

1



Agenda

- Introduction
- Mathematical Foundations
- Maximum Likelihood Estimation (MLE)
- Interpreting & Evaluating Model Coefficients

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Brief Recap of Logistic Regression Basics

- Logistic Regression is a statistical method for binary classification. Unlike linear regression, it predicts the probability of a binary outcome.
- Real World Examples:
 - disease presence
 - customer churn
 - loan defaults
 - spam detection

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Discrete Distributions for Binary Cases

Bernoulli Distribution



$$Y \sim \text{Bern}(p)$$

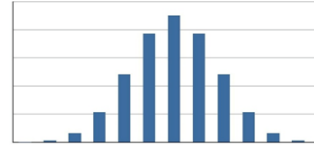
Characteristics

- Consists of a single trial
- 2 possible outcomes
- $E(Y) = p$
- $\text{Var}(Y) = p \times (1 - p)$

Uses

- Guessing a single True/False question.

Binomial Distribution



$$Y \sim B(n, p)$$

Characteristics

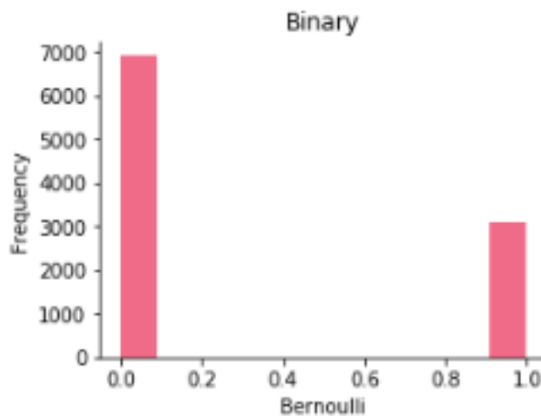
- Over the n trials, it measures the frequency of occurrence of one of the possible result.
- $E(Y) = n \times p$
- $P(Y = y) = C(y, n) \times p^y \times (1 - p)^{n-y}$
- $\text{Var}(Y) = n \times p \times (1 - p)$

Uses

- How many heads obtained if a coin is flipped a coin n times.
- Predict an event occur over a series of trials

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Binary Data → Logistic Regression



Data type: binary

Domain: 0, 1

Examples: True/False

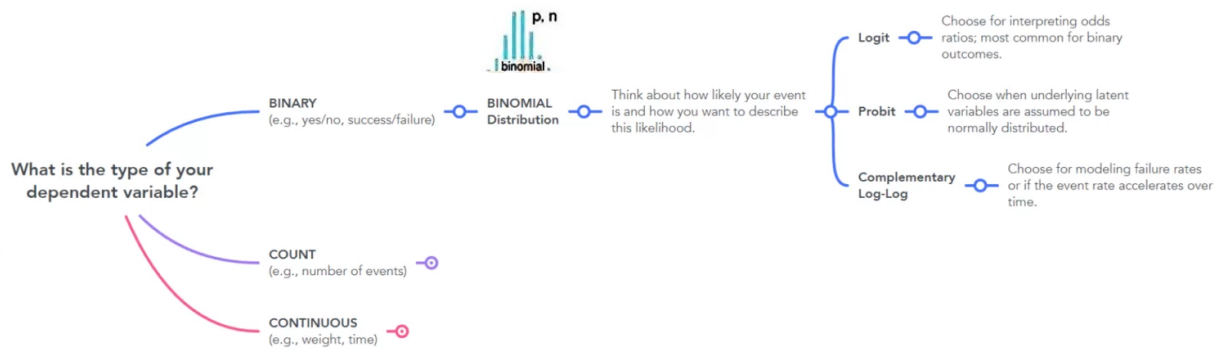
Family: Binomial()

Link: logit

Model = Logistic regression

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GLM: Binary Variables, Binomial Distribution & Link Functions



<https://statisticseasily.com/generalized-linear-model-distribution-and-link-function/>

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Summary Table of Different GLMs

Response Variable Type	Suggested Distribution	Common Link Functions	Use Case
Binary Outcome (e.g., success/failure)	Binomial	Logit, Probit, Complementary Log-Log	Modeling probabilities of binary outcomes, such as presence/absence of a disease.
Count Data (e.g., number of events)	Poisson	Log, Identity, Square Root	Counting occurrences in fixed intervals, such as the number of calls received by a call center per hour.
Count Data with Overdispersion	Negative Binomial	Log, Identity	Count data that exhibit variability exceeding Poisson assumptions, such as the number of insurance claims per client.
Continuous Proportions	Beta	Logit, Probit	Proportions that vary between 0 and 1, such as the fraction of an area affected by a certain condition.
Positive Continuous Data	Gamma	Inverse, Log, Identity	Modeling waiting times or service times, where the response variable is always positive.
Normally Distributed Data	Normal (Gaussian)	Identity	Continuous outcomes that are symmetrically distributed, such as test scores or heights.

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Logistic Regression

- Objective
 - Making a predictive model for classification
- Extension of a Linear Regression (think GLM)
 - When the output Y is categorical.
- Classification
 - Classifying a new record, where its class is unknown, into one of the two classes, based on the values of its predictor variables \mathbf{X} .
- Feature Selection
 - Finding factors distinguishing between records in different classes in terms of their predictor variables \mathbf{X} , or “predictor profile” (odds).

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Linear Regression vs Logistic Regression

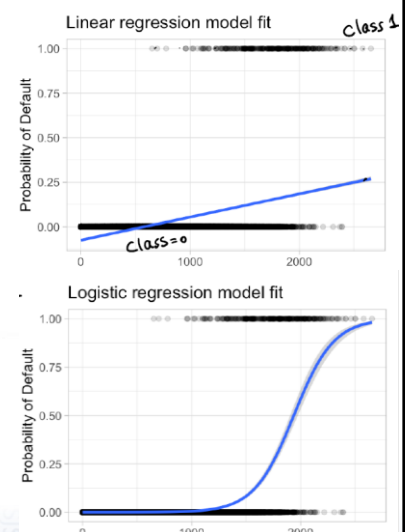
- Linear Regression (Prediction)
 - Y : continuous value $(-\infty, +\infty)$

$$Y = \mathbf{X}^T \boldsymbol{\beta} = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p$$

$$Y|\mathbf{X} \sim N(\mathbf{X}^T \boldsymbol{\beta}, \sigma^2 \mathbf{I})$$

- Logistic Regression (Classification)
 - Y : discrete value from M classes

$$P(Y=C_j | \mathbf{x}; \boldsymbol{\beta}) \in [0,1] \text{ and } \sum_j P(Y=C_j | \mathbf{x}; \boldsymbol{\beta}) = 1$$

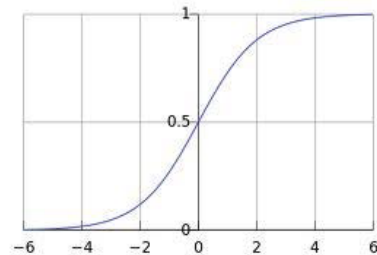


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Logistic Function

- Logistic Function / Sigmoid Function:
 - map any real-valued number R into $[0, 1]$

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$



- Note that the 1st derivative is simply:

$$\sigma'(x) = \left(\frac{1}{1 + e^{-x}} \right)' = \frac{e^{-x}}{(1 + e^{-x})^2} = \frac{1}{1 + e^{-x}} \frac{e^{-x}}{1 + e^{-x}} = \sigma(x) (1 - \sigma(x))$$

$P(1-P)$

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Modeling Probabilities of Two Classes

- The probabilities of the 2 classes (0 and 1) are based on the logistic function $\sigma(x)$:

$$P(Y = 1|X; \beta) = \sigma(X^T \beta) = \frac{1}{1 + e^{-X^T \beta}} = \frac{e^{X^T \beta}}{1 + e^{X^T \beta}}$$

$$P(Y = 0|X; \beta) = 1 - P(Y = 1|X; \beta) = 1 - \sigma(X^T \beta) = \frac{e^{-X^T \beta}}{1 + e^{-X^T \beta}} = \frac{1}{1 + e^{X^T \beta}}$$

- So, it's just the Bernoulli distribution:

$$Y|X \sim \text{Bern}(\sigma(X^T \beta))$$

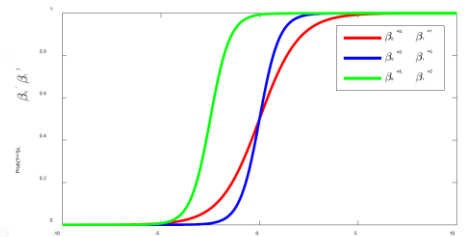
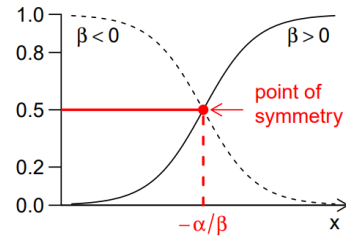
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1D (One Variable) Example

- Here's a simple logistic regression model for a single explanatory variable X_1 :

$$P(Y=1 | X_1, \beta_0, \beta_1) = \sigma(\beta_0 + \beta_1 X_1) = \frac{1}{1 + e^{-\beta_0 - \beta_1 X_1}}$$

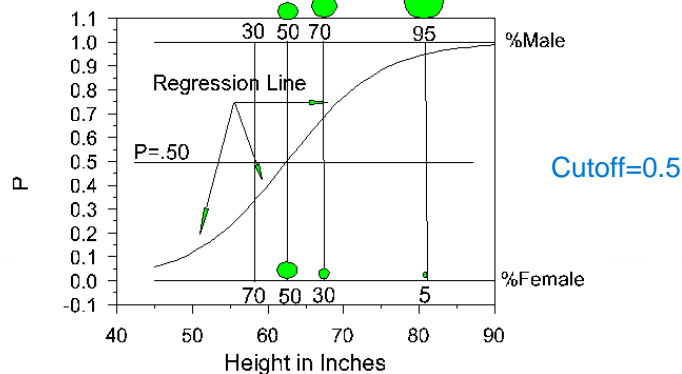
- What happens when β_1 increases?
- What does the coefficient β_0 represent?



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Example

Regression of Sex on Height



What do we know about β_0 ? Positive or negative?

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Probability and Odds

- Probability (of class 1):

$$P(Y = 1) = \frac{P(Y = 1)}{P(Y = 0) + P(Y = 1)}$$

where

$$P(Y = 1|X; \beta) = \sigma(X^T \beta) = \frac{1}{1 + e^{-X^T \beta}}$$

- Odds - Ratio of $P(Y = 1)$ to $P(Y = 0)$:

$$\text{Odds}(Y = 1) = \frac{P(Y = 1)}{P(Y = 0)} = \frac{P(Y = 1)}{1 - P(Y = 1)} \quad \text{Odds} = \frac{P}{1 - P} \quad \Rightarrow \quad P = \frac{\text{Odds}}{1 + \text{Odds}}$$

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Probability and Odds

- Odds

$$\text{Odds} = \frac{P}{1 - P} = \frac{\frac{1}{1 + e^{-X^T \beta}}}{1 - \frac{1}{1 + e^{-X^T \beta}}} = \frac{1}{e^{-X^T \beta}} = e^{X^T \beta}$$

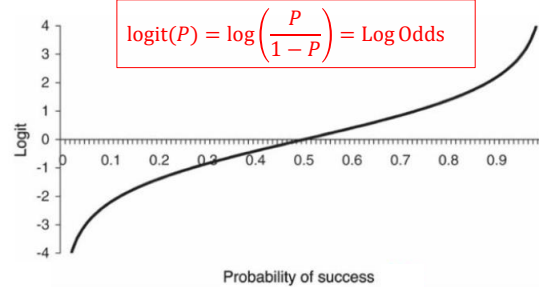
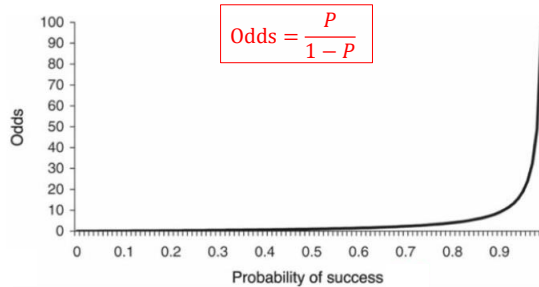
$$\text{logit}(P) = \log\left(\frac{P}{1 - P}\right)$$

- Log Transformation of Odds $\log(\text{Odds}(Y = 1))$ aka "Logit (Transformation)":

$$\underbrace{\log(\text{Odds}(Y = 1))}_{\substack{\text{log odds} \\ \text{or} \\ \text{logit}(P)}} = \log(e^{X^T \beta}) = X^T \beta = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p \quad \underbrace{\hspace{10em}}_{\text{linear combination of } X}$$

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Relationship between Odds and Logit



logit function: $P(Y = 1|X; \beta) \Rightarrow \text{Odds}$

logistic function: $\sigma(X^T\beta) \in [0, 1] \Rightarrow P(Y = 1)$ using cutoff

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Parameter Estimation with MLE

Maximum Likelihood Estimation (MLE)

- Given a dataset with N data points
- For a single data object with predictors X_i , and binary outcome Y_i
 - Let $p_i = P(Y_i = 1 | X_i; \beta)$: the probability of i in class 1
 - The probability of observing Y_i would be:

$$p_i^{Y_i}(1-p_i)^{1-Y_i} \begin{cases} \text{if } Y_i = 1, \text{ then } P_i \\ \text{if } Y_i = 0, \text{ then } 1 - P_i \end{cases}$$

- Combining the two cases and include all datapoints \rightarrow Likelihood $L(\beta)$:

$$L(\beta) = \prod_i p_i^{Y_i}(1-p_i)^{1-Y_i} = \prod_i \left(\frac{e^{X_i^T\beta}}{1+e^{X_i^T\beta}} \right)^{Y_i} \left(\frac{1}{1+e^{X_i^T\beta}} \right)^{1-Y_i}$$

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Parameter Estimation with MLE

- To find the coefficients β_i , it's more straightforward to maximize the log likelihood:

$$\begin{aligned}
 \log L(\boldsymbol{\beta}) &= \sum_i Y_i \log p_i + (1 - Y_i) \log(1 - p_i) \\
 &= \sum_i Y_i \log \left(\frac{e^{X_i^T \boldsymbol{\beta}}}{1 + e^{X_i^T \boldsymbol{\beta}}} \right) + (1 - Y_i) \log \left(\frac{1}{1 + e^{X_i^T \boldsymbol{\beta}}} \right) \\
 &= \sum_i Y_i X_i^T \boldsymbol{\beta} - \log(1 + e^{X_i^T \boldsymbol{\beta}}) \quad \rightarrow \quad \frac{\partial \log L}{\partial \beta_j} = \sum_i (Y_j - p_j) X_{ij}
 \end{aligned}$$

argmax of above

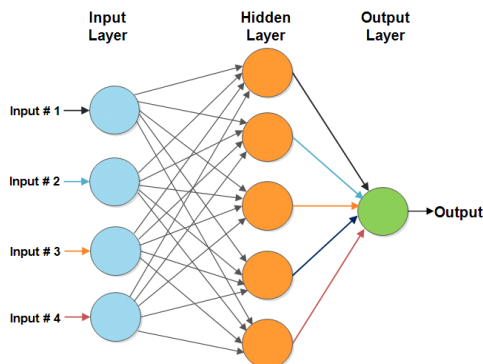
- Use gradient ascend update to compute β_i numerically, :

$$\beta_i^{new} = \beta_i^{old} + \eta \frac{\partial \log L}{\partial \beta_j}$$

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Logistic Regression and Neural Network

- Basic Neural Network



Activation function	Equation	Example	1D Graph
Unit step (Heaviside)	$\phi(z) = \begin{cases} 0, & z < 0, \\ 1, & z \geq 0, \end{cases}$	Perceptron variant	
Sign (Signum)	$\phi(z) = \begin{cases} -1, & z < 0, \\ 0, & z = 0, \\ 1, & z > 0, \end{cases}$	Perceptron variant	
Linear	$\phi(z) = z$	Adaline, linear regression	
Piece-wise linear	$\phi(z) = \begin{cases} 1, & z \geq \frac{1}{2}, \\ z + \frac{1}{2}, & -\frac{1}{2} < z < \frac{1}{2}, \\ 0, & z \leq -\frac{1}{2}, \end{cases}$	Support vector machine	
Logistic (sigmoid)	$\phi(z) = \frac{1}{1 + e^{-z}}$	Logistic regression, Multi-layer NN	
Hyperbolic tangent	$\phi(z) = \frac{e^z - e^{-z}}{e^z + e^{-z}}$	Multi-layer Neural Networks	
Rectifier, ReLU (Rectified Linear Unit)	$\phi(z) = \max(0, z)$	Multi-layer Neural Networks	
Rectifier, softplus	$\phi(z) = \ln(1 + e^z)$	Multi-layer Neural Networks	

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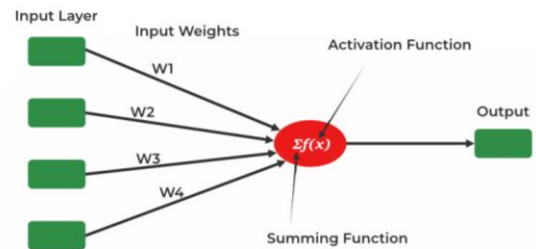
Logistic Regression and Neural Network

- Logistic Regression is similar to a single layer Neural Network:

- Activation function → Sigmoid function
- Input nodes → Predictor variables X
- Weights → Regression coefficients β

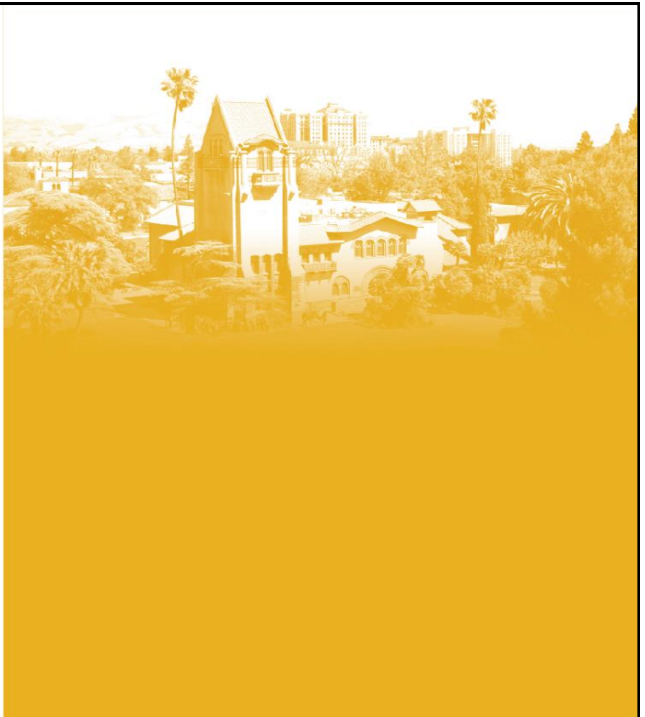
- Different optimizers normally used:

- MLE for Logistic Regression
- Adam, BP, ... for Neural Network
- Linear model (LR) vs usually nonlinear (NN)



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Interpreting Coefficients



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Model Coefficients

- The model coefficients $\hat{\beta}_i$ are computed from the maximum likelihood.

Generalized Linear Model Regression Results

```

=====
Dep. Variable:                y                No. Observations:                173
Model:                        GLM              Df Residuals:                  171
Model Family:                 Binomial         Df Model:                    1
Link Function:                 logit           Scale:                        1.0000
Method:                       IRLS           Log-Likelihood:                -97.226
Date:                         Thu, 26 Sep 2024 Deviance:                      194.45
Time:                         14:36:09       Pearson chi2:                  165.
No. Iterations:               4              Pseudo R-squ. (CS):           0.1655
Covariance Type:              nonrobust
=====

```

	coef	std err	z	P> z	[0.025	0.975]
Intercept	-12.3508	2.629	-4.698	0.000	-17.503	-7.199
width	0.4972	0.102	4.887	0.000	0.298	0.697

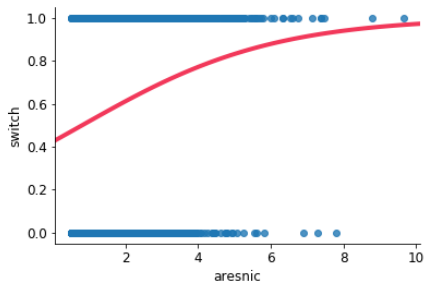
The intercept coefficient of -12.3508 denotes the baseline log odds $\exp(-12.3508) = 0.0004326$ are the odds when $width = 0$

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Model Coefficients

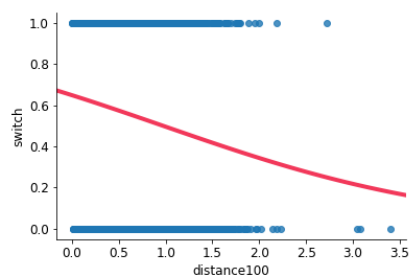
$$\beta > 0$$

- Ascending curve



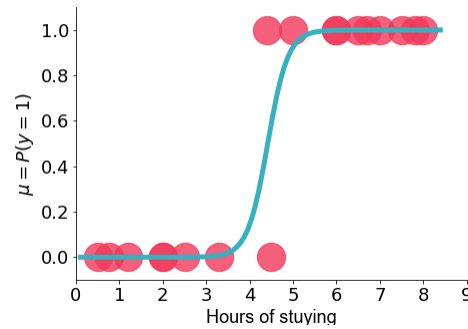
$$\beta < 0$$

- Descending curve



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Probability vs Logistic Fit



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Log Odds Interpretation

- Logistic Model

$$\text{logit}(P) = \log\left(\frac{P}{1-P}\right) = \mathbf{X}^T \boldsymbol{\beta} = \beta_0 + \beta_1 X_1$$

- If X_1 is increased by one-unit

$$\text{logit}(P) = \log\left(\frac{P}{1-P}\right) = \beta_0 + \beta_1 (X_1 + 1)$$



$$\text{Odds} = \frac{P}{1-P} = e^{\beta_0 + \beta_1 (X_1 + 1)} = e^{\beta_0 + \beta_1 X_1} e^{\beta_1}$$

odds are multiplied by e^{β_1}

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Profiling with Odds Ratio in Logistic Regression

Odds Ratio for a given predictor variable X_i quantifies the change in odds of the outcome occurring for a one-unit increase in that predictor, holding all other variables constant.

- For X_i , the odds ratio (OR) is given as:

$$OR(X_i) = \frac{\text{odds}_{new}}{\text{odds}_{orig}} = e^{\beta_i}$$

	coef	std err	z	P> z	[0.025	0.975]
Intercept	-12.3508	2.629	-4.698	0.000	-17.503	-7.199
width	0.4972	0.102	4.887	0.000	0.298	0.697

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Standard Error (SE)

The standard error measures the variability or precision of an estimated coefficient. It helps in assessing the reliability of the coefficient estimates. It's given by:

$$SE(\beta_i) = \sqrt{\text{Var}(\hat{\beta}_i)}$$

estimated variance of the coefficient

- It's used to construct confidence intervals and conduct hypothesis tests
- Smaller SE → more precise estimate of β_i

	coef	std err	z	P> z	[0.025	0.975]
Intercept	-12.3508	2.629	-4.698	0.000	-17.503	-7.199
width	0.4972	0.102	4.887	0.000	0.298	0.697

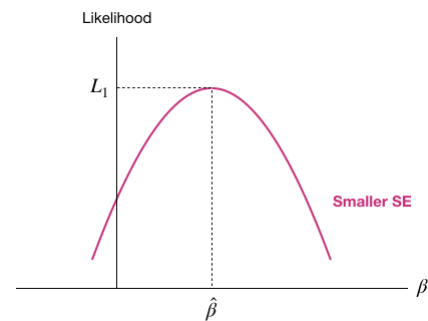
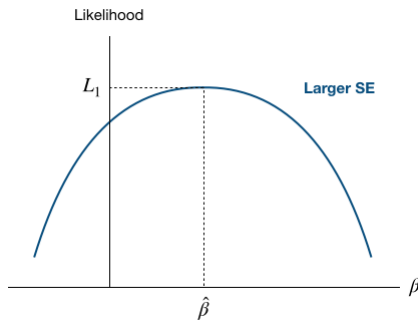
	Intercept	width
Intercept	6.910	-0.267
width	-0.267	0.010

covariance matrix

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Standard Error (SE)

- Flatter Peak
 - Maximum location harder to define
 - Larger SE
- Sharper Peak
 - Maximum location more clearly defined
 - Smaller SE



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Evaluation of Coefficients (z values)

The Z-statistic is used to test the significance of individual coefficients in a model:

$$z = \frac{\hat{\beta}_i}{SE(\hat{\beta}_i)}$$

- Larger $z \rightarrow z \neq 0 \rightarrow \beta_i$ significant
- Rule of Thumb: cut-off value $\rightarrow \sim 2$

	coef	std err	z	P> z	[0.025	0.975]
Intercept	-12.3508	2.629	-4.698	0.000	-17.503	-7.199
width	0.4972	0.102	4.887	0.000	0.298	0.697

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Evaluation of Coefficients (p values)

The p values can be used to determine the significance of individual coefficient β_i :

Null Hypothesis $H_0: \beta_i = 0$ (no impact to outcome)

Alternate Hypothesis $H_1: \beta_i \neq 0$ (important)

- P-Value $\leq \alpha \rightarrow$ **reject the null hypothesis**
 - This indicates that the predictor X_i has a statistically significant relationship with outcome Y
- P-Value $> \alpha \rightarrow$ **cannot reject the null hypothesis**
 - This suggest insufficient evidence to conclude that the predictor variable X_i is statistically associated with outcome Y

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Example: Feature Selection using P Values

Feature Selection using the p values

Null Hypothesis $H_0: \beta_i = 0$ (no impact to outcome)

Alternate Hypothesis $H_1: \beta_i \neq 0$ (important)

- If 95% confidence level, $p < 0.05$



Reject H_0

- If 99% confidence level, $p < 0.01$



Reject H_0

	Coef.	Std.Err.	z	P> z	[0.025	0.975]
Age	-0.0359	0.0673	-0.5340	0.5934	-0.1678	0.0959
Experience	0.0450	0.0668	0.6740	0.5003	-0.0859	0.1760
Income	0.0602	0.0030	20.2888	0.0000	0.0544	0.0660
Family	0.6182	0.0770	8.0239	0.0000	0.4672	0.7692
CCAvg	0.1634	0.0441	3.7078	0.0002	0.0770	0.2497
Mortgage	0.0007	0.0006	1.1961	0.2316	-0.0005	0.0019
SecuritiesAccount	-0.8701	0.3007	-2.8938	0.0038	-1.4595	-0.2808
CDAccount	3.8389	0.3416	11.2393	0.0000	3.1695	4.5084
Online	-0.7605	0.1657	-4.5886	0.0000	-1.0854	-0.4357
CreditCard	-1.0382	0.2131	-4.8720	0.0000	-1.4559	-0.6205
Education_Prof	0.0987	0.1888	0.5226	0.6012	-0.2714	0.4687
Education_Under	-3.9654	0.2696	-14.7084	0.0000	-4.4938	-3.4370
Intercept	-8.3452	1.7916	-4.6579	0.0000	-11.8567	-4.8337

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Evaluation of Coefficients (Confidence Intervals)

The confidence intervals can be used to determine the uncertainty of individual coefficients:

$$[\hat{\beta}_i - z_{\alpha/2} \times \text{SE}(\hat{\beta}_i), \hat{\beta}_i + z_{\alpha/2} \times \text{SE}(\hat{\beta}_i)]$$

- For 95% confidence intervals for β_i :

$$[\hat{\beta}_i - 1.96 \times \text{SE}(\hat{\beta}_i), \hat{\beta}_i + 1.96 \times \text{SE}(\hat{\beta}_i)]$$

Confidence Interval	z
80%	1.282
85%	1.440
90%	1.645
95%	1.960
99%	2.576
99.5%	2.807
99.9%	3.291

	coef	std err	z	P> z	[0.025	0.975]
Intercept	-12.3508	2.629	-4.698	0.000	-17.503	-7.199
width	0.4972	0.102	4.887	0.000	0.298	0.697

95% CI

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Example: Recap all the quantities

Generalized Linear Model Regression Results

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Model Family:                 Binomial Df Model:                      1
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Time:                          14:36:09 Pearson chi2:                  165.
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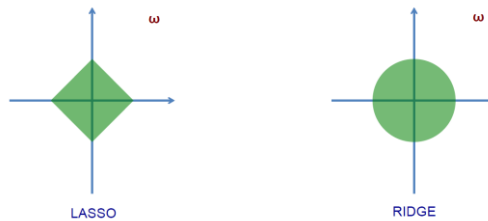
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width	0.4972	0.102	4.887	0.000	0.298	0.697

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Regularization

- L1 (Lasso) Regularization
- L2 (Ridge) Regularization
- Elastic Net: Combining L1 and L2 regularization.



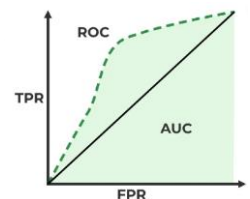
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Model Evaluation

These are the standard model evaluation metrics for classification problems:

- Confusion Matrix
 - Summarizes the performance of the classification model.
- ROC Curve
 - Plots the true positive rate vs the false positive rate at various threshold/cutoff settings.
- AUC (Area Under the Curve)
 - Measures the overall performance of the model.

		Predicted	
		0	1
Actual	0	TN	FP
	1	FN	TP



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Summary

- **Logistic Regression** is a powerful tool for binary classification problems, providing interpretable results through odds ratios and p-values.
- Formal mathematical formulation including using the MLE to estimate parameters.
- Logistic regression is similar to a single layer neural network with sigmoid function as the activation function.
- Hypothesis testing can be used to determine the significance of individual coefficients.
- L_1 , L_2 and Elastic Net regularization can be used with logistic regression.
- Confusion matrix, ROC and AUC are popular model evaluation metrics for logistic regression.