CMSC 678 Statistical Learning & Fuzzy Logic Algorithms

Intro to

Machine Learning

Basic Ideas, Problems, Examples and Approaches

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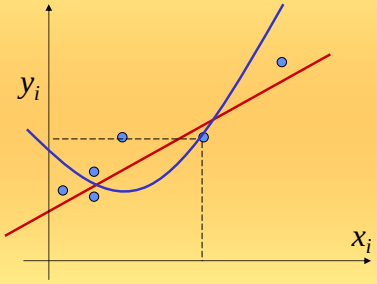
Motivations for these lectures

- There is no part of human activities left untouched by both the need for and the desire to collect **data** today
- The consequences are - we are **surrounded by**, in fact, we are **immersed in an ocean of all kinds of data** (a.k.a. measurements, images, patterns, sounds, samples, web pages, tunes, x-rays or ct images, etc.)
- **Humans can't handle ultra-large data** sets but,
- we must **develop algorithms able to learn from such datasets** and to mine them efficiently

What is the Learning from Data, or Data Mining, about?

- The Math in the last 2,000 years was playing with such models:
- $A = \pi r^2 = w_1 r^2$, $v = \text{sqrt}(2gh) = w_1 \text{sqrt}(h)$,
- $y = 3x - 2 = w_1 x + w_2$, $z = -x + y - 3 = w_1 x + w_2 y + w_3$ Parameters w_i **of the relations are known**, and given the independent variable(s) the task is to find the dependent one(s)!
- **TODAY; we want to learn from the pairs (x_i, y_i) of the measured data sets, in order to infere i.e., learn the UNKNOWN parameter values w_i .**
- **This is an INVERSE PROBLEM stated as:**
- **having the pairs (x_i, y_i) find the parameters w_i, of the model. In other words, LEARN the dependency between the x_i and y_i!**

or, the problems to solve are a kind of this one: having the data points find weights (parameters) which define a function assumed (here linear and quadratic ones are assumed)



In a real life, examples are same in character but much larger in DIMENSIONS!!!

Contents

Examples of Applications in Diverse Fields, Comparisons with classic approximation and NN, Basics of a Bias–Variance Dilemma, Learning from sparse data, Distribution-free learning

Support Vector Machines - a QP based learning

Linear Maximal Hard Margin Classifier, Linear Soft Margin Classifier for Overlapping Classes

The Nonlinear Classifier – Kernels and 'NN' representation, Regression by SVMs

The talk today will be on how one learns from experimental data.

WHY?

Because we live in an information age? - Possibly!
Because we live in a knowledge society? - Possibly YES!

Because we live surrounded by an **OCEAN OF 'DATA'?**
YES, FOR SURE!

And, I mean **ALL** possible '**data**' because, we and our devices are surrounded by all imaginable **measurements**, **images**, **sounds**, **smells**, **records**, etc.

We want - to produce data, to transfer it, to compress it, to use it, to process it, to reuse it, to filter it, etc .

But primarily, we want to LEARN FROM DATA, a.k.a., examples, samples, measurements, records, observations, patterns

CLASSIC applications:

- increase in sleep depending on the drug,
- pulmonary function modeling by measuring oxygen consumption,
- head length and breadths of brothers,
- classification of the Brahmin, Artisan and Korwa caste based on physical measurements,
- biting flies (genus: *Leptoconops*) data for classification of the two species of flies,
- battery-failure data dependency and regression,
- various financial and market analysis (bankruptcy, stock market prediction, bonds, goods transportation cost data, production cost data, etc.),
- study of love and marriage regarding the relationships and feelings of couples,
- air pollution data classification, college test score classification and prediction, crude oil consumption modeling, closeness between 11 different languages, and so on.

(all of the above were **linear** models, taken from 20 years old statistics books)

TODAYS (primarily **NON-linear**) applications:

Note the following strong fact -> there is no field of human activities today, left untouched by learning from data!!!

Statistical learning is very, very hot nowdays - find patterns, identify, control, make prediction, make decisions, develop models, search, filter, compress, …, and some <u>today's applications are:</u>

- **computer graphics, animations,**
- **image analysis & compression, face detection, face recognition,**
- **text categorization, media news classification, multimedia (sound video) analysis**
- **bioinformatics - gene analysis, disease's study**
- **time series identification - financial, meteorological, hydro,**
- **biomedicine signals, all possible engineering signal processing**
- **predictions - sales, TV audience share, investments needed, ..etc**

Few more examples:

- Banks: Fraud checks detection
- Google, Microsoft et al: Targeted advertising
- Supermarkets: Promotion planning
- Call centers: Speech recognition
- Scanners: Optical character recognition
- Web pages classification, Text categorization
- Post office: Zipcode handwriting recognition
- Credit cards: Loan default prediction
- Stock market: Statistical arbitrage
- Drug design: Drug candidate screening
- Large Hadron Collider: Particle screening
- Airport scanner: Explosives, Drugs, Arm, Faces

On the basic notations in this class:

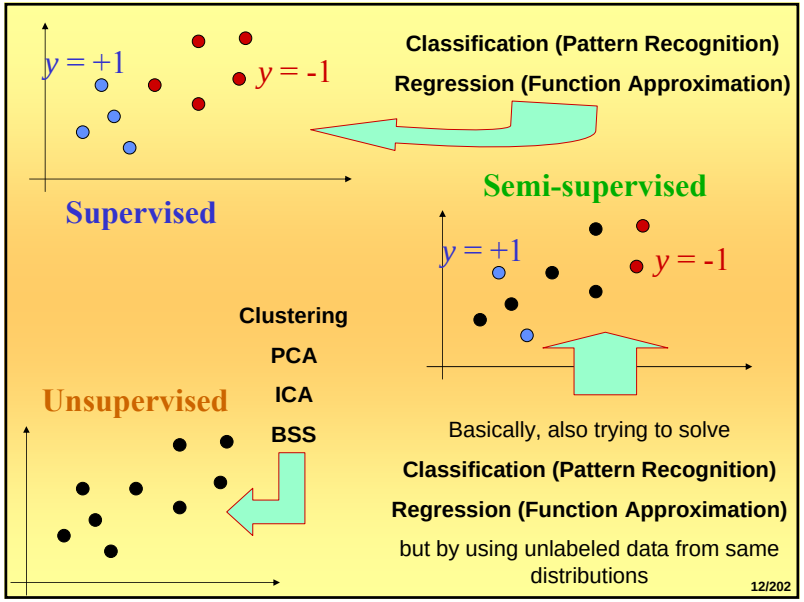
- Unless clear from the context, or defined otherwise, the following applies:
- *scalars* are low-case italics – $w, y, a, b, \ldots$
- **vectors** are low-case bold – $\mathbf{x}, \mathbf{y}, \mathbf{w}, \ldots$
- **MATRICES** are capitals bold – $\mathbf{X}, \mathbf{A}, \mathbf{G}, \ldots$

- **Vectors** are always column vectors say $\mathbf{x}(n, 1)$. Hence, $\mathbf{x}' = \mathbf{x}^T$ is an $(1, n)$ vector

Let's first set the stage, there are three (3) machine learning (ML) settings

- Supervised (pairs x_i, y_i are given for **all** data pairs, where x_i are the values of the independent variables, features, inputs, attributes and y_i are class labels)
- Semi-supervised (pairs x_i, y_i are given for **just a fraction** of data pairs)
- Unsupervised (only inputs x_i, are given and no single label y_i is known)

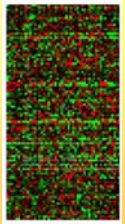
Here, we deal only with **SUPERVISED** ML problems!

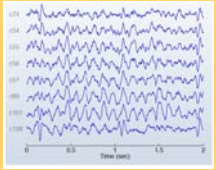


Data sets variety

X and **Y**, or **X** only

	Legs	Wings	Fur	Feathers
cat	4	no	yes	no
crow	2	yes	no	yes
frog	4	no	no	no
bat	4	yes	yes	no
barstool	3	no	no	no

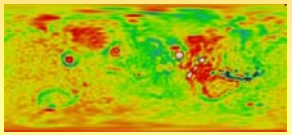




Play golf dataset

Independent variables				Dep. var
OUTLOOK	TEMPERATURE	HUMIDITY	WINDY	PLAY
sunny	85	85	FALSE	Don't Play
sunny	80	90	TRUE	Don't Play
overcast	83	78	FALSE	Play
rain	70	96	FALSE	Play
rain	68	80	FALSE	Play
rain	65	70	TRUE	Don't Play
overcast	64	65	TRUE	Play
sunny	72	95	FALSE	Don't Play
sunny	69	70	FALSE	Play
rain	75	80	FALSE	Play
sunny	75	70	TRUE	Play
overcast	72	90	TRUE	Play
overcast	81	75	FALSE	Play
rain	71	80	TRUE	Don't Play

1	-0.66242	-0.03596
2	101.07	100.04
2	100.28	99.692
2	102.26	99.244
2	100.27	99.729
1	-1.2924	0.31328
1	1.4643	0.63647
2	100.24	99.294



Mars magnetic field

Hence, our data is given as:

1st data pair

$$\mathbf{X}=\begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1n} \\ x_{21} & x_{21} & \cdots & x_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ x_{l1} & x_{l2} & \cdots & x_{ln} \end{bmatrix}, \quad \mathbf{Y}_{Class}=\begin{bmatrix} +1 \\ -1 \\ \vdots \\ -1 \end{bmatrix}, \text{ or } \quad \mathbf{Y}_{Regress}=\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_l \end{bmatrix}$$

l^{st} data pair

First, let's clarify basic similarities and differences between ML (represented by NN&SVMs) and Fuzzy Logic!

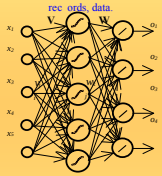
NN (SVM) AND FL MODELING

NNs stand for SVMs here too

Neural Networks

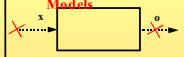
Black-Box

No previous knowledge, but there are measurements, observations, rec ords, data.



Behind NN stands the idea of **learning** from the data.

Fuzzy Logic Models



White-Box

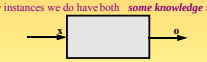
Structured knowledge (*experience, expertise or heuristics*). **IF - THEN** rules are the most typical ex amples of the structured knowledge.

Example: Controlling the distance between two cars.

R1 : IF the speed is *low* AND the distance is *small* THEN the force on brake should be *small*
R2 : IF the speed is *medium* AND the di s tance is *small* THEN the force on brake should be *big*
R3 : IF the speed is *high* AND the distance is *small* THEN the force on brake should be *very big*

Behind FLM stands the idea of **embedding hu man knowledge** into workable alg o rithms.

At many instances we do have both ***some knowledge*** and ***some data.***



This is the most common **gray box** situation covered by the paradigm of **Neuro-Fuzzy** *or* **Fuzzy-Neuro** models.
If we do not have any prior knowledge AND we do not have any measurements (*by all accounts very hopeless situation indeed)* it may be hard to expect or believe that the problem at hand may be approached and solved easily. This is a **no-color box** situa tion.

Machine Learning is concerned by solving two (out of three) classic statistics problems:

Classification (Pattern Recognition)

Regression (Curve, Surface, Fitting, i.e., Function Approximation)

one more statistics' problem, we will not be playing with in this course, is the **Density Estimation Problem**

Classification (Pattern Recognition)

- Classification (Pattern Recognition) setting is as follows – **(see also my Chap 1)**

You want your model, i.e., function implemented in software, i.e., NN, i.e., Decision Function, i.e., SVM

to be trained on training data sets comprised of the training pairs ($\mathbf{x}_i$, y_i), and

to be used on the new, previously unseen inputs $\mathbf{x}_i$, in order to recognize it i.e., classify it.

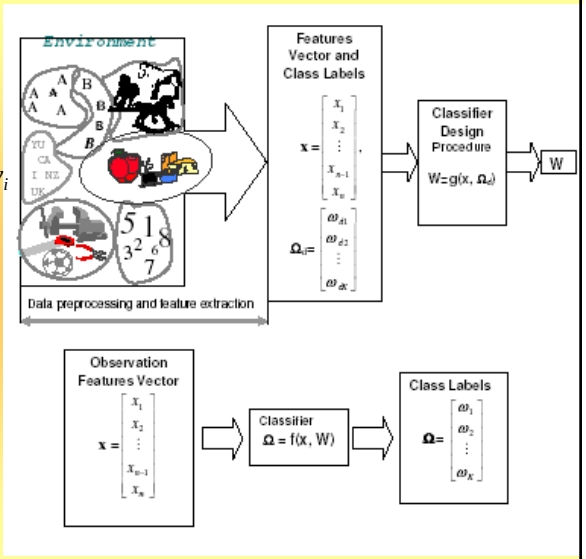
$\mathbf{x}_i$ is called an input vector of features, or just the feature vector

y_i is called the output, i.e., desired or target value, or just label

Training Phase:

$\mathbf{w} = f(\mathbf{x}, \mathbf{y})$

class label $\omega_i = y_i$



Test Phase:

$\omega_i = g(\mathbf{x}_i, \mathbf{w})$

Just one simple example: **LINEAR CLASSIFIER**

- We are designing **linear** classifier by using **sum-of-error-squares** cost (merit, loss, fitness) function (norm). i.e. we work under L_2-*norm*
- A problem is 1-dimensional for visualization's purposes only
- All math is same for any-dimensional input vector **x**
- Notation: **x** is an ***m****-dimensional* sample or a measurement, **X**(*n, m*) is an input data matrix having *n* **x**-es as rows, **y** or **Y**, i.e., **D** is a label vector with + or -1 as a label. **Y=D**, and **D** stands for **d**esired output value, called the label in the classification.

See also my The MIT Press book, Chapter 3, Section 3.2,

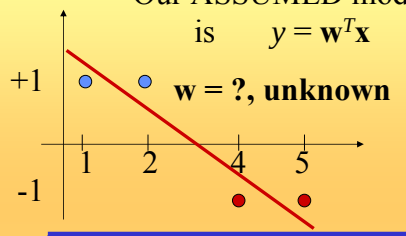
Let's solve an 1-dimensional problem, *m* = 1

Training pairs (x_i, y_i) are given:

$\mathbf{x}$=[1 2 4 5]', $\mathbf{y}$=[1 1 -1 -1]'

We are after decision function. Assume linear one -> then we are after **weights** (intercept and slope)

Our ASSUMED model is $y = \mathbf{w}^T\mathbf{x}$



w = ?, unknown

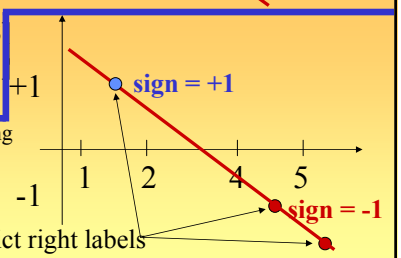
$$\mathbf{X} = \begin{bmatrix} 1 & 1 \\ 2 & 1 \\ 4 & 1 \\ 5 & 1 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 1 \\ 1 \\ -1 \\ -1 \end{bmatrix}, \quad \mathbf{w} = \mathbf{X}^*\mathbf{y}, \quad \mathbf{w} = \begin{bmatrix} -0.6 \\ 1.8 \end{bmatrix}$$

After, the training we can discard the training data and given new (test, application) data

$y_{itest} = \mathbf{w}^t\, \mathbf{x}_{ites}$, say for

$\mathbf{x}$=[1.5 4.5 5.5], our model will predict right labels

$\mathbf{y}$ = sign([0.9 -0.9 -1.5]^T)



How the solutions has actually been obtained?

What's $\mathbf{X}^*$??

Well, it is an old good math technique for solving both **over-** and **under-determined** systems. However, be extremely cautious – solutions for the two different cases have entirely different meanings!

Classical Linear Regression (i.e., Classification)

n = number of data, *m* = number of features, attributes, inputs, ***x = input, y = output***

$$\mathbf{X}_{nm}\mathbf{w}_{m1} = \mathbf{y}_{n1} \qquad /*_{left}\ \mathbf{X}^T_{mn}$$

$$\mathbf{X}^T_{mn}\mathbf{X}_{nm}\mathbf{w}_{m1} = \mathbf{X}^T_{mn}\mathbf{y}_{n1}$$

$$\boxed{\left(\mathbf{X}^T_{mn}\mathbf{X}_{nm}\right)\mathbf{w}_{m1} = \mathbf{X}^T_{mn}\mathbf{y}_{n1}}$$

NORMAL SYSTEM

$$\left(\mathbf{X}^T_{mn}\mathbf{X}_{nm}\right)^{-1}\left(\mathbf{X}^T_{mn}\mathbf{X}_{nm}\right)\mathbf{w}_{m1} = \left(\mathbf{X}^T_{mn}\mathbf{X}_{nm}\right)^{-1}\mathbf{X}^T_{mn}\mathbf{y}_{n1}$$

$$\mathbf{w}_{m1} = \boxed{\left(\mathbf{X}^T_{mn}\mathbf{X}_{nm}\right)^{-1}\mathbf{X}^T_{mn}}\mathbf{y}_{n1}$$

Pseudoinverse X*

At this point, the TRAINING is OVER. You are DONE, and you can use your model!!!

$$\hat{\mathbf{y}}_{test,1} = \mathbf{X}_{test,m}\mathbf{w}_{m1}$$

Application or usage of your Model. Given any NEW (or OLD) data points, predict the output

It looks simple, but it is a very tricky story about the meaning of the solution depending on whether *n* > *m, or n* < *m*

Usually, *n* > *m* - **overdetermined** system and if *n* < *m* - **underdetermined** system

The differences in a meaning of the solution **w** in two cases?

See my book, pages 225, 226 and so on for the **overdetermined case**

In the case of an **overdetermined** system **w** results in a solution providing the **minimal sum of errors squares**,

and you should look up into the meaning of the solution **w** in the case of an **underdetermined** system

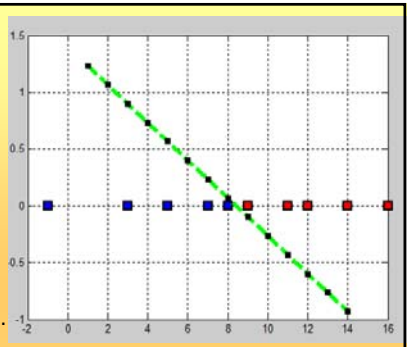
Matlab code for previous example

```
x1=[-1;3;5;7;8;9;11;12;14;16];
i1=ones(10,1);
x=[x1 i1]
d=[1 1 1 1 1 -1 -1 -1 -1 -1]
d=d'

w=pinv(x)*d
plot(x1(1:5),zeros(size(x1)/2,1),'bs',...
                'LineWidth',2,...
                 'MarkerEdgeColor','k',...
                 'MarkerFaceColor','b',...
                 'MarkerSize',10)
hold on
plot(x1(6:10),zeros(size(x1)/2,1),'rs',...
                'LineWidth',2,...
                 'MarkerEdgeColor','k',...
                 'MarkerFaceColor','r',...
                 'MarkerSize',10)


i2=1:1:14;
plot((w(1)*i2+w(2)),'--gs','LineWidth',4,...
                 'MarkerEdgeColor','k',...
                 'MarkerFaceColor','y',...
                 'MarkerSize',2)

grid on
```



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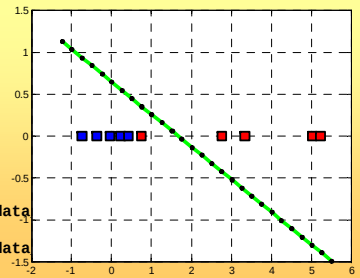
More general matlab code

```
% linclass_lect_RS
close all, clear all
num_data_per_class = 5;   shift=3;
% the smaller the shift of the means,
% the bigger overlapping of classes
x1=[randn(num_data_per_class,1);
randn(num_data_per_class,1)+shift];
i1=ones(2*num_data_per_class,1);
x=[x1 i1];
d=[ones(num_data_per_class,1);-ones(num_data
w=pinv(x)*d
plot(x1(1:num_data_per_class),zeros(num_data
                'LineWidth',2,...
                 'MarkerEdgeColor','k',...
                 'MarkerFaceColor','b',...
                 'MarkerSize',10)
hold on
plot(x1(num_data_per_class+1:2*num_data_per_class),zeros(num_data_per_class,1),'r
s',...
                'LineWidth',2,...
                 'MarkerEdgeColor','k',...
                 'MarkerFaceColor','r',...
                 'MarkerSize',10)
x2=[min(x1)-0.5:0.25:max(x1)+0.5]';i2=ones(length(x2),1);
plot(x2,[x2 i2]*w,'--gs','LineWidth',4,...
                 'MarkerEdgeColor','k',...
                 'MarkerFaceColor','y',...
                 'MarkerSize',2)
grid on
```



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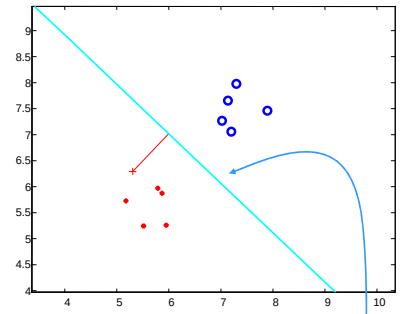
A simple example how this algorithm works:



$$\mathbf{X} = \begin{bmatrix} 5.7948 & 5.9797 & 1.0000 \\ 5.9568 & 5.2714 & 1.0000 \\ 5.5226 & 5.2523 & 1.0000 \\ 5.8801 & 5.8757 & 1.0000 \\ 5.1730 & 5.7373 & 1.0000 \\ 7.1365 & 7.6614 & 1.0000 \\ 7.0118 & 7.2844 & 1.0000 \\ 7.8939 & 7.4692 & 1.0000 \\ 7.1991 & 7.0648 & 1.0000 \\ 7.2987 & 7.9883 & 1.0000 \end{bmatrix} \qquad \mathbf{D} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ -1 \\ -1 \\ -1 \\ -1 \\ -1 \end{bmatrix}$$

$\mathbf{w} = \mathbf{X}^{*}\,\mathbf{D} \longrightarrow \mathbf{w}_{opt} = [-0.5209 \quad -0.5480 \quad 6.9731]^T$, and

the separation boundary equals

$$x_2 = -0.951x_1 + 12.725$$

MATLAB EXERCISE

- Learn how to create random data by 2 different distributions, uniform (UD) and normal (ND)
- Create 3, 2 dimensional ND classes with means (centers) at [0 0], [3 2] and [-3 -2] , having variances [1 2], [2 1] and [3 3]. Create 10 data in each class, and plot them in different colors and shapes.
- Create 3, 2 dimensional UD classes between the following boundaries; Class1: [-1 2] and [0 1], Class2: [1.5 3] and [-1 0.25], and Class3 – [1 2] and [1 3]. Create 100 data in each class, and plot them in different colors and shapes.

Hint: Go to matlab, type in, help help, choose doc help, search for randn or rand, also look at graphics

In this course, SVMs will be the tool used, but what are the alternatives?

Basic, the most popular and powerful, ones would be:

- **The least squares classifiers**, (Gauss and Legendre, ~ 200 years ago, today **FFT** and **JPEG** are still using it),
- **Linear discriminant analysis**, LDA (R.A. Fisher, 1936), for multivariate normal distributions; it uses hyperplanes as decision functions. A generalization of LDA is
- **Quadratic discriminant analysis**, which allows quadratic decision functions. Both methods are still used by many practitioners often with good success.
- **k-nearest-neighbor, KNN,** introduced in 1951; see Fix and Hodges (1951, 1952). Many followers and it's still in use. It was the first method for which universal consistency was established; see Stone (1977)

- **Cluster analysis** is an **UNsupervised** approach to recognize clusters in unlabeled data. Check the books by Hartigan (1975) and Kaufman and Rousseeuw (2005) for an introduction to cluster analysis techniques. K-means cluster analysis.
- **Parametric logistic regression** proposed by D. R. Cox to model binomial distributed outputs; see Cox and Snell (1989). This method is based on linear decision functions but **does not make specific assumptions on the distribution of the inputs**. Parametric logistic regression is **a special case of generalized linear**, see McCullagh and Nelder (1989). Hastie and Tibshirani (1990) proposed a semi-parametric generalization called **generalized additive models** where the inputs may influence the outputs in an additive but not necessarily linear manner. The **lasso** (Tibshirani, 1996) is a method for regularizing a least squares regression. It minimizes the usual sum of squared errors, with a bound on the sum of the absolute values of the coefficients.
- Other 'classic' methods for classification and regression are **trees**, Breiman et al. (1984). Trees often produce not only accurate results but are also able to uncover the predictive structure of the problem.
- **Neural networks** are **non-linear statistical data modeling tools** that can be used to model complex relationships between inputs and outputs or to find patterns in data sets. The motivation for neural networks, which were very popular in the 1990s, goes back to McCullogh and Pitts (1943) and Rosenblatt (1962). We refer also to Bishop (1996), Anthony and Bartlett (1999), and Vidyasagar (2002).

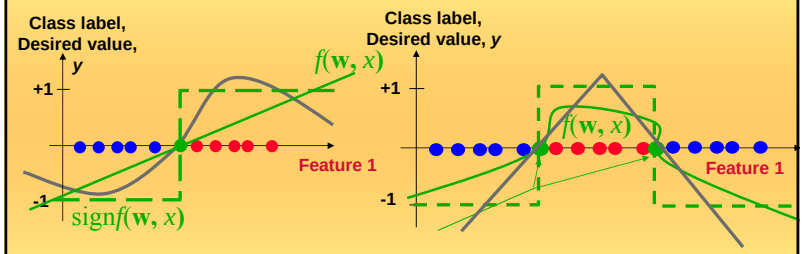
- There also exist various other **kernel-based methods**. For **wavelets**, we refer to Daubechies (1991), and for **splines** to Wahba (1990). Recent developments for kernel-based methods in the context of **SVMs** are also described by Cristianini and Shawe-Taylor (2000), Schoelkopf and Smola (2002), and Shawe-Taylor and Cristianini (2004).
- **Boosting algorithms** are based on an adaptive aggregation to construct from a set of weak learners a strong learner; see Schapire (1990), Freund (1995), and Freund and Schapire (1997). Finally, the books by Hastie et al. (2001, 2009), Duda et al. (2001), and Bishop (2006) give a broad overview of various techniques used in statistical machine learning, whereas both Devroye et al. (1996) and Gyoerfi et al. (2002) treat several classification and regression methods in a mathematically more rigorous way.

Well, fine,
let's go back to our problem of classification.
Here we show what we can see, meaning 1-dimensional or 2-dimensional (1D or 2D) problems
(1D or 2D means the input vector $\boldsymbol{x}$ is either 1D or 2D)

Let's analyze a very low dimensional problem of classifying two classes based on a single feature.

Thus, we believe that the Feature 1 **only** can be useful for classification!

Label classes as: y = +1 for class 1, y = -1 for class 2



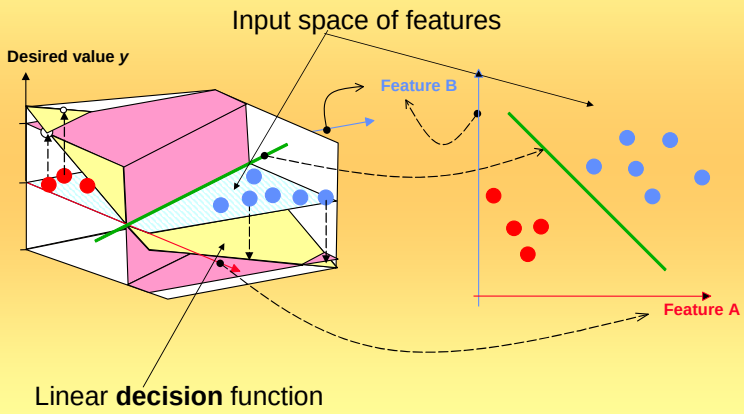
This is an EASY problem

This is a very COMPLEX problem

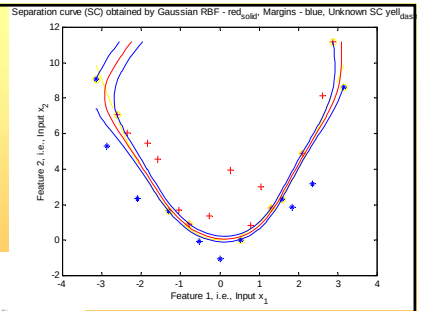
What about solving such a complex NONLINEAR problem

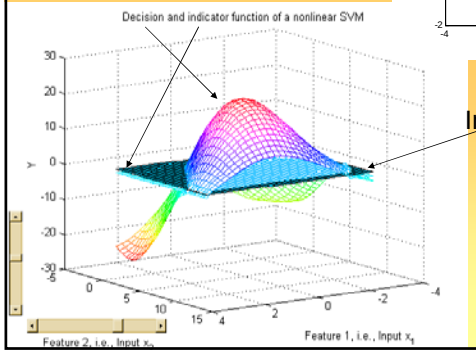
There are many possibilities, and we'll talk about them extensively!

For two dimensional problem: classifying two classes based on 2 features, we can show the **decision** function, but when number of features > 2, we deal with HYPER-surfaces, that can not be seen. However, the algorithms can 'see' in high-dimensional spaces and **they will be the same.**



VERY OFTEN the decision function and separating boundary are NON-LINEAR

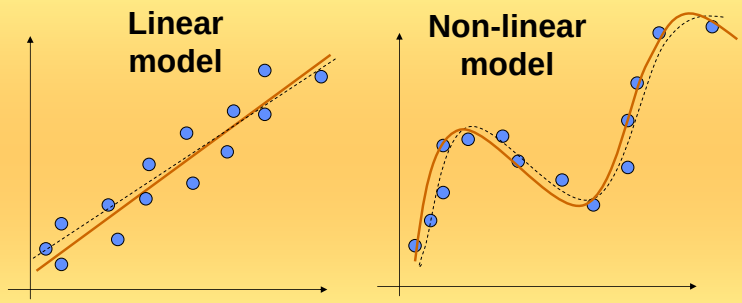




Indicator function (the term Vapnik & Chervonenkis use) is just a

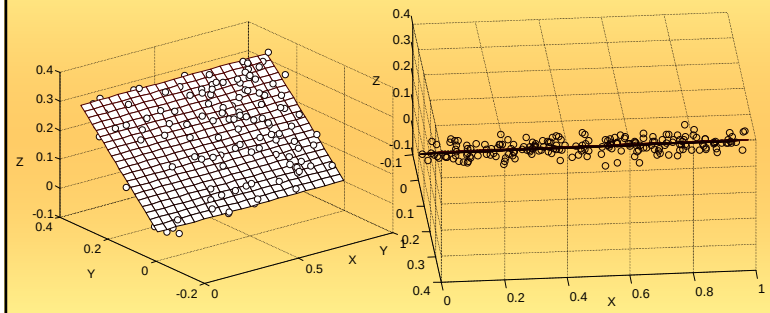
sign(Decision Function)

Regression (Curve, Surface, Fitting, i.e., Function Approximation)



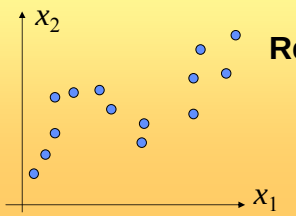
True, but unknown, function
Regression curve
Measured data points

Linear regression (function approximation, surface fitting) over two-dimensional input space



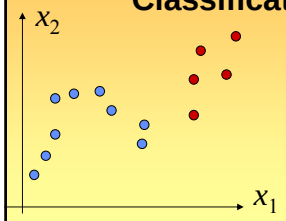
A view along the plane

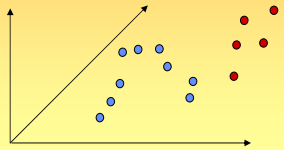
What is a basic labeling for classification and regression?



Regression DATA: X = x_1, Y = x_2
$x_2 = f(x_1)$ i.e. Y = $f(x_1)$

Classification DATA: X = [x_1 x_2], Y=[+1 or -1]
Y = $f(x_1, x_2)$





Now, some basics of a

Bias – Variance - Dilemma!

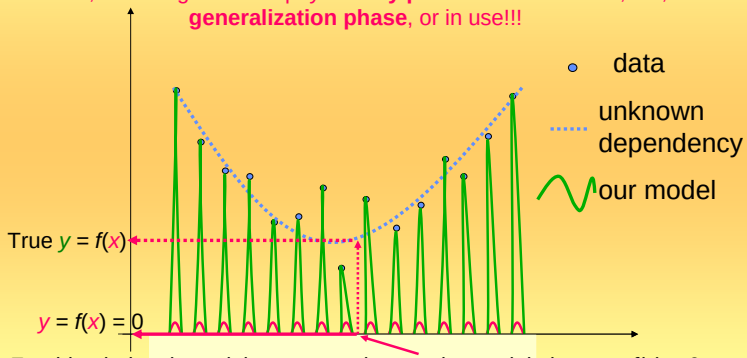
It is **the must piece of the knowledge** in order to get an idea of the relationship between the data, models and errors!

It will be **intuitive**, without math or any equation and it will serve for warming up! Check Kecman's book (there are many others better and more specialized too) if you prefer math.

Training and Generalization

Today, having powerful computers and good math software it is easy to be **'great** and **perfect'** on the training data set!

However, such a 'greatness' pays **heavy price at unseen data**, i.e., in a **generalization phase**, or in use!!!



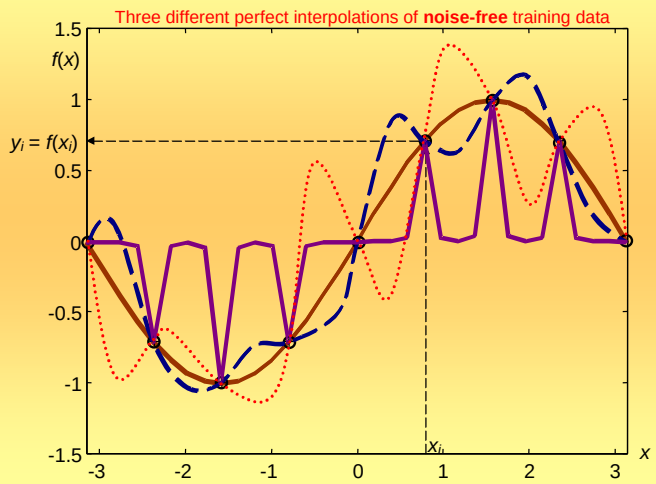
For this, during the training unseen, input x the model gives $y = f(x) = 0$

This is (deliberately chosen) extremely bad modeling, **but real!**

The same or similar phenomena will be present in the high dimensional cases, too!

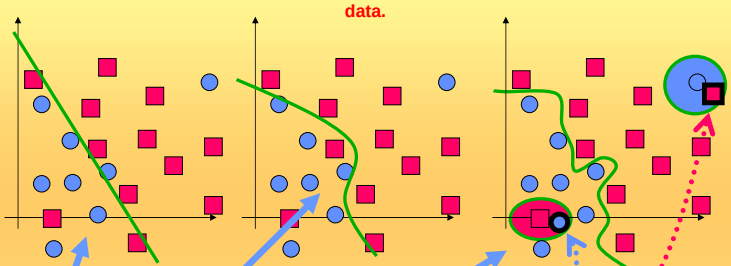
One more example showing **the perfect training results,** but **very bad generalization ones.**

Note that all three models have the training error equal zero! Bias = 0! Perfect interpolants!



And, still one more example, but now from the PATTERN RECOGNITION (CLASSIFICATION) task, showing various models and their performances.

Note that the last model (learning machine) learns perfectly, i.e., **separates all the training data.**



On the left, the separation boundary is linear, and it misses not only the outliers, but some 'easy' points. The solution on the right does not miss anything. By having high capacity, it learns each data belongings 'by heart', but it is unlikely that it will perform well on the new data, say this one

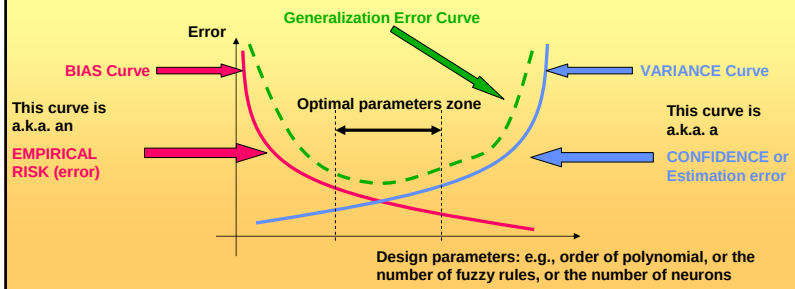
Or, this one

Central solution is of an intermediate capacity, separating most of the points, without putting too much trust into any particular training data point!!!

Obviously, we need much <u>more</u> than being good (or even excellent) on the training data set!

This 'more' means, we want that our models perform well on all future, previously unseen data, generated by the same data generator (i.e., plant, system, process, probability distribution).

The whole statistical learning fights (optimizes) the following two curves!



Although the graph looks very simple, finding the optimal modeling parameters is an

EXTREMALY DIFFICULT task!!!

and, this is due to the following facts:

- **we never (or, rarely only) know the underlying probability distribution, meaning the data generation, function,**
- **we never know the space of (target) functions, or to which class of functions our f. belongs**
- **we always have scarce (insufficient, not enough) data,**
- **our data are always high- (or/and extremely high-) dimensional,**
- **there is always the noise, or data are corrupted**

Bias & Variance

In modeling an **unknown dependency (regression or discrimination function)**, without knowledge of its mathematical form (**target space**), our **models (functions from hypothesis space**) produce **approximating functions**, which may be incapable of representing the **target function** behavior.

A difference between the model output and unknown target function is called **the bias.**

When there are not sufficient data, (or even if there appears to be sufficient representative data, **noise** contamination can still contribute that) **the sample of data** that is **available for training** *may not be representative of* ***average*** *data generated by the target function*.

Consequently, there may be a difference between a network output **for a particular data set**, and network function output **for the average of all data sets** produced by the target function.

The *square* of this difference is called **the variance.**

In other words, model's **bias** is a measure of **how well we can model the underlying unknown function with some function from hypothesis space H .**

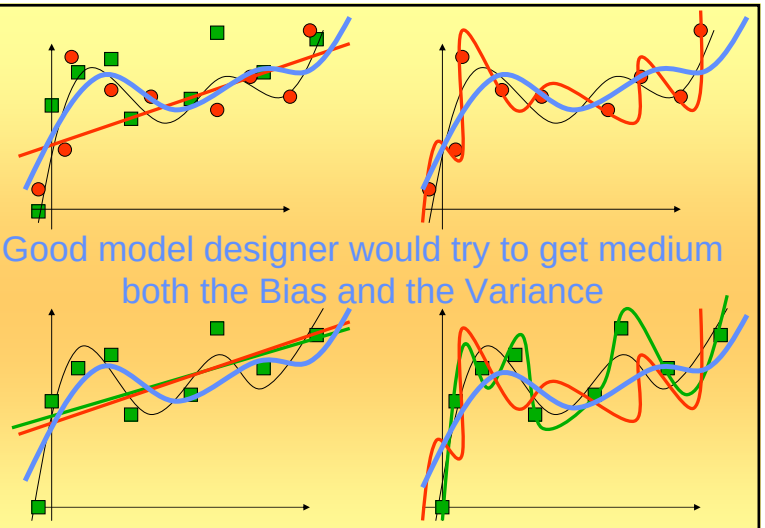
If the underlying function can be modeled perfectly with a model from our hypothesis space, i.e. if the underlying model is a member of our hypothesis space **H** , **then we say that our hypothesis space has zero model bias, or that it is unbiased.**

If the underlying function is not a member of the hypothesis space, then we say that **our model family is biased.**

Model's **variance** is a measure of how much our models **vary** when we train them with different training sets. If the hypothesis space **H** is very 'small', then there will be small differences between models trained with different training sets and we say that the model variance is small.

On the other hand, if the model family is 'large', then there can be (*and according to Murphy's law there will be*) large differences between models trained with different training sets and we say that the model variance is large.

We explain the above, by presenting the geometrical (graphical) meaning of BIAS and VARIANCE! Corresponding math doesn't fit here!



Good model designer would try to get medium both the Bias and the Variance

High Bias - Low Variance

Low Bias - High Variance

The mathematics of the Bias - Variance decomposition is to be found in many sources, inclusive my, The MIT Press published, book (Kecman, 2001).

And now, back to NNs & SVMs

In the rest of presentation we tightly follow The MIT Press published book (Kecman, 2001), as well as our the most recent results.

Check the book's site **http://www.support-vector.ws** for the newest paper's and software's downloads.

Some connections between

NNs *i.e./or/and* SVMs

and

classic techniques such as Fourier series and Polynomial approximations

Classic approximation techniques in NN graphical appearance

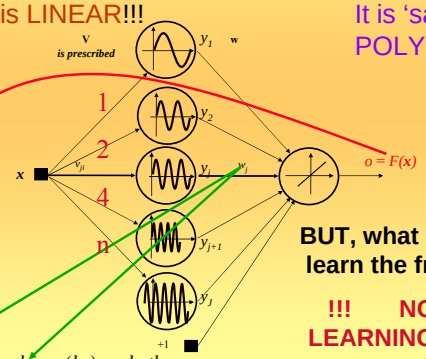
FOURIER SERIES

AMPLITUDES and PHASES of sine (cosine) waves are unknown, but frequencies are known because

Mr Joseph Fourier has selected frequencies for us -> they are INTEGER multiplies of some pre-selected base frequency.

And the problem is LINEAR!!!

It is 'same' with POLYNOMIALS

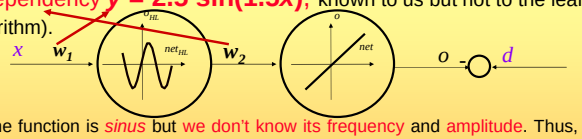


$$F(x) = \sum_{k=1}^{N} a_k \sin(kx),\ or\ b_k \cos(kx),\ or\ both$$

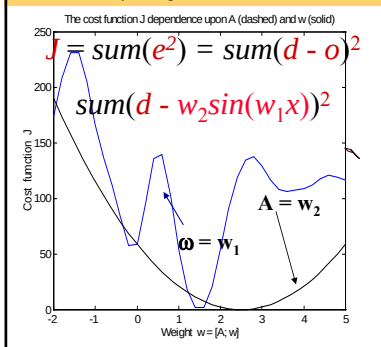
BUT, what if we want to learn the frequencies?

!!! NONLINEAR LEARNING PROBLEM !!!

Now, we want to find Fourier 'series' model $o = y = w_2 \sin(w_1 x)$ of the underlying dependency $y = 2.5 \sin(1.5x)$, known to us but not to the learning machine (algorithm).



We know that the function is *sinus* but we don't know its frequency and amplitude. Thus, by using the training data set {**x**, *d*}, we want to model this system with the NN model consisting of a single neuron in HL (having *sinus* as an activation function) as given above.



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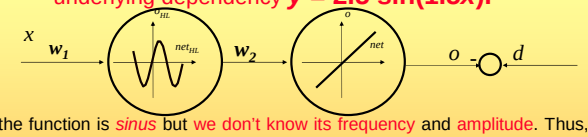

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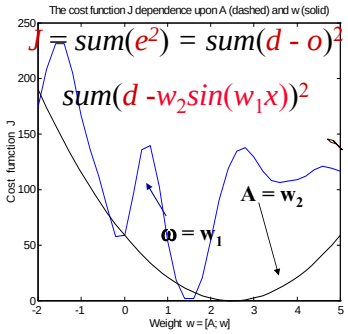
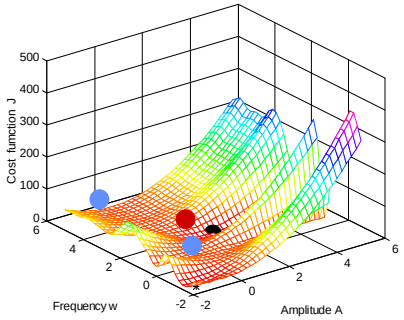
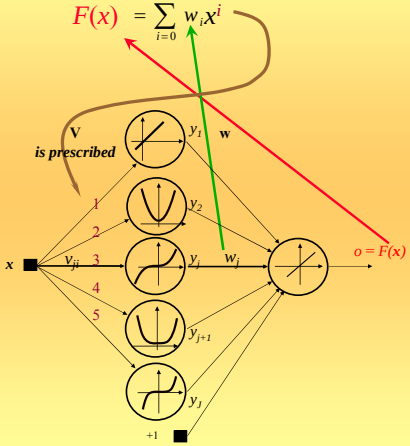




Another classic approximation scheme is a

POLYNOMIAL SERIES

$$F(x) = \sum_{i=0}^{N} w_i x^i$$



Another classic approximation scheme is a

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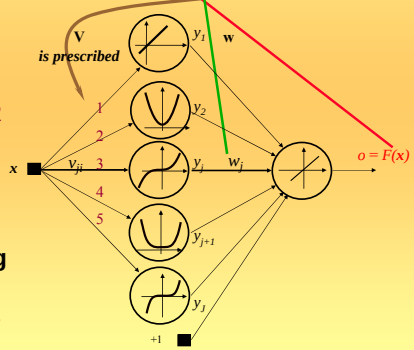
With a prescribed (integer) exponents this is again LINEAR APPROXIMATION SCHEME. Linear in terms of parameters to learn and not in terms of the resulting approximation function. This one is NL function for *i* > 1.



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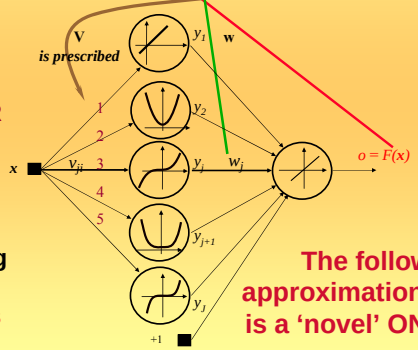


The following approximation scheme is a 'novel' ONE called RBF network here.

Approximation of some

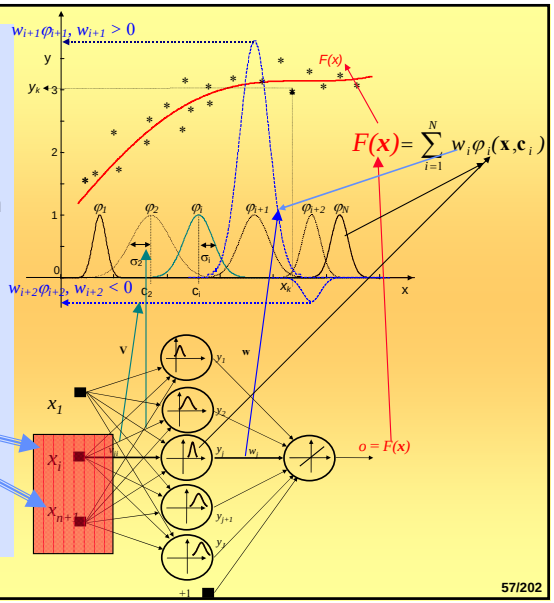
NL 1D function by

Gaussian

Radial Basis Function

(RBF)

In 1-D case forget these two inputs. They are here just to denote that the basic structure of the NN is the same for ANY-DIMENSIONAL INPUT



Approximation of some NL 2D function by

Gaussian Radial Basis Function (RBF)

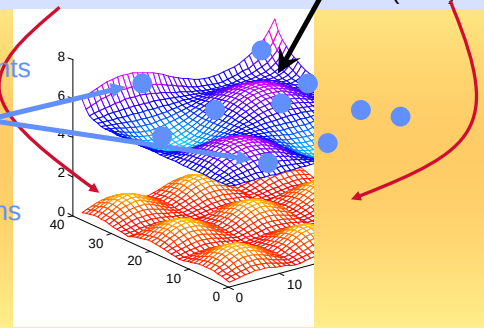
Measurements

Images

Records

Observations

Data



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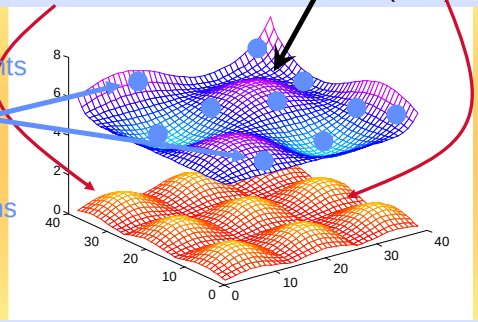

For FIXED Gaussian RBFs a LEARNING FROM DATA is a LINEAR PROBLEM. If the Centers and Covariance matrices are the subjects of learning, the problem becomes NONLINEAR.

Read it - **extremely difficult!**

The learning machine that uses data to find the APPROXIMATING FUNCTION (in regression problems) or the SEPARATION BOUNDARY (in classification, pattern recognition problems), is the same in high-dimensional situations.

Here, it will be either the so-called **SVM** or the **NN**

(however remember, there are other models too).

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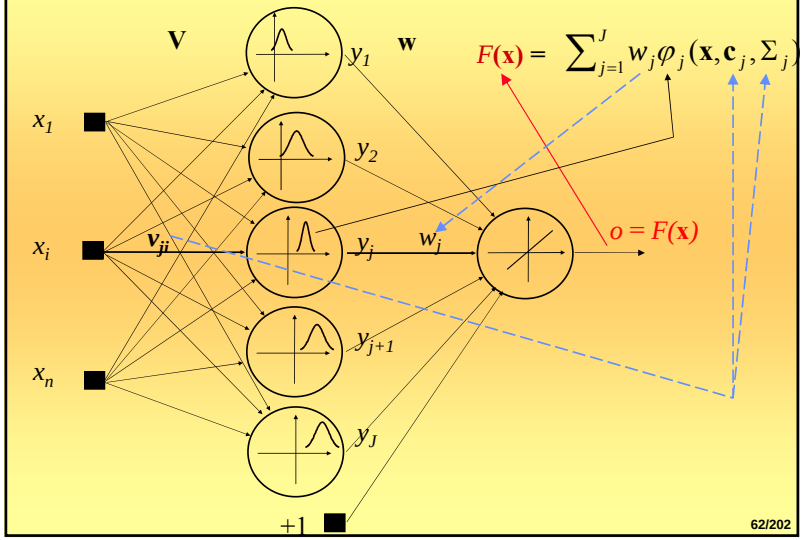
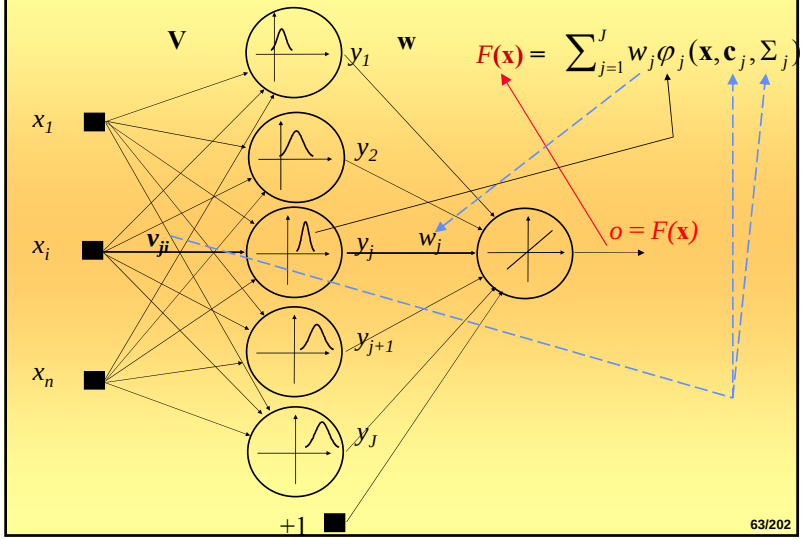
WHAT are DIFFERENCES and SIMILARITIES?

WHATCH CAREFULLY NOW !!!

This is a Neural Network,



and, this is a Support Vector Machine.



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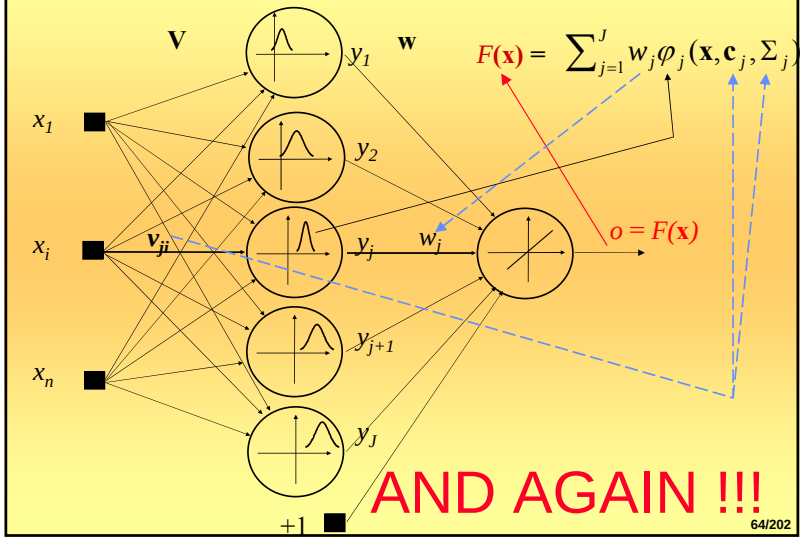
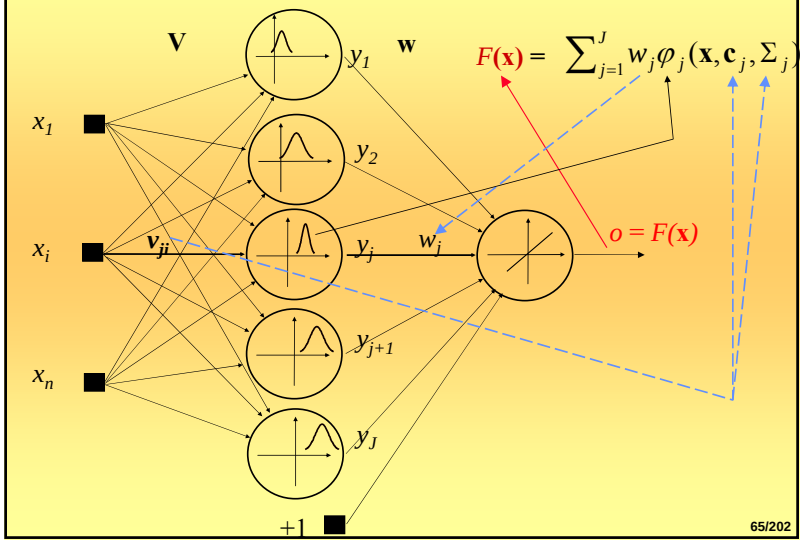


AND AGAIN !!!

This is a Neural Network,



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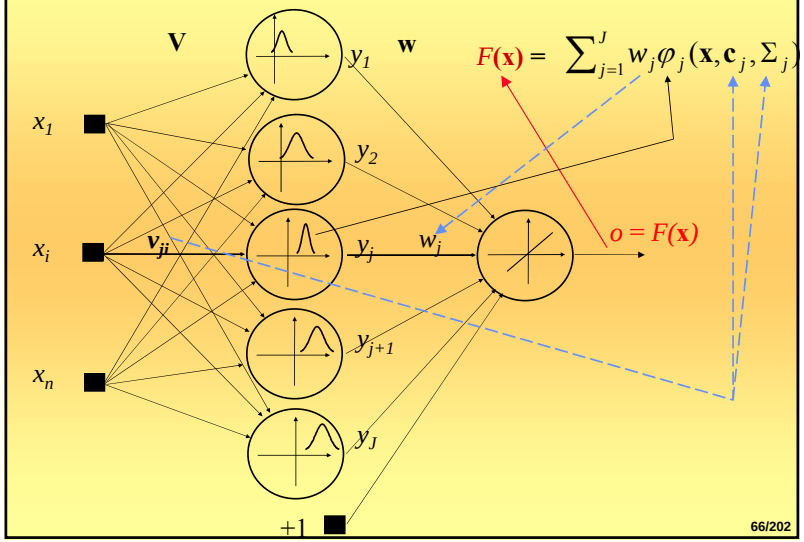

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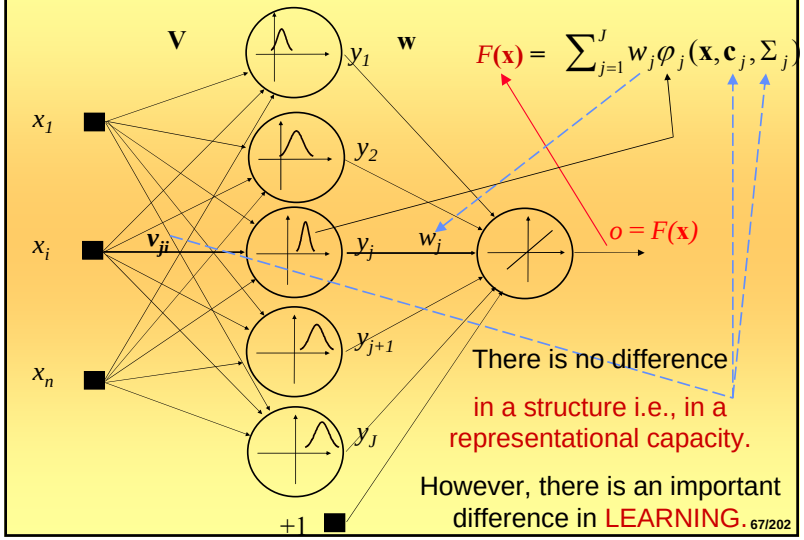

There is no difference

in a structure i.e., in a representational capacity.

However, there is an important difference in LEARNING.

Where then the
BASIC DIFFERENCES between
NNs and SVMs

(*in fact among all the other various ML models*)

are coming from?

Well ! There are two fundamental pieces in any ML modeling

- They are the questions of:
- the **FORM**

  and
- the **NORM**

FORM

- covers – the type of the model and in particular the type of the kernel (SVM), i.e., activation (NN), i.e., basis (RBF), i.e., membership (FL) function used

NORM

- covers – the type of the cost, i.e., merit, i.e., loss, i.e., fitness, i.e., objective, function **which is minimized over the parameters of interest** (here, we call them **weights**)

FORM

- **'All'** our models in ML are 'same' i.e. they are the

SUM OF THE WEIGHTED BASIS FUNCTIONS

$$o = f(\mathbf{x}) = \sum_{j=1}^{J} w_j \varphi_j(\mathbf{x}, \mathbf{c}_j, \Sigma_j)$$

Hyperparameters to be found during the learning (training) phase

Hence,

ONE MODEL = MANY MODELS

Polynomial approximations, Fourier expansions, NN, SVMs, wavelets, JPEG, MPEG, Fuzzy Logic models, …, many others … they ALL are

NORM

- **Basically, we use primarily (or a soft only) two NORMs (cost functions)** in ML which are the
- **MINIMIZATION** of the **SUM OF ERROR SQUARES in the OUTPUT space** (linear standard classifier, FFT, JPEG, MPEG, MLP NN and RBF NN) – L_2 norm

  and the
- **MAXIMIZATION of the MARGIN in the INPUT space** expressed as a **MINIMIZATION** of the **SUM OF WEIGHTS SQUARES** (SVMs)

(a variant of both may be the L_1 norm or some composite norm)

Norms (Loss Functions) of NNs and SVMs

$$E = \sum_{i=1}^{P} (d_i - f(\mathbf{x}_i, \mathbf{w}))^2$$

Closeness to data

A classic multilayer perceptron (MLP), FFT, polynomial models

$$E = \sum_{i=1}^{P} (d_i - f(\mathbf{x}_i, \mathbf{w}))^2 + \lambda \| \mathbf{P} f \|^2$$

Closeness to data *Smoothness*

Regularization (RBF) NN

$$E = \sum_{i=1}^{P} L_{\varepsilon i} + \lambda \| \mathbf{P} f \|^2 = \underbrace{\sum_{i=1}^{P} L_{\varepsilon i}}_{\text{Clossenes to data}} + \underbrace{\Omega(h, l)}_{\text{Capacity of machine}}$$

Support Vector Machines

In the last expression the SRM principle uses the VC dimension *h* (defining model capacity) as a controlling parameter for minimizing *E*

Therefore,

let's say a little more about basics of the learning from data first.

Note that you may find different names for the L from D:

identification, estimation, regression, classification, pattern recognition, function approximation, curve or surface fitting etc.

All these tasks used to be solved previously.

Thus, THERE IS THE QUESTION:

Is there anything new in respect to the classic statistical inference?

The classic regression and (Bayesian) classification statistical techniques are based on the very strict assumption that probability distribution models or probability-density functions are known.

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*In the most of real-life problems, a stochastic component of data is the normal probability distribution law, i.e., the underlying joint probability distribution is Gaussian.
*Due to the second assumption, the induction paradigm for parameter estimation is the maximum likelihood method that is reduced to the minimization of the sum-of-errors-squares cost function in most engineering applications.

All three assumptions on which the classic statistical paradigm relied, turned out to be inappropriate for many contemporary real-life problems (Vapnik, 1998) due to the facts that:

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***the underlying real-life data generation laws may typically be very far from the normal distribution and a model-builder must consider this difference in order to construct an effective learning algorithm,**

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***the underlying real-life data generation laws may typically be very far from the normal distribution and a model-builder must consider this difference in order to construct an effective learning algorithm,**

***from the first two objections it follows that the maximum likelihood estimator (and consequently the sum-of-error-squares cost function) should be replaced by a new induction paradigm that is uniformly better, in order to model non-Gaussian distributions.**

There is a real life fact

the probability-density functions are TOTALLY unknown,

and there is the question

HOW TO PERFORM a ***distribution-free***

***REGRESSION* or *CLASSIFICATION* ?**

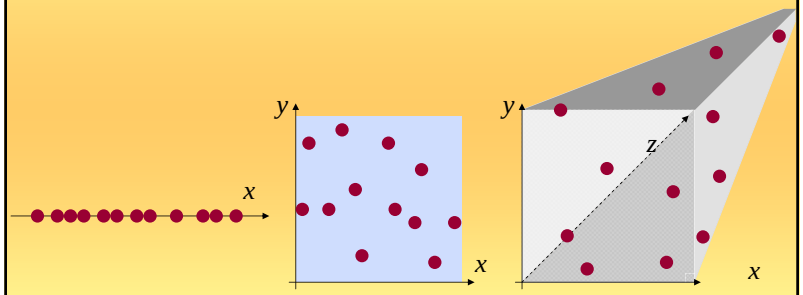
Mostly, all we have are recorded **EXPERIMENTAL DATA** (training patterns, samples, observations, records, examples):
Data is high-dimensional and **scarce (always too little data)!!!**

High-dimensional spaces seem to be **terrifyingly empty** and our learning algorithms (i.e., machines) should be able to operate in such spaces and to **learn from such a sparse data**.
There is an old saying that ***redundancy provides knowledge***.
Stated simpler
the more data pairs we have the better results will be.

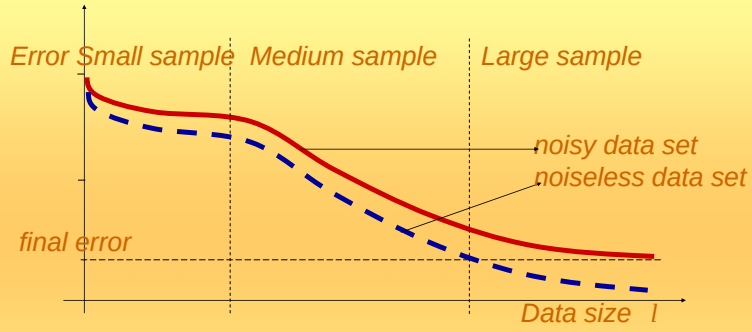
Terrifying emptiness and/or data sparseness

Just a first simple example

Imagine sampling some 1D $y = f(x)$, 2D $z = f(x, y)$, and 3D $u = f(x, y, z)$, functions and taking 10 samples on the domain (0, 1)!



Data points in 1D, 2D and 3D domains are less and less dense, and the average distance between the points increases with the dimensionality!!!



Dependency of the modeling error on the training data set size

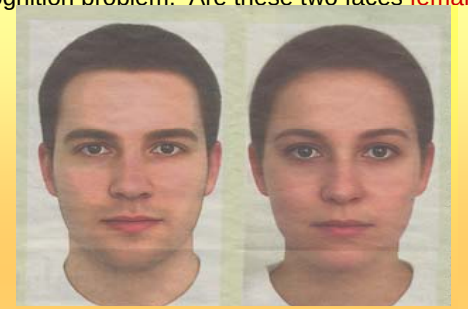
Thus, the main characteristics of all MODERN problems is the mapping between the high-dimensional spaces, but

where are HIGH-DIMENSIONAL problems coming from?

Let's exemplify this by the following (extremely simple) pattern recognition (classification) example!

Gender recognition problem: Are these two faces female or male?

F or M?

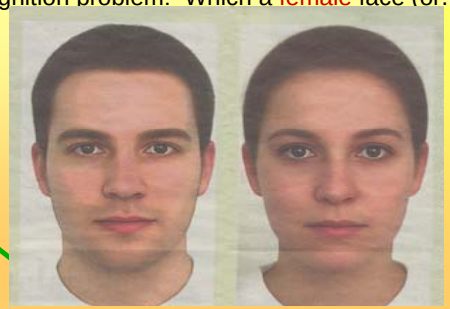


M or F?

Gender recognition problem: Which a female face (or, male one)?

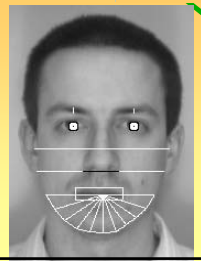
F or M?

There must be something in the geometry of our faces. Here, 18 input variables, features, were chosen!



M or F?

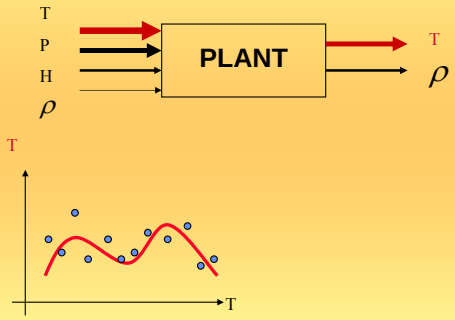
A problem from **Brunelli & Poggio**, 1993.



Nr	Feature
1	pupil to nose vertical distance
2	pupil to mouth vertical distance
3	pupil to chin vertical distance
4	nose width
5	mouth width
6	zygomatic breadth
7	bigonial breadth
8-13	chin radii
14	mouth height
15	upper lip thickness
16	lower lip thickness
17	pupil to eyebrow separation
18	eyebrow thickness

Approximation and classification are 'same' for any dimensionality of the input space. **Nothing (!) but size changes.** But the **change is DRASTIC.** High dimensionality means both an **EXPLOSION in a number OF PARAMETERS** to learn and a **SPARSE training data set.**

High dimensional spaces seem to be terrifyingly empty.



$\Re \Rightarrow \Re$

N data

Approximation and classification are 'same' for any dimensionality of the input space. **Nothing (!) but size changes.** But the **change is DRASTIC.** High dimensionality means both an **EXPLOSION in a number OF PARAMETERS** to learn and a **SPARSE training data set.**

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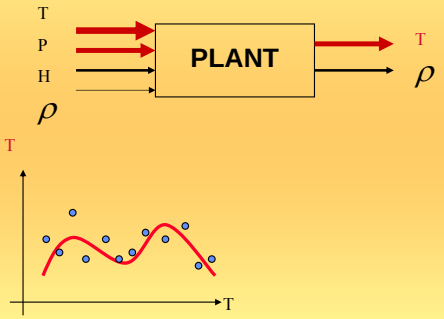

$\Re \Rightarrow \Re$ **However, for 2 inputs (T and P)**

N data **do we need 2N or N^2 data?**

Approximation and classification are 'same' for any dimensionality of the input space. **Nothing (!) but size changes.** But the **change is DRASTIC.** High dimensionality means both an **EXPLOSION in a number OF PARAMETERS** to learn and a **SPARSE training data set.**

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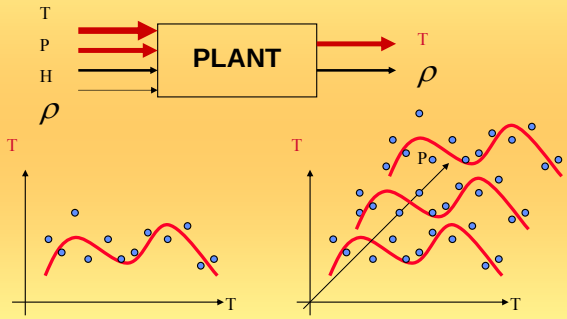


$\Re \Rightarrow \Re$ $\Re^2 \Rightarrow \Re$ $\Re^n \Rightarrow \Re$

N data **N^2 data** **N^n data**

CURSE of DIMENSIONALITY and SPARSITY OF DATA.

The newest promising tool FOR WORKING UNDER THESE CONSTRAINTS are the SUPPORT VECTOR MACHINES based on the STATISTICAL LEARNING THEORY (VLADIMIR VAPNIK and ALEKSEI CHERVONENKIS).

WHAT IS THE contemporary BASIC LEARNING PROBLEM???

LEARN THE DEPENDENCY (FUNCTION, MAPPING) from SPARSE DATA, under NOISE, in HIGH DIMENSIONAL SPACE!

Recall - the redundancy provides the knowledge!

A lot of data - 'easy' problem.

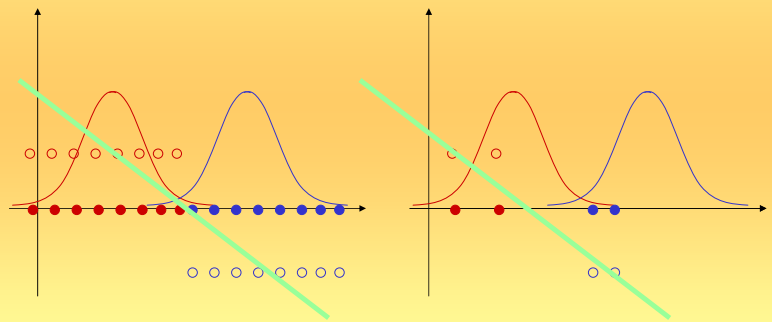
LET'S EXEMPLIFY

THE INFLUENCE OF A DATA SET SIZE ON THE SIMPLEST RECOGNITION PROBLEM

BINARY CLASSIFICATION, i.e., DICHOTOMIZATION.

First, the simplest case – 1-dim feature (i.e. input), generated by normal, Gaussian distribution

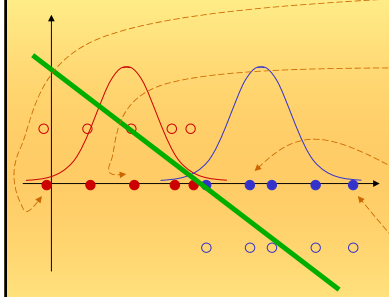
a) enough data b) sparse data



Sum of error squares will work in the left hand side graph, and it will make BIG error in the right hand side one

How this algorithm works?

Note that a decision function here is given as: $y_i = w_1 x_i + w_2$



$$\mathbf{X}\ \mathbf{w} = \mathbf{D}$$

$$\begin{bmatrix} -1 & 1.0000 \\ 3 & 1.0000 \\ 5 & 1.0000 \\ 7 & 1.0000 \\ 8 & 1.0000 \\ 9 & 1.0000 \\ 11 & 1.0000 \\ 12 & 1.0000 \\ 14 & 1.0000 \\ 16 & 1.0000 \end{bmatrix} \mathbf{w} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ -1 \\ -1 \\ -1 \\ -1 \\ -1 \end{bmatrix}$$

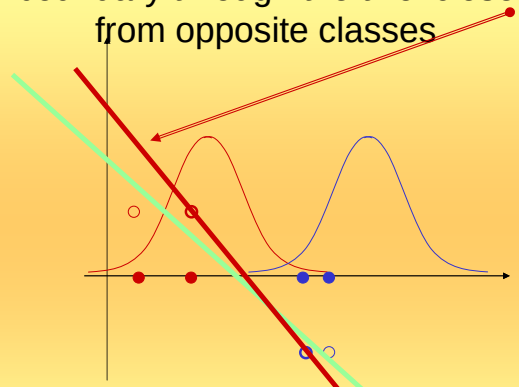
The solution here is given by

$$\mathbf{w} = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{D} = \mathbf{X}^*\mathbf{D}$$

$\mathbf{X}^*$ is known as the **pseudoinverse**

(we'll show later why is it this way)

However, what about this idea – draw the decision boundary through the two 'closest' points from opposite classes

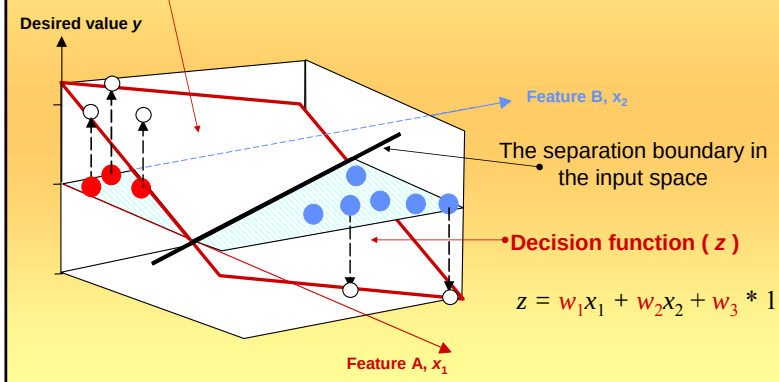


Actually, similar results will be obtained for SVMs, where we **don't bother with the sum of error squares** in the output space

Let's check now the **2-dimensional input case**, and this is the last example where we can represent the decision function graphically.

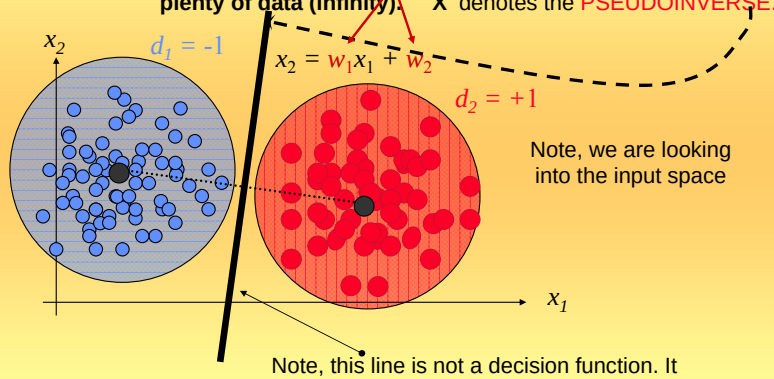
Nevertheless, the algorithms will work for **any-dimensional input**, but following the results visually will not be possible!!!

Decision function in 2-dim case is shown below



CLASSIFICATION or PATTERN RECOGNITITON EXAMPLE

Assume - Normally distributed classes, same covariance matrices. Solution is 'easy' - decision boundary is linear and defined by parameter **w = X* D when there is plenty of data (infinity).** **X*** denotes the PSEUDOINVERSE.



Note, we are looking into the input space

Note, this line is not a decision function. It is the separation boundary in the input space obtained from $z = 0$

CLASSIFICATION or PATTERN RECOGNITITON EXAMPLE

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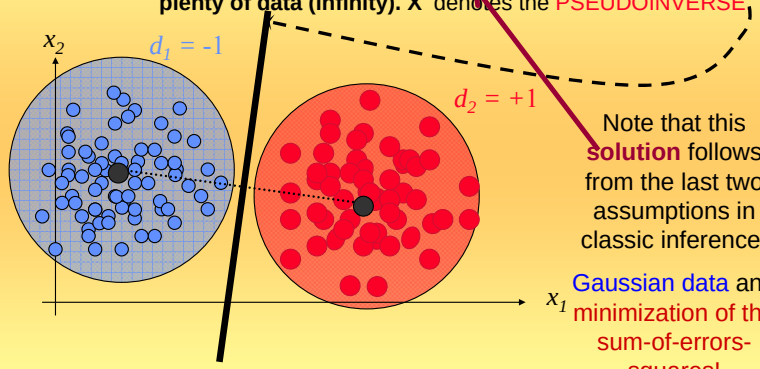
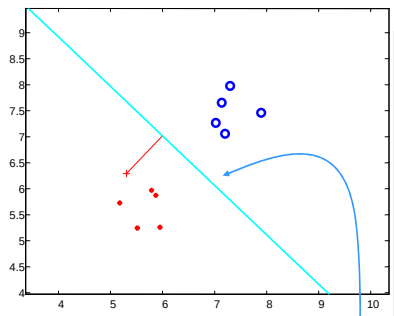


Note that this **solution** follows from the last two assumptions in classic inference!

Gaussian data and minimization of the sum-of-errors-squares!

A simple example how this algorithm works:



$$\mathbf{X} = \begin{bmatrix} 5.7948 & 5.9797 & 1.0000 \\ 5.9568 & 5.2714 & 1.0000 \\ 5.5226 & 5.2523 & 1.0000 \\ 5.8801 & 5.8757 & 1.0000 \\ 5.1730 & 5.7373 & 1.0000 \\ 7.1365 & 7.6614 & 1.0000 \\ 7.0118 & 7.2844 & 1.0000 \\ 7.8939 & 7.4692 & 1.0000 \\ 7.1991 & 7.0648 & 1.0000 \\ 7.2987 & 7.9883 & 1.0000 \end{bmatrix} \qquad \mathbf{D} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ -1 \\ -1 \\ -1 \\ -1 \\ -1 \end{bmatrix}$$

$\mathbf{w} = \mathbf{X}^{*}\mathbf{D}$ $\longrightarrow$ $\mathbf{w}_{opt} = [-0.5209 \quad -0.5480 \quad 6.9731]^T$, and

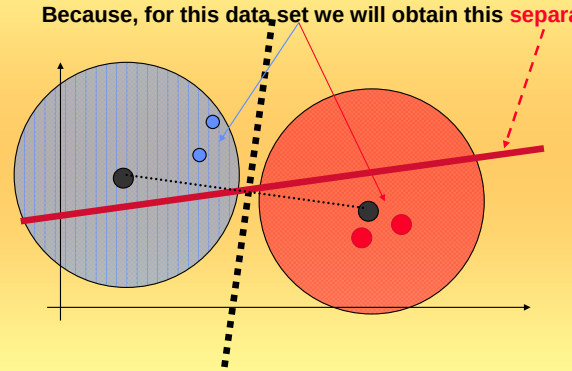
the separation boundary equals

$$x_2 = -0.951x_1 + 12.725$$

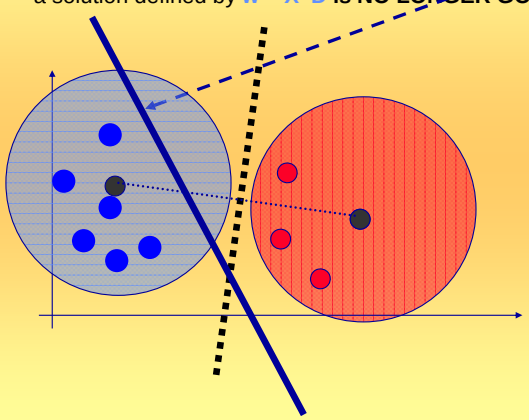
However, for a small sample - The **First** training datasets

Solution defined by **$\mathbf{w} = \mathbf{X}^{*}\mathbf{D}$ is NO LONGER GOOD ONE !!!**

Because, for this data set we will obtain this separation line,



and,
for The **Second** training datasets **we will obtain another separation line.**
Again, for small sample -
a solution defined by **$\mathbf{w} = \mathbf{X}^{*}\mathbf{D}$ is NO LONGER GOOD ONE !!!**

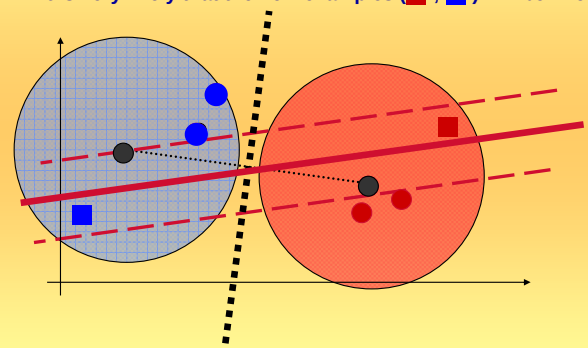


What is common for both separation lines, obtain from 2 different datasets the red and the blue one.

Both have a SMALL MARGIN.

WHAT'S WRONG WITH SMALL MARGIN? Look at the RED line!

It is very likely that the new examples (■ , ■) will be wrongly classified.

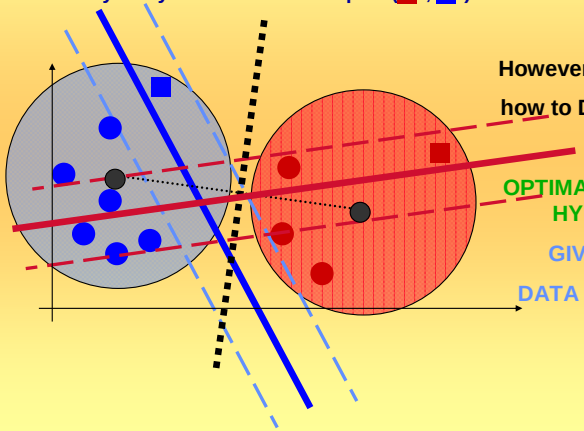


What is common for both separation lines the red and the blue one.

Both have a SMALL MARGIN.

WHAT'S WRONG WITH SMALL MARGIN? Look at the BLUE line!

It is very likely that the new examples (,) will be wrongly classified.



However, the question is how to DEFINE and FIND the

OPTIMAL SEPARATION HYPERPLANE

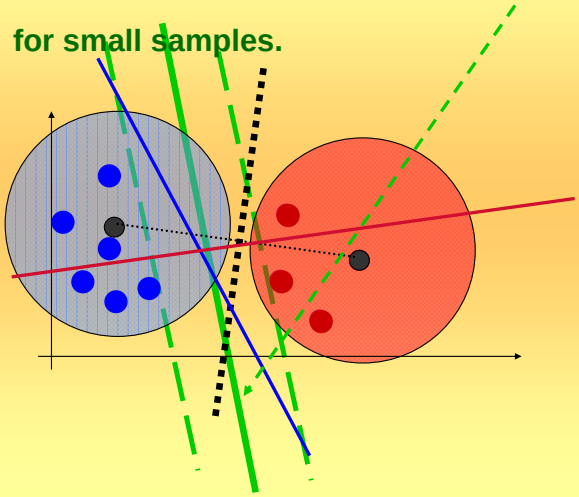
GIVEN (scarce)

DATA SAMPLES ???

The STATISTICAL LEARNING THEORY IS DEVELOPED TO SOLVE

PROBLEMS of FINDING THE OPTIMAL SEPARATION HYPERPLANE

for small samples.



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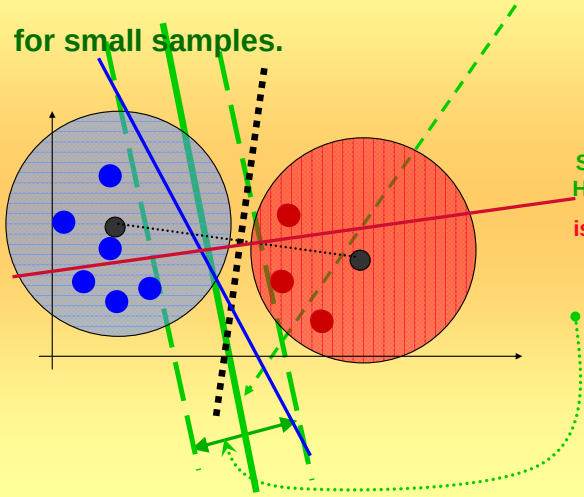


OPTIMAL SEPARATION HYPERPLANE

is the one that has the

LARGEST MARGIN

on given

DATA SET

One more intuitive presentation why the maximal margin idea may be a good statistical approach follows on the next slide!

Note, however, that the intuition only, does not qualify for, and does not guarantee, a broad acceptance of a maximal margin approach in a statistical learning.

There are both the strong theoretical proofs about the errors, bounds and generalization properties of SVMs based on a maximal margin idea, and convincing experimental performances on various benchmark data sets..

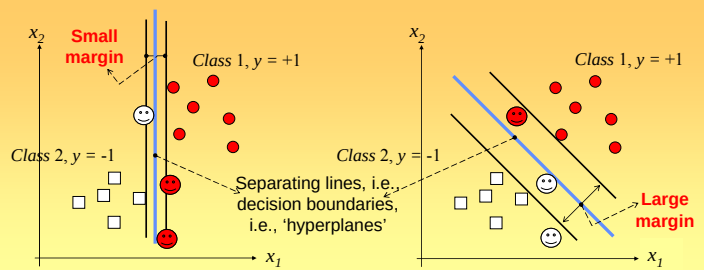
SUPPORT VECTOR MACHINE

is a MAXIMAL MARGIN CLASSIFIER

• it aims at finding the separating hyperplane with the maximal geometric margin (and not any one, that is the perceptron solution)

• WHY maximal margin?

Suppose we wan to separate two linearly separable classes, and we did it by two different decision functions.



Thus, the larger the margin, the smaller the probability of misclassification!

Before presenting the math of SVMs, just a few more 'similarities' between NNs and SVMs follow

$$E = \sum_{i=1}^{P} (d_i - f(\mathbf{x}_i, \mathbf{w}))^2$$

$\underbrace{}_{Closeness\,to\,data}$

A classic multilayer perceptron

$$E = \sum_{i=1}^{P} (d_i - f(\mathbf{x}_i, \mathbf{w}))^2 + \lambda \| \mathbf{P}f \|^2$$

$\underbrace{}_{Closeness\,to\,data}$ $\underbrace{}_{Smoothness}$

Regularization (RBF) NN

$$E = \sum_{i=1}^{P} L_{\varepsilon i} + \lambda \| \mathbf{P}f \|^2 = \underbrace{\sum_{i=1}^{P} L_{\varepsilon i}}_{Clossenes\ to\ data} + \underbrace{\Omega(h,l)}_{Capacity\ of\ machine}$$

Support Vector Machines

In the last expression the SRM principle uses the VC dimension *h* (defining model capacity) as a controlling parameter for minimizing the generalization error E (i.e., risk R).

There are two basic, constructive approaches to the minimization of the right hand side of previous equations (Vapnik, 1995 and 1998):

-choose an appropriate structure (order of polynomials, number of HL neurons, number of rules in the FL model) and, keeping the confidence interval fixed in this way, minimize the training error (i.e., empirical risk), or

-keep the value of the training error fixed (equal to zero or equal to some acceptable level) and minimize the confidence interval.

classic NNs implement the first approach (or some of its sophisticated variants) and SVMs implement the second strategy. In both cases the resulting model should resolve the trade-off between under-fitting and over-fitting the training data. The final model structure (order) should ideally *match the learning machines capacity with training data complexity*.

We don't go into SVMs right now

- First, we show what are the features and capacities of a classic linear classifiers, parameters of which are determined by **minimizing sum-of-errors-squares**
- The task for you now, is the **read about the NORM and FORM of approximation** (either classification or regression) in **my book – section 1.3.1**
  - As for us, we continue with **chapter 3** on both a **perceptron** and **linear classifier**.

O.K. now, back to SVMs

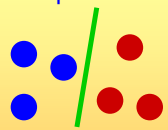
Let us do some more formal,

meaning,

mathematical analysis of SVMs learning!

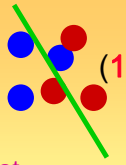
We follow an idea of a **gentle SVMs introduction**, **i.e., of a gradual proceeding** from the 'simple' cases to the more complex ones!

1) ***Linear Maximal Margin Classifier for Linearly Separable Data*** - no samples overlapping (late **1960-ties** and early **70-ties**).



3) ***Nonlinear Classifier*** (1992)

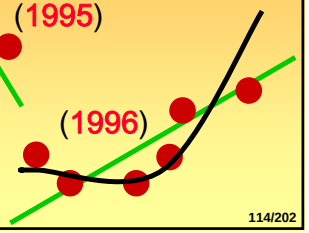
2) ***Linear Soft Margin Classifier for Overlapping Classes.***



(1995)

4) ***Regression by SV Machines*** that can be both **linear** and **nonlinear**!

(1996)



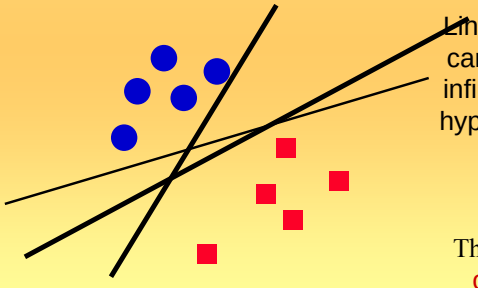
1) Linear Maximal Margin Classifier for Linearly Separable Data

Binary classification - no samples overlapping

Given some training data

$$(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_l, y_l), \quad y_i \in \{-1, +1\}$$

find the function $f(\mathbf{x}, \mathbf{w}_0) \in f(\mathbf{x}, \mathbf{w})$ which best approximates the unknown discriminant (separation) function $y = f(\mathbf{x})$.



Linearly separable data can be separated by in infinite number of linear hyperplanes that can be written as

$$f(\mathbf{x}, \mathbf{w}) = \mathbf{w}^{\mathrm{T}}\mathbf{x} + b$$

The problem is: find the optimal separating hyperplane

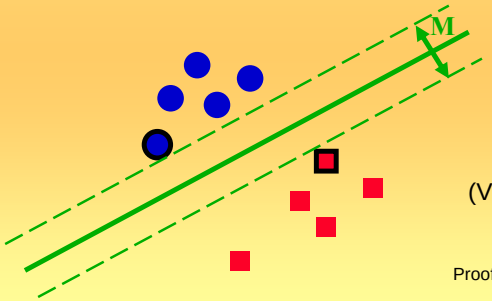
1) Vapnik-Chervonenkis: Optimal separating hyperplane is the one with

MAXIMAL MARGIN **!**

This hyperplane is uniquely determined by the vectors on the margin

the support vectors!

MARGIN IS DEFINED by **w** as follows:

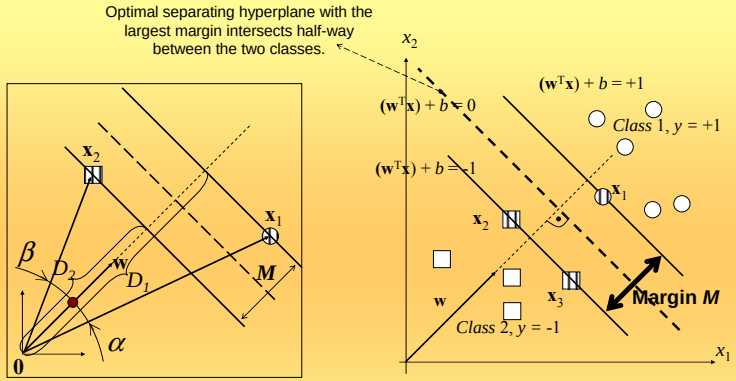


$$M = \frac{2}{\|\mathbf{w}\|}$$

(Vapnik, Chervonenkis '74)

Proof for *M* is on the next two slides

The relation between the weight vector w and the margin *M*



The margin M that is to be maximized during the training stage is a projection, onto the separating hyperplane's normal (weight) vector direction, of a distance between any two support vectors belonging to **different** classes. In the example above this margin M can be found as follows:

$$M = (\mathbf{x}_1 - \mathbf{x}_2)_{\mathbf{w}} = (\mathbf{x}_1 - \mathbf{x}_3)_{\mathbf{w}},$$

where the subscript $_{\mathbf{w}}$ denotes the projection onto the weight vector $\mathbf{w}$ direction. The margin M can now be found by using support vectors $\mathbf{x}_1$ and $\mathbf{x}_2$ as follows

$$D_1 = \|\mathbf{x}_1\|\cos(\alpha),\ D_2 = \|\mathbf{x}_2\|\cos(\beta) \text{ and } M = D_1 - D_2,$$

where α and β are the angles between $\mathbf{w}$ and $\mathbf{x}_1$ and between $\mathbf{w}$ and $\mathbf{x}_2$ respectively as given on page 4 e.g.,

$$\cos(\alpha) = \frac{\mathbf{x}_1^T\mathbf{w}}{\|\mathbf{x}_1^T\|\|\mathbf{w}\|}$$

Substituting cosines into the expression for M above results in

$$M = (\mathbf{x}_1^T\mathbf{w} - \mathbf{x}_2^T\mathbf{w}) / \|\mathbf{w}\|$$

and by using the fact that $\mathbf{x}_1$ and $\mathbf{x}_2$ are support vectors satisfying

$y_j|\mathbf{w}^T\mathbf{x}_j + b| = 1,\ j = 1, 2,$ that is

$\mathbf{w}^T\mathbf{x}_1 + b = 1$ and $\mathbf{w}^T\mathbf{x}_2 + b = -1$

we finally obtain $$M = \frac{2}{\|\mathbf{w}\|}$$ **!!!!!!**

The optimal canonical separating hyperplane (OCSH), i.e., a separating hyperplane with the largest margin (defined by $M = 2 / \|\mathbf{w}\|$), specifies *support vectors,* i.e., training data points closest to it, which satisfy $y_j[\mathbf{w}^T\mathbf{x}_j + b] \equiv 1,\ j = 1, N_{SV}$. **At the same time, the OCSH must separate data correctly, i.e., it should satisfy inequalities**

$$y_i[\mathbf{w}^T\mathbf{x}_i + b] \geq 1, \qquad i = 1, l$$

where l denotes a # of training data and N_{SV} stands for a # of SV. See the next slide about the meaning of the inequality above!

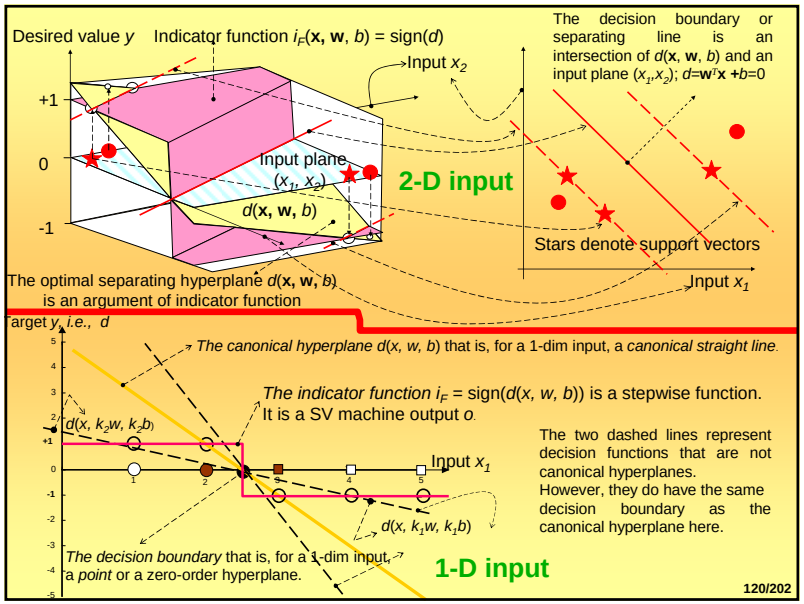
Note that maximization of M means a minimization of $\|\mathbf{w}\|$.

Minimization of a norm of a hyperplane normal weight vector $\|\mathbf{w}\| = \sqrt{\mathbf{w}^T\mathbf{w}} = \sqrt{w_1^2 + w_2^2 + \ldots + w_n^2}$ leads to a maximization of a margin M. Because *sqrt*(*f*) is a monotonic function, its minimization is equivalent to a minimization of *f* .

Consequently, a minimization of norm $\|\mathbf{w}\|$ equals a minimization of

$$\mathbf{w}^T\mathbf{w} = w_1^2 + w_2^2 + \ldots + w_n^2$$

and this leads to a maximization of a margin M.



Thus the problem to solve is:

minimize

$$J = \mathbf{w}^T \mathbf{w} = \| \mathbf{w} \|^2$$

subject to constraints

$$y_i[\mathbf{w}^T \mathbf{x}_i + b] \geq 1$$

and this is a classic QP problem with constraints that ends in forming and solving of a primal and/or dual Lagrangian.

Thus the problem to solve is:

minimize

Margin maximization!

$$J = \mathbf{w}^T \mathbf{w} = \| \mathbf{w} \|^2$$

subject to constraints

Correct classification!

$$y_i[\mathbf{w}^T \mathbf{x}_i + b] \geq 1$$

Note that # of constraining **in**equalities = # of training data *l*

and this is a classic QP problem with constraints that ends in forming and solving of a primal and/or dual Lagrangian.

Now, from the one sphere of mathematics (say, an intuitive geometric one) we should jump into the another sphere, into the sphere of a nonlinear optimization (say, into an algebraic sphere).

Basics of the General Optimization Problem

Optimize $f(\mathbf{w})$

Subject To (s.t.) $g(\mathbf{w}) = 0$

$\mathbf{w} > \mathbf{0}$, or $\mathbf{w} >= \mathbf{0}$

LINEAR PROGRAMMING problem: when $f(\mathbf{w})$ and $g(\mathbf{w})$ are linear and w_i's > 0

INTEGER PROGRAMMING problem: when w_i**'s should take only** integer **values.**

QUADRATIC PROGRAMMING problem $f(\mathbf{w})$ quadratic, $g(\mathbf{w})$ is linear.

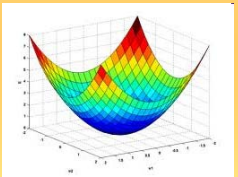
NONLINEAR PROGRAMMING problem, $f(\mathbf{w})$ **and** $g(\mathbf{w})$ are general nonlinear functions!

Remind basic QUADRICS in 2D

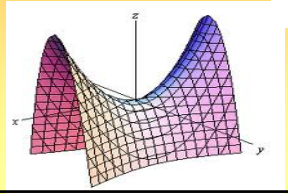
$$J = \mathbf{x}^T \mathbf{H} \mathbf{x} + \mathbf{v}^T \mathbf{x} + C$$

Eigenvalues of **H** define the shape

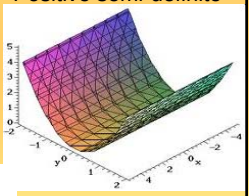
All EVal > 0
Positive definite



Some EVal > 0
Some EVal < 0
Indefinite, Saddle point



All EVal >= 0
Positive semi-definite



How one solves such QP problems with constraints:

Step 1) Forming a Primal Lagrangian in terms of primal (original) variables *w-s, b and* α-s (by an augmenting of the cost function by the constraints multiplied by dual variables α-s).

Step 2) Using the Karush-Kuhn-Tucker (KKT) conditions and forming a Dual Lagrangian in terms of α-s only.

Step 3) Solving a Dual Lagrangian for α-s.

Step 4) Using the KKT conditions for calculation of primal variables *w*-s and *b*.

Step 5) Creating the decision function for a classification problem, or the regression one for the function approximation task.

Step 6) Applying the SVM's model obtained.

A QP problem $J = \mathbf{w}^T \mathbf{w} = \| \mathbf{w} \|^2$, subject to constraints $y_i[\mathbf{w}^T \mathbf{x}_i + b] \geq 1$ is solved by **the *saddle point*** of the Lagrange functional (Lagrangian).

(In forming the Lagrangian for constraints of the form $g_i > 0$, the inequality constraints equations are multiplied by nonnegative Lagrange multipliers α_i (i.e., $\alpha_i > 0$) and subtracted from the objective function).

Step 1) Thus, a *primal variables Lagrangian* $L(\mathbf{w}, b, \alpha)$ is,

$$L(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\mathbf{w}^T\mathbf{w} - \sum_{i=1}^{l} \alpha_i \{y_i[\mathbf{w}^T \mathbf{x}_i + b] - 1\}$$

where the α_i are Lagrange multipliers. The search for an *optimal* **saddle point** ($\mathbf{w}_o$, b_o, α_0) is necessary because Lagrangian L must be *minimized* with respect to **w** and *b*, and has to be *maximized* with respect to nonnegative α_i (i.e., maximal $\alpha_i \geq 0$ should be found). This problem can be solved either in **a *primal space*** (which is the space of parameters **w** and *b*) or in **a *dual space*** (which is the space of Lagrange multipliers α_i).

The second approach gives insightful results and we will consider this solution in a dual space below. In order to do that, we use the Karush-Kuhn-Tucker (KKT) conditions for the optimum of a constrained function.

Step 2) Karush-Kuhn-Tucker (KKT) conditions are:

-at the saddle point ($\mathbf{w}_o$, b_o, α_o), **derivatives** of Lagrangian L with respect to primal variables should vanish (**NOTE, THERE ARE NO CONSTRAINTS on w** and *b* whatsoever) which leads to,

$$\frac{\partial L}{\partial \mathbf{w}_o} = 0, \qquad \text{i.e.,} \qquad \mathbf{w}_o = \sum_{i=1}^{l} \alpha_i y_i \mathbf{x}_i \qquad \text{(a)}$$

$$\frac{\partial L}{\partial b_o} = 0, \qquad \text{i.e.,} \qquad \sum_{i=1}^{l} \alpha_i y_i = 0 \qquad \text{(b)}$$

- and, in addition, the complementarity conditions

$$\alpha_i \{y_i[\mathbf{w}^T \mathbf{x}_i + b] - 1\} = 0, \quad i = 1, l.$$

must be satisfied.

Substituting (a) and (b) in a *primal variables Lagrangian* $L(\mathbf{w}, b, \alpha)$ (on previous page), we change to the *dual variables Lagrangian* $L_d(\alpha)$

Step 2-3)

$$L_d(\alpha) = \sum_{i=1}^{l} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{l} y_i y_j \alpha_i \alpha_j \mathbf{x}_i^T \mathbf{x}_j$$

Step 3) Such a *standard quadratic optimization problem* can be expressed in a ***matrix notation*** and formulated as follows:

Maximize

$$L_d(\alpha) = -0.5\boldsymbol{\alpha}^T\mathbf{H}\,\boldsymbol{\alpha} + \mathbf{1}^T\boldsymbol{\alpha},$$

subject to

$$\mathbf{y}^T\boldsymbol{\alpha} = 0,$$ Note that there are 1 equality constraint here

$$\boldsymbol{\alpha} \geq \mathbf{0},$$ Note that there are *l* inequality constraints here

where, **H** denotes the Hessian matrix ($H_{ij} = y_i y_j(\mathbf{x}_i\mathbf{x}_j) = y_i y_j \mathbf{x}^T_i\mathbf{x}_j$) of this problem and **1** is a unit vector $\mathbf{1} = [1\ 1\ .\ .\ .\ 1]^T$.

Some standard optimization programs typically ***minimize*** given objective function. Obviously, we can apply such programs and the same solution would be obtained if we

minimize

$$L_d(\alpha) = 0.5\boldsymbol{\alpha}^T\mathbf{H}\boldsymbol{\alpha} - \mathbf{1}^T\boldsymbol{\alpha},$$

subject to the same constraints namely

$$\mathbf{y}^T\boldsymbol{\alpha} = 0, \qquad \boldsymbol{\alpha} \geq \mathbf{0}.$$

Step 4) **Solutions α_{oi}** of the dual optimization problem above determine the parameters of the optimal hyperplane $\mathbf{w}_o$ (according to (a)) and b_o (according to the complementarity conditions) as follows,

$$\mathbf{w}_o = \sum_{i=1}^{N_{SV}} \alpha_{oi} y_i \mathbf{x}_i, \qquad i = 1, N_{SV}$$

All Support Vectors

For b, **we use only FREE, i.e., unbounded, SVecs** for which

$$0 < \alpha_i < C$$

Story about C comes in few slides!!!

$$b_o = \frac{1}{N_{freeeSV}}\left(\sum_{s=1}^{N_{freeSV}}\left(\frac{1}{y_s} - \mathbf{x}_s^T\mathbf{w}_o\right)\right), \; s = 1, N_{SV}.$$

N_{SV} denotes the number of support vectors. Note that an optimal weight vector $\mathbf{w}_o$, the same as the bias term b_0, is calculated by **using support vectors only**. This is because Lagrange multipliers for all non-support vectors equal zero ($\alpha_{oi} = 0$, $i = N_{SV} + 1, l$). Finally, having calculated $\mathbf{w}_o$ and b_o we obtain a decision hyperplane $d(\mathbf{x})$ and an indicator function $i_F = o = \text{sign}(d(\mathbf{x}))$ as given below

Step 5-6)

Remember this scalar product

$$d(\mathbf{x}) = \sum_{i=1}^{l} w_{oi}x_i + b_o = \sum_{i=1}^{l} y_i\alpha_i\left(\mathbf{x}_i^T\mathbf{x}\right) + b_o \qquad i_F = o = \text{sign}(d(\mathbf{x})).$$

Both the beauty and the power of working with SVMs can be seen below too

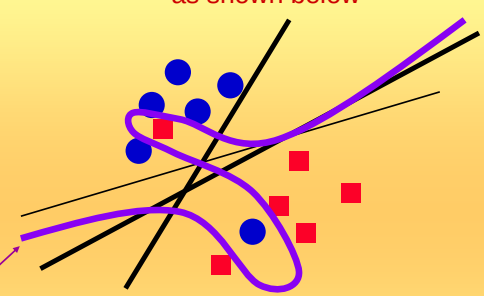
Once the support vectors have been found, we can calculate the bound on the expected probability of committing an error on a test example as follows

$$E_n\left[P(\text{error})\right] \leq \frac{E\left[\text{number of support vectors}\right]}{n}, \qquad (2.20)$$

where E_n denotes expectation over all training data sets of size n. Note how easy it is to estimate this bound that is independent of the dimensionality of the input space. Therefore, an SV machine having a small number of support vectors will have good generalization ability even in a very high-dimensional space.

My Springer book, page 30

However, the previous algorithm **will not work for linearly NOT separable classes** i.e., in the case when there is data overlapping as shown below



There is no single hyperplane that can perfectly separate all data!

But, separation can now be done in two ways:

- 1) allow some misclassified data
- 2) try to find NONLINEAR separation boundary

2) Linear Soft Margin Classifier for Overlapping Classes

(allowing misclassification)

Possible idea!

Minimize $\frac{1}{2}\mathbf{w}^T\mathbf{w} + C(\#\ of\ training\ errors)$

where C is a penalty parameter, trading off the margin size for the number of misclassified data points. Large C leads to small number of misclassification and smaller margin and vice versa.

HOWEVER!!! There is a serious problem! **Counting errors can't be accommodated within the NICE (meaning reliable, well understood and well developed) quadratic programming approach.**
Also, **it doesn't distinguish between disastrous errors and near misses)!**

SOLUTION! Minimize

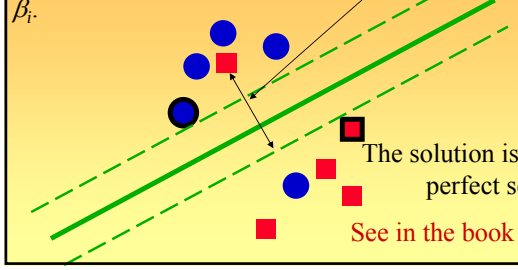
$$\frac{1}{2}\mathbf{w}^T\mathbf{w} + C(distance\ of\ \ error\ points\ to\ their\ correct\ side)$$

2) Linear Soft Margin Classifier for Overlapping Classes

Now one minimizes: $J(\mathbf{w},\xi) = \frac{1}{2}\mathbf{w}^T\mathbf{w} + C(\sum_{i=1}^{l}\xi_i)^k$

s.t. $\mathbf{w}^T\mathbf{x}_i + b \geq +1 - \xi_i$, for $y_i = +1$,
$\mathbf{w}^T\mathbf{x}_i + b \leq -1 + \xi_i$, for $y_i = -1$.

The problem is no longer convex and the solution is given by the saddle point of the primal Lagrangian $L_p(\mathbf{w}, b, \boldsymbol{\xi}, \boldsymbol{\alpha}, \boldsymbol{\beta})$ where α_i and β_i are the Lagrange multipliers. Again, we should find an *optimal* saddle point ($\mathbf{w}_o$, b_o, $\boldsymbol{\xi}_o$, $\boldsymbol{\alpha}_o$, $\boldsymbol{\beta}_o$) because the Lagrangian L_p has to be *minimized* with respect to $\mathbf{w}$, b and $\boldsymbol{\xi}$, and *maximized* with respect to nonnegative α_i and β_i.



The solution is a **hyperplane again**. No perfect separation however!

See in the book the details of the solution!

For overlapping classes dual problem is formulated as

$$L_d = -\tfrac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j y_i y_j \mathbf{x}_i^T\mathbf{x}_j + \sum_{i=1}^{N}\alpha_i \rightarrow \max_{\boldsymbol{\alpha}}$$

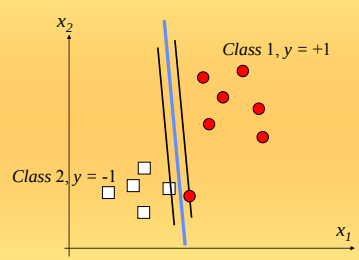
s.t. $0 \leq \alpha_i \leq C$ for $i = 1, \ldots, N$

$$\sum_{i=1}^{N}\alpha_i y_i = \alpha^T\mathbf{y} = 0$$

This C is the NOVELTY in respect to the hard margin classifier

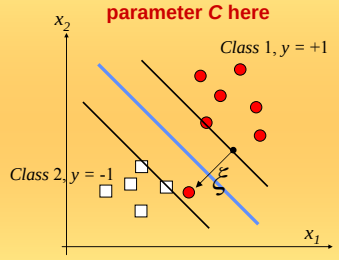
See in my Springer book the details of the solution!

Hard vs. Soft Margin SVMs an example on robustness



Hard Margin SVM leads to small margin

Use of penalty parameter *C* here



Soft Margin SVM leads to large margin

QP setting of a LINEAR SVM learning problem:

PRIMAL: minimize $J = \mathbf{w}^T \mathbf{w} = \| \mathbf{w} \|^2$, s.t. $y_i[\mathbf{w}^T \mathbf{x}_i + b] \geq 1$!

HARD MARGIN:

DUAL: minimize $\sum_{i=1}^{l} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{l} y_i y_j \alpha_i \alpha_j \mathbf{x}_i^T \mathbf{x}_j$ s.t. $\alpha_i \geq 0$, $\sum_{i=1}^{l} \alpha_i y_i = 0$

SOFT MARGIN:

DUAL: minimize $\sum_{i=1}^{l} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{l} y_i y_j \alpha_i \alpha_j \mathbf{x}_i^T \mathbf{x}_j$ s.t. $C \geq \alpha_i \geq 0$, $\sum_{i=1}^{l} \alpha_i y_i = 0$

Learning is expressed **in terms of training data** and it depends *only* on **the scalar products of input patterns** ($\mathbf{x}_i^T \mathbf{x}_j$).

Comments: Solving primal results in the same weight vector **w** as in the dual solution, but 'primal' **w** is composed of all training data. Primal does not select relevant points - support vectors (i.e., it does not compress the information as the dual does). $\alpha_i > 0$ only for SVs, in a dual setting!!!

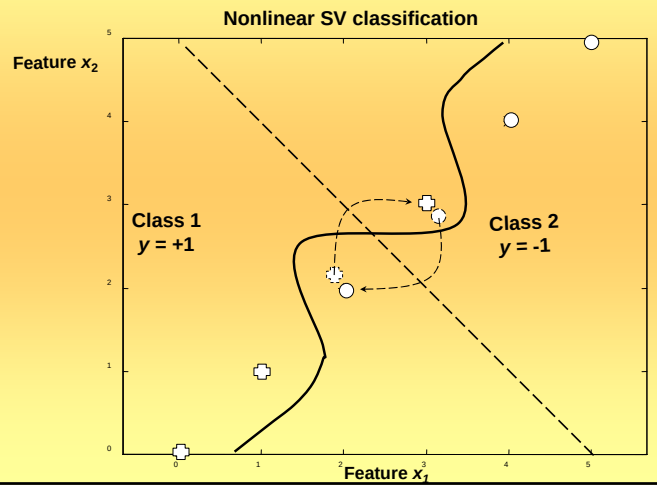
Just a fraction of relevant data (SVs) composes a decision hyperplane.

Here the LINEAR SVM models story ends!!!

What to do, and how to go about, when the true decision function (i.e., separation boundary) is NONLINEAR???

Remind, for example, that even if data are generated by normal (Gaussian) distribution but with different covariance matrices, the true decision function will be a quadratic function (see Example 1.10 on page 95, in chapter 1 of my The MIT book)

Hence, the hyperplanes cannot be the solutions when the decision boundaries are TRULY nonlinear, SAY AS IN THE CASE OF TWO GAUSSIAN CLASSES HAVING DIFFERENT COVARIANCE MATRICES or AS IN THE EXAMPLE SHOWN BELOW



Now, the SVM should be constructed by

i) mapping input vectors nonlinearly into a high dimensional feature space and,

ii) by constructing the OCSH in the high dimensional feature space.

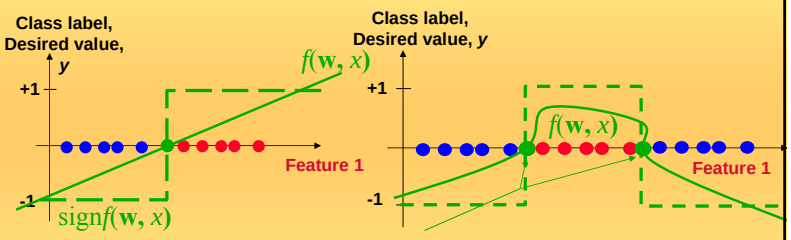
Check my Springer Verlag book

for all the derivations!!!

Let's analyze a very low dimensional problem of classifying two classes based on a single feature.

Thus, we believe that the Feature 1 **only** can be useful for classification!

Label classes as: y = +1 for class 1, y = -1 for class 2



This is an EASY problem

This is a very COMPLEX problem

What about solving such a complex NONLINEAR problem

There are two possibilities:

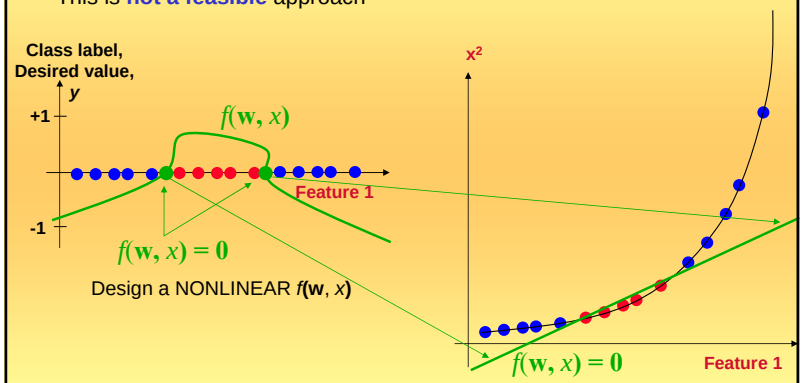
Example 1:

1) Solve in original *x domain*

This is **not a feasible** approach

2) Map data into an **extended features' *domain***

This is **an RIGHT** approach

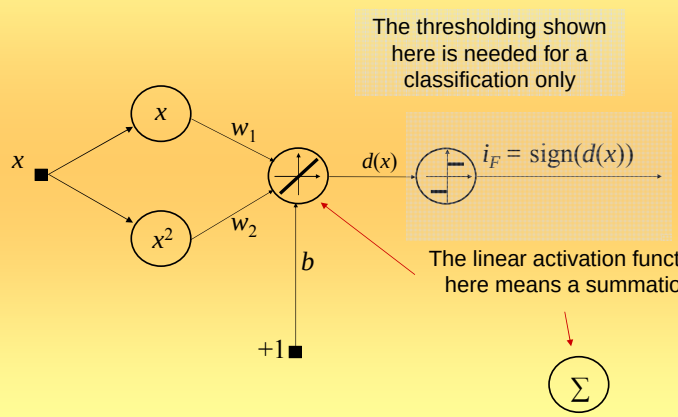


Design a NONLINEAR $f(\mathbf{w}, x)$

Design a LINEAR decision function in a NEW features plane.

Note that we do not see Class Labels here!

An extension (mapping) of an input space x into the feature one $[x \quad x^2]$ can be given the graphical representation in the form of a 'neural' network below

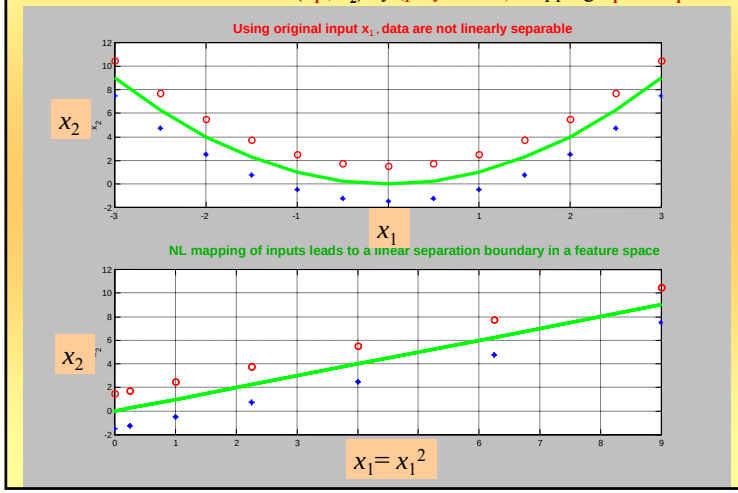


The thresholding shown here is needed for a classification only

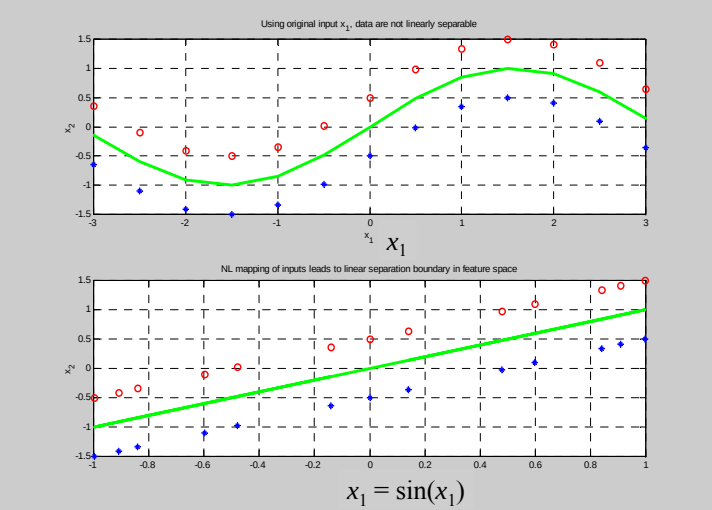
The linear activation function here means a summation

Why may the mapping of input space **X** (x_1, x_2) into feature space **F** $(f(x_1), f(x_2))$ be useful?

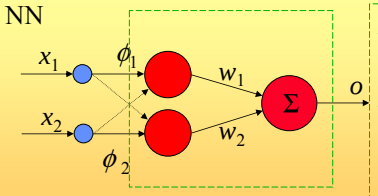
Example 2: Nonlinear (quadratic) separation boundary in **X** (x_1, x_2) is transformed into linear one in **F** (x_1^2, x_2) by (polynomial) mapping x_1 into x_1^2



Example 3: Nonlinear (sinusoidal) separation boundary in **X** (x_1, x_2) is transformed into linear one in **F** $(\sin(x_1), x_2)$ by (trigonometric) mapping x_1 into $\sin(x_1)$



In both cases the mapping performed can be represented as the following SVM i.e., NN



After the mapping Φ is chosen, the linear margin classifier, i.e., the SVM, is to be designed **in a feature space** with the hard, or soft learning algorithms presented so far!

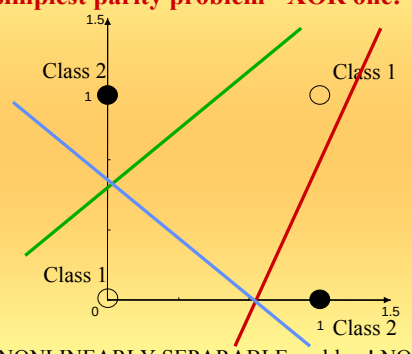
Despite the fact that NL mapping works nicely, there are two basic comments needed now:

a) We decided in advance which NL mapping to perform, **for we knew the nonlinearity.** Generally we do not know the very character of separation (hyper)surfaces and we will try to solve each problem with a few standard mappings (polynomial and RBF Gaussian ones primarily).

b) The dimension of a feature space in two previous examples is same as the one of the original input space. This is, however, not typical and we will usually map input space into much richer space (space of the much higher dimension, **possibly into space of infinite dimension(!)**)

Solution of a problem, regarding both the nonlinear mapping and a dimensionality of the feature space (that is related to the number of neurons in a hidden layer) used, **is usually not unique.**

Consider the simplest parity problem - XOR one:

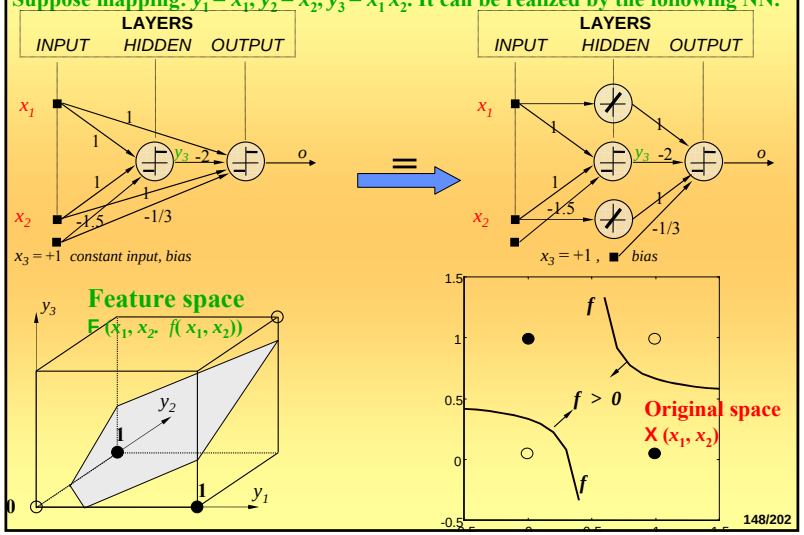


This is a classic NONLINEARLY SEPARABLE problem! NO linear separation line!

We show solutions by using both **a polynomial** and **an RBF** approach.
Other polynomial and RBF solutions, as well as other NL ones are possible, too!!!

XOR problem - polynomial solution: $f(\mathbf{x}) = x_1 + x_2 - 2\,x_1 x_2 - 1/3$

Suppose mapping: $y_1 = x_1, y_2 = x_2, y_3 = x_1 x_2$. **It can be realized by the following NN.**

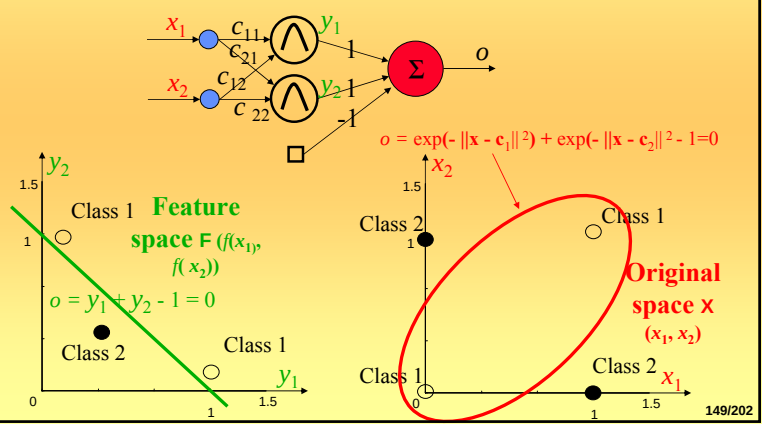


XOR problem - Gaussian RBF solution. We choose two Gaussians only, i.e., a dimension of a feature space is 2: $c_1 = [1\ 1]^T$ and $c_2 = [0\ 0]^T$.

This is a following mapping: $\mathbf{y} = [\exp(-\|\mathbf{x} - \mathbf{c}_1\|^2)\quad \exp(-\|\mathbf{x} - \mathbf{c}_2\|^2)]^T$. Hence, **x -> y:**

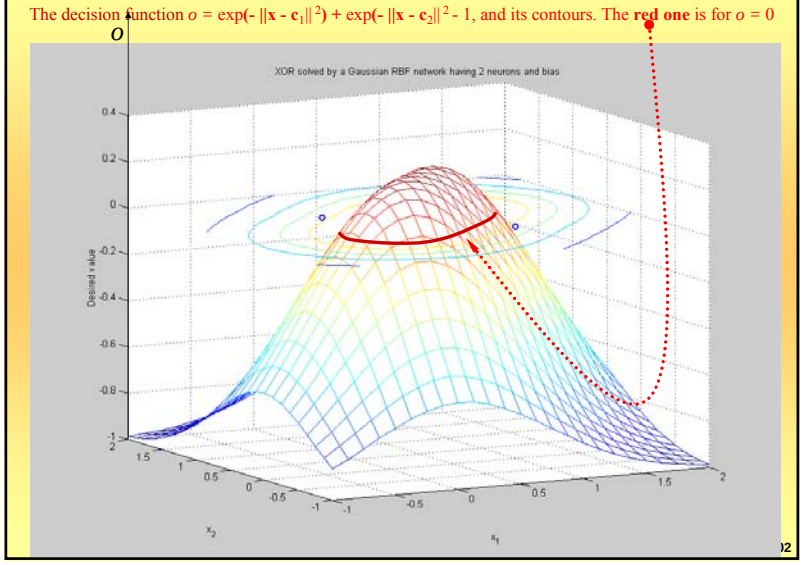
[0 0] -> [0.135 1], [1 1] -> [1 0.135], [1 0] -> [0.368 0.368], [0 1] -> [0.368 0.368].

The following NN, will produce linear separation boundary in a feature space and the NL one in the original space.

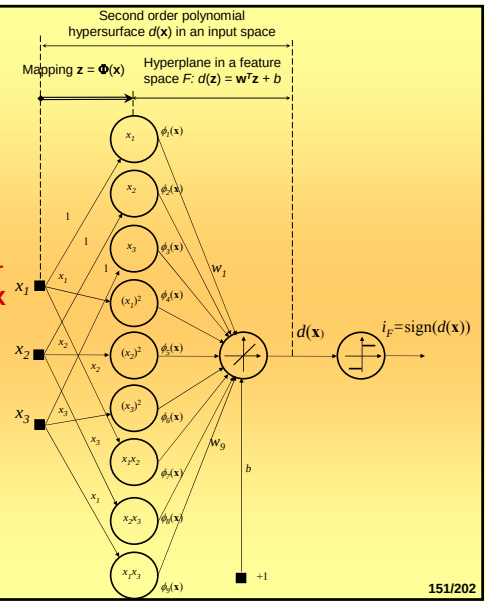


cont. **XOR problem - Gaussian RBF solution;**

The decision function $o = \exp(-\|\mathbf{x} - \mathbf{c}_1\|^2) + \exp(-\|\mathbf{x} - \mathbf{c}_2\|^2 - 1$, and its contours. The **red one** is for $o = 0$



SVMs arise from more complex mapping of an n-dimensional input vector $\mathbf{x} = [x_1\ x_2\ \ldots\ x_n]^T$ into a feature vector $\mathbf{z} = \Phi(\mathbf{x})$.



Now, we apply a '**kernel trick**'.

One basic idea in designing nonlinear SV machines is to map input vectors $\mathbf{x} \in \Re^n$ into vectors $\mathbf{z}$ of a higher dimensional *feature space* $F(\mathbf{z}) = \Phi(\mathbf{x})$ where Φ represents mapping: $\Re^n \to \Re^f$ and to solve a linear classification problem in this feature space

$$\mathbf{x} \in \Re^n \to \mathbf{z}(\mathbf{x}) = [a_1\phi_1(\mathbf{x}), a_2\phi_2(\mathbf{x}), \ldots, a_f\phi_f(\mathbf{x})]^T \in \Re^f$$

The solution for an indicator function $i_F(\mathbf{x}) = \mathrm{sign}(\mathbf{w}^T\mathbf{z}(\mathbf{x}) + b)$, which is a linear classifier in a feature space F, will create a nonlinear separating hypersurface in the original input space given by

$$i_F(\mathbf{x}) = \mathrm{sign}\left(\sum_{i=1}^{l} \alpha_i y_i \mathbf{z}^T(\mathbf{x})\mathbf{z}(\mathbf{x}_i) + b\right)$$

$$K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{z}_i^T\mathbf{z}_j = \Phi^T(\mathbf{x}_i)\Phi(\mathbf{x}_j).$$

Note that a *kernel function* $K(\mathbf{x}_i, \mathbf{x}_j)$ is a function in input space.

POLYNOMIAL KERNELS:

Let $x \in \Re^2$ i.e., $\mathbf{x} = [x_1 \quad x_2]^T$, and if we choose $\boldsymbol{\Phi}(\mathbf{x}) = [x_1^2 \quad \sqrt{2}x_1x_2 \quad x_2^2]^T$ (i.e., there is an $\Re^2 \to \Re^3$ mapping), then the dot product

$$\begin{aligned}\boldsymbol{\Phi}^T(\mathbf{x}_i)\boldsymbol{\Phi}(\mathbf{x}_j) &= [x_{i1}^2 \ \sqrt{2}x_{i1}x_{i2} \ x_{i2}^2][x_{j1}^2 \ \sqrt{2}x_{j1}x_{j2} \ x_{j2}^2]^T \\ &= [x_{i1}^2x_{j1}^2 + 2x_{i1}x_{i2}x_{j1}x_{i2} + x_{i2}^2x_{j2}^2] = (\mathbf{x}_i^T\mathbf{x}_j)^2 = K(\mathbf{x}_i,\mathbf{x}_j), \text{ or} \\ K(\mathbf{x}_i,\mathbf{x}_j) &= (\mathbf{x}_i^T\mathbf{x}_j)^2 = \boldsymbol{\Phi}^T(\mathbf{x}_i)\boldsymbol{\Phi}(\mathbf{x}_j)\end{aligned}$$

Note that in order to calculate the scalar product in a feature space $\boldsymbol{\Phi}^T(\mathbf{x}_i)\boldsymbol{\Phi}(\mathbf{x}_j)$ we do not need to perform the mapping $\boldsymbol{\Phi}(\mathbf{x}) = [x_1^2 \ \sqrt{2}x_1x_2 \ x_2^2]^T$ at all. Instead, we calculate this product directly in the input space by computing $(\mathbf{x}_i^T\mathbf{x}_j)^2$. This is very well known under the popular name of *the kernel trick*. Interestingly, note also that other mappings such as an

$\Re^2 \to \Re^3$ mapping given by $\boldsymbol{\Phi}(\mathbf{x}) = [x_1^2 - x_2^2 \ \ 2x_1x_2 \ \ x_1^2 + x_2^2]$, or an

$\Re^2 \to \Re^4$ mapping given by $\boldsymbol{\Phi}(\mathbf{x}) = [x_1^2 \ \ x_1x_2 \ \ x_1x_2 \ \ x_2^2]$

also accomplish the same task as $(\mathbf{x}_i^T\mathbf{x}_j)^2$.

Now, assume the following mapping

$$\boldsymbol{\Phi}(\mathbf{x}) = [1 \ \ \sqrt{2}x_1 \ \ \sqrt{2}x_2 \ \ \sqrt{2}x_1x_2 \ \ x_1^2 \ \ x_2^2],$$

i.e., there is an $\Re^2 \to \Re^5$ mapping plus bias term as the constant 6th dimension's value. Then the dot product in a feature space $\mathcal{S}$ is given as

$$\begin{aligned}\boldsymbol{\Phi}^T(\mathbf{x}_i)\boldsymbol{\Phi}(\mathbf{x}_j) &= 1 + 2x_{i1}x_{j1} + 2x_{i2}x_{j2} + 2x_{i1}x_{i2}x_{j1}x_{i2} + x_{i1}^2x_{j1}^2 + x_{i2}^2x_{j2}^2 \\ &= 1 + 2(\mathbf{x}_i^T\mathbf{x}_j) + (\mathbf{x}_i^T\mathbf{x}_j)^2 = (\mathbf{x}_i^T\mathbf{x}_j + 1)^2 = K(\mathbf{x}_i,\mathbf{x}_j), \text{ or} \\ K(\mathbf{x}_i,\mathbf{x}_j) &= (\mathbf{x}_i^T\mathbf{x}_j + 1)^2 = \boldsymbol{\Phi}^T(\mathbf{x}_i)\boldsymbol{\Phi}(\mathbf{x}_j)\end{aligned}$$

Thus, the last mapping leads to the second order *complete* polynomial.

The Curse of Dimensionality

Note that **over the *n* dimensional input space**, the number of monomial terms of degree less than or equal to *d* (i.e. **the feature space dimensionality**) explodes, and it can be calculated as

$$Feat\_Space\_Dim = \binom{n+d}{d}$$

n \ ***Degree d***	**2**	**3**	**4**
2	6	10	15
5	21	56	126
10	66	286	1001
50	1,326	23,426	316251
100	5,151	176,851	4,598,126
256	33,153	2,862,209	**186,043,585**

Kernel functions	**Type of classifier**
$K(\mathbf{x}, \mathbf{x}_i) = [(\mathbf{x}^T\mathbf{x}_i) + 1]^d$	Polynomial of degree *d*
$K(\mathbf{x},\mathbf{x}_i) = e^{-\frac{1}{2}[(\mathbf{x}-\mathbf{x}_i)^T\Sigma^{-1}(\mathbf{x}-\mathbf{x}_i)]}$	Gaussian RBF
$K(\mathbf{x}, \mathbf{x}_i) = \tanh[(\mathbf{x}^T\mathbf{x}_i) + b]^*$	Multilayer perceptron

*only for certain values of *b*

The learning procedure is the same as the construction of a 'hard' and 'soft' margin classifier in **x**-space previously.

Now, in **z**-space, the dual Lagrangian that should be maximized is

$$L_d(\alpha) = \sum_{i=1}^{l}\alpha_i - \frac{1}{2}\sum_{i,j=1}^{l} y_iy_j\alpha_i\alpha_j\mathbf{z}_i^T\mathbf{z}_j \qquad \text{or,}$$

$$L(\alpha) = -0.5\boldsymbol{\alpha}'\mathbf{H}\,\boldsymbol{\alpha} + \mathbf{1}'\boldsymbol{\alpha},$$

$$L_d(\alpha) = \sum_{i=1}^{l}\alpha_i - \frac{1}{2}\sum_{i,j=1}^{l} y_iy_j\alpha_i\alpha_jK(\mathbf{x}_i,\mathbf{x}_j)$$

$$\mathbf{H} = \mathbf{YY'}.*\mathbf{K}$$

and the constraints are

$$\alpha_i \geq 0, \qquad i = 1, l$$

In a more general case, because of a noise or generic class' features, there will be an overlapping of training data points. Nothing but constraints change as for the soft margin classifier above. Thus, the nonlinear 'soft' margin classifier will be the solution of the quadratic optimization problem given above subject to constraints

$$C \geq \alpha_i \geq 0, \qquad i = 1, l \qquad \text{and} \qquad \sum_{i=1}^{l}\alpha_iy_i = 0$$

The decision hypersurface is given by

$$\boxed{d(\mathbf{x}) = \sum_{i=1}^{l} y_i\alpha_iK(\mathbf{x},\mathbf{x}_i) + b}$$

We see that the final structure of the SVM is equal to the NN model.

In essence it is a weighted linear combination of some kernel (basis) functions. We'll show this (hyper)surfaces in simulations later.

In the case of NL SVMs we never, or only rarely, calculate a weight vector **w**. Solving NL SVM is performed in the so-called feature space which is of a very high, including infinite, dimension. In fact we don't need **w!!!** Instead we use *alphas* as follows (in S. Abe's book):

$$b = \frac{1}{|U|} \sum_{j \in U} \left(y_j - \sum_{i \in S} \alpha_i y_i K(\mathbf{x}_i, \mathbf{x}_j) \right)$$

$$D(\mathbf{x}) = \sum_{i \in S} \alpha_i \, y_i \, K(\mathbf{x}_i, \mathbf{x}) + b$$

where, U is a set of all *free* i.e., ***u**nbounded* SVecs, and S is a set of ***all*** SVecs

Regression

by

Support Vector Machines

Comparisons of some popular regression schemes

d is a dimension of the model. For NL models it corresponds to the # of HL neurons, i.e., to the # of SVs!

Method	Functional to minimize	Solution
Linear regression	$\Sigma e^2 = \Sigma(y - f(\mathbf{x}, \mathbf{w}))^2$ $d << l$	$f(\mathbf{x}, \mathbf{w}) = \mathbf{x}^T\mathbf{w}$ $\mathbf{w} = \mathbf{X}^+\mathbf{y}$
Ridge regression	$\Sigma e^2 = \Sigma(y - f(\mathbf{x}, \mathbf{w}))^2 + \lambda\|\|\mathbf{w}\|\|^2$ $d << l$	$f(\mathbf{x}, \mathbf{w}) = \mathbf{x}^T\mathbf{w}$ $\mathbf{w} = (\mathbf{X}\mathbf{X}^T + \lambda\mathbf{I})^{-1}\,\mathbf{X}^T\mathbf{y}$
RBF networks, **approximation**	$\Sigma e^2 = \Sigma(y - f(\mathbf{x}, \mathbf{w}))^2$ $d << l$	$f(\mathbf{x}, \mathbf{w}) = \Sigma_{i=1,d}\, w_i g(\mathbf{x} - \mathbf{c}_i)$ $\mathbf{w} = \mathbf{G}^+\mathbf{y}$, $\mathbf{c}_i$ is predefined
RBF networks, **interpolation**	$\Sigma e^2 = \Sigma(y - f(\mathbf{x}, \mathbf{w}))^2$ $d = l$	$f(\mathbf{x}, \mathbf{w}) = \Sigma_{i=1,l}\, w_i g(\|\|\mathbf{x} - \mathbf{x}_i\|\|)$ $\mathbf{w} = \mathbf{G}^{-1}\mathbf{y}$, $\mathbf{c}_i = \mathbf{x}_i$
Regularization Networks (RNs)	$\Sigma(y - f(\mathbf{x}, \mathbf{w}))^2 + \lambda\|\|f\|\|_{FS}^2$ $d = l$	$f(\mathbf{x}, \mathbf{w}) = \Sigma_{i=1,l}\, w_i g(\|\|\mathbf{x} - \mathbf{x}_i\|\|)$ $\mathbf{w} = (\mathbf{G} + \lambda\mathbf{I})^{-1}\mathbf{y}$, $\mathbf{c}_i = \mathbf{x}_i$
SVMs	$L_\varepsilon + \lambda\|\|f\|\|_{FS}^2$ # of SV << l	$f(\mathbf{x}, \mathbf{w}) = \Sigma_{i=1,l}\, w_i g(\|\|\mathbf{x} - \mathbf{x}_i\|\|)$ $\mathbf{w}$ by **QP**, $\mathbf{c}_i = \mathbf{x}_i$, but note that many $w_i = 0$, SPARSENESS

The crucial difference between RNs and SVMs is in a loss function used! Note that an **application of Vapnik's ε-insensitivity loss function L_ε** leads to QP learning and to the **sparse solution**. Only a fraction of data points is important! They are SVs! → Data compression!

Regression by SVMs

Initially developed for solving classification problems, SV techniques can be successfully applied in regression, i.e., for a functional approximation problems (Drucker et al, (1996), Vapnik et al, (1997)).

Unlike pattern recognition problems (where the desired outputs y_i are discrete values e.g., Boolean), here we deal with *real valued* functions.

Now, the general regression learning problem is set as follows;

the learning machine is given l training data from which it attempts to learn the input-output relationship (dependency, mapping or function) $f(\mathbf{x})$.

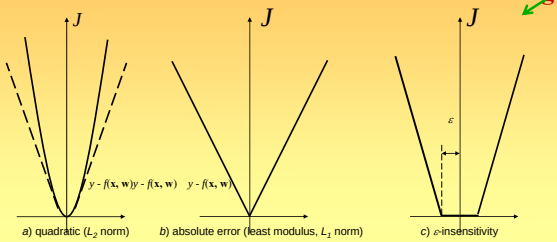
A training data set $D = \{[\mathbf{x}(i), y(i)] \in \Re^n \times \Re, i = 1,...,l\}$ consists of l pairs $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_l, y_l)$, where the inputs $\mathbf{x}$ are n-dimensional vectors $\mathbf{x} \in \Re^n$ and system responses $y \in \Re$, are continuous values. The SVM considers approximating functions of the form

$$f(\mathbf{x}, \mathbf{v}) = \sum_{i=1}^{N} v_i \varphi_i(\mathbf{x})$$

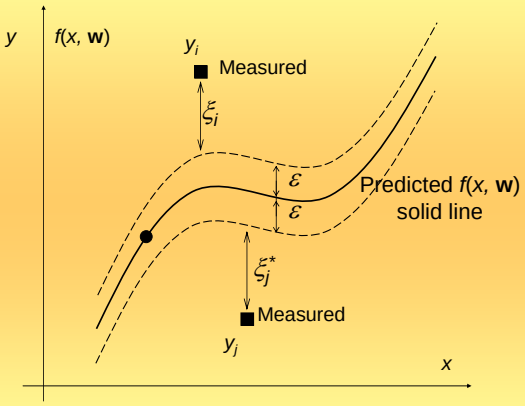
Vapnik introduced a more general error (loss) function - the so-called **ε-insensitivity loss function**

$$|y - f(\mathbf{x}, \mathbf{w})|_\varepsilon = \begin{cases} 0 & \text{if } |y - f(\mathbf{x}, \mathbf{w})| \le \varepsilon \\ |y - f(\mathbf{x}, \mathbf{w})| - \varepsilon, & \text{otherwise.} \end{cases}$$

Thus, the loss is equal to 0 if the difference between the predicted $f(\mathbf{x}, \mathbf{w})$ and the measured value is less than ε. Vapnik's ε-insensitivity loss function **defines an ε tube** around $f(\mathbf{x}, \mathbf{w})$. If the predicted value is within the tube the loss (error, cost) is zero. For all other predicted points outside the tube, the loss equals the magnitude of the difference between the predicted value and the radius ε of the tube. **See the next figure.**



a) quadratic (L_2 norm) b) absolute error (least modulus, L_1 norm) c) ε-insensitivity



The parameters used in (1-dimensional) support vector regression.

Now, minimizing risk R equals

$$R_{\mathbf{w}, \xi, \xi^*} = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_{i=1}^{l}\xi_i + C\sum_{i=1}^{l}\xi_i^*$$

and the constraints are,

$y_i - \mathbf{w}^T\mathbf{x}_i - b \le \varepsilon + \xi_i$, $\quad i = 1, l$,
$\mathbf{w}^T\mathbf{x}_i + b - y_i \le \varepsilon + \xi_i^*$, $\quad i = 1, l$,
$\xi_i \ge 0$ $\quad i = 1, l$,
$\xi_i^* \ge 0$ $\quad i = 1, l$,

where ξ and ξ^* are slack variables shown in previous figure for measurements **'above'** and **'below'** an ε-tube respectively. Both slack variables are positive values. Lagrange multipliers (that will be introduced during the minimization) α_i and α_i^* corresponding to ξ and ξ^* will be nonzero values for training points 'above' and 'below' an ε-tube respectively. Because no training data can be on both sides of the tube, either α_i or α_i^* will be nonzero. For data points inside the tube, both multipliers will be equal to zero.

Similar to procedures applied to SV classifiers, we solve this constrained optimization problem by forming a *primal variables Lagrangian* $L_p(\mathbf{w}, \xi, \xi^*)$ Step 1

$$L_p(\mathbf{w}, b, \xi, \xi^*, \alpha_i, \alpha_i^*, \beta_i, \beta_i^*) = \frac{1}{2}\mathbf{w}^T\mathbf{w} + C\sum_{i=1}^{l}\xi + \sum_{i=1}^{l}\xi^* - \sum_{i=1}^{l}\alpha_i^*\left[y_i - \mathbf{w}^T\mathbf{x}_i - b + \varepsilon + \xi_i^*\right]$$

$$-\sum_{i=1}^{l}\alpha_i\left[\mathbf{w}^T\mathbf{x}_i + b - y_i + \varepsilon + \xi_i\right] - \sum_{i=1}^{l}(\beta_i^*\xi_i^* + \beta_i\xi_i)$$

A primal variables Lagrangian $L_p(w_i, b, \xi, \xi^*, \alpha, \alpha^*, \beta, \beta^*)$ has to be *minimized* with respect to primal variables $\mathbf{w}$, b, ξ and ξ^* and *maximized* with respect to nonnegative LaGrange multipliers α, α^*, β and β^*. This problem can be solved again either in a ***primal space*** or in a ***dual*** one. Below, we consider a solution in a dual space. Applying Karush-Kuhn-Tucker (KKT) conditions for regression, we will *maximize a dual variables Lagrangian* $L_d(\alpha, \alpha^*)$ Step 3

$$L_d(\alpha, \alpha^*) = -\varepsilon\sum_{i=1}^{l}(\alpha_i^* + \alpha_i) + \sum_{i=1}^{l}(\alpha_i^* - \alpha_i)y_i - \frac{1}{2}\sum_{i,j=1}^{l}(\alpha_i^* - \alpha_i)(\alpha_j^* - \alpha_j)\mathbf{x}_i^T\mathbf{x}_j$$

subject to constraints

$$\sum_{i=1}^{l} \alpha_i^* = \sum_{i=1}^{l} \alpha_i$$
$$0 \le \alpha_i^* \le C \qquad i = 1, l,$$
$$0 \le \alpha_i \le C \qquad i = 1, l.$$

Note that **a dual variables Lagrangian $L_d(\boldsymbol{\alpha}, \boldsymbol{\alpha}^*)$ is expressed in terms of LaGrange multipliers $\boldsymbol{\alpha}$ and $\boldsymbol{\alpha}^*$ only**, and that - the size of the problem, with respect to the size of an SV classifier design task, is doubled now.

There are $2l$ unknown multipliers for linear regression and the Hessian matrix **H** of the quadratic optimization problem in the case of regression is a $(2l, 2l)$ matrix.

The ***standard quadratic optimization problem*** above can be expressed in a ***matrix notation*** and formulated as follows:

Maximize Step 3 in a matrix form

$$L_d(\alpha) = -0.5\boldsymbol{\alpha}^T\mathbf{H}\,\boldsymbol{\alpha} + \mathbf{f}^T\boldsymbol{\alpha},$$

subject to constraints above where for a **linear regression**,

$\mathbf{G} = [\mathbf{x}^T\mathbf{x} + 1]$, $\mathbf{f} = [\varepsilon - y_1\ \varepsilon - y_2, \ldots, \varepsilon - y_l, \varepsilon + y_1, \varepsilon + y_2, \ldots, \varepsilon + y_{2l}]$.

More interesting, common and challenging problem is to aim at solving the ***nonlinear regression tasks***. Here, similar as in the case of nonlinear classification, this will be achieved by considering a linear regression hyperplane in the so-called *feature space.*

Thus, we use the same basic idea in designing SV machines for creating a nonlinear regression function.

We map input vectors $\mathbf{x} \in \Re^n$ into vectors **z** of a higher dimensional *feature space F* ($\mathbf{z} = \boldsymbol{\Phi}(\mathbf{x})$ where $\boldsymbol{\Phi}$ represents mapping: $\Re^n \rightarrow \Re^f$) and **we solve a linear regression problem in this feature space.**

A mapping $\boldsymbol{\Phi}(\mathbf{x})$ is again chosen in advance. Such an approach again leads to solving a quadratic optimization problem with inequality constraints in a **z**-space. The solution for an regression hyperplane $f = \mathbf{w}^T\mathbf{z}(\mathbf{x}) + b$ which is linear in a feature space F, will create a nonlinear regressing hypersurface in the original input space. In the case of nonlinear regression, after calculation of LaGrange multiplier vectors $\boldsymbol{\alpha}$ and $\boldsymbol{\alpha}^*$, we can find an optimal desired weight vector of the *kernels expansion* $\mathbf{v}_o$ as Step 4

$$\mathbf{v}_o = \boldsymbol{\alpha}^* - \boldsymbol{\alpha},$$

and an optimal bias b_o can be found from $b_o = \frac{1}{l}\sum_{i=1}^{l}(y_i - g_i)$.

where $\mathbf{g} = \mathbf{G}\,\mathbf{v}_o$ and the matrix **G** is a corresponding design matrix of given RBF kernels.

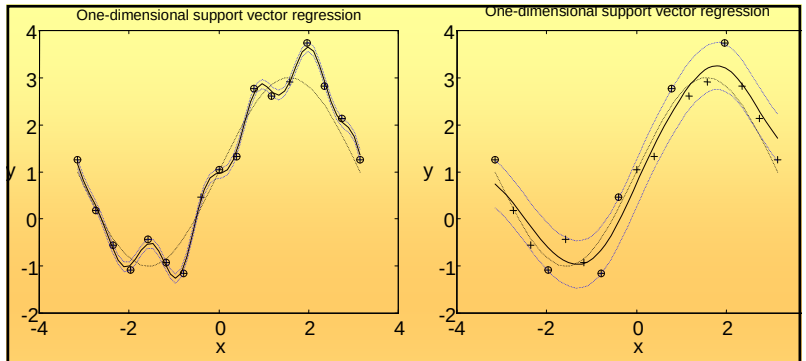
Step 5

The best nonlinear regression hyperfunction is given by

$$z = f(\mathbf{x}, \mathbf{v}) = \mathbf{G}\mathbf{v} + b.$$

There are a few learning parameters in constructing SV machines for regression. The two most relevant are **the insensitivity zone *e*** and the **penalty parameter *C*** that determines the trade-off between the training error and VC dimension of the model. **Both parameters should be chosen by the user.**

Generally, an increase in an insensitivity zone *e* has smoothing effects on modeling highly noisy polluted data. Increase in *e* means a reduction in requirements on the accuracy of approximation. It decreases the number of SVs leading to data compression too. See the next figures.



The influence of **a insensitivity zone *e* on modeling quality.** *A* nonlinear SVM creates a regression function with **Gaussian kernels** and models a highly polluted (25% noise) sinus function (dashed). 17 measured training data points (plus signs) are used.

Left: *e* = 0.1. 15 SV are chosen (encircled plus signs).

Right: *e* = 0.5. 6 chosen SV produced a much better regressing function.

Some of the constructive problems:

The SV training works almost perfectly for not too large data basis.

However, when the number of data points is large (say $l > 2000$) the QP problem becomes extremely difficult to solve with standard methods. For example, a training set of **50,000 examples amounts to a Hessian matrix H with $2.5*10^9$ (2.5 billion) elements. Using an 8-byte floating-point representation we need 20,000 Megabytes = 20 Gigabytes of memory** (Osuna et al, 1997). This cannot be easily fit into memory of present standard computers.

There are three, now classic, approaches that resolve the QP for large data sets. Vapnik in (**Vapnik, 1995**) proposed the ***chunking method*** that is the decomposition approach. Another decomposition approach is proposed in (**Osuna, Girosi, 1997**). The sequential minimal optimization (**Platt, 1997**) algorithm is of different character (works with 2 data points at the time) and it seems to be an 'error back propagation' for a SVM learning.

The newest iterative single data (per-pattern) algorithm (Kecman, Vogt, Huang, 2003; Huang, Kecman, 2004) seems to be the fastest for a huge data sets (say, for more than a few hundred thousands data pairs) at the moment!

Let us conclude the presentation of SVMs by summarizing the basic constructive steps that lead to SV machine:

- **selection of the kernel function that determines the shape of the decision and regression function in classification and regression problems respectively,**
- **selection of the 'shape', i.e., 'smoothing' parameter in the kernel function (for example, polynomial degree and variance of the Gaussian RBF for polynomials and RBF kernels respectively),**
- **choice of the penalty factor *C* and selection of the desired accuracy by defining the insensitivity zone *e*,**
- **solution of the QP problem in *l* and 2*l* variables in the case of classification and regression problems respectively.**

Now, we introduce and discuss the iterative algorithm known as Iterative Single Data Algorithm ISDA aimed at solving huge data set problems iteratively.

There is also an interesting approach for medium sized data sets based on an Active Set method see the chapters below

Kecman, V., T. M. Huang, M. Vogt, Chapter 'Iterative Single Data Algorithm for Training Kernel Machines from Huge Data Sets: Theory and Performance', in a Springer-Verlag book, 'Support Vector Machines: Theory and Applications', Ed. L. Wang, 2005

Vogt, M., V. Kecman, Chapter 'Active-Set Methods for Support Vector Machines', in a Springer-Verlag book, 'Support Vector Machines: Theory and Applications', Ed. L. Wang, 2005

Both chapters are downloadable from: http://www.support-vector.ws

Lecture on ISDA will be focused on*:

- **Classification und Regression Settings of SVMs**
- **QP Based Learning,**
  - **Huge Data Sets Issues,**
  - **Implementation and Tools**
- **Per-Pattern (Single Data) Learning for SVMs**
  - **Without the Bias Term**
  - **With the Bias Term**
- **Summary**

*** First few slides are taken from M. Vogt's presentation of our joint ESANN 2003 paper**

SVMs Linear Classification Learning Setting

Dual Problem:

$$L_{\mathrm{d}} = -\tfrac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}\alpha_i\alpha_j y_i y_j \mathbf{x}_i^{\mathrm{T}}\mathbf{x}_j + \sum_{i=1}^{N}\alpha_i = \max_{\boldsymbol{\alpha}}$$

s.t. $0 \le \alpha_i \le C$ for $i = 1, \ldots, N$

$$\sum_{i=1}^{N}\alpha_i y_i = 0$$

SVMs Linear Regression Learning Setting

Dual Problem:

$$L_{\mathrm{d}} = -\tfrac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N}(\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*)\mathbf{x}_i^{\mathrm{T}}\mathbf{x}_j - \varepsilon\sum_{i=1}^{N}(\alpha_i + \alpha_i^*) + \sum_{i=1}^{N}(\alpha_i - \alpha_i^*)\, y_i = \max_{\boldsymbol{\alpha}}$$

s.t. $0 \le \alpha_i, \alpha_i^* \le C$ for $i = 1, \ldots, N$

$$\sum_{i=1}^{N}(\alpha_i - \alpha_i^*) = 0$$

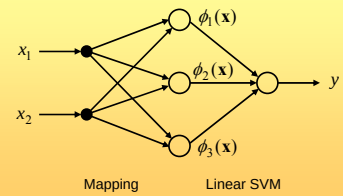
Final solution is:

$$f(\mathbf{x}) = \sum_{i=1}^{N}\left\{\begin{matrix}\alpha_i y_i \\ \alpha_i - \alpha_i^*\end{matrix}\right\} * \mathbf{x}_i^T\mathbf{x} + b$$

classification

regression

Nonlinear SVMs



Kernel-Function: $k(\mathbf{x},\mathbf{y}) = \boldsymbol{\Phi}^{\mathrm{T}}(\mathbf{x})\cdot\boldsymbol{\Phi}(\mathbf{y})$

New at NL SVM:
- Scalar product is replaced by the Kernel-Function.
- Kernel-Function is usually **positive definite.**
- Support Vectors Representation of an NL SVM is:

$$f(\mathbf{x}) = \sum_{i=1}^{N}\left\{\begin{matrix}\alpha_i y_i \\ \alpha_i - \alpha_i^*\end{matrix}\right\} k(\mathbf{x}_i, \mathbf{x}) + b$$

classification

regression

Solving the SVM QP-Problems

Matrix formulation: maximize $L_d(\boldsymbol{\alpha}) = -\tfrac{1}{2}\boldsymbol{\alpha}^T\mathbf{K}\boldsymbol{\alpha} + \mathbf{f}^T\boldsymbol{\alpha}$

subject to 1) $0 \le \alpha_i, \alpha_i^* \le C,\ i = 1, \ldots, l$

and 2) equality constraint if working with bias *b*

Various Solution's Methods Possible:

- Interior-Point: precise, batch, not suitable for huge data sets.
- Active-Set (NNLS): robust, relative slow, memory prop. to # of SVecs.
- Gradient projection: fast in finding active sets (M. Vogt).
- Working-Set (chunking, SMO, ISDA): for huge data sets, iterative.

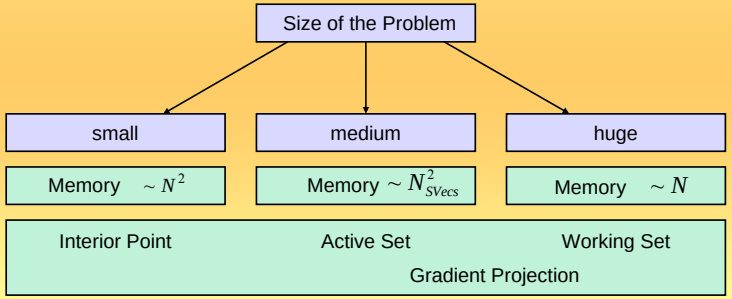
Available Software:

- Interior-Point: Universal-Routines, e.g., LOQO, CPLEX, MOSEK, Quadprog in matlab, ...
- Working-Set: SVM^{light}, mySVM, SVMTorch, (Hero-SVMs (?))...

  SMO, 2 data only: LibSVM, NodeLib, ...
- Partly available (acc. to M. Vogt): ν-SVM
- Special routines, e.g., LS-SVMlab.

Optimizing Algorithms*

Goals:
- Speed
- Memory requirements
- Accuracy
- Suitability for SVMs-Problems



* Graph taken from M. Vogt

What follows is an exploitition of the ‘nice‘(?) property of the

POSITIVE DEFINITE kernels

that they do not require bias term *b*

in an NL SVM model

$$f(\mathbf{x}) = \sum_{i=1}^{N} \begin{Bmatrix} \alpha_i y_i \\ \alpha_i - \alpha_i^* \end{Bmatrix} k(\mathbf{x}_i, \mathbf{x}) + \cancel{b}$$

classification

regression

First, however, just an attempt to visualize the mapping to the feature space by using Gaussians with and without bias.

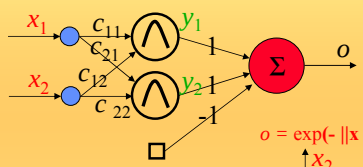
It should necessarily be **only two SVecs** so that the visualization is possible,

and it will be the beloved XOR example!

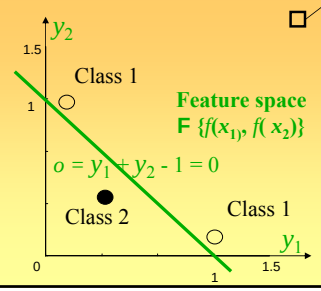
XOR problem - Gaussian RBF solution WITH BIAS TERM. We choose two Gaussians only, i.e., a dimension of a feature space is 2: $c_1 = [1\ 1]^T$ and $c_2 = [0\ 0]^T$.

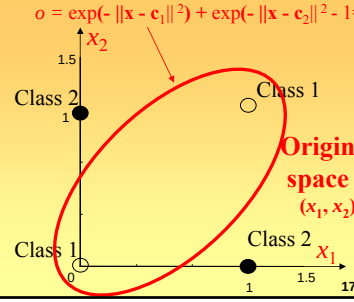
This is a following mapping: y = [exp(- ||x - c$_1$||^2) exp(- ||x - c$_2$||^2)]^T. Hence, **x -> y:**

[0 0] -> [0.135 1], [1 1] -> [1 0.135], [1 0] -> [0.368 0.368], [0 1] -> [0.368 0.368]. The following NN, will produce linear separation boundary in a feature space and the NL one in the original space.



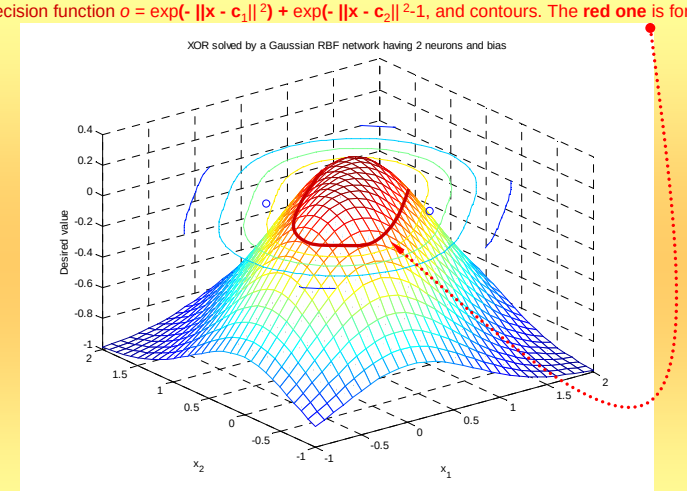
$o = \exp(- \|x - c_1\|^2) + \exp(- \|x - c_2\|^2 - 1 = 0$





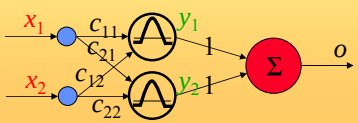
cont. **XOR problem - Gaussian RBF solution WITH EXPLICIT BIAS;**

The decision function o = exp(- ||x - c$_1$||^2) + exp(- ||x - c$_2$||^2-1, and contours. The **red one** is for o=0

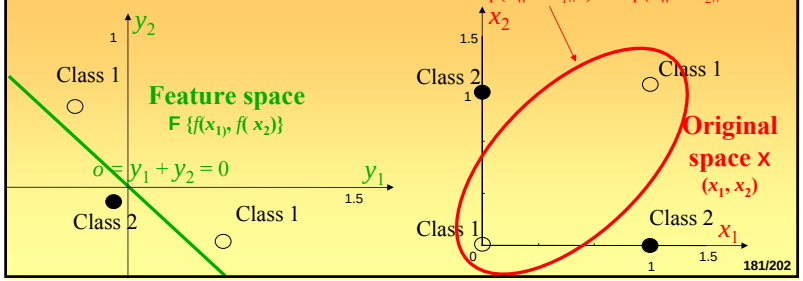


XOR problem - Gaussian RBF solution WITHOUT EXPLICIT BIAS TERM. Two Gaussians only, i.e., a dimension of a feature space is 2: $c_1 = [1\ 1]^T$ and $c_2 = [0\ 0]^T$.

Mapping now is: $y = [\exp(-\|x - c_1\|^2)-0.5 \quad \exp(-\|x - c_2\|^2)-0.5]^T$. Hence, **x -> y:**
[0 0] -> [-0.365 0.5], [1 1] -> [0.5 -0.365], [1 0] -> [-0.132 -0.132], [0 1]->[-0.132 -0.132].
The following NN, will also produce linear separation boundary in a feature space and the same (because of adding -0.5) NL one in the original space.

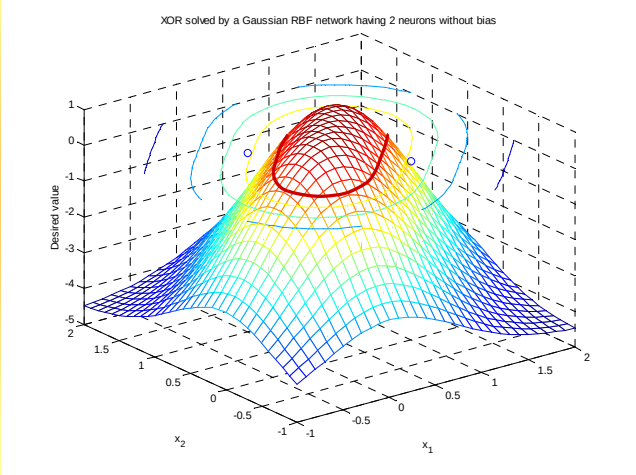


$o = \exp(-\|x - c_1\|^2) + \exp(-\|x - c_2\|^2 - 1=0$



cont. **XOR problem - Gaussian RBF solution WITHOUT EXPLICIT BIAS term *b*;**

The decision function $o = w_1(\exp(-\|x - c_1\|^2)-0.5) + w_2(\exp(-\|x - c_2\|^2)-0.5)$, and its contours. The red one is for $o = 0$, $w_1=w_2=4.5335$



We first show the equality of three (actually four) approaches (Kecman, Vogt, Huang, 2003, ESANN conference) in an iterative machine learning, namely the equality of the

KERNEL ADATRON ALGORITHM,

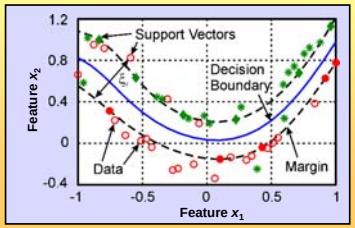
SEQUENTIAL MINIMAL OPTIMIZATION,

GAUSS-SEIDEL (GS) METHOD for solving a system of linear equations,

and its derivative SUCCESSIVE-OVER-RELAXATION (SOR) METHOD for solving a system of linear equations.

Support Vector Machine Classification

	SVM	SMO	KA	GS
Class.	✓			
Regr.				



SVM Output: Decision function

$$y = \sum_{i=1}^{l} \alpha_i y_i K(\mathbf{x}_i, \mathbf{x}) + \cancel{b}$$

$K(\mathbf{x}_i, \mathbf{x})$: Kernel function

α_i: Dual variables

maximize $$L_d(\boldsymbol{\alpha}) = \sum_{i=1}^{l} \alpha_i - \frac{1}{2}\sum_{i=1}^{l}\sum_{j=1}^{l} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

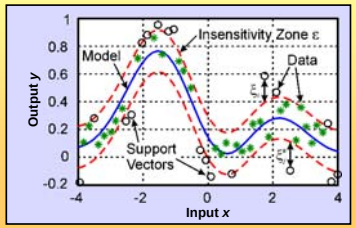
subject to $0 \le \alpha_i \le C, \quad i = 1, \ldots, l$

$$\cancel{\sum_{i=1}^{l} \alpha_i y_i = 0}$$

SVM classification without bias term:
- for positive definite kernels
- equality constraint vanishes

Support Vector Machine Regression

	SVM	SMO	KA	GS
Class.				
Regr.	✓			



SVM Output: Regression function

$$y = \sum_{i=1}^{l} (\alpha_i - \alpha_i^*) K(\mathbf{x}_i, \mathbf{x}) + \cancel{b}$$

$K(\mathbf{x}_i, \mathbf{x})$: Kernel function

α_i, α_i^*: Dual variables, $\alpha_i \cdot \alpha_i^* = 0$

maximize $$L_\mathrm{d} = \sum_{i=1}^{l} (\alpha_i - \alpha_i^*) y_i - \varepsilon \sum_{i=1}^{l} (\alpha_i + \alpha_i^*) - \frac{1}{2} \sum_{i=1}^{l} \sum_{j=1}^{l} (\alpha_i - \alpha_i^*)(\alpha_j - \alpha_j^*) K(\mathbf{x}_i, \mathbf{x}_j)$$

subject to $0 \le \alpha_i, \alpha_i^* \le C, \quad i = 1, \ldots, l$

$$\cancel{\sum_{i=1}^{l} (\alpha_i - \alpha_i^*) = 0}$$

SVM regression without bias term:
- for positive definite kernels
- equality constraint vanishes

Sequential Minimal Optimization for SVM Classification without Bias Term

	SVM	SMO	KA	GS
Class.		✓		
Regr.				

Concept: QP optimization of a subset of $\alpha_1, \ldots, \alpha_l$
- Standard SMO: 2 parameters per step
- SMO without bias term: 1 parameter per step

(Suggested by V. Kecman and developed by M. Vogt)

Update rule:

$$\Delta\alpha_i = -\frac{y_i E_i}{K(\mathbf{x}_i, \mathbf{x}_i)}$$
$$\alpha_i \leftarrow \min\{\max\{\alpha_i + \Delta\alpha_i, 0\}, C\}$$

with $E_i = f_i - y_i$

Optimality check: Karush-Kuhn-Tucker (KKT) conditions

$$\alpha_i < C \quad \wedge \quad y_i E_i < -\tau$$
$$\alpha_i > 0 \quad \wedge \quad y_i E_i > \tau$$

Kernel AdaTron Optimization for SVM Classification without Bias Term

	SVM	SMO	KA	GS
Class.			✓	
Regr.				

Concept: Gradient method for $\alpha_1, \ldots, \alpha_l$

Update rule:

$$\Delta\alpha_i = -\eta_i \frac{\partial L_\mathrm{d}}{\partial \alpha_i} = -\eta_i \cdot y_i E_i$$
$$\alpha_i \leftarrow \min\{\max\{\alpha_i + \Delta\alpha_i, 0\}, C\}$$

with $E_i = f_i - y_i$

Optimality check: Change in dual variables

Equality: Update rules for SMO and KA are identical for classification

- if SVMs are used without bias term
- optimal learning rate $\eta_i = \dfrac{1}{K(\mathbf{x}_i, \mathbf{x}_i)}$

Sequential Minimal Optimization for SVM Regression without Bias Term

	SVM	SMO	KA	GS
Class.				
Regr.		✓		

Concept: QP optimization of a subset of $(\alpha_1, \alpha_1^*), \ldots, (\alpha_l, \alpha_l^*)$
- Standard SMO: 2 parameters per step
- SMO without bias term: 1 parameter per step

(Suggested by V. Kecman and developed by M. Vogt)

Update rule:

$$\Delta\alpha_i = -\alpha_i^* - \frac{\varepsilon + E_i}{K(\mathbf{x}_i, \mathbf{x}_i)}, \quad \Delta\alpha_i^* = -\alpha_i - \frac{\varepsilon - E_i}{K(\mathbf{x}_i, \mathbf{x}_i)}$$
$$\alpha_i \leftarrow \min\{\max\{\alpha_i + \Delta\alpha_i, 0\}, C\}$$
$$\alpha_i^* \leftarrow \min\{\max\{\alpha_i^* + \Delta\alpha_i^*, 0\}, C\}$$

Optimality check: Karush-Kuhn-Tucker (KKT) conditions

$$\alpha_i < C \quad \wedge \quad \varepsilon + E_i < -\tau$$
$$\alpha_i > 0 \quad \wedge \quad \varepsilon + E_i > \tau$$
$$\alpha_i^* < C \quad \wedge \quad \varepsilon - E_i < -\tau$$
$$\alpha_i^* > 0 \quad \wedge \quad \varepsilon - E_i > \tau$$

Kernel AdaTron Optimization for SVM Regression without Bias Term

	SVM	SMO	KA	GS
Class.				
Regr.			✓	

Developed by K. Veropoulos

Concept: Gradient method for $(\alpha_1, \alpha_1^*), \ldots, (\alpha_l, \alpha_l^*)$

Update rule:

$$\Delta\alpha_i = -\eta_i \frac{\partial L_d}{\partial \alpha_i} = -\eta_i(\varepsilon + E_i)$$

$$\Delta\alpha_i^* = -\eta_i \frac{\partial L_d}{\partial \alpha_i^*} = -\eta_i(\varepsilon - E_i)$$

$$\alpha_i \leftarrow \min\{\max\{\alpha_i + \Delta\alpha_i, 0\}, C\}$$

$$\alpha_i^* \leftarrow \min\{\max\{\alpha_i^* + \Delta\alpha_i^*, 0\}, C\}$$

Note that this is slightly different from our SMO algorithm because Veropoulos did not care for the geometrical fact that $\alpha_i \alpha_i^* = 0$

Optimality check: Change in dual variables

Equality: Update rules for SMO and our adaptation of the KA are identical for regression

- if SVMs are used without bias term
- optimal learning rate $\eta_i = \dfrac{1}{K(\mathbf{x}_i, \mathbf{x}_i)}$

Gauss-Seidel Method for Support Vector Machines

	SVM	SMO	KA	GS
Class.				✓
Regr.				✓

Matrix formulation: maximize $L_d(\boldsymbol{\alpha}) = -\frac{1}{2}\boldsymbol{\alpha}^T \mathbf{K}\boldsymbol{\alpha} + \mathbf{f}^T\boldsymbol{\alpha}$

subject to $0 \le \alpha_i \le C, \quad i = 1, \ldots, l$

Gauss-Seidel: Coordinate-ascent based method for $\dfrac{\partial L_d}{\partial \boldsymbol{\alpha}} = \mathbf{0} \Leftrightarrow \mathbf{K}\boldsymbol{\alpha} = \mathbf{f}$

Update rule:

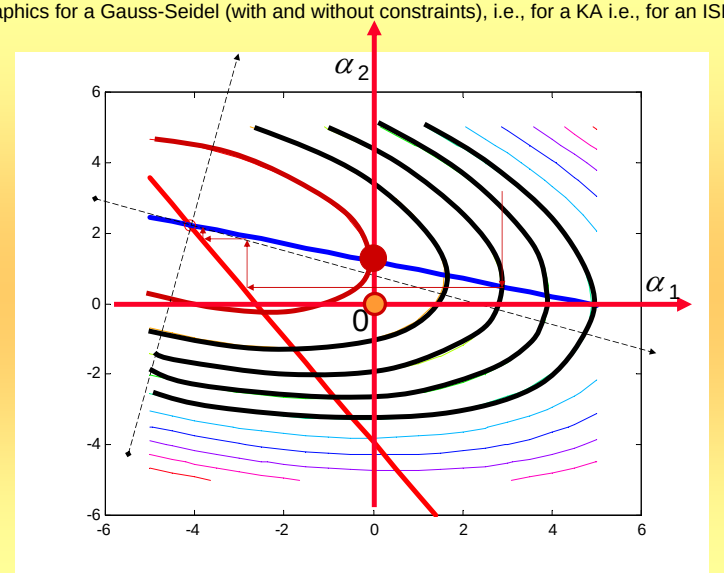
$$\Delta\alpha_i = -\frac{1}{K(\mathbf{x}_i, \mathbf{x}_i)} \cdot \frac{\partial L_d}{\partial \alpha_i}$$

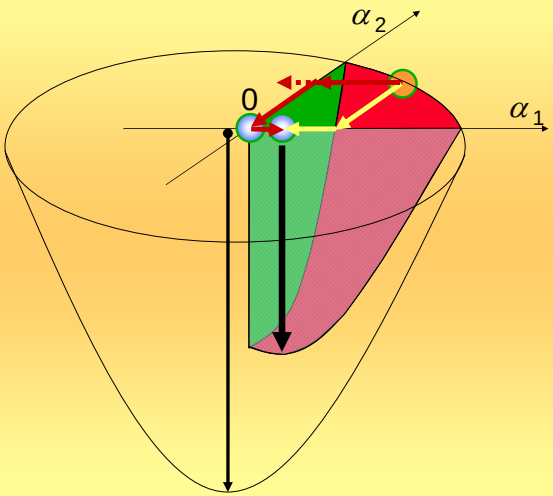
Equality: GS is equal to SMO and KA, if box constraints are considered

Convergence:

- Standard proof for positive definite matrices
- Adaptions for inequality constraints
- Also valid for SMO and KA (w.b.t.)

Graphics for a Gauss-Seidel (with and without constraints), i.e., for a KA i.e., for an ISDA





Conclusions on Equality of SMO, KA and GS (SOR) for an ISDA without the Bias Term

- SMO and KA are equal for **a classification**
  - if SVMs are used without bias term
  - and optimal learning rate $\eta_i = 1/K(\mathbf{x}_i, \mathbf{x}_i)$
- SMO and KA are equal for **an regression**
  - for the same conditions as above
  - and adapted version of the KA algorithm
- Gauss-Seidel Method
  - is also equal to SMO and KA
  - allows the proof of the convergence of all 3 methods

However, the very first comparisons of our ISDA algorithm with the LIBSVM on MNIST data (60,000 train.; 10,000 test) and other data sets, have shown similar generalizations properties but there were **about 25 % more SVecs** in our **models without bias term!**

* Having less SVecs is often very desirable for the sake of data (information) compression.

* At the same time, more SVecs prolonged the training time.

And, thus, in order to

- **reduce the number of SVecs as well as to,**
- **speed up the learning stage,**

we incorporated the bias term *b* and its calculation into the ISDA.

(this is shown in a submitted paper to ESANN 2004).

Iterative Single Data Algorithm (ISDA) for SVMs with Bias

Our original QP problem in NL classification is to solve

$$\min\ 0.5\mathbf{w}^T\mathbf{w} \qquad \textbf{(CF)}$$

$$\text{s.t.} \quad y_i[\ \mathbf{w}^T\Phi(\mathbf{x}_i)+b\ ] \geq 1, \qquad i = 1, \ldots, l$$

which can be transformed into its dual form by minimizing the primal Lagrangian in respect to **w** and *b*, by using $\partial L_p / \partial \mathbf{w} = 0$ and $\partial L_p / \partial b = 0$.

The standard change to a dual problem is to substitute **w** into the primal Lagrangian and this leads to a dual Lagrangian problem below,

$$L_d(\alpha) = \sum_{i=1}^{l} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{l} y_i y_j \alpha_i \alpha_j K(\mathbf{x}_i, \mathbf{x}_j) - \sum_{i=1}^{l} \alpha_i y_i b$$

subject to the box constraints and, in a standard SVMs formulation, also to the equality constraint as given below:

$$0 \leq \alpha_i \leq C, \quad i = 1, \ldots, l \qquad \sum_{i=1}^{l} \alpha_i y_i = 0$$

There are ***three major avenues*** (procedures, algorithms) possible in solving the dual problem above:

1. The first method is **the standard SVMs algorithm** which **needs at least 2 data**, imposes the equality constraint during the optimization and in this way ensures that the solution never leaves a feasible region. **In this case the last term in a dual Lagrangian above vanishes.**

   After the dual problem is solved, the bias term is calculated by using the *unbounded* support vectors.

2. The second method augments the cost function (CF) with the term $0.5kb^2$ (where $k > 0$). This step **equals to solving the dual problem by penalty method** where a decrease in *k* leads to the stronger imposing of equality constraints (see comments in a paper). After forming the primal Lagrangian one arrives at the **dual one, not containing the explicit bias *b*,** and

   ISDA for the classification boils down to iterative solving the following Lin. Syst.

$$\mathbf{K}_k \boldsymbol{\alpha} = \mathbf{1}_l, \qquad s.t. \qquad 0 \leq \alpha_i \leq C,\ i = 1, \ldots, l$$

   where

$$K_k(\mathbf{x}_i, \mathbf{x}_j) = y_i y_j \left(K(\mathbf{x}_i, \mathbf{x}_j) + \frac{1}{k} \right)$$

   after α_i-s are found one finds the bias *b* from or as in method 1.

$$b = \frac{1}{k} \sum_{j=1}^{\#SVecs} \alpha_j y_j$$

3. ***The third method*** in implementing the ISDA for SVMs with the bias term *b* is to work with original cost function (CF) and keep imposing the equality constraints during the iterations as suggested in (Veropoulos, 2001). The learning starts with ***b* = 0** and **after each epoch** the bias *b* is updated by applying a secant method as follows

$$b^k = b^{k-1} - \omega^{k-1} \frac{b^{k-1} - b^{k-2}}{\omega^{k-1} - \omega^{k-2}}$$

where $\omega = \sum_{i=1}^{l} \alpha_i y_i$ in the classification, and

$\omega = \sum_{i=1}^{l} \left(\alpha_i - \alpha_i^*\right)$ in the regression.

Now, some experimental results on the MNIST benchmark data set

576 dimensional input, 60,000tr, 10,000 test data

Table 1: Simulation time for different algorithms

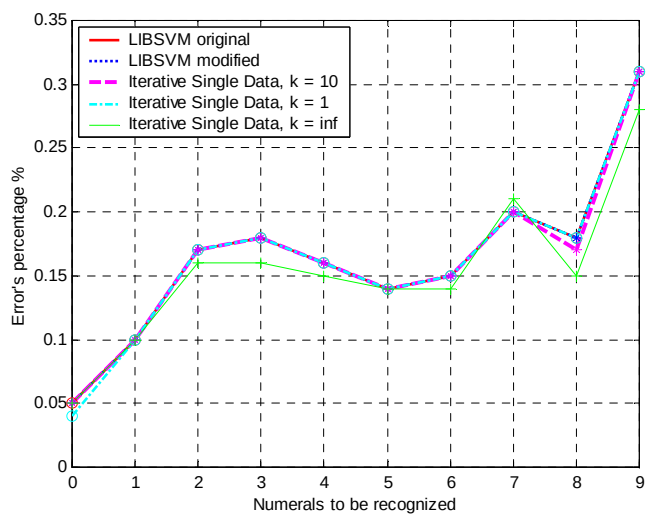
	LIBSVM original	LIBSVM modified	Iterative single data algorithm (ISDA) $k = 10$	$k = 1$	$k = \infty$
Class	Time(sec)	Time(sec)	Time(sec)	Time(sec)	Time(sec)
0	1606	885	**794**	800	1004
1	740	**465**	491	490	855
2	2377	1311	**1181**	1398	1296
3	2321	1307	**1160**	1318	1513
4	1997	1125	**1028**	1206	1235
5	2311	1289	**1143**	1295	1328
6	1474	818	**754**	808	1045
7	2027	1156	**1026**	2137	1250
8	2591	1499	**1321**	1631	1764
9	2255	1266	**1185**	1410	1651
Time Increase	**+95.3%**	**+10.3%**	**0**	**+23.9%**	**+28.3%**

Table 2: Number of support vectors for each algorithm

	LIBSVM original	LIBSVM modified	Iterative single data algorithm (ISDA) $k = 10$	$k = 1$	$k = \infty$
Class	# SV (BSV)	# SV (BSV)	# SV (BSV)	# SV (BSV)	# SV (BSV)
0	2172 (0)	2172 (0)	2132 (0)	2162 (0)	**2682** (0)
1	1440 (4)	1440 (4)	1453 (4)	1429 (4)	**2373** (4)
2	3055 (0)	3055 (0)	3017 (0)	3047 (0)	**3327** (0)
3	2902 (0)	2902 (0)	2897 (0)	2888 (0)	**3723** (0)
4	2641 (0)	2641 (0)	2601 (0)	2623 (0)	**3096** (0)
5	2900 (0)	2900 (0)	2856 (0)	2884 (0)	**3275** (0)
6	2055 (0)	2055 (0)	2037 (0)	2042 (0)	**2761** (0)
7	2651 (4)	2651 (4)	2609 (4)	3315 (4)	**3139** (4)
8	3222 (0)	3222 (0)	3226 (0)	3267 (0)	**4224** (0)
9	2702 (2)	2702 (2)	2756 (2)	2733 (2)	**3914** (2)
Average # of SV	**2574**	**2574**	**2558**	**2639**	**3151**

BSV = Bounded SVs

The percentage of the error on the test data



SUMMARY

- The per-pattern (ISDA) based learning for the SVMs is possible for both the classification and regression, and can be very effective for the huge data sets.
- In the case of positive definite kernels, ISDA without a bias term equals to KA, SMO, GS and SOR algorithm.
- The models generated by ISDAs (either with or without the bias term *b*) seem to be as good as the standard QP (i.e., SMO) based algorithms in terms of a generalization performance.
- Moreover, ISDAs with an appropriate *k* value are faster than the standard SMO algorithms on large scale classification problems.
- The behavior and performance of the ISDA should be tested on other (notably, positive semidefinite) kernels.

Let us conclude the part on a comparisons between the SVMs and NNs

- both the NNs and SVMs learn from experimental data,
- both the NNs and SVMs are universal approximators in the sense that they can approximate any function to any desired degree of accuracy,
- after the learning they are given with the same mathematical model, as the sum of weighted basis (kernel) funstions, and they can be presented graphically with the same so-called NN's graph,
- they differ by the learning method used. While NNs typically use either EBP (or some more sophisticated gradient descent algorithm) or some other linear algebra based approach, the SVMs learn by solving the QP or LP problem.