

# Follow the Gradient

# The power of differentiation

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- The big idea: optimisation by following gradients
- Recap: what are gradients and how do we find them?
- Recap: Singular Value Decomposition and its applications
- Example: Computing SVD using gradients - The Netflix Challenge

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  - How do we select those parameters?
- In deep learning/differentiable programming we typically define an objective function that we *minimise* (or *maximise*) with respect to those parameters
- This implies that we're looking for points at which the gradient of the objective function is zero w.r.t the parameters

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  - First order methods, second order methods, subgradient methods...
- With deep learning we're primarily interested in first-order methods<sup>1</sup>.
  - Primarily using variants of gradient descent: a function  $F(\mathbf{x})$  has a minima<sup>2</sup> (or a saddle-point) at a point  $\mathbf{x} = \mathbf{a}$  where  $\mathbf{a}$  is given by applying  $\mathbf{a}_{n+1} = \mathbf{a}_n - \alpha \nabla F(\mathbf{a}_n)$  until convergence from some initial point  $\mathbf{a}_0$ .

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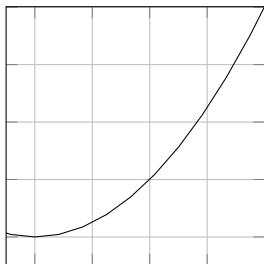
<sup>2</sup>not necessarily global or unique

# Recap: what are gradients and how do we find them?

## The derivative in 1D

- Recall that the gradient of a straight line is

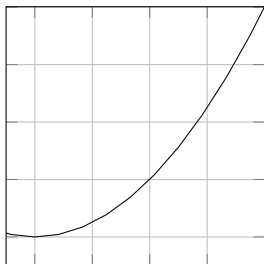
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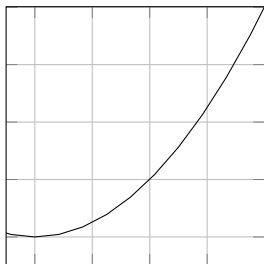
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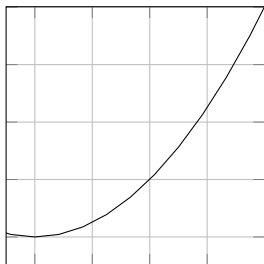
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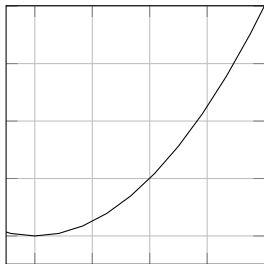


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- This expression is 'Newton's Quotient' or 'Fermat's Difference Quotient'.
- As  $h$  becomes smaller, the approximated derivative becomes more accurate.
- If we take the limit as  $h \rightarrow 0$ , then we have an exact expression for the derivative: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





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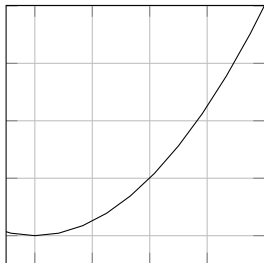
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Aside: numerical approximation of the derivative

- For numerical computation of derivatives it is better to use a “centralised” definition of the derivative:

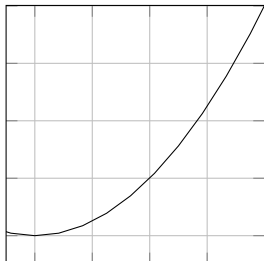
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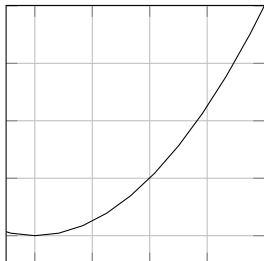




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  - The bit inside the limit is known as the *symmetric difference quotient*
  - For small values of  $h$  this has less error than the standard one-sided difference quotient.



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Aside: numerical approximation of the derivative

- If you are going to use difference quotients to estimate derivatives you need to be aware of potential rounding errors due to floating point representations.
  - Calculating derivatives this way using less than 64-bit precision is rarely going to be useful. (Numbers are not represented exactly, so even if  $h$  is represented exactly,  $x + h$  will probably not be)
  - You need to pick an appropriate  $h$  - too small and the subtraction will have a large rounding error!

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## Derivatives of deeper functions

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  - e.g.  $z = f \circ g(x) = f(g(x))$

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- Deep learning is all about optimising deeper functions; functions that are compositions of other functions
  - e.g.  $z = f \circ g(x) = f(g(x))$
- The chain rule of calculus tells us how to differentiate compositions of functions:
  - $\frac{dz}{dx} = \frac{dz}{dy} \frac{dy}{dx}$

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Example: differentiating  $z = x^4$

Note that this is a silly example that just serves to demonstrate the principle!

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Equivalently, from first principles:

$$z = x^4$$

$$\frac{dz}{dx} = \lim_{h \rightarrow 0} \frac{(x+h)^4 - x^4}{h}$$

$$\frac{dz}{dx} = \lim_{h \rightarrow 0} \frac{h^4 + 4h^3x + 6h^2x^2 + 4hx^3 + x^4 - x^4}{h}$$

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  - Thus the derivative is a vector (the 'tangent vector'),  
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  - Equivalently,  $\mathbf{y}'(t) = \lim_{h \rightarrow 0} \frac{\mathbf{y}(t+h) - \mathbf{y}(t)}{h}$  if the limit exists.

# Recap: what are gradients and how do we find them?

Functions of multiple variables: partial differentiation

- What if the function we're trying to deal with has multiple variables<sup>3</sup> (e.g.  $f(x, y) = x^2 + xy + y^2$ )?
  - This expression has a pair of *partial derivatives*,  $\frac{\partial f}{\partial x} = 2x + y$  and  $\frac{\partial f}{\partial y} = x + 2y$ , computed by differentiating with respect to each variable  $x$  and  $y$  whilst holding the other(s) constant.

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  - This is the **gradient** of  $f$  at  $a$ .
- In the case of a vector-valued multivariate function, the partial derivatives form a matrix called the **Jacobian**.

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  - **How will we find the gradients of these?**

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## The chain rule for vectors

Suppose that  $\mathbf{x} \in \mathbb{R}^m$ ,  $\mathbf{y} \in \mathbb{R}^n$ ,  $g$  maps from  $\mathbb{R}^m$  to  $\mathbb{R}^n$  and  $f$  maps from  $\mathbb{R}^n$  to  $\mathbb{R}$ .

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If  $\mathbf{y} = g(\mathbf{x})$  and  $z = f(\mathbf{y})$ , then

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Equivalently, in vector notation:

$$\nabla_{\mathbf{x}} z = \left( \frac{\partial \mathbf{y}}{\partial \mathbf{x}} \right)^\top \nabla_{\mathbf{y}} z$$

where  $\frac{\partial \mathbf{y}}{\partial \mathbf{x}}$  is the  $n \times m$  Jacobian matrix of  $g$ .



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  - Indices into  $\mathbf{X}$  now have multiple coordinates, but we can generalise by using a single variable  $i$  to represent the complete tuple of indices.
    - For all index tuples  $i$ ,  $(\nabla_{\mathbf{X}} z)_i$  gives  $\frac{\partial z}{\partial \mathbf{x}_i}$ .

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- Conceptually, the simplest way to think about gradients of tensors is to imagine flattening them into vectors, computing the vector-valued gradient and then reshaping the gradient back into a tensor.
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- More formally, consider the gradient of a scalar  $z$  with respect to a tensor  $\mathbf{X}$  to be denoted as  $\nabla_{\mathbf{X}} z$ .
  - Indices into  $\mathbf{X}$  now have multiple coordinates, but we can generalise by using a single variable  $i$  to represent the complete tuple of indices.
    - For all index tuples  $i$ ,  $(\nabla_{\mathbf{X}} z)_i$  gives  $\frac{\partial z}{\partial \mathbf{x}_i}$ .
  - Thus, if  $\mathbf{Y} = g(\mathbf{X})$  and  $z = f(\mathbf{Y})$  then  $\nabla_{\mathbf{X}} z = \sum_j (\nabla_{\mathbf{X}} \mathbf{Y}_j) \frac{\partial z}{\partial \mathbf{Y}_j}$ .

# Recap: what are gradients and how do we find them?

Example:  $\nabla_{\mathbf{W}} f(\mathbf{XW})$

- Let  $\mathbf{D} = \mathbf{XW}$  where the rows of  $\mathbf{X} \in \mathbb{R}^{n \times m}$  contain some fixed *features*, and  $\mathbf{W} \in \mathbb{R}^{m \times h}$  is a matrix of weights.
- Also let  $\mathcal{L} = f(\mathbf{D})$  be some scalar function of  $\mathbf{D}$  that we wish to minimise.

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- What are the derivatives of  $\mathcal{L}$  with respect to the weights  $\mathbf{W}$ ?



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- Start by considering a specific weight,  $W_{uv}$ :  $\frac{\partial \mathcal{L}}{\partial W_{uv}} = \sum_{i,j} \frac{\partial \mathcal{L}}{\partial D_{ij}} \frac{\partial D_{ij}}{\partial W_{uv}}$ .

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$$\begin{aligned} D_{iv} &= \sum_{k=1}^m X_{ik} W_{kv} \\ \frac{\partial D_{iv}}{\partial W_{uv}} &= \frac{\partial}{\partial W_{uv}} \sum_{k=1}^m X_{ik} W_{kv} = \sum_{k=1}^m \frac{\partial}{\partial W_{uv}} X_{ik} W_{kv} \\ \therefore \frac{\partial D_{iv}}{\partial W_{uv}} &= X_{iu} \end{aligned}$$

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- We can then see that if we want this for all values of  $\mathbf{W}$  it simply generalises to:  $\frac{\partial \mathcal{L}}{\partial \mathbf{W}} = \mathbf{X}^\top \frac{\partial \mathcal{L}}{\partial \mathbf{D}}$ .

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- But, it isn't a particularly useful way to think about the gradients of a loss with respect to the weights of a parameterised function.
  - **The gradient of the loss with respect to a parameter tells you how much the loss will change with a small perturbation to that parameter.**

# Recap: Singular Value Decomposition and its applications

Let's now change direction — we're going to look at an early success story resulting from using some differentiation and the Singular Value Decomposition (SVD).

For complex  $\mathbf{A}$  :

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^*$$

where  $\mathbf{V}^*$  is the *conjugate transpose* of  $\mathbf{V}$ .

For real  $\mathbf{A}$  :

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^{\top}$$



# Recap: Singular Value Decomposition and its applications

- SVD has many uses:
  - Computing the Eigendecomposition:
    - Eigenvectors of  $\mathbf{A}\mathbf{A}^\top$  are columns of  $\mathbf{U}$ ,
    - Eigenvectors of  $\mathbf{A}^\top\mathbf{A}$  are columns of  $\mathbf{V}$ ,
    - and the non-zero values of  $\mathbf{\Sigma}$  are the square roots of the non-zero eigenvalues of both  $\mathbf{A}\mathbf{A}^\top$  and  $\mathbf{A}^\top\mathbf{A}$ .

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  - Low-rank approximation and matrix completion
    - if you take the  $\rho$  columns of  $\mathbf{U}$ , and the  $\rho$  rows of  $\mathbf{V}^\top$  corresponding to the  $\rho$  largest singular values, you can form the matrix  $\mathbf{A}_\rho = \mathbf{U}_\rho \Sigma_\rho \mathbf{V}_\rho^\top$  which will be the *best* rank- $\rho$  approximation of the original  $\mathbf{A}$  in terms of the Frobenius norm.

# Example: Computing SVD using gradients - The Netflix Challenge

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  - e.g. computing the SVD of a sparse matrix with 17770 rows, 480189 columns and 100480507 non-zero entries!
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- OK, so what can you do?
  - The 'Simon Funk' solution: realise that there is a really simple (and quick) way to compute the SVD by following gradients...

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Deriving a gradient-descent solution to SVD

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- Without loss of generality we can write SVD as a 2-matrix decomposition  $\mathbf{A} = \hat{\mathbf{U}}\hat{\mathbf{V}}^T$  by rolling in the square roots of  $\Sigma$  to both  $\hat{\mathbf{U}}$  and  $\hat{\mathbf{V}}$ :  $\hat{\mathbf{U}} = \mathbf{U}\Sigma^{0.5}$  and  $\hat{\mathbf{V}}^T = \Sigma^{0.5}\mathbf{V}^T$ .

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- Then we can define the decomposition as finding  $\min_{\hat{\mathbf{U}}, \hat{\mathbf{V}}} (\|\mathbf{A} - \hat{\mathbf{U}}\hat{\mathbf{V}}^T\|_F^2)$

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Start by expanding our optimisation problem:

$$\begin{aligned}\min_{\hat{\mathbf{U}}, \hat{\mathbf{V}}}(\|\mathbf{A} - \hat{\mathbf{U}}\hat{\mathbf{V}}^{\top}\|_{\text{F}}^2) &= \min_{\hat{\mathbf{U}}, \hat{\mathbf{V}}}(\sum_r \sum_c (A_{rc} - \hat{U}_r \hat{V}_{:,c}^{\top})^2) \\ &= \min_{\hat{\mathbf{U}}, \hat{\mathbf{V}}}(\sum_r \sum_c (A_{rc} - \sum_{p=1}^{\rho} \hat{U}_{rp} \hat{V}_{cp})^2)\end{aligned}$$

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Let  $e_{rc} = A_{rc} - \sum_{p=1}^{\rho} \hat{U}_{rp} \hat{V}_{cp}$  denote the error. Then, our problem becomes:

$$\text{Minimise } \mathcal{L} = \sum_r \sum_c e_{rc}^2$$

We can then differentiate with respect to specific variables  $\hat{U}_{rq}$  and  $\hat{V}_{cq}$

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$$\frac{\partial \mathcal{L}}{\partial \hat{U}_{rq}} = \sum_r \sum_c 2e_{rc} \frac{\partial e}{\partial \hat{U}_{rq}} = -2 \sum_r \sum_c \hat{V}_{cq} e_{rc}$$
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and use this as the basis for a gradient descent algorithm:

$$\hat{U}_{rq} \leftarrow \hat{U}_{rq} + \lambda \sum_r \sum_c \hat{V}_{cq} e_{rc}$$

$$\hat{V}_{cq} \leftarrow \hat{V}_{cq} + \lambda \sum_r \sum_c \hat{U}_{rq} e_{rc}$$



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- A stochastic version of this algorithm (updates on one single item of  $\mathbf{A}$  at a time) helped win the Netflix Challenge competition in 2009.

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- A stochastic version of this algorithm (updates on one single item of  $\mathbf{A}$  at a time) helped win the Netflix Challenge competition in 2009.
- It was both *fast* and *memory efficient*