The power of differentiation

Jonathon Hare

Topics

- 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[1].
  - Primarily using variants of gradient descent: a function $F(\boldsymbol{x})$ has *a* minima[2] (or a saddle-point) at a point $\boldsymbol{x} = \boldsymbol{a}$ where $\boldsymbol{a}$ is given by applying $\boldsymbol{a}_{n+1} = \boldsymbol{a}_n - \alpha \nabla F(\boldsymbol{a}_n)$ until convergence from some initial point $\boldsymbol{a}_0$.

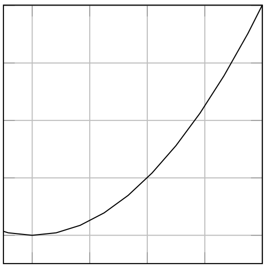
Recap: what are gradients and how do we find them?

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

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

[2] not necessarily global or unique



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

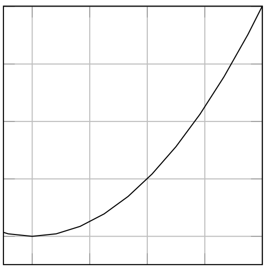
The derivative of $y = x^2$ from first principles

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

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:
  - $f'(a) = \lim_{h \to 0} \frac{f(a+h) - f(a-h)}{2h}$
  - 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.



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

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!

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!

$$
\begin{aligned}
z &= x^4 \\
z &= (x^2)^2 = y^2 \quad \text{where} \quad y = x^2 \\
\frac{dz}{dx} &= \frac{dz}{dy}\frac{dy}{dx} = (2y)(2x) = (2x^2)(2x) = 4x^3
\end{aligned}
$$

Equivalently, from first principles:

$$
\begin{aligned}
z &= x^4 \\
\frac{dz}{dx} &= \lim_{h \to 0} \frac{(x+h)^4 - x^4}{h} \\
\frac{dz}{dx} &= \lim_{h \to 0} \frac{h^4 + 4h^3x + 6h^2x^2 + 4hx^3 + x^4 - x^4}{h} \\
\frac{dz}{dx} &= \lim_{h \to 0} h^3 + 4h^2x + 6hx^2 + 4x^3 = 4x^3
\end{aligned}
$$

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

Vector functions

- What if we're dealing with a *vector* function, $\boldsymbol{y}(t)$?
  - This can be split into its constituent coordinate functions: $\boldsymbol{y}(t) = (y_1(t), \dots, y_n(t))$.
  - Thus the derivative is a vector (the 'tangent vector'), $\boldsymbol{y}'(t) = (y_1'(t), \dots, y_n'(t))$, which consists of the derivatives of the coordinate functions.
  - Equivalently, $\boldsymbol{y}'(t) = \lim_{h \to 0} \frac{\boldsymbol{y}(t+h) - \boldsymbol{y}(t)}{h}$ 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[3] (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: $\frac{\partial f}{\partial x_i}(a_1, \dots, a_n) = \lim_{h \to 0} \frac{f(a_1, \dots, a_i + h, \dots, a_n) - f(a_1, \dots, a_i, \dots, a_n)}{h}$.
- 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: $\nabla f(a_1, \dots, a_n) = \big(\frac{\partial f}{\partial x_1}(a_1, \dots, a_n), \dots, \frac{\partial f}{\partial x_n}(a_1, \dots, a_n)\big)$.
  - 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**.

[3] 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 $\boldsymbol{x} \in \mathbb{R}^m$, $\boldsymbol{y} \in \mathbb{R}^n$, g maps from $\mathbb{R}^m$ to $\mathbb{R}^n$ and f maps from $\mathbb{R}^n$ to $\mathbb{R}$.

If $\boldsymbol{y} = g(\boldsymbol{x})$ and $z = f(\boldsymbol{y})$, 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:

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

where $\frac{\partial \boldsymbol{y}}{\partial \boldsymbol{x}}$ 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 $\frac{\partial z}{\partial \mathsf{X}_i}$.
  - Thus, if $\mathbf{Y} = g(\mathbf{X})$ and $z = f(\mathbf{Y})$ then $\nabla_{\mathbf{X}} z = \sum_j (\nabla_{\mathbf{X}} \mathsf{Y}_j) \frac{\partial z}{\partial \mathsf{Y}_j}$.

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

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

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

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

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

- 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 $\boldsymbol{X}$ and column j of $\boldsymbol{W}$.

- 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 $\frac{\partial D_{iv}}{\partial W_{uv}}$?

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

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

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

- 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 $\boldsymbol{W}$ it simply generalises to: $\frac{\partial \mathcal{L}}{\partial \boldsymbol{W}} = \boldsymbol{X}^\top \frac{\partial \mathcal{L}}{\partial \boldsymbol{D}}$.

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

STOP! What does a gradient actually mean?

- In your early calculus lessons you likely had it hammered into you that gradients represent rates of change of functions.
- This is of course totally true...
- 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). [1em] For complex $\boldsymbol{A}$:

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

where $\boldsymbol{V}^*$ is the *conjugate transpose* of $\boldsymbol{V}$.[1em] For real $\boldsymbol{A}$:

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

Recap: Singular Value Decomposition and its applications

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

  - Dimensionality reduction
    * ...use to compute PCA
  - Computing the Moore-Penrose Pseudoinverse
    * for real $\boldsymbol{A}$: $\boldsymbol{A}^{+} = \boldsymbol{V}\boldsymbol{\Sigma}^{+}\boldsymbol{U}^{\top}$ where $\boldsymbol{\Sigma}^{+}$ 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 ρ columns of $\boldsymbol{U}$, and the ρ rows of $\boldsymbol{V}^{\top}$ corresponding to the ρ largest singular values, you can form the matrix $\boldsymbol{A}_{\rho} = \boldsymbol{U}_{\rho}\boldsymbol{\Sigma}_{\rho}\boldsymbol{V}_{\rho}^{\top}$ which will be the *best* rank-ρ approximation of the original $\boldsymbol{A}$ 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-ρ SVD of a matrix $\boldsymbol{A}$ 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 $\boldsymbol{A} = \hat{\boldsymbol{U}}\hat{\boldsymbol{V}}^{T}$ by rolling in the square roots of $\boldsymbol{\Sigma}$ to both $\hat{\boldsymbol{U}}$ and $\hat{\boldsymbol{V}}$: $\hat{\boldsymbol{U}} = \boldsymbol{U}\boldsymbol{\Sigma}^{0.5}$ and $\hat{\boldsymbol{V}}^{\top} = \boldsymbol{\Sigma}^{0.5}\boldsymbol{V}^{\top}$.
- Then we can define the decomposition as finding $\min_{\hat{\boldsymbol{U}},\hat{\boldsymbol{V}}}(\|\boldsymbol{A} - \hat{\boldsymbol{U}}\hat{\boldsymbol{V}}^{\top}\|_{\mathrm{F}}^{2})$

Example: Computing SVD using gradients - The Netflix Challenge

Deriving a gradient-descent solution to SVD

Start by expanding our optimisation problem:

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

Let $e_{rc} = A_{rc} - \sum_{p=0}^{\rho}\hat{U}_{rp}\hat{V}_{cp}$ 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 $\hat{V}_{cq}$:

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

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

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

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 $\boldsymbol{A}$ at a time) helped win the Netflix Challenge competition in 2009.
- It was both *fast* and *memory efficient*