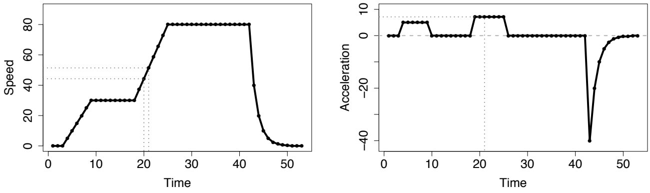
Appendix C Differentiation Techniques for Machine Learning

John D. Kelleher and Brian Mac Namee and Aoife D'Arcy

Imagine a car journey where we start out driving on a minor road at about 30mph and then move onto a highway where we drive at about 80mph before noticing an accident and braking suddenly.



(a) (b)

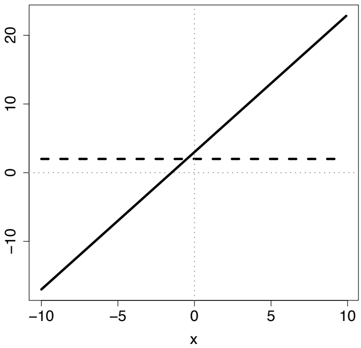
Figure: (a) the speed of a car during a journey along on the minor road before joining a motorway and finally coming to a sudden (safe) halt. (b) shows acceleration, the derivative of speed with respect to time, during this journey.

- Acceleration is a measure of the rate of change of speed over time.
- We can say more formally that acceleration is, in fact, the **derivative** of speed *with respect to* time.
- **Differentiation** is the set of techniques from **calculus** (the branch of mathematics that deals with how things change) that allows us to calculate **derivatives**.

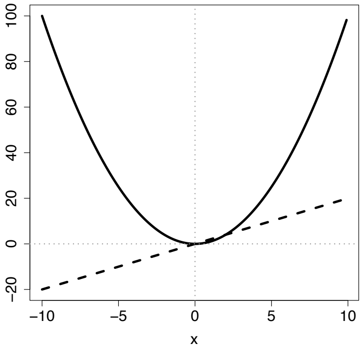
- A **continuous function**, $f(x)$, generates an output for every value of a variable x based on some expression involving x. For example:

$$\begin{aligned} f(x) &= 2x + 3 \\ f(x) &= x^2 \\ f(x) &= 3x^3 + 2x^2 - x - 2 \end{aligned}$$

- The first function is known as a **linear function** as the output is a combination of only additions and multiplications
- The other two functions are known as **polynomial functions** as they include addition, multiplication and raising to exponents (we show a **second order polynomial function**, also known as a **quadratic function** and a **third order polynomial function**, also known as **cubic function**.



(a) $f(x) = 2x + 3$



(b) $f(x) = x^2$

Figure: (a) - (b) Some examples of continuous functions, shown as solid lines, and their derivatives, shown as dashed lines.

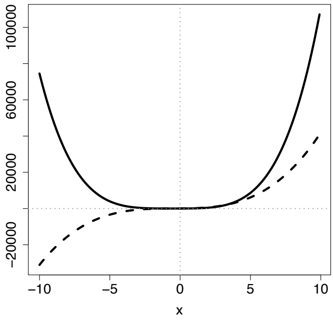
Derivatives and Slopes!

- The derivative of a function $f(x)$ with respect to x also gives us the slope of the function at that value of x.

- To actually calculate the derivative, referred to as $\frac{d}{dx}f(x)$, of a simple continuous function, $f(x)$, we use a small number of differentiation rules:

1)	$\dfrac{d}{dx}\alpha$	$=$	0	(where α is any constant)
2)	$\dfrac{d}{dx}\alpha x^n$	$=$	$\alpha \times n \times x^{n-1}$	
3)	$\dfrac{d}{dx}a+b$	$=$	$\dfrac{d}{dx}a+\dfrac{d}{dx}b$	(where a and b are expressions that may or may not contain x)
4)	$\frac{d}{dx}\alpha \times c$	$=$	$\alpha \times \dfrac{d}{dx}c$	(where α is any constant and c is an expression containing x)

- The function $f(x) = (x^2 + 1)^2$ cannot be differentiated using the rules just described because it is a **composite function** - it is a *function of a function*.



(a) $f(x) = (x^2 + 1)^2$

Figure: A composite function and it's derivative.

- We can rewrite $f(x)$ as $f(x) = (g(x))^2$ where $g(x) = x^2 + 1$.
- The differentiation chain rule allows us to differentiate functions of this kind of function.

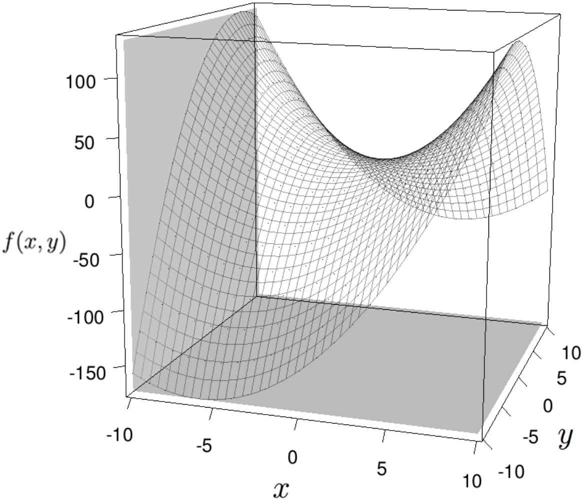
The Chain Rule

$$\frac{d}{dx} f(g(x)) = \frac{d}{d\, g(x)} f(g(x)) \times \frac{d}{dx} g(x) \tag{1}$$

- Applying this to the example $f(x) = (x^2+1)^2$ we get:

$$\begin{aligned}\frac{d}{dx}(x^2+1)^2 &= \frac{d}{d\,(x^2+1)}(x^2+1)^2 \times \frac{d}{dx}(x^2+1)\\ &= \Big(2\times(x^2+1)\Big)\times(2x)\\ &= 4x^3+4x\end{aligned}$$

- Some functions are not defined in terms of just one variable.
- For example, $f(x, y) = x^2 - y^2 + 2x + 4y - xy + 2$ is a function defined in terms of two variables x and y.
- Rather than defining a curve (as was the case for all of the previous examples) this function defines a surface.

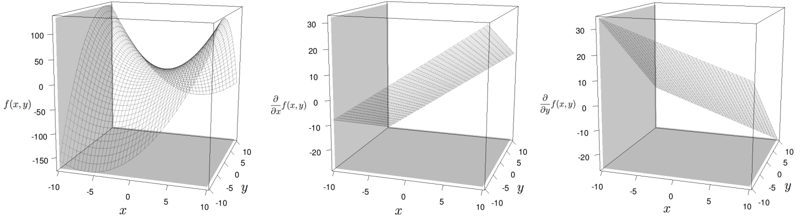


(a) $f(x, y) = x^2 - y^2 + 2x + 4y - xy + 2$

Figure: A continuous function in two variables, x and y.

- Using **partial derivatives** offers us an easy way to calculate the derivative of a function like this.
- A partial derivative (denoted by the symbol ∂) of a function of more than one variable is its derivative with respect to one of those variables with the other variables held constant.

- For the example function $f(x, y) = x^2 - y^2 + 2x + 4y - xy + 2$ we get two partial derivatives:
$$\frac{\partial}{\partial x}(x^2 - y^2 + 2x + 4y - xy + 2) \quad = \quad 2x + 2 - y$$
where the terms y^2 and $4y$ are treated as constants as they do not include x, and:
$$\frac{\partial}{\partial y}(x^2 - y^2 + 2x + 4y - xy + 2) = -2y + 4 - x$$
where the terms x^2 and $2x$ are treated as constants as they do not include y. Figures 5(b) [16] and 5(c) [16] show these partial derivatives.



(a) $f(x,y) = x^2 - y^2 + 2x + 4y - xy + 2$ (b) $\dfrac{\partial}{\partial x} f(x,y) = 2x + 2 - y$ (c) $\dfrac{\partial}{\partial y} f(x,y) = -2y + 4 - x$

Figure: (a) a continuous function in two variables, x and y. (b) the partial derivative of this function with respect to x. (c) the partial derivative of this function with respect to y.

Summary