Follow the Gradient

VLC = $\iiint$ Vision Learning Control $dV\,dL\,dC$

The power of differentiation

Jonathon Hare

Vision, Learning and Control
University of Southampton

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

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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

The big idea: optimisation by following gradients

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- 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 $\boldsymbol{a}_0$.

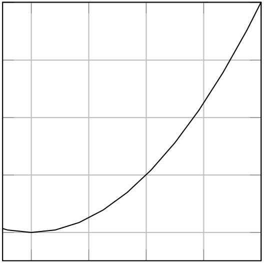
[1] Second order gradient optimisers are potentially better, but for systems with many variables are currently impractical as they require computing the Hessian.

[2] not necessarily global or unique

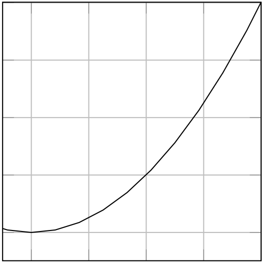
Recap: what are gradients and how do we find them?

The derivative in 1D

- Recall that the gradient of a straight line is $\frac{\Delta y}{\Delta x}$.



- 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 $(a+h, f(a+h))$: $f'(a) \approx \frac{f(a+h)-f(a)}{h}$.



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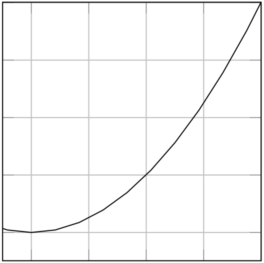

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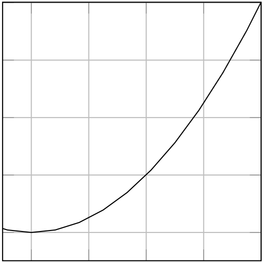

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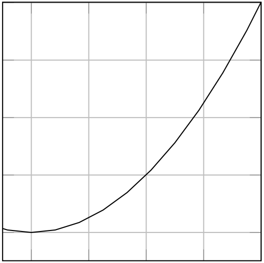
  - This expression is 'Newton's Difference Quotient'.
  - As h becomes smaller, the approximated derivative becomes more accurate.
  - If we take the limit as $h \to 0$, then we have an exact expression for the derivative: $\frac{df}{da} = f'(a) = \lim_{h\to 0} \frac{f(a+h)-f(a)}{h}$.



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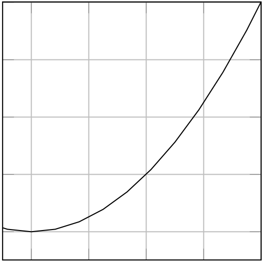
- For numerical computation of derivatives it is better to use a "centralised" definition of the derivative:
  - $f'(a) = \lim_{h \to 0} \frac{f(a+h) - f(a-h)}{2h}$



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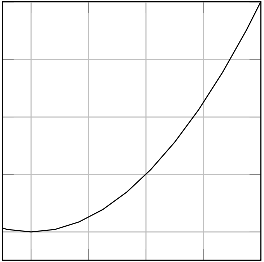

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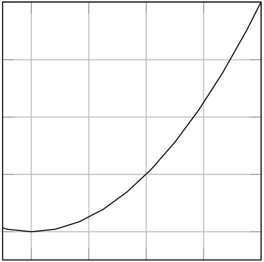
  - For small values of h this has less error than the standard one-sided difference quotient.



- 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!

- Deep learning is all about optimising deeper functions; functions that are compositions of other functions
  - e.g. $z = f \circ g(x) = f(g(x))$

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

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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, $\boldsymbol{y}'(t) = \lim_{h\to 0} \frac{\boldsymbol{y}(t+h) - \boldsymbol{y}(t)}{h}$ if the limit exists.

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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.

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- The vector of partial derivatives of a scalar-value multivariate function, $f(x_1, \ldots, x_n)$ at a point $(a_1, \ldots, a_n)$, can be arranged into a vector: $\nabla f(a_1, \ldots, a_n) = (\frac{\partial f}{\partial x_1}(a_1, \ldots, a_n), \ldots, \frac{\partial f}{\partial x_n}(a_1, \ldots, a_n))$.

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- 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?**

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 $\mathbb{R}$.

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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.

- 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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    - 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 $\nabla_{\mathbf{X}} z = \sum_j (\nabla_{\mathbf{X}} \mathsf{Y}_j) \frac{\partial z}{\partial \mathsf{Y}_j}$.

- 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.
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- 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}: $\frac{\partial \mathcal{L}}{\partial W_{uv}} = \sum_{i,j} \frac{\partial \mathcal{L}}{\partial D_{ij}} \frac{\partial D_{ij}}{\partial W_{uv}}$.

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- Therefore, we can simplify the summation to only consider cases where $j = v$: $\sum_{i,j} \frac{\partial \mathcal{L}}{\partial D_{ij}} \frac{\partial D_{ij}}{\partial W_{uv}} = \sum_{i} \frac{\partial \mathcal{L}}{\partial D_{iv}} \frac{\partial D_{iv}}{\partial W_{uv}}$.

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$$\therefore \frac{\partial D_{iv}}{\partial W_{uv}} = X_{iu}$$

- Putting every together, we have: $\frac{\partial \mathcal{L}}{\partial W_{uv}} = \sum_i \frac{\partial \mathcal{L}}{\partial D_{iv}} X_{iu}$.

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- and note that the sum over i is doing a dot product with row u and column v if we transpose X_{iu} to $X_{ui}^\top$: $\frac{\partial \mathcal{L}}{\partial W_{uv}} = \sum_i X_{ui}^\top \frac{\partial \mathcal{L}}{\partial D_{iv}}$.

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

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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).

For complex $\boldsymbol{A}$:

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

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

For real $\boldsymbol{A}$:

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

Recap: Singular Value Decomposition and its applications

- SVD has many uses:
  - Computing the Eigendecomposition:
    - Eigenvectors of $\boldsymbol{A}\boldsymbol{A}^\top$ 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 $\boldsymbol{A}\boldsymbol{A}^\top$ and $\boldsymbol{A}^\top\boldsymbol{A}$.

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  - 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.

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  - 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

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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

- 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.

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- 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 $\hat{\boldsymbol{V}}^\top = \boldsymbol{\Sigma}^{0.5}\boldsymbol{V}^\top$.

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- Then we can define the decomposition as finding $\min_{\hat{\boldsymbol{U}},\hat{\boldsymbol{V}}}(\|\boldsymbol{A} - \hat{\boldsymbol{U}}\hat{\boldsymbol{V}}^\top\|_{\mathrm{F}}^2)$

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Deriving a gradient-descent solution to SVD

Start by expanding our optimisation problem:

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

Let $e_{rc} = A_{rc} - \sum_{p=0}^{\rho} \hat{U}_{rp} \hat{V}_{cp}$ denote the error. Then, our problem becomes:

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

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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 $\boldsymbol{A}$ at a time) helped win the Netflix Challenge competition in 2009.

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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*