

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...

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)
- 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:

$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} \mathcal{L}$$

- 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 \mathbf{D} and model g with learnable parameters θ .
- Define how many passes over the data to make (each one known as an Epoch)
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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:

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for each Epoch:  
    for each  $(\mathbf{x}, y) \in \mathbf{D}$ :  
         $\theta \leftarrow \theta - \eta \nabla_{\theta} \ell$ 
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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)

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 \mathbf{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** \mathbf{D}_b , \mathcal{L}_b by the learning rate η multiplied by the gradient:

partition the dataset \mathbf{D} into an array of subsets of size b
for each Epoch:

for each $\mathbf{D}_b \in \text{partitioned}(\mathbf{D})$:
$$\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} \mathcal{L}_b$$

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- Mini-batch Stochastic Gradient Descent has reasonable statistical properties (much lower variance than SGD)
- Allows for computational 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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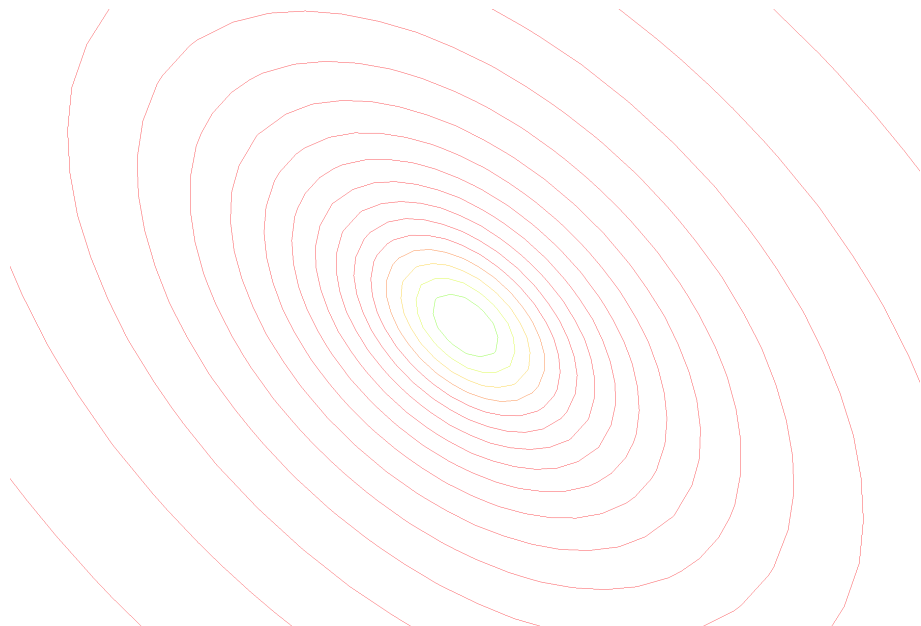
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 - Symmetries (permutation, etc)
 - Certainly no single global minima

*GD in the convex case: failure modes



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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

Momentum I

It's common for the 'leaky' average (the 'velocity', v_t) to be an 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'.

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

- 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

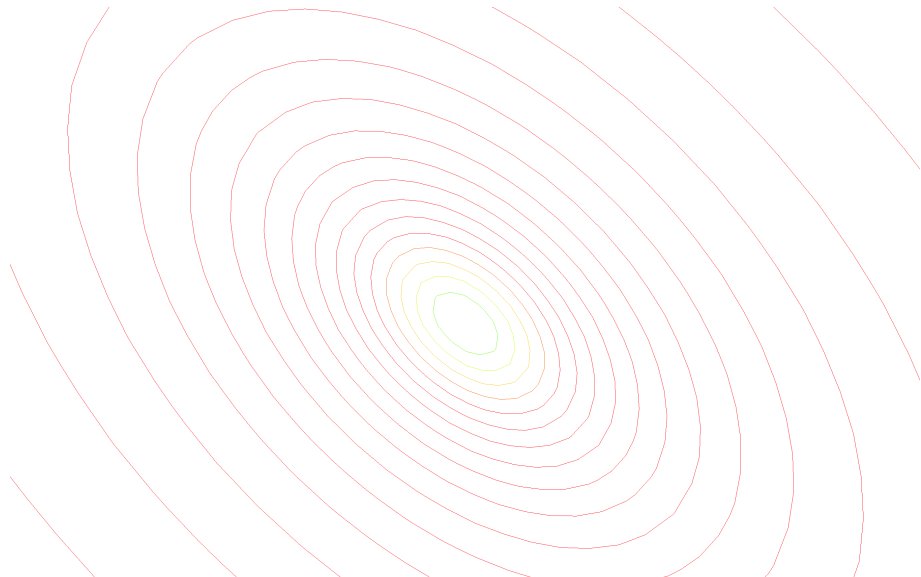
Learning with momentum on iteration t (batch at t denoted by $b(t)$) is given by:

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

$$\theta_t \leftarrow \theta_{t-1} - \eta \mathbf{v}_t$$

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

SGD with Momentum - potentially better convex convergence



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- Smaller steps will help you get closer to the minima
- But don't do it too early, else you might get stuck
- Something of an art form!
 - 'Grad Student Descent' or GDGS ('Gradient Descent by Grad Student')

Reduce LR on plateau

- 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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 - Modifies Adagrad to decouple learning rate from gradient magnitude scaling
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 - LR would typically follow a predefined schedule
- Adam
 - Essentially takes all the best ideas from RMSProp and SGD+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!