Machine Learning and Intelligent Systems

Linear Models for Classification: Logistic Regression

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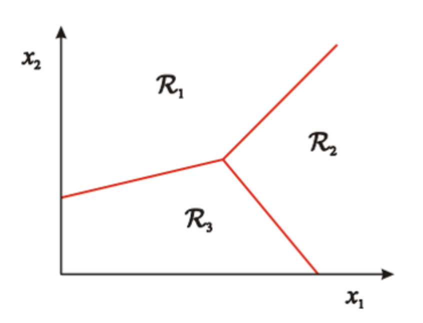
Quick recap

Supervised Learning: Classification

- **Assumption 1:** The target variable (output) y is now binary



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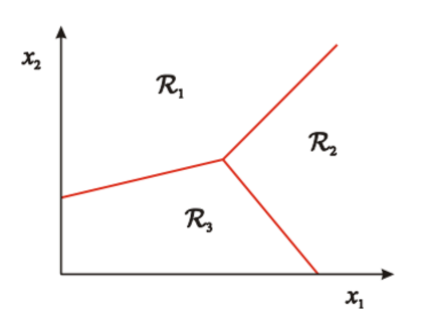
- **Assumption 2:** The input data x is separable



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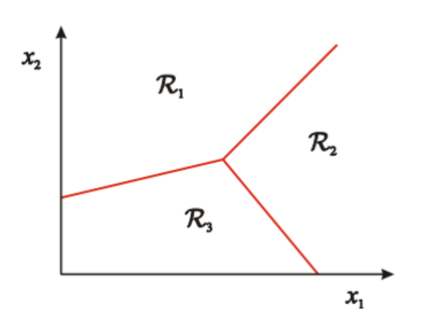
- **Definition:** We will denote $\mathcal{C}$ the set of possible classes that y can take



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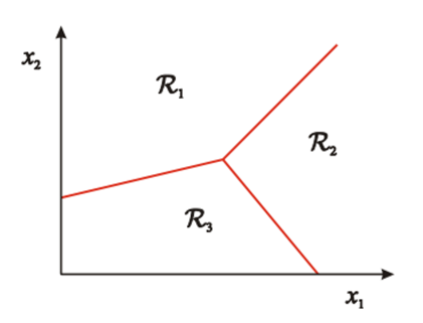

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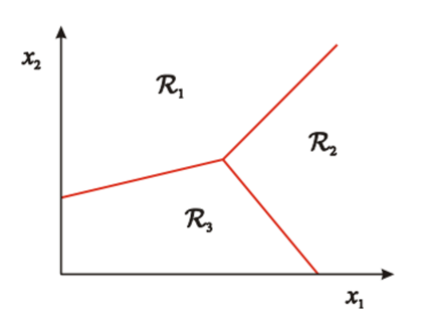

The boundaries of the **decision regions** are called **decision boundaries** or **surfaces**.

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The Zero-one loss function

- We derived an expression for the decision rule that minimizes the expected loss:

$$\min \sum_k L_{kj} p(\mathcal{C}_k | \mathbf{x})$$

The Bayes Classifier

- Using the 0-1 loss, we derived the Bayes Classifier.
- It classifies x to the most likely class using the conditional distribution

$$\begin{aligned}\hat{y} &= \arg\min_j 1 - p(\mathcal{C}_j|\mathbf{x}) \\ &= \arg\max_j p(\mathcal{C}_j|\mathbf{x})\end{aligned}$$

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  - Linear Discriminant Analysis - Generative approach
- **Now:** A second method - Logistic regression (discriminative approach)

Logistic Regression

Probability Refresher: The Odds

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- Example: Odds that a randomly chosen day of the week is a weekend
- What about chances of choosing a day that is a weekend?

Odds & Probabilities: Relationship[1]

- Odds can be expressed as a ratio of two numbers:

$$1:1 \quad \text{or} \quad 100:100,$$

  which leads to a non-unique representation

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- or as a number, by dividing the terms in the ratio (unique representation)
- Odds and probabilities are related by simple formulas
- Odds range from 0 to infinity, whereas probabilities go from 0 to 1

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Odds & Probabilities: Relationship[2]

- Given the odds as the ratio $W : L$ (Wins:Losses), the odds in favor (as a number) o_f and odds against (as a number) o_a can be computed by:

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o_f &= W/L, \\
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- Analogously, given odds as a ratio, the probability of success p or failure q can be computed by:

$$p = W/(W + L),$$
$$q = L/(W + L),$$
$$p + q = 1$$

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$$p = o_f/(o_f + 1) = 1/(o_a + 1),$$
$$q = o_a/(o_a + 1) = 1/(o_f + 1)$$

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Odds & Probabilities: Summary Table

odds (ratio)	o_f	o_a	p	q
1:1	1	1	50%	50%
0:1	0	∞	0%	100%
1:0	∞	0	100%	0%
2:1	2	0.5	67%	33%
1:2	0.5	2	33%	67%
4:1	4	0.25	80%	20%
1:4	0.25	4	20%	80%
9:1	9	$0.\overline{1}$	90%	10%
10:1	10	0.1	$90.\overline{90}\%$	$9.\overline{09}\%$
99:1	99	$0.\overline{01}$	99%	1%
100:1	100	0.01	$99.\overline{0099}\%$	$0.\overline{9900}\%$

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Linear Discriminant Analysis: Quick recap

- **Assumption:** Data within each class is normally distributed

$$p(\mathbf{x}|\mathcal{C}_k) \sim \mathcal{N}(\mu_k, \mathbf{\Sigma})$$

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$$\frac{P(E)}{P(\bar{E})} = \frac{p(\mathcal{C}_1|\mathbf{x})}{p(\mathcal{C}_2|\mathbf{x})}$$

- As the log is monotonic we can estimate the log-odds:

$$\log\left(\frac{p(\mathcal{C}_1|\mathbf{x})}{p(\mathcal{C}_2|\mathbf{x})}\right)$$

The Log-odds

Using the Bayes' theorem:

$$\log\left(\frac{p(\mathcal{C}_1|\mathbf{x})}{p(\mathcal{C}_2|\mathbf{x})}\right) = \log\left(\frac{p(\mathbf{x}|\mathcal{C}_1)p(\mathcal{C}_1)/p(\mathbf{x})}{p(\mathbf{x}|\mathcal{C}_2)p(\mathcal{C}_2)/p(\mathbf{x})}\right)$$

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$$= \log\left(\frac{C\exp\left(-\frac{1}{2}(\mathbf{x}-\mu_1)^T\mathbf{\Sigma}^{-1}(\mathbf{x}-\mu_1)\right)}{C\exp\left(-\frac{1}{2}(\mathbf{x}-\mu_2)^T\mathbf{\Sigma}^{-1}(\mathbf{x}-\mu_2)\right)}\right) + \log\left(\frac{\pi_1}{\pi_2}\right)$$

C : Common constant value to both terms. Why?

The Log-odds: Derivation

$$\log\left(\frac{p(\mathcal{C}_1|\mathbf{x})}{p(\mathcal{C}_2|\mathbf{x})}\right) = -\frac{1}{2}\left(\mathbf{x}-\mu_1\right)^T \boldsymbol{\Sigma}^{-1}\left(\mathbf{x}-\mu_1\right) + \frac{1}{2}\left(\mathbf{x}-\mu_2\right)^T \boldsymbol{\Sigma}^{-1}\left(\mathbf{x}-\mu_2\right) + \log\left(\frac{\pi_1}{\pi_2}\right)$$

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Exercise: Prove that

$$\log\left(\frac{p(\mathcal{C}_1|\mathbf{x})}{p(\mathcal{C}_2|\mathbf{x})}\right) = \log\left(\frac{\pi_1}{\pi_2}\right) - \frac{1}{2}\left(\mu_1+\mu_2\right)^T \boldsymbol{\Sigma}^{-1}\left(\mu_1-\mu_2\right) + \mathbf{x}^T\boldsymbol{\Sigma}^{-1}\left(\mu_1-\mu_2\right)$$

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Having a closer look at the expression we just obtained:

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Instead of estimating μ, $\boldsymbol{\Sigma}$ and π, we can directly estimate $\hat{w}_0$ and $\hat{\mathbf{w}}$. This is:

Logistic Regression

Model Assumptions

Assumption:

$$\log\left(\frac{p(\mathcal{C}_j|\mathbf{x})}{p(\mathcal{C}_k|\mathbf{x})}\right) = w_0 + \mathbf{w}^T\mathbf{x}$$

where

$$p(\mathcal{C}_j|\mathbf{x}) = \frac{\exp(w_0 + \mathbf{w}^T\mathbf{x})}{1 + \exp(w_0 + \mathbf{w}^T\mathbf{x})}$$

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\log\frac{p}{1-p} &= w_0 + \mathbf{w}^T\mathbf{x} \\
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Model Assumptions

Assumption:

$$\log\left(\frac{p(\mathcal{C}_j|\mathbf{x})}{p(\mathcal{C}_k|\mathbf{x})}\right) = w_0 + \mathbf{w}^T\mathbf{x}$$

where

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with $p = p(\mathcal{C}_j|\mathbf{x})$

The Sigmoid function

Our model assumption about the posterior probabilities $p(\mathcal{C}_j|\mathbf{x})$ is represented by the sigmoid function:

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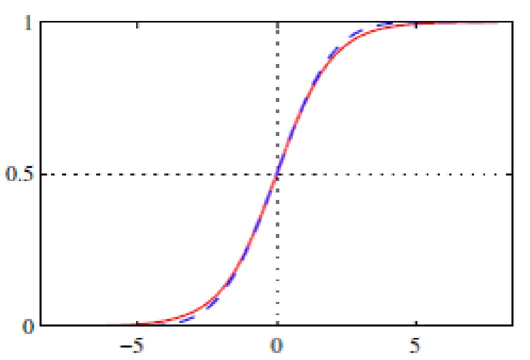

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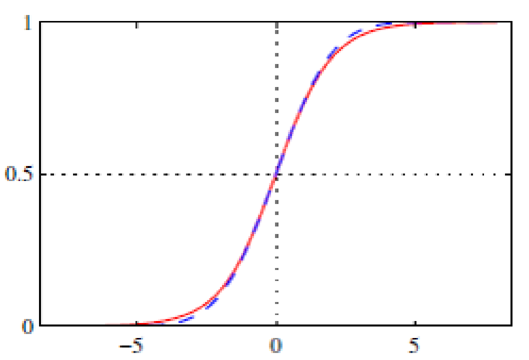

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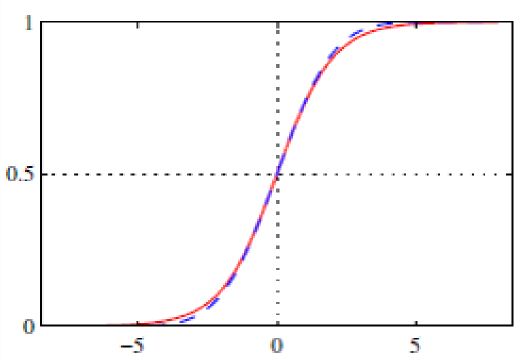

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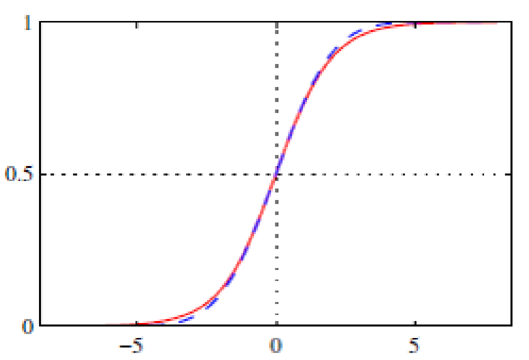

Sigmoid means S-shaped. Also called squashing function because it maps the whole real axis into a finite interval

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Note that the inverse represents the log ratio of probabilities, which is nothing else than the log-odds:

$$\log\left(\frac{p(\mathcal{C}_1|\mathbf{x})}{p(\mathcal{C}_2|\mathbf{x})}\right)$$

Data Assumptions

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The Learning Process

- We will make use of the Maximum Likelihood Estimator (MLE) to fit our model.
- In other words, using a training dataset $\mathcal{D} = \{\mathbf{x}_i, y_i\}_{i=1}^{N}$, we use MLE to choose parameters that maximize the conditional likelihood:

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- **Question:** How?

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$$p(\mathcal{C}_2|\mathbf{x}_i;\mathbf{w}) = 1 - p(\mathcal{C}_1|\mathbf{x}_i;\mathbf{w})$$

3. and we made some assumptions about the underlying model for $p(\mathcal{C}_j|\mathbf{x}_i;\mathbf{w})$.

Let's put all together to derive an expression for the log-likelihood in terms of $\mathbf{y}$, $\mathbf{X}$ and $\mathbf{w}$.

The Learning Process (3)

- From point 1, we can rewrite the log-likelihood:

$$\ell(\mathbf{w}) = \sum_{i=1}^{N} y_i \log p(\mathcal{C}_1 | \mathbf{x}_i; \mathbf{w}) + (1 - y_i) \log p(\mathcal{C}_2 | \mathbf{x}_i; \mathbf{w})$$

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- From point 2, we can write everything in terms of $p(\mathcal{C}_1|\mathbf{x}_i;\mathbf{w})$:

$$\ell(\mathbf{w}) = \sum_{i=1}^{N} y_i \log p(\mathcal{C}_1|\mathbf{x}_i;\mathbf{w}) + (1-y_i)\log\left(1 - p(\mathcal{C}_1|\mathbf{x}_i;\mathbf{w})\right)$$

- Finally, thanks to point 3, we make use of our model assumption:

$$\ell(\mathbf{w}) = \sum_{i=1}^{N} y_i \log \sigma(w_0 + \mathbf{w}^T\mathbf{x}_i) + (1-y_i)\log\left(1 - \sigma(w_0 + \mathbf{w}^T\mathbf{x}_i)\right)$$

Cross-Entropy Loss Function

Instead of maximizing, we can take the negative of the previous expression to obtain a loss or error function[4]:

$$E(\mathbf{w}) = -\sum_{i=1}^{N} y_i \log \sigma(\mathbf{w}^T \mathbf{x}_i) + (1 - y_i) \log \left(1 - \sigma(\mathbf{w}^T \mathbf{x}_i)\right) \tag{1}$$

This expression is denoted the **cross-entropy loss function**

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To obtain the optimal $\mathbf{w}$, we need to derive the above expression and equal it to zero.

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Derivation

We will make use of the following property:

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Deriving Eq. 1:

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&= \sum_{i=1}^{N} \left(\sigma(\mathbf{w}^T \mathbf{x}_i) - y_i\right) \mathbf{x}_i
\end{aligned}
$$

Warning

After equating to zero, there is no way to obtain a closed-form solution for $\hat{\mathbf{w}}$

Predictions

- Formally, the parameters for logistic regression are estimated via:

$$\hat{w}_0, \hat{\mathbf{w}} = \arg\min_{\mathbf{w}} \; -\sum_{i=1}^{N} y_i \log \sigma(w_0 + \mathbf{w}^T \mathbf{x}_i) + (1 - y_i) \log \left(1 - \sigma(w_0 + \mathbf{w}^T \mathbf{x}_i)\right)$$

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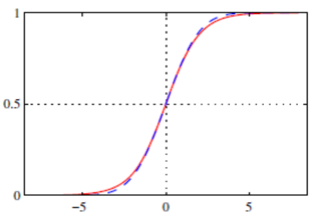
- We will not cover their estimation for now.
- Assuming we have $\hat{w}_0, \hat{\mathbf{w}}$, given a new sample $\mathbf{x}_{new}$, we will use what we know about the sigmoid function to assign y_{new}:

$$\begin{aligned} y_{new} &= p(\mathcal{C}_1 | \mathbf{x}_{new}; \hat{\mathbf{w}}) = \sigma(\hat{w}_0 + \hat{\mathbf{w}}^T \mathbf{x}_{new}) \\ &= \begin{cases} 1 & \text{if } \hat{w}_0 + \hat{\mathbf{w}}^T \mathbf{x}_{new} > 0 \\ 0 & \text{if } \hat{w}_0 + \hat{\mathbf{w}}^T \mathbf{x}_{new} \leq 0 \end{cases} \end{aligned}$$



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- **Exercise:** Verify that this is correct and that $\sum_k p(\mathcal{C}_k|\mathbf{x})$ sums to 1.

Recap

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What we have seen so far...

- We introduced more formally the classification task
- We presented linear discriminant analysis (LDA)
- and we covered logistic regression
- Differently from LDA, it is a discriminative approach
- We saw that by relying in the log-odds logistic regression avoids to estimate the parameters of the generative model (as LDA)
- We have introduced the sigmoid function

What we have NOT seen...

- How to estimate the model parameters $\hat{\mathbf{w}}$ of the logistic regression model

References

Further Reading and Useful Material

Source	Notes
Pattern Recognition and Machine Learning	Ch. 4
The Elements of Statistical Learning	Ch. 2 and 4
Machine Learning - Tom Mitchel	Chapter 3 (link)