

# Follow the Gradient

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## 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

## The big idea: optimisation by following gradients

- Fundamentally, we're interested in machines that we train by optimising parameters
  - 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

# The big idea: optimisation by following gradients

- Gradient based optimisation is a *big* field!
  - 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> 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  $\mathbf{a}_0$ .

<sup>1</sup>Second order gradient optimisers are potentially better, but for systems with many variables are currently impractical as they require computing the Hessian.

<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  $\frac{\Delta y}{\Delta x}$ .
- 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  $(a + h, f(a + h))$ :
$$f'(a) \approx \frac{f(a+h) - f(a)}{h}.$$
  - This expression is 'Newton'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:  $\frac{df}{da} = f'(a) = \lim_{h \rightarrow 0} \frac{f(a+h) - f(a)}{h}$ .

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

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

$$\begin{aligned}y &= x^2 \\ \frac{dy}{dx} &= \lim_{h \rightarrow 0} \frac{(x+h)^2 - x^2}{h} \\ \frac{dy}{dx} &= \lim_{h \rightarrow 0} \frac{x^2 + h^2 + 2hx - x^2}{h} \\ \frac{dy}{dx} &= \lim_{h \rightarrow 0} \frac{h^2 + 2hx}{h} \\ \frac{dy}{dx} &= \lim_{h \rightarrow 0} (h + 2x) \\ \frac{dy}{dx} &= 2x\end{aligned}$$

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

Aside: numerical approximation of the derivative

- For numerical computation of derivatives it is better to use a “centralised” definition of the derivative:
  - $f'(a) = \lim_{h \rightarrow 0} \frac{f(a+h) - f(a-h)}{2h}$
  - 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.
- If you are going to use this 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!

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

## Derivatives of deeper functions

- 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:
  - $\frac{dz}{dx} = \frac{dz}{dy} \frac{dy}{dx}$

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

Example: differentiating  $z = x^4$

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

$$z = x^4$$

$$z = (x^2)^2 = y^2 \quad \text{where} \quad y = x^2$$

$$\frac{dz}{dx} = \frac{dz}{dy} \frac{dy}{dx} = (2y)(2x) = (2x^2)(2x) = 4x^3$$

Equivalently, from first principles:

$$z = x^4$$

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

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

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

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

## Vector functions

- What if we're dealing with a *vector* function,  $\mathbf{y}(t)$ ?
  - This can be split into its constituent coordinate functions:  
 $\mathbf{y}(t) = (y_1(t), \dots, y_n(t))$ .
  - Thus the derivative is a vector (the 'tangent vector'),  
 $\mathbf{y}'(t) = (y_1'(t), \dots, y_n'(t))$ , which consists of the derivatives of the coordinate functions.
  - 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.
- In general, the partial derivative of a function  $f(x_1, \dots, x_n)$  at a point  $(a_1, \dots, a_n)$  is given by:  
$$\frac{\partial f}{\partial x_i}(a_1, \dots, a_n) = \lim_{h \rightarrow 0} \frac{f(a_1, \dots, a_i + h, \dots, a_n) - f(a_1, \dots, a_i, \dots, a_n)}{h}.$$
- The vector of partial derivatives of a scalar-value multivariate function,  $f((x_1, \dots, x_n)$  at a point  $(a_1, \dots, a_n)$ , can be arranged into a vector:  $\nabla f(a_1, \dots, a_n) = (\frac{\partial f}{\partial x_1}(a_1, \dots, a_n), \dots, \frac{\partial f}{\partial x_n}(a_1, \dots, a_n))$ .
  - 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**.

<sup>3</sup>A multivariate function

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

Functions of vectors and matrices: partial differentiation

- For the kinds of functions (and programs) that we'll look at *optimising* in this course have a number of typical properties:
  - They are scalar-valued
    - We'll look at programs with *multiple losses*, but ultimately we can just consider optimising with respect to the *sum* of the losses.
  - They involve multiple variables, which are often wrapped up in the form of vectors or matrices, and more generally tensors.
  - **How will we find the gradients of these?**

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

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  $\mathbb{R}$ .

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

$$\frac{\partial z}{\partial x_i} = \sum_j \frac{\partial z}{\partial y_j} \frac{\partial y_j}{\partial x_i}.$$

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  $g$ .

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

## The chain rule for Tensors

- 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.
  - In this way we're still just multiplying Jacobians by gradients.
- 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  $\frac{\partial z}{\partial x_i}$ .
  - Thus, if  $\mathbf{Y} = g(\mathbf{X})$  and  $z = f(\mathbf{Y})$  then  $\nabla_{\mathbf{X}} z = \sum_j (\nabla_{\mathbf{X}} Y_j) \frac{\partial z}{\partial Y_j}$ .

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



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

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

- Start by considering a specific weight,  $W_{uv}$ :  $\frac{\partial \mathcal{L}}{\partial W_{uv}} = \sum_{i,j} \frac{\partial \mathcal{L}}{\partial D_{ij}} \frac{\partial D_{ij}}{\partial W_{uv}}$ .
- We know that  $\frac{\partial D_{ij}}{\partial W_{uv}} = 0$  if  $j \neq v$  because  $D_{ij}$  is the dot product of row  $i$  of  $\mathbf{X}$  and column  $j$  of  $\mathbf{W}$ .
- Therefore, we can simplify the summation to only consider cases where  $j = v$ :  $\sum_{i,j} \frac{\partial \mathcal{L}}{\partial D_{ij}} \frac{\partial D_{ij}}{\partial W_{uv}} = \sum_i \frac{\partial \mathcal{L}}{\partial D_{iv}} \frac{\partial D_{iv}}{\partial W_{uv}}$ .
- What is  $\frac{\partial D_{iv}}{\partial W_{uv}}$ ?

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

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

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

- Putting every together, we have:  $\frac{\partial \mathcal{L}}{\partial W_{uv}} = \sum_i \frac{\partial \mathcal{L}}{\partial D_{iv}} X_{iu}$ .
- As we're summing over multiplications of scalars, we can change the order:  $\frac{\partial \mathcal{L}}{\partial W_{uv}} = \sum_i X_{iu} \frac{\partial \mathcal{L}}{\partial D_{iv}}$ .
- and note that the sum over  $i$  is doing a dot product with row  $u$  and column  $v$  if we transpose  $X_{iu}$  to  $X_{ui}^\top$ :  $\frac{\partial \mathcal{L}}{\partial W_{uv}} = \sum_i X_{ui}^\top \frac{\partial \mathcal{L}}{\partial D_{iv}}$ .
- We can then see that if we want this for all values of  $\mathbf{W}$  it simply generalises to:  $\frac{\partial \mathcal{L}}{\partial \mathbf{W}} = \mathbf{X}^\top \frac{\partial \mathcal{L}}{\partial \mathbf{D}}$ .

## 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  $\mathbf{A}^\top\mathbf{A}$ .
  - Dimensionality reduction
    - ...use to compute PCA
  - Computing the Moore-Penrose Pseudoinverse
    - for real  $\mathbf{A}$ :  $\mathbf{A}^+ = \mathbf{V}\mathbf{\Sigma}^+\mathbf{U}^\top$  where  $\mathbf{\Sigma}^+$  is formed by taking the reciprocal of every non-zero diagonal element and transposing the result.
  - 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  $\mathbf{A}_\rho = \mathbf{U}_\rho\mathbf{\Sigma}_\rho\mathbf{V}_\rho^\top$  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

- There are many standard ways of computing the SVD:
  - e.g. 'Power iteration', or 'Arnoldi iteration' or 'Lanczos algorithm' coupled with the 'Gram-Schmidt process' for orthonormalisation
- but, these don't necessarily scale up to really big problems
  - e.g. computing the SVD of a sparse matrix with 17770 rows, 480189 columns and 100480507 non-zero entries!
  - this corresponds to the data provided by Netflix when they launched the *Netflix Challenge* in 2006.
- 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...

## Example: Computing SVD using gradients - The Netflix Challenge

Deriving a gradient-descent solution to SVD

- One of the definitions of rank- $\rho$  SVD of a matrix  $\mathbf{A}$  is that it minimises reconstruction error in terms of the Frobenius norm.
- 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  $\hat{\mathbf{V}}^T = \Sigma^{0.5}\mathbf{V}^T$ .
- Then we can define the decomposition as finding  $\min_{\hat{\mathbf{U}}, \hat{\mathbf{V}}} (\|\mathbf{A} - \hat{\mathbf{U}}\hat{\mathbf{V}}^T\|_{\text{F}}^2)$

# Example: Computing SVD using gradients - The Netflix Challenge

Deriving a gradient-descent solution to SVD

Start by expanding our optimisation problem:

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

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

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

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

# Example: Computing SVD using gradients - The Netflix Challenge

Deriving a gradient-descent solution to SVD

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

$$\begin{aligned}\frac{\partial J}{\partial \hat{U}_{rq}} &= \sum_r \sum_c 2e_{rc} \frac{\partial e}{\partial \hat{U}_{rq}} = -2 \sum_r \sum_c \hat{V}_{cq} e \\ \frac{\partial J}{\partial \hat{V}_{cq}} &= \sum_r \sum_c 2e_{rc} \frac{\partial e}{\partial \hat{V}_{cq}} = -2 \sum_r \sum_c \hat{U}_{rq} e\end{aligned}$$

and use this as the basis for a gradient descent algorithm:

$$\begin{aligned}\hat{U}_{rq} &\Leftarrow \hat{U}_{rq} + \lambda \sum_r \sum_c \hat{V}_{cq} e_{rc} \\ \hat{V}_{cq} &\Leftarrow \hat{V}_{cq} + \lambda \sum_r \sum_c \hat{U}_{rq} e_{rc}\end{aligned}$$

# Example: Computing SVD using gradients - The Netflix Challenge

Deriving a gradient-descent solution to SVD

- 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*