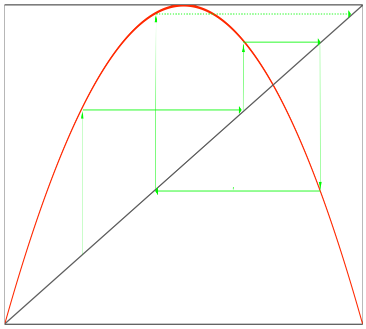
This is the case of the Euclidean space $\mathbb{R}^d$, the linear space of vectors $x = (x_1, \ldots, x_d)$ equipped with the Euclidean distance $\text{dist}(x, y) := \|x - y\|$, where the Euclidean norm is $\|x\| := \sqrt{\langle x, y\rangle}$ and the Euclidean inner product is $\langle x, y\rangle := x_1y_1 + \cdots + x_dy_d$.

A function/map $f : X \to Y$ between two metric spaces (X, dist_X) and (Y, dist_Y) is *continuous* if whenever $x_n \to x$ in X we also have $f(x_n) \to f(x)$ in Y (that is, we are allowed to exchange limits with the map). Equivalently, if for any $x \in X$ and any "precision" $\varepsilon > 0$ there exists an allowed "error" $\delta > 0$ such that $\text{dist}_X(x, x') < \delta$ implies $\text{dist}_Y(f(x), f(x')) < \varepsilon$.

help: The RSolve command of Mathematica finds analytic solutions of recurrent sequations/systems, if possible.

help: The Nest command of Mathematica also does iterations.

Análise gráfica. Se o espaço dos estados é um intervalo $X \subset \mathbb{R}$, as trajetórias podem ser observadas no plano x-y esboçando o caminho poligonal (*cobweb plot*)



$$(x_0, x_0) \mapsto (x_0, x_1) \mapsto (x_1, x_1) \mapsto (x_1, x_2) \mapsto (x_2, x_2) \mapsto (x_2, x_3) \mapsto \ldots$$

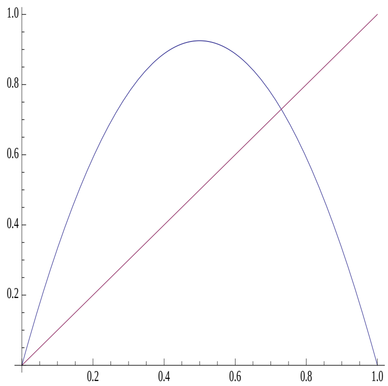
entre o gráfico da transformação, $y = f(x)$, e a diagonal, $y = x$.

help: You may find a GeoGebra code and the derived applet in my web page.

help: With `Mathematica®8` , you may plot the graphs of both the map $y = f(x)$ and the identity $y = x$ with the "Plot" command

```
Plot[{3.7 x (1 - x), x}, {x, 0, 1}]
```

and get



help: A cobweb plot with `Maxima` is obtained with the "staircase" commands, as

```
(%i1) load("dynamics")$
(%i2) staircase(3*x*(1-x), 0, 10, [x, 0, 1]);
```

ex: Estude as trajetórias (ou seja, determine os estados de equilíbrio, as trajetórias periódicas, e o comportamento assimptótico de algumas das outras trajetórias) dos sistemas dinâmicos definidos pelas seguintes transformações do intervalo

$$f(x) = \frac{1}{3}x \qquad f(x) = 7x \qquad f(x) = -x$$

$$f(x) = 3x + 1 \qquad f(x) = 2x - 7 \qquad f(x) = \frac{1}{2}x + 5$$

$$f(x) = |1 - x| \qquad f(x) = x^2 - \frac{1}{4} \qquad f(x) = x^2 - 2$$

$$f(x) = x^3 \qquad f(x) = -x^3 \qquad f(x) = x^{1/3}$$

$$f(x) = x - x^3 \qquad f(x) = x + x^3$$

e.g. **Equilíbrio de Hardy-Weinberg.** Considere a transmissão hereditária de um gene com dois alelos, A e a. Sejam P_0, Q_0 e $Z_0 = 1 - (P_0 + Q_0)$ as frequências dos genótipos AA, aa e Aa, respectivamente, numa dada população inicial. Então as probabilidades de ter o alelo A ou a na formação de um gameta são

$$p_0 = P_0 + \frac{1}{2}Z_0 \qquad \text{e} \qquad q_0 = 1 - p_0 = Q_0 + \frac{1}{2}Z_0\,,$$

respectivamente. Na fecundação, logo na primeira geração, teremos os genótipos AA, aa e Aa com probabilidades/frequências

$$P_1 = p_0^2\,, \qquad Q_1 = q_0^2 \qquad \text{e} \qquad Z_1 = 2p_0q_0\,,$$

respectivamente. Sucessivamente, as probabilidades de ter os alelos A ou a na formação de um gameta na primeira geração são

$$p_1 = P_1 + \frac{1}{2}Z_1 \qquad \text{e} \qquad q_1 = Q_1 + \frac{1}{2}Z_1\,.$$

respectivamente. Mas $p_1 = p_0^2 + p_0q_0 = p_0$ e $q_1 = q_0^2 + p_0q_0 = q_0$. Consequentemente, as frequências dos três genótipos na segunda geração serão

$$P_2 = p_1^2 = P_1\,, \qquad Q_2 = q_1^2 = Q_1 \qquad \text{e} \qquad Z_2 = 2p_1q_1 = Z_1\,.$$

Ou seja, a distribuição dos três genótipos atinge um valor estacionário a partir da primeira geração (*Hardy*[6]*-Weinberg*[7] *equilibrium/principle/law*) This is a physically interesting dynamical system with (mathematically) trivial dynamics.

e.g. **Seleção natural, modelo de Fisher, Wright e Haldane.** Um modelo simples de seleção natural, proposto por Ronald Fisher[8], Sewall Wright[9] e John Burdon Haldane[10], considera apenas um gene com dois alelos, A e a. A vantagem ou desvantagem competitiva dos diferentes genótipos, AA, Aa e aa, é modelada por coeficientes de "sucesso biológico" (*fitness*), ϕ_{AA}, ϕ_{Aa} e ϕ_{aa}, que determinam as diferentes taxas de sobrevivência, e portanto de reprodução. Sejam $0 \leqslant p_n \leqslant 1$ e $q_n = 1 - p_n$ as frequências dos alelos A e a, respetivamente, na n-ésima geração. Então a frequência do alelo A na $(n+1)$-ésima geração é dada por

$$p_{n+1} = \frac{\alpha p_n^2 + p_nq_n}{\alpha p_n^2 + 2p_nq_n + \beta q_n^2}$$

onde $\alpha = \phi_{AA}/\phi_{Aa} > 0$ e $\beta = \phi_{aa}/\phi_{Aa} > 0$.

As soluções estacionárias são as soluções triviais 0 e 1, e, quando α e β são os dois superiores ou os dois inferiores a 1,

$$\overline{p} = \frac{|\beta - 1|}{|\alpha - 1| + |\beta - 1|}\,.$$

Quando $\alpha < 1 < \beta$ ou $\beta < 1 < \alpha$, na população assimptótica apenas sobrevive o alelo favorecido.

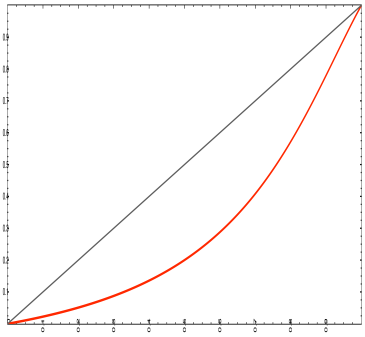
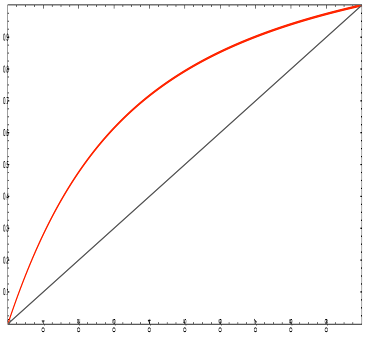
[6] G.H. Hardy, Mendelian proportions in a mixed population, *Science* **28** (1908), 49-50.

[7] W. Weinberg, Über den Nachweis der Vererbung beim Menschen, *Jahreshefte des Vereins für vaterländische Neturkunde in Württemberg* **64** (1908), 368-382.

[8] R.A. Fisher, *Genetical Theory of Natural Selection*, Clarendon Press, 1930.

[9] S. Wright, Evolution in Mendelian populations, *Genetics* **16** (1931), 97-159.

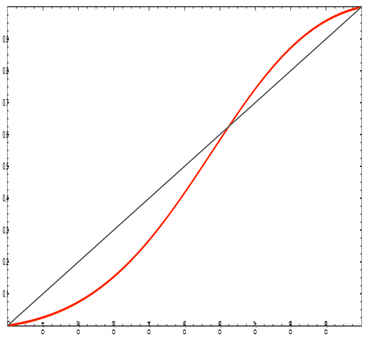
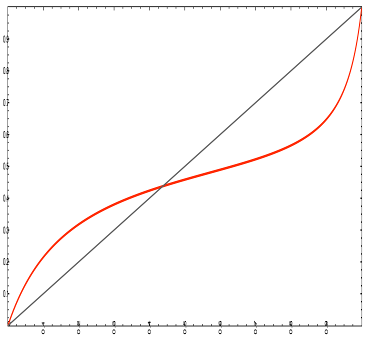
[10] J.B.S. Haldane, A Mathematical Theory of Natural and Artificial Selection (1924-1934). J.B.S. Haldane, The effect of variation on fitness, *Am. Nat.* **71** (1937), 337-349.

$\alpha < 1 < \beta$ $\beta < 1 < \alpha$

Quando $\alpha > 1$ e $\beta > 1$ (ou seja, os genótipos AA e aa têm uma vantagem competitiva em relação ao genótipo Aa), o estado estacionário $\overline{p}$ é instável, e pequenas perturbações $x_0 = \overline{p} \pm \varepsilon$ do equilíbrio produzem comportamentos assimptóticos diferentes, a extinção de A ou a extinção de a, dependendo do sinal de $\pm\varepsilon$ (*disruptive selection*).

Quando $\alpha < 1$ e $\beta < 1$ (ou seja, o genótipo Aa é o favorecido), o estado estacionário $\overline{p}$ é estável, e portanto os dois alelos convivem na população assimptótica (*heterosis*).

Disruptive selection: $1 < \alpha < \beta$. *Heterosis*: $\alpha < \beta < 1$.

e.g. Hénon map. The *Hénon map*[11] is the recursive map of the plane

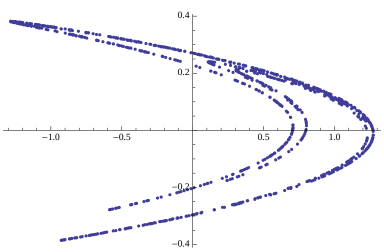
$$\begin{cases} x_{n+1} = 1 + y_n - \alpha x_n^2 \\ y_{n+1} = \beta x_n \end{cases}$$

Depending on the values of its parameters, its trajectories show regular, "intermittent" or "chaotic" behavior. If you choose the parameters $\alpha \simeq 1.4$ and $\beta \simeq 0.3$, you see the "Hénon attractor".

help: With Mathematica®8 , you may use the commands

```
RecurrenceTable[{x[n + 1] == y[n] + 1 - 1.4 x[n]^2,
                                y[n + 1] == 0.3 x[n], x[0] == 0.6, y[0] == 0.2},
                                {x, y}, {n, 1, 1000}] // Short
ListPlot[%, PlotRange -> All]
```

to get the following picture of the "Henón attractor".



[11] M. Hénon, A two-dimensional mapping with a strange attractor, *Comm. Math. Phys.* **50** (1976), 69-77.

help: Two-dimensional orbits may be obtained with `Maxima` using the "evolution2d" command, as

```
(%i1) load("dynamics")$
(%i2) f:  1+y+1.4*x^2$
(%i3) g:  0.3*x$
(%i4) evolution2d([f,g], [x,y], [0,6, 0.2],  1000, [style,dots]);
```

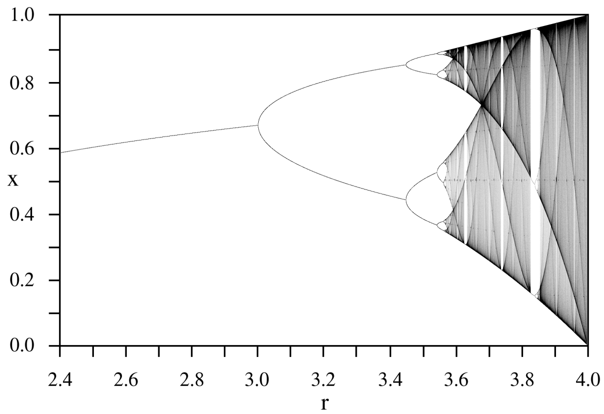
e.g. **Cigarras periódicas.** As cigarras passam quase toda a vida, um periódo de $1 \leqslant c \leqslant 17$ anos (dependendo da espécie), no chão como ninfas, e depois saem durante as poucas semanas ou meses de vida adulta (acasalar, pôr ovos e morrer). Se os predadores têm ciclos de vida de p_k anos, a escolha de c que minimiza os encontros é um número primo diferente dos p_k's. As *magicidada* (uma cigarra americana) saem da terra cada 13 ou 17 anos, aproximadamente sincronizadas em diferentes lugares do continente. Modelos matemáticos que sugerem "explições" do fenómeno, descrito por Stephen Jay Gould em [Gou77], foram propostos a partir dos anos '70 [12] [13] [14].

A game on prime number and cicadas is in Marcus du Sautoy's page Music of the primes.

Orbit diagram. Consider a family of transformations

$$x_{n+1} = f_\lambda(x_n) \, ,$$

depending on a parameter λ. The behavior of a typical orbit may change as λ changes. An interesting picture is obtained if we plot the parameter λ, within some interval, versus a typical orbit of f_λ, say $\{x_{100}, x_{101}, \dots, x_{200}\}$ starting from a random initial point x_0.



Orbit diagram for the logistic family (from the Wikipedia).

help: A orbit diagram with `Maxima` is obtained with the "orbits" command, as

```
(%i1) load("dynamics")$
(%i2) orbits(a*x*(1-x), 0, 10, 100, [a, 0, 4], [style, dots]);
```

[12]F.C. Hoppensteadt and J.B. Keller, Syncronization of Periodical Cicada Emergences, *Sciences*, New Series, **194** (1976), 335-337.

[13]R.M. May, Periodical cicadas, *Nature*, **277** (1979), 347-349.

[14]E. Goles, O. Schulz and M. Markus, Prime number selection of cycles in a predator-prey mode, *Complexity* **6** (2001), 33-38.

3 Derivadas e aplicações

ref: [Ap69, RHB06]

e.g. **Movimento rectilíneo uniforme.** A lei do movimento rectilíneo uniforme num referencial inercial é

$$q(t) = q_0 + v_0 t \, ,$$

onde $q(t) = (x(t), y(t), z(t))$ denota a posição no tempo t, $v_0 \in \mathbb{R}^3$ a velocidade e $q_0 \in \mathbb{R}^3$ a posição inicial.

- Determine a velocidade média no intervalo de tempos entre t e $t+\varepsilon$, e a velocidade instantânea no tempo t.
- Determine a lei horária de uma partícula que viaja com velocidade de 3 m/s e que no instante $t = 10$ s está na posição $q(10) = 10$ m. Quando estava na origem?

e.g. **Aquiles e a tartaruga.** Aquiles (or Usain Bolt?) começa a correr com velocidade de 10 m/s em direcção de uma tartaruga que a sua vez foge com velocidade de 0.1 m/s. A distância inicial entre Aquiles e a tartaruga é de 100 m.

- Determine quanto tempo demora Aquiles a percorrer $1/2$, $1/2 + 1/4$, $1/2 + 1/4 + 1/8$, ..., da distância inicial, e passado quanto tempo chega ao ponto onde estava inicialmente a tartaruga.
- Determine a distância $d(t)$ entre Aquiles e a tartaruga no tempo t.
- Aquiles alcança a tartaruga? Se sim, em quanto tempo?

e.g. **Queda livre.** A queda livre de uma partícula próxima da superfície terrestre é modelada pela lei horária

$$z(t) = z_0 + v_0 t - \frac{1}{2} g t^2 \, ,$$

onde $z(t)$ denota a altura da partícula no tempo t, z_0 é a altura inicial,v_0 é velocidade inicial, e $g \simeq 980$ cm/s^2 é a aceleração da gravidade próximo da superfície terrestre.

- Determine a velocidade média
$$\overline{v}_{t_0,t_1} := \frac{z(t_1) - z(t_0)}{t_1 - t_0}$$
no intervalo de tempos entre $t_0 = t$ e $t_1 = t+\varepsilon$, e a velocidade (instantânea), ou seja, o limite
$$v(t) := \lim_{\varepsilon \to 0} \frac{z(t+\varepsilon) - z(t)}{\varepsilon}$$
- Determine a aceleração da partícula, ou seja, o limite
$$a(t) := \lim_{\varepsilon \to 0} \frac{v(t+\varepsilon) - v(t)}{\varepsilon}$$
- Uma pedra é deixada cair do topo da torre de Pisa, que tem $\simeq 56$ metros de altura, com velocidade inicial nula. Calcule a altura da pedra após 1 segundo, o tempo necessário para a pedra atingir o chão e a sua velocidade no instante do impacto.
- Com que velocidade inicial deve uma pedra ser atirada para cima de forma a atingir a altura de 20 metros, relativamente ao ponto inicial?
- Com que velocidade inicial deve uma pedra ser atirada para cima de forma a voltar de novo ao ponto de partida ao fim de 10 segundos?

Derivative. Let $f : I \to \mathbb{R}$ be a real valued function defined in some open interval $I = (a, b) \subset \mathbb{R}$. The function f is *differentiable* at the point $x \in I$ if there exists the limit

$$f'(x) := \lim_{\varepsilon \to 0} \frac{f(x+\varepsilon) - f(x)}{\varepsilon}, \tag{3.1}$$

called *derivative* of f at x. Equivalently, the function f is differentiable at the point x if there exists a number λ, called derivative of f at x and denoted by $\lambda = f'(x)$, such that for all sufficiently small "variations" ε we may write

$$f(x+\varepsilon) - f(x) = \lambda \cdot \varepsilon + r(\varepsilon) \tag{3.2}$$

where the "remainder" $r(\varepsilon)$ satisfies $\lim_{\varepsilon \to 0} \frac{r(\varepsilon)}{\varepsilon} = 0$. Thus, the derivative $\lambda = f'(x)$ is the "slope" of the best linear approximation

$$f(x+\varepsilon) \simeq f(x) + \lambda \cdot \varepsilon \tag{3.3}$$

to the function f near the point x. Geometrically, this is as well the tangent line at the graph $\mathcal{G}_f := \{(x, f(x)),\ x \in I\} \subset \mathbb{R}^2$ of f at the point $(x, f(x))$.

Taking the limit as $\varepsilon \to 0$ in (3.2), we see that $f(x+\varepsilon) \to f(x)$. Thus, a function which is differentiable at x is also continuous at x.

A function $f : I \to \mathbb{R}$ is *differentiable* if it admits a derivative $f'(x)$ at all points $x \in I$.

Successive derivatives. If $f : I \to \mathbb{R}$ admits derivatives for all x in its domain, we may regard the derivative f' as a function, say $f' : I \to \mathbb{R}$, hence try to compute its derivative. The derivative of the derivative of f is called *second derivative* of f, and denoted by $f'' := (f')'$. In the same manner we may define the successive derivatives f''', f'''' and so on, whenever they exist.

Leibniz' notation. We may write $y = f(x)$, hence denote by $\delta y := f(x+\delta x) - f(x)$ the variation of y due to a variation δx of x. Then the derivative is the limit

$$\lim_{\delta x \to 0} \frac{f(x+\delta x) - f(x)}{\delta x} = \lim_{\delta x \to 0} \frac{\delta y}{\delta x} := \frac{dy}{dx}$$

This is *Leibniz' notation* for derivatives. The second derivative is then $\frac{d^2y}{dx^2}$, the third $\frac{d^3y}{dx^3}$, and so on.

Observe that if we rescale both variables as $\tilde{x} = \lambda x$ and $\tilde{y} = \mu y$, with $\lambda > 0$ and $\mu > 0$, then the derivatives change according to

$$\frac{d\tilde{y}}{d\tilde{x}} = \frac{\mu}{\lambda}\frac{dy}{dx} \qquad \frac{d^2\tilde{y}}{d\tilde{x}^2} = \frac{\mu}{\lambda^2}\frac{d^2y}{dx^2} \qquad \dots \qquad \frac{d^k\tilde{y}}{d\tilde{x}^k} = \frac{\mu}{\lambda^k}\frac{d^ky}{dx^k}$$

This explain the different use of the exponents in Leibniz' notation.

Derivative as velocity, physicists' notation. When the independent variable has the meaning of "time", hence is denoted by $t \in I \subset \mathbb{R}$, a function $t \mapsto x(t)$ represents a *trajectory*, or a *time law*, the way some observable called x is changing in time. Its time derivative is then denoted using a "dot", as

$$\dot{x} := \frac{dx}{dt}$$

and referred to as a *velocity* $v := \dot{x}$, or "time variation", or "taxa de variação". The second derivative $a := \ddot{x}$ is also meaningful, and it is called *acceleration*. Very few (not to say none!) physical phenomena require the use of higher order time derivatives.

ex: Calcule as derivadas $f'(x)$ e $f''(x)$ de cada uma das seguintes funções $f(x)$ nos pontos onde existem.

$$f(x) = 2x - 3 \qquad f(x) = x^2 \qquad f(x) = |x| \qquad f(x) = \begin{cases} \frac{x}{|x|} & \text{se } x \neq 0 \\ 0 & \text{se } x = 0 \end{cases}$$

Derivatives of elementary functions. It is clear that the derivative of a constant function $f(x) = c$ is $f'(x) = 0$. Moreover, in high school you learn to derive positive integer powers, $(x^n)' = nx^{n-1}$, and the trigonometric functions $\sin' = \cos$ and $\cos' = -\sin$.

ex: Use the binomial formula to prove the above formula for the derivative of powers.

help: With `Mathematica®8` , you may define a function $f(x) = e\ -x^2 \cos(3x)$ with

```
f[x_] :=  Exp[-x^2] Cos[3 x]
```

and then derive with a "prime", as

```
f'[x]
```

to get

$$-2e^{-x^2} x \cos(3x) - 3e^{-x^2} \sin(3x)$$

Algebra of derivatives. It is clear that the derivative is linear, namely

$$(\lambda f)' = \lambda f' \qquad \text{and} \qquad (f+g)' = f' + g' \tag{3.4}$$

whenever f and g are differentiable functions (defined in a common interval) and $\lambda \in \mathbb{R}$ is an arbitrary constant.

The product $f \cdot g$ of two differentiable functions f and g is also differentiable, and its derivative is given by *Leibniz' rule*

$$(fg)' = f'g + fg' \tag{3.5}$$

Indeed, let $y = f(x)$ and $z = g(x)$. A small variation δx induces variations $\delta y := f(x+\delta x) - f(x)$ and $\delta z := g(x+\delta x) - g(x)$. Summing and subtracting $y \cdot (z + \delta z)$ to the variation of $f \cdot g$ below, we get

$$\begin{aligned} \frac{(y+\delta y)\cdot(z+\delta z) - yz}{\delta x} &= \frac{(y+\delta y)\cdot(z+\delta z) - y\cdot(z+\delta z) + y\cdot(z+\delta z) - yz}{\delta x} \\ &= \frac{\delta y}{\delta x}\cdot(z+\delta z) + y\cdot\frac{\delta z}{\delta x} \\ &\to_{\delta x\to 0} \frac{dy}{dx}\cdot z + y\cdot\frac{dz}{dx} \end{aligned}$$

since $\delta z \to 0$ (because g is continuous).

The quotient f/g of two differentiable functions f and g is also differentiable where the denominator is $g(x) \neq 0$, and its derivative is given by the formula

$$(f/g)' = \frac{f'g - fg'}{g^2}\,. \tag{3.6}$$

To see this, we first compute the derivative of $1/g(x)$ at a point where $g(x) \neq 0$. If $z = g(x)$ and $\delta z = g(x+\delta x) - g(x)$, then

$$\frac{1/g(x+\delta x) - 1/g(x)}{\delta x} = \frac{1}{(z+\delta z)\cdot z}\cdot\frac{z-(z+\delta z)}{\delta x} \to_{\delta x\to 0} -\frac{1}{z^2}\frac{dz}{dx}\,.$$

Finally, we apply Leibniz' rule to the product $f(x)\cdot(1/g(x))$, to get (3.6).

ex: Calcule a derivada $f'(x)$ de cada uma das seguintes funções $f(x)$ nos pontos onde podem ser definidas.

$$\begin{array}{ccc} f(x) = 3x & f(x) = x\sin(x) & f(x) = 17 \\ f(x) = x^3 - 3x + 1 & f(x) = \sqrt{x} & f(x) = x^{-1} - x^{5/3} \\ f(x) = \dfrac{1}{x} & f(x) = \dfrac{x-1}{x^3+2} & f(x) = \dfrac{1}{\sqrt{x}} \\ \tan(x) = \dfrac{\sin(x)}{\cos(x)} & \sec(x) = \dfrac{1}{\cos(x)} & \mathrm{cosec}(x) = \dfrac{1}{\sin(x)} \end{array}$$

ex: Calcule as derivadas $P'(0)$, $P''(0)$, $P'''(0)$, ..., $P^{(n)}(0)$, $P^{(n+1)}(0)$, de um polinómio

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

ex: Estime os seguintes valores, usando a aproximação linear $f(x+\varepsilon) \simeq f(x) + f'(x) \cdot \varepsilon$.

$$\sin(0.01) \qquad \sqrt{1.1} \qquad \cos(\pi - 0.03) \qquad \frac{1}{1+0.001}$$

Chain rule. Let $g : I \subset \mathbb{R} \to \mathbb{R}$ and $f : J \subset \mathbb{R} \to \mathbb{R}$ be differentiable functions, with $f(I) \subset J$, so that we may form the composition $(f \circ g) : I \to \mathbb{R}$, the function $x \mapsto f(g(x))$. If both f and g are differentiable, then $f \circ g$ also is differentiable, and its derivative is given by the *chain rule*

$$(f \circ g)'(x) = f'(g(x)) \cdot g'(x) . \tag{3.7}$$

Here Leibniz' notation is particularly meaningful. If $y = g(x)$ and $z = f(y) = f(g(x))$, then

$$\frac{dz}{dx} = \frac{dz}{dy} \cdot \frac{dy}{dx}$$

That is, you may act as if you could divide by "dy".

For the proof, we use Leibniz' notation again. For small δx, we define the corresponding variations $\delta y = g(x+\delta x) - g(x)$, hence $\delta z = f(y+\delta y) - f(y)$. By (3.2), there exists a function $e(\varepsilon)$, which converges to 0 when $\varepsilon \to 0$, such that

$$\delta z = \frac{dz}{dy} \cdot \delta y + e(\delta y) \cdot \delta y$$

for sufficiently small δy. Consequently,

$$\frac{\delta z}{\delta x} = \left(\frac{dz}{dy} + e(\delta y) \right) \cdot \frac{\delta y}{\delta x} \to_{\delta x \to 0} \frac{dz}{dy} \cdot \frac{dy}{dx}$$

since $\delta y \to 0$ when $\delta x \to 0$.

ex: Calcule a derivada $f'(x)$ de cada uma das seguintes funções $f(x)$ nos pontos onde podem ser definidas.

$$f(x) = \cos(x^2) \qquad f(x) = \sqrt{2x-1} \qquad f(x) = \sin\left(\sqrt{x}\right)$$

$$f(x) = (\sin(x))^2 \qquad f(x) = \sin(\cos(x^3)) \qquad f(x) = \frac{\cos(2x) - x}{\sqrt{x}}$$

Derivatives of inverse function. Let $f : I \subset \mathbb{R} \to \mathbb{R}$ be one-to-one function onto $J = f(I)$, and let $h : J \to I$ be its inverse, so that $h(f(x)) = x$ for all $x \in I$ and $f(h(y)) = y$ for all $y \in J$. If f is differentiable at $x \in I$ and h is continuous at $y = f(x)$, then h is differentiable at y if and only if $f'(x) \neq 0$, and if this is the case, its derivative is

$$h'(y) = \frac{1}{f'(h(y))} . \tag{3.8}$$

Indeed, if h is differentiable at y, we may apply the chain rule to $h(f(x)) = x$ to get $h'(y) \cdot f'(x) = 1$, hence (3.8) whenever $f'(x) \neq 0$. Conversely, given a variation δy, let $\delta x = h(y+\delta y) - h(y)$ be the corresponding variation of x. Since h is continuous at y, $\delta x \to 0$ whenever $\delta y \to 0$. Therefore,

$$\frac{\delta x}{\delta y} = \left(\frac{\delta y}{\delta x} \right)^{-1} \to_{\delta x \to 0} \left(\frac{dy}{dx} \right)^{-1}$$

provided $f'(x) \neq 0$.

ex:

- Show that the derivative of $x^{1/n}$, for $x > 0$ and $n = 1, 2, 3, \dots$, is $\frac{1}{n} x^{1/n-1}$.
- Calcue as derivadas das seguintes funções nos pontos onde podem ser definidas.

$$f(x) = \arcsin(x) \qquad f(x) = \arccos(x) \qquad f(x) = \arctan(x)$$

- Calcule a derivada da função inversa de $f(x) = x + x^3$ no ponto $y = 0$.

ex: Taxas de variação. Determine a taxa de variação

- $\frac{dA}{dr}$, onde A é a área de uma circunferência e r o seu raio,
- $\frac{dV}{dr}$, onde V é o volume de uma bola e r o seu raio,
- $\frac{dV}{d\ell}$, onde V é o volume de um cubo e ℓ o seu lado.

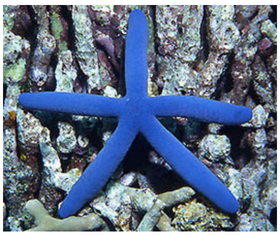
e.g. Growth of a spherical cell. A spherical cell grows absorbing raw material (necessary for its metabolism) from its surface, hence at a rate αS proportional to the surface S. On the other hand, the rate of raw material necessary for the metabolism is proportional to the volume V of the cell, say βV. Therefore, the cell can survive only when $\beta V \leqslant \alpha S$, i.e until its surface area to volume ratio (SA:V) ratio S/V is grater than some lower limit β/α. The SA:V of a sphere of radius r is $3/r$, therefore the limit size of the cell is $\overline{r} \simeq 3\alpha/\beta$.

If the density ρ is assumed constant, then the mass ρV of the cell grows according to $\rho\dot{V} = \alpha S$. If r denotes the radius of the cell, we get $\rho\, 4\pi r^2 \dot{r} = \alpha\, 4\pi r^2$, i.e.

$$\dot{r} = \alpha/\rho$$

and therefore the radius increases linearly with time t according to $r(t) = r(0) + (\alpha/\rho) \cdot t$. Correspondingly, the SA:V ratio decreases as $S/V \simeq 3/r(t)$, until a certain limit $3/\overline{r}$ when the incoming material can no longer support the cell metabolism.

e.g. Surface Area to volume ratio and shapes. The SA:V ratio of an organism depends on the shape and on the linear dimensions, and Nature offers a huge variety of selected shapes.[15]



(from Life at the Edge of Reef and Wikipedia)

For example, the "sahuaro" cactus (*Carnegiea gigantea*), from the Sonora desert of México, optimize their surface area to volume ratio, hence minimize transpiration, assuming a cylindrical shape.

Derivative and growth. A differentiable function $f(x)$ is striclty increasing in intervals where $f'(x) > 0$, strictly decreasing in intervals where $f'(x) < 0$, and constant in intervals where its derivative vanishes. Consequently, if c is a local maximum or minimum of a differentiable function f defined in a neighborhood $(c - \varepsilon, c + \varepsilon)$ of c, then c is a *critical point* of f, i.e. a point where $f'(c) = 0$.

[15] K. Schmidt-Nielson, *Scaling: Why is Animal Size so Important?* Cambridge University Press, 1984.

ex:

- Esboce os gráficos das seguintes funções, definidas em oportunos domínios.

$$f(x) = 1 - \frac{x^2}{2} \qquad f(x) = x + \frac{1}{x} \qquad f(x) = 1 + x + \frac{x^2}{2}$$

$$f(x) = \frac{1}{(x-1)(x-2)} \qquad f(x) = (x-1)(x-2)(x-3)$$

$$f(x) = x - \sin(x) \qquad f(x) = \sin(x) + \sin(2x) \qquad f(x) = \frac{\sin(x)}{x}$$

- Mostre que, entre todos os rectângulos de perímetro P fixado, o quadrado é o que tem área maior.

- Mostre que, dados n números $a_1, a_2, ..., a_n$, o valor de x que minimiza a soma dos "erros quadráticos"
$$(x-a_1)^2 + (x-a_2)^2 + ... + (x-a_n)^2$$
é a média aritmética
$$\overline{a} = \frac{a_1 + a_2 + ... + a_n}{n} \, .$$

Mean value theorem and inequality. Let $f : [a,b] \to \mathbb{R}$ be a continuous function with $f(a) = f(b)$, and assume that f differentiable in (a,b). Indeed, by Weierstrass theorem, the function attains its maximum and minimum values, say M and m, respectively. If both are attained at the endpoints, then the function is constant and its derivative is everywhere zero at $c(a,b)$. If, on the other side, its maximum or its minimum is attained at an internal point $c \in (a,b)$, then this must be a critical point. Therefore, there always exists a point $c \in (a,b)$ where $f'(c) = 0$ (*Rolle's theorem*). If we apply Rolle's theorem to the function $f(a) + \frac{f(b)-f(a)}{b-a}x$, we get the

Theorem 3.1. (Mean value theorem). *If $f : [a,b] \to \mathbb{R}$ is a continuous function which is differentiable in (a,b), then there is a point $c \in (a,b)$ where*

$$f(b) - f(a) = f'(c) \cdot (b-a) \, .$$

In particular, if $f'(x) = 0$ for all $c \in (a,b)$, then $f(b) = f(a)$. Thus, a function with zero derivative for all points in an interval is constant. More interesting (and physically obvious!) is that a bound on the derivative implies a bound on the displacement: if $|f'(c)| \leqslant \lambda$ for all $c \in (a,b)$, then we have the inequality
$$|f(b) - f(a)| \leqslant \lambda \cdot |b-a| \, .$$

ex:

- Mostre que, se $f(x)$ é um polinómio de segundo grau, então a recta que une os pontos $(a, f(a))$ e $(b, f(b))$ é paralela à recta tangente ao gráfico de f no ponto médio $\frac{a+b}{2}$.

- Mostre que para todos os x e y
$$|\sin(x) - \sin(y)| \leqslant |x-y|$$

- Mostre que para todos $0 < y \leqslant x$
$$ny^{n-1}(x-y) \leqslant x^n - y^n \leqslant nx^{n-1}(x-y)$$

4 Aproximação

ref: [Ap69, Li06, RHB06]

Polynomial approximation. The value $f(a)$ is the best constant approximation

$$f(x) \simeq f(a)$$

to a continuous function $f(x)$ near the point a, in the sense that the "error" $e(x-a) := f(x)-f(a)$ goes to $e(\varepsilon) \to 0$ as $\varepsilon := x-a \to 0$. The derivative $f'(a)$ is the slope of the best linear approximation

$$f(x) \simeq f(a) + f'(a)(x-a)$$

to a differentiable function $f(x)$ near the point a, since by the very definition of derivative the "error" $e(x-a) := f(x) - f(a) - f'(a)(x-a)$ is so small that $e(\varepsilon)/\varepsilon \to 0$ as $\varepsilon \to 0$. If f has n derivatives at the point a, we may as well look for the polynomial of degree $\leqslant n$ which best approximate $f(x)$ for small $\varepsilon = x - a$, hoping to get better approximations. After all, the only functions that human beings and machines can compute are polynomials (since we only can do finite sums and multiplications), and we need means to estimate the other functions which, we believe, describe Nature.

A n-times differentiable function $e(\varepsilon)$ satisfies $\lim_{\varepsilon\to 0} e(\varepsilon)/\varepsilon^n = 0$ iff its value and its first n derivatives vanishes at zero, i.e. $e^{(k)}(0) = 0$ for all $k = 0, 1, \dots, n$ (this is not trivial, and is a consequence of the mean value theorem, see [Li06]). If we apply this to the error $r(x-a) = f(x) - P(x-a)$, where P is any polynomial of degree $\leqslant n$, we see that the it goes to zero as $r(\varepsilon)/\varepsilon^n \to_{\varepsilon\to 0} 0$ if and only if P is the *Taylor polynomial* (of the function f at the point a)

$$P_n(x-a) := f(a) + f'(a)\cdot(x-a) + \frac{f''(a)}{2}\cdot(x-a)^2 + \frac{f'''(a)}{6}\cdot(x-a)^3 + \cdots + \frac{f^{(n)}(a)}{n!}\cdot(x-a)^n .$$

If, moreover, the derivative $f^{(n)}$ is continuos in the closed interval $[a, x]$ (if $a < x$, or $[x, a]$ if $x < a$) and $f^{n+1}(y)$ exists for all $y \in (a, x)$, then there is a point $c \in (a, x)$ such that the error is

$$e_n(\varepsilon) := f(a+\varepsilon) - P_n(\varepsilon) = \frac{f^{(n+1)}(c)}{(n+1)!}\,\varepsilon^{n+1}$$

i.e.

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2}(x-a)^2 + \ldots + \frac{f^{(n)}(a)}{n!}(x-a)^n + \frac{f^{(n+1)}(c)}{(n+1)!}\,(x-a)^{n+1}$$

This generalizes the mean value theorem.

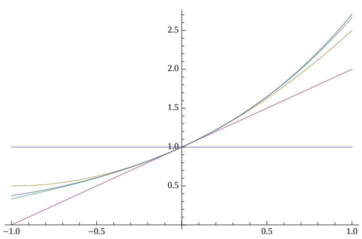
e.g. The exponential. We already saw that the exponential is the function defined by the power series

$$\exp(x) := \sum_{n=0}^{\infty} \frac{x^n}{n!} .$$

If we limit the sum to finite degree n, we obtain a sequence of polynomial approximations

$$\exp x \simeq 1 + x + \frac{1}{2}x^2 + \frac{1}{6}x^3 + \cdots + \frac{1}{n!}x^n .$$

This is what a machine computes when asked to produce e^x, once chosen an n so large that the successive terms give no appreciable difference to the sum.



Taylor polynomials of the exponential near $a = 0$, with degrees $n = 0, 1, 2, 3, 4$.

e.g. Trigonometric functions. The Taylor polynomials of the trigonometric functions cos and sin centered at 0 start with

$$\cos(x) \simeq 1 - \frac{1}{2}x^2 + \frac{1}{24}x^4 + \dots \qquad \text{and} \qquad \sin(x) \simeq x - \frac{1}{6}x^3 + \frac{1}{120}x^5 + \dots$$

ex:

- Prove as seguintes aproximações, validas para x suficientemente pequeno,

$$e^x \simeq 1 + x + \frac{x^2}{2} + \dots \qquad \log(1+x) \simeq x - \frac{x^2}{2} + \dots$$
$$\sin(x) \simeq x - \frac{x^3}{6} + \dots \qquad \cos(x) \simeq 1 - \frac{1}{2}x^2 + \dots$$

- e determine estas outras

$$\frac{1}{1-x} \simeq 1 + x + \dots \qquad \sqrt{1+x} \simeq 1 + \frac{1}{2}x + \dots$$
$$\log(1+x^2) \simeq \dots \qquad \sin(\pi e^{-x}) \simeq \dots$$

- Aproxime e, e estime o erro na sua aproximação, usando os polinómios de Taylor

$$e^x = 1 + x + \frac{x^2}{2!} + \dots + \frac{x^n}{n!} + r_n(x)$$

(observe que $1 \leqslant e^x \leqslant 3$ no intervalo $x \in [0,1]$).

Contraction principle. A *contraction* of an interval $X \subset \mathbb{R}$ is a transformation $f : X \to X$ such that there exists a constant $0 \leqslant \lambda < 1$ such that

$$|f(x) - f(x')| \leqslant \lambda \cdot |x - x'| \tag{4.1}$$

for all $x, x' \in X$ (this definition extends to a generic metric space (X, dist) if we replace the absolute value of the difference with the distance). For example, a differentiable transformation $f : X \to X$ of a (closed) interval $X \subset \mathbb{R}$ such that $|f'(x)| \leqslant \lambda < 1$ for all $x \in X$ is a contraction, since, by the mean value theorem,

$$|f(x) - f(y)| = |f'(c) \cdot (x-y)| \leqslant \lambda \cdot |x-y| \, .$$

where c is some point between x and y. Observe that a contraction is (uniformly) continuous, since for any $|x-y| < \delta = \varepsilon/\lambda$ we have $|f(x) - f(y)| < \lambda \cdot \delta < \varepsilon$.

Proposition 4.1. (Contraction principle) *A contraction $f : X \to X$ of a closed interval $X \subset \mathbb{R}$ (or a complete metric space) has one and only one fixed point p. Moreover, all trajectories defined recursively by $x_{n+1} = f(x_n)$ given an arbitrary initial condition $x_0 \in X$ converge exponentially fast to the fixed point p.*

Indeed, let $x_0 \in X$ and let (x_n) be its trajectory, so that $x_{n+1} = f(x_n)$. If we iterate (4.1), we see that $|x_{k+1} - x_k| \leqslant \lambda^k \cdot |x_1 - x_0|$. Using k times the triangular inequality, and then the convergence of the geometric series of ratio λ, we see that

$$\begin{aligned} |x_{n+k} - x_n| &\leqslant \sum_{j=0}^{k-1} |x_{n+j+1} - x_{n+j}| \leqslant |x_1 - x_0| \cdot \sum_{j=0}^{k-1} \lambda^{n+j} \\ &\leqslant |x_1 - x_0| \cdot \lambda^n \cdot \sum_{j=0}^{\infty} \lambda^j \leqslant \frac{\lambda^n}{1-\lambda} \cdot |x_1 - x_0| \, . \end{aligned}$$

Therefore, (x_n) is a Cauchy (or fundamental) sequence. The limit $p = \lim_{n\to\infty} x_n$ exists because X is a closed interval, and is a fixed point of f because

$$f(p) = f(\lim_{n\to\infty} x_n) = \lim_{n\to\infty} f(x_n) = \lim_{n\to\infty} x_{n+1} = p \, ,$$

by the continuity of f. Uniqueness of the fixed point is obvious, since if p and p' are both fixed points, then $|p - p'| = |f(p) - f(p')| \leqslant \lambda \cdot |p - p'|$ with $\lambda < 1$, and therefore $|p - p'| = 0$. On the other side, iteration of (4.1) implies that $|x_n - p| \leqslant \lambda^n \cdot |x_0 - p|$, so that the convergence $x_n \to p$ is exponential.

Estabilidade dos estados estacionários. Seja $\overline{x}$ um estado estacionário da equação recursiva

$$x_{n+1} = f(x_n)$$

ou seja, um ponto tal que $f(\overline{x}) = \overline{x}$. Se a transformação $f(x)$ é diferenciável, o príncipio das contrações permite decidir sobre a estabilidade do estado estacionário.

Se $|f'(\overline{x})| < 1$, então o ponto fixo é *atrativo*. Existe uma vizinhança $B = [\overline{x} - \varepsilon, \overline{x} + \varepsilon]$ de p tal que a restrição $f|_B : B \to B$ é uma contração, e $\overline{x}$ é o seu único ponto fixo. As trajetórias de todo o ponto x_0 suficientemente próximo de $\overline{x}$ (ou seja, em B) convergem exponencialmente para $\overline{x}$, ou seja $x_n \to \overline{x}$.

Se $|f'(\overline{x})| > 1$, então o ponto fixo é *repulsivo*: as trajetórias de todo o ponto $x_0 \neq \overline{x}$ numa vizinhança suficientemente pequena de $\overline{x}$ saem da vizinhança em tempo finito.

Se $f'(\overline{x}) = 0$, o ponto fixo $\overline{x}$ é dito *super-atrativo*. Usando o polinómio de Taylor de grau 1 com resto, vê-se que, se x_0 está numa vizinhança suficientemente pequena de $\overline{x}$, então a trajetória de x_0 converge para o ponto fixo $\overline{x}$ e a velocidade de convergência é "quadrática", ou seja,

$$|x_{n+1} - \overline{x}| \leqslant \beta \cdot |x_n - \overline{x}|^2$$

onde β é uma constante.

ex:

- Estude a natureza dos pontos fixos das seguintes transformações

  $$f(x) = \alpha x \qquad f(x) = \alpha x^3 \qquad f(x) = \alpha x + \beta x^2$$

  ao variar os parâmetros.

- Digite 0.1 na sua máquina de calcular, e pressione repetidamente a tecla "cos". O que acontece?

- Estude a natureza do ponto fixo não trivial do modelo logístico

  $$x_{n+1} = \lambda x_n (1 - x_n)$$

  ao variar o parâmetro λ.

e.g. **Babylonian-Heron algorithm.** Considere o problema de determinar o lado ℓ de um quadrado dada a sua área $a > 0$, ou seja, o número que chamamos $\ell = \sqrt{a}$. Um método, descrito por Heron [16], mas utilizado provavelmente pelos babilónios [17] [18], consiste em construir recursivamente rectângulos de área a com lados cada vez mais próximos. Se x_1 e y_1 são a base e a altura do primeiro rectângulo, e portanto $x_1 y_1 = a$, então o segundo rectângulo tem como base a média aritmética $b_2 = (x_1 + y_1)/2$ de base e altura do primeiro, o terceiro rectângulo tem como base a média aritmética $x_3 = (x_2 + y_2)/2$ da base e a altura do segundo, e assim sucessivamente. A equação recursiva para as bases é

$$x_{n+1} = \frac{1}{2}\left(x_n + \frac{a}{x_n}\right) .$$

Observe que se a e a conjectura inicial são racionais, então todos os x_n são números racionais. We could, as the babylonians, put an initial guess $x_1 = 3/2$ for $\sqrt{2}$ (since $1^2 < 2 < 2^2$), and find

$$x_2 = \frac{17}{12} \simeq 1.41666666666 \qquad x_3 = \frac{577}{408} \simeq 1.41421568627 \qquad x_4 = \frac{665857}{470832} \simeq 1.41421356237$$

As you see, the sequence stabilizes quite fast.

[16] Heron of Alexandria, *Metrica*, Book I.
[17] C.B. Boyer, *A history of mathematics*, John Wiley & Sons, 1968.
[18] O. Neugebauer, *The exact sciences in antiquity*, Dover, 1969.

As a first attempt to explain this miracle, we could start looking at the recursive equations for the bases and the heights of the rectangles:

$$x_{n+1} = \frac{x_n + y_n}{2} \qquad y_{n+1} = \frac{2}{1/x_n + 1/y_n}$$

(so, the next height is the "harmonic mean" of the base and height). We see that the x_n's and the y_n's form decreasing and increasing sequences, respectively (disregarding the first guess, of course), namely

$$y_2 \leqslant y_3 \leqslant \dots \leqslant y_n \leqslant \dots \leqslant x_n \leqslant \dots \leqslant x_3 \leqslant x_2 \,,$$

The real root is somewhere between, namely $y_n \leqslant \sqrt{a} \leqslant x_n$. Hence, we have an explicit control of the error. A computation shows that the lenghts of those intervals, the differences $\varepsilon_n = x_n - y_n$ satisfy the recursion

$$\varepsilon_{n+1} < \frac{1}{2} \cdot \varepsilon_n$$

So, and initial "error" $\varepsilon_1 \leqslant 1$ (an easy achievement, since we easily recognize squares of integers) reduces to at least $\varepsilon_n \leqslant 2^{-n}$ after n iterations. The true error is actually much smaller. Indeed, in our example we may compute

$$\varepsilon_2 = \frac{17}{12} - 2\frac{12}{17} = \frac{1}{204} \simeq .005 \qquad \text{and} \qquad \varepsilon_3 = \frac{577}{408} - 2\frac{408}{577} = \frac{1}{235416} \simeq 0.000004$$

So that the first improved guess x_2 has already one correct decimals, and the second, x_3 has already four correct decimals!

Irrationals. What babylonians didn't suspect is that if you start with a rational guess for $\sqrt{2}$, you get an infinite sequence of rational approximations, but the process never stops. This is due to

Pythagoras theorem. *The square root of* 2 *is not rational.*

ex:

- A fórmula de Heron diz que a área de um triângulo de lados a, b e c, e semi-perímetro $s = (a+b+c)/2$ é

  $$\text{área} = \sqrt{s(s-a)(s-b)(s-c)}$$

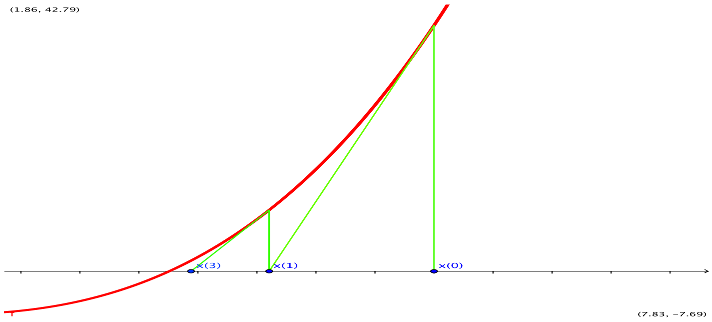
  Estime a área de um triângulo de lados 7, 8 e 9.
- Estime $\sqrt{13}$ com um erro < 0.01 e 0.001.
- Estime quantas iterações é preciso fazer para obter os primeiros n dígitos decimais de $\sqrt{2}$ usando o método dos babilónios.
- Prove o teorema se Pitágoras: $\sqrt{2}$ não é racional.

e.g. **Newton-Raphson iterative scheme.** Finding $\sqrt{a}$ means solving the polynomial equation $z^2 - a = 0$. What about finding roots of a generic polynomial $p(x) \in \mathbb{R}[x]$?

Newton's idea consists in improving an initial guess x_0 using the root of the linear approximation $p(x) \simeq p(x_0) + p'(x_0)(x - x_0)$, which is $x_1 = x_0 - p(x_0)/p'(x_0)$. This amounts to the iterative scheme

$$x_{n+1} = x_n - \frac{p(x_n)}{p'(x_n)} \,. \tag{4.2}$$

If the trajectory converges, i.e. $x_n \to x_\infty$, and if $p'(x_\infty) \neq 0$, then clearly the limit x_∞ is a root of p. On the other hand, if c is a root where $p'(c) \neq 0$, then c is a super-attractive fixed point of the map $x \mapsto f(x) ;= x - p(x)/p'(x)$. Therefore, an initial guess x_0 sufficiently near c will produce a trajectory (x_n) which converges to c (quadratically fast, i.e. such that $|x_{n+1} - c| \leqslant \beta \cdot |x_n - c|^2$ for some constant $\beta > 0$).



Search for a root of $x^3 - 2x - 5$ using Newton iterations.

help: `Mathematica®8` search for a root of an equation like $x^7 - 13x^5 + 9 = 0$ (or even more complicated equations, involving transcendental functions!) using the Newton iterative scheme starting with the initial guess $x_0 = 10$ with the instruction

```
FindRoot [x^7 - 13 x^5 + 9 == 0, {x, 10}]
{x -> 3.6035}
```

ex: **Exercícios.**

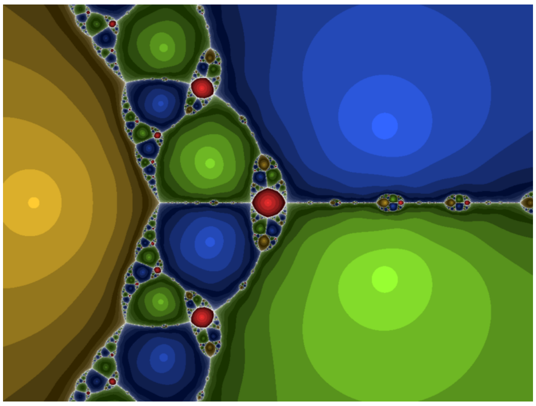
- Use Newton method to solve Newton's problem, i.e. find the roots of $x^3 - 2x - 5$.
- Show that Newton method to solve $x^2 - a = 0$ corresponds to babylonian-Heron iterative scheme.
- Use o método de Newton para aproximar a "razão", a raiz positiva de $x^2 - x - 1$. Then, compare with the babylonian-Heron method (i.e., estimate $\sqrt{5}$, then sum 1 and divide by 2).
- Write and implement Newton method to find n-th roots, i.e. to solve $x^n - a = 0$.
- Utilize o método de Newton para estimar raizes de

$$z^2 + 1 + z \qquad z^3 - z - 1 \qquad z^5 + z + 1 \qquad z^3 - 2z - 5$$

e.g. **Newton's fractals.** Em 1879 Cayley observou que o método pode ser utilizado também para aproximar raízes complexas de polinómios $p(z) \in \mathbb{C}[z]$. A receita consiste em iterar a função racional

$$f(z) = z - \frac{p(z)}{p'(z)}$$

O problema é decidir quando, ou seja para quais valores da conjetura inicial z_0, a sucessão (z_n), com $z_{n+1} = f(z_n)$, converge para uma raiz de $p(z)$. As bacias de atração das diferentes raizes desenham padrões surprendentes no plano complexo



Basins of attraction of the three roots of $2z^3 - 2z + 2$ in the complex plane.
(from http://en.wikipedia.org/wiki/Newton_fractal).

Iteração de funções racionais na esfera de Riemann. É natural considerar iterações de funções racionais $f(z) \in \mathbb{C}(z)$ arbitrárias (os endomorfismos da esfera de Riemann $\overline{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$), e querer descrever as trajecórias definidas pela equação recursiva $z_{n+1} = f(z_n)$.

O exemplo mais estudado consiste nas iterações da família de polinómios quadráticos

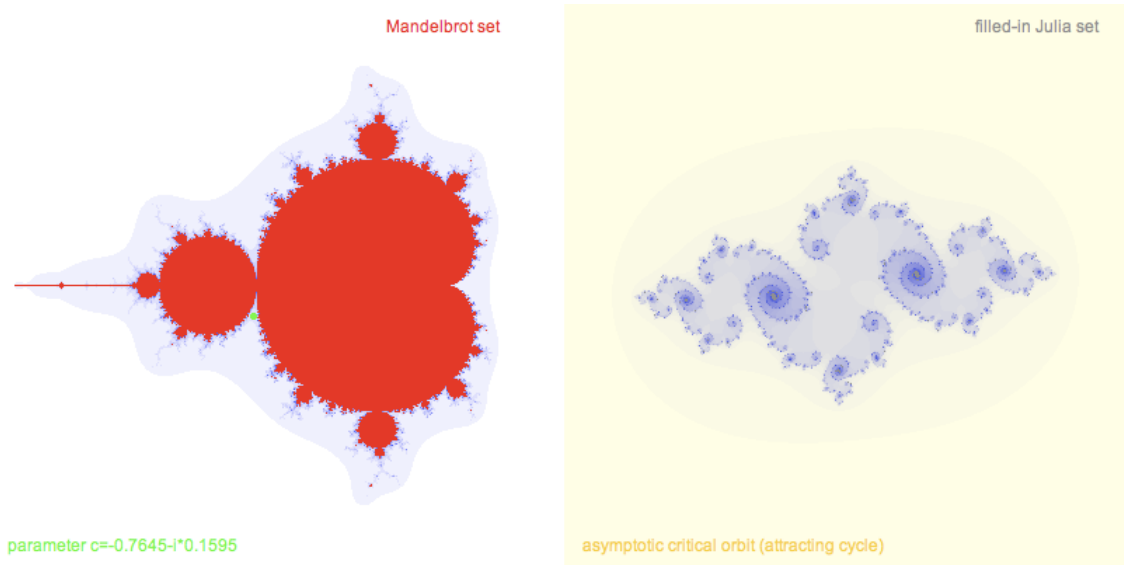
$$f(z) = z^2 + c$$

ao variar o parâmetro $c \in \mathbb{C}$. A sua beleza foi intuida por Gaston Julia[19] e Pierre Fatou[20] no princípio do século XX, desvendada com o auxílio dos computadores modernos por Benoît Madelbrot, e estudada por uma multidão de excelentes matemáticos (como Adrian Douady, Dennis Sullivan, John Milnor, Misha Lyubich, Jean-Christophe Yoccoz, Curtis McMullen, . . .) a partir dos anos '80 do século passado.

Nice pictures. Em baixo, está uma imagem que nos tempos de Julia e Fatou apenas era possível ver com uns olhos matemáticos bem afinados (um applet Java que produz a figura está no meu bestiario). O laço de corações vermelhos à esquerda, chamado *Mandelbrot set*, consiste nos valores do parâmetro complexo c tais que a órbita do ponto crítico $z_0 = 0$ permanece limitada. A região cinzenta à direita, chamada *filled-in Julia set*, consiste no conjunto das condições iniciais z_0 cuja órbita é limitada. As outras côres (que permitem ver os conjuntos "invisíveis" de Cantor) são escolhidas dependendo da velocidade com que as trajectórias z_n fogem para o infinito.

[19] G. Julia, Mémoire sur l'iteration des fonctions rationnelles, *Journal de Mathématiques Pures et Appliquées*, **8** (1918), 47-245.

[20] P. Fatou, Sur les substitutions rationnelles, *Comptes Rendus de l'Académie des Sciences de Paris*, **164** (1917) 806-808, and **165** (1917), 992-995.



Mandelbrot set (left) and Julia set of the polynomial $z^2 + c$, with $c \simeq -0.7645 - i \cdot 0.1595$ (right).
(from http://w3.math.uminho.pt/~scosentino/bestiario/julia.html)

5 Área, integral e métodos de integração

The problem posed by Newton equation. If you derive twice a trajectory $t \mapsto q(t) \in \mathbb{R}^3$, you get the velocity $v(t) := \dot{q}(t)$ and then then acceleration $a(t) := \ddot{q}(t)$. Physicists know the acceleration of a particle in an inertial frame, it is proportional to the force, according to Newton equation

$$m\ddot{q} = F(q, \dot{q}, t) .$$

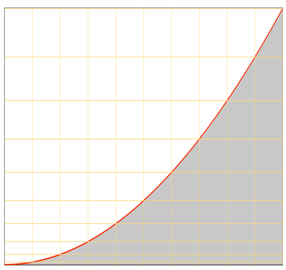
Therefore, they have the problem to deduce the trajectory from its second derivative.

Work. The work done by a constant force field F to move a particle from the position q_0 to the position q_1, hence a distance $\delta q = q_1 - q_0$, is $\mathrm{W} = F \cdot \delta q$. If we make a path through the points q_0, q_1, ..., q_n, with increments $\delta q_k = q_k - q_{k-1}$, and assume that the force is piece-wise constant, we are led to an expression

$$\mathrm{W} = F(q_1) \cdot \delta q_1 + F(q_2) \cdot \delta q_2 + \cdots + F(q_n) \cdot \delta q_n .$$

This is a sum of signed areas (i.e. positive or negative depending on the sign of the force) of rectangles with bases δq_k and heights $F(q_k)$. If we plot the graph of $F(q)$, this is the signed area of the region bounded by such a graph, the q-axis, and the vertical lines q_0 and q_n. For a generic force $F(q)$, say continuous, it is natural to call work such an area, and pose the problem to compute it.

e.g. **Area of a parabolic segment according to Eudoxo and Arquimedes.** O *método de exaustão*, utilizado por Eudoxo e Arquimedes, para calcular a área de uma figura geométrica consiste em aproximar a região com reuniões de figuras simples, como rectângulos e triângulos. Por exemplo, a área do "segmento parabólico"



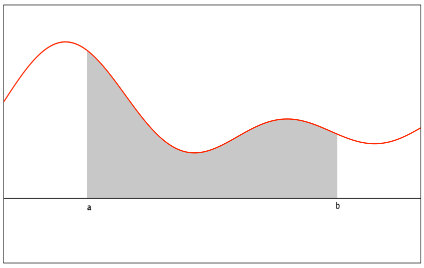
$$A = \{(x, y) \in \mathbb{R}^2 \text{ t.q. } 0 \leqslant x \leqslant 1 \text{ e } 0 \leqslant y \leqslant x^2\},$$

pode ser aproximada dividindo o intervalo $[0, 1]$ em n subintervalos de comprimento $1/n$, e observando que área(A) é superior à soma $s_n(A)$ das áreas dos rectângulos de bases $[\frac{k}{n}, \frac{k+1}{n}]$ e alturas $(k/n)^2$, e inferior à soma $S_n(A)$ das áreas dos rectângulos de bases $[\frac{k}{n}, \frac{k+1}{n}]$ e alturas $((k+1)/n)^2$, onde $k = 0, 1, 2, ..., n-1$. Ou seja,

$$\sum_{k=0}^{n-1} \frac{k^2}{n^3} = s_n(A) \leqslant \text{área}(A) \leqslant S_n(A) = \sum_{k=1}^{n} \frac{k^2}{n^3}$$

- Mostre que a diferença $S_n(A) - s_n(A) \to 0$ quando $n \to \infty$.
- Use a identidade
$$1^2 + 2^2 + 3^2 + ... + n^2 = \frac{n^3}{3} + \frac{n^2}{2} + \frac{n}{6}$$
para mostrar que, quando $n \to \infty$, as aproximações $s_n(A)$ e $S_n(A)$ convergem para $1/3$.

Riemann integral. Let $f : [a, b] \to \mathbb{R}$ be a bounded function. We want to define the signed area between the graph of $y = f(x)$, the x-axis (i.e. $y = 0$), and the vertical lines $x = a$ and $x = b$. For example, if $f(x) \geqslant 0$, this is the area



$$\text{area}\left(\{(x,y)\in\mathbb{R}^2 \text{ t.q. } a\leqslant x\leqslant b \text{ e } 0\leqslant y\leqslant f(x)\}\right) \quad ,$$

The strategy is to approximate the area from below and from above, namely fill and cover the region by unions of rectangles with smaller and smaller bases.

A *partition* of the interval $[a,b]$ is a finite collection $P\subset[a,b]$ of points (that we may order according to their natural order) $a = x_0 < x_1 < x_2 < \cdots < x_k < x_{k+1} < \cdots < x_n = b$ dividing the interval in a finite number (in this case n) of subintervals $[x_k, x_{k+1}]$ of lengths $\delta x_k := x_{k+1} - x_k$. Given a partition P, we denote by m_k and M_k the minimum and the maximum of f in the subinterval $[x_k, x_{k+1}]$, respectively, hence define the *lower sum* and the *upper sum* of f w.r.t. the partition P as

$$s(f;P) := \sum_{k=0}^{n-1} m_k\cdot\delta x_k \qquad \text{and} \qquad S(f;P) := \sum_{k=0}^{n-1} M_k\cdot\delta x_k\,,$$

respectively. It is clear that the signed area (as the work, if f represents a force) we are trying to compute should be somewhere between $s(f;P)\leqslant$ "area" $\leqslant S(f;P)$. It is also clear that if we "refine" the partition P, i.e. if we define a partition P' containing more points than P (hence $P\subset P'$ as subsets of $[a,b]$), then $s(f;P)\leqslant s(f;P')$ and $S(f;P')\leqslant S(f;P)$. In particular, we always have the inequality $s(f;P)\leqslant S(f;Q)$ for all partitions P and Q (just consider the common refinement $P\cup Q$ and use the previous observations).

We say that the bounded function f is *(Riemann) integrable* in the interval $[a,b]$ if there exists a unique number A such that $s(f;P)\leqslant A\leqslant S(f;Q)$ for all partitions P and Q. Equivalently, if $\sup_P s(f;P) = A = \inf_P S(f;P)$ (if you know what sup and inf are). Equivalently, if for any precision $\varepsilon > 0$ one may find two partitions P and Q such that $S(f;Q) - s(f;P) < \varepsilon$, hence a partition R (for example $R = P\cup Q$) such that $S(f;R) - s(f;R) < \varepsilon$. If this happens, we call such number "*integral* of f in $[a,b]$", and denote it as

$$A := \int_a^b f(x)\,dx\,.$$

About the notation. The notation $\int_a^b f(x)\,dx$ reminds you that the integral should be thought as a sort of limit of the finite sums $\sum_k f(x_k)\cdot\delta x_k$ as the partition gets finer, i.e. as the maximal $|\delta x_k|$ goes to zero. Actually, the notation, to be compared with Leibniz notation dy/dx for derivatives, is useful to state and remind some recipes to compute integrals, as will appear clear in the following.

Also, the variable x inside the integral may be replaced by any other symbol, so that you can also write $\int_a^b f(t)\,dt$, or $\int_a^b f(\clubsuit)\,d\clubsuit$, or $\int_a^b f(🐟)\,d🐟$, ...or whatever you want. The only forbidden symbols are those that you already used somewhere else: so, for example, you can't write $\int_a^b f(b)\,db$.

Integrability of continuous and monotone functions. Which function are Riemann integrable? The final answer is somehow technical. Here, you may be satisfied with knowing that continuous (or also piece-wise continuous) or monotone functions are.

Theorem 5.1. *Any continuos function $f(x)$ in a closed and bounded interval $[a,b]$ is integrable.*

Indeed, a continuous function in a closed and bounded (i.e. compact) interval is uniformly continuous. In particular, for any $\varepsilon > 0$ there exists a $\delta > 0$ such that $|x - x'| < \delta$ implies

$|f(x) - f(x')| \leqslant \varepsilon/(b-a)$. Consequently, if P is a partition of $[a,b]$ into n subintervals of length $x_{k+1} - x_k < \delta$, we see that $S(f,P) - s(f,P) \leqslant n \cdot \delta \cdot \varepsilon/(b-a) \leqslant \varepsilon$.

It is clear that also a function $f : [a,b] \to \mathbb{R}$ with a finite number of discontinuities and finite limits on both sides is integrable (just repeating the argument in any closed subinterval where it is continuous).

Theorem 5.2. *Any monotone function $f(x)$ in a closed and bounded interval $[a,b]$ is integrable.*

Indeed, assume that $f(x)$ is non-decreasing (otherwise take $-f(x)$), and take any $\varepsilon > 0$. If P is a partition of $[a,b]$ into n subintervals of length $|x_{k+1} - x_k| \leqslant \varepsilon/(f(b) - f(a))$, then, since $m_k = f(x_k)$ and $M_k = f(x_{k+1})$,

$$S(f,P) - s(f,P) \leqslant \frac{\varepsilon}{f(b) - f(a)} \sum_{k=0}^{n-1} (f(x_{k+1}) - f(x_k)) \leqslant \varepsilon\,,$$

because the above sum is telescopic and equal to $f(b) - f(a)$.

Elementary properties. The following elementary properties of the integral are obvious for integrals of constant functions, namely for areas of rectangles. But the Riemann integral is defined using rectangles, so it is not surprising that they continue to hold for all integrable functions. You may want to draw pictures to understand their meanings and to convince yourself of their validity.

It is clear that the integral is linear, namely

$$\int_a^b (f(x) + g(x))\,dx = \int_a^b f(x)\,dx + \int_a^b g(x)\,dx \tag{5.1}$$

and

$$\int_a^b \lambda \cdot f(x)\,dx = \lambda \cdot \int_a^b f(x)\,dx \quad . \tag{5.2}$$

for all integrable function $f(x)$ and $g(x)$ and all constants $\lambda \in \mathbb{R}$. It is clear that

$$\int_a^b f(x)\,dx = \int_a^c f(x)\,dx + \int_c^b f(x)\,dx\,, \tag{5.3}$$

whenever $a < c < b$. If we define

$$\int_a^a f(x)\,dx := 0\,,$$

and

$$\int_b^a f(x)\,dx := -\int_a^b f(x)\,dx\,,$$

then formula (5.3) holds for all a, b, c, independently of their order. The integral, being a signed area, behaves well under translations and dilatations of the independent variable, namely:

$$\int_a^b f(x)\,dx = \int_{a+c}^{b+c} f(x-c)\,dx \tag{5.4}$$

for all $c \in \mathbb{R}$, and

$$\int_{\lambda a}^{\lambda b} f(x/\lambda)\,dx = \lambda \int_a^b f(x)\,dx \tag{5.5}$$

for all $\lambda > 0$. The integral is monotone:

$$f(x) \leqslant g(x) \quad \forall x \in [a,b] \qquad \Rightarrow \qquad \int_a^b f(x)\,dx \leqslant \int_a^b g(x)\,dx\,. \tag{5.6}$$

In particular,

$$\int_a^b f(x)\,dx \leqslant \int_a^b |f(x)|\,dx\,. \tag{5.7}$$

Finally, it can be (crudely) estimated as

$$m \leqslant f(x) \leqslant M \quad \forall x \in [a,b] \qquad \Rightarrow \qquad m \cdot (b-a) \leqslant \int_a^b f(x)dx \leqslant M \cdot (b-a)\,. \tag{5.8}$$

An interesting consequence is the

Theorem 5.3. (Mean value theorem). *If $f : [a,b] \to \mathbb{R}$ is a continuous function, then there is a point $c \in [a,b]$ such that*

$$\int_a^b f(x)\,dx = f(c) \cdot (b-a)\,.$$

Indeed, let m and M be the minimum and maximum of $f(x)$ in the interval $[a,b]$, respectively. From (5.8), we see that there exists some value $m \leqslant d \leqslant M$ such that $\int_a^b f(x)\,dx = d \cdot (b-a)$. By continuity (i.e. Bolzano theorem), there exists a point $c \in [a,b]$ where $f(c) = d$.

Observe that the value

$$f(c) = \frac{1}{b-a} \cdot \int_a^b f(x)\,dx$$

must be thought as an average of the values $f(x)$ for $a \leqslant x \leqslant b$.

ex: Compute the following integrals drawing a picture and using the elementary formulas for areas.

$$\int_0^1 3dx \qquad \int_{-2}^2 7\,dx \qquad \int_1^{10} x\,dx \qquad \int_{-2}^3 (-2x)\,dx$$

$$\int_{-2}^2 |x|\,dx \qquad \int_0^3 (5x-2)\,dx \qquad \int_{-33}^{33} (11-x)\,dx$$

$$\int_0^{n+1} [x]\,dx\,^{21} \qquad \int_6^x 7t\,dt \qquad \int_x^{x^2} (1-t)\,dt$$

Derivative of an integral. Here is Newton's and Leibniz' discovery:

Theorem 5.4. (fundamental theorem of calculus) *Let $f(x)$ be a continuous function defined in some interval $I \subset \mathbb{R}$. Given a point $a \in I$, define the function $F(x)$ as the integral*

$$F(x) := \int_a^x f(t)\,dt\,,$$

for $x \in I$. Then $F(x)$ is differentiable, and its derivative is $F'(x) = f(x)$, i.e

$$\frac{d}{dx}\left(\int_a^x f(t)\,dt\right) = f(x)\,.$$

Indeed, the difference $F(x+\delta) - F(x)$ is equal to the integral $\int_x^{x+\delta} f(t)\,dt$. Therefore,

$$\frac{F(x+\delta)-F(x)}{\delta} - f(x) = \frac{1}{\delta}\int_x^{x+\delta} (f(t)-f(x))\,dt\,. \tag{5.9}$$

If f is continuous at the point x (just at the point x!), for any $\varepsilon > 0$ there exists $\delta > 0$ such that $|t-x| < \delta$ implies $|f(t)-f(x)| < \varepsilon$. Therefore, for such small $\delta > 0$, the r.h.s. of (5.9) above is bounded by $\frac{1}{\delta} \cdot \varepsilon \cdot \delta = \varepsilon$. Consequently, $(F(x+\delta)-F(x))/\delta \to f(x)$ when $\delta \to 0$.

[21] $[x]$ denotes the "integer part of x", i.e. the unique integer $n \in \mathbb{Z}$ such that $n \leqslant x < n+1$.

Logarithm and exponential. The *logarithm* is the function $\log : \mathbb{R}_+ \to \mathbb{R}$ defined by the integral

$$\log(x) := \int_1^x \frac{dt}{t}$$

for $x \in \mathbb{R}_+ =]0, \infty[$. By the fundamental theorem of calculus 5.4, the derivative is

$$\log'(x) = \frac{1}{x}$$

so that the logarithm is strictly increasing. It is clear that $\log(1) = 0$. Moreover, for any $x, y > 0$

$$\int_1^{xy} \frac{dt}{t} = \int_1^x \frac{dt}{t} + \int_x^{xy} \frac{dt}{t} = \int_1^x \frac{dt}{t} + \int_1^y \frac{ds}{s},$$

(using (5.5) in the second integral above), therefore

$$\log(xy) = \log(x) + \log(y). \tag{5.10}$$

Also, for any $x > 0$

$$\int_1^{1/x} \frac{dt}{t} = \int_x^1 \frac{ds}{s} = -\int_1^x \frac{ds}{s}$$

(using (5.5)), therefore

$$\log(1/x) = -\log(x). \tag{5.11}$$

In particular, $\log(x) \to \infty$ when $x \to \infty$, and $\log(x) \to -\infty$ when $x \to 0$. Thus, $\log(\mathbb{R}_+) = \mathbb{R}$.

The *exponential* is the inverse function of the logarithm, the function $\exp : \mathbb{R} \to \mathbb{R}_+$ such that $\exp(\log x) = x$ for all $x \in \mathbb{R}_+$ and $\log(\exp(y)) = y$ for all $y \in \mathbb{R}$. In particular, $\exp(0) = 1$. The value $\exp(x)$ is also denoted by e^x, where $e = \exp(1)$, hence $\log(e) = 1$. The derivative of the exponential is

$$\exp'(x) = \exp(x).$$

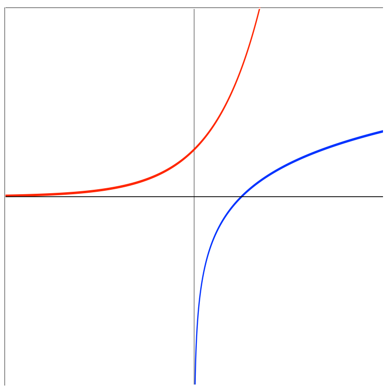
From (5.10) we get

$$\exp(x + y) = \exp(x)\exp(y) \tag{5.12}$$

for all $x, y \in \mathbb{R}$, and from (5.11) we get

$$\exp(-x) = 1/\exp(x) \tag{5.13}$$

for all $x \in \mathbb{R}$.



Graphs of the logarithm (blue) and the exponential (red).

Primitives and integration. A differentiable function $F(x)$ is called a *primitive* ("a" primitive, and not "the" primitive!) of the continuous function $f(x)$ if

$$F'(x) = f(x)$$

for any x in a common interval of definition. Leibniz' notation for a primitive of $f(x)$ is $\int f(x)\,dx$. Thus, for example, $\log(x)$ is a primitive of $1/x$, and e^x is a primitive of e^x itself.

We already know a primitive of a continuous function $f(x)$, this is $G(x) = \int_a^x f(t)\,dt$, according to theorem 5.4. If $F(x)$ is any other primitive of the same function $f(x)$, then the difference $F(x) - G(x)$ has zero derivatives, hence is constant by the mean value theorem. Therefore, there is some constant $c \in \mathbb{R}$ such that $F(x) = G(x) + c$ for any x (in some domain). In particular, if we take $x = a$ and then $x = b$, we see that $F(a) = c$ and $F(b) = G(b) + c$, so that $G(b) = F(b) - F(a)$. Therefore, we may state the following recipe to compute integrals:

Theorem 5.5. *If $F(x)$ is any primitive of $f(x)$, then*

$$\int_a^b f(x)\,dx = [F(x)]_a^b := F(b) - F(a)\,. \tag{5.14}$$

Thus, to any derivative that you know there corresponds an integral that you can compute.

ex: Compute the following primitives.

$$\int dx \qquad \int x^2 dx \qquad \int \frac{1}{x^3} dx \qquad \int \sqrt{2x-1}dx$$

$$\int (x^2 - 2x + 5)dx \qquad \int \sin(\theta)d\theta \qquad \int \left(\cos(\pi x) - 2x^3\right)dx \qquad \int \frac{dx}{\sqrt{x}}$$

$$\int \frac{d\theta}{\cos^2(\theta)} \qquad \int \frac{dx}{1+x^2} \qquad \int \frac{dx}{\sqrt{1-x^2}}$$

ex: Compute the following integrals.

$$\int_0^3 (x-1)dx \qquad \int_{-1}^1 (1-|x|)dx \qquad \int_0^{10} \sqrt{x}dx \qquad \int_{-\pi}^{\pi} \cos(x)dx$$

$$\int_{-3}^2 \sqrt{x^2}dx \qquad \int_{-\pi}^{\pi/2} \sin(2x)dx \qquad \int_1^2 \frac{1}{x^2}dx \qquad \int_3^5 \left(x^{1/3} - x^{1/5}\right)dx$$

$$\int_{-5}^5 \left(1 + 399x - x^2\right)dx \qquad \int_0^{2\pi} |\sin(x)|dx \qquad \int_{-1}^1 (33-11x)^{66}\,dx$$

$$\int_2^3 \frac{dx}{x} \qquad \int_{\log 1}^{\log 2} e^x dx \qquad \int \frac{dx}{x-1} \qquad \int_1^2 e^{x-1}dx$$

$$\int 2e^{3x}dx \qquad \int_0^7 e^{-x}dx \qquad \int \frac{1}{x(1-x)}dx$$

ex: Compute the derivative of

$$F(x) = \int_0^x \frac{dt}{1+t^2} \qquad F(x) = \int_0^{x^2} \sin(t)dt \qquad F(x) = \int_{2x}^{x^3} (t-t^2)dt$$

ex: Compute the area of the planar region bounded by the curves

$$y = x^2 \quad \text{e} \quad y = x^3\,, \qquad \text{com } 0 \leqslant x \leqslant 1$$

$$y = \sin(x) \quad \text{e} \quad y = -\sin(x)\,, \qquad \text{com } 0 \leqslant x \leqslant \pi$$

$$y = x^{1/3} \quad \text{e} \quad y = x^{1/2}\,, \qquad \text{com } 0 \leqslant x \leqslant 1$$

e.g. **Potential energy and work.** Let $f(x)$ be a continuous force field, defined in an interval of the real line. Any function $V(x)$ such that $V'(x) = -f(x)$ (i.e. minus a primitive of $f(x)$) is called *potential energy*. Theorem 5.5 says that the work done when displacing a particle from a to b is

$$W(a \to b) = \int_a^b f(x)\, dx = V(a) - V(b)\,.$$

thus equal to the difference between the potential energies of the initial and the final points. Observe that in dimension one all (continuous) forces are conservative! Indeed, any $-\int_a^x f(t)\, dt$ is a potential.

Substitutions. Let $F(x)$ be a primitive of the continuous function $f : I \to \mathbb{R}$. If $g : I \to \mathbb{R}$ is a continuous function, then by (5.14)

$$\int_{g(a)}^{g(b)} f(y)\, dy = F(g(b)) - F(g(a))\,.$$

If, moreover, g is differentiable, by the chain rule $F(g(x))$ is a primitive of $f(g(x))\, g'(x)$, hence by (5.14) again, the r.h.s. above is also equal to

$$F(g(b)) - F(g(a)) = \int_a^b f(g(x))\, g'(x)\, dx\,.$$

Therefore, we may state the following recipe to transform one integral into another, hopefully simpler, integral: the "substitution" $y = g(x)$, with $dy = g'(x)dx$ (this means $dy/dx = g'(x)$), transforms $f(g(x))\, g'(x)\, dx$ into $f(y)\, dy$, so that

$$\int_a^b f(g(x))\, g'(x)\, dx = \int_{g(a)}^{g(b)} f(y)\, dy \qquad (5.15)$$

e.g. For example, the substitution $y = x^2$, with $dy = 2xdx$, sends

$$\int_a^b x e^{x^2}\, dx = \frac{1}{2}\int_{a^2}^{b^2} e^y\, dy = \frac{e^{b^2} - e^{a^2}}{2}$$

ex: Compute

$$\int_0^1 x e^{x^2} dx \qquad \int \frac{\cos(\log x)}{x} dx \qquad \int \frac{\cos(\theta)}{\sqrt{5 + 2\sin(\theta)}} d\theta \qquad \int \tan(\theta) d\theta$$

$$\int 3x^2 \cos(x^3) dx \qquad \int_\pi^{2\pi} \frac{\sin(\sqrt{x})}{\sqrt{x}} dx \qquad \int_{-1/2}^{1/2} \frac{x}{\sqrt{1 - x^2}} dx$$

$$\int \cos(x) e^{\sin(x)} dx \qquad \int \frac{x}{x^2 - 1} dx \qquad \int_{\log 1}^{\log 2} \frac{e^x}{\sqrt{1 + e^x}} dx \qquad \int \frac{\sin(\sqrt{x})}{\sqrt{x}} dx$$

Integration by parts. Let f and g be two differentiable functions. The derivative of the product fg is $(fg)' = f'g + fg'$. Therefore, by (5.14),

$$\int_a^b f(x) g'(x) dx = [f(x)g(x)]_a^b - \int_a^b f'(x) g(x) dx\,. \qquad (5.16)$$

This is useful when the integral on the left seems difficult, but the one on the right is simple.

e.g. For example, from $(x \sin x)' = \sin x + x \cos x$, we get

$$\int x \cos(x)\, dx = x \sin x - \int \sin(x)\, dx = x \sin(x) + \cos(x)\,.$$

ex: Calcule

$$\int_0^1 xe^{-x}\,dx \qquad \int \sin(\log(x))\,dx \qquad \int_1^{e^3} \log(x)\,dx$$
$$\int x\sin(x)\,dx \qquad \int x^2\sin(x)\,dx \qquad \int e^x\sin(x)\,dx$$

ex: Compute

$$\int_0^1 xe^{x^2}\,dx \qquad \int \frac{\cos(\log x)}{x}dx \qquad \int \frac{\cos(\theta)}{\sqrt{5+2\sin(\theta)}}d\theta \qquad \int \tan(\theta)d\theta$$
$$\int \cos(x)e^{\sin(x)}dx \qquad \int \frac{x}{x^2-1}dx \qquad \int_{\log 1}^{\log 2} \frac{e^x}{\sqrt{1+e^x}}dx$$

help: `Mathematica®8` computes primitives as

```
Integrate[1/ Sin[2 x], x]
-(1/2) Log[Cos[x]] + 1/2 Log[Sin[x]]
```

or (definite) integrals as

```
Integrate[x^2 - Sin[x], {x, 0, 3}]
8 + Cos[3]
```

e.g. Velocity/acceleration + initial conditions ⇒ time law) If we know the velocity $v(t) = \dot{q}(t)$ of a particle (moving in one dimension) and its initial condition $q(0)$, we may find its trajectory as

$$q(t) = q(0) + \int_0^t v(s)\,ds\,.$$

If we know the acceleration $a(t) = \dot{v}(t)$ and the initial velocity $v(0)$, we may integrate once to get

$$v(t) = v(0) + \int_0^t a(s)\,ds\,,$$

and then integrate once again to get the trajectory $q(t)$ as above.

e.g. Work of a perfect gas. The work done by a perfect gas expanding from an initial volume V_0 to a final volume V_1 is given by the integral of the pressure $p(V)$

$$W = \int_{V_0}^{V_1} p(V)\,dV\,.$$

If the pressure is mantained constant, this is simply $W = p\cdot(V_1 - V_0)$. If the expansion occurs at constant temperature T, we get from the equation of state $pV = nRT$ (here n is the number of moles, $R \simeq 8.314\times 10^7$ J/K mol, and T the absolute temperature)

$$W = nRT\int_{V_0}^{V_1}\frac{dV}{V} = nRT\log(V_1/V_0)\,.$$

Improper integrals. It is useful to integrate a function in an infinite domain like $[a,\infty)$, the definition being

$$\int_a^\infty f(x)\,dx := \lim_{K\to\infty}\int_a^K f(x)\,dx\,,$$

or in a domain $(a,b]$ bounded by a point a where the function is not defined, the definition being

$$\int_{a^+}^b f(x)\,dx := \lim_{\varepsilon\searrow 0}\int_{a+\varepsilon}^b f(x)\,dx\,.$$

These limits are called *improper integrals*.

e.g. **Gaussian and error function.** An important function in many areas of mathematics and applied sciences is the *Gaussian* $g(x) := e^{-x^2}$ (and its variations, obtained by a linear change of coordinates, or multidimensional ones). One knows that the improper integral

$$\int_{-\infty}^{\infty} e^{-x^2}\, dx = \sqrt{\pi}$$

(we'll compute it later), thus $\frac{1}{\sqrt{\pi}} e^{x^2}$ is a probability distribution, indeed a most fundamental one. A primitive of the Gaussian cannot be computed in terms of elementary functions (polynomials, trigonometric, exponential, ...), hence deserves a name. It is called *error function*, and usually normalized according to

$$\mathrm{erf}(x) := \frac{2}{\sqrt{\pi}} \int_0^x e^{t^2}\, dt\,.$$

Thus, $\mathrm{erf}(x) \to \pm 1$ as $x \to \pm\infty$.

Formulário primitivas

	(função)	("uma" primitiva)
	$f(x) = F'(x)$	$\int f(x)dx = F(x)$
(por substituição)	$f(y(x))y'(x)$	$\int f(y(x))y'(x)dx = \int f(y)dy$
(por partes)	$f(x)g'(x)$	$\int f(x)g'(x)dx = f(x)g(x) - \int f'(x)g(x)dx$
(constantes)	λ	$\int \lambda dx = \lambda x$
(potências, $\alpha \neq -1$)	x^α	$\int x^\alpha dx = \frac{1}{\alpha+1}x^{\alpha+1}$
(logaritmo)	$1/x$	$\int \frac{dx}{x} = \log \lvert x \rvert$
(exponencial)	e^x	$\int e^x dx = e^x$
(seno)	$\sin(x)$	$\int \sin(x)dx = -\cos(x)$
(coseno)	$\cos(x)$	$\int \cos(x)dx = \sin(x)$
(tangente)	$\frac{1}{\cos^2(x)}$	$\int \frac{dx}{\cos^2(x)} = \tan(x)$
(cotangente)	$\frac{1}{\sin^2(x)}$	$\int \frac{dx}{\sin^2(x)} = -\text{cotan}(x)$
(arco cujo seno)	$\frac{1}{\sqrt{1-x^2}}$	$\int \frac{dx}{\sqrt{1-x^2}} = \arcsin(x)$
(arco cuja tangente)	$\frac{1}{1+x^2}$	$\int \frac{dx}{1+x^2} = \arctan(x)$
(exponencial $\times$ seno)	$e^{\alpha x}\sin(\beta x)$	$\int e^{\alpha x}\sin(\beta x)dx = \frac{e^{\alpha x}(\alpha\sin(\beta x)-\beta\cos(\beta x))}{\alpha^2+\beta^2}$
(exponencial $\times$ coseno)	$e^{\alpha x}\cos(\beta x)$	$\int e^{\alpha x}\cos(\beta x)dx = \frac{e^{\alpha x}(\alpha\cos(\beta x)+\beta\sin(\beta x))}{\alpha^2+\beta^2}$
(coseno $\times$ coseno, $n^2 \neq m^2$)	$\cos(nx)\cos(mx)$	$\int \cos(nx)\cos(mx)dx = \frac{\sin((n+m)x)}{2(n+m)} + \frac{\sin((n-m)x)}{2(n-m)}$
(seno $\times$ seno, $n^2 \neq m^2$)	$\sin(nx)\sin(mx)$	$\int \sin(nx)\sin(mx)dx = -\frac{\sin((n+m)x)}{2(n+m)} - \frac{\sin((n-m)x)}{2(n-m)}$
(seno $\times$ coseno, $n^2 \neq m^2$)	$\sin(nx)\cos(mx)$	$\int \sin(nx)\cos(mx)dx = -\frac{\cos((n+m)x)}{2(n+m)} - \frac{\cos((n-m)x)}{2(n-m)}$
(x $\times$ coseno, $n \neq 0$)	$x\cos(nx)$	$\int x\cos(nx)dx = \frac{\cos(nx)}{n^2} + \frac{x\sin(nx)}{n}$
(x $\times$ seno, $n \neq 0$)	$x\sin(nx)$	$\int x\sin(nx)dx = \frac{\sin(nx)}{n^2} - \frac{x\cos(nx)}{n}$
(x^k $\times$ coseno, $n \neq 0$)	$x^k\cos(nx)$	$\int x^k\cos(nx)dx = \frac{x^k\sin(nx)}{n} - \frac{k}{n}\int x^{k-1}\sin(nx)dx$
(x^k $\times$ seno, $n \neq 0$)	$x^k\sin(nx)$	$\int x^k\sin(nx)dx = -\frac{x^k\cos(nx)}{n} + \frac{k}{n}\int x^{k-1}\cos(nx)dx$

6 Equações diferenciais ordinárias

e.g. Free particle. The trajectory $t \mapsto q(t) \in \mathbb{R}^3$ of a free particle of mass m in an inertial frame is modeled by the Newton equation

$$\frac{d}{dt}(mv) = 0\,, \qquad \text{i.e., if } m \text{ is constant,} \qquad ma = 0\,,$$

where $v(t) := \dot{q}(t)$ denotes the *velocity* and $a(t) := \ddot{q}(t)$ denotes the *acceleration* of the particle. In particular, the *linear momentum* $p := mv$ is a constant of the motion (i.e. $\frac{d}{dt}p = 0$), in accordance with Galileo's principle of inertia or Newton's first law[22].

The solutions of Newton equation are the affine lines

$$q(t) = s + vt\,,$$

where $s, v \in \mathbb{R}^3$ are arbitrary vectors, the initial position and the initial velocity.

Thus, for example, the trajectory of a free particle starting at $q(0) = (3,2,1)$ with velocity $\dot{q}(0) = (1,2,3)$ is $q(t) = (3,2,1) + (1,2,3)t$.

e.g. Free fall near the Earth surface. The Newton equation

$$m\ddot{x} \simeq -G\frac{mM_\oplus}{R_\oplus^2}$$

models the free fall of a particle of mass m near the Earth surface. Here $x(t)$ is the height of the particle at time t (measured from some reference height, e.g. the sea level), $G \simeq 6.67$ m^3 kg^{-1} s^{-2} is the gravitational constant, $M_\oplus$ and $R_\oplus$ are the mass and radius of the Earth, respectively. We are assuming that $x \ll R_\oplus$. Since inertial and gravitational masses are (experimentally) equal, the mass m cancels out and we get the equation

$$\ddot{x} = g\,,$$

where $g := GM_\oplus/R_\oplus^2 \simeq 9.8$ m s^{-2} is the the gravitational acceleration near the Earth surface, independent on the falling object!

A function with constant second derivative equal to $-g$ is $-gt^2/2$. But it is not the unique solution. We may add to it any function with zero second derivative, that is any constant s and any linear function vt. This means that also any

$$x(t) = s + vt - \frac{1}{2}gt^2$$

is a solution of our Newton equation, for any s and any v. The first arbitrary constant s is the initial position $x(0)$ (and this physically corresponds to the homogeneity of space: Newtonian physics is independent on the place where the laboratory is placed). The second arbitrary constant v is the initial velocity $\dot{x}(0)$ (and this physically corresponds to Galilean invariance: we cannot distinguish between two inertial laboratories moving at constant speed one from each other).

The moral is that the Newton equation alone does not have a "unique" solution. It has a whole "family of solutions", depending on two parameters s and v. On the other side, once we fix the initial position $x(0)$ and the initial velocity $\dot{x}(0)$, the solution turns out to be unique (we'll prove it soon! meanwhile, you may try to prove that the difference of any two solutions with the same initial conditions is constant and equal to zero). In other words, once known the initial "state" of the particle, i.e. its position and its velocity, the Newton equation uniquely determines the "future" and "past" history of the particle.

e.g. A differential equation for the exponential function. Consider the first order ODE

$$\dot{x} = x$$

[22] "Corpus omne perseverare in statu suo quiescendi vel movendi uniformiter in directum, nisi quatenus a viribus impressis cogitur statum illum mutare" [Isaac Newton, *Philosophiae Naturalis Principia Mathematica*, 1687.]

where $\dot{x}$ denotes the derivative of $x(t)$ w.r.t. the real variable t.

An obvious solution is $x(t) = 0$. Besides, computation shows that the exponential function e^t satisfies the equation. Indeed, the (natural) exponential is defined by the power series

$$\exp(t) := \sum_{n\geqslant 0} \frac{t^n}{n!} = 1 + t + \frac{t^2}{2} + \frac{t^3}{6} + \dots$$

(remember that $0! = 1$), which converges uniformly in any bounded interval. You may check, deriving the power series term by term, that $\exp' = \exp$.

But we can multiply it by any constant b and still get a solution, hence any function $x(t) = be^t$ satisfies the above identity. If we set $t = 0$, we notice that b is the value of $x(0)$.

We claim that $x(t) = x_0 e^t$ is the "unique" solution of the differential equation $\dot{x} = x$ with initial data $x(0) = x_0$. Indeed, let $y(t)$ be any other solution. Since the exponential is never zero, we can divide by e^t and define the function $h(t) = y(t)e^{-t}$. Deriving we get

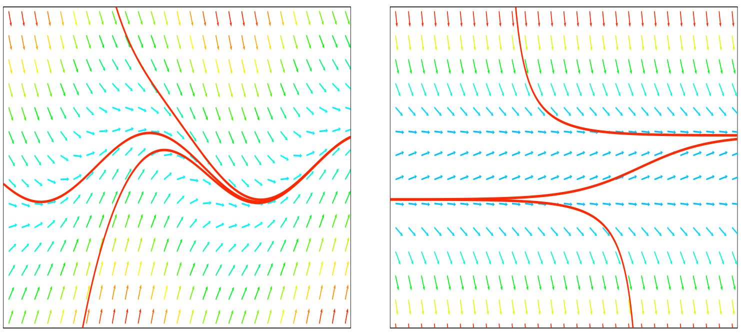
$$\dot{h} = (\dot{y} - y)\, e^{-t}\,.$$

But y solves the equation, hence the first derivative of h is everywhere zero. By the mean value theorem h is a constant function, and, since $y(0) = x_0$ too, its value at the origin is $h(0) = y(0)e^{-0} = x_0$. This implies that $y(t)$ is indeed equal to $x(t)$.

Equações diferenciais ordinárias. Uma *equação diferencial ordinária (EDO)* de primeira ordem (resolúvel para a derivada) é uma lei

$$\dot{x} = v(t, x)$$

para a trajectória $t \mapsto x(t) \in \mathbb{R}$ de um sistema dinâmico, onde $\dot{x} = \frac{dx}{dt}$ denota a derivada do observável x em ordem ao tempo t, e $v(t, x)$ é um *campo de direções* dado (ou seja, uma recta com declive $v(t, x)$ para cada ponto (t, x)). Uma *solução* da EDO é uma função $t \mapsto x(t)$ tal que $\dot{x}(t) = v(t, x(t))$ para cada tempo t num certo intervalo, ou seja, uma função cujo gráfico é tangente ao campo de direções em cada ponto $(t, x(t))$ do gráfico. Se o campo $v(t, x)$ é suficientemente regular (por exemplo, diferenciável), para cada ponto (t_0, x_0) passa uma única solução com condição inicial $x(t_0) = x_0$.



Slope fields and some solutions of $\dot{x} = \sin(t) - x$ and of $\dot{x} = x(1 - x)$.

ex: A função $x(t) = t^3$ é solução da equação diferencial $t\dot{x} - 3x = 0$? E a função $x(t) = 0$?

Simple ODEs. The simplest case occurs when the velocity field v does not depend on the phase space variable x, so the equation is

$$\dot{x} = v(t)\,,$$

where $v(t)$ is some given function of time. This just says that x is a primitive of v, and the fundamental theorem of calculus (i.e. Leibniz and/or Newton's discovery) tells us how to compute such a primitive: just integrate the function v from some initial time t_0 up to a final time t. Indeed, provided v is a continuous function, the derivative of $\int_{t_0}^{t} v(s)ds$ at the point t is $v(t)$. This explains the current use of the expression "integrate" a differential equation instead of "solving" a differential equation, as well as the meaning of Newton's quoted anagram.

Primitives are not unique, but are defined modulo an additive constant. This arbitrary constant can be matched with the initial condition, so that the solution of $\dot{x} = v(t)$ with initial condition $x(t_0) = x_0$ is

$$x(t) = x_0 + \int_{t_0}^{t} v(s)ds\,.$$

Here you may observe that this class of ODEs have "symmetries". The line field does not depend on x, hence slopes of solutions are the same along horizontal lines (t = constant) in the extended phase space. There follows that any translate $\varphi(t) + c$ of a solution $\varphi(t)$ is still a solution. This is but a geometrical interpretation of the arbitrary constant in the primitive of v.

ex: **Newtonian motion in a time dependent force field.** The one-dimensional motion of a particle of mass m subject to a time-dependent force $F(t)$ is modeled by the Newton equation

$$m\ddot{x} = F(t)\,.$$

Call $v = \dot{x}$ the velocity of the particle, and derive the first order ODE satisfied by the velocity v. Solve the equation for the velocity, given a force $F(t) = F_0 \sin(\gamma t)$ and an initial condition $v(0) = v_0$. Use the above solution $v(t)$ to find the trajectory $x(t)$ of the particle, given an initial position $x(0) = x_0$.

ex: **Rockets.** Se um foguetão (no espaço vazio, sem forças gravitacionais!) expulsa combustível a uma velocidade relativa constante $-V$ e a uma taxa constante $\dot{m} = -\alpha$, então a sua trajectória num referencial inercial (uni-dimensional) é modelada pela equação de Newton

$$\frac{d}{dt}(mv) = \alpha(V - v)\,, \qquad \text{ou seja}\ , \qquad \dot{m}v + m\dot{v} = \alpha(V - v)\,.$$

Resolva a EDO $\dot{m} = -\alpha$ para a massa do foguetão, com massa inicial $m(0) = m_0$, e substitua o resultado na equação de Newton, obtendo

$$\dot{v} = \frac{\alpha V}{m_0 - \alpha t}$$

(valida se $0 \leqslant t < m_0/\alpha$). Calcule a trajectória do foguetão com velocidade inicial $v(0) = v_0$ e posição inicial $q(0) = 0$, válida para tempos t inferiores ao tempo necessário para acabar o combustível.

Autonomous ODEs. A first order ODE of the form

$$\dot{x} = v(x)\,,$$

where the velocity field v does not depend on time, is called *autonomous*. Most fundamental equations of physics (those describing closed systems, without external forces) can be written as autonomous first order ODEs, and this corresponds to time-invariance of physical laws.

Here you may notice symmetries again. The line field v of an autonomous equation is constant along vertical lines (x = constant) of the extended phase space. Hence any translate $\varphi(t + s)$ of a solution $\varphi(t)$ is still a solution. This is the manifestation of time-invariance of a law codified by an autonomous ODE. This also implies that there is no loss of generality in restricting to initial value problems with initial time $t_0 = 0$.

Equilibrium solutions. First, we observe that an autonomous equation may admit constant solutions. Indeed, if x_0 is a *singular point* of the vector field v, i.e. a point where $v(x_0) = 0$, then the constant function

$$x(t) = x_0$$

obviously solves the equation. Such solutions, which do not change with time, are called *equilibrium*, or *stationary*, solutions.

Solutions near non-singular points. Let x_0 be a *non-singular point* of the velocity field $v(x)$, i.e. a point x_0 where $v(x_0) \neq 0$. We want to solve $\dot{x} = v(x)$ with initial condition $x(t_0) = x_0$. First, rewrite the equation $dx/dt = v(x)$ formally as "$dx/v(x) = dt$" (multiply by dt and divide by $v(x)$, so that all x's are on the left and all t's are on the right). Instead of trying to make sense to this last expression (which is possible, of course, and here you can appreciate the beauty of Leibniz' notation dx/dt for derivatives!), observe that it is suggesting that $\int dx/v(x) = \int dt$. Now assume that the velocity field v is continuous and let $J = (x_-, x_+)$ be the maximal interval containing x_0 where v is different from zero. Integrating, from x_0 to $x \in J$ on the left and from t_0 to t on the right, we obtain a differentiable function $x \mapsto t(x)$ defined as

$$t(x) - t_0 = \int_{x_0}^{x} \frac{dy}{v(y)}$$

for any $x \in J$. Now, observe that the derivative dt/dx is equal to $1/v$. Since, by continuity, $1/v$ does not change its sign in J, our $t(x)$ is a strictly monotone continuously differentiable function. We can invoke the inverse function theorem and conclude that the function $t(x)$ is invertible. This prove that the above relation defines actually a continuously differentiable function $t \mapsto x(t)$ in some interval $I = t(J)$ of times around t_0. Finally, you may want to check that the function $t \mapsto x(t)$ solves the Cauchy problem: just compute the derivative (using the inverse function theorem),

$$\begin{aligned} \dot{x}(t) &= 1/\left(\frac{dt}{dx}(x(t))\right) \\ &= v(x), \end{aligned}$$

and check the initial condition. Observe that the function $t(x) - t_0$ has then the interpretation of the "time needed to go from x_0 to x".

At the end of the story, if you are lucky enough and know how to invert the function $t(x)$, you'll get an explicit solution as

$$x(t) = F^{-1}\left(t - t_0 + F(x_0)\right),$$

where F is any primitive of $1/v$. Close inspection of the above reasoning shows that the local solution you've found is indeed the unique one. Namely, we have the following

Proposition 6.1. (Existence and uniqueness theorem for autonomous ODEs near a non-singular point) *Let $v(x)$ be a continuous velocity field and let x_0 be a point where $v(x_0) \neq 0$. Then there exist one and only one solution of $\dot{x} = v(x)$ with initial condition $x(t_0) = x_0$ in some sufficiently small interval I around t_0. Moreover, the solution $x(t)$ is given implicitly by*

$$\int_{x_0}^{x} \frac{dy}{v(y)} = \int_{t_0}^{t} ds,$$

defined in some small interval J around x_0.

On the failure of uniqueness near singular points. The interval $I = t(J)$ where the solution is defined need not be the entire real line: solutions may reach the boundary of J, i.e. one of the singular points $x_\pm$ of the velocity field, in finite time. Since singular points are themselves equilibrium solutions, this imply that solutions of the initial value problem at singular points may not be unique, under such mild conditions (continuity) for the velocity field. Picard's theorem prescribes stronger regularity conditions on v under which the initial value problem admits unique solutions for any initial condition in the extended phase space.

e.g. **Two solutions with the same initial condition!** Both the curves $x(t) = 0$ and $x(t) = t^3$ solve the equation

$$\dot{x} = 3x^{2/3}$$

with initial condition $x(0) = 0$. The problem here is that the velocity field $v(x) = 3x^{2/3}$, although continuous, is not differentiable and not even Lipschitz at the origin. You may notice that the solution starting, for example, at $x_0 = 1$ reaches (or better comes from) the singular point $x_- = 0$ in finite time, since

$$\begin{aligned} t(x_-) - t(x_0) &= \int_1^0 \frac{1}{3} y^{-2/3} dy \\ &= -1 . \end{aligned}$$

help: O Mathematica® pode resolver analiticamente equações diferenciais. Por exemplo,

```
DSolve[x'[t] + 2 x[t] == Sin[t], x[t], t]
{{x[t] -> E^(-2 t) C[1] + 1/5 (-Cos[t] + 2 Sin[t])}}
```

e.g. **Radioactive decay.** Radioactive matter (such as ^{14}C or ^{238}U) decay according to the law

$$\dot{N} = -\beta N$$

where $N(t)$ denotes the number of nuclei (assumed large so that the law of large number applies), and $1/\beta$ is the *mean life*, the average time life of one single nucleus. The solution with initial condition $N(0) = N_0 > 0$ is

$$N(t) = N_0 e^{-\beta t}$$

In particular, the initial quantity is reduced to one half after a time $T = (\log 2)/\beta$, called *half-life*. For example, ^{14}C has an average time of $1/\beta \simeq 8033$ years.

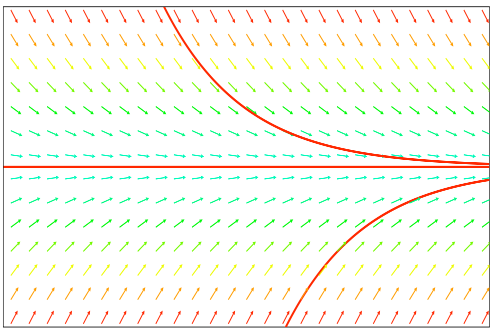
If cosmic radiation produces ^{14}C in Earth's atmosphere at a rate α, then the quantity of ^{14}C in the atmosphere follows a law

$$\dot{N} = -\beta N + \alpha .$$

The equilibrium is $\overline{N} = \alpha/\beta$. The difference $x(t) = N(t) - \overline{N}$ follows the law $\dot{x} = -\beta x$, hence $x(t) = x(0)e^{-\beta t}$, and therefore

$$N(t) = \overline{N} + \left(N(0) - \overline{N}\right) e^{-\beta t} .$$

In particular, $N(t) \to \overline{N}$ as $t \to \infty$, independently from the initial condition $N(0)$.



Direction field and some solutions of $\dot{x} = -2x + 1$.

e.g. **Exponential growth.** The growth of a population in a (virtually) unlimited medium is modeled by

$$\dot{N} = \lambda N$$

where $N(t)$ denotes the population size at time t, and $\lambda > 0$ is some growth rate. The solution is an exponential growth like

$$N(t) = N(0)e^{\lambda t} .$$

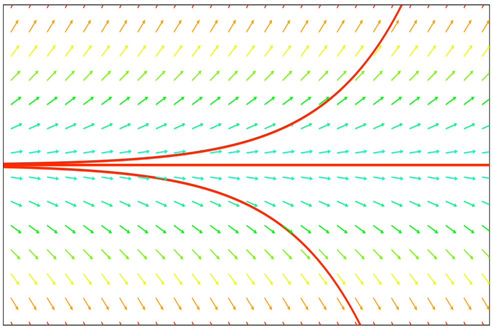
If we retire aportion of the population at constant rate $\alpha > 0$, we get

$$\dot{N} = \lambda N - \alpha$$

Now the stationary solution is $\overline{N} = \alpha/\lambda$, and the general solution

$$N(t) = \overline{N} + \left(N(0) - \overline{N}\right) e^{\lambda t} .$$

Now, the non-constant solutions diverge or disappear.



Direction field and some solutions of $\dot{x} = 2x - 1$.

e.g. Logistic equation. A more realistic model of the growth of a population in a limited environment is the *logistic equation*[23]

$$\dot{N} = \lambda N(1 - N/M)$$

where $\lambda > 0$ and the number $M > 0$ is a maximal population. Observe that $\dot{N} \simeq \lambda N$ when $N \ll M$, and that $\dot{N} \to 0$ when $N \to M$. It is convenient to define the relative population $x(t) := N(t)/M$, which satisfies the adimensional logistic equation

$$\dot{x} = \lambda x(1 - x) .$$

Equilibrium solutions are $x = 0$ e $x = 1$. To find solutions with initial condition $x(0) = x_0 \neq 0, 1$, we may integrate

$$\int_{x_0}^{x} \frac{dy}{y(1-y)} = \int_0^t ds ,$$

using the identity

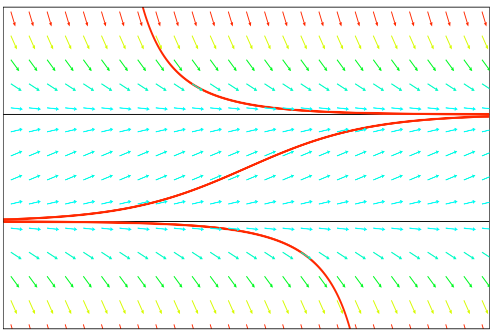
$$\frac{1}{y(1-y)} = \frac{1}{y} + \frac{1}{1-y} .$$

The result is

$$\log \left| \frac{x \cdot (x_0 - 1)}{x_0 \cdot (x - 1)} \right| = t$$

which may be solved for $x(t)$, giving, when $0 < x_0 < 1$,

$$x(t) = \frac{1}{1 + \left(\frac{1}{x_0} - 1\right) e^{-\lambda t}} .$$



[23]Pierre François Verhulst, Notice sur la loi que la population pursuit dans son accroissement, *Correspondance mathématique et physique* **10** (1838), 113-121.

Campo de direções e soluções da equação logística.

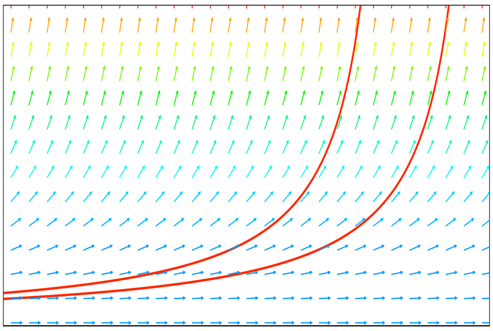
e.g. Super-exponential growth. Um outro modelo de dinâmica populacional em meio ilimitado é

$$\dot{N} = \alpha N^2 .$$

onde $\alpha > 0$. A solução com condição inicial $N(0) = N_0 > 0$ é

$$N(t) = \frac{1}{1/N_0 - \alpha t} .$$

Observe que as soluções não estão definidas para todos os tempos: este modelo prevê uma catástrofe (população infinita) após um intervalo de tempo finito (o tempo $\bar{t} = 1/(\alpha N_0)$) !



Campo de direções e soluções da equação $\dot{x} = x^2$.

Separable ODEs. A first order ODE $\dot{x} = v(t, x)$ is said *separable* when the velocity field v is a product of a function which only depends on t and another function which only depends on x. So it has the form

$$\dot{x} = \frac{f(x)}{g(t)}$$

for some known functions f and g. We assume that both f and g are continuous functions on some intervals of the phase space and the real line, respectively, and that $g(t)$ does not vanishes. Observe that both simple ODEs like $\dot{x} = v(t)$ and autonomous ODEs like $\dot{x} = v(x)$ fall in this class.

If x_0 is a zero of f, then $x(t) = x_0$ is an equilibrium solution. The recipe to find other solutions is known as "separation of variables". Take point x_0 where $f(x_0) \neq 0$, and an initial time t_0 where $g(t_0) \neq 0$. Choose a maximal interval J containing x_0 where f is different from zero, rewrite the equation formally as "$dx/f(x) = dt/g(t)$", and then integrate from x_0 to $x \in J$ the r.h.s. and from t_0 to t the l.h.s. You'll get

$$\int_{x_0}^{x} \frac{dy}{f(y)} = \int_{t_0}^{t} \frac{ds}{g(s)} .$$

As we did for autonomous equations, we can see that any continuously differentiable solution $t \mapsto x(t)$ of the equation passing through the non-singular point (t_0, x_0) must satisfy the above relation, as long as x is sufficiently near to x_0.

e.g. Solve $\dot{x} = tx^3$.

An obvious solution is the equilibrium solution $x(t) = 0$. For a positive initial condition $x(t_0) = x_0 > 0$, rewrite the equation as $dx/x^3 = tdt$ and integrate

$$\int_{x_0}^{x} \frac{dy}{y^3} = \int_{t_0}^{t} s ds$$

for $x > 0$. You'll find

$$1/x^2 - 1/x_0^2 = t^2 - t_0^2 ,$$

and, solving for x, the solution

$$x(t) = \frac{1}{\sqrt{t_0^2 + 1/x_0^2 - t^2}} .$$

defined for times t in the interval $|t| < \sqrt{t_0^2 + 1/x_0^2}$. In the same way you'll find solutions with negative initial condition $x_0 < 0$.

Linear first order ODEs. A *first order linear differential equation* is a differential equation which can be written in the "canonical form"

$$\dot{x} + p(t)x = q(t) , \tag{6.1}$$

where p and q are (known) functions of the real variable t in some interval I of the real line, called *coefficients*. We assume that both p and q are continuous functions, and we look for solutions $t \mapsto x(t)$ defined on I. Eventually we will want to solve the problem with some initial condition $x(t_0) = x_0$.

The equation

$$\dot{y} + p(t)y = 0 \tag{6.2}$$

is said the *homogeneous* equation associated with the general, hence *non-homogeneous*, equation (6.1) above. The word "homogeneous" is due to the fact that any constant multiple $\lambda \cdot y(t)$ of a solution y of the homogeneous equation (6.2) is again a solution. Also, any linear combination (with real coefficients) $ay_1(t) + by_2(t)$ of solutions $y_1(t)$ and $y_2(t)$ of the homogeneous equation (6.2) is still a solution of the homogeneous equation. This means that the space of solutions of the homogeneous equation is a linear space, actually a one-dimensional vector space $\mathcal{H} \simeq \mathbb{R}$.

Also interesting is that the difference $y(t) = x_1(t) - x_2(t)$ of any two solutions $x_1(t)$ and $x_2(t)$ of the non-homogeneous equation (6.1) is a solution of the associated homogeneous equation (6.2), hence belongs to the linear space $\mathcal{H}$. Therefore, the space of solutions of the non-homogeneous equation (6.1) is an affine space $x + \mathcal{H}$, where $x(t)$ is any (particular) solution of (6.1).

Solutions of the homogeneous equation are obtained separating the variables, and are given by the following

Proposition 6.2. (Existence and uniqueness theorem for homogeneous first order linear ODEs) *Let p be a continuous function on some interval of the real line. Then the unique solution of the hmogeneous equation $\dot{y} + p(t)y = 0$ with initial condition $y(t_0) = y_0$ is given by*

$$y(t) = y_0 e^{-\int_{t_0}^t p(s)ds} .$$

Indeed, let $z(t)$ be a second solution of the Cauchy problem above, and define

$$h(t) = z(t)e^{\int_{t_0}^t p(s)ds} .$$

Its value for t_0 is y_0. Its derivative is

$$\dot{h}(t) = e^{\int_{t_0}^t p(s)ds} \left(\dot{z}(t) + p(t)z(t)\right) .$$

Since z is supposed to solve the equation, the derivative of h is equal to zero for any t in the chosen interval, and the mean value theorem says that then $h(t)$ is constant and equal to y_0. There follows that $z(t)$ is indeed equal to our solution $y(t)$.

e.g. Solve $t\dot{x} - 2x = 0$ for $t \in (0, \infty)$ with initial condition $x(t_0) = x_0$.

If $x_0 = 0$, the solution is the equilibrium solution $x(t) = 0$. If $x_0 > 0$, write the equation as $dx/x = 2dt/t$, integrate

$$\int_{x_0}^x dy/y = \int_{t_0}^t 2ds/s ,$$

for positive x, obtain

$$\log x - \log x_0 = \log(t^2) - \log\left(t_0^2\right) ,$$

and solve it for x, the solution being

$$x(t) = \left(x_0/t_0^2\right) t^2 .$$

Finally observe that this formula gives the solutions for any initial condition x_0.

Back to the non-homogeneous equation. To solve the non-homogeneous equation

$$\dot{x} + p(t)x = q(t)\,,$$

we use the following trick, a first and elementary instance of a much more general method named "variation of parameters" (or, sometimes, with the oxymoron "variation of constants"). We already know that any function proportional to $e^{-\int_a^t p(s)ds}$ solves the homogeneous equation. We look for a solution of the non-homogeneous equation having the form

$$x(t) = \lambda e^{-\int_{t_0}^t p(s)ds}\,,$$

but, instead of treating the parameter λ as a constant, we allow it to depend on t. Putting our guess into the non-homogeneous equation, we get

$$\frac{d}{dt}\left(\lambda(t)e^{-\int_{t_0}^t p(s)ds}\right) + p(t)\lambda(t)e^{-\int_{t_0}^t p(s)ds} = q(t)\,.$$

Computing the derivative, we get

$$\dot{\lambda}(t)e^{-\int_{t_0}^t p(s)ds} - \cancel{p(t)\lambda(t)e^{-\int_{t_0}^t p(s)ds}} + \cancel{p(t)\lambda(t)e^{-\int_{t_0}^t p(s)ds}} = q(t)\,,$$

the two terms containing $p(t)$ do cancel, and we are left with

$$\dot{\lambda}(t)e^{-\int_{t_0}^t p(s)ds} = q(t)\,.$$

This can be solved for $\dot{\lambda}$ (because exponentials are never zero), and integration gives

$$\lambda(t) = \lambda(t_0) + \int_{t_0}^t e^{\int_{t_0}^s p(u)du}q(s)ds$$

for some constant $\lambda(t_0)$ equal to the value of $x(t_0)$ (this depends on our choice for $y(t)$, such that $y(t_0) = 1$). Finally, we get a solution

$$x(t) = \lambda(t)e^{-\int_{t_0}^t p(s)ds}\,,$$

and you may check that it has initial value $x(t_0) = x_0$. Since the difference of any two solutions of the general equation is a solution of the associated homogeneous equation, and since (as follows from the uniqueness theorem above) the only solution of the homogeneous equation with initial condition $x(t_0) = 0$ is the zero solution, we just proved the following

Proposition 6.3. (Existence and uniqueness theorem for first order linear ODEs) *Let p and q be continuous functions in some interval I. Then the unique solution of the linear differential equation $\dot{x} + p(t)x = q(t)$ with initial condition $x(t_0) = x_0$ for $t_0 \in I$ is given by*

$$x(t) = e^{-\int_{t_0}^t p(u)du}\left(x_0 + \int_{t_0}^t e^{\int_{t_0}^s p(u)du}q(s)ds\right)\,.$$

Suggestion. Perhaps, instead of fixing the unpleasant formula in the above theorem, you could simply remember the strategy used to derive it: find one non-trivial solution $y(t)$ of the associated homogeneous equation (which is separable!), and then make the conjecture $x(t) = \lambda(t)y(t)$ for some other unknown function $\lambda(t)$. You'll get a simple differential equation for λ, and integration gives you the solution.

e.g. Solve $t\dot{x} - 2x = t$ for $t \in (0, \infty)$ with initial condition $x(t_0) = x_0$.

You already know that the solution of the associated homogeneous equation $ty' - 2y = 0$ with initial condition $y(t_0) = 1$ is $y(t) = t^2/t_0^2$. Make the conjecture $x(t) = \lambda(t)t^2/t_0^2$, insert your guess into the non-homogeneous equation, and get

$$\dot{\lambda} = t_0^2/t^2\,.$$

Integrate and find

$$\lambda(t) - \lambda(t_0) = t_0 - t_0^2/t\,,$$

and, since $\lambda(t_0) = x(t_0)$, finally find the solution

$$x(t) = \frac{x_0 + t_0}{t_0^2}t^2 - t\,.$$

ex: Determine a solução geral das EDOs lineares de primeira ordem

$$2\dot{x} - 6x = e^{2t} \qquad \dot{x} + 2x = t \qquad \dot{x} + x/t^2 = 1/t^2 \qquad \dot{x} + tx = t^2$$

definidas em oportunos intervalos da recta real.

ex: Resolva os seguintes problemas nos intervalos indicados:

$$\begin{array}{ccc} 2\dot{x} - 3x = e^{2t} & t \in (-\infty, \infty) & \text{com } x(0) = 1 \\ \dot{x} + x = e^{3t} & t \in (-\infty, \infty) & \text{com } x(1) = 2 \\ t\dot{x} - x = t^3 & t \in (0, \infty) & \text{com } x(1) = 3 \\ \dot{x} + tx = t^3 & t \in (-\infty, \infty) & \text{com } x(0) = 0 \\ dr/d\theta + r\tan\theta = \cos\theta & t \in (-\pi/2, \pi/2) & \text{com } r(0) = 1 \end{array}$$

e.g. **Free fall with friction.** Friction may be modeled as a force $-kv$ proportional and contrary to velocity, where $k > 0$ is a friction coefficient (which depends on the shape of the falling body, and on many other things!). Therefore, free fall near the Earth's surface may be modeled by the Newton equation

$$m\dot{v} = -kv - mg$$

This is a linear ODE for the velocity, whose solution is

$$v(t) = \frac{gm}{k} + e^{-(k/m)t}\left(v(0) - \frac{gm}{k}\right) .$$

In particular, the velocity is asymptotic to the equilibrium value $\overline{v} = gm/k$.

e.g. **Circuito RL.** A corrente $I(t)$ num circuito RL, de resistência R e indutância L, é determinada pela EDO

$$L\dot{I} + RI = V$$

onde $V(t)$ é a tensão que alimenta o circuito.

- Escreva a solução geral como função da corrente inicial $I(0) = I_0$.
- Resolva a equação para um circuito alimentado com tensão constante $V(t) = E$. Esboce a representação gráfica de algumas das soluções e diga o que acontece para grandes intervalos de tempo.
- Resolva a equação para um circuito alimentado com uma tensão alternada $V(t) = E\sin(\omega t)$. Se não conseguir, mostre que a solução com $I(0) = 0$ tem a forma

  $$I(t) = \frac{E}{\sqrt{R^2 + \omega^2 L^2}}\sin(\omega t - \alpha) + \frac{E\omega L}{R^2 + \omega^2 L^2} e^{-\frac{R}{L}t}$$

  onde α é uma constante que depende de ω, L e R.

e.g. **Lei do arrefecimento de Newton.** Numa primeira aproximação, a temperatura $T(t)$ no instante t de um corpo num meio ambiente cuja temperatura no instante t é $M(t)$ segue a *lei do arrefecimento de Newton*

$$\dot{T} = -k\,(T - M(t))$$

onde k é uma constante positiva (que depende do material do corpo).

- Escreva a solução $T(t)$ como função da temperatura inicial $T(0) = T_0$ e de $M(s)$ com $0 \leqslant s \leqslant t$.
- Resolva a equação quando a temperatura do meio ambiente é mantida constante $M(t) = M$. Esboce a representação gráfica de algumas das soluções e diga o que acontece para grandes intervalos de tempo.
- Uma chávena de café, com temperatura inicial de 100^oC, é colocada numa sala cuja temperatura é de 20^oC. Sabendo que o café atinge uma temperatura de 60^oC em 10 minutos, determine a constante k do café e o tempo necessário para o café atingir a temperatura de 40^oC.

7 Curvas

e.g. **Spaces and coordinates.** The space where we think we live in is the 3-dimensional space $\mathbb{R}^3$. This means that we need 3 numbers, for example the Cartesian coordinates x, y and z in a fixed reference frame, to uniquely define/indicate the position of a planet at a given time. A rattlesnake in the Sonora desert thinks she lives in a plane, since she need just two coordinates, say x and y, to say her friend where she lives. Similarly, a chemist who is describing a reaction like

$$A + 2B + 3C \leftrightarrows 4D + 5E + 6F + 7G$$

needs 7 numbers, the concentrations $a = [A]$, $b = [B]$, ..., $g = [G]$ of the seven reagents, to describe to his collegues the state of the reaction at a given time.

Espaço Euclidiano. $\mathbb{R}^n$ denota o espaço Euclidiano de dimensão n. Fixada a base canónica $\mathbf{e}_1 = (1, 0, \dots, 0)$, $\mathbf{e}_2 = (0, 1, 0, \dots, 0)$, ..., $\mathbf{e}_n = (0, \dots, 0, 1)$, os pontos de $\mathbb{R}^n$ são os vetores

$$\mathbf{x} = (x_1, x_2, \dots, x_n) := x_1\mathbf{e}_1 + x_2\mathbf{e}_2 + \cdots + x_n\mathbf{e}_n \,,$$

de coordenadas $x_i \in \mathbb{R}$, com $i = 1, 2, \dots, n$. Outra notação usada nos manuais para os vetores é $\vec{x}$.

As coordenadas no plano Euclidiano ou no espaço 3-dimensional são também denotadas, conforme a tradição, por $\mathbf{r} = (x, y) = x\,\mathbf{i} + y\,\mathbf{j} \in \mathbb{R}^2$ ou $\mathbf{r} = (x, y, z) = x\,\mathbf{i} + y\,\mathbf{j} + z\,\mathbf{k} \in \mathbb{R}^3$.

O *produto interno Euclidiano* em $\mathbb{R}^n$, denotado por $\langle \mathbf{x}, \mathbf{y} \rangle$ ou $\mathbf{x} \cdot \mathbf{y}$, é

$$\langle \mathbf{x}, \mathbf{y} \rangle := x_1y_1 + x_2y_2 + \cdots + x_ny_n \,,$$

e a *norma Euclidiana* é

$$\|\mathbf{x}\| := \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle}\,.$$

Dois vetores x e y são ditos *ortogonais* se $\langle \mathbf{x}, \mathbf{y} \rangle = 0$. A desigualdade de Schwarz diz que

$$|\langle \mathbf{x}, \mathbf{y} \rangle| \leqslant \|\mathbf{x}\| \cdot \|\mathbf{y}\|\,.$$

(para provar a desigualdade no caso não trivial em que $\mathbf{x} \neq 0$ e $\mathbf{y} \neq 0$, basta definir $\mathbf{u} = \mathbf{x}/\|\mathbf{x}\|$ e $\mathbf{v} = \mathbf{y}/\|\mathbf{y}\|$, e observar que $0 \leqslant \|\mathbf{u} \pm \mathbf{v}\|^2 = 2(1 \pm \langle \mathbf{u}, \mathbf{v} \rangle)$, donde $-1 \leqslant \langle \mathbf{u}, \mathbf{v} \rangle \leqslant 1$). O *ângulo* $\theta \in [0, \pi]$ entre os vetores não nulos $\mathbf{x}$ e $\mathbf{y}$ é definido pela identidade $\langle \mathbf{x}, \mathbf{y} \rangle = \|\mathbf{x}\| \cdot \|\mathbf{y}\| \cdot \cos(\theta)$. A *distância Euclidiana* entre os pontos $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ é definida por

$$\mathrm{d}(\mathbf{x}, \mathbf{y}) := \|\mathbf{x} - \mathbf{y}\|\,.$$

Em particular, o comprimento do vetor $\mathbf{x}$, a distância entre $\mathbf{x}$ e 0, é dado pelo teorema de Pitágoras

$$\mathrm{d}(\mathbf{x}, 0) = \|\mathbf{x}\| = \sqrt{x_1^2 + \cdots + x_n^2}\,.$$

A desigualdade de Schwarz implica a desigualdade do triângulo

$$\mathrm{d}(\mathbf{x}, \mathbf{y}) \leqslant \mathrm{d}(\mathbf{x}, \mathbf{z}) + \mathrm{d}(\mathbf{z}, \mathbf{y})$$

(para provar a desigualdade, calcule $\|x + y\|^2$ e use a desigualdade de Schwarz).

A bola aberta de centro $\mathbf{a} \in \mathbb{R}^n$ e raio $r > 0$ é o conjunto $B_r(\mathbf{a}) := \{\mathbf{x} \in \mathbb{R}^n \text{ s.t. } \|\mathbf{x} - \mathbf{a}\| < r\}$. Um subconjunto $A \subset \mathbb{R}^n$ é aberto em $\mathbb{R}^n$ se cada seu ponto $\mathbf{a} \in A$ é o centro de uma bola $B_\varepsilon(a) \subset A$, com $\varepsilon > 0$ suficientemente pequeno.

A reta que passa pelo ponto $\mathbf{a} \in \mathbb{R}^n$ na direção do vetor não nulo $\mathbf{v} \in \mathbb{R}^n$ é

$$\mathbf{a} + [\mathbf{v}] := \{\mathbf{a} + t\mathbf{v} \text{ com } t \in \mathbb{R}\}\,.$$

A reta perpendicular/normal ao vetor não nulo $n \in \mathbb{R}^2$ que passa pelo ponto $a \in \mathbb{R}^2$ é

$$\mathbf{a} + [\mathbf{n}]^\perp := \{\mathbf{x} \in \mathbb{R}^2 \text{ t.q. } \langle \mathbf{x} - \mathbf{a}, \mathbf{n} \rangle = 0\}$$

O plano gerado pelos vectores linearmente independentes v e w que passa pelo ponto $a \in \mathbb{R}^n$ é

$$\mathbf{a} + [\mathbf{v}, \mathbf{w}] := \{\mathbf{a} + t\mathbf{v} + s\mathbf{w} \text{ com } (t, s) \in \mathbb{R}^2\}$$

O plano ortogonal/perpendicular/normal ao vetor não nulo $\mathbf{n} \in \mathbb{R}^3$ que passa pelo ponto $\mathbf{a} \in \mathbb{R}^3$ é

$$\mathbf{a} + [\mathbf{n}]^\perp := \{\mathbf{x} \in \mathbb{R}^3 \text{ t.q. } \langle \mathbf{x} - \mathbf{a}, \mathbf{n} \rangle = 0\}$$

($\mathbf{n}$ é dito *vector normal* ao plano).

Coordenadas polares. As coordenadas polares (ρ, θ), com $\rho \in \mathbb{R}_+$ e $\theta \in [0, 2\pi[$, no plano estão definidas por

$$\begin{aligned} x &= \rho \cos(\theta) \\ y &= \rho \sin(\theta) \end{aligned}$$

onde x e y são as coordenadas cartesianas de $\mathbb{R}^2$. Em particular, $\rho = \sqrt{x^2 + y^2}$ é a norma do vetor (x, y).

Caminhos. Um *caminho* em $\mathbb{R}^n$ é uma função $\mathbf{c} : I \to \mathbb{R}^n$,

$$t \mapsto \mathbf{c}(t) = (c_1(t), c_2(t), ..., c_n(t)),$$

definida num intervalo $I \subset \mathbb{R}$. Se $\mathbf{c}$ é uma função continua (ou seja, se as suas coordenadas $c_k : I \to \mathbb{R}$, com $k = 1, 2, \dots, n$, são funções contínuas), o caminho é dito *contínuo* e a sua imagem, o subconjunto $c(I) := \{\mathbf{c}(t), \text{ com } t \in I\} \subset \mathbb{R}^n$, é dita *curva*. Se $I = [a, b]$ é um intervalo fechado e $\mathbf{c}(a) = \mathbf{c}(b)$, então $\mathbf{c}$ é dito *caminho fechado*, ou *laço*.

Por exemplo, um caminho no plano $\mathbb{R}^2$ ou no espaço $\mathbb{R}^3$, é uma função

$$t \mapsto \mathbf{r}(t) = (x(t), y(t)) \in \mathbb{R}^2 \qquad \text{ou} \qquad t \mapsto \mathbf{r}(t) = (x(t), y(t), z(t)) \in \mathbb{R}^3$$

definida num intervalo (de tempos) $t \in I \subset \mathbb{R}$.

O parâmetro $t \in I$ tem a interpretação de um "tempo", o espaço $\mathbb{R}^n$ a interpretaçao dos possíveis "estados" de um sistema físico (a posição e o momento de um planeta, as concentrações dos n reagentes de uma reação química, ...). Assim, o caminho $t \mapsto \mathbf{c}(t)$ representa uma "trajetória", ou "lei horária", uma lei que determina o estado $c(t)$ do sistema em cada tempo $t \in I$. A curva $\mathbf{c}(I)$, o conjunto dos estados pelos quais passa a trajetória, é dita "órbita" do sistema.

e.g. Retas e segmentos. A reta que passa pelo ponto $a \in \mathbb{R}^n$ (no tempo 0) na direção do vetor não nulo $v \in \mathbb{R}^n$ é o caminho

$$t \mapsto \mathbf{a} + t\mathbf{v} \qquad \text{com} \qquad t \in \mathbb{R}.$$

O segmento que une os pontos $\mathbf{a}$ e $\mathbf{b}$ de $\mathbb{R}^n$ é, por exemplo, o caminho

$$t \mapsto \mathbf{a} + (\mathbf{b} - \mathbf{a})t \qquad \text{com} \qquad t \in [0, 1].$$

Warning! As strange as it may look, a generic continuous path may be much different from the idea we have in mind when drawing a curve in our blackboard. This was discovered by Giuseppe Peano, who shocked the mathematical community back in 1890 exhibiting a continuous image of the unit interval $[0, 1]$ which covered the entire unit square $[0, 1] \times [0, 1]$. More amazingly, you may want to know that the "obvious" statement that a closed curve without self-intersections divides the plane in two "pieces" requires a very long and delicate proof!, and deserves the name of *Jordan curve theorem*.

Caminhos diferenciáveis. Dado o caminho $\mathbf{c} : I \to \mathbb{R}^n$, o vetor $(\mathbf{c}(t + \varepsilon) - \mathbf{c}(t)) / \varepsilon$ representa a velocidade média entre os "tempos" $t + \varepsilon$ e t. O caminho é dito *diferenciável* no ponto $t \in I$ quando existe o limite

$$\dot{\mathbf{c}}(t) := \lim_{\varepsilon \to 0} \frac{\mathbf{c}(t + \varepsilon) - \mathbf{c}(t)}{\varepsilon}.$$

O vetor $\frac{d\mathbf{c}}{dt}(t) := \dot{\mathbf{c}}(t) \in \mathbb{R}^n$ é dito *derivada* do caminho c no ponto t, ou *velocidade* do caminho c no tempo t.

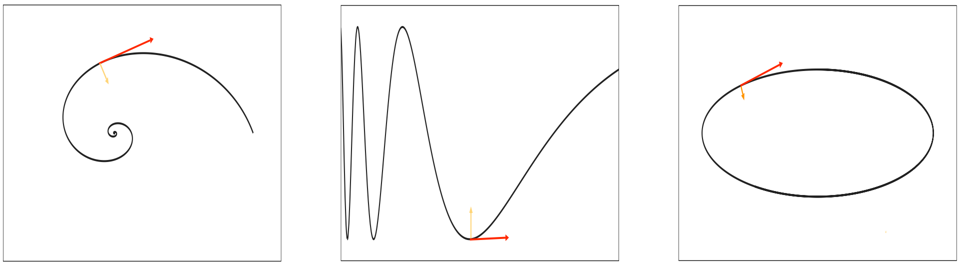
A diferenciabilidade do caminho em t, ou seja a existência do limite $\dot{\mathbf{c}}(t)$, é equivalente à diferenciabilidade das n funções reais $t \mapsto c_k(t)$ em t, onde $k = 1, 2, ..., n$. A derivada $\dot{\mathbf{c}}(t)$ é portanto um vetor de coordenadas $\dot{\mathbf{c}}(t) = (\dot{c}_1(t), \dot{c}_2(t), ..., \dot{c}_n(t))$.

O caminho $\mathbf{c} : I \to X$ é dito *diferenciável* quando é diferenciável para todo tempo $t \in I$.

Se $t \mapsto \mathbf{c}(t) = (c_1(t), c_2(t), \dots, c_n(t)) \in \mathbb{R}^n$ é um caminho diferenciável, então a sua derivada $\dot{\mathbf{c}} : I \to \mathbb{R}^n$ é também um caminho, e faz sentido definir as derivadas sucessivas, como

$$\dot{\mathbf{c}} = \frac{d\mathbf{c}}{dt}, \qquad \ddot{\mathbf{c}} = \frac{d^2\mathbf{c}}{dt^2} := \frac{d}{dt}\left(\frac{d\mathbf{c}}{dt}\right), \qquad \dddot{\mathbf{c}} = \frac{d^3\mathbf{c}}{dt^3} := \frac{d}{dt}\left(\frac{d^2\mathbf{c}}{dt^2}\right), \qquad \dots$$

Em particular, a primeira derivada $\mathbf{v}(t) := \dot{\mathbf{c}}(t)$ é dita "velocidade", a sua norma $v(t) := \|\mathbf{v}(t)\|$ "velocidade escalar", e a segunda derivada $\mathbf{a}(t) := \dot{\mathbf{v}}(t) = \ddot{\mathbf{c}}(t)$ é dita "aceleração".



As curvas $(e^t \cos(3t), e^t \sin(3t))$, $(t, \sin(1/t))$, e $(2\cos(t), \sin(-t)$.

Reparametrizatons. A curve, seen as a subset of some $\mathbb{R}^n$, may have different paramerizations. Namely, if $\mathbf{c} : I \to \mathbb{R}^n$ is a continuous path, and $\varphi : J \to I$, sending $s \mapsto t(s)$, is a continuous function from the interval J onto the interval I, then the composition $\mathbf{c} \circ \varphi : s \mapsto \mathbf{c}(t(s))$ is a continuous path from J onto the same curve $\mathbf{c}(I)$. If both the path c and the reparametrization φ are differentiable, the velocity of the path $s \mapsto \mathbf{c}(t(s))$ is $\frac{d\mathbf{c}}{dt}(t(s)) \cdot \frac{dt}{ds}$.

e.g. Uniform circular motion. *Uniform circular motion* in the Euclidean plane is described by the path

$$t \mapsto \mathbf{r}(t) = (R\cos(\omega t), R\sin(\omega t)) \ .$$

Here $R > 0$ is a fixed radius, and $\omega > 0$ is an angular velocity. Indeed, the trajectory describes a circle $\{x^2 + y^2 = R^2\}$ of radius R around the origin. The velocity is

$$\mathbf{v}(t) = \frac{d\mathbf{r}}{dt}(t) = (-R\omega\sin(\omega t), R\omega\cos(\omega t)) \ ,$$

and the acceleration is

$$\mathbf{a}(t) = \frac{d^2\mathbf{r}}{dt^2}(t) = \left(-R\omega^2\cos(\omega t), -R\omega^2\sin(\omega t)\right) \ .$$

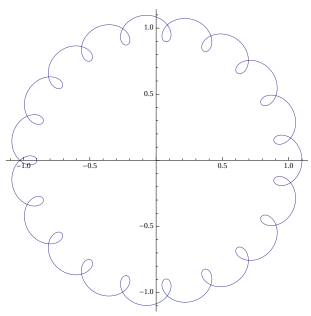
In particular, $\langle \mathbf{a}(t), \mathbf{v}(t) \rangle = 0$, i.e. the acceleration is orthogonal to the velocity, and it is directed towards the center of the orbit, since $\mathbf{a}(t) = -\omega^2 r(t)$. The quotient between the scalar velocity $v(t) = \|\mathbf{v}(t)\| = R\omega$ and the radius of the circle is the *angular velocity* ω.

e.g. Epicycles. According to Aristotle and Plato, "all movements are combinations of circular uniform motions". This idea is at the basis of the cosmology of Hipparchus and Ptolemy, as transmitted to us in the *Almagest*. "Fixed" stars describe circles in the sky. "Wandering" (i.e. *planets*, from the greek πλανήτης) stars describe a circle (*epicycle*) around a circle, which again describe a circle around a circle, . . . , which describes a circle around a first circle (*deferent*).

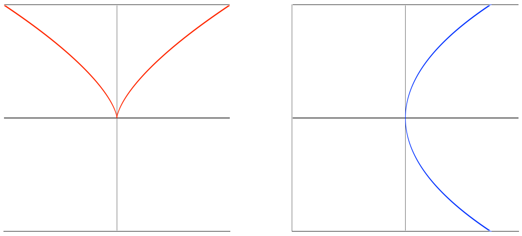
help: Mathematica®8 plots parametric curves. For example, the command

```
ParametricPlot[{Cos[t] + 0.1 Cos[20 t], Sin[t] + 0.1 Sin[20 t]}, {t,  0, 2 Pi}]
```

produces the following pictures of an epicycle



e.g. Cusps. Differentiability depends on the parametrization of the path, i.e. on the time law, and not on the curve! For example, the path $t \mapsto (t^3, t^2)$, with $t \in [-1, 1]$, describe the *cusp* $y^3 = x^2$ in the plane. Nevertheless, it is differentiable, and its velocity is the path $t \mapsto (3t^2, 2t)$. The apparent singularity at $t = 0$ is reached with zero velocity!



The cusp $t \mapsto (t^3, t^2)$ and its velocity.

ex: Esboce as seguintes curvas no plano, e calcule velocidade e aceleração, nos pontos onde podem ser definidas.

$$\mathbf{r}(t) = \left(t, t^2\right) \quad \text{com } t \in \mathbb{R}\,, \qquad \mathbf{r}(t) = \left(t^3, t^2\right) \quad \text{com } t \in \mathbb{R}\,,$$
$$\mathbf{r}(t) = (t, |t|) \quad \text{com } t \in [-1, 1]\,, \qquad \mathbf{r}(t) = (\cos\theta, \sin\theta) \quad \text{com } \theta \in [0, 2\pi]\,,$$
$$\mathbf{r}(t) = (t, [t]) \quad \text{com } t \in [-2, 2]\,, \qquad \mathbf{r}(t) = (t, \sin(1/t)) \quad \text{com } t \in]0, \infty[\,.$$
$$\mathbf{r}(t) = (|\sin(5t)|\cos(2t), |\sin(5t)|\sin(2t)) \quad \text{com } t \in [0, 2\pi]\,,$$
$$\mathbf{r}(t) = (\cos(t) + 0.1\cos(17t), \sin(t) + 0.1\sin(17t)) \quad \text{com } t \in [0, 2\pi]\,.$$

ex: Verifique que a trajetória

$$t \mapsto \mathbf{r}(t) = (a\cos t, b\sin t)\,,$$

com $t \in \mathbb{R}$ e $a, b > 0$, descreve a elipse $x^2/a^2 + y^2/b^2 = 1$.

ex: Esboce a trajetória

$$t \mapsto \mathbf{r}(t) = (R\cos t, R\sin t, bt)\,,$$

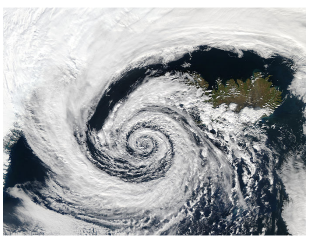
com $t \in \mathbb{R}$ e $R, b > 0$, descrita por uma partícula em movimento numa *hélice circular*.

ex: Determine umas equações paramétricas para a parábola $x = y^2 + 1$ e para a hipérbole $x^2 - y^2 = 1$ com $x > 0$ (lembre a identidade $\cosh^2\theta - \sinh^2\theta = 1$ entre as funções "hiperbólicas").

Smooth paths. A path is said of *class* $\mathcal{C}^0$ if it is continuous, of *class* $\mathcal{C}^1$ if its derivative is continuous. Using induction, it is said of class $\mathcal{C}^{k+1}$ if its derivative is of class $\mathcal{C}^k$. It is said of class $\mathcal{C}^\infty$ if it is of class $\mathcal{C}^k$ for any k, namely if all its derivatives are continuous.

Trajectories of physics used to have so many derivatives as we want (simply because most physical laws are written in terms of derivatives!), and we'll refer to them as "smooth", without specifying their regularity. Meanwhile, you must keep in mind that there are continuous paths which are nowhere differentiable. Actually, as shown by Weierstrass, almost all continuous paths are like that! They play a role in models of phenomena like the Brownian motion or turbolence ...

e.g. Espiral logarítmica. A recurrent pattern in Nature is the *logarithmic spiral*.

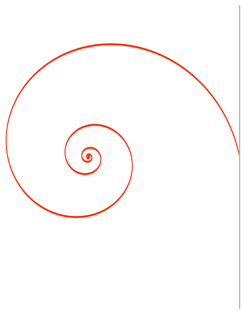


It is defined in polar coordinates, r and θ, by the law

$$r = c \cdot \lambda^{\theta} ,$$

for some constants $c > 0$ and $\lambda > 0$. We may parametrize the angle as $t \mapsto \theta(t) = \omega t$, for some angular velocity $\omega > 0$. Then, the logarithmic spiral is the curve drown by the path

$$t \mapsto \left(A e^{-\alpha t} \cos(\omega t), A e^{-\alpha t} \sin(\omega t) \right) .$$



Theorem 7.1. (Teorema do valor médio) *Seja* $\mathbf{c} : [a, b] \to \mathbb{R}^n$ *um caminho contínuo, diferenciável em* $]a, b[$ *e com derivada limitada por*

$$\|\dot{\mathbf{c}}(t)\| \leqslant K$$

para todo $t \in]a, b[$*. Então*

$$\|\mathbf{c}(b) - \mathbf{c}(a)\| \leqslant K \cdot |b - a| \ .$$

De fato, o teorema do valor médio aplicado à função real $t \mapsto \langle \mathbf{c}(t), \mathbf{c}(b) - \mathbf{c}(a) \rangle$, implica que existe um tempo $\bar{t} \in]a, b[$ tal que

$$\|\mathbf{c}(b) - \mathbf{c}(a)\|^2 = \left\langle \dot{\mathbf{c}}\left(\bar{t}\right), \mathbf{c}(b) - \mathbf{c}(a) \right\rangle \cdot (b - a) \ .$$

Pela desigualdade de Cauchy-Schwarz

$$\|\mathbf{c}(b) - \mathbf{c}(a)\|^2 \leqslant K \cdot \|\mathbf{c}(b) - \mathbf{c}(a)\| \cdot |b - a| \ ,$$

e portanto, ou $\|\mathbf{c}(b) - \mathbf{c}(a)\| = 0$, ou $\|\mathbf{c}(b) - \mathbf{c}(a)\| \leqslant K \cdot |b - a|$.

Comprimento de uma curva. The length of the segment between the vectors $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{y} \in \mathbb{R}^n$, the curve $\overline{\mathbf{xy}} := \{\mathbf{x} + t\mathbf{y}, t \in [0, 1]\}$ is, by definition, the norm of the vector $\mathbf{y} - \mathbf{x}$, namely

$$\ell(\overline{\mathbf{xy}}) := \|\mathbf{y} - \mathbf{x}\| .$$

If $\mathbf{c} : [a, b] \to \mathbb{R}^n$ is a path made of straight segments between the points $\mathbf{x}_n = \mathbf{c}(t_n)$ and $\mathbf{x}_{n+1} = \mathbf{c}(t_{n+1})$, given the sequence of times $a = t_0 < t_1 < \dots t_n < t_{n+1} < \dots t_N = b$, it is natural to define its length as the sum $\sum_{n=0}^{N-1} \|\mathbf{c}(t_{n+1}) - \mathbf{c}(t_n)\|$. Therefore, a natural definition of *length* of a continuous path $\mathbf{c} : [a, b] \to \mathbb{R}^n$ is

$$\ell(\mathbf{c}) := \sup \sum_{n=0}^{N-1} \|\mathbf{c}(t_{n+1}) - \mathbf{c}(t_n)\| ,$$

where the "sup" is taken over all finite partitions $a = t_0 < t_1 < \dots t_n < t_{n+1} < \dots t_N = b$ of the time interval $[a, b]$. It is obvious from this definition that the length does not depend on the parametrization of the path. The curve is called *rectifiable* when $\ell(\mathbf{c}) < \infty$.

If we try to approximate a differentiable path $\mathbf{c} : [a, b] \to \mathbb{R}^n$ by a polygonal path between the points $\mathbf{c}(t_k)$ and $\mathbf{c}(t_{k+1})$, we may observe that the length of the portion of the path between t_k and $t_{k+1} = t_k + dt$ is, to a first approximation, $\simeq \|\dot{\mathbf{c}}(t_k)\| \cdot dt$. It turns out (but it is not obvious!)

that the length of a differentiable curve may equivalently be computed/defined as the integral of its scalar velocity:

$$\ell(\mathbf{c}) = \int_a^b \|\dot{\mathbf{c}}(t)\| \, dt \,.$$

For example, a planar path like $t \mapsto \mathbf{r}(t) = (x(t), y(t))$, or a 3-dimensional path like $t \mapsto \mathbf{r}(t) = (x(t), y(t), z(t))$, with times $t \in [a, b]$, have length

$$\int_a^b \sqrt{\dot{x}(t)^2 + \dot{y}(t)^2} \, dt \qquad \text{or} \qquad \int_a^b \sqrt{\dot{x}(t)^2 + \dot{y}(t)^2 + \dot{z}(t)^2} \, dt \,.$$

ex: Calcule o comprimento ...

... do arco de circunferência $\theta \mapsto (\cos\theta, \sin\theta)$ com $\theta \in [\pi/2, 2\pi]$,

... da espiral logarítmica $t \mapsto (e^{-t}\cos t, e^{-t}\sin t)$ com $t \in [0, \infty[$,

... do arco de parábola $t \mapsto \left(t, t^2/2\right)$ com $t \in [0, 1]$ (considere a susbtituição $t = \sinh s$).

Comprimento de um gráfico. Seja $f(t)$ uma função real com derivada contínua definida no intervalo $[a, b]$. O gráfico de f, o conjunto

$$\Gamma_f = \left\{(t, f(t)) \in \mathbb{R}^2 \ \text{ com } \ t \in [a, b]\right\} \subset \mathbb{R}^2 \,,$$

é a imagem do caminho $t \mapsto (t, f(t))$ com $t \in [a, b]$. Em particular, o seu comprimento é

$$\ell\left(\Gamma_f\right) = \int_a^b \sqrt{1 + f'(t)^2} \, dt \,.$$

8 Campos escalares

Scalar fields. A *scalar field* is a real valued function $f : X \subset \mathbb{R}^n \to \mathbb{R}$ defined in some domain $X \subset \mathbb{R}^n$. We use both the notations $f(\mathbf{x}) = f(x_1, x_2, \dots, x_n)$ for the value of the field f at the point $\mathbf{x} = (x_1, x_2, \dots, x_n) \in \mathbb{R}^n$.

Thus, a scalar field is a number $f(\mathbf{x})$ attached to any point $\mathbf{x} \in X$. For example, the "coordinate functions" $\mathbf{x} = (x_1, x_2, \dots, x_n) \mapsto x_k$, for $k = 1, 2, \dots, n$, are scalar fields, which give the values of the different coordinates attached to a given point $\mathbf{x} \in \mathbb{R}^n$.

A scalar field $f : X \subset \mathbb{R}^n \to \mathbb{R}$ is said *continuous at the point* $\mathbf{x} \in X$ if for any $\varepsilon > 0$ there exists $\delta > 0$ such that $\|\mathbf{y} - \mathbf{x}\| < \delta$ implies $|f(\mathbf{y}) - f(\mathbf{x})| < \varepsilon$. This is the same as saying that $f(\mathbf{x}_n) \to f(\mathbf{x})$ for any sequence $\mathbf{x}_n \to \mathbf{x}$. A scalar field f is said *continuous* if it is continuous at all points $\mathbf{x} \in X$ of its domain.

e.g. Temperature. The temperature of a ideal gas, as a function of the pressure P and the volume V, is

$$T(P, V) = \frac{1}{nR} PV .$$

where n is the number of moles, and $R \simeq 8.314 \times 10^7$ J/K·mol. Curves with constant temperature are hyperbolas $PV =$ constant.

Level sets. Let $f : X \subset \mathbb{R}^n \to \mathbb{R}$ be a scalar field, and λ one of the values of f. The λ-*level set* of f is the subset

$$\Sigma_\lambda = f^{-1}(\{\lambda\}) := \{\mathbf{x} \in X \text{ such that } f(\mathbf{x}) = \lambda\} \subset X .$$

It may be one single point, or even all of X (if f is a constant function). For reasonable (i.e. sufficiently smooth) fields and generic values λ (in some precise meaning), it is a *hypersurface*, a set of "dimension" $n - 1$ inside $\mathbb{R}^n$. The *graph* of f is the set

$$\mathcal{G}_f := \{(\mathbf{x}, \lambda) \in X \times \mathbb{R} \text{ t.q. } f(\mathbf{x}) = \lambda\} \subset X \times \mathbb{R} .$$

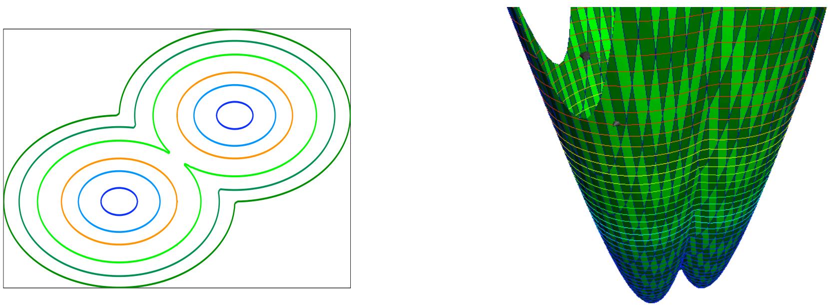
For example, if $f(x, y)$ is a smooth scalar field defined in $X \subset \mathbb{R}^2$, then

$$\Sigma_\lambda := \left\{(x, y) \in X \subset \mathbb{R}^2 \text{ t.q. } f(x, y) = \lambda\right\}$$

is, for generic values of λ, a *level curve*. The graph of f is the surface

$$\mathcal{G}_f := \{(x, y, z) \in X \times \mathbb{R} \text{ t.q. } f(x, y) = z\} \subset \mathbb{R}^3 .$$

Of course, it is not easy to draw the graph of a function defined on $\mathbb{R}^n$ when $n \geqslant 3$!



Curvas de nível e gráfico.

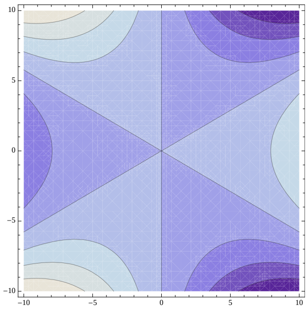
help: With Mathematica®8 , we may visualize level sets or plot the graphic of the absolute value of a function like $f(x, y) = x^3 - 3xy^2$ with the commands

```
ContourPlot[x^3 - 3 x y^2, {x, -10, 10}, {y, -10, 10}]
```

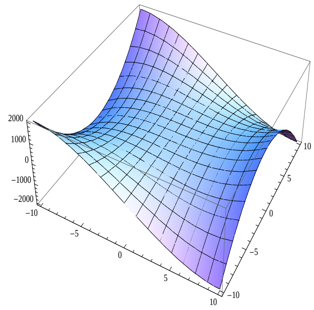
and

```
Plot3D[x^3 - 3 x y^2, {x, -10, 10}, {y, -10, 10}]
```

and get



and



respectively.

ex: Esboce as curvas de nível e os gráficos das seguintes funções, nos domínios onde podem ser definidas:

$$f(x,y) = x + y \qquad f(x,y) = xy \qquad f(x,y) = x^2 + 2y^2 \qquad f(x,y) = \sqrt{1 - x^2 - y^2}$$

$$f(x,y) = \log\left(x^2 + y\right) \qquad f(x,y) = x^2 - y^2 \qquad f(x,y) = \sin(xy)$$

e.g. Equação de Van der Waals.

$$\left(P + \frac{a}{V^2}\right)(V - b) = nRT$$

onde b representa o efeito das dimensões finitas das moléculas e a/V^2 o efeito das forças moleculares de coesão.

Directional and partial derivatives. Let $f : X \subset \mathbb{R}^n \to \mathbb{R}$ be a scalar field. Given any point $\mathbf{x} \in \mathbb{R}^n$, a non-zero vector $\mathbf{v} \in \mathbb{R}^n$ defines a straight line $t \mapsto \mathbf{x} + t\mathbf{v}$ passing through the point $\mathbf{x}$ at time $t = 0$ with velocity $\mathbf{v}$. The *directional derivative* of the field f at the point $\mathbf{x} \in X$ along the direction of the vector $\mathbf{v} \in \mathbb{R}^n$ is the derivative of the real valued function $t \mapsto f(\mathbf{x} + t\mathbf{v})$ computed at time $t = 0$, namely

$$\frac{\partial f}{\partial \mathbf{v}}(\mathbf{x}) := \left.\frac{d}{dt} f(\mathbf{x} + t\mathbf{v})\right|_{t=0} .$$

Another notation for the directional derivative is $\pounds_{\mathbf{v}} f(\mathbf{x})$ (called *Lie derivative* of the scalar field f along the constant vector field $\mathbf{v}$). Some authors reserve the name of directional derivative to the case when $\mathbf{v}$ is a unit vector, i.e. when $\|\mathbf{v}\| = 1$.

If we compute the directional derivative of f w.r.t. the direction $\mathbf{v} = \mathbf{e}_k$, the k-th vector of the canonical basis $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_n$ of $\mathbb{R}^n$, we get the *partial derivative* of f at the point $\mathbf{x}$ with respect to the variable x_k, denoted as

$$\frac{\partial f}{\partial x_k}(x) := \lim_{t \to 0} \frac{f(\mathbf{x} + t\mathbf{e}_k) - f(\mathbf{x})}{t} .$$

Thus, in order to compute the partial derivative $\frac{\partial f}{\partial x_k}(\mathbf{x})$, you "freeze" all the remaining coordinates x_i, with $i \neq k$, to their values at the point $\mathbf{x}$, and compute the usual derivative of the real valued function $t \mapsto f(x_1, \ldots, x_{k-1}, t, x_{k+1}, \ldots, x_n)$ at the point $t = x_k$.

For example, the partial derivatives of the scalar field $f(x,y)$ defined in some domain of the Cartesian plane $\mathbb{R}^2$ with coordinates (x,y) are the limits

$$\frac{\partial f}{\partial x}(x,y) = \lim_{\varepsilon \to 0} \frac{f(x+\varepsilon, y) - f(x,y)}{\varepsilon} \qquad \text{and} \qquad \frac{\partial f}{\partial y}(x,y) = \lim_{\varepsilon \to 0} \frac{f(x, y+\varepsilon) - f(x,y)}{\varepsilon} .$$

Higher order derivatives and smooth fields. Partial derivatives of a scalar field are themselves scalar fields, so it make sense to compute their partial derivatives,

$$\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right) = \frac{\partial^2 f}{\partial y \partial x}, \qquad \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right) = \frac{\partial^2 f}{\partial x^2}, \qquad \dots$$

and so on.

A scalar field is said of *class* $\mathcal{C}^0$ if it is continuous, of *class* $\mathcal{C}^1$ if its partial derivatives are continuous. Using induction, it is said of class $\mathcal{C}^{k+1}$ if its partial derivatives are of class $\mathcal{C}^k$. It is said of class $\mathcal{C}^\infty$ if it is of class $\mathcal{C}^k$ for any k, namely if all its partial derivatives exist and are continuous. According to *Schwarz theorem*, if a scalar field f is of class $\mathcal{C}^k$ in some domain, then its partial derivatives up to order $\leqslant k$ commute. Thus, for example,

$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_j \partial x_i}$$

if the field f is of class $\mathcal{C}^2$.

Differentiable scalar fields. A scalar field $f : X \subset \mathbb{R}^n \to \mathbb{R}$ is *differentiable* at the point $\mathbf{x} \in X$ if there exists a linear map $L : \mathbb{R}^n \to \mathbb{R}$ such that, for any $\mathbf{v} \in \mathbb{R}^n$ with sufficiently small norm,

$$f(\mathbf{x} + \mathbf{v}) = f(\mathbf{x}) + L \cdot \mathbf{v} + e(\mathbf{v})$$

where the “error” $e(\mathbf{v})$ is so small that

$$\lim_{\|\mathbf{v}\| \to 0} \frac{e(\mathbf{v})}{\|\mathbf{v}\|} = 0 .$$

The linear map L is called *differential of f at* $\mathbf{x}$, and denoted by $df(\mathbf{x})$ (or also $Df(\mathbf{x})$, or $f'(\mathbf{x})$). Above, we used the notation $L \cdot \mathbf{v} = L_1 v_1 + L_2 v_2 + \cdots + L_n v_n$ for the value of the linear map L at the vector $\mathbf{v}$.

It is clear that a linear map L as above, if it exists, must be unique. It also immediate to see that a differentiable field is continuous, since both $L \cdot \mathbf{v} \to 0$ and $e(\mathbf{v}) \to 0$, and consequently $f(\mathbf{x} + v) \to f(\mathbf{x})$, as $\|\mathbf{v}\| \to 0$.

If f is differentiable at $\mathbf{x}$, its directional and partial derivatives may be computed as

$$\frac{\partial f}{\partial \mathbf{v}}(\mathbf{x}) = df(\mathbf{x}) \cdot \mathbf{v} \qquad \text{and} \qquad \frac{\partial f}{\partial x_k}(\mathbf{x}) = df(\mathbf{x}) \cdot \mathbf{e}_k .$$

Therefore, the *differential* of a scalar field $f : X \subset \mathbb{R}^n \to \mathbb{R}$ at the point $\mathbf{x} \in X$ is the linear form $df(\mathbf{x}) : \mathbb{R}^n \to \mathbb{R}$ given in coordinates by

$$df(\mathbf{x}) := \frac{\partial f}{\partial x_1}(\mathbf{x})\, dx_1 + \frac{\partial f}{\partial x_2}(\mathbf{x})\, dx_2 + \cdots + \frac{\partial f}{\partial x_n}(\mathbf{x})\, dx_n$$

where dx_k, the differential of the coordinate function $\mathbf{x} \mapsto x_k$, is the linear form which takes the vector $\mathbf{v} = (v_1, v_2, \dots, v_n) \in \mathbb{R}^n$ into the scalar $dx_k \cdot \mathbf{v} := v_k$.

Gradient. A convenient way to write the differential of a scalar field is the following. The *gradient* of the scalar field $f : X \subset \mathbb{R}^n \to \mathbb{R}$ at the point $\mathbf{x} \in X$ is the vector whose components are the partial derivatives of f at $\mathbf{x}$, namely

$$\nabla f(\mathbf{x}) := \left(\frac{\partial f}{\partial x_1}(x), \frac{\partial f}{\partial x_2}(x), \dots, \frac{\partial f}{\partial x_n}(x)\right) .$$

An alternative notation, also used by physicists, is $\operatorname{grad} f(\mathbf{x})$.

In particular, the directional derivative of the differentiable field f along the direction of $\mathbf{v} \in \mathbb{R}^n$ at the point $\mathbf{x}$ is

$$\frac{\partial f}{\partial \mathbf{v}}(x) = df(\mathbf{x}) \cdot v = \langle \nabla f(\mathbf{x}), \mathbf{v} \rangle .$$

If $\mathbf{v}$ is a unit vector, i.e. $\|\mathbf{v}\| = 1$, then the Schwarz inequality says that

$$-\|\nabla f(\mathbf{x})\| \leqslant \frac{\partial f}{\partial \mathbf{v}}(\mathbf{x}) \leqslant \|\nabla f(\mathbf{x})\| \,.$$

More precisely,

$$\frac{\partial f}{\partial \mathbf{v}}(\mathbf{x}) = \|\nabla f(\mathbf{x})\| \cdot \cos(\theta)$$

where θ is the angle between $\nabla f(\mathbf{x})$ and $\mathbf{v}$. Therefore, the directional derivative is the component of $\mathbf{v}$ along the direction of the gradient $\nabla f(\mathbf{x})$. In particular, the directional derivative is maximal in the direction of the gradient, namely for $v = \nabla f(\mathbf{x})/\|\nabla f(\mathbf{x})\|$, and minimal in the opposite direction, for $\mathbf{v} = -\nabla f(\mathbf{x})/\|\nabla f(\mathbf{x})\|$. Thus, the gradient points to the direction along which the function increases most rapidly.

Computation of the gradient may be simplified using the following properties, easy consequences of the corresponding properties of the derivative:

$$\nabla f = 0 \qquad \text{if } f \text{ is constant}$$

$$\nabla(f+g) = \nabla f + \nabla f$$

$$\nabla(fg) = f\,\nabla g + g\,\nabla f$$

$$\nabla(f/g) = \left(g\,\nabla f - f\,\nabla g\right)/g^2$$

Vector fields. A *vector field* is a vector valued function $\mathbf{F} : X \subset \mathbb{R}^n \to \mathbb{R}^k$ defined in some domain $X \subset \mathbb{R}^n$, with coordinates $F_1(x), F_2(x), \ldots, F_k(x)$ which are k scalar fields. Continuity of a vector field is defined component-wise. Thus, a vector field $\mathbf{F}$ is continuous if all its coordinates F_i are continuous scalar fields.

The gradient of a differentiable scalar field $f : X \subset \mathbb{R}^n \to \mathbb{R}$, thought as a function $\nabla f : X \subset \mathbb{R}^n \to \mathbb{R}^n$, sending $x \mapsto \nabla f(x)$, is an example (actually a most important one!) of a vector field.

A vector field $\mathbf{F} : X \subset \mathbb{R}^n \to \mathbb{R}^k$ is *differentiable* at the point $x \in X$ if there exists a linear map $\mathbf{L} : \mathbb{R}^n \to \mathbb{R}^k$ such that, for any $\mathbf{v} \in \mathbb{R}^n$ with sufficiently small norm,

$$\mathbf{F}(\mathbf{x}+\mathbf{v}) = \mathbf{F}(\mathbf{x}) + \mathbf{L} \cdot \mathbf{v} + \mathbf{E}(\mathbf{v})$$

where the error $\mathbf{E}(\mathbf{v})$ is so small that

$$\lim_{\|\mathbf{v}\| \to 0} \frac{\mathbf{E}(\mathbf{v})}{\|\mathbf{v}\|} = 0 \,.$$

The linear map $\mathbf{L}$ is called *differential of* $\mathbf{F}$ *at* $\mathbf{x}$, and denoted by $D\mathbf{F}(\mathbf{x})$, or $\mathbf{F}'(\mathbf{x})$.

Thus, if $\mathbf{F}$ is differentiable at $\mathbf{x}$, its directional and partial derivatives may be computed as

$$\frac{\partial \mathbf{F}}{\partial \mathbf{v}}(\mathbf{x}) = D\mathbf{F}(\mathbf{x}) \cdot \mathbf{v} \qquad \text{and} \qquad \frac{\partial \mathbf{F}}{\partial x_k}(\mathbf{x}) = D\mathbf{F}(\mathbf{x}) \cdot \mathbf{e}_k \,.$$

Therefore, the matrix which represents the differential $D\mathbf{F}(\mathbf{x})$ in the canonical basis of $\mathbb{R}^n$ and $\mathbb{R}^k$ is the *Jacobian matrix*

$$J\mathbf{F}(\mathbf{x}) := \left(\frac{\partial F_i}{\partial x_j}(\mathbf{x}) \right) \in \mathrm{Mat}_{k \times n}(\mathbb{R}) \,.$$

Differentiability classes. The existence of partial derivatives does not implies differentiability. For example, the function $f(x,y)$ equal to 1 for $xy = 0$ (i.e. on the two coordinate axis) and equal to 0 for $xy \neq 0$ (i.e. outside the axis) does admit partial derivatives at the origin, but it is not even continuous there. Even the existence of directional derivatives for all non-zero directions does not implies differentiability.

More interesting is that the existence and continuity of all first partial derivatives in some domain does implies differentiability. The class of real valued functions having continuous partial derivatives inside the domain $X \subset \mathbb{R}^n$ is named the class of $\mathcal{C}^1(X, \mathbb{R})$ functions.

Chain rule for scalar fields and paths. Let $\mathbf{r} : I \subset \mathbb{R} \to X \subset \mathbb{R}^n$ be a differentiable path, given explicitly by $t \mapsto \mathbf{c}(t) = (x_1(t), x_2(t), \dots, x_n(t))$, and let $f : X \subset \mathbb{R}^n \to \mathbb{R}$ be a differentiable scalar field. The composite function $f \circ \mathbf{c} : I \to \mathbb{R}$ (which is a real valued function of a real variable) is differentiable and its derivative may be computed as

$$\begin{aligned}\frac{d}{dt} f(\mathbf{c}(t)) &= \langle \nabla f(\mathbf{c}(t)), \dot{\mathbf{c}}(t) \rangle \\ &= \frac{\partial f}{\partial x_1}(\mathbf{c}(t)) \cdot \frac{dx_1}{dt}(t) + \frac{\partial f}{\partial x_2}(\mathbf{c}(t)) \cdot \frac{dx_2}{dt}(t) + \cdots + \frac{\partial f}{\partial x_n}(\mathbf{c}(t)) \cdot \frac{dx_n}{dt}(t)\end{aligned}$$

Por exemplo, se $t \mapsto \mathbf{r}(t) = (x(t), y(t)) \in \mathbb{R}^2$ é um caminho com velocidade $\mathbf{v}(t) = (\dot{x}(t), \dot{y}(t))$, e $f(x, y)$ um campo escalar, então

$$\frac{d}{dt} f(\mathbf{r}(t)) = \langle \nabla f(\mathbf{r}(t)), \mathbf{v}(t) \rangle = \frac{\partial f}{\partial x}(\mathbf{r}(t)) \cdot \dot{x}(t) + \frac{\partial f}{\partial y}(\mathbf{r}(t)) \cdot \dot{y}(t) \, .$$

e.g. **Linear field.** Inner product by a fixed vector $\mathbf{w} \in \mathbb{R}^3$ (or in any other $\mathbb{R}^n$) defines a linear scalar field according to $f(\mathbf{r}) = \langle \mathbf{w}, \mathbf{r} \rangle$. One easily compute that

$$\nabla f(\mathbf{r}) = \mathbf{w} \qquad \text{and therefore} \qquad \frac{\partial f}{\partial \mathbf{v}}(\mathbf{r}) = \langle \mathbf{w}, \mathbf{v} \rangle$$

for any direction $\mathbf{v} \in \mathbb{R}^3$ and any point $\mathbf{r} \in \mathbb{R}^3$. Level surfaces of f are the affine planes orthogonal to the vector $\mathbf{w} \neq 0$, namely

$$\Sigma_\lambda = \{\mathbf{x} \in \mathbb{R}^3 \text{ such that } \langle \mathbf{w}, \mathbf{x} - \mathbf{a} \rangle = 0\} = \mathbf{a} + \mathbf{w}^\perp \, ,$$

if $\mathbf{a} \in \Sigma_\lambda$ is any point where $f(\mathbf{a}) = \langle \mathbf{w}, \mathbf{a} \rangle = \lambda$.

e.g. **Norm and its powers.** The norm may be viewed as a scalar field $\mathbf{r} \mapsto r := \|\mathbf{r}\|$. One computes, for any $k = 1, \dots, n$,

$$\frac{\partial r}{\partial x_k}(\mathbf{r}) = \frac{2x_k}{2\sqrt{x_1 + x_2^2 + \cdots + x_n^2}} = \frac{x_k}{r} \, ,$$

and consequently

$$\nabla r(\mathbf{r}) = \frac{\mathbf{r}}{r}$$

for $\mathbf{r} \neq 0$. The gradient of the N-th power $f(\mathbf{r}) = r^N$ is therefore

$$\nabla f(\mathbf{r}) = N r^{N-1} \nabla r = N \frac{\mathbf{r}}{r^{2-N}} \, .$$

In particular, for $\varphi(\mathbf{r}) = \|\mathbf{r}\|^2$,

$$\nabla \varphi(\mathbf{r}) = 2\mathbf{r} \qquad \text{and therefore} \qquad \frac{\partial \varphi}{\partial \mathbf{v}}(\mathbf{r}) = 2 \langle \mathbf{r}, \mathbf{v} \rangle \, .$$

for any direction $\mathbf{v} \in \mathbb{R}^3$. Observe that level surfaces of $\varphi(\mathbf{r}) = r^2$ in $\mathbb{R}^3$ are the spheres $\Sigma_\lambda = \{\mathbf{x} \in \mathbb{R}^3 \text{ such that } \|\mathbf{x}\|^2 = \lambda\}$ of radius $\sqrt{\lambda}$, for $\lambda \geqslant 0$.

Thus, if a particle moves inside a fixed sphere, i.e. if $t \mapsto \mathbf{r}(t)$ is a path with constant $\|\mathbf{r}(t)\|^2 = \lambda$, then $\langle \dot{\mathbf{r}}(t), \mathbf{r}(t) \rangle = 0$, so that the velocity $\mathbf{v}(t) = \dot{\mathbf{r}}(t)$ is orthogonal to the position vector $\mathbf{r}(t)$ at every time t.

ex: Calcule as derivadas parciais de primeira e segunda ordem das seguintes funções, nos domínios onde podem ser definidas:

$$f(x,y) = \sqrt{x^2 + y^2} \qquad f(x,y,z) = x^3 + y^2 + zxy \qquad f(x,y) = \log\left(x^2 + y^2\right)$$

$$f(x,y) = e^{x+y} \qquad f(x,y) = \frac{\sin(x^2)}{y} \qquad f(x,y) = e^{y \log x}$$

ex: Calcule o gradiente das seguintes funções, nos domínios onde podem ser definidas:

$$f(x,y) = \sqrt{x^2+y^2+z^2} \qquad f(x,y) = x^2 - y^2 \qquad f(x,y) = \sin\left(x^2+y^2\right)$$

$$f(x,y) = e^{-x^2-y^2} \qquad f(x,y,z) = xyz \qquad f(x,y) = e^{y\log x}$$

ex: Calcule a derivada $\frac{d}{dt}f(\mathbf{r}(t))$ dos seguintes campos $f(\mathbf{r})$ ao longo dos respetivos caminhos $t \mapsto \mathbf{r}(t)$ nos tempos indicados.

$$f(x,y) = x^3y - xy^2 \qquad t \mapsto (t^2, t^3) \qquad t = 0\,,$$

$$f(x,y) = xy \qquad t \mapsto (2e^t\cos(t), 2e^t\sin(t)) \qquad t = 1\,,$$

$$f(x,y,z) = x^2+y^2+z^2 \qquad t \mapsto (\cos(t), \sin(t), t) \qquad t = \pi\,,$$

e.g. **Gravitational field.** The gravitational force field produced by a star of mass M placed at the origin of $\mathbb{R}^3$ is

$$\mathbf{F}(\mathbf{r}) = -GM\frac{\mathbf{r}}{\|\mathbf{r}\|^3}$$

where $G \simeq 6.670 \times 10^{-8}$ dina-cm^2/gm^2. It is the gradient of the *gravitational potential*

$$\varphi(\mathbf{r}) = \frac{GM}{\|\mathbf{r}\|}\,.$$

ex: Mostre que o potencial Newtoniano $\varphi(\mathbf{r}) = 1/\|\mathbf{r}\|$ em $\mathbb{R}^3\backslash\{(0,0,0)\}$ satisfaz a *equação de Laplace*

$$\frac{\partial\varphi}{\partial x^2} + \frac{\partial\varphi}{\partial y^2} + \frac{\partial\varphi}{\partial z^2} = 0\,.$$

ex: A temperatura do mar num ponto $\mathbf{r} = (x,y,z)$ é dada por $T(x,y,z) = x^3 - xy + yz^2$. Uma sardinha encontra-se no ponto $\mathbf{a} = (3,2,1)$. Em que direcção e sentido a sardinha tem de nadar para arrefecer mais rapidamente?

ex: Seja $f(t)$ uma função real diferenciável. Mostre que a função $u(x,y) = f(xy)$ satisfaz a equação

$$x\frac{\partial u}{\partial x} - y\frac{\partial u}{\partial y} = 0$$

e que a função $v(x,y) = f(x/y)$ satisfaz a equação

$$x\frac{\partial v}{\partial x} + y\frac{\partial v}{\partial y} = 0$$

ex: **(aproximação linear)** Estime os seguintes valores, usando a aproximação linear

$$f(x+dx, y+dy) \simeq f(x,y) + \frac{\partial f}{\partial x}(x,y)\cdot dx + \frac{\partial f}{\partial y}(x,y)\cdot dy$$

$$e^{0.01}\sqrt{3.999} \qquad \frac{\log(1.01)}{1+0.001} \qquad \sqrt[3]{7.99}\sqrt{36.01}$$

e.g. Kinetic energy and conservative systems. Let $t \to \mathbf{r}(t) \in \mathbb{R}^2$ (or $\mathbb{R}^3$) the trajectory of a particle of mass $m > 0$, $\mathbf{v}(t) = \dot{\mathbf{r}}(t)$ its velocity and $\mathbf{a}(t) = \dot{\mathbf{v}}(t) = \ddot{\mathbf{r}}(t)$ its acceleration. The *kinetic energy* of the particle is

$$K := \frac{1}{2} m \|\mathbf{v}\|^2 .$$

Its time variation is

$$\frac{d}{dt}\left(\frac{1}{2} m \|\mathbf{v}(t)\|^2\right) = \langle m\,\mathbf{a}(t), \mathbf{v}(t)\rangle .$$

Thus, if the particle is subject to a force $\mathbf{F} = m\,\mathbf{a}$ which is orthogonal to the velocity (as a magnetic force acting on a moving charged particle) then the kinetic energy is a constant of the motion.

A force field $\mathbf{F}(\mathbf{r})$ is said *conservative* if there exists a scalar field $V(\mathbf{r})$, called potential, such that $\mathbf{F}(\mathbf{r}) = -\nabla V(\mathbf{r})$. The name is justified by the fact that the *(total) energy*, defined as

$$E := K + V = \frac{1}{2} m \|\mathbf{v}\|^2 + V(\mathbf{r}) ,$$

is a constant of the motion. Indeed

$$\begin{aligned} \frac{d}{dt} E(\mathbf{r}(t), \mathbf{v}(t)) &= \langle m\mathbf{a}(t), \mathbf{v}(t)\rangle + \langle \nabla V(\mathbf{r})(t), \mathbf{v}(t)\rangle \\ &= \langle m\mathbf{a}(t) - \mathbf{F}, \mathbf{v}(t)\rangle = 0 \end{aligned}$$

if the acceleration satisfies Newton equation $\mathbf{F} = m\mathbf{a}$.

Tangent space to a level set. Let Σ_λ be a non-empty level set of the differentiable scalar field $f : X \subset \mathbb{R}^n \to \mathbb{R}$, and $\mathbf{x} \in \Sigma_\lambda$ one of its points. If $\mathbf{c} :]-\varepsilon, \varepsilon[\to \Sigma_\lambda$ is any differentiable curve lying entirely on the level set Σ_λ and passing through $\mathbf{c}(0) = \mathbf{x}$ at time 0, then the composite function $t \mapsto f(\mathbf{c}(t))$ is constant and equal to λ, and therefore, by the chain rule,

$$0 = \frac{d}{dt} f(\mathbf{c}(t))\Big|_{t=0} = \langle \nabla f(\mathbf{x}), \dot{\mathbf{c}}(0)\rangle .$$

If the gradient of f at $\mathbf{x}$ is different from the zero vector, i.e. $\nabla f(\mathbf{x}) \neq 0$, we deduce the the space of all such velocities $\dot{\mathbf{c}}(0)$, which we call *tangent space* to Σ_λ at $\mathbf{x}$, is the normal space to the gradient of f at $\mathbf{x}$.

For example, If $f(x, y, z)$ is a scalar field defined in some $X \subset \mathbb{R}^3$, then the tangent plane to the level surface Σ_λ at some point $\mathbf{r}$ is the affine plane orthogonal to the gradient $\nabla f(\mathbf{r})$ and passing through the point $\mathbf{r}$, namely

$$\{\mathbf{v} \in \mathbb{R}^3 \text{ such that } \langle \nabla f(\mathbf{r}), \mathbf{v} - \mathbf{r}\rangle = 0\} .$$

The Cartesian equation of such a plane is

$$\frac{\partial f}{\partial x}(\mathbf{r}) \cdot (x - a) + \frac{\partial f}{\partial y}(\mathbf{r}) \cdot (y - b) + \frac{\partial f}{\partial z}(\mathbf{r}) \cdot (z - c) = 0 ,$$

where $\mathbf{v} = (x, y, z)$ and $\mathbf{r} = (a, b, c)$.

ex: Considere as seguintes funções:

$$f(x,y) = x^2 + y^2 \qquad f(x,y) = x^2 - y^2 \qquad f(x,y) = x^2$$

$$f(x,y) = xy \qquad f(x,y) = e^{x^2+y^2} \qquad f(x,y) = 1 - y - x^2$$

$$f(x,y,z,) = x^2 + y^2 + z^2 \qquad f(x,y,z) = x^2 + y^2 - z^2 \qquad f(x,y,z) = x^2 + y^2 - z$$

Calcule o gradiente num ponto genérico onde estão definidas. Determine a recta/superfície tangente à curva/superfície de nível no ponto $\mathbf{r} = (1,1)$ (ou $\mathbf{r} = (1,1,1)$).

Critical points and local extrema. Let $f : X \to \mathbb{R}$ be a differentiable scalar field defined in some domain $X \subset \mathbb{R}^n$. *Critical points* (or *stationary points*) of f are points $\mathbf{a} \in X$ where the differential (hence the gradient) vanishes, i.e. where

$$df(\mathbf{a}) = 0.$$

Observe that this means that all partial derivatives vanish.

If f has a local maximum or minimum at some interior point $\mathbf{a} \in X$ (as, for example, the origin for $f(x,y) = -x^2 - y^2$ or $f(x,y) = x^2 + y^2$), then it must be a critical point, since the directional derivative $\frac{\partial f}{\partial \mathbf{v}}(\mathbf{a})$ must vanishes there for any vector $\mathbf{v} \in \mathbb{R}^n$. The converse is, of course, false already in dimension one. Critical points such that in any neighborhood $B_\varepsilon(\mathbf{a})$ there exists points $\mathbf{x}, \mathbf{y}$ such that $f(\mathbf{x}) < f(\mathbf{a}) < f(\mathbf{y})$ are said *saddle points*. The simplest example in the plane is the origin for $f(x,y) = xy$.

To decide if a critical point $\mathbf{a}$ is indeed a local minimum or maximum we must look at least at the second derivatives of f, namely its *Hessian matrix*

$$\mathcal{H}f(\mathbf{a}) := \left(\frac{\partial^2 f}{\partial x_i \partial x_j}(\mathbf{a}) \right) .$$

It follows from Schwarz theorem that, if f is of class $\mathcal{C}^2$, this is a symmetric matrix. But this implies that $\mathcal{H}f(\mathbf{a})$ is diagonalizable, namely that there exist n linear independent eigenvectors $\mathbf{w}_1, \dots, \mathbf{w}_n$, forming a base of $\mathbb{R}^n$, and corresponding eigenvalues $\lambda_1, ..., \lambda_n$, such that

$$\mathcal{H}f(\mathbf{a}) \cdot \mathbf{w}_k = \lambda_k \mathbf{w}_k$$

Now, given any direction $\mathbf{v} = \sum_{k=1}^n v_k \mathbf{w}_k$, Taylor formula for the restriction $t \mapsto g(t) = f(a + t\mathbf{v})$ gives

$$g(t) = g(0) + \sum_i \lambda_k v_k^2 t^2 + \text{ higher order terms} .$$

There follows

Proposition 8.1. *Let $\mathbf{a} \in X$ be a critical point of a scalar field $f : X \subset \mathbb{R}^n \to \mathbb{R}$ of class $\mathcal{C}^2$. If all the eigenvalues of the Hessian matrix $\mathcal{H}f(\mathbf{a})$ are positive/negative then a is a local minimum/maximum of f. If the Hessian matrix has both positive and negative eigenvalues, then $\mathbf{a}$ is a saddle point.*

Observe also that if our scalar field is defined on the plane $\mathbb{R}^2$, then the Hessian matrix is two-by-two matrix, and the task to detect its signature is much easier. In this case we can state the recipe: a critical point of a scalar field $f(x,y)$ is a local extremum iff the determinant $\det(\mathcal{H}f(\mathbf{a}))$ is positive; moreover, the local extremum is a maximum/minimum iff one of the diagonal entries of $\mathcal{H}f(\mathbf{a})$ is negative/positive.

ex: Compute critical points of the following fields, and decide if they are maxima, minima or saddle points.

$$f(x,y) = (x-1)(y-2) \qquad f(x,y) = x^2 + (y-3)^2 \qquad f(x,y) = x^2 - y^2 + 7$$

$$f(x,y) = x^3 y^2 \qquad f(x,y = \sin(x)\cos(y) \qquad f(x,y) = e^{-x^2-y^2}$$

e.g. Geometric center. Given N points $\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N \in \mathbb{R}^n$, we may try to minimize the sum

$$S(\mathbf{r}) = \sum_{k=1}^N \|\mathbf{x}_k - \mathbf{r}\|^2$$

of the square distances from a given point $\mathbf{r}$. The minimum is attained for $\mathbf{r}$ equal to the *(geometric) center*

$$\overline{\mathbf{x}} := \frac{1}{N} \sum_{k=1}^N \mathbf{x}_k .$$

e.g. Least squares. We measure n times an observable y in correspondence of another observable x, obtaining the set of data

$$x_1,\, y_1, \qquad x_2,\, y_2 \qquad \dots \qquad x_n,\, y_n$$

We conjecture a law $y = f(x, \mathbf{a})$, depending on certain parameters $\mathbf{a} = (\alpha_1, \dots, \alpha_k) \in \mathbb{R}^k$, and pose the problem to find the "best" values of the parameters that fit the experimental results. One popular answer, called *least square fitting*, consists in choosing those values of the parameters that minimize the sum

$$Q(\mathbf{a}) = \sum_{k=1}^{n} (y_k - f(x_k, \mathbf{a}))^2$$

of the squares of the errors. In general, the condition $\nabla Q(\mathbf{a}) = 0$ being nonlinear, cannot be solved by exact methods. Computational softwares, in particular statistics software, use to have routines dedicated to estimate a solution.

The answer is easy when we conjecture a linear law $y = \alpha + \beta x$, In this case, computing the partial derivatives $\partial Q/\partial\alpha$ and $\partial Q/\partial\beta$, we get the two equations

$$\sum_{k=1}^{n} (y_k - (\alpha + \beta x_k)) = 0 \qquad \text{and} \qquad \sum_{k=1}^{n} (y_k - (\alpha + \beta x_k))\, x_k = 0\,,$$

hence the system

$$\begin{cases} \beta\,\overline{x} + \alpha = \overline{y} \\ n\,\alpha + \beta\left(\overline{\sigma}^2_{xx} + n\overline{x}^2\right) = \overline{\sigma}^2_{xy} + n\overline{xy} \end{cases}$$

for α and β, where we used the notations $\overline{x} = \frac{1}{n}(x_1 + x_2 + \cdots + x_n)$ and $\overline{y} = \frac{1}{n}(y_1 + y_2 + \cdots + y_n)$ for the mean values, and

$$\overline{\sigma}^2_{xx} := \sum_{k=1}^{n} (x_k - \overline{x})^2 = \left(\sum_{k=1}^{n} x_k^2\right) - n\overline{x}^2$$

$$\overline{\sigma}^2_{xy} := \sum_{k=1}^{n} (x_k - \overline{x})(y_k - \overline{y}) = \left(\sum_{k=1}^{n} x_k y_k\right) - n\overline{xy}$$

for the covariances. After some rearrangement, we see that the critical point of $Q(\alpha, \beta)$, hence the answer according to the least squares principle, is given by the recipe

$$\beta = \frac{\overline{\sigma}^2_{xy}}{\overline{\sigma}^2_{xx}} \qquad \text{and} \qquad \alpha = \overline{y} - \beta\overline{x}\,.$$

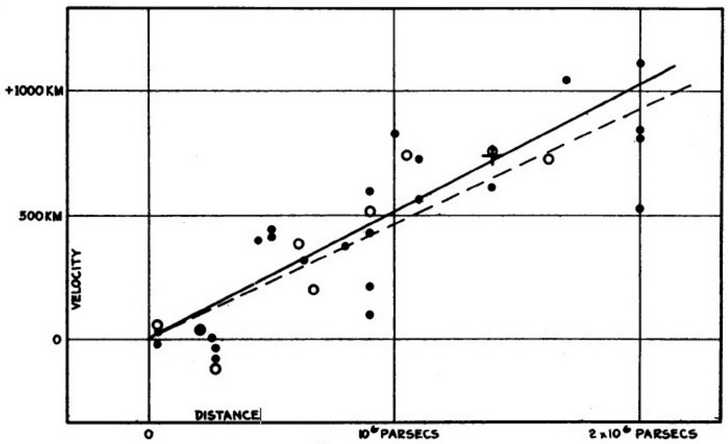


FIGURE 1

Velocity-Distance Relation among Extra-Galactic Nebulae.

Picture from the original paper by Hubble[24], showing the velocity-distance relation $v = Hd$, therefore suggesting the expansion of our Universe.

[24] E. Hubble, A relation between distance and radial velocity among extra-galactic nebulae, *Proc. N. A. S.* **15** (1929), 168-173.

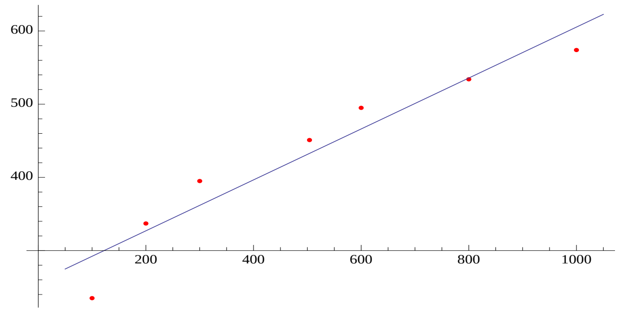
It must be said that minima of $Q(\mathbf{a})$ always exist, hence the method produces values of the parameters for all laws we may conjecture, true or false! The actual value of the minimum, together with some knowledge of the statistical errors in the data, gives a measure of the significance of the result. You may learn more in any good manual on statistics.

help: With `Mathematica`®`8` you may define your data and fit a line with the commands

```
data = {{100, 235}, {200, 337}, {300, 395}, {504, 451}, {600,  495}, {800, 534}, {1000, 574}};
line = Fit[data, {1, x}, x]
```

and produce the picture

```
Show[ListPlot[data, PlotStyle -> Red], Plot[{line}, {x, 50, 1050}]]
```



ex: Na seguinte amostra, obtida por Galileo, foram registadas as coordenadas (altura x e distância y) da trajectória de um objecto lançado com uma força horizontal,

x	100	200	300	450	600	800	1000
y	235	337	395	451	495	534	574

Ajuste uma recta.

ex: Na seguinte tabela, colecionada por Jaques Cassini, foram registadas as obliquidades da eclíptica (o ângulo entre o plano equatorial da Terra e o seu plano orbital) $(y + 23)°$ em diferentes datas t,

t	−140	−140	390	880	1070	1300	1460
y	0.853	0.856	0.500	0.583	0.567	0.533	0.500

t	1500	1500	1570	1570	1600	1656	1672	1738
y	0.473	0.488	0.499	0.525	0.517	0.484	0.482	0.472

Ajuste uma recta. Retire os dados anteriores ao ano 1500, e ajuste outra recta. Discuta o resultado.

9 Modelos contínuos e simulações

Systems of ordinary differential equations. Meaningful models of many physical, chemical, biological ... systems are written in the language of systems of differential equations

$$\dot{\mathbf{x}} = \mathbf{v}(t, \mathbf{x}) \tag{9.1}$$

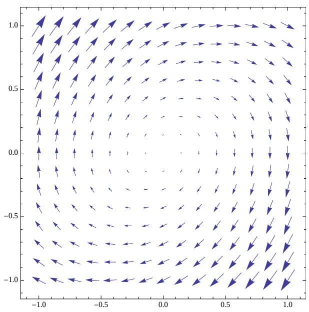
where $\mathbf{x}(t) = (x_1(t), x_2(t), \dots, x_n(t)) \in X \subset \mathbb{R}^n$ is a vector of values of certain observables at time t, and $\mathbf{v}(t, \mathbf{x})$ is a given direction field in the extended phase space $T \times X \subset \mathbb{R} \times \mathbb{R}^n$.

e.g. **Chemical reactions.** The modern approach to the kinetics of chemical reactions is discussed in the article Chemical reaction kinetics of the Scholarpedia.

help: O campo vetorial do oscilador harmónico com atrito pode ser desenhado, no Mathematica®, usando a instrução

```
VectorPlot[{y, -x + 0.5 y}, {x, -1, 1}, {y, -1, 1}]
```

O resultado é



Simulations. It is in general hopeless to find "exact" solutions of systems of differential equations, as long as they are not linear. For this reason, we must content with making simulations.

Euler method. Considere o problema de simular as soluções da EDO

$$\dot{\mathbf{x}} = \mathbf{v}(t, \mathbf{x}) \, .$$

O *método de Euler* consiste em utilizar recursivamente a aproximação linear

$$\mathbf{x}(t + dt) - \mathbf{x}(t) \simeq \mathbf{v}(t, \mathbf{x}) \cdot dt \, ,$$

dado um "passo" dt suficientemente pequeno. Portanto, a solução $\mathbf{x}(t_0 + n \cdot dt)$ com condição inicial $\mathbf{x}(t_0) = \mathbf{x}_0$, é estimada pela sucessão (x_n) definida recursivamente por

$$x_{n+1} = x_n + v(t_n, x_n) \cdot dt \, , \tag{9.2}$$

onde $t_n = t_0 + n \cdot dt$. Numa linguagem como `c++` ou `Java`, o ciclo para obter uma aproximação de $x(t)$, dado $x(t_0) =$ `x`, é

```
while (time < t)
  {
    x += v(time, x) * dt ;
    time += dt ;
  }
```

e.g. The exponential. Considere a equação diferencial

$$\dot{x} = x$$

com condição inicial $x(0) = 1$. Mostre que, se o passo é $dt = \varepsilon$, então o método de Euler fornece a aproximação

$$x(t) \simeq (1+\varepsilon)^n$$

onde $n \simeq t/\varepsilon$ é o número de passos. Deduza que, no limite quando o passo $\varepsilon \to 0$, as aproximações convergem para a solução e^t, pois

$$\lim_{\varepsilon \to 0} (1+\varepsilon)^{t/\varepsilon} = \lim_{n\to\infty} \left(1 + \frac{t}{n}\right)^n$$

Método RK-4. O *método de Runge-Kutta* (de ordem) *4* para simular a solução de

$$\dot{x} = v(t,x) \qquad \text{com condição inicial} \qquad x(t_0) = x_0$$

consiste em escolher um "passo" dt, e aproximar $x(t_0 + n \cdot dt)$ com a sucessão (x_n) definida recursivamente por

$$\boxed{x_{n+1} = x_n + \tfrac{dt}{6}\left(k_1 + 2k_2 + 2k_3 + k_4\right)}$$

onde $t_n = t_0 + n \cdot dt$, e os coeficientes k_1, k_2, k_3 e k_4 são definidos recursivamente por

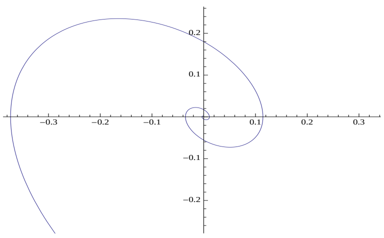
$$\boxed{k_1 = v(t_n, x_n) \quad k_2 = v\left(t_n + \tfrac{dt}{2}, x_n + \tfrac{dt}{2} \cdot k_1\right) \quad k_3 = v\left(t_n + \tfrac{dt}{2}, x_n + \tfrac{dt}{2} \cdot k_2\right) \quad k_4 = v(t_n + dt, x_n + dt \cdot k_3)}$$

- Implemente um código para simular sistemas de EDOs usando o método RK-4.

help: O pêndulo com atrito pode ser simulado, no Mathematica®, usando as instruções

```
s = NDSolve[{x'[t] == y[t], y'[t] == -Sin[x[t]] - 0.7 y[t],
   x[0] == y[0] == 1}, {x, y}, {t, 20}]
ParametricPlot[Evaluate[{x[t], y[t]} /. s], {t, 0, 20}]
```

O resultado é



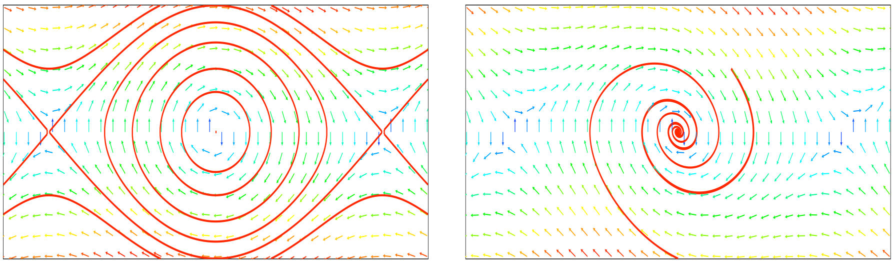
e.g. Pêndulo matemático. Considere a equação de Newton que modela as oscilações de um *pêndulo*,

$$\ddot{\theta} = -\omega^2 \sin(\theta) - \alpha\dot{\theta}\,.$$

onde $\omega = \sqrt{g/\ell}$, g é a aceleração gravitacional, ℓ o comprimento do pêndulo, e $\alpha \geqslant 0$ um coeficiente de atrito. No espaço de fase, de coordenadas θ e $p = \dot{\theta}$, a equação assume a forma do sistema

$$\begin{aligned} \dot{\theta} &= p \\ \dot{p} &= -\omega^2 \sin(\theta) - \alpha p \end{aligned}$$

- Simule o sistema, e esboçe as trajectórias e as curvas de fase.



Retrato de fase do pêndulo (sem e com atrito).

e.g. Oscilador harmónico. As pequenas oscilações de um pêndulo em torno da posição de equilíbrio estável $\theta = 0$ são descrita pela equação do *oscilador harmónico*

$$\ddot{q} = -\omega^2 q \, .$$

onde ω é a frequência característica. No espaço de fase, de coordenadas q e $p = \dot{q}$, a equação assume a forma do sistema

$$\begin{aligned} \dot{q} &= p \\ \dot{p} &= -\omega^2 q \end{aligned}$$

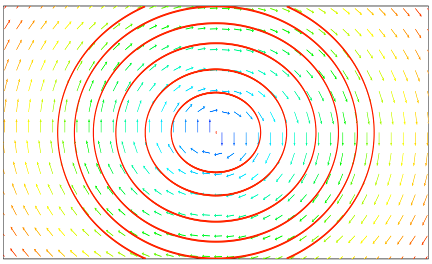
As tsoluç oes são

$$q(t) = A \sin(\omega t + \varphi) \qquad \text{ou} \qquad A \cos(\omega t + \phi) \, ,$$

onde a amplitude A e as fases φ e ϕ dependem dos dados iniciais $q(0) = q_0$ e $\dot{q}(0) = v_0$. A energia

$$E(q,p) = \frac{1}{2}p^2 + \frac{1}{2}\omega^2 q^2$$

é uma constante do movimento, ou seja, $\frac{d}{dt}E\left(q(t), p(t)\right) = 0$.



Retrato de fase do oscilador harmónico.

e.g. Circuito LRC. A corrente $I(t)$ num circuito RLC, de resistência R, indutância L e capacidade C, é determinada pela EDO

$$L\ddot{I} + R\dot{I} + \frac{1}{C}I = \dot{V} \, ,$$

onde $V(t)$ é a tensão que alimenta o circuito.

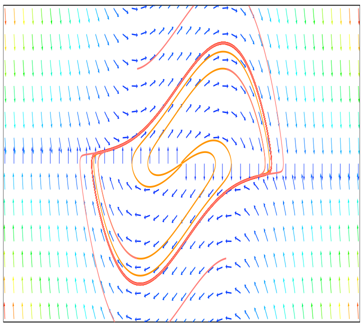
- Simule a corrente num circuito alimentado com uma tensão constante $V(t) = V_0$.
- Simule a corrente num circuito alimentado com uma tensão alternada $V(t) = V_0 \sin(\gamma t)$ (compare com a equação das oscilações forçadas amortecidas).

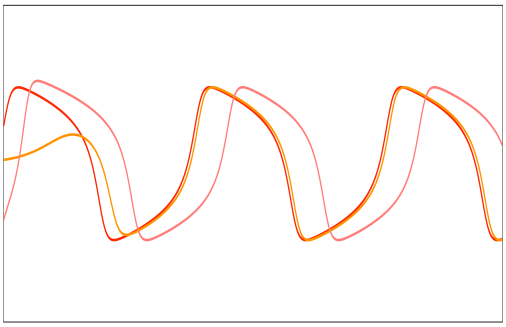
e.g. Oscilador de van der Pol. Considere o *oscilador de van der Pol*[25]

$$\ddot{q} - \mu(1 - q^2)\dot{q} + q = 0$$

que modela a corrente num circuito com um elemento não-linear.

- Simule o sistema e discuta o comportamento das soluções ao variar o parâmetro μ.





Retrato de fase e trajectórias do oscilador de van der Pol.

- Simule o oscilador forçado

$$\ddot{q} - \mu(1 - q^2)\dot{q} + q = F_0 \sin(\omega t)$$

ao variar o parâmetro μ e a frequência ω.

e.g. Sistema de Lotka-Volterra. Considere o *sistema de Lotka-Volterra*

$$\begin{aligned} \dot{x} &= ax - bxy \\ \dot{y} &= -cy + dxy \end{aligned}$$

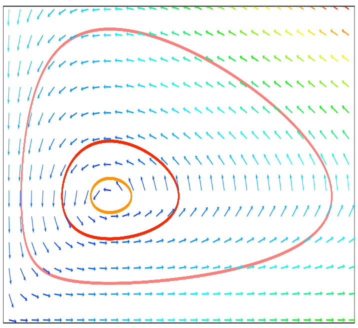
Foi proposto por Vito Volterra[26] para modelar a competição entre x presas e y predadores, e por Alfred J. Lotka[27] para modelar o comportamento cíclico de certas reacções químicas, como o esquema abstracto

$$A + X \to 2X \qquad X + Y \to 2Y \qquad Y \to B$$

Stationary solutions are found solving the system $\dot{x} = 0$ and $\dot{y} = 0$. This gives the trivial solution $(0, 0)$, and the point $(c/d, a/b)$. To understand the other solutions, one observes that the function

$$H(x, y) = dx + by - c \log x - a \log y$$

is a constant of the motion, i.e. $\frac{d}{dt} H(x(t), y(t)) = 0$. Therefore, orbits of the Lotka-Volterra system are contained in the level curves $H(x, y) = c$.



[25] B. van der Pol, A theory of the amplitude of free and forced triode vibrations, *Radio Review* **1** (1920), 701-710 and 754-762. B. van der Pol and J. van der Mark, Frequency demultiplication, *Nature* **120** (1927), 363-364.

[26] Vito Volterra, Variazioni e fluttuazioni del numero d'individui in specie di animali conviventi, *Mem. Acad. Lincei* **2** (1926), 31-113. Vito Volterra, *Leçons sur la Théorie Mathématique de la Lutte pour la Vie*, Paris 1931.

[27] Alfred J. Lotka, *J. Amer. Chem. Soc* **27** (1920), 1595. Alfred J. Lotka, *Elements of physical biology*, Williams & Wilkins Co. 1925.

Phase portrait of the Lotka-Volterra system.

e.g. Rock-paper-scissor game. Consider the reaction

$$X + Y \xrightarrow{\gamma} 2X \qquad Y + Z \xrightarrow{\alpha} 2Y \qquad Z + X \xrightarrow{\beta} 2Z$$

modeled by the system

$$\begin{aligned}\dot{x} &= x(\gamma y - \beta z)\\ \dot{y} &= y(\alpha z - \gamma x)\\ \dot{z} &= z(\beta x - \alpha y)\end{aligned}$$

e.g. Double-negative feedback. The interplay between two mutually repressing genes is described by the system[28]

$$\begin{aligned}\dot{x} &= \frac{\alpha}{1+y^\gamma} - x\\ \dot{y} &= \frac{\beta}{1+x^\delta} - y\end{aligned}$$

e.g. Brusselator. O *Brusselator* é um modelo autocatalítico proposto por Ilya Prigogine e colaboradores[29] que consiste na reacção abstracta

$$A \to X \qquad B + X \to Y + C \qquad 2X + Y \to 3X \qquad X \to D$$

- Simule o sistema

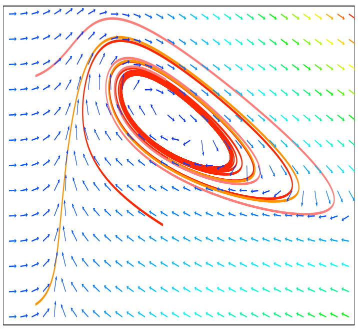
$$\begin{aligned}\dot{x} &= \alpha - (\beta+1)x + x^2 y\\ \dot{y} &= \beta x - x^2 y\end{aligned}$$

  para as concentrações das espécies catalíticas X e Y, obtido quando as concentrações $[A] \sim \alpha$ e $[B] \sim \beta$ são mantidas constantes.

- Simule o sistema

$$\begin{aligned}\dot{x} &= \alpha - (b+1)x + x^2 y\\ \dot{y} &= bx - x^2 y\\ \dot{b} &= -bx + \delta\end{aligned}$$

  para as concentrações de X, Y e B, obtido quando a concentração $[A] \sim \alpha$ é mantida constante e B é injectado a uma velocidade constante $v \sim \delta$.



Rerato de fase do Brusselator.

[28] T.S. Gardner, C.R. Cantor and J.J. Collins, Construction of a genetic toggle switch in *Escherichia coli*, *Nature* **403** (2000) 339-342.

[29] I. Prigogine and R. Lefever, Symmetry breaking instabilities in dissipative systems, *J. Chem. Phys.* **48** (1968), 1655-1700. P. Glansdorff and I. Prigogine, *Thermodynamic theory of structure, stability and fluctuations*, Wiley, New York 1971. G. Nicolis and I. Prigogine, *Self-organization in non-equilibrium chemical systems*, Wiley, New York 1977.

e.g. Reacção de Schnakenberg. Considere a *reacção de Schnakenberg*[30]

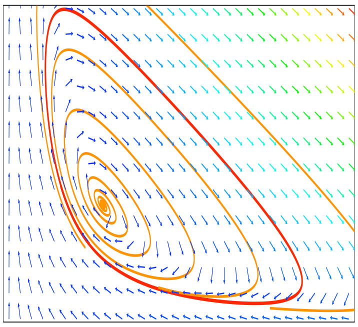
$$2X + Y \to 3X \qquad A \to Y \qquad X \to B$$

modelada pelo sistema

$$\begin{aligned} \dot{x} &= x^2 y - x + \beta \\ \dot{y} &= -x^2 y + \alpha \end{aligned}$$

para as concentrações $x \sim [X]$ e $y \sim [Y]$.

- Simule o sistema e discuta o comportamento das soluções ao variar so parâmetros.



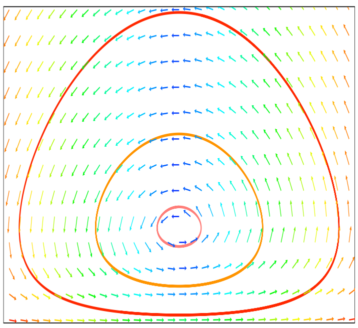
Retrato de fase do sistema de Schnakenberg.

e.g. Oscilador bioquímico de Goodwin. Um modelo de interações proteinas-mRNA proposto por Goodwin[31] é

$$\begin{aligned} \dot{M} &= \frac{1}{1+P} - \alpha \\ \dot{P} &= M - \beta \end{aligned}$$

onde M e P denotam as concentrações relativas de mRNA e proteina, respectivamente.

- Simule o sistema e discuta o comportamento das soluções ao variar so parâmetros.



Retrato de fase do sistema de Goodwin.

- Simule o sistema[32]

$$\begin{aligned} \dot{M} &= \frac{1}{1+P^n} - \alpha M \\ \dot{P} &= M^m - \beta P \end{aligned}$$

[30] J. Schnakenberg, Simple chemical reaction with limit cycle behavior, *J. Theor. Biol.* **81** (1979), 389-400.

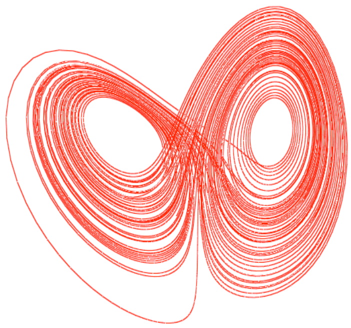
[31] B.C. Goodwin, *Temporal organization in cells*, Academic Press, London/New York 1963. B.C. Goodwin, Oscillatory behaviour in enzymatic control processes, *Adv. Enzyme Regul.* **3** (1965), 425-438.

[32] T. Scheper, D. Klinkenberg, C. Pennartz and J. van Pelt, A Mathematical Model for the Intracellular Cicardian Rhythm Generator, *J. Neuroscience* **19** (1999), 40-47.

e.g. **Atrator de Lorenz.** Considere o *sistema de Lorenz*[33]

$$\dot{x} = \sigma(y - x)$$
$$\dot{y} = x(\rho - z) - y$$
$$\dot{z} = xy - \beta z$$

- Analize o comportamento assimptótico das trajectórias ao variar os parâmetros σ, ρ e β.
- Observe o comportamento das trajectórias quando $\sigma \simeq 10$, $\rho \simeq 28$ e $\beta \simeq 8/3$.



Atractor de Lorenz.

[33] E.N. Lorenz, Deterministic nonperiodic flow, *J. Atmspheric Science* **20** (1963), 130-141.

References

[Ap69] T.M. Apostol, *Calculus*, John Wiley & Sons, 1969 [*Cálculo*, Editora Reverté, 1999].

[Ar78] V.I. Arnold, *Equações diferenciais ordinárias*, MIR, 1985.

[Be62] C. Kittel, W.D. Knight and M.A. Ruderman, *Berkeley Physics: Mechanics*, McGraw-Hill 1962.

[Co04] V. Comincioli, *Modelli Matematici: elementi introduttivi*, Università degli studi di Pavia, 2004.

[Ei88] M. Eisen, *Mathematical Methods and Models in the Biological Sciences*, Prentice Hall, 1988.

[EK05] L. Edelstein-Keshet, *Mathematical Models in Biology*, SIAM, 2005 [Random House, 1988].

[Go77] H.J. Gold, *Mathematical Modeling of Biological Systems - An Introduction Guidebook*, Wiley Interscinece, 1977.

[Gou77] S.J. Gould, *Ever Since Darwin: Reflections in Natural History*, Norton, New York, 1977.

[HK03] B. Hasselblatt and A. Katok, *A first course in dynamics, with a panorama of recent developments*, Cambridge University Press, 2003.

[HS74] M.W. Hirsch and S. Smale, *Differential equations, dynamical systems and linear algebra*, Academic Press, 1974.

[KR85] D. Kleppner and N. Ramsey, *Quick calculus: a self-teaching guide*, Wiley 1985.

[Li06] E.L. Lima, *Análise Real*, Coleção Matemática Universitária, IMPA, 2006.

[MF05] Philip McCord Morse and Herman Feshbach, *Methods of Theoretical Physics*, McGraw-Hill 1953 or Feshbach Publishing, 2005.

[RHB06] K.F. Riley, M.P. Hobson and S. J. Bence, *Mathematical Methods for Physics and Engineering*, Third Edition, Cambridge University Press, 2006.

[Ri04] S.H. Rice, *Evolutionary Theory: Mathematical and Conceptual Foundations*, Sinauer, 2004.

[Ro04] J.C. Robinson, *An introduction to ordinary differential equations*, Cambridge University Press, 2004.

[Ros84] S.L. Ross, *Differential equations*, John Wiley & Sons, 1984.

[Si91] G.F. Simmons, *Differential equations with applications and historical notes*, McGraw-Hill, 1991.

[Wae91] B.L. van der Waerden, *Algebra*, Springer 1991.

[Wr69] S. Wright, *Evolution and the Genetic of Populations*, The University of Chicago Press, 1969.