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

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

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

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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  $\ell$ , dataset **D** and model g with learnable parameters  $\theta$ .
- Define how many passes over the data to make (each one known as an Epoch)
- ullet Define a learning rate  $\lambda$

Stochastic Gradient Descent updates the parameters  $\theta$  by moving them in the direction of the negative gradient with respect to the loss of a **single** item  $\ell$  by the learning rate  $\lambda$  multiplied by the gradient:

```
for each Epoch:  \text{for each } (\textbf{\textit{x}}, y) \in \textit{shuffle}(\textbf{\textit{D}}) \text{:} \\  \theta \leftarrow \theta - \lambda \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  $\ell$  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)
- ullet Define a learning rate  $\lambda$

Mini-batch Gradient Descent updates the parameters  $\theta$  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  $\lambda$  multiplied by the gradient:

for each Epoch:

shuffle & partition dataset D into an array of subsets of size b for each  $D_b \in partitioned(shuffle(D))$ :

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \lambda \nabla_{\boldsymbol{\theta}} \mathcal{L}_{\boldsymbol{b}}$$

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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)

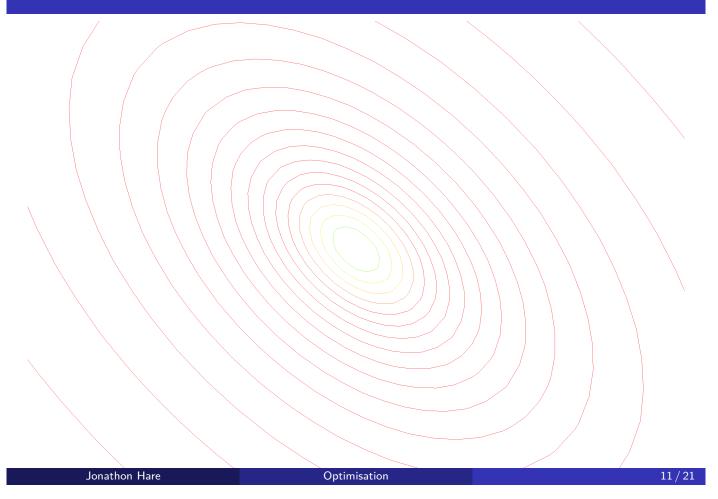
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### So, what about the learning rate?

- 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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## \*GD in the convex case: failure modes



#### **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 velocity<sup>1</sup>:

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

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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<sup>&</sup>lt;sup>1</sup>There are quite a few variants of this; here we're following the PyTorch variant

## MB-SGD with Momentum

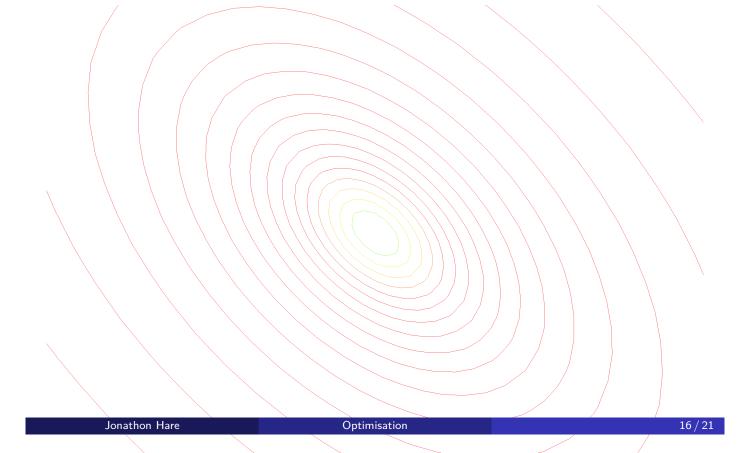
Learning with momentum on iteration t (batch at t denoted by b(t)) is given by:

$$oldsymbol{v}_t \leftarrow eta oldsymbol{v}_{t-1} + 
abla_{oldsymbol{ heta}} \mathcal{L}_{b(t)}$$
 $oldsymbol{ heta}_t \leftarrow oldsymbol{ heta}_{t-1} - \lambda oldsymbol{v}_t$ 

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

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# SGD with Momentum - potentially better convex convergence



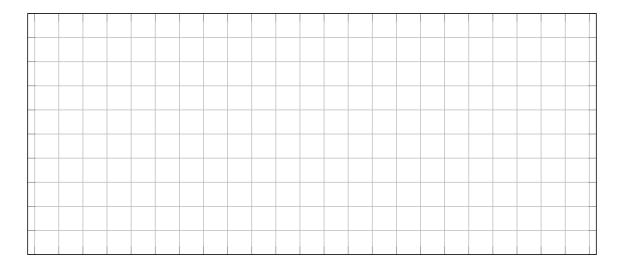
## Learning rate schedules

- 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 lr 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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