Optimization Techniques for Big Data Analysis

Chapter 2. Machine Learning Contextualization

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Basic problems in supervised learning

We will be focused on two basic problems:

- Linear regression
- Linear classification

Considering a sample $\mathbf{x}_i = [x_{i1}, x_{i2}, \cdots, x_{id}]$, the model will be a form of: $f(\mathbf{x}_i) = w_1 x_{i1} + w_2 x_{i2} + \cdots + w_d x_{id} + w_0 = \mathbf{w}^T \mathbf{x}_i + w_0$.

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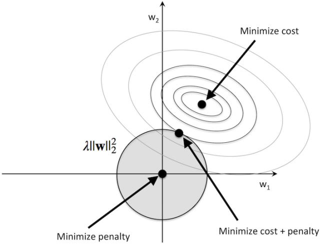
The optimization problem in those cases takes the form:

$$\arg\min_{\bar{\mathbf{w}}} \frac{1}{n} \sum_{i=1}^{n} \ell(\bar{\mathbf{w}}^T \bar{\mathbf{x}}_i, y_i) + r(\bar{\mathbf{w}}) \tag{1}$$

Regularizer

The regularizer adds an extra term (usually a norm) that penalizes/enforces certain characteristics of $\mathbf{w}$.

$$r(\mathbf{w}) = \frac{\lambda}{2}\|\mathbf{w}\|_2^2 = \frac{\lambda}{2}\sum_{j=1}^{d} w_j^2$$



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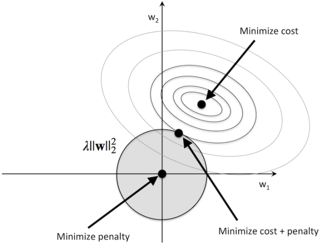
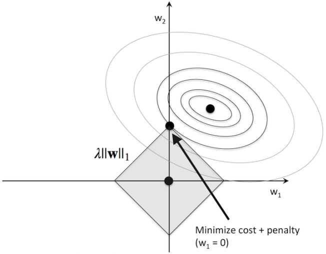


$$r(\mathbf{w}) = \lambda\|\mathbf{w}\|_1 = \lambda\sum_{i=j}^{d} |w_j|$$



Linear regression from a Statistical Signal Processing view

In the general case of an arbitrary observable distribution $\hat{y} = g(\mathbf{x}) = \mathbb{E}(Y|X = \mathbf{x})$. If we assume that variables (Y, X) are jointly Gaussian, $p(y|\mathbf{x}) \sim \mathcal{N}(y|\mu_{y|\mathbf{x}}, \Sigma_{y|\mathbf{x}})$, where:

$$\mu_{y|\mathbf{x}} = \mu_Y + \Sigma_{X,Y}^T \Sigma_Y^{-1} (\mathbf{x} - \mu_X)$$

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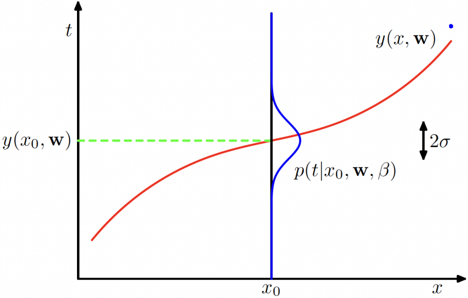
Equivalently:

$$\begin{aligned} p(y|\mathbf{x}, \mathbf{w}, \beta) &= \mathcal{N}\left(f(\mathbf{x}, \mathbf{w}), \beta^{-1}\right) \\ &= \mathcal{N}\left(\mathbf{w}^T\mathbf{x}, \beta^{-1}\right) \end{aligned}$$



Least Square Error

Given a data set $\mathcal{D} = \{(\mathbf{x}_i, y_i)_{i=1}^n\}$, of $i.i.d$ samples, the **likelihood** function is [1]:

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$$\ln p(\mathbf{y}|\mathbf{X}, \mathbf{w}, \beta) = -\frac{\beta}{2}\sum_{i=1}^{n}\left(\mathbf{w}^T\mathbf{x}_i - y_i\right)^2 + \frac{n}{2}\ln\beta - \frac{n}{2}\ln(2\pi)$$

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This is equivalent to minimizing:

$$\mathcal{L}(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{n}\left(\mathbf{w}^T\mathbf{x}_i - y_i\right)^2$$

Linear Regression as a Least Square problem

$$\arg\min_{\mathbf{w}\in\mathbb{R}^{d+1}} \frac{1}{n}\sum_{i=1}^{n} \ell(\mathbf{w}^T\mathbf{x}_i, y_i) = \arg\min_{\mathbf{w}\in\mathbb{R}^{d+1}} \frac{1}{n}\sum_{i=1}^{n}(\mathbf{w}^T\mathbf{x}_i - y_i)^2$$

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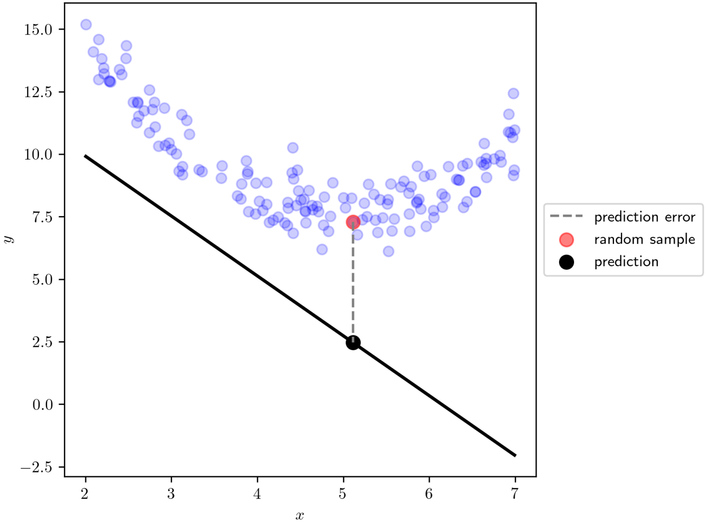
Whose analytical solution is:

$$\frac{1}{n}\mathbf{X}^T(\mathbf{X}\mathbf{w} - \mathbf{y}) = 0;\ \mathbf{w}^* = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y}$$

Error in Least Square



Ridge regression

$$\mathcal{L}(\mathbf{w}) = \underset{\mathbf{w}\in\mathbb{R}^{d+1}}{\arg\min}\ \frac{1}{n}\|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2 + \frac{\lambda}{2}\|\mathbf{w}\|_2^2$$

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LASSO regression

LASSO (Least Absolute Shrinkage and Selection Operator) looks similar but uses a L_1 regularizer instead:

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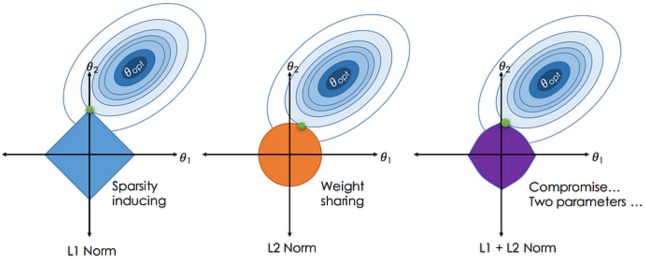

Basis pursuit

1. Basis pursuit is a similar problem to linear regression but with a different goal: the idea now is to find a good fit for the given data as a linear combination of a small number of the basis functions.
2. In this context, the basis family use to be referred to as a dictionary.
3. The goal now is that we seek a function ϕ that fits the data well:

$$\Phi\left(\mathbf{x}_i\right) \approx y_i \qquad \forall i$$

such that this function can be expressed as a linear combination of a particular basis:

$$\Phi\left(\mathbf{x}\right) = \sum_{j=0}^{d} \mathbf{w}_j \phi_j\left(\mathbf{x}\right)$$

Basis Pursuit

The formulation is well known to us (typically an L1-norm is added):

$$\underset{\mathbf{w}\in\mathbb{R}^{d+1}}{\arg\min}\left(\frac{1}{n}\sum_{i=1}^{n}\left(\underbrace{\sum_{j=0}^{d} w_j\phi_j\left(\mathbf{x}_i\right)}_{\Phi(\mathbf{x}_i)} - y_i\right)^2 + \lambda\left\|\mathbf{w}\right\|_1\right)$$

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In matrix form, we define:

$$\mathbf{X} = \begin{bmatrix} \phi_0\left(\mathbf{x}_1\right) & \cdots & \phi_d\left(\mathbf{x}_1\right) \\ \vdots & \ddots & \vdots \\ \phi_0\left(\mathbf{x}_n\right) & & \phi_d\left(\mathbf{x}_n\right) \end{bmatrix}$$

and we reach the standard LASSO-like expression:

$$\mathcal{L}(\mathbf{w}) = \underset{\mathbf{w}\in\mathbb{R}^{d+1}}{\arg\min}\,\frac{1}{n}\|\mathbf{X}\mathbf{w}-\mathbf{y}\|_2^2 + \lambda\|\mathbf{w}\|_1$$

Basis Pursuit. Example 2_1

Let us suppose that our observable has the following structure

$$y = w_1 \phi_1 (x) + w_2 \phi_2 (x) + \varepsilon$$

where $x \in (0, 10)$ and the two arbitrary basis are

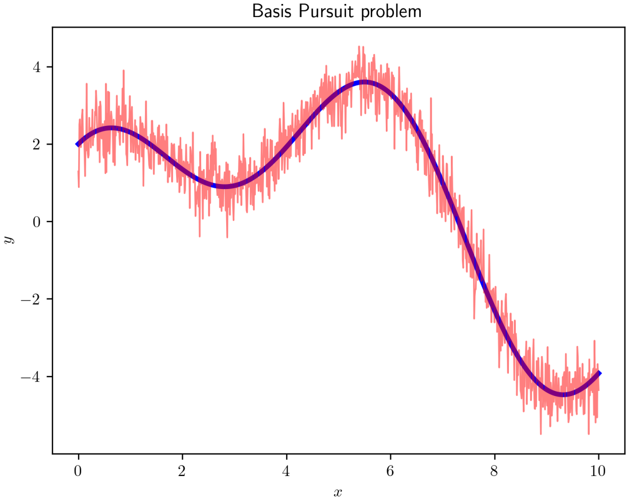
$$\phi_1 (x) = \cos \frac{\pi}{3} x, \phi_2 (x) = \sin \frac{\pi}{7} x$$

and ε a white Gaussian noise with power σ_n^2. The objective is to write a Python code to calculate coefficients w_1, w_2 from y according to

$$\min_{\mathbf{x} \in \mathbb{R}^d} \left(\frac{1}{N} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2 \right)$$

Next figure shows the case where $w_1 = 2$, $w_2 = 3$ and σ_n^2=0.25.

Example 2_1 (Denoising)



Classification. Basic ideas

The classification problem is just like the regression problem, except that the values y_i that we want to predict take on only a small number of discrete values.

We will show two very popular approaches:

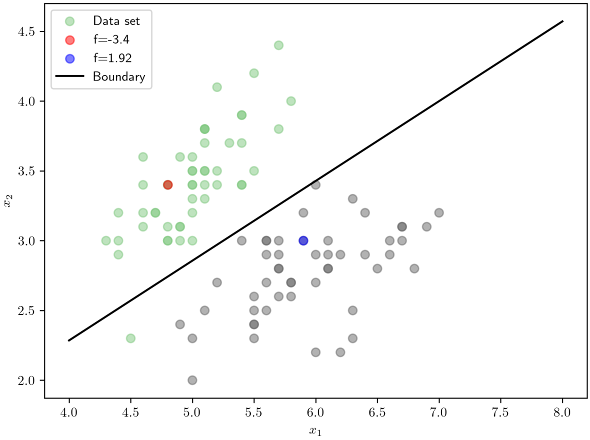
- Logistic Regression
- Support Vector Machines (SVM)

We will be just focused on the binary case, $y_i \in \{+1, -1\}$, in order to simplify the interpretations.

Extensions to more classes are straightforward.

Classification. Basic ideas

In this case, we talk about *discriminative functions* as those that represent the borders of decision regions.



Optimum Bayesian boundary

Defining the probability of a certain hypothesis conditioned to a certain observable

$$P(H_i \mid \mathbf{x}) = \frac{p(\mathbf{x} \mid H_i)P(H_i)}{p(\mathbf{x})}$$

after the Bayes rule and, since $p(\mathbf{x}) \geq 0$ and it does not depend on i, to maximize the likelihood *a posteriori* is equivalent to maximize the numerator resulting in the rule based on the likelihood functions

$$\text{Accept } H_i \text{ iff } p(X \mid H_i)P(H_i) > p(X \mid H_j)P(H_j),\ \forall j \neq i$$

or, taking logarithms

$$\text{Accept } H_i \text{ iff } \ln p(X \mid H_i) + \ln P(H_i) > \ln p(X \mid H_j) + \ln P(H_j), \forall j \neq i$$

Optimum Bayesian classification in the Gaussian case

Therefore, in general, a Bayesian classifier will use a decision rule type

$$\text{Accept } H_i \text{ iff } g_i(X) > g_j(X),\ \forall j \neq i$$

where $g_i(\mathbf{x})$, $i = 0, 1, \ldots, M-1$ ($M = 2$ for the binary case) are called *discriminant functions*. For a two-class, we can define a single discriminant function

$$g(\mathbf{x}) \equiv g_1(\mathbf{x}) - g_2(\mathbf{x})$$

which decides H_1 if $g(\mathbf{x}) > 0$; otherwise decide H_2. The *borders* between the decision regions of the hypotheses is the set of points $\mathbf{x} \in \mathbb{R}^d$ where $g(\mathbf{x}) = 0$.

Linear classifier

Suppose that the observation vector follows a multivariate Gaussian distribution: $X \sim \mathcal{N}(\mu, \Sigma)$.

The discriminative function for the i-th class will be [2]:

$$g_i(\mathbf{x}) = -\frac{d}{2}\ln 2\pi - \frac{1}{2}\ln|\Sigma_i| - \frac{1}{2}\mathbf{x}^T\Sigma_i^{-1}\mathbf{x} + \mu_i^T\Sigma_i^{-1}\mathbf{x} - \frac{1}{2}\mu_i^T\Sigma_i^{-1}\mu_i + \ln P(H_i)$$

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- Case 1: $\Sigma_i = \sigma^2\mathbf{I}$

$$g_i(\mathbf{x}) = \mathbf{w}_i^T\mathbf{x} + w_{i0} \rightarrow \mathbf{w}_i = \frac{1}{\sigma^2}\mu_i; \;\; w_{i0} = \frac{-1}{2\sigma^2}\mu_i^T\mu_i + \ln P(H_i)$$

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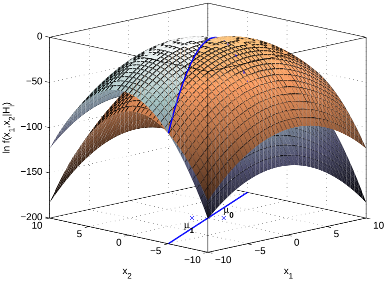
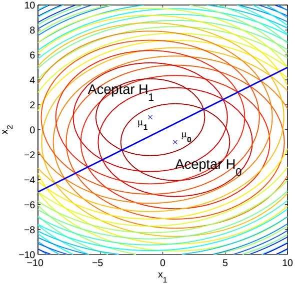
- Case 2: $\Sigma_i = \Sigma$

$$g_i(\mathbf{x}) = \mathbf{w}_i^T\mathbf{x} + w_{i0} \rightarrow \mathbf{w}_i = \sigma^{-1}\mu_i; \;\; w_{i0} = \frac{-1}{2}\mu_i^T\Sigma^{-1}\mu_i + \ln P(H_i)$$

Linear classifier





$P(H_0) = P(H_1) = 1/2$. Border regions decision

Quadratic Classifier

- Case 3: Σ_i = arbitrary

$$g_i(\mathbf{x}) = \mathbf{x}^T \mathbf{W}_i \mathbf{x} + \mathbf{w}_i^T \mathbf{x} + w_{i0}$$

$$\mathbf{W}_i = -\frac{1}{2}\Sigma_i^{-1}$$

$$\mathbf{w}_i = \Sigma_i^{-1}\mu_i$$

$$w_{i0} = \frac{-1}{2}\mu_i^T\Sigma_i^{-1}\mu_i - \frac{1}{2}\ln|\Sigma_i| + \ln P(H_i)$$

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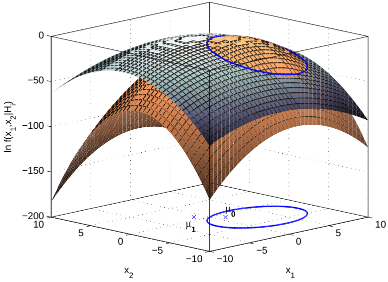
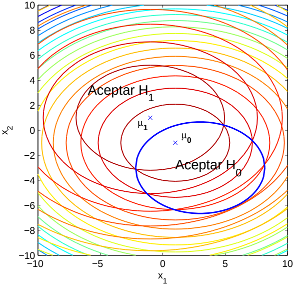
There is an additional case where you assume that Σ_i is arbitrary but diagonal, which is call Naïve Bayes Classifier.

Quadratic classifier

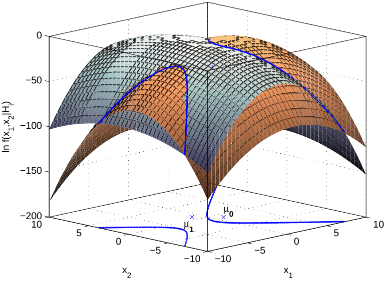


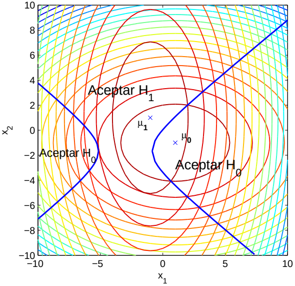


$$P(H_0) = P(H_1) = 1/2,\ \mu_0 = [1, -1]^T,\ \mu_1 = [-1, 1]^T,$$
$$\Sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{2} \end{bmatrix},\ \Sigma_1 = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}$$

The border is an ellipse

Quadratic classifier

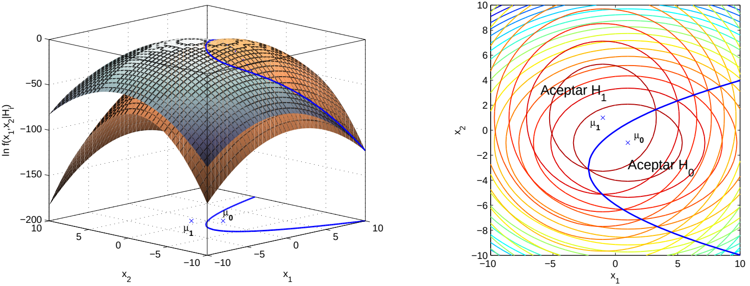




$$P(H_0) = P(H_1) = 1/2,\ \mu_0 = [1, -1]^T,\ \mu_1 = [-1, 1]^T,$$
$$\Sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & \frac{1}{2} \end{bmatrix},\ \Sigma_1 = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & 2 \end{bmatrix}$$

The border is a hyperbola

Quadratic classifier



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The border is a parabola

Logistic Regression

Like Linear regression, we can apply the maximum likelihood criterion to a classification problem. Assuming a Bernoulli distribution (2-class problem):

$$\max \mathcal{L} = \log \left(\prod_{i=1}^{n} p_i^{y_i} (1 - p_i)^{(1-y_i)} \right); \quad y_i \in \{0, 1\}$$

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To model $p_i = p(\mathbf{x}_i; \mathbf{w}, w_0) = P(Y = 1 | X = \mathbf{x}_i; \mathbf{w}, w_0)$, logistic

regression uses the inverse of a *logit* function to map the output of a linear function to the interval $(0, 1)$.

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$$p(\mathbf{x}_i; \mathbf{w}, w_0) = \frac{1}{1+\exp\left(-(\mathbf{w}^T\mathbf{x}_i + w_0)\right)} = g(\bar{\mathbf{w}}^T\bar{\mathbf{x}}_i)$$

Logistic loss

$$
\begin{aligned}
\arg\max_{\mathbf{w}} \mathcal{L} &= \sum_{i=1}^{n} \log\left((g(\mathbf{w}^T\mathbf{x}_i))^{y_i}\right) + \log\left((1 - g(\mathbf{w}^T\mathbf{x}_i))^{(1-y_i)}\right) \\
&= \sum_{i=1}^{n} y_i \log\left(g(\mathbf{w}^T\mathbf{x}_i)\right) + (1 - y_i)\log\left(1 - g(\mathbf{w}^T\mathbf{x}_i)\right)
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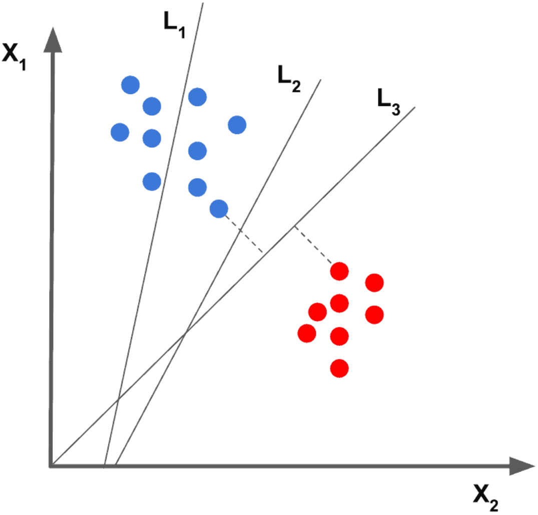
\end{aligned}
$$

It is straightforward to add a regularisation term $r(\mathbf{w})$.

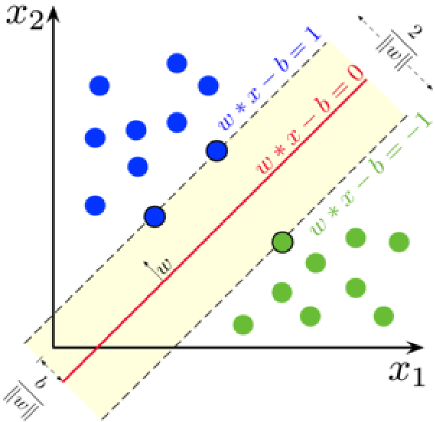
Support Vector Machines



Which one do you prefer?

Support Vector Machines

SVM provides a solution based on the idea of maximising the **margin** between the closest points of the classes.



Support Vector Machines

- Suppose that we find among all the points of the two classes those that are the most critical because they are the closest.
- We draw two hyperplanes over these points and define the discriminant function as the hyperplane in between.
- The equation of this hyperplane is

$$\mathbf{w}^T\mathbf{x} + b = 0$$

  where $\mathbf{w}$ is a vector orthogonal to the hyperplane and b is an offset parameter.
- The other two hyperplanes parallel to the first one are denoted by

$$\mathbf{w}^T\mathbf{x} + b = \gamma$$

  and

$$\mathbf{w}^T\mathbf{x} + b = -\gamma$$

However, we can normalize just the hyperplane equation:

$$c\left(\mathbf{w}^T\mathbf{x}+b\right)=0$$

where c is an arbitrary constant.
Let us choose this constant $c=\gamma$, so the two parallel hyperplanes become

$$\mathbf{w}^T\mathbf{x}+b=\pm 1$$

Clearly, the intention is to design $\mathbf{w}^T, b$ so that

$$\mathbf{w}^T\mathbf{x}+b\geq 1\Rightarrow y_i=1 \qquad \mathbf{w}^T\mathbf{x}+b\leq -1\Rightarrow y_i=-1$$

Support Vector Machines

The aim is then to maximise the margin, which corresponds to the distance between the points and the decision hyperplane:

$$\frac{y_i f(\mathbf{x}_i)}{\|\mathbf{w}\|} = \frac{y_i(\mathbf{w}^T \mathbf{x}_i + b)}{\|\mathbf{w}\|}$$

which can be rewrite as [3]:

$$\arg\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|^2 \ \text{ Subject to } \ y_i(\mathbf{w}^T \mathbf{x}_i + b) \geq 1$$

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In practice, we must relax the restrictions because the problem cannot be linearly separable.

$$\begin{gathered}
\underset{\mathbf{w},b,\zeta_i \geq 0}{\arg\min} \tfrac{1}{2} \|\mathbf{w}\|_2^2 + \alpha \textstyle\sum_{i=1}^n \zeta_i \\
s.t. : y_i \left(\mathbf{w}^T \mathbf{x}_i + b\right) \geq 1 - \zeta_i \\
\zeta_i \geq 0
\end{gathered}$$

Hinge loss

If we transform the inequality constraints in an approximate unconstrained problem, we get:

$$y_i\left(\mathbf{w}^T\mathbf{x}_i + b\right) = 1 - \zeta_i \rightarrow \zeta_i = \max\left\{0, 1 - y_i\left(\mathbf{w}^T\mathbf{x}_i + b\right)\right\}$$

so, we have:

$$\underset{\mathbf{w}\in\mathbb{R}^d, b\in\mathbb{R}}{\arg\min}\left(\frac{1}{2}\|\mathbf{w}\|_2^2 + \alpha\sum_{i=1}^{n}\max\left(1 - y_i\left(\mathbf{w}^T\mathbf{x}_i + b\right), 0\right)\right)$$

Hinge loss

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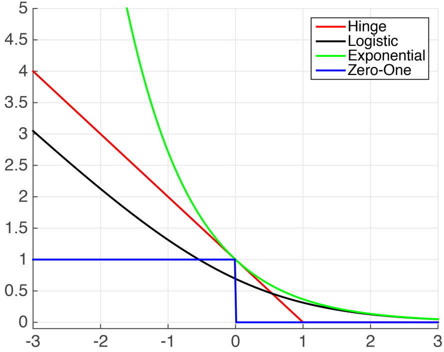
where α intends to penalize deviations from the feasibility region. It could also be rewritten as:

$$\underset{\mathbf{w}\in\mathbb{R}^d, b\in\mathbb{R}}{\arg\min}\left(\frac{1}{n}\sum_{i=1}^{n}\max\left(1 - y_i\left(\mathbf{w}^T\mathbf{x}_i + b\right), 0\right) + \frac{\lambda}{2}\|\mathbf{w}\|_2^2\right)$$

SVM loss function



As we have already mentioned, in practice, we will use an equivalent definition by compacting model parameters:

$$\underset{\mathbf{w}\in\mathbb{R}^{d+1}}{\arg\min}\left(\frac{1}{n}\sum_{i=1}^{n}\max\left(1-y_i\left(\mathbf{w}^T\mathbf{x}_i\right),0\right)^p+\frac{\lambda}{2}\|\mathbf{w}\|_2^2\right)$$

Code repository

Some functions must be reviewed in detail:

- **Generation**: `Get_data_reg`, `Scenarios_regression`, `Get_data_class`, `Scenarios_classification`. (Have a look at Examples 2_3 and 2_5)

SSR

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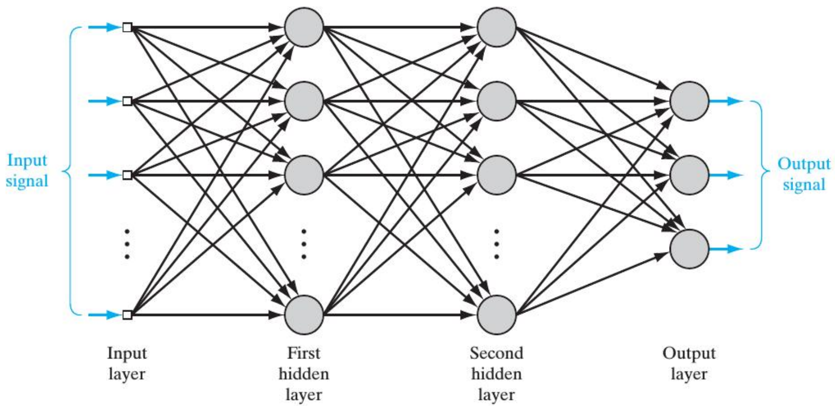
- **Case_studies**: Compilation of topics.
  - `case_study_2_1` (Regression): Understand how the data is generated, training and testing datasets, and the effect of regularization in the error surface.
  - `case_study_2_2` (Classification): What can we expect if the class means are asymmetric? See the effect of regularization in the loss function.

Neural networks. General architecture



Questions?

References

[1] Christopher M. Bishop. *Pattern Recognition and Machine Learning*. Springer, 2006.

[2] Richard O Duda, Peter E Hart, et al. *Pattern classification*. John Wiley & Sons, 2000.

[3] Bernhard Schölkopf and Alexander J Smola. *Learning with kernels: support vector machines, regularization, optimization, and beyond*. MIT press, 2002.

Thank You

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