Machine Learning

Logistic Regression

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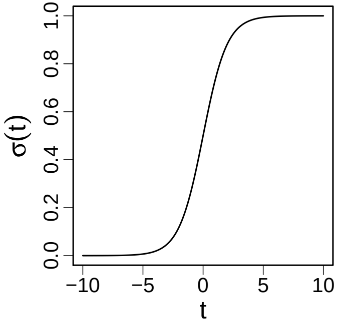
Logistic regression

- For simplicity we first consider classification for 2 classes $Y \in \{0, 1\}$.
- We assume the feature vector X is such that $X_1 = 1$ (intercept), so that we can simply write $x^\top \beta$ instead of $\beta_0 + \beta_1 x_1 + \cdots + \beta_p x_p$.
- Logistic regression links the probability of class 1 to $x^\top \beta$ by

$$\Pr(Y = 1 \mid X = x) = \sigma(x^\top \beta) \quad \text{where} \quad \sigma(t) = \frac{\exp(t)}{1 + \exp(t)}.$$

- The function σ is called the `logistic function`: it maps $\mathbb{R}$ to $(0, 1)$.



Logistic regression: interpretation

- We observe

$$\Pr(Y = 1 \mid X = x) = \sigma(x^\top \beta) \quad \Leftrightarrow \quad \sigma^{-1}\left(\Pr(Y = 1 \mid X = x)\right) = x^\top \beta,$$

  where $\sigma^{-1}(u) = \log\{u/(1-u)\}$ called the `logit function`.
- Logistic regression thus implies that `log-odds` are linear

$$\log \frac{\Pr(Y = 1 \mid X = x)}{\Pr(Y = 0 \mid X = x)} = \log \frac{\sigma(x^\top \beta)}{1 - \sigma(x^\top \beta)} = x^\top \beta,$$

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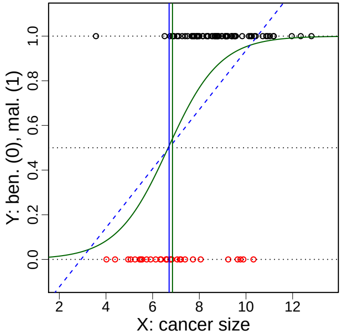
- Note that this implies that the decision boundary from logistic regression is linear.
- Figure: Logistic regression (green) versus linear regression (blue).



Logistic regression: estimation

- We estimate the parameter β by maximizing the conditional log-likelihood of the sample $(x_1, y_1), \ldots, (x_n, y_n)$ where $y_i \in \{0, 1\}$.
- By the logistic model assumption $Y \mid X = x_i$ is Bernoulli distributed with success probability $\sigma(x_i^\top \beta)$. This gives the log-likelihood for the sample

$$\ell(\beta) = \sum_{i=1}^{n} \log \Pr(Y = y_i \mid X = x_i) = \sum_{i=1}^{n} y_i x_i^\top \beta - \log(1 + e^{x_i^\top \beta}).$$

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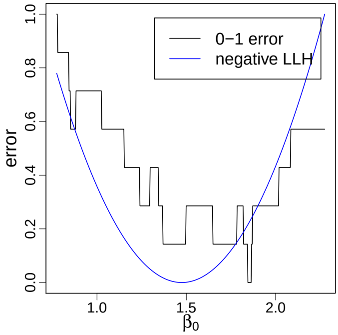
- The maximum likelihood estimator (MLE) $\widehat{\beta} = \operatorname{argmax}_\beta \ell(\beta)$ has no explicit formula; ℓ must be maximized numerically (Newton–Raphson, gradient descent, etc.).



Logistic regression: estimation

- Prediction: From $\widehat{\beta}$ we estimate for a new input $x_0 \in \mathbb{R}^p$

$$\widehat{\Pr}(Y = 1 \mid X = x_0) = \sigma(x_0^\top \widehat{\beta}).$$

We use the Bayes classifier based on these estimates to predict the class

$$\widehat{y}_0 = \begin{cases} 1 & \text{if } \sigma(x_0^\top \widehat{\beta}) > 1/2, \\ 0 & \text{otherwise.} \end{cases}$$

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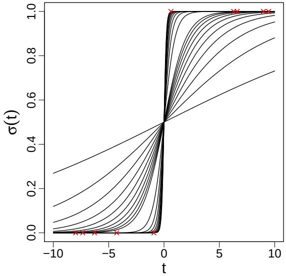
- Careful: The MLE $\widehat{\beta}$ does not exist when the classes are perfectly separable.
- The figure illustrate the problem of perfect separation. The observations are in red.
- The two classes can be perfectly separated by letting $\beta_1 \to \infty$.



Multiclass logistic regression: multinomial regression

- Logistic regression extends to the multiclass case $Y \in \{1, \ldots, q\}$ by specifying

$$
\begin{aligned}
\Pr(Y = j \mid X = x) &= \frac{e^{x^\top \beta^{(j)}}}{1 + \sum_{l=1}^{q-1} e^{x^\top \beta^{(l)}}}, \qquad j = 1, \ldots, q-1, \\
\Pr(Y = q \mid X = x) &= \frac{1}{1 + \sum_{l=1}^{q-1} e^{x^\top \beta^{(l)}}},
\end{aligned}
$$

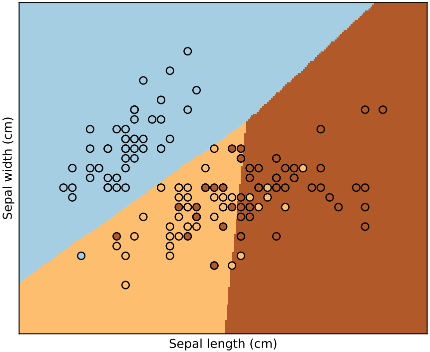
  where $\beta^{(1)}, \ldots, \beta^{(q-1)} \in \mathbb{R}^p$ are parameter vectors to be estimated.
- The model uses $q-1$ equations for q classes: this is because of the constraint that the probabilities must sum to one.
- Maximum likelihood estimation: the distribution of $Y \mid X$ is multinomial and we can obtain the likelihood

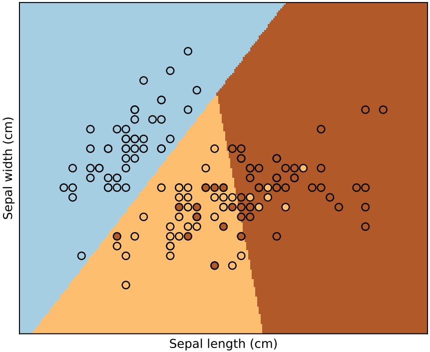
$$
\ell(\beta) = \sum_{i=1}^{n} \log \Pr(Y = y_i \mid X = x_i).
$$

Iris data set: multinomial (logistic) regression

For 150 measured plants; $p = 4$ predictors as response the three Iris species $\mathcal{G} = \{\texttt{setosa}, \texttt{versicolor}, \texttt{virginica}\}$ the plant belongs. We only use two predictors here.

```
from sklearn.linear_model import LogisticRegression
iris = sklearn.datasets.load_iris()
X, y = iris.data[:, :2], iris.target  # we only keep the first two features: 'Sepal length', 'Sepal width'
logreg = LogisticRegression(penalty="none")
logreg.fit(X, y)
x_min, x_max = X[:, 0].min() - .5, X[:, 0].max() + .5
y_min, y_max = X[:, 1].min() - .5, X[:, 1].max() + .5
h = .02  # step size in the mesh
xx, yy = np.meshgrid(np.arange(x_min, x_max, h), np.arange(y_min, y_max, h))
Z = logreg.predict(np.c_[xx.ravel(), yy.ravel()]).reshape(xx.shape)
```





Comments

- Other link functions than σ can be used to map responses $x^\top \beta$ to probabilities, e.g., the so-called `probit regression`

  $$\Pr(Y = 1 \mid X = x) = \Phi(x^\top \beta),$$

  where Φ is the univariate Gaussian distribution function. Logistic is usually preferable to probit regression: it is more robust to outliers.
- Logistic regression is a special case of a `generalized linear model` (GLM).

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Logistic regression vs. LDA

- For both models the log-odds between any two classes are linear in x.
- The difference between LDA and logistic regression comes from the `estimation` of their parameters.
- LDA models the joint distribution of (Y, X), while logistic regression only models $Y \mid X$. If the Gaussian assumption for the conditional class densities is reasonable then LDA may perform better. If the Gaussian assumption is clearly unreasonable then logistic regression will outperform LDA.
- Often they have similar performance.