Regression

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CHULA ENGINEERING
Foundation toward Innovation
COMPUTER

Chula Big Data and IoT
Center of Excellence (CUBIC)

DataMind

Linear Regression

Build a supervised learning model using Excel

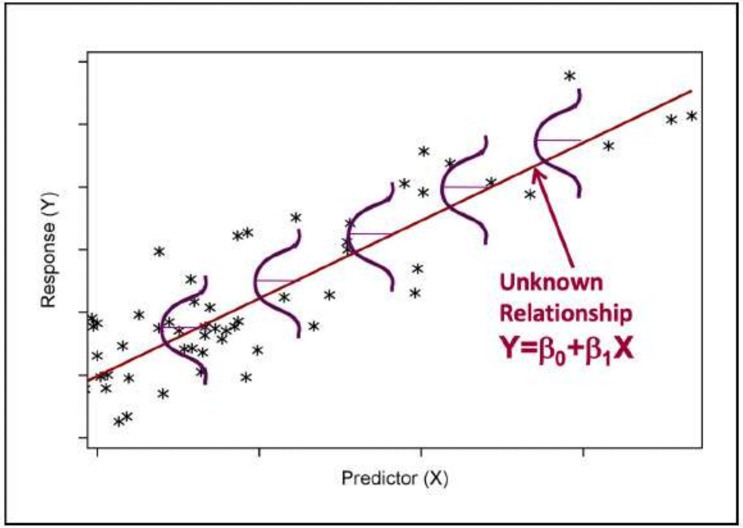
Type of Predictors / Type of Response	Categorical	Continuous	Continuous and Categorical
Continuous	Analysis of Variance (ANOVA)	Ordinary Least Squares (OLS) Regression	Analysis of Covariance (ANCOVA)
Categorical	Contingency Table Analysis or Logistic Regression	Logistic Regression	Logistic Regression

Linear Regression: Model

- Main Idea: **to obtain a line that best fits the data** where its overall prediction error from all data points are as small as possible.

- Simple Linear Regression (1 feature):
  - $y(x) = \theta_0 + \theta_1 x_1$
- Multiple Linear Regression (n features):
  - $y(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + ... + \theta_n x_n$

- 4 key assumptions of linear regression:
  - Linear relationship
  - Multivariate normality
  - No or little multicollinearity (no auto-correlation)
  - Homoscedasticity



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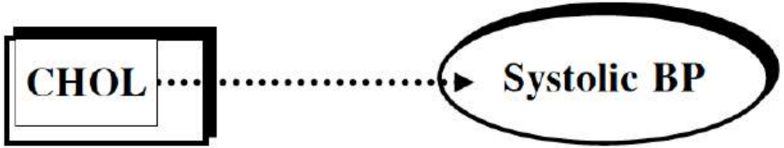
Simple Linear Regression

Problem: 1 input (predictor) & 1 output

- Collect data of 7 patients
- Systolic Blood Pressure (y) & Cholesterol (x)

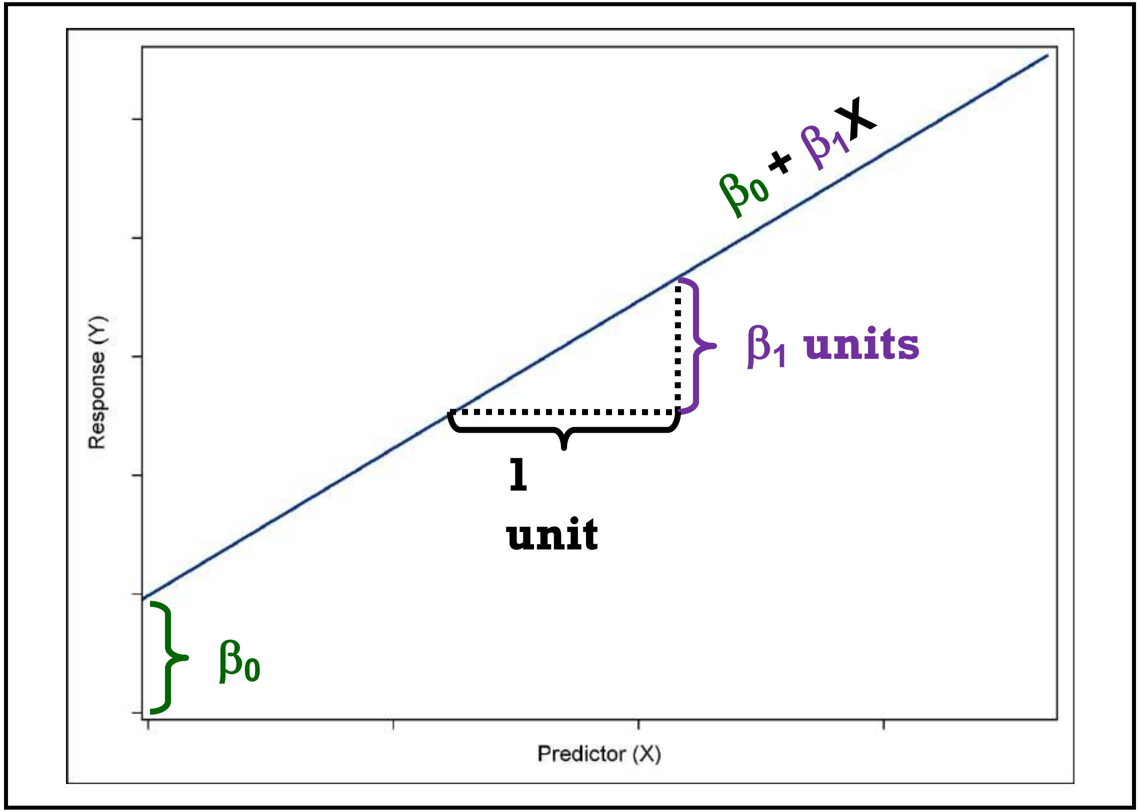
idno	chol (x)	sysbp (y)
1	437	194
2	264	121
3	249	131
4	297	159
5	243	123
6	272	161
7	161	115
รวม	1923	1004



$$\hat{y} = \beta_0 + \beta_1 x$$

$$\widehat{bp} = \beta_0 + \beta_1 chol$$

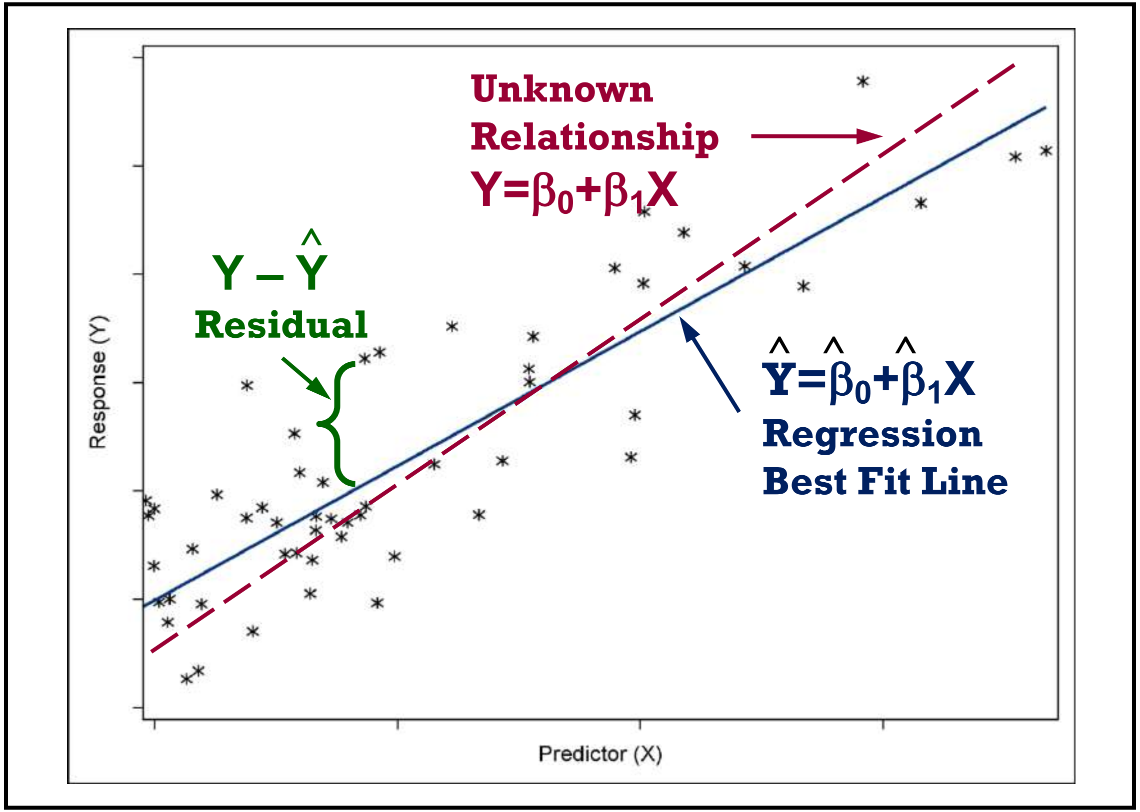
Simple Linear Regression Model



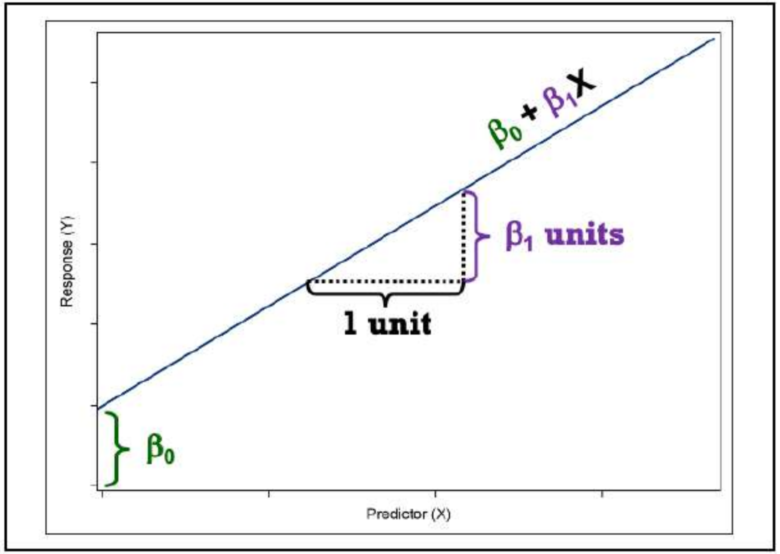
$$\hat{y} = \beta_0 + \beta_1 x$$

$$\widehat{bp} = \beta_0 + \beta_1 chol$$

Ordinary Least Squares (OLS) Regression



How to estimate parameters



$$\hat{y} = \beta_0 + \beta_1 x$$

$$\beta_0 = \bar{y} - \beta_1\,\bar{x}$$

$$\beta_1 = \frac{s_{xy}}{s_{xx}} = \frac{\left(\sum x_i y_i - \frac{\sum x_i \sum y_i}{n}\right)}{\left(\sum x_i^2 - \frac{(\sum x_i)^2}{n}\right)}$$

$$[Y] = [X][\beta]$$
$$[\beta]=[X]^{-1}[Y]$$

Example

$$\hat{y} = \beta_0 + \beta_1 x$$

$$\beta_0 = \bar{y} - \beta_1\,\bar{x}$$

$$\beta_1 = \frac{s_{xy}}{s_{xx}} = \frac{\left(\sum x_i y_i - \frac{\sum x_i \sum y_i}{n}\right)}{\left(\sum x_i^2 - \frac{(\sum x_i)^2}{n}\right)}$$

- Systolic Blood Pressure (y)
- Cholesterol (x)

idno	chol (x)	sysbp (y)	x^2	xy	y^2
1	437	194	190969	84778	37636
2	264	121	69696	31944	14641
3	249	131	62001	32619	17161
4	297	159	88209	47223	25281
5	243	123	49049	29889	15129
6	272	161	73984	43792	25921
7	161	115	25921	18515	13225
รวม	1923	1004	569829	288760	148994

$$\bar{x} = \frac{1923}{7} = 247.7143, \bar{y} = \frac{1004}{7} = 143.4286$$

$$\beta_1 = \frac{s_{xy}}{s_{xx}} = \frac{\left(288760 - \frac{1923 \times 1004}{7}\right)}{\left(569829 - \frac{(1923)^2}{7}\right)} = 0.3116$$

$$\beta_0 = 143.4286 - (0.3116)(247.7143) = 57.8355$$

$$\hat{y} = 57.8355 + 0.3116x$$

How to read an equation

$$\widehat{bp} = 57.8355 + 0.3116 \times chol$$

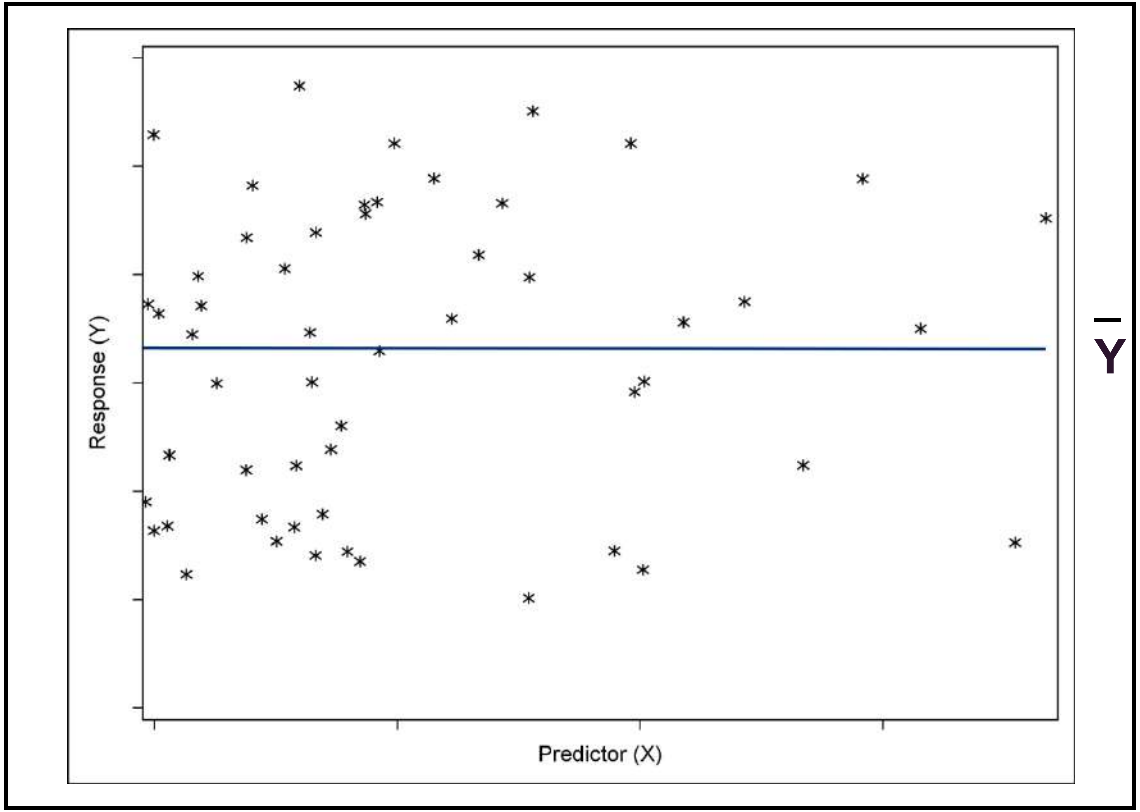
Example: Prediction

- Systolic Blood Pressure (y)
- Cholesterol (x)

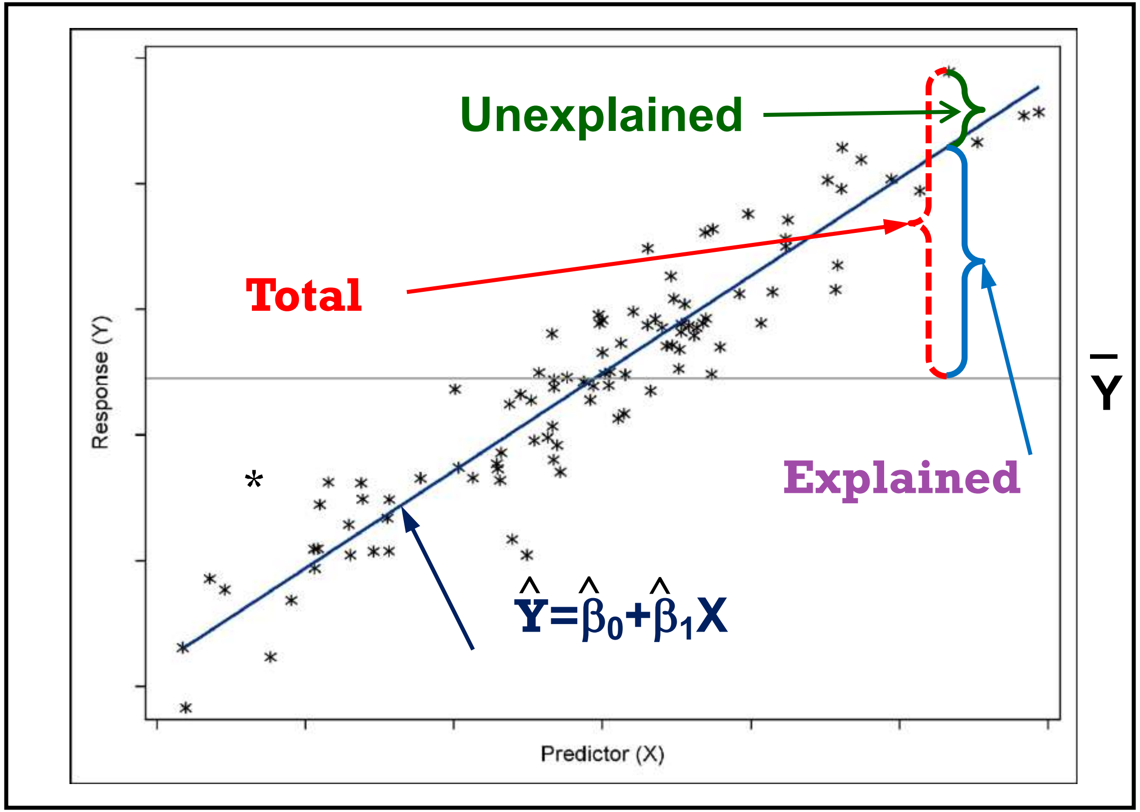
$$\widehat{bp} = 57.8355 + 0.3116 \times chol$$

idno	chol (x)	sysbp (y)	predict
1	437	194	196.1897
2	264	121	141.4179
3	249	131	136.6689
4	297	159	151.8657
5	243	123	134.7693
6	272	161	143.9507
7	161	115	108.8081
รวม	1923	1004	

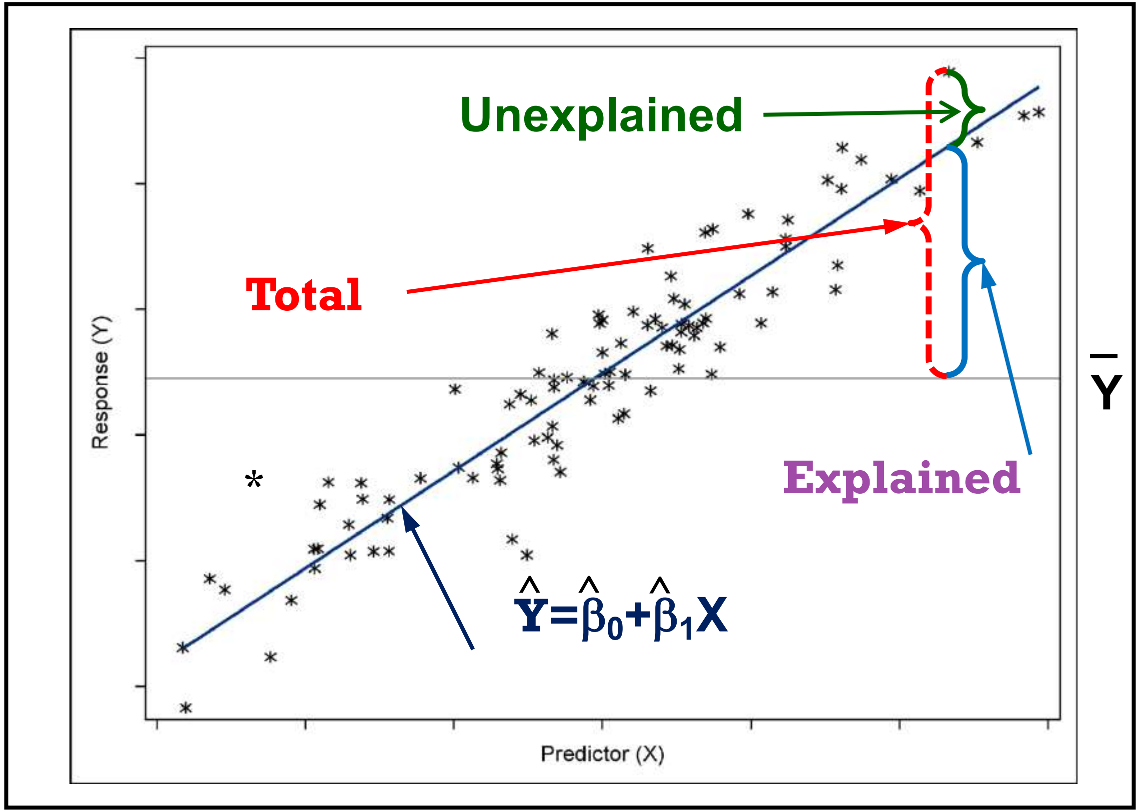
The Baseline Model (Null Hypothesis)



Explained versus Unexplained Variability



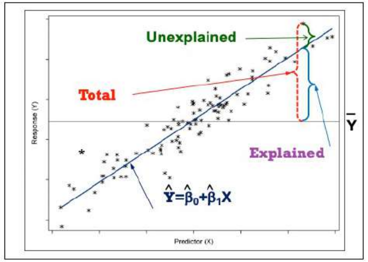
Coefficient of Determination



$$R^2 = \frac{SSM}{SST} = 1 - \frac{SSE}{SST}$$

- "Proportion of variance accounted for by the model"

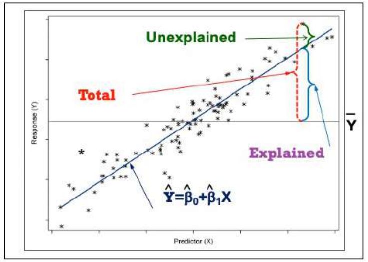
Coefficient of Determination (cont.)



$$R^2 = \frac{SSM}{SST} = 1 - \frac{SSE}{SST}$$

id	chol (x)	bp (y)	predict	error	squred error (SE)	guess	(y - y_bar)	squred total (ST)
1	437	194	196.1897	(2.1897)	4.7948	143.4286	50.5714	2,557.4694
2	264	121	141.4179	(20.4179)	416.8906	143.4286	(22.4286)	503.0408
3	249	131	136.6689	(5.6689)	32.1364	143.4286	(12.4286)	154.4694
4	297	159	151.8657	7.1343	50.8982	143.4286	15.5714	242.4694
5	243	123	134.7693	(11.7693)	138.5164	143.4286	(20.4286)	417.3265
6	272	161	143.9507	17.0493	290.6786	143.4286	17.5714	308.7551
7	161	115	108.8081	6.1919	38.3396	143.4286	(28.4286)	808.1837
average	274.7143	143.4286		SSE	972.2548		SST	4,991.7143
				MSE	138.8935			
				RMSE	**11.7853**			
	R^2	**1 - (SSE/SST)**	**0.8052**					

Coefficient of Determination (cont.)



- Train: R^2, RMSE
- Test: R^2, RMSE (honest estimate)

Training Data

Testing Data

id	chol (x)	bp (y)	predict	error	squred error (SE)	guess	(y - y_bar)	squred total (ST)
1	437	194	196.1897	(2.1897)	4.7948	143.4286	50.5714	2,557.4694
2	264	121	141.4179	(20.4179)	416.8906	143.4286	(22.4286)	503.0408
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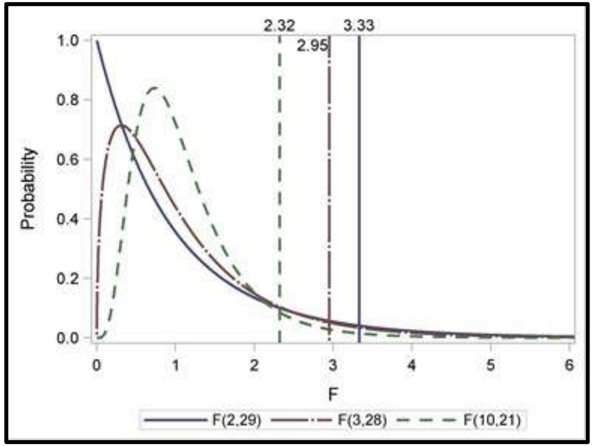
average	274.7143	143.4286		SSE	972.2548		SST	4,991.7143
				MSE	138.8935			
				RMSE	**11.7853**			
	R^2	**1 - (SSE/SST)**	**0.8052**					

Model Hypothesis Test
F Statistic and Critical Values at α=0.05

- Null Hypothesis:
  - The simple linear regression model does not fit the data better than the baseline model.
  - $\beta_1=0$
- Alternative Hypothesis:
  - The simple linear regression model does fit the data better than the baseline model.
  - $\beta_1\neq0$

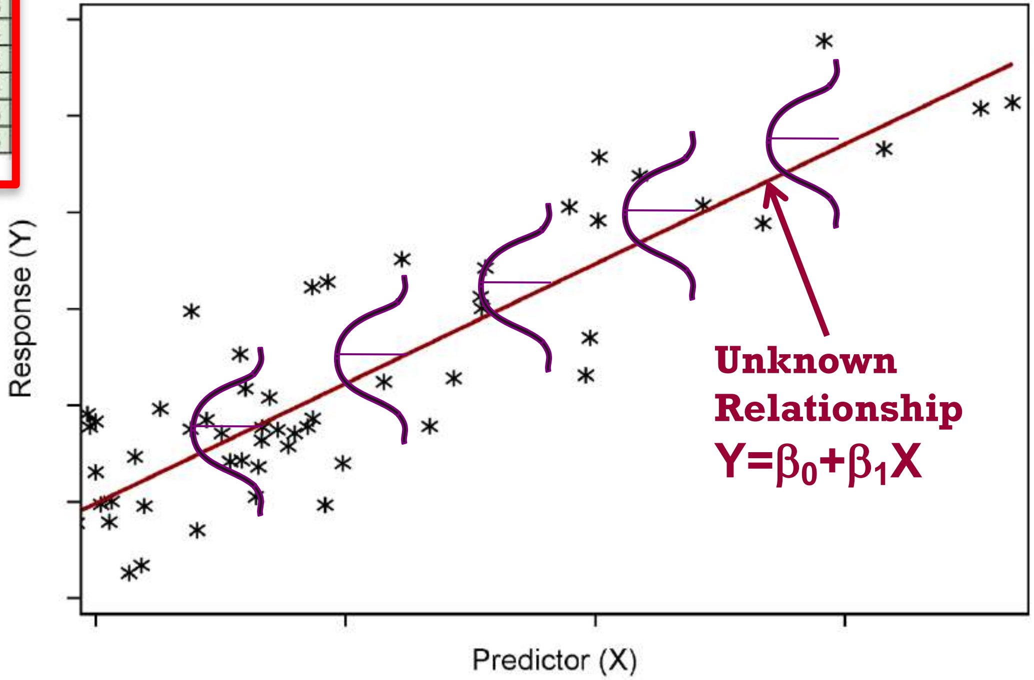


F(Model df, Error df)=MS_M / MS_E

Assumptions of Simple Linear Regression

id	chol (x)	bp (y)	predict	error	squred error (SE)
1	437	194	196.1897	(2.1897	4.7948
2	264	121	141.4179	(20.4179	416.8906
3	249	131	136.6689	(5.6689	32.1364
4	297	159	151.8657	7.1343	50.8982
5	243	123	134.7693	(11.7693	138.5164
6	272	161	143.9507	17.0493	290.6786
7	161	115	108.8081	6.1919	38.3396

- The mean of the Ys is accurately modeled by a linear function of the X.
- The random error term, ε, is assumed to have a normal distribution with a mean of zero.
- The random error term, ε, is assumed to have a constant variance, σ^2.
  - Not skew
- The errors are independent.



Multiple Linear Regression

Multiple Linear Regression with Two Variables

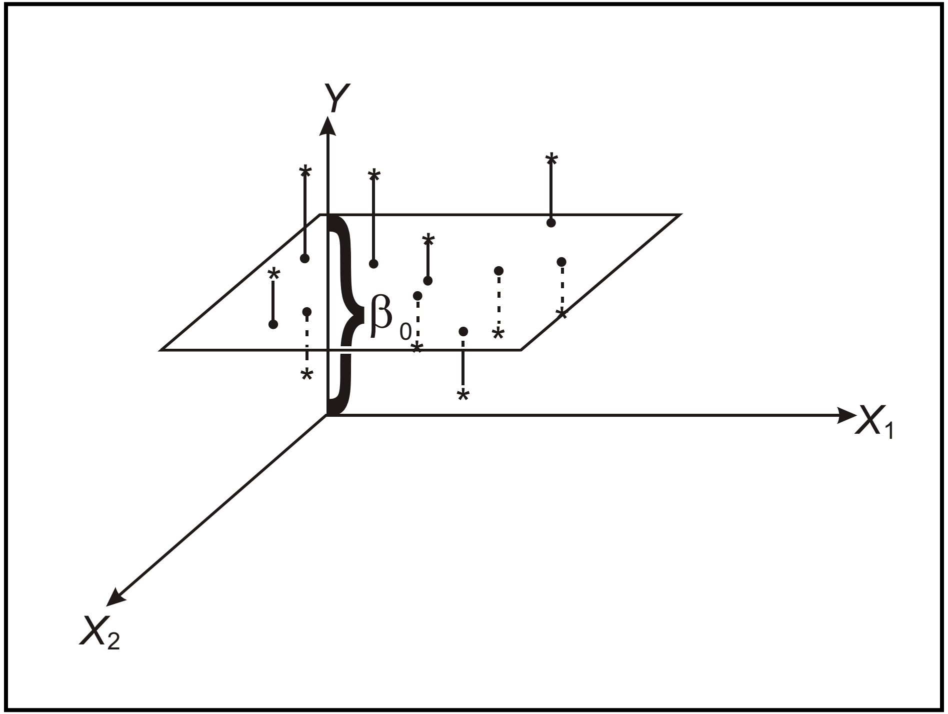
- Consider the two-variable model

$$Y=\beta_0+\beta_1X_1+\beta_2X_2+\varepsilon$$

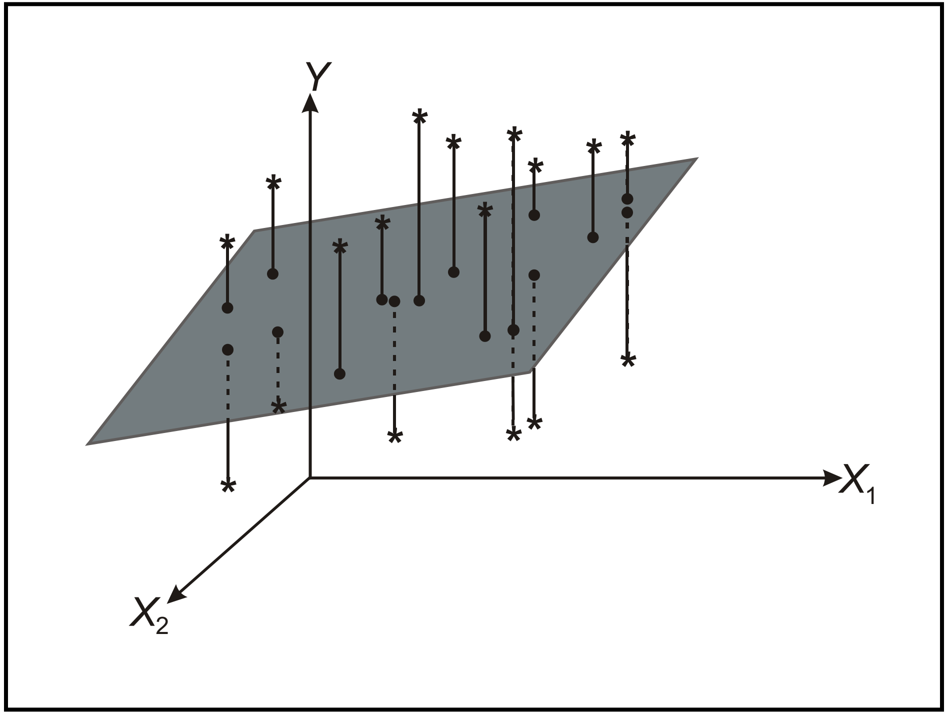
- where

Y	is the dependent variable.
X_1 and X_2	are the independent or predictor variables.
ε	is the error term.
β_0, β_1, and β_2	are unknown parameters.

Picturing the Model: No Relationship



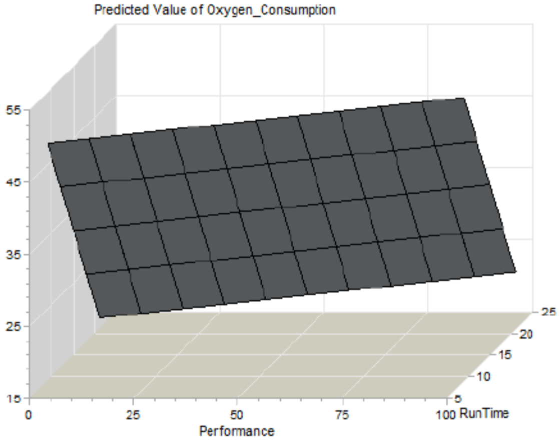
Picturing the Model: A Relationship

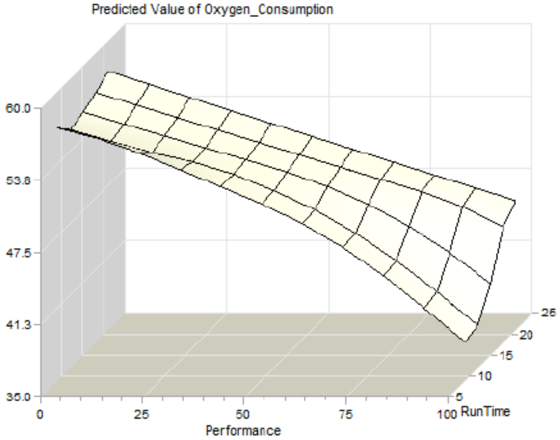


The Multiple Linear Regression Model

- In general, you model the dependent variable, Y, as a linear function of k independent variables, X_1 through X_k:

$$Y=\beta_0+\beta_1X_1+\ldots+\beta_kX_k+\varepsilon$$





$$Y=\beta_0+\beta_1X_1+\beta_2X_2+\varepsilon$$

Linear Model with only Linear Effects

$$Y=\beta_0+\beta_1X_1+\beta_2X_1^2+\beta_3X_2+\beta_4X_2^2+\varepsilon$$

Linear Model with Nonlinear Effects

The Multiple Linear Regression Model (cont.) Matrix Multiplication Approach

inputs target

Age	Income	Spending
25	25,000	400
35	50,000	500
32	35,000	550

$$Y=\beta_0(1)+\beta_1 X_1+\beta_2 X_2+\varepsilon$$

$$[Y] = [X][\beta]$$
$$[\beta]=[X]^{-1}[Y]$$

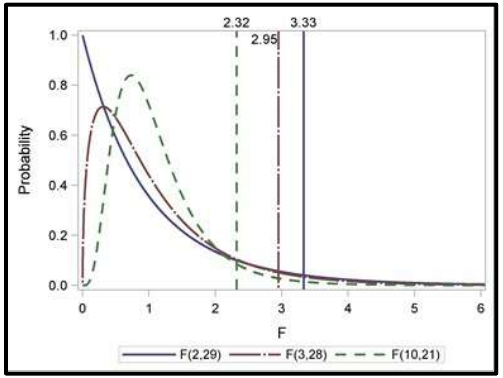
$$\begin{bmatrix}400\\500\\550\end{bmatrix} = \begin{bmatrix}25 & 25000\\35 & 50000\\32 & 35000\end{bmatrix}\begin{bmatrix}\beta_1\\\beta_2\\\beta_3\end{bmatrix}$$

https://sites.google.com/site/mystatistics01/regression-correlation-analysis/multiple-linear-regression-step

Model Hypothesis Test (F-Test)

- Null Hypothesis:
  - The regression model does not fit the data better than the baseline model.
  - $\beta_1=\beta_2=\ldots=\beta_k=0$

- Alternative Hypothesis:
  - The regression model does fit the data better than the baseline model.
  - Not all β_is equal zero.



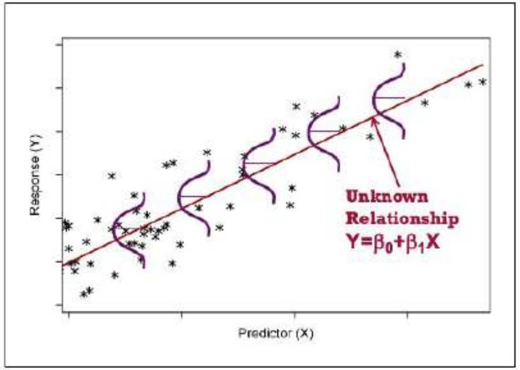
$F(\text{Model df, Error df})=MS_M / MS_E$

Assumptions for Linear Regression

- The mean of the Ys is accurately modeled by a linear function of the X_i.
  - (y, x_i) = linear relationship (correlation)

- The random error term, ε, is assumed to have a normal distribution with a mean of zero.
- The random error term, ε, is assumed to have a constant variance, σ^2.
  - Not skew

- The errors are independent.



Multiple Linear Regression versus Simple Linear Regression

- **Main Advantage**
- Multiple linear regression enables you to investigate the relationship among Y and several independent variables simultaneously.
- **Main Disadvantages**
- Increased complexity makes it more difficult to do the following:
  - ascertain which model is "best"
  - interpret the models

Common Applications of Multiple Regression

- Multiple linear regression is a powerful tool for the following tasks:
  - Prediction – to develop a model to predict future values of a response variable (Y) based on its relationships with other predictor variables (Xs)
  - Analytical or Explanatory Analysis – to develop an understanding of the relationships between the response variable and predictor variables

Prediction

- The terms in the model, the values of their coefficients, and their statistical significance are of secondary importance.
- The focus is on producing a model that is the best at predicting future values of Y as a function of the Xs. The predicted value of Y is given by this formula:

$$\hat{Y} = \hat{\beta}_0 + \hat{\beta}_1 X_1 + \ldots + \hat{\beta}_k X_k$$

Analytical or Explanatory Analysis

- The focus is on understanding the relationship between the dependent variable and the independent variables.
- Consequently, the statistical significance of the coefficients is important as well as the magnitudes and signs of the coefficients.

$$\hat{Y} = \underline{\hat{\beta}_0} + \underline{\hat{\beta}_1} X_1 + \ldots + \underline{\hat{\beta}_k} X_k$$

$$R^2 = \frac{SSM}{SST} = 1 - \frac{SSE}{SST}$$

Adjusted R Square

$$\boxed{R^2_{ADJ} = 1 - \frac{(n-i)(1-R^2)}{n-p}}$$

- i=1 if there is an intercept and 0 otherwise
- n=the number of observations used to fit the model
- p=the number of parameters in the model

$$R^2_{ADJ} = 1 - \frac{(100-1)(1-0.7)}{(100-1)} = 0.70; R^2 = 0.7, n = 100, p = 1$$

$$R^2_{ADJ} = 1 - \frac{(100-1)(1-0.7)}{(100-3)} = 0.69; R^2 = 0.7, n = 100, p = 3$$

$$R^2_{ADJ} = 1 - \frac{(100-1)(1-0.7)}{(100-10)} = 0.67; R^2 = 0.7, n = 100, p = 10$$

https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LinearRegression.html

sklearn.linear_model.LinearRegression

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

Ordinary least squares Linear Regression.

LinearRegression fits a linear model with coefficients w = (w1, ..., wp) to minimize the residual sum of squares between the observed targets in the dataset, and the targets predicted by the linear approximation.

Parameters:

fit_intercept : *bool, optional, default True*
Whether to calculate the intercept for this model. If set to False, no intercept will be used in calculations (i.e. data is expected to be centered).

normalize : *bool, optional, default False*
This parameter is ignored when `fit_intercept` is set to False. If True, the regressors X will be normalized before regression by subtracting the mean and dividing by the l2-norm. If you wish to standardize, please use

Methods

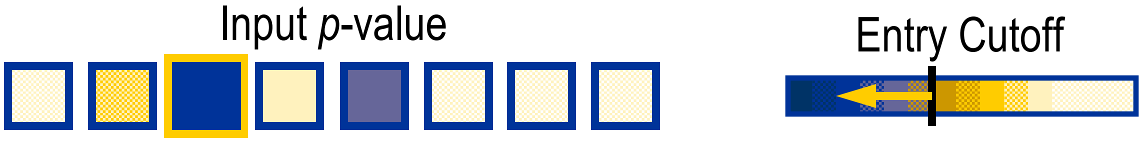
`fit`(self, X, y[, sample_weight])	Fit linear model.
`get_params`(self[, deep])	Get parameters for this estimator.
`predict`(self, X)	Predict using the linear model.
`score`(self, X, y[, sample_weight])	Return the coefficient of determination $\boxed{R^2}$ of the prediction.
`set_params`(self, **params)	Set the parameters of this estimator.

Feature Selection

Feature Selection

- Forward
- Backward
- Stepwise

Sequential Selection: Forward



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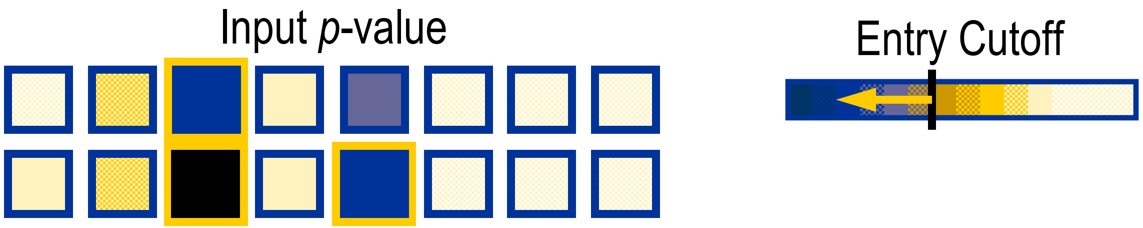
Sequential Selection: Forward



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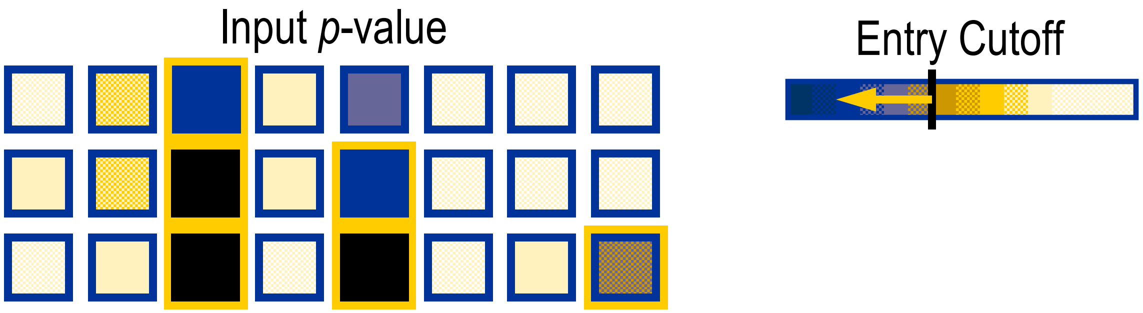
Sequential Selection: Forward



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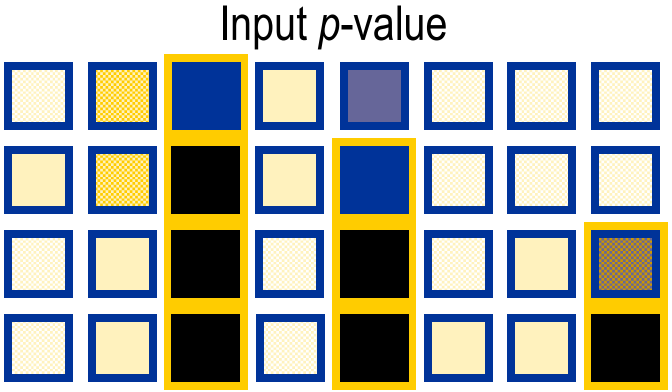
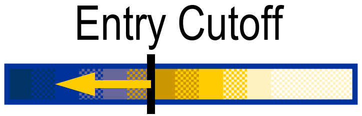
Sequential Selection: Forward





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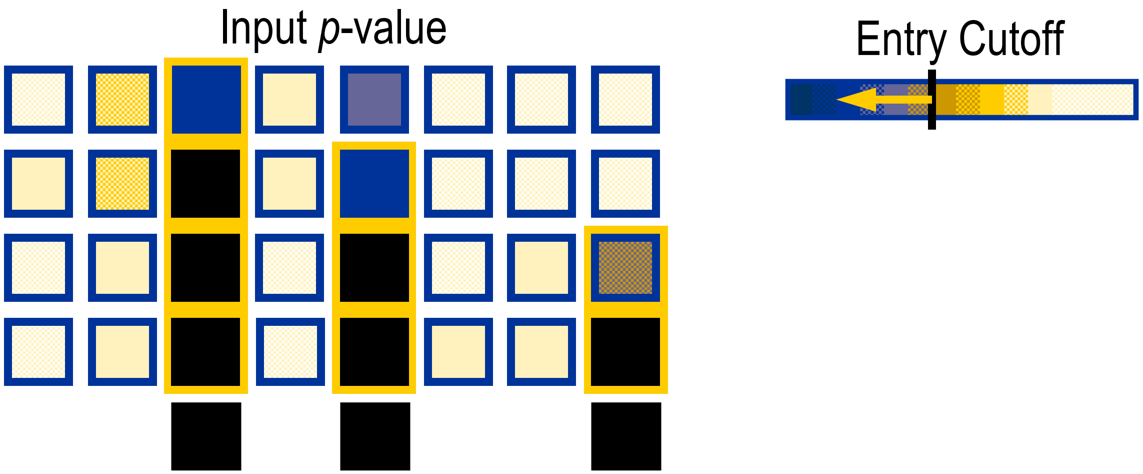
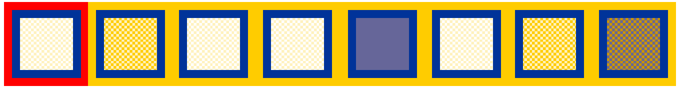
Sequential Selection: Forward



Sequential Selection: Backward

Input *p*-value



Stay Cutoff

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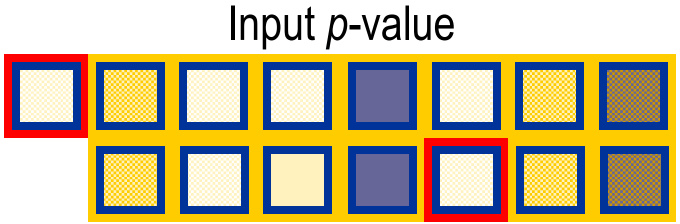
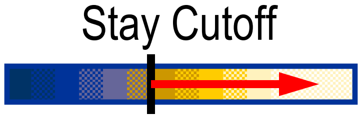
Sequential Selection: Backward





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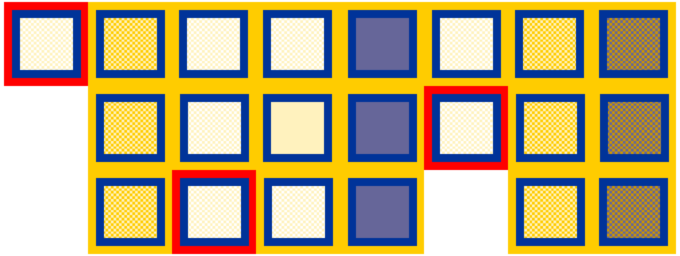
Sequential Selection: Backward



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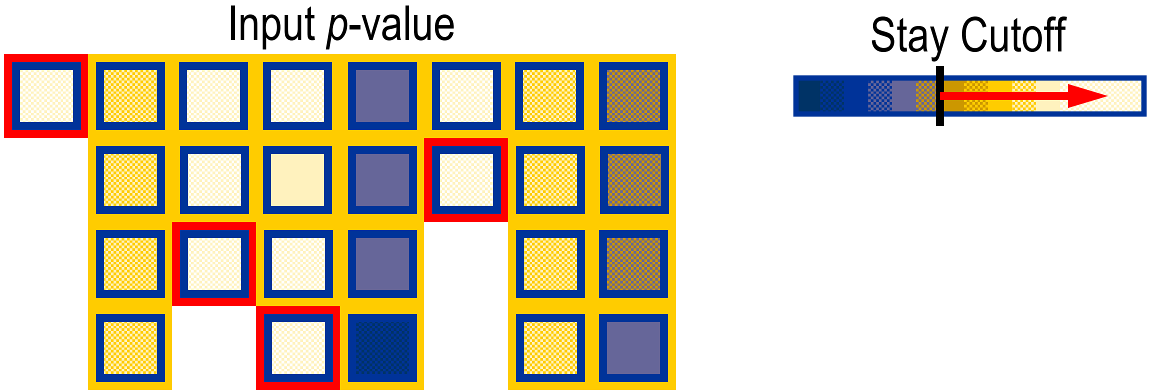
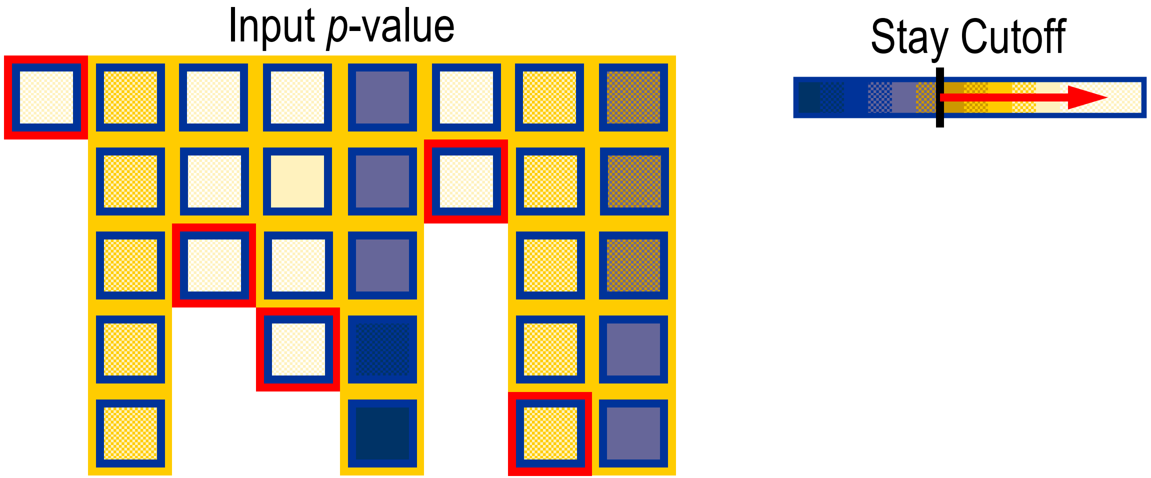
Sequential Selection: Backward



Sequential Selection: Backward



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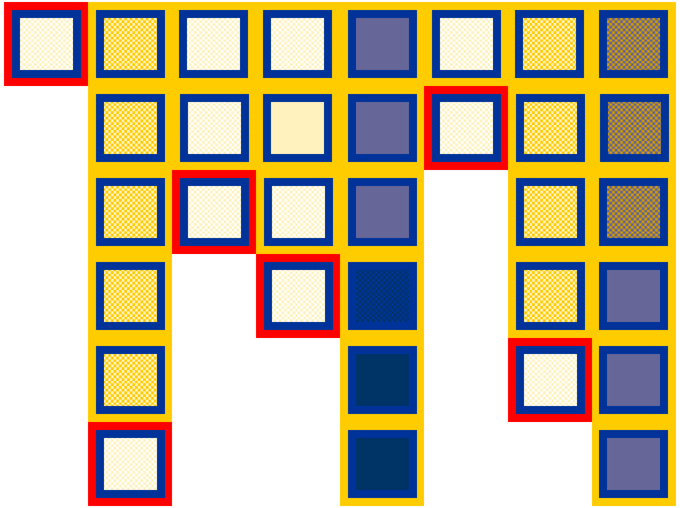
Sequential Selection: Backward

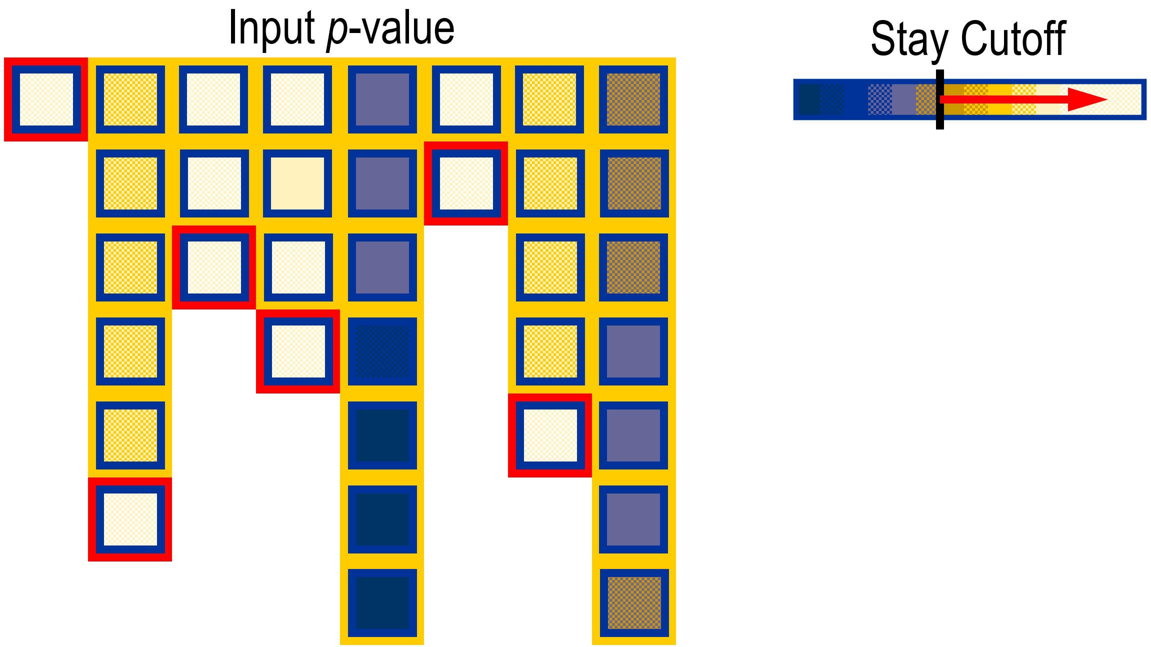
Input p-value



Stay Cutoff

...

Sequential Selection: Backward



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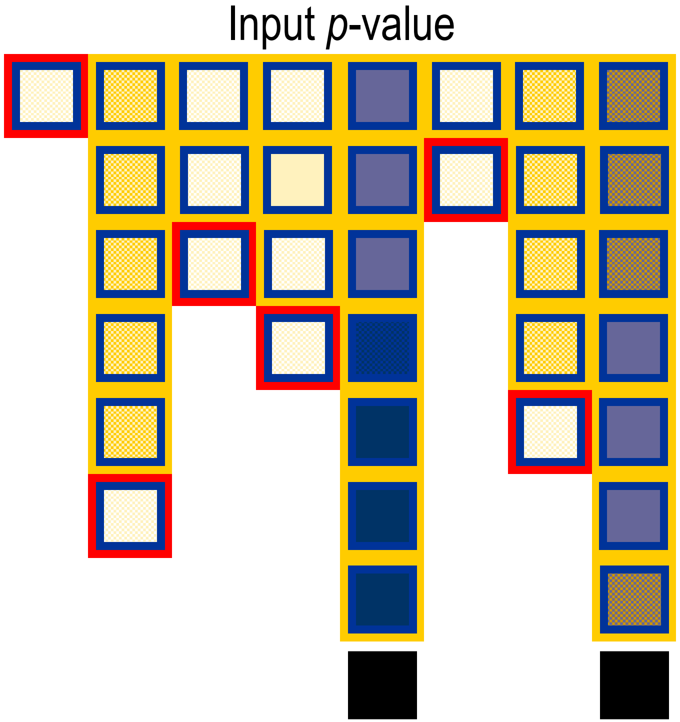
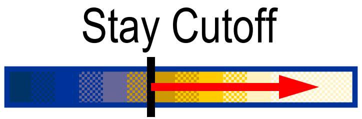
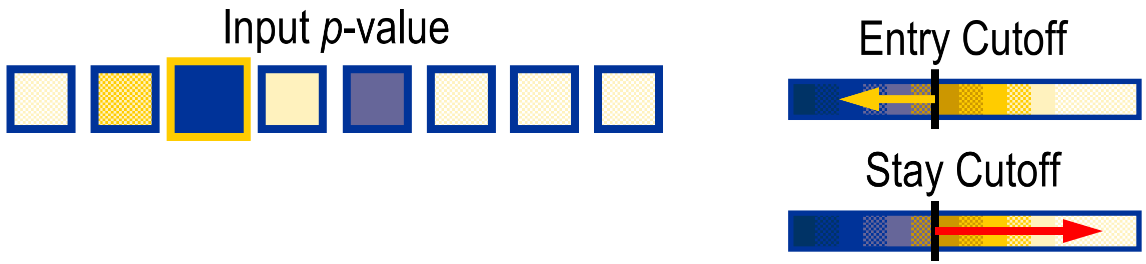
Sequential Selection: Backward



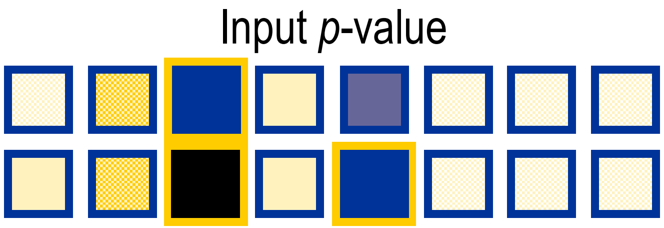


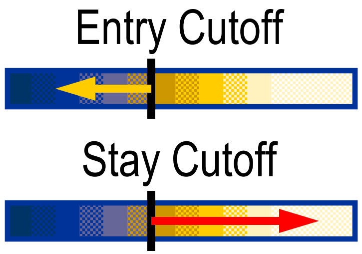
Sequential Selection: Stepwise



...

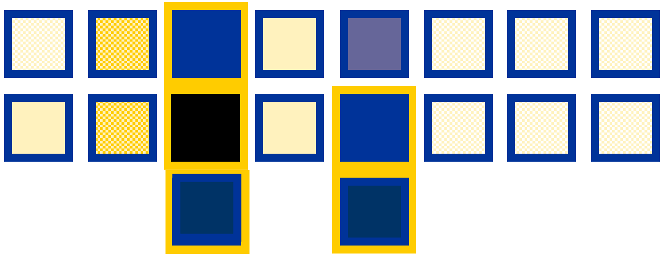
Sequential Selection: Stepwise

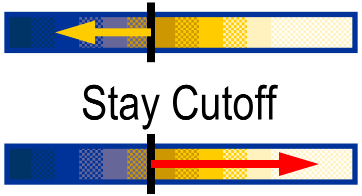




...

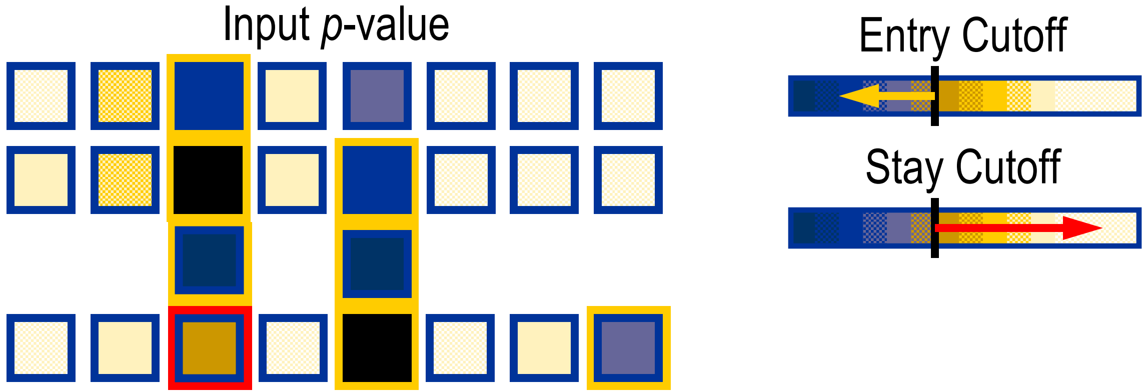
Sequential Selection: Stepwise





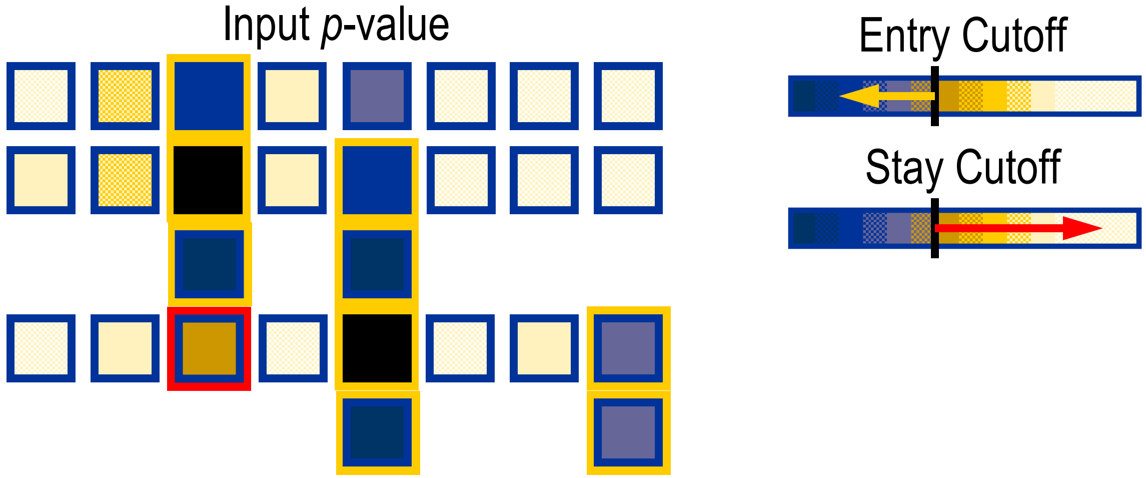
...

Sequential Selection: Stepwise



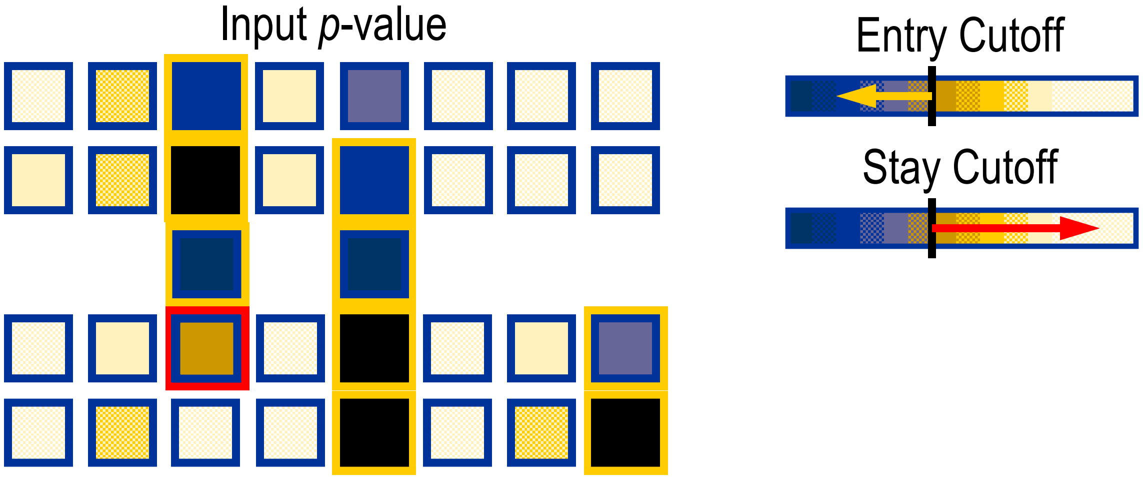
…

Sequential Selection: Stepwise



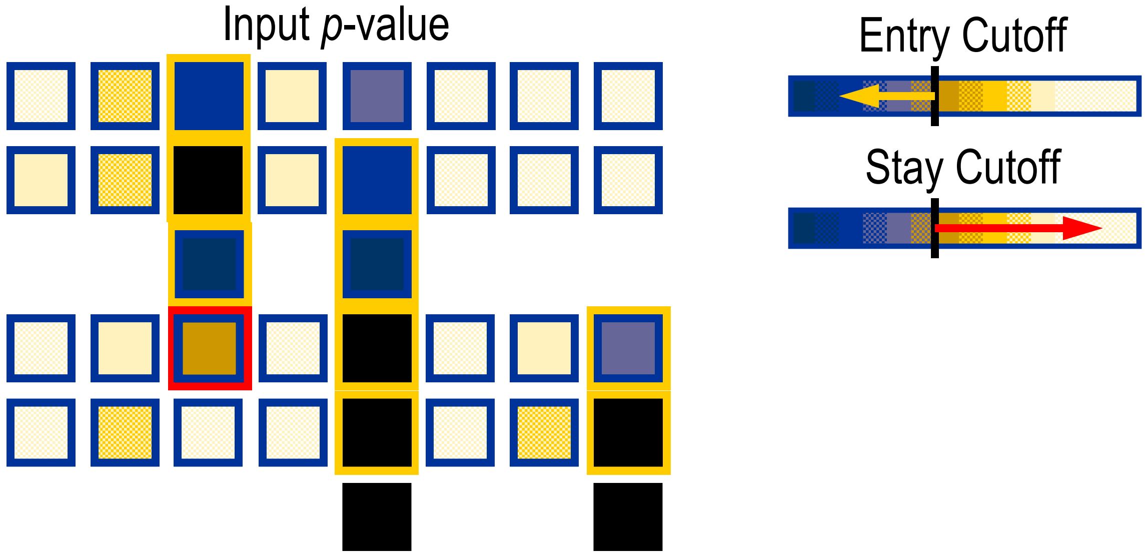
...

Sequential Selection: Stepwise



...

Sequential Selection: Stepwise



mlxtend Home User Guide API Installation About Search GitHub

Sequential Feature Selector

Implementation of *sequential feature algorithms* (SFAs) -- greedy search algorithms -- that have been developed as a suboptimal solution to the computationally often not feasible exhaustive search.

```
from mlxtend.feature_selection import SequentialFeatureSelector
```

- Sequential feature selection algorithms are a family of greedy search algorithms that are used to reduce an initial d-dimensional feature space to a k-dimensional feature subspace where $k < d$.
- In a nutshell, SFAs remove or add one feature at the time based on the classifier performance (such as, accuracy) until a feature subset of the desired size k is reached.
- Sequential Forward Selection (SFS)
- Sequential Backward Selection (SBS)
- Sequential Forward Floating Selection (SFFS)
- Sequential Backward Floating Selection (SBFS)

- `scoring` : str, callable, or None (default: None)

  If None (default), uses 'accuracy' for sklearn classifiers and 'r2' for sklearn regressors. If str, uses a sklearn scoring metric string identifier, for example {accuracy, f1, precision, recall, roc_auc} for classifiers, {'mean_absolute_error', 'mean_squared_error'/'neg_mean_squared_error', 'median_absolute_error', 'r2'} for regressors. If a callable object or function is provided, it has to be conform with sklearn's signature `scorer(estimator, X, y)`; see http://scikit-learn.org/stable/modules/generated/sklearn.metrics.make_scorer.html for more information.
- `cv` : int (default: 5)

  Integer or iterable yielding train, test splits. If cv is an integer and `estimator` is a classifier (or y consists of integer class labels) stratified k-fold. Otherwise regular k-fold cross-validation is performed. No cross-validation if cv is None, False, or 0.

http://rasbt.github.io/mlxtend/user_guide/feature_selection/SequentialFeatureSelector/

+ Seqeuntial Feature Selector (cont.)

- The ***floating*** variants, SFFS and SBFS, can be considered as extensions to the simpler SFS and SBS algorithms.
- The dimensionality of the subset during the search can be thought to be "floating" up and down. (somewhat similar to stepwise)
  - Sequential Forward Floating Selection (SFFS)
  - Sequential Backward Floating Selection (SBFS)

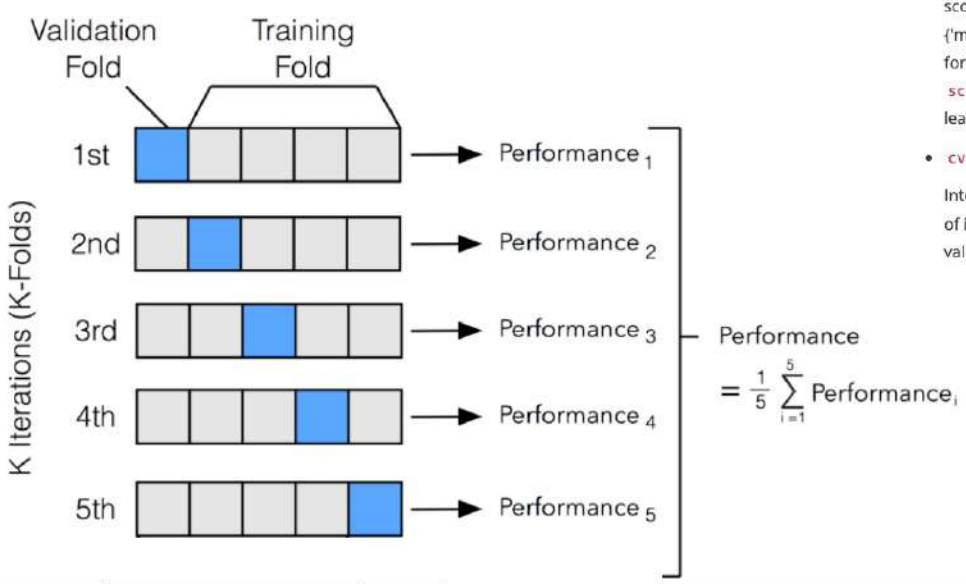
```python
# Build RF classifier to use in feature selection
clf = LogisticRegression()

# Build step forward feature selection
sfs1 = sfs(clf,
           k_features=5,
           forward=True,
           floating=False,
           verbose=2,
           scoring='accuracy',
           cv=5)

# Perform SFFS
sfs1 = sfs1.fit(bank_final, y)
```

```python
# Which features?
feat_cols = list(sfs1.k_feature_idx_)
print(feat_cols)
```

```
[6, 10, 15, 16, 17]
```



- `scoring` : str, callable, or None (default: None)

  If None (default), uses 'accuracy' for sklearn classifiers and 'r2' for sklearn regressors. If str, uses a sklearn scoring metric string identifier, for example {accuracy, f1, precision, recall, roc_auc} for classifiers, {'mean_absolute_error', 'mean_squared_error'/'neg_mean_squared_error', 'median_absolute_error', 'r2'} for regressors. If a callable object or function is provided, it has to be conform with sklearn's signature `scorer(estimator, X, y)`; see http://scikit-learn.org/stable/modules/generated/sklearn.metrics.make_scorer.html for more information.

- `cv` : int (default: 5)

  Integer or iterable yielding train, test splits. If cv is an integer and `estimator` is a classifier (or y consists of integer class labels) stratified k-fold. Otherwise regular k-fold cross-validation is performed. No cross-validation if cv is None, False, or 0.

Now it is available in scikit-learn now.

Please **cite us** if you use the software.

sklearn.feature_selection.SequentialFeatureSelector

class sklearn.feature_selection.**SequentialFeatureSelector**(*estimator, *, n_features_to_select='warn', tol=None, direction='forward', scoring=None, cv=5, n_jobs=None*) [source]

Transformer that performs Sequential Feature Selection.

This Sequential Feature Selector adds (forward selection) or removes (backward selection) features to form a feature subset in a greedy fashion. At each stage, this estimator chooses the best feature to add or remove based on the cross-validation score of an estimator. In the case of unsupervised learning, this Sequential Feature Selector looks only at the features (X), not the desired outputs (y).

Read more in the User Guide.

New in version 0.24.

Parameters:

estimator : *estimator instance*
An unfitted estimator.

n_features_to_select : *"auto", int or float, default='warn'*
If "auto", the behaviour depends on the tol parameter:

tol : *float, default=None*
If the score is not incremented by at least tol between two consecutive feature additions or removals, stop adding or removing. tol is enabled only when n_features_to_select is "auto".

New in version 1.1.

direction : *{'forward', 'backward'}, default='forward'*
Whether to perform forward selection or backward selection.

scoring : *str or callable, default=None*
A single str (see The scoring parameter: defining model evaluation rules) or a callable (see Defining your scoring strategy from metric functions) to evaluate the predictions on the test set.

NOTE that when using a custom scorer, it should return a single value.

If None, the estimator's score method is used.

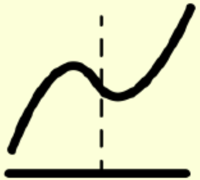
cv : *int, cross-validation generator or an iterable, default=None*
Determines the cross-validation splitting strategy. Possible inputs for cv are:

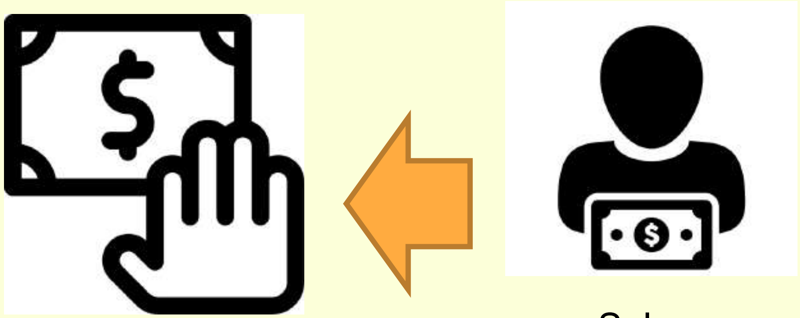
https://scikit-learn.org/stable/modules/generated/sklearn.feature_selection.SequentialFeatureSelector.html#sklearn.feature_selection.SequentialFeatureSelector.

Examples

```
>>> from sklearn.feature_selection import SequentialFeatureSelector
>>> from sklearn.neighbors import KNeighborsClassifier
>>> from sklearn.datasets import load_iris
>>> X, y = load_iris(return_X_y=True)
>>> knn = KNeighborsClassifier(n_neighbors=3)
>>> sfs = SequentialFeatureSelector(knn, n_features_to_select=3)
>>> sfs.fit(X, y)
SequentialFeatureSelector(estimator=KNeighborsClassifier(n_neighbors=3),
                          n_features_to_select=3)
>>> sfs.get_support()
array([ True, False,  True,  True])
>>> sfs.transform(X).shape
(150, 3)
```

Logistic Regression



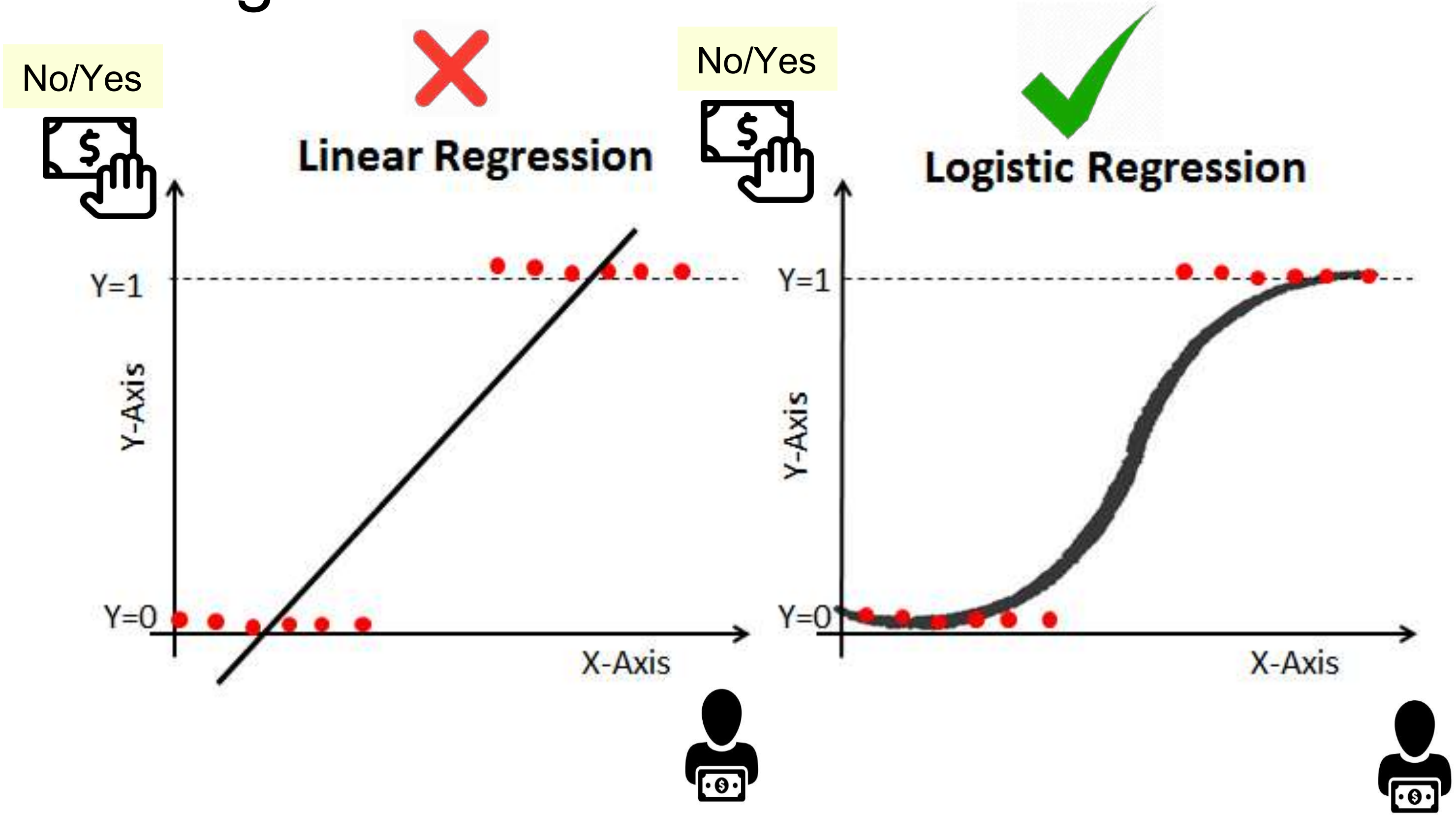


Purchase
(No/Yes)

Salary

Type of Predictors / Type of Response	Categorical	Continuous	Continuous and Categorical
Continuous	Analysis of Variance (ANOVA)	Ordinary Least Squares (OLS) Regression	Analysis of Covariance (ANCOVA)
Categorical	Contingency Table Analysis or Logistic Regression	Logistic Regression	Logistic Regression

Logistic Regression

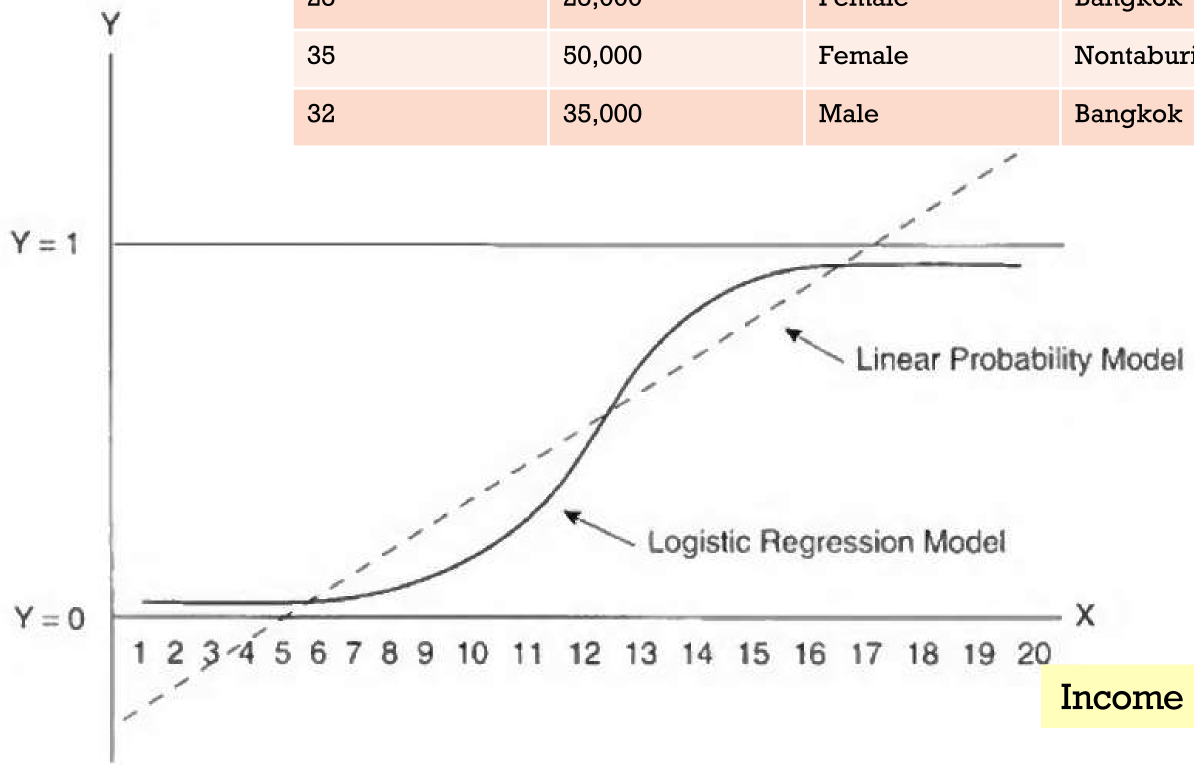


https://medium.com/@ODSC/logistic-regression-with-python-ede39f8573c7

Classification Task

Prob. of purchase

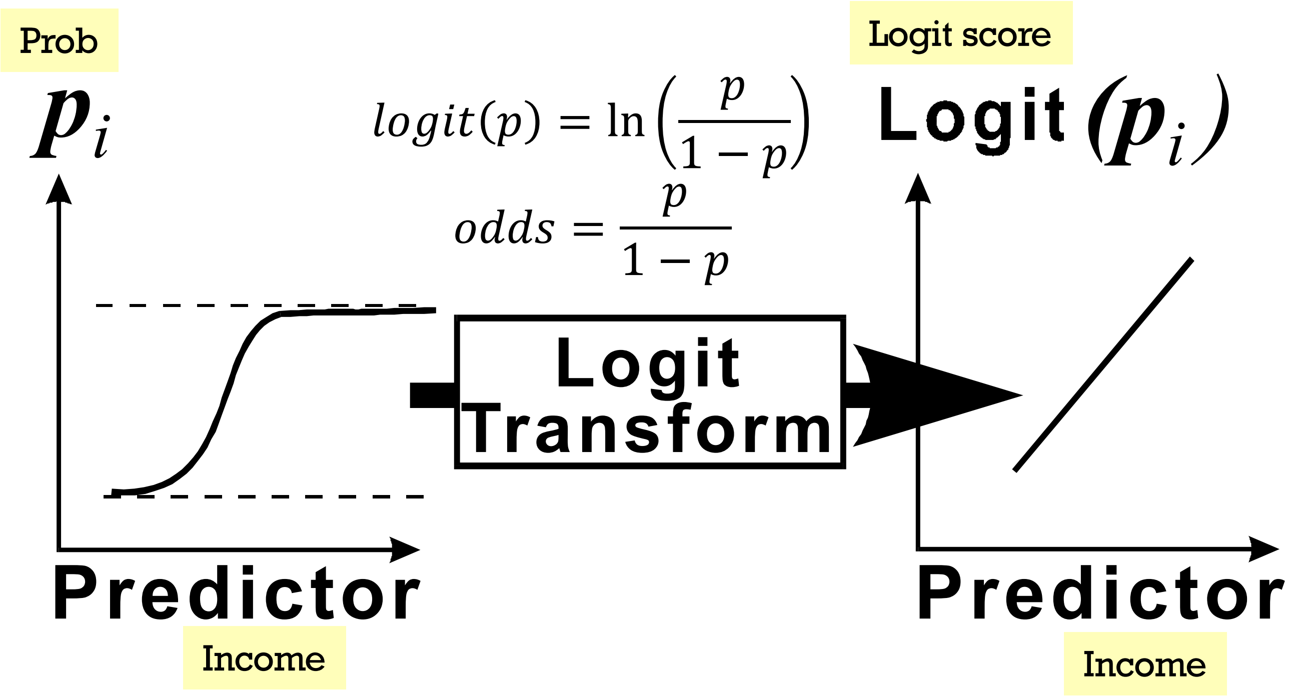
Age	Income	Gender	Province	Purchase
25	25,000	Female	Bangkok	Yes (1)
35	50,000	Female	Nontaburi	Yes (1)
32	35,000	Male	Bangkok	No (0)



Income

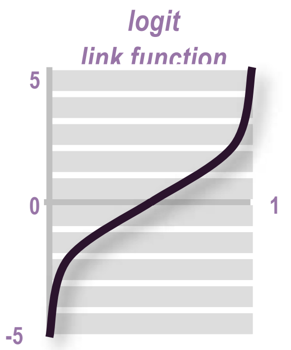
Logistic function
Sigmoid function

Logistic Regression
Logit link function: Non-linear to Linear

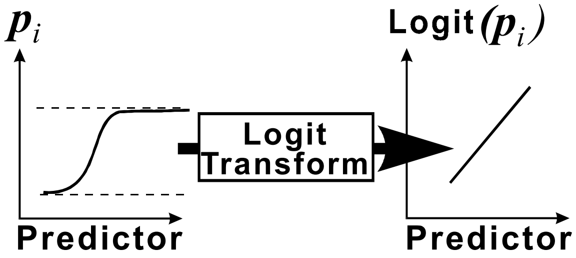


Logistic Regression Prediction Formula

$$\log\left(\frac{\hat{p}}{1-\hat{p}}\right) = \hat{w}_0 + \hat{w}_1 x_1 + \hat{w}_2 x_2$$ *logit scores*



The logit link function transforms probabilities (between 0 and 1) to logit scores (between −∞ and +∞).



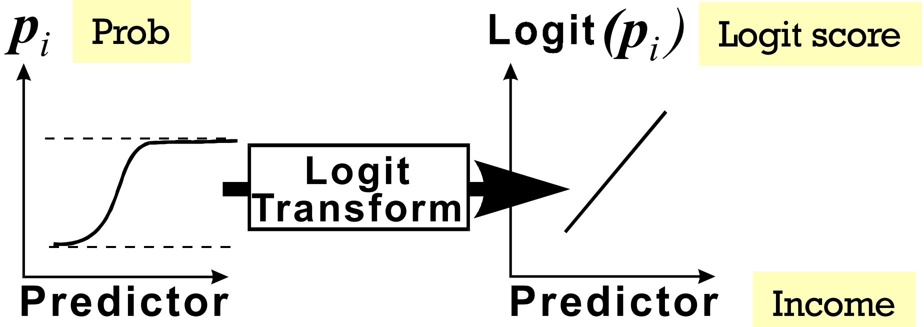
...

Logit Link Function

$$\log\left(\frac{\hat{p}}{1-\hat{p}}\right) = \hat{w}_0 + \hat{w}_1 x_1 + \hat{w}_2 x_2 = \text{logit}(\hat{p})$$

$$\hat{p} = \frac{1}{1 + e^{-\text{logit}(\hat{p})}}$$

To obtain prediction estimates, the logit equation is solved for $\hat{p}$.



…

Training Phase: Regressions
Maximum Log-Likelihood Estimation (MLE)

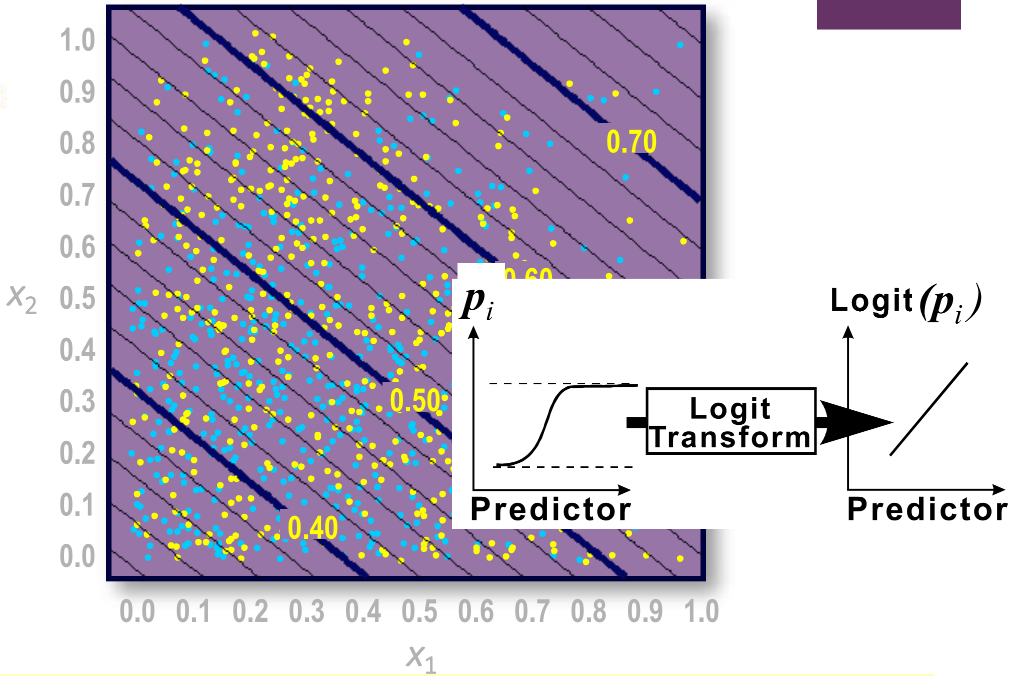
$$\text{logit}(\hat{p}) = \boxed{\hat{w}_0} + \boxed{\hat{w}_1} \cdot x_1 + \boxed{\hat{w}_2} \cdot x_2$$

$$\hat{p} = \frac{1}{1 + e^{-\text{logit}(\hat{p})}}$$

Find parameter estimates by *maximizing*

$$\underbrace{\sum \log(\hat{p}_i)}_{\text{primary outcome training cases}} + \underbrace{\sum \log(1 - \hat{p}_i)}_{\text{secondary outcome training cases}}$$

log-likelihood function



For each set of parameters (w0, w1, w2), we can calculate log-likelihood (LL) of the whole training data.
So, pick the set of parameters with a maximum LL (MLE).

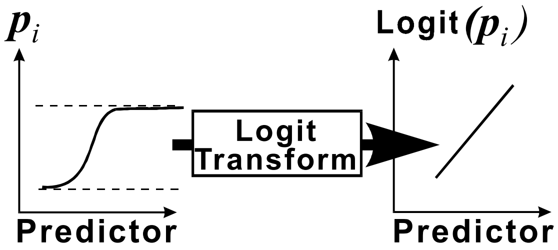
…

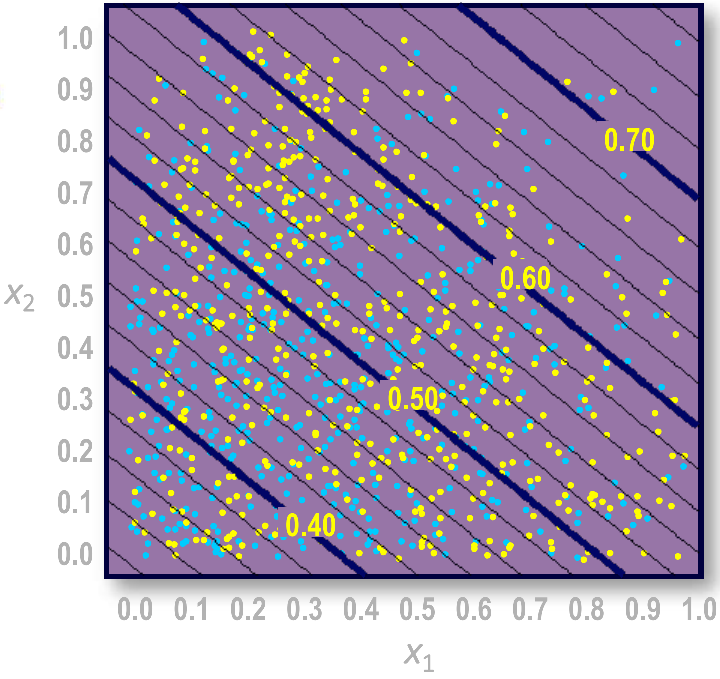
Testing Phase: Regressions

$$\text{logit}(\hat{p}) = -0.81 + 0.92\,x_1 + 1.11\,x_2$$

$$\hat{p} = \frac{1}{1 + e^{-\text{logit}(\hat{p})}}$$

Using the maximum likelihood estimates, the prediction formula assigns a logit score to each x_1 and x_2.

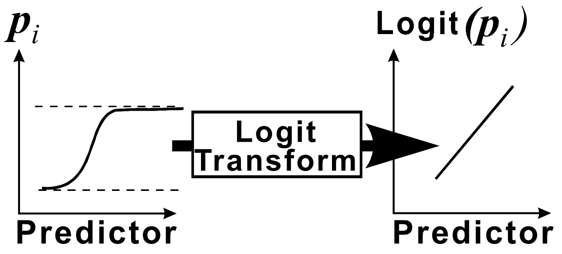




...

+

Quiz



- What is the logistic regression prediction for the indicated point?

a. 0.243

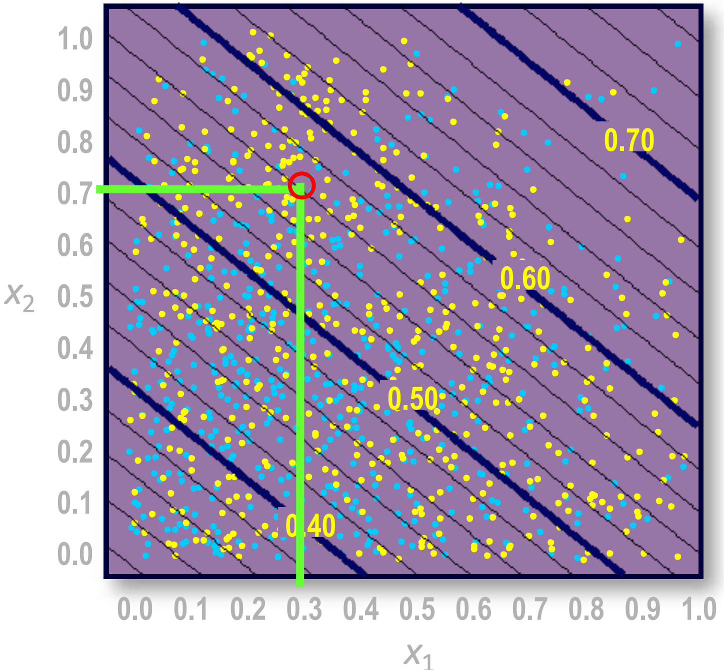
b. 0.56

c. yellow

d. It depends.

$$\text{logit}(\hat{p}) = -0.81 + 0.92\, x_1 + 1.11\, x_2$$

$$\hat{p} = \frac{1}{1 + e^{-\text{logit}(\hat{p})}}$$



Training Phase: Regressions (Recap) Maximum Log-Likelihood Estimation (MLE)

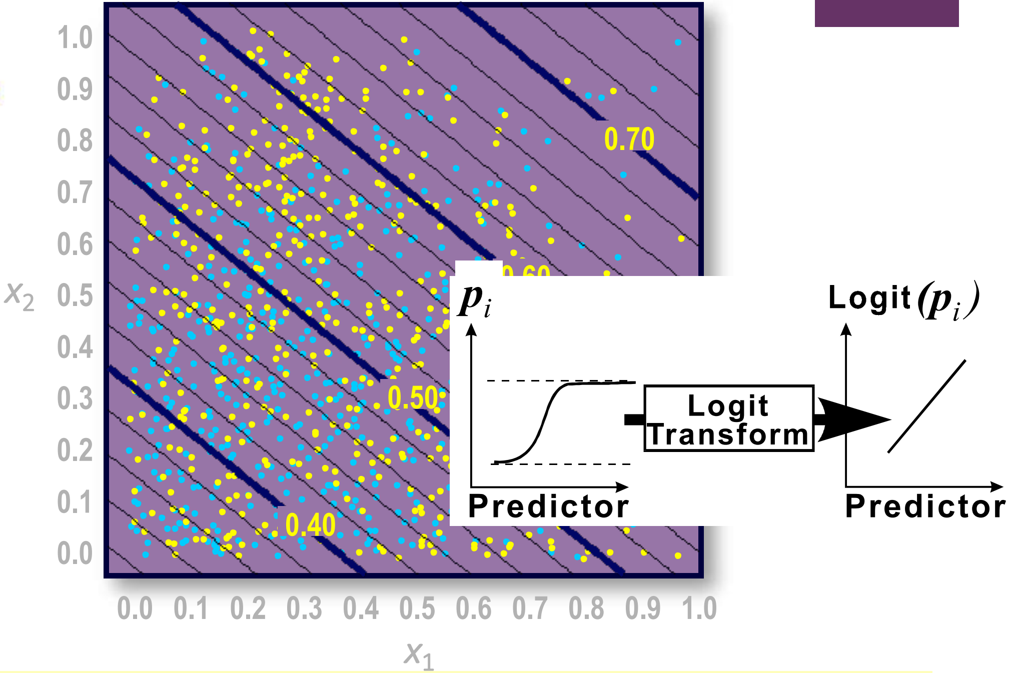
$$\text{logit}(\hat{p}) = \boxed{\hat{w}_0} + \boxed{\hat{w}_1} x_1 + \boxed{\hat{w}_2} x_2$$

$$\hat{p} = \frac{1}{1 + e^{-\text{logit}(\hat{p})}}$$

Find parameter estimates by *maximizing*

$$\underbrace{\sum \log(\hat{p}_i)}_{\text{primary outcome training cases}} + \underbrace{\sum \log(1 - \hat{p}_i)}_{\text{secondary outcome training cases}}$$

log-likelihood function



For each set of parameters (w0, w1, w2), we can calculate log-likelihood (LL) of the whole training data.
So, pick the set of parameters with a maximum LL (MLE).

…

$$P(Y = y) = p^y(1-p)^{1-y}, y = 0,1$$

$$P(Y = 1) = p^1(1-p)^0 = p$$

$$P(Y = 0) = p^0(1-p)^{1-0} = (1-p)$$

$$Likelihood = \prod_{i=1}^{n} p^{y_i}(1-p)^{1-y_i}$$

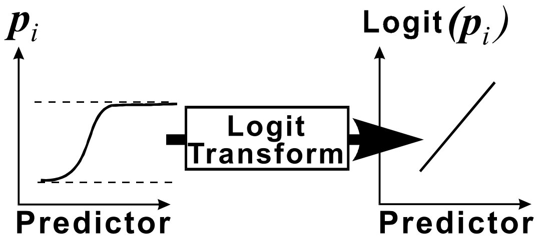
$$Log - Likelihood\ (LL) = \sum_{i=1}^{n} y_i \ln(p_i) + (1-y_i)ln(1-p_i)$$

Outcome	Predicted Probability	
y_i	p_i	$(1-p_i)$
1	.899	.101
1	.540	.460
0	.317	.683
1	.516	.439
1	.698	.302
0	.457	.543
0	.234	.766
1	.899	.101
1	.451	.439
1	.764	.236
0	.457	.543
0	.561	.439
1	.698	.302
1	.457	.543
0	.899	.101

$$\text{logit}(\hat{p}) = \hat{w}_0 + \hat{w}_1 x_1 + \hat{w}_2 x_2$$

$$\text{logit}(\hat{p}) = -0.81 + 0.92\, x_1 + 1.11\, x_2$$

$$\hat{p} = \frac{1}{1 + e^{-\text{logit}(\hat{p})}}$$



[a]–2 * log-likelihood = 17.48.

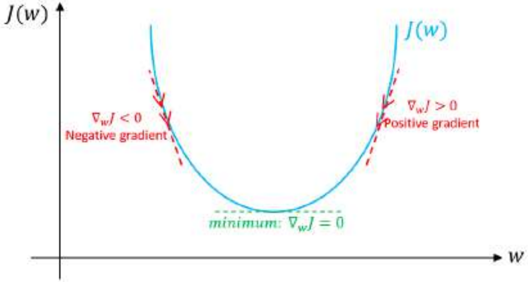
-2LL can be considered as error (loss), so smaller is better.

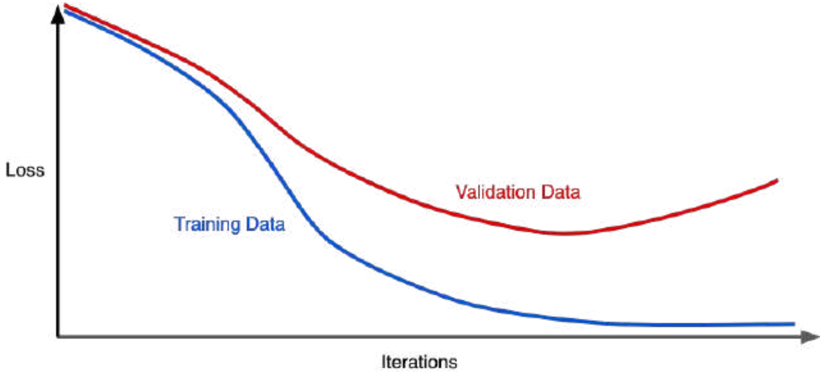
MLE Solver

$$\text{logit}(\hat{p}) = \hat{w}_0 + \hat{w}_1 x_1 + \hat{w}_2 x_2$$

$$\text{logit}(\hat{p}) = -0.81 + 0.92\, x_1 + 1.11\, x_2$$

- Maximum Log-Likelihood Estimation (MLE) refers to **maximize LL**
- Or **minimize -2LL (loss)**
- Gradient descent optimization
  - Stochastic Average Gradient solver





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]

Logistic Regression (aka logit, MaxEnt) classifier.

In the multiclass case, the training algorithm uses the one-vs-rest (OvR) scheme if the 'multi_class' option is set to 'ovr', and uses the cross-entropy loss if the 'multi_class' option is set to 'multinomial'. (Currently the 'multinomial' option is supported only by the 'lbfgs', 'sag', 'saga' and 'newton-cg' solvers.)

solver : *{'newton-cg', 'lbfgs', 'liblinear', 'sag', 'saga'}, default='lbfgs'*

Algorithm to use in the optimization problem.

- For small datasets, 'liblinear' is a good choice, whereas 'sag' and 'saga' are faster for large ones.
- For multiclass problems, only 'newton-cg', 'sag', 'saga' and 'lbfgs' handle multinomial loss; 'liblinear' is limited to one-versus-rest schemes.
- 'newton-cg', 'lbfgs', 'sag' and 'saga' handle L2 or no penalty
- 'liblinear' and 'saga' also handle L1 penalty
- 'saga' also supports 'elasticnet' penalty
- 'liblinear' does not support setting `penalty='none'`

Note that 'sag' and 'saga' fast convergence is only guaranteed on features with approximately the same scale. You can preprocess the data with a scaler from sklearn.preprocessing.

New in version 0.17: Stochastic Average Gradient descent solver.

New in version 0.19: SAGA solver.

Changed in version 0.22: The default solver changed from 'liblinear' to 'lbfgs' in 0.22.

max_iter : *int, default=100*

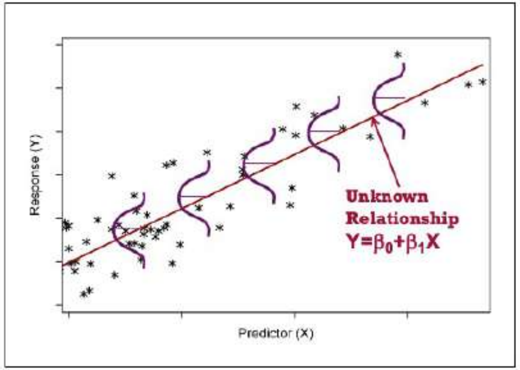
Maximum number of iterations taken for the solvers to converge.

Assumptions for Linear Regression (recap)

- The mean of the Ys is accurately modeled by a linear function of the X_i.
  - (y, x_i) = linear relationship (correlation)

- The random error term, ε, is assumed to have a normal distribution with a mean of zero.
- The random error term, ε, is assumed to have a constant variance, σ^2.
  - Not skew

- The errors are independent.

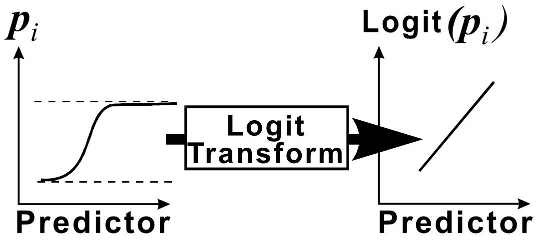


Assumptions for Logistic Regression

- The mean of the logit is accurately modeled by a linear function of the X_i.
  - (logit, x_i) = linear relationship

- ~~The random error term, ε, is assumed to have a normal distribution with a mean of zero.~~
- ~~The random error term, ε, is assumed to have a constant variance, σ^2.~~
  - ~~Not skew~~

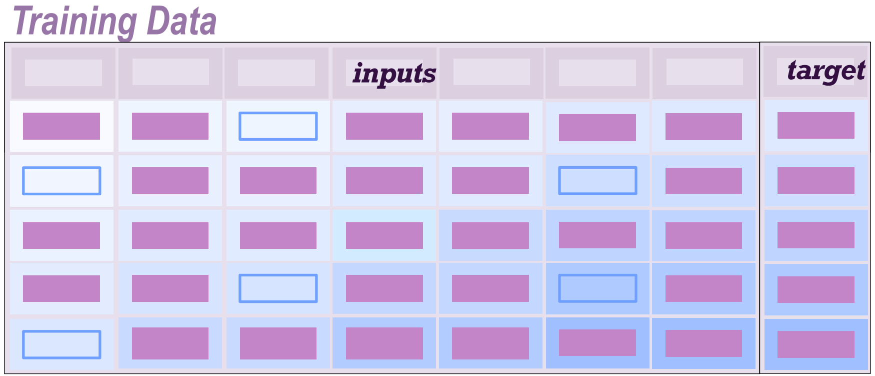
- The errors are independent.



Beyond the prediction

- Manage missing values
- Interpret the model
- Handle outliers
- Use nonnumeric inputs

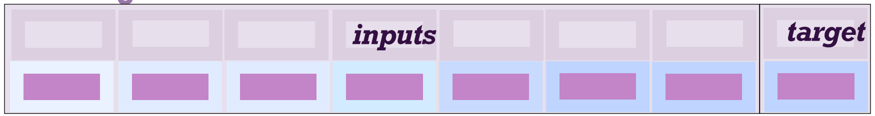
Missing Values and Regression Modeling



Problem 1: Training data cases with missing values on inputs used by a regression model are ignored.

Missing Values and Regression Modeling

Training Data



Consequence: Missing values can significantly reduce your amount of training data for regression modeling!

Missing Values and the Prediction Formula

$$\mathrm{logit}(\hat{p}) = -0.81 + 0.92 \cdot x_1 + 1.11 \cdot x_2$$

Predict: (x1, x2) = (0.3, ?)

Problem 2: **Prediction formulas cannot score cases with missing values.**

…

Missing Values and the Prediction Formula

$$\text{logit}(\hat{p}) = -0.81 + 0.92 \cdot 0.3 + 1.11 \cdot ?$$

Predict: (x1, x2) = (0.3, ?)

Problem 2: **Prediction formulas cannot score cases with missing values.**

...

Interpret the model: Positive effect (income)

Recap how to interpret "regression"

$$logit(p) = 500 + 0.2 \times Income - 0.8 \times Age$$

$$\ln(odds) = 500 + 0.2 \times Income - 0.8 \times Age$$

$$\ln(odds(Income = 1)) = 0.2 \times 1 = 0.2$$

$$odds(Income = 1) = e^{0.2} = 1.22$$

$$\ln(odds(Income = 0)) = 0.2 \times 0 = 0$$

$$odds(Income = 0) = e^{0} = 1$$

$$Odss\ Ratio(Income) = \frac{odds(Income = 1)}{odds(Income = 0)} = \frac{1.22}{1} = 1.22\ (+22\%) = \exp(w_1)$$

- OR(Income) = 1.22 (22% increase)
- When income increases by 1THB, it has higher chance (odds) to purchase for 22%

Interpret the model: Negative effect (age)

Recap how to interpret "regression"

$$logit(p) = 500 + 0.2 \times Income - 0.8 \times Age$$

$$\ln(odds) = 500 + 0.2 \times Income - 0.8 \times Age$$

$$\ln(odds(Age = 1)) = -0.8 \times 1 = -0.8$$
$$odds(Age = 1) = e^{-0.8} = 0.45$$

$$\ln(odds(Age = 0)) = -0.8 \times 0 = 0$$
$$odds(Age = 0) = e^{0} = 1$$

$$Odss\ Ratio(Age) = \frac{odds(Age = 1)}{odds(Age = 0)} = \frac{0.45}{1} = 0.45\ (-55\%) = \exp(w_1)$$

- OR(Age) = 0.45 (55% decrease)
- When age increases by 1 year, it has lower chance (odds) to purchase for 55%.

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]

Logistic Regression (aka logit, MaxEnt) classifier.

In the multiclass case, the training algorithm uses the one-vs-rest (OvR) scheme if the 'multi_class' option is set to 'ovr', and uses the cross-entropy loss if the 'multi_class' option is set to 'multinomial'. (Currently the 'multinomial' option is supported only by the 'lbfgs', 'sag', 'saga' and 'newton-cg' solvers.)

This class implements regularized logistic regression usin
regularization is applied by default. It can handle both d
64-bit floats for optimal performance; any other input for

The 'newton-cg', 'sag', and 'lbfgs' solvers support only L2
solver supports both L1 and L2 regularization, with a dual
supported by the 'saga' solver.

Read more in the User Guide.

Examples

```
>>> from sklearn.datasets import load_iris
>>> from sklearn.linear_model import LogisticRegression
>>> X, y = load_iris(return_X_y=True)
>>> clf = LogisticRegression(random_state=0).fit(X, y)
>>> clf.predict(X[:2, :])
array([0, 0])
>>> clf.predict_proba(X[:2, :])
array([[9.8...e-01, 1.8...e-02, 1.4...e-08],
       [9.7...e-01, 2.8...e-02, ...e-08]])
>>> clf.score(X, y)
0.97...
```

Parameters: **penalty : {'l1', 'l2', 'elasticnet', 'none'},**

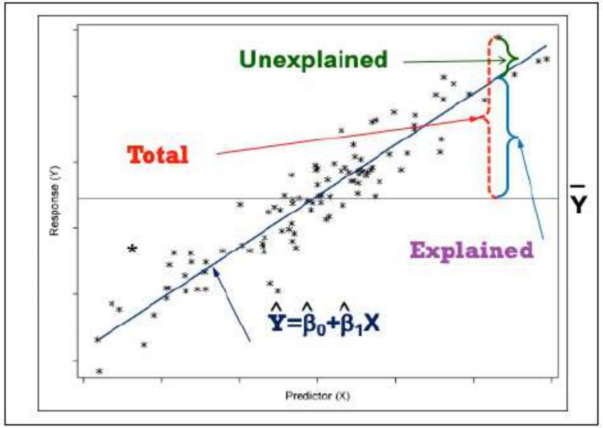
Used to specify the norm used in the penalization. The 'newton-cg', 'sag' and 'lbfgs' solvers support only l2 penalties. 'elasticnet' is only supported by the 'saga' solver. If 'none' (not supported by the liblinear solver), no regularization is applied.

New in version 0.19: l1 penalty with SAGA solver (allowing 'multinomial' + L1)

https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LogisticRegression.html

Evaluation

Pseudo R^2
TP, TN, FP, FN
Precision, Recall, F1



R^2 (recap)

$$R^2 = \frac{SSM}{SST} = 1 - \frac{SSE}{SST}$$

id	chol (x)	bp (y)	predict	error	squred error (SE)	guess	(y - y_bar)	squred total (ST)
1	437	194	196.1897	(2.1897)	4.7948	143.4286	50.5714	2,557.4694
2	264	121	141.4179	(20.4179)	416.8906	143.4286	(22.4286)	503.0408
3	249	131	136.6689	(5.6689)	32.1364	143.4286	(12.4286)	154.4694
4	297	159	151.8657	7.1343	50.8982	143.4286	15.5714	242.4694
5	243	123	134.7693	(11.7693)	138.5164	143.4286	(20.4286)	417.3265
6	272	161	143.9507	17.0493	290.6786	143.4286	17.5714	308.7551
7	161	115	108.8081	6.1919	38.3396	143.4286	(28.4286)	808.1837
average	274.7143	143.4286		SSE	972.2548		SST	4,991.7143
				MSE	138.8935			
				RMSE	11.7853			
	R^2	1 - (SSE/SST)	0.8052					

Pseudo R²

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2}$$

Outcome	Predicted Probability	
Y	$\hat{Y}$	$1 - \hat{Y}$
1	.899	.101
1	.540	.460
0	.317	.683
1	.516	.439
1	.698	.302
0	.457	.543
0	.234	.766
1	.899	.101
1	.451	.439
1	.764	.236
0	.457	.543
0	.561	.439
1	.698	.302
1	.457	.543
0	.899	.101

$\bar{y} = 0.6$

[a]–2 * log-likelihood = 17.48.

Confusion Matrix

n=165	Predicted: NO	Predicted: YES	
Actual: NO	TN = 50	FP = 10	60
Actual: YES	FN = 5	TP = 100	105
	55	110	

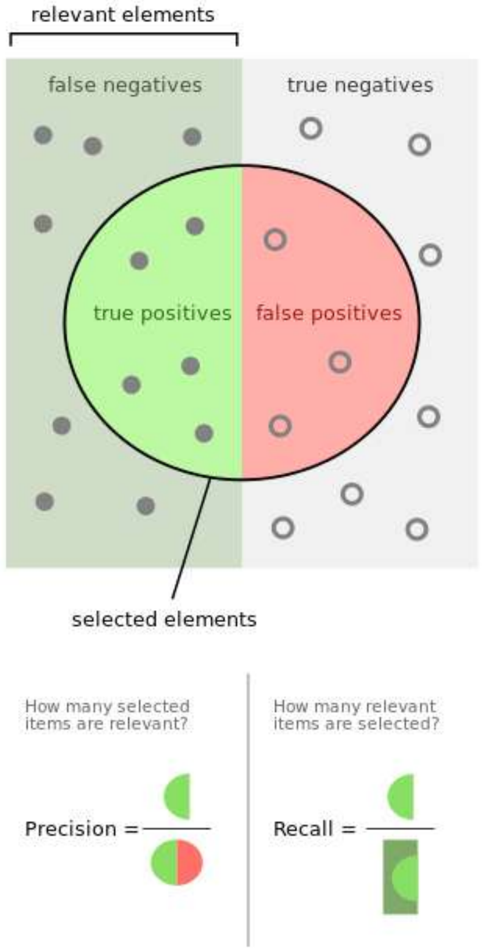
- True Positive (TP)
- True Negative (TN)
- False Positive (FP)
- False Negative (FN)

- Accuracy = (TP + TN) / total
- Misclassification = (FP + FN) / total

Precision, Recall, F1

n=165	Predicted: NO	Predicted: YES	
Actual: NO	TN = 50	FP = 10	60
Actual: YES	FN = 5	TP = 100	105
	55	110	

- Precision = correctly predict = TP / (TP + FP)
- Recall = coverage = TP / (TP + FN)
- F1 = (2*pre*rec) / (pre + rec)



Precision, Recall, F1: Average

n=165	Predicted: NO	Predicted: YES	
Actual: NO	TN = 50	FP = 10	60
Actual: YES	FN = 5	TP = 100	105
	55	110	

- Precision = correctly predict = TP / (TP + FP)
- Recall = coverage = TP / (TP + FN)
- F1 = (2*pre*rec) / (pre + rec)

- What is a positive class?
  - 1) Direct target marketing? Yes
  - 2) Intelligent diagnosis to predict "Corona" or "Flu" – both are important.
- If there is no positive (all classes are important)
  - Macro Average
  - Weighted Average (Micro Average) by the amount of data in that class

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sklearn.metrics.confusion_matrix
Examples using sklearn.metrics.confusion_matri

sklearn.metrics.confusion_matrix

`sklearn.metrics.confusion_matrix`(*y_true, y_pred, labels=None, sample_weight=None, normalize=None*) [source]

Compute confusion matrix to evaluate the accuracy of a classification.

By definition a confusion matrix C is such that $C_{i,j}$ is equal to the number of observations known to be in group i and predicted to be in group j.

Thus in binary classification, the count of true negatives is $C_{0,0}$, false negatives is $C_{1,0}$, true positives is $C_{1,1}$ and false positives is $C_{0,1}$.

Read more in the User Guide.

Parameters:

y_true : *array-like of shape (n_samples,)*
Ground truth (correct) target values.

f shape (n_samples,)
s returned by a classifier.

shape (n_classes), default=None
ex the matrix. This may be used to reorder or select a subset of labels. If `None` is given, those once in `y_true` or `y_pred` are used in sorted order.

y-like of shape (n_samples,), default=None

normalize : *{'true', 'pred', 'all'}, default=None*
Normalizes confusion matrix over the true (rows), predicted (columns) conditions or all the population. If None, confusion matrix will not be normalized.

```
>>> from sklearn.metrics import confusion_matrix
>>> y_true = [2, 0, 2, 2, 0, 1]
>>> y_pred = [0, 0, 2, 2, 0, 2]
>>> confusion_matrix(y_true, y_pred)
array([[2, 0, 0],
       [0, 0, 1],
       [1, 0, 2]])
```

https://scikit-learn.org/stable/modules/generated/sklearn.metrics.confusion_matrix.html

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`sklearn.metrics.classification_report`
Examples using
`sklearn.metrics.classification_`

sklearn.metrics.classification_report

`sklearn.metrics.`**`classification_report`**(*y_true, y_pred, labels=None, target_names=None, sample_weight=None, digits=2, output_dict=False, zero_division='warn'*) [source]

Build a text report showing the main classification metrics

Read more in the User Guide.

Parameters:

y_true : *1d array-like, or label in*
Ground truth (correct) target va

y_pred : *1d array-like, or label in*
Estimated targets as returned b

labels : *array, shape = [n_labels*
Optional list of label indices to i

target_names : *list of strings*
Optional display names matchin

sample_weight : *array-like of sh*
Sample weights.

digits : *int*
Number of digits for formatting
the returned values will not be rounded.

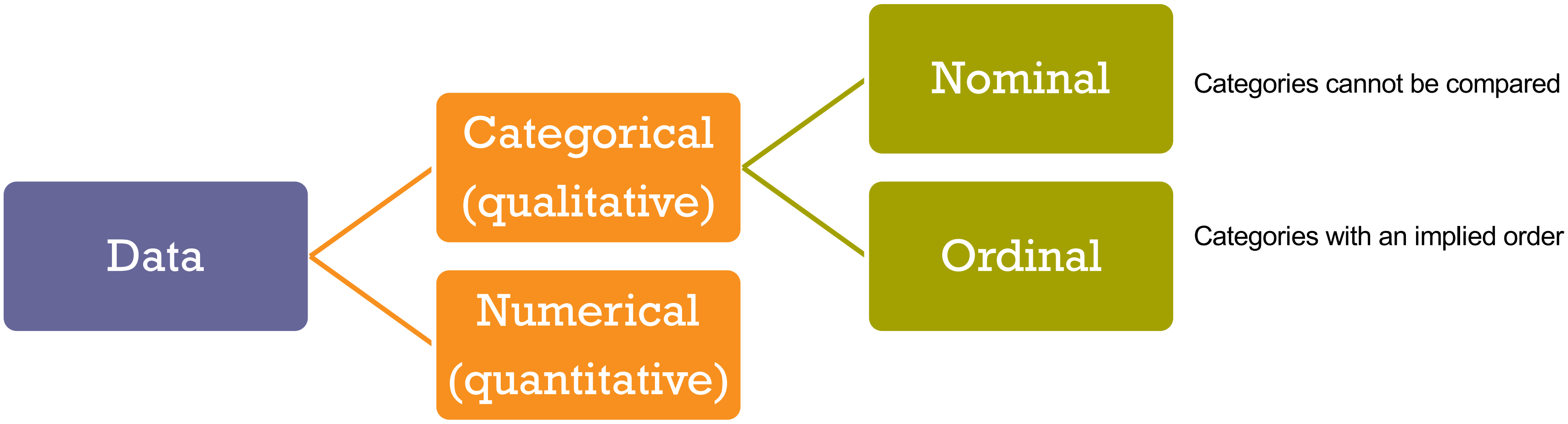
Examples

```
>>> from sklearn.metrics import classification_report
>>> y_true = [0, 1, 2, 2, 2]
>>> y_pred = [0, 0, 2, 2, 1]
>>> target_names = ['class 0', 'class 1', 'class 2']
>>> print(classification_report(y_true, y_pred, target_names=target_names))
              precision    recall  f1-score   support
<BLANKLINE>
     class 0       0.50      1.00      0.67         1
     class 1       0.00      0.00      0.00         1
     class 2       1.00      0.67      0.80         3
<BLANKLINE>
    accuracy                           0.60         5
   macro avg       0.50      0.56      0.49         5
weighted avg       0.70      0.60      0.61         5
<BLANKLINE>
>>> y_pred = [1, 1, 0]
>>> y_true = [1, 1, 1]
>>> print(classification_report(y_true, y_pred, labels=[1, 2, 3]))
              precision    recall  f1-score   support
<BLANKLINE>
           1       1.00      0.67      0.80         3
           2       0.00      0.00      0.00         0
           3       0.00      0.00      0.00         0
<BLANKLINE>
   micro avg       1.00      0.67      0.80         3
   macro avg       0.33      0.22      0.27         3
weighted avg       1.00      0.67      0.80         3
<BLANKLINE>
```

https://scikit-learn.org/stable/modules/generated/sklearn.metrics.classification_report.html

Non-numeric variables (Model M2)

Terminology: Kinds of data (recap)



Ordinal: Recode

Grade	GradeNum
A	4.00
B+	3.50
B	3.00
C+	2.50
C	2.00
D+	1.50
D	1.00
F	0.00

Size	SizeNum
XL	5
L	4
M	3
S	2
XS	1

Categorical

- Dummy coding = (n-1) dummy codes

Branch		BranchNum		D_BKK	B_Patum	D_Non		D_BKK	B_Patum	
BKK		1		1	0	0		1	0	
Patumtani		2		0	1	0		0	1	
Nontaburi		3		0	0	1		0	0	reference

pandas.get_dummies

`pandas.get_dummies`(*data, prefix=None, prefix_sep='_', dummy_na=False, columns=None, sparse=False, drop_first=False, dtype=None*) → 'DataFrame' [source]

Convert categorical variable into dummy/indicator variables.

Parameters: **data** : *array-like, Series, or DataFrame*

Data of which to get dummy indicators.

prefix : *str, list of str, or dict of str, default None*

String to append DataFrame column names. Pass a list with length equal to the number of columns when calling get_dummies on a DataFrame. Alternatively, *prefix* can be a dictionary mapping column names to prefixes.

prefix_sep : *str, default '_'*

If appending prefix, separator/delimiter to use. Or pass a list or dictionary as with *prefix*.

dummy_na : *bool, default False*

Add a column to indicate NaNs, if False NaNs are ignored.

ke, default None

es in the DataFrame to be encoded. If *columns* is None then all the columns with *object* or *category* converted.

efault False

dummy-encoded columns should be backed by a `SparseArray` (True) or a regular NumPy array (False).

```
>>> pd.get_dummies(pd.Series(list('abcaa')), drop_first=True)
   b  c
0  0  0
1  1  0
2  0  1
3  0  0
4  0  0
```

https://pandas.pydata.org/pandas-docs/stable/reference/api/pandas.get_dummies.html