Lecture 2: Basic Artificial Neural Networks

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Logistics

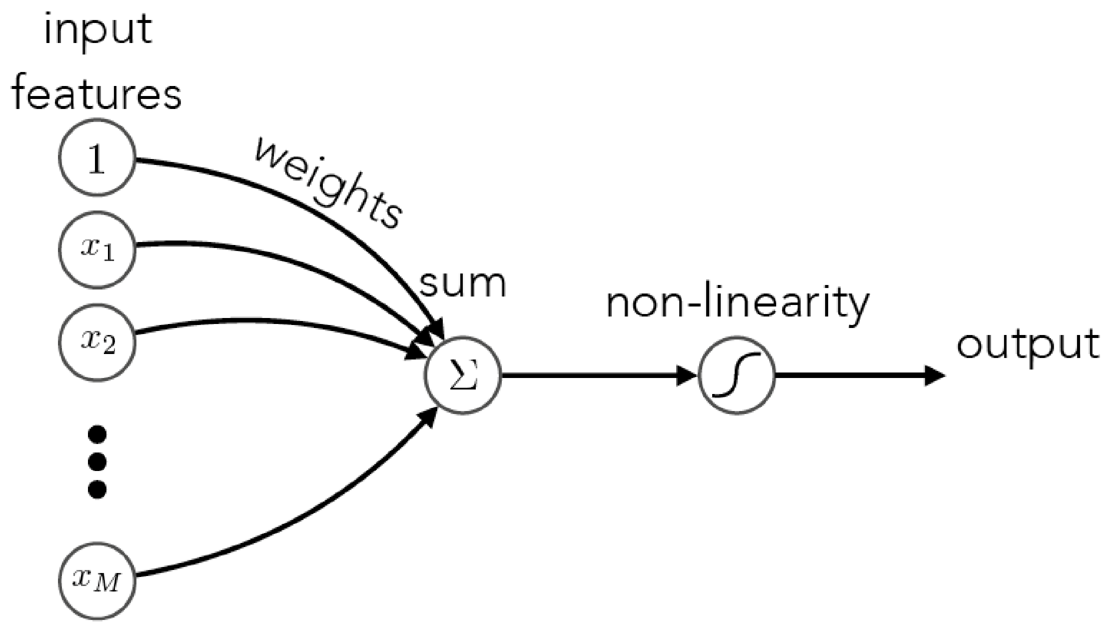
- Course project
  - Each team consists of 4~5 members
  - You may make exceptions if you are among top 10% in first 4 quizzes
- Full course schedule on Piazza
  - HW1 out next Monday
  - Tutorial schedule: please vote on Piazza
- TA office hours
  - See Piazza for detailed schedule and location

Outline

- 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



artificial neuron: *weighted sum and non-linearity*

bias input features

$$s = b + w_1 x_1 + w_2 x_2 + \cdots + w_M x_M = \mathbf{w}^{\mathsf{T}}\mathbf{x}$$

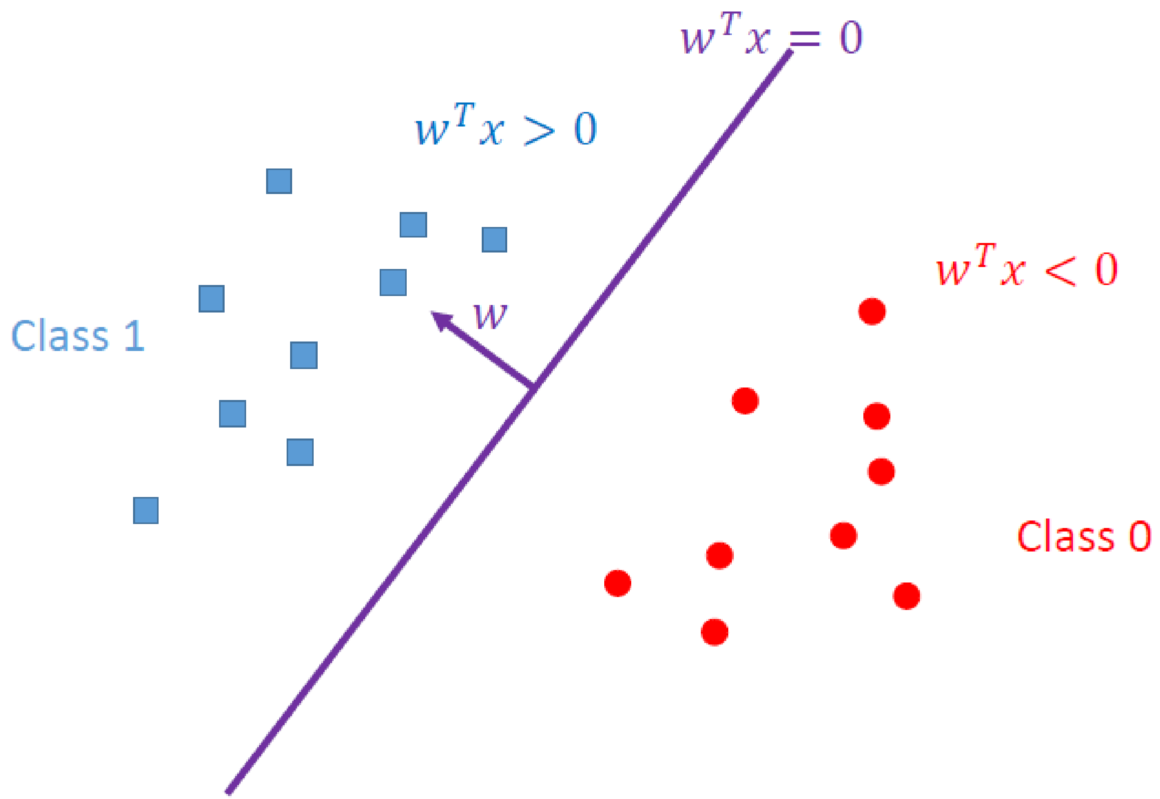
sum weights

$$h = g(s)$$

output non-linearity sum

Single neuron as a linear classifier

- Binary classification



How do we determine the weights?

- Learning problem
  - Given training data $\{(x_i, y_i): 1 \leq i \leq n\}$ i.i.d. from distribution D
  - Hypothesis $f_w(x) = w^T x$
    - $y = 1$ 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 $\mathcal{H}$

Linear classification

- Learning problem: simple approach

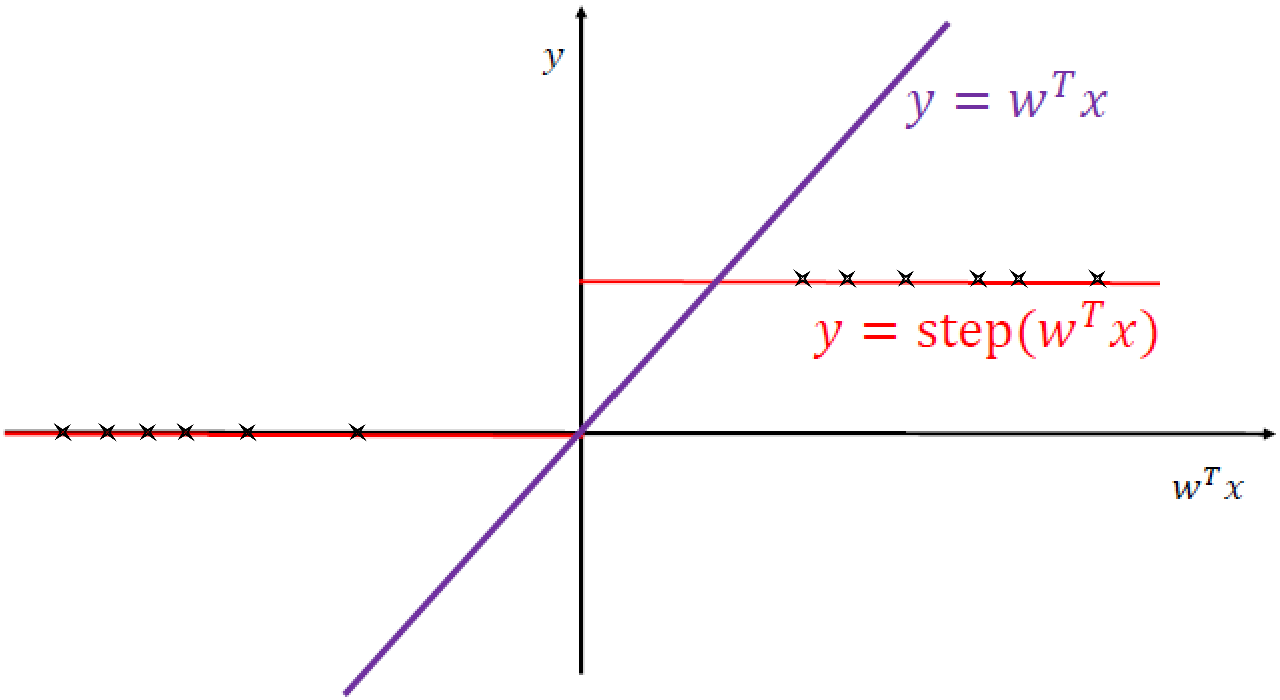
  - Given training data $\{(x_i, y_i): 1 \leq i \leq n\}$ i.i.d. from distribution D
  - Find $f_w(x) = w^T x$ that minimizes $\hat{L}(f_w) = \frac{1}{n}\sum_{i=1}^{n}(w^T x_i - y_i)^2$

  - Drawback: Sensitive to “outliers”

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

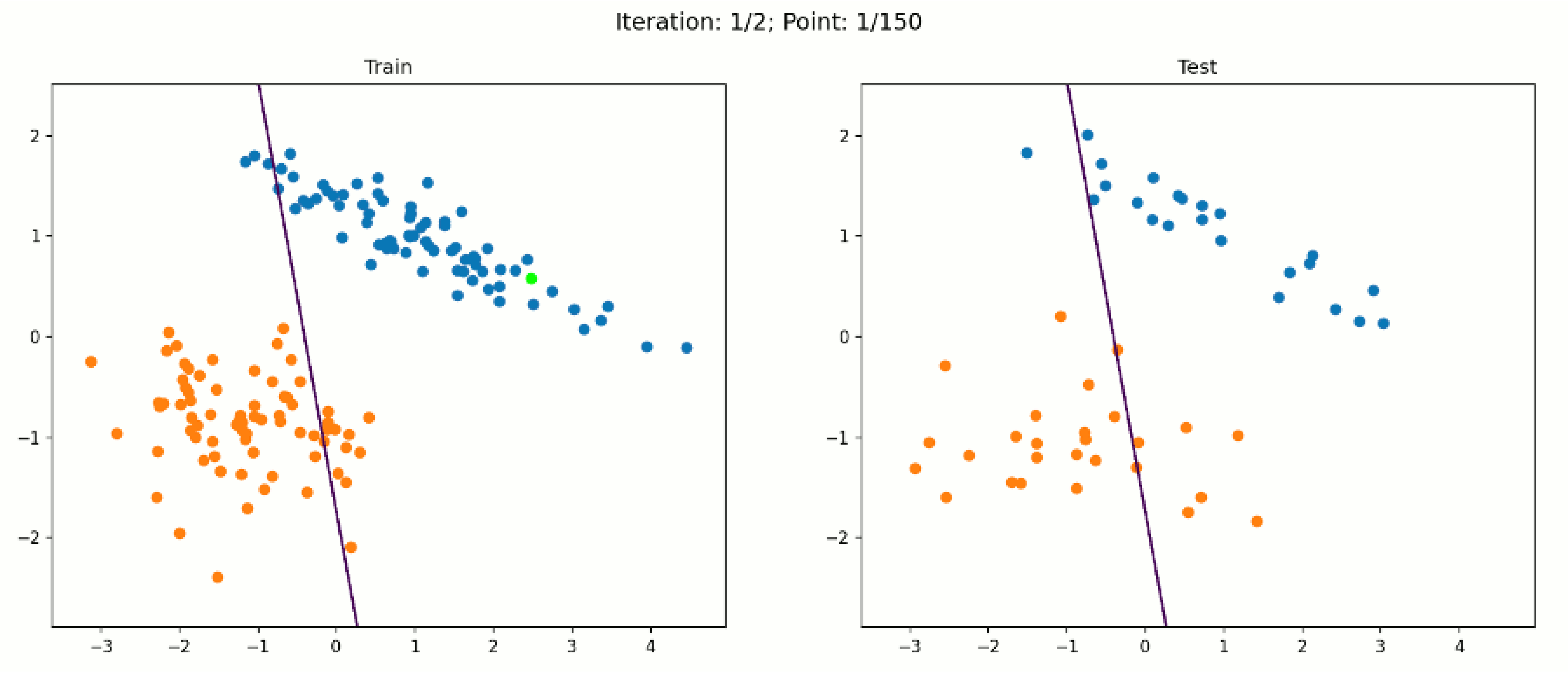
1D Example

- Compare two predictors



Perceptron algorithm

- Learn a single neuron for binary classification



https://towardsdatascience.com/perceptron-explanation-implementation-and-a-visual-example-3c8e76b4e2d1

Perceptron algorithm

- Learn a single neuron for binary classification

- Task formulation

  - Given training data $\{(x_i, y_i): 1 \leq i \leq n\}$ i.i.d. from distribution D
  - Hypothesis $f_w(x) = w^T x$
    - $y = +1$ 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

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

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

Perceptron algorithm

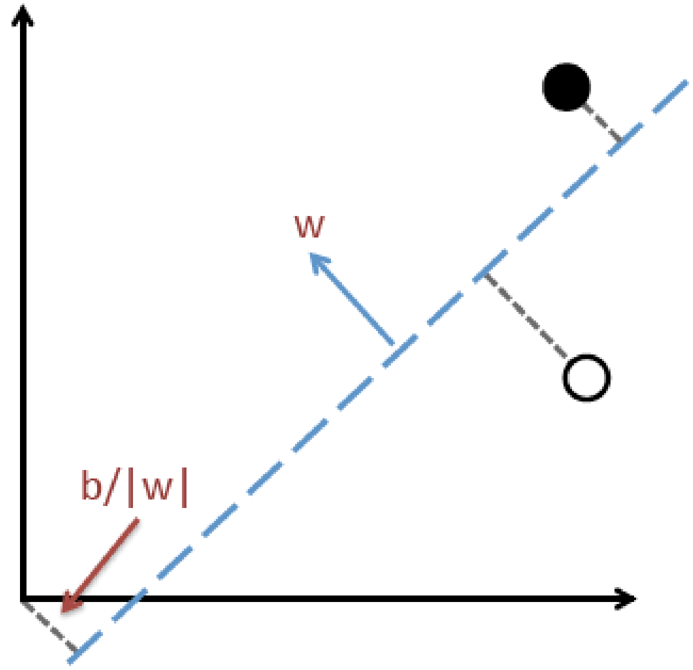
- The Perceptron theorem
  - Suppose there exists w^* that correctly classifies $\{(x_i, y_i)\}$
  - W.L.O.G., all x_i and w^* have length 1, so the minimum distance of any example to the decision boundary is

$$\gamma = \min_i |(w^*)^T x_i|$$

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

Hyperplane Distance

- Line is a 1D, Plane is 2D
- Hyperplane is many D
  - Includes Line and Plane
- Defined by (w,b)
- Distance: $\dfrac{|w^T x - b|}{\|w\|}$
- Signed Distance: $\dfrac{w^T x - b}{\|w\|}$



Linear Model = un-normalized signed distance!

Perceptron algorithm

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

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

  - If mistake on a negative example

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

Perceptron algorithm

- The Perceptron theorem: proof
  - Next look at the quantity $||w_t||$
  - Claim 2: $||w_{t+1}||^2 \leq ||w_t||^2 + 1$
  - Proof: If mistake on a positive example x

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

Negative since we made a mistake on x

Perceptron algorithm

- The Perceptron theorem: proof intuition
  - Claim 1: $w_{t+1}^T w^* \geq w_t^T w^* + \gamma$
  - Claim 2: $||w_{t+1}||^2 \leq ||w_t||^2 + 1$

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"

Perceptron algorithm

- The Perceptron theorem: proof

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

  After M mistakes:

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

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

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

$$\gamma = \min_i |(w^*)^T x_i|$$

Need not be i.i.d. !

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

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

Perceptron Learning problem

- What loss function is minimized?
  - Given training data $\{(x_i, y_i): 1 \leq i \leq n\}$ 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

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

Perceptron algorithm

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

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

$$\hat{L}(w) = -\sum_t y_t w^T x_t \; \mathbb{I}[\text{mistake on } x_t]$$

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

Perceptron algorithm

- 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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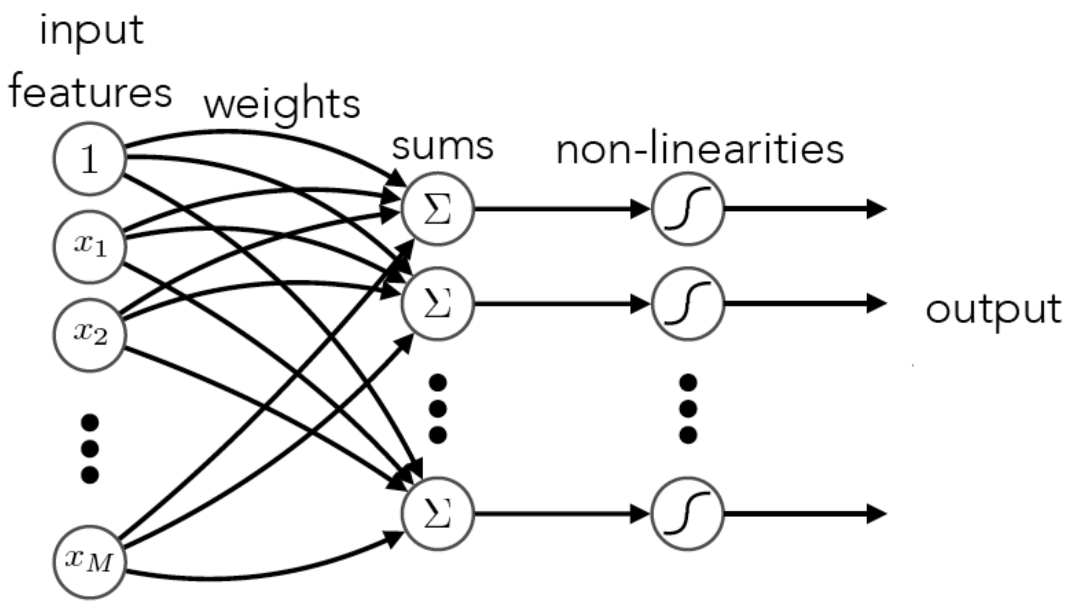
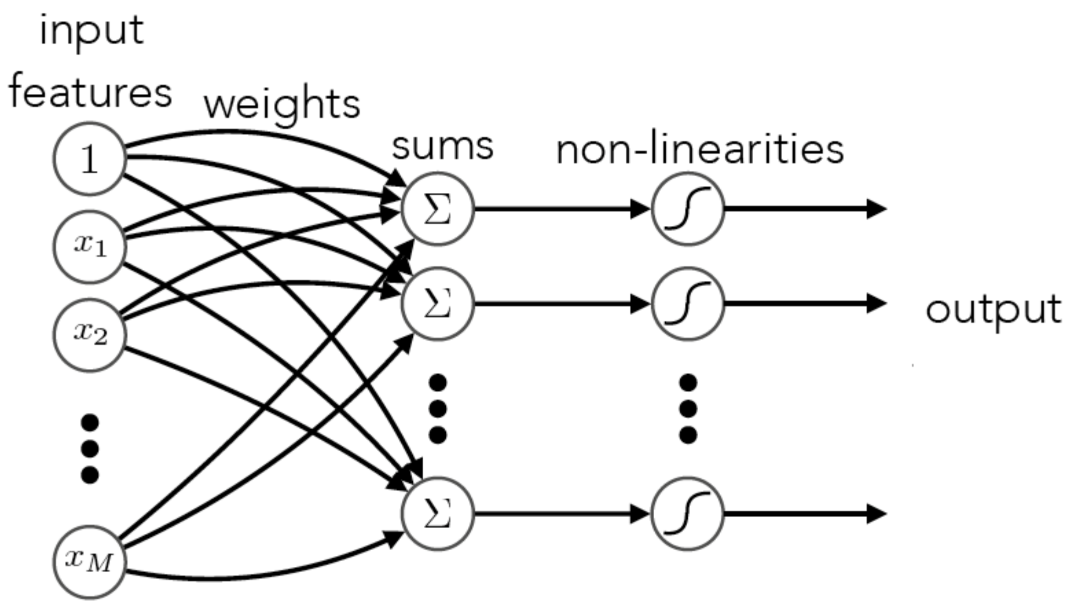
Single layer neural network



Single layer neural network

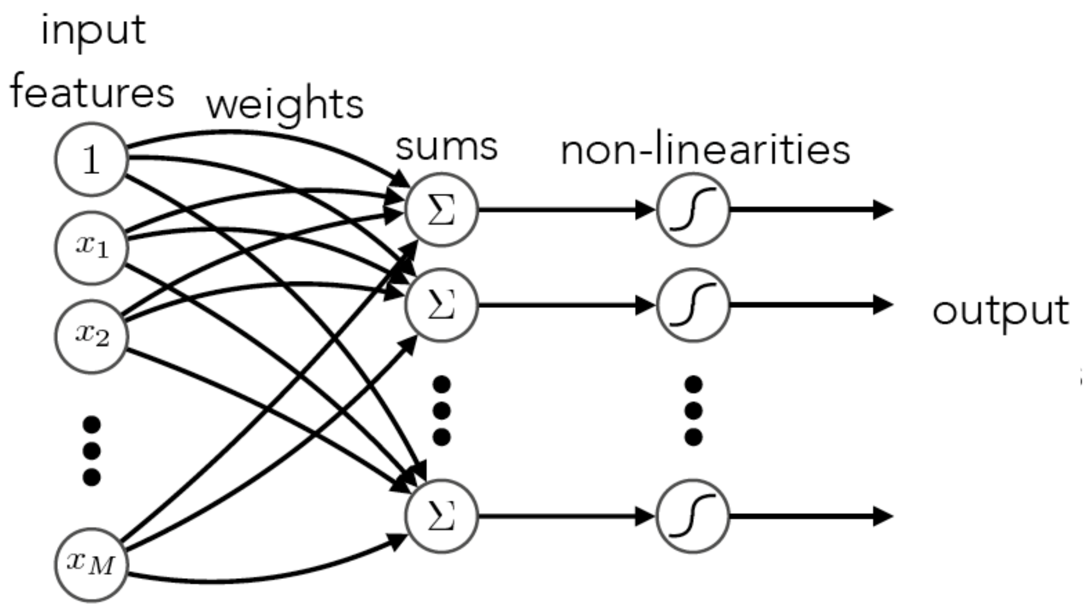


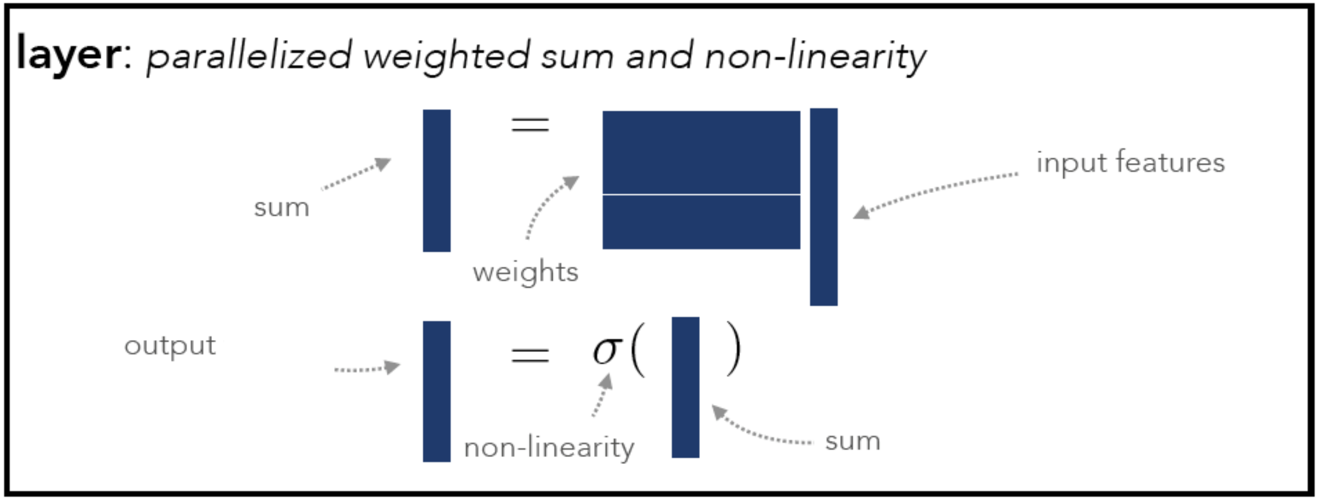
layer: *parallelized weighted sum and non-linearity*

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

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

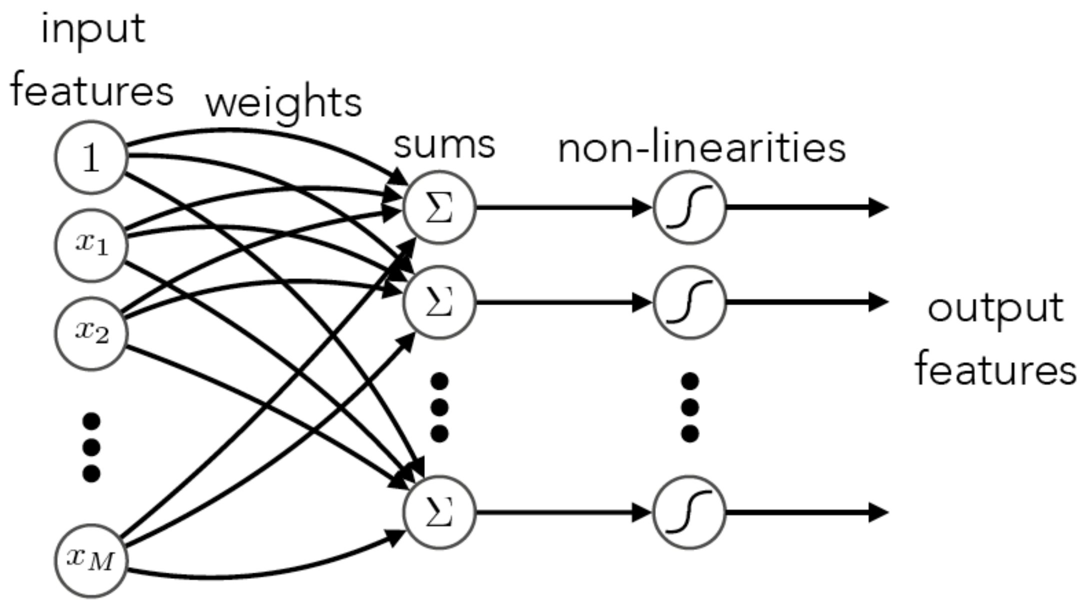
Single layer neural network





What is the output?

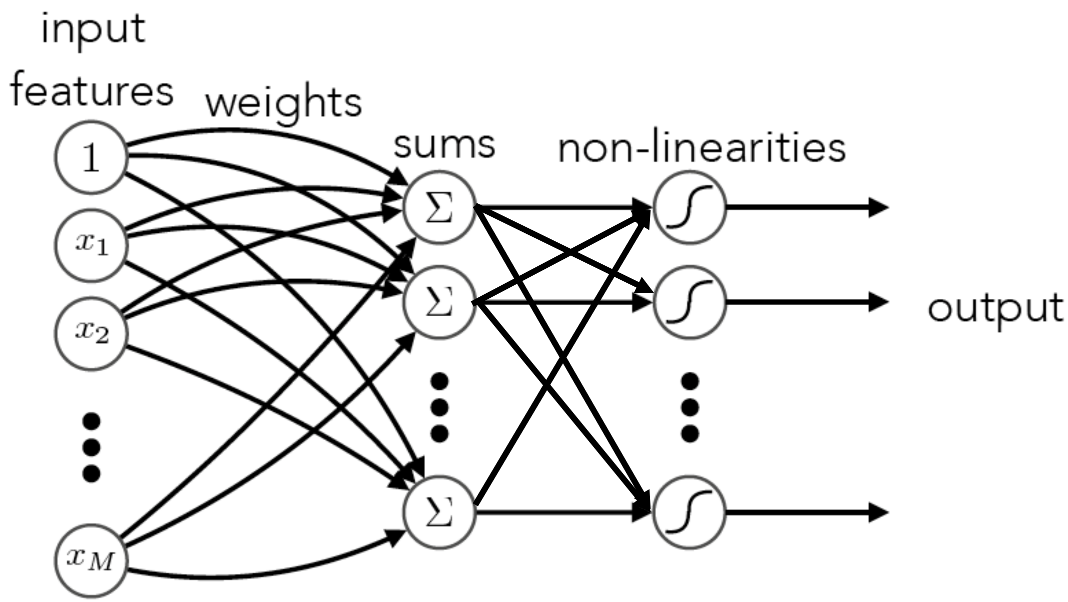
- Element-wise nonlinear functions
  - Independent feature/attribute detectors



$$\mathbf{h} = [h_j] \qquad h_j = \sigma(s_j) = \sigma(\mathbf{w}_j^\intercal \mathbf{x})$$

What is the output?

- Nonlinear functions with vector input
  - Competition between neurons

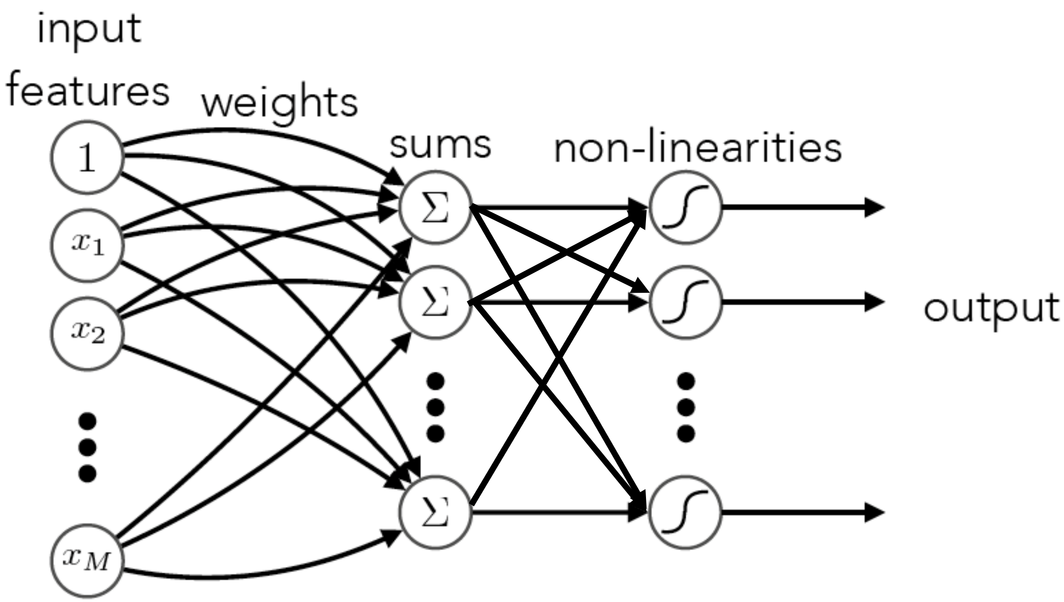


$$\mathbf{h} = [h_j]$$

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

What is the output?

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

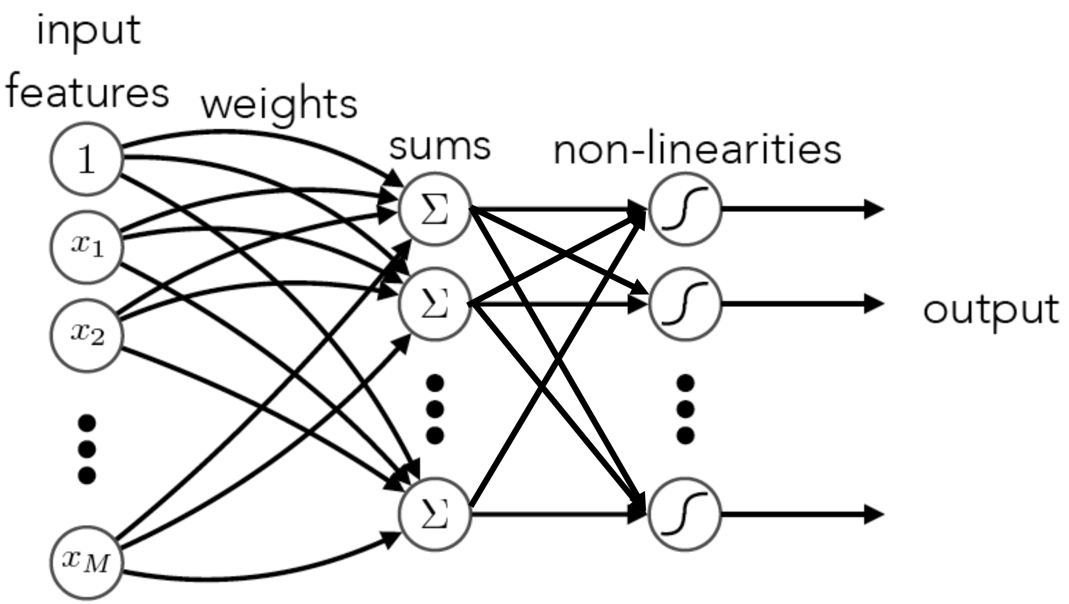


$$\mathbf{h} = [h_j]$$

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

A probabilistic perspective

- Change the output nonlinearity



  - From WTA to Softmax function

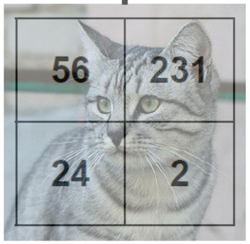
scores = unnormalized log probabilities of the classes.

$$P(Y = k|X = x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}} \quad \text{where} \quad s = f(x_i; W)$$

Multiclass linear classifiers

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

Stretch pixels into column



Input image

$$\underbrace{\begin{bmatrix} 0.2 & -0.5 & 0.1 & 2.0 \\ 1.5 & 1.3 & 2.1 & 0.0 \\ 0 & 0.25 & 0.2 & -0.3 \end{bmatrix}}_{W} \begin{bmatrix} 56 \\ 231 \\ 24 \\ 2 \end{bmatrix} + \begin{bmatrix} 1.1 \\ 3.2 \\ -1.2 \end{bmatrix} = \begin{bmatrix} -96.8 \\ 437.9 \\ 61.95 \end{bmatrix} \begin{array}{l} \text{Cat score} \\ \text{Dog score} \\ \text{Ship score} \end{array}$$

- 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.

$$P(Y=k|X=x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}} \quad \text{where} \quad s = f(x_i; W)$$

unnormalized probabilities

	unnormalized log probabilities		unnormalized probabilities		probabilities
cat	**3.2**	exp →	**24.5**	normalize →	**0.13**
car	5.1		164.0		0.87
frog	-1.7		0.18		0.00

unnormalized log probabilities

probabilities

How to learn a multiclass classifier?

- Define a loss function and do minimization
  - Given training data $\{(x_i, y_i): 1 \leq i \leq n\}$ 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

Learning a multiclass linear classifier

- Design a loss function for multiclass classifiers
  - Perceptron?
    - Yes, see homework
  - Hinge loss
    - The SVM and max-margin (see CS231n)
  - Probabilistic formulation
    - Log loss and logistic regression
- Generalization issue
  - Avoid overfitting by regularization

Example: Logistic Regression

- Learning loss: negative log likelihood

scores = unnormalized log probabilities of the classes.

$$\boxed{P(Y=k|X=x_i) = \frac{e^{s_k}}{\sum_j e^{s_j}}} \quad \text{where} \quad \boxed{s = f(x_i; W)}$$

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

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

Logistic Regression

- Learning loss: example

$$L_i = -\log\left(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}}\right)$$

unnormalized probabilities

	unnormalized log probabilities	exp →	unnormalized probabilities	normalize →	probabilities
cat	**3.2**		**24.5**		**0.13**
car	5.1		164.0		0.87
frog	-1.7		0.18		0.00

→ L_i = -log(0.13)
= **0.89**

unnormalized log probabilities

probabilities

Logistic Regression

- Learning loss: questions

$$L_i = -\log\left(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}}\right)$$

unnormalized probabilities

Q: What is the min/max possible loss L_i?

cat	**3.2**	**24.5**	**0.13**
car	5.1	164.0	0.87
frog	-1.7	0.18	0.00

exp → normalize →

→ L_i = -log(0.13)
= **0.89**

unnormalized log probabilities

probabilities

Logistic Regression

- Learning loss: questions

$$L_i = -\log\left(\frac{e^{s_{y_i}}}{\sum_j e^{s_j}}\right)$$

unnormalized probabilities

Q2: Usually at initialization W is small so all s ≈ 0.
What is the loss?

	unnormalized log probabilities		unnormalized probabilities		probabilities
cat	**3.2**	exp →	**24.5**	normalize →	**0.13**
car	5.1		164.0		0.87
frog	-1.7		0.18		0.00

→ L_i = -log(0.13)
= **0.89**

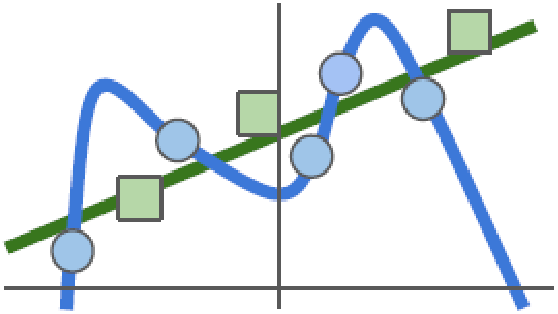
Learning with regularization

- Constraints on hypothesis space
  - Similar to Linear Regression

$$\underbrace{L(W) = \frac{1}{N}\sum_{i=1}^{N} L_i(f(x_i, W), y_i)}_{\text{Data loss}} + \underbrace{\lambda R(W)}_{\text{Regularization}}$$

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

L1 vs L2 regularization

https://www.youtube.com/watch?v=jEVh0uheCPk

L1 vs L2 regularization

- Sparsity

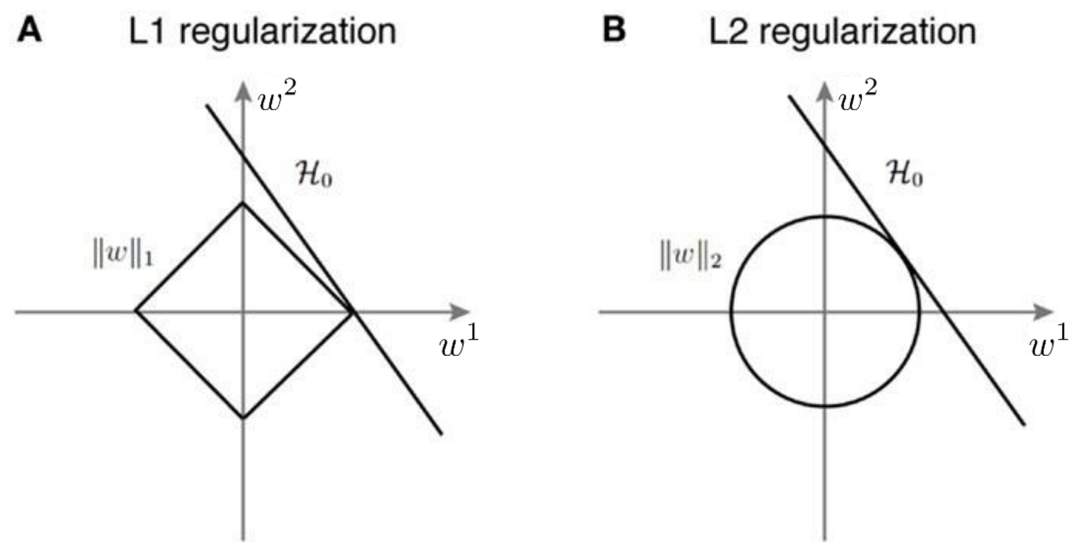
$$x = [1, 1, 1, 1]$$

$$w_1 = [1, 0, 0, 0]$$
$$w_2 = [0.25, 0.25, 0.25, 0.25]$$
$$w_3 = [0.5, 0.5, 0, 0]$$

$$f(x) = w^\intercal x$$

$$w_1^\intercal x = w_2^\intercal x = w_3^\intercal x$$

$$\|w_1\|^2 = |w_1| = 1$$
$$\|w_2\|^2 = 4/16 = 1/4, |w_2| = 1$$
$$\|w_3\|^2 = 2/4 = 1/2, |w_3| = 1$$



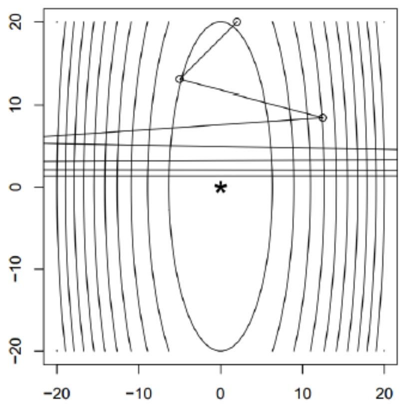
Optimization: gradient descent

- Gradient descent

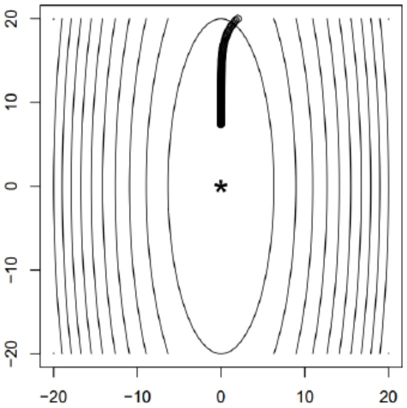
```
# Vanilla Gradient Descent

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

- Learning rate matters

$\eta_t = t$, it is too big



too small η_t, after 100 iterations



Optimization: gradient descent

- Stochastic gradient descent

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

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

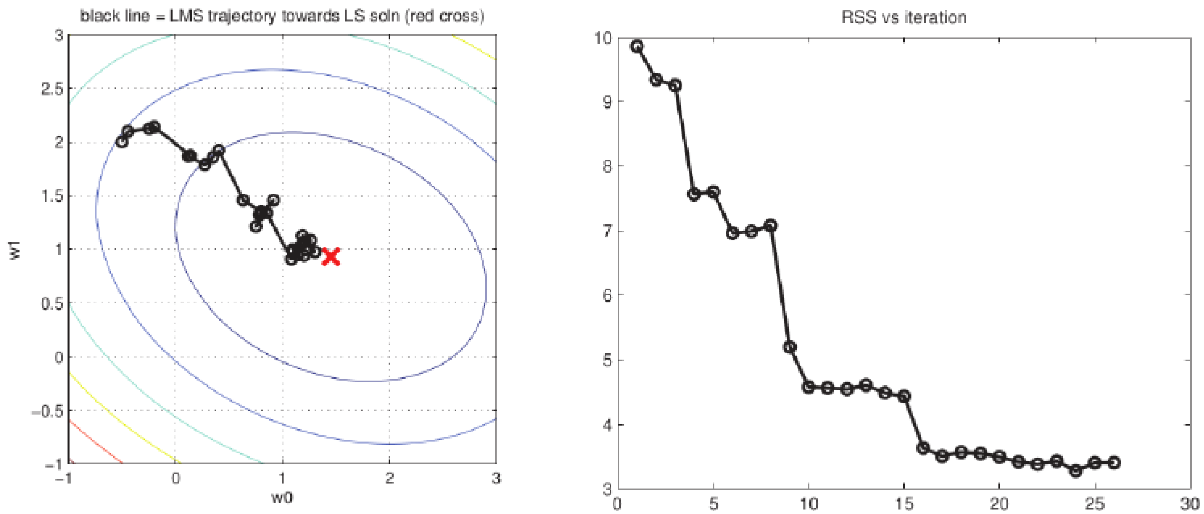
Full sum expensive when N is large!

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

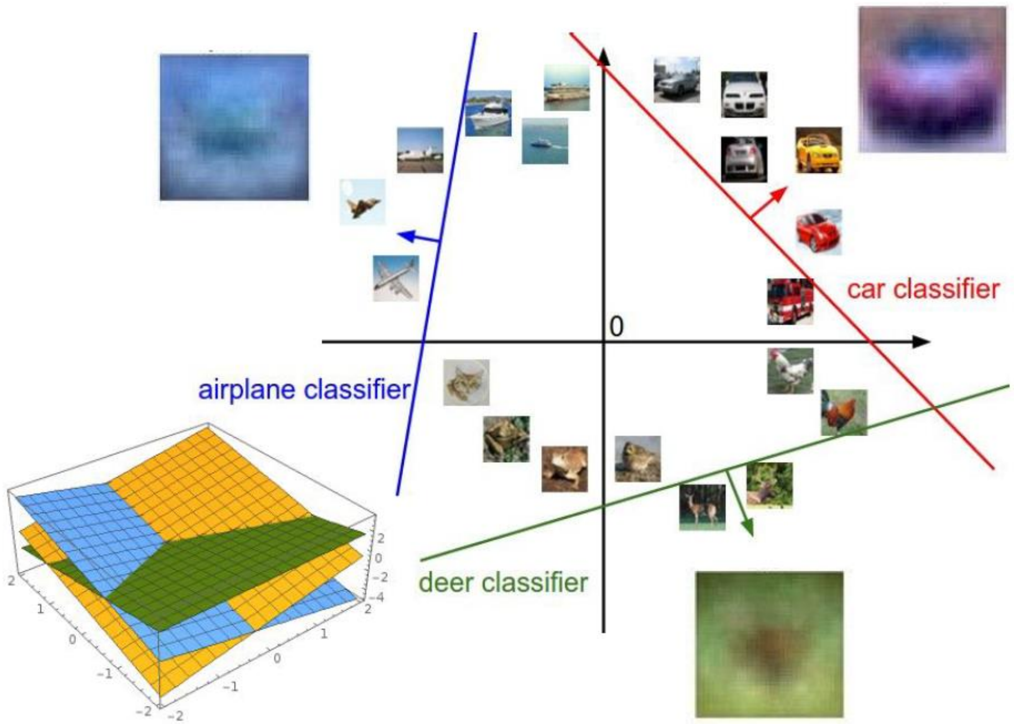
- Stochastic gradient descent



- 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

Interpreting network weights

- What are those weights?



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

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

Summary

- Artificial neurons
- Single-layer network
- Next time
  - Multi-layer neural networks
  - Computation in neural networks