大数据计算及应用

Large-Scale Machine Learning: k-NN, Perceptron

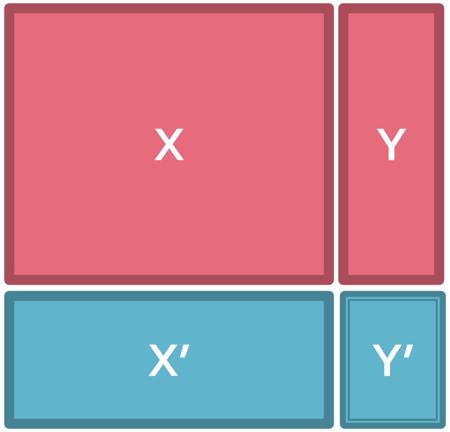
New Topic: Machine Learning!

High dim. data	Graph data	Infinite data	Machine learning	Apps
Locality sensitive hashing	**PageRank,** SimRank	Filtering data streams	SVM	Recommender systems
Clustering	Community Detection	Web advertising	Decision Trees	Association Rules
Dimensionality reduction	Spam Detection	Queries on streams	Perceptron, kNN	Duplicate document detection

Supervised Learning

- **Would like to do prediction:**
  estimate a function **f(x)** so that ***y = f(x)***

- **Where *y* can be:**
  - **Real number**: Regression
  - **Categorical**: Classification
  - Complex object:
    - Ranking of items, Parse tree, etc.



Training and test set

Estimate *y = f(x)* on *X,Y.*
Hope that the same *f(x)*
also works on unseen X', Y'

- **Data is labeled:**
  - Have many pairs **{(x, y)}**
    - **x** … vector of binary, categorical, real valued features
    - **y** … class ({+1, -1}, or a real number)

Large Scale Machine Learning

- **We will talk about the following methods:**
  - **k**-Nearest Neighbor (Instance based learning)
  - Perceptron and Winnow algorithms
  - Support Vector Machines
  - Decision trees
- **Main question:**
  How to efficiently train
  (build a model/find model parameters)**?**

Instance Based Learning

- **Instance based learning**
- **Example: Nearest neighbor**
  - Keep the whole training dataset: **{(x, y)}**
  - A query example (vector) ***q*** comes
  - Find closest example(s) $\mathbf{x}^*$
  - Predict $\mathbf{y}^*$
- **Works both for regression and classification**
  - **Collaborative filtering** is an example of k-NN classifier
    - Find ***k*** most similar people to user **x** that have rated movie **y**
    - Predict rating $\mathbf{y}_x$ of **x** as an average of $\mathbf{y}_k$

Item-Item CF (|N|=2)

users

movies	1	2	3	4	5	6	7	8	9	10	11	12
1	1		3			5			5		4	
2			5	4			4			2	1	3
3	2	4		1	2		3		4	3	5	
4		2	4		5			4			2	
5			4	3	4	2					2	5
6	1		3		3			2			4	

- unknown rating

- rating between 1 to 5

Item-Item CF (|N|=2)

users

movies	1	2	3	4	**5**	6	7	8	9	10	11	12
1	1		3		?	5			5		4	
2			5	4			4			2	1	3
3	2	4		1	2		3		4	3	5	
4		2	4		5			4			2	
5			4	3	4	2					2	5
6	1		3		3			2			4	

- estimate rating of movie **1** by user **5**

Item-Item CF (|N|=2)

users

movies	1	2	3	4	**5**	6	7	8	9	10	11	12	sim(1,m)
1	1		3		?	5			5		4		1.00
2			5	4			4			2	1	3	-0.18
<u>**3**</u>	2	4		1	2		3		4	3	5		<u>0.41</u>
4		2	4		5			4			2		-0.10
5			4	3	4	2					2	5	-0.31
<u>**6**</u>	1		3		3			2			4		<u>0.59</u>

Neighbor selection:
Identify movies similar to movie **1**, **rated by user 5**

Here we use Pearson correlation as similarity:
1) Subtract mean rating m_i from each movie i
$m_1 = (1+3+5+5+4)/5 = \mathbf{3.6}$
row 1: *[-2.6, 0, -0.6, 0, 0, 1.4, 0, 0, 1.4, 0, 0.4, 0]*
2) Compute cosine similarities between rows

Item-Item CF (|N|=2)

movies \ users	1	2	3	4	5	6	7	8	9	10	11	12	sim(1,m)
1	1		3		?	5			5		4		**1.00**
2			5	4			4			2	1	3	**-0.18**
3	2	4		1	2		3		4	3	5		**0.41**
4		2	4		5			4			2		**-0.10**
5			4	3	4	2					2	5	**-0.31**
6	1		3		3			2			4		**0.59**

Compute similarity weights:

$s_{1,3}=0.41$, $s_{1,6}=0.59$

Item-Item CF (|N|=2)

users

movies	1	2	3	4	5	6	7	8	9	10	11	12
1	1		3		**2.6**	5			5		4	
2			5	4			4			2	1	3
3	2	4		1	2		3		4	3	5	
4		2	4		5			4			2	
5			4	3	4	2					2	5
6	1		3		3			2			4	

Predict by taking weighted average:

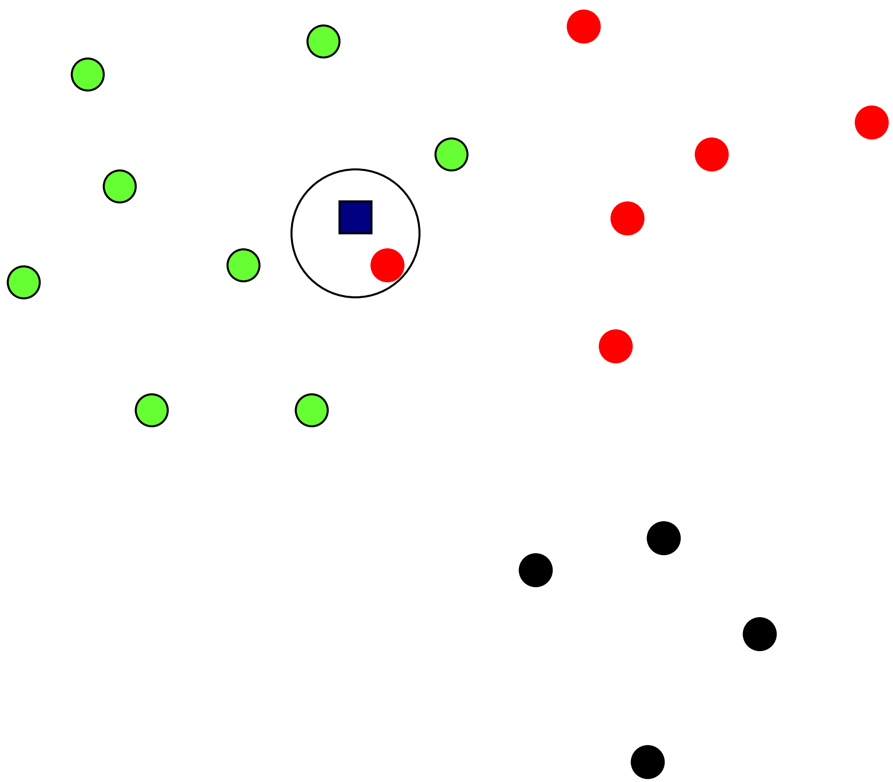
$r_{1.5}$ = **(0.41*2 + 0.59*3) / (0.41+0.59) = 2.6**

$$r_{ix} = \frac{\sum_{j \in N(i;x)} s_{ij} \cdot r_{jx}}{\sum s_{ij}}$$

1-Nearest Neighbor

- **To make Nearest Neighbor work we need 4 things:**
  - **Distance metric:**
    - Euclidean
  - **How many neighbors to look at?**
    - One
  - **Weighting function (optional):**
    - Unused
  - **How to fit with the local points?**
    - Just predict the same output as the nearest neighbor

Example: k=1 (1NN)

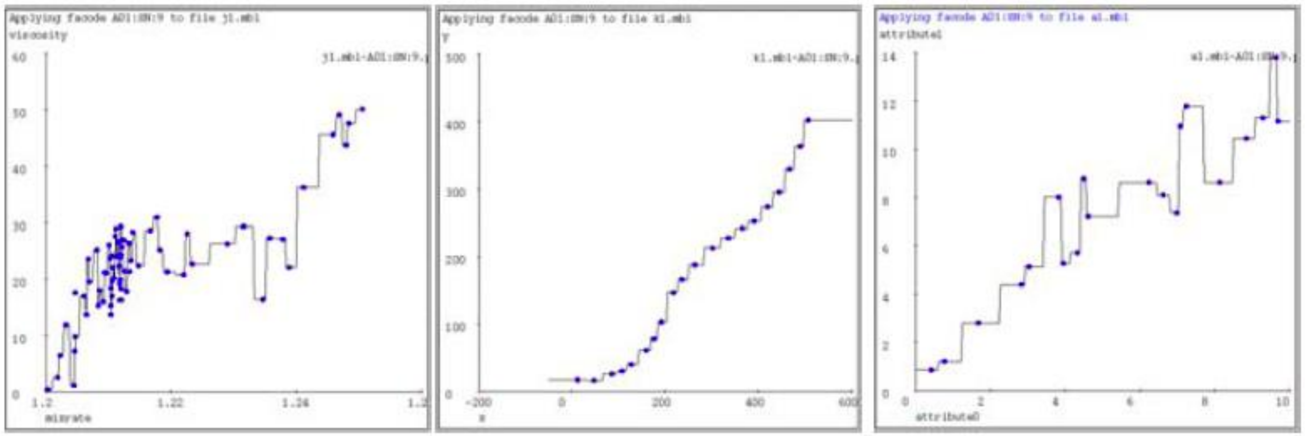


- Car
- Book
- Clothes

■ which class?
Book

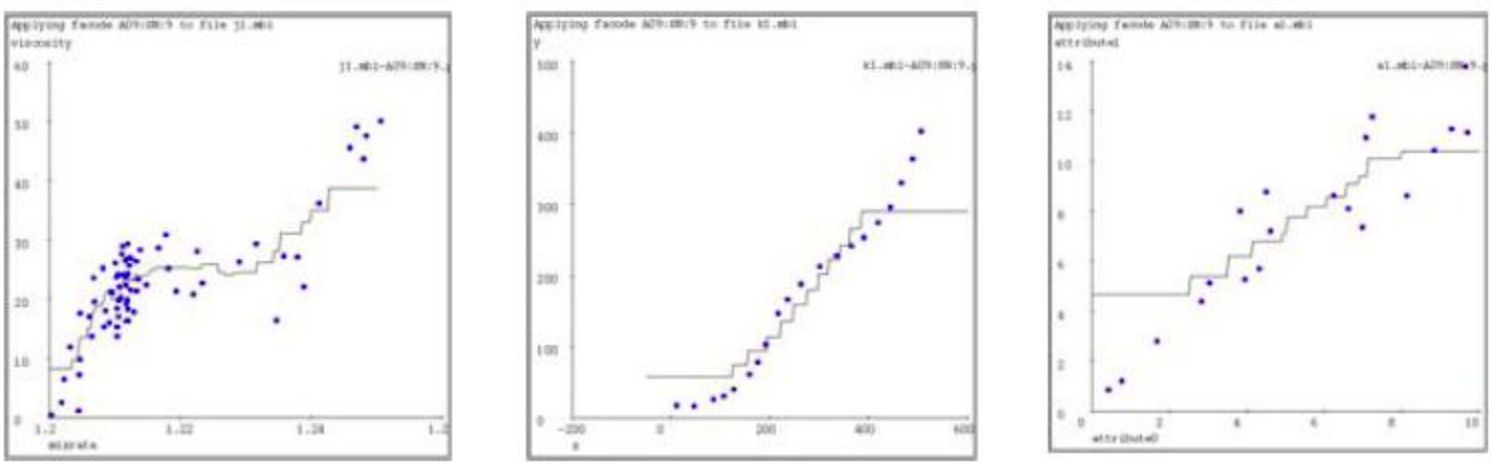
1-Nearest Neighbor

- **To make Nearest Neighbor work we need 4 things:**
  - **Distance metric:**
    - Euclidean
  - **How many neighbors to look at?**
    - One
  - **Weighting function (optional):**
    - Unused
  - **How to fit with the local points?**
    - Just predict the same output as the nearest neighbor



k-Nearest Neighbor

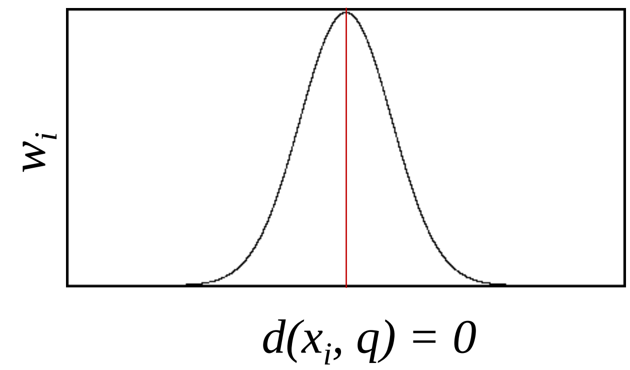
- **Distance metric:**
  - Euclidean
- **How many neighbors to look at?**
  - ***k***
- **Weighting function (optional):**
  - Unused
- **How to fit with the local points?**
  - Just predict the average output among *k* nearest neighbors

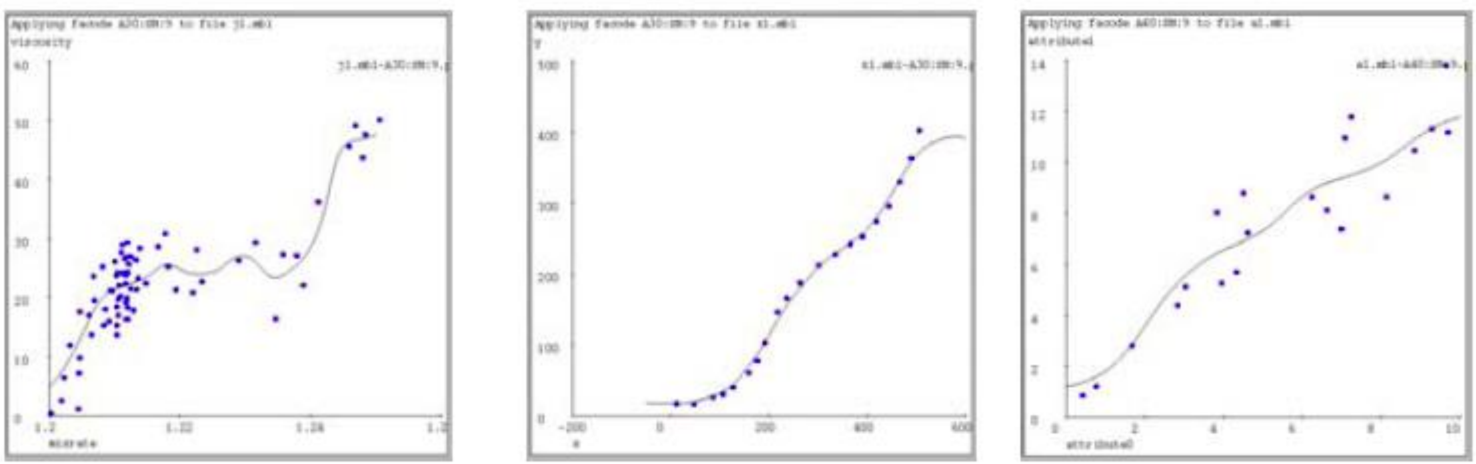


k=9

Kernel Regression

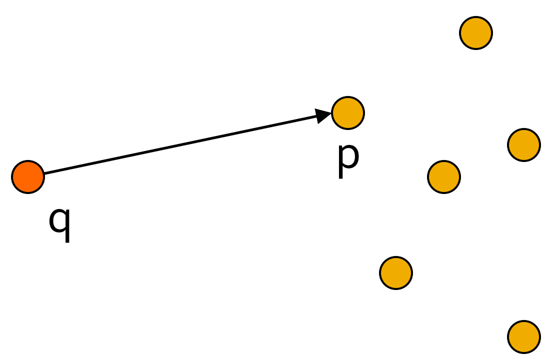
- **Distance metric:**
  - Euclidean
- **How many neighbors to look at?**
  - **All of them (!)**
- **Weighting function:**
  - $w_i = \exp\left(-\frac{d(x_i,q)^2}{K_w}\right)$
    - Nearby points to query q are weighted more strongly. K_w…kernel width.
- **How to fit with the local points?**
  - **Predict weighted average:** $\frac{\sum_i w_i y_i}{\sum_i w_i}$





How to find nearest neighbors?

- **Given:** a set ***P*** of ***n*** points in $\boldsymbol{R^d}$
- **Goal: Given a query point *q***
  - **NN:** Find the *nearest neighbor* ***p*** of ***q*** in ***P***
  - **Range search:** Find one/all points in ***P*** within distance ***r*** from ***q***



Algorithms for NN

- **Main memory:**
  - **Linear scan**
  - **Tree based:**
    - Quadtree
    - kd-tree
  - **Hashing:**
    - Locality-Sensitive Hashing
- **Secondary storage:**
  - R-trees

(1958)
F. Rosenblatt

The perceptron: a probabilistic model
for information storage and organization in the brain
Psychological Review 65:386–408

Perceptron

Linear models: Perceptron

- **Example: Spam filtering**

	viagra	learning	the	dating	nigeria	*spam?*
$\vec{x}_1 = ($	1	0	1	0	0 $)$	$y_1 = 1$
$\vec{x}_2 = ($	0	1	1	0	0 $)$	$y_2 = -1$
$\vec{x}_3 = ($	0	0	0	0	1 $)$	$y_3 = 1$

- **Instance space x ∈ X** (|**X**|= **n** data points)
  - **Binary or real-valued feature vector *x* of word occurrences**
  - ***d*** features (words + other things, **d**~100,000)
- **Class y ∈ Y**
  - ***y***: Spam (+1), Ham (-1)

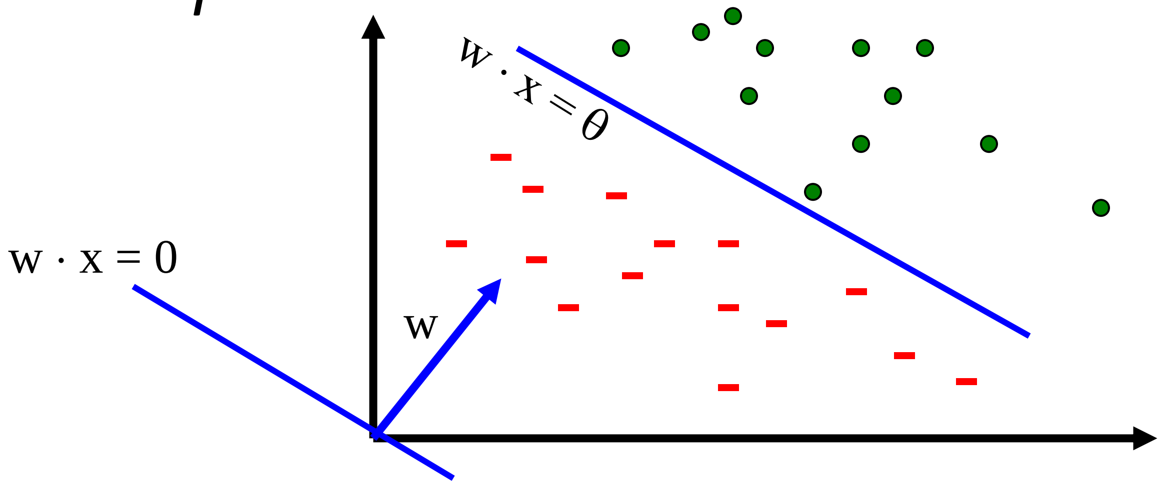
Linear models for classification

- **Binary classification:**

$$f(\mathbf{x}) = \begin{cases} +1 & \text{if} \quad \mathbf{w}_1\, \mathbf{x}_1 + \mathbf{w}_2\, \mathbf{x}_2 + \ldots \mathbf{w}_d\, \mathbf{x}_d \geq \theta \\ -1 & \text{otherwise} \end{cases}$$

Decision boundary is **linear**

- **Input:** Vectors $\boldsymbol{x}^{(j)}$ and labels $\boldsymbol{y}^{(j)}$
  - Vectors $\boldsymbol{x}^{(j)}$ are real valued where $\|x\|_2 = 1$
- **Goal:** Find vector $\boldsymbol{w} = (w_1, w_2, \ldots, w_d)$
  - Each $\boldsymbol{w}_i$ is a real number



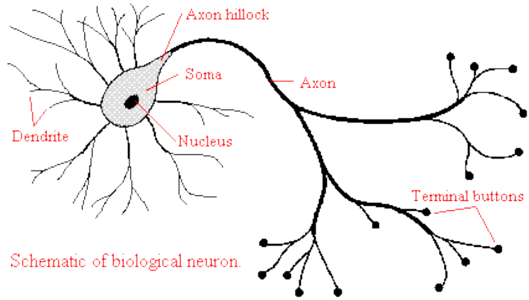
Note:

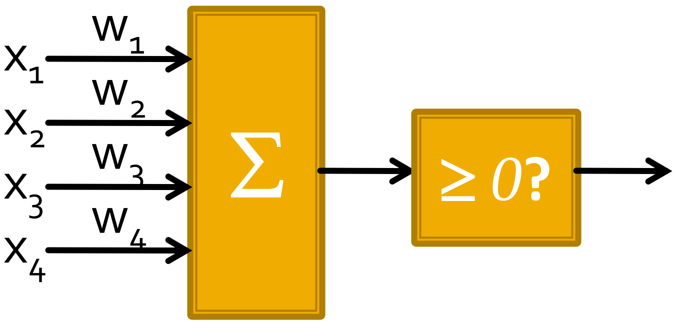
$$\mathbf{x} \Leftrightarrow \langle \mathbf{x}, 1 \rangle \quad \forall \mathbf{x}$$

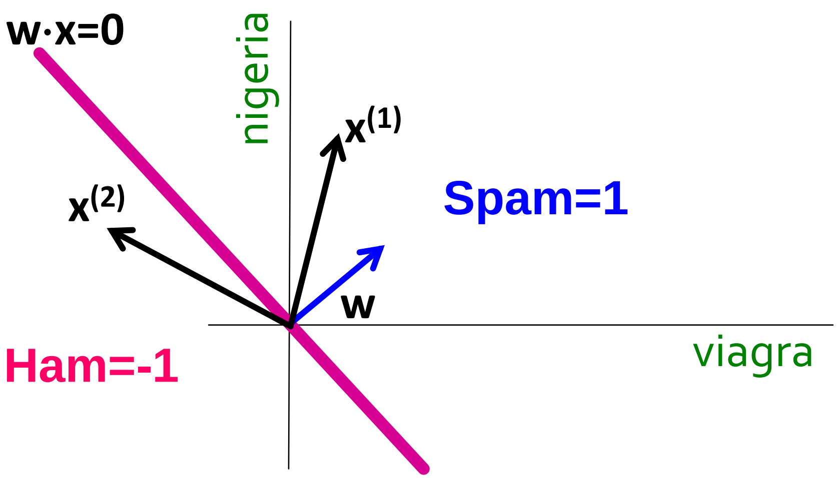
$$\mathbf{w} \Leftrightarrow \langle \mathbf{w}, -\theta \rangle$$

Perceptron [Rosenblatt '58]

- **(very) Loose motivation: Neuron**
- Inputs are feature values
- Each feature has a weight $\boldsymbol{w_i}$
- **Activation is the sum:**
  - $f(x) = \Sigma_i w_i x_i = w \cdot x$
- If the ***f(x)*** is:
  - **Positive:** Predict **+1**
  - **Negative:** Predict **-1**







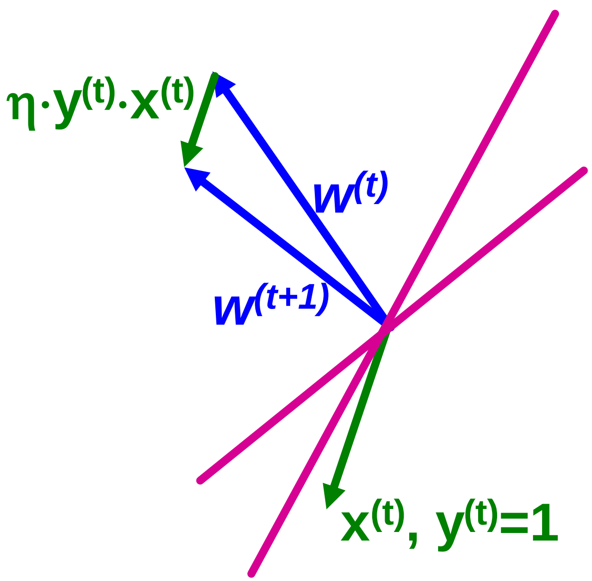
Perceptron: Estimating w

Note that the Perceptron is a conservative algorithm: it ignores samples that it classifies correctly.

- **Perceptron:** $y' = sign(w \cdot x)$
- **How to find parameters w?**
  - Start with $w_0 = 0$
  - Pick training examples $x^{(t)}$ **one by one (from disk)**
  - Predict class of $x^{(t)}$ using current weights
    - $y' = sign(w^{(t)} \cdot x^{(t)})$
  - **If y' is correct (i.e., $y_t = y'$)**
    - No change: $w^{(t+1)} = w^{(t)}$
  - **If y' is wrong:** adjust $w^{(t)}$

$$w^{(t+1)} = w^{(t)} + \eta \cdot y^{(t)} \cdot x^{(t)}$$

- η is the learning rate parameter
- $x^{(t)}$ is the t-th training example
- $y^{(t)}$ is true t-th class label ({+1, -1})

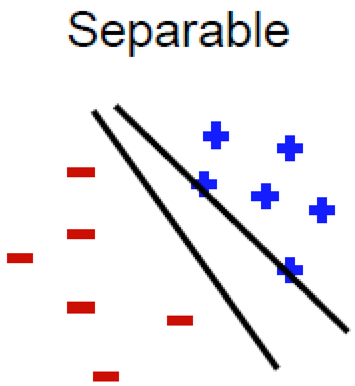


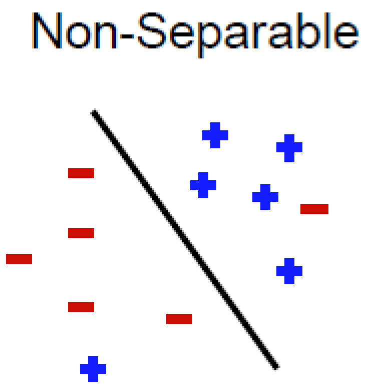
Perceptron Convergence

- **Perceptron Convergence Theorem:**
  - If there exist a set of weights that are consistent (i.e., the data is linearly separable) the Perceptron learning algorithm will converge
- **How long would it take to converge?**
- **Perceptron Cycling Theorem:**
  - If the training data is not linearly separable the Perceptron learning algorithm will eventually repeat the same set of weights and therefore enter an infinite loop
- **How to provide robustness, more expressivity?**

Properties of Perceptron

- **Separability:** Some parameters get training set perfectly
- **Convergence:** If training set is separable, perceptron will converge
- **(Training) Mistake bound:**
  Number of mistakes $< \frac{1}{\gamma^2}$
  - **where** $\gamma = \min_{t,u} |x^{(t)} u|$
    and $\|u\|_2 = 1$
    - Note we assume **x** Euclidean length **1**, then **γ** is the minimum distance of any example to plane **u**





Updating the Learning Rate

- **Perceptron will oscillate and won't converge**
- **When to stop learning?**
- **(1)** Slowly decrease the learning rate η
  - A classic way is to: $\eta = \mathbf{c_1/(t + c_2)}$
    - But, we also need to determine constants $\mathbf{c_1}$ and $\mathbf{c_2}$
- **(2)** Stop when the training error stops chaining
- **(3)** Have a small test dataset and stop when the test set error stops decreasing
- **(4)** Stop when we reached some maximum number of passes over the data

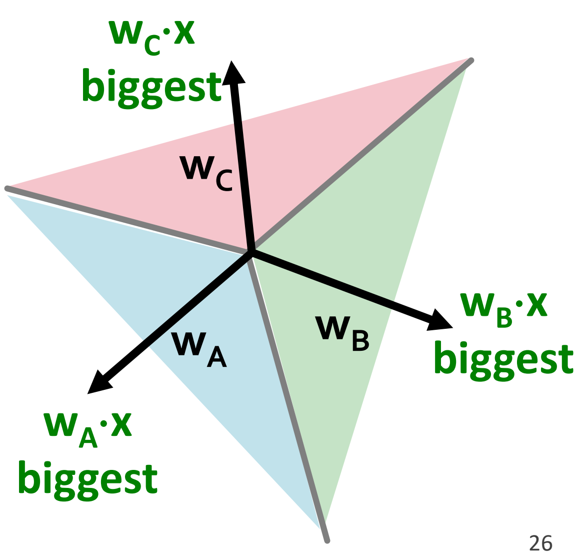
Multiclass Perceptron

- **What if more than 2 classes?**
- Weight vector $\boldsymbol{w_c}$ for each class **c**
  - **Train one class vs. the rest:**
    - Example: 3-way classification **y = {A, B, C}**
    - Train 3 classifiers: $\mathbf{w_A}$: A vs. B,C; $\mathbf{w_B}$: B vs. A,C; $\mathbf{w_C}$: C vs. A,B
- **Calculate activation for each class**

$$f(x,c) = \Sigma_i \; w_{c,i} \, x_i \; = \; w_c \cdot x$$

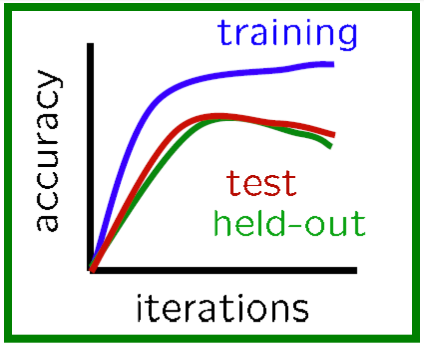
- **Highest activation wins**

$$c = \arg\max_c f(x,c)$$

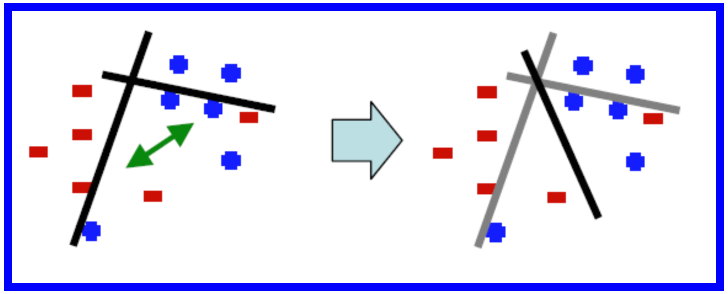


Issues with Perceptrons

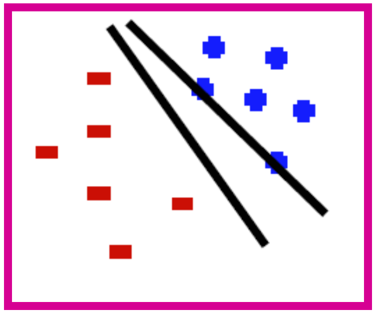
- **Overfitting:**



- **Regularization:** If the data is not separable weights dance around



- **Mediocre generalization:**
  - Finds a "barely" separating solution



Improvement: Winnow Algorithm

- **Winnow :** Predict **f(x) = +1** iff $\boldsymbol{w} \cdot \boldsymbol{x} \geq \boldsymbol{\theta}$
  - Similar to perceptron, just different updates
  - **Assume *x* is a real-valued feature vector,** $\|x\|_2 = 1$

> - Initialize: $\boldsymbol{\theta} = \frac{d}{2},\ \boldsymbol{w} = \left[\frac{1}{d}, \dots, \frac{1}{d}\right]$
> - **For every training example $x^{(t)}$**
>   - **Compute $\boldsymbol{y}' = \boldsymbol{f}(\boldsymbol{x}^{(t)})$**
>   - If no mistake ($\boldsymbol{y}^{(t)} = \boldsymbol{y}'$): do nothing
>   - If mistake then: $\boldsymbol{w_i} \leftarrow \boldsymbol{w_i} \frac{\exp\left(\eta y^{(t)} x_i^{(t)}\right)}{Z^{(t)}}$

  - **w** … weights **(can never get negative!)**
  - $\boldsymbol{Z^{(t)}} = \sum_i \boldsymbol{w_i} \mathbf{exp}\left(\boldsymbol{\eta y^{(t)} x_i^{(t)}}\right)$ is the normalizing const.

Improvement: Winnow Algorithm

- **About the update:** $\boldsymbol{w_i \leftarrow w_i \frac{\exp\left(\eta y^{(t)} x_i^{(t)}\right)}{Z^{(t)}}}$
  - If **x** is false negative, increase $\mathbf{w}_i$ **(promote)**
  - If **x** is false positive, decrease $\mathbf{w}_i$ **(demote)**

- **In other words:** Consider $\boldsymbol{x_i^{(t)}} \in \{-1, +1\}$
- Then $\boldsymbol{w_i^{(t+1)}} \propto \boldsymbol{w_i^{(t)}} \cdot \begin{cases} \boldsymbol{e^{\eta}} & if\ x_i^{(t)} = y^{(t)} \\ \boldsymbol{e^{-\eta}} & else \end{cases}$
  - **Notice: This is a weighted majority algorithm of "experts" x_i agreeing with y**

Extensions: Winnow

- **Problem: All w_i can only be >0**
- **Solution:**
  - For every feature $\mathbf{x_i}$, introduce a new feature $\boldsymbol{x_i' = -x_i}$
  - Learn Winnow over ***2d*** features
- **Example:**
  - Consider: $\boldsymbol{x} = [1, .7, -.4], \boldsymbol{w} = [.5, .2, .3]$
  - Then new $\boldsymbol{x}$ and $\boldsymbol{w}$ are $\boldsymbol{x} = [1, .7, -.4, -1, -.7, .4], \mathbf{w} = [.5, .2, 0, 0, 0, -.3]$
  - Note this results in the same dot values as if we used original $\boldsymbol{x}$ and $\mathbf{w}$
- New algorithm is called **Balanced Winnow**

Extensions: Balanced Winnow

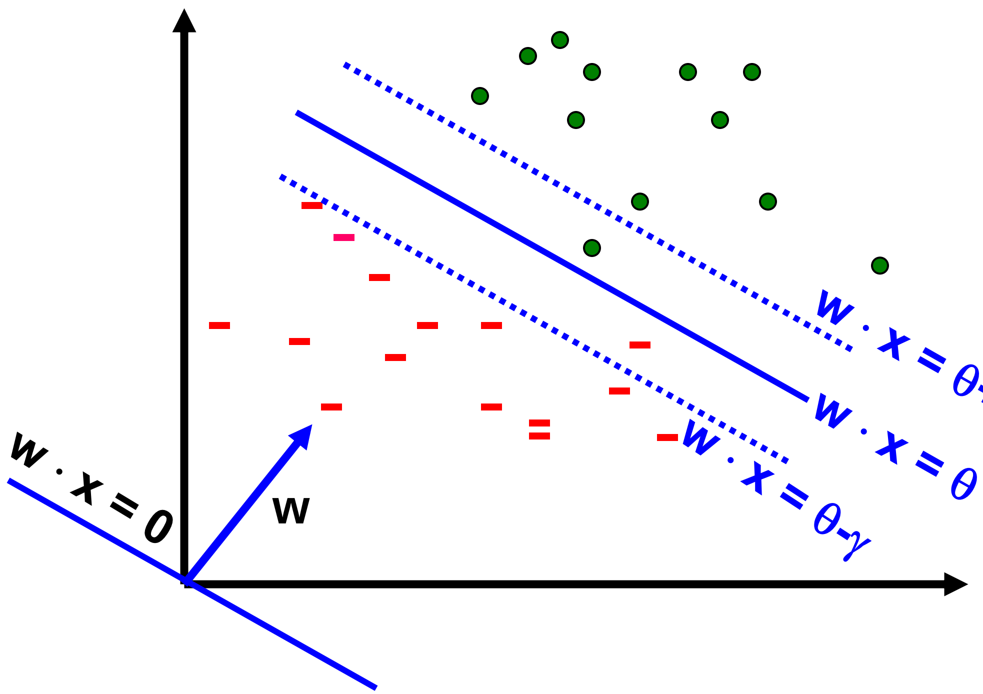
- **In practice we implement Balanced Winnow:**
  - **2** weight vectors **w⁺, w⁻**; effective weight is the difference

- **Classification rule:**
  - f(x) =+1 if (w⁺-w⁻)·x ≥ θ
- **Update rule:**
  - **If mistake:**
    - $$\mathbf{w}_i^+ \leftarrow \mathbf{w}_i^+ \frac{\exp\left(\eta y^{(t)} x_i^{(t)}\right)}{Z^{+(t)}}$$
    - $$\mathbf{w}_i^- \leftarrow \mathbf{w}_i^- \frac{\exp\left(-\eta y^{(t)} x_i^{(t)}\right)}{Z^{-(t)}}$$

$$Z^{-(t)} = \sum_i w_i \exp\left(-\eta y^{(t)} x_i^{(t)}\right)$$

Extensions: Thick Separator

- **Thick Separator** (aka **Perceptron with Margin**) (Applies both to Perceptron and Winnow)
  - Set margin parameter γ
  - **Update** if **y=+1** but $\mathbf{w} \cdot \mathbf{x} < \theta + \gamma$
  - **or** if **y=-1** but $\mathbf{w} \cdot \mathbf{x} > \theta - \gamma$



Note: γ is a functional margin. Its effect could disappear as ***w*** grows. Nevertheless, this has been shown to be a very effective algorithmic addition.

Summary of Algorithms

- **Setting:**
  - **Examples:** $x \in \{0, 1\}$, **weights** $w \in R^d$
  - **Prediction:** $f(x) = +1$ iff $w \cdot x \geq \theta$ else -1
- **Perceptron:** Additive weight update

$$\boxed{\mathbf{w} \leftarrow \mathbf{w} + \eta\, \mathbf{y}\, \mathbf{x}}$$

  - **If y=+1 but w·x ≤ θ then $w_i \leftarrow w_i + 1$ (if x_i=1)** **(promote)**
  - **If y=-1 but w·x > θ then $w_i \leftarrow w_i - 1$ (if x_i=1)** **(demote)**
- **Winnow:** Multiplicative weight update

$$\boxed{\mathbf{w} \leftarrow \mathbf{w}\, \exp\{\eta\, \mathbf{y}\, \mathbf{x}\}}$$

  - **If y=+1 but w·x ≤ θ then $w_i \leftarrow 2 \cdot w_i$ (if x_i=1)** **(promote)**
  - **If y=-1 but w·x > θ then $w_i \leftarrow w_i / 2$ (if x_i=1)** **(demote)**

Perceptron vs. Winnow

- **How to compare learning algorithms?**
- **Considerations:**
  - Number of features **d** is **very large**
  - **The instance space is sparse**
    - Only few features per training example are non-zero
  - **The model is sparse**
    - Decisions depend on a small subset of features
    - In the “true” model on a few $\mathbf{w}_i$ are non-zero
  - Want to learn from a number of examples that is small relative to the dimensionality **d**

Perceptron vs. Winnow

Perceptron

- **Online**: Can adjust to changing target, over time
- **Advantages**
  - Simple
  - Guaranteed to learn a linearly separable problem
  - **Advantage with few relevant features per training example**
- **Limitations**
  - Only linear separations
  - Only converges for linearly separable data
  - Not really "efficient with many features"

Winnow

- **Online**: Can adjust to changing target, over time
- **Advantages**
  - Simple
  - Guaranteed to learn a linearly separable problem
  - **Suitable for problems with many irrelevant attributes**
- **Limitations**
  - Only linear separations
  - Only converges for linearly separable data
  - Not really "efficient with many features"

Online Learning

- **New setting: Online Learning**
  - Allows for modeling problems where we have a continuous stream of data
  - We want an algorithm to learn from it and slowly adapt to the changes in data
- **Idea: Do slow updates to the model**
  - Both our methods Perceptron and Winnow make updates if they misclassify an example
  - **So:** First train the classifier on training data. Then for every example from the stream, if we misclassify, update the model (using small learning rate)

Example: Shipping Service

- **Protocol:**
  - User comes and tell us origin and destination
  - We offer to ship the package for some money ($10 - $50)
  - Based on the price we offer, sometimes the user uses our service (**y = 1**), sometimes they don't (**y = -1**)
- **Task:** Build an algorithm to optimize what price we offer to the users
- **Features *x* capture:**
  - Information about user
  - Origin and destination
- **Problem: Will user accept the price?**

Example: Shipping Service

- **Model whether user will accept our price:**
  $y = f(x; w)$
  - **Accept: $y = 1$**, **Not accept: $y = -1$**
  - Build this model with say Perceptron or Winnow
- **The website that runs continuously**
- **Online learning algorithm would do something like**
  - User comes
  - She is represented as an **(x,y)** pair where
    - **x:** Feature vector including price we offer, origin, destination
    - **y:** If they chose to use our service or not
  - The algorithm updates **w** using just the **(x,y)** pair
  - Basically, we update the **w** parameters every time we get some new data

Example: Shipping Service

- We discard this idea of a data "set"
- Instead we have a continuous stream of data
- **Further comments:**
  - For a major website where you have a massive stream of data then this kind of algorithm is pretty reasonable
  - Don't need to deal with all the training data
  - If you had a small number of users you could save their data and then run a normal algorithm on the full dataset
    - Doing multiple passes over the data

Online Algorithms

- An online algorithm can adapt to changing user preferences
- For example, over time users may become more price sensitive
- **The algorithm adapts and learns this**
- So the system is dynamic

Acknowledgement

- Slides are adapted from:
  - Prof. Jeffrey D. Ullman
  - Dr. Anand Rajaraman
  - Dr. Jure Leskovec