CSMMA16

Mathematics and Statistics

Calculus

28th September 2016

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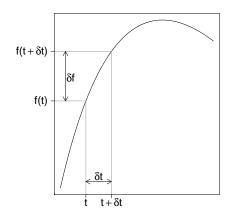
Second Order Systems

Matrix calculus

Optimisation

Differentiation

Differentiation is a measure of change. Consider a function f varying over time t.



Approximate gradient over the interval $(t, t + \delta t)$ is

$$\frac{\delta f}{\delta t} = \frac{f(t + \delta t) - f(t)}{\delta t}$$

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Definition (Derivative)

The (first) derivative of f(t) at point t, denoted f'(t) or $\frac{df}{dt}$, is

$$\frac{df}{dt} = \lim_{\delta t \to 0} \frac{f(t + \delta t) - f(t)}{\delta t}$$

- ▶ The derivative of the derivative of f is $\frac{d^2f}{dt^2}$ or f''(t)
- ▶ The n'th derivative is $\frac{d^n f}{dt^n}$ or $f^n(t)$
- ▶ If y is function of x, do $\frac{dy}{dx}$, etc

Some Simple Rules

- 1. For f(t) and any constant k, $\frac{d(kf)}{dt} = k \times \frac{df}{dt}$
- 2. For f(t) and g(t), $\frac{d(f+g)}{dt} = \frac{df}{dt} + \frac{dg}{dt}$
- 3. For u(t) and v(t),

$$\frac{duv}{dt} = v\frac{du}{dt} + u\frac{dv}{dt}$$
$$\frac{du/v}{dt} = \frac{v\frac{du}{dt} - u\frac{dv}{dt}}{v^2}$$

4. For inverse functions

$$\frac{dt}{dy} = \frac{1}{\frac{dy}{dt}}$$

5. If a function is defined as a function of another variable, eg y = f(x) where x = g(t),

Use chain rule:

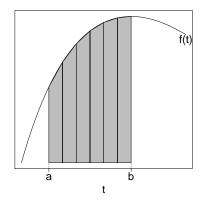
$$\frac{dy}{dt} = \frac{dy}{dx} \times \frac{dx}{dt}$$

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Integration

Integration is a type of sum.

Consider again a function f varying over time t.



Divide area into strips and sum

$$Sum \approx \sum_{r=a}^{b} f(r) * \delta t$$

Definition (Integral)

The integral of f over the interval (a, b) is

$$\int_{a}^{b} f(t)dt = \lim_{\delta t \to 0} \sum_{r=a}^{b} f(r) * \delta t$$

Theorem (First Fundamental Theorem of Calculus)

Suppose that f is continuous on the closed interval [a, b] and F(t) is defined by

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

for all t in [a, b]. Then F is differentiable on the open interval (a, b) and

$$F'(t) = f(t).$$

This shows that integration can be viewed as the inverse of differentiation and provides a way of working out integrals.

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Integral over limits provides the definite integral

$$\int_{a}^{b} f(t)dt = [F(t)]_{a}^{b} = F(b) - F(a) .$$

If no limits are specified, we get the indefinite integral,

$$\int f(t)dt = F(t) + c.$$

This result follows from the first fundamental theorem of calculus and the fact that

$$\frac{d(F(t)+c)}{dt}=\frac{d(F(t))}{dt}.$$

Integration Rules

Follow from those of differentiation

$$\int kf(t)dt = k \int f(t)dt$$

$$\int (f(t) + g(t))dt = \int f(t)dt + \int g(t))dt$$

$$\int u \frac{dv}{dt}dt = uv - \int v \frac{du}{dt}dt \qquad \int_{q}^{p} u \frac{dv}{dt}dt = [uv]_{q}^{p} - \int_{q}^{p} v \frac{du}{dt}dt$$

When integrating $u \times \frac{dv}{dt}$, choose which is u and which $\frac{dv}{dt}$ so

$$\int v \frac{du}{dt} dt$$
 is easier to solve than $\int u \frac{dv}{dt} dt$.

If a function is defined as a function of another variable eg x=f(z) and z=g(t)

$$\int f(z)dt = \int f(z)dz \times \frac{dt}{dz}.$$

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Standard Differentials and Integrals

$f(t) = \frac{dF}{dt}$	$F(t) = \int \frac{f(t)}{dt}$	$f(t) = \frac{dF}{dt}$	$F(t) = \int f(t)dt$
0	С	cos(at)	sin(at)/a + c
1	t+c	sin(at)	$-\cos(at)/a + c$
t	$t^2/2 + c$	sec ² (at)	tan(at) + c
$t^n(n \neq 1)$	$\frac{t^{n+1}}{n+1}+c$	$\frac{1}{\sqrt{1-a^2t^2}}$	$sin^{-1}(at)/a+c$
1/t	In(t)+c	$-\frac{1}{\sqrt{1-a^2t^2}}$	$\cos^{-1}(at)/a + c$
e ^{at}	$\frac{1}{a}e^{at}+c$	$\frac{1}{1+a^2t^2}$	$tan^{-1}(at)/a+c$
sinh(at)	$\cosh(at)/a + c$	cosh(at)	sinh(at)/a + c

Applications of Differentiation

- 1. Finding local maxima/minima of f(t)
 - ▶ Before maximum, f(t) rising, after f(t) falling, at maximum f(t) const

 - ► Hence at maximum $\frac{df}{dt} = 0$ and $\frac{d^2f}{dt^2} < 0$ ► Similarly at minimum $\frac{df}{dt} = 0$ and $\frac{d^2f}{dt^2} > 0$
- 2. Newton-Raphson: iterative method of finding t satisfying f(t) = 0
 - ▶ Suppose t_n is n' th estimate, then next one is found by

$$t_{n+1} = t_n - \frac{f(t_n)}{f'(t_n)}$$

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Applications of Integration

1. Mean of function f(t) between t = a and t = b is

$$\frac{1}{b-a}\int_{a}^{b}f(t)dt$$

2. root mean square of f(t),

$$rms = \sqrt{\frac{\int_{a}^{b} f^{2}(t)dt}{b - a}}$$

If f(t) is a repetitive function of period T, that is f(t) = f(t + T)then

Mean of f(t) is

$$\frac{1}{T} \int_0^T f(t) dt.$$

rms of f(t) is

$$\sqrt{\frac{1}{T} \int_0^T f^2(t) dt}$$

On Lines and Solids of Revolution

Suppose y = f(x)

Length of f(x) from x = a to b is:

$$s = \int_{a}^{b} \sqrt{1 + \left(\frac{dy}{dx}\right)^2} dx$$

If y = f(x) is rotated 360° about x axis, Volume of solid from x=a to b is

$$V = \int_{a}^{b} \pi y^2 dx$$

Surface area of solid from x=a to b is

$$S = \int_{a}^{b} 2\pi y \sqrt{1 + \left(\frac{dy}{dx}\right)^2} dx$$

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Example

Find the surface area between x = 0 and x = 0.5 when $y = x^3$ is rotated about the x axis.

$$\frac{dy}{dx} = 3x^2 \quad \text{so}$$

$$S = \int_0^{0.5} 2\pi x^3 \sqrt{1 + 9x^4} dx$$

Make the substitution $t=x^4$ so $\frac{dt}{dx}=4x^3$ or $dx=\frac{dt}{4x^3}$. Then

$$S = \int_{x=0}^{x=0.5} 2\pi x^3 \sqrt{1+9t} \frac{dt}{4x^3} = \int_{t=0}^{t=0.0625} \frac{\pi}{2} \sqrt{1+9t} dt$$
$$= \left[\frac{\pi}{18} \frac{(1+9t)^{3/2}}{3/2} \right]_0^{1/16} = \frac{\pi(1+9/16)^{3/2}}{27} - \frac{\pi}{27}$$
$$= \frac{\pi}{27} ((25/16)^{3/2} - 1) = \frac{61\pi}{1728}$$

Integration by Trig Substitution

Find mean of function $f(t) = \frac{1}{4+t^2}$ between t = 0 and t = a. Mean given by :

$$\overline{f} = \int_0^a \frac{1}{4+t^2} dt$$

Let $t = 2\tan(x)$ so $\frac{dt}{dx} = 2\sec^2(x)$ and substitute to get

$$\bar{f} = \int_{x=0}^{x=\tan^{-1}(\frac{a}{2})} \frac{1}{4+4\tan^{2}(x)} 2\sec^{2}(x) dx$$

$$= \int_{0}^{\tan^{-1}(\frac{a}{2})} \frac{1}{4\sec^{2}(x)} 2\sec^{2}(x) dx$$

$$= \left[\frac{1}{2}x\right]_{0}^{\tan^{-1}(\frac{a}{2})}$$

$$= \frac{1}{2}tan^{-1}\left(\frac{a}{2}\right)$$

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Differentiation of Product

The output position x of a computer controlled motor is given by

$$x = 3 - e^{-0.5t}(2\sin(2t) + 8\cos(2t))$$

What is its velocity?

$$\begin{aligned} \frac{dx}{dt} &= 0 - e^{-0.5t} (4\cos(2t) - 16\sin(2t)) \\ &- [-0.5e^{-0.5t} (2\sin(2t) + 8\cos(4t))] \\ &= e^{-0.5t} (-4\cos(2t) + 16\sin(2t) + \sin(t) + 4\cos(t)) \\ &= 17e^{-0.5t} \sin(2t) \end{aligned}$$

Using Integration By Parts

To integrate
$$2te^{-2t}$$
, let $u=2t$ and $\frac{dv}{dt}=e^{-2t}$
Then $\frac{du}{dt}=2$ and $v=\int e^{-2t}dt=-\frac{1}{2}e^{-2t}$

So

$$\int 2te^{-2t}dt = 2t(-\frac{1}{2}e^{-2t}) - \int -\frac{1}{2}e^{-2t}2dt$$
$$= -te^{-2t} - \frac{1}{2}e^{-2t} + c$$

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Ordinary Differential Equations

An ordinary differential equation (ODE) is an equation with one or more differentials of a dependent variable.

- ▶ The order of the ODE is the degree of the highest derivative
- An ODE is linear if the dependent variable and its derivatives
 - 1. are of first degree only
 - 2. do not appear as products in the equation
 - 3. do not appear in any transcendental (non-algebraic) function.

General form of an ODE:

$$\frac{d^{n}y}{dt^{n}} + A_{1}(t)\frac{d^{n-1}y}{dt^{n-1}} + \cdots + A_{n-1}(t)\frac{dy}{dt} + A_{n}(t)y = g(t) ,$$

where $A_i(t)$, i = 0, ..., n and g(t) are functions of t.

NOTE: A differential equation with more than one dependent variable is called a partial differential equation (PDE)

Homogeneous ODE

Each term in the linear differential equation must contain the dependent variable or a derivative of the dependent variable.

Thus, it is sufficient that

$$g(t) = 0$$

Examples:

$$\frac{dy}{dt} + 4y = 0$$

- First order, linear, homogenous

$$\frac{d^2y}{dt^2} + 4\frac{dy}{dt} + 3y = 4\sin(t)$$

- Second order, linear, inhomogenous

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Solving ODEs

The solution of a differential equation expresses the dependent variable y in terms of t.

Solving an ODE involves integration

There are many ways of solving ODEs, we will concentrate on a few.

Note, solutions can have two forms

General solution

like indefinite integral, with constant(s)

Particular solution

where use information to find constant(s)

We can also use computers to solve ODEs numerically

Simple Example

The velocity at time t of a moving object, with initial velocity 3 and constant acceleration 8, is given by

$$\frac{dy}{dt} = 3 + 8t$$

What is y, its position at time t?

Can integrate both sides wrt t: as RHS of equation is f(t)

$$\int \frac{dy}{dt}dt = y = \int (3+8t)dt = 3t + 4t^2 + c$$

This is the general solution.

With extra information, such as the position is 5 at t = 0, we get

$$5 = 0 + 0 + c$$
, so $c = 5$

Hence the particular solution is

$$y = 5 + 3t + 4t^2$$

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Separable Differential Equations

Here $\frac{dy}{dt} = f(y, t)$ which can be manipulated into $\frac{dy}{dt} = \frac{h(t)}{g(y)}$

This is solved by $\int g(y)dy = \int h(t)dt + c$

Previous slide - simple example of this type

Example: Lotka-Volterra equations for predator-prey system.

Let F=number of foxes, R=number of rabbits at time t.

$$\frac{dR}{dt} = R(a - bF)$$
 and $\frac{dF}{dt} = F(cR - d) \Rightarrow \frac{dR}{dF} = \frac{R(a - bF)}{F(cR - d)}$

Hence

$$\int \frac{cR - d}{R} dR = \int \frac{a - bF}{F} dF$$

Or

$$cR - d \ln(R) = a \ln(F) - bF + k$$

Integrating Factor Method

Suppose
$$\frac{dy}{dx} + P(x)y = Q(x)$$

Given that,

$$\frac{d}{dx}\left(ye^{\int P(x)dx}\right) = \frac{dy}{dx}e^{\int P(x)dx} + P(x)ye^{\int P(x)dx}$$

If we multiply the original equation by $e^{\int P(x)dx}$ we get

$$e^{\int P(x)dx} \frac{dy}{dx} + P(x)ye^{\int P(x)dx} = \frac{d}{dx}(ye^{\int P(x)dx}) = Q(x)e^{\int P(x)dx}$$

Hence

$$ye^{\int P(x)dx} = \int Q(x)e^{\int P(x)dx}dx$$

So

$$y = e^{-\int P(x)dx} \int Q(x)e^{\int P(x)dx}dx$$

 $e^{\int P(x)dx}$ is the integrating factor

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Linear Equations with constant coefficients

Consider

$$RC\frac{dV}{dt} + V = E$$

The solution to these has two parts:

- 1. The complementary function is the solution of the homogenous equation.
- 2. The particular integral is any solution of the inhomogenous ODE.

Alternatively:

$$V_{ss}(V_{PI}) =$$
Steady state : final function of V

$$V_T(V_{CF}) = \text{transient}$$
: defines how V gets to V_{ss}

The complete solution is

$$V = V_{ss} + V_T \quad (V_{PI} + V_{CF})$$

Complementary Function - Transient Solution

Set RHS of equation to 0 to get (in general):

$$(a_n \frac{d^n V}{dt^n} + a_{n-1} \frac{d^{n-1} V}{dt^{n-1}} + \dots + a_1 \frac{dV}{dt} + a_0 V = 0$$

This has solution of the form $V=ke^{rt}$ for constants k and r. Substitute derivatives of V and replace $\frac{d^i V}{dt^i}$ by m^i , $i=1,\ldots,n$ to form the auxiliary equation:

$$(a_n m^n + a_{n-1} m^{n-1} + ... + a_1 m + a_0)V = 0$$

Each root r of this yields component in CF of the form ke^{rt} For the example:

$$RC\frac{dV}{dt} + V = 0 \Rightarrow RCmV + V = 0 \text{ or } RCm + 1 = 0$$

Clearly one root,

$$m=-rac{1}{RC},$$

SO

$$V_{CF} = ke^{-\frac{1}{RC}t}$$

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Particular Integral- Steady State Solution

Consider

$$RC\frac{dV}{dt} + V = E$$

The integrating factor is $e^{\int \frac{1}{RC}dt} = e^{\frac{t}{RC}}$, hence

$$V_{PI} = e^{-\frac{t}{RC}} \int \frac{E}{RC} e^{\frac{t}{RC}} dt = e^{-\frac{t}{RC}} \frac{E}{RC} RC e^{\frac{t}{RC}} = E$$

Therefore complete solution is

$$V = E + ke^{-\frac{t}{RC}}$$

If, for instance, V = 0 at time t = 0, then k = -E and

$$V = E - Ee^{-\frac{t}{RC}}$$

Trial solution method

Consider the second order differential equation of the form

$$a\frac{d^2O}{dt^2} + b\frac{dO}{dt} + cO = f(t)$$

As before, the complementary function for

$$a\frac{d^2O}{dt^2} + b\frac{dO}{dt} + ct = 0$$

is found using the roots of the auxiliary equation $am^2 + bm + c = 0$ Different forms are used if roots are real or complex

For the particular integral a suitable general form (say O = g(t)) based on the term f(t) is selected.

The associated constants of g(t) are then found by substitution in the original differential equation as

$$a\frac{d^2g}{dt^2} + b\frac{dg}{dg} + cg = f(t)$$

As before, general solution is complementary function plus particular integral. $^{27/54}$

Example

$$0.01\frac{d^2O}{dt^2} + \frac{dO}{dt} + 9O = 9$$

Aux Eqn $0.01m^2 + m + 9 = 0$

Factorise as (0.1m+9)(0.1m+1) = 0 So m = -90 or -10

So Complimentary Function (Transient Response) is

$$O_{CF} = Ae^{-90t} + Be^{-10t}$$

The RHS is a constant, so Particular Integral (Steady State

Solution) is of form O_{PI} =constant (k), say.

$$0.01\frac{d^2O_{PI}}{dt^2} + \frac{dO_{PI}}{dt} + 9O_{PI} = 0 + 0 + 9k = 9;$$

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Hence, k = 1.

$$\therefore O_{PI} = 1$$

General Solution is therefore $O = 1 + Ae^{-90t} + Be^{-10t}$

Particular Solution

General Solution is

$$O = 1 + Ae^{-90t} + Be^{-10t}$$

Suppose O and $\frac{dO}{dt} = 0$ at t = 0

$$\frac{dO}{dt} = -90Ae^{-90t} - 10Be^{-10t}$$

So at t = 0

$$0 = 1 + A + B$$

 $0 = -90A - 10B$

From 2nd equation, B = -9A

Hence 1st equation, 0 = 1+A-9A = 1-8A, so A = 1/8

Thus B = -9/8

Particular Solution is

$$O = 1 + \frac{1}{8}e^{-90t} - \frac{9}{8}e^{-10t}$$

Example with complex roots

$$\frac{1}{4}\frac{d^2O}{dt^2} + \frac{dO}{dt} + 10O = 10$$

Aux Eqn $\frac{1}{4}m^2 + m + 10 = 0$

So
$$m = \frac{-1 \pm \sqrt{1 - 4 \times 0.25 \times 10}}{0.5} = \frac{-1 \pm 3j}{0.5} = -2 \pm 6j$$

So

$$O_{CF} = Ae^{-2t}\cos(6t) + Be^{-2t}\sin(6t)$$

As before $O_{PI} = 1$ so general solution is

$$O = 1 + Ae^{-2t}\cos(6t) + Be^{-2t}\sin(6t)$$

Particular Solution

Have

$$O = 1 + Ae^{-2t}\cos(6t) + Be^{-2t}\sin(6t)$$

Suppose O and $\frac{dO}{dt} = 0$ at t = 0

$$\frac{dO}{dt} = e^{-2t} \frac{d}{dt} \left(A\cos(6t) + B\sin(6t) \right) - 2e^{-2t} \left(A\cos(6t) + B\sin(6t) \right)
= e^{-2t} \left(-6A\sin(6t) + 6B\cos(6t) \right) - 2e^{-2t} \left(A\cos(6t) + B\sin(6t) \right)
= e^{-2t} \left((6B - 2A)\cos(6t) - (6A + 2B)\sin(6t) \right)$$

So at t = 0

$$\begin{array}{c} 0=1+\text{A and }0\text{=}6\text{B-}2\text{A};\\ \text{so A}=\text{-}1\\ \text{and B}\text{=}-\frac{1}{3}; \end{array}$$

Therefore

$$O = 1 - e^{-2t}\cos(6t) - \frac{1}{3}e^{-2t}\sin(6t)$$

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Example with repeated roots

$$\frac{1}{36}\frac{d^2O}{dt^2} + \frac{dO}{dt} + 9O = 9$$

Aux Eqn $\frac{1}{36}m^2 + m + 9 = 0$

Factorise as $(\frac{1}{6}m+3)^2=0$ So m = -18

So Complimentary Function or Transient Response is

$$O_{CF} = (A + Bt)e^{-18t}$$

 $O_{PI}=1$ as before so general solution is

$$O = 1 + (A + Bt)e^{-18t}$$

Particular Solution

Have

$$O = 1 + (A + Bt)e^{-18t}$$

Suppose O and $\frac{dO}{dt}=0$ at t=0

$$\frac{dO}{dt} = -18(A + Bt)e^{-18t} + Be^{-18t}$$

So at t = 0

$$0 = 1 + A;$$

so $A = -1$
 $0 = -18A + B;$
so $B = -18$

Therefore

$$O = 1 - (1 + 18Bt)e^{-18t}$$

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f(t) exponential

For example, consider

$$0.01\frac{d^2O}{dt^2} + \frac{dO}{dt} + 9O = 9e^{-5t}$$

Complimentary Function will be the same as before

Particular Integral is of the form $O_{PI} = Ce^{-5t}$

$$0.01 \frac{d^{2}O_{PI}}{dt^{2}} + \frac{dO_{PI}}{dt} + 9O_{PI} = 0.01 \times 25Ce^{-5t} - 5Ce^{-5t} + 9Ce^{-5t}$$

$$= 4.25Ce^{-5t}$$

$$9e^{-5t} = 4.25Ce^{-5t}$$

$$\therefore C = \frac{9e^{-5t}}{4.25e^{-5t}} = \frac{9}{4.25} = 2.1176$$

General Solution is therefore

$$O = 2.1176e^{-5t} + Ae^{-90t} + Be^{-10t}$$

f(t) exponential-another example

Now consider,

$$0.01\frac{d^2O}{dt^2} + \frac{dO}{dt} + 9O = 9e^{-10t}$$

Here the RHS has the same power as comp. function. So if try

$$O_{PI} = Ce^{-10t}$$

$$\begin{array}{l} 0.01 \frac{d^2 O_{PI}}{dt^2} + \frac{d O_{PI}}{dt} + 9 O_{PI} = 0.01 (100 C e^{-10t}) - 10 C e^{-10t} + 9 C e^{-10t} \\ = 0 C e^{-10t} \end{array}$$

As we can't have 0C = 9, instead try $O_{PI} = Cte^{-10t}$ to get

$$\frac{dO_{PI}}{dt} = Ce^{-10t} - 10Cte^{-10t} = C(1 - 10t)e^{-10t}$$

$$\frac{d^2O_{PI}}{dt^2} = -10Ce^{-10t} - 10C(1 - 10t)e^{-10t} = C(100t - 20)e^{-10t}$$

$$0.01\frac{d^2O_{PI}}{dt^2} + \frac{dO_{PI}}{dt} + 9O_{PI}$$

$$= 0.01C(100t - 20)e^{-10t} + C(1 - 10t)e^{-10t} + 9Cte^{-10t}$$

$$= C(t - 0.2 + 1 - 10t + 9t)e^{-10t} = 0.8Ce^{-10t}$$

So 0.8C = 9, or $O_{PI} = \frac{45}{4} t e^{-10t}$

Numerical Solution of ODEs

R can be used to provide numerical solutions to initial value problems for some types of ODE's.

It has an add-on package 'deSolve' consisting of functions that provide interfaces to various FORTRAN functions and C-implementation of solvers of the Runge-Kutta family.

Syntax:

Return value of func must be a list.

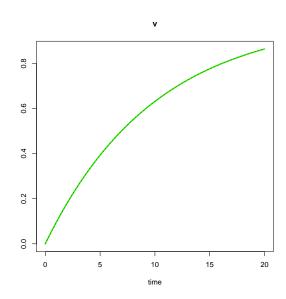
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Example:

$$RC\frac{dV}{dt} + V = E$$

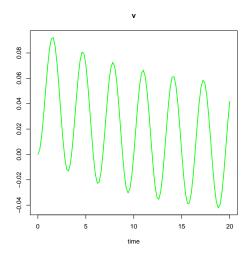
```
library(deSolve)
```

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Another Example

$$RC\frac{dV}{dt} + V = E\sin(\omega t) \implies \frac{dV}{dt} = \frac{(E \times \sin(\omega t) - V)}{RC}$$



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Second Order Systems

R can also solve second order systems by re-organising it into two first order equations

Consider

$$a\frac{d^2O}{dt^2} + b\frac{dO}{dt} + cO = f(t)$$

If we let $v = \frac{dO}{dt}$ so that $\frac{d^2O}{dt^2} = \frac{dv}{dt}$

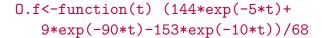
We can then write the ODE as

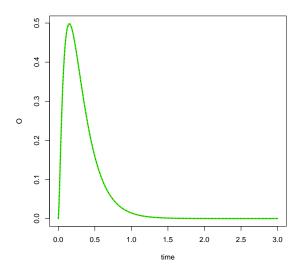
$$a\frac{d^2O}{dt^2} + b\frac{dO}{dt} + cO = f(t) \Rightarrow a\frac{dv}{dt} + bv + cO = f(t)$$

In other words,

$$\frac{d}{dt}\left(\left[\begin{array}{c}O\\v\end{array}\right]\right) = \left[\begin{array}{c}v\\\frac{f(t)-cO-bv}{a}\end{array}\right]$$

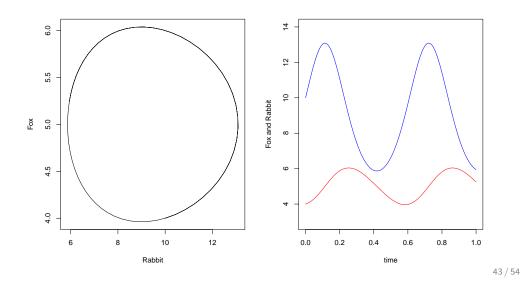
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Fox and Rabbit example

$$\frac{dR}{dt} = R(a - bF)$$
 and $\frac{dF}{dt} = F(cR - d)$



Partial Differentiation

Suppose function f depends upon variables x, y, z

Partial differentiation is where differentiate wrt to one variable, assuming the other variables are constant.

Use ∂ rather than d to indicate partial differentiation

$$eg f = x^2 + xsin(3y) + yz$$

►
$$\frac{\partial f}{\partial x} = 2x + \sin(3y)$$

► $\frac{\partial f}{\partial y} = 3x \cos(3y) + z$

$$ightharpoonup \frac{\partial f}{\partial z} = y$$

Note notation on second derivatives

$$\frac{\partial^2 f}{\partial x^2} = 2;$$
 $\frac{\partial^2 f}{\partial x \partial y} = 3\cos(3y);$ $\frac{\partial^2 f}{\partial y \partial x} = 3\cos(3y)$

Differentiation of Matrices

If $\mathbf{x} = [x_1, x_2, ..., x_n]^T$ and L(x) is a scalar function, then

$$\mathbf{L_x} = \frac{\partial \mathbf{L}}{\partial \mathbf{x}} = \left[\frac{\partial L}{\partial x_1}, \frac{\partial L}{\partial x_2}, ..., \frac{\partial L}{\partial x_n} \right]$$

The gradient of L(x) is a column vector : $\nabla_{\mathbf{x}} \mathbf{L} = \frac{\partial \mathbf{L}^T}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial L}{\partial x_1} \\ \frac{\partial L}{\partial x_2} \\ \vdots \\ \frac{\partial L}{\partial x_n} \end{bmatrix}$

The second derivative of L(x) is an n*n matrix, called the Hessian matrix

$$\mathbf{L}_{\mathbf{xx}} = \begin{bmatrix} \frac{\partial^2 L}{\partial x_1^2} & \cdots & \frac{\partial^2 L}{\partial x_1 \partial x_n} \\ \vdots & & \vdots \\ \frac{\partial^2 L}{\partial x_n \partial x_1} & \cdots & \frac{\partial^2 L}{\partial x_n^2} \end{bmatrix}$$

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More On Matrix Calculus

If $\mathbf{x} = [x_1, x_2, ..., x_n]^T$ and f(x) is a differentiable vector function

$$\mathbf{f} = [f_1, f_2, \cdots, f_m]^T$$

Then the partial differential of f wrt x is an $m \times n$ matrix called the Jacobian matrix

$$\mathbf{f_x} = \frac{\partial \mathbf{f}}{\partial \mathbf{x}} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \vdots & & \vdots \\ \frac{\partial f_m}{\partial x_1} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}$$

If f is a function of an $m \times n$ matrix **A**

$$\frac{\partial f}{\partial \mathbf{A}} = \begin{bmatrix} \frac{\partial f}{\partial a_{11}} & \dots & \frac{\partial f}{\partial a_{1m}} \\ \vdots & & \vdots \\ \frac{\partial f}{\partial a_{n1}} & \dots & \frac{\partial f}{\partial a_{nm}} \end{bmatrix}$$

Differentiate matrix wrt scalar

If y is a vector function of t, then

$$\mathbf{y}(t) = \left[egin{array}{c} y_1(t) \ dots \ y_n(t) \end{array}
ight] \Rightarrow rac{d\mathbf{y}}{dt} = \left[egin{array}{c} rac{dy_1}{dt} \ dots \ rac{dy_n}{dt} \end{array}
ight]$$

If **A** is a matrix function of t, then

$$\mathbf{A}(t) = \begin{bmatrix} a_{11}(t) & a_{1m}(t) \\ \vdots & \dots & \vdots \\ a_{n1}(t) & a_{nm}(t) \end{bmatrix} \Rightarrow \frac{d\mathbf{A}}{dt} = \begin{bmatrix} \frac{da_{11}}{dt} & \frac{da_{1m}}{dt} \\ \vdots & \dots & \vdots \\ \frac{da_{n1}}{dt} & \frac{da_{nm}}{dt} \end{bmatrix}$$

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Some Rules

For $n \times n$ matrix **A**, and n-dimensional vectors x and y:

$$\frac{\partial}{\partial x}(\mathbf{A}x) = \mathbf{A}$$

$$\frac{\partial}{\partial x}(x^T y) = \frac{\partial}{\partial x}(y^T x) = y^T \qquad \frac{\partial}{\partial x}(x^T \mathbf{A}y) = \frac{\partial}{\partial x}(y^T \mathbf{A}x) = y^T \mathbf{A}$$

$$\frac{\partial}{\partial x}(x^T \mathbf{A}x) = x^T (\mathbf{A} + \mathbf{A}^T) \qquad \frac{\partial^2}{\partial x^2}(x^T \mathbf{A}x) = \mathbf{A} + \mathbf{A}^T$$

If matrix **A** is symmetric:

$$\frac{\partial}{\partial x}(x^T \mathbf{A} x) = 2x^T \mathbf{A}$$
$$\frac{\partial^2}{\partial x^2}(x^T \mathbf{A} x) = 2\mathbf{A}$$

Linearisation

Approximating a function by a straight line at a point

For f(t) approx at t = a, the straight line has gradient of f(t) at t = a

Can show that straight line defined by

$$f(t) \approx f(a) + (t - a) \times f'(a)$$

An extension of this : approximate a function by a quadratic at t=a

Here approximation has same gradient and second derivative at a.

$$f(t) \approx f(a) + (t-a) \times f'(a) + \frac{(t-a)^2}{2!} \times f''(a)$$

The n^{th} order model, the n^{th} order Taylor's series, is :

$$f(t) \approx f(a) + (t-a) \times f'(a) + \frac{(t-a)^2}{2!} \times f''(a) + \dots + \frac{(t-a)^n}{n!} \times f^n(a)$$

Multi Variable Taylors Series

Suppose f(x) is a differentiable scalar function where $\mathbf{x} = [x_1, x_2, ..., x_n]^T$ then its partial derivative is

$$\frac{\partial f}{\partial \mathbf{x}} = \mathbf{f}_{\mathbf{x}} = \left[\frac{\partial f}{\partial x_1} \frac{\partial f}{\partial x_2} ... \frac{\partial f}{\partial x_n} \right]$$

The gradient vector of f(x) is

$$abla \mathbf{f} = f_{x}^{T} = \left[egin{array}{c} rac{\partial f}{\partial x_{1}} \\ rac{\partial f}{\partial x_{2}} \\ dots \\ rac{\partial f}{\partial x_{n}} \end{array}
ight]$$

The values at which $f_x = 0$ are called stationary points.

The Hessian matrix of f(x) is

$$f_{xx} = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \vdots & & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

Assuming f has first and second order partial derivatives, the second order Taylor series expansion of f about some point \mathbf{a} (in n-dimensions) is approximately

$$f(\mathbf{x}) = f(\mathbf{a}) + f_{\mathbf{x}}(\mathbf{x} - \mathbf{a}) + \frac{(\mathbf{x} - \mathbf{a})^T}{2!} f_{\mathbf{x}\mathbf{x}}(\mathbf{x} - \mathbf{a})$$

Here the partial derivatives $f_{\mathbf{x}}$ and $f_{\mathbf{xx}}$ are computed at $\mathbf{x} = \mathbf{a}$.

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Optimisation

Just as the differentiation of f(x) wrt x can be used to find local maxima or minima, and hence work out optimum values, the concept can be extended for functions of many variables.

For some vector x, it is determined where f_x is 0.

The function f has a maximum if Hessian f_{xx} is negative definite and a minimum if f_{xx} is positive definite.

A minimum occurs, for instance, if all eigenvalues of Hessian f_{xx} at the local optima are positive (see matrix material)

If Hessian has positive and negative eigenvalues, it is a saddle point Similar to turning points for functions of one variable

Example 1

$$f(x_1, x_2) = x_1^2 + x_2^2$$

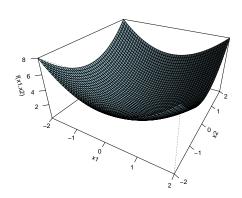
$$\frac{\partial f}{\partial x} = f_x = [2x_1, 2x_2]$$

A critical point is therefore [0,0]

Hessian at [0,0] is $f_{xx} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$, whose eigenvalues are 2,2

Clearly $f_{xx}>0$, $f_x=0$, so f has a minimum at (0,0)-plot confirms

$$f(x_1, x_2) = x_1^2 + x_2^2$$



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Example 2

$$f(x_1, x_2) = x_1^2 + x_2^2 \frac{\partial f}{\partial x} = f_x = [2x_1 - 2x_2]$$

$$f(x_1, x_2) = x_1^2 + x_2^2 \frac{\partial f}{\partial x} = f_x = [2x_1 - 2x_2]$$
Hessian $f_{xx} = \begin{bmatrix} 2 & 0 \\ 0 & -2 \end{bmatrix}$, eigenvalues 2,-2

Hence we have a saddle point

$$f(x_1, x_2) = x_1^2 - x_2^2$$

