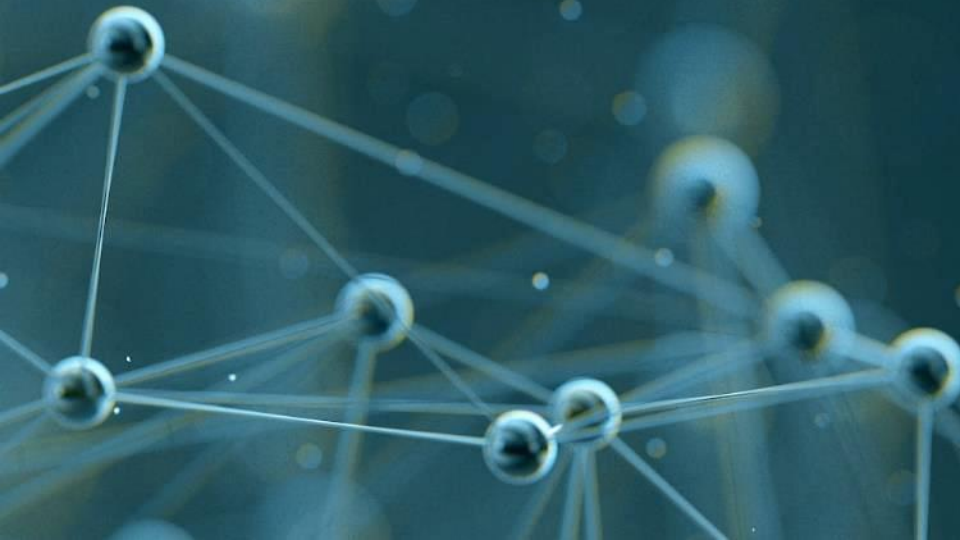
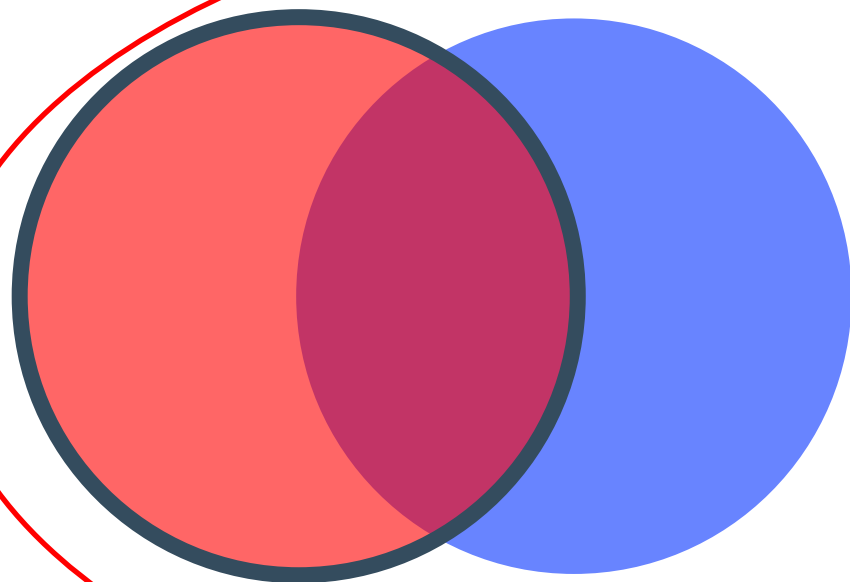


NAÏVE BAYES



PROBABILITY BASICS



LinSingle event probability:

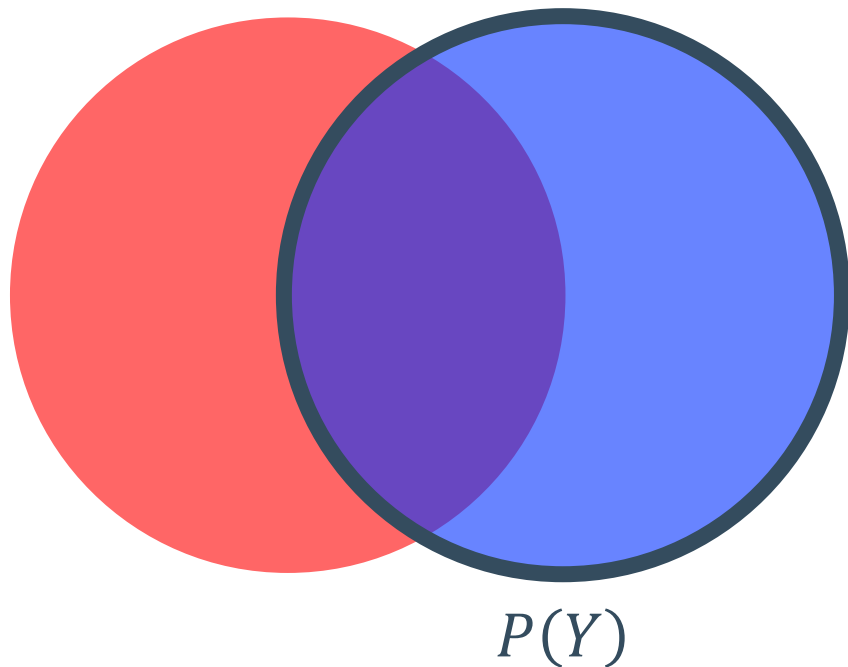
$$P(X)$$

$$P(X) = |X| / |U|$$

Universe

$$P(X)$$

PROBABILITY BASICS

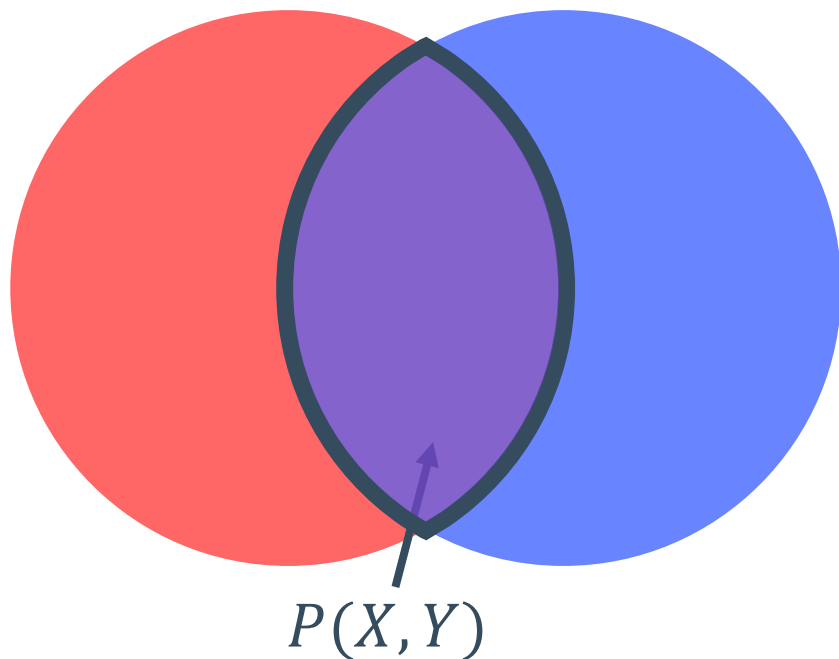


Single event probability:

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

$$P(Y) = |Y| / |U|$$

PROBABILITY BASICS



Single event probability:

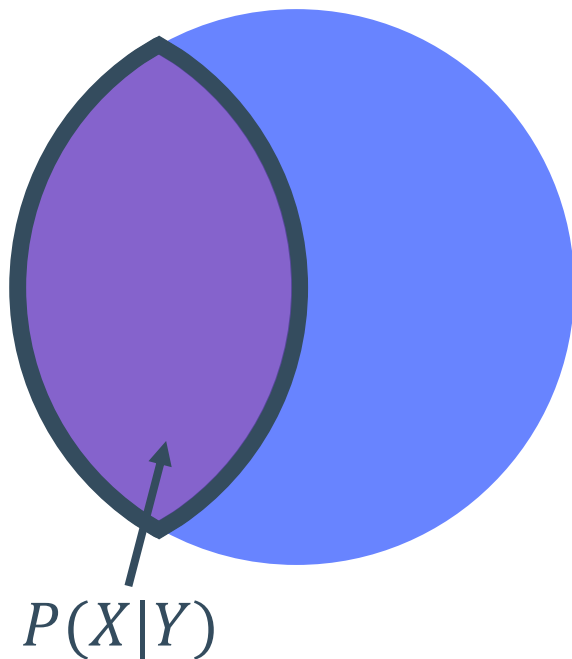
$$P(X), P(Y)$$

Joint event probability:

$$P(X, Y)$$

$$P(X, Y) = |X, Y| / |U|$$

PROBABILITY BASICS



Single event probability:

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

Joint event probability:

$$P(X, Y)$$

Conditional probability:

$$P(X|Y)$$

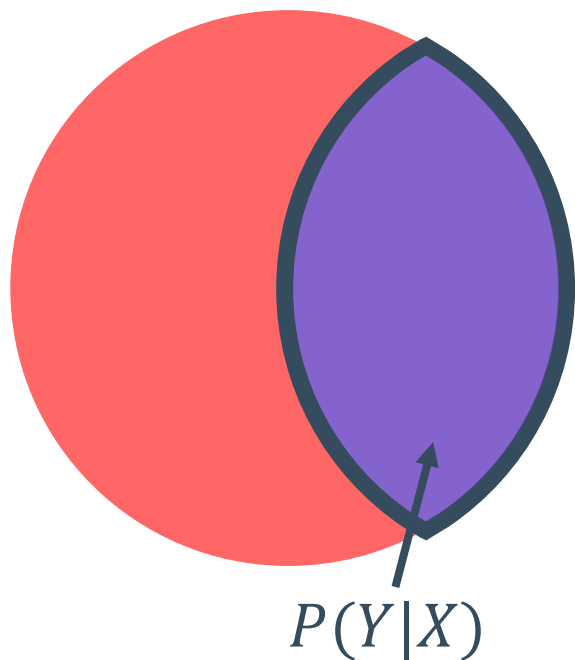
$$P(X|Y) = |X \cap Y| / |Y|$$

And if we divide both the numerator and the denominator by $|U|$

$$P(X/Y) = (|X, Y| / |U|) / (|Y| / |U|) = P(X, Y) / P(Y)$$

Source

PROBABILITY BASICS



Single event probability:

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

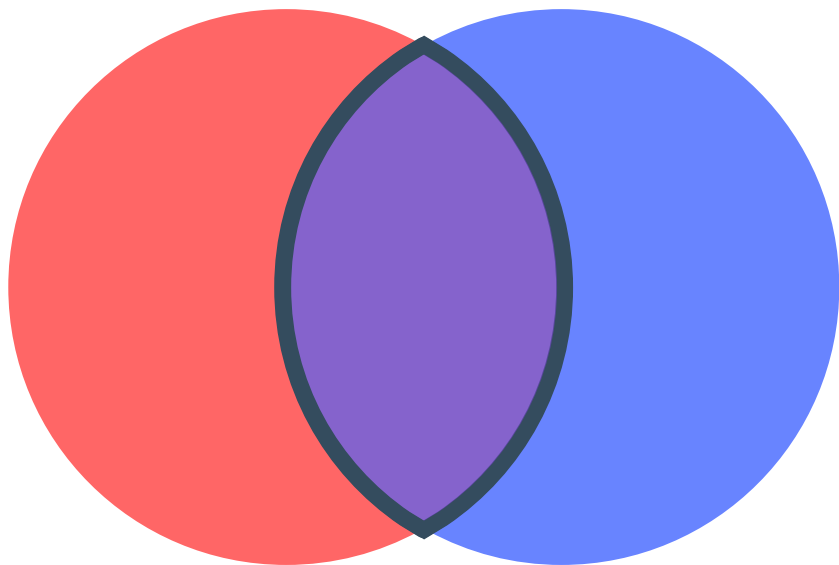
Joint event probability:

$$P(X, Y)$$

Conditional probability:

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

PROBABILITY BASICS



Single event probability:

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Joint event probability:

$$P(X, Y)$$

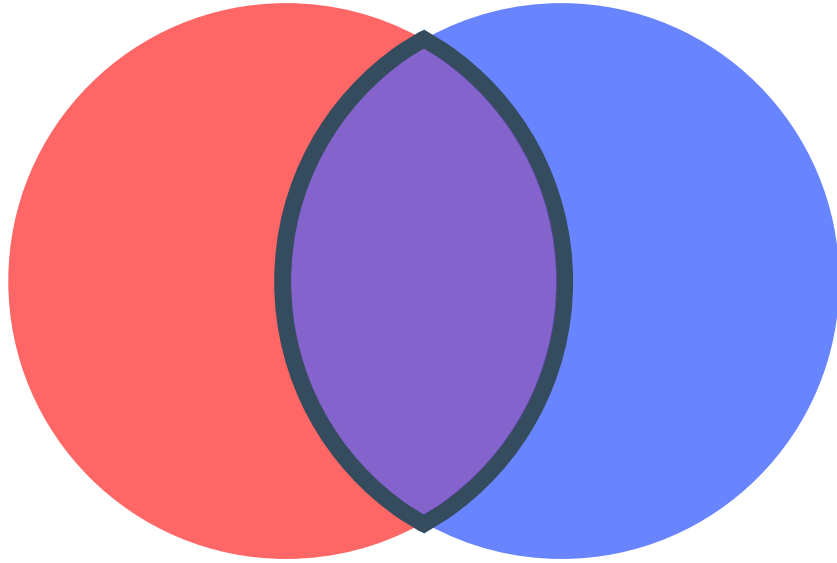
Conditional probability:

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

Joint and conditional relationship:

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

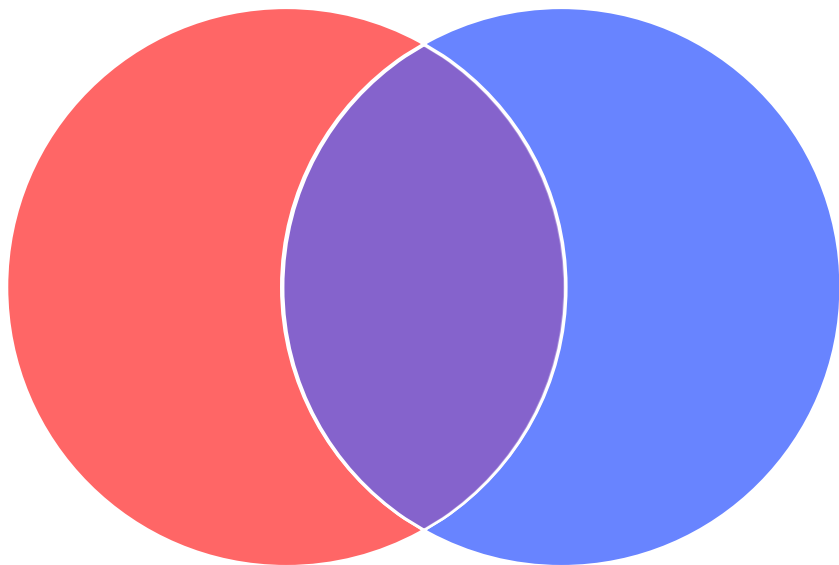
BAYES THEOREM DERIVATION



By conditional and joint relationship:

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

BAYES THEOREM DERIVATION



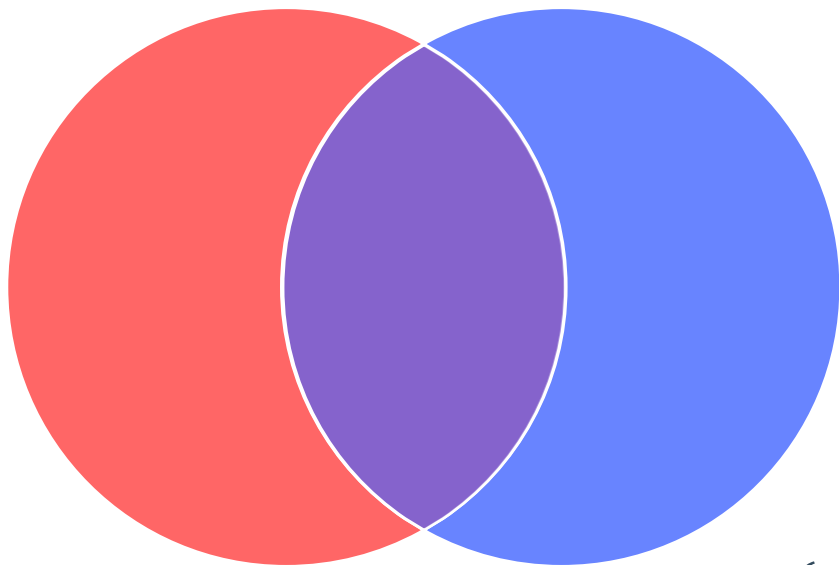
By conditional and joint relationship:

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

To invert conditional probability:

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

BAYES THEOREM DERIVATION



By conditional and joint relationship:

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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

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

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

TRAINING NAÏVE BAYES

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

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


The diagram illustrates the components of the Naïve Bayes formula. Below the equation, the word "Class" is written in red and "Features" in blue. Two black arrows point from these words to the variables in the formula: one arrow points from "Class" to the red C in $P(C|X)$, and another arrow points from "Features" to the blue X in $P(C|X)$.

TRAINING NAÏVE BAYES: THE NAÏVE ASSUMPTION

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

Difficult to calculate
joint probabilities
produced by expanding
for all features

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

$$\begin{aligned} P(C|X) &= P(X_1, X_2, \dots, X_n|C) * P(C) \\ &= P(X_1|X_2, \dots, X_n, C) * P(X_2, \dots, X_n|C) * P(C) \\ &\dots \end{aligned}$$

TRAINING NAÏVE BAYES: THE NAÏVE ASSUMPTION

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

Solution: assume all
features independent
of each other

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

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

TRAINING NAÏVE BAYES: THE NAÏVE ASSUMPTION

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

Solution: assume all
features independent
of each other

This is the “**naïve**”
assumption

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

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

$$P(C|X) = P(C) \prod_{i=1}^n P(X_i|C)$$

TRAINING NAÏVE BAYES

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

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

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

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

TRAINING NAÏVE BAYES

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

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



Means select potential
class with largest value

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

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

THE LOG TRICK

Multiplying many values
together causes
computational instability
(underflows)

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

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

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

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

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

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

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

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

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

Wind	Play=Yes	Play=No
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:

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

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

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

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:

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

Feature	Play=Yes	Play=No
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Wind=Strong	3/9	3/5
Overall Label	9/14	5/14

EXAMPLE: PREDICTING TENNIS WITH NAÏVE BAYES

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Probability	0.0053	0.0206

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LAPLACE SMOOTHING

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

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

LAPLACE SMOOTHING

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

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

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

0

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

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

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

TYPES OF NAÏVE BAYES

Naïve Bayes Model

Bernoulli

Data Type

Binary (T/F)

TYPES OF NAÏVE BAYES

Naïve Bayes Model

Bernoulli

Multinomial

Data Type

Binary (T/F)

Discrete (e.g. count)

TYPES OF NAÏVE BAYES

Naïve Bayes Model

Bernoulli

Multinomial

Gaussian

Data Type

Binary (T/F)

Discrete (e.g. count)

Continuous

COMBINING FEATURE TYPES

Problem

Model features contain different data types (continuous and categorical)

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Solution

- **Option 1:** Bin continuous features to create categorical ones and fit multinomial model

COMBINING FEATURE TYPES

Problem

Model features contain different data types (continuous and categorical)

Solution

- **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

```
from sklearn.naive_bayes import BernoulliNB
```

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Create an instance of the class

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BNB = BernoulliNB(alpha=1.0)
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Laplace smoothing
parameter

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Laplace smoothing
parameter

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

```
BNB = BNB.fit(X_train, y_train)  
y_predict = BNB.predict(X_test)
```

NAÏVE BAYES: THE SYNTAX

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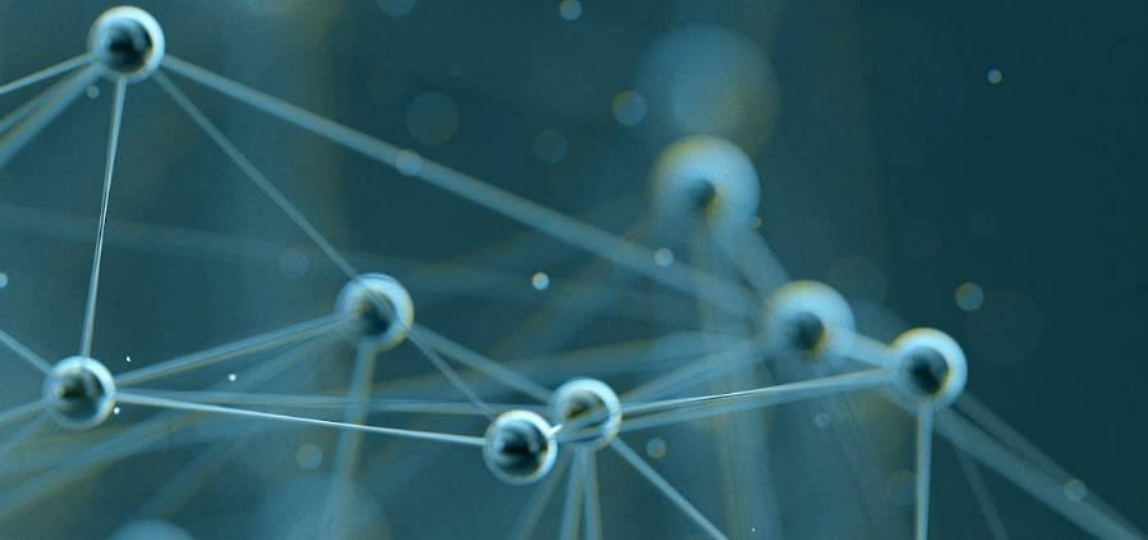
Laplace smoothing
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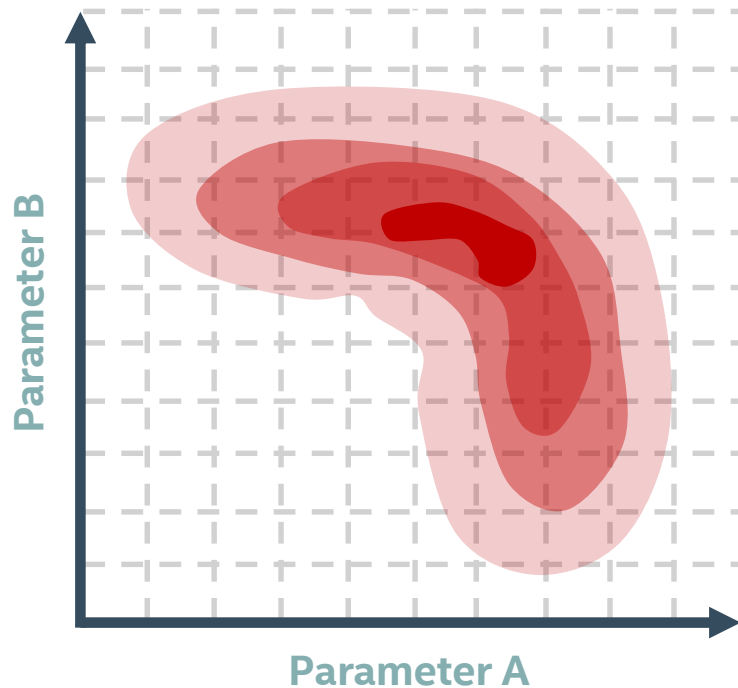
Other naïve Bayes models: `MultinomialNB`, `GaussianNB`.

GRID SEARCH AND PIPELINES



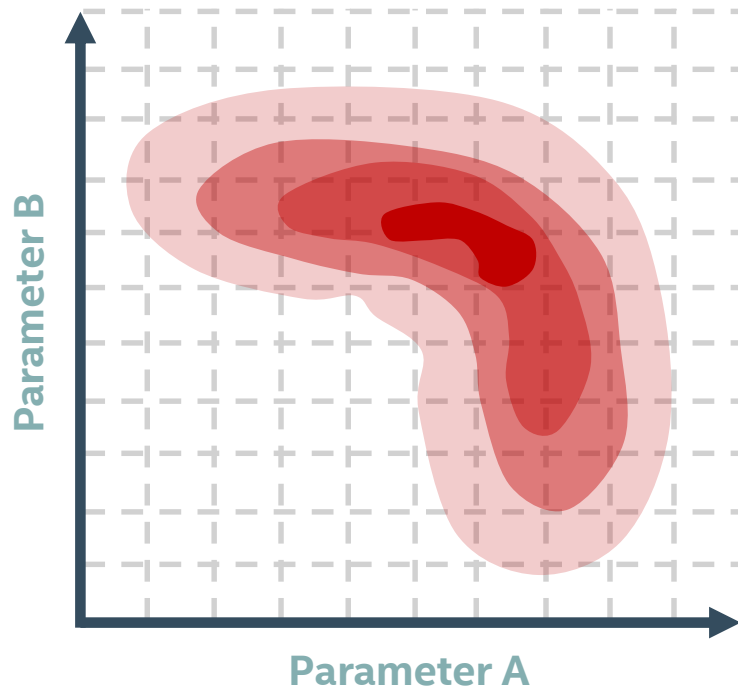
GENERALIZED HYPERPARAMETER GRID SEARCH

- 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

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from sklearn.linear_model import LogisticRegression
from sklearn.model_selection import GridSearchCV
```

GRID SEARCH WITH CROSS VALIDATION: THE SYNTAX

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Create an instance of the estimator and grid search class

```
LR = LogisticRegression(penalty='l2')
GS = GridSearchCV(LR, param_grid={'c':[0.001, 0.01, 0.1]},
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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

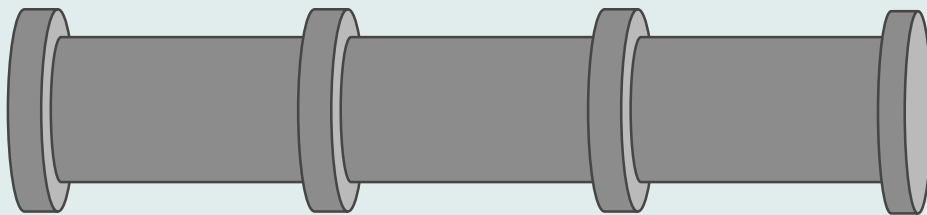
- Grid searches enable model parameters to be optimized

OPTIMIZING THE REST OF THE PIPELINE

- Grid searches enable model parameters to be optimized
- How can this be incorporated with other steps of the process (e.g. feature extraction and transformation)?

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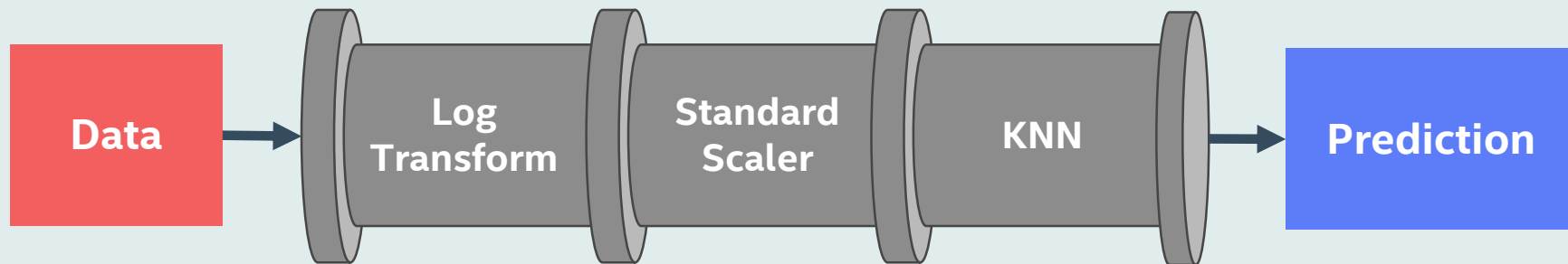
- Grid searches enable model parameters to be optimized
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Pipelines!

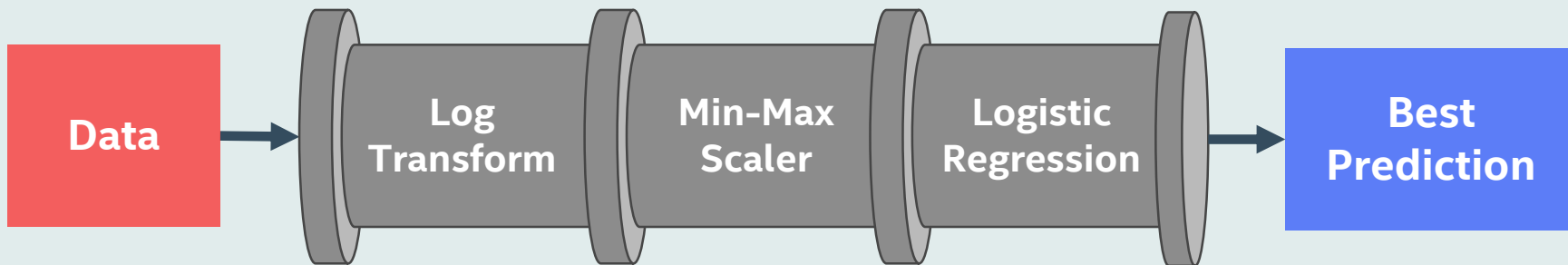
AUTOMATING MACHINE LEARNING WITH PIPELINES

- Machine learning models often selected empirically



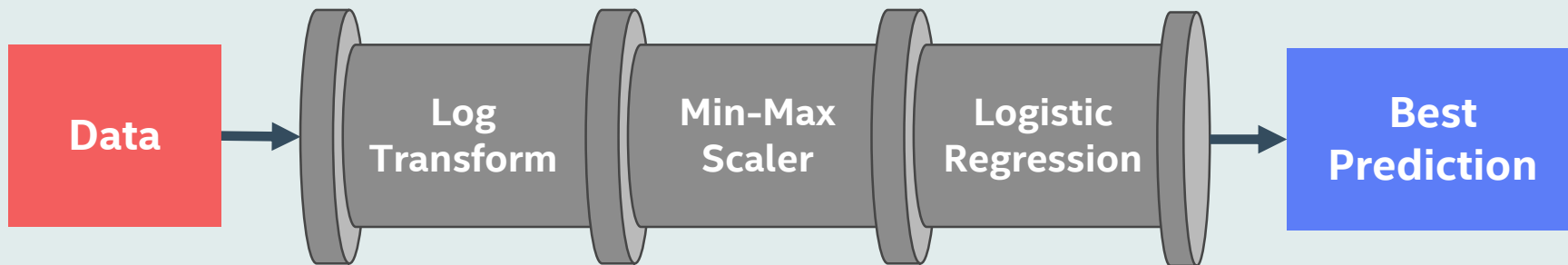
AUTOMATING MACHINE LEARNING WITH PIPELINES

- Machine learning models often selected empirically
- By trying different processing methods and tuning multiple models



AUTOMATING MACHINE LEARNING WITH PIPELINES

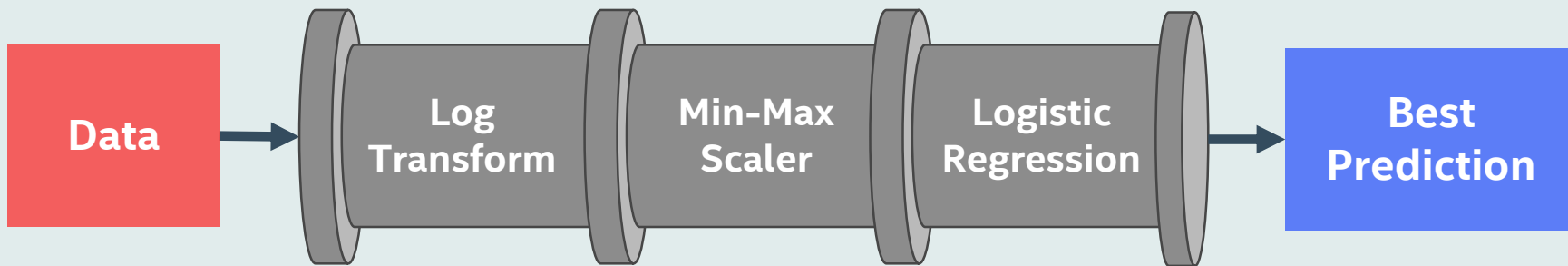
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How to automate this process?

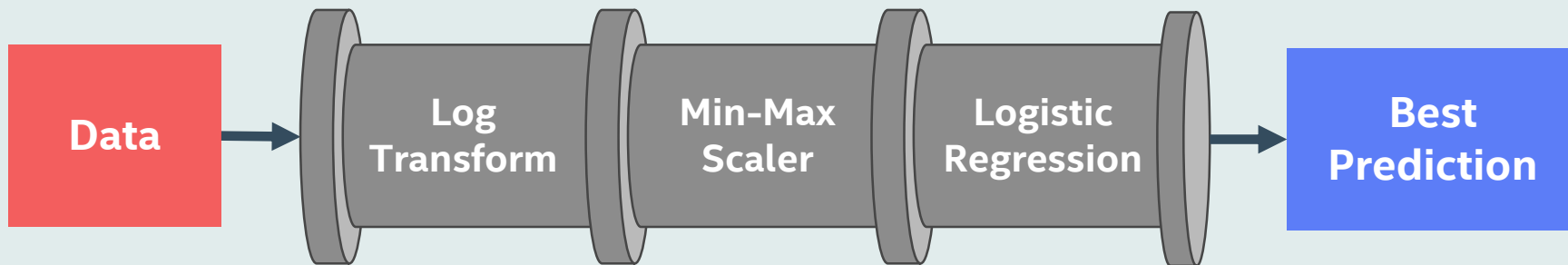
AUTOMATING MACHINE LEARNING WITH PIPELINES

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



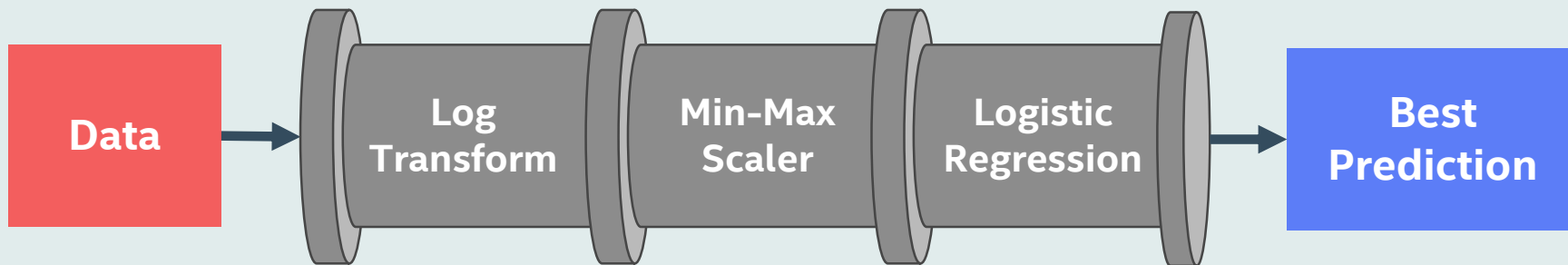
AUTOMATING MACHINE LEARNING WITH PIPELINES

- Pipelines in Scikit-Learn allow feature transformation steps and models to be chained together
- Successive steps perform 'fit' and 'transform' before sending data to the next step



AUTOMATING MACHINE LEARNING WITH PIPELINES

- Pipelines in Scikit-Learn allow feature transformation steps and models to be chained together
- Successive steps perform 'fit' and 'transform' before sending data to the next step



Pipelines make automation and reproducibility easier!

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feature
scaler class



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lasso
model
class



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```

Features can be combined from different transform method using
`FeatureUnion`

