Deep Neural Networks (2)
Tanh & ReLU layers; Generalisation and Regularisation

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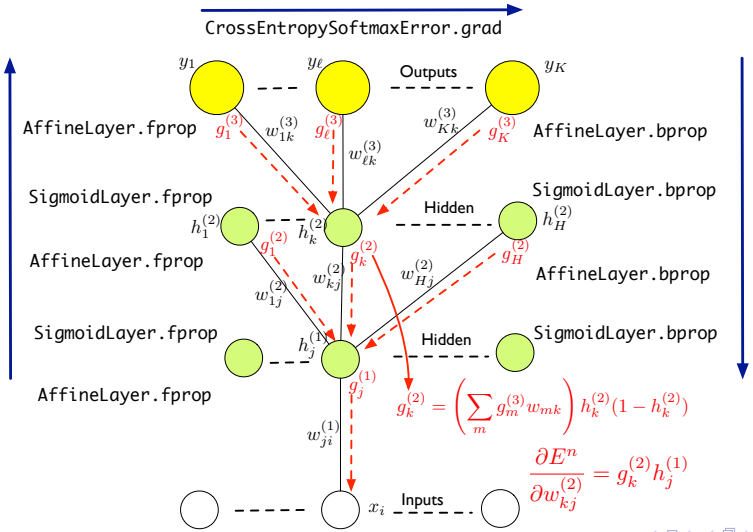
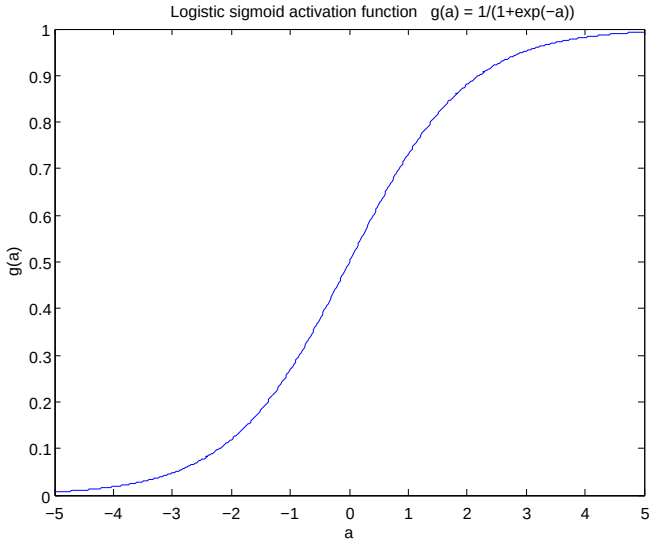
Machine Learning Practical — MLP Lecture 4
9 October 2018

Recap: Training multi-layer networks



Are there alternatives to Sigmoid Hidden Units?

Sigmoid function



Sigmoid Hidden Units (`SigmoidLayer`)

- Compress unbounded inputs to (0,1), saturating high magnitudes to 1
- Interpretable as the probability of a feature defined by their weight vector
- Interpretable as the (normalised) firing rate of a neuron

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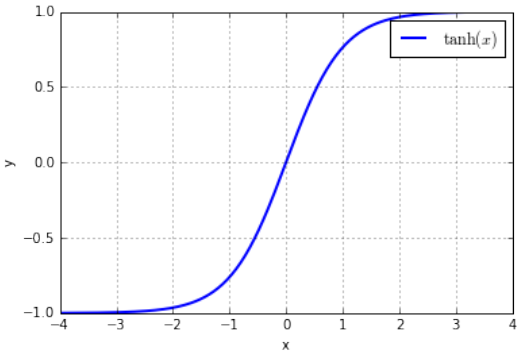
However...

- Saturation causes gradients to approach 0
  - If the output of a sigmoid unit is h, then the gradient is $h(1-h)$ which approaches 0 as h saturates to 0 or 1 – hence the gradients it multiplies into approach 0.
  - Small gradients result in small parameter changes, so learning becomes slow
- Outputs are not centred at 0
  - The output of a sigmoid layer will have mean> 0 – numerically undesirable.

tanh



$$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$$

$$\text{sigmoid}(x) = \frac{1 + \tanh(x/2)}{2}$$

Derivative:

$$\frac{d}{dx}\tanh(x) = 1 - \tanh^2(x)$$

tanh hidden units (TanhLayer)

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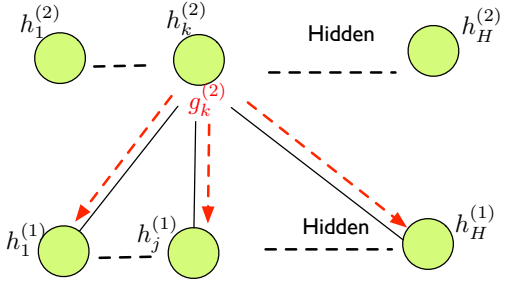

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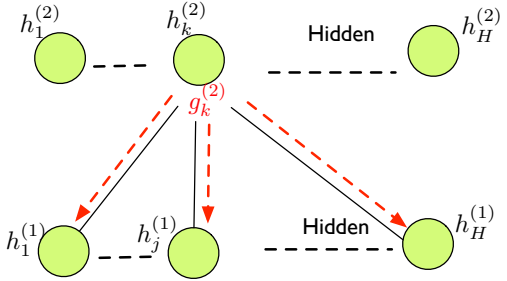
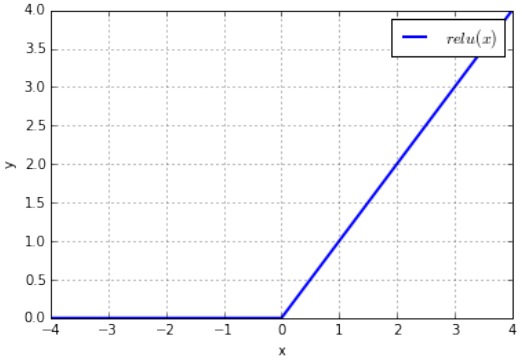
- Saturation still a problem



Rectified Linear Unit – ReLU



$$\text{relu}(x) = \max(0, x)$$

Derivative:

$$\frac{d}{dx}\text{relu}(x) = \begin{cases} 0 & \text{if } x \leq 0 \\ 1 & \text{if } x > 0 \end{cases}$$

ReLU hidden units (`ReluLayer`)

- Similar approximation results to tanh and sigmoid hidden units
- Empirical results for speech and vision show consistent improvements using relu over sigmoid or tanh
- Unlike tanh or sigmoid there is no positive saturation – saturation results in very small derivatives (and hence slower learning)

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- Negative input to relu results in zero gradient (and hence no learning)
- Relu is computationally efficient: $\max(0, x)$
- Relu units can "die" (i.e. respond with 0 to everything)
- Relu units can be very sensitive to the learning rate

Generalisation

Generalization

- Generalization:
  - what is the expected error on a test set?
  - how to compare the accuracy of different networks trained on the same data?
- Causes of error
  - Network too flexible: Too many weights compared with number of training examples
  - Network not flexible enough: Not enough weights (hidden units) to represent the desired mapping

  When comparing models, it can be helpful to compare systems with the same number of *trainable parameters* (i.e. the number of trainable weights in a neural network)
- Optimizing training set performance does not necessarily optimize test set performance....

Training / Test / Validation Data

- Partitioning the data...
  - **Training** data – data used for training the network
  - **Validation** data – frequently used to measure the error of a network on "unseen" data (e.g. after each epoch)
  - **Test** data – less frequently used "unseen" data, ideally only used once
- Frequent use of the same test data can indirectly "tune" the network to that data (e.g. by influencing choice of *hyperparameters* such as learning rate, number of hidden units, number of layers, ...)

Measuring generalisation

- Generalization Error – The predicted error on unseen data. How can the generalization error be estimated?
  - Training error?

$$E_{\text{train}} = - \sum_{\text{training set}} \sum_{k=1}^{K} t_k^n \ln y_k^n$$

  - Validation error?

$$E_{\text{val}} = - \sum_{\text{validation set}} \sum_{k=1}^{K} t_k^n \ln y_k^n$$

Cross-validation

- Optimize network performance given a fixed training set
- *Hold out* a set of data (validation set) and predict generalization performance on this set
  1. Train network in usual way on training data
  2. Estimate performance of network on validation set
- If several networks trained on the same data, choose the one that performs best on the validation set (**not** the training set)
- *n-fold* Cross-validation: divide the data into n partitions; select each partition in turn to be the validation set, and train on the remaining $(n-1)$ partitions. Estimate generalization error by averaging over all validation sets.

Overtraining

- Overtraining corresponds to a network function too closely fit to the training set (too much flexibility)
- Undertraining corresponds to a network function not well fit to the training set (too little flexibility)
- Solutions
  - If possible increasing both network complexity in line with the training set size
  - Use prior information to constrain the network function
  - Control the flexibility: **Structural Stabilization**
  - Control the *effective flexibility*: **early stopping** and **regularization**

Structural Stabilization

Directly control the number of weights:

- Compare models with different numbers of hidden units
- Start with a large network and reduce the number of weights by pruning individual weights or hidden units
- Weight sharing — use prior knowledge to constrain the weights on a set of connections to be equal.
  $\rightarrow$ Convolutional Neural Networks

Lab 4: 04_Generalisation_and_overfitting

Lab 4 explores overfitting and how we can measure how well the models we train generalise their predictions to unseen data.

- Setting up a 1-dimension regression problem
- Using a radial basis functions (RBF) network as a model for this problem
- Exploring the behaviour of the RBF network as the number of model parameters (basis functions) increases

Early Stopping

- Use validation set to decide when to stop training
- Training Set Error monotonically decreases as training progresses

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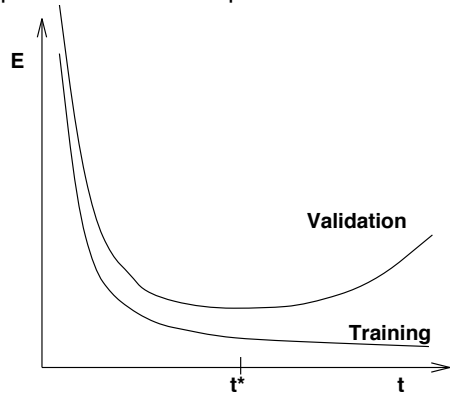

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- "Effective Flexibility" increases as training progresses
- Network has an increasing number of "effective degrees of freedom" as training progresses
- Network weights become more tuned to training data
- Very effective — used in many practical applications such as speech recognition and optical character recognition

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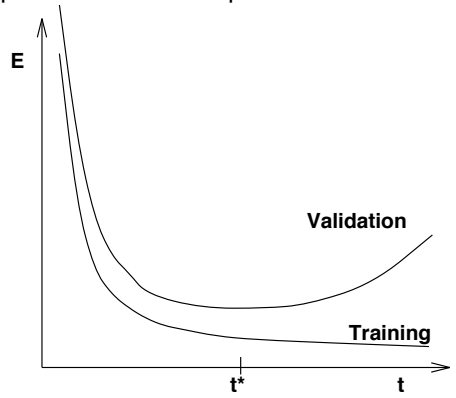

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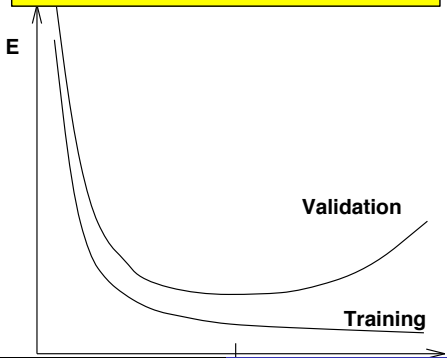
Why does early stopping improve generalisation?



Generalisation by design

- Regularisation – penalise the weights: L1 (sparsity), L2 (weight decay)
- Data augmentation – generate additional (noisy) training data
- Model combination – smooth together multiple networks
- Dropout – randomly delete a fraction of hidden units each minibatch
- Parameter sharing – e.g. convolutional networks

Weight Decay (L2 Regularisation)

- Weight decay puts a "spring" on weights
- If training data puts a consistent force on a weight, it will outweigh weight decay
- If training does not consistently push weight in a direction, then weight decay will dominate and weight will decay to 0
- Without weight decay, weight would walk randomly without being well determined by the data
- Weight decay can allow the data to determine how to reduce the effective number of parameters

Penalizing Complexity

- Consider adding a *complexity term* E_w to the network error function, to encourage smoother mappings:

$$E^n = \underbrace{E^n_{\text{train}}}_{\text{data term}} + \underbrace{\beta E_W}_{\text{prior term}}$$

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- E_W should be a differentiable flexiblity/complexity measure, e.g.

$$E_W = E_{L2} = \frac{1}{2}\sum_i w_i^2$$

$$\frac{\partial E_{L2}}{\partial w_i} = w_i$$

Gradient Descent Training with Weight Decay

$$\frac{\partial E^n}{\partial w_i} = \frac{\partial (E^n_{\text{train}} + E_{L2})}{\partial w_i} = \left(\frac{\partial E^n_{\text{train}}}{\partial w_i} + \beta \frac{\partial E_{L2}}{\partial w_i} \right)$$

$$= \left(\frac{\partial E^n_{\text{train}}}{\partial w_i} + \beta w_i \right)$$

$$\Delta w_i = -\eta \left(\frac{\partial E^n_{\text{train}}}{\partial w_i} + \beta w_i \right)$$

- Weight decay corresponds to adding $E_{L2} = 1/2 \sum_i w_i^2$ to the error function
- Addition of complexity terms is called *regularisation*
- When used with gradient descent, weight decay corresponds to L2 regularisation

L1 Regularisation

- **L1 Regularisation** corresponds to adding a term based on summing the absolute values of the weights to the error:

$$\begin{aligned} E^n &= \underbrace{E^n_{\text{train}}}_{\text{data term}} + \underbrace{\beta E^n_{L1}}_{\text{prior term}} \\ &= E^n_{\text{train}} + \beta |w_i| \end{aligned}$$

- Gradients

$$\begin{aligned} \frac{\partial E^n}{\partial w_i} &= \frac{\partial E^n_{\text{train}}}{\partial w_i} + \beta \frac{\partial E_{L1}}{\partial w_i} \\ &= \frac{\partial E^n_{\text{train}}}{\partial w_i} + \beta \, \text{sgn}(w_i) \end{aligned}$$

Where $\text{sgn}(w_i)$ is the sign of w_i:
$\text{sgn}(w_i) = 1$ if $w_i > 0$ and $\text{sgn}(w_i) = -1$ if $w_i < 0$

L1 vs L2

- L1 and L2 regularisation both have the effect of penalising larger weights
  - In L2 they shrink to 0 at a rate proportional to the size of the weight (βw_i)
  - In L1 they shrink to 0 at a constant rate ($\beta \operatorname{sgn}(w_i)$)
- Behaviour of L1 and L2 regularisation with large and small weights:
  - when $|w_i|$ is large L2 shrinks faster than L1
  - when $|w_i|$ is small L1 shrinks faster than L2
- So L1 tends to shrink some weights to 0, leaving a few large important connections – L1 encourages *sparsity*
- $\partial E_{L1}/\partial w$ is undefined when $w = 0$; assume it is 0 (i.e. take $\operatorname{sgn}(0) = 0$ in the update equation)

Data Augmentation – Adding "fake" training data

- Generalisation performance goes with the amount of training data (change `MNISTDataProvider` to give training sets of 1 000 / 5 000 / 10 000 examples to see this)
- Given a finite training set we could *create* further training examples...
  - Create new examples by making small rotations of existing data
  - Add a small amount of random noise
- Using "realistic" distortions to create new data is better than adding random noise

Model Combination

- Combining the predictions of multiple models can reduce overfitting
- Model combination works best when the component models are *complementary* – no single model works best on all data points
- Creating a set of diverse models
  - Different NN architectures (number of hidden units, number of layers, hidden unit type, input features, type of regularisation, ...)
  - Different models (NN, SVM, decision trees, ...)
- How to combine models?
  - Average their outputs
  - Linearly combine their outputs
  - Train another "combiner" neural network whose input is the outputs of the component networks
  - Architectures designed to create a set of specialised models which can be combined (e.g. mixtures of experts)

Lab 5: 05_Regularisation

Lab 5 explores different methods for regularising networks to reduce overfitting and improve generalisation

In the context of a feed-forward network using ReLU hidden layers, the lab explores

- L1 and L2 regularisation
- Data augmentation

Summary

- Tanh and ReLU
- Generalisation and overfitting
- Preventing overfitting
  - L2 regularisation – weight decay
  - L1 regularisation – sparsity
  - Creating additional training data
  - Model combination
- Reading:
  - Nielsen, chapter 3 (section on overfitting and regularization) of *Neural Networks and Deep Learning*
    http://neuralnetworksanddeeplearning.com/chap3.html#overfitting_and_regularization
  - Goodfellow et al, chapter 7 *Deep Learning* (sections 7.1–7.5)
    http://www.deeplearningbook.org/contents/regularization.html