MSc Computational Methods in Ecology and Evolution: Maths for Biology

Differentiation, limits, & Taylor series

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Information needed for this tutorial:

1. You will be asked to calculate limits of the form $\lim_{x\to a}\{f(x)\}$. Note that limits of the sum of a number of terms is a sum of their limits:

$$\lim_{x\to a}\{f(x)+g(x)\} = \lim_{x\to a}\{f(x)\} + \lim_{x\to a}\{g(x)\}\,.$$

   Using this rule you can calculate limits of products, by expanding out brackets and evaluating the limit of each term.

2. The first principles (limit) definition of a derivative is

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

3. A Taylor series is a series expansion of a function $f(x)$ about some specific value a in terms of monomials of increasing order:

$$f(x-a) = f(a) + \left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x=a}(x-a) + \left.\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}\right|_{x=a}(x-a)^2 + \left.\frac{\mathrm{d}^3 f}{\mathrm{d}x^3}\right|_{x=a}(x-a)^3 + ...$$

   .

   Typically, we want to expand about $x = 0$ ($a = 0$), which gives

$$f(x) = f(0) + \left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x=0}x + \left.\frac{\mathrm{d}^2 f}{\mathrm{d}x^2}\right|_{x=0}x^2 + \left.\frac{\mathrm{d}^3 f}{\mathrm{d}x^3}\right|_{x=0}x^3 + ...$$

   .

4. When asked to specify a Taylor series in x to a certain order n the $O(x^m)$ notation is used to signify the remaining terms starting with the highest *non-zero* term of order $m > n$.

5. Useful Taylor series about $x = 0$ to know (specified to 5^{th} order)

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \frac{x^4}{4!} + \frac{x^5}{5!} + O(x^6)$$

$$\sin x = x - \frac{x^3}{3!} + \frac{x^5}{5!} + O(x^7)$$

$$\cos x = 1 - \frac{x^2}{2!} + \frac{x^4}{4!} + O(x^6)$$

QUESTION 1

Differentiation of x^2 as change in area

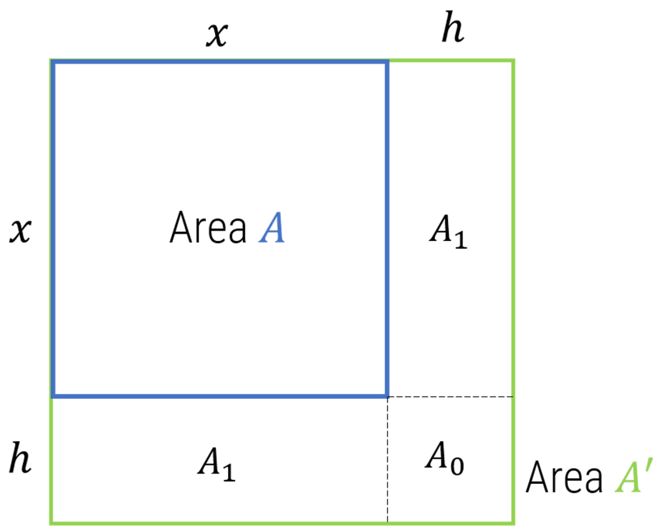

FIG. 1. Differentiating x^2

a) The area of the smaller square is $A = x^2$. What is the area of the bigger square A' in terms of the areas A, A_0, A_1?

b) What is the area of the bigger square A' in terms of x and h?

c) Expand out this expression for A' and identify each term with areas A, A_0, xA_1.

d) Evaluate all these areas for $x = 1$ and $h = 0.3$.

e) i) Show that the change in area with respect to the change in length is

$$\frac{\Delta A}{\Delta x} = \frac{A' - A}{h} = 2x + h$$

and ii) evaluate $\frac{\Delta A}{\Delta x}$ for $x = 1$ and $h = 0.3$.

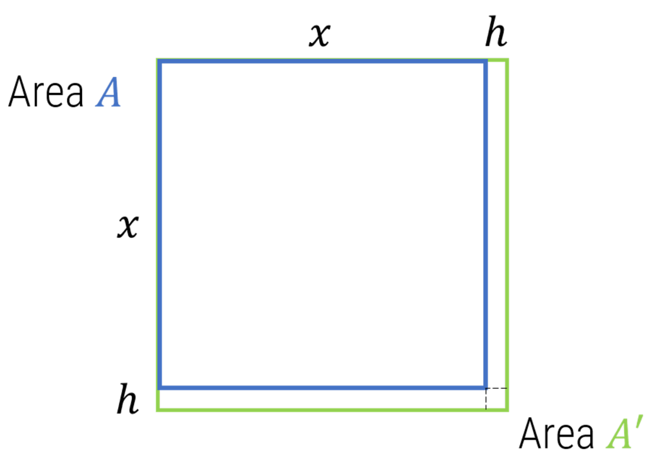

FIG. 2. Smaller h

f) Now imagine the two squares are more similar in size as in diagram above; i) calculate the different areas again and evaluate $\frac{\Delta A}{\Delta x}$ for $x = 1$ and $h = 0.05$. ii) Repeat for $x = 1$ and $h = 10^(- 6)$.

g) This demonstrates that

$$\lim_{h \to 0} \left\{ \frac{\Delta A}{\Delta x} \right\} = \frac{\mathrm{d}A}{\mathrm{d}x} = \frac{\mathrm{d}x^2}{\mathrm{d}x} = 2x;$$

which parts of the diagram or which areas does this $2x$ correspond? Why is there a coefficient 2? Why are the other terms not important?

QUESTION 2

Derivatives of trigonometric functions

a) Use the first principles (limit) definition of a derivative and the Taylor series expansion of the exponential function to show

$$\frac{\mathrm{d}e^{\alpha x}}{\mathrm{d}x} = \lim_{h\to 0}\left\{\frac{e^{\alpha(x+h)} - e^{\alpha x}}{h}\right\} = \alpha e^{\alpha x}$$

b) Using Eulers formula it can be shown that

$$\cos x = \frac{1}{2}(e^{ix} + e^{-ix})$$

$$\sin x = \frac{1}{2i}(e^{ix} - e^{-ix}).$$

Using these results show that

$$\frac{\mathrm{d}\sin x}{\mathrm{d}x} = \cos x$$

$$\frac{\mathrm{d}\cos x}{\mathrm{d}x} = -\sin x$$

(Hint: $\frac{1}{i} = -i$)

c) Use the product (or quotient) rule and chain rule to show that

$$\frac{\mathrm{d}\cot x}{\mathrm{d}x} = -\csc^2 x$$

where $\cot x = 1/\tan x$ and $\csc x = \frac{1}{\sin x}$ (N.B. Not the same as $\sin^{-1} x = \arcsin x$).
(Hint: $\sin^2 x + \cos^2 x = 1$)

QUESTION 3

Properties of the Gaussian function

The Gaussian function $y = e^{-x^2}$ is ubiquitous in statistics and probability theory, as it describes the Normal/Gaussian distribution.

a) Plot/sketch this function and indicate values x^* for which $\frac{\mathrm{d}y}{\mathrm{d}x} = 0$ (there is one obvious value of x^* where $\frac{\mathrm{d}y}{\mathrm{d}x} = 0$, and two less obvious values).

b) Sketch $\frac{\mathrm{d}y}{\mathrm{d}x}$ qualitatively. (Hint: The Gaussian is a symmetric/even function ($f(-x) = f(x)$) and so its derivative will be an anti-symmetric/odd function ($f'(-x) = -f'(x)$) — in other words the derivative of a Gaussian should be equal and opposite in sign when reflected about the y-axis)

c) Using the chain rule, show $\frac{\mathrm{d}y}{\mathrm{d}x} = -2xe^{-x^2}$, and plot your result; verify that your sketch in b) is qualitatively accurate.

d) Solve $\frac{\mathrm{d}y}{\mathrm{d}x} = 0$ and verify your answer agrees with the answer from a).

e) Which solution x^* of $\frac{\mathrm{d}y}{\mathrm{d}x} = 0$ corresponds to where y is at maximum. Argue qualitatively why this must be a maximum from the plot of $\frac{\mathrm{d}y}{\mathrm{d}x}$.

f) We can show this mathematically, by examining the *curvature* of y, which is defined to be the 2nd derivative $\frac{\mathrm{d}^2y}{\mathrm{d}x^2}$. Show that $\frac{\mathrm{d}^2y}{\mathrm{d}x^2} = 2e^{-x^2}(x^2 - 1)$ and that the curvature is negative at the point x^* where y is maximum; why does this mean y is at maximum?

QUESTION 4

Taylor series

a) i) Use the Taylor series of $\sin\theta$ to show

$$\lim_{\theta\to 0}\left\{\frac{\sin\theta}{\theta}\right\} = 1$$

Compare this to simply evaluating $\frac{\sin\theta}{\theta}$ at $\theta = 0$ is it even possible to evaluate this?

ii) Plot $\frac{\sin\theta}{\theta}$ and verify that it asymptotes to 1 as $\theta \to 0$.

b) The following formula is the probability of fixation of a mutant with selective advantage s and initial frequency $1/N$ in a population of N haploid individuals (Kimura, Genetics, 1962)

$$p_{fix} = \frac{1 - e^{-2s}}{1 - e^{-2Ns}}.$$

i) Show using the Taylor expansion of the exponential function that

$$\lim_{s\to 0}\{p_{fix}\} = \frac{1}{N},$$

which is the probability of fixation of a neutral mutant.

ii) Plot p_{fix} vs s for $0 < s \leq 0.1$ on a log-linear scale with $N = 10$ and $N = 100$ and verify that the y-intercept is $1/N$.

c) Discrete time and continuous time evolutionary models use two different definitions of fitness, the *Wrightian* fitness w and *Malthusian* fitness f, which are related by $f = \ln(w)$. The Wrightian fitness is often described in terms of the selective advantage s of a mutant, where $w = 1 + s$.

i) Show the Taylor series expansion of $f(s) = \ln(1 + s)$ to 3rd order about $s = 0$ is

$$\ln(1+s) = s - \frac{1}{2}s^2 + \frac{1}{3}s^3 + O(s^4)$$

ii) Using this result, show that the Malthusian fitness difference (compared to wild type) is equivalent to the selective advantage s, when $|s| \ll 1$, by showing

$$f = \ln(w) = \ln(1+s) \approx s$$

(Hint: when $s \ll 1$, consider how big is s^2 compared to s, and how big is s^3 compared to s^2, and so on)

ii) Plot $\ln(1 + s)$ and s for $-0.5 \leq s \leq 0.5$ to verify this approximation works well for $|s| \ll 1$.

d) The hyperbolic sine and cosine are part of a group of functions (hyperbolic functions), which are analogous to the trigonometric sine and cosine, but for geometry on the unit hyperbola $x^2 - y^2 = 1$, instead of on the unit circle $(x^2 + y^2 = 1)$. They have many applications including solutions to certain differential equations. They are defined by

$$\cos i\theta = \cosh\theta = \frac{1}{2}(e^{\theta} + e^{-\theta})$$

$$\sin i\theta = \sinh\theta = \frac{1}{2}(e^{\theta} - e^{-\theta})$$

i) Using these equations show that

$$\frac{\mathrm{d}\sinh\theta}{\mathrm{d}\theta} = \cosh\theta$$

$$\frac{\mathrm{d}\cosh\theta}{\mathrm{d}\theta} = \sinh\theta$$

ii) Show that the Taylor series for $\sinh\theta$ to 3rd order is

$$\sinh\theta = \theta + \frac{\theta^3}{6} + O(\theta^5)$$

iii) Now consider $f(\theta) = \sinh\theta - \sin\theta$. For small θ, to lowest order their respective Taylor series are

$$sin\theta = \theta + O(\theta^3)$$

$$\sinh\theta = \theta + O(\theta^3)$$

from this can we conclude that the $f(\theta) = \sinh\theta - \sin\theta = 0$ as $\theta \ll 1$?

Use the Taylor expansion of $\sinh\theta$ and $\sin\theta$ to third order to show that the Taylor series expansion of $f(\theta)$ to lowest order is

$$f(\theta) = \sinh\theta - \sin\theta = \frac{\theta^3}{3}$$

iv) Plot $f(\theta) = \sinh\theta - \sin\theta$, and $\frac{\theta^3}{3}$ for $0 < \theta < 3$ and verify that they are the same for small θ.

e) *Derive Eulers formula:

$$e^{i\theta} = \cos\theta + i\sin\theta,$$

using the Taylor series expansion of $e^{i\theta}$ and comparing to the Taylor expansion of $\cos\theta$ and $\sin\theta$.
(Hint: $i^2 = -1;\ i^3 = i^2 \times i = -i;\ i^4 = i^2 \times i^2 = 1;\ i^5 = i \times i^4 = i;\ i^6 = i^4 \times i^2 = -1;\ i^7 = i^4 \times i^3 = -i...$)

Supplementary (completely optional) Questions

QUESTION 5

Differentiation of x^3 as change in volume

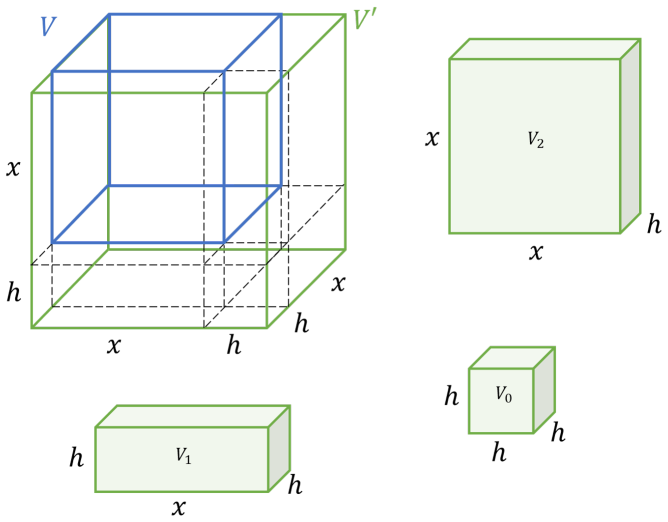

FIG. 3. Differentiating x^3

a) What is the volume of the bigger cube V' in terms of the volumes V,V_0,V_1,V_2?

b) What is the volume of the bigger cube V' in terms of x and h?

c) Expand out this expression for V' and identify each term with volumes V,V_0,V_1,V_2.

d) Evaluate all these volumes for $x = 1$ and $h = 0.3$.

e) i) Show that the change in volume with respect to the change in length is

$$\frac{\Delta V}{\Delta x} = \frac{V' - V}{h} = 3x^2 + 3xh + h^2$$

And ii) evaluate $\frac{\Delta V}{\Delta x}$ for $x = 1$ and $h = 0.3$.

f) Repeat d) and e)ii) for $x = 1$ and $h = 0.05$ and $h = 10^{-6}$.

g) This demonstrates that

$$\lim_{h \to 0} \left\{ \frac{\Delta V}{\Delta x} \right\} = \frac{\mathrm{d}V}{\mathrm{d}x} = \frac{\mathrm{d}x^3}{\mathrm{d}x} = 3x^2;$$

which parts of the diagram or which volumes does this $3x^2$ correspond? Why is there a coefficient 3? Why are the other terms not important?

h) *Using the binomial theorem, show that the change in (hyper)volume of a hypercube of dimension n, $\Delta\Omega = x^n$ is dominated by n hypersurfaces of area x^{n-1} and hence in the limit of an infinitesimal change h

$$\lim_{h\to 0}\left\{\frac{\Delta\Omega}{\Delta x}\right\} = \frac{\mathrm{d}\Omega}{\mathrm{d}x} = \frac{\mathrm{d}x^n}{\mathrm{d}x} = nx^{n-1};$$

(Hint: Binomial theorem is

$$\begin{aligned}(x+h)^n &= \sum_{k=0}^{n}\binom{n}{k}x^{n-k}h^k\\ &= \binom{n}{0}x^n + \binom{n}{1}x^{n-1}h + \binom{n}{2}x^{n-2}h^2 + \ldots\end{aligned}$$

)

QUESTION 6

Derivative of $\sqrt[n]{x} = x^{1/n}$

There isnt a nice (conventional) geometric interpretation of what the quantity $\sqrt[n]{x} = x^{1/n}$ represents if x represents a length along a line.

a) However, if $\Omega = x^n$ is the "volume" of a hypercube in n-dimensions, then what does $\sqrt[n]{\Omega} = \Omega^{1/n}$ represent?

b) With $x = \Omega^{1/n}$ and using fact that $\frac{\mathrm{d}x}{\mathrm{d}\Omega} = \left(\frac{\mathrm{d}\Omega}{\mathrm{d}x}\right)^{-1}$ show that

$$\frac{\mathrm{d}x^{1/n}}{\mathrm{d}x} = \frac{1}{n}x^{\frac{1}{n}-1}.$$