CSE276C - Regression and Classification

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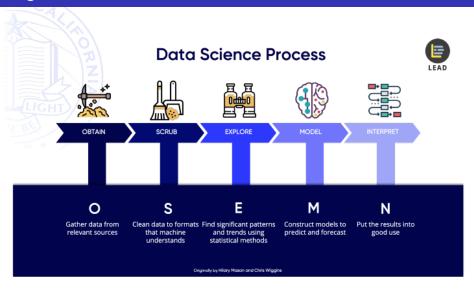
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Introduction

- Data science is a big part of robotics
- Many aspects of robotics rely on data analysis
 - Recognition of objects
 - Adpative Control
 - Clean-up of sensor information

• ..

A general framework



Outline

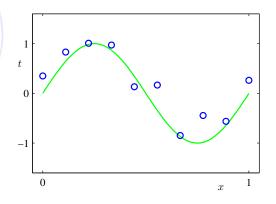
- Introduction Regression
- 2 Preliminaries
- 3 Linear Basis Function Models
- 4 Bayesian Linear Regression
- 5 Bayesian Model Comparison
- 6 Regression Summary
- Classification
- 8 Linear Discriminant Functions
- Use LSQ for Classification
- Fisher's Discriminant Method
- Perceptrons
- Summary

Introduction

- The objective of regression is to enable prediction of a value based on modeling over a dataset X.
- Consider a set of D observations over a space
- How can we generate estimates for the future?
 - Battery time?
 - Time to completion?
 - Position of doors?

Introduction (2)

Example



$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_m x^m = \sum_{i=0}^m w_i x^i$$

Introduction (3)

- In general the functions could be beyond simple polynomials
- The "components" $(\phi_i(x))$ are termed basis functions, i.e.

$$y(x, \mathbf{w}) = \sum_{i=0}^{m} w_i \phi_i(x) = \vec{w}^T \phi(\vec{x})$$

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Loss Function

For optimization we need a penalty / loss function

Expected loss is then

$$E[L] = \int \int L(t, y(x)) p(x, t) dx dt$$

• For the squared loss function we have

$$E[L] = \int \int \{y(x) - t\}^2 p(x, t) dx dt$$

• Goal: choose y(x) to minimize expected loss (E[L])

Loss Function

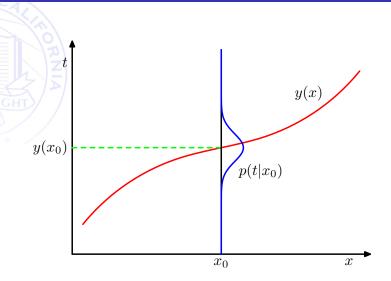
Derivation of the extrema

$$\frac{\delta E[L]}{\delta y(x)} = 2 \int \{y(x) - t\} p(x, t) dt = 0$$

• Implies that

$$y(x) = \frac{\int tp(x,t)dt}{p(x)} = \int tp(t|x)dt = E[t|x]$$

Loss Function - Interpretation



Alternative

Consider a small rewrite

$${y(x) - t}^2 = {y(x) - E[t|x] + E[t|x] - t}^2$$

The expected loss is then

$$E[L] = \int \{y(x) - E[t|x]\}^2 p(x) dx + \int \{E[t|x] - t\}^2 p(x) dx$$

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Outline

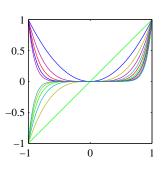
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Polynomial Basis Functions

Basic Definition:

$$\phi_i(x) = x^i$$

Global functions Small change in x affects all of them



Gaussian Basis Functions

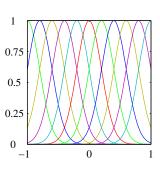
Basic Definition:

$$\phi_i(x) = e^{-\frac{(x-\mu_i)^2}{2s^2}}$$

A way to Gaussian mixtures, local impact

Not required to have probabilistic interpretation.

 μ control position and s control scale



Sigmoid Basis Functions

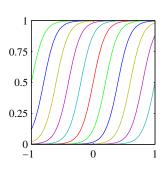
Basic Definition:

$$\phi_i(x) = \sigma\left(\frac{x - \mu_i}{s}\right)$$

where

$$\sigma(a) = \frac{1}{1 + e^{-a}}$$

 $\boldsymbol{\mu}$ controls location and \boldsymbol{s} controls slope



Maximum Likelihood & Least Squares

 Assume observation from a deterministic function contaminated by Gaussian Noise

$$t = y(x, w) + \epsilon$$
 $p(\epsilon|\beta) = N(\epsilon|0, \beta^{-1})$

the problem at hand is then

$$p(t|x, w, \beta) = N(t|y(x, w), \beta^{-1})$$

• From a series of observations we have the likelihood

$$p(\mathbf{t}|\mathbf{X}, w, \beta) = \prod_{i=1}^{N} N(t_i|w^T\phi(x_i), \beta^{-1})$$

Maximum Likelihood & Least Squares (2)

This results in

$$\ln p(\mathbf{t}|\mathbf{w},\beta) = \frac{N}{2} \ln \beta - \frac{N}{2} \ln(2\pi) - \beta E_D(\mathbf{w})$$

where

$$E_D(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^{N} \{t_i - \mathbf{w}^T \phi(x_i)\}^2$$

is the sum of squared errors

Maximum Likelihood & Least Squares (3)

Computing the extrema yields:

$$\mathbf{w}_{\mathit{ML}} = \left(\Phi^{\mathit{T}}\Phi\right)^{-1}\Phi^{\mathit{T}}\mathbf{t}$$

where

$$\Phi = \begin{pmatrix} \phi_0(x_1) & \phi_1(x_1) & \cdots & \phi_{M-1}(x_1) \\ \phi_0(x_1) & \phi_1(x_2) & \cdots & \phi_{M-1}(x_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_0(x_N) & \phi_1(x_N) & \cdots & \phi_{M-1}(x_N) \end{pmatrix}$$

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Line Estimation

- Least square minimization:
 - Line equation: y = ax + b
 - Error in fit: $\sum_{i} (y_i ax_i b)^2$
 - Solution:

$$\left(\begin{array}{c} \bar{y^2} \\ \bar{y} \end{array}\right) = \left(\begin{array}{cc} \bar{x^2} & \bar{x} \\ \bar{x} & 1 \end{array}\right) \left(\begin{array}{c} a \\ b \end{array}\right)$$

• So what is the problem?

Line Estimation

- Least square minimization:
 - Line equation: y = ax + b
 - Error in fit: $\sum_{i} (y_i ax_i b)^2$
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- So what is the problem?
- Minimizes vertical errors. Non-robust!

LSQ on Lasers

- Line model: $r_i \cos(\phi_i \theta) = \rho$
- Error model: $d_i = r_i \cos(\phi_i \theta) \rho$
- Optimize: $\operatorname{argmin}_{(\rho,\theta)} \sum_{i} (r_i \cos(\phi_i \theta) \rho)^2$
- Error model derived in (author?) [1]
- Well suited for "clean-up" of Hough lines

Total Least Squares

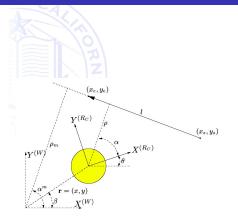
- Line equation: ax + by + c = 0
- Error in fit: $\sum_{i} (ax_i + by_i + c)^2$ where $a^2 + b^2 = 1$.
- Solution:

$$\left(\begin{array}{cc} \bar{x^2} - \bar{x}\bar{x} & \bar{x}\bar{y} - \bar{x}\bar{y} \\ \bar{x}\bar{y} - \bar{x}\bar{y} & \bar{y^2} - \bar{y}\bar{y} \end{array}\right) \left(\begin{array}{c} a \\ b \end{array}\right) = \mu \left(\begin{array}{c} a \\ b \end{array}\right)$$

where μ is a scale factor.

• $c = -a\bar{x} - b\bar{y}$

Line Representations



- The line representation is crucial
- Often a redundant model is adopted
- Line parameters vs end-points
- Important for fusion of segments.
- End-points are less stable

Sequential Adaptation

- In some cases one at a time estimation is more suitable
- Also known as gradient descent

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E_n$$

=
$$\mathbf{w}^{(\tau)} - \eta (t_n - \mathbf{w}^{(\tau)T} \phi(x_n)) \phi(x_n)$$

• Knows as least-mean square (LMS). An issue is how to choose η ?

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Regularized Least Squares

- As seen in previous lecture sometime control of parameters might be useful.
- Consider the error function:

$$E_D(\mathbf{w}) + \lambda E_W(\mathbf{w})$$

which generates

$$\frac{1}{2}\sum_{i=1}^{N}\{t_i-w^t\phi(x_i)\}^2+\frac{\lambda}{2}\mathbf{w}^T\mathbf{w}$$

which is minimized by

$$w = \left(\lambda I + \Phi^T \Phi\right)^{-1} \Phi^T \mathbf{t}$$

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Bayesian Linear Regression

Define a conjugate prior over w

$$p(w) = N(w|m_0, S_0)$$

• given the likelihood function and regular from Bayesian analysis we can derive

$$p(w|t) = N(w|m_N, S_N)$$

where

$$m_N = S_N \left(S_0^{-1} m_0 + \beta \Phi^T t \right)$$

$$S_N^{-1} = S_0^{-1} + \beta \Phi^T \Phi$$

Bayesian Linear Regression (2)

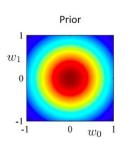
- A common choice is
- So that

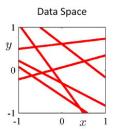
$$p(w) = N(w|0,\alpha^{-1}I)$$

$$m_N = \beta S_N \Phi^T t$$

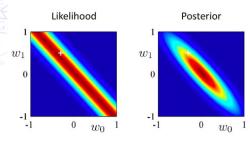
 $S_N^{-1} = \alpha I + \beta \Phi^T \Phi$

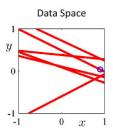
Example - No Data



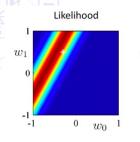


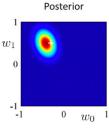
Example - 1 Data Point

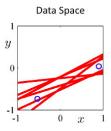




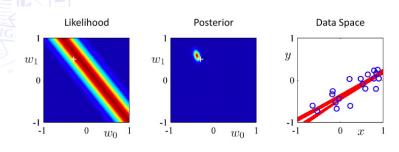
Example - 2 Data Points







Example - 20 Data Points



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Bayesian Model Comparison

- How does one select an appropriate model?
- Assume for a minute we want to compare a set of models M_i , $i \in {1,...L}$ for a dataset D
- We could compute

$$p(M_i|D) \propto p(D|M_i)p(M_i)$$

Bayes Factor: Ratio of evidence for two models

$$\frac{p(D|M_i)}{p(D|M_j)}$$

The mixture distribution approach

• We could use all the models:

$$p(t|x,D) = \sum_{i=1}^{L} p(t|x,M_i,D)p(M_i|D)$$

• Or simply go with the most probably/best model.

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Model Evidence

We can compute model evidence

$$p(D|M_i) = \int p(D|w, M_i)p(w|M_i)dw$$

Allow computation of model fit based on parameter range

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Evaluation of Parameters



$$p(w|D,M_i) = \frac{P(D|w,M_i)p(w|M_i)}{P(D|M_i)}$$

• There is a need to understand how good is a model?

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Model Comparison

Consider evaluation of a model w. parameters w

$$p(D) = \int p(D|w)p(w)dw \approx p(D|w_{map}) \frac{\sigma_{posterior}}{\sigma_{prior}}$$

Then

$$\ln p(D) \approx \ln p(D|w_{map}) + \ln \left(\frac{\sigma_{posterior}}{\sigma_{prior}}\right)$$

Model Comparison as Kullback-Leibler

From earlier we have comparison of distributions

$$KL = \int p(D|M_1) \ln \frac{p(D|M_1)}{p(D|M_2)} dD$$

• Enables comparison of two different models

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Regression Summary

- Brief intro to linear methods for estimation of models
- Prediction of values and models
 - Needed for adaptive selection of models (black-box/grey-box)
 - Evaluation of sensor models, . . .
- Consideration of batch and recursive estimation methods
- Significant discussion of methods for evaluation of models and parameters.
- This far purely a discussion of linear models

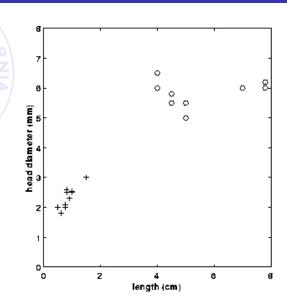
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Classification Introduction

- Linear classification of data
 - Basic pattern recognition
 - Separation of data: buy/sell
 - Segmentation of line data, ...

Simple Example - Bolts or Needles



Classification

- Given
 - An input vector: X
 - A set of classes: $c_i \in \mathcal{C}, \quad i = 1, \dots, k$
- Mapping $m: X \to \mathcal{C}$
- Separation of space into decision regions
- Boundaries termed decision boundaries/surfaces

Basis Formulation

- It is a 1-of-K coding problem
- Target vector: $\mathbf{t} = (0, \dots, 1, \dots, 0)$
- Consideration of 3 different approaches
 - Optimization of discriminant function
 - 2 Bayesian Formulation: $p(c_i|x)$
 - Learning & Decision fusion

Code for experimentation

- There are data sets and sample code available
 - NETLAB: http://www.ncrg.aston.ac.uk/netlab/index.php
 - Kaggle: https://www.kaggle.com
 - Lots of good robotics datasets too

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Discriminant Functions

- Objective: input vector x assigned to a class c_i
- Simple formulation:

$$y(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + w_0$$

- w is termed a weight vector
- w_0 is termed a bias
- Two class example: c_1 if $y(\mathbf{x}) \geq 0$ otherwise c_2

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Basic Design

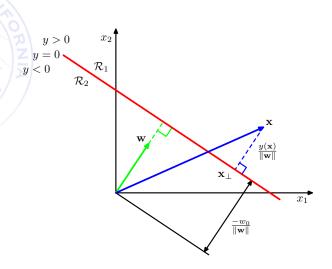
- Two points on decision surface x_a and x_b
- $y(\mathbf{x}_a) = y(\mathbf{x}_b) = 0 \Rightarrow \mathbf{w}^T(\mathbf{x}_a \mathbf{x}_b) = 0$
- w perpendicular to decision surface

$$\frac{\mathbf{w}^T \mathbf{x}}{||\mathbf{w}||} = -\frac{w_0}{||\mathbf{w}||}$$

• Define: $\tilde{w} = (w_0, \mathbf{w})$ and $\tilde{x} = (1, \mathbf{x})$ so that:

$$y(\mathbf{x}) = \tilde{\mathbf{w}}^T \tilde{\mathbf{x}}$$

Linear discriminant function



Multi Class Discrimination

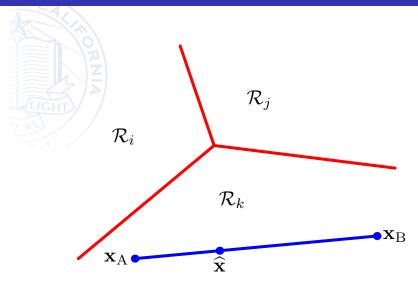
Generation of multiple decision functions

$$y_k(\mathbf{x}) = \mathbf{w}_k^T \mathbf{x} + w_{k0}$$

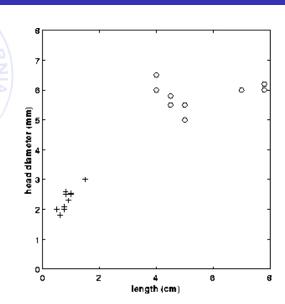
Decision strategy

$$j = \arg\max_{i \in 1..k} y_i(\mathbf{x})$$

Multi-Class Decision Regions



Example - Bolts or Needles



Minimum distance classification

- Suppose we have computed the mean value for each of the classes
- $m_{needle} = [0.86, 2.34]^T$ and $m_{bolt} = [5.74, 5, 85]^T$
- We can then compute the minimum distance

$$d_j(x) = ||x - m_j||$$

- $argmin_i d_i(x)$ is the best fit
- Decision functions can be derived

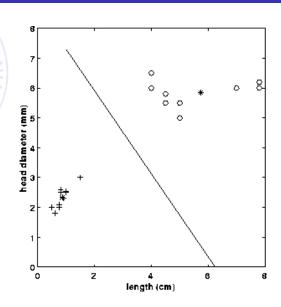
Bolts / Needle Decision Functions

Needle
$$d_{needle}(x) = 0.86x_1 + 2.34x_2 - 3.10$$

Bolt $d_{bolt}(x) = 5.74x_1 + 5.85x_2 - 33.59$
Decision boundary $d_i(x) - d_j(x) = 0$
 $d_{needle/bolt}(x) = -4.88x_1 - 3.51x_2 + 30.49$

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Example decision surface



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Least Squares for Classification

- ullet Just like we could do LSQ for regression we can perform an approximation to the classification vector $\mathcal C$
- Consider again

$$y_k(\mathbf{x}) = \mathbf{w}_k^T \mathbf{x} + w_{k0}$$

Rewrite to

$$\mathbf{y}(\mathbf{x}) = \tilde{\mathbf{W}}^T \tilde{\mathbf{x}}$$

Assuming we have a target vector T

Least Squares for Classification

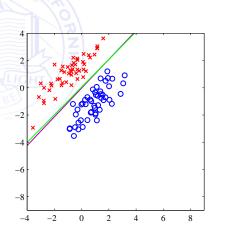
• The error is then:

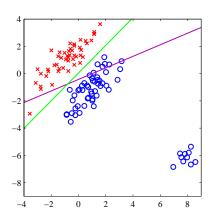
$$E_D(\tilde{\mathbf{W}}) = \frac{1}{2} Tr \left\{ (\tilde{\mathbf{X}} \tilde{\mathbf{W}} - \mathbf{T})^T (\tilde{\mathbf{X}} \tilde{\mathbf{W}} - \mathbf{T}) \right\}$$

• The solution is then

$$\tilde{\mathbf{W}} = \left(\tilde{\mathbf{X}}^T \tilde{\mathbf{X}} \right)^{-1} \tilde{\mathbf{X}}^T \mathbf{T}$$

LSQ and Outliers





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Fisher's linear discriminant

- Selection of a decision function that maximizes distance between classes
- Assume for a start

$$y = \mathbf{W}^T \mathbf{x}$$

• Compute m_1 and m_2

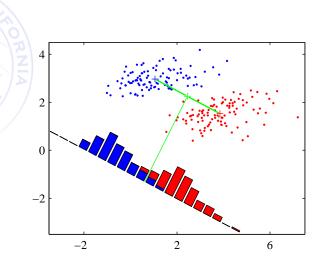
$$\mathbf{m}_1 = \frac{1}{N_1} \sum_{i \in C_1} \mathbf{x}_i \quad \mathbf{m}_2 = \frac{1}{N_2} \sum_{j \in C_2} \mathbf{x}_j$$

Distance:

$$m_2 - m_1 = \mathbf{w}^T (\mathbf{m}_2 - \mathbf{m}_1)$$

• where $m_i = \mathbf{wm}_i$

The suboptimal solution



The Fisher criterion

Consider the expression

$$J(w) = \frac{\mathbf{w}^T \mathbf{S}_B \mathbf{w}}{\mathbf{w}^T \mathbf{S}_W \mathbf{w}}$$

• where S_B is the between class covariance and S_W is the within class covariance, i.e.

$$\mathbf{S}_B = (\mathbf{m}_1 - \mathbf{m}_2)(\mathbf{m}_1 - \mathbf{m}_2)^T$$

and

$$\mathbf{S}_W = \sum_{i=\mathcal{C}_1} (\mathbf{x}_i - \mathbf{m}_1) (\mathbf{x}_i - \mathbf{m}_1)^T + \sum_{i=\mathcal{C}_2} (\mathbf{x}_i - \mathbf{m}_2) (\mathbf{x}_i - \mathbf{m}_2)^T$$

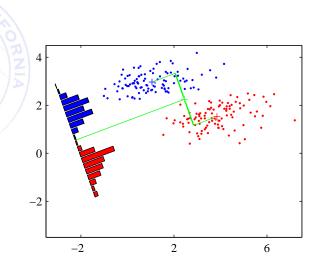
Optimized when

$$(\mathbf{w}^T \mathbf{S}_B \mathbf{w}) \mathbf{S}_w \mathbf{w} = (\mathbf{w}^T \mathbf{S}_W \mathbf{w}) \mathbf{S}_B \mathbf{w}$$

or

$$\mathbf{w} \propto \mathbf{S}_w^{-1} (\mathbf{m}_2 - \mathbf{m}_1)$$

The Fisher result



Generalization to N > 2

Define a stacked weight factor

$$\mathbf{y} = \mathbf{W}^T \mathbf{x}$$

• The within class covariance generalizes to

$$\mathbf{S}_w = \sum_{k=1}^K \mathbf{S}_k$$

• The between class covariance is

$$\mathbf{S}_B = \sum_{k=1}^K N_k (\mathbf{m}_k - \mathbf{m}) (\mathbf{m}_k - \mathbf{m})^T$$

• It can be shown that $J(\mathbf{w})$ is optimized by the eigenvectors to the equation

$$S = \mathbf{S}_W^{-1} \mathbf{S}_B$$

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Perceptron Algorithm

- Developed by Rosenblatt (1962)
- Formed an important basis for neural networks
- Use a non-linear transformation $\phi(x)$
- Construct a decision function

$$y(\mathbf{x}) = f\left(\mathbf{w}^T \phi(\mathbf{x})\right)$$

where

$$f(a) = \begin{cases} +1, & a \ge 0 \\ -1, & a < 0 \end{cases}$$

The perceptron criterion

Normally we want

$$w^t \phi(x_n) > 0$$

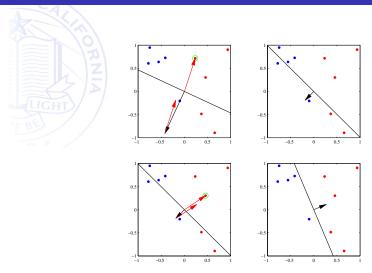
Given the target vector definition

$$E_p(\mathbf{w}) = -\sum_{n \ in\mathcal{M}} \mathbf{w}^T \phi_n t_n$$

- ullet Where ${\mathcal M}$ represents all the mis-classified samples
- We can make this a gradient descent as seen in last lecture

$$\mathbf{w}^{(\tau+1)} = \mathbf{w}^{(\tau)} - \eta \nabla E_P(\mathbf{w}) = \mathbf{w}^{(\tau)} + \eta \phi_n t_n$$

Perceptron learning example



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Classification Summary

- Basics for discrimination / classification
- Obviously not all problems are linear
- Optimization of the distance/overlap between classes
 - Minimizing the probability of error classification
- Basic formulation as an optimization problem
- How to optimize between cluster distance? Covariance Weighted
- Basic recursive formulation
- Could we make it more robust?

Summary

- Data models are anchored in pure data driven or model based evaluation
- How can we use models to interpret data and extrapolate beyond the basic data?
- Covered basic models for regression and classification.