Minimise your Loss

Optimisation

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

Reminder: Gradient Descent

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

Gradient Descent updates the parameters $\boldsymbol{\theta}$ 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:
    θ ← θ − η∇θℒ
```

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)

Reminder: Stochastic Gradient Descent

- Define loss function ℓ, dataset $\boldsymbol{D}$ and model g with learnable parameters $\boldsymbol{\theta}$.
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Stochastic Gradient Descent updates the parameters $\boldsymbol{\theta}$ 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:
    for each (x, y) ∈ D:
        θ ← θ − η∇θℓ
```

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)

Mini-batch Stochastic Gradient Descent

- Define a batch size b
- Define batch loss as $\mathcal{L}_b = -\sum_{(\boldsymbol{x},y) \in \boldsymbol{D}_b} \ell(g(\boldsymbol{x}, \boldsymbol{\theta}), y)$ for some loss function ℓ and model g with learnable parameters $\boldsymbol{\theta}$. $\boldsymbol{D}_b$ 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 $\boldsymbol{\theta}$ by moving them in the direction of the negative gradient with respect to the loss of a **mini-batch $\boldsymbol{D}_b$**, $\mathcal{L}_b$ by the learning rate η multiplied by the gradient:

> partition the dataset $\boldsymbol{D}$ into an array of subsets of size b
> ```
> for each Epoch:
>     for each Db ∈ partitioned(D):
>         θ ← θ − η∇θLb
> ```

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- 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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    - Symmetries (permutation, etc)
    - Certainly no single global minima
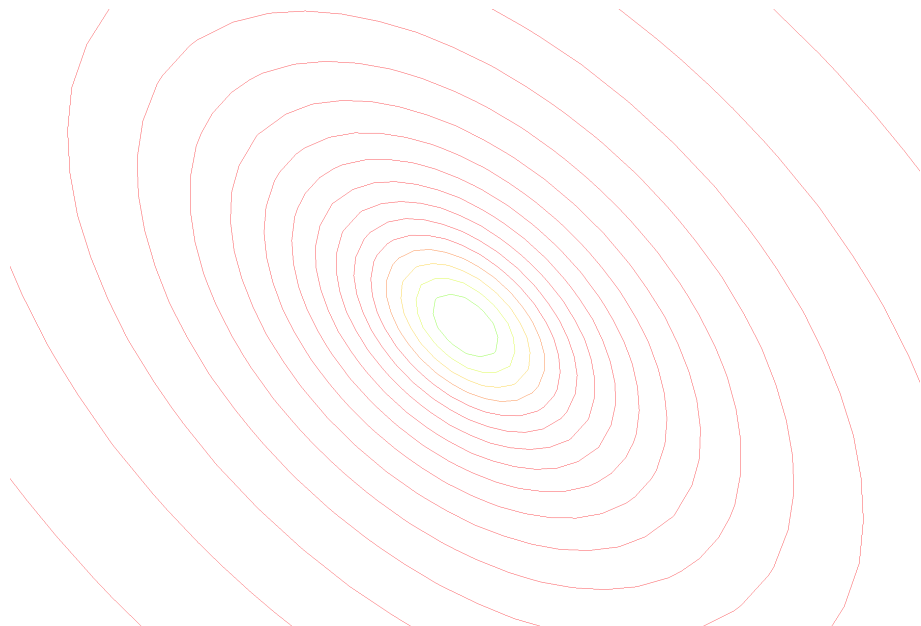
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- A physical analogy would be one of the momentum a ball picks up rolling down a hill...
- As you'll see, this helps address the *GD failure modes, but also helps avoid getting stuck in local minima

It's common for the 'leaky' average (the 'velocity', v_t) to be a weighted average of the instananeous gradient g_t and the past velocity[1]:

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

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

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

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
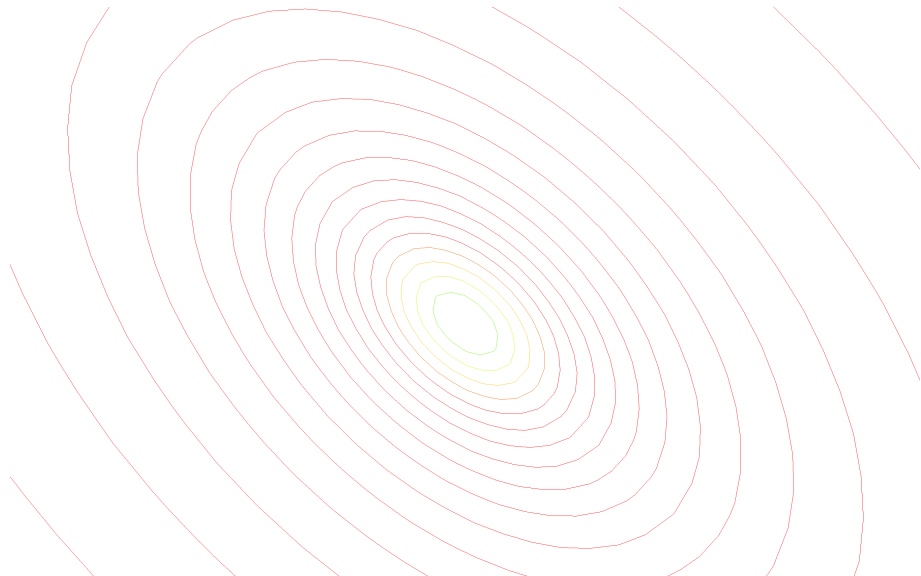
MB-SGD with Momentum

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

$$\mathbf{v}_t \leftarrow \mathbf{v}_{t-1} + \nabla_\theta \mathcal{L}_{b(t)}$$
$$\boldsymbol{\theta}_t \leftarrow \boldsymbol{\theta}_{t-1} - \eta \mathbf{v}_t$$

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

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- Something of an art form!
  - 'Grad Student Descent' or GDGS ('Gradient Descent by Grad Student')

- Common Heuristic approach:
  - 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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- See `https://arxiv.org/abs/1506.01186`

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.
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- 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)

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!