Minimise your Loss



Optimisation

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Gradient descent and SGD (again), and mini-batch SGD

We'll start up by looking again at gradient descent algorithms and their behaviours...

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Reminder: Gradient Descent

- Define total loss as $\mathcal{L} = -\sum_{(\mathbf{x},y)\in \mathbf{D}} \ell(g(\mathbf{x},\boldsymbol{\theta}),y)$ for some loss function ℓ , dataset \mathbf{D} and model g with learnable parameters $\boldsymbol{\theta}$.
- Define how many passes over the data to make (each one known as an Epoch)
- ullet Define a learning rate η

Gradient Descent updates the parameters θ by moving them in the direction of the negative gradient with respect to the **total loss** $\mathcal L$ by the learning rate η multiplied by the gradient:

for each Epoch:
$$oldsymbol{ heta} \leftarrow oldsymbol{ heta} - \eta
abla_{oldsymbol{ heta}} \mathcal{L}$$

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Gradient Descent

- Gradient Descent has good statistical properties (very low variance)
- But is very data inefficient (particularly when data has many similarities)
- Doesn't scale to effectively infinite data (e.g. with augmentation)

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Reminder: Stochastic Gradient Descent

- Define loss function ℓ , dataset **D** and model g with learnable parameters θ .
- Define how many passes over the data to make (each one known as an Epoch)
- Define a learning rate η

Stochastic Gradient Descent updates the parameters θ by moving them in the direction of the negative gradient with respect to the loss of a **single** item ℓ by the learning rate η multiplied by the gradient:

for each Epoch:
$$\text{for each } (\textbf{\textit{x}}, \textbf{\textit{y}}) \in \textbf{\textit{D}} \colon \\ \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} \ell$$

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Stochastic Gradient Descent

- Stochastic Gradient Descent has poor statistical properties (very high variance)
- But is computationally inefficient (poor utilisation of resources particularly with respect to vectorisation)

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Mini-batch Stochastic Gradient Descent

- Define a batch size b
- Define batch loss as $\mathcal{L}_b = -\sum_{(\mathbf{x},y)\in \mathbf{D}_b} \ell(g(\mathbf{x},\boldsymbol{\theta}),y)$ for some loss function ℓ and model g with learnable parameters $\boldsymbol{\theta}$. \mathbf{D}_b is a subset of dataset \boldsymbol{D} of cardinality b.
- Define how many passes over the data to make (each one known as an Epoch)
- Define a learning rate η

Mini-batch Gradient Descent updates the parameters θ by moving them in the direction of the negative gradient with respect to the loss of a **mini-batch** D_b , \mathcal{L}_b by the learning rate η multiplied by the gradient:

partition the dataset D into an array of subsets of size b for each Epoch:

for each
$$m{D}_b \in \mathit{partitioned}(m{D})$$
 : $m{ heta} \leftarrow m{ heta} - \eta
abla_{m{ heta}} \mathcal{L}_b$

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Mini-batch Stochastic Gradient Descent

- Mini-batch Stochastic Gradient Descent has reasonable statistical properties (much lower variance than SGD)
- Allows for computationally efficiency (good utilisation of resources)
- Ultimately we would normally want to make our batches as big as possible for lower variance gradient estimates, but:
 - Must still fit in RAM (e.g. on the GPU)
 - Must be able to maintain throughput (e.g. pre-processing on the CPU; data transfer time)

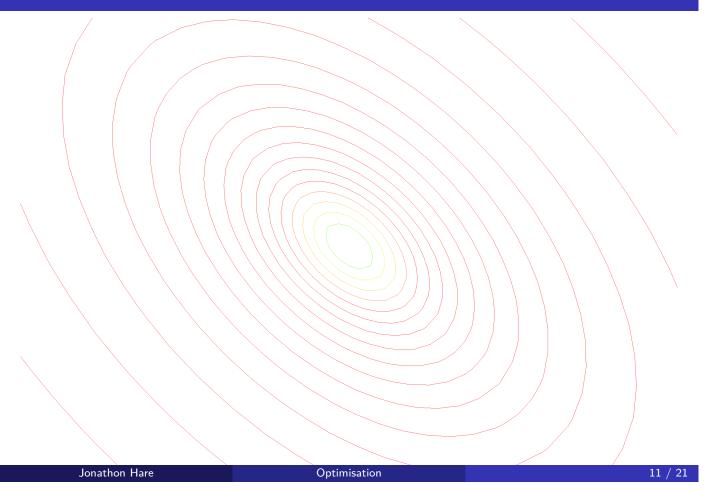
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So, what about the learning rate?

- Choice of learning rate is extremely important
- But we have to reason about the 'loss landscape'
 - Most convergence analysis of optimisation algorithms assumes a convex loss landscape
 - Easy to reason about
 - Can be shown that (S)GD will converge to the optimal solution for a variety of learning rates
 - Can give insights into potential problems in the non-convex case
 - Deep Learning is highly non-convex
 - Many local minima
 - Plateaus
 - Saddle points
 - Symmetries (permutation, etc)
 - Certainly no single global minima

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Accelerated Gradient Methods

- Accelerated gradient methods use a leaky average of the gradient, rather than the instantaneous gradient estimate at each time step
- A physical analogy would be one of the momentum a ball picks up rolling down a hill...
- As you'll see, this helps address the *GD failure modes, but also helps avoid getting stuck in local minima

Momentum I

It's common for the 'leaky' average (the 'velocity', v_t) to be a weighted average of the instantaneous gradient g_t and the past velocity¹:

$$v_t = \beta v_{t-1} + g_t$$

where $\beta \in [0,1]$ is the 'momentum'.

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Momentum II

- The momentum method allows to accumulate velocity in directions of low curvature that persist across multiple iterations
- This leads to accelerated progress in low curvature directions compared to gradient descent

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¹There are quite a few variants of this; here we're following the PyTorch variant

MB-SGD with Momentum

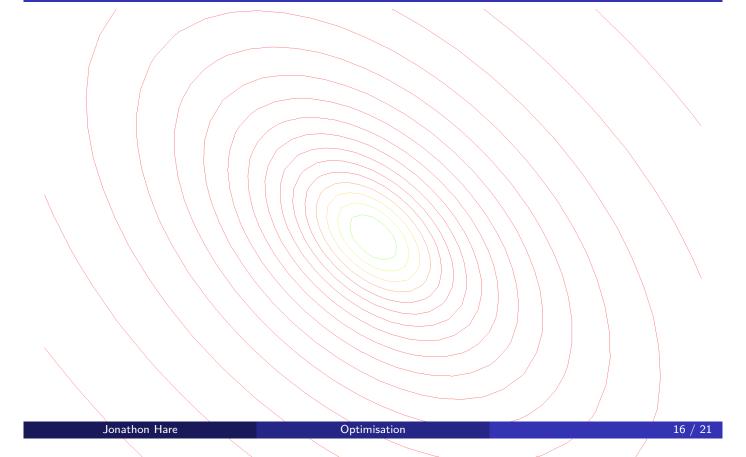
Learning with momentum on iteration t (batch at t denoted by b(t)) is given by:

$$\begin{aligned} & \mathbf{v}_t \leftarrow \beta \mathbf{v}_{t-1} + \nabla_{\theta} \mathcal{L}_{b(t)} \\ & \mathbf{\theta}_t \leftarrow \mathbf{\theta}_{t-1} - \eta \mathbf{v}_t \end{aligned}$$

Note $\beta = 0.9$ is a good choice for the momentum parameter.

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SGD with Momentum - potentially better convex convergence



Learning rate schedules

- In practice you want to decay your learning rate over time
- Smaller steps will help you get closer to the minima
- But don't do it to early, else you might get stuck
- Something of an art form!
 - 'Grad Student Descent' or GDGS ('Gradient Descent by Grad Student')

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Reduce LR on plateau

- Common Heuristic approach:
 - ullet if the loss hasn't improved (within some tolerance) for k epochs
 - then drop the Ir by a factor of 10
- Remarkably powerful!

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Cyclic learning rates

- Worried about getting stuck in a non-optimal local minima?
- Cycle the learning rate up and down (possibly annealed), with a different Ir on each batch
- See https://arxiv.org/abs/1506.01186

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More advanced optimisers

Adagrad

- Decrease learning rate dynamically per weight.
- Squared magnitude of the gradient (2nd moment) used to adjust how quickly progress is made - weights with large gradients are compensated with a smaller learning rate.
- Particularly effective for sparse features.

RMSProp

- Modifies Adagrad to decouple learning rate from gradient magnitude scaling
- Incorporates leaky averaging of squared gradient magnitudes
- LR would typically follow a predefined schedule

Adam

- Essentially takes all the best ideas from RMSProp and SDG+Momentum
- Bias corrected momentum and second moment estimation
- Shown that it might still diverge (or be non optimal, even in convex settings)...
- LR is still a hyperparameter (you might still schedule)

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Take-away messages

- The loss landscape of a deep network is complex to understand (and is far from convex)
- If you're in a hurry to get results use Adam
- If you have time (or a Grad Student at hand), then use SGD (with momentum) and work on tuning the learning rate
- If you're implementing something from a paper, then follow what they did!

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