Machine Learning

Perceptron and Extensions

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Kernels and Dual Perceptron

One of the main limitation of linear models is, well.. ***linearity***!
This means that certain concepts cannot be represented.

One way to deal with this problem is to manually construct new features, or alternatively, systematically project the features to a new, higher dimensional space.

This presents two problems – ***computationally***, it is costly, and ***overfitting*** is more likely to happen (more data is needed).
We will introduce ***Kernels*** *as a way to efficiently learn in a high dimensional space (i.e., the first problem).*

Perceptron

- We learn f:X→ {-1,+1} represented as f =sgn{w•x)
- Where X= $\{0,1\}^n$ or X= R^n and w ² R^n
- Given Labeled examples: $\{(x_1, y_1), (x_2, y_2),\ldots(x_m, y_m)\}$

1. Initialize w=0 ϵ $\mathbf{R}^n$
2. Cycle through all examples

   a. Predict the label of instance x to be y' = sgn{w•x)

   b. If *y'≠y*, update the weight vector:

   w = w + r y x (r - a constant, learning rate)

   Otherwise, if y'=y, leave weights unchanged.

Note: this is the same as writing an "if-then-else" statement:

If (y=1): **w = w + r x**
If (y=-1): **w = w - r x**

Margin

- Given a dataset D, a weight vector w that separates D
- **Margin(w,D)**: distance between w and the nearest point

$$\min_{(x,y)\in D} y(wx)/|||w||$$

  - *Essentially the point with minimum activation (absolute value)*
    - *Similar to distance when* ||w|| = 1 (*functional margin = geometric margin*)

- **The margin of a dataset (Margin(D))**

$$margin(D) = \sup_w margin(D,w)$$

  - *The margin of a data set is the largest attainable margin on this data*
- *Perceptron mistake bound depends on Margin(D)*

Perceptron Mistake Bound

- Let D be a linearly separable data set with a margin $\gamma > 0$. Assume the $||x|| \leq 1$ for all $x \in D$. Then the algorithm will converge after at most $1/\gamma^2$

  - The theorem is connects the margin of the dataset with the number of mistakes, **not examples!**
  - In practice, practical considerations often determine performance:
    - We often prefer not to run the algorithm to convergence
      - Stop early, especially if the data is not linearly separable
    - Different classifiers with no (or similar) error on the training data, would behave differently on the test data

Getting Perceptron to work well!

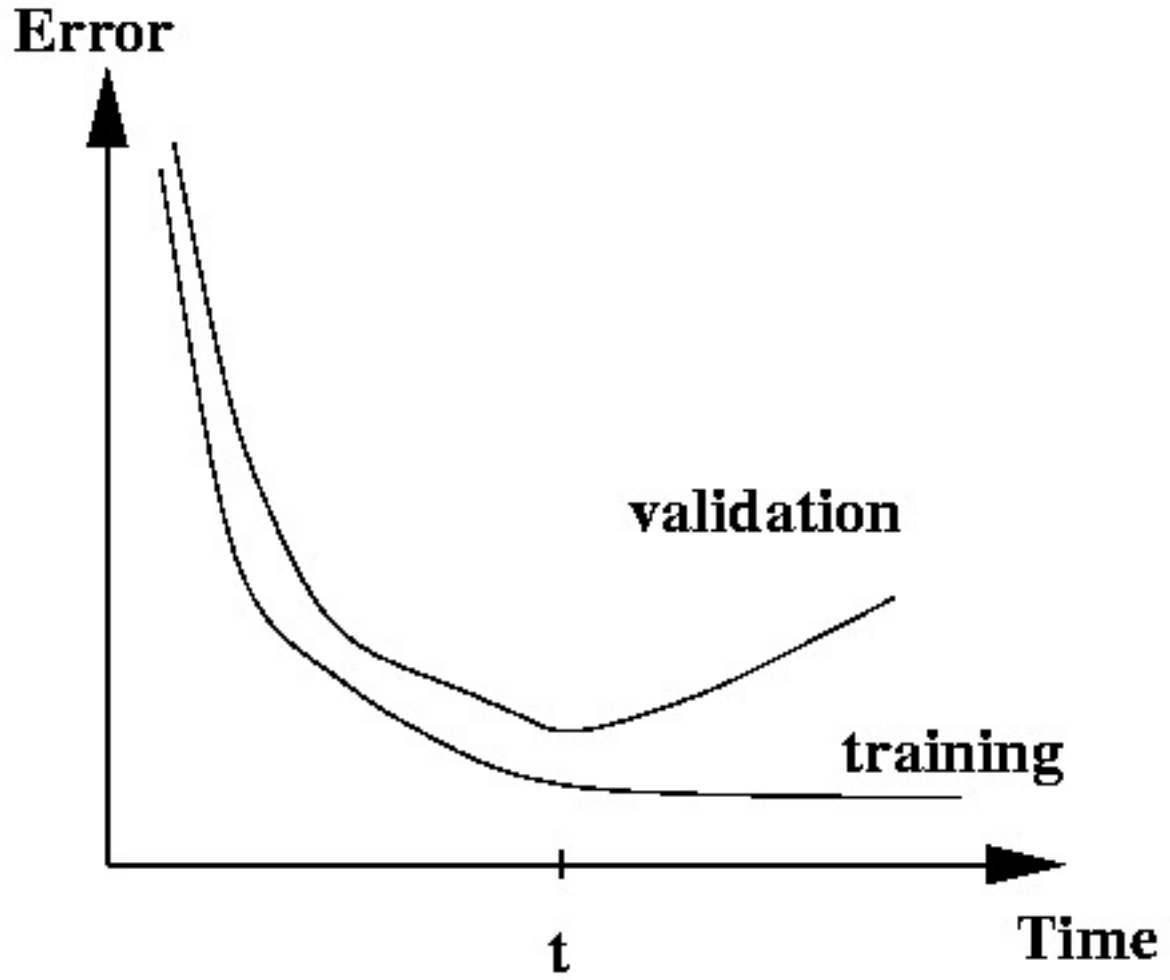
- **Randomize order of examples**
  - Even between epochs
- **Initialize W to small random weights**
- **Tune hyperparameters**
  - Learning rate
  - Number of iterations (can be fixed, or adapted using validation data)
- **Use extensions**
  - Perceptron with margin
  - Averaged perceptron

Perceptron in Practice: hyperparameters

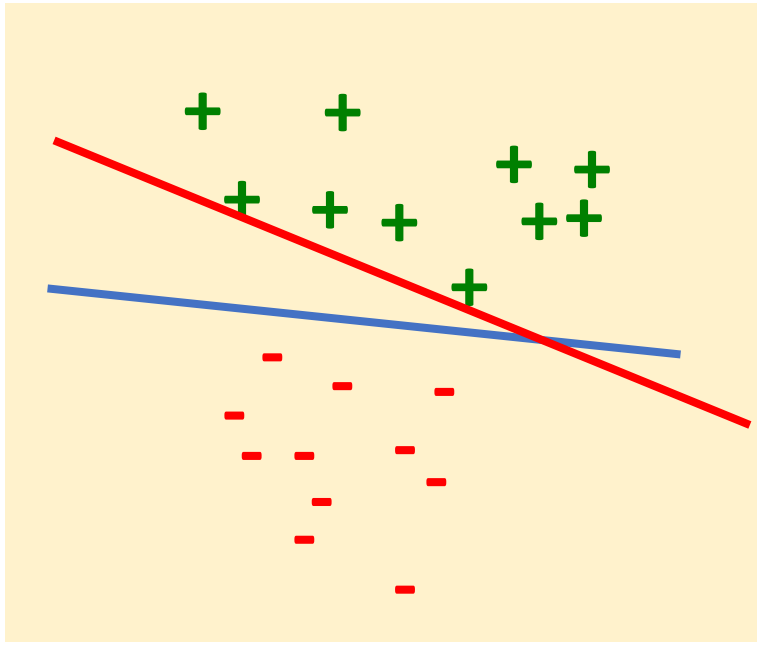
1. Initialize w with random weights close to 0
2. Cycle ***max_iter*** times through the examples
   a. **Predict** the label of instance x to be $y' = \text{sgn}\{w \bullet x\}$
   b. If $y' \neq y$, **update** the weight vector:
   $w = w + r\, y\, x$ (r - a constant, learning rate)
   Otherwise, if $y' = y$, leave weights unchanged.

- Iterating over the data until convergence might not be a good idea (***why***?)
- Introduce a new hyperparamter: `max_iter`
- *How can we find the best assignment for it?*

Overfitting and the Perceptron Algorithm



Which one is *better*?



The margin of a classifier captures this difference, but perceptron is not aiming for the larger margin one!

Regularization: *Perceptron with Margin*

- *Weights with better margin generalize better*
  - Perceptron finds *any* separating hyperplane
- Thick Separator (aka as Perceptron with Margin)

- **Predict positive**

  $w \cdot x - \theta > \gamma$

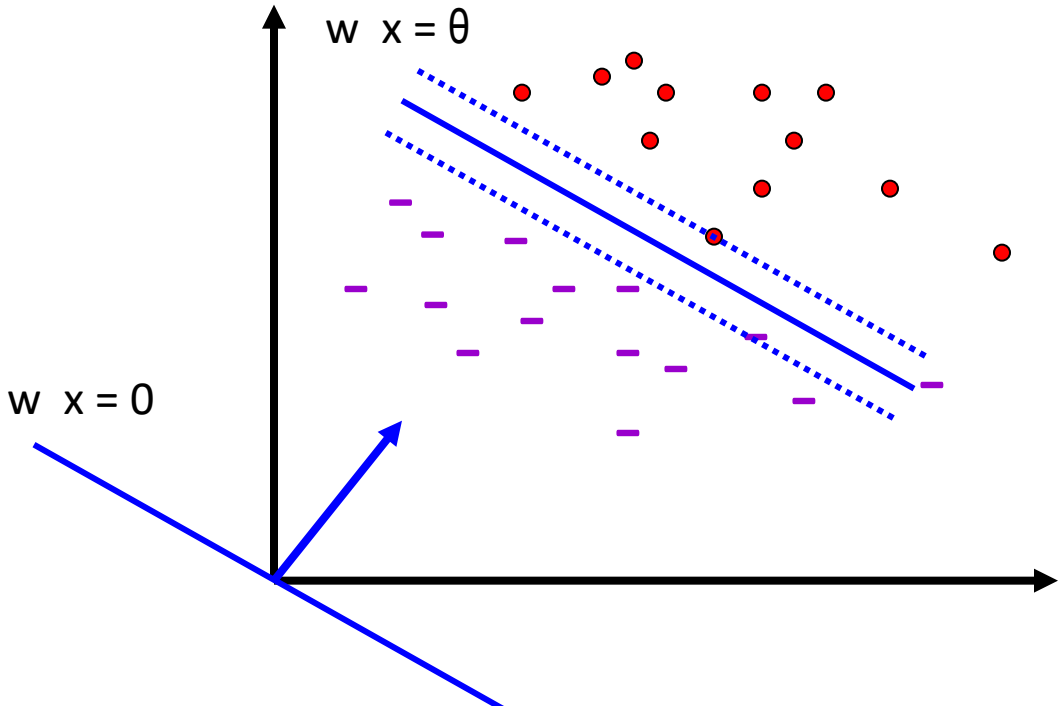
- **Predict negative**

  $w \cdot x - \theta < -\gamma$

- **Mistake:**

  $\gamma > (w \cdot x - \theta) > -\gamma$

Note: only at training time!



Averaged Perceptron

- **Training**: *Maintain a running weighted average of survived hypotheses*
- **Test**: *Predict according to the averaged weight vector*

Voted Perceptron $\longrightarrow$ $\hat{y} = \text{sign}\left(\sum_{k=1}^{K} c^{(k)} \text{sign}\left(\boldsymbol{w}^{(k)} \cdot \hat{\boldsymbol{x}} + b^{(k)}\right)\right)$

$\hat{y} = \text{sign}\left(\sum_{k=1}^{K} c^{(k)} \left(\boldsymbol{w}^{(k)} \cdot \hat{\boldsymbol{x}} + b^{(k)}\right)\right)$ $\longleftarrow$ Averaged Perceptron

- *An efficient approximation of voted perceptron*
- *Almost always better than regular perceptron!*

Averaged Perceptron

1. Initialize w=0 $\mathbf{R}^n$
2. Cycle through the examples

   a. Predict the label of instance x to be y' = sgn{w•x)

   b. If $y' \neq y$, update the weight vector:

   $$w = w + r\ y\ x \qquad \text{(r - a constant, learning rate)}$$

   a = a+w

3. Return a

Summary: Perceptron/ Winnow

- Examples: $x \in \{0,1\}^n$; Hypothesis: $w \in R^n$
- Prediction: $y \in \{-1,+1\}$: $y = 1$ iff $w\ x > \mu$
- Additive weight update algorithm
  - (Perceptron, Rosenblatt, 1958. Variations exist)

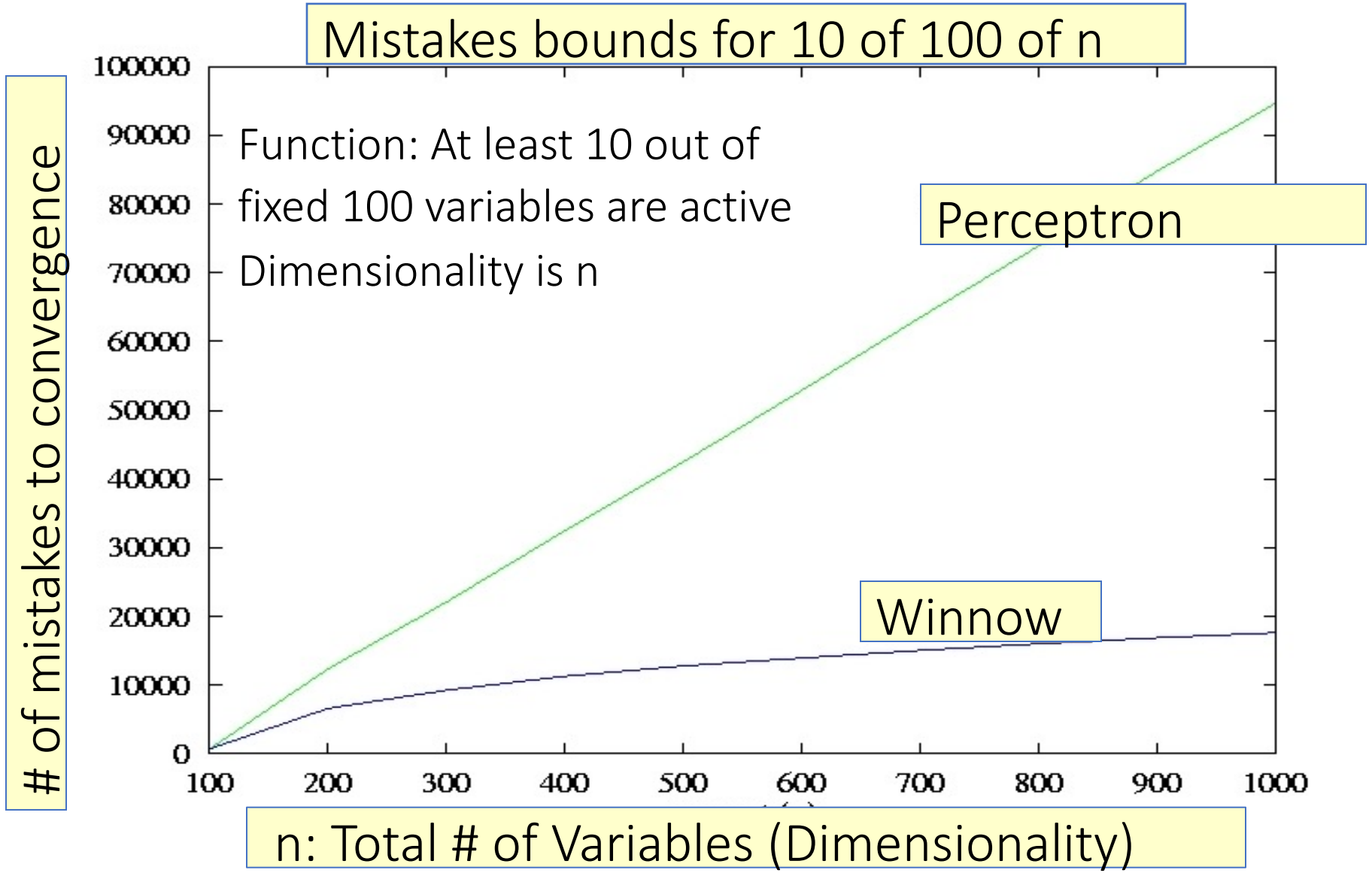
$$\text{If Class} = 1 \text{ but } w \bullet x \le \theta \text{ , } w_i \leftarrow w_i + 1 \text{ (if } x_i = 1) \text{ (promotion)}$$
$$\text{If Class} = 0 \text{ but } w \bullet x \ge \theta \text{ , } w_i \leftarrow w_i - 1 \text{ (if } x_i = 1) \text{ (demotion)}$$

- Multiplicative weight update algorithm
  - (Winnow, Littlestone, 1988. Variations exist)

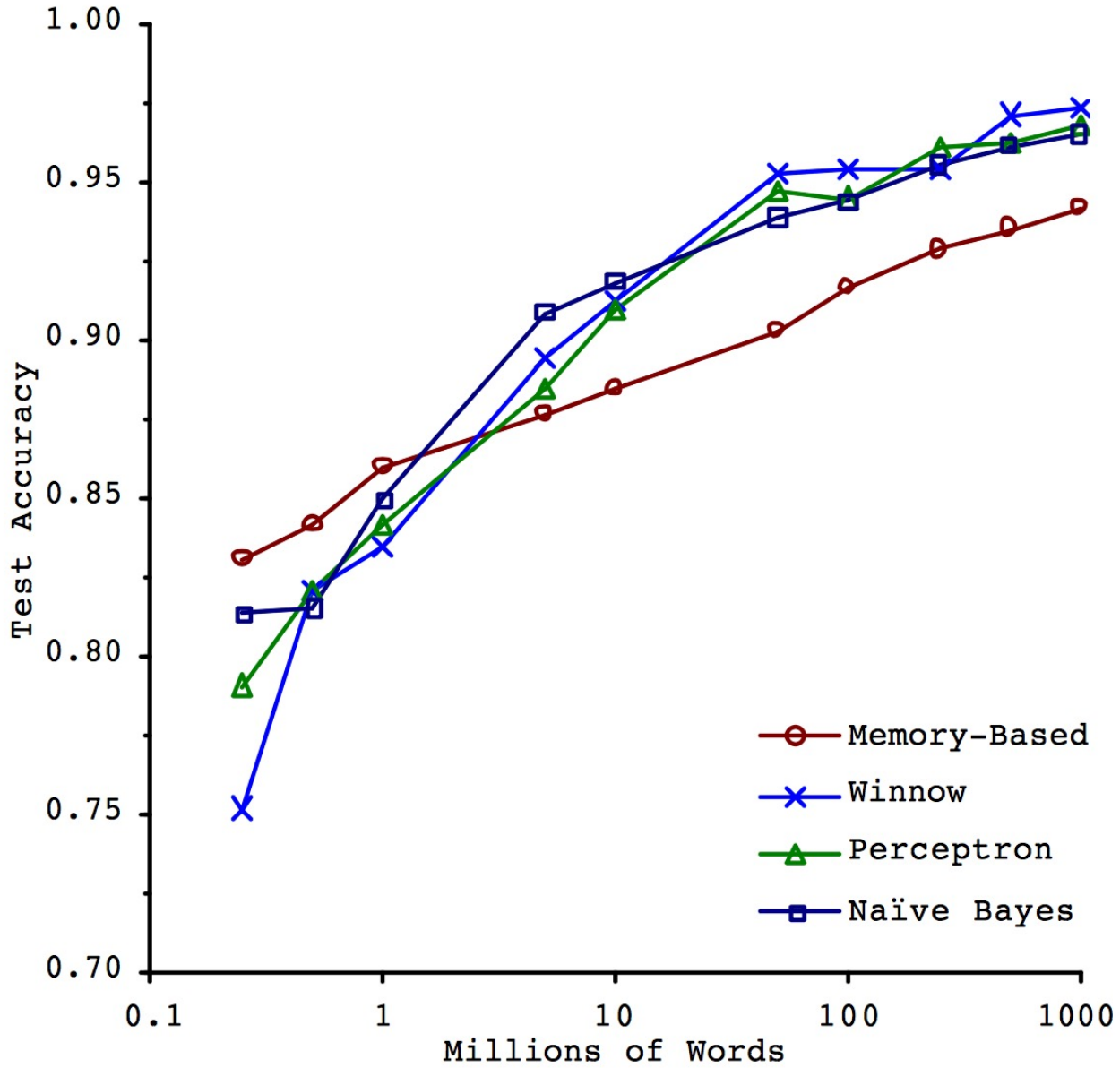
$$\text{If Class} = 1 \text{ but } w \bullet x \le \theta \text{ , } w_i \leftarrow 2w_i \text{ (if } x_i = 1) \text{ (promotion)}$$
$$\text{If Class} = 0 \text{ but } w \bullet x \ge \theta \text{ , } w_i \leftarrow w_i/2 \text{ (if } x_i = 1) \text{ (demotion)}$$

How to Compare the Algorithms?

- **Fair Question!**
  - **Same representation**, comparison pertains to the algorithms
  - Both mistake bound algorithm
- *Both algorithms are robust to noise*
  - *Small variations to for the noisy settings*
- ***Which algorithm should you choose?***
  - ***Multiplicative:*** *many irrelevant attributes (sparse target functions)*



Sparseness in the function space



Scaling to Very Very Large Corpora for Natural Language Disambiguation. Banko Brill 2001

Kernels and Dual Perceptron

Expressivity

- *The perceptron algorithm is very easy to implement and when few modifications are added, it performs well.*
- Tends to converge quickly

- **Easy to interpret**
  - How can you diagnose what is really being captured by the output classifier?
  - **Hint**: *How could you do it for decision trees?*

- This simplicity also comes with a price..

Feature Extraction

$$\text{Linear models: } w \cdot x \geq \theta$$

- Features*: words*
- *"John likes cake and hates carrots"*
- *(1,0,..,1,0,…,1,0,…,1,0,..,1,0,… 0)*

The value of the feature representing the word "John"

Most of the feature vector has zero valued entries
(efficient implementation do not carry the zero elements)

Feature Extraction

$$\text{Linear models: } w \cdot x \geq \theta$$

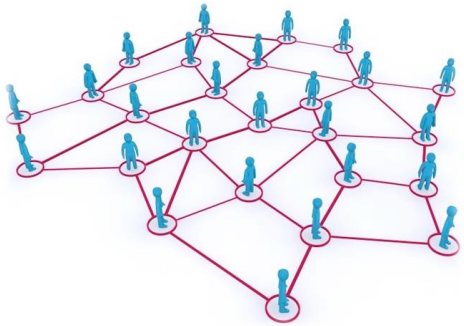
- Let's build a *food recommendation* classifier
  - Features*: words*
  - ***"John likes cake and hates carrots"***
  - ***"John likes carrots and hates cake"***
- What can you say about the feature vectors of the two sentences?

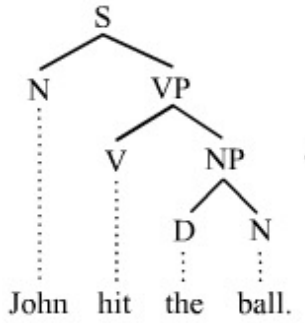
Feature Representation

- We cannot learn anything when different labels are represented using similar feature vectors
- ***How can we fix it?***
  - Move to a more meaningful representation!
  - *Encode the structure of the input object*
- **How about word conjunctions?**
  - ***(likes_cake, …, hates_carrots)***
  - ***(likes_carrots,.., hates_cake)***
- ***What can we say about the new feature space?***

Features over input Objects

- Word n-grams are a simple way to represent structured input objects
- We often need to learn over complex objects
  - Social networks, language semantics, protein structures
- *As we saw* – learning works only when we capture meaningful aspects of this structure
  - Define: feature functions mapping over inputs structures

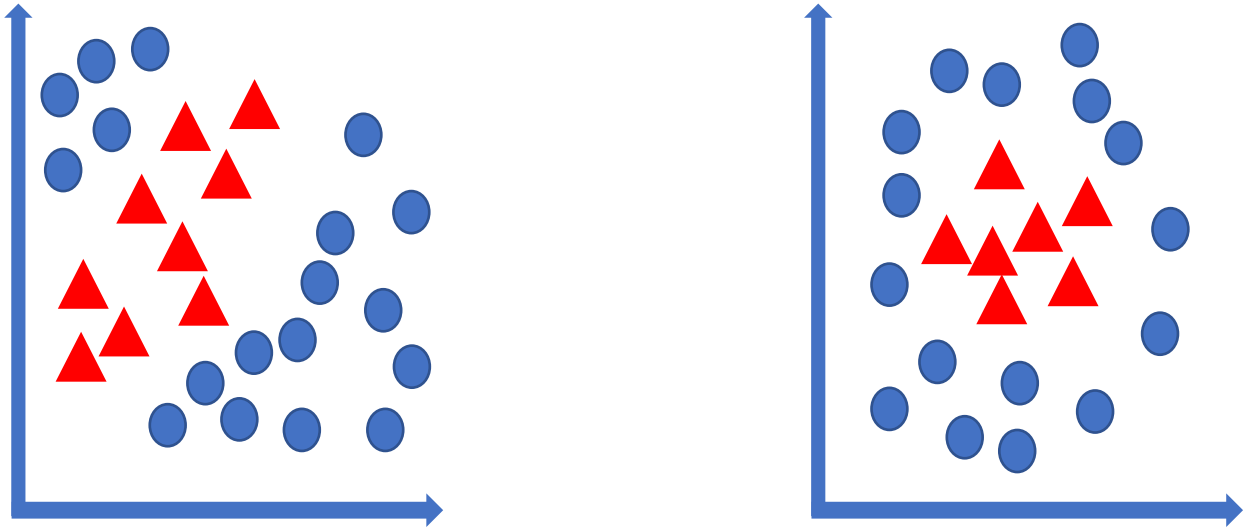




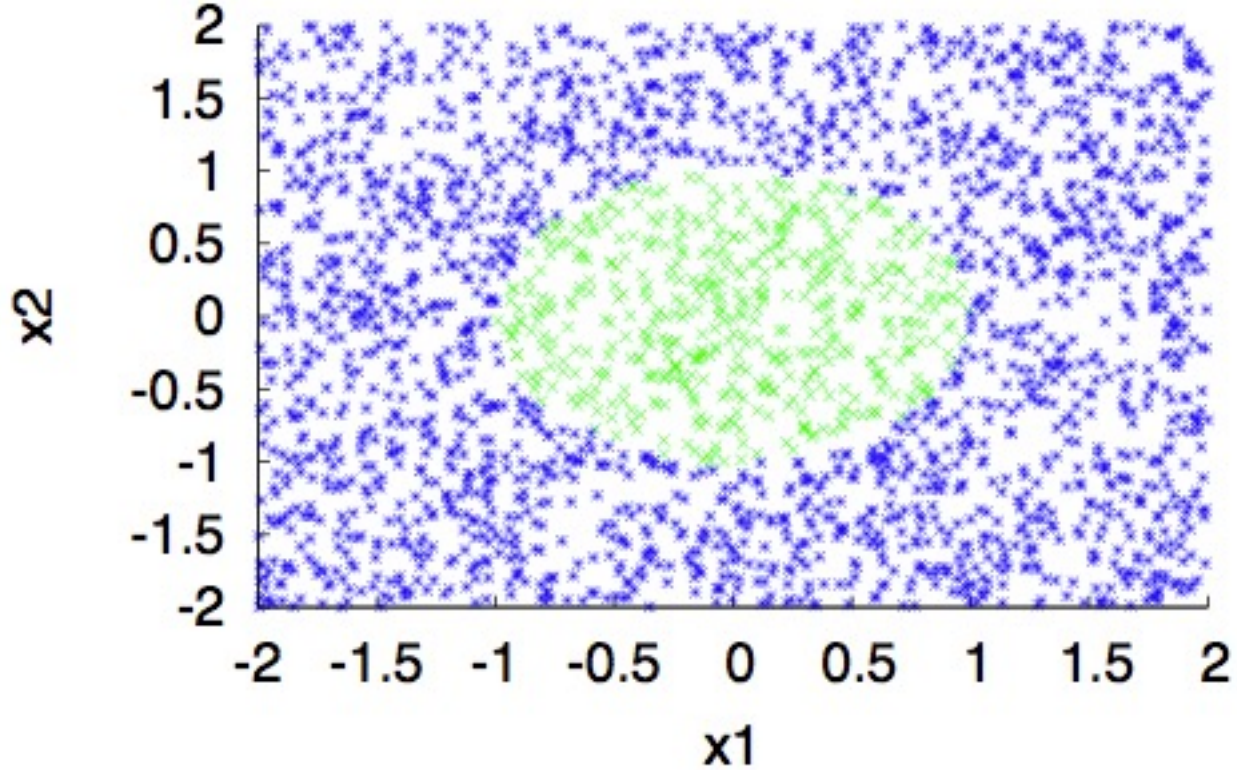
Constituency-based parse tree

Linear Separability

- Finding a good representation is especially relevant when we learn linear models
- *We often run into problems*

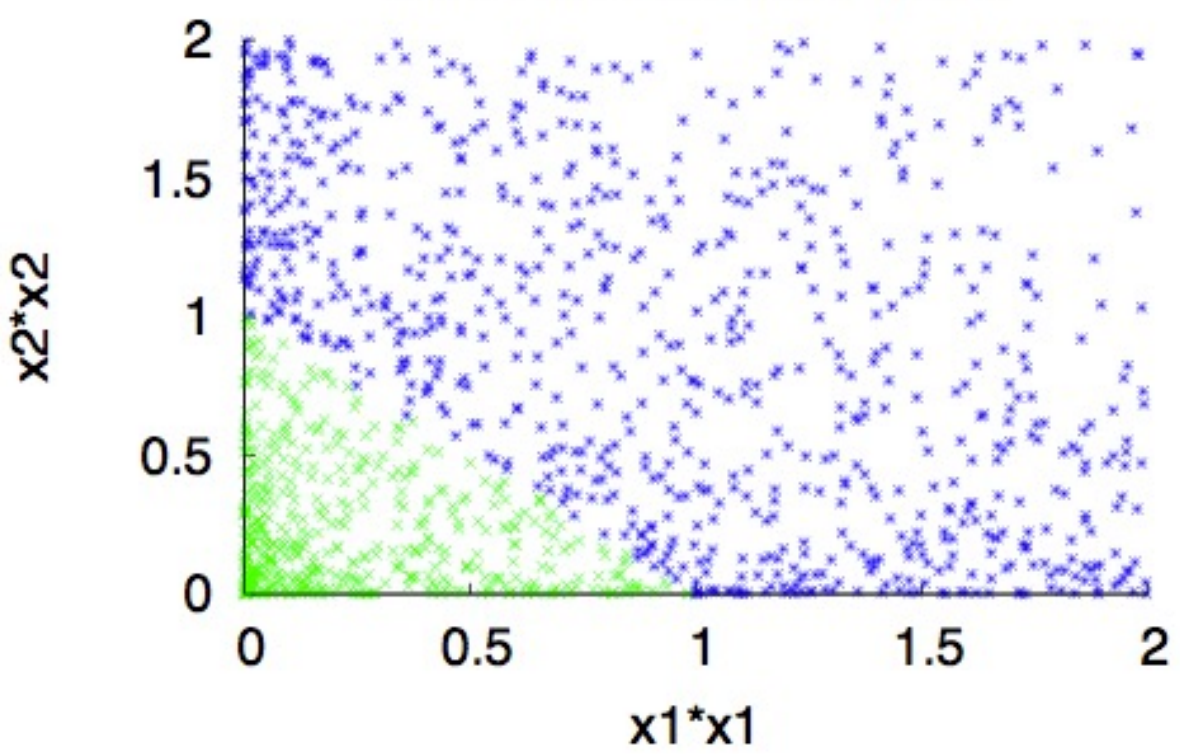


Linear Separability



$$f(x) = 1 \quad \text{iff} \quad x_1^2 + x_2^2 \leqslant 1$$

Linear Separability



$$x = (x_1, x_2) \rightarrow \; x' = (x_1^2, x_2^2)$$

$$f(x') = 1 \quad \text{iff} \;\; x'_1 + x'_2 \leqslant 1$$

Linear Separability

- **Problem**: *The data might not be linearly separable in the original feature space*
- **Solution**: add new features making the data linearly separable in the new space
  - Transform the original space and capture interactions between features
- **Caution**: this may blow up the feature space!
- **Why is this a problem?**
  - ***Efficiency***
  - ***Generalization***

Simple example: *Bigram features*

- **Let's build a Shakespeare classifier!**

- We will define a classification task over all the works of Shakespeare.
- Corpus size: N=884,647, V = 29,066
- So far, so good..
- But when moving to Bigram features -
- V^2= 844,000,000
- **Why is this a problem?**

Dual Perceptron

- ***Primal** vs. **Dual** representation*
  - Difference: weights (**primal**) vs. examples (**dual**)
- Dual representation allows for a more **efficient** feature computation
- **Key idea:**
  - Blow up the feature space (e.g., all conjunction of features)
  - Find an **efficient** way to compute the features in the dual representation (complexity depends on the original feature space)
  - Kernel function: efficiently computes the similarity between examples in the blown up space

Dual Representation

Examples : $x \in \{0,1\}^n$

Hypothesis : $w \in R^n$

$$f(x) = Th_\theta \left(\sum_{i \in I} w_i x_i(x) \right)$$

Primal

- Let w be an initial weight vector for perceptron.
- Let (x^1,+), (x^2,+), (x^3,-), (x^4,-) be examples
  - assume mistakes are made on x^1, x^2, x^4
- What is the resulting weight vector? **$w = w + x^1 + x^2 - x^4$**
- ➔ *The weight vector is a linear combination of examples*

$$w = \sum_{1,..,m} r \alpha_i y_i x_i$$

- α_i is the #mistakes of x_i , r is the learning rate (assume r=1)

Dual Representation

Examples : $x \in \{0,1\}^n$

Hypoth

- Let w be a
  (x^3,-), (x^4,-
- What is th
- The weigh
- α_i is the n

Prediction: *compute the dot-product between the weights and a new example*

$$f(x) = w \cdot x =$$

$$(\sum_{1,..,m} r\alpha_i y_i x_i) \cdot x =$$

Dual

$$\sum_{1,..,m} r\alpha_i y_i (x_i \cdot x)$$

Linear sum of dot products between x (new example) and previous ``mistake" examples

Kernel Based Methods

- A method to learn on a very large feature set in the dual representation, without incurring the cost of keeping a very large weight vector.
  - *Computing the weight vector can still be done in the original feature space.*
- **Notice**: *this pertains only to efficiency: The classifier is identical to the one you get by blowing up the feature space*.

- Generalization is still relative to the real dimensionality

Kernel Based Methods

We want to learn a function in a blown up space

- Let I be the set $t_1, t_2, t_3 \ldots$ of conjunctions over the feature space $x_1, x_2 \ldots x_n$.
- Then we can write a linear function over this new feature space.

$$f(x) = Th_\theta\left(\sum_{i \in I} w_i x_i(x)\right) \quad \Rightarrow \quad f(x) = Th_\theta\left(\sum_{i \in I} w_i t_i(x)\right)$$

Example: $\mathbf{x_1 \wedge x_2 \wedge x_4(11010) = 1}$

$\mathbf{x_3 \wedge x_4(11010) = 0}$

For brevity we'll denote these as $x_1x_2x_4$

Kernel Based Methods

$$f(x) = Th_\theta \left(\sum_{i \in I} w_i t_i(x) \right)$$

- **Great** Increase in expressivity
- **The size of *w* is exponential in *n* (HUGE)**
  - *Storage* consideration
- Computing the dot product $w \cdot t$ is **not** efficient
  - Computationally intractable
- *Can run perceptron but the convergence bound may suffer exponential growth*
  - Exponential number of conjunctions are true in each example

The Kernel Trick (1)

$$f(x) = Th_\theta \left(\sum_{i \in I} w_i t_i(x) \right)$$

- *Consider the value of w used in the prediction*
  - Each previous mistake, on example z, makes an additive contribution of +/-1 to w, iff t(z) = 1.
- **The value of w is determined by the number of mistakes on which t() was satisfied.**

The Kernel Trick(2)

- **P** – set of examples on which we Promoted
- **D** – set of examples on which we Demoted
- M = **P** U **D**

$$f(x) = Th_\theta\left(\sum_{i\in I} w_i t_i(x)\right) \Rightarrow f(x) = Th_\theta\left(\sum_{i\in I}\left[\sum_{z\in P, t_i(z)=1} 1 - \sum_{z\in D, t_i(z)=1} 1\right] t_i(x)\right) =$$

Where S(z)=1 if $z \in P$ and S(z)=-1 if $z \in D$

- Reordering:

$$Th_\theta\left(\sum_{z\in M} S(z)\sum_{i\in I} t_i(z)t_i(x)\right)$$

The Kernel Trick(3)

- So far we saw:
  - A *mistake* on z contributes the value +/-1 to *all conjunctions* satisfied by z.
- Given an example *x* ,the contribution of z to the sum is the *number of conjunctions satisfying both x and z.*
- Define a dot product in the t-space:

$$K(x,z) = \sum_{i \in I} t_i(z) t_i(x)$$

- We get the standard notation:

$$Th_\theta \left(\sum_{z \in M} S(z) \sum_{i \in I} t_i(z) t_i(x) \right) \Rightarrow f(x) = Th_\theta \left(\sum_{z \in M} S(z) K(x,z) \right)$$

Kernel Based Methods

- What does this representation give us?

$$f(x) = Th_\theta \left(\sum_{z \in M} S(z) K(x,z) \right)$$

$$K(x,z) = \sum_{i \in I} t_i(z) t_i(x)$$

- *We can view this Kernel as the distance between x,z* ***in the t-space***
  - sum of common active conjunctions in x,z
- But, K(x,z) can be measured in the **original space**, *without explicitly writing the t-representation of x, z*

Kernel Based Methods

$$f(x) = Th_\theta\left(\sum_{z \in Z} S(z)K(x,z)\right) \qquad K(x,z) = \sum_{i \in I} t_i(z)t_i(x)$$

- Consider the space of all 3^n conjunctions (allowing both positive and negative literals). Then,

$$K(x,z) = \sum_{i \in I} t_i(z)t_i(x) = 2^{same(x,z)}$$

- **same(x,z)** : *the number of features that have the same value for both x and z (computed over the original feature space)*
- We get:

$$f(x) = Th_\theta\left(\sum_{z \in M} S(z)2^{same(x,z)}\right)$$

Example (**all** conjunctions over x)

$n = 2 \qquad v = (0, 0), \qquad z = (0, 1)$

What is the new feature space?

Write down the set of all conjunctions

How are v,z represented in the new space?

Write the values of v,z in the new representation

What is their dot-product?

What is the value of kernel function?

Calculate the value of your kernel function

Example (**all** conjunctions over x)

$$n = 2 \qquad v = (0, 0), \qquad z = (0, 1)$$

$$\text{I}= (\emptyset, x_1, x_2, \neg x_1, \neg x_2, \neg x_1 x_2, x_1 \neg x_2, x_1 x_2, \neg x_1 \neg x_2)$$

$v \in \{0, 1\}^2$ In the new space: $v^i \in \{0, 1\}^9$

$v^i = (1, 0, 0, 1, 1, 0, 0, 0, 1)$

$z^i = (1, 0, 1, 1, 0, 0, 1, 0, 0)$

$v^i \cdot z^i = 2^{same(v,z)}$

$same(v, z) = 1$

Example (**all** conjunctions over x)

$$n = 2 \qquad v = (0, 0), \qquad z = (0, 1)$$

$$\text{I}= (\emptyset, x_1, x_2, \neg x_1, \neg x_2, \neg x_1 x_2, x_1 \neg x_2, x_1 x_2, \neg x_1 \neg x_2)$$

$v \in \{0, 1\}^2$ In the new space: $v^i \in \{0, 1\}^9$

$v^i = (1, 0, 0, 1, 1, 0, 0, 0, 1)$

$z^i = (1, 0, 1, 1, 0, 0, 1, 0, 0)$

$v^i \cdot z^i = 2^{same(v,z)}$

$same(v, z) = 1$

Kernel Based Methods

Proof:

- let k=same(x,z);
- construct a “surviving” conjunctions by
  - (1) choosing to include one of these k literals with the right polarity in the conjunction, or
  - (2) choosing to not include it at all.
- Conjunctions with literals outside this set disappear.

Example II

- Let's look at a different feature mapping
- Let I be the set $t_1, t_2, t_3 \ldots$ of **monotone** conjunctions over the feature space $x_1, x_2 \ldots x_n$.

- How can we calculate the dot product **efficiently**?

$$K(x, z) = \sum_{i \in I} t_i(z) t_i(x)$$

- *How does the monotone requirement change the Boolean kernel we just saw?*

Example II: **Monotone** conjunctions over x

$n = 2 \qquad v = (1, 0), \qquad z = (1, 1)$

What is the new feature space?
Write down the set of all monotone conjunctions

How are v,z represented in the new space?
Write the values of v,z in the new representation
What is their dot-product?

What is the value of kernel function?
Calculate the value of your kernel function

Example II: **Monotone** conjunctions over x

$$n = 2 \qquad v = (1, 0), \qquad z = (1, 1)$$

$$\mathrm{I} = (\emptyset,\ x_1,\ x_2,\ x_1 x_2)$$

$v \in \{0, 1\}^2$ In the new space: $v^i \in \{0, 1\}^4$

$v^i = (1, 1, 0, 0)$

$z^i =$ `(1,1,1,1)`

$v^i \cdot z^i = 2^{samePos(v,z)}$

$same(v, z) = 1$

Kernel Perceptron: Implementation

$$f(x) = Th_\theta\left(\sum_{z\in M} S(z)K(x,z)\right) \qquad K(x,z) = \sum_{i\in I} t_i(z)t_i(x)$$

- Simply run Perceptron in an on-line mode, but keep track of the set M.
- Keeping the set M allows us to keep track of S(z).
- Rather than remembering the weight vector w, remember the set M (P and D) – all those examples on which we made mistakes

Primal and Dual Representations

- **Primal Representation**
  - Works in the transformed space (high dimension)
  - Explicitly compute feature values
  - Maintain a large weight vector
- **Dual Representation**
  - Original space
  - Kernel trick
  - Weight examples (mistakes)

$$f(x) = Th_\theta\left(\sum_{i\in I} w_i t_i(x)\right)$$

$$f(x) = Th_\theta\left(\sum_{z\in M} S(z)K(x,z)\right)$$

$$K(x,z) = \sum_{i\in I} t_i(z)t_i(x)$$

Kernel trick

- Define a feature function $\varphi(x)$ which maps items x into a **high dimensional** space

- The kernel function $K(x_i, x_j)$ computes the inner-product between $\varphi(x_i)$ and $\varphi(x_j)$

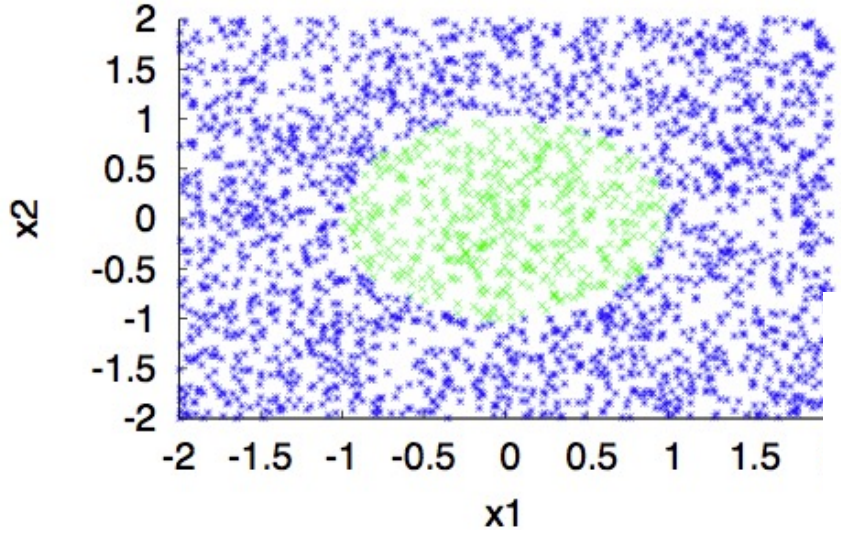
$$K(x_i, x_j) = \varphi(x_i)\varphi(x_j)$$

- Kernel function can be computed efficiently
  - No need to work with high dimensional *w*

Polynomial Kernel

A function $K(x,z)$ is a valid **kernel function** if it corresponds to an inner product in some (perhaps infinite dimensional) feature space.

Reminder..


x2
x1
2
1.5
1
0.5
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-1
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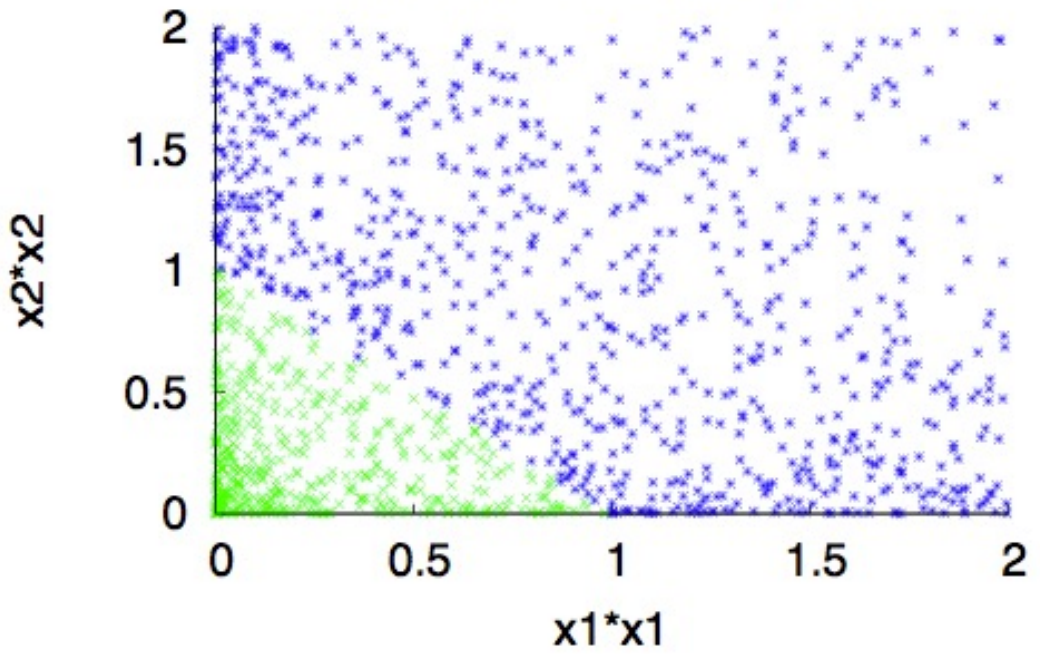
x2*x2
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2
1.5
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0 0.5 1 1.5 2

Polynomial Kernel

$$K(\mathbf{x}, \mathbf{y}) = (\mathbf{xy} + \mathbf{c})^{\mathbf{2}}$$

Example:

$$\mathbf{x} = (\mathbf{x_1}, \mathbf{x_2}) \in \mathbf{R^2} :$$

$$(\mathbf{x_1},\ \mathbf{x_2},\ \mathbf{x_1x_1},\ \mathbf{x_1x_2},\ \mathbf{x_1x_2},\ \mathbf{x_2x_2})$$

Polynomial Kernels

We can extend the quadratic kernel to any (higher) degree polynomial $(xz)^d$

Linear Kernel:

$$k(x, y) = xy$$

Polynomial Kernel:

$$k(x, y) = (xy)^d$$

Polynomial Kernel *up to degree n*:

$$k(x, y) = (xy + c)^d \ , \quad c > 0$$

The Kernel Matrix

The Kernel matrix of D $=\{\mathbf{x_1}...\mathbf{x_n}\}$,

defined by a kernel function $\mathbf{k}(\mathbf{x},\mathbf{z}) = \phi(\mathbf{x})\phi(\mathbf{z})$

is the $\mathbf{n} \times \mathbf{n}$ matrix $\mathbf{K}$, $\mathbf{K_{i,j}} = \mathbf{k}(\mathbf{x_i},\mathbf{x_j})$

The **Gram matrix** of the vectors $\mathbf{x_1}..\ \mathbf{x_n}$

$\mathbf{K}$ is symmetric: $\mathbf{K_{i,j}} = \mathbf{k}(\mathbf{x_i},\mathbf{x_j}) = \phi(\mathbf{x})\phi(\mathbf{z}) = \mathbf{k}(\mathbf{x_j},\mathbf{x_i}) = \mathbf{K_{j,i}}$

$\mathbf{K}$ is positive semi-definite: $(\forall \mathbf{v} : \mathbf{v^T K v} \geq \mathbf{0})$

$$\mathbf{v^T K v} = \sum_{\mathbf{i=0}}^{\mathbf{D}} \sum_{\mathbf{j=0}}^{\mathbf{D}} v_i v_j \mathbf{K_{i,j}} = \sum_{\mathbf{i=0}}^{\mathbf{D}} \sum_{\mathbf{j=0}}^{\mathbf{D}} v_i v_j \langle \phi(\mathbf{x_i})\phi(\mathbf{x_j}) \rangle =$$

$$\sum_{\mathbf{i=0}}^{\mathbf{D}} \sum_{\mathbf{j=0}}^{\mathbf{D}} v_i v_j \sum_{\mathbf{k=1}}^{\mathbf{N}} \phi(\mathbf{x_i})\phi(\mathbf{x_j}) = \sum_{\mathbf{i=0}}^{\mathbf{D}} \sum_{\mathbf{j=0}}^{\mathbf{D}} \sum_{\mathbf{k=1}}^{\mathbf{N}} v_i \phi(\mathbf{x_i})\ v_j \phi(\mathbf{x_j}) =$$

$$\sum_{\mathbf{k=1}}^{\mathbf{N}} \left(\sum_{\mathbf{i=1}}^{\mathbf{D}} v_i \right)^{\mathbf{2}} \geq \mathbf{0}$$

Constructing New Kernels

- You can construct new kernels $k'(\mathbf{x}, \mathbf{x}')$ from existing ones:
  - Multiplying $k(\mathbf{x}, \mathbf{x}')$ by a constant c: $k'(\mathbf{x}, \mathbf{x}') = ck(\mathbf{x}, \mathbf{x}')$
  - Multiplying $k(\mathbf{x}, \mathbf{x}')$ by a function f applied to $\mathbf{x}$ and $\mathbf{x}'$:

    $k'(\mathbf{x}, \mathbf{x}') = f(\mathbf{x})k(\mathbf{x}, \mathbf{x}')f(\mathbf{x}')$
  - Applying a polynomial (w\ non-neg. coeffs.) to $k(\mathbf{x}, \mathbf{x}')$:

    $k'(\mathbf{x}, \mathbf{x}') = P(\ k(\mathbf{x}, \mathbf{x}')\ )$ with $P(z) = \sum_i a_i z^i$ and $a_i \geq \mathbf{0}$
  - Exponentiating $k(\mathbf{x}, \mathbf{x}')$: $k'(\mathbf{x}, \mathbf{x}') = \exp(k(\mathbf{x}, \mathbf{x}'))$

Constructing New Kernels

- You can construct $k'(\mathbf{x}, \mathbf{x'})$ from $k_1(\mathbf{x}, \mathbf{x'})$, $k_2(\mathbf{x}, \mathbf{x'})$:
  - Adding $k_1(\mathbf{x}, \mathbf{x'})$ and $k_2(\mathbf{x}, \mathbf{x'})$: $k'(\mathbf{x}, \mathbf{x'}) = k_1(\mathbf{x}, \mathbf{x'}) + k_2(\mathbf{x}, \mathbf{x'})$
  - Multiplying $k_1(\mathbf{x}, \mathbf{x'})$ and $k_2(\mathbf{x}, \mathbf{x'})$: $k'(\mathbf{x}, \mathbf{x'}) = k_1(\mathbf{x}, \mathbf{x'})k_2(\mathbf{x}, \mathbf{x'})$

  - If $\phi(\mathbf{x}) \in R^m$ and $k_m(\mathbf{z}, \mathbf{z'})$ a valid kernel in R^m, $k(\mathbf{x}, \mathbf{x'}) = k_m(\phi(\mathbf{x}), \phi(\mathbf{x'}))$ is also a valid kernel
  - If $\mathbf{A}$ is a symmetric positive semi-definite matrix, $k(\mathbf{x}, \mathbf{x'}) = \mathbf{x}\mathbf{A}\mathbf{x'}$ is also a valid kernel

Gaussian Kernel (*radial basis function kernel*)

$$k(x, z) = \exp\left(-\frac{||\mathbf{x} - \mathbf{z}||^2}{c}\right)$$

- $||x - z||^2$: squared Euclidean distance between **x** and **z**
- $c = 2\sigma^2$: a free parameter

- Intuition:
  - k(**x**, **z**) ≈ 1 when **x**, **z** close
  - k(**x**, **z**) ≈ 0 when **x**, **z** dissimilar

  - **very small c:** every item is different
  - **very large c**: all items are the same

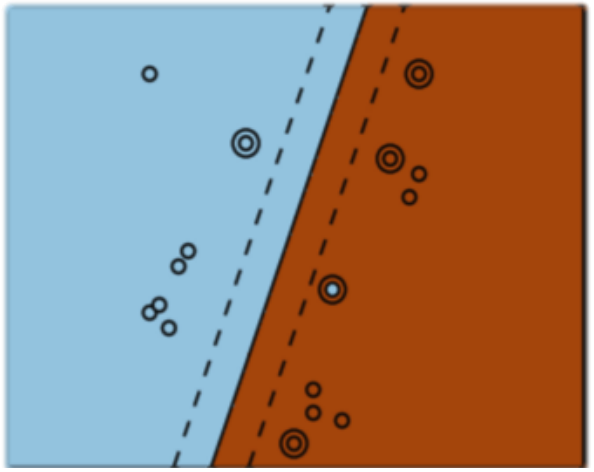
Gaussian Kernel (*radial basis function kernel*)

- k(x, z) = $\exp\left(-\frac{||\mathbf{x}-\mathbf{z}||^2}{c}\right)$ ***Is this a kernel?***

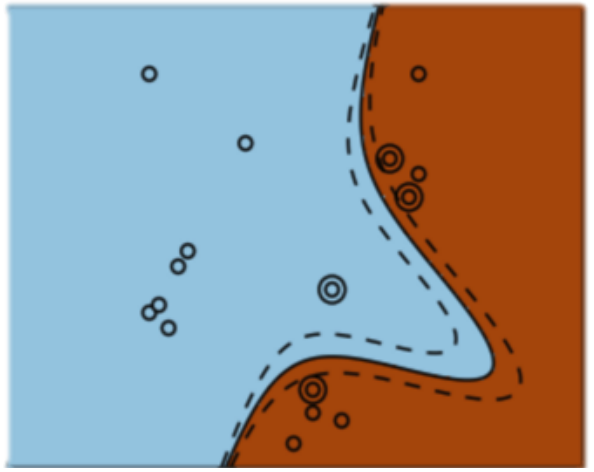
- $k(\mathbf{x}, \mathbf{z}) = \exp(-(\mathbf{x}-\mathbf{z})^2/2\sigma^2)$
  $= \exp(-(\mathbf{xx} + \mathbf{zz} - 2\mathbf{xz})/2\sigma^2)$
  $= \exp(-\mathbf{xx}/2\sigma^2)\ \exp(\mathbf{xz}/\sigma^2)\ \exp(-\mathbf{zz}/2\sigma^2)$
  $= f(\mathbf{x})\ \exp(\mathbf{xz}/\sigma^2)\ f(\mathbf{z})$

- **$\exp(\mathbf{xz}/\sigma^2)$ is a valid kernel:**
  - **xz** is the linear kernel;
  - we can multiply kernels by constants ($1/\sigma^2$)
  - we can exponentiate kernels

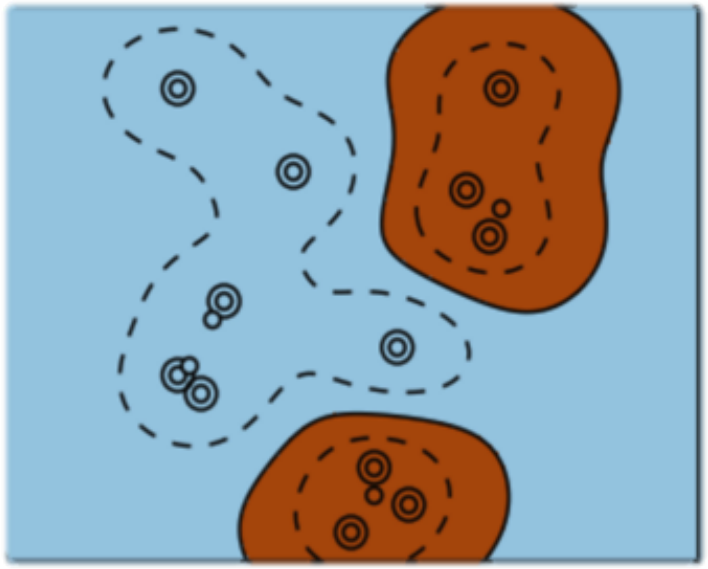
Linear Kernel



Polynomial Kernel



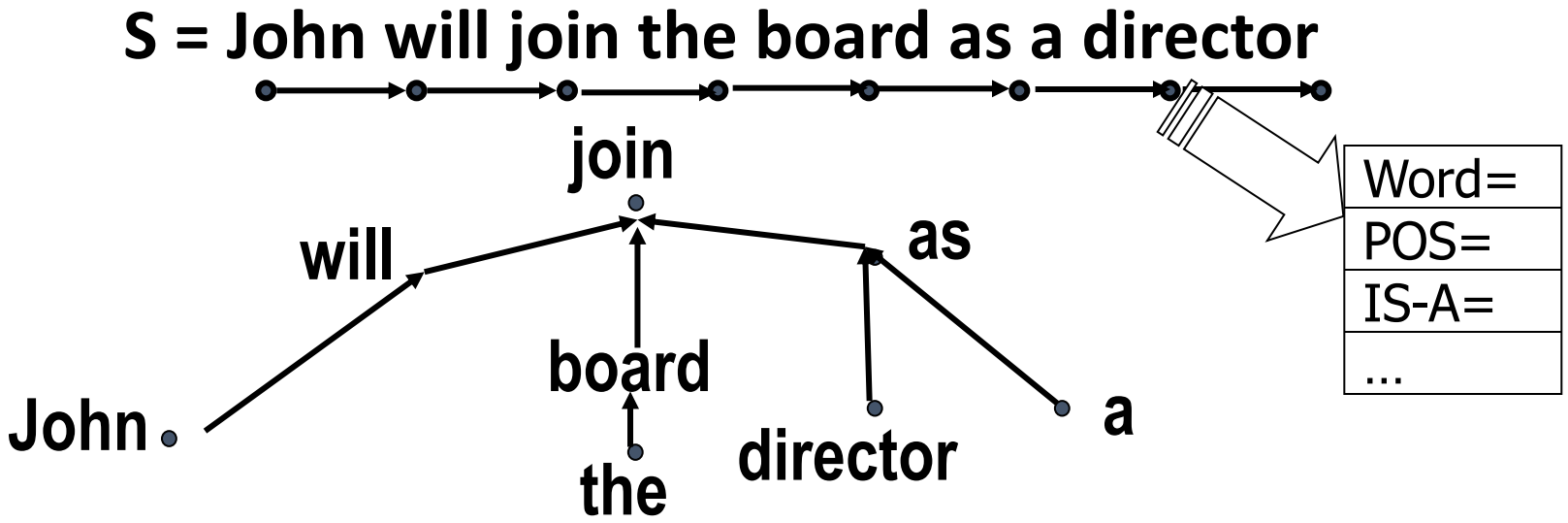
Gaussian (RBF) Kernel



Learning From Structured Input

- Extract features from ***structured domain elements***
  - their internal (hierarchical) structure should be encoded.
- A feature is a mapping from the **instance space** to *{0,1}* or *an integer/real number*
  - It is possible to represent expressive features that constitute an infinite dimensional space
  - ***Learning can be done in the infinite attribute domain.***
- What does it mean to extract features over structured inputs?
  - **Conceptually**: different data instantiations may be abstracted to yield the same representation
  - **Computationally**: graph matching process (graph isomorphism)

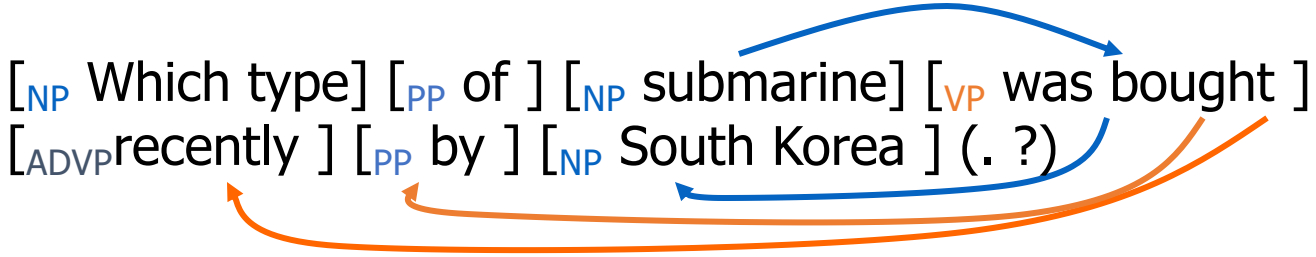
Structured Input



We want to unify the representation for all examples:

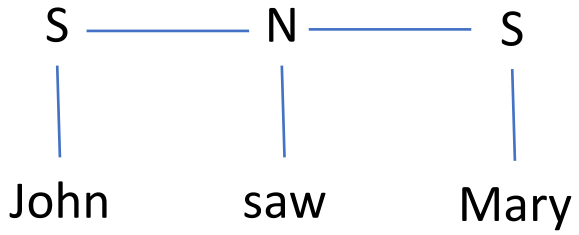
"John will join" , "John joins", "John joined"

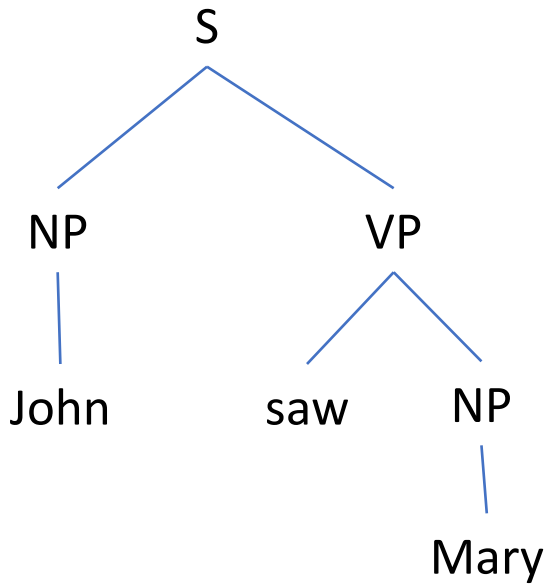
Define patterns (feature functions) that will determine the representation



Extracting features from Input Structures

- Tree structures are useful representations of hierarchical data
  - *NLP*: Syntactic/semantic aspects can be represented using trees
  - Other examples: social networks, protein structures
- **Issue**: how can we capture structural properties?





Extracting features from Input Structures

- Define a feature function Φ mapping input structures into a feature vector
  - Represent interesting ***structural properties***
  - ***Example:*** ***sub-tree counting feature***

$h_1(x)$: *how many times does* 

appear in x*?*

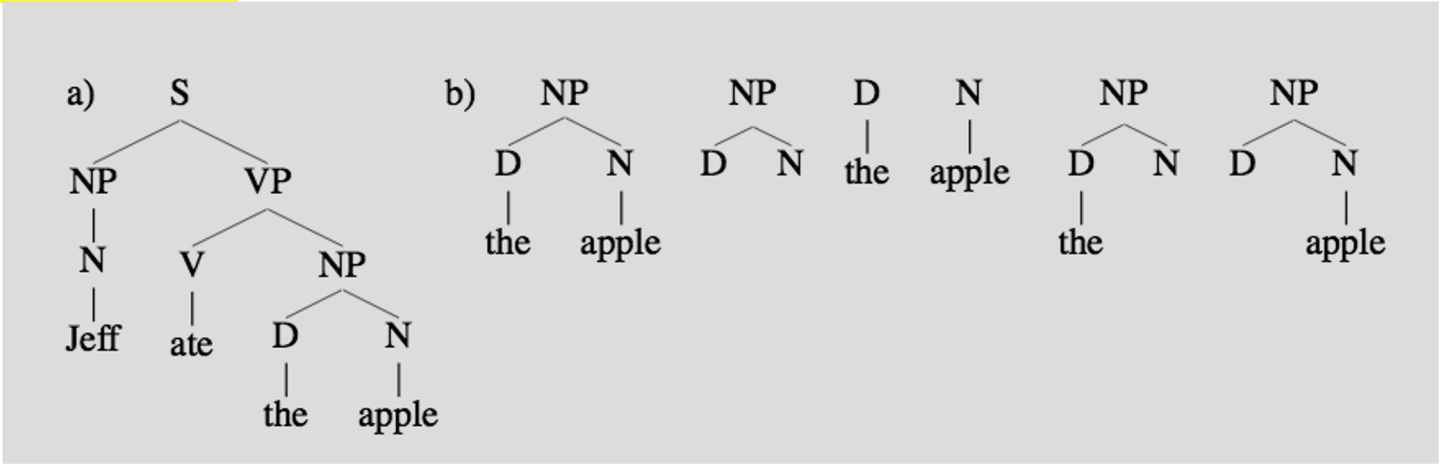
Extracting features from Input Structures

Given a set of Non-Terminal symbols $\{A, B, ..\}$
and Terminal Symbols {a,b,c}

The functions $h_1, ..., h_d$ *define a feature vector*

Each h_i corresponds to a different subtree!

$\Phi(x)=(h_1(x), ..., h_d(x))$



Convolution Kernels for Natural Language. Collins and Duffy. NIPS 2001

Extracting features from Input Structures

$$\Phi(x) = \langle h_1(x), h_2(x), .., h_d(x) \rangle$$

The dot product between two input structures T_1 and T_2

$$\Phi(T_1) \cdot \Phi(T_2) = \sum_{i=1}^{d} h_i(T_1) h_i(T_2)$$

Intuition:

- Two trees are "close" if they share many sub-trees

Dot product can be computed efficiently using dynamic programming

Kernels: Complexity Tradeoff

- It's possible to define kernels for structured data
  - *Equivalent to blowing up the feature space by generating functions of primitive features*
- Is it worth doing in structured domains?
  - *Tree*: not all sub-trees are that important
  - Small matches are more interesting (large trees→ overfits)
  - Increased dimensionality
- **Computationally**: *Dual space* ***vs.*** *Primal Space*
  - Dual space: #examples while the primal: blown up feature space
  - **Consideration**: *the number of examples one needs to use relative to the growth in dimensionality.*

Kernels: Generalization

- ***Do we want to use the most expressive kernels we can?***
  - No; this is equivalent to working in a larger feature space, and will lead to overfitting.
  - You add a lot of irrelevant features
- **In practice, many applications use a linear kernel/work in the primal**
  - Explicitly extend the feature space

Representing Structured Input

- Can determine the success of learning!
  - Necessity in many real world application
    - Social networks
    - Natural Language analysis
    - Planning
    - …
- Key question: *What are the relevant structural attributes?*
  - Define feature functions mapping attributes to features
  - You will have to use these in the **final project**