Machine learning tools: learning to classify

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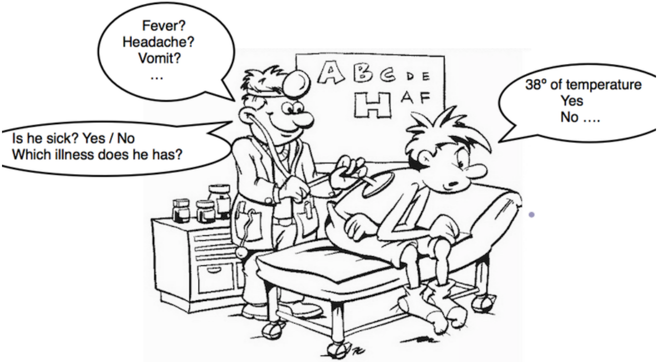
Summary

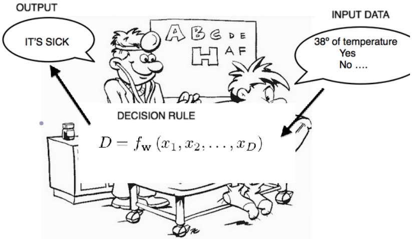
The classification problem



Machines can learn to classify

Machine learning...

designs algorithms that allow computers to learn tasks based on empirical data



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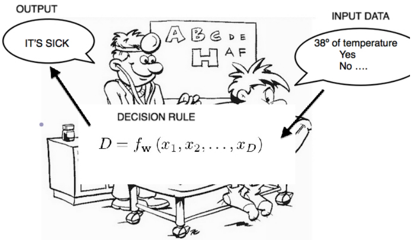


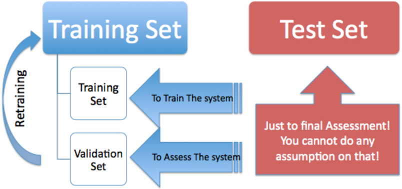
Final goal

Then machine needs to obtain good results in new patterns; this is known as **GENERALIZATION** (**OVERFITTING** problems has to be avoided).

Ingredients of the classification problem

The data

- Training data: input samples $\left\{\mathbf{x}^{(l)}\right\}_{l=1}^{L} \in \Re^{M}$ and their labels $\left\{y^{(l)}\right\}_{l=1}^{L}$ which belong to the set of categories $\{C_1, C_2, ...C_J\}$.
- Validation data: useful to adjust free parameters.
- Test data: to evaluate the final performance of the classifier.



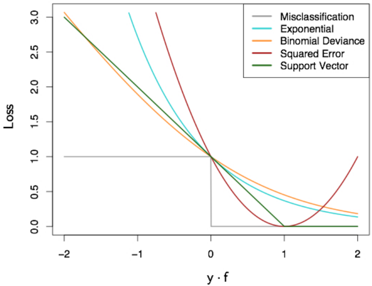
Ingredients of the classification problem

The loss function

Parametric models fix a decision function:

$$D = f_{\mathbf{w}}(\mathbf{x})$$

and need to adjust their free parameters ($\mathbf{w}$) minimizing a loss function. In the ideal case, this cost would be the **classification rate**; however, this cost function is not differentiable, so upper-bounds are preferred.



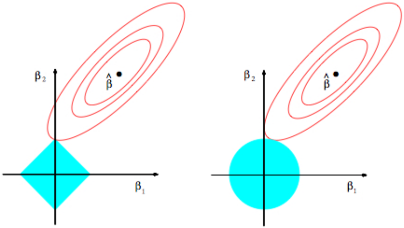
- Exponential: $\exp\left(-yf(\mathbf{x})\right)$
- Binomial Deviance: $\log\left[1 + \exp\left(-yf(\mathbf{x})\right)\right]$
- Squared error: $\left(y - f(\mathbf{x})\right)^2 = \left(1 - yf(\mathbf{x})\right)^2$
- SVM Hinge loss: $\left[1 - yf(\mathbf{x})\right]_+$

Ingredients of the classification problem

The regularization term

It's typical to include a regularization term during the optimization of the cost function to add some properties to the solution:

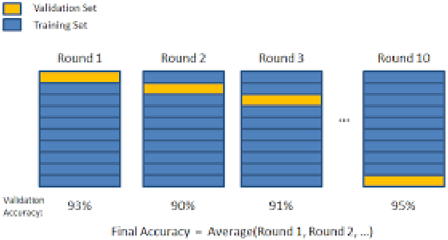
- An L2 term helps to avoid overfitting problems (it maximizes the classifier margin).
- An L1 term provides sparsity to the solution.



Ingredients of the classification problem

Hiperparameter selection

- The training process depends on hyperparameter values.
- These values are critical in the generalization capability.
- **Cross validation** (CV): divides the data set in K subsets without replacement and successively train K models with all the subsets but one which is used to validate.



Criteria to classify classifiers

- Binary vs. multiclass (and multilabel)
- Linear vs. non-linear
- Parametric vs. non-parametric
- Discriminative vs. generative
- Single vs. ensembles

Strategies in multiclass problems

One vs. one

- It trains a binary classifier per pair of classes.
- At prediction time, the class which receives the most votes is selected.
- It requires to train $n_{classes} * (n_{classes} - 1)/2$ classifiers.
- Each individual learning problem involves a small subset of the data.

One vs. all

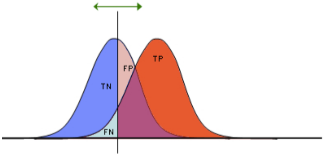
- It defines binary problems fitting each class against the remaining classes.
- Only $n_{classes}$ classifiers are trained (computational efficiency).
- A gain of interpretability (each class is represented by one classifier).
- This is the most commonly used strategy.

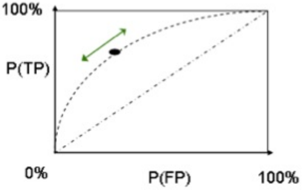
Performance evaluation in binary problems

- Classification error or accuracy
- False positive (FP) rate, True positive (TP) or detection rate, ...

	$D = 1$	$D = 0$
$H = 1$	TP	FP
$H = 0$	TN	FN

- ROC curve (AUC)





Performance evaluation in multiclass problems

- Classification error or accuracy
- Confusion matrix: It analyzes the number of errors by class

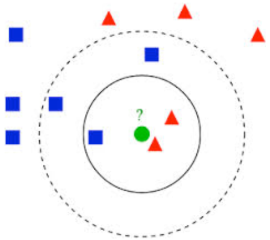
		ACTUAL			Prediction Totals	Prediction Error%
		Setosa	Versicolour	Virginica		
PRED	Setosa	50	0	0	50	0.00%
PRED	Versicolour	0	48	1	49	2.04%
PRED	Virginica	0	2	49	51	3.92%
Actual Totals		50	50	50	150	2.00%
Actual Error%		0.00%	4.00%	2.00%	2.00%	

K-Nearest Neighbours

It is a **non-parametric** classifier, i.e, there are not parameters to be learned.

To classify a test data $\mathbf{x}^*$:

- Select the value of K.
- Search, among the training data, the K nearest neighbours of $\mathbf{x}^*$.
- Decide that $\mathbf{x}^*$ belongs to the majority class of the neighbours.



It's intrinsically a **multiclass** classifier.

The support vector machine

- It is the reference (baseline) **binary** classifier.
- It is characterized for **maximizing the classification margin**.
- It minimizes the *hinge-loss*.
- Its formulation can be reduced to a convex optimization problem (**unique solution**).
- Its linear formulation can provide **non linear** classifiers by means of the *kernel trick*.
- There are multiple extensions: for regression and novelty-detection, with different cost functions, different regularizations....

The linear SVM: separable case

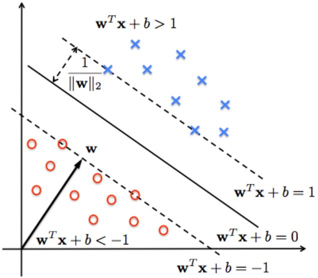
Let's start considering that training data are linearly separable...

- We want a **maximum margin** classifier

$$\rho = \frac{1}{\|\mathbf{w}\|_2}$$

- which is able to classify all training data:

$$\min_{\mathbf{w},b} \quad \|\mathbf{w}\|_2^2$$
$$\text{st.}y^{(l)}\left(\mathbf{w}^T\mathbf{x}^{(l)}+b\right) \geq 1; \quad \forall l$$



The linear SVM: separable case

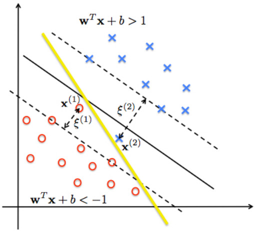
When training data aren't linearly separable or we let some data be misclassified...

- We can add some slack variables in the formulation
- Linear binary classifier

$$\min_{\mathbf{w},b,\xi_{(l)}} \quad \|\mathbf{w}\|_\mathbf{2}^\mathbf{2} + \mathbf{C}\sum_{\mathbf{l=1}}^{\mathbf{L}} \xi^{(\mathbf{l})}$$

$$\text{st.} \quad y^{(l)}\left(\mathbf{w}^T\mathbf{x}^{(l)} + b\right) \geq 1 - \xi^{(l)}; \quad \forall l$$

$$\xi^{(l)} \geq 0; \quad \forall l$$



The linear support vector machine

- The training of the linear SVM relies on solving

$$\min_{\mathbf{w},b,\xi_{(l)}} \quad \|\mathbf{w}\|_2^2 + \mathbf{C}\sum_{l=1}^{L} \xi^{(l)}$$
$$\text{st.} \quad y^{(l)}\left(\mathbf{w}^T\mathbf{x}^{(l)} + b\right) \geq 1 - \xi^{(l)}; \quad \forall l$$
$$\xi^{(l)} \geq 0; \quad \forall l$$

  an optimization problem with a **unique solution**.
- The value of C has to be properly selected.
- The soft-output of the classifier is given by

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

  if $f(\mathbf{x}^*) > 0$ (< 0) the datum is assigned to class $+1$ (-1).
- This optimization problem can be reformulated by means of the Lagrangian multipliers, providing a dual formulation... (next).

The SVM dual formulation

- Previous SVM optimization problem can be reformulated by means of the Lagrangian multipliers, providing a dual formulation

$$\max_{\alpha^{(1)},\dots,\alpha^{(L)}} \quad \sum_{l=1}^{L} \alpha^{(l)} - \frac{1}{2} \sum_{l=1}^{L} \sum_{l'=1}^{L} y^{(l)} y^{(l')} \alpha^{(l)} \alpha^{(l')} \mathbf{x}^{(l)T} \mathbf{x}^{(l')}$$

$$\text{st.} \quad 0 < \alpha^{(l)} < C \quad \forall l$$

$$\sum_{l=1}^{L} \alpha^{(l)} y_{(l)} = 0; \quad \forall l$$

where now the optimization has to be solved regarding to the dual variables $\alpha^{(l)}$.

- The problem complexity is given by the number of data (L).

The SVM dual formulation

- Once $\left\{\alpha^{(l)}\right\}_{l=1}^{L}$ values are obtain, one can compute the weight vector as:

$$\mathbf{w}^T = \sum_{l=1}^{L} y^{(l)} \alpha^{(l)} \mathbf{x}^{(l)}$$

- Then, the soft-output of the classifier for a new data $\mathbf{x}^*$ is given by

$$f(\mathbf{x}^*) = \mathbf{w}^T \mathbf{x}^* + b = \sum_{l=1}^{L} y^{(l)} \alpha^{(l)} \mathbf{x}^{(l)} \mathbf{x}^* + b$$

- Sparsity of the SVM solution:
    - Most dual variables are zero;
    - The SVM output is given by a linear combination of just few input data
    - These data, which support the solution of the classifier, are call **support vectors**.

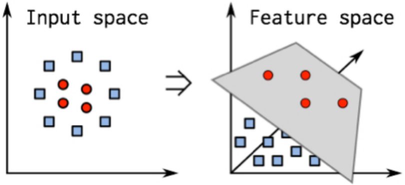
No-linear SVM

Mapping the data

- When we cannot find linear solutions in the input space
- We can map the data to a high dimensional space (even of infinitive dimension)

$$\mathbf{x} \longrightarrow \phi(\mathbf{x})$$

- then, a liner solution of the problem can be found in this high dimensional space



No-linear SVM

Kernel trick

- In most cases, you cannot compute the kernel transformation explicitly.
- But you can compute the dot product of the data in the feature space.

$$K\left(\mathbf{x}, \mathbf{x}'\right) = \phi\left(\mathbf{x}\right)^T \phi\left(\mathbf{x}'\right)$$

- $K\left(\cdot, \cdot\right)$, which is called *kernel function*, measures similarities between the data.

Some examples

- Linear kernel: $K\left(\mathbf{x}, \mathbf{x}'\right) = \mathbf{x}^T \mathbf{x}'$
- Polynomial kernel: $K\left(\mathbf{x}, \mathbf{x}'\right) = \left(\mathbf{x}^T \mathbf{x}' + c\right)^d$
- Gaussian kernel: $K\left(\mathbf{x}, \mathbf{x}'\right) = \exp\left(-\gamma \|\mathbf{x} - \mathbf{x}'\|^2\right)$

No-linear SVM

- We can obtain no-linear classification boundaries by replacing the dot products of the dual formulation by a kernel function.

$$\max_{\alpha^{(1)},\dots,\alpha^{(L)}} \quad \sum_{l=1}^{L} \alpha^{(l)} - \frac{1}{2} \sum_{l=1}^{L} \sum_{l'=1}^{L} y^{(l)} y^{(l')} \alpha^{(l)} \alpha^{(l')} K\left(\mathbf{x}^{(l)}, \mathbf{x}^{(l')}\right)$$

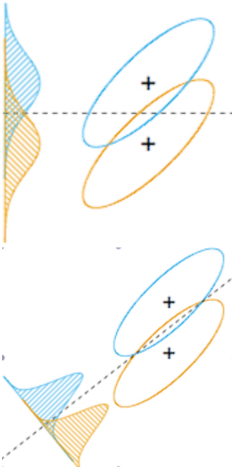
$$\begin{aligned} \text{st.} \quad & 0 < \alpha^{(l)} < C \quad \forall l \\ & \sum_{l=1}^{L} \alpha^{(l)} y_{(l)} = 0; \quad \forall l \end{aligned}$$

- Now, the SVM weight cannot be explicitly computed.
- But, the SVM output can be obtained as:

$$f(\mathbf{x}^*) = \mathbf{w}^T \mathbf{x}^* + b = \sum_{l=1}^{L} y^{(l)} \alpha^{(l)} K\left(\mathbf{x}^{(l)}, \mathbf{x}^*\right) + b$$

Linear Discriminant Analysis

- It is a **generative** classification model.
- It considers that the data follow a gaussian distribution with the same covariance matrix.
- Then, the optimum classifier is **linear**.
- It finds the direction of minimum overlap among the classes. We can project the data over this direction and classify them in this new space.
- Fisher discriminant generalizes it to any data set.



Linear Discriminant Analysis

- Let's consider that the data follow a gaussian distribution with the same covariance matrix.

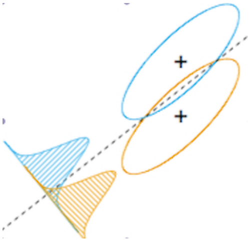
$$p(\mathbf{x}|y=-1) \sim G(\mathbf{m}_0, V) \qquad p(\mathbf{x}|y=1) \sim G(\mathbf{m}_1, V)$$

- Then, the optimum classifier is

$$\hat{y} = \text{sign}\left(\mathbf{w}^T\mathbf{x}\right)$$

where $\mathbf{w} = V^{-1}(\mathbf{m}_1 - \mathbf{m}_0)$.

- To decide, we project the input data over $\mathbf{w}$, i.e., for each multidimensional input data, a unidimensional value is obtained and a threshold is applied.
- In multiclass problems there are as many linear discrimination functions as number of classes minus one.



Logistic Regression

- Define the posterior probabilities (for the binary case) as:

$$P(Y = 1|\mathbf{x}) = \frac{\exp(\mathbf{w}^T\mathbf{x})}{1 + \exp(\mathbf{w}^T\mathbf{x})} = \frac{1}{1 + \exp(-\mathbf{w}^T\mathbf{x})}$$

$$P(Y = 0|\mathbf{x}) = 1 - P(Y = 1|\mathbf{x}) = \frac{1}{1 + \exp(\mathbf{w}^T\mathbf{x})}$$

- In this way, the MAP classifier is linear:

$$\log \frac{P(Y = 1|\mathbf{x})}{P(Y = 0|\mathbf{x})} = \mathbf{w}^T\mathbf{x}$$

- Taking into account that the probability that Y is 1 is given by $P(Y = 1|\mathbf{x}) = p(\mathbf{x})$ and $1 - p(\mathbf{x})$ is the probability of being 0, the joint likelihood over all training data is:

$$L(\mathbf{w}) = \prod_{l=1}^{L} p(\mathbf{x}_l)^{y_l} \left(1 - p(\mathbf{x}_l)\right)^{y_l}$$

Logistic Regression

- Then, to learn the parameters of the model, we can maximize the log-likelihood for N observations:

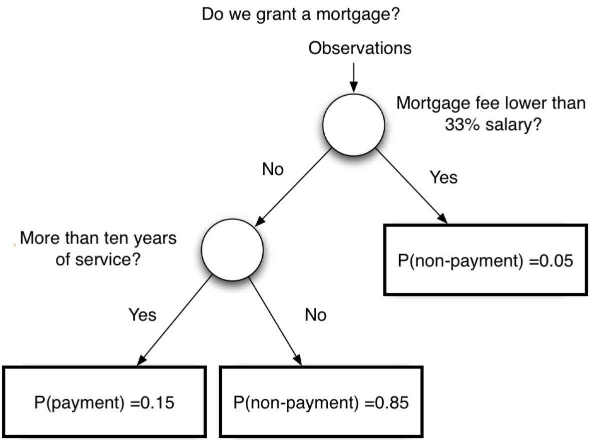
$$l(\mathbf{w}) = \sum_{l=1}^{L} \{y_l \log\left(p(\mathbf{x}_l)\right) + (1 - y_l)\log\left(1 - p(\mathbf{x}_l)\right)\}$$

$$l(\mathbf{w}) = \sum_{l=1}^{L} \left\{y_l(\mathbf{w}^T\mathbf{x}) - \log\left(1 + \exp(\mathbf{w}^T\mathbf{x}_l)\right)\right\}$$

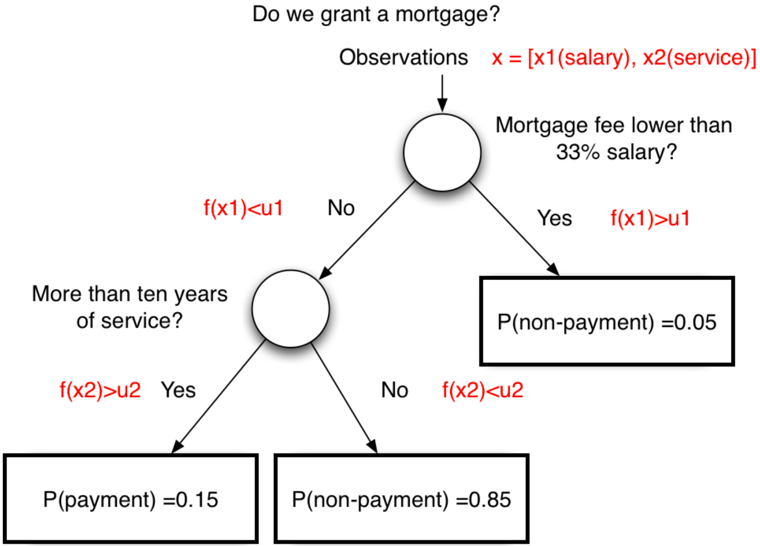
- A Newton method is used to find the maximum of this loss function.
- **Regularized Logistic Regression**: we can minimize the equivalent loss function with a regularization term

$$\min_{\mathbf{w}} - \sum_{l=1}^{L} \left\{y_l(\mathbf{w}^T\mathbf{x}) - \log\left(1 + \exp(\mathbf{w}^T\mathbf{x}_l)\right)\right\} + C\|\mathbf{w}\|_2^2$$

Decision trees: working principles



Decision trees: working principles



Training a decision tree

- Inputs: $\left\{\mathbf{x}^{(l)}\right\}_{l=1}^{L} \in \Re^M$ and $\left\{y^{(l)}\right\}_{l=1}^{L} \in \{C_1, C_2, ...C_J\}$.
- for $d = 1 : DM$ # *For each feature*
    - for $u_{d,l} \in$ all values of x_d # *Exploring thresholds*
        - Evaluate the index Gini :

$$g(u_{d,l}) = \sum_{j=1}^{J} P_j(u_{d,l})\,(1 - P_j(u_{d,l}))$$

being $P_j(u_{d,l})$ the fraction of items classified in the class C_j by the threshold $u_{d,l}$

- Select threshold $(u_{d,l})$ and feature (x_d) minimizing $g(u_{d,l})$
- Split the data according to x_d and threshold $u_{d,l}$
- Apply recursively

The minimization of Gini index aims at getting leaves “pure enough”.

Random Forest

Working principles

- Build many trees (forest) randomizing samples and features
- Key points:
    - Low correlation among trees
    - Strength of each tree

Test data classification

- Then, each test data ($\mathbf{x}^*$) is classified by all the tree
- The forest classification rule is given by:

$$C_j^* = \underset{j}{\operatorname{argmax}} \frac{1}{T} \sum_{t=1}^{T} P_t(C_j|\mathbf{x}^*)$$

where $P_t(C_j|\mathbf{x}^*)$ is the probability output of each tree.

Training a Random Forest

- Inputs: $\left\{\mathbf{x}^{(l)}\right\}_{l=1}^{L} \in \Re^M$ and $\left\{y^{(l)}\right\}_{l=1}^{L} \in \{C_1, C_2, ...C_J\}$.
- For each tree $(1, \ldots, T)$:
  - Sample with replacement from the original data set (boostrap sampling) : $L?(< L)$ data
  - Randomly select $D'(< D)$ features
  - Train a tree optimizing the index Gini with the data matrix $(L? \times D')$.
  - Once the forest is trained, each leaf of the tree has the class probabilities: $P_t(C_j|\mathbf{x})$

Introduction to ensembles

Goal

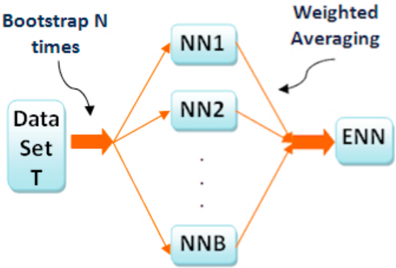
- Combine a set of weak learners to build a strong one
- Exploit the diversity among the base learners

Kind of ensembles

- Bagging, boosting, mixture of experts...
- Random forests is set of bagged trees

Bagging: Boostrap Aggregating

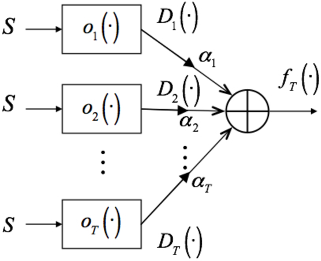
- Generate T data subsets by subsampling the training data with replacement.
- Train T models, one model for each training subset
- Classification: obtain T outputs and majority vote



Boosting

Idea

Iteratively pay more attention to the misclassified data (-¿ emphasis function).



- Emphasis function:

$$D_{t+1}(\mathbf{x}^{(l)}) = \frac{D_t(\mathbf{x}^{(l)}) \exp\left(-\alpha_t o_t(\mathbf{x}^{(l)}) y^{(l)}\right)}{Z_t}$$

- Output weights (α_t) can be analytically computed
- Final output:

$$f(\mathbf{x}^*) = \sum_{t=1}^{T} \alpha_t o_t(\mathbf{x}^*)$$