Mathematical Methods

for Computer Science

Peter Harrison and Jeremy Bradley
Email: {pgh,jb}@doc.ic.ac.uk

Web page: http://www.doc.ic.ac.uk/∼jb/teaching/145/

Room 372. Department of Computing, Imperial College London

Produced with prosper and LaTeX

Differential Equations: Contents

- What are differential equations used for?
- Useful differential equation solutions:
  - 1st order, constant coefficient
  - 1st order, variable coefficient
  - 2nd order, constant coefficient
  - Coupled ODEs, 1st order, constant coefficient
- Useful for:
  - Performance modelling (3rd year)
  - Simulation and modelling (3rd year)

Differential Equations: Background

- Used to model how systems evolve over time:
  - e.g. computer systems, biological systems, chemical systems
- Terminology:
  - Ordinary differential equations (ODEs) are *first order* if they contain a $\frac{\mathrm{d}y}{\mathrm{d}x}$ term but no higher derivatives
  - ODEs are *second order* if they contain a $\frac{\mathrm{d}^2y}{\mathrm{d}x^2}$ term but no higher derivatives

Ordinary Differential Equations

- First order, constant coefficients:
  - For example, $2\frac{\mathrm{d}y}{\mathrm{d}x} + y = 0 \quad (*)$
  - Try: $y = e^{mx}$

    $\Rightarrow 2me^{mx} + e^{mx} = 0$

    $\Rightarrow e^{mx}(2m+1) = 0$

    $\Rightarrow e^{mx} = 0$ or $m = -\frac{1}{2}$
  - $e^{mx} \neq 0$ for any x, m. Therefore $m = -\frac{1}{2}$
  - General solution to $(*)$:

$$y = Ae^{-\frac{1}{2}x}$$

Ordinary Differential Equations

- First order, variable coefficients of type:

$$\frac{\mathrm{d}y}{\mathrm{d}x} + f(x)y = g(x)$$

- Use *integrating factor* (IF): $e^{\int f(x)\,\mathrm{d}x}$
  - For example: $\frac{\mathrm{d}y}{\mathrm{d}x} + 2xy = x \quad (*)$
  - Multiply throughout by IF: $e^{\int 2x\,\mathrm{d}x} = e^{x^2}$

  $\Rightarrow e^{x^2}\frac{\mathrm{d}y}{\mathrm{d}x} + 2xe^{x^2}y = xe^{x^2}$
  $\Rightarrow \frac{\mathrm{d}}{\mathrm{d}x}(e^{x^2}y) = xe^{x^2}$
  $\Rightarrow e^{x^2}y = \frac{1}{2}e^{x^2} + C$ So, $y = Ce^{-x^2} + \frac{1}{2}$

Ordinary Differential Equations

- Second order, constant coefficients:
  - For example, $\frac{\mathrm{d}^2y}{\mathrm{d}x^2} + 5\frac{\mathrm{d}y}{\mathrm{d}x} + 6y = 0 \quad (*)$
  - Try: $y = e^{mx}$

  $\Rightarrow m^2e^{mx} + 5me^{mx} + 6e^{mx} = 0$
  $\Rightarrow e^{mx}(m^2 + 5m + 6) = 0$
  $\Rightarrow e^{mx}(m + 3)(m + 2) = 0$
  - $m = -3, -2$
  - i.e. two possible solutions
  - General solution to $(*)$:

$$y = Ae^{-2x} + Be^{-3x}$$

Ordinary Differential Equations

- Second order, constant coefficients:
  - If $y = f(x)$ and $y = g(x)$ are distinct solutions to $(*)$
  - Then $y = Af(x) + Bg(x)$ is also a solution of $(*)$ by following argument:
    - $\frac{\mathrm{d}^2}{\mathrm{d}x^2}(Af(x) + Bg(x)) + 5\frac{\mathrm{d}}{\mathrm{d}x}(Af(x) + Bg(x)) + 6(Af(x) + Bg(x)) = 0$
    - $A\underbrace{\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}f(x) + 5\frac{\mathrm{d}}{\mathrm{d}x}f(x) + 6f(x)\right)}_{=0} + B\underbrace{\left(\frac{\mathrm{d}^2}{\mathrm{d}x^2}g(x) + 5\frac{\mathrm{d}}{\mathrm{d}x}g(x) + 6g(x)\right)}_{=0} = 0$

Ordinary Differential Equations

- Second order, constant coefficients (repeated root):
  - For example, $\frac{\mathrm{d}^2y}{\mathrm{d}x^2} - 6\frac{\mathrm{d}y}{\mathrm{d}x} + 9y = 0 \quad (*)$
  - Try: $y = e^{mx}$

  $\Rightarrow m^2e^{mx} - 6me^{mx} + 9e^{mx} = 0$
  $\Rightarrow e^{mx}(m^2 - 6m + 9) = 0$
  $\Rightarrow e^{mx}(m - 3)^2 = 0$
  - $m = 3$ (twice)
  - General solution to $(*)$ for repeated roots:

$$y = (Ax + B)e^{3x}$$

Applications: Coupled ODEs

- Coupled ODEs are used to model massive state-space physical and computer systems
- Coupled Ordinary Differential Equations are used to model:
  - chemical reactions and concentrations
  - biological systems
  - epidemics and viral infection spread
  - large state-space computer systems (e.g. distributed publish-subscribe systems

Coupled ODEs

- Coupled ODEs are of the form:

$$\begin{cases} \frac{\mathrm{d}y_1}{\mathrm{d}x} &= ay_1 + by_2 \\ \frac{\mathrm{d}y_2}{\mathrm{d}x} &= cy_1 + dy_2 \end{cases}$$

- If we let $\vec{y} = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}$, we can rewrite this as:

$$\begin{pmatrix} \frac{\mathrm{d}y_1}{\mathrm{d}x} \\ \frac{\mathrm{d}y_2}{\mathrm{d}x} \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix} \text{ or } \frac{\mathrm{d}\vec{y}}{\mathrm{d}x} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \vec{y}$$

Coupled ODE solutions

- For coupled ODE of type: $\frac{\mathrm{d}\vec{y}}{\mathrm{d}x} = A\vec{y} \quad (*)$
- Try $\vec{y} = \vec{v}e^{\lambda x}$ so, $\frac{\mathrm{d}\vec{y}}{\mathrm{d}x} = \lambda\vec{v}e^{\lambda x}$
- But also $\frac{\mathrm{d}\vec{y}}{\mathrm{d}x} = A\vec{y}$, so $A\vec{v}e^{\lambda x} = \lambda\vec{v}e^{\lambda x}$
- Now solution of $(*)$ can be derived from an eigenvector solution of $A\vec{v} = \lambda\vec{v}$
- For n eigenvectors $\vec{v}_1, \dots, \vec{v}_n$ and corresp. eigenvalues $\lambda_1, \dots, \lambda_n$: general solution of $(*)$ is $\vec{y} = B_1\vec{v}_1e^{\lambda_1 x} + \cdots + B_n\vec{v}_ne^{\lambda_n x}$

Coupled ODEs: Example

- Example coupled ODEs:

$$\begin{cases} \frac{\mathrm{d}y_1}{\mathrm{d}x} &= 2y_1 + 8y_2 \\ \frac{\mathrm{d}y_2}{\mathrm{d}x} &= 5y_1 + 5y_2 \end{cases}$$

- So $\frac{\mathrm{d}\vec{y}}{\mathrm{d}x} = \begin{pmatrix} 2 & 8 \\ 5 & 5 \end{pmatrix} \vec{y}$
- Require to find eigenvectors/values of

$$A = \begin{pmatrix} 2 & 8 \\ 5 & 5 \end{pmatrix}$$

Coupled ODEs: Example

- Eigenvalues of A: $\left|\begin{pmatrix} 2-\lambda & 8 \\ 5 & 5-\lambda \end{pmatrix}\right| =$
  $\lambda^2 - 7\lambda - 30 = (\lambda - 10)(\lambda + 3) = 0$
- Thus eigenvalues $\lambda = 10, -3$
- Giving:
  $\lambda_1 = 10, \vec{v}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}; \lambda_2 = -3, \vec{v}_2 = \begin{pmatrix} 8 \\ -5 \end{pmatrix}$
- Solution of ODEs:
  $\vec{y} = B_1 \begin{pmatrix} 1 \\ 1 \end{pmatrix} e^{10x} + B_2 \begin{pmatrix} 8 \\ -5 \end{pmatrix} e^{-3x}$

Partial Derivatives

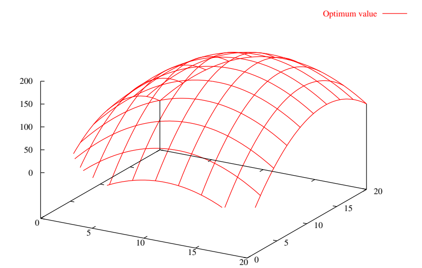
- Used in (amongst others):
  - Computational Techniques (2nd Year)
  - Optimisation (3rd Year)
  - Computational Finance (4th Year)

Differentiation Contents

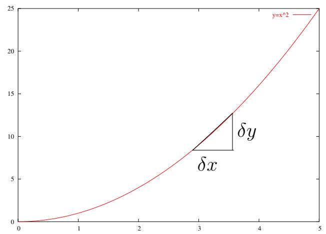
- What is a (partial) differentiation used for?
- Useful (partial) differentiation tools:
  - Differentiation from first principles
  - Partial derivative chain rule
  - Derivatives of a parametric function
  - Multiple partial derivatives

Optimisation

- Example: look to find best predicted gain in portfolio given different possible share holdings in portfolio



Differentiation



- Gradient on a curve $f(x)$ is approximately:

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

Definition of derivative

- The derivative at a point x is defined by:

$$\frac{\mathrm{d}f}{\mathrm{d}x} = \lim_{\delta x \to 0} \frac{f(x+\delta x) - f(x)}{\delta x}$$

- Take $f(x) = x^n$
  - We want to show that:

$$\frac{\mathrm{d}f}{\mathrm{d}x} = nx^{n-1}$$

Derivative of x^n

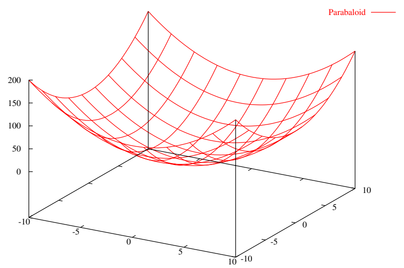
- $\frac{\mathrm{d}f}{\mathrm{d}x} = \lim_{\delta x \to 0} \frac{f(x+\delta x)-f(x)}{\delta x}$

$$
\begin{aligned}
&= \lim_{\delta x \to 0} \frac{(x+\delta x)^n - x^n}{\delta x} \\
&= \lim_{\delta x \to 0} \frac{\sum_{i=0}^{n} \binom{n}{i} x^{n-i} \delta x^i - x^n}{\delta x} \\
&= \lim_{\delta x \to 0} \frac{\sum_{i=1}^{n} \binom{n}{i} x^{n-i} \delta x^i}{\delta x} \\
&= \lim_{\delta x \to 0} \sum_{i=1}^{n} \binom{n}{i} x^{n-i} \delta x^{i-1} \\
&= \lim_{\delta x \to 0} \Big(\binom{n}{1} x^{n-1} + \underbrace{\sum_{i=2}^{n} \binom{n}{i} x^{n-i} \delta x^{i-1}}_{\to 0 \text{ as } \delta x \to 0} \Big) \\
&= \frac{n!}{1!(n-1)!} x^{n-1} = nx^{n-1}
\end{aligned}
$$

Partial Differentiation

- Ordinary differentiation $\frac{\mathrm{d}f}{\mathrm{d}x}$ applies to functions of one variable i.e. $f \equiv f(x)$
- What if function f depends on one or more variables e.g. $f \equiv f(x_1, x_2)$
- Finding the derivative involves finding the gradient of the function by varying one variable and keeping the others constant
- For example for $f(x,y) = x^2 y + xy^3$; partial derivatives are written:
  - $\frac{\partial f}{\partial x} = 2xy + y^3$ and $\frac{\partial f}{\partial y} = x^2 + 3xy^2$

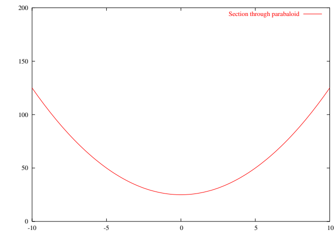
Partial Derivative: example



- $f(x, y) = x^2 + y^2$

Partial Derivative: example

- $f(x, y) = x^2 + y^2$
  - Fix $y = k \Rightarrow g(x) = f(x, k) = x^2 + k^2$
  - Now $\frac{\mathrm{d}g}{\mathrm{d}x} = \frac{\partial f}{\partial x} = 2x$



Further Examples

- $f(x, y) = (x + 2y^3)^2$
  $\Rightarrow \frac{\partial f}{\partial x} = 2(x + 2y^3)\frac{\partial}{\partial x}(x + 2y^3) = 2(x + 2y^3)$
- If x and y are themselves functions of t then

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\partial f}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}t} + \frac{\partial f}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}t}$$

- So if $f(x, y) = x^2 + 2y$ where $x = \sin t$ and $y = \cos t$ then:
  - $\frac{\mathrm{d}f}{\mathrm{d}t} = 2x\cos t - 2\sin t = 2\sin t(\cos t - 1)$

Extended Chain Rule

- If f is a function of x and y where x and y are themselves functions of s and t then:
  - $\frac{\partial f}{\partial s} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial s} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial s}$
  - $\frac{\partial f}{\partial t} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial t} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial t}$
- which can be expressed as a matrix equation:

$$\begin{pmatrix} \frac{\partial f}{\partial s} \\ \frac{\partial f}{\partial t} \end{pmatrix} = \begin{pmatrix} \frac{\partial x}{\partial s} & \frac{\partial y}{\partial s} \\ \frac{\partial x}{\partial t} & \frac{\partial y}{\partial t} \end{pmatrix} \begin{pmatrix} \frac{\partial f}{\partial x} \\ \frac{\partial f}{\partial y} \end{pmatrix}$$

- Useful for changes of variable e.g. to polar coordinates

Jacobian

- The modulus of this matrix is called the *Jacobian*:

$$J = \begin{vmatrix} \frac{\partial x}{\partial s} & \frac{\partial y}{\partial s} \\ \frac{\partial x}{\partial t} & \frac{\partial y}{\partial t} \end{vmatrix}$$

- Just as when performing a substitution on the integral:

$$\int f(x)\,\mathrm{d}x$$

  we would use: $\mathrm{d}u \equiv \frac{\mathrm{d}f(x)}{\mathrm{d}x}\,\mathrm{d}x$
- So if converting between multiple variables in an integration, we would use $\mathrm{d}u \equiv J\mathrm{d}x$.

Formal Definition

- Similar to ordinary derivative. For a two variable function $f(x,y)$:

$$\frac{\partial f}{\partial x} = \lim_{\delta x \to 0} \frac{f(x+\delta x, y) - f(x,y)}{\delta x}$$

- and in the y-direction:

$$\frac{\partial f}{\partial y} = \lim_{\delta y \to 0} \frac{f(x, y+\delta y) - f(x,y)}{\delta y}$$

Further Notation

- Multiple partial derivatives (as for ordinary derivatives) are expressed:
  - $\frac{\partial^2 f}{\partial x^2}$ is the second partial derivative of f
  - $\frac{\partial^n f}{\partial x^n}$ is the nth partial derivative of f
  - $\frac{\partial^2 f}{\partial x \partial y}$ is the partial derivative obtained by first partial differentiating by y and then x
  - $\frac{\partial^2 f}{\partial y \partial x}$ is the partial derivative obtained by first partial differentiating by x and then y
- If $f(x,y)$ is a *nice* function then: $\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x}$