# Machine Learning for Computational Advertising <br> L3: Linear Models 

Alexander J. Smola

Yahoo! Labs<br>Santa Clara, CA 95051<br>alex@smola.org

UC Santa Cruz, April 2009

## Overview

L1: Machine learning and probability theory
Introduction to pattern recognition, classification, regression, novelty detection, probability theory, Bayes rule, density estimation
L2: Instance based learning
Nearest Neighbor, Kernels density estimation, Watson
Nadaraya estimator, crossvalidation

## L3: Linear models

Hebb's rule, perceptron algorithm, regression, classification, feature maps

## L3 Linear Models

Hebb's rule

- positive feedback
- perceptron convergence rule

Hyperplanes

- Linear separability
- Inseparable sets

Features

- Explicit feature construction
- Implicit features via kernels

Kernels

- Examples
- Kernel perceptron


## Biology and Learning

## Basic Idea

- Good behavior should be rewarded, bad behavior punished (or not rewarded).
This improves the fitness of the system.
- Example: hitting a tiger should be rewarded ...
- Correlated events should be combined.
- Example: Pavlov's salivating dog.


## Training Mechanisms

- Behavioral modification of individuals (learning): Successful behavior is rewarded (e.g. food).
- Hard-coded behavior in the genes (instinct): The wrongly coded animal dies.


## Perceptron



## Perceptrons

## Weighted combination

- Output of the perceptron is a linear combination of the inputs.
- Rescale output (e.g. by sigmoid or threshold function)


## Decision Function

- Results results are combined into

$$
\sigma\left(\sum_{i=1}^{n} w_{i} x_{i}+b\right)=\sigma(\langle w, x\rangle+b)
$$

## Linear Function Classes

## Expansion

$$
f(x)=\langle w, x\rangle+b \text { where } w, x \in \mathbb{R}^{m} \text { and } b \in \mathbb{R} .
$$

## Applications

- Spam filtering (e-mail)
- Echo cancellation (old analog overseas cables)
- Click probability
- Bid value for advanced match
- Machine learning ranking
- Collaborative filtering

Learning
Weights are "plastic" - adapted via the training data.

## Linear Separation



## Perceptron Algorithm

```
argument: \(\quad X:=\left\{x_{1}, \ldots, x_{m}\right\} \subset \mathcal{X}\) (data)
\(Y:=\left\{y_{1}, \ldots, y_{m}\right\} \subset\{ \pm 1\}\) (labels)
function \((w, b)=\operatorname{Perceptron}(X, Y)\)
    initialize \(w, b=0\)
    repeat
        Pick \(\left(x_{i}, y_{i}\right)\) from data
        if \(y_{i}\left(w \cdot x_{i}+b\right) \leq 0\) then
        \(w^{\prime}=w+y_{i} x_{i}\)
        \(b^{\prime}=b+y_{i}\)
    until \(y_{i}\left(w \cdot x_{i}+b\right)>0\) for all \(i\)
end
```


## Interpretation

## Algorithm

- Do nothing if we classify $\left(x_{i}, y_{i}\right)$ correctly
- For incorrectly classified observation update
$(w, b)+=\left(y_{i} x_{i}, y_{i}\right)$.
- Positive reinforcement of observations.


## Solution

- Weight vector is linear combination of observations $x_{i}$ :

$$
w \longleftarrow w+y_{i} x_{i}
$$

- Classification can be written in terms of dot products:

$$
w \cdot x+b=\sum_{j \in E} y_{j} x_{j} \cdot x+b
$$

## Theoretical Analysis

Incremental Algorithm
Already while the perceptron is learning, we can use it.
Convergence Theorem (Rosenblatt and Novikoff)
Suppose that there exists a $\rho>0$, a weight vector $w^{*}$ satisfying $\left\|w^{*}\right\|=1$, and a threshold $b^{*}$ such that

$$
y_{i}\left(\left\langle w^{*}, x_{i}\right\rangle+b^{*}\right) \geq \rho \text { for all } 1 \leq i \leq m .
$$

Then the hypothesis maintained by the perceptron algorithm converges to a linear separator after no more than

$$
\frac{\left(b^{* 2}+1\right)\left(R^{2}+1\right)}{\rho^{2}}
$$

updates, where $R=\max _{i}\left\|x_{i}\right\|$.

## Proof, Part I

## Starting Point

We start from $w_{1}=0$ and $b_{1}=0$.

## Step 1: Bound on the increase of alignment

Denote by $w_{i}$ the value of $w$ at step $i$ (analogously $b_{i}$ ).

$$
\text { Alignment: }\left\langle\left(w_{i}, b_{i}\right),\left(w^{*}, b^{*}\right)\right\rangle
$$

For error in observation $\left(x_{i}, y_{i}\right)$ we get

$$
\begin{aligned}
& \left\langle\left(w_{j+1}, b_{j+1}\right) \cdot\left(w^{*}, b^{*}\right)\right\rangle \\
& =\left\langle\left[\left(w_{j}, b_{j}\right)+y_{i}\left(x_{i}, 1\right)\right],\left(w^{*}, b^{*}\right)\right\rangle \\
& =\left\langle\left\langle\left(w_{j}, b_{j}\right),\left(w^{*}, b^{*}\right)\right\rangle+y_{i}\left(\left(x_{i}, 1\right) \cdot\left(w^{*}, b^{*}\right)\right\rangle\right. \\
& \geq\left\langle\left(w_{j}, b_{j}\right),\left(w^{*}, b^{*}\right)\right\rangle+\rho \\
& \geq j \rho .
\end{aligned}
$$

Alignment increases with number of errors.

## Proof, Part II

Step 2: Cauchy-Schwartz for the Dot Product

$$
\begin{aligned}
\left\langle\left(w_{j+1}, b_{j+1}\right) \cdot\left(w^{*}, b^{*}\right)\right\rangle & \leq\left\|\left(w_{j+1}, b_{j+1}\right)\right\|\left\|\left(w^{*}, b^{*}\right)\right\| \\
& =\sqrt{1+\left(b^{*}\right)^{2}}\left\|\left(w_{j+1}, b_{j+1}\right)\right\|
\end{aligned}
$$

Step 3: Upper Bound on $\left\|\left(w_{j}, b_{j}\right)\right\|$
If we make a mistake we have

$$
\begin{aligned}
\left\|\left(w_{j+1}, b_{j+1}\right)\right\|^{2} & =\left\|\left(w_{j}, b_{j}\right)+y_{i}\left(x_{i}, 1\right)\right\|^{2} \\
& =\left\|\left(w_{j}, b_{j}\right)\right\|^{2}+2 y_{i}\left\langle\left(x_{i}, 1\right),\left(w_{j}, b_{j}\right)\right\rangle+\left\|\left(x_{i}, 1\right)\right\|^{2} \\
& \leq\left\|\left(w_{j}, b_{j}\right)\right\|^{2}+\left\|\left(x_{i}, 1\right)\right\|^{2} \\
& \leq j\left(R^{2}+1\right) .
\end{aligned}
$$

Step 4: Combination of first three steps

$$
j \rho \leq \sqrt{1+\left(b^{*}\right)^{2}}\left\|\left(w_{j+1}, b_{j+1}\right)\right\| \leq \sqrt{j\left(R^{2}+1\right)\left(\left(b^{*}\right)^{2}+1\right)}
$$

Solving for $j$ proves the theorem.

## Solutions of the Perceptron



## Interpretation

## Learning Algorithm

We perform an update only if we make a mistake.
Convergence Bound

- Bounds the maximum number of mistakes in total. We will make at most $\left(b^{* 2}+1\right)\left(R^{1}+1\right) / \rho^{2}$ mistakes in the case where a "correct" solution $w^{*}, b^{*}$ exists.
- This also bounds the expected error (if we know $\rho, R$, and $\left.\left|b^{*}\right|\right)$.
Dimension Independent
Bound does not depend on the dimensionality of $X$.


## Sample Expansion

We obtain $w$ as a linear combination of $x_{i}$.

## Mini Summary

## Perceptron

- Separating halfspaces
- Perceptron algorithm
- Convergence theorem
- Only depends on margin, dimension independent

Pseudocode

$$
\begin{aligned}
& \text { for i in range }(m): \\
& \text { ytest }=\text { numpy. } \operatorname{dot}(w, x[:, i])+b \\
& \text { if ytest } * y[i]<=0: \\
& w+=y[i] * x[: i] \\
& b+=y[i]
\end{aligned}
$$

## Nonlinearity via Preprocessing

## Problem

Linear functions are often too simple to provide good estimators.

Idea

- Map to a higher dimensional feature space via $\Phi: x \rightarrow \Phi(x)$ and solve the problem there.
- Replace every $\left\langle x, x^{\prime}\right\rangle$ by $\left\langle\Phi(x), \Phi\left(x^{\prime}\right)\right\rangle$ in the perceptron algorithm.


## Consequence

- We have nonlinear classifiers.
- Solution lies in the choice of features $\Phi(x)$.


## Nonlinearity via Preprocessing



Features
Quadratic features correspond to circles, hyperbolas and ellipsoids as separating surfaces.

## Constructing Features

Idea
Construct features manually. E.g. for OCR we could use

|  | I | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 0 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Loops | 0 | 0 | 0 | 1 | 0 | 1 | 0 | 2 | 1 | 1 |
| 3 Joints | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 1 | 0 |
| 4 Joints | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 0 |
| Angles | 0 | 1 | 1 | 1 | 1 | 0 | 1 | 0 | 0 | 0 |
| Ink | 1 | 2 | 2 | 2 | 2 | 2 | 1 | 3 | 2 | 2 |

## More Examples

## Two Interlocking Spirals

If we transform the data $\left(x_{1}, x_{2}\right)$ into a radial part
( $r=\sqrt{x_{1}^{2}+x_{2}^{2}}$ ) and an angular part ( $x_{1}=r \cos \phi$,
$x_{1}=r \sin \phi$ ), the problem becomes much easier to solve (we only have to distinguish different stripes).
Japanese Character Recognition
Break down the images into strokes and recognize it from the latter (there's a predefined order of them).
Medical Diagnosis
Include physician's comments, knowledge about unhealthy combinations, features in EEG, ...
Suitable Rescaling
If we observe, say the weight and the height of a person, rescale to zero mean and unit variance.

## Perceptron on Features

argument: $X:=\left\{x_{1}, \ldots, x_{m}\right\} \subset \mathcal{X}$ (data)

$$
Y:=\left\{y_{1}, \ldots, y_{m}\right\} \subset\{ \pm 1\} \text { (labels) }
$$

function $(w, b)=\operatorname{Perceptron}(X, Y, \eta)$ initialize $w, b=0$ repeat

Pick ( $x_{i}, y_{i}$ ) from data

$$
\begin{aligned}
& \text { if } \begin{aligned}
& y_{i}\left(w \cdot \Phi\left(x_{i}\right)+b\right) \leq 0 \text { then } \\
& w^{\prime}=w+y_{i} \Phi\left(x_{i}\right) \\
& b^{\prime}=b+y_{i}
\end{aligned}
\end{aligned}
$$

until $y_{i}\left(w \cdot \Phi\left(x_{i}\right)+b\right)>0$ for all $i$
end
Important detail

$$
w=\sum_{j} y_{j} \Phi\left(x_{j}\right) \text { and hence } f(x)=\sum_{j} y_{j}\left(\Phi\left(x_{j}\right) \cdot \Phi(x)\right)+b
$$

## Problems with Constructing Features

## Problems

- Need to be an expert in the domain (e.g. OCR).
- Features may not be robust (e.g. postman drops letter).
- Can be expensive to compute.


## Solution

- Use shotgun approach.
- Compute many features and hope ...
- Do this efficiently.


## Polynomial Features

Quadratic Features in $\mathbb{R}^{2}$

$$
\Phi(x):=\left(x_{1}^{2}, \sqrt{2} x_{1} x_{2}, x_{2}^{2}\right)
$$

## Dot Product

$$
\begin{aligned}
\left\langle\Phi(x), \Phi\left(x^{\prime}\right)\right\rangle & =\left\langle\left(x_{1}^{2}, \sqrt{2} x_{1} x_{2}, x_{2}^{2}\right),\left(x_{1}^{\prime 2}, \sqrt{2} x_{1}^{\prime} x_{2}^{\prime}, x_{2}^{\prime 2}\right)\right\rangle \\
& =\left\langle x, x^{\prime}\right\rangle^{2} .
\end{aligned}
$$

## Insight

Trick works for any polynomials of order $d$ via $\left\langle x, x^{\prime}\right\rangle^{d}$.



## Kernels

## Problem

- Extracting features can sometimes be very costly.
- Example: second order features in 1000 dimensions. This leads to 5005 numbers. For higher order polynomial features much worse.


## Solution

Don't compute the features, try to compute dot products implicitly. For some features this works ...
Definition
A kernel function $k: X \times X \rightarrow \mathbb{R}$ is a symmetric function in its arguments for which the following property holds

$$
k\left(x, x^{\prime}\right)=\left\langle\Phi(x), \Phi\left(x^{\prime}\right)\right\rangle \text { for some feature map } \Phi .
$$

If $k\left(x, x^{\prime}\right)$ is much cheaper to compute than $\Phi(x) \ldots$

## Polynomial Kernels in $\mathbb{R}^{n}$

## Idea

- We want to extend $k\left(x, x^{\prime}\right)=\left\langle x, x^{\prime}\right\rangle^{2}$ to

$$
k\left(x, x^{\prime}\right)=\left(\left\langle x, x^{\prime}\right\rangle+c\right)^{d} \text { where } c \geq 0 \text { and } d \in \mathbb{N} .
$$

- Prove that such a kernel corresponds to a dot product.


## Proof strategy

Simple and straightforward: compute the explicit sum given by the kernel, i.e.

$$
k\left(x, x^{\prime}\right)=\left(\left\langle x, x^{\prime}\right\rangle+c\right)^{d}=\sum_{i=0}^{m}\binom{d}{i}\left(\left\langle x, x^{\prime}\right\rangle\right)^{i} c^{d-i}
$$

Individual terms $\left(\left\langle x, x^{\prime}\right\rangle\right)^{i}$ are dot products for some $\Phi_{i}(x)$

## Kernel Perceptron

argument: $X:=\left\{x_{1}, \ldots, x_{m}\right\} \subset \mathcal{X}$ (data)

$$
Y:=\left\{y_{1}, \ldots, y_{m}\right\} \subset\{ \pm 1\} \text { (labels) }
$$

function $f=\operatorname{Perceptron}(X, Y, \eta)$
initialize $f=0$
repeat
Pick $\left(x_{i}, y_{i}\right)$ from data
if $y_{i} f\left(x_{i}\right) \leq 0$ then

$$
f(\cdot) \leftarrow f(\cdot)+y_{i} k\left(x_{i}, \cdot\right)+y_{i}
$$

until $y_{i} f\left(x_{i}\right)>0$ for all $i$
end

Important detail

$$
w=\sum_{j} y_{j} \Phi\left(x_{j}\right) \text { and hence } f(x)=\sum_{j} y_{j} k\left(x_{j}, x\right)+b
$$

## Are all $k\left(x, x^{\prime}\right)$ good Kernels?

## Computability

We have to be able to compute $k\left(x, x^{\prime}\right)$ efficiently (much cheaper than dot products themselves).
"Nice and Useful" Functions
The features themselves have to be useful for the learning problem at hand. Quite often this means smooth functions.
Symmetry
Obviously $k\left(x, x^{\prime}\right)=k\left(x^{\prime}, x\right)$ due to the symmetry of the dot product $\left\langle\Phi(x), \Phi\left(x^{\prime}\right)\right\rangle=\left\langle\Phi\left(x^{\prime}\right), \Phi(x)\right\rangle$.
Dot Product in Feature Space
Is there always a $\phi$ such that $k$ really is a dot product?
Mercer's theorem
$k$ needs to correspond to a positive integral operator ...

## Some Good Kernels

Examples of kernels $k\left(x, x^{\prime}\right)$

Linear<br>Laplacian RBF<br>Gaussian RBF<br>Polynomial<br>B-Spline<br>Cond. Expectation

$$
\begin{aligned}
& \left\langle x, x^{\prime}\right\rangle \\
& \exp \left(-\lambda\left\|x-x^{\prime}\right\|\right) \\
& \exp \left(-\lambda\left\|x-x^{\prime}\right\|^{2}\right) \\
& \left.\left(\left\langle x, x^{\prime}\right\rangle+c\right\rangle\right)^{d}, c \geq 0, d \in \mathbb{N} \\
& B_{2 n+1}\left(x-x^{\prime}\right) \\
& \mathbf{E}_{c}\left[p(x \mid c) p\left(x^{\prime} \mid c\right)\right]
\end{aligned}
$$

Simple trick for checking Mercer's condition
Compute the Fourier transform of the kernel and check that it is nonnegative.

## Linear Kernel



## Laplacian Kernel



## Gaussian Kernel



## Polynomial (Order 3)



## $B_{3}$-Spline Kernel



## Mini Summary

## Features

- Prior knowledge, expert knowledge
- Shotgun approach (polynomial features)
- Kernel trick $k\left(x, x^{\prime}\right)=\left\langle\phi(x), \phi\left(x^{\prime}\right)\right\rangle$
- Mercer's theorem


## Applications

- Kernel Perceptron
- Nonlinear algorithm automatically by query-replace

Examples of Kernels

- Gaussian RBF
- Polynomial kernels


## Risk Minimization

## General Problem

Find $f(x)=\langle w, x\rangle+b$ such that loss $I(y, f(x))$ is minimized. Learning as optimization

Minimize the average risk on training set via

$$
\underset{(w, b)}{\operatorname{minimize}} \sum_{i=1}^{m} l\left(y_{i},\left\langle w, x_{i}\right\rangle+b\right)+\frac{\lambda}{2}\|w\|^{2}
$$

Here $\frac{\lambda}{2}\|w\|^{2}$ is a regularizer penalizing how steep the function $f$ is.

## Applications

Regression - Least Mean Squares

- Bid estimation: $y$ is bid, $x=$ (keyword, query)
- Collaborative filtering: $y$ is rating, $x=$ (product, user)

$$
I(y, f(x))=\frac{1}{2}(y-f(x))^{2}
$$

Classification - Logistic Regression

- Click probability estimation: $y$ is click/no click, $x$ is ad
- Spam filtering: $y$ is spam/no spam, $x$ is webpage

$$
I(y, f(x))=-\log p(y \mid x)=\log \left(1+e^{-y f(x)}\right)
$$

equivalently $p(y \mid x)=\frac{1}{1+e^{-y f(x)}}$

## Applications

Classification - Hinge loss

$$
I(y, f(x))=\max (0,-y f(x))
$$

This will give us the Perceptron algorithm
Classification - Soft margin loss

$$
I(y, f(x))=\max (0,1-y f(x))
$$

This will give us the Support Vector Machines loss. We want to ensure that we classify with confidence: loss only vanishes if $y f(x) \geq 1$.
Regression - Absolute Value Loss
Want to penalize absolute deviation from observation

$$
I(y, f(x))=|y-f(x)|
$$

## Stochastic Gradient Descent

$$
\begin{array}{ll}
\text { argument: } & X:=\left\{x_{1}, \ldots, x_{m}\right\} \subset \mathcal{X} \text { (data) } \\
& Y:=\left\{y_{1}, \ldots, y_{m}\right\} \subset \mathcal{y} \text { (labels) }
\end{array}
$$

function $(w, b)=$ StochasticGradientDescent $(X, Y)$ initialize $w, b=0$
initialize counter $n=n_{0}$, scale $\eta_{0}$ repeat

Pick $(x, y)$ from data
Compute prediction $f\left(x_{i}\right)$
Compute learning rate $\eta=\frac{\eta_{0}}{\sqrt{n}}$

$$
(w, b)=(1-\lambda \eta)(w, b)-\eta(x, 1) \cdot \partial_{f(x)} I\left(y, f\left(x_{i}\right)\right)
$$

Increment $n=n+1$
until all data read
end

## Key Theorem

## Convergence

Under general conditions stochastic gradient descent converges at rate $O\left(n^{-\frac{1}{2}}\right)$ to the optimal solution.
Practical hack
Set regularization $\lambda=0$ if we have lots of data.

## Summary

Hebb's rule

- positive feedback
- perceptron convergence rule, kernel perceptron


## Features

- Explicit feature construction
- Implicit features via kernels

Kernels

- Examples
- Mercer's theorem

Risk Minimization

- Stochastic gradient descent algorithm
- Simple to implement
- Fast convergence

