Modul 215: Machine Learning

Linear Regression Methods: Linear & Logistic Regression

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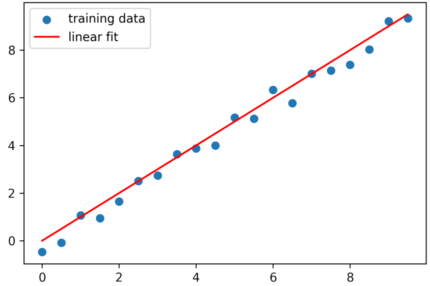
Recap: Regression

- **Goal:** Find a function f (in most cases a set of parameters) to predict a quantity y for input x by using training data:

$$\left((x^{(1)}, y^{(1)}), \ldots, (y^{(N)}, x^{(N)})\right) \tag{1}$$

- where $(x^{(i)}, y^{(i)})$ is one data sample
- e.g (kaggle.com):
  1. House prices (given location, size, etc.)
  2. Sales prediction (given advertisement)
  3. $C0_2$ emission (given engine size, etc.)
  4. Diabetes (disease progression)
  5. ...



Linear Regression

- **Goal**: Model the relationship between input and target by a linear equation:

$$\hat{y} = f(x_1, \dots, x_p) = \hat{\beta}_0 + \sum_{j=1}^{p} \hat{\beta}_j x_j \tag{2}$$

- $\hat{\beta}_0$: Intercept, bias
- $\hat{\beta}_j$: Slope, weight for dimension j
- $\hat{y}$: Prediction for target y given input x
- Multiple approaches available to fit a linear model e.g.:
  1. Closed form solution: ordinary least squares
  2. Locally weighted linear regression
  3. Gradient descent
  4. ...

Ordinary Least Squares (OLS): Residual Sum of Squares

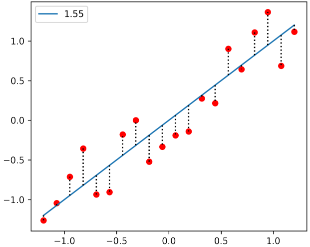
- **Goal:** find a function f that minimizes residual sum of squares:

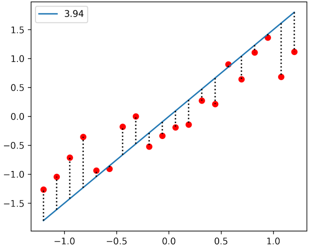
$$RSS(\hat{\beta}) = \sum_{i=1}^{N} \Big(\underbrace{y^{(i)} - f(x^{(i)})}_{residual} \Big)^2 \tag{3}$$

- with

$$f(x_1^{(i)}, \dots x_p^{(i)}) = \hat{\beta}_0 + \sum_{j=1}^{p} \hat{\beta}_j x_j^{(i)} \tag{4}$$

- with target value $y^{(i)}$ for input $x^{(i)}$ and model parameters $\hat{\beta} = \{\hat{\beta}_0, \{\hat{\beta}_j\}_{1:p}\}$





Ordinary Least Squares (OLS): Matrix Representations I

- We can replace the sum of $x_j\hat{\beta}_j$ terms (linear combination) with inner product of vector x^T and $\hat{\beta}$:

$$\hat{y} = \hat{\beta}_0 + \sum_{j=1}^{p} x_j\hat{\beta}_j = \hat{\beta}_0 + \underbrace{x_1\hat{\beta}_1 + \cdots + x_j\hat{\beta}_j}_{\begin{pmatrix} x_1 & \dots & x_j \end{pmatrix}\begin{pmatrix} \hat{\beta}_1 \\ \vdots \\ \hat{\beta}_j \end{pmatrix}} \tag{5}$$

- Which gives us:

$$\hat{y} = \hat{\beta}_0 + x^T\hat{\beta} \tag{6}$$

Ordinary Least Squares (OLS): Matrix Representations II

- Further, we can combine:

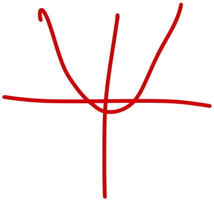
$$1\,\hat{\beta}_0 + x'^T\hat{\beta} = \begin{pmatrix} 1 & x_1 & \dots & x_j \end{pmatrix} \begin{pmatrix} \hat{\beta}_0 \\ \hat{\beta}_1 \\ \vdots \\ \hat{\beta}_j \end{pmatrix} \tag{7}$$

- Which gives us the following expression for multiple datapoints:

$$\hat{y} = \mathbf{X}'^T\hat{\beta} \tag{8}$$

- where $\mathbf{X}'$ is a $N\times$ (p+1) matrix containing N feature vectors, $\hat{\beta}$ is a vector containing all parameters and $\hat{y}$ is a vector containing all predictions

Ordinary Least Square (OLS): Closed Form Solution



- Now we can reformulate the RSS objective as:

$$RSS(\hat{\beta}) = \left(y - \mathbf{X}'^T\hat{\beta}\right)^T \left(y - \mathbf{X}'^T\hat{\beta}\right) \tag{9}$$

- By differentiating $RSS(\hat{\beta})$ w.r.t. $\hat{\beta}$, setting the equation to zero, it gives us an unique solution for $\hat{\beta}$ ($\mathbf{X}'^T\mathbf{X}'$) must be invertible):

$$\hat{\beta} = \left(\mathbf{X}'^T\mathbf{X}'\right)^{-1}\mathbf{X}'^T y \tag{10}$$

Ordinary Least Square (OLS): Solving OLS Manually I

- Consider the following dataset $\mathcal{D} = \{(-1,-2),(1,0),(2,1)\}$ where each tuple $(x^{(i)}, y^{(i)})$ consists of a one-dimensional (scalar) feature $x^{(i)}$ and a scalar target $y^{(i)}$. Find the parameters β for a linear regression model using OLS.

$$X = \begin{pmatrix} -1 \\ 1 \\ 2 \end{pmatrix} \quad y = \begin{pmatrix} -2 \\ 0 \\ 1 \end{pmatrix} \quad \begin{pmatrix} 1 & -1 \\ 1 & 1 \\ 1 & 2 \end{pmatrix} = X' \quad AA^{-1} = I$$

$$\begin{pmatrix} 1 & & \\ & 1 & \\ & & 1 \end{pmatrix}$$

$$X' = \begin{pmatrix} 1 & -1 \\ 1 & 1 \\ 1 & 2 \end{pmatrix} \quad X'^T = \begin{pmatrix} 1 & 1 & 1 \\ -1 & 1 & 2 \end{pmatrix}$$

$$X'^T X' = \begin{pmatrix} 3 & 2 \\ 2 & 6 \end{pmatrix} = A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad A^{-1} = \frac{1}{a \cdot d - bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

$$= \frac{1}{14} \begin{pmatrix} 6 & -2 \\ -2 & 3 \end{pmatrix}$$

Ordinary Least Square (OLS): Solving OLS Manually II

$$X^T y = \begin{pmatrix} -1 \\ 4 \end{pmatrix}$$

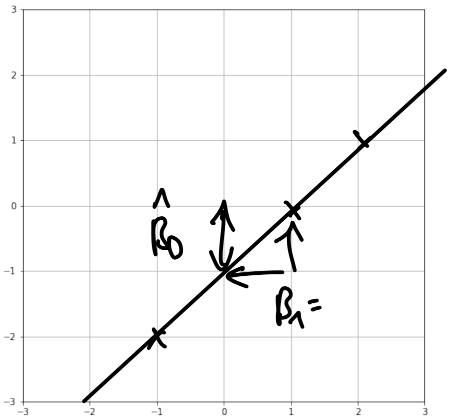
$$A^{-1} X^T y = \frac{1}{14} \begin{pmatrix} 6 & -2 \\ -2 & 3 \end{pmatrix} \begin{pmatrix} -1 \\ 4 \end{pmatrix}$$

$$= 1/14 \begin{pmatrix} -14 \\ 14 \end{pmatrix}$$

$$\hat{\beta} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

Ordinary Least Square (OLS): Solving OLS Manually III

$$\hat{\beta} = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$



Ordinary Least Square (OLS): Scikit Learn I

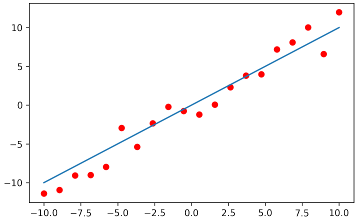
sklearn.linear_model.LinearRegression

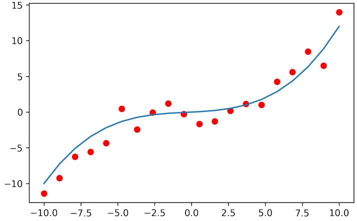
class sklearn.linear_model.LinearRegression(*, *fit_intercept=True*, *normalize='deprecated'*, *copy_X=True*, *n_jobs=None*, *positive=False*) [source]

- fit_intercept (bool): Use parameter β_0 during data fit. (Recommended in most use-cases, data must be centered otherwise)
- normalize: $\rightarrow$ will be removed in v1.2
- copy_X: if true, X will be copied (otherwise it might be overwritten)
- n_jobs: The number of jobs to use for the computation. Requires sufficiently large task.
- positive: When set to True, forces the coefficients to be positive.

Going Beyond Linear Functions: Nonlinear Features I

- In reality observed data is often not linear (e.g. quadratic, polynomial, etc.) $\rightarrow$ we still want to use our linear model
- How to extend our previous OLS framework to deal with this kind of data?





Going Beyond Linear Functions: Nonlinear Features II (Polynomial)

- **Single feature x with polynomial target y:**

  Suppose: $\mathcal{D} = \{(x^{(j)}, y^{(j)})\}_{1:N}$ $\qquad$ $y(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$

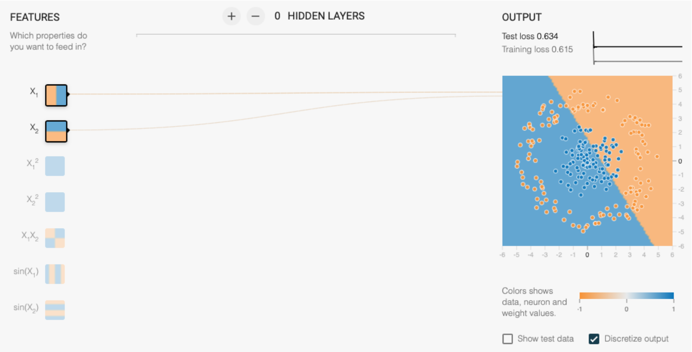
- **Polynomial features x with linear target y:**

  Now: $\mathcal{D} = \{([x^{(j)}, (x^{(j)})^2, (x^{(j)})^3], y^{(j)})\}_{1:N}$ $\qquad$ $y(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3$

- Data is now linear separable in higher dimensional feature space
- General notation: "polynomial feature transform" $\phi(x) = [1, x, x^2, x^3, \dots]$
- Can be expanded to any kind of nonlinear transformation (e.g sin, cosine, sqrt)

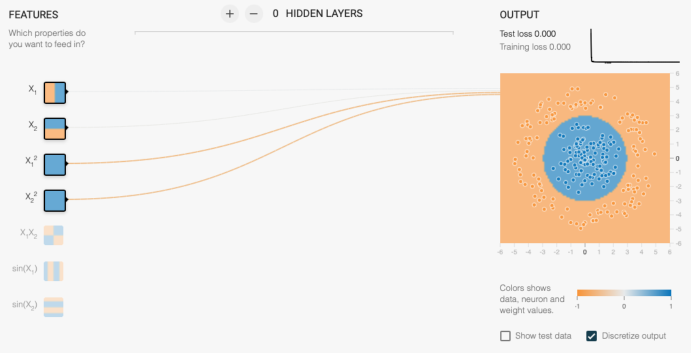
Tensorflow Playground[1] - Polynomial Features I

- **Usage**: Taking only input feature without hidden dimension and linear activation function corresponds to linear model optimized using gradient descent.



[1] http://playground.tensorflow.org/

- **Summary**: By using nonlinear transformation X_1^2, X_2^2 we can fit our dataset without any modification of the linear model.



- **Consider**:

$$y = \beta + \beta_1 x_1 + \beta_2 x_2 \tag{11}$$

- **Following**:

$$\frac{\partial y}{\partial x_1} = \beta_1 \tag{12}$$

- This means changing x_1 by one unit will change y by β_1 $\rightarrow$ we cannot capture any dependence on x_2 (independent variables)

Exclusive-Or Gate: XOR

Input		Output
x_1	x_2	$x_1 \oplus x_2$
0	0	0
0	1	1
1	0	1
1	1	0

Going Beyond Linear Functions: Interactions II

- **In Contrast**:

$$y = \beta + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1 X_2 \tag{13}$$

- **Following**:

$$\frac{\partial y}{\partial x_1} = \beta_1 + \beta_3 X_2 \tag{14}$$

- Modeled interactions (combinations) of x_1 with x_2 captures dependencies between those two variables

Exclusive-Or Gate: XOR

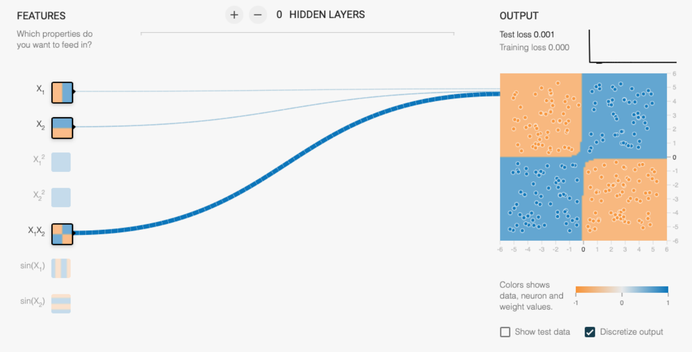
Input		Output
x_1	x_2	$x_1 \oplus x_2$
0	0	0
0	1	1
1	0	1
1	1	0

Tensorflow Playgroud - Interactions I

- **Recap**: Taking only input feature without hidden dimension and linear activation function corresponds to linear model optimized using gradient descent.

Tensorflow Playground - Interactions II

- **Summary**: By using interaction term X_1X_2 we can fit XOR dataset without any modification of the linear model.



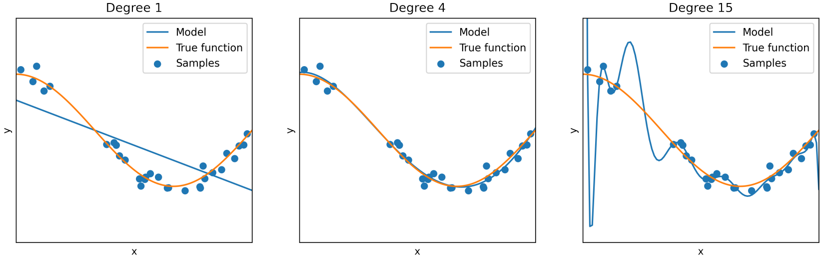
Going Beyond Linear Functions: Scikit-Learn

sklearn.preprocessing.PolynomialFeatures

class sklearn.preprocessing.PolynomialFeatures(*degree=2, *, interaction_only=False, include_bias=True, order='C'*) [source]

- degree (int): Maximal degree of the polynomial features (e.g. x_1, x_2 with degree=2: $[x_1, x_2, x_1^2, x_2^2, x_1 x_2]$)
- intearaction_only (bool): If True, only interaction features are produced.
- include_bias (bool): If True (default), then include a bias column.

Going Beyond Linear Functions: Final Notes



Parametric vs. Nonparametric Learning Algorithms

- **"Parametric" learning algorithm**: fit a fixed set of parameters to data $\leftarrow$ e.g. Linear Regression, Neural Networks, Naive Bayes
- **"Nonparametric" learning algorithm**: amount of data/parameters you need to keep grows (linearly) w.r.t size of data $\rightarrow$ **do not make strong assumptions about the form of the mapping function** (stay flexible). $\leftarrow$ e.g. Locally Weighted Regression,

Going Beyond Linear Functions: Locally Weighted Linear Regression

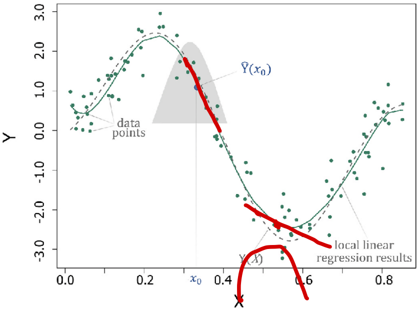
- Find a set of parameter β' for each point in test set that minimizes weighted sum of squares:

$$WRSS(\hat{\beta}) = \sum_{i}^{m} w^{(i)} \left(y^{(i)} - \hat{\beta}^T x^{(i)} \right)^2 \tag{15}$$

- where w is a non-negative weight (scaling factor) with

$$w^{(i)} = \exp\left(-\frac{(x^{(i)} - x)^2}{2\tau^2} \right) \tag{16}$$

- Requires no training phase. Instead coefficients are calculated for each sample during prediction.



Summary: Linear Regression

- Ordinary Least Squares Regression
  - RSS objective and closed form solution for OLS
  - How to solve linear regression problems by hand
- Nonlinear features
  - Polynomial features + how they solve the nonlinearity problem
  - Interactions + how they work
  - Overadaption of linear models to highly nonlinear features
- Locally Weighted Linear Regression
  - Non-parametric machine learning model
  - Requires no specific assumption about function mapping

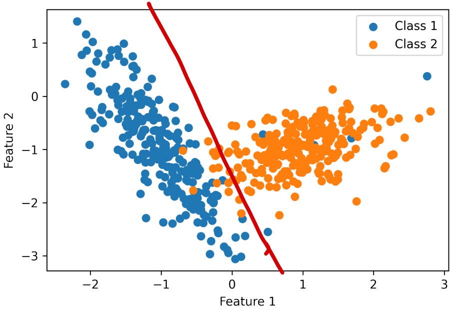
Any Questions ?

Recap: Classification

- **Goal:** Find a function f that divides the input space (feature space) X into decision regions separating all classes contained in Y using data $\rightarrow$ discrete outcome:

$$(y^{(1)}, x^{(1)}), \ldots \ldots, (y^{(N)}, x^{(N)}) \qquad (17)$$

- with $y^{(i)} \in \mathbb{N}$ and $x^{(i)} \in \mathbb{R}^n$
- e.g (kaggle.com):
  1. Optical character recognition (given image of character)
  2. Heart attack classification (given ECG)
  3. Skin cancer classification (given skin image)
  4. ...



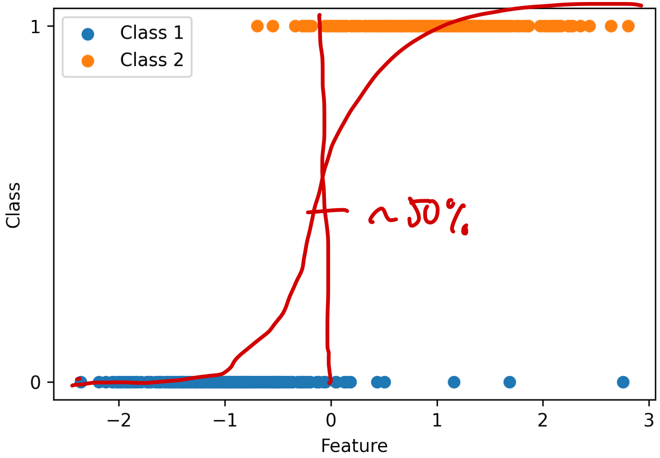
Logistic Regression I: Binary Classification and Class Probabilities

- In contrast to linear regression the type of the dependent (predicted) variable is binary instead of continuous $\rightarrow$ we need some modification to the existing framework.
- Additional we want to calculate class probabilities using linear functions.
- Given a **binary classification** problem with features $x \in \mathbb{R}^p$, the class probabilities are defined formally as:

$$P(Y = 0|X = x) \tag{18}$$

$$P(Y = 1|X = x) \tag{19}$$

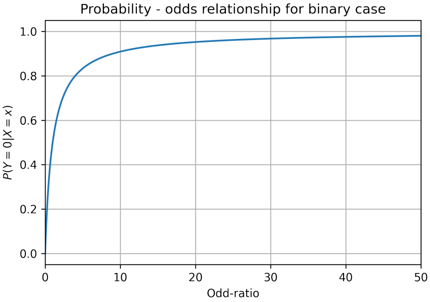
Binary Classification - Features, Target Relationship



Logistic Regression II: Class Probabilities and Odd-Ratio

- Consider ratio between odds of events (odd-ratio):

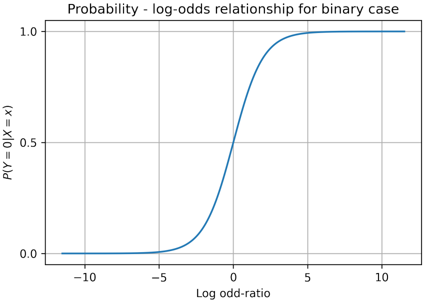
$$\text{odd-ratio} = \frac{P(Y=0|X=x)}{P(Y=1|X=x)} = \frac{P(Y=0|X=x)}{1-P(Y=0|X=x)} \tag{20}$$



- Non-symmetric function
- Odd-ratios for $P \in [0,1]$ ranges from 0 to infinity

Logistic Regression II: Class Probabilities and Log Odd-Ratio

- Now consider log odd ratio (log-odds) log(odd-ratio)
- Symmetric function $\rightarrow$ log-odds against (-) and in (+) favour while value stays the same



$$P(Y=0|X=x)\begin{cases} > & P(Y=1|X=x): \quad \text{the log odd-ratio is positive} \\ = & P(Y=1|X=x): \quad \text{the log odd-ratio is zero} \\ < & P(Y=1|X=x): \quad \text{the log odd-ratio is negative} \end{cases} \tag{21}$$

Logistic Regression III: From Log-Odds to Probabilities

- Suppose event with binary outcome with $p = 0.2$ and $\overline{p} = 0.8$ we can get the following conversion rules:

$$odds = \frac{0.2}{0.8} = 0.25 \quad \rightarrow \quad p = \frac{odds}{1 + odds} = 0.2 \tag{22}$$

$$\log(odds) = \ln \frac{0.2}{0.8} = -1.3863 \quad \rightarrow \quad p = \frac{\exp(\log(odds))}{1 + \exp(\log(odds))} = 0.2 \tag{23}$$

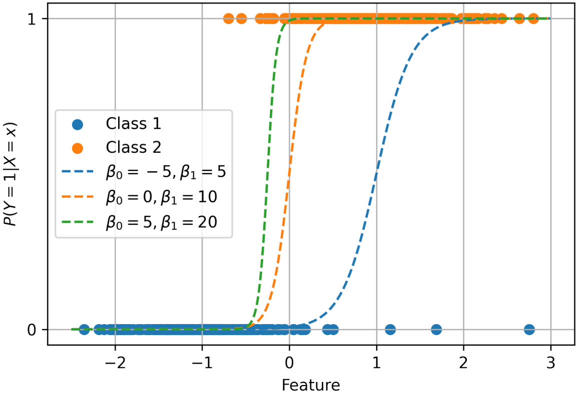
Logistic Regression V

- Decision boundaries is defined by the hyperplane where the log-odds are zero $\{x|\beta_0 + \beta^T x = 0\}$
- Leaves us with:

$$P(Y = 0|X = x) = \frac{\exp(\beta_0 + \beta^T x)}{1 + exp(\beta_0 + \beta^T x)} \tag{24}$$

$$P(Y = 1|X = x) = \frac{1}{1 + \exp(\beta_0 + \beta^T x)} \tag{25}$$

Logistic Regression VI: Examples for Different Linear Functions



Interactive demo in *logistic_regression_interactive.ipynb*

Logistic Regression VII: Maximum Likelihood Fit

- **Likelihood**: Factorized probability of a set of N observations as a function of β

$$\mathcal{L}(\beta) = \prod_{i=0}^{N} P_\beta(Y = y_i | X = x_i) \tag{26}$$

- **Maximum Likelihood**: Find the best fitting parameter β that maximizes the likelihood:

$$\hat{\beta} = \arg\max_\beta \mathcal{L}(\beta) \tag{27}$$

Logistic Regression VIII: Maximum Likelihood Fit (Log Likelihood)

- Consider the likelihood for $N \to \infty$ events:

$$\lim_{N\to\infty} \mathcal{L}(\beta) = \lim_{N\to\infty} \prod_{i=1}^{N} P(Y = y_i|X = x_i) \quad \begin{cases} 1 & P(Y = y_i|X = x_i) = 1 \\ 0 & P(Y = y_i|X = x_i) < 1 \end{cases} \tag{28}$$

- Numerical instabilities $\to$ It is often more convenient to maximize the **log likelihood**
- **Log likelihood:**

$$\ell(\beta) = \log \mathcal{L}(\beta) = \sum_{i=1}^{N} \log P(Y = y_i|X = x_i) \tag{29}$$

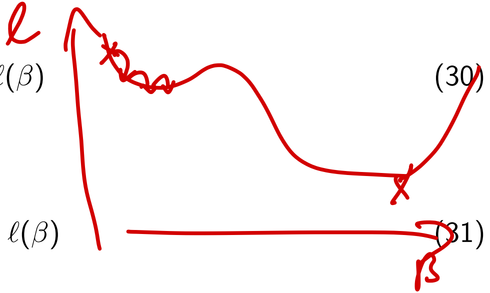
Logistic Regression VIII: Maximum Likelihood Fit (Iterative Solutions)

- No closed form solution for logistic regression $\rightarrow$ instead iterative optimization $\rightarrow$ convergence to optimal solution not guaranteed.

$$\hat{\beta} = \arg\max_{\beta} \ell(\beta) \tag{30}$$

- or equalently

$$\hat{\beta} = \arg\min_{\beta} \; -\ell(\beta) \tag{31}$$



- Many algorithms to find a good maximum likelihood fit: (https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html)

Logistic Regression VIV: Maximum Likelihood - Improved Loss Function

- **Recap**: The loss function of the log-likelihood ℓ is defined as:

$$\ell(\beta) = \log \mathcal{L}(\beta) = \sum_{i=1}^{N} \log P(Y = y_i | X = x_i) \tag{32}$$

- where y_i is the target class for y_i.

$$P(Y = y_i | X = x_i) = \begin{cases} \log P(Y = 1 | X = x_i) & \text{if } y_i = 1 \\ \log\left(1 - P(Y = 1 | X = x_i)\right) & \text{if } y_i = 0 \end{cases} \tag{33}$$

- This gives us :

$$\ell = \sum_{i=1}^{N} \{y_i \log P(y = 1 \, | X = x) + (1 - y_i) \log(1 - P(Y = 1 | X = x))\} \tag{34}$$

Logistic Regression X: Dealing with $K \geq 2$ Classes I

- Let $\mathrm{Y} = \{\ 1,\ 2,\ 3,\ \ldots,\ \mathrm{K}\ \}$
- We want a logistic regression model that provides the posterior probabilities of all K classes.
- **Requirements**:
  1. Sum to one
  2. All outputs remain in [0, 1]

Logistic Regression X: Dealing with $K \geq 2$ Classes II

- We can define K-1 log-odds using K-1 linear models with:

$$\log \frac{P(Y=1|X=x)}{P(Y=K|X=x)} = \beta_{10} + \beta_1^T x \tag{35}$$

$$\log \frac{P(Y=2|X=x)}{P(Y=K|X=x)} = \beta_{20} + \beta_2^T x \tag{36}$$

$$\log \frac{P(Y=K-1|X=x)}{P(Y=K|X=x)} = \beta_{(K-1)0} + \beta_{K-1}^T x \tag{37}$$

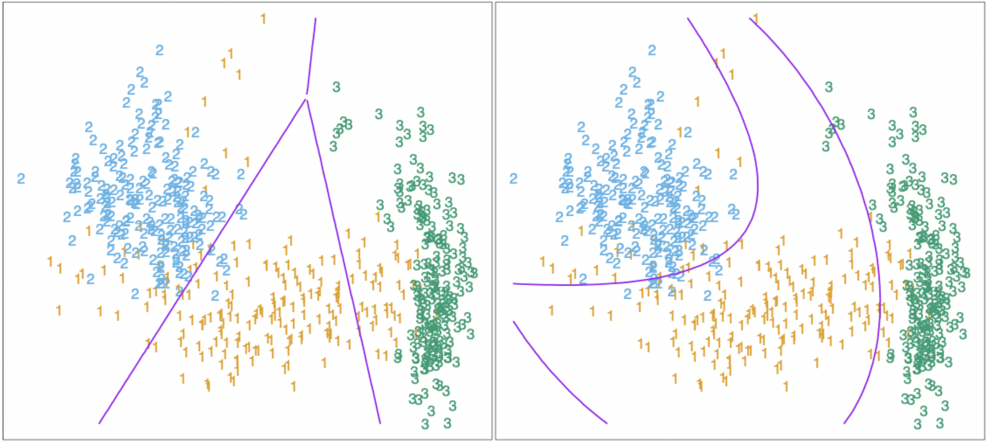
- where the choice of denominator (last class) is arbitrary.

Logistic Regression XI: Dealing with $K \geq 2$ Classes III

- Further we can transform our log-odds to posterior probabilities, respectively as

$$P(Y = 1|X = x) = \frac{\exp(\beta_{k0} + \beta_k^T x)}{1 + \sum_{l=1}^{K-1} \exp(\beta_{l0} + \beta_l^T x)}, k = 1, \dots K - 1 \tag{38}$$

$$P(Y = K|X = x) = \frac{1}{1 + \sum_{l=1}^{K-1} \exp(\beta_{l0} + \beta_l^T x)} \tag{39}$$



Source: Hastie et al.

Notes on Using Linear Regression

- Remember that you can expand your feature space $\rightarrow$ non-linear dependencies
- For nominal features: use one-hot-encoding:
  - Suppose $X \in \{red, green, blue\}$
  - Instead of X use transformed feature: $I(X = x)$
  - red = (1,0,0), green = (0,1,0), blue = (0, 0, 1)

Logistic Regression: Scikit-Learn

sklearn.linear_model.LogisticRegression ¶

class sklearn.linear_model.LogisticRegression(*penalty='l2'*, ***, *dual=False*, *tol=0.0001*, *C=1.0*, *fit_intercept=True*, *intercept_scaling=1*, *class_weight=None*, *random_state=None*, *solver='lbfgs'*, *max_iter=100*, *multi_class='auto'*, *verbose=0*, *warm_start=False*, *n_jobs=None*, *l1_ratio=None*) [source]

- penalty: Regularization method (we cover this next lecture).
- tol: Tolerance for stopping criteria.
- fit_intercept: Specifies if a constant (a.k.a. bias or intercept) should be added to the decision function.
- class_weight: Weights associated with classes in the form class_label: weight. If not given, all classes are supposed to have weight one.
- solver: Algorithm to use in the optimization problem
- max_iter: Maximum number of iterations taken for the solvers to converge.

Summary: Logistic Regression

- Relationship between posterior probabilities, odds, and log-odds.
- Modeling of log-odd$\rightarrow$posterior relationships with linear models.
- Optimization of logistic regression models using maximum likelihood estimation.
- Logistic regression for $K \geq 2$ classes.

Any Questions ?

References

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Figures:

1. https://www.researchgate.net/figure/Schematic-depiction-of-the-locally-weighted-least-squares-kernel-regressi fig3_351477495