Lecture 2: Basic Artificial Neural Networks

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9/12/2019



Logistics

- Course project
 - □ Each team is up to 3 members
 - You should form the team right after the National holiday week
- Homework
 - Programming: not the same as CS231n
 - □ Write-up: problem set
 - ☐ HW1 out next Tuesday
- Quiz
 - □ ~20 mins
 - □ Q1 next Tuesday ~30 mins

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Outline

- Review: Supervised learning
 - □ Linear regression
- Artificial neuron
 - Neuron models
 - □ Perceptron algorithm
- Single layer neural networks
 - Network models

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



Learning problem

Problem setup

- 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

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



Formulation

- Given training data $\{(x_i, y_i): 1 \le i \le n\}$ i.i.d. from distribution D
- Find $f_{w}(x) = w^{T}x$ that minimizes $\hat{L}(f_{w}) = \frac{1}{n}\sum_{i=1}^{n}(w^{T}x_{i} y_{i})^{2}$

l₂ loss; also called mean square error

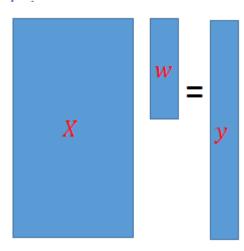
Hypothesis class ${m {\mathcal H}}$



Optimization

- Given training data $\{(x_i, y_i): 1 \le i \le n\}$ i.i.d. from distribution D
- Find $f_w(x) = w^T x$ that minimizes $\hat{L}(f_w) = \frac{1}{n} \sum_{i=1}^n (w^T x_i y_i)^2$
- Let X be a matrix whose i-th row is x_i^T , y be the vector $(y_1, ..., y_n)^T$

$$\widehat{L}(f_w) = \frac{1}{n} \sum_{i=1}^{n} (w^T x_i - y_i)^2 = \frac{1}{n} ||Xw - y||_2^2$$





Optimization

Set the gradient to 0 to get the minimizer

$$\nabla_{w} \hat{L}(f_{w}) = \nabla_{w} \frac{1}{n} ||Xw - y||_{2}^{2} = 0$$

$$\nabla_{w} [(Xw - y)^{T} (Xw - y)] = 0$$

$$\nabla_{w} [w^{T} X^{T} X w - 2w^{T} X^{T} y + y^{T} y] = 0$$

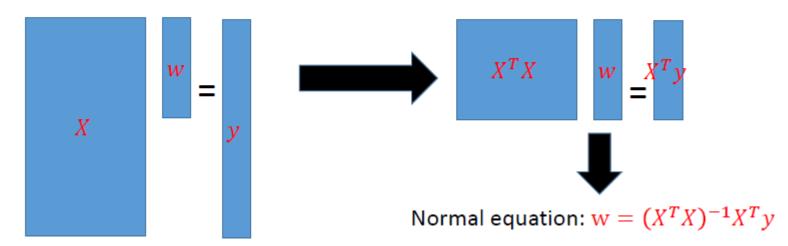
$$2X^{T} X w - 2X^{T} y = 0$$

$$w = (X^{T} X)^{-1} X^{T} y$$



Optimization

- Algebraic view of the minimizer
 - If X is invertible, just solve Xw = y and get $w = X^{-1}y$
 - But typically X is a tall matrix



□ What if not invertible?



With bias term

Bias term

- Given training data $\{(x_i, y_i): 1 \le i \le n\}$ i.i.d. from distribution D
- Find $f_{w,b}(x) = w^T x + b$ to minimize the loss
- Reduce to the case without bias:
 - Let w' = [w; b], x' = [x; 1]
 - Then $f_{w,b}(x) = w^T x + b = (w')^T (x')$



■ Why l₂ loss?

- Why not choose another loss
 - l_1 loss, hinge loss, exponential loss, ...
- Empirical: easy to optimize
 - For linear case: $w = (X^T X)^{-1} X^T y$
- Theoretical: a way to encode prior knowledge

Questions:

- What kind of prior knowledge?
- Principal way to derive loss?



- Maximum likelihood estimation (MLE)
 - Given training data $\{(x_i, y_i): 1 \le i \le n\}$ i.i.d. from distribution D
 - Let $\{P_{\theta}(x,y): \theta \in \Theta\}$ be a family of distributions indexed by θ
 - Would like to pick θ so that $P_{\theta}(x, y)$ fits the data well



- Maximum likelihood estimation (MLE)
 - Given training data $\{(x_i, y_i): 1 \le i \le n\}$ i.i.d. from distribution D
 - Let $\{P_{\theta}(x,y): \theta \in \Theta\}$ be a family of distributions indexed by θ
 - "fitness" of θ to one data point (x_i, y_i) likelihood $(\theta; x_i, y_i) := P_{\theta}(x_i, y_i)$



- Maximum likelihood estimation (MLE)
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- Maximum likelihood estimation (MLE)
 - Given training data $\{(x_i, y_i): 1 \le i \le n\}$ i.i.d. from distribution D
 - Let $\{P_{\theta}(x,y): \theta \in \Theta\}$ be a family of distributions indexed by θ
 - MLE: maximize "fitness" of θ to i.i.d. data points $\{(x_i, y_i)\}$ $\theta_{ML} = \operatorname{argmax}_{\theta \in \Theta} \prod_i P_{\theta}(x_i, y_i)$



- Maximum likelihood estimation (MLE)
 - Given training data $\{(x_i, y_i): 1 \le i \le n\}$ i.i.d. from distribution D
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\theta_{ML} = \operatorname{argmax}_{\theta \in \Theta} \log[\prod_i P_{\theta}(x_i, y_i)]
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 $\theta_{ML} = \operatorname{argmax}_{\theta \in \Theta} \sum_{i} \log[P_{\theta}(x_i, y_i)]$



- Maximum likelihood estimation (MLE)
 - Given training data $\{(x_i, y_i): 1 \le i \le n\}$ i.i.d. from distribution D
 - Let $\{P_{\theta}(x,y): \theta \in \Theta\}$ be a family of distributions indexed by θ
 - MLE: negative log-likelihood loss

$$\theta_{ML} = \operatorname{argmax}_{\theta \in \Theta} \sum_{i} \log(P_{\theta}(x_{i}, y_{i}))$$
$$l(P_{\theta}, x_{i}, y_{i}) = -\log(P_{\theta}(x_{i}, y_{i}))$$
$$\hat{L}(P_{\theta}) = -\sum_{i} \log(P_{\theta}(x_{i}, y_{i}))$$



- MLE: conditional log-likelihood
 - Given training data $\{(x_i, y_i): 1 \le i \le n\}$ i.i.d. from distribution D
 - Let $\{P_{\theta}(y|x): \theta \in \Theta\}$ be a family of distributions indexed by θ
 - MLE: negative conditional log-likelihood loss

$$\theta_{ML} = \operatorname{argmax}_{\theta \in \Theta} \sum_{i} \log(P_{\theta}(y_i|x_i))$$

$$l(P_{\theta}, x_i, y_i) = -\log(P_{\theta}(y_i|x_i))$$

$$\hat{L}(P_{\theta}) = -\sum_i \log(P_{\theta}(y_i|x_i))$$

Only care about predicting y from x; do not care about p(x)



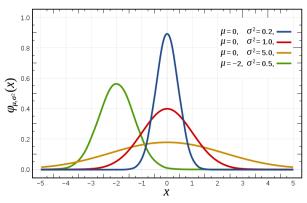
MLE example: Regression

Regression with I2 Loss

- Given training data $\{(x_i, y_i): 1 \le i \le n\}$ i.i.d. from distribution D
- Find $f_{\theta}(x)$ that minimizes $\hat{L}(f_{\theta}) = \frac{1}{n} \sum_{i=1}^{n} (f_{\theta}(x_i) y_i)^2$

 l_2 loss: Normal + MLE

- Define $P_{\theta}(y|x) = \text{Normal}(y; f_{\theta}(x), \sigma^2)$
- $\log(P_{\theta}(y_i|x_i)) = \frac{-1}{2\sigma^2}(f_{\theta}(x_i) y_i)^2 \log(\sigma) \frac{1}{2}\log(2\pi)$
- $\theta_{ML} = \operatorname{argmin}_{\theta \in \Theta} \frac{1}{n} \sum_{i=1}^{n} (f_{\theta}(x_i) y_i)^2$

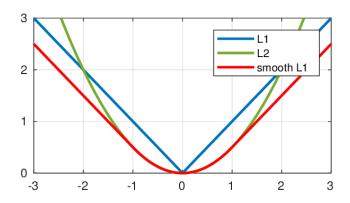


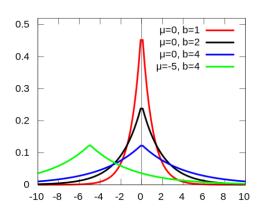


Outliers

- L2 loss = Gaussian distribution
- What if we have outliers?
 - Some data points lie far away from the linear structure
- Robust estimation
 - □ L1 loss: Laplace distribution

$$\hat{L}(f_w) = \frac{1}{n} \sum_{i=1}^n |w^{\mathsf{T}} x_i - y_i|$$







Generalization

- Overfitting or under-determined?
 - □ Ridge regression

$$\hat{L}(f_w) = \frac{1}{n} \sum_{i=1}^n \|w^{\mathsf{T}} x_i - y_i\|^2 + \lambda \sum_{j=1}^d w_j^2$$

- The optimal weights $w^* = (X^\intercal X + \lambda I)^{-1} X^\intercal Y$
- □ Lasso regression

$$\hat{L}(f_w) = \frac{1}{n} \sum_{i=1}^n \|w^{\mathsf{T}} x_i - y_i\|^2 + \lambda \sum_{j=1}^d |w_j|$$

- Convex optimization: proximal gradient descent
- oxdot The hyper-parameter λ controls the model complexity



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Artificial Neuron

Biological inspiration

 \bullet Our brain has $\sim 10^{11}$ neurons, each of which communicates (is connected) to $\sim 10^4$ other neurons

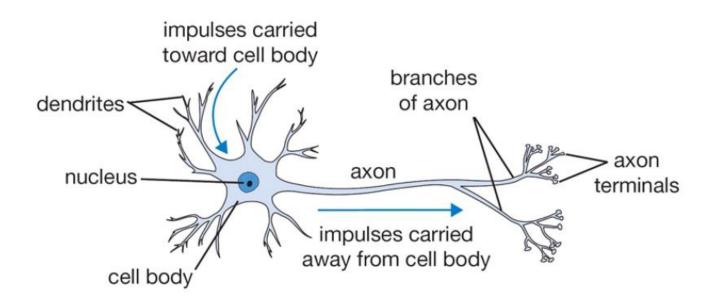
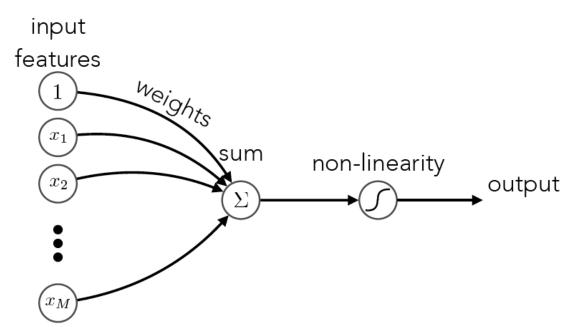
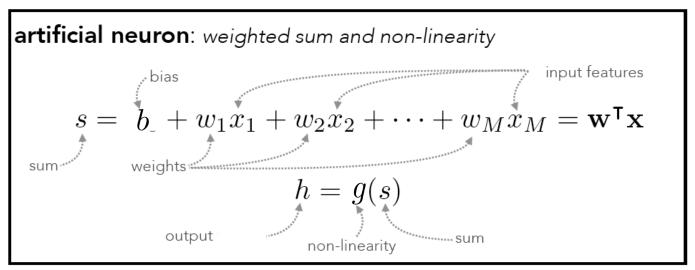


Figure: The basic computational unit of the brain: Neuron

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Mathematical model of a neuron







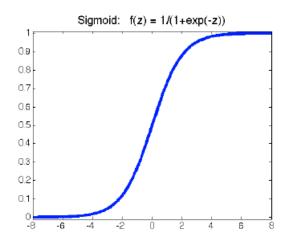
Activation functions

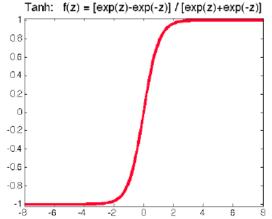
Most commonly used activation functions:

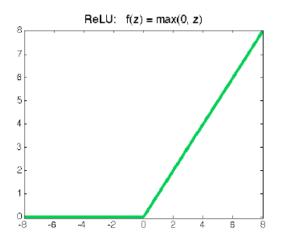
• Sigmoid:
$$\sigma(z) = \frac{1}{1 + \exp(-z)}$$

• Tanh:
$$\tanh(z) = \frac{\exp(z) - \exp(-z)}{\exp(z) + \exp(-z)}$$

• ReLU (Rectified Linear Unit): ReLU(z) = max(0, z)

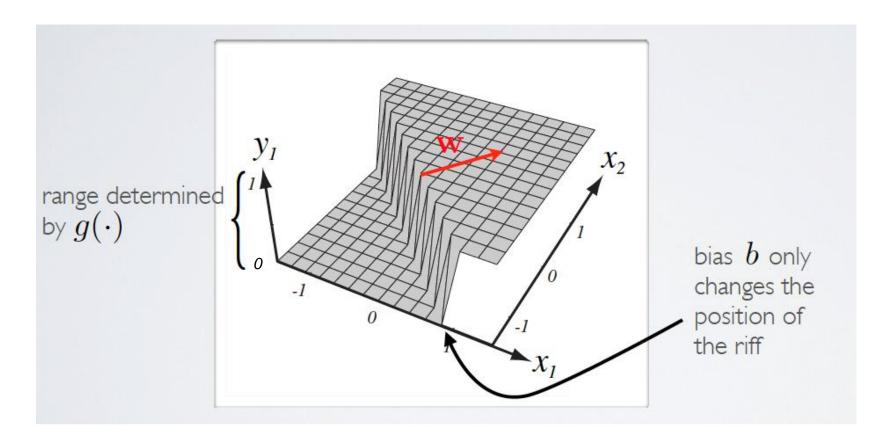






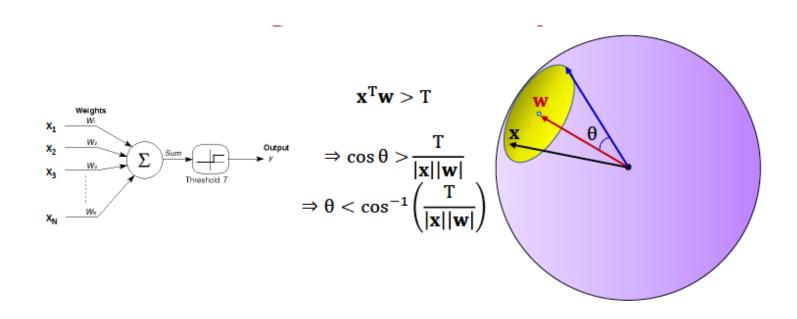
Capacity of single neuron

Sigmoid activation function



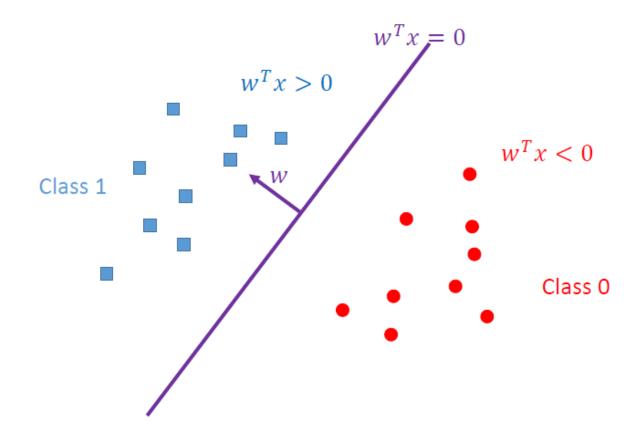
What a single neuron does?

- A neuron (perceptron) fires if its input is within a specific angle of its weight
 - If the input pattern matches the weight pattern closely enough



Single neuron as a linear classifier

Binary classification





How do we determine the weights?

Learning problem

- Given training data $\{(x_i, y_i): 1 \le i \le n\}$ i.i.d. from distribution D
- Hypothesis $f_w(x) = w^T x$
 - $y = 1 \text{ if } w^T x > 0$
 - y = 0 if $w^T x < 0$
- Prediction: $y = \text{step}(f_w(x)) = \text{step}(w^T x)$

Linear model ${\cal H}$



Linear classification

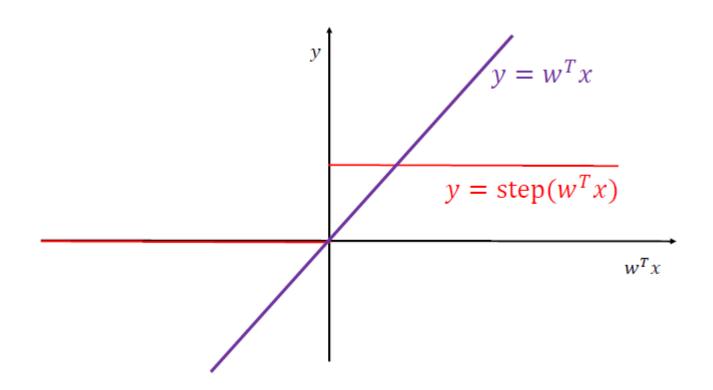
- Learning problem: simple approach
 - Given training data $\{(x_i, y_i): 1 \le i \le n\}$ i.i.d. from distribution D
 - Find $f_w(x) = w^T x$ that minimizes $\hat{L}(f_w) = \frac{1}{n} \sum_{i=1}^n (w^T x_i y_i)^2$
 - Drawback: Sensitive to "outliers"

Reduce to linear regression; ignore the fact $y \in \{0,1\}$



1D Example

Compare two predictors





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Perceptron algorithm

- Learn a single neuron for binary classification
- Task formulation
 - Given training data $\{(x_i, y_i): 1 \le i \le n\}$ i.i.d. from distribution D
 - Hypothesis $f_w(x) = w^T x$
 - $y = +1 \text{ if } w^T x > 0$
 - y = -1 if $w^T x < 0$
 - Prediction: $y = \text{sign}(f_w(x)) = \text{sign}(w^T x)$
 - Goal: minimize classification error

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Perceptron algorithm

- Algorithm outline
- Assume for simplicity: all x_i has length 1
 - 1. Start with the all-zeroes weight vector $\mathbf{w}_1 = \mathbf{0}$, and initialize t to 1.
 - 2. Given example \mathbf{x} , predict positive iff $\mathbf{w}_t \cdot \mathbf{x} > 0$.
 - 3. On a mistake, update as follows:
 - Mistake on positive: $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t + \mathbf{x}$.
 - Mistake on negative: $\mathbf{w}_{t+1} \leftarrow \mathbf{w}_t \mathbf{x}$.

$$t \leftarrow t + 1$$
.

Perceptron: figure from the lecture note of Nina Balcan



Perceptron algorithm

- Intuition: correct the current mistake
 - If mistake on a positive example

$$w_{t+1}^T x = (w_t + x)^T x = w_t^T x + x^T x = w_t^T x + 1$$

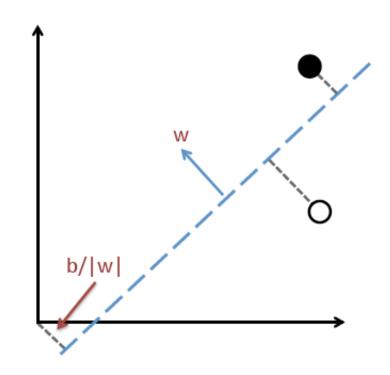
If mistake on a negative example

$$w_{t+1}^T x = (w_t - x)^T x = w_t^T x - x^T x = w_t^T x - 1$$

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Hyperplane Distance

- Line is a 1D, Plane is 2D
- Hyperplane is many D
 - Includes Line and Plane
- Defined by (w,b)
- Distance: $\frac{|w'x w'|}{\|w\|}$
- Signed Distance: $\frac{w^T x b}{\|w\|}$





Perceptron algorithm

The Perceptron theorem

- Suppose there exists w^* that correctly classifies $\{(x_i, y_i)\}$
- W.L.O.G., all x_i and w^* have length 1, so the minimum distance of any example to the decision boundary is

$$\gamma = \min_{i} |(w^*)^T x_i|$$

• Then Perceptron makes at most $\left(\frac{1}{\gamma}\right)^2$ mistakes



The Perceptron theorem

- Suppose there exists w^* that correctly classifies $\{(x_i, y_i)\}$
- W.L.O.G., all x_i and w^* have length 1, so the minimum distance of any example to the decision boundary is

$$\gamma = \min_{i} |(w^*)^T x_i|$$

Need not be i.i.d.!

• Then Perceptron makes at most $\left(\frac{1}{\nu}\right)^2$ mistakes

Do not depend on n, the length of the data sequence!



- The Perceptron theorem: proof
 - First look at the quantity $w_t^T w^*$
 - Claim 1: $w_{t+1}^T w^* \ge w_t^T w^* + \gamma$
 - Proof: If mistake on a positive example x

$$w_{t+1}^T w^* = (w_t + x)^T w^* = w_t^T w^* + x^T w^* \ge w_t^T w^* + \gamma$$

If mistake on a negative example

$$w_{t+1}^T w^* = (w_t - x)^T w^* = w_t^T w^* - x^T w^* \ge w_t^T w^* + \gamma$$



- The Perceptron theorem: proof
 - Next look at the quantity $||w_t||$

Negative since we made a mistake on x

- Claim 2: $||w_{t+1}||^2 \le ||w_t||^2 + 1$
- ullet Proof: If mistake on a positive example x

$$||w_{t+1}||^2 = ||w_t + x||^2 = ||w_t||^2 + ||x||^2 + 2w_t^T x$$



■ The Perceptron theorem: proof intuition

- Claim 1: $w_{t+1}^T w^* \ge w_t^T w^* + \gamma$
- Claim 2: $\left|\left|w_{t+1}\right|\right|^2 \leq \left|\left|w_{t}\right|\right|^2 + 1$

The correlation gets larger. Could be:

- 1. W_{t+1} gets closer to W^*
- 2. w_{t+1} gets much longer

Rules out the bad case "2. w_{t+1} gets much longer"



The Perceptron theorem: proof

- Claim 1: $w_{t+1}^T w^* \ge w_t^T w^* + \gamma$
- Claim 2: $||w_{t+1}||^2 \le ||w_t||^2 + 1$

After M mistakes:

- $w_{M+1}^T w^* \ge \gamma M$
- $||w_{M+1}|| \leq \sqrt{M}$
- $w_{M+1}^T w^* \le ||w_{M+1}||$

So $\gamma M \leq \sqrt{M}$, and thus $M \leq \left(\frac{1}{\gamma}\right)^2$



Perceptron Learning problem

- What loss function is minimized?
 - 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 $\widehat{L}(f) = \frac{1}{n} \sum_{i=1}^{n} l(f, x_i, y_i)$
 - s.t. the expected loss is small

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

Learning as iterative optimization

Gradient descent

• choose initial $w^{(0)}$, repeat

$$w^{(t+1)} = w^{(t)} - \eta_t \cdot \nabla L(w^{(t)})$$

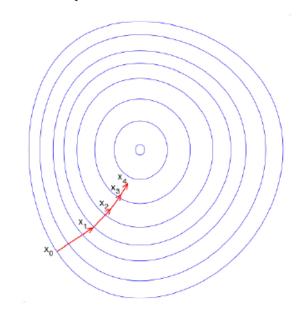
until stop

 \triangleright η_t is the learning rate, and

$$\nabla L(w^{(t)}) = \frac{1}{n} \sum_{i} \nabla_{w} L_{i}(w^{(t)}; y_{i}, x_{i})$$

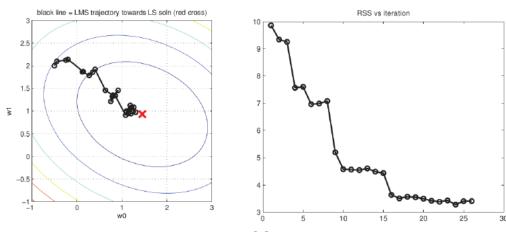
► How to stop? $||w^{(t+1)} - w^{(t)}|| \le \epsilon$ or $||\nabla L(w^{(t)})|| \le \epsilon$

Two dimensional example:





- Stochastic gradient descent (SGD)
 - Suppose data points arrive one by one
 - $\hat{L}(\mathbf{w}) = \frac{1}{n} \sum_{t=1}^n l(\mathbf{w}, x_t, y_t)$, but we only know $l(\mathbf{w}, x_t, y_t)$ at time t
 - Idea: simply do what you can based on local information
 - Initialize W₀
 - $\mathbf{w}_{t+1} = \mathbf{w}_t \eta_t \nabla l(\mathbf{w}_t, x_t, y_t)$





- What loss function is minimized?
 - Hypothesis: $y = \text{sign}(w^T x)$
 - Define hinge loss

$$l(w, x_t, y_t) = -y_t w^T x_t \mathbb{I}[\text{mistake on } x_t]$$

$$\widehat{L}(w) = -\sum_{t} y_{t} w^{T} x_{t} \mathbb{I}[\text{mistake on } x_{t}]$$

$$w_{t+1} = w_t - \eta_t \nabla l(w_t, x_t, y_t) = w_t + \eta_t y_t x_t \mathbb{I}[\text{mistake on } x_t]$$



- What loss function is minimized?
 - Hypothesis: $y = \text{sign}(w^T x)$ $w_{t+1} = w_t - \eta_t \nabla l(w_t, x_t, y_t) = w_t + \eta_t y_t x_t \mathbb{I}[\text{mistake on } x_t]$
 - Set $\eta_t = 1$. If mistake on a positive example

$$w_{t+1} = w_t + y_t x_t = w_t + x$$

If mistake on a negative example

$$w_{t+1} = w_t + y_t x_t = w_t - x$$

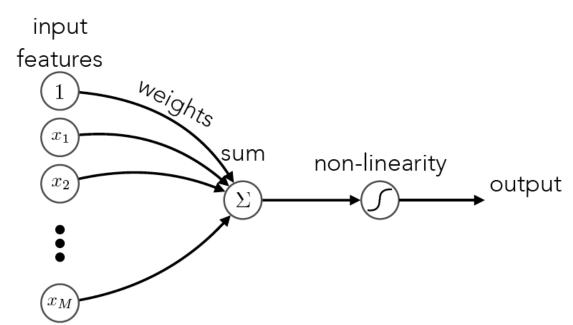


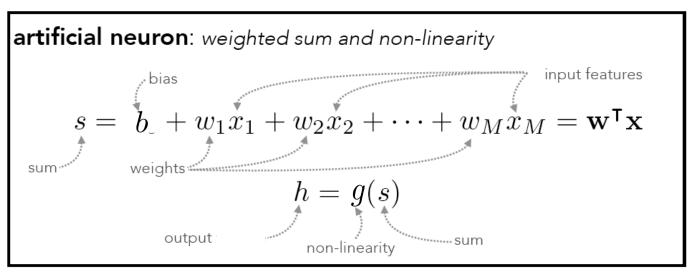
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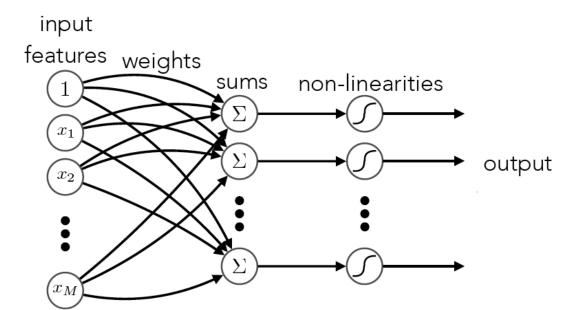
Mathematical model of a neuron







Single layer neural network

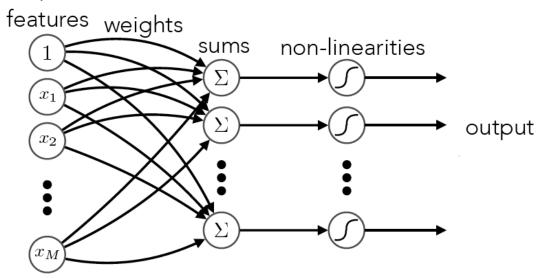


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Single layer neural network

input

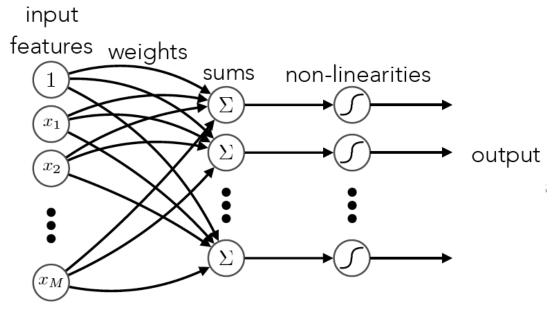


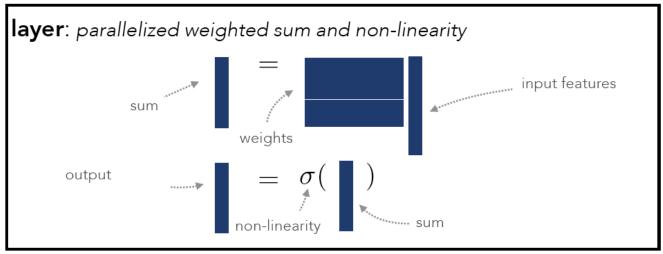
layer: parallelized weighted sum and non-linearity

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

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

Single layer neural network



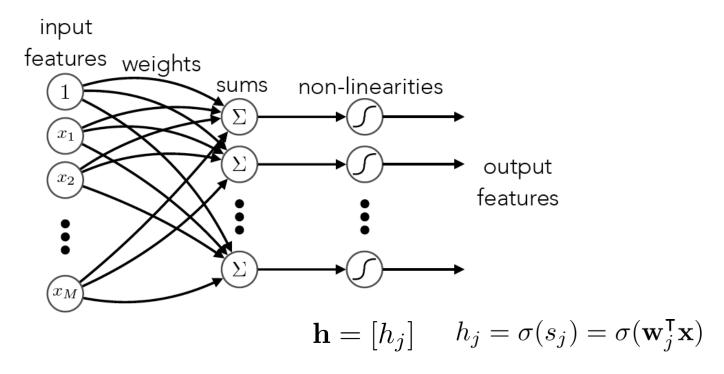


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What is the output?

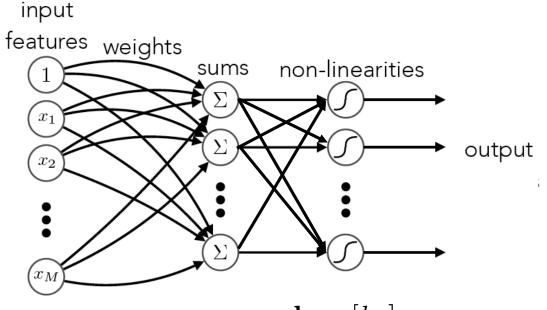
- Element-wise nonlinear functions
 - □ Independent feature/attribute detectors





What is the output?

- Nonlinear functions with vector input
 - Competition between neurons



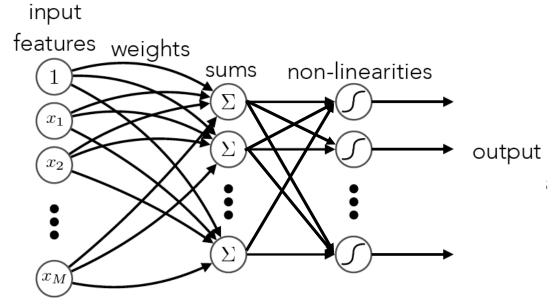
$$\mathbf{h} = [h_j]$$

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



What is the output?

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



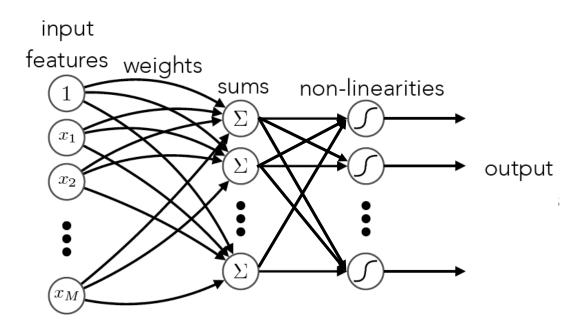
$$\mathbf{h} = [h_j]$$

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



A probabilistic perspective

Change the output nonlinearity



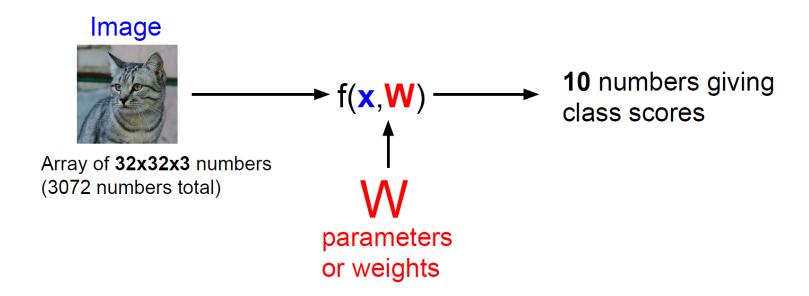
□ From WTA to Softmax function

scores = unnormalized log probabilities of the classes.

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

Example: Multiclass classification

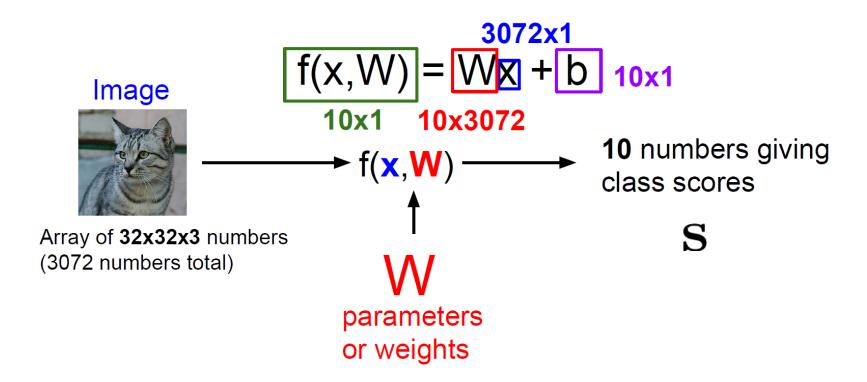
CIFAR10 as an example



The output/prediction: WTA

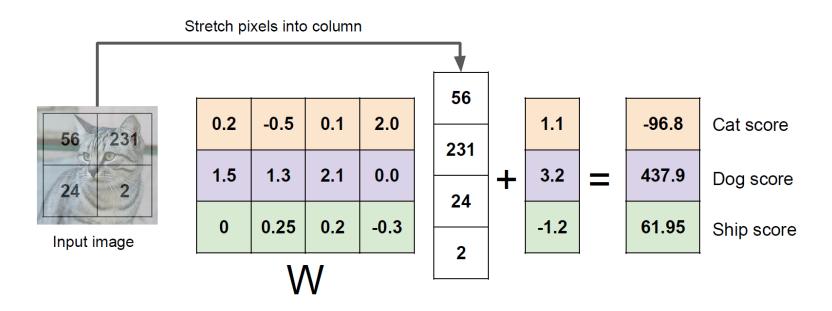
Multiclass linear classifiers

Extending linear classifier in binary case



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

scores = unnormalized log probabilities of the classes.



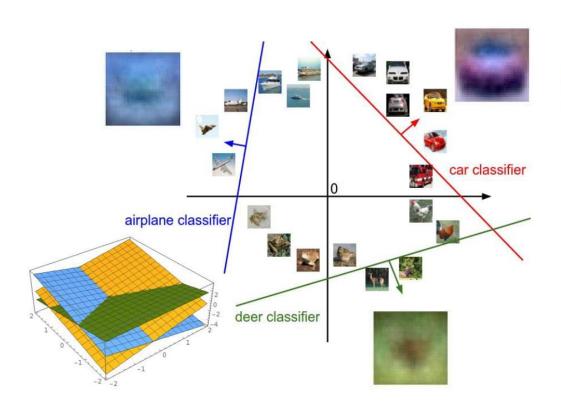
$$P(Y=k|X=x_i)=rac{e^{s_k}}{\sum_j e^{s_j}}$$

where
$$s=f(x_i;W)$$

unnormalized probabilities

Interpreting network weights

What are those weights?



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



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



How to learn a multiclass classifier?

- 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 $\widehat{L}(f) = \frac{1}{n} \sum_{i=1}^{n} l(f, x_i, y_i)$
 - s.t. the expected loss is small

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

Empirical loss

Learning a multiclass linear classifier

- Design a loss function for multiclass classifiers
 - □ Perceptron?
 - Yes, see homework
 - ☐ Hinge loss
 - The SVM and max-margin
 - □ Probabilistic formulation
 - Log loss and logistic regression
- Generalization issue
 - Avoid overfitting by regularization
- To be covered next time



Summary

- Supervised learning
 - □ Linear models
- Artificial neurons
- Single-layer network
 - Multi-class predictions
- Next time ...
 - □ Learning single-layer network
 - ☐ Multi-layer neural networks