

Deep Learning (CS324)

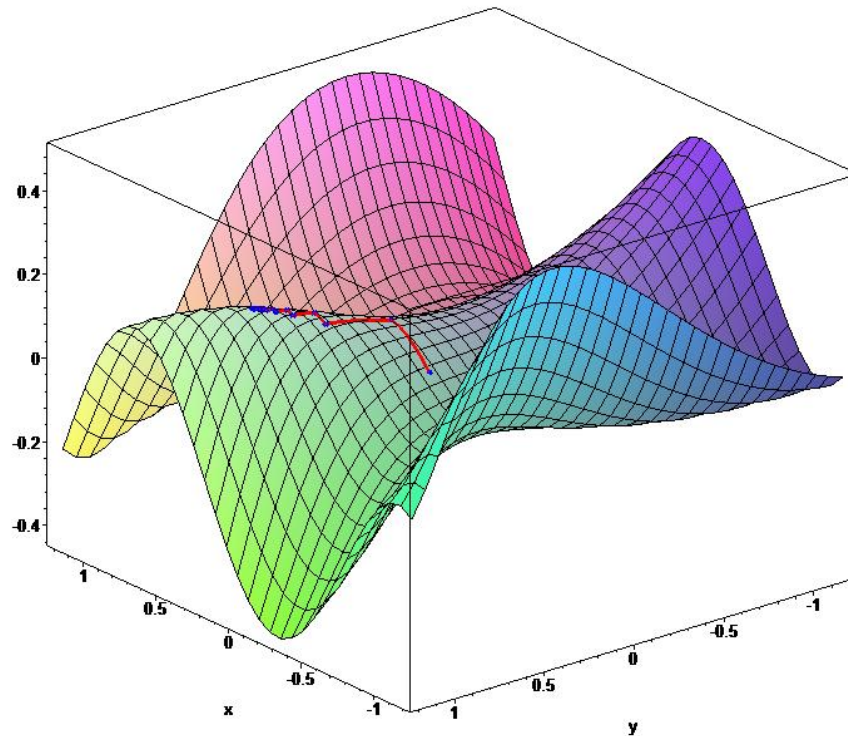
4. Optimisation and regularisation*

Prof. Jianguo Zhang
SUSTech

Gradient descent

- We've already learned how gradient descent works...

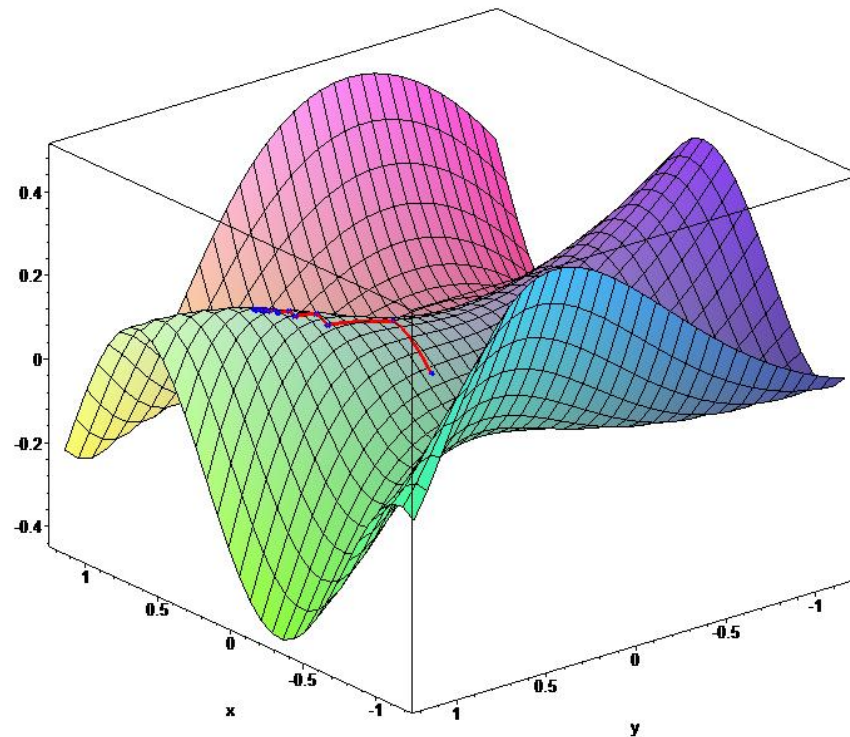
$$w^{(t+1)} = w^{(t)} - \eta_t \nabla_{w^{(t)}} L$$



Gradient descent

- ...but actually there are many versions of it!

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Batch gradient descent

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- If we compute the gradient on the full training set we are doing **batch gradient descent**

$$\nabla_{w^{(t)}} L = \frac{1}{m} \sum_{i=1}^m \nabla_{w^{(t)}} L(w; x_i, y_i)$$

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m training samples (x_i, y_i)

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But note that this is just a sample gradient, an estimate that is likely to be different from the true gradient if we knew the real data distribution

Batch gradient descent

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$$\nabla_{w^{(t)}} L = \frac{1}{m} \sum_{i=1}^m \nabla_{w^{(t)}} L(w; x_i, y_i)$$

In practice we compute the loss as the average loss over all the training samples and then we compute the gradient of this number wrt w

$$L = \frac{1}{m} \sum_{i=1}^m L(x_i, y_i)$$

Batch GD: advantages

- Acceleration techniques based on second order derivatives (Hessian) can be used
- We can measure not only the gradient but also the curvature of the loss function
- It's possible to do a simple theoretical analysis of the convergence rate

Batch GD: disadvantages

- Datasets can be too large for a complete gradient computation to be feasible
- Loss surfaces are highly non-convex and high dimensional

Stochastic gradient descent

- An alternative is to compute the gradient and use it to update the weights as we input the training samples one by one
- This is called **Stochastic Gradient Descent** (SGD)
- Instead of doing...

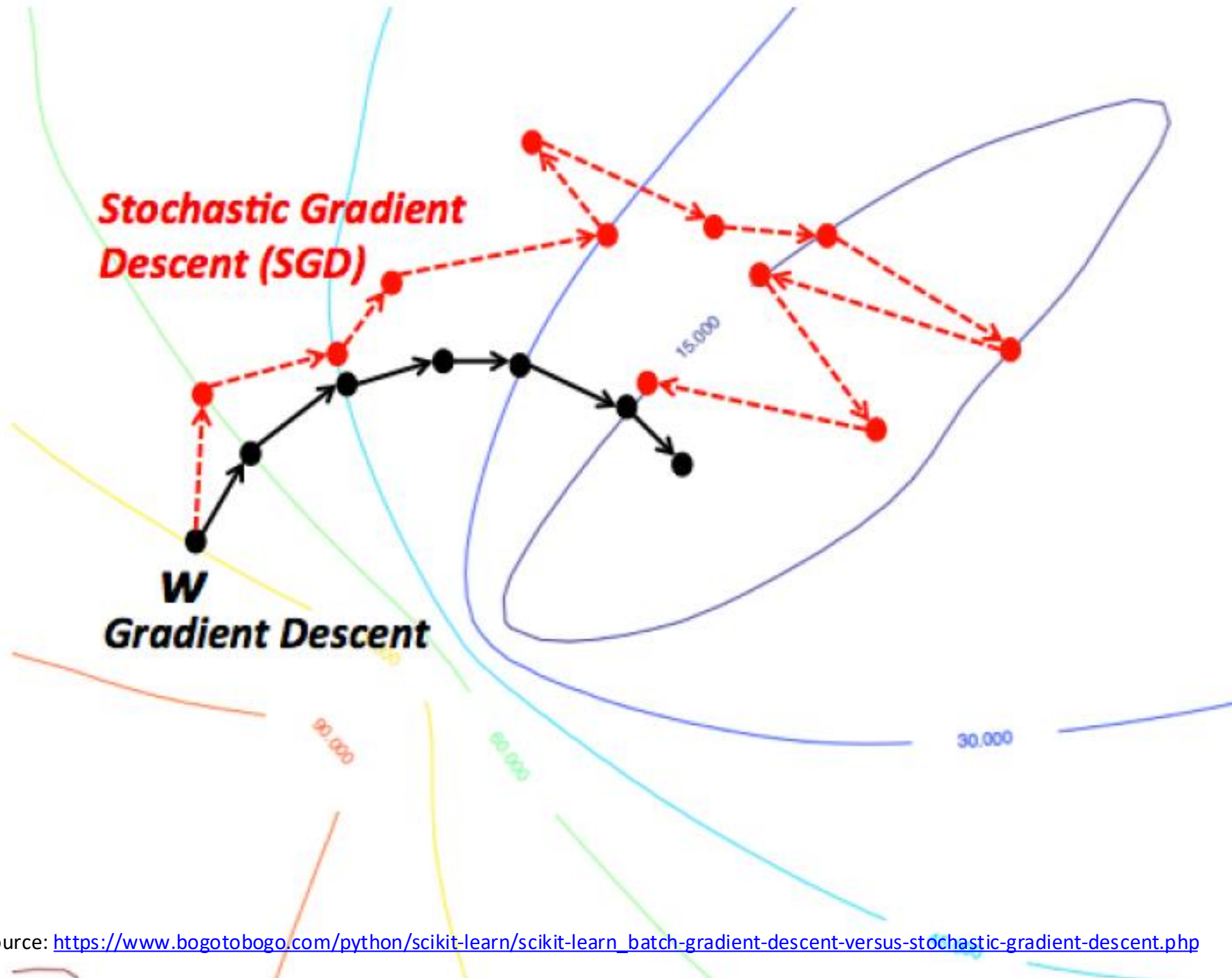
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Stochastic gradient descent

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Stochastic gradient descent

- An alternative is to compute the gradient and use it to update the weights as we input the training samples one by one
- This is called **Stochastic Gradient Descent** (SGD)
- We do...
$$w^{(t+1)} = w^{(t)} - \eta_t \nabla_{w^{(t)}} L(w; x_i, y_i)$$
 - Choose an initial vector of parameters w and learning rate η .
 - Repeat until an approximate minimum is obtained:
 - Randomly shuffle examples in the training set.
 - For $i = 1, 2, \dots, n$, do:
 - $w := w - \eta \nabla Q_i(w)$.



SGD: advantages

- Faster than gradient descent
 - Start improving from first sample rather than waiting; also, there may be redundant when considering whole training data
- Randomness helps to avoid overfitting, which in turn can improve the accuracy
- Suitable for datasets that change over time

SGD: disadvantages

- Mostly, it's an approximation of an approximation so it's bound to be imperfect
 - But in practice this is not a problem, in fact it's an advantage (noise helps against overfitting)
- The main problem is that with samples of size 1 we can't take advantage of massive parallelism...

Mini-batch gradient descent

- So why not using more than 1 data sample to compute the gradient, but less than the entire training set?
- This is called **mini-batch gradient descent**

$$w^{(t+1)} = w^{(t)} - \frac{\eta_t}{|B|} \sum_{b \in B} \nabla_{w^{(t)}} L(w; b)$$

- where B is a sample of the data
- More general version of stochastic gradient descent (so often called SGD)

Mini-batch gradient descent

Algorithm 8.1 Stochastic gradient descent (SGD) update

Require: Learning rate schedule $\epsilon_1, \epsilon_2, \dots$

Require: Initial parameter θ

$k \leftarrow 1$

while stopping criterion not met **do**

 Sample a minibatch of m examples from the training set $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ with corresponding targets $\mathbf{y}^{(i)}$.

 Compute gradient estimate: $\hat{\mathbf{g}} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

 Apply update: $\theta \leftarrow \theta - \epsilon_k \hat{\mathbf{g}}$

$k \leftarrow k + 1$

end while

SGD vs GD

- SGD works well when the data changes over time, while GD is biased toward “past” samples
- SGD can choose samples with maximum information content
- SGD can also choose samples that generated the largest errors in the previous epoch, to yield larger gradients and thus faster learning

SGD vs GD

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Challenges in optimisation

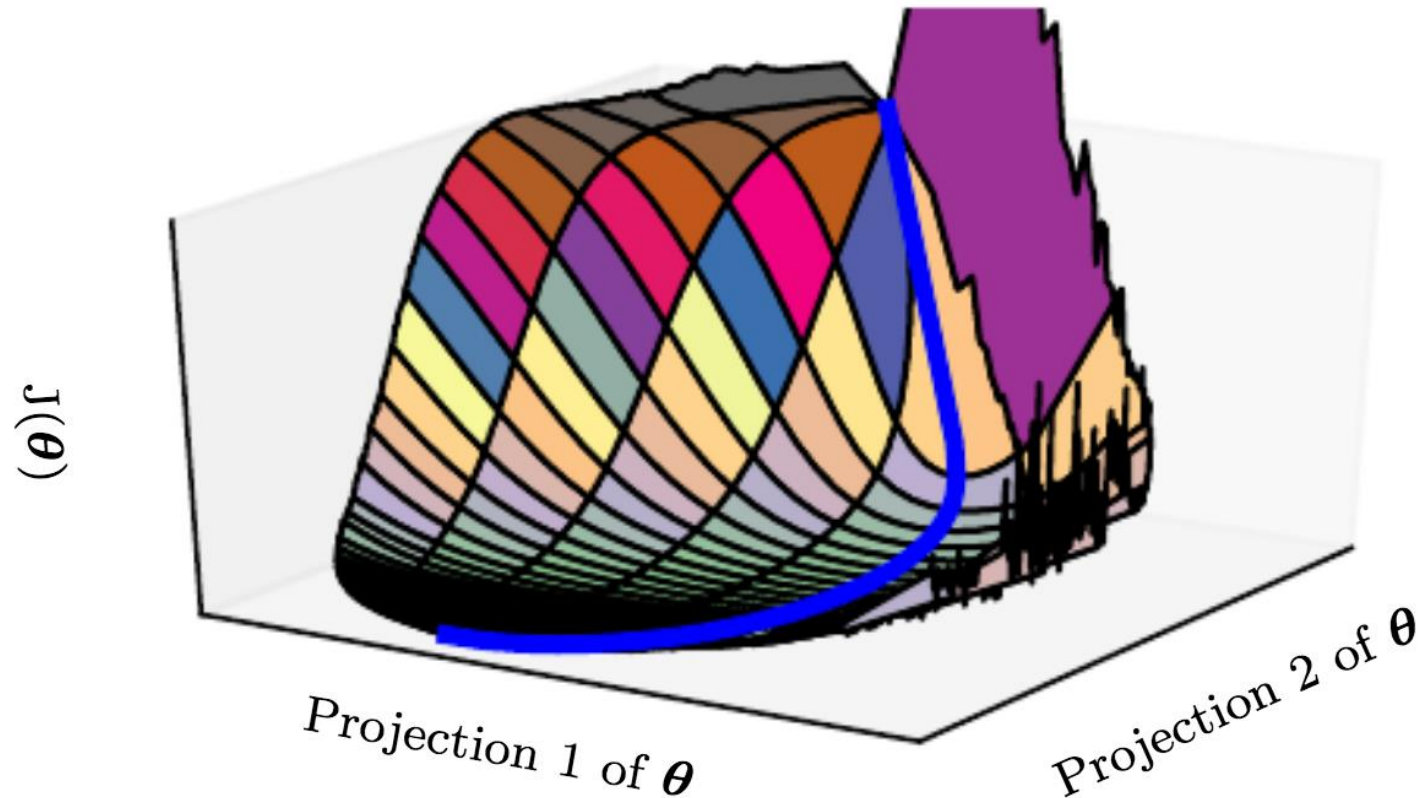
- Ill-conditioning

$$f(\mathbf{x}) \approx f(\mathbf{x}^{(0)}) + (\mathbf{x} - \mathbf{x}^{(0)})^\top \mathbf{g} + \frac{1}{2}(\mathbf{x} - \mathbf{x}^{(0)})^\top \mathbf{H}(\mathbf{x} - \mathbf{x}^{(0)})$$

$$f(\mathbf{x}^{(0)} - \epsilon \mathbf{g}) \approx f(\mathbf{x}^{(0)}) - \epsilon \mathbf{g}^\top \mathbf{g} + \frac{1}{2}\epsilon^2 \mathbf{g}^\top \mathbf{H} \mathbf{g}.$$

- Local minima
- Plateaus, saddle points, and other flat regions

Challenges in optimisation



Challenges in optimisation

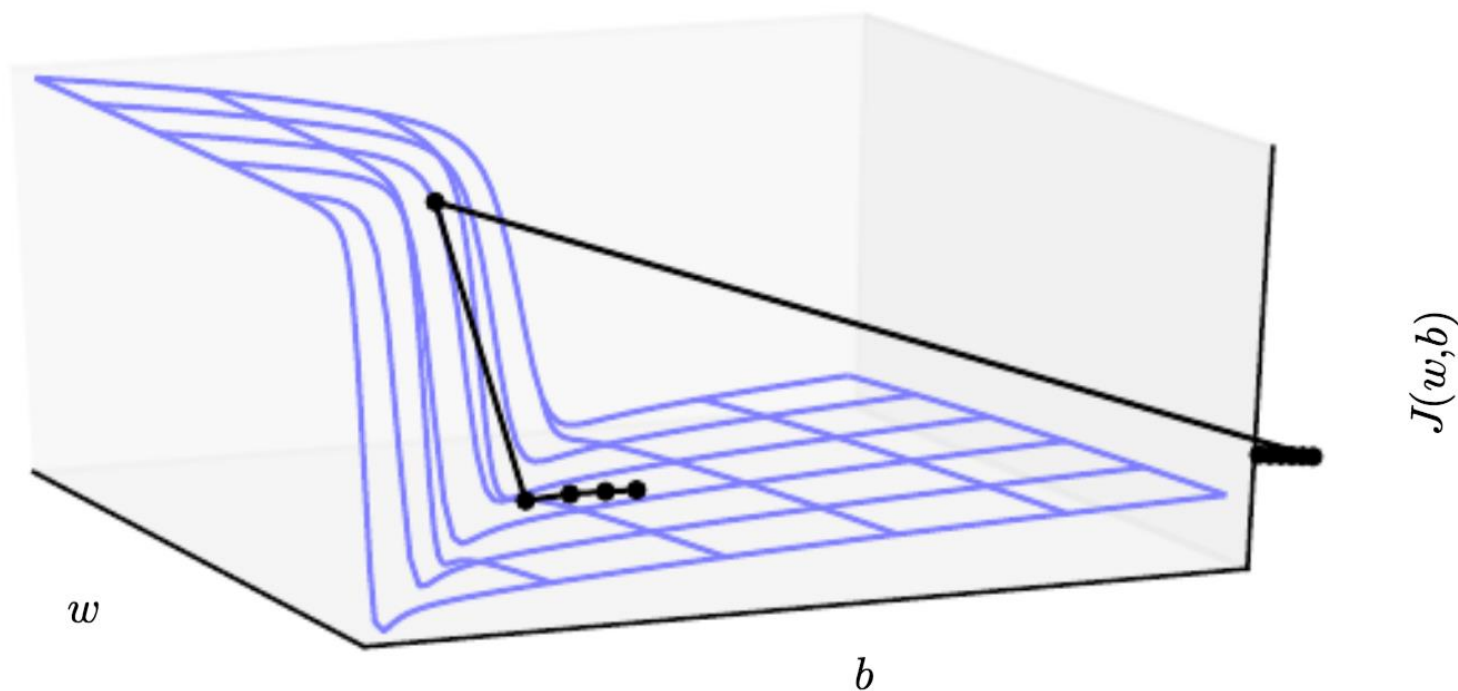
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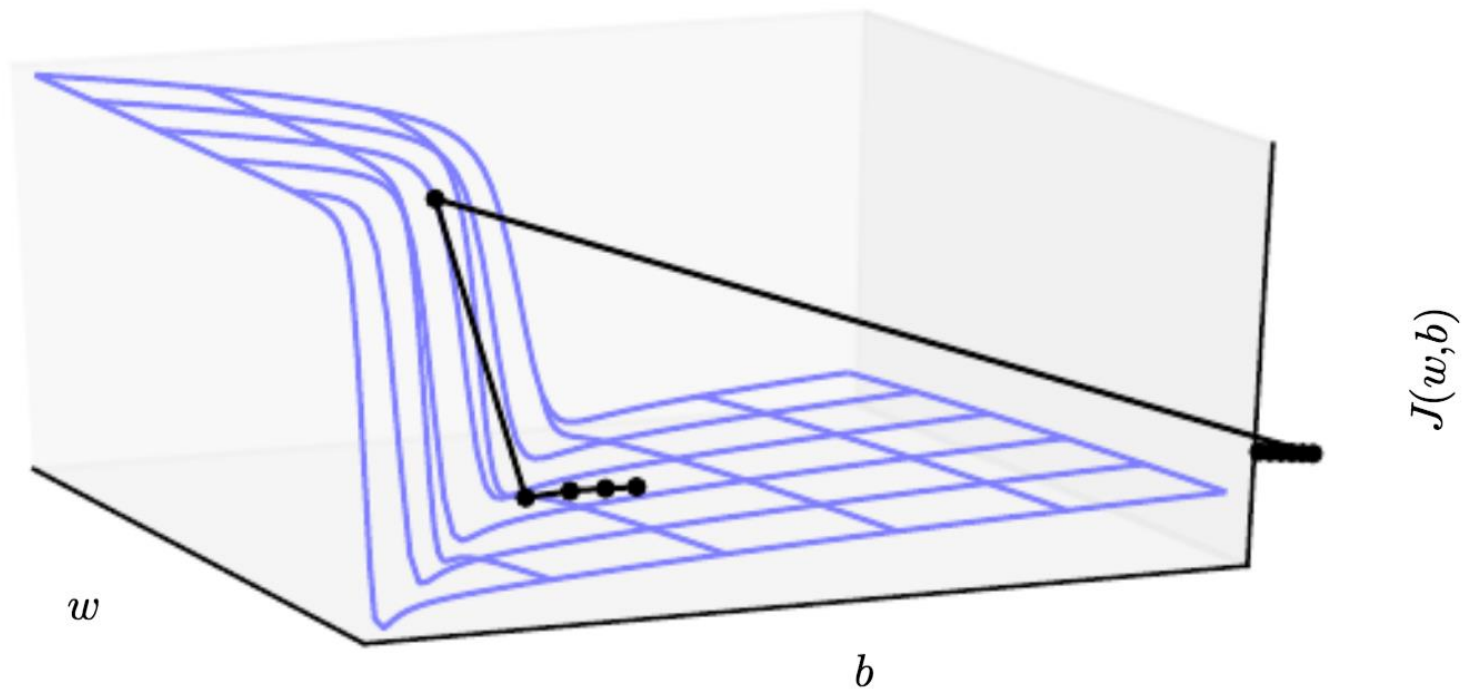
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- Local minima
- Plateaus, saddle points, and other flat regions
- Cliffs and exploding gradients

Challenges in optimisation



Challenges in optimisation



See <https://www.cs.umd.edu/~tomg/projects/landscapes/>
for more cool visualisations

Momentum

- Analogy with physical momentum
- Keep taking into account past gradients but let their contribution decay exponentially with time
- This is performed through a **velocity** parameter which accumulates the value of previous gradients
- This dampens oscillations, yielding a more robust gradients which in turn leads to faster convergence

SGD with momentum

Algorithm 8.2 Stochastic gradient descent (SGD) with momentum

Require: Learning rate ϵ , momentum parameter α

Require: Initial parameter θ , initial velocity v

while stopping criterion not met **do**

 Sample a minibatch of m examples from the training set $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ with corresponding targets $\mathbf{y}^{(i)}$.

 Compute gradient estimate: $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$.

 Compute velocity update: $\mathbf{v} \leftarrow \alpha \mathbf{v} - \epsilon \mathbf{g}$.

 Apply update: $\theta \leftarrow \theta + \mathbf{v}$.

end while

SGD with momentum

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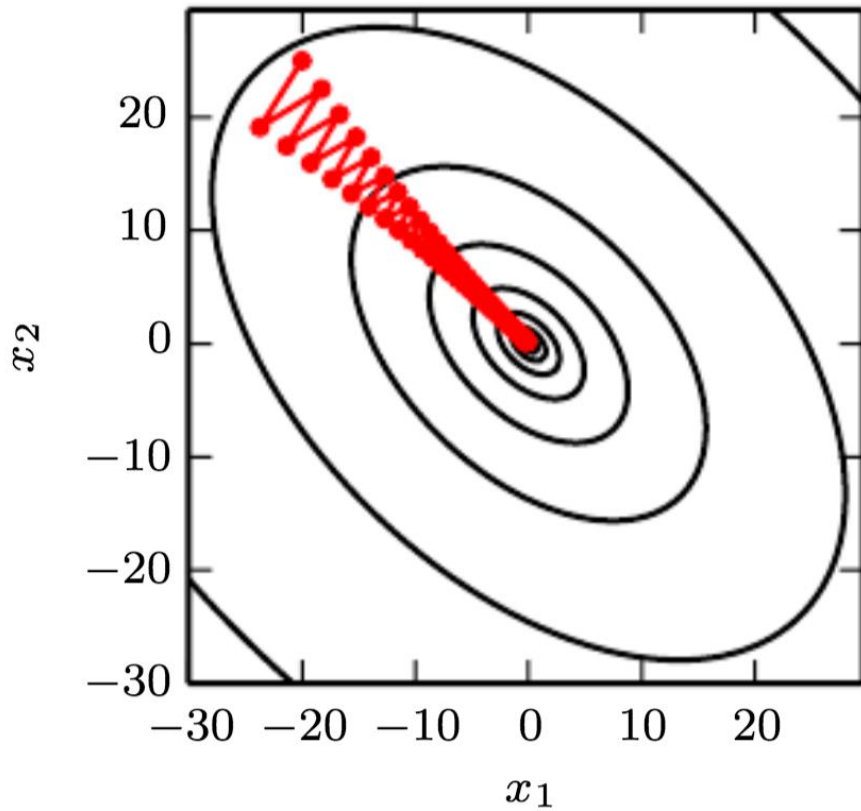
 Apply update: $\theta \leftarrow \theta + \mathbf{v}$.

end while

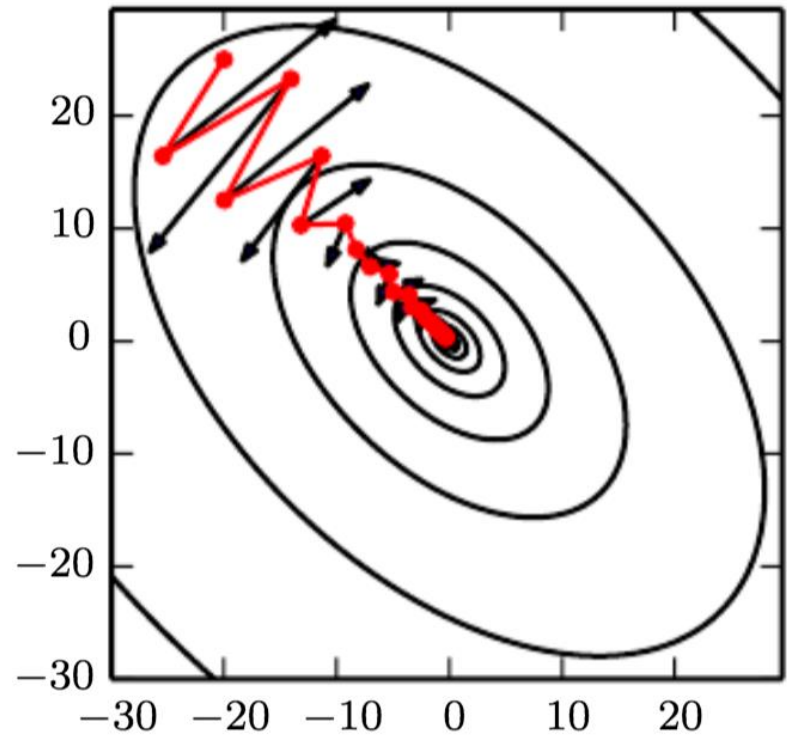
Typical values are 0.5, 0.9, or 0.99.

Usually it starts at a low value that is then raised with time

Momentum



Without momentum



With momentum

Nesterov momentum

梯度计算在施加当前速度之后

- Just like standard momentum, but **use the future gradient** (which results in better convergence)

Algorithm 8.3 Stochastic gradient descent (SGD) with Nesterov momentum

Require: Learning rate ϵ , momentum parameter α

Require: Initial parameter θ , initial velocity v

while stopping criterion not met **do**

 Sample a minibatch of m examples from the training set $\{x^{(1)}, \dots, x^{(m)}\}$ with corresponding labels $y^{(i)}$.

 Apply interim update: $\tilde{\theta} \leftarrow \theta + \alpha v$.

 Compute gradient (at interim point): $g \leftarrow \frac{1}{m} \nabla_{\tilde{\theta}} \sum_i L(f(x^{(i)}; \tilde{\theta}), y^{(i)})$.

 Compute velocity update: $v \leftarrow \alpha v - \epsilon g$.

 Apply update: $\theta \leftarrow \theta + v$.

end while

Adaptive learning rates

- Learning rate hard to set as it significantly affects the model performance
 - Loss function can change in very different ways in different directions
 - Momentum helps, but it's yet another hyper parameter
- We can try to learn individual learning rates for each parameter and automatically adapt them

Delta-bar-delta

- One the first heuristics (1988) to adapt individual learning rates during training
- If the sign of the partial derivative of the loss with respect to a given model parameter remains the same, then the learning rate should increase
- If it changes, the learning rate should decrease
- Works only with batch gradient descent (can you guess why?)

AdaGrad

- Adapt learning rates of model parameters by scaling them inversely proportional to the square root of the sum of all the past squared values of the gradient
- Learning rate of parameters with large (small) value of partial derivative of loss decreases (increases)
 - Faster progress in gently sloped directions
- But long history of gradients can slow things down

AdaGrad

Algorithm 8.4 The AdaGrad algorithm

Require: Global learning rate ϵ

Require: Initial parameter θ

Require: Small constant δ , perhaps 10^{-7} , for numerical stability

Initialize gradient accumulation variable $\mathbf{r} = \mathbf{0}$

while stopping criterion not met **do**

 Sample a minibatch of m examples from the training set $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ with corresponding targets $\mathbf{y}^{(i)}$.

 Compute gradient: $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$.

 Accumulate squared gradient: $\mathbf{r} \leftarrow \mathbf{r} + \mathbf{g} \odot \mathbf{g}$.

 Compute update: $\Delta \theta \leftarrow -\frac{\epsilon}{\delta + \sqrt{\mathbf{r}}} \odot \mathbf{g}$. (Division and square root applied element-wise)

 Apply update: $\theta \leftarrow \theta + \Delta \theta$.

end while

RMSprop

- RMSprop is an (unpublished) modification of AdaGrad that accumulates past gradients using an exponential moving average*
- While AdaGrad is designed to work well for convex functions, RMSprop works better in non-convex settings (typical of deep learning)

*https://en.wikipedia.org/wiki/Moving_average#Exponential_moving_average

RMSprop

Algorithm 8.5 The RMSProp algorithm

Require: Global learning rate ϵ , decay rate ρ

Require: Initial parameter θ

Require: Small constant δ , usually 10^{-6} , used to stabilize division by small numbers

Initialize accumulation variables $\mathbf{r} = 0$

while stopping criterion not met **do**

 Sample a minibatch of m examples from the training set $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ with corresponding targets $\mathbf{y}^{(i)}$.

 Compute gradient: $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$.

 Accumulate squared gradient: $\mathbf{r} \leftarrow \rho \mathbf{r} + (1 - \rho) \mathbf{g} \odot \mathbf{g}$.

 Compute parameter update: $\Delta \theta = -\frac{\epsilon}{\sqrt{\delta + \mathbf{r}}} \odot \mathbf{g}$. ($\frac{1}{\sqrt{\delta + \mathbf{r}}}$ applied element-wise)

 Apply update: $\theta \leftarrow \theta + \Delta \theta$.

end while

Adam

- Best understood as a way of combining RMSprop with SGD + momentum
- Uses square gradients to scale learning rate like RMSprop + moving average of gradient for momentum
- Turns out to be fairly robust to choice of hyperparameters

Adam

Algorithm 8.7 The Adam algorithm

Require: Step size ϵ (Suggested default: 0.001)

Require: Exponential decay rates for moment estimates, ρ_1 and ρ_2 in $[0, 1)$.
(Suggested defaults: 0.9 and 0.999 respectively)

Require: Small constant δ used for numerical stabilization (Suggested default: 10^{-8})

Require: Initial parameters θ

Initialize 1st and 2nd moment variables $\mathbf{s} = \mathbf{0}$, $\mathbf{r} = \mathbf{0}$

Initialize time step $t = 0$

while stopping criterion not met **do**

 Sample a minibatch of m examples from the training set $\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(m)}\}$ with corresponding targets $\mathbf{y}^{(i)}$.

 Compute gradient: $\mathbf{g} \leftarrow \frac{1}{m} \nabla_{\theta} \sum_i L(f(\mathbf{x}^{(i)}; \theta), \mathbf{y}^{(i)})$

$t \leftarrow t + 1$

 Update biased first moment estimate: $\mathbf{s} \leftarrow \rho_1 \mathbf{s} + (1 - \rho_1) \mathbf{g}$

 Update biased second moment estimate: $\mathbf{r} \leftarrow \rho_2 \mathbf{r} + (1 - \rho_2) \mathbf{g} \odot \mathbf{g}$

 Correct bias in first moment: $\hat{\mathbf{s}} \leftarrow \frac{\mathbf{s}}{1 - \rho_1^t}$

 Correct bias in second moment: $\hat{\mathbf{r}} \leftarrow \frac{\mathbf{r}}{1 - \rho_2^t}$

 Compute update: $\Delta \theta = -\epsilon \frac{\hat{\mathbf{s}}}{\sqrt{\hat{\mathbf{r}} + \delta}}$ (operations applied element-wise)

 Apply update: $\theta \leftarrow \theta + \Delta \theta$

end while

What's the optimal optimiser?

- There's still not a generally accepted answer to this question, unfortunately
- For a visualisation of different optimisers seeking the minimise various landscapes see the excellent visualisations at <https://github.com/Jaewan-Yun/optimizer-visualization>
- See also <http://runder.io/optimizing-gradient-descent/> for a good summary of the different optimisers available

Also check: <https://blog.paperspace.com/intro-to-optimization-momentum-rmsprop-adam/>

Second order optimisation

- The methods seen so far rely only on first-order information (gradient)
- Using second-order information (Hessian) can help to improve convergence
- Based on Newton's method

$$J(\boldsymbol{\theta}) \approx J(\boldsymbol{\theta}_0) + (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \mathbf{H}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)$$

$$\boldsymbol{\theta}^* = \boldsymbol{\theta}_0 - \mathbf{H}^{-1} \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0)$$

Second order optimisation

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$$\boldsymbol{\theta}^* = \boldsymbol{\theta}_0 - \mathbf{H}^{-1} \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0)$$

- If J is locally quadratic (\mathbf{H} is positive definite) then we can jump directly to the minimum
- Otherwise, iterate steps 1) quadratic approximation & 2) update parameters
- However if \mathbf{H} has negative eigenvalues we may end up moving in the wrong direction

Second order optimisation

- We need to modify the Hessian

$$J(\boldsymbol{\theta}) \approx J(\boldsymbol{\theta}_0) + (\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \nabla_{\boldsymbol{\theta}} J(\boldsymbol{\theta}_0) + \frac{1}{2}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)^\top \mathbf{H}(\boldsymbol{\theta} - \boldsymbol{\theta}_0)$$

$$\boldsymbol{\theta}^* = \boldsymbol{\theta}_0 - [\mathbf{H}(f(\boldsymbol{\theta}_0)) + \alpha \mathbf{I}]^{-1} \nabla_{\boldsymbol{\theta}} f(\boldsymbol{\theta}_0)$$

- But when curvature is very high we may need to increase alpha to the point that diagonal dominates and method becomes standard gradient descent with small step size
- Also, inverting the Hessian is expensive
 - $O(k^3)$ where k is the number of parameters

Regularisation

- Deep networks can have millions of parameters, often more than the size of the training data, which can lead to overfitting!
 - Need to regularise the loss function

$$w^* = \operatorname{argmin}_{x,y} \sum L(w_1, \dots, w_L; x, y) + \lambda \Omega(\theta)$$

- Possible methods include L1 regularisation, L2 regularisation, and Dropout
- The goal is to *reduce the model capacity*

L1 regularisation

- L1 regularisation enforces sparse weights, i.e., more weights become 0 (i.e., delete connections)
- Performs feature selection (which features of the input data should we retain?)

$$w^* = \operatorname{argmin}_{x,y} \sum L(w_1, \dots, w_L; x, y) + \lambda \sum_l |w_l|$$

Why sparse?

<https://medium.com/mlreview/l1-norm-regularization-and-sparsity-explained-for-dummies-5b0e4be3>

L1 regularisation

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$$w^* = \operatorname{argmin}_{x,y} \sum L(w_1, \dots, w_L; x, y) + \lambda \sum_l |w_l|$$

$$w_l = w_l - \lambda \eta \frac{w_l}{|w_l|} - \eta \nabla_w L$$

Sign function (+1 or -1)

L2 regularisation

- Most popular type of regression, drives weights closer to the origin
- Nice analytical form (can derive and thus compute gradient)
- Usually lambda is 10^{-1} or 10^{-2}

$$w^* = \operatorname{argmin}_{x,y} \sum L(w_1, \dots, w_L; x, y) + \frac{\lambda}{2} \sum_l ||w_l||_2^2$$

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$$w^* = \operatorname{argmin}_{x,y} \sum L(w_1, \dots, w_L; x, y) + \frac{\lambda}{2} \sum_l ||w_l||_2^2$$

$$w_l = (1 - \lambda\eta)w_l - \eta_t \nabla_{w_l} L$$

The gradient descent step changes to this
Note the “weight decay”

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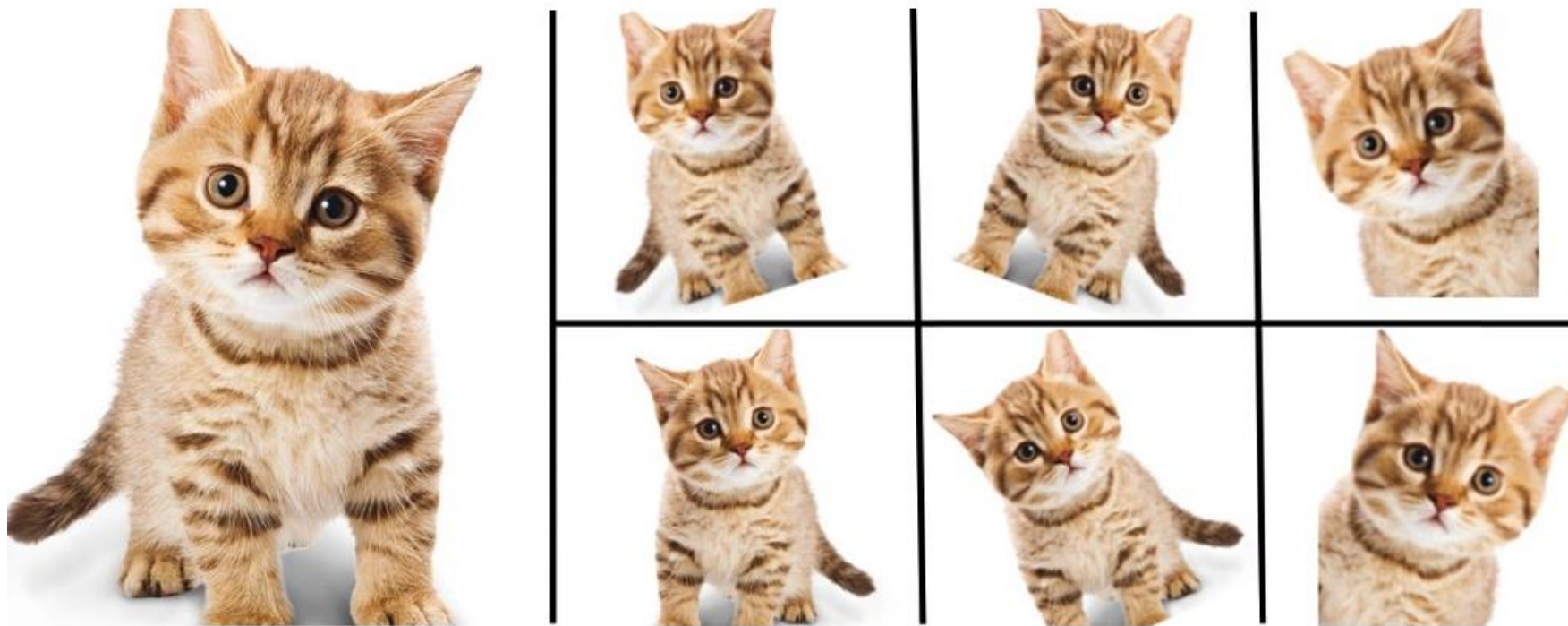
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$$w_l = (1 - \lambda\eta)w_l - \eta_t \nabla_{w_l} L$$

Practically what happens is that we decrease the weight on features that have low covariance with the output target (i.e., less important features)

Dataset augmentation

- Instead of reducing the capacity of the model, another way to reduce overfitting is to **have more training data!**
- This approach is particularly easy to apply on object recognition tasks, where we can take input data and generate transformed version of it that simulate real-world scenarios (e.g., occlusion, rotation, etc.)

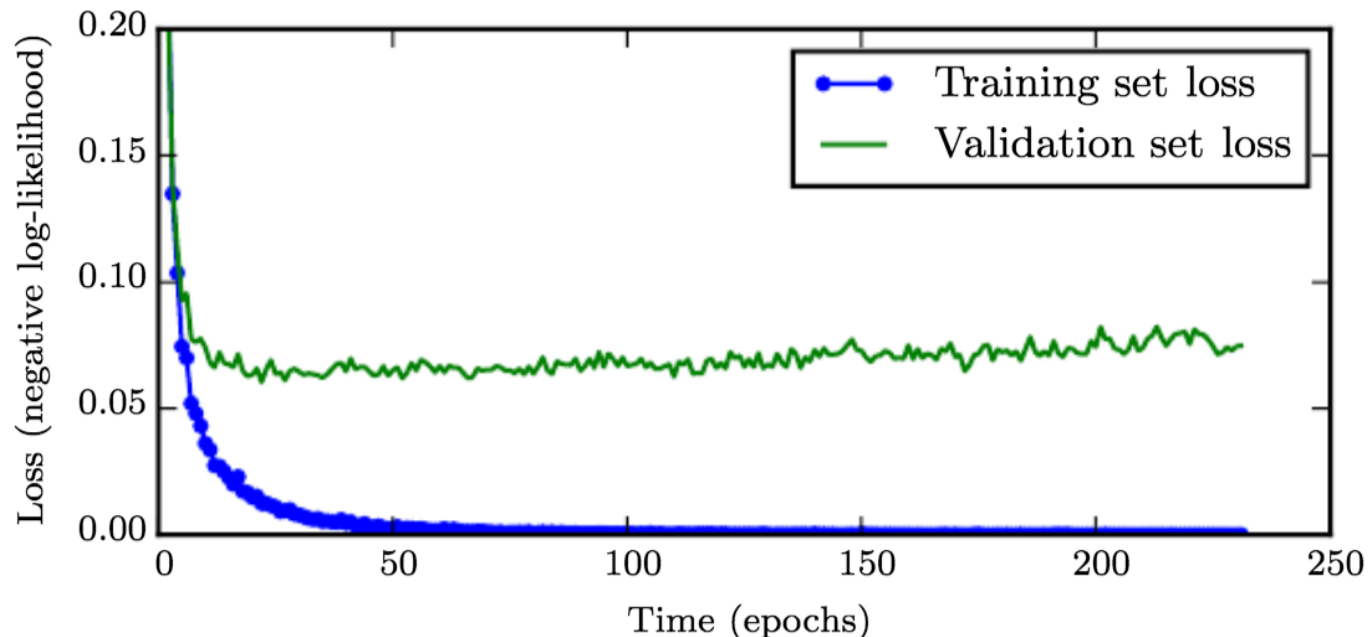


Enlarge your Dataset

Source: <https://medium.com/nanonets/how-to-use-deep-learning-when-you-have-limited-data-part-2-data-augmentation-c26971dc8ced>

Early stopping

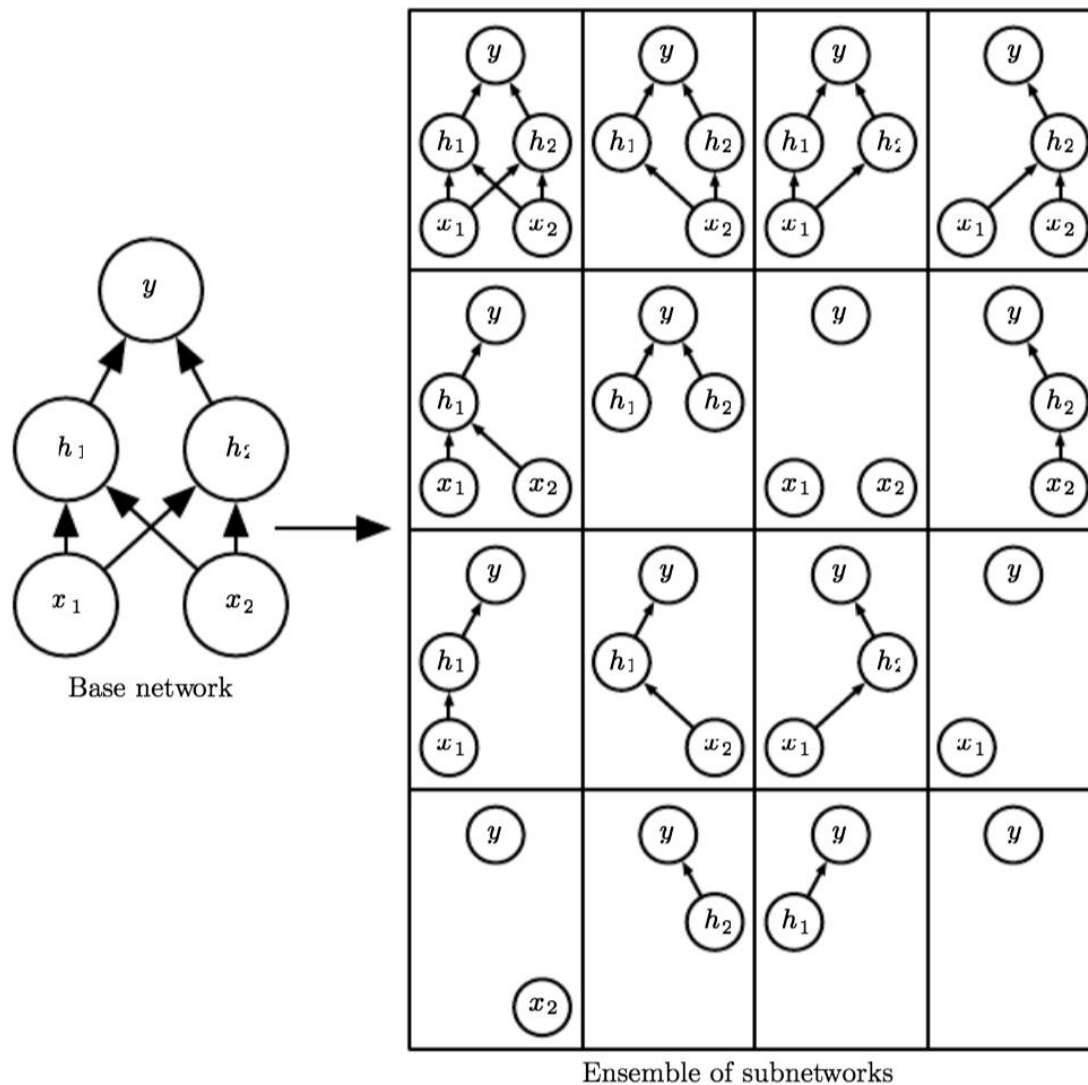
- Simple idea: to avoid overfitting, stop training when validation set error starts increasing, even if training error is still decreasing



Number of epochs can be seen as hyper-parameter to optimise

Dropout

- During training, randomly “deactivate” some units according to a probability p
- At test time, use all units with activations weighted by p
- Advantages include:
 - Faster training
 - Less overfitting
 - Units become more robust



In each epoch we randomly “deactivate” some units, effectively training a different subnetwork of the base network

Other common practices

- Apart from choosing the optimisation scheme and applying regularisations, there are other standard practices we can use to initialise the parameters of the networks and pre-process the input data

Weight initialisation

- Deep learning training is iterative and strongly depends on the initialisation point (i.e., how we initialise the parameters of the network)
- Important principle: **weight asymmetry**
 - *Why?* Because if 2 units share the same activation, same weights, and same inputs, they will be updated in the same way (no learning)
 - So, **don't** give same value to all weights (e.g., 0)
 - Sample weights from Gaussian or uniform dists

Weight initialisation

- But, be careful:
 - **Large weights** will have strong symmetry-breaking effect and help to propagate strong signal during forward and backward propagation
 - However they may also cause exploding values, saturation of units
 - But we also don't want **small weights**...
 - **Also**, we want to maintain the same variance for input and output (because outputs are inputs of next layer)

Weight initialisation

- Uniform distribution initialisation (tanh)

$$W_{ij} \sim U\left(-\sqrt{\left(\frac{6}{m+n}\right)}, \sqrt{\left(\frac{6}{m+n}\right)}\right)$$

- Xavier initialisation (tanh)

$$W_{ij} \sim N\left(0, \sqrt{\frac{1}{m}}\right)$$

Where m is the number of inputs and n is the number of outputs of the layer

Weight initialisation

- Uniform distribution initialisation (sigmoid)

$$W_{ij} \sim U \left(-4\sqrt{\left(\frac{6}{m+n}\right)}, 4\sqrt{\left(\frac{6}{m+n}\right)} \right)$$

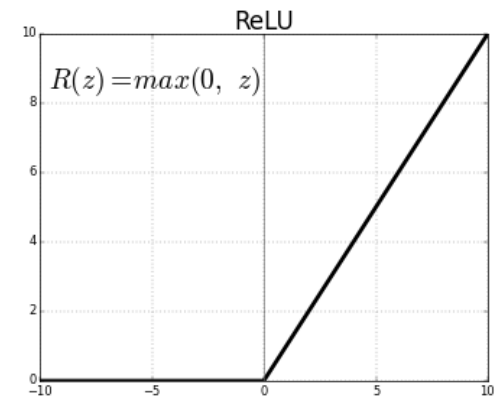
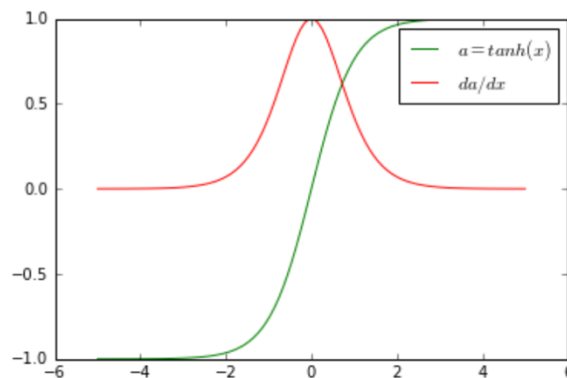
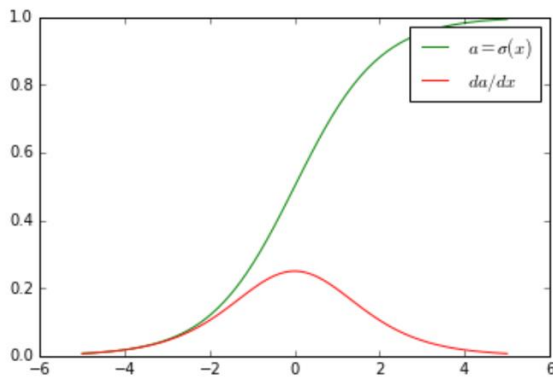
- ReLU initialisation

$$W_{ij} \sim N \left(0, \sqrt{\frac{2}{m}} \right)$$

Where m is the number of inputs and n is the number of outputs of the layer

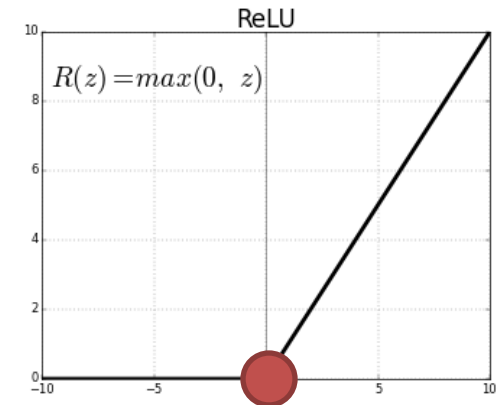
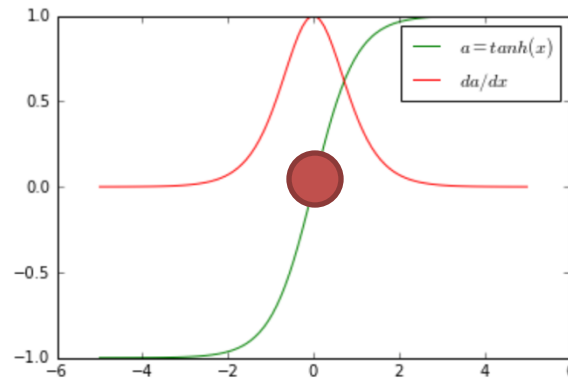
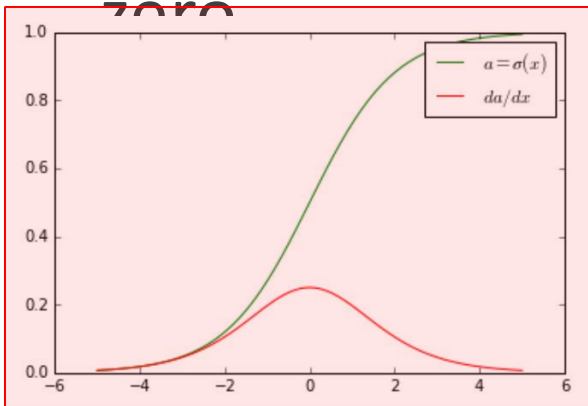
Data pre-processing

- Activation functions are usually centred around zero



Data pre-processing

- Activation functions are usually centred around



Not the sigmoid :(...

Data pre-processing

- Activation functions are usually centred around zero
- This is a good thing because it helps us to avoid saturation, which leads to **vanishing gradients**
- At the same time, we like **one-sided saturations** because they help to avoid variance due to noise

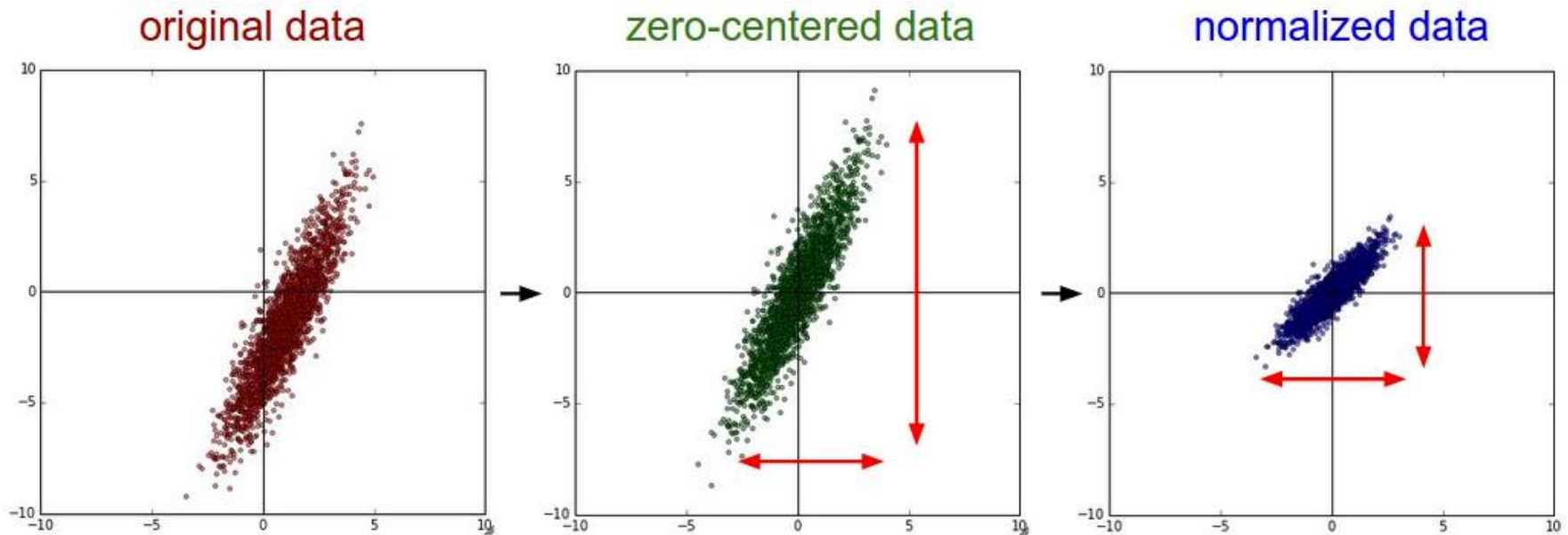
More about this here: <https://blog.paperspace.com/vanishing-gradients-activation-function/>

Data pre-processing

- Subtract mean so that training data is centred around zero as well
 - Otherwise may cause vanishing gradients
- Scale inputs to have similar diagonal covariances
 - Otherwise input samples with very different covariances can generate very different gradients and make the gradient update harder

Unit normalisation

- When input variables are normally distributed, subtract mean and **divide by** standard deviation



Source: <http://cs231n.github.io/neural-networks-2/>

Batch normalisation

- Two important principles. The distribution of the data fed to the layers of a network should be:
 - zero-centred
 - constant through time and data (mini-batches)

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 - Normalise the activations of each layer!

Batch normalisation

$$\mathbf{Z} = \mathbf{X}\mathbf{W}$$

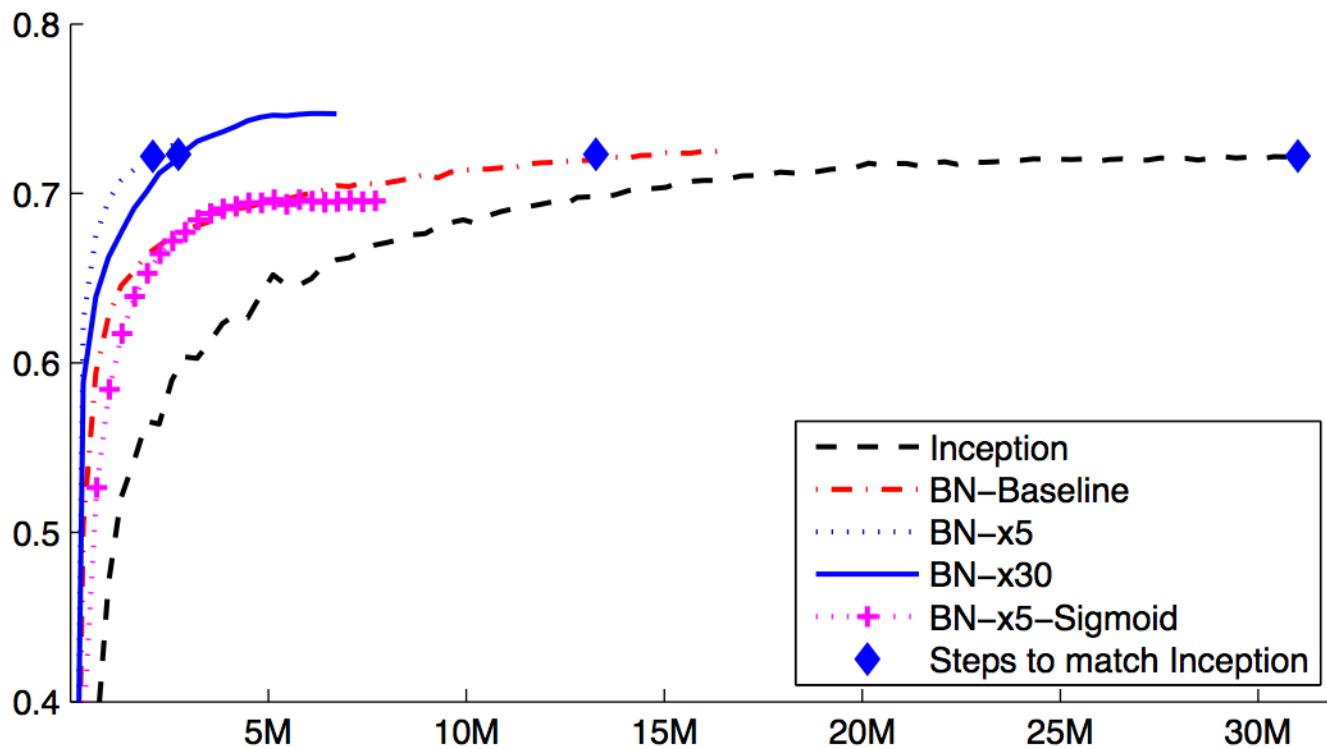
$$\tilde{\mathbf{Z}} = \mathbf{Z} - \frac{1}{m} \sum_{i=1}^m \mathbf{Z}_{i,:}$$

$$\hat{\mathbf{Z}} = \frac{\tilde{\mathbf{Z}}}{\sqrt{\epsilon + \frac{1}{m} \sum_{i=1}^m \tilde{\mathbf{Z}}_{i,:}^2}}$$

$$\mathbf{H} = \max\{0, \gamma \hat{\mathbf{Z}} + \beta\}$$

“Batch Normalization: Accelerating Deep Network Training by Reducing Internal Covariate Shift”
Ioffe and Szegedy 2015

Batch normalisation



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Summary

- Gradient descent and variants
- Momentum and learning rate
- Regularisation
- Parameters initialisation
- Input normalisation
- Batch normalisation