

Differentiate your Objective

Differentiable Programming

How does pre-university calculus relate to AI and the future of computer programming?

Jonathon Hare & Antonia Marcu

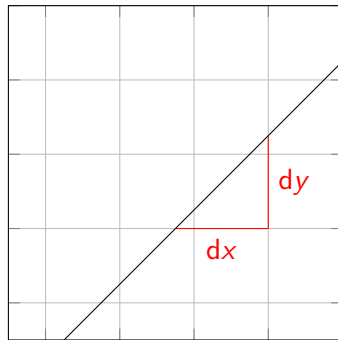
Vision, Learning and Control
University of Southampton

Differentiation

Recap: what is the derivative of a function of one variable?

The derivative in 1D

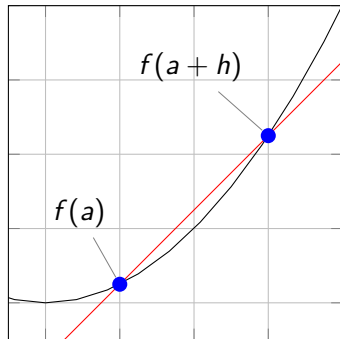
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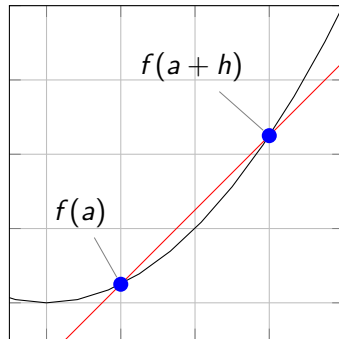
- Recall that the gradient of a straight line is $\frac{dy}{dx}$.
- For an arbitrary real-valued function, $f(a)$, we can approximate the derivative, $f'(a)$ using the gradient of the *secant line* defined by $(a, f(a))$ and a point a small distance, h , away $(a + h, f(a + h))$: $f'(a) \approx \frac{f(a+h)-f(a)}{h}$.



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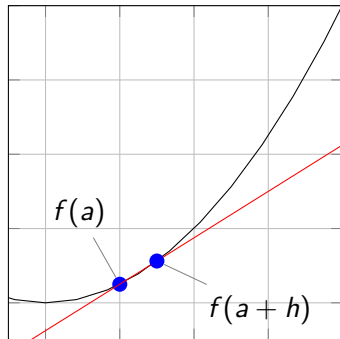
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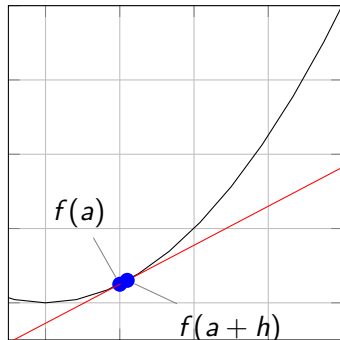
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 - This expression is *Newton's Quotient*.
 - As h becomes smaller, the approximated derivative becomes more accurate.
 - If we take the limit as $h \rightarrow 0$, then we have an exact expression for the derivative:
$$\frac{df}{da} = f'(a) = \lim_{h \rightarrow 0} \frac{f(a+h)-f(a)}{h}.$$



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The derivative of $y = x^2$ from first principles

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$$\frac{dy}{dx} = 2x$$

Intuition: What does the gradient dy/dx tell us

- The 'rate of change' of y with respect to x .

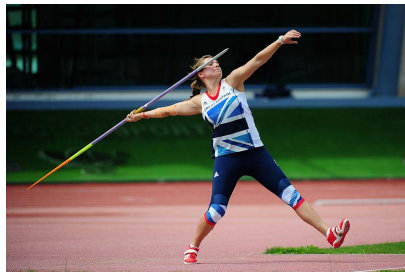
Intuition: What does the gradient dy/dx tell us

- The 'rate of change' of y with respect to x .
- By how much does y change if I make a small change to the x .

Why should we care?

Solving a simple problem with differentiation

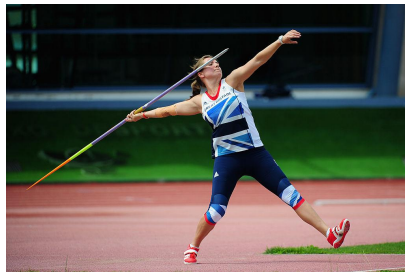
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- At what angle should a javelin be thrown to maximise the distance travelled?
- Assume initial velocity $u = 28 \text{ m s}^{-1}$ and $g = 9.8 \text{ m s}^{-2}$
- Choose to ignore launch height as it is negligible compared to distance travelled.



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- Assume initial velocity $u = 28 \text{ m s}^{-1}$ and $g = 9.8 \text{ m s}^{-2}$
- Choose to ignore launch height as it is negligible compared to distance travelled.
- Kinematics equations:

$$x = ut \cos(\theta) = 28t \cos(\theta)$$

$$y = ut \sin(\theta) - 0.5gt^2 = 28t \sin(\theta) - 4.9t^2$$



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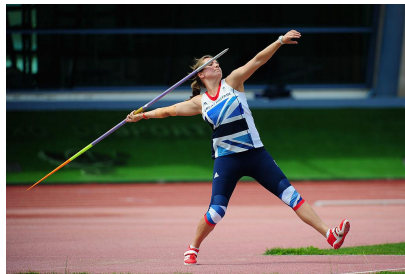
- Javelin hits ground when $y = 0$ and we only care about $t > 0$:

$$0 = 28t \sin(\theta) - 4.9t^2$$

$$\implies t = \frac{28}{4.9} \sin(\theta)$$

- Substituting into the horizontal component:

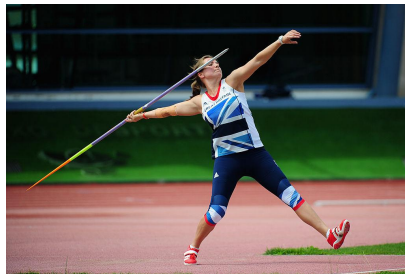
$$x = 28 \frac{28}{4.9} \sin(\theta) \cos(\theta) = 80 \sin(2\theta)$$



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Solving a simple problem with differentiation

$$\begin{aligned} \max_{\theta} \quad & 80 \sin(2\theta) \\ \text{s.t.} \quad & 0 \leq \theta \leq \frac{\pi}{2} \end{aligned}$$



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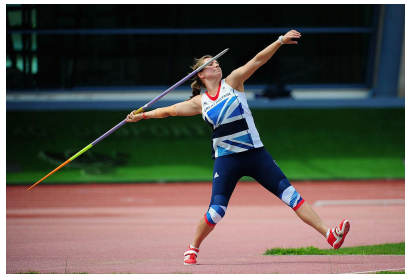
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Compute derivative w.r.t θ and set to zero:

$$0 = \frac{d(80 \sin(2\theta))}{d\theta}$$

$$= 160 \cos(2\theta)$$

$$\implies \theta = \frac{1}{2} \cos^{-1}(0) = \frac{\pi}{4}$$



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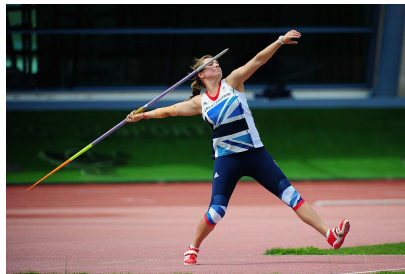
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Irrespective of the initial velocity maximum distance is achieved at 45° .



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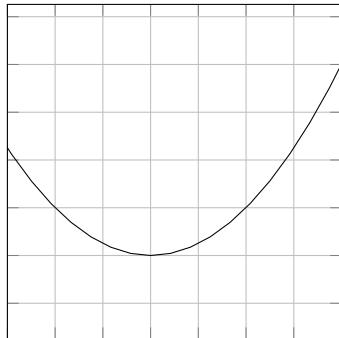
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- We can solve all kinds of problems if we can:
 - **formulate** a *loss* or *cost* function.
 - **minimise** the loss with respect to the parameter(s)¹.
- Problems:
 - The loss must be differentiable (or rather you must be able to compute or estimate its gradient somehow).
 - Some loss functions might have many minima; you might have to settle for finding a sub-optimal one (or a saddle-point).
 - The loss function could be arbitrarily complex... you might not be able to analytically compute the solution (or the gradient).

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A simple algorithm for minimising a function

Gradient Decent

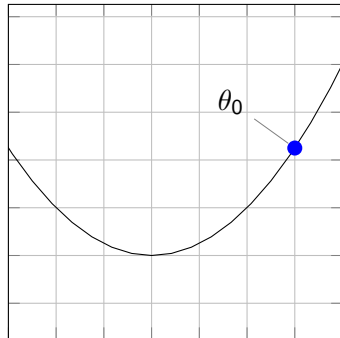
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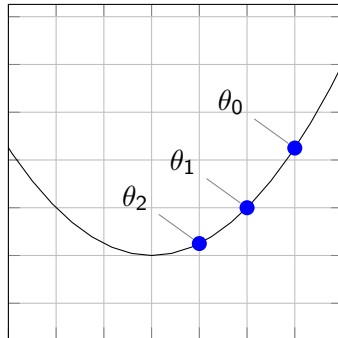
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Gradient Descent:

$$\theta_{i+1} = \theta_i - \gamma \frac{d\ell}{d\theta} \text{ where } \gamma \text{ is the } \textit{learning rate}$$



Javelin throwing again, but with Python code

Derivatives of more general functions

- Almost all complex functions can be broken into simpler parts (often with very simple derivatives).
- You can add (or subtract) sub-functions, multiply (or divide) sub-functions and make functions of functions.
 - The sum rule, product rule and chain rule tell you how to differentiate these.

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- You can add (or subtract) sub-functions, multiply (or divide) sub-functions and make functions of functions.
 - The sum rule, product rule and chain rule tell you how to differentiate these.
- If you break down functions into their constituent parts computing the derivative becomes very easy
- Example: the sin function can be written in terms of exponentials (Euler's formula) and the derivative of an exponential e^x is just $e^x \dots$

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 - In many real applications it can be *millions* of parameters.
- Partial derivatives $\frac{\partial f}{\partial x_i}$ let us compute the gradient of the i -th parameter by holding the other parameters constant.

Back to programming

Programming is really just function composition and control statements

- At the end of the day computer programs are just compositions of really simple functions that computer processors can compute: arithmetic operations (add, multiply, divide, ...), logical operations (and, or, not, comparisons...), operations that move data, etc.

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- The chain rule tells us how to compute gradients of composite functions.

So, in principle we can find the optimal “parameters” of a computer program designed to solve a specific task by following the gradients to optimise it.

Differentiating Branches

Code - *if-else* statement

```
if a > 0.5:  
    b = 0  
else:  
    b = 2 * a
```

Math

$$b(a) = \begin{cases} 0 & \text{if } a > 0.5 \\ 2a & \text{if } a \leq 0.5 \end{cases}$$

$$\frac{\partial b}{\partial a} = \begin{cases} 0 & \text{if } a > 0.5 \\ 2 & \text{if } a \leq 0.5 \end{cases}$$

Differentiating Loops

Code - *for* loop statement

```
b = 1
for i in range(3):
    b = b + b * a
```

Math

$$b_0 = 1$$

$$b_1 = b_0 + b_0 a = 1 + a$$

$$b_2 = b_1 + b_1 a = 1 + 2a + a^2$$

$$b_3 = b_2 + b_2 a = 1 + 3a + 3a^2 + a^3$$

$$\frac{\partial b}{\partial a} = 3 + 6a + 3a^2$$

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- We can differentiate through lots of types of programs and algorithms (even the Gradient Descent algorithm is itself differentiable!), but...
- not every operation or function has *useful* gradients
 - discontinuities, large areas of zero-gradient, ...
- Computer science researchers are actively developing mathematical ‘tricks’ to circumvent many of these problems.
 - *Relaxations* of functions that behave almost the same, but have well defined gradients.
 - *Reparameterisations* of functions involving randomness.
 - *Approximations* of useable gradients for functions that have ill-posed gradients.

What kinds of functional building blocks are common?

- Today, the most common operations with parameters are:
 - *Vector addition*: the input vector to a function is added to a vector of weights.
 - *Vector-Matrix multiplication*: the input vector to the function is multiplied with a matrix of weights.
 - *Convolution*: the input vector (or matrix...) is 'convolved' with a set of weights.
 - (in all these cases 'weights' are the parameters which are learned)

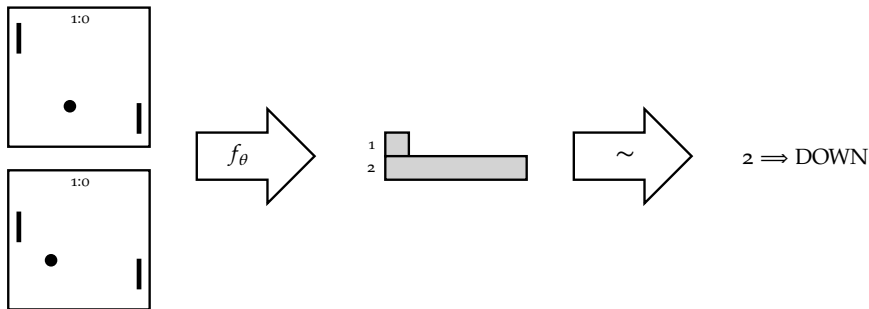
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- The above operations are *linear*, so they are often combined with element-wise nonlinearities; e.g.:
 - $\max(0, x)$ aka ReLU.
 - $\tanh(x)$.
 - $\frac{1}{1+e^{-x}}$ aka *sigmoid* or the *logistic* function.

Real Examples of Differentiable Programming

Playing Games

- You can use differentiable programming to write (and train) ‘agents’ that can play games.
- It can be hard to get a gradient from a single game involving many moves, but there is a clever trick which allows good estimates of gradients to be created over the average of *many* games.
- This is broadly the area of what is called *reinforcement learning*.

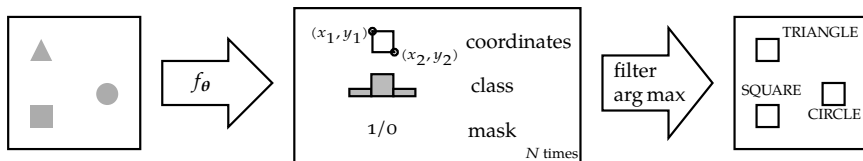


Playing Games

Demo: AlphaStar

Object detection

- Consider a function that takes an image as input and produces an array of *bounding boxes* and corresponding *labels*.
- With enough *training data* we can learn the parameters required to detect objects in images.



Object detection

Demo

- We could envisage a differentiable function that takes in a set of line coordinates and turns them into an image...
- With such a function we can optimise the line coordinates so they e.g. match a photograph, thus automatically creating a *sketch*.

Drawing

Demo



Drawing

Demo

Where is this all going?

Software 2.0

There is a revolution happening and you're going to be part of it!

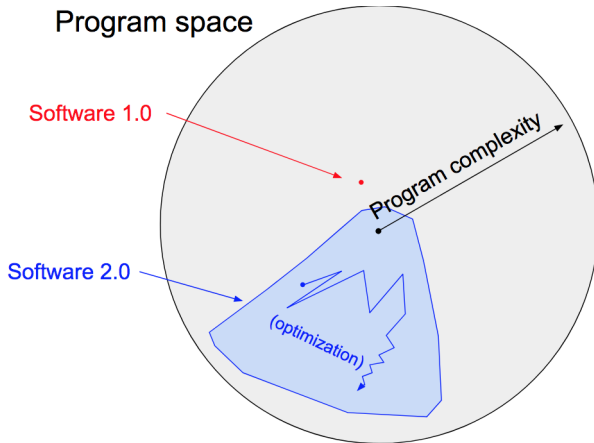


Image credit: Andrei Karpathy

<https://karpathy.medium.com/software-2-0-a64152b37c35>

Any Questions?