EE 628
Deep Learning
Fall 2019

Lecture 5

02/20/2019

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Overview

- Last lecture we covered
    - Multilayer Perceptron

- Today, we will cover
    - Overfitting/underfitting
    - Backpropagation

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- The phenomena of fitting our training data more closely than we fit the underlying distribution is called **overfitting**.
- The techniques used to combat overfitting are called **generalization**.

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- Example: a student memorizing all exam questions to prepare an exam in future

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- Sometimes we can get away with minor violations of the i.i.d assumption
- But some violations can cause trouble

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- The number of training examples.
  - It’s trivially easy to overfit a dataset containing only one or two examples even if your model is simple

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- What if we cannot afford to holdout enough data
  - Solution: K-fold Cross Validation

Underfitting or Overfitting

- Underfitting:
  - when our training error and validation error are both substantial but there is a little gap between them
  - If the model is unable to reduce the training error, that could mean that our model is too simple
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- Overfitting:
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- Whether we overfit or underfit can depend both on the complexity of our model and the size of the available training datasets

Model Complexity

- An example using polynomials $\hat{y} = \sum_{i=0}^{d} x^i w_i$

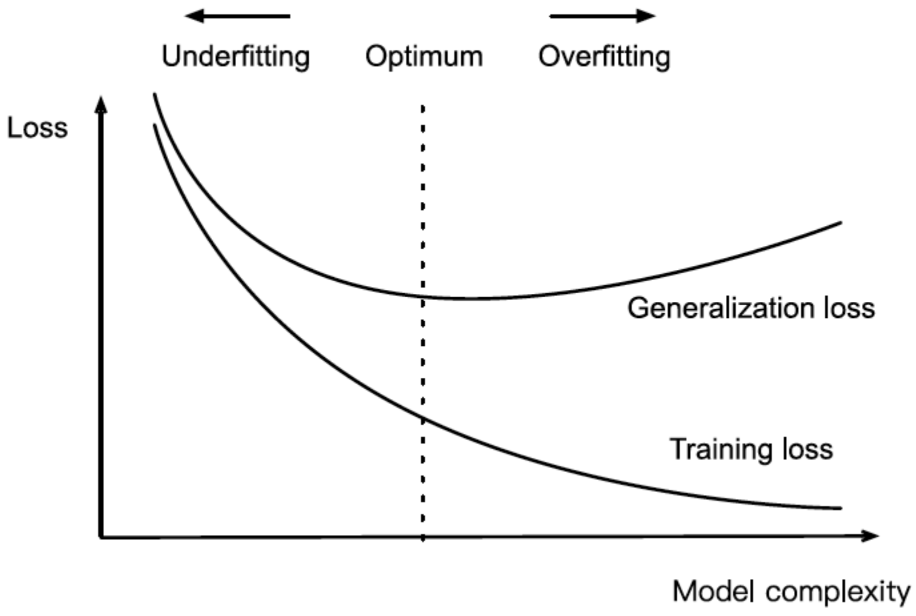

Fig. 6.4.1: Influence of Model Complexity on Underfitting and Overfitting

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- In part, the current success of deep learning owes to the current abundance of massive datasets due to internet companies, cheap storage, connected devices, and the broad digitization of the economy.

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- We can add this as penalty term to our loss function
- For linear regression problem, our loss becomes:

$$l(\mathbf{w}, b) + \frac{\lambda}{2}\|w\|^2$$

Regularization constant $\lambda \geq 0$ governs the amount of regularization

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- Why not other norms?
- In fact, several other choices are valid and popular in statistics.
  - L2 regularized regression is called ridge regression
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- What is the SGD update for L2 regularized regression?

Dropout

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  - The function should be robust under small changes in the input
- In 1995, Christopher Bishop showed that training with input noise is equivalent to Tikhonov regularization
- In 2014, Siravastana applied Bishop's idea to internal layers of the network
  - Dropout – widely used in neural networks
  - On each iteration, drop out zeroes out some fraction of the nodes in each layer before calculating the subsequent layer in training

Dropout

- The key challenge: how to inject noise without introducing bias?
  - i.e. we want to perturb the inputs to each layer during training in such a way that the expected value of the layer is equal to the value it would have taken had we not introduced any noise at all.

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- Show the expectations remain unchanged!

Dropout in Practice

- In the image below h_2 and h_5 are removed
- This way, calculation of the output cannot be overly dependent on any one element of h_1, h_2, h_3, h_4, h_5.

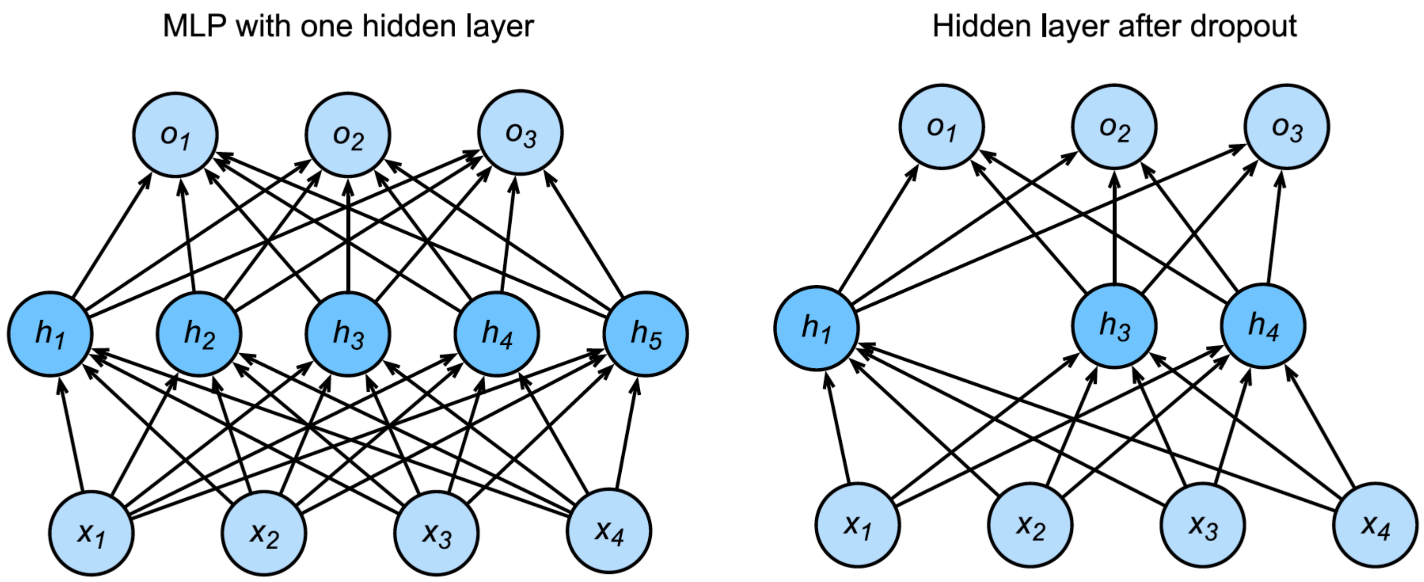

Fig. 6.6.1: MLP before and after dropout

- At test time, we typically do not use dropout.

Implementation of dropout

- From scratch
- concise

Forward Propagation, Backward Propagation, and Computational Graphs

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- The automatic calculation of gradients profoundly simplifies the implementation of deep learning algorithms
- Now, we will discuss some of the details of backward propagation
- To start, we will focus our exposition on a simple multilayer perceptron with
  - a single hidden layer and
  - $\ell 2$ norm regularization.

Really simple example

- We want
  - $\frac{\partial f}{\partial x}, \frac{\partial f}{\partial y}, \frac{\partial f}{\partial z}$
  - for $\mathrm{f(x, y, z) = (x + y)z}$
  - where $x = -2, y = 5, z = -4$
- Draw the computation graph

Reference: http://cs231n.stanford.edu/slides/2019/cs231n_2019_lecture04.pdf

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- The regularization term is $s = \frac{\lambda}{2}(||\mathbf{W}^{(1)}||_F^2 + ||\mathbf{W}^{(2)}||_F^2)$
- Finally, the model's regularized loss (*objective function*) on a given data example is $J = L + s$

Computational Graph of Forward Propagation

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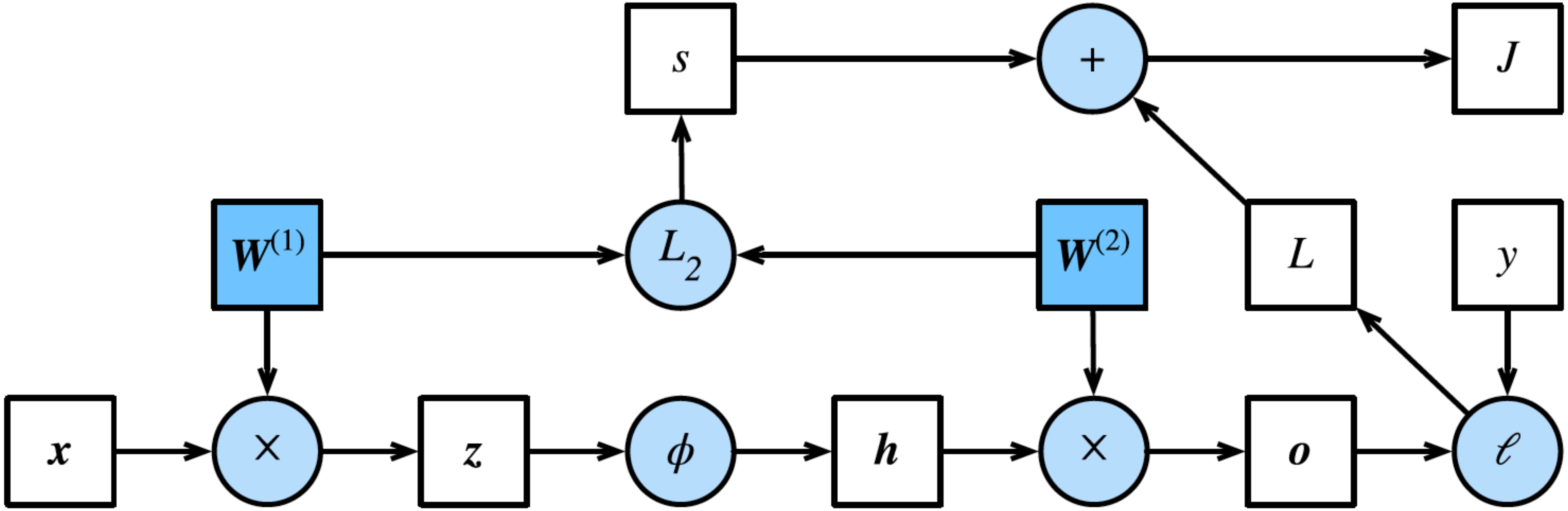

Fig. 6.7.1: Computational Graph

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- What gradients do we need in our example?

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- To obtain the gradient with respect to $\mathbf{W}^{(1)}$, we need to continue backpropagation along the output layer to the hidden layer $\frac{\partial J}{\partial \mathbf{h}} = prod\ \left(\frac{\partial J}{\partial \mathbf{o}}, \frac{\partial \mathbf{o}}{\partial \mathbf{h}}\right) = W^{(2)T} \frac{\partial J}{\partial \mathbf{o}}$. Calculating gradient with respect to $\mathbf{z}$, requires derivative of the activation function $\frac{\partial J}{\partial z} = prod\ \left(\frac{\partial J}{\partial \mathbf{h}}, \frac{\partial \mathbf{h}}{\partial \mathbf{z}}\right) = \frac{\partial J}{\partial \mathbf{h}} \odot \phi'(\mathbf{z})$.

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- Finally we obtain $\frac{\partial J}{\partial \mathbf{W}^{(1)}} = prod\left(\frac{\partial J}{\partial \mathbf{z}}, \frac{\partial \mathbf{z}}{\partial \mathbf{W}^{(1)}}\right) + prod\ \left(\frac{\partial J}{\partial s}, \frac{\partial s}{\partial \mathbf{W}^{(1)}}\right) = \frac{\partial J}{\partial \mathbf{z}} \mathbf{x}^T + \lambda \mathbf{W}^{(1)}$.

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- we need to retain the intermediate values until backpropagation is complete
- This is also one of the reasons why backpropagation requires significantly more memory

Numerical Stability and Initialization

- Which nonlinearity function we use
- How we decide to initialize our parameters
- can play important role in convergence

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$$\partial_{\mathbf{W}_t} \mathbf{o} = \underbrace{\partial_{\mathbf{h}^{d-1}} \mathbf{h}^d}_{:=\mathbf{M}_d} \cdot \ldots \cdot \underbrace{\partial_{\mathbf{h}^t} \mathbf{h}^{t+1}}_{:=\mathbf{M}_t} \underbrace{\partial_{\mathbf{W}_t} \mathbf{h}^t}_{:=\mathbf{v}_t} .$$

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$$\partial_{\mathbf{W}_t} \mathbf{o} = \underbrace{\partial_{\mathbf{h}^{d-1}} \mathbf{h}^d}_{:= \mathbf{M}_d} \cdot \ldots \cdot \underbrace{\partial_{\mathbf{h}^t} \mathbf{h}^{t+1}}_{:= \mathbf{M}_t} \underbrace{\partial_{\mathbf{W}_t} \mathbf{h}^t}_{:= \mathbf{v}_t}.$$

- In other words, it is the product of $d - t$ matrices and a gradient vector

Vanishing and Exploding Gradients

- Consider a deep neural network with d layers, input $\mathbf{x}$ and output $\mathbf{o}$.
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- In other words, it is the product of $d - t$ matrices and a gradient vector
- This product might be too large or too small!

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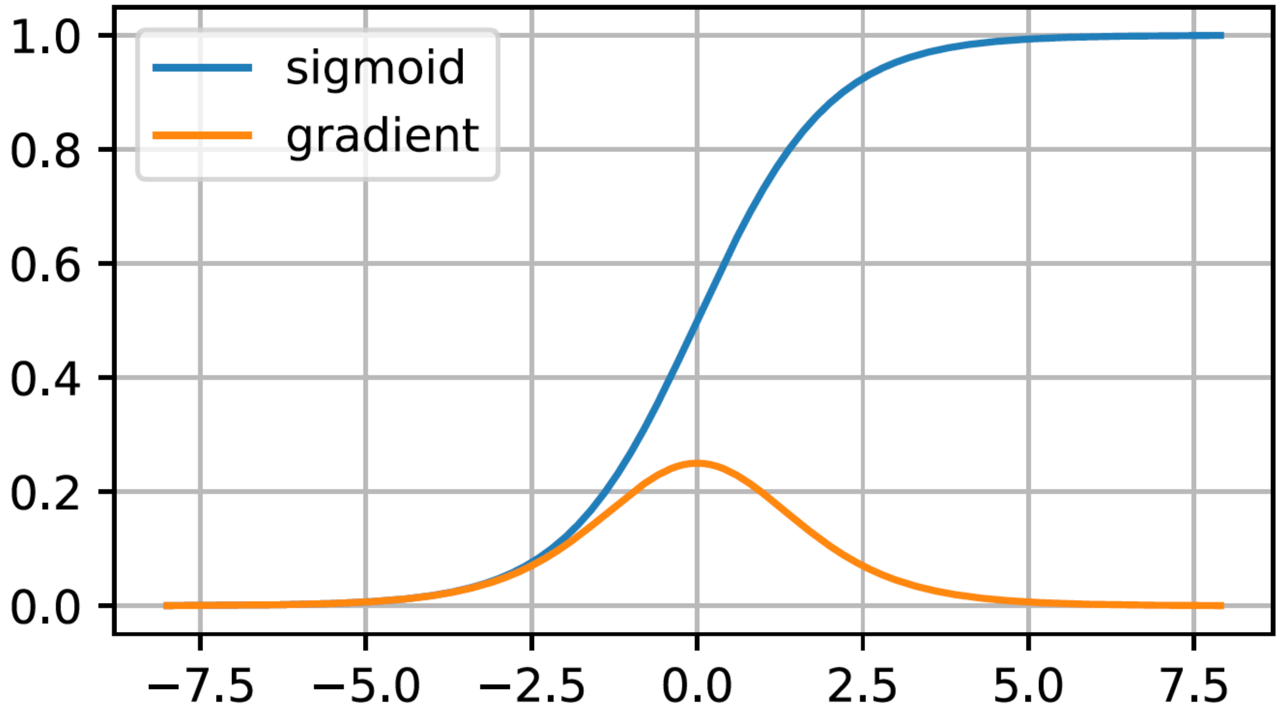
- Sigmoid function outputs 0 gradients unless we are in a perfect zone.
- That is why ReLUs have become the default choice !



Exploding Gradients

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Exploding Gradients

- The opposite problem of vanishing gradients
- Let’s draw 100 Gaussian random matrices and multiply them with some initial matrix 100 times.
- The matrix product explodes

```
A single matrix
[[ 2.2122064   0.7740038   1.0434405   1.1839255 ]
 [ 1.8917114  -1.2347414  -1.771029   -0.45138445]
 [ 0.57938355 -1.856082   -1.9768796  -0.20801921]
 [ 0.2444218  -0.03716067 -0.48774993 -0.02261727]]
<NDArray 4x4 @cpu(0)>
After multiplying 100 matrices
[[ 3.1575275e+20 -5.0052276e+19  2.0565092e+21 -2.3741922e+20]
 [-4.6332600e+20  7.3445046e+19 -3.0176513e+21  3.4838066e+20]
 [-5.8487235e+20  9.2711797e+19 -3.8092853e+21  4.3977330e+20]
 [-6.2947415e+19  9.9783660e+18 -4.0997977e+20  4.7331174e+19]]
<NDArray 4x4 @cpu(0)>
```

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- In this case, the gradients for all dimensions are identical
- SGD would never break symmetry but dropout regularization would.

Parameter Initialization

- One way of addressing the issues raised above is through careful initialization of the weight vectors
- PyTorch uses uniform initialization by default for Linear layers

```
Attributes:
    weight: the learnable weights of the module of shape
        :math:`(\text{out\_features}, \text{in\_features})`. The values are
        initialized from :math:`\mathcal{U}(-\sqrt{k}, \sqrt{k})`, where
        :math:`k = \frac{1}{\text{in\_features}}`
    bias:   the learnable bias of the module of shape :math:`(\text{out\_features})`.
            If :attr:`bias` is ``True``, the values are initialized from
            :math:`\mathcal{U}(-\sqrt{k}, \sqrt{k})` where
            :math:`k = \frac{1}{\text{in\_features}}`
```

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- Similarly, we need $n_{out}\sigma^2 = 1$ for backpropagation which leaves us in a dilemma.
- Xavier initialization simply tries to satisfy: $\frac{1}{2}(n_{in} + n_{out})\sigma^2 = 1$