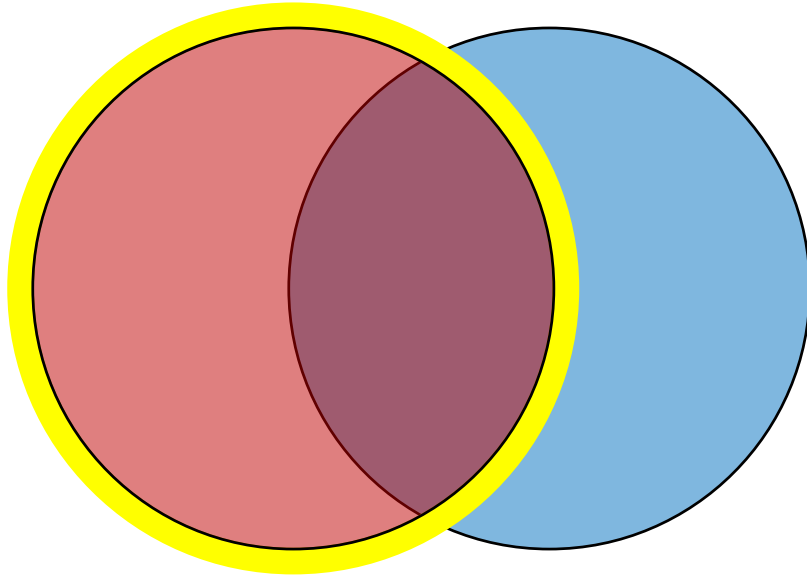


# Chapter 6

## Naïve Bayes Grid Search & Pipelines

# Naïve Bayes

# Probability Basics

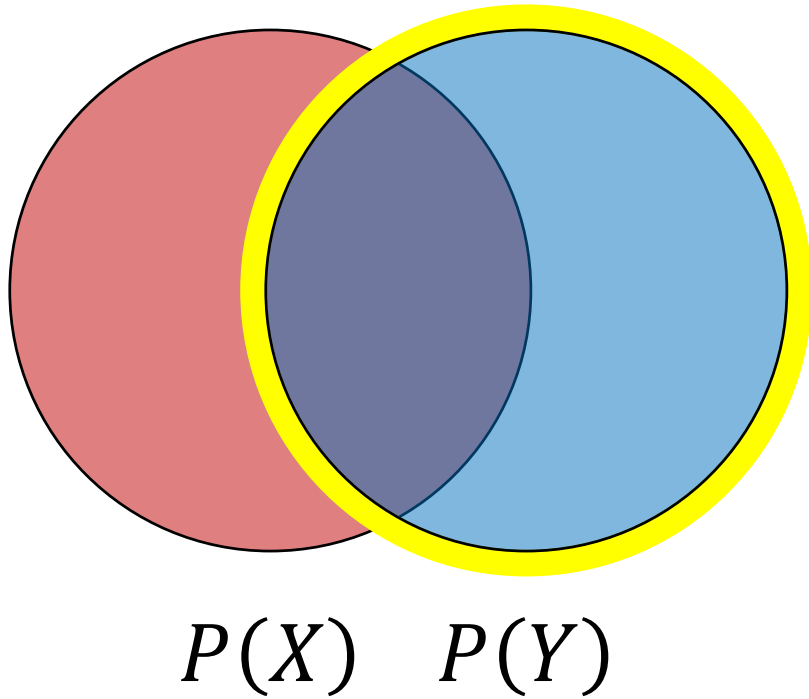


$P(X)$

- Single event probability:

$P(X)$

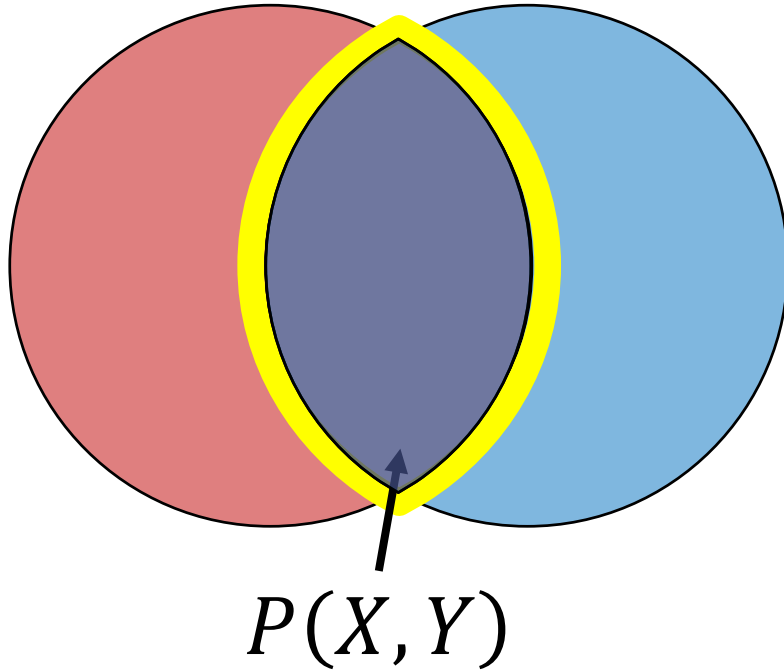
# Probability Basics



- Single event probability:

$$P(X), P(Y)$$

# Probability Basics



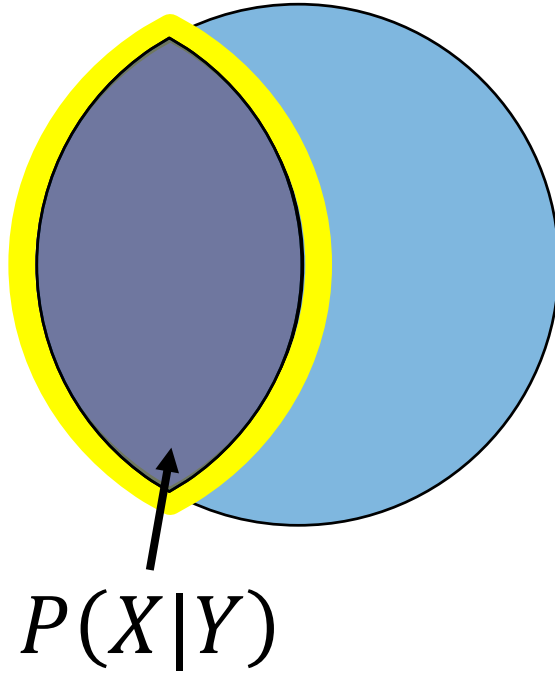
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$$P(X, Y)$$

# Probability Basics



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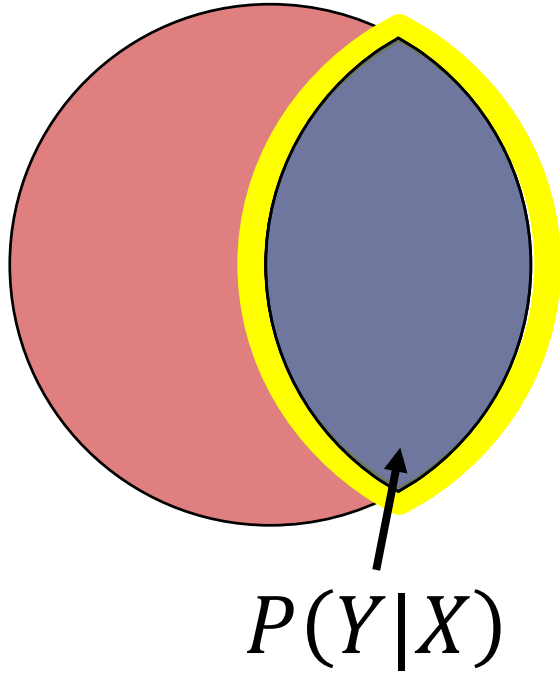
- Joint event probability:

$$P(X, Y)$$

- Conditional probability:

$$P(X|Y)$$

# Probability Basics



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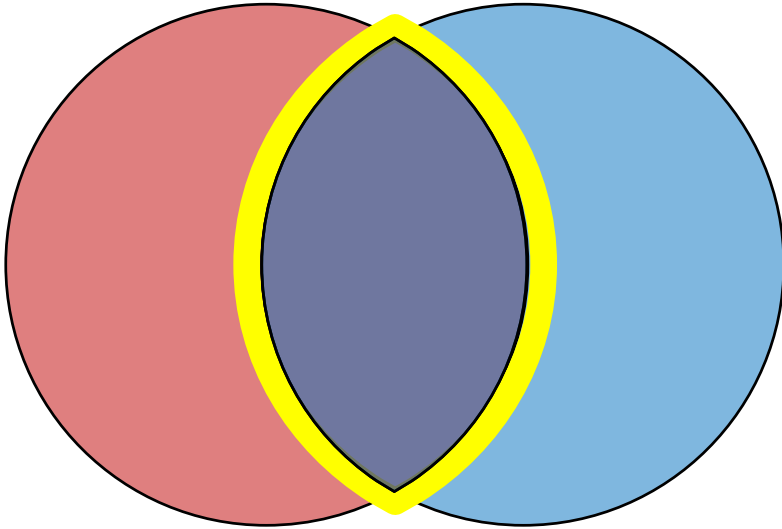
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# Probability Basics



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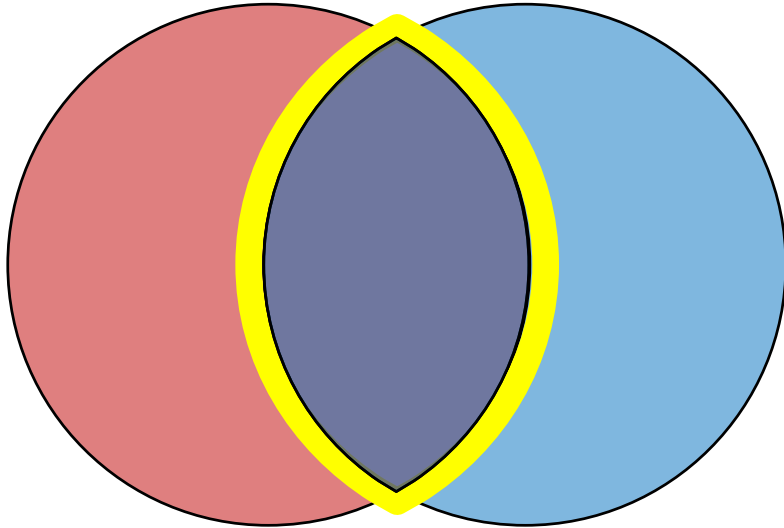
$$P(X|Y), P(Y|X)$$

- Joint and conditional relationship:

$$P(X, Y) = P(Y|X) * P(X) = P(X|Y) * P(Y)$$



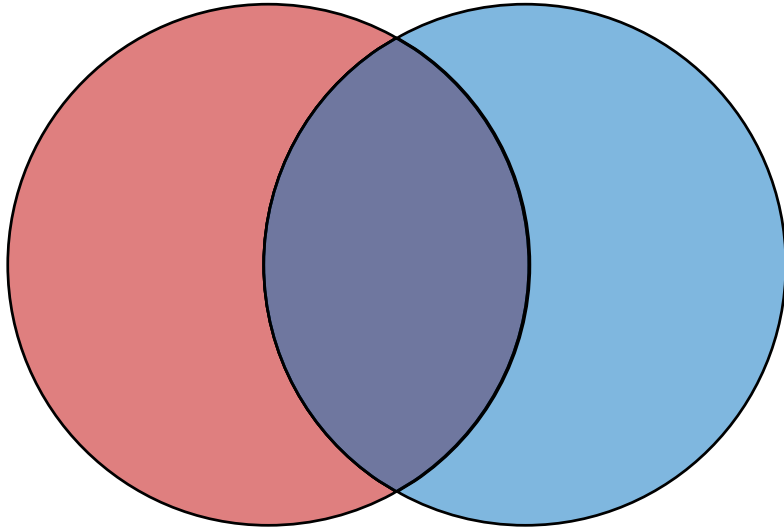
# Bayes Theorem Derivation



- By conditional and joint relationship:

$$P(Y|X) * P(X) = P(X|Y) * P(Y)$$

# Bayes Theorem Derivation



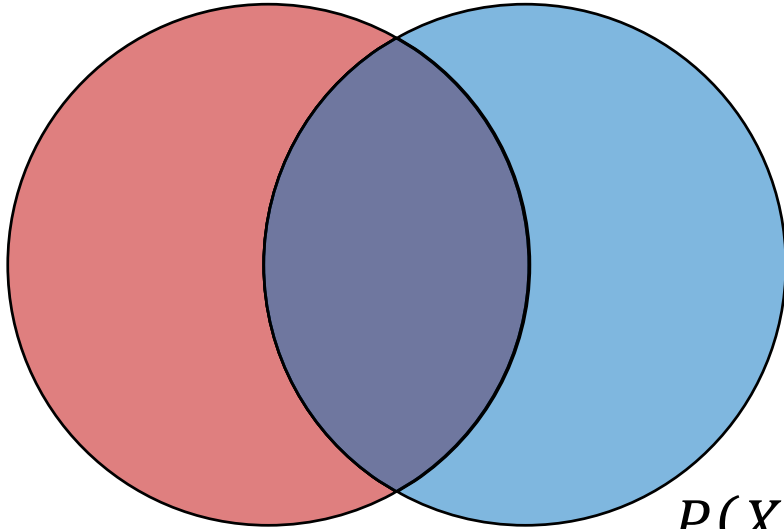
- Use conditional and joint relationship:

$$P(Y|X) * P(X) = P(X|Y) * P(Y)$$

- To invert conditional probability:

$$P(Y|X) = \frac{P(X|Y) * P(Y)}{P(X)}$$

# Bayes Theorem Derivation



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$$P(Y|X) * P(X) = P(X|Y) * P(Y)$$

- To invert conditional probability:

$$P(Y|X) = \frac{P(X|Y) * P(Y)}{P(X)}$$

$$P(X) = \sum_Z P(X, Z) = \sum_Z P(X|Z) * P(Z)$$

# Bayes Theorem


$$P(Y|X) = \frac{P(X|Y) * P(Y)}{P(X)}$$


# Bayes Theorem

$$P(Y|X) = \frac{P(X|Y) * P(Y)}{P(X)}$$

$$\textit{posterior} = \frac{\textit{likelihood} * \textit{prior}}{\textit{evidence}}$$

# Naïve Bayes Classification

$$P(Y|X) = \frac{P(X|Y) * P(Y)}{P(X)}$$


$$posterior = \frac{likelihood * prior}{evidence}$$


# Training Naïve Bayes

- For each class ( $C$ ), calculate probability given features ( $X$ )

$$P(\textcolor{red}{C}|\textcolor{blue}{X}) = P(\textcolor{blue}{X}|\textcolor{red}{C}) * P(\textcolor{red}{C})$$

**Class** **Feature**

# Training Naïve Bayes: The Naïve Assumption

- For each class ( $C$ ),  
calculate probability  
given features ( $X$ )  
$$P(C|X) = P(X|C) * P(C)$$
- Difficult to calculate joint  
probabilities produced  
by expanding for all  
features  
$$P(C|X) = P(X_1, X_2, \dots, X_n|C) * P(C)$$
$$P(X_1|X_2, \dots, X_n, C) * P(X_2, \dots, X_n|C) * P(C)$$
$$\dots$$



# Training Naïve Bayes: The Naïve Assumption

- For each class ( $C$ ),  
calculate probability  
given features ( $X$ )  
$$P(C|X) = P(X|C) * P(C)$$
- **Solution:** assume all  
features independent  
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$$P(C|X) = P(X_1|C) * P(X_2|C) * P(X_n|C) * P(C)$$

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- For each class ( $C$ ), calculate probability given features ( $X$ )  
$$P(C|X) = P(X|C) * P(C)$$
- **Solution:** assume all features independent of each other  
$$P(C|X) = P(X_1|C) * P(X_2|C) * P(X_n|C) * P(C)$$
- This is the "naïve" assumption  
$$P(C|X) = P(C) \prod_{i=1}^n P(X_i|C)$$

# Training Naïve Bayes

- For each class ( $C$ ), calculate probability given features ( $X$ )

$$P(C|X) = P(X|C) * P(C)$$

- Class assignment is selected based on *maximum a posteriori* (MAP) rule

$$\underset{k \in \{1, \dots, K\}}{\operatorname{argmax}} P(C_k) \prod_{i=1}^n P(X_i|C_k)$$

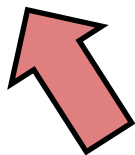
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- Class assignment is selected based on *maximum a posteriori* (MAP) rule

$$\underset{k \in \{1, \dots, K\}}{\operatorname{argmax}} P(C_k) \prod_{i=1}^n P(X_i|C_k)$$



Means select potential class with largest value

# The Log Trick

- Multiplying many values together causes computational instability (underflows)

$$\underset{k \in \{1, \dots, K\}}{\operatorname{argmax}} P(\textcolor{red}{C}_k) \prod_{i=1}^n P(\textcolor{blue}{X}_i | \textcolor{red}{C}_k)$$

# The Log Trick

- Multiplying many values together causes computational instability (underflows)
- Work with log values and sum the results

$$\underset{k \in \{1, \dots, K\}}{\operatorname{argmax}} P(\mathbf{C}_k) \prod_{i=1}^n P(X_i | \mathbf{C}_k)$$

$$\log(P(\mathbf{C}_k)) \sum_{i=1}^n \log(P(X_i | \mathbf{C}_k))$$

# Example: Predicting Tennis With Naïve Bayes

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

# Example: Training Naïve Bayes Tennis Model

$$P(\text{Play}=\text{Yes}) = 9/14 \quad P(\text{Play}=\text{No}) = 5/14$$

Create probability lookup tables based on training data



# Example: Training Naïve Bayes Tennis Model

$$P(\text{Play}=\text{Yes}) = 9/14$$

Outlook	Play=Yes	Play=No
Sunny	2/9	3/5
Overcast	4/9	0/5
Rain	3/9	2/5

$$P(\text{Play}=\text{No}) = 5/14$$

Temperature	Play=Yes	Play=No
Hot	2/9	2/5
Mild	4/9	2/5
Cool	3/9	1/5

Create probability lookup tables based on training data

# Example: Training Naïve Bayes Tennis Model

$$P(\text{Play}=\text{Yes}) = 9/14$$

$$P(\text{Play}=\text{No}) = 5/14$$

<b>Outlook</b>	<b>Play=Yes</b>	<b>Play=No</b>
Sunny	2/9	3/5
Overcast	4/9	0/5
Rain	3/9	2/5

<b>Humidity</b>	<b>Play=Yes</b>	<b>Play=No</b>
High	3/9	4/5
Normal	6/9	1/5

<b>Temperature</b>	<b>Play=Yes</b>	<b>Play=No</b>
Hot	2/9	2/5
Mild	4/9	2/5
Cool	3/9	1/5

<b>Wind</b>	<b>Play=Yes</b>	<b>Play=No</b>
Strong	3/9	3/5
Weak	6/9	2/5

Create probability lookup tables based on training data

# Example: Predicting Tennis With Naïve Bayes

Predict outcome for the following:

$x' = (\text{Outlook}=\text{Sunny}, \text{Temperature}=\text{Cool}, \text{Humidity}=\text{High}, \text{Wind}=\text{Strong})$

$$P(\text{yes}|\text{sunny}, \text{cool}, \text{high}, \text{strong}) = P(\text{sunny}|\text{yes}) * P(\text{cool}|\text{yes}) * \\ P(\text{high}|\text{yes}) * P(\text{strong}|\text{yes}) * P(\text{yes})$$

$$P(\text{no}|\text{sunny}, \text{cool}, \text{high}, \text{strong}) = P(\text{sunny}|\text{no}) * P(\text{cool}|\text{no}) * \\ P(\text{high}|\text{no}) * P(\text{strong}|\text{no}) * P(\text{no})$$

# Example: Predicting Tennis With Naïve Bayes

Predict outcome for the following:

$x' = (\text{Outlook}=\text{Sunny}, \text{Temperature}=\text{Cool}, \text{Humidity}=\text{High}, \text{Wind}=\text{Strong})$

Feature	Play=Yes	Play=No
Outlook=Sunny	2/9	3/5

# Example: Predicting Tennis With Naïve Bayes

Predict outcome for the following:

$x' = (\text{Outlook}=\text{Sunny}, \text{Temperature}=\text{Cool}, \text{Humidity}=\text{High}, \text{Wind}=\text{Strong})$

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Outlook=Sunny	2/9	3/5
Temperature=Cool	3/9	1/5
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<b>Overall Label</b>	<b>9/14</b>	<b>5/14</b>

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Predict outcome for the following:

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# Example: Predicting Tennis With Naïve Bayes

Predict outcome for the following:

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# Laplace Smoothing

- **Problem:** categories with no entries result in a value of "0" for conditional probability

$$P(C|X) = P(X_1|C) * P(X_2|C) * P(C)$$



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# Laplace Smoothing

- **Problem:** categories with no entries result in a value of "0" for conditional probability
- **Solution:** add "1" to numerator and denominator of empty categories

$$P(C|X) = \overset{0}{\boxed{P(X_1|C)}} * P(X_2|C) * P(C)$$

$$P(X_1|C) = \frac{1}{\text{Count}(C) + n}$$

$$P(X_2|C) = \frac{\text{Count}(X_2 \& C) + 1}{\text{Count}(C) + m}$$

# Types of Naïve Bayes

Naïve Bayes Model

Bernoulli

Data Type

Binary (T/F)

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Gaussian

Continuous

# Combining Feature Types

## Problem

- Model features contain different data types (continuous and categorical)

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## Problem

- Model features contain different data types (continuous and categorical)

## Solutions

- **Option 1:** Bin continuous features to create categorical ones and fit multinomial model
- **Option 2:** Fit Gaussian model on continuous features and multinomial on categorical features; combine to create "meta model" (week 10)



# Distributed Computing with Naïve Bayes

- Well-suited for large data and distributed computing—limited parameters and log probabilities are a summation
- Scikit-Learn implementations contain a "partial\_fit" method designed for out-of-core calculations

# Naïve Bayes: The Syntax

**Import the class containing the classification method**

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from sklearn.naive_bayes import BernoulliNB
```

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BNB = BernoulliNB(alpha=1.0)
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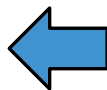
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Laplace  
smoothing  
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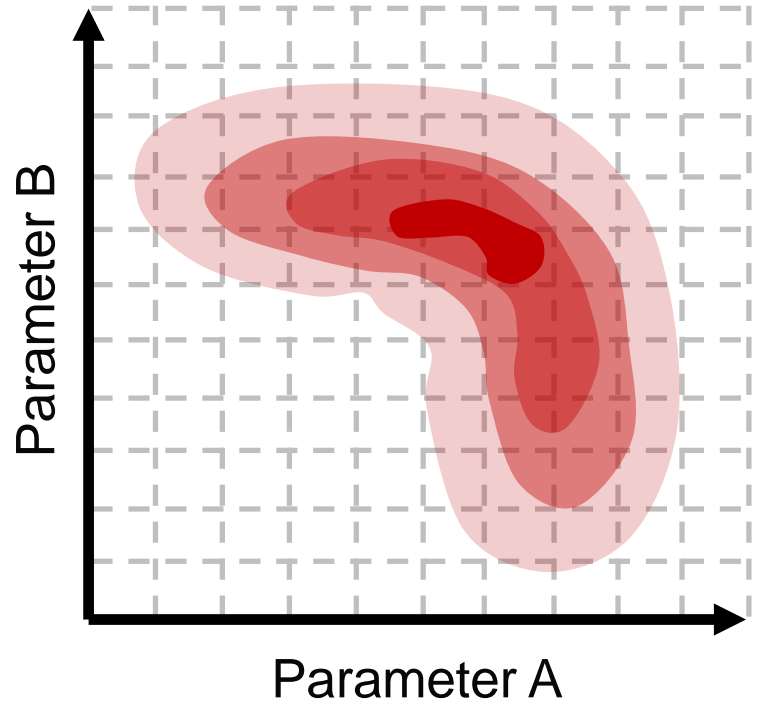
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BNB = BNB.fit(X_train, y_train)  
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```

Other naïve Bayes models: [MultinomialNB](#), [GaussianNB](#).

# Grid Search & Pipelines

# Generalized Hyperparameter Grid Search

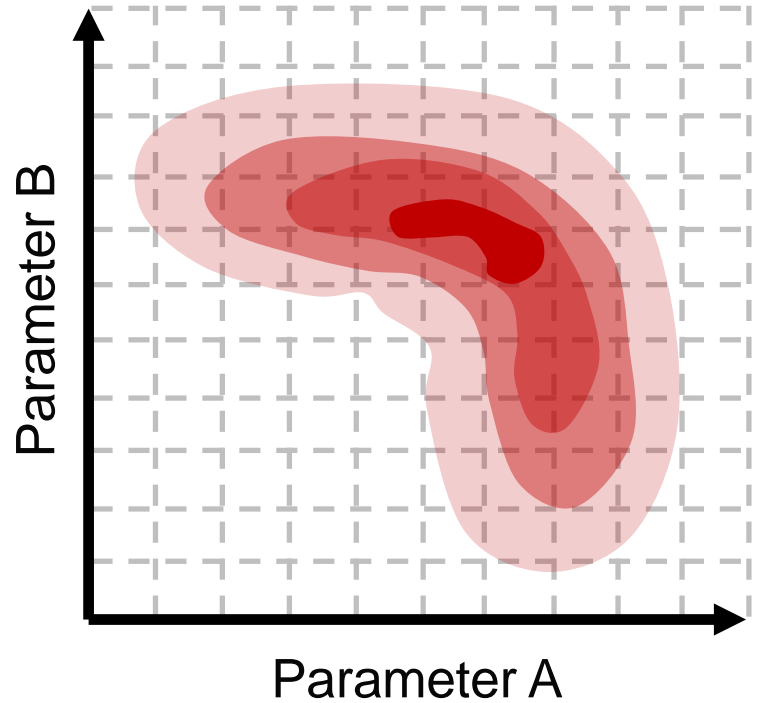
- Hyperparameter selection for regularization / better models requires cross validation on training data
- Linear and logistic regression methods have classes devoted to grid search (e.g. LassoCV)





# Generalized Hyperparameter Grid Search

- Grid search can be useful for other methods too, so a generalized method is desirable
- Scikit-learn contains GridSearchCV, which performs a grid search with parameters using cross validation



# Grid Search with Cross Validation: The Syntax

**Import the class containing the grid search method**

```
from sklearn.linear_model import LogisticRegression
```

```
from sklearn.model_selection import GridSearchCV
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# Grid Search with Cross Validation: The Syntax

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Create an instance of the estimator and grid search class

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LR = LogisticRegression(penalty='l2')  
GS = GridSearchCV(LR, param_grid={'c':[0.001, 0.01, 0.1]},  
                    scoring='accuracy', cv=4)
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logistic  
regression  
method



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                    scoring='accuracy', cv=4)
```

Fit the instance on the data to find the best model and then predict

```
GS = GS.fit(X_train, y_train)  
y_train = GS.predict(X_test)
```

# Optimizing the Rest of the Pipeline

- Grid searches enable model parameters to be optimized

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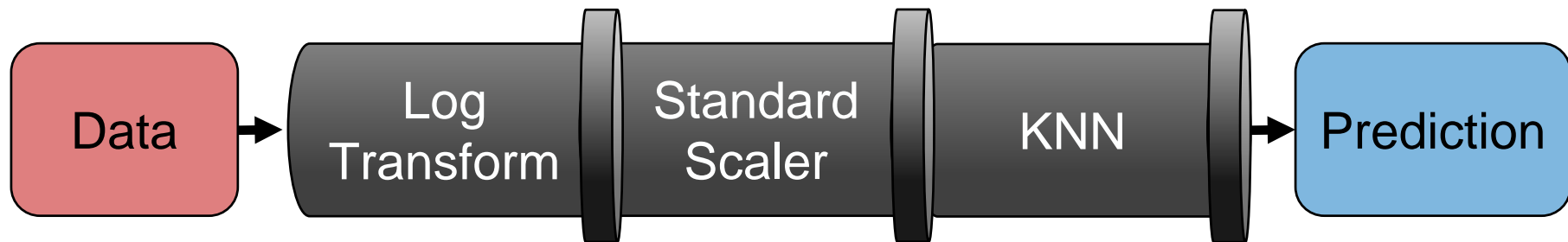


## Pipelines!



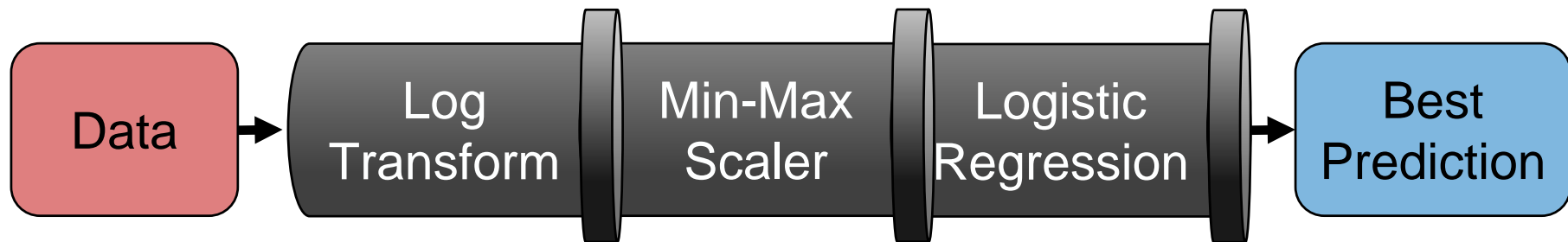
# Automating Machine Learning with Pipelines

- Machine learning models often selected empirically



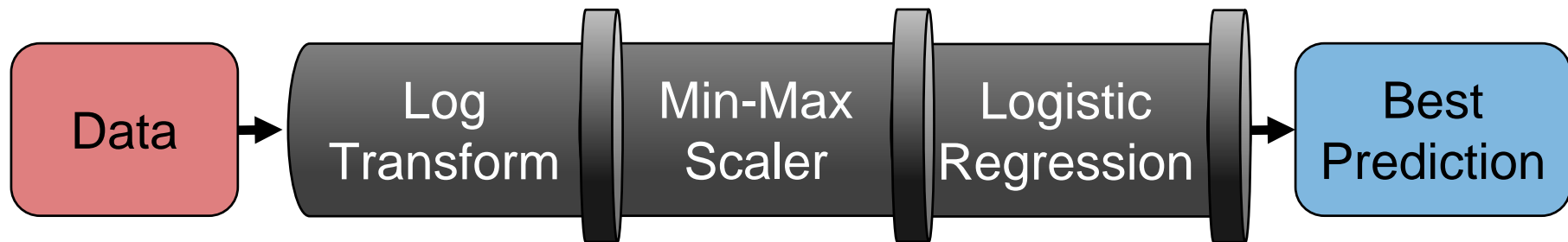
# Automating Machine Learning with Pipelines

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# Automating Machine Learning with Pipelines

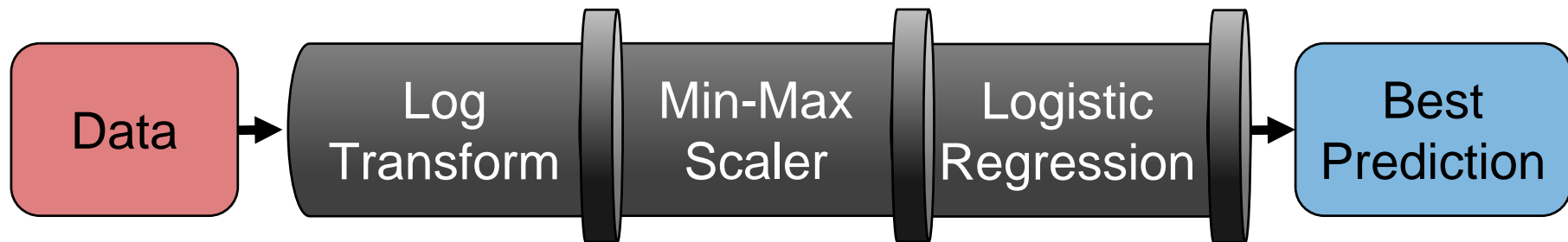
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How to automate this process?

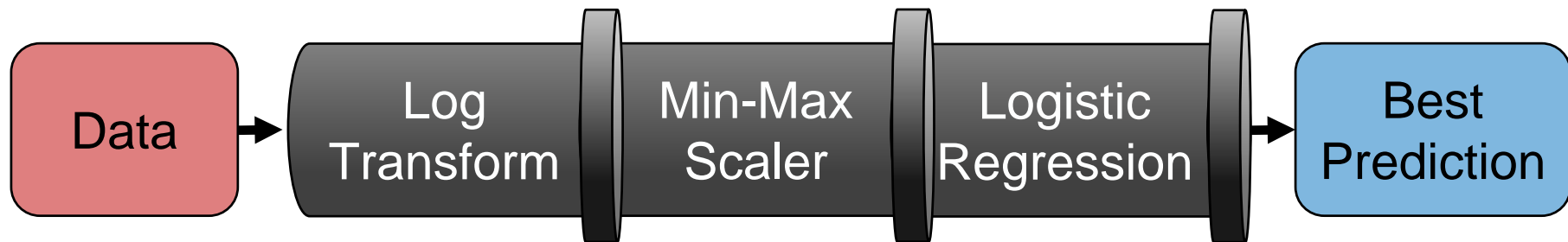
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- Pipelines in Scikit-Learn allow feature transformation steps and models to be chained together



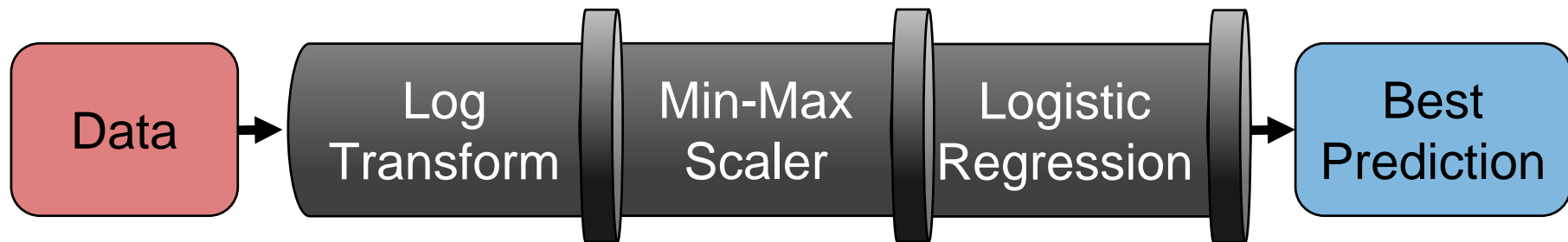
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Pipelines make automation and reproducibility easier!

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```
estimators = [('scaler', MinMaxScaler()), ('lasso', Lasso())]
```

```
Pipe = Pipeline(estimators)
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feature scaler  
class



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lasso model  
class

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Fit the instance on the data and then predict the expected value

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Pipe = Pipe.fit(X_train, y_train)
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y_predict = Pipe.predict(X_test)
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Features can be combined from different transform method using FeatureUnion

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