Approximate Functions



Going Deep

Jonathon Hare

Vision, Learning and Control University of Southampton

- No free lunch and universal approximation
- Why go deep?
- Problems of going deep
- Some fixes:
 - Improving gradient flow with skip connections
 - Regularising with Dropout

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No Free Lunch

- Statistical learning theory claims that a machine can generalise well from a finite training set.
- This contradicts basic inductive reasoning which says to derive a rule describing every member of a set one must have information about every member.
- Machine learning avoids this problem by learning probabilistic¹ rules which are probably correct about most members of the set they concern.
- But, no free lunch theorem states that every possible classification machine has the same error when averaged over all possible data-generating distributions.
 - No machine learning algorithm is universally better than any other!
 - Fortunately, in the real world, data is generated by a small subset of generating distributions...

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 $^{^{1}}$ or perhaps more generally rules which are not certain

The Universal Approximation Theorem

Let $\psi: \mathbb{R} \to \mathbb{R}$ be a nonconstant, bounded, and continuous function. Let I_m denote the m-dimensional unit hypercube $[0,1]^m$. The space of real-valued continuous functions on I_m is denoted by $C(I_m)$. Then, given any $\varepsilon > 0$ and any function $f \in C(I_m)$, there exist an integer N, real constants $v_i, b_i \in \mathbb{R}$ and real vectors $w_i \in \mathbb{R}^m$ for $i = 1, \ldots, N$, such that we may define:

 $F(x) = \sum_{i=1}^{N} v_i \psi(w_i^T x + b_i)$ as an approximate realization of the function f; that is,

$$|F(x)-f(x)|<\varepsilon\ \forall\ x\in I_m.$$

⇒ simple neural networks can represent a wide variety of interesting functions when given appropriate parameters.

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So a single hidden layer network can approximate most functions?

- Yes!
- But, ...
 - to get the precision you require (small ε), you might need a really large number of hidden units (very large N).
 - worse-case analysis shows it might be exponential (possibly one hidden unit for every input configuration)
 - We've not said anything about learnability...
 - The optimiser might not find a good solution².
 - The training algorithm might just choose the wrong solution as a result of overfitting.
 - There is no known universal procedure for examining a set of examples and choosing a function that will generalise to points out of the training set.

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²note that it has been shown that the gradients of the function are approximated by the network to an arbitrary precision

Then Why Go Deep?

- There are functions you can compute with a deep neural network that shallow networks require exponentially more hidden units to compute.
 - The following function is more efficient to implement using a deep neural network: $y = x_1 \oplus x_2 \oplus x_3 \oplus \cdots \oplus x_n$
- We should care about the data generating distribution (c.f. NFL).
 - Real-world data has significant structure; often believed to be generated by (relatively) simple low-dimensional latent processes.
 - Implies a prior belief that the underlying factors of variation in data can be explained by a hierarchical composition of increasingly simple latent factors
- Alternatively, one could just consider that a deep architecture just expresses that the function we wish to learn is a program made of multiple steps where each step makes use of the previous steps outputs.
- Empirically, deeper networks just seem to generalise better!

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What are the problems?

- Learnability is still hard
 - Problems of gradient flow
 - Horrible symmetries in the loss landscape
 - Overfitting

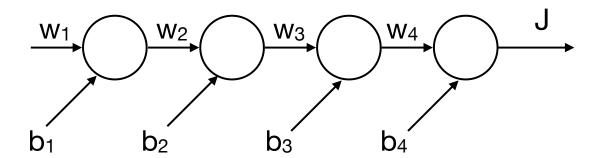
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Vanishing and Exploding Gradients

- The vanishing and exploding gradient problem is a difficulty found in training NN with gradient-based learning methods and backpropagation.
- In training, the gradient may become vanishingly small (or large), effectively preventing the weight from changing its value (or exploding in value).
- This leads to the neural network not being able to train.
- This issue affects many-layered networks (feed-forward), as well as recurrent networks.
- In principle, optimisers that rescale the gradients of each weight should be able to deal with this issue (as long as numeric precision doesn't become problematic).

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Issues with Going Deep



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Residual Connections

- One of the most effective ways to resolve diminishing gradients is with residual neural networks (ResNets)³.
- ResNets are artificial neural networks that use *skip connections* to jump over layers.
- The vanishing gradient problem is mitigated in ResNets by reusing activations from a previous layer.
- Is this the full story though? Skip connections also break symmetries, which could be much more important...

³K. He, X. Zhang, S. Ren and J. Sun, "Deep Residual Learning for Image Recognition,"

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Residual Connections

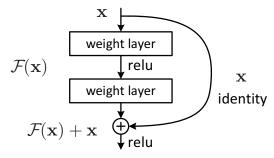


Figure 2. Residual learning: a building block.

K. He, X. Zhang, S. Ren and J. Sun, "Deep Residual Learning for Image Recognition," CVPR, Las Vegas, NV, 2016, pp. 770-778.

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CVPR, Las Vegas, NV, 2016, pp. 770-778.

Residual Connections

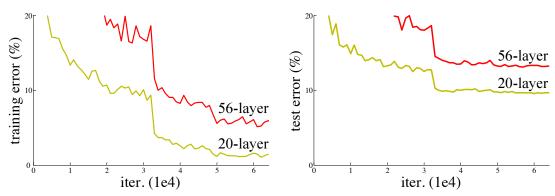


Figure 1. Training error (left) and test error (right) on CIFAR-10 with 20-layer and 56-layer "plain" networks. The deeper network has higher training error, and thus test error. Similar phenomena on ImageNet is presented in Fig. 4.

CVPR, Las Vegas, NV, 2016, pp. 770-778.

K. He, X. Zhang, S. Ren and J. Sun, "Deep Residual Learning for Image Recognition,"

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Residual Connections

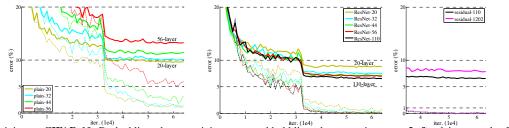


Figure 6. Training on **CIFAR-10**. Dashed lines denote training error, and bold lines denote testing error. **Left**: plain networks. The error of plain-110 is higher than 60% and not displayed. **Middle**: ResNets. **Right**: ResNets with 110 and 1202 layers.

K. He, X. Zhang, S. Ren and J. Sun, "Deep Residual Learning for Image Recognition," CVPR, Las Vegas, NV, 2016, pp. 770-778.

Overfitting

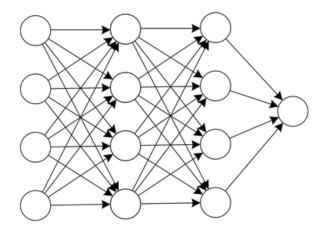
- Neural networks with a large number of parameters (and hidden layers) are powerful, however, overfitting is a serious problem in such systems.
- Just as you've seen in simple machines (e.g. Ridge Regression and LASSO), regularisation can help mitigate overfitting
- In deep networks, we might:
 - Use the architecture to regularise (e.g. ConvNets)
 - Use weight regularisers (L1, L2 [weight decay], etc, ...)
 - Use a stochastic weight regulariser (like dropout)
 - Regularise by smoothing the optimisation landscape (e.g. Batch Normalisation)

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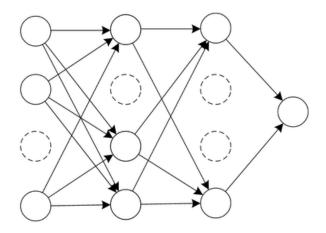
Dropout

- Dropout is a form of regularisation
- The key idea in dropout is to randomly drop neurons, including all of the connections, from the neural network during training.
- Motivation: the best way to regularise a fixed size model is to average predictions over all possible parameter settings, weighting each setting by the posterior probability given the training data.
 - Clearly this isn't actually tractable dropout is an approximation of this idea.
 - The idea of averaging predictions to resolve the bias-variance dilemma is called ensembling.

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(b) Network after Dropout

Image from: https://www.researchgate.net/figure/
Dropout-neural-network-model-a-is-a-standard-neural-network-b-is-the-same-network_fig3_309206911

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How Does Dropout Work?

- In the learning phase, we set a dropout probability for each layer in the network.
- For each batch we then randomly decide whether or not a given neuron in a given layer is removed.
- **Inverse Dropout** scales the activations with their probability to maintain the overall magnitude of the response when dropout is disabled at evaluation/test time.

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How is Inverted Dropout implemented?

- We define a random binary mask $m^{(l)}$ which is used to remove neurons and is generated by sampling a Bernoulli distribution with P(x=1)=p, and note, $m^{(l)}$ changes for each iteration of the backpropagation algorithm.
- The forward pass of a Dropout layer (function) during **training** is given by $f(x) = x \odot m/p$.
- The forward pass of a Dropout layer (function) during **inference** is given by f(x) = x.
- This can be applied to any layer(s) of the network except the output layer!
- It's not common to put it everywhere; just a couple of select places (empirically chosen).
- The gradient (during training) is simply the hadamard product of the incoming gradient with m/p.

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Why Does Dropout Work?

- Neurons cannot co-adapt to other units (they cannot assume that all of the other units will be present).
- By breaking co-adaptation, each unit will ultimately find more general features.
- By ensembling (averaging) multiple networks, each relying on different (but overlapping) features we get a more effective machine.

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