Machine Learning II

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Course Announcements

Assignment 1 is released and due October 7 **No class** on Tues, October 15 due to holiday as per SFU guidelines **Midterm** is set for Tues, October 29 in class.

Course Overview

Week 1: Getting to know you

Week 2: Introduction to Artificial Intelligence

Week 3: Machine Learning I: Basic Supervised Models (Classification)

Week 4: Machine Learning II: Supervised Regression, Classification and Gradient Descent

Week 5: Machine Learning III: Neural Networks and Unsupervised Learning

Week 6: Search

Week 7: Markov Decision Processes

Week 8: Midterm

Week 9: Reinforcement Learning

Week 10: Games

Week 11: Hidden Markov Models and Bayesian Networks

Week 12: Constraint Satisfaction Problems

Week 13: Ethics and Explainability

Search Markov decision processes Games

State-based

models

Constraint satisfaction problems Markov networks Bayesian networks

Variable-based models

Logic-based models

Reflex-based models



Today's Plan

Supervised Learning

- 19.6 Linear Regression
- 19.4.2 Loss functions
- 19.6.2 Gradient Descent
- 19.6.4 Linear Classification
- 19.6.2 Stochastic Gradient Descent

Recall

Supervised Learning

Last time, we learned about 2 non-parametric classification methods: K-Nearest Neighbors and Decision Trees.

Today we'll learn about parametric regression and classification.

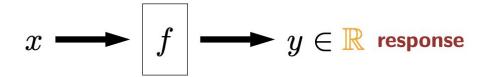


Supervised Learning

Linear Regression



Regression



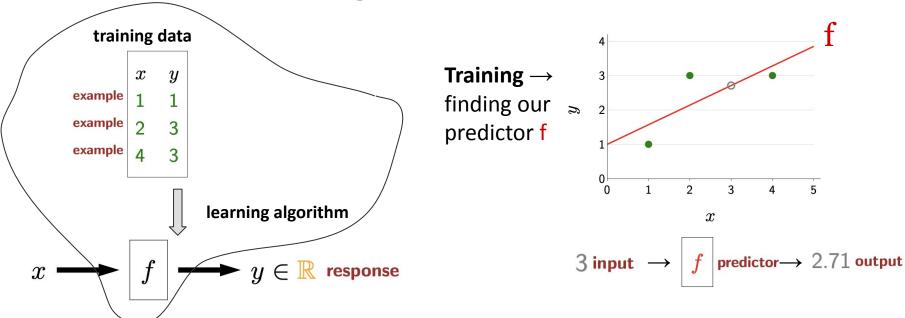
Housing: information about house \rightarrow price

Arrival times: destination, weather, time \rightarrow time of arrival

Robotic vision: image, xy-coord → distance



Linear regression framework



Which predictors **f** is the learning algorithm **allowed** to produce?

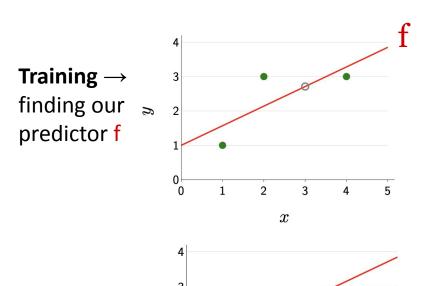
Decide the **hypothesis class** \Rightarrow *here, linear function*

How **good** is a predictor? Decide the **loss function** \Rightarrow here, squared loss

How to **find** the best predictor? Decide the **optimization algorithm** \Rightarrow here, gradient descent



Hypothesis class for Linear Regression: Linear Functions



 \boldsymbol{x}

 \mathcal{S}

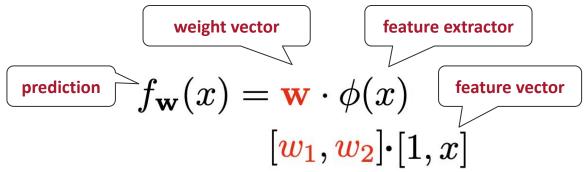
$$f(x) = 1 + 0.57x$$

$$f(x) = 2 + 0.2x$$

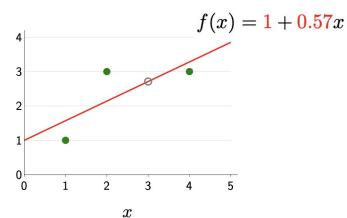
$$f(x) = w_1 + w_2 x$$

Here, we opt for a **linear** function, as opposed to a nonlinear function such as a polynomial

Linear Regression



These are the parameters we want to tweak for the problem.



We might hypothesize that $\mathbf{w} = [1,0.57]$ produces a good model that fits our training data. If so, we could use this model to predict the outcome of x=3.

$$f_{\mathbf{w}}(3) = [1, 0.57] \cdot [1,3]$$

= 1 + 0.57·3
= **2.71**

But how do we know if **w** is any good?

 \mathcal{L}

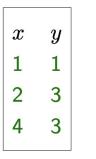
Linear Regression: How to evaluate a weight vector?

For each sample in our training set, find the difference between the **predicted output** $f_{\mathbf{w}}(\mathbf{x})$ and the **actual** output y. This difference is called the **residual**, $f_{\mathbf{w}}(\mathbf{x}) - \mathbf{y}$

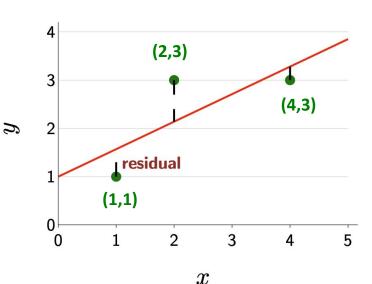
Let's square the residual to ensure the difference is positive, to later sum them. We will call the squared value $(f_{\mathbf{w}}(\mathbf{x})-\mathbf{y})^2$ the **squared** error loss also called **L2** loss.

Remember Gauss' method of least squares? It minimized the sum of the squares of the residuals.

training data $\mathcal{D}_{\mathsf{train}}$



$$f_{\mathbf{w}}(x) = \mathbf{w} \cdot \phi(x)$$
$$\mathbf{w} = \begin{bmatrix} 1, 0.57 \end{bmatrix}$$
$$\phi(x) = \begin{bmatrix} 1, x \end{bmatrix}$$



Loss(x,y,w)=
$$(f_{\mathbf{w}}(x)-y)^2$$

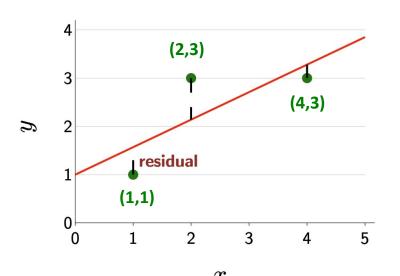
Loss(2,3,w)= $(f_{\mathbf{w}}(x)-3)^2$
= $(\mathbf{w}\cdot\phi(x)-3)^2$
= $([1,0.57]\cdot[1,2]-3)^2$
= $(1\cdot1+0.57\cdot2-3)^2=0.74$

Do this for all the samples in your training set and find the average

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Linear Regression: How to evaluate a weight vector?



Loss(x,y,w)=
$$(f_{\mathbf{w}}(x)-y)^2$$

Loss(2,3,w)= $(f_{\mathbf{w}}(x)-3)^2$ x is 2 here
= $(\mathbf{w}\cdot\phi(x)-3)^2$
= $([1,0.57]\cdot[1,2]-3)^2$
= $(1\cdot1+0.57\cdot2-3)^2=0.74$

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 $\begin{aligned} \mathsf{TrainLoss}(\mathbf{w}) &= \frac{1}{|\mathcal{D}_{\mathsf{train}}|} \sum_{(x,y) \in \mathcal{D}_{\mathsf{train}}} \mathsf{Loss}(x,y,\mathbf{w}) \\ f_{\mathbf{w}}(\mathbf{x}) &= \mathbf{w} \cdot \boldsymbol{\phi}(\mathbf{x}) \\ \mathbf{w} &= [1,0.57] \\ \boldsymbol{\phi}(\mathbf{x}) &= [1,\mathbf{x}] \end{aligned}$

Loss(1,1,**w**)=(**w**·
$$\phi$$
(1)-1)²=0.32
Loss(2,3,**w**)=(**w**· ϕ (2)-3)²=0.74
Loss(4,3,**w**)=(**w**· ϕ (4)-3)²=0.08

TrainLoss([1,0.57]) =
$$(.32+.74+.08)/3 = 0.38$$

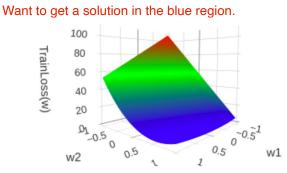
You could use a grid search to find an optimal w with lowest TrainLoss

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Finding the optimal predictor using a Loss

$$\mathsf{TrainLoss}(\mathbf{w}) = rac{1}{|\mathcal{D}_{\mathsf{train}}|} \sum_{(x,y) \in \mathcal{D}_{\mathsf{train}}} (f_{\mathbf{w}}(x) - y)^2$$

We can minimize this value using gradients.



$\min_{\mathbf{w}} \mathsf{TrainLoss}(\mathbf{w})$

The best predictor is the one with the lowest training loss. We need to solve this optimization problem.

What is grid search?

You could perform a grid search over w1 and w2 to find a w with a minimum training loss, but this will get unwieldy for higher dimensions.

80

Gradient Descent: Faster than Grid Search

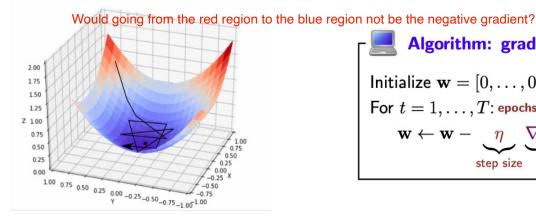
Goal: $\min_{\mathbf{w}} \mathsf{TrainLoss}(\mathbf{w})$

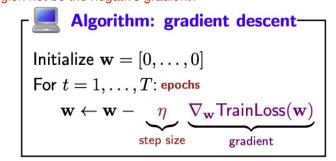
Potentially faster? In which cases is it slower



Definition: gradient-

The gradient $\nabla_{\mathbf{w}} \operatorname{TrainLoss}(\mathbf{w})$ is the direction that increases the training loss the most.





Note that in the textbook, you

may see $(y-w\cdot \varphi(x))$

Computing the gradient

Objective function:

$$\mathsf{TrainLoss}(\mathbf{w}) = \frac{1}{|\mathcal{D}_{\mathsf{train}}|} \sum_{(x,y) \in \mathcal{D}_{\mathsf{train}}} (\mathbf{w} \cdot \phi(x) - y)^2$$

Review gradient descent.

Gradient (use chain rule):

Remember, we're taking the gradient w.r.t. w, so everything else is treated as a constant

$$\nabla_{\mathbf{w}} \mathsf{TrainLoss}(\mathbf{w}) = \frac{1}{|\mathcal{D}_{\mathsf{train}}|} \sum_{(x,y) \in \mathcal{D}_{\mathsf{train}}} 2(\underbrace{\mathbf{w} \cdot \phi(x) - y}_{\mathsf{prediction-target}}) \phi(x)$$

training data $\mathcal{D}_{\mathsf{train}}$

Gradient Descent example

 $egin{array}{cccc} x & y \ 1 & 1 \ 2 & 3 \ 4 & 3 \ \end{array}$

Residual multiplied by the feature vector!

$$\nabla_{\mathbf{w}} \mathsf{TrainLoss}(\mathbf{w}) = \frac{1}{|\mathcal{D}_{\mathsf{train}}|} \sum_{(x,y) \in \mathcal{D}_{\mathsf{train}}} 2(\underbrace{\mathbf{w} \cdot \phi(x) - y}_{\mathsf{prediction-target}}) \phi(x)$$

Gradient update: $\mathbf{w} \leftarrow \mathbf{w} - 0.1 \nabla_{\mathbf{w}} \text{TrainLoss}(\mathbf{w})$

Step size

t **w** $\nabla_{\mathbf{w}}$ TrainLoss(w)

1
$$[0,0]$$
 $2([0,0]\cdot[1,1]-1)[1,1] + 2([0,0]\cdot[1,2]-3)[2,3] + 2([0,0]\cdot[1,4]-3)[4,3]$
3

= [-4.67, -12.67] //then update **w** with step size (learning rate)

[0.47, 1.27]

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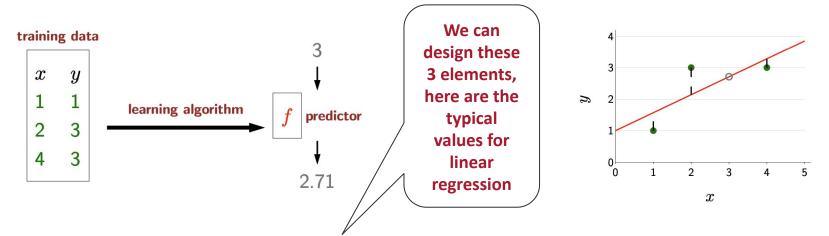
Gradient Descent example

```
\nabla_{w} TrainLoss(w)
      W
                     2([0,0]\cdot[1,1]-1)[1,1] + 2([0,0]\cdot[1,2]-3)[2,3] + 2([0,0]\cdot[1,4]-3)[4,3]
     [0,0]
                                                      = [-4.67, -12.67]
      [0.47, 1.27]
                     2([.47,1.27]\cdot[1,1]-1)[1,1] + 2([.47,1.27]\cdot[1,2]-3)[2,3] + 2([.47,1.27]\cdot[1,4]-3)[4,3]
                                                      = [2.18, 7.24]
      [0.25, 0.54]
200 [1, 0.57]
                     2([1,57]\cdot[1,1]-1)[1,1] + 2([1,57]\cdot[1,2]-3)[2,3] + 2([1,57]\cdot[1,4]-3)[4,3]
                                                                     Until gradient is zero and there
                                                                     is no more change, i.e.
```

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algorithm has converged

Summary: Linear Regression



Hypothesis class: Linear functions

$$\mathcal{F} = \{ f_{\mathbf{w}}(x) = \mathbf{w} \cdot \phi(x) \}, \phi(x) = [1, x]$$

Loss function: Squared loss

$$\mathsf{Loss}(x, y, \mathbf{w}) = (f_{\mathbf{w}}(x) - y)^2$$

Optimization algorithm: Gradient descent $\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla \mathsf{TrainLoss}(\mathbf{w})$

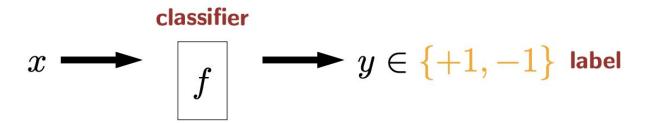


Supervised Learning

Linear Classification



Binary Classification



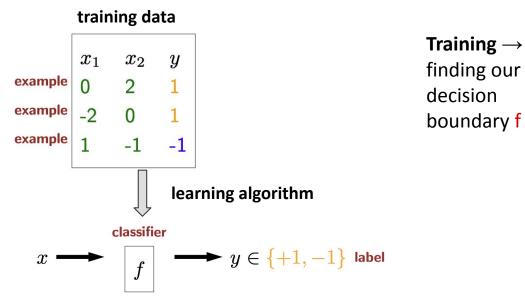
Spam detection: online comment \rightarrow toxic or not toxic

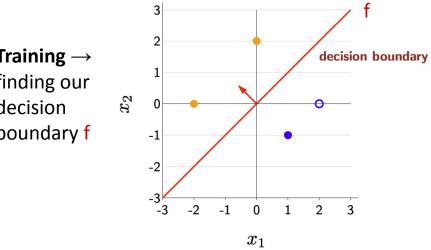
Earthquake: measurements of event \rightarrow earthquake or explosion

Melanoma: mole size and color \rightarrow cancerous or non-cancerous

Extension: multiclass classification $y \in \{1, \dots, K\}$

Linear classification framework





$$[2, 0]$$
 input $\rightarrow \boxed{f}$ predictor \rightarrow -1 label

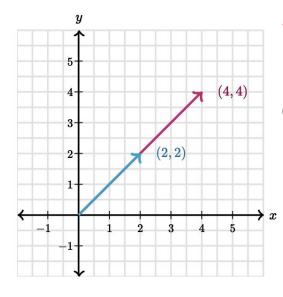
Which predictors **f** is the learning algorithm **allowed** to produce?

Decide the **hypothesis class** \Rightarrow here, linear function with sign(prediction)

How **good** is a predictor? Decide the **loss function** \Rightarrow here, zero-one loss (or hinge, or logistic) How to **find** the best predictor? Decide the **optimization algorithm** \Rightarrow here, gradient descent

Recall: Dot Product

$$ec{a} \cdot ec{b} = \|ec{a}\| \|ec{b}\| \cos(heta)$$

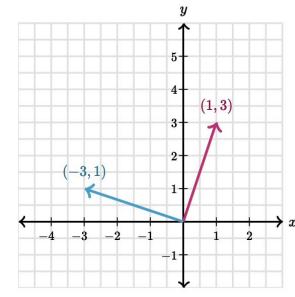


this will help us for determining what class our input falls into

$$\theta = 0$$

$$cos(0)=1$$

When vectors are pointing in the same direction, their dot product will be 1



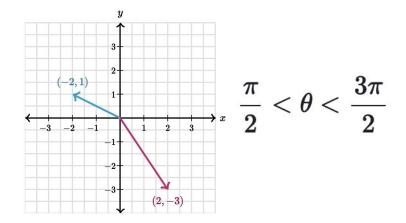
$$heta=rac{\pi}{2}$$

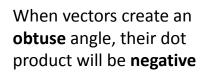
$$\cos\left(rac{\pi}{2}
ight) = 0$$

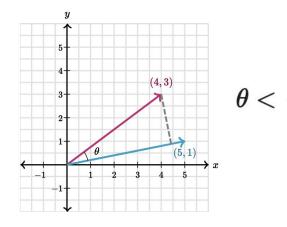
When vectors are perpendicular, their dot product will be 0.

Recall: Dot Product

$$ec{a} \cdot ec{b} = \|ec{a}\| \|ec{b}\| \cos(heta)$$

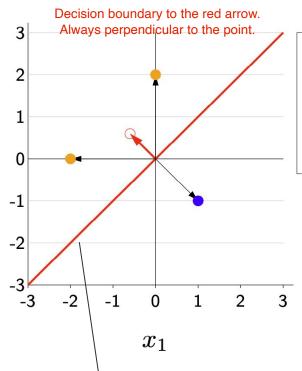






When vectors create an **acute** angle, their dot product will be **positive**

An example linear classifier



$$\operatorname{sign}(z) = \begin{cases} +1 & \text{if } z > 0 \\ -1 & \text{if } z < 0 \\ 0 & \text{if } z = 0 \end{cases}$$

Reminder:

$$\vec{a}=(a_1,a_2,a_3)$$

$$ec{b}=(b_1,b_2,b_3)$$

$$ec{a}\cdotec{b}=a_1b_1+a_2b_2+a_3b_3$$

$$f(x) = sign(\mathbf{w} \cdot \phi(x))$$

$$f([0,2]) = sign([-0.6,0.6] \cdot [0,2])$$

$$=$$
sign $(-0.6*0+0.6*2)$ = sign (1.2) = 1

$$f([0,2]) = sign([-0.6,0.6] \cdot [-2,0])$$

$$=$$
sign $(-0.6*-2+0.6*0)$ = sign (1.2) = 1

$$f([0,2]) = sign([-0.6,0.6] \cdot [1,-1])$$

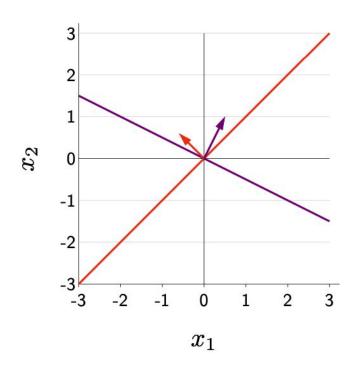
$$=$$
sign $(-0.6*1+0.6*-1)$ = sign (-1.2) = -1

Decision boundary:

X such that $\mathbf{W}^{\mathsf{L}} \phi(\mathbf{X}) = 0$



Binary classification



$$\boldsymbol{\phi}(\mathbf{x}) = [\mathbf{x}_{\scriptscriptstyle 1}, \mathbf{x}_{\scriptscriptstyle 2}]$$

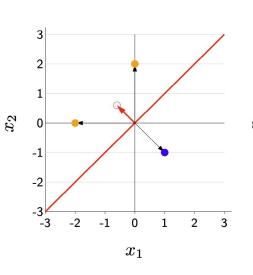
$$f(x) = \text{sign}([-0.6, 0.6] \cdot \phi(x))$$

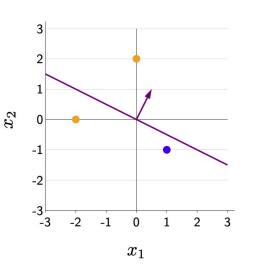
$$f(\mathbf{x}) = \operatorname{sign}([0.5, 1] \cdot \phi(\mathbf{x}))$$

General binary $f_{\mathbf{w}}(x) = \operatorname{sign}(\mathbf{w} \cdot \phi(x))$ classifier:

Hypothesis class:
$$\mathcal{F} = \{f_{\mathbf{w}} : \mathbf{w} \in \mathbb{R}^2\}$$

Zero-one Loss





training data $\mathcal{D}_{\mathsf{train}}$

$$f_{\mathbf{w}}(x) = \mathbf{w} \cdot \phi(x)$$
$$\mathbf{w} = [0.5, 1]$$
$$\phi(x) = [x_1, x_2]$$

y is the target value.

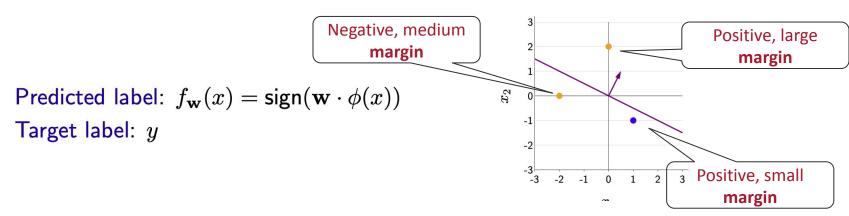
$$\mathsf{Loss}_{0\text{-}1}(x,y,\mathbf{w}) = \mathbf{1}[f_{\mathbf{w}}(x) \neq y]$$

- Remember, we want to minimize the loss (better if close to 0).
- 1 if it's incorrect, and 0 if correct.
- Total loss is the average over all training samples.

$$\begin{aligned} & \mathsf{Loss}([0,2], \mathbf{1}, [0.5,1]) = \mathbf{1}[\mathsf{sign}([0.5,1] \cdot [0,2]) \neq \mathbf{1}] = 0 \\ & \mathsf{Incorrectly \ classified} \\ & \mathsf{Loss}([-2,0], \mathbf{1}, [0.5,1]) = \mathbf{1}[\mathsf{sign}([0.5,1] \cdot [-2,0]) \neq \mathbf{1}] = 1 \\ & \mathsf{Loss}([1,-1], -1, [0.5,1]) = \mathbf{1}[\mathsf{sign}([0.5,1] \cdot [1,-1]) \neq -1] = 0 \end{aligned}$$

TrainLoss(
$$[0.5, 1]$$
) = $1/3 = 0.33$

Score and margin





Definition: margin-

The margin on an example (x,y) is $(\mathbf{w} \cdot \phi(x))y$, how **correct** we are.



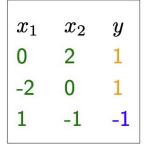


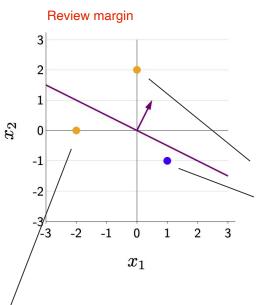
Correct by a large

(positive) margin

Margin example







Margin(
$$[0.5, 1]$$
 · $[-2,0]$, 1) = $[0.5,1]$ [-2,0](1) = -1

Margin($\mathbf{w} \cdot \phi(\mathbf{x})$,y)

Margin([0.5, 1] [x1,x2],y)

Margin([0.5, 1], [0.2], [0.5, 1], [0.5, 1], [0.2], [0.5, 1]

Margin([0.5, 1]•[1,-1],-[0.5,1][[1,-1](-1)= **0.5**

Negative margin when **incorrectly** classified

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Zero-one loss with margin

 $\mathsf{Loss}_{0\text{--}1}(x,y,\mathbf{w}) = \mathbf{1}[f_{\mathbf{w}}(x) \neq y]$

1 if it's incorrect, and 0 if correct.

Rewriting the 0-1 loss in terms of **margin**

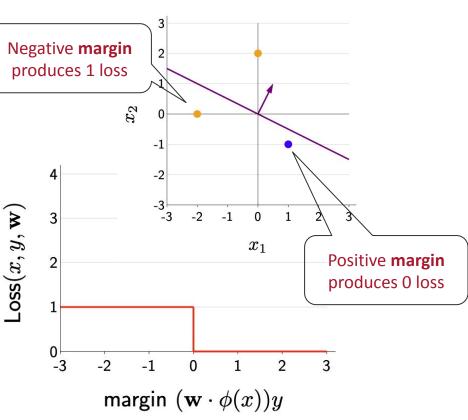


Definition: zero-one loss-

 $\mathsf{Loss}_{0\text{-}1}(x,y,\mathbf{w}) = \mathbf{1}[f_{\mathbf{w}}(x) \neq y]$

$$= \mathbf{1}[\underbrace{(\mathbf{w} \cdot \phi(x))y} \le 0]$$





Gradient descent: Problem with zero-one loss 30

$$\begin{aligned} \mathsf{Loss}_{0\text{-}1}(x, y, \mathbf{w}) &= \mathbf{1}[f_{\mathbf{w}}(x) \neq y] \\ &= \mathbf{1}[(\mathbf{w} \cdot \phi(x))y \leq 0] \end{aligned}$$

If you do this, you will not converge to a specific value.

This loss function does not give a nice differentiable function.

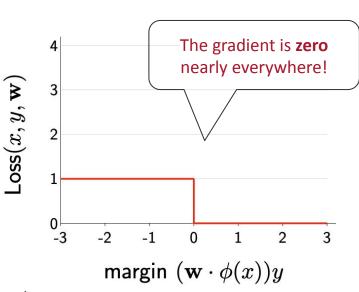
Goal: min_wTrainLoss(w)

To run gradient descent, compute the gradient:

$$\nabla_{\mathbf{w}} \mathsf{Loss}_{0\text{-}1}(x, y, \mathbf{w}) = \nabla \mathbf{1}[(\mathbf{w} \cdot \phi(x))y \leq 0]$$

Gradient of training loss: average over the sample losses.

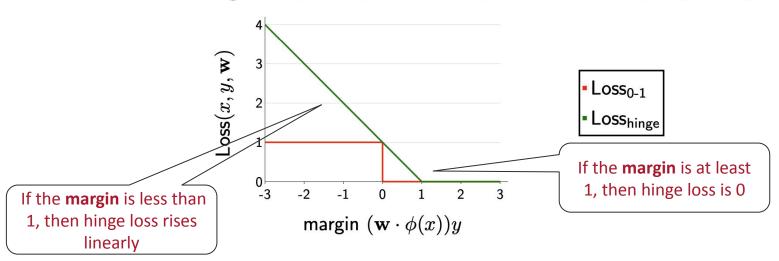
$$\textstyle \nabla_{\mathbf{w}} \mathsf{TrainLoss}(\mathbf{w}) = \frac{1}{|\mathcal{D}_{\mathsf{train}}|} \textstyle \sum_{(x,y) \in \mathcal{D}_{\mathsf{train}}} \nabla \mathsf{Loss}_{\mathsf{0-1}}(x,y,\mathbf{w})$$



Hinge Loss

What does hinge loss represent?

$$\mathsf{Loss}_{\mathsf{hinge}}(x, y, \mathbf{w}) = \max\{1 - (\mathbf{w} \cdot \phi(x))y, 0\}$$

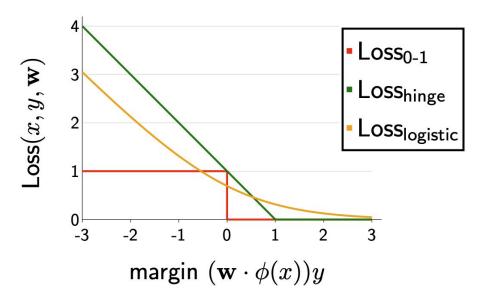


Intuition: The 1 is to provide buffer to predict not only correctly but with a positive margin of safety. The 1 ~ regularization strength.



Logistic regression

$$\mathsf{Loss}_{\mathsf{logistic}}(x, y, \mathbf{w}) = \log(1 + e^{-(\mathbf{w} \cdot \phi(x))y})$$



Intuition: Try to increase margin even when it already exceeds 1



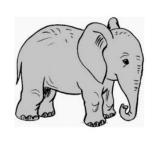
Supervised Learning

Stochastic Gradient Descent



Gradient Descent is Slow

$$\mathsf{TrainLoss}(\mathbf{w}) = \frac{1}{|\mathcal{D}_{\mathsf{train}}|} \sum_{(x,y) \in \mathcal{D}_{\mathsf{train}}} \mathsf{Loss}(x,y,\mathbf{w})$$





Algorithm: gradient descent

$$\begin{aligned} & \text{Initialize } \mathbf{w} = [0, \dots, 0] \\ & \text{For } t = 1, \dots, T \text{:} \\ & \mathbf{w} \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} \mathsf{TrainLoss}(\mathbf{w}) \end{aligned}$$

Problem: each iteration requires going over all training examples — expensive when have lots of data!

Stochastic gradient descent

Review stochastic gradient descent.

$$\frac{\mathsf{TrainLoss}(\mathbf{w})}{|\mathcal{D}_{\mathsf{train}}|} \sum_{(x,y) \in \mathcal{D}_{\mathsf{train}}} \mathsf{Loss}(x,y,\mathbf{w})$$
 Stochastic gradient descent gets to a solution quicker since

your weight parameter decreases more quickly, reaching a gradient of zero more quickly

What is the difference between this algorithm and the previous algorithm for gradient descent?



You still go over all the samples, no?

Algorithm: stochastic gradient descent

You end up reusing the same data points. How does this help?

Initialize
$$\mathbf{w} = [0, \dots, 0]$$

For
$$t = 1, ..., T$$
:

For
$$(x,y) \in \mathcal{D}_{\mathsf{train}}$$
:

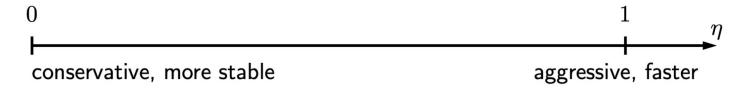
$$\mathbf{w} \leftarrow \mathbf{w} - \eta \nabla_{\mathbf{w}} \mathsf{Loss}(x, y, \mathbf{w})$$



Step size

$$\mathbf{w} \leftarrow \mathbf{w} - \underbrace{\eta}_{\text{step size}} \nabla_{\mathbf{w}} \mathsf{Loss}(x, y, \mathbf{w})$$

Question: what should η be?



Strategies:

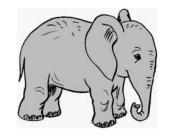
- Constant: $\eta = 0.1$
- Decreasing: $\eta = 1/\sqrt{\#}$ updates made so far

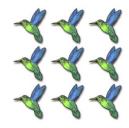
Start with larger step sizes, and decrease over time

Is this to avoid overshooting the minimum?

Summary

$$\frac{\mathsf{TrainLoss}(\mathbf{w})}{|\mathcal{D}_{\mathsf{train}}|} \sum_{(x,y) \in \mathcal{D}_{\mathsf{train}}} \mathsf{Loss}(x,y,\mathbf{w})$$





gradient descent

stochastic gradient descent



Key idea: stochastic updates-

It's not about quality, it's about quantity.

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Unsupervised Learning

K-Means Clustering



A Clustering Problem





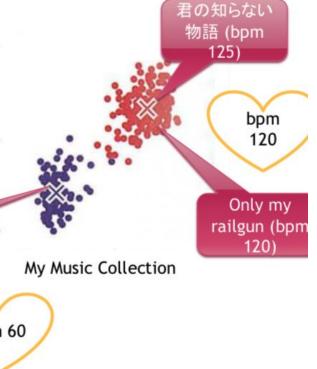
A Clustering Problem

• Recommend me some music!

Discover groups of similar songs...

> Bach Sonata #1 (bpm 60)

> > bpm 60

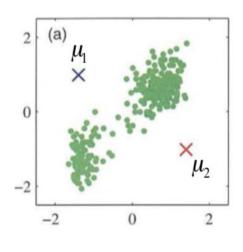


Unsupervised Learning

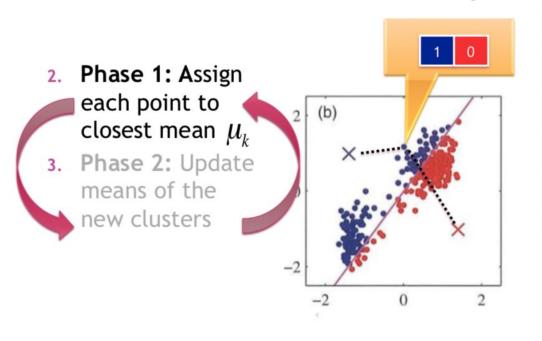
K-Means Clustering

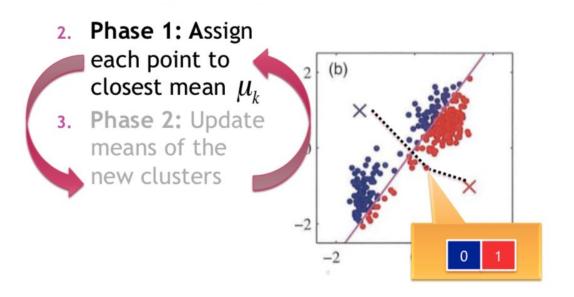


- 1. Initialize K "means" μ_k , one for each class
 - Eg. Use random starting points, or choose k random points from the set



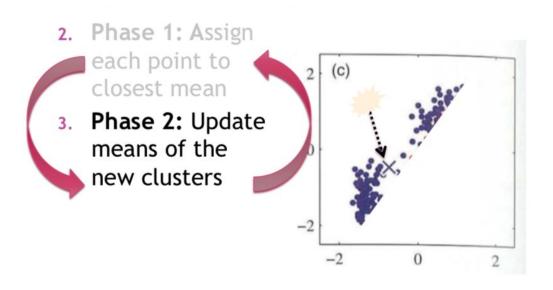
K=2



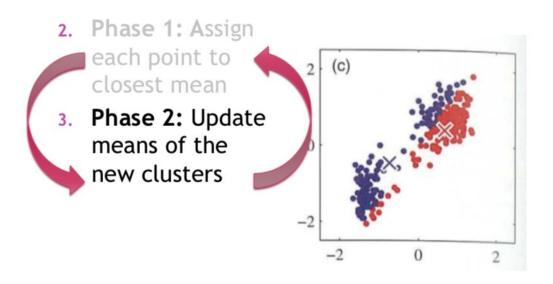


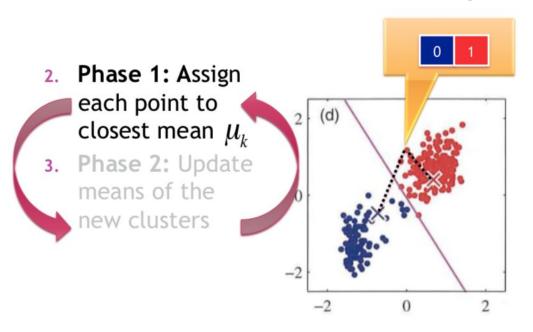
When you update the means of the new clusters, how are we doing this?





2. Phase 1: Assign
each point to closest mean
3. Phase 2: Update means of the new clusters

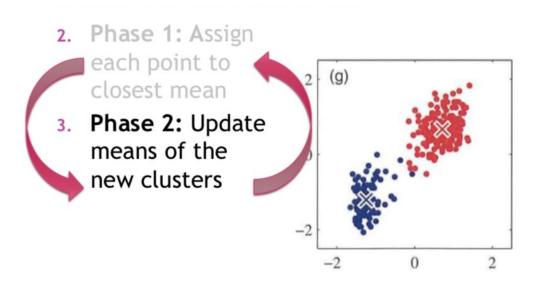




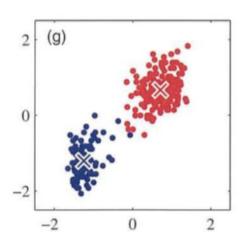
Review K-means algorithm

2. Phase 1: Assign
each point to closest mean
3. Phase 2: Update means of the new clusters

2. Phase 1: Assign each point to closest mean μ_k 3. Phase 2: Update means of the new clusters



 When means do not change anymore → clustering DONE.



Problem with K-Means

- In K-means, a point can only have 1 class
- But what about points that lie in between groups? eg. Jazz + Classical

