

Lecture 2: Basic Artificial Neural Networks and MLP

Yujiao Shi SIST, ShanghaiTech Spring, 2024



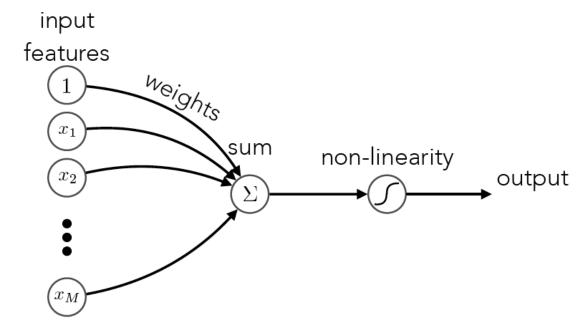


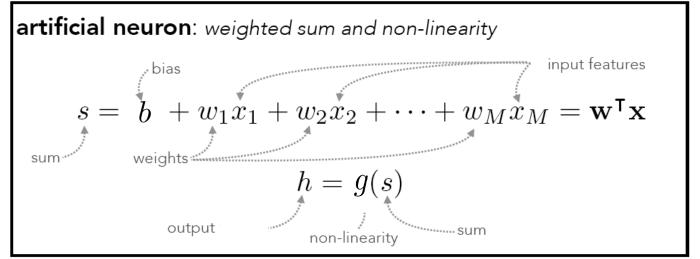
- Artificial neuron
 - □ Perceptron algorithm
- Single layer neural networks
 - Network models
 - □ Example: Logistic Regression
- Multi-layer neural networks
 - ☐ Limitations of single layer networks
 - Networks with single hidden layer

Acknowledgement: Hugo Larochelle's, Mehryar Mohri@NYU's & Yingyu Liang@Princeton's course notes

Mathematical model of a neuron 上海科技大学



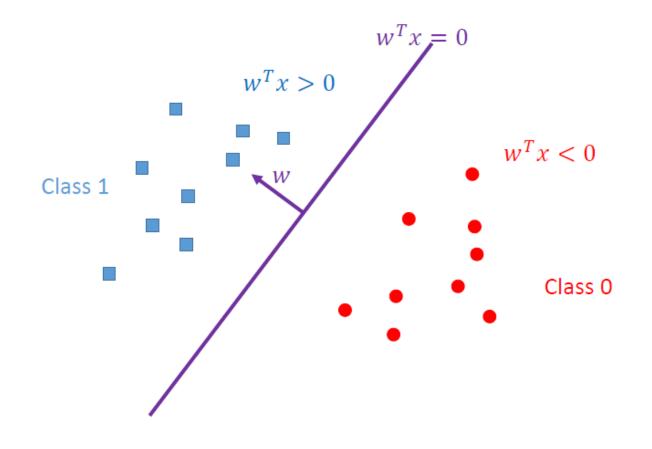




Single neuron as a linear classifier 上海科技大学

上海科技大学 ShanghaiTech University

Binary classification







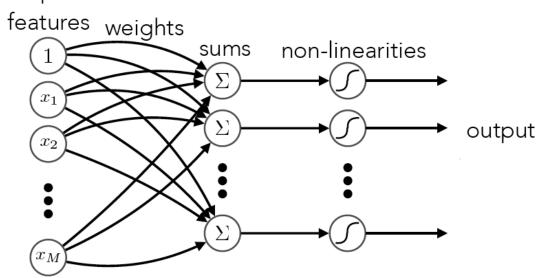
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input



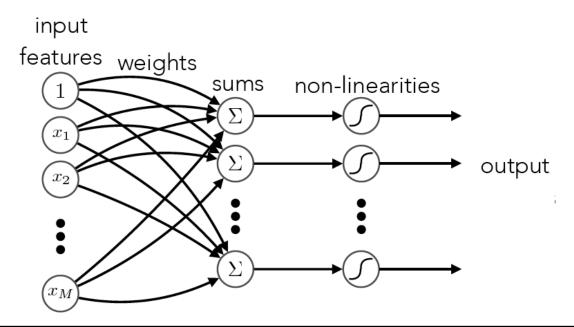
layer: parallelized weighted sum and non-linearity

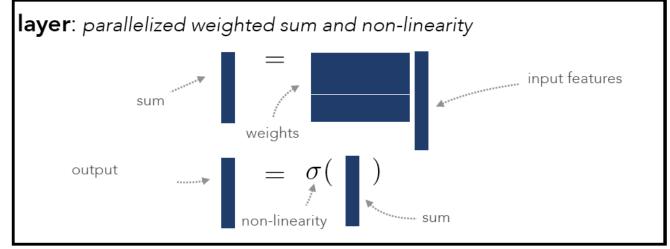
one sum per weight vector
$$s_j = \mathbf{w}_j^\intercal \mathbf{x}$$
 ———— $\mathbf{s} = \mathbf{W}^\intercal \mathbf{x}$ from weight matrix

$$\mathbf{h} = \sigma(\mathbf{s})$$

Single layer neural network





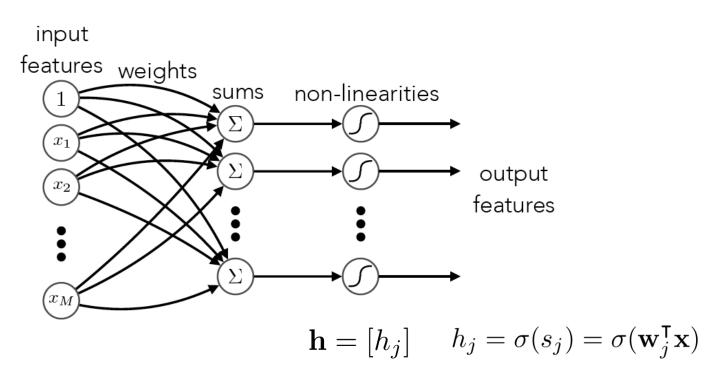




What is the output?



- Element-wise nonlinear functions
 - □ Independent feature/attribute detectors

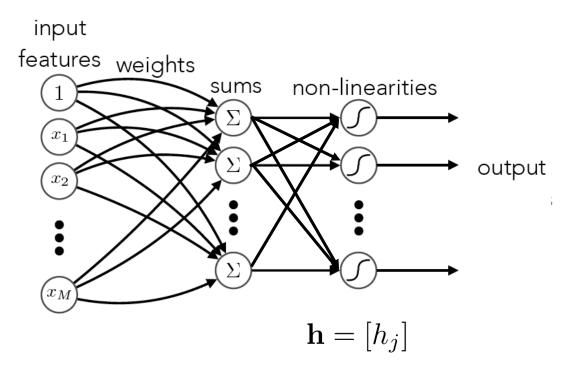




What is the output?



- Nonlinear functions with vector input
 - □ Competition between neurons



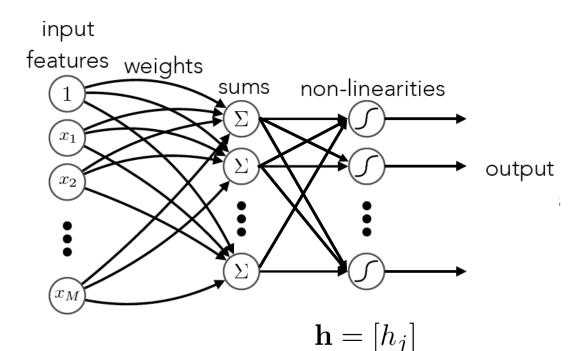
$$h_j = g(\mathbf{s}) = g(\mathbf{w}_1^\mathsf{T} \mathbf{x}, \cdots, \mathbf{w}_m^\mathsf{T} \mathbf{x})$$



What is the output?



- Nonlinear functions with vector input
 - □ Example: Winner-Take-All (WTA)



$$\mathbf{n} = [n_{\mathcal{I}}]$$

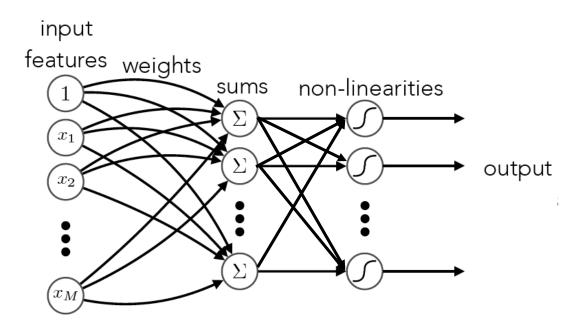
$$h_j = g(\mathbf{s}) = \begin{cases} 1 & \text{if } j = \arg\max_i \mathbf{w}_i^\mathsf{T} \mathbf{x} \\ 0 & \text{if otherwise} \end{cases}$$

10

A probabilistic perspective



Change the output nonlinearity



□ From WTA to Softmax function

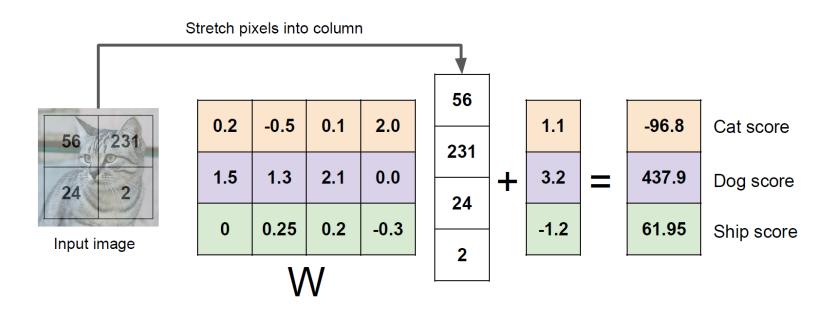
scores = unnormalized log probabilities of the classes.

$$P(Y=k|X=x_i) = rac{e^{s_k}}{\sum_j e^{s_j}}$$
 where $egin{aligned} oldsymbol{s} = f(x_i;W) \end{aligned}$

Multiclass linear classifiers



Example with an image with 4 pixels, and 3 classes (cat/dog/ship)

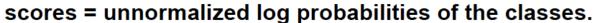


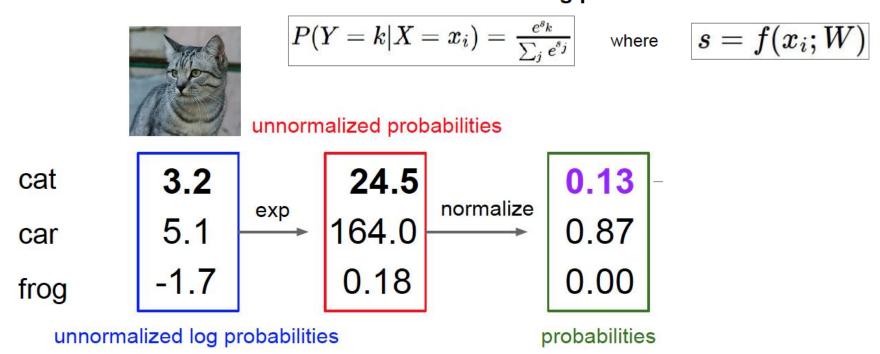
The WTA prediction: one-hot encoding of its predicted label

$$y = 1 \Leftrightarrow y = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \qquad y = 2 \Leftrightarrow y = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \qquad y = 3 \Leftrightarrow y = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

Probabilistic outputs









How to learn a multiclass classifier? 上海科技大学



Define a loss function and do minimization

- Given training data $\{(x_i, y_i): 1 \le i \le n\}$ i.i.d. from distribution D
- Find $y = f(x) \in \mathcal{H}$ that minimizes $\hat{L}(f) = \frac{1}{n} \sum_{i=1}^{n} l(f, x_i, y_i)$
- s.t. the expected loss is small

$$L(f) = \mathbb{E}_{(x,y) \sim D}[l(f,x,y)]$$

Empirical loss



Example: Logistic Regression



Learning loss: negative log likelihood

scores = unnormalized log probabilities of the classes.

$$P(Y=k|X=x_i) = rac{e^{s_k}}{\sum_j e^{s_j}}$$
 where $egin{aligned} oldsymbol{s} = f(x_i;W) \end{aligned}$

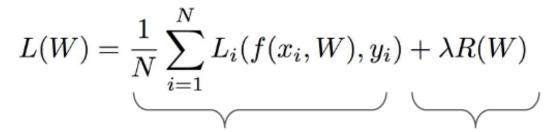
Want to maximize the log likelihood, or (for a loss function) to minimize the negative log likelihood of the correct class:

$$|L_i| = -\log P(Y=y_i|X=x_i)$$



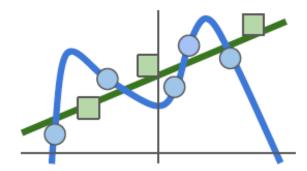
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- Constraints on hypothesis space
 - □ Similar to Linear Regression



Data loss: Model predictions should match training data

Regularization: Model should be "simple", so it works on test data





Learning with regularization



Regularization terms

In common use:

L2 regularization $R(W) = \sum_k \sum_l W_{k,l}^2$ L1 regularization $R(W) = \sum_k \sum_l |W_{k,l}|$ Elastic net (L1 + L2) $R(W) = \sum_k \sum_l \beta W_{k,l}^2 + |W_{k,l}|$ Max norm regularization (might see later)

- Priors on the weights
 - □ Bayesian: integrating out weights
 - □ Empirical: computing MAP estimate of W

Optimization: gradient descent

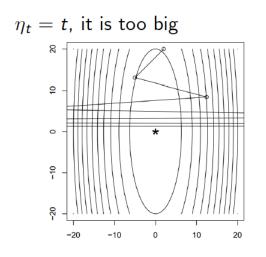


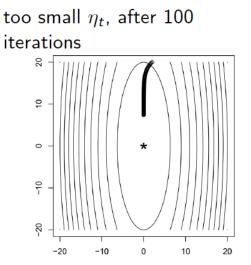
Gradient descent

```
# Vanilla Gradient Descent

while True:
    weights_grad = evaluate_gradient(loss_fun, data, weights)
    weights += - step_size * weights_grad # perform parameter update
```

Learning rate matters









Stochastic gradient descent

$$L(W) = \frac{1}{N} \sum_{i=1}^{N} L_i(x_i, y_i, W) + \lambda R(W)$$

$$\nabla_W L(W) = \frac{1}{N} \sum_{i=1}^{N} \nabla_W L_i(x_i, y_i, W) + \lambda \nabla_W R(W)$$

Full sum expensive when N is large!

Approximate sum using a minibatch of examples 32 / 64 / 128 common

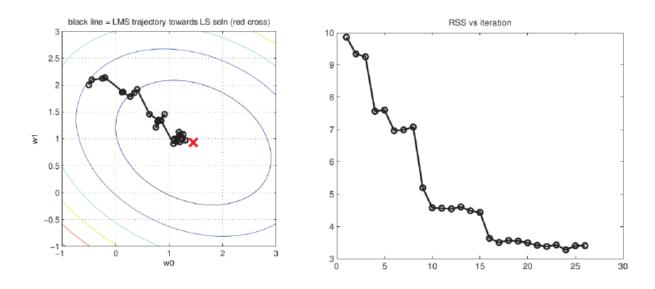
```
# Vanilla Minibatch Gradient Descent

while True:
   data_batch = sample_training_data(data, 256) # sample 256 examples
   weights_grad = evaluate_gradient(loss_fun, data_batch, weights)
   weights += - step_size * weights_grad # perform parameter update
```

Optimization: gradient descent



Stochastic gradient descent

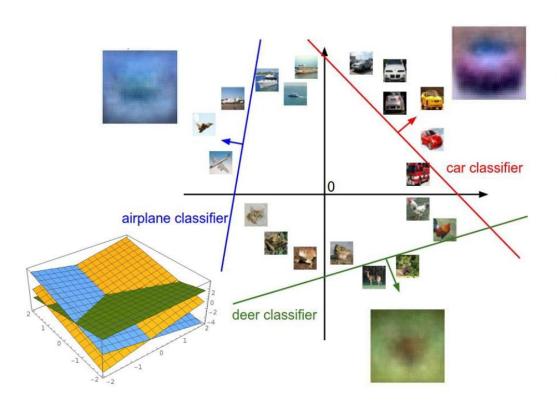


- the objective does not always decrease for each step
- comparing to GD, SGD needs more steps, but each step is cheaper
- mini-batch, say pick up 100 samples and do average, may accelerate the convergence





What are those weights?



$$f(x,W) = Wx + b$$



Array of **32x32x3** numbers (3072 numbers total)

Outline



- Single layer neural networks
 - Network models
 - □ Example: Logistic Regression
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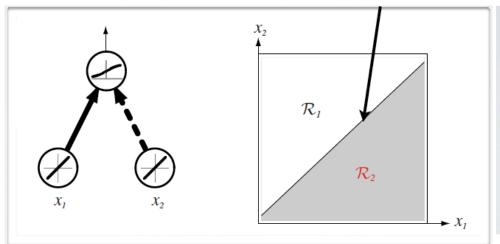
Capacity of single neuron

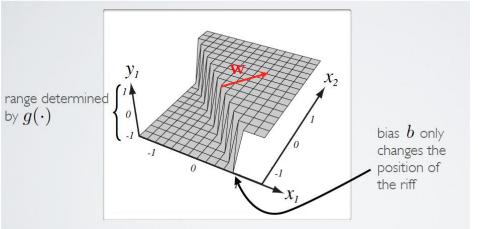


- Binary classification
 - □ A neuron estimates

$$P(y=1|\mathbf{x}) = \sigma(\mathbf{w}^{\mathsf{T}}\mathbf{x})$$

□ Its decision boundary is linear, determined by its weights





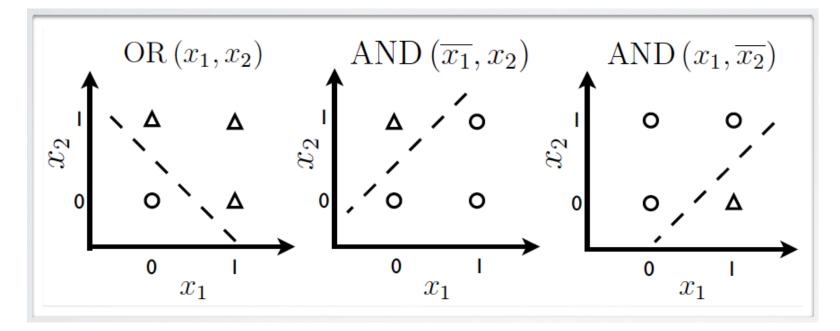


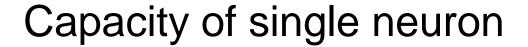


Can solve linearly separable problems

$$\mathcal{D} = \mathcal{D}^{+} \cup \mathcal{D}^{-}$$
$$\exists \mathbf{w}^{*}, \mathbf{w}^{*T}\mathbf{x} > 0, \ \forall \mathbf{x} \in \mathcal{D}^{+}$$
$$\mathbf{w}^{*T}\mathbf{x} < 0, \ \forall \mathbf{x} \in \mathcal{D}^{-}$$

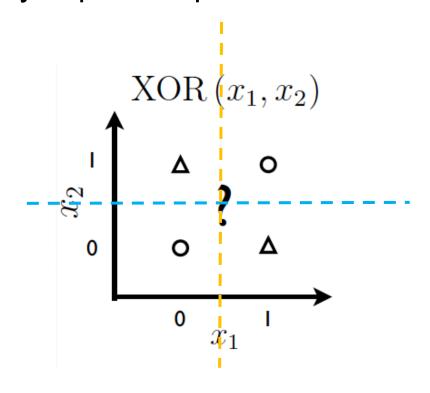
Examples







Can't solve non linearly separable problems



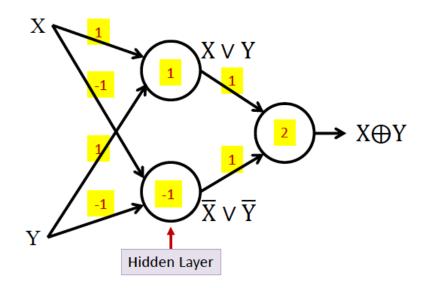
Can we use multiple neurons to achieve this?



Capacity of single neuron



- Can't solve non linearly separable problems
- Unless the input is transformed in a better representation

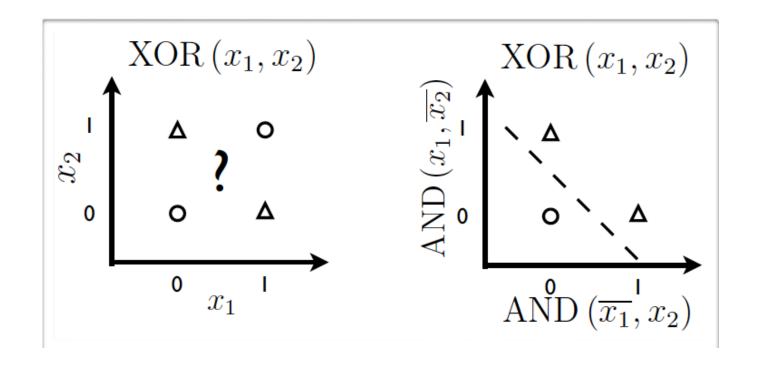




Capacity of single neuron



Can't solve non linearly separable problems



Unless the input is transformed in a better representation

Adding one more layer



- Single hidden layer neural network
 - □ 2-layer neural network: ignoring input units

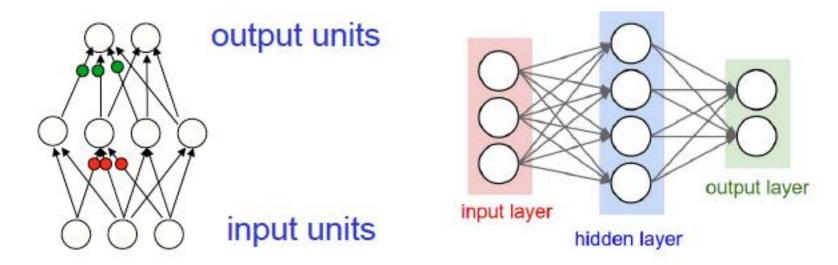


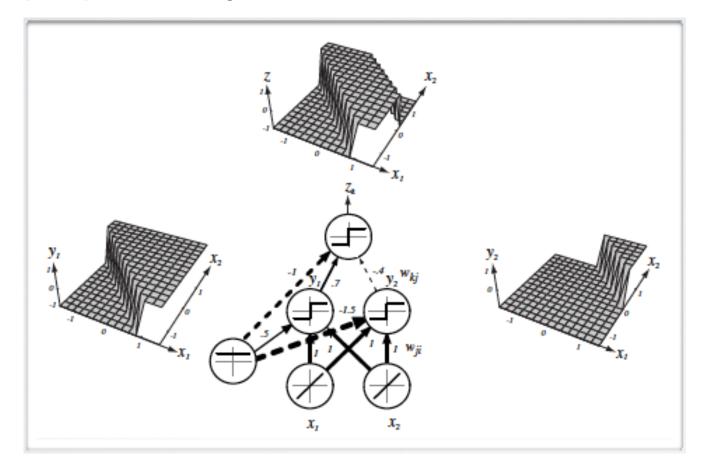
Figure: Two different visualizations of a 2-layer neural network. In this example: 3 input units, 4 hidden units and 2 output units

Q: What if using linear activation in hidden layer?





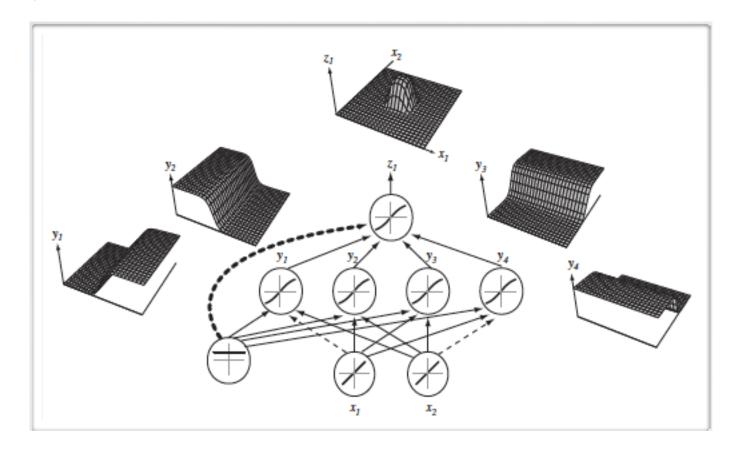
- Single hidden layer neural network
 - □ Partition the input space into regions







- Single hidden layer neural network
 - ☐ Form a stump/delta function





Capacity of neural network



- Universal approximation
 - ☐ Theorem (Hornik, 1991)
 - A single hidden layer neural network with a linear output unit can approximate any continuous function arbitrarily well, given enough hidden units.
 - □ The result applies for sigmoid, tanh and many other hidden layer activation functions
 - Caveat: good result but not useful in practice
 - ☐ How many hidden units?
 - How to find the parameters by a learning algorithm?

General neural network



Multi-layer neural network

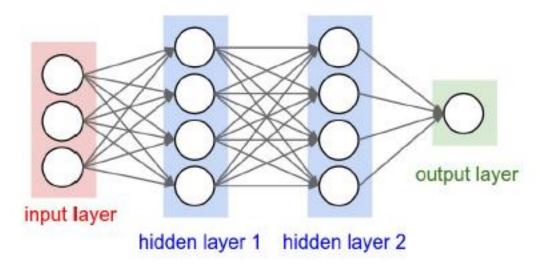
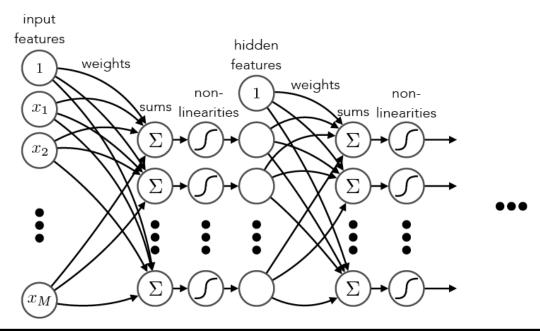


Figure: A 3-layer neural net with 3 input units, 4 hidden units in the first and second hidden layer and 1 output unit

- Naming conventions; a N-layer neural network:
 - N − 1 layers of hidden units
 - One output layer







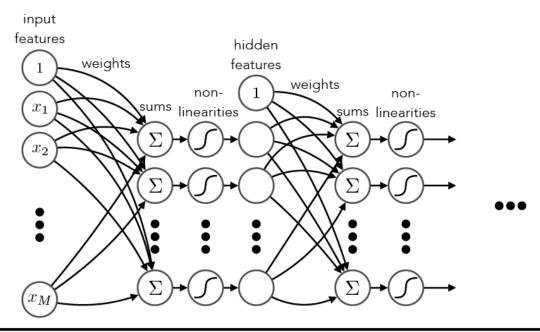
network: sequence of parallelized weighted sums and non-linearities

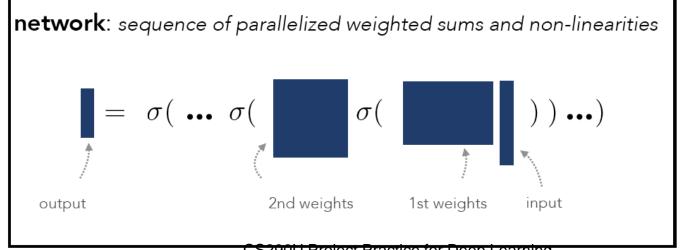
DEFINE
$$\mathbf{x}^{(0)} \equiv \mathbf{x}$$
, $\mathbf{x}^{(1)} \equiv \mathbf{h}$, etc.

$$\mathbf{s}^{(1)} = \mathbf{W}^{(1)} \mathbf{T} \mathbf{x}^{(0)}$$
 $\mathbf{s}^{(2)} = \mathbf{W}^{(2)} \mathbf{T} \mathbf{x}^{(1)}$ $\mathbf{x}^{(1)} = \sigma(\mathbf{s}^{(1)})$ $\mathbf{x}^{(2)} = \sigma(\mathbf{s}^{(2)})$

Multilayer networks







Other network connectivity



sequential connectivity: information must flow through the entire sequence to reach the output

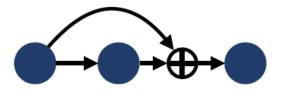


information may not be able to propagate easily

→ make shorter paths to output

residual & highway connections

dense (concatenated) connections

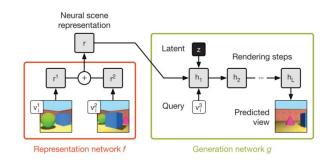


Deep residual learning for image recognition, He et al., 2016 Highway networks, Srivastava et al., 2015 Densely connected convolutional networks, Huang et al., 2017

Modern MLP as Implicit Representation海科技大学

ShanghaiTech University

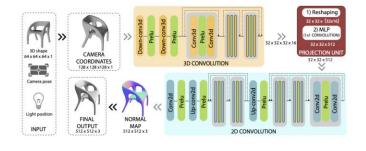




Generative Query Networks [Eslami et al. 2018]



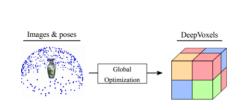
[Flynn et al., 2016; Zhou et al., 2018b; Mildenhall et al. 2019]



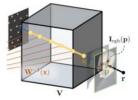
RenderNet [Nguyen-Phuoc et al. 2018]

Voxel Grids + CNN decoder

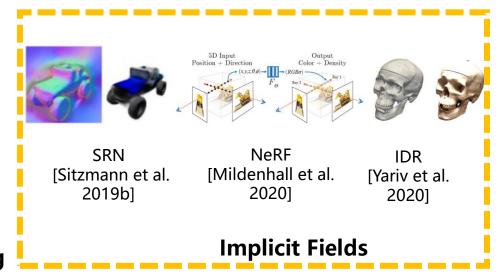
Multiplane Images (MPIs)



DeepVoxels
[Sitzmann et al. 2019]



Neural Volumes [Lombardi et al. 2019]

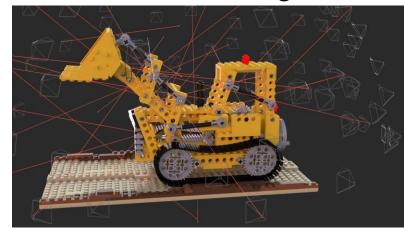


Voxel Grids + Ray Marching

Modern MLP in NeRF

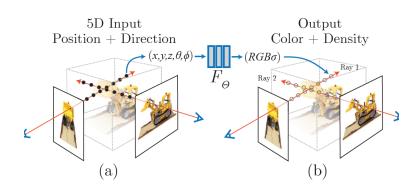


- Color + Density
- Positional Encoding
- Volume Rendering



Representing Scenes as Neural Radiance Fields for View Synthesis, Mildenhall et al., ECCV 2020 Oral - Best Paper Honorable Mention





Outline



- Single layer neural networks
 - □ Network models; Example: Logistic Regression
- Multi-layer neural networks
 - ☐ Limitations of single layer networks
 - □ Neural networks with single hidden layer
 - □ Sequential network architecture and variants
- Inference and learning
 - □ Forward and Backpropagation
 - □ Examples: one-layer network
 - ☐ General BP algorithm





- We only need to know two algorithms
 - □ Inference/prediction: simply forward pass
 - □ Parameter learning: needs backward pass
- Basic fact:
 - ☐ A neural network is a function of composed operations

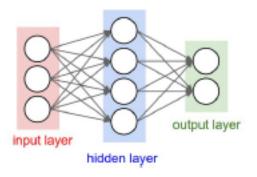
$$f_L(\mathbf{w}_L, f_{L-1}(\mathbf{w}_{L-1}, \dots f_1(\mathbf{w}_1, \mathbf{x}) \dots))$$

□ All the f functions are linear + (simple) nonlinear (differentiable a.e.) operators

Inference example: Forward Pass 上海科技大学



What does the network compute?



Output of the network can be written as:

$$h_j(x) = f(v_{j0} + \sum_{i=1}^{D} x_i v_{ji})$$

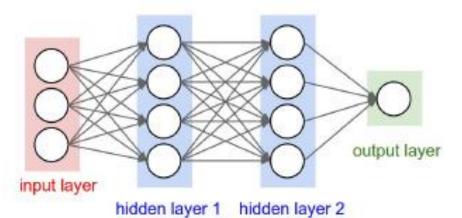
 $o_k(x) = g(w_{k0} + \sum_{j=1}^{J} h_j(x) w_{kj})$

(j indexing hidden units, k indexing the output units, D number of inputs)

Forward Pass in Python



Example code for a forward pass for a 3-layer network in Python:



forward-pass of a 3-layer neural network:
f = lambda x: 1.0/(1.0 + np.exp(-x)) # activation function (use sigmoid)
x = np.random.randn(3, 1) # random input vector of three numbers (3x1)
h1 = f(np.dot(W1, x) + b1) # calculate first hidden layer activations (4x1)
h2 = f(np.dot(W2, h1) + b2) # calculate second hidden layer activations (4x1)
out = np.dot(W3, h2) + b3 # output neuron (1x1)

Can be implemented efficiently using matrix operations

Parameter learning: Backward Pass 上海科技大学

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- Supervised learning framework
 - Find weights:

$$\mathbf{w}^* = \underset{\mathbf{w}}{\operatorname{argmin}} \sum_{n=1}^N \operatorname{loss}(\mathbf{o}^{(n)}, \mathbf{t}^{(n)})$$

where $\mathbf{o} = f(\mathbf{x}; \mathbf{w})$ is the output of a neural network

- Define a loss function, eg:
 - Squared loss: $\sum_{k} \frac{1}{2} (o_k^{(n)} t_k^{(n)})^2$
 - Cross-entropy loss: $-\sum_k t_k^{(n)} \log o_k^{(n)}$
- Gradient descent:

$$\mathbf{w}^{t+1} = \mathbf{w}^t - \eta \frac{\partial E}{\partial \mathbf{w}^t}$$

where η is the learning rate (and E is error/loss)

Gradient descent iteration



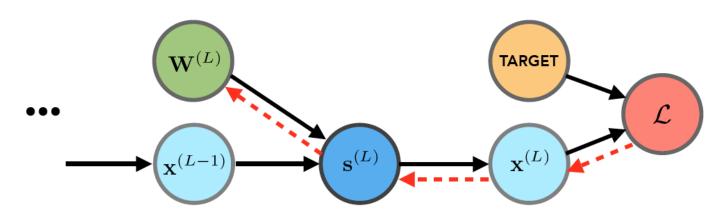
Forward pass

$$\mathbf{s}^{(1)} = \mathbf{W}^{(1)\intercal}\mathbf{x}^{(0)}$$
 $\mathbf{s}^{(2)} = \mathbf{W}^{(2)\intercal}\mathbf{x}^{(1)}$ $\mathbf{x}^{(1)} = \sigma(\mathbf{s}^{(1)})$ $\mathbf{x}^{(2)} = \sigma(\mathbf{s}^{(2)})$

Backward pass

calculate $\, \nabla_{W^{(1)}} \mathcal{L}, \nabla_{W^{(2)}} \mathcal{L}, \dots \,$ let's start with the final layer: $\nabla_{W^{(L)}} \mathcal{L}$

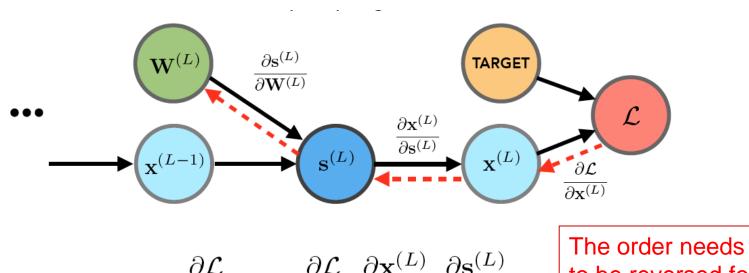
to determine the chain rule ordering, we'll draw the dependency graph



Gradient descent iteration



Backward pass



$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{(L)}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}^{(L)}} \frac{\partial \mathbf{x}^{(L)}}{\partial \mathbf{s}^{(L)}} \frac{\partial \mathbf{s}^{(L)}}{\partial \mathbf{W}^{(L)}}$$
 to be reversed for Jacobians!
$$\frac{\partial}{\partial \mathbf{W}^{(L)}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}^{(L)}} \frac{\partial \mathbf{x}^{(L)}}{\partial \mathbf{w}^{(L)}} \frac{\partial \mathbf{s}^{(L)}}{\partial \mathbf{w}^{(L)}} = \mathbf{x}^{(L-1)\mathsf{T}}$$

note
$$abla_{\mathbf{W}^{(L)}}\mathcal{L}\equiv \frac{\partial \mathcal{L}}{\partial \mathbf{W}^{(L)}}$$
 is notational convention

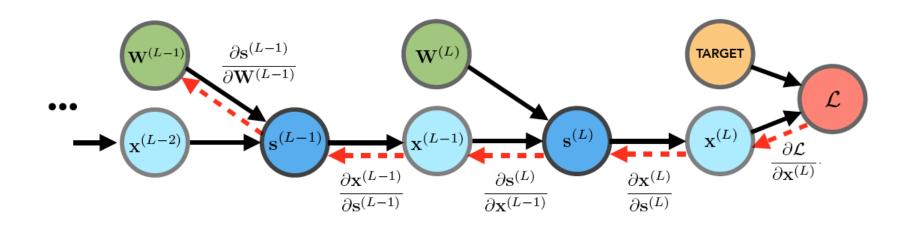
Gradient descent iteration



Backward pass

now let's go back one more layer...

again we'll draw the dependency graph:



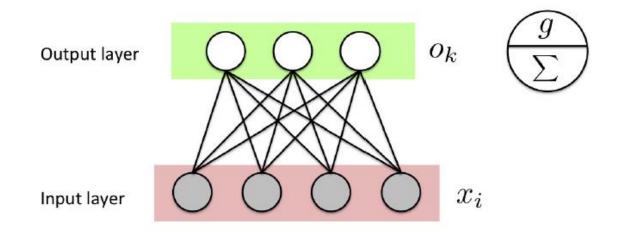
$$\frac{\partial \mathcal{L}}{\partial \mathbf{W}^{(L)}} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}^{(L)}} \frac{\partial \mathbf{x}^{(L)}}{\partial \mathbf{s}^{(L)}} \frac{\partial \mathbf{s}^{(L)}}{\partial \mathbf{x}^{(L-1)}} \frac{\partial \mathbf{x}^{(L-1)}}{\partial \mathbf{s}^{(L-1)}} \frac{\partial \mathbf{s}^{(L-1)}}{\partial \mathbf{W}^{(L-1)}}$$

The order needs to be reversed for Jacobians!





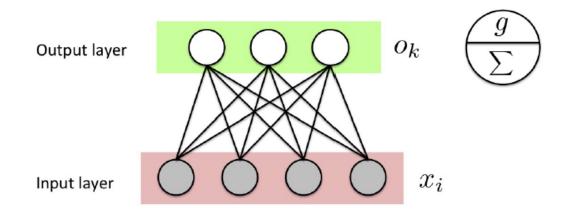
Let's take a single layer network

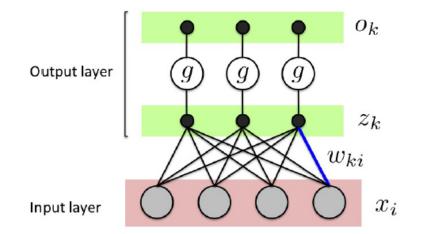


Example: Single Layer Network



• Let's take a single layer network and draw it a bit differently





Output of unit k

Output layer activation function

Net input to output unit k

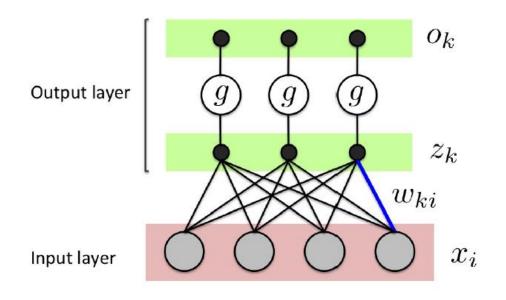
Weight from input i to k

Input unit i



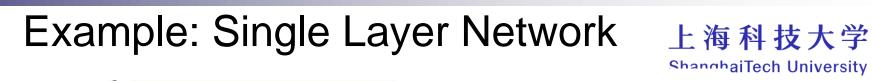
Example: Single Layer Network



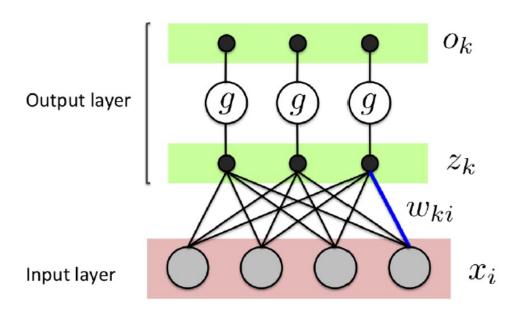


• Error gradients for single layer network:

$$\frac{\partial E}{\partial w_{ki}} =$$







• Error gradients for single layer network:

$$\frac{\partial E}{\partial w_{ki}} = \frac{\partial E}{\partial o_k} \frac{\partial o_k}{\partial z_k} \frac{\partial z_k}{\partial w_{ki}}$$

• Error gradient is computable for any continuous activation function g(), and any continuous error function

Outline



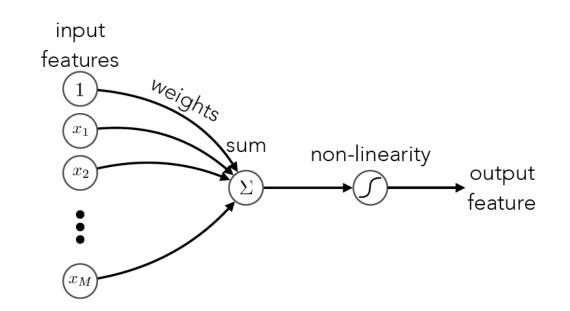
- Multi-layer neural networks
 - ☐ Limitations of single layer networks
 - □ Neural networks with single hidden layer
 - □ Sequential network architecture and variants
- Inference and learning
 - □ Forward and Backpropagation
 - □ Examples: one-layer network
 - □ General BP algorithm





Example: Univariate logistic least square model

$$s = wx + b$$
$$y = \sigma(s)$$
$$\mathcal{L} = \frac{1}{2}(y - t)^2$$







- A structured way to implement it
 - ☐ The goal is to write a program that efficiently computes the derivatives

Computing the loss:

$$s = wx + b$$
$$y = \sigma(s)$$
$$\mathcal{L} = \frac{1}{2}(y - t)^{2}$$

Computing the derivatives:

$$\frac{d\mathcal{L}}{dy} = y - t$$

$$\frac{d\mathcal{L}}{ds} = \frac{d\mathcal{L}}{dy}\sigma'(s)$$

$$\frac{d\mathcal{L}}{dw} = \frac{d\mathcal{L}}{ds}x$$

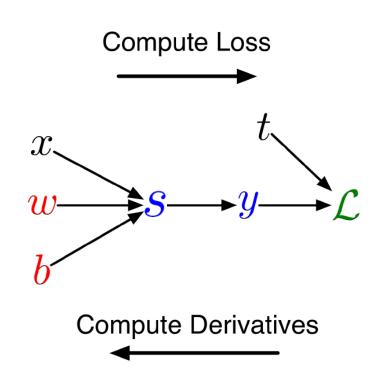
$$\frac{d\mathcal{L}}{db} = \frac{d\mathcal{L}}{ds}$$



Computation graph



- Represent the computations using a computation graph
 - □ Nodes: inputs & computed quantities
 - □ Edges: which nodes are computed directly as function of which other nodes



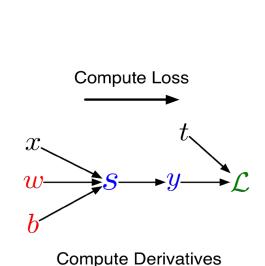
Univariate chain rule



- A shorthand notation
 - \square Use $\delta_y := d\mathcal{L}/dy$, called the error signal
 - □ Note that the error signals are values computed by the program

Computing the loss:

$$s = wx + b$$
$$y = \sigma(s)$$
$$\mathcal{L} = \frac{1}{2}(y - t)^2$$



Computing the derivatives:

$$\delta_y = y - t$$

$$\delta_s = \delta_y \sigma'(s)$$

$$\delta_w = \delta_s x$$

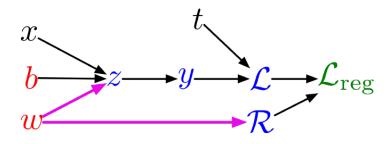
$$\delta_b = \delta_s$$

Multivariate chain rule



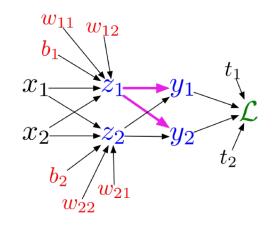
The computation graph has fan-out > 1

*L*₂-Regularized regression



$$z = wx + b$$
 $y = \sigma(z)$
 $\mathcal{L} = \frac{1}{2}(y - t)^2$
 $\mathcal{R} = \frac{1}{2}w^2$
 $\mathcal{L}_{reg} = \mathcal{L} + \lambda \mathcal{R}$

Multiclass logistic regression

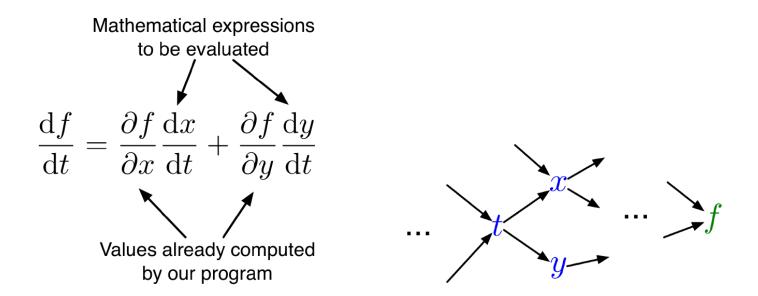


$$z_{\ell} = \sum_{j} w_{\ell j} x_{j} + b_{\ell}$$
 $y_{k} = \frac{e^{z_{k}}}{\sum_{\ell} e^{z_{\ell}}}$
 $\mathcal{L} = -\sum_{j} t_{k} \log y_{k}$

Multivariable chain rule



Recall the distributed chain rule



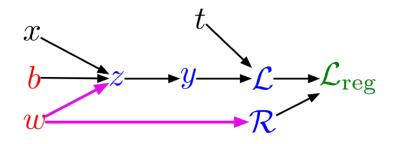
■ The shorthand notation:

$$\delta_t = \delta_x \frac{dx}{dt} + \delta_y \frac{dy}{dt}$$

General Backpropagation



Example: univariate logistic least square regression



Forward pass:

$$z = wx + b$$
 $y = \sigma(z)$
 $\mathcal{L} = \frac{1}{2}(y - t)^2$
 $\mathcal{R} = \frac{1}{2}w^2$
 $\mathcal{L}_{reg} = \mathcal{L} + \lambda \mathcal{R}$

Backward pass:

$$\delta_{\mathcal{L}_{reg}} = 1$$

$$\delta_{\mathcal{R}} = \delta_{\mathcal{L}_{reg}} \frac{d\mathcal{L}_{reg}}{d\mathcal{R}}$$

$$= \delta_{\mathcal{L}_{reg}} \lambda$$

$$\delta_{z} = \delta_{y} \frac{dy}{dz}$$

$$= \delta_{y} \sigma'(z)$$

$$\delta_{w} = \delta_{z} \frac{dz}{dw} + \delta_{z} \frac{dz}{dw}$$

$$= \delta_{\mathcal{L}_{reg}}$$

$$\delta_{w} = \delta_{z} \frac{dz}{dw} + \delta_{z} \frac{dz}{dw}$$

$$= \delta_{z} x + \delta_{z} w$$

$$\delta_{z} = \delta_{z} \frac{dz}{dw} + \delta_{z} \frac{dz}{dw}$$

$$= \delta_{z} x + \delta_{z} w$$

$$\delta_{z} = \delta_{z} \frac{dz}{dw} + \delta_{z} \frac{dz}{dw}$$

$$= \delta_{z} x + \delta_{z} w$$

$$\delta_{z} = \delta_{z} \frac{dz}{dz}$$

$$= \delta_{z} \frac{dz}{dz}$$

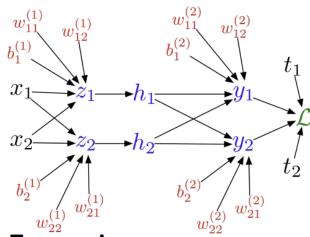
$$= \delta_{z} \frac{dz}{dz}$$

$$= \delta_{z} \frac{dz}{dz}$$

General Backpropagation

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Example: Multilayer Perceptron (multiple outputs)



Forward pass:

$$z_i = \sum_{j} w_{ij}^{(1)} x_j + b_i^{(1)}$$
 $h_i = \sigma(z_i)$
 $y_k = \sum_{i} w_{ki}^{(2)} h_i + b_k^{(2)}$
 $\mathcal{L} = \frac{1}{2} \sum_{k} (y_k - t_k)^2$

Backward pass:

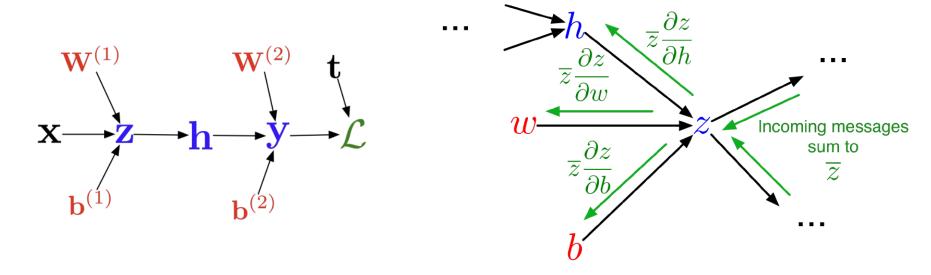
$$egin{aligned} \overline{\mathcal{L}} &= 1 \ \overline{y_k} &= \overline{\mathcal{L}} \left(y_k - t_k
ight) \ \overline{w_{ki}^{(2)}} &= \overline{y_k} \ h_i \ \overline{b_k^{(2)}} &= \overline{y_k} \ \overline{h_i} &= \sum_k \overline{y_k} w_{ki}^{(2)} \ \overline{z_i} &= \overline{h_i} \ \sigma'(z_i) \ \overline{w_{ij}^{(1)}} &= \overline{z_i} \ x_j \ \overline{b_i^{(1)}} &= \overline{z_i} \end{aligned}$$



General Backpropagation



Backprop as message passing:



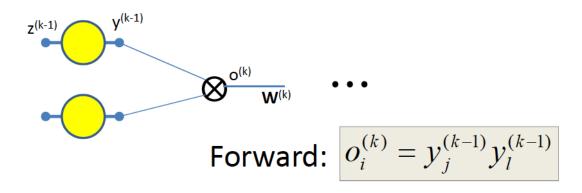
- Each node receives a set of messages from its children, which are aggregated into its error signal, then it passes messages to its parents
- Modularity: each node only has to know how to compute derivatives w.r.t. its arguments local computation in the graph



Patterns in backward flow



Multiplicative node

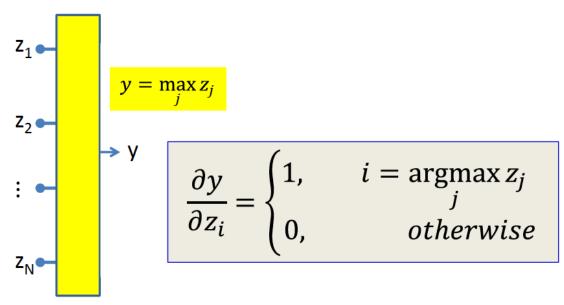


$$rac{\partial L}{\partial y_j^{(k-1)}} = rac{\partial L}{\partial o_i^{(k)}} rac{\partial o_i^{(k)}}{\partial y_j^{(k-1)}} = y_l^{(k-1)} rac{\partial L}{\partial o_i^{(k)}}$$

Patterns in backward flow



Max node



- Vector equivalent of subgradient
 - 1 w.r.t. the largest incoming input
 - Incremental changes in this input will change the output
 - 0 for the rest
 - Incremental changes to these inputs will not change the output



Backpropagation



- Backprop is used to train the majority of neural nets
 - □ Even generative network learning, or advanced optimization algorithms (second-order) use backprop to compute the update of weights
- However, backprop seems biologically implausible
 - □ No evidence for biological signals analogous to error derivatives
 - ☐ All the existing biologically plausible alternatives learn much more slowly on computers.
 - □ So how on earth does the brain learn???



Summary



- Artificial neurons, Single-layer network
- Multi-layer neural networks
- Inference and learning
 - □ Forward and Backpropagation
- Next time ...
 - ☐ Modern topics about CNN

Reference:

- □ d2l.ai: 4.1-4.3, 4.7
- □ DLBook: Chapter 6