Neural Networks and Non-convex Optimisation

Machine Learning Theory (MLT)
Edinburgh
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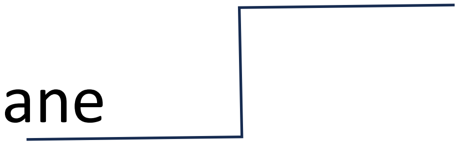
Course matters

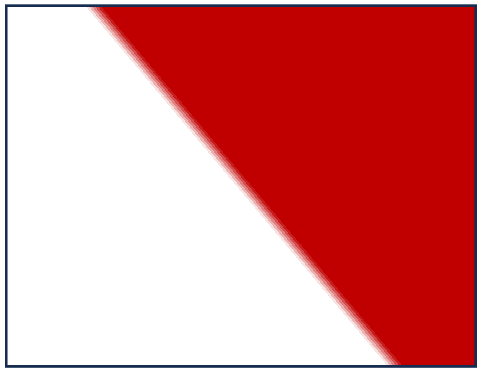
- Please attend tutorials!
- Solutions to tutorial 1 will be up soon

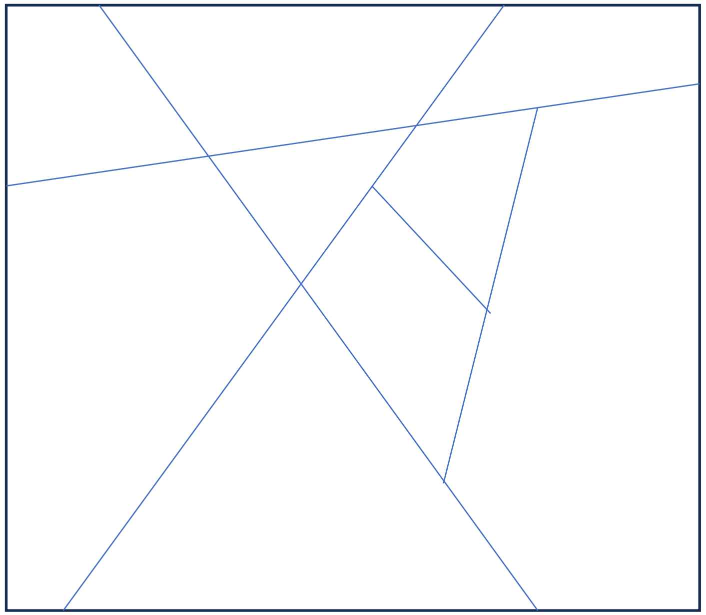
- Coursework will be out by end of day on Friday.

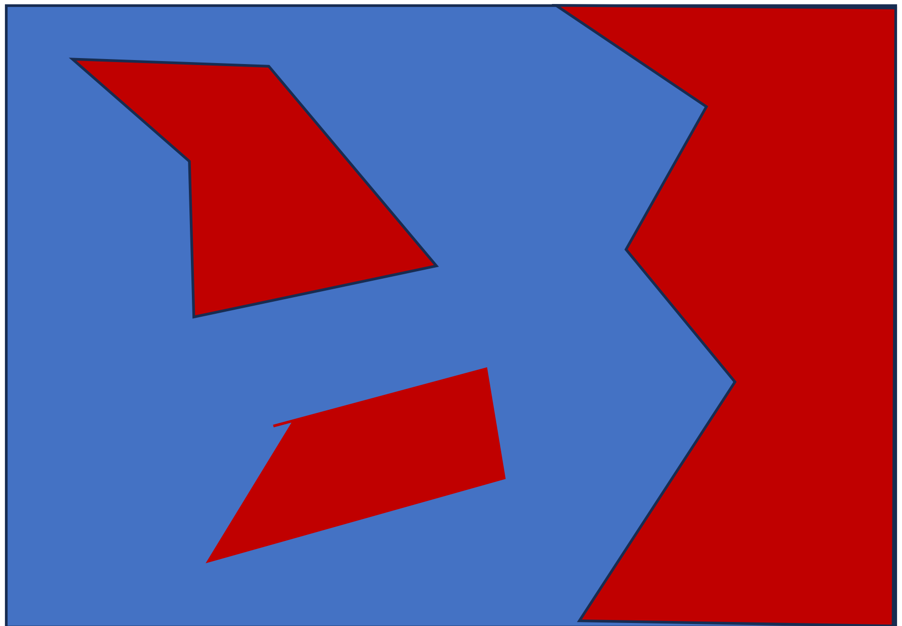
Neural networks

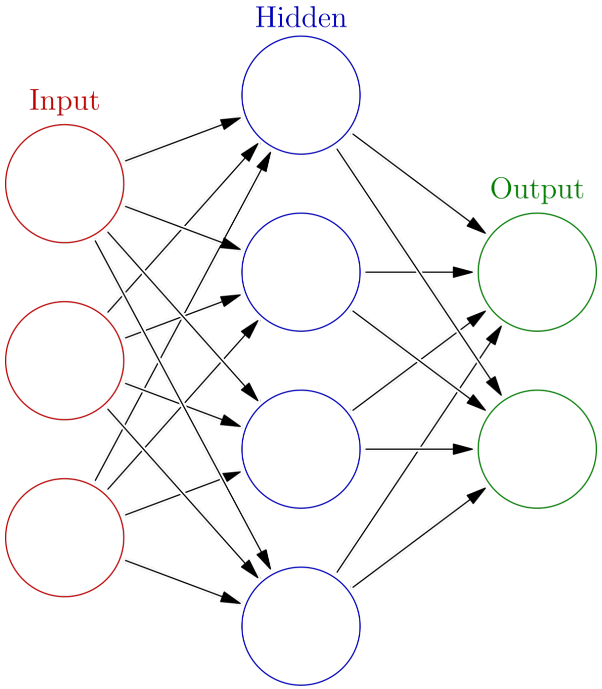
- Perceptron activation functions
- Each perceptron defines a half plane
- Together they can form complex boundaries using arrangements of half spaces
- More perceptrons, more options for regions available in the arrangement of half spaces









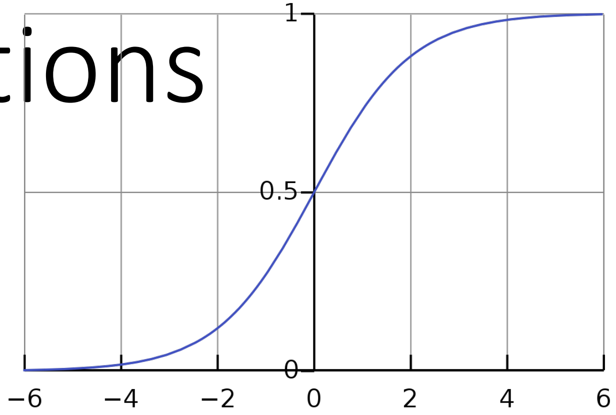


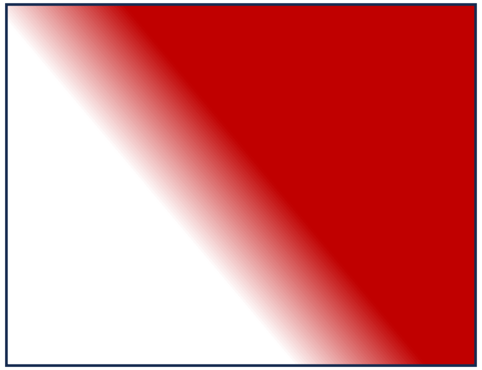
Challenges with perceptron and 0-1 values

- Gradients are not always useful
  - Eg. If a small change does not change the classification of any point
  - Hard to apply SGD type methods

- Sometimes it is useful to have real values

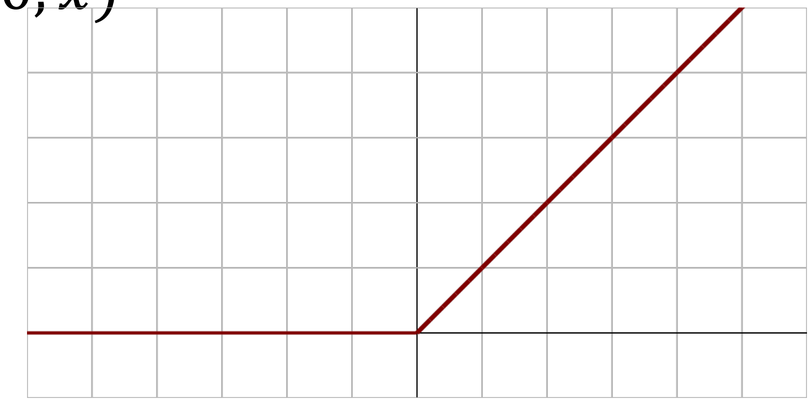
Other activations





- Sigmoid
  - $f(x) = \frac{1}{1+e^{x}}$

- ReLU
  - $f(x) = \max(0, x)$



Neural network structure

- Use ReLU or similar activation functions
  - More compatible with gradients
  - Easy to compute
- The middle layers produce a vector $\boldsymbol{y}$ of ”scores” for each class, called logit values
- Final layer: apply “softmax” to logits:
  - $softmax(\boldsymbol{y}_i) = \frac{e^{y_i}}{\sum e^{y_j}}$ (improved the notation from the lecture)

Question: Why softmax?

Hard max or exact max

- Take a vector of values eg. [2,3,5,2,6,4,9,2,2,4]
- Make one indicating the position of the max eg. [0,0,0,0,0,0,1,0,0,0]

Softmax

- Substitute for hard-max, but differentiable
- Normalized, can be treated as probability p_i for each class

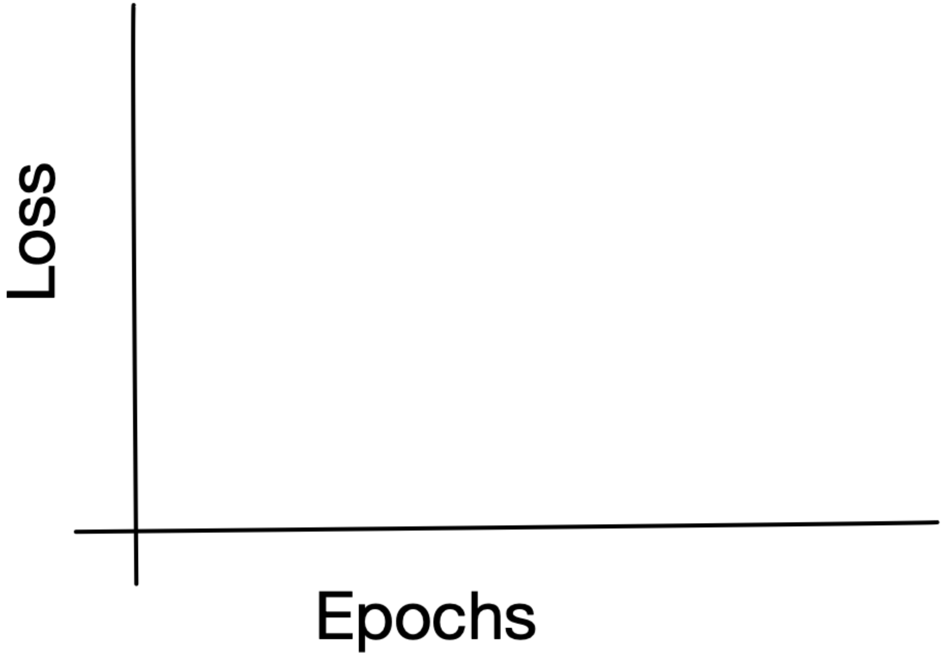
Cross entropy loss

- Neural networks are usually trained on the cross entropy loss of their output p
- Given:
  - Data point x
  - Probability estimate vector p
  - Truth label vector t: indicator vector or one-hot encoding where only the true class has value 1.
- Cross entropy loss: $\ell_{CE} = -\sum t_i \ln p_i$
  - Measures difference between the two probability distributions

p=[0.1, 0.5, 0.2, 0.2]
t= [0.0, 1.0, 0.0, 0.0]

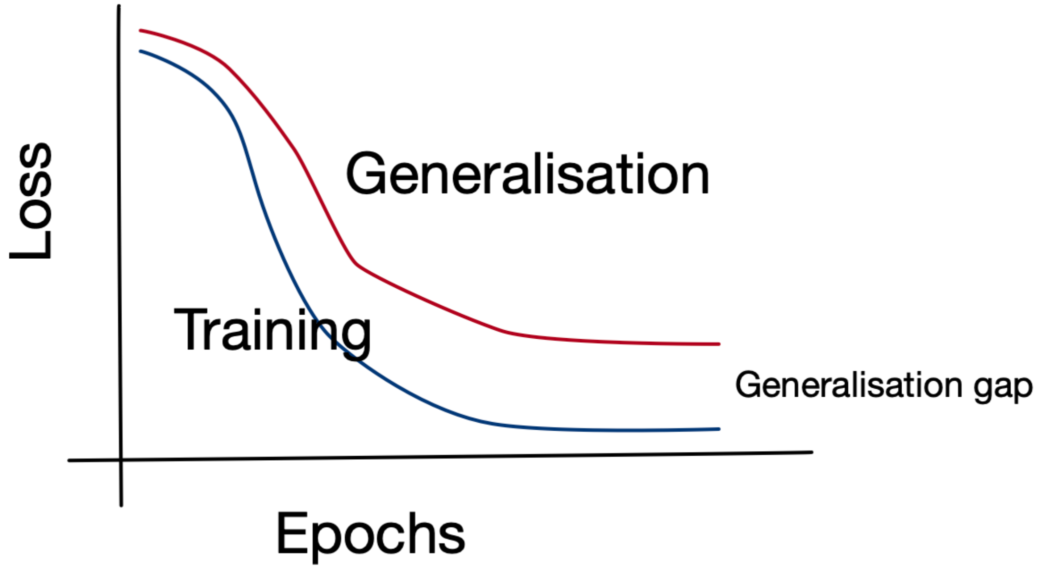
Generalisation gap for neural networks: How does is grow?

- What do curves look like for training loss and test loss?

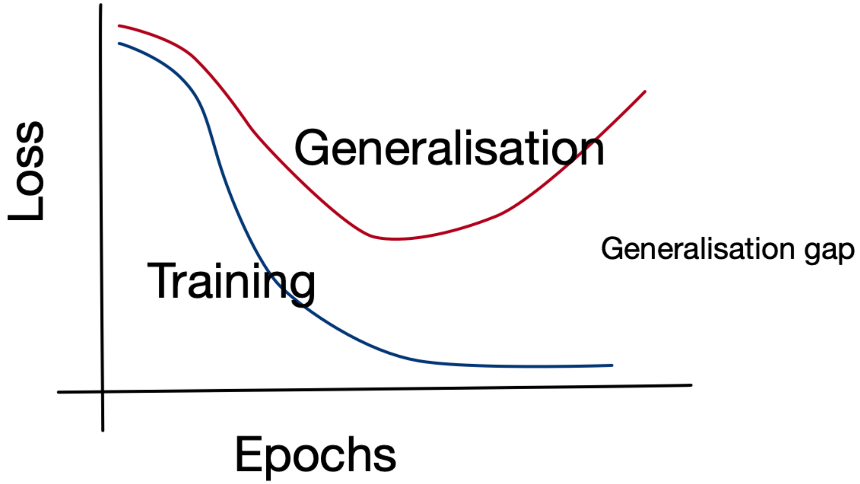


Generalisation gap for neural networks

What we might expect

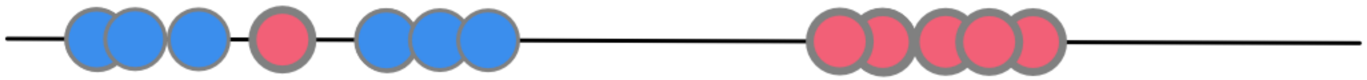


What we find



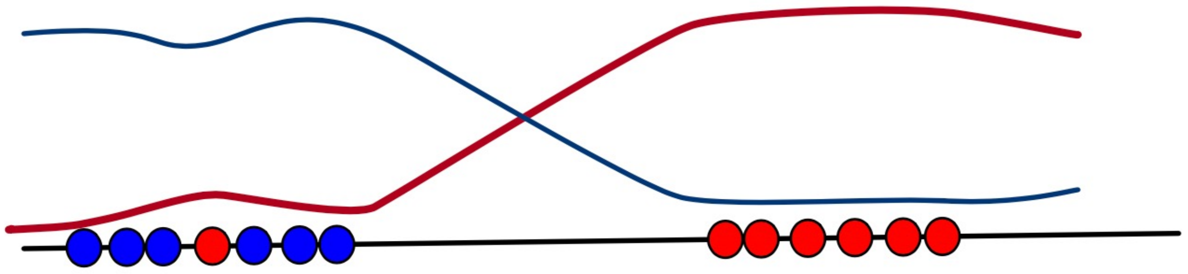
Overfitting in neural networks

- The role of cross entropy loss
- Consider probability outputs for this data and this data space
  - One curve for each class
- What should the curves look like?



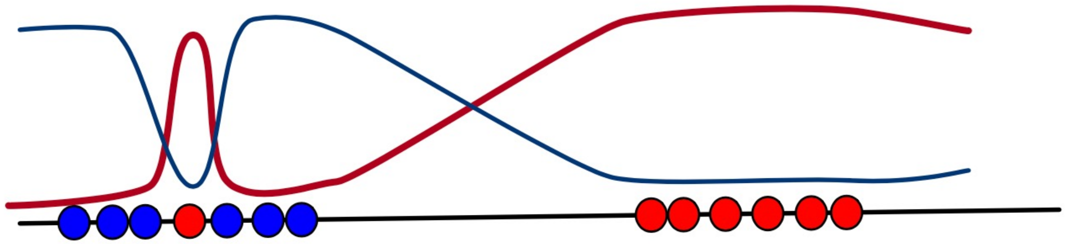
Probability curves for classification

- A reasonable model sacrifices the outlier for better generalization
- But what is the cross entropy loss at the outlier?



Overfitting

- Optimiser tries to modify probability curves
- Such that large CE losses become smaller



What prevents the NN from overfitting too much to every point?

- The NN architecture restricts the possible arrangements of hyperplanes
- The architecture and activation functions restrict

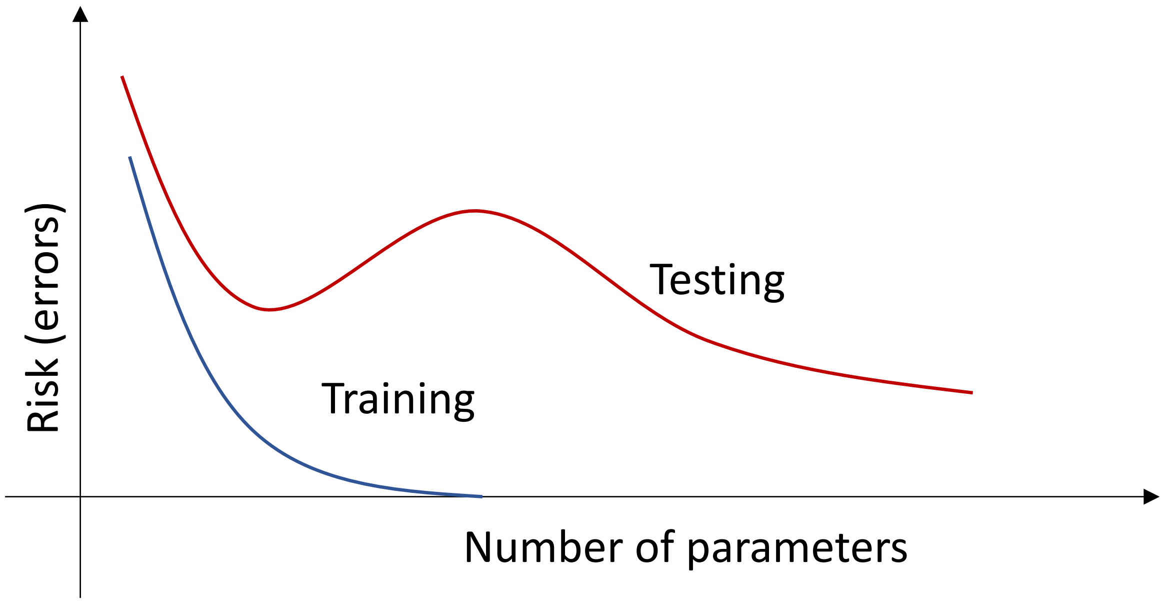
Overparameterised neural networks

- Idea:
  - More neurons/weights/parameters: more unknown variables
  - More data points: More information (similar to more equations)
- Recap of statistical ML: data requirements grow with parameters/complexity
- Modern neural networks:
  - Many more parameters than data points
  - High complexity and therefore high estimation error
  - We expect heavy overfitting and high test/generalization loss/error

Double descent

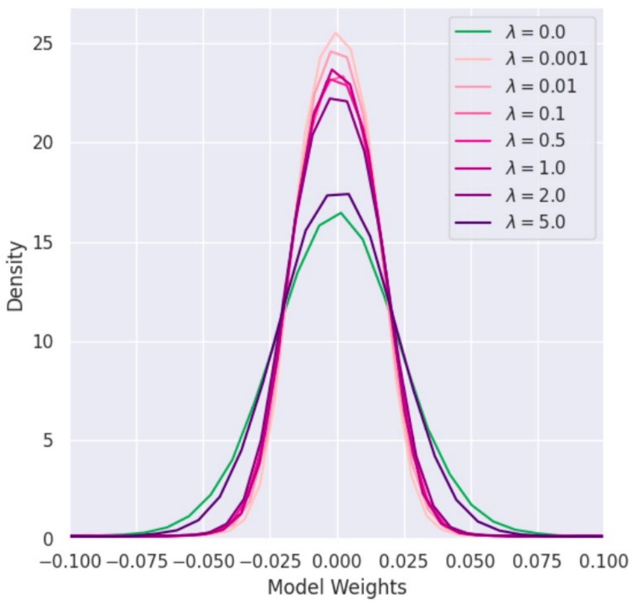
- With very large number of parameters (more than number of data points) testing performs well again!
- Out of many possible models with low training loss, SGD is finding ones that have low test loss!

- See also (optional): Neural Tangent kernels



Distribution of weights on trained NNs

- A large fraction of weights are close to zero
- Small fraction is far from zero
- Observation:
  - Zero weight edges have no effect – do not conduct information
  - Almost zero weights: Little effect



- Conclusion: While NNs have large number of parameters, after training, many of them have little to no effect!

Pruning

- Idea: take all the edges that are tiny weights, and remove them!
- Observations
  - Can sometimes remove 80% - 90% of edges
  - Retains comparable performance and sometimes better generalization

Lottery ticket hypothesis

- Hypothesis: A randomly initialised dense NN already contains a subnetwork (a winning ticket) that can give good performance.

- Algorithm to find the winning ticket
  - Initialise a network to random weights
  - Train for some iterations
  - Prune p% of edges with small weights
  - Reset the remaining edge to their original random weights

- Works surprisingly well on MNIST, CIFAR with test performance comparable to a well trained network [Frankle and Carbin, 2019]

Standard pruning methods

- One shot:
  - Train
  - Remove small weights
  - Return to initialization weights and retrain
  - Stop

- Iterative
  - Set random weights
  - Train
  - Remove edges with small weights
  - Start over

Other results

- Theoretical proofs (special cases, few layers etc)
  - [Malach et al. 2020, Bartoldson et al. 2020]

- Pruning and finding winning tickets without data
  - [Wang et al. 2020, Tanaka et al. 2020]

Pruning and dimension

- The dimension of $\mathcal{H}$ is determined by the number of parameters
- The pruning and lottery tickets papers suggest that there are lowe dimensional subspaces of $\mathcal{H}$ that contain good solutions

Question

- If a small network is good enough, why are we using a large one?

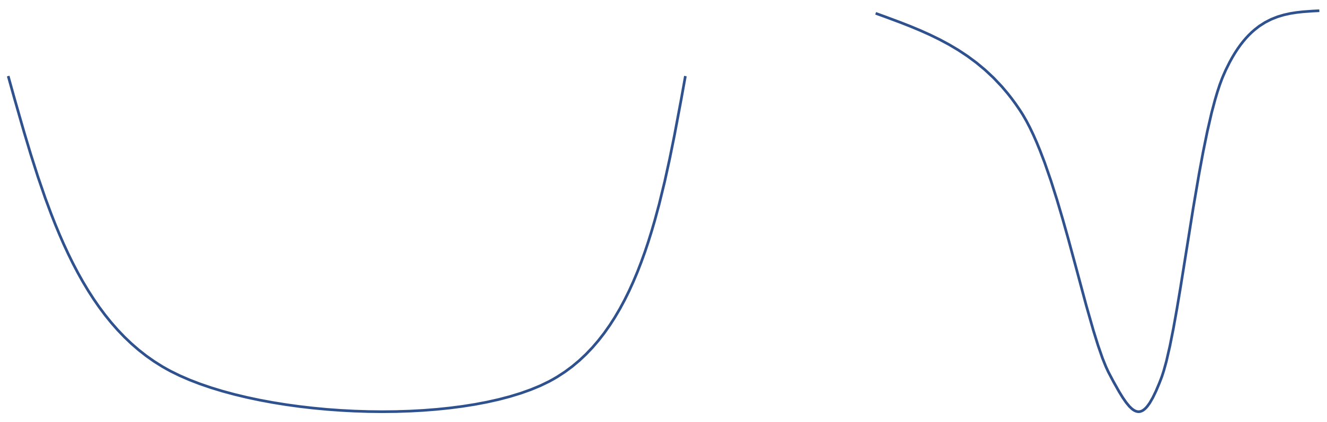
Shape of minima

- Why it is good
- Hessians and eps

Flat and sharp minima

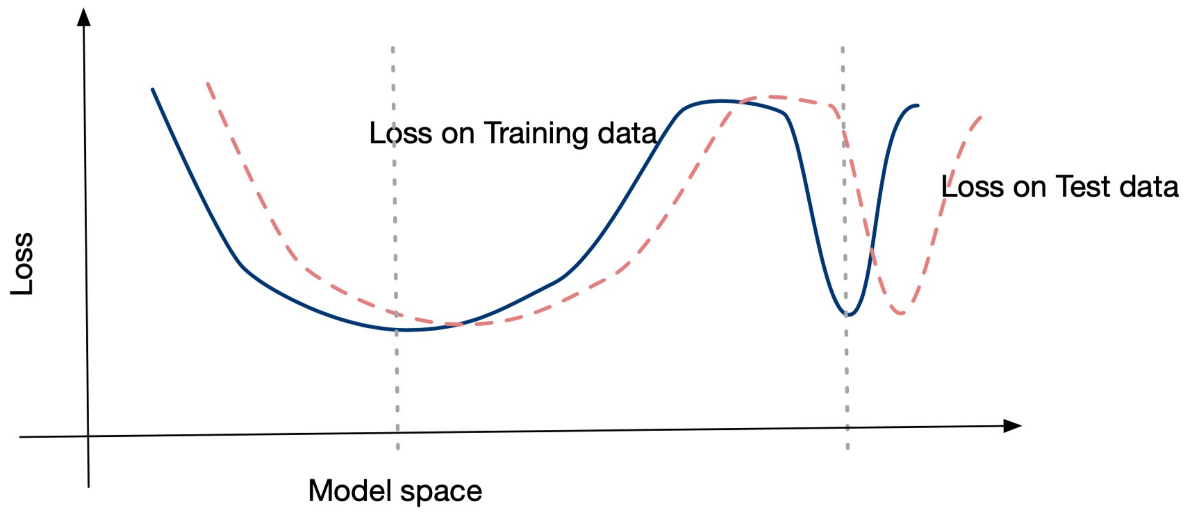
- A minimum of the loss function can be flat or sharp

- Which is better?

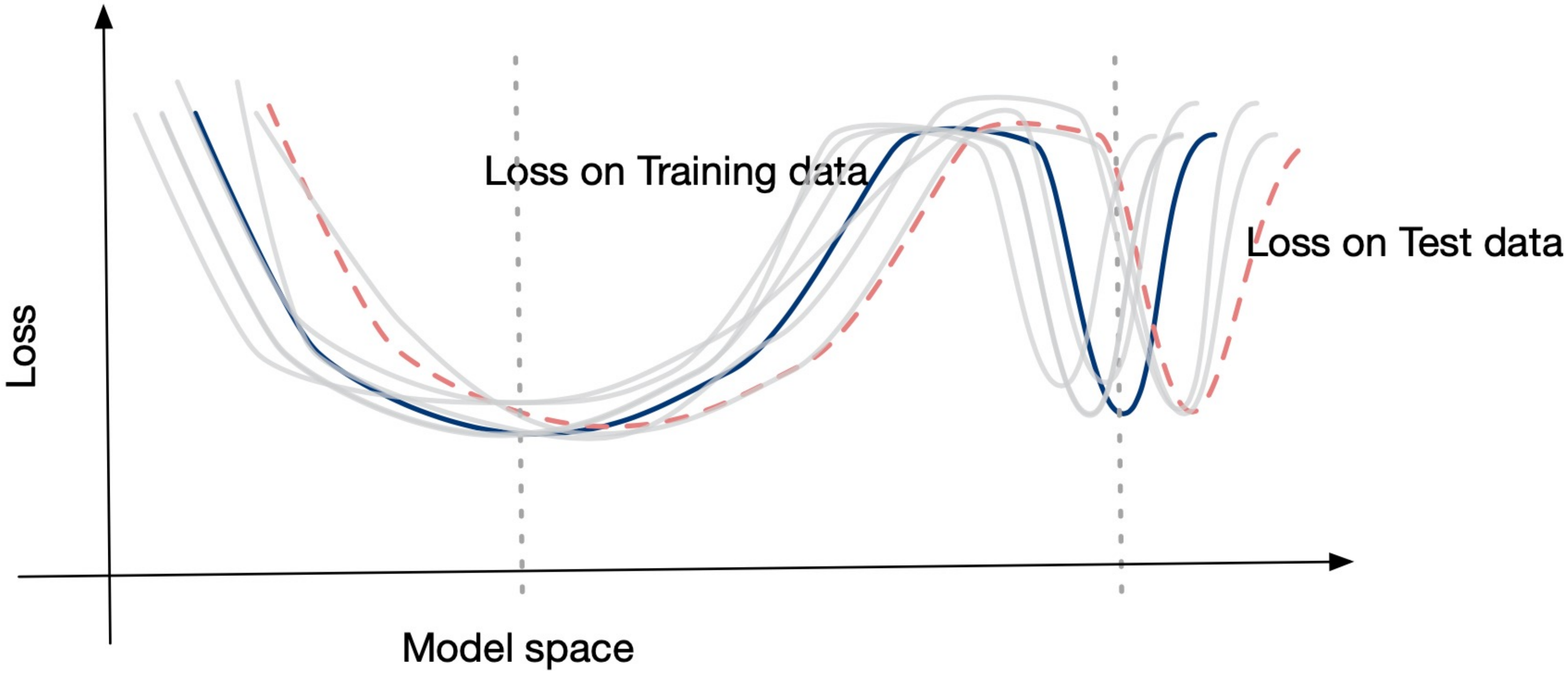


Flat and sharp minima

- Flat minima generalize better
- Sharper minima likely to represent overfitting



Flat minima are also more likely to be stable



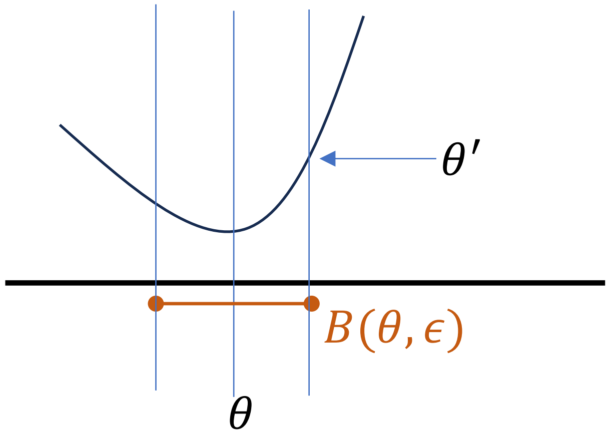
Curvature as a sharpness measure

- For the min of a real valued function in 1-D we can measure curvature as the second derivative
  - $\frac{d^2y}{dx^2}$
- For loss over models
  - $\frac{d^2L}{dw^2}$
- Larger second derivative => sharper min

ϵ-Sharpness

- At min θ take ball $B(\theta, \epsilon)$ of radius ϵ
  - Set of all points within a distance ϵ of θ
- Sharpness is:

$$\frac{\max_{\theta' \in B_2(\epsilon, \theta)} \left(L(\theta') - L(\theta)\right)}{1 + L(\theta)}$$



Model spaces are high dimensional

- ϵ – Sharpness definition applies directly

- Curvature requires considering the Hessian – high dim representation of 2nd derivative

Partial derivatives

- Suppose f is a function of many variables $x, y, z, \ldots$
- We can ask how f changes with x. This is written as $\frac{\partial f}{\partial x}$
  - Same as $\frac{df}{dx}$, but implying that there are other variables to potentially consider
  - And we can write the curvature along x as $\frac{\partial^2 f}{\partial x^2}$: how $\frac{\partial f}{\partial x}$ changes with x

Partial derivatives

- Now we can also ask how $\frac{\partial f}{\partial x}$ changes with y
- This is written as $\frac{\partial^2 f}{\partial y \partial x}$
- Hessian is just a collection of all these written as a matrix
- With two variable models:
- $\begin{pmatrix} \frac{\partial^2 f}{\partial w_1^2} & \frac{\partial^2 f}{\partial w_1 \partial w_2} \\ \frac{\partial^2 f}{\partial w_2 \partial w_1} & \frac{\partial^2 f}{\partial w_2^2} \end{pmatrix}$

$$\mathbf{H}_f = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1\,\partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1\,\partial x_n} \\ \frac{\partial^2 f}{\partial x_2\,\partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2\,\partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n\,\partial x_1} & \frac{\partial^2 f}{\partial x_n\,\partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}.$$

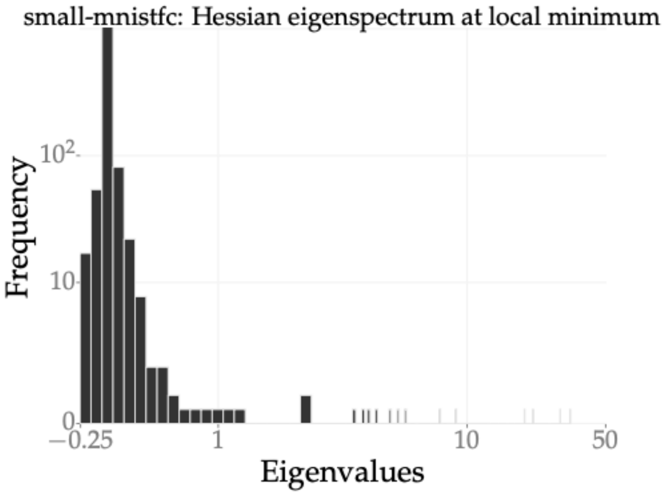
Curvature directions

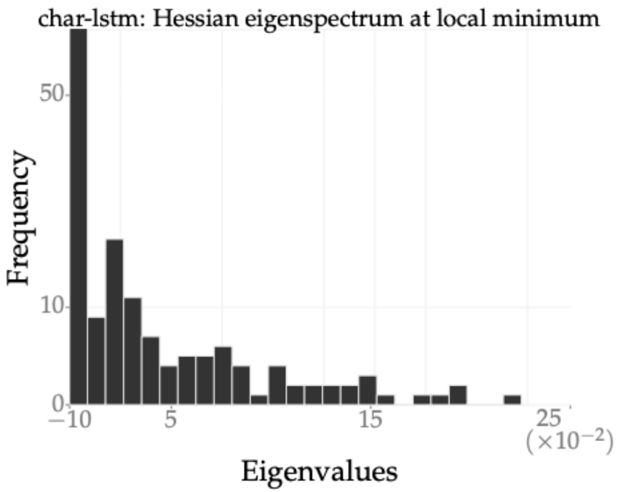
- The problem is that strongest directions of curvature may not align exactly with w_1, w_2 etc
- So, we need to take eigen values and eigen vectors of the hessian
- The eigen values represent the principal curvatures
  - Corresponding eigen vectors represent the directions of these curvatures
- Larger eigen values of hessian imply sharper minima

- (Think Principal components of curvature matrix)

So, the method is

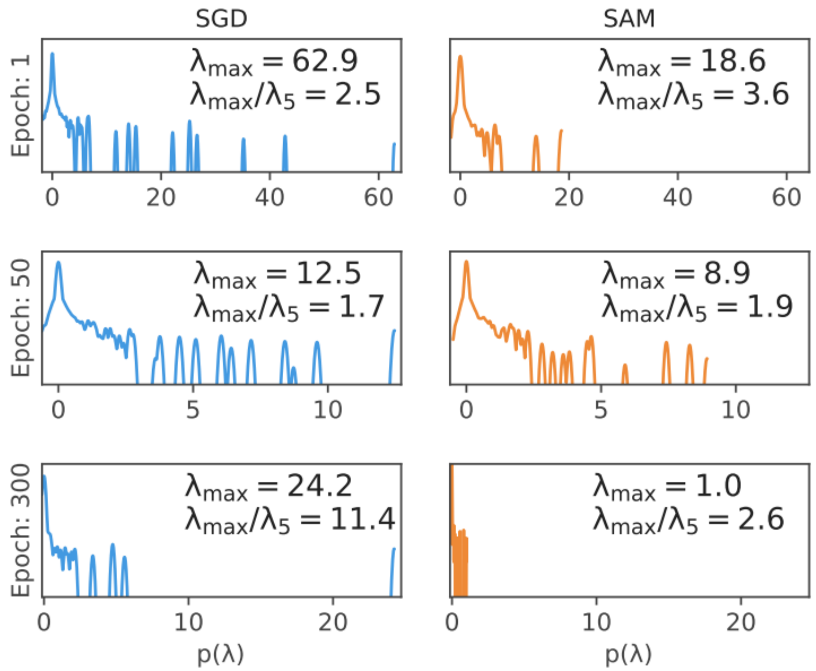
- Take the hessian
- Compute its eigen values
- Look at their distributions
- If there are more of large values, that implies a sharper min





Algorithms

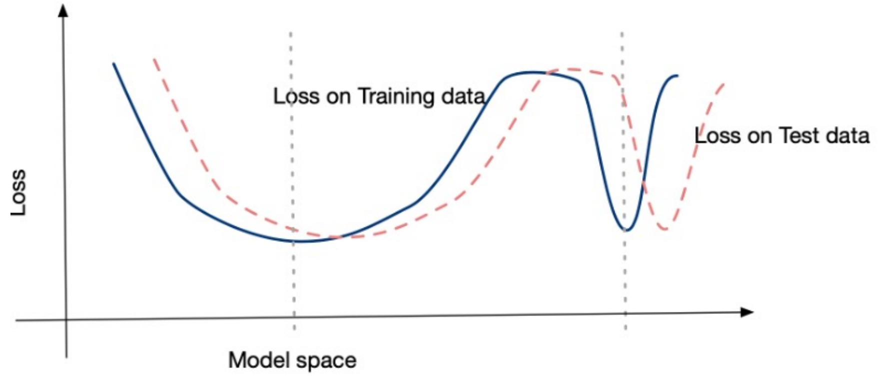
- Shapness aware minimization
  - Use ϵ sharpness
  - Minimize $L(\theta) + [L(\theta + \epsilon') - L(\theta)]$
- Entropy SGD
  - Optimise a different function
  - Computationally very expensive
- Stochastic weight averaging
  - Average the weights of the last c models
  - Shown to produce flat minima



Flat minima

- Current topic of research
- While flat minima are generally agreed to be good, the full picture is not clear
- There are works showing that sometimes sharp minima can work well
- Neural nets are highly redundant (e.g. symmetric) and many possible weight assignments achieve the same effective function
  - It is possible to reconfigure weights such that the effective prediction function is same, therefore loss is same, but the curvature is different

SGD and Flat minima



- SGD is known to have a bias toward flat and well generalizable min
- Large batch sizes and small learning rate approximates a smooth gradient
  - And more likely to find a sharp min
- Small batch sizes and larger learning rate makes a more random, jumpy trajectory that can skip over sharp min.
  - Also easy to jump away from sharp min neighborhood since that is likely a small region
- However, a flat min means that even after step away from it, SGD is likely in the same basin