pomegranate Documentation

Release 0.6.0

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Jun 16, 2018

Contents

pomegranate

pomegranate is a python package which implements fast, efficient, and extremely flexible probabilistic models ranging from probability distributions to Bayesian networks to mixtures of hidden Markov models. The most basic level of probabilistic modeling is the a simple probability distribution. If we're modeling language, this may be a simple distribution over the frequency of all possible words a person can say.

1. *Probability Distributions*

The next level up are probabilistic models which use the simple distributions in more complex ways. A markov chain can extend a simple probability distribution to say that the probability of a certain word depends on the word(s) which have been said previously. A hidden Markov model may say that the probability of a certain words depends on the latent/hidden state of the previous word, such as a noun usually follows an adjective.

2. *Markov Chains*
3. *Bayes Classifiers and Naive Bayes*
4. *General Mixture Models*
5. *Hidden Markov Models*
6. *Bayesian Networks*
7. *Factor Graphs*

The third level are stacks of probabilistic models which can model even more complex phenomena. If a single hidden Markov model can capture a dialect of a language (such as a certain persons speech usage) then a mixture of hidden Markov models may fine tune this to be situation specific. For example, a person may use more formal language at work and more casual language when speaking with friends. By modeling this as a mixture of HMMs, we represent the persons language as a "mixture" of these dialects.

8. GMM-HMMs
9. Mixtures of Models
10. Bayesian Classifiers of Models

CHAPTER 1

Installation

pomegranate is pip installable using `pip install pomegranate`. You can get the bleeding edge from github using the following:

```
git clone https://github.com/jmschrei/pomegranate
cd pomegranate
python setup.py install
```

On Windows machines you may need to download a C++ compiler. For Python 2 this minimal version of Visual Studio 2008 works well. For Python 3 this version of the Visual Studio build tools has been reported to work.

No good project is done alone, and so I'd like to thank all the previous contributors to YAHMM and all the current contributors to pomegranate as well as the graduate students whom I have pestered with ideas. Contributions are eagerly accepted! If you would like to contribute a feature then fork the master branch and be sure to run the tests before changing any code. Let us know what you want to do on the issue tracker just in case we're already working on an implementation of something similar. Also, please don't forget to add tests for any new functions.

1.1 FAQ

Can I create a usable model if I already know the parameters I want, but don't have data to fit to?

Yes! pomegranate has two ways of initializing models, either by starting off with pre-initialized distributions or by using the `Model.from_samples` class method. In the case where you have a model that you'd like to use you can create the model manually and use it to make predictions without the need to fit it to data.

How do I create a model directly from data?

pomegranate attempts to closely follow the scikit-learn API. However, a major area in which it diverges is in the initialization of models directly from data. Typically in scikit-learn one would create an estimator and then call the `fit` function on the training data. In pomegranate one would use the `Model.from_samples` class method, such as `BayesianNetwork.from_samples(X)`, to learn a model directly from data.

What is the difference between ''fit'' and ''from_samples''?

The `fit` method trains an initialized model, whereas the `from_samples` class method will first initialize the model and then train it. These are separated out because frequently a person already knows a good initialization, such as the structure of the Bayesian network but maybe not the parameters, and wants to fine-tune that initialization instead of learning everything directly from data. This also simplifies the backend by allowing the `fit` function to assume that the model is initialized instead of having to check to see if it is initialized, and if not then initialize it. This is particularly useful in structured models such as Bayesian networks or hidden Markov models where the `Model.from_samples` task is really structure learning + parameter learning, because it allows the `fit` function to be solely parameter learning.

How can I use pomegranate for semi-supervised learning?

When using one of the supervised models (such as naive Bayes or Bayes classifiers) simply pass in the label -1 for samples that you do not have a label for.

How can I use out-of-core learning in pomegranate?

Once a model has been initialized the `summarize` method can be used on arbitrarily sized chunks of the data to reduce them into their sufficient statistics. These sufficient statistics are additive, meaning that if they are calculated for all chunks of a dataset and then added together they can yield exact updates. Once all chunks have been summarized then `from_summaries` is called to update the parameters of the model based on these added sufficient statistics. Out-of-core computing is supported by allowing the user to load up chunks of data from memory, summarize it, discard it, and move on to the next chunk.

Does pomegranate support parallelization?

Yes! pomegranate supports parallelized model fitting and model predictions, both in a data-parallel manner. Since the backend is written in cython the global interpreter lock (GIL) can be released and multi-threaded training can be supported via joblib. This means that parallelization is utilized time isn't spent piping data from one process to another nor are multiple copies of the model made.

Does pomegranate support GPUs?

Currently pomegranate does not support GPUs.

Does pomegranate support distributed computing?

Currently pomegranate is not set up for a distributed environment, though the pieces are currently there to make this possible.

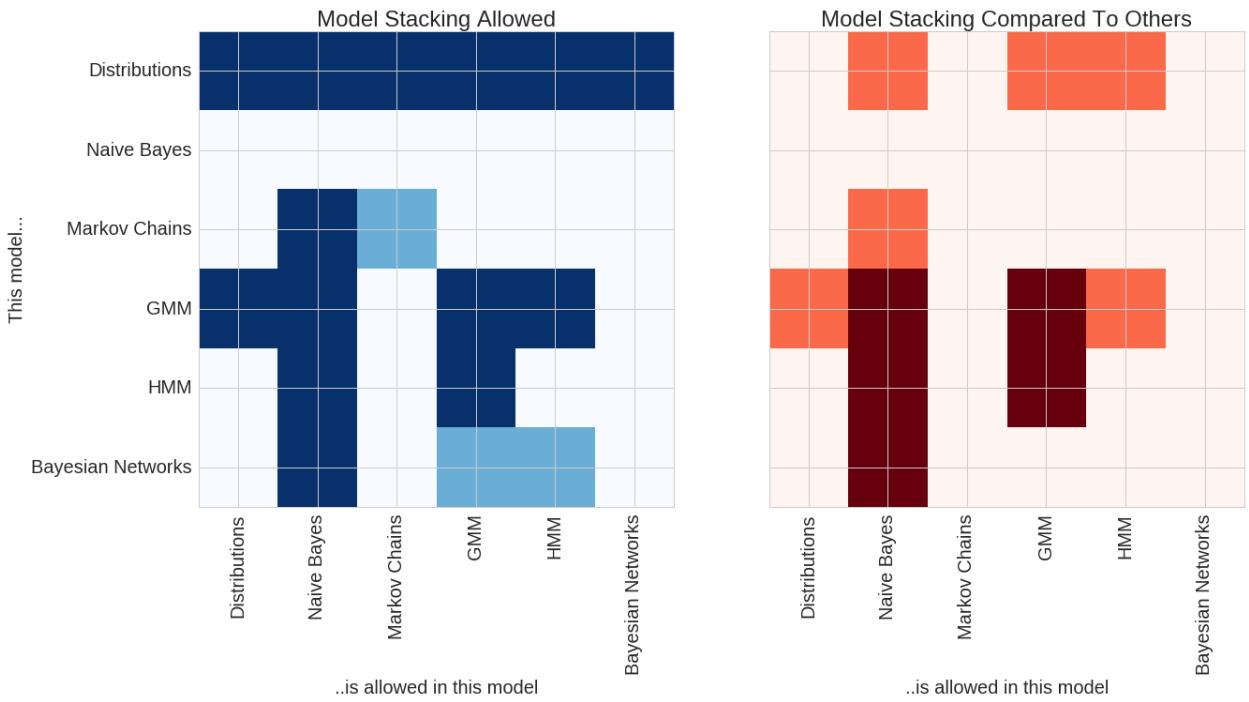
How can I cite pomegranate?

I don't currently have a research paper which can be cited, but the GitHub repository can be.

```
@misc{Schreiber2016,
        author = {Jacob Schreiber},
        title = {pomegranate},
        year = {2016},
        publisher = {GitHub},
        journal = {GitHub repository},
        howpublished = {\url{https://github.com/jmschrei/pomegranate}},
        commit = {enter commit that you used}
}
```

How does pomegranate compare to other packages?

A comparison of the features between pomegranate and others in the python ecosystem can be seen in the following two plots.



The plot on the left shows model stacks which are currently supported by pomegranate. The rows show each model, and the columns show which models those can fit in. Dark blue shows model stacks which currently are supported, and light blue shows model stacks which are currently being worked on and should be available soon. For example, all models use basic distributions as their main component. However, general mixture models (GMMs) can be fit into both Naive Bayes classifiers and hidden Markov models (HMMs). Conversely, HMMs can be fit into GMMs to form mixtures of HMMs. Soon pomegranate will support models like a mixture of Bayesian networks.

The plot on the right shows features compared to other packages in the python ecosystem. Dark red indicates features which no other package supports (to my knowledge!) and orange shows areas where pomegranate has an expanded feature set compared to other packages. For example, both pomegranate and sklearn support Gaussian naive Bayes classifiers. However, pomegranate supports naive Bayes of arbitrary distributions and combinations of distributions, such as one feature being Gaussian, one being log normal, and one being exponential (useful to classify things like ionic current segments or audio segments). pomegranate also extends naive Bayes past its "naivity" to allow for features to be dependent on each other, and allows input to be more complex things like hidden Markov models and Bayesian networks. There's no rule that each of the inputs to naive Bayes has to be the same type though, allowing you to do things like compare a markov chain to a HMM. No other package supports a HMM Naive Bayes! Packages like hmmlearn support the GMM-HMM, but for them GMM strictly means Gaussian mixture model, whereas in pomegranate it ~can~ be a Gaussian mixture model, but it can also be an arbitrary mixture model of any types of distributions. Lastly, no other package supports mixtures of HMMs despite their prominent use in things like audio decoding and biological sequence analysis.

Models can be stacked more than once, though. For example, a "naive" Bayes classifier can be used to compare multiple mixtures of HMMs to each other, or compare a HMM with GMM emissions to one without GMM emissions. You can also create mixtures of HMMs with GMM emissions, and so the most stacking currently supported is a "naive" Bayes classifier of mixtures of HMMs with GMM emissions, or four levels of stacking.

How can pomegranate be faster than numpy?

pomegranate has been shown to be faster than numpy at updating univariate and multivariate gaussians. One of the reasons is because when you use numpy you have to use `numpy.mean(X)` and `numpy.cov(X)` which requires two full passes of the data. pomegranate uses additive sufficient statistics to reduce a dataset down to a fixed set of numbers which can be used to get an exact update. This allows pomegranate to calculate both mean and covariance in a single pass of the dataset. In addition, one of the reasons that numpy is so fast is its use of BLAS. pomegranate also

uses BLAS, but uses the cython level calls to BLAS so that the data doesn't have to pass between cython and python multiple times.

1.2 Out of Core

Sometimes datasets which we'd like to train on can't fit in memory but we'd still like to get an exact update. pomegranate supports out of core training to allow this, by allowing models to summarize batches of data into sufficient statistics and then later on using these sufficient statistics to get an exact update for model parameters. These are done through the methods `model.summarize` and `model.from_summaries`. Let's see an example of using it to update a normal distribution.

```
>>> from pomegranate import *
>>> import numpy
>>>
>>> a = NormalDistribution(1, 1)
>>> b = NormalDistribution(1, 1)
>>> X = numpy.random.normal(3, 5, size=(5000,))
>>>
>>> a.fit(X)
>>> a
{
    "frozen" :false,
    "class" :"Distribution",
    "parameters" :[
        3.012692830297519,
        4.972082359070984
    ],
    "name" :"NormalDistribution"
}
>>> for i in range(5):
>>>     b.summarize(X[i*1000:(i+1)*1000])
>>> b.from_summaries()
>>> b
{
    "frozen" :false,
    "class" :"Distribution",
    "parameters" :[
        3.01269283029752,
        4.972082359070983
    ],
    "name" :"NormalDistribution"
}
```

This is a simple example with a simple distribution, but all models and model stacks support this type of learning. Lets next look at a simple Bayesian network.

We can see that before fitting to any data, the distribution in one of the states is equal for both. After fitting the first distribution they become different as would be expected. After fitting the second one through summarize the distributions become equal again, showing that it is recovering an exact update.

It's easy to see how one could use this to update models which don't use Expectation Maximization (EM) to train, since it is an iterative algorithm. For algorithms which use EM to train there is a `fit` wrapper which will allow you to load up batches of data from a numpy memory map to train on automatically.

1.3 Probability Distributions

IPython Notebook Tutorial

While probability distributions are frequently used as components of more complex models such as mixtures and hidden Markov models, they can also be used by themselves. Many data science tasks require fitting a distribution to data or generating samples under a distribution. pomegranate has a large library of both univariate and multivariate distributions which can be used with an intuitive interface.

Univariate Distributions

`UniformDistribution`	A uniform distribution between two values.
`BernoulliDistribution`	A Bernoulli distribution describing the probability of a binary variable.
`NormalDistribution`	A normal distribution based on a mean and standard deviation.
`LogNormalDistribution`	Represents a lognormal distribution over non-negative floats.
`ExponentialDistribution`	Represents an exponential distribution on non-negative floats.
`PoissonDistribution`	A discrete probability distribution which expresses the probability of a number of events occuring in a fixed time window.
`BetaDistribution`	This distribution represents a beta distribution, parameterized using alpha/beta, which are both shape parameters.
`GammaDistribution`	This distribution represents a gamma distribution, parameterized in the alpha/beta (shape/rate) parameterization.
`DiscreteDistribution`	A discrete distribution, made up of characters and their probabilities, assuming that these probabilities will sum to 1.0.

Kernel Densities

`GaussianKernelDensity`	A quick way of storing points to represent a Gaussian kernel density in one dimension.
`UniformKernelDensity`	A quick way of storing points to represent an Exponential kernel density in one dimension.
`TriangleKernelDensity`	A quick way of storing points to represent an Exponential kernel density in one dimension.

Multivariate Distributions

`IndependentComponentsDistribution`	Allows you to create a multivariate distribution, where each distribution is independent of the others.
`MultivariateGaussianDistribution`	
`DirichletDistribution`	A Dirichlet distribution, usually a prior for the multinomial distributions.
`ConditionalProbabilityTable`	A conditional probability table, which is dependent on values from at least one previous distribution but up to as many as you want to encode for.

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Table 3 – continued from previous page

`JointProbabilityTable`	A joint probability table.

While there is a large variety of univariate distributions, multivariate distributions can be made from univariate distributions by using `` `IndependentComponentsDistribution` `` with the assumption that each column of data is independent from the other columns (instead of being related by a covariance matrix, like in multivariate gaussians). Here is an example:

```
d1 = NormalDistribution(5, 2)
d2 = LogNormalDistribution(1, 0.3)
d3 = ExponentialDistribution(4)
d = IndependentComponentsDistribution([d1, d2, d3])
```

1.3.1 Initialization

Initializing a distribution is simple and done just by passing in the distribution parameters. For example, the parameters of a normal distribution are the mean (mu) and the standard deviation (sigma). We can initialize it as follows:

```
from pomegranate import *
a = NormalDistribution(5, 2)
```

However, frequently we don't know the parameters of the distribution beforehand or would like to directly fit this distribution to some data. We can do this through the *from_samples* class method.

```
b = NormalDistribution.from_samples([3, 4, 5, 6, 7], weights=[0.5, 1, 1.5, 1, 0.5])
```

If we want to fit the model to weighted samples, we can just pass in an array of the relative weights of each sample as well.

```
b = NormalDistribution.from_samples([3, 4, 5, 6, 7], weights=[0.5, 1, 1.5, 1, 0.5])
```

1.3.2 Probability

Distributions are typically used to calculate the probability of some sample. This can be done using either the *probability* or *log_probability* methods.

```
a = NormalDistribution(5, 2)
a.log_probability(8)
-2.737085713764219
a.probability(8)
0.064758797832971712
b = NormalDistribution.from_samples([3, 4, 5, 6, 7], weights=[0.5, 1, 1.5, 1, 0.5])
b.log_probability(8)
-4.437779569430167
```

These methods work for univariate distributions, kernel densities, and multivariate distributions all the same. For a multivariate distribution you'll have to pass in an array for the full sample.

```
d1 = NormalDistribution(5, 2)
d2 = LogNormalDistribution(1, 0.3)
d3 = ExponentialDistribution(4)
d = IndependentComponentsDistribution([d1, d2, d3])
>>>
```

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```
X = [6.2, 0.4, 0.9]
d.log_probability(X)
-23.205411733352875
```

1.3.3 Fitting

We may wish to fit the distribution to new data, either overriding the previous parameters completely or moving the parameters to match the dataset more closely through inertia. Distributions are updated using maximum likelihood estimates (MLE). Kernel densities will either discard previous points or downweight them if inertia is used.

```
d = NormalDistribution(5, 2)
d.fit([1, 5, 7, 3, 2, 4, 3, 5, 7, 8, 2, 4, 6, 7, 2, 4, 5, 1, 3, 2, 1])
d
{
    "frozen" :false,
    "class" :"Distribution",
    "parameters" :[
        3.9047619047619047,
        2.13596776114341
    ],
    "name" :"NormalDistribution"
}
```

Training can be done on weighted samples by passing an array of weights in along with the data for any of the training functions, like the following:

```
d = NormalDistribution(5, 2)
d.fit([1, 5, 7, 3, 2, 4], weights=[0.5, 0.75, 1, 1.25, 1.8, 0.33])
d
{
    "frozen" :false,
    "class" :"Distribution",
    "parameters" :[
        3.538188277087034,
        1.954149818564894
    ],
    "name" :"NormalDistribution"
}
```

Training can also be done with inertia, where the new value will be some percentage the old value and some percentage the new value, used like *d.from_sample([5,7,8], inertia=0.5)* to indicate a 50-50 split between old and new values.

1.3.4 API Reference

class pomegranate.distributions.**Distribution**

A probability distribution.

Represents a probability distribution over the defined support. This is the base class which must be subclassed to specific probability distributions. All distributions have the below methods exposed.

Parameters

Varies on distribution.

Attributes

name [str] The name of the type of distributioon.

summaries [list] Sufficient statistics to store the update.

frozen [bool] Whether or not the distribution will be updated during training.

d [int] The dimensionality of the data. Univariate distributions are all 1, while multivariate distributions are > 1.

clear_summaries()
Clear the summary statistics stored in the object. Parameters ———- None Returns ——- None

copy()
Return a deep copy of this distribution object.

This object will not be tied to any other distribution or connected in any form.

Returns

distribution [Distribution] A copy of the distribution with the same parameters.

from_json()
Read in a serialized distribution and return the appropriate object.

Parameters

s [str] A JSON formatted string containing the file.

Returns

model [object] A properly initialized and baked model.

from_samples()
Fit a distribution to some data without pre-specifying it.

from_summaries()
Fit the distribution to the stored sufficient statistics. Parameters ———- inertia : double, optional

The weight of the previous parameters of the model. The new parameters will roughly be old_param*inertia + new_param*(1-inertia), so an inertia of 0 means ignore the old parameters, whereas an inertia of 1 means ignore the new parameters. Default is 0.0.

None

log_probability()
Return the log probability of the given X under this distribution.

Parameters

X [double] The X to calculate the log probability of (overriden for DiscreteDistributions)

Returns

logp [double] The log probability of that point under the distribution.

marginal()
Return the marginal of the distribution.

Parameters

***args** [optional] Arguments to pass in to specific distributions

****kwargs** [optional] Keyword arguments to pass in to specific distributions

Returns

distribution [Distribution] The marginal distribution. If this is a multivariate distribution then this method is filled in. Otherwise returns self.

plot()
Plot the distribution by sampling from it.

This function will plot a histogram of samples drawn from a distribution on the current open figure.

Parameters

n [int, optional] The number of samples to draw from the distribution. Default is 1000.

****kwargs** [arguments, optional] Arguments to pass to matplotlib's histogram function.

Returns

None

summarize()
Summarize a batch of data into sufficient statistics for a later update. Parameters ———- items : array-like, shape (n_samples, n_dimensions)

This is the data to train on. Each row is a sample, and each column is a dimension to train on. For univariate distributions an array is used, while for multivariate distributions a 2d matrix is used.

weights [array-like, shape (n_samples,), optional] The initial weights of each sample in the matrix. If nothing is passed in then each sample is assumed to be the same weight. Default is None.

None

to_json()
Serialize the distribution to a JSON.

Parameters

separators [tuple, optional] The two separaters to pass to the json.dumps function for formatting. Default is (',', ' : ').

indent [int, optional] The indentation to use at each level. Passed to json.dumps for formatting. Default is 4.

Returns

json [str] A properly formatted JSON object.

1.4 General Mixture Models

IPython Notebook Tutorial

General Mixture models (GMMs) are an unsupervised probabilistic model composed of multiple distributions (commonly referred to as components) and corresponding weights. This allows you to model more complex distributions corresponding to a singular underlying phenomena. For a full tutorial on what a mixture model is and how to use them, see the above tutorial.

1.4.1 Initialization

General Mixture Models can be initialized in two ways depending on if you know the initial parameters of the model or not: (1) passing in a list of pre-initialized distributions, or (2) running the `from_samples` class method on data. The initial parameters can be either a pre-specified model that is ready to be used for prediction, or the initialization for expectation-maximization. Otherwise, if the second initialization option is chosen, then k-means is used to initialize the distributions. The distributions passed for each component don't have to be the same type, and if an

`IndependentComponentDistribution` object is passed in, then the dimensions don't need to be modeled by the same distribution.

Here is an example of a traditional multivariate Gaussian mixture where we pass in pre-initialized distributions. We can also pass in the weight of each component, which serves as the prior probability of a sample belonging to that component when doing predictions.

```
from pomegranate import *
d1 = MultivariateGaussianDistribution([1, 6, 3], [[1, 0, 0], [0, 1, 0], [0, 0, 1]])
d2 = MultivariateGaussianDistribution([2, 8, 4], [[1, 0, 0], [0, 1, 0], [0, 0, 2]])
d3 = MultivariateGaussianDistribution([0, 4, 8], [[2, 0, 0], [0, 3, 0], [0, 0, 1]])
model = GeneralMixtureModel([d1, d2, d3], weights=[0.25, 0.60, 0.15])
```

Alternatively, if we want to model each dimension differently, then we can replace the multivariate Gaussian distributions with `IndependentComponentsDistribution` objects.

```
from pomegranate import *
d1 = IndependentComponentsDistributions([NormalDistribution(5, 2),␣
↪ExponentialDistribution(1), LogNormalDistribution(0.4, 0.1)])
d2 = IndependentComponentsDistributions([NormalDistribution(3, 1),␣
↪ExponentialDistribution(2), LogNormalDistribution(0.8, 0.2)])
model = GeneralMixtureModel([d1, d2], weights=[0.66, 0.34])
```

If we do not know the parameters of our distributions beforehand and want to learn them entirely from data, then we can use the `from_samples` class method. This method will run k-means to initialize the components, using the returned clusters to initialize all parameters of the distributions, i.e. both mean and covariances for multivariate Gaussian distributions. Afterwards, execptation-maximization is used to refine the parameters of the model, iterating until convergence.

```
from pomegranate import *
model = GeneralMixtureModel.from_samples(MultivariateGaussianDistribution, n_
↪components=3, X=X)
```

If we want to model each dimension using a different distribution, then we can pass in a list of callables and they will be initialized using k-means as well.

```
from pomegranate import *
model = GeneralMixtureModel.from_samples([NormalDistribution, ExponentialDistribution,
↪ LogNormalDistribution], n_components=5, X=X)
```

1.4.2 Probability

The probability of a point is the sum of its probability under each of the components, multiplied by the weight of each component c, $P = \sum_{i \in M} P(D|M_i)P(M_i)$. The `probability` method returns the probability of each sample under the entire mixture, and the `log_probability` method returns the log of that value.

1.4.3 Prediction

The common prediction tasks involve predicting which component a new point falls under. This is done using Bayes rule $P(M|D) = \frac{P(D|M)P(M)}{P(D)}$ to determine the posterior probability $P(M|D)$ as opposed to simply the likelihood $P(D|M)$. Bayes rule indicates that it isn't simply the likelihood function which makes this prediction but the likelihood function multiplied by the probability that that distribution generated the sample. For example, if you have a distribution which has 100x as many samples fall under it, you would naively think that there is a ~99% chance that

any random point would be drawn from it. Your belief would then be updated based on how well the point fit each distribution, but the proportion of points generated by each sample is important as well.

We can get the component label assignments using `model.predict(data)`, which will return an array of indexes corresponding to the maximally likely component. If what we want is the full matrix of $P(M|D)$, then we can use `model.predict_proba(data)`, which will return a matrix with each row being a sample, each column being a component, and each cell being the probability that that model generated that data. If we want log probabilities instead we can use `model.predict_log_proba(data)` instead.

1.4.4 Fitting

Training GMMs faces the classic chicken-and-egg problem that most unsupervised learning algorithms face. If we knew which component a sample belonged to, we could use MLE estimates to update the component. And if we knew the parameters of the components we could predict which sample belonged to which component. This problem is solved using expectation-maximization, which iterates between the two until convergence. In essence, an initialization point is chosen which usually is not a very good start, but through successive iteration steps, the parameters converge to a good ending.

These models are fit using `model.fit(data)`. A maximimum number of iterations can be specified as well as a stopping threshold for the improvement ratio. See the API reference for full documentation.

1.4.5 API Reference

class pomegranate.gmm.**GeneralMixtureModel**

A General Mixture Model.

This mixture model can be a mixture of any distribution as long as they are all of the same dimensionality. Any object can serve as a distribution as long as it has fit(X, weights), log_probability(X), and summarize(X, weights)/from_summaries() methods if out of core training is desired.

Parameters

distributions [array-like, shape (n_components,) or callable] The components of the model. If array, corresponds to the initial distributions of the components. If callable, must also pass in the number of components and kmeans++ will be used to initialize them.

weights [array-like, optional, shape (n_components,)] The prior probabilities corresponding to each component. Does not need to sum to one, but will be normalized to sum to one internally. Defaults to None.

Examples

```
>>> from pomegranate import *
>>> clf = GeneralMixtureModel([
>>>     NormalDistribution(5, 2),
>>>     NormalDistribution(1, 1)])
>>> clf.log_probability(5)
-2.304562194038089
>>> clf.predict_proba([[5], [7], [1]])
array([[ 0.99932952,  0.00067048],
       [ 0.99999995,  0.00000005],
       [ 0.06337894,  0.93662106]])
>>> clf.fit([[1], [5], [7], [8], [2]])
>>> clf.predict_proba([[5], [7], [1]])
```

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```
array([[ 1.        ,  0.        ],
       [ 1.        ,  0.        ],
       [ 0.00004383,  0.99995617]])
>>> clf.distributions
array([ {
    "frozen" :false,
    "class" :"Distribution",
    "parameters" :[
        6.6571359101390755,
        1.2639830514274502
    ],
    "name" :"NormalDistribution"
},
       {
    "frozen" :false,
    "class" :"Distribution",
    "parameters" :[
        1.498707696758334,
        0.4999983303277837
    ],
    "name" :"NormalDistribution"
}], dtype=object)
```

Attributes

distributions [array-like, shape (n_components,)] The component distribution objects.

weights [array-like, shape (n_components,)] The learned prior weight of each object

clear_summaries()

Remove the stored sufficient statistics.

Parameters

None

Returns

None

copy()

Return a deep copy of this distribution object.

This object will not be tied to any other distribution or connected in any form.

Parameters

None

Returns

distribution [Distribution] A copy of the distribution with the same parameters.

fit()

Fit the model to new data using EM.

This method fits the components of the model to new data using the EM method. It will iterate until either max iterations has been reached, or the stop threshold has been passed.

This is a sklearn wrapper for train method.

Parameters

X [array-like, shape (n_samples, n_dimensions)]

This is the data to train on. Each row is a sample, and each column is a dimension to train on.

weights [array-like, shape (n_samples,), optional] The initial weights of each sample in the matrix. If nothing is passed in then each sample is assumed to be the same weight. Default is None.

inertia [double, optional] The weight of the previous parameters of the model. The new parameters will roughly be old_param*inertia + new_param*(1-inertia), so an inertia of 0 means ignore the old parameters, whereas an inertia of 1 means ignore the new parameters. Default is 0.0.

stop_threshold [double, optional, positive] The threshold at which EM will terminate for the improvement of the model. If the model does not improve its fit of the data by a log probability of 0.1 then terminate. Default is 0.1.

max_iterations [int, optional, positive] The maximum number of iterations to run EM for. If this limit is hit then it will terminate training, regardless of how well the model is improving per iteration. Default is 1e8.

pseudocount : double, optional, positive

A pseudocount to add to the emission of each distribution. This

effectively smoothes the states to prevent 0. probability symbols

if they don't happen to occur in the data. Only effects mixture

models defined over discrete distributions. Default is 0.

verbose [bool, optional] Whether or not to print out improvement information over iterations. Default is False.

Returns

improvement [double] The total improvement in log probability P(D|M)

freeze()

Freeze the distribution, preventing updates from occuring.

from_samples()

Create a mixture model directly from the given dataset.

First, k-means will be run using the given initializations, in order to define initial clusters for the points. These clusters are used to initialize the distributions used. Then, EM is run to refine the parameters of these distributions.

A homogenous mixture can be defined by passing in a single distribution callable as the first parameter and specifying the number of components, while a heterogeneous mixture can be defined by passing in a list of callables of the appropriate type.

Parameters

distributions [array-like, shape (n_components,) or callable]

The components of the model. If array, corresponds to the initial distributions of the components. If callable, must also pass in the number of components and kmeans++ will be used to initialize them.

n_components [int] If a callable is passed into distributions then this is the number of components to initialize using the kmeans++ algorithm.

X [array-like, shape (n_samples, n_dimensions)] This is the data to train on. Each row is a sample, and each column is a dimension to train on.

weights [array-like, shape (n_samples,), optional] The initial weights of each sample in the matrix. If nothing is passed in then each sample is assumed to be the same weight. Default is None.

n_init [int, optional] The number of initializations of k-means to do before choosing the best. Default is 1.

init [str, optional] The initialization algorithm to use for the initial k-means clustering. Must be one of 'first-k', 'random', 'kmeans++', or 'kmeans||'. Default is 'kmeans++'.

max_kmeans_iterations [int, optional] The maximum number of iterations to run kmeans for in the initialization step. Default is 1.

inertia [double, optional] The weight of the previous parameters of the model. The new parameters will roughly be old_param*inertia + new_param*(1-inertia), so an inertia of 0 means ignore the old parameters, whereas an inertia of 1 means ignore the new parameters. Default is 0.0.

stop_threshold [double, optional, positive] The threshold at which EM will terminate for the improvement of the model. If the model does not improve its fit of the data by a log probability of 0.1 then terminate. Default is 0.1.

max_iterations [int, optional, positive] The maximum number of iterations to run EM for. If this limit is hit then it will terminate training, regardless of how well the model is improving per iteration. Default is 1e8.

pseudocount : double, optional, positive

A pseudocount to add to the emission of each distribution. This

effectively smoothes the states to prevent 0. probability symbols

if they don't happen to occur in the data. Only effects mixture

models defined over discrete distributions. Default is 0.

verbose [bool, optional] Whether or not to print out improvement information over iterations. Default is False.

from_summaries()

Fit the model to the collected sufficient statistics.

Fit the parameters of the model to the sufficient statistics gathered during the summarize calls. This should return an exact update.

Parameters

inertia [double, optional] The weight of the previous parameters of the model. The new parameters will roughly be old_param*inertia + new_param*(1-inertia), so an inertia of 0 means ignore the old parameters, whereas an inertia of 1 means ignore the new parameters. Default is 0.0.

pseudocount [double, optional] A pseudocount to add to the emission of each distribution. This effectively smoothes the states to prevent 0. probability symbols if they don't happen to occur in the data. If discrete data, will smooth both the prior probabilities of each

component and the emissions of each component. Otherwise, will only smooth the prior probabilities of each component. Default is 0.

Returns

None

log_probability()

Calculate the log probability of a point under the distribution.

The probability of a point is the sum of the probabilities of each distribution multiplied by the weights. Thus, the log probability is the sum of the log probability plus the log prior.

This is the python interface.

Parameters

X [numpy.ndarray, shape=(n, d) or (n, m, d)] The samples to calculate the log probability of. Each row is a sample and each column is a dimension. If emissions are HMMs then shape is (n, m, d) where m is variable length for each obervation, and X becomes an array of n (m, d)-shaped arrays.

Returns

log_probability [double] The log probabiltiy of the point under the distribution.

predict()

Predict the most likely component which generated each sample.

Calculate the posterior P(M|D) for each sample and return the index of the component most likely to fit it. This corresponds to a simple argmax over the responsibility matrix.

This is a sklearn wrapper for the maximum_a_posteriori method.

Parameters

X [array-like, shape (n_samples, n_dimensions)] The samples to do the prediction on. Each sample is a row and each column corresponds to a dimension in that sample. For univariate distributions, a single array may be passed in.

Returns

y [array-like, shape (n_samples,)] The predicted component which fits the sample the best.

predict_log_proba()

Calculate the posterior log P(M|D) for data.

Calculate the log probability of each item having been generated from each component in the model. This returns normalized log probabilities such that the probabilities should sum to 1

This is a sklearn wrapper for the original posterior function.

Parameters

X [array-like, shape (n_samples, n_dimensions)] The samples to do the prediction on. Each sample is a row and each column corresponds to a dimension in that sample. For univariate distributions, a single array may be passed in.

Returns

y [array-like, shape (n_samples, n_components)] The normalized log probability log P(M|D) for each sample. This is the probability that the sample was generated from each component.

predict_proba()
Calculate the posterior P(M|D) for data.

Calculate the probability of each item having been generated from each component in the model. This returns normalized probabilities such that each row should sum to 1.

Since calculating the log probability is much faster, this is just a wrapper which exponentiates the log probability matrix.

Parameters

X [array-like, shape (n_samples, n_dimensions)] The samples to do the prediction on. Each sample is a row and each column corresponds to a dimension in that sample. For univariate distributions, a single array may be passed in.

Returns

probability [array-like, shape (n_samples, n_components)] The normalized probability P(M|D) for each sample. This is the probability that the sample was generated from each component.

probability()
Return the probability of the given symbol under this distribution.

Parameters

symbol [object] The symbol to calculate the probability of

Returns

probability [double] The probability of that point under the distribution.

sample()
Generate a sample from the model.

First, randomly select a component weighted by the prior probability, Then, use the sample method from that component to generate a sample.

Parameters

n [int, optional] The number of samples to generate. Defaults to 1.

Returns

sample [array-like or object] A randomly generated sample from the model of the type modelled by the emissions. An integer if using most distributions, or an array if using multivariate ones, or a string for most discrete distributions. If n=1 return an object, if n>1 return an array of the samples.

summarize()
Summarize a batch of data and store sufficient statistics.

This will run the expectation step of EM and store sufficient statistics in the appropriate distribution objects. The summarization can be thought of as a chunk of the E step, and the from_summaries method as the M step.

Parameters

X [array-like, shape (n_samples, n_dimensions)] This is the data to train on. Each row is a sample, and each column is a dimension to train on.

weights [array-like, shape (n_samples,), optional] The initial weights of each sample in the matrix. If nothing is passed in then each sample is assumed to be the same weight. Default is None.

Returns

logp [double] The log probability of the data given the current model. This is used to speed up EM.

thaw()
Thaw the distribution, re-allowing updates to occur.

to_json()
Serialize the model to a JSON.

Parameters

separators [tuple, optional] The two separaters to pass to the json.dumps function for formatting. Default is (',', ' : ').

indent [int, optional] The indentation to use at each level. Passed to json.dumps for formatting. Default is 4.

Returns

json [str] A properly formatted JSON object.

1.5 Hidden Markov Models

- IPython Notebook Tutorial
- IPython Notebook Sequence Alignment Tutorial

Hidden Markov models (HMMs) are a structured probabilistic model that forms a probability distribution of sequences, as opposed to individual symbols. It is similar to a Bayesian network in that it has a directed graphical structure where nodes represent probability distributions, but unlike Bayesian networks in that the edges represent transitions and encode transition probabilities, whereas in Bayesian networks edges encode dependence statements. A HMM can be thought of as a general mixture model plus a transition matrix, where each component in the general Mixture model corresponds to a node in the hidden Markov model, and the transition matrix informs the probability that adjacent symbols in the sequence transition from being generated from one component to another. A strength of HMMs is that they can model variable length sequences whereas other models typically require a fixed feature set. They are extensively used in the fields of natural language processing to model speech, bioinformatics to model biosequences, and robotics to model movement.

The HMM implementation in pomegranate is based off of the implementation in its predecessor, Yet Another Hidden Markov Model (YAHMM). To convert a script that used YAHMM to a script using pomegranate, you only need to change calls to the `Model` class to call `HiddenMarkovModel`. For example, a script that previously looked like the following:

```
from yahmm import *
model = Model()
```

would now be written as

```
from pomegranate import *
model = HiddenMarkovModel()
```

and the remaining method calls should be identical.

1.5.1 Initialization

Hidden Markov models can be initialized in one of two ways depending on if you know the initial parameters of the model, either (1) by defining both the distributions and the graphical structure manually, or (2) running the `from_samples` method to learn both the structure and distributions directly from data. The first initialization method can be used either to specify a pre-defined model that is ready to make predictions, or as the initialization to a training algorithm such as Baum-Welch. It is flexible enough to allow sparse transition matrices and any type of distribution on each node, i.e. normal distributions on several nodes, but a mixture of normals on some nodes modeling more complex phenomena. The second initialization method is less flexible, in that currently each node must have the same distribution type, and that it will only learn dense graphs. Similar to mixture models, this initialization method starts with k-means to initialize the distributions and a uniform probability transition matrix before running Baum-Welch.

If you are initializing the parameters manually, you can do so either by passing in a list of distributions and a transition matrix, or by building the model line-by-line. Let's first take a look at building the model from a list of distributions and a transition matrix.

```
from pomegranate import *
dists = [NormalDistribution(5, 1), NormalDistribution(1, 7), NormalDistribution(8,2)]
trans_mat = numpy.array([[0.7, 0.3, 0.0],
                         [0.0, 0.8, 0.2],
                         [0.0, 0.0, 0.9]])
starts = numpy.array([1.0, 0.0, 0.0])
ends = numpy.array([0.0, 0.0, 0.1])
model = HiddenMarkovModel.from_matrix(trans_mat, dists, starts, ends)
```

Next, let's take a look at building the same model line by line.

```
from pomegranate import *
s1 = State(Distribution(NormalDistribution(5, 1)))
s2 = State(Distribution(NormalDistribution(1, 7)))
s3 = State(Distribution(NormalDistribution(8, 2)))
model = HiddenMarkovModel()
model.add_states(s1, s2, s3)
model.add_transition(model.start, s1, 1.0)
model.add_transition(s1, s1, 0.7)
model.add_transition(s1, s2, 0.3)
model.add_transition(s2, s2, 0.8)
model.add_transition(s2, s3, 0.2)
model.add_transition(s3, s3, 0.9)
model.add_transition(s3, model.end, 0.1)
model.bake()
```

Initially it may seem that the first method is far easier due to it being fewer lines of code. However, when building large sparse models defining a full transition matrix can be cumbersome, especially when it is mostly 0s.

Models built in this manner must be explicitly "baked" at the end. This finalizes the model topology and creates the internal sparse matrix which makes up the model. This step also automatically normalizes all transitions to make sure they sum to 1.0, stores information about tied distributions, edges, pseudocounts, and merges unneccesary silent states in the model for computational efficiency. This can cause the *bake* step to take a little bit of time. If you want to reduce this overhead and are sure you specified the model correctly you can pass in *merge="None"* to the bake step to avoid model checking.

The second way to initialize models is to use the `from_samples` class method. The call is identical to initializing a mixture model.

```
from pomegranate import *
model = HiddenMarkovModel.from_samples(NormalDistribution, n_components=5, X=X)
```

Much like a mixture model, all arguments present in the `fit` step can also be passed in to this method. Also like a mixture model, it is initialized by running k-means on the concatenation of all data, ignoring that the symbols are part of a structured sequence. The clusters returned are used to initialize all parameters of the distributions, i.e. both mean and covariances for multivariate Gaussian distributions. The transition matrix is initialized as uniform random probabilities. After the components (distributions on the nodes) are initialized, the given training algorithm is used to refine the parameters of the distributions and learn the appropriate transition probabilities.

1.5.2 Log Probability

There are two common forms of the log probability which are used. The first is the log probability of the most likely path the sequence can take through the model, called the Viterbi probability. This can be calculated using `model.viterbi(sequence)`. However, this is $P(D|S_{ML}, S_{ML}, S_{ML})$ not $P(D|M)$. In order to get $P(D|M)$ we have to sum over all possible paths instead of just the single most likely path. This can be calculated using `model.log_probability(sequence)` and uses the forward algorithm internally. On that note, the full forward matrix can be returned using `model.forward(sequence)` and the full backward matrix can be returned using `model.backward(sequence)`, while the full forward-backward emission and transition matrices can be returned using `model.forward_backward(sequence)`.

1.5.3 Prediction

A common prediction technique is calculating the Viterbi path, which is the most likely sequence of states that generated the sequence given the full model. This is solved using a simple dynamic programming algorithm similar to sequence alignment in bioinformatics. This can be called using `model.viterbi(sequence)`. A sklearn wrapper can be called using `model.predict(sequence, algorithm='viterbi')`.

Another prediction technique is called maximum a posteriori or forward-backward, which uses the forward and backward algorithms to calculate the most likely state per observation in the sequence given the entire remaining alignment. Much like the forward algorithm can calculate the sum-of-all-paths probability instead of the most likely single path, the forward-backward algorithm calculates the best sum-of-all-paths state assignment instead of calculating the single best path. This can be called using `model.predict(sequence, algorithm='map')` and the raw normalized probability matrices can be called using `model.predict_proba(sequence)`.

1.5.4 Fitting

A simple fitting algorithm for hidden Markov models is called Viterbi training. In this method, each observation is tagged with the most likely state to generate it using the Viterbi algorithm. The distributions (emissions) of each states are then updated using MLE estimates on the observations which were generated from them, and the transition matrix is updated by looking at pairs of adjacent state taggings. This can be done using `model.fit(sequence, algorithm='viterbi')`.

However, this is not the best way to do training and much like the other sections there is a way of doing training using sum-of-all-paths probabilities instead of maximally likely path. This is called Baum-Welch or forward-backward training. Instead of using hard assignments based on the Viterbi path, observations are given weights equal to the probability of them having been generated by that state. Weighted MLE can then be done to updates the distributions, and the soft transition matrix can give a more precise probability estimate. This is the default training algorithm, and can be called using either `model.fit(sequences)` or explicitly using `model.fit(sequences, algorithm='baum-welch')`.

Fitting in pomegranate also has a number of options, including the use of distribution or edge inertia, freezing certain states, tying distributions or edges, and using pseudocounts. See the tutorial linked to at the top of this page for full details on each of these options.

1.5.5 API Reference

class pomegranate.hmm.**HiddenMarkovModel**

A Hidden Markov Model

A Hidden Markov Model (HMM) is a directed graphical model where nodes are hidden states which contain an observed emission distribution and edges contain the probability of transitioning from one hidden state to another. HMMs allow you to tag each observation in a variable length sequence with the most likely hidden state according to the model.

Parameters

name [str, optional] The name of the model. Default is None.

start [State, optional] An optional state to force the model to start in. Default is None.

end [State, optional] An optional state to force the model to end in. Default is None.

Examples

```
>>> from pomegranate import *
>>> d1 = DiscreteDistribution({'A' : 0.35, 'C' : 0.20, 'G' : 0.05, 'T' : 40})
>>> d2 = DiscreteDistribution({'A' : 0.25, 'C' : 0.25, 'G' : 0.25, 'T' : 25})
>>> d3 = DiscreteDistribution({'A' : 0.10, 'C' : 0.40, 'G' : 0.40, 'T' : 10})
>>>
>>> s1 = State(d1, name="s1")
>>> s2 = State(d2, name="s2")
>>> s3 = State(d3, name="s3")
>>>
>>> model = HiddenMarkovModel('example')
>>> model.add_states([s1, s2, s3])
>>> model.add_transition(model.start, s1, 0.90)
>>> model.add_transition(model.start, s2, 0.10)
>>> model.add_transition(s1, s1, 0.80)
>>> model.add_transition(s1, s2, 0.20)
>>> model.add_transition(s2, s2, 0.90)
>>> model.add_transition(s2, s3, 0.10)
>>> model.add_transition(s3, s3, 0.70)
>>> model.add_transition(s3, model.end, 0.30)
>>> model.bake()
>>>
>>> print model.log_probability(list('ACGACTATTCGAT'))
-4.31828085576
>>> print ", ".join(state.name for i, state in model.viterbi(list('ACGACTATTCGAT
↪'))[1])
example-start, s1, s2, s2, s2, s2, s2, s2, s2, s2, s2, s2, s2, s3, example-end
```

Attributes

start [State] A state object corresponding to the initial start of the model

end [State] A state object corresponding to the forced end of the model

start_index [int] The index of the start object in the state list

end_index [int] The index of the end object in the state list

silent_start [int] The index of the beginning of the silent states in the state list

states [list] The list of all states in the model, with silent states at the end

add_edge()
Add a transition from state a to state b which indicates that B is dependent on A in ways specified by the distribution.

add_model()
Add the states and edges of another model to this model.

Parameters

other [HiddenMarkovModel] The other model to add

Returns

None

add_node()
Add a node to the graph.

add_nodes()
Add multiple states to the graph.

add_state()
Add a state to the given model.

The state must not already be in the model, nor may it be part of any other model that will eventually be combined with this one.

Parameters

state [State] A state object to be added to the model.

Returns

None

add_states()
Add multiple states to the model at the same time.

Parameters

states [list or generator] Either a list of states which are entered sequentially, or just comma separated values, for example model.add_states(a, b, c, d).

Returns

None

add_transition()
Add a transition from state a to state b.

Add a transition from state a to state b with the given (non-log) probability. Both states must be in the HMM already. self.start and self.end are valid arguments here. Probabilities will be normalized such that every node has edges summing to 1. leaving that node, but only when the model is baked. Psueodocounts are allowed as a way of using edge-specific pseudocounts for training.

By specifying a group as a string, you can tie edges together by giving them the same group. This means that a transition across one edge in the group counts as a transition across all edges in terms of training.

Parameters

a [State] The state that the edge originates from

b [State] The state that the edge goes to

probability [double] The probability of transitioning from state a to state b in [0, 1]

pseudocount [double, optional] The pseudocount to use for this specific edge if using edge pseudocounts for training. Defaults to the probability. Default is None.

group [str, optional] The name of the group of edges to tie together during training. If groups are used, then a transition across any one edge counts as a transition across all edges. Default is None.

Returns

None

add_transitions()

Add many transitions at the same time,

Parameters

a [State or list] Either a state or a list of states where the edges originate.

b [State or list] Either a state or a list of states where the edges go to.

probabilities [list] The probabilities associated with each transition.

pseudocounts [list, optional] The pseudocounts associated with each transition. Default is None.

groups [list, optional] The groups of each edge. Default is None.

Returns

None

Examples

```
>>> model.add_transitions([model.start, s1], [s1, model.end], [1., 1.])
>>> model.add_transitions([model.start, s1, s2, s3], s4, [0.2, 0.4, 0.3, 0.9])
>>> model.add_transitions(model.start, [s1, s2, s3], [0.6, 0.2, 0.05])
```

backward()

Run the backward algorithm on the sequence.

Calculate the probability of each observation being aligned to each state by going backward through a sequence. Returns the full backward matrix. Each index i, j corresponds to the sum-of-all-paths log probability of starting at the end of the sequence, and aligning observations to hidden states in such a manner that observation i was aligned to hidden state j. Uses row normalization to dynamically scale each row to prevent underflow errors.

If the sequence is impossible, will return a matrix of nans.

See also:

- Silent state handling taken from p. 71 of "Biological

Sequence Analysis" by Durbin et al., and works for anything which does not have loops of silent states.

- Row normalization technique explained by

http://www.cs.sjsu.edu/~stamp/RUA/HMM.pdf on p. 14.

Parameters

sequence [array-like] An array (or list) of observations.

Returns

matrix [array-like, shape (len(sequence), n_states)] The probability of aligning the sequences to states in a backward fashion.

bake()

Finalize the topology of the model.

Finalize the topology of the model and assign a numerical index to every state. This method must be called before any of the probability- calculating methods.

This fills in self.states (a list of all states in order) and self.transition_log_probabilities (log probabilities for transitions), as well as self.start_index and self.end_index, and self.silent_start (the index of the first silent state).

Parameters

verbose [bool, optional] Return a log of changes made to the model during normalization or merging. Default is False.

merge ["None", "Partial, "All"] Merging has three options: "None": No modifications will be made to the model. "Partial": A silent state which only has a probability 1 transition

to another silent state will be merged with that silent state. This means that if silent state "S1" has a single transition to silent state "S2", that all transitions to S1 will now go to S2, with the same probability as before, and S1 will be removed from the model.

"All": A silent state with a probability 1 transition to any other state, silent or symbol emitting, will be merged in the manner described above. In addition, any orphan states will be removed from the model. An orphan state is a state which does not have any transitions to it OR does not have any transitions from it, except for the start and end of the model. This will iteratively remove orphan chains from the model. This is sometimes desirable, as all states should have both a transition in to get to that state, and a transition out, even if it is only to itself. If the state does not have either, the HMM will likely not work as intended.

Default is 'All'.

Returns

None

clear_summaries()

Clear the summary statistics stored in the object.

Parameters

None

Returns

None

concatenate()

Concatenate this model to another model.

Concatenate this model to another model in such a way that a single probability 1 edge is added between self.end and other.start. Rename all other states appropriately by adding a suffix or prefix if needed.

Parameters

other [HiddenMarkovModel] The other model to concatenate

suffix [str, optional] Add the suffix to the end of all state names in the other model. Default is ‘’.

prefix [str, optional] Add the prefix to the beginning of all state names in the other model. Default is ‘’.

Returns

None

copy()
Returns a deep copy of the HMM.

Parameters

None

Returns

model [HiddenMarkovModel] A deep copy of the model with entirely new objects.

dense_transition_matrix()
Returns the dense transition matrix.

Parameters

None

Returns

matrix [numpy.ndarray, shape (n_states, n_states)] A dense transition matrix, containing the log probability of transitioning from each state to each other state.

edge_count()
Returns the number of edges present in the model.

fit()
Fit the model to data using either Baum-Welch, Viterbi, or supervised training.

Given a list of sequences, performs re-estimation on the model parameters. The two supported algorithms are “baum-welch”, “viterbi”, and “labeled”, indicating their respective algorithm. “labeled” corresponds to supervised learning that requires passing in a matching list of labels for each symbol seen in the sequences.

Training supports a wide variety of other options including using edge pseudocounts and either edge or distribution inertia.

Parameters

sequences [array-like] An array of some sort (list, numpy.ndarray, tuple..) of sequences, where each sequence is a numpy array, which is 1 dimensional if the HMM is a one dimensional array, or multidimensional if the HMM supports multiple dimensions.

weights [array-like or None, optional] An array of weights, one for each sequence to train on. If None, all sequences are equaly weighted. Default is None.

labels [array-like or None, optional] An array of state labels for each sequence. This is only used in ‘labeled’ training. If used this must be comprised of n lists where n is the number of sequences to train on, and each of those lists must have one label per observation. Default is None.

stop_threshold [double, optional] The threshold the improvement ratio of the models log probability in fitting the scores. Default is 1e-9.

min_iterations [int, optional] The minimum number of iterations to run Baum-Welch training for. Default is 0.

max_iterations [int, optional] The maximum number of iterations to run Baum-Welch training for. Default is 1e8.

algorithm ['baum-welch', 'viterbi', 'labeled'] The training algorithm to use. Baum-Welch uses the forward-backward algorithm to train using a version of structured EM. Viterbi iteratively runs the sequences through the Viterbi algorithm and then uses hard assignments of observations to states using that. Default is 'baum-welch'. Labeled training requires that labels are provided for each observation in each sequence.

verbose [bool, optional] Whether to print the improvement in the model fitting at each iteration. Default is True.

pseudocount [double, optional] A pseudocount to add to both transitions and emissions. If supplied, it will override both transition_pseudocount and emission_pseudocount in the same way that specifying *inertia* will override both *edge_inertia* and *distribution_inertia*. Default is None.

transition_pseudocount [double, optional] A pseudocount to add to all transitions to add a prior to the MLE estimate of the transition probability. Default is 0.

emission_pseudocount [double, optional] A pseudocount to add to the emission of each distribution. This effectively smoothes the states to prevent 0. probability symbols if they don't happen to occur in the data. Only effects hidden Markov models defined over discrete distributions. Default is 0.

use_pseudocount [bool, optional] Whether to use the pseudocounts defined in the *add_edge* method for edge-specific pseudocounts when updating the transition probability parameters. Does not effect the *transition_pseudocount* and *emission_pseudocount* parameters, but can be used in addition to them. Default is False.

inertia [double or None, optional, range [0, 1]] If double, will set both edge_inertia and distribution_inertia to be that value. If None, will not override those values. Default is None.

edge_inertia [bool, optional, range [0, 1]] Whether to use inertia when updating the transition probability parameters. Default is 0.0.

distribution_inertia [double, optional, range [0, 1]] Whether to use inertia when updating the distribution parameters. Default is 0.0.

n_jobs [int, optional] The number of threads to use when performing training. This leads to exact updates. Default is 1.

Returns

improvement [double] The total improvement in fitting the model to the data

forward()

Run the forward algorithm on the sequence.

Calculate the probability of each observation being aligned to each state by going forward through a sequence. Returns the full forward matrix. Each index i, j corresponds to the sum-of-all-paths log probability of starting at the beginning of the sequence, and aligning observations to hidden states in such a manner that observation i was aligned to hidden state j. Uses row normalization to dynamically scale each row to prevent underflow errors.

If the sequence is impossible, will return a matrix of nans.

See also:

- Silent state handling taken from p. 71 of "Biological

Sequence Analysis" by Durbin et al., and works for anything which does not have loops of silent states.

- Row normalization technique explained by

http://www.cs.sjsu.edu/~stamp/RUA/HMM.pdf on p. 14.

Parameters

sequence [array-like] An array (or list) of observations.

Returns

matrix [array-like, shape (len(sequence), n_states)] The probability of aligning the sequences to states in a forward fashion.

forward_backward()

Run the forward-backward algorithm on the sequence.

This algorithm returns an emission matrix and a transition matrix. The emission matrix returns the normalized probability that each each state generated that emission given both the symbol and the entire sequence. The transition matrix returns the expected number of times that a transition is used.

If the sequence is impossible, will return (None, None)

See also:

- Forward and backward algorithm implementations. A comprehensive

description of the forward, backward, and forward-background algorithm is here: http://en.wikipedia.org/wiki/Forward%E2%80%93backward_algorithm

Parameters

sequence [array-like] An array (or list) of observations.

Returns

emissions [array-like, shape (len(sequence), n_nonsilent_states)] The normalized probabilities of each state generating each emission.

transitions [array-like, shape (n_states, n_states)] The expected number of transitions across each edge in the model.

freeze()

Freeze the distribution, preventing updates from occuring.

freeze_distributions()

Freeze all the distributions in model.

Upon training only edges will be updated. The parameters of distributions will not be affected.

Parameters

None

Returns

None

from_json()

Read in a serialized model and return the appropriate classifier.

Parameters

s [str] A JSON formatted string containing the file.

Returns

———-

model [object] A properly initialized and baked model.

from_matrix()

Create a model from a more standard matrix format.

Take in a 2D matrix of floats of size n by n, which are the transition probabilities to go from any state to any other state. May also take in a list of length n representing the names of these nodes, and a model name. Must provide the matrix, and a list of size n representing the distribution you wish to use for that state, a list of size n indicating the probability of starting in a state, and a list of size n indicating the probability of ending in a state.

Parameters

transition_probabilities [array-like, shape (n_states, n_states)] The probabilities of each state transitioning to each other state.

distributions [array-like, shape (n_states)] The distributions for each state. Silent states are indicated by using None instead of a distribution object.

starts [array-like, shape (n_states)] The probabilities of starting in each of the states.

ends [array-like, shape (n_states), optional] If passed in, the probabilities of ending in each of the states. If ends is None, then assumes the model has no explicit end state. Default is None.

state_names [array-like, shape (n_states), optional] The name of the states. If None is passed in, default names are generated. Default is None

name [str, optional] The name of the model. Default is None

verbose [bool, optional] The verbose parameter for the underlying bake method. Default is False.

merge ['None', 'Partial', 'All', optional] The merge parameter for the underlying bake method. Default is All

Returns

model [HiddenMarkovModel] The baked model ready to go.

Examples

matrix = [[0.4, 0.5], [0.4, 0.5]] distributions = [NormalDistribution(1, .5), NormalDistribution(5, 2)] starts = [1., 0.] ends = [.1., .1] state_names= ["A", "B"]

model = Model.from_matrix(matrix, distributions, starts, ends, state_names, name="test_model")

from_samples()

Learn the transitions and emissions of a model directly from data.

This method will learn both the transition matrix, emission distributions, and start probabilities for each state. This will only return a dense graph without any silent states or explicit transitions to an end state. Currently all components must be defined as the same distribution, but soon this restriction will be removed.

If learning a multinomial HMM over discrete characters, the initial emisison probabilities are initialized randomly. If learning a continuous valued HMM, such as a Gaussian HMM, then kmeans clustering is used first to identify initial clusters.

Regardless of the type of model, the transition matrix and start probabilities are initialized uniformly. Then the specified learning algorithm (Baum-Welch recommended) is used to refine the parameters of the model.

Parameters

distributions [callable] The emission distribution of the components of the model.

n_components [int] The number of states (or components) to initialize.

X [array-like] An array of some sort (list, numpy.ndarray, tuple..) of sequences, where each sequence is a numpy array, which is 1 dimensional if the HMM is a one dimensional array, or multidimensional if the HMM supports multiple dimensions.

weights [array-like or None, optional] An array of weights, one for each sequence to train on. If None, all sequences are equaly weighted. Default is None.

labels [array-like or None, optional] An array of state labels for each sequence. This is only used in 'labeled' training. If used this must be comprised of n lists where n is the number of sequences to train on, and each of those lists must have one label per observation. Default is None.

stop_threshold [double, optional] The threshold the improvement ratio of the models log probability in fitting the scores. Default is 1e-9.

min_iterations [int, optional] The minimum number of iterations to run Baum-Welch training for. Default is 0.

max_iterations [int, optional] The maximum number of iterations to run Baum-Welch training for. Default is 1e8.

algorithm ['baum-welch', 'viterbi', 'labeled'] The training algorithm to use. Baum-Welch uses the forward-backward algorithm to train using a version of structured EM. Viterbi iteratively runs the sequences through the Viterbi algorithm and then uses hard assignments of observations to states using that. Default is 'baum-welch'. Labeled training requires that labels are provided for each observation in each sequence.

verbose [bool, optional] Whether to print the improvement in the model fitting at each iteration. Default is True.

pseudocount [double, optional] A pseudocount to add to both transitions and emissions. If supplied, it will override both transition_pseudocount and emission_pseudocount in the same way that specifying *inertia* will override both *edge_inertia* and *distribution_inertia*. Default is None.

transition_pseudocount [double, optional] A pseudocount to add to all transitions to add a prior to the MLE estimate of the transition probability. Default is 0.

emission_pseudocount [double, optional] A pseudocount to add to the emission of each distribution. This effectively smoothes the states to prevent 0. probability symbols if they don't happen to occur in the data. Only effects hidden Markov models defined over discrete distributions. Default is 0.

use_pseudocount [bool, optional] Whether to use the pseudocounts defined in the *add_edge* method for edge-specific pseudocounts when updating the transition probability parameters. Does not effect the *transition_pseudocount* and *emission_pseudocount* parameters, but can be used in addition to them. Default is False.

inertia [double or None, optional, range [0, 1]] If double, will set both edge_inertia and distribution_inertia to be that value. If None, will not override those values. Default is None.

edge_inertia [bool, optional, range [0, 1]] Whether to use inertia when updating the transition probability parameters. Default is 0.0.

distribution_inertia [double, optional, range [0, 1]] Whether to use inertia when updating the distribution parameters. Default is 0.0.

n_jobs [int, optional] The number of threads to use when performing training. This leads to exact updates. Default is 1.

Returns

model [HiddenMarkovModel] The model fit to the data.

from_summaries()

Fit the model to the stored summary statistics.

Parameters

inertia [double or None, optional] The inertia to use for both edges and distributions without needing to set both of them. If None, use the values passed in to those variables. Default is None.

pseudocount [double, optional] A pseudocount to add to both transitions and emissions. If supplied, it will override both transition_pseudocount and emission_pseudocount in the same way that specifying *inertia* will override both *edge_inertia* and *distribution_inertia*. Default is None.

transition_pseudocount [double, optional] A pseudocount to add to all transitions to add a prior to the MLE estimate of the transition probability. Default is 0.

emission_pseudocount [double, optional] A pseudocount to add to the emission of each distribution. This effectively smoothes the states to prevent 0. probability symbols if they don't happen to occur in the data. Only effects hidden Markov models defined over discrete distributions. Default is 0.

use_pseudocount [bool, optional] Whether to use the pseudocounts defined in the *add_edge* method for edge-specific pseudocounts when updating the transition probability parameters. Does not effect the *transition_pseudocount* and *emission_pseudocount* parameters, but can be used in addition to them. Default is False.

edge_inertia [bool, optional, range [0, 1]] Whether to use inertia when updating the transition probability parameters. Default is 0.0.

distribution_inertia [double, optional, range [0, 1]] Whether to use inertia when updating the distribution parameters. Default is 0.0.

Returns

None

log_probability()

Calculate the log probability of a single sequence.

If a path is provided, calculate the log probability of that sequence given the path.

Parameters

sequence [array-like] Return the array of observations in a single sequence of data

check_input [bool, optional] Check to make sure that all emissions fall under the support of the emission distributions. Default is True.

Returns

logp [double] The log probability of the sequence

maximum_a_posteriori()
Run posterior decoding on the sequence.

MAP decoding is an alternative to viterbi decoding, which returns the most likely state for each observation, based on the forward-backward algorithm. This is also called posterior decoding. This method is described on p. 14 of http://ai.stanford.edu/~serafim/CS262_2007/ notes/lecture5.pdf

WARNING: This may produce impossible sequences.

Parameters

sequence [array-like] An array (or list) of observations.

Returns

logp [double] The log probability of the sequence under the Viterbi path

path [list of tuples] Tuples of (state index, state object) of the states along the posterior path.

node_count()
Returns the number of nodes/states in the model

plot()
Draw this model's graph using NetworkX and matplotlib.

Note that this relies on networkx's built-in graphing capabilities (and not Graphviz) and thus can't draw self-loops.

See networkx.draw_networkx() for the keywords you can pass in.

Parameters

precision [int, optional] The precision with which to round edge probabilities. Default is 4.

****kwargs** [any] The arguments to pass into networkx.draw_networkx()

Returns

None

predict()
Calculate the most likely state for each observation.

This can be either the Viterbi algorithm or maximum a posteriori. It returns the probability of the sequence under that state sequence and the actual state sequence.

This is a sklearn wrapper for the Viterbi and maximum_a_posteriori methods.

Parameters

sequence [array-like] An array (or list) of observations.

algorithm ["map", "viterbi"] The algorithm with which to decode the sequence

Returns

logp [double] The log probability of the sequence under the Viterbi path

path [list of tuples] Tuples of (state index, state object) of the states along the Viterbi path.

predict_log_proba()
Calculate the state log probabilities for each observation in the sequence.

Run the forward-backward algorithm on the sequence and return the emission matrix. This is the log normalized probability that each each state generated that emission given both the symbol and the entire sequence.

This is a sklearn wrapper for the forward backward algorithm.

See also:

- Forward and backward algorithm implementations. A comprehensive

description of the forward, backward, and forward-background algorithm is here: http://en.wikipedia.org/wiki/Forward%E2%80%93backward_algorithm

Parameters

sequence [array-like] An array (or list) of observations.

Returns

emissions [array-like, shape (len(sequence), n_nonsilent_states)] The log normalized probabilities of each state generating each emission.

predict_proba()

Calculate the state probabilities for each observation in the sequence.

Run the forward-backward algorithm on the sequence and return the emission matrix. This is the normalized probability that each each state generated that emission given both the symbol and the entire sequence.

This is a sklearn wrapper for the forward backward algorithm.

See also:

- Forward and backward algorithm implementations. A comprehensive

description of the forward, backward, and forward-background algorithm is here: http://en.wikipedia.org/wiki/Forward%E2%80%93backward_algorithm

Parameters

sequence [array-like] An array (or list) of observations.

Returns

emissions [array-like, shape (len(sequence), n_nonsilent_states)] The normalized probabilities of each state generating each emission.

probability()

Return the probability of the given symbol under this distribution.

Parameters

symbol [object] The symbol to calculate the probability of

Returns

probability [double] The probability of that point under the distribution.

sample()

Generate a sequence from the model.

Returns the sequence generated, as a list of emitted items. The model must have been baked first in order to run this method.

If a length is specified and the HMM is infinite (no edges to the end state), then that number of samples will be randomly generated. If the length is specified and the HMM is finite, the method will attempt to generate a prefix of that length. Currently it will force itself to not take an end transition unless that is the only path, making it not a true random sample on a finite model.

WARNING: If the HMM has no explicit end state, must specify a length to use.

Parameters

length [int, optional] Generate a sequence with a maximal length of this size. Used if you have no explicit end state. Default is 0.

path [bool, optional] Return the path of hidden states in addition to the emissions. If true will return a tuple of (sample, path). Default is False.

Returns

sample [list or tuple] If path is true, return a tuple of (sample, path), otherwise return just the samples.

state_count()
Returns the number of states present in the model.

summarize()
Summarize data into stored sufficient statistics for out-of-core training. Only implemented for Baum-Welch training since Viterbi is less memory intensive.

Parameters

sequences [array-like] An array of some sort (list, numpy.ndarray, tuple..) of sequences, where each sequence is a numpy array, which is 1 dimensional if the HMM is a one dimensional array, or multidimensional if the HMM supports multiple dimensions.

weights [array-like or None, optional] An array of weights, one for each sequence to train on. If None, all sequences are equaly weighted. Default is None.

labels [array-like or None, optional] An array of state labels for each sequence. This is only used in 'labeled' training. If used this must be comprised of n lists where n is the number of sequences to train on, and each of those lists must have one label per observation. Default is None.

algorithm ['baum-welch', 'viterbi', 'labeled'] The training algorithm to use. Baum-Welch uses the forward-backward algorithm to train using a version of structured EM. Viterbi iteratively runs the sequences through the Viterbi algorithm and then uses hard assignments of observations to states using that. Default is 'baum-welch'. Labeled training requires that labels are provided for each observation in each sequence.

n_jobs [int, optional] The number of threads to use when performing training. This leads to exact updates. Default is 1.

parallel [joblib.Parallel or None, optional] The joblib threadpool. Passed between iterations of Baum-Welch so that a new threadpool doesn't have to be created each iteration. Default is None.

check_input [bool, optional] Check the input. This casts the input sequences as numpy arrays, and converts non-numeric inputs into numeric inputs for faster processing later. Default is True.

Returns

logp [double] The log probability of the sequences.

thaw()
Thaw the distribution, re-allowing updates to occur.

thaw_distributions()
Thaw all distributions in the model.

Upon training distributions will be updated again.

Parameters

None

Returns

None

to_json()
Serialize the model to a JSON.

Parameters

separators [tuple, optional] The two separaters to pass to the json.dumps function for formatting.

indent [int, optional] The indentation to use at each level. Passed to json.dumps for formatting.

Returns

json [str] A properly formatted JSON object.

viterbi()
Run the Viteri algorithm on the sequence.

Run the Viterbi algorithm on the sequence given the model. This finds the ML path of hidden states given the sequence. Returns a tuple of the log probability of the ML path, or (-inf, None) if the sequence is impossible under the model. If a path is returned, it is a list of tuples of the form (sequence index, state object).

This is fundamentally the same as the forward algorithm using max instead of sum, except the traceback is more complicated, because silent states in the current step can trace back to other silent states in the current step as well as states in the previous step.

See also:

- Viterbi implementation described well in the wikipedia article

http://en.wikipedia.org/wiki/Viterbi_algorithm

Parameters

sequence [array-like] An array (or list) of observations.

Returns

logp [double] The log probability of the sequence under the Viterbi path

path [list of tuples] Tuples of (state index, state object) of the states along the Viterbi path.

pomegranate.hmm.**log**()
Return the natural log of the value or -infinity if the value is 0.

1.6 Bayes Classifiers and Naive Bayes

IPython Notebook Tutorial

Bayes classifiers are simple probabilistic classification models based off of Bayes throerom. See the above tutorial for a full primer on how they work, and what the distinction between a naive Bayes classifier and a Bayes classifier is. Essentially, each class is modeled by a probability distribution and classifications are made according to what distribution fits the data the best. They are a supervised version of general mixture models, in that the `predict`, `predict_proba`, and `predict_log_proba` methods return the same values for the same underlying distributions, but that instead of using expectation-maximization to fit to new data they can use the provided labels directly.

1.6.1 Initialization

Bayes classifiers and naive Bayes can both be initialized in one of two ways depending on if you know the parameters of the model beforehand or not, (1) passing in a list of pre-initialized distributions to the model, or (2) using the `from_samples` class method to initialize the model directly from data. For naive Bayes models on multivariate data, the pre-initialized distributions must be a list of `IndependentComponentDistribution` objects since each dimension is modeled independently from the others. For Bayes classifiers on multivariate data a list of any type of multivariate distribution can be provided. For univariate data the two models produce identical results, and can be passed in a list of univariate distributions. For example:

```
from pomegranate import *
d1 = IndependentComponentsDistribution([NormalDistribution(5, 2),␣
↪NormalDistribution(6, 1), NormalDistribution(9, 1)])
d2 = IndependentComponentsDistribution([NormalDistribution(2, 1),␣
↪NormalDistribution(8, 1), NormalDistribution(5, 1)])
d3 = IndependentComponentsDistribution([NormalDistribution(3, 1),␣
↪NormalDistribution(5, 3), NormalDistribution(4, 1)])
model = NaiveBayes([d1, d2, d3])
```

would create a three class naive Bayes classifier that modeled data with three dimensions. Alternatively, we can initialize a Bayes classifier in the following manner

```
from pomegranate import *
d1 = MultivariateGaussianDistribution([5, 6, 9], [[2, 0, 0], [0, 1, 0], [0, 0, 1]])
d2 = MultivariateGaussianDistribution([2, 8, 5], [[1, 0, 0], [0, 1, 0], [0, 0, 1]])
d3 = MultivariateGaussianDistribution([3, 5, 4], [[1, 0, 0], [0, 3, 0], [0, 0, 1]])
model = BayesClassifier([d1, d2, d3])
```

The two examples above functionally creatte the same model, as the Bayes classifier uses multivariate Gaussian distributions with the same means and a diagonal covariance matrix containing only the variances. However, if we were to fit these models to data later on, the Bayes classifier would learn a full covariance matrix while the naive Bayes would only learn the diagonal.

If we instead wish to initialize our model directly onto data, we use the `from_samples` class method.

```
from pomegranate import *
import numpy
X = numpy.load('data.npy')
y = numpy.load('labels.npy')
model = NaiveBayes.from_samples(NormalDistribution, X, y)
```

This would create a naive Bayes model directly from the data with normal distributions modeling each of the dimensions, and a number of components equal to the number of classes in `y`. Alternatively if we wanted to create a model with different distributions for each dimension we can do the following:

```
model = NaiveBayes.from_samples([NormalDistribution, ExponentialDistribution], X, y)
```

This assumes that your data is two dimensional and that you want to model the first distribution as a normal distribution and the second dimension as an exponential distribution.

We can do pretty much the same thing with Bayes classifiers, except passing in a more complex model.

```
model = BayesClassifier.from_samples(MultivariateGaussianDistribution, X, y)
```

One can use much more complex models than just a multivariate Gaussian with a full covariance matrix when using a Bayes classifier. Specifically, you can also have your distributions be general mixture models, hidden Markov models, and Bayesian networks. For example:

```
model = BayesClassifier.from_samples(BayesianNetwork, X, y)
```

That would require that the data is only discrete valued currently, and the structure learning task may be too long if not set appropriately. However, it is possible. Currently, one cannot simply put in GeneralMixtureModel or HiddenMarkovModel despite them having a `from_samples` method because there is a great deal of flexibility in terms of the structure or emission distributions. The easiest way to set up one of these more complex models is to build each of the components separately and then feed them into the Bayes classifier method using the first initialization method.

```
d1 = GeneralMixtureModel.from_samples(MultivariateGaussianDistribution, n_
↪components=5, X=X[y==0])
d2 = GeneralMixtureModel.from_samples(MultivariateGaussianDistribution, n_
↪components=5, X=X[y==1])
model = BayesClassifier([d1, d2])
```

1.6.2 Prediction

Bayes classifiers and naive Bayes supports the same three prediction methods that the other models support, `predict`, `predict_proba`, and `predict_log_proba`. These methods return the most likely class given the data (argmax_m P(M|D)), the probability of each class given the data (P(M|D)), and the log probability of each class given the data (log P(M|D)). It is best to always pass in a 2D matrix even for univariate data, where it would have a shape of (n, 1).

The `predict` method takes in samples and returns the most likely class given the data.

```
from pomegranate import *
model = NaiveBayes([NormalDistribution(5, 2), UniformDistribution(0, 10),␣
↪ExponentialDistribution(1.0)])
model.predict( np.array([[0], [1], [2], [3], [4]]))
[2, 2, 2, 0, 0]
```

Calling `predict_proba` on five samples for a Naive Bayes with univariate components would look like the following.

```
from pomegranate import *
model = NaiveBayes([NormalDistribution(5, 2), UniformDistribution(0, 10),␣
↪ExponentialDistribution(1)])
model.predict_proba(np.array([[0], [1], [2], [3], [4]]))
[[ 0.00790443  0.09019051  0.90190506]
 [ 0.05455011  0.20207126  0.74337863]
 [ 0.21579499  0.33322883  0.45097618]
 [ 0.44681566  0.36931382  0.18387052]
 [ 0.59804205  0.33973357  0.06222437]]
```

Multivariate models work the same way.

```
from pomegranate import *
d1 = MultivariateGaussianDistribution([5, 5], [[1, 0], [0, 1]])
d2 = IndependentComponentsDistribution([NormalDistribution(5, 2),␣
↪NormalDistribution(5, 2)])
model = BayesClassifier([d1, d2])
clf.predict_proba(np.array([[0, 4],
                                                    [1, 3],
                                                    [2, 2],
                                                    [3, 1],
                                                    [4, 0]]))
```

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```
array([[ 0.00023312,  0.99976688],
       [ 0.00220745,  0.99779255],
       [ 0.00466169,  0.99533831],
       [ 0.00220745,  0.99779255],
       [ 0.00023312,  0.99976688]])
```

`predict_log_proba` works the same way, returning the log probabilities instead of the probabilities.

1.6.3 Fitting

Both naive Bayes and Bayes classifiers also have a `fit` method that updates the parameters of the model based on new data. The major difference between these methods and the others presented is that these are supervised methods and so need to be passed labels in addition to data. This change propogates also to the `summarize` method, where labels are provided as well.

```
from pomegranate import *
d1 = MultivariateGaussianDistribution([5, 5], [[1, 0], [0, 1]])
d2 = IndependentComponentsDistribution(NormalDistribution(5, 2), NormalDistribution(5,
↪ 2)])
model = BayesClassifier([d1, d2])
X = np.array([[6.0, 5.0],
                           [3.5, 4.0],
                           [7.5, 1.5],
                               [7.0, 7.0 ]])
y = np.array([0, 0, 1, 1])
model.fit(X, y)
```

As we can see, there are four samples, with the first two samples labeled as class 0 and the last two samples labeled as class 1. Keep in mind that the training samples must match the input requirements for the models used. So if using a univariate distribution, then each sample must contain one item. A bivariate distribution, two. For hidden markov models, the sample can be a list of observations of any length. An example using hidden markov models would be the following.

```
d1 = HiddenMarkovModel...
d2 = HiddenMarkovModel...
d3 = HiddenMarkovModel...
model = BayesClassifier([d1, d2, d3])
X = np.array([list('HHHHHTHTHTTTTH'),
                                              list('HHTHHTTHHHHHTH'),
                                              list('TH'),
                                              list('HHHHT')])
y = np.array([2, 2, 1, 0])
model.fit(X, y)
```

1.6.4 API Reference

class pomegranate.NaiveBayes.**NaiveBayes**

A naive Bayes model, a supervised alternative to GMM.

A naive Bayes classifier, that treats each dimension independently from each other. This is a simpler version of the Bayes Classifier, that can use any distribution with any covariance structure, including Bayesian networks and hidden Markov models.

Parameters

models [list] A list of initialized distributions.

weights [list or numpy.ndarray or None, default None] The prior probabilities of the components. If None is passed in then defaults to the uniformly distributed priors.

Examples

```
>>> from pomegranate import *
>>> X = [0, 2, 0, 1, 0, 5, 6, 5, 7, 6]
>>> y = [0, 0, 0, 0, 0, 1, 1, 0, 1, 1]
>>> clf = NaiveBayes.from_samples(NormalDistribution, X, y)
>>> clf.predict_proba([6])
array([[0.01973451,  0.98026549]])
```

```
>>> from pomegranate import *
>>> clf = NaiveBayes([NormalDistribution(1, 2), NormalDistribution(0, 1)])
>>> clf.predict_log_proba([[0], [1], [2], [-1]])
array([[-1.1836569 , -0.36550972],
           [-0.79437677, -0.60122959],
           [-0.26751248, -1.4493653],
           [-1.09861229, -0.40546511]])
```

Attributes

models [list] The model objects, either initialized by the user or fit to data.

weights [numpy.ndarray] The prior probability of each component of the model.

clear_summaries()
Remove the stored sufficient statistics.

Parameters

None

Returns

None

copy()
Return a deep copy of this distribution object.

This object will not be tied to any other distribution or connected in any form.

Parameters

None

Returns

distribution [Distribution] A copy of the distribution with the same parameters.

fit()
Fit the Naive Bayes model to the data by passing data to their components.

Parameters

X [numpy.ndarray or list] The dataset to operate on. For most models this is a numpy array with columns corresponding to features and rows corresponding to samples. For markov chains and HMMs this will be a list of variable length sequences.

y [numpy.ndarray or list or None, optional] Data labels for supervised training algorithms. Default is None

weights [array-like or None, shape (n_samples,), optional] The initial weights of each sample in the matrix. If nothing is passed in then each sample is assumed to be the same weight. Default is None.

n_jobs [int] The number of jobs to use to parallelize, either the number of threads or the number of processes to use. Default is 1.

inertia [double, optional] Inertia used for the training the distributions.

pseudocount [double, optional] A pseudocount to add to the emission of each distribution. This effectively smoothes the states to prevent 0. probability symbols if they don't happen to occur in the data. Default is 0.

stop_threshold [double, optional, positive] The threshold at which EM will terminate for the improvement of the model. If the model does not improve its fit of the data by a log probability of 0.1 then terminate. Only required if doing semisupervised learning. Default is 0.1.

max_iterations [int, optional, positive] The maximum number of iterations to run EM for. If this limit is hit then it will terminate training, regardless of how well the model is improving per iteration. Only required if doing semisupervised learning. Default is 1e8.

verbose [bool, optional] Whether or not to print out improvement information over iterations. Only required if doing semisupervised learning. Default is False.

Returns

self [object] Returns the fitted model

freeze()

Freeze the distribution, preventing updates from occuring.

from_samples()

Create a mixture model directly from the given dataset.

First, k-means will be run using the given initializations, in order to define initial clusters for the points. These clusters are used to initialize the distributions used. Then, EM is run to refine the parameters of these distributions.

A homogenous mixture can be defined by passing in a single distribution callable as the first parameter and specifying the number of components, while a heterogeneous mixture can be defined by passing in a list of callables of the appropriate type.

Parameters

distributions [array-like, shape (n_components,) or callable]

The components of the model. If array, corresponds to the initial distributions of the components. If callable, must also pass in the number of components and kmeans++ will be used to initialize them.

n_components [int] If a callable is passed into distributions then this is the number of components to initialize using the kmeans++ algorithm.

X [array-like, shape (n_samples, n_dimensions)] This is the data to train on. Each row is a sample, and each column is a dimension to train on.

weights [array-like, shape (n_samples,), optional] The initial weights of each sample in the matrix. If nothing is passed in then each sample is assumed to be the same weight. Default is None.

pseudocount : double, optional, positive

A pseudocount to add to the emission of each distribution. This

effectively smoothes the states to prevent 0. probability symbols

if they don't happen to occur in the data. Only effects mixture

models defined over discrete distributions. Default is 0.

stop_threshold [double, optional, positive] The threshold at which EM will terminate for the improvement of the model. If the model does not improve its fit of the data by a log probability of 0.1 then terminate. Only required if doing semisupervised learning. Default is 0.1.

max_iterations [int, optional, positive] The maximum number of iterations to run EM for. If this limit is hit then it will terminate training, regardless of how well the model is improving per iteration. Only required if doing semisupervised learning. Default is 1e8.

verbose [bool, optional] Whether or not to print out improvement information over iterations. Only required if doing semisupervised learning. Default is False.

Returns

model [NaiveBayes] The fit naive Bayes model.

from_summaries()

Fit the model to the collected sufficient statistics.

Fit the parameters of the model to the sufficient statistics gathered during the summarize calls. This should return an exact update.

Parameters

inertia [double, optional] The weight of the previous parameters of the model. The new parameters will roughly be old_param*inertia + new_param*(1-inertia), so an inertia of 0 means ignore the old parameters, whereas an inertia of 1 means ignore the new parameters. Default is 0.0.

pseudocount [double, optional] A pseudocount to add to the emission of each distribution. This effectively smoothes the states to prevent 0. probability symbols if they don't happen to occur in the data. If discrete data, will smooth both the prior probabilities of each component and the emissions of each component. Otherwise, will only smooth the prior probabilities of each component. Default is 0.

Returns

None

log_probability()

Calculate the log probability of a point under the distribution.

The probability of a point is the sum of the probabilities of each distribution multiplied by the weights. Thus, the log probability is the sum of the log probability plus the log prior.

This is the python interface.

Parameters

X [numpy.ndarray, shape=(n, d) or (n, m, d)] The samples to calculate the log probability of. Each row is a sample and each column is a dimension. If emissions are HMMs then shape is (n, m, d) where m is variable length for each obervation, and X becomes an array of n (m, d)-shaped arrays.

Returns

log_probability [double] The log probabiltiy of the point under the distribution.

predict()

Predict the most likely component which generated each sample.

Calculate the posterior P(M|D) for each sample and return the index of the component most likely to fit it. This corresponds to a simple argmax over the responsibility matrix.

This is a sklearn wrapper for the maximum_a_posteriori method.

Parameters

X [array-like, shape (n_samples, n_dimensions)] The samples to do the prediction on. Each sample is a row and each column corresponds to a dimension in that sample. For univariate distributions, a single array may be passed in.

Returns

y [array-like, shape (n_samples,)] The predicted component which fits the sample the best.

predict_log_proba()

Calculate the posterior log P(M|D) for data.

Calculate the log probability of each item having been generated from each component in the model. This returns normalized log probabilities such that the probabilities should sum to 1

This is a sklearn wrapper for the original posterior function.

Parameters

X [array-like, shape (n_samples, n_dimensions)] The samples to do the prediction on. Each sample is a row and each column corresponds to a dimension in that sample. For univariate distributions, a single array may be passed in.

Returns

y [array-like, shape (n_samples, n_components)] The normalized log probability log P(M|D) for each sample. This is the probability that the sample was generated from each component.

predict_proba()

Calculate the posterior P(M|D) for data.

Calculate the probability of each item having been generated from each component in the model. This returns normalized probabilities such that each row should sum to 1.

Since calculating the log probability is much faster, this is just a wrapper which exponentiates the log probability matrix.

Parameters

X [array-like, shape (n_samples, n_dimensions)] The samples to do the prediction on. Each sample is a row and each column corresponds to a dimension in that sample. For univariate distributions, a single array may be passed in.

Returns

probability [array-like, shape (n_samples, n_components)] The normalized probability P(M|D) for each sample. This is the probability that the sample was generated from each component.

probability()
Return the probability of the given symbol under this distribution.

Parameters

symbol [object] The symbol to calculate the probability of

Returns

probability [double] The probability of that point under the distribution.

sample()
Generate a sample from the model.

First, randomly select a component weighted by the prior probability, Then, use the sample method from that component to generate a sample.

Parameters

n [int, optional] The number of samples to generate. Defaults to 1.

Returns

sample [array-like or object] A randomly generated sample from the model of the type modelled by the emissions. An integer if using most distributions, or an array if using multivariate ones, or a string for most discrete distributions. If n=1 return an object, if n>1 return an array of the samples.

summarize()
Summarize data into stored sufficient statistics for out-of-core training.

Parameters

X [array-like, shape (n_samples, variable)] Array of the samples, which can be either fixed size or variable depending on the underlying components.

y [array-like, shape (n_samples,)] Array of the known labels as integers

weights [array-like, shape (n_samples,) optional] Array of the weight of each sample, a positive float

n_jobs [int] The number of jobs to use to parallelize, either the number of threads or the number of processes to use. Default is 1.

Returns

None

thaw()
Thaw the distribution, re-allowing updates to occur.

to_json()
Serialize the model to a JSON.

Parameters

separators [tuple, optional] The two separaters to pass to the json.dumps function for formatting. Default is (',', ' : ').

indent [int, optional] The indentation to use at each level. Passed to json.dumps for formatting. Default is 4.

Returns

json [str] A properly formatted JSON object.

class pomegranate.BayesClassifier.**BayesClassifier**

A Naive Bayes model, a supervised alternative to GMM.

Parameters

models [list or constructor] Must either be a list of initialized distribution/model objects, or the constructor for a distribution object:

- Initialized : NaiveBayes([NormalDistribution(1, 2), NormalDistribution(0, 1)])
- Constructor : NaiveBayes(NormalDistribution)

weights [list or numpy.ndarray or None, default None] The prior probabilities of the components. If None is passed in then defaults to the uniformly distributed priors.

Examples

```
>>> from pomegranate import *
>>> clf = NaiveBayes( NormalDistribution )
>>> X = [0, 2, 0, 1, 0, 5, 6, 5, 7, 6]
>>> y = [0, 0, 0, 0, 0, 1, 1, 0, 1, 1]
>>> clf.fit(X, y)
>>> clf.predict_proba([6])
array([[ 0.01973451,  0.98026549]])
```

```
>>> from pomegranate import *
>>> clf = NaiveBayes([NormalDistribution(1, 2), NormalDistribution(0, 1)])
>>> clf.predict_log_proba([[0], [1], [2], [-1]])
array([[-1.1836569 , -0.36550972],
           [-0.79437677, -0.60122959],
           [-0.26751248, -1.4493653 ],
           [-1.09861229, -0.40546511]])
```

Attributes

models [list] The model objects, either initialized by the user or fit to data.

weights [numpy.ndarray] The prior probability of each component of the model.

clear_summaries()

Remove the stored sufficient statistics.

Parameters

None

Returns

None

copy()

Return a deep copy of this distribution object.

This object will not be tied to any other distribution or connected in any form.

Parameters

None

Returns

distribution [Distribution] A copy of the distribution with the same parameters.

fit()

Fit the Naive Bayes model to the data by passing data to their components.

Parameters

X [numpy.ndarray or list] The dataset to operate on. For most models this is a numpy array with columns corresponding to features and rows corresponding to samples. For markov chains and HMMs this will be a list of variable length sequences.

y [numpy.ndarray or list or None, optional] Data labels for supervised training algorithms. Default is None

weights [array-like or None, shape (n_samples,), optional] The initial weights of each sample in the matrix. If nothing is passed in then each sample is assumed to be the same weight. Default is None.

n_jobs [int] The number of jobs to use to parallelize, either the number of threads or the number of processes to use. Default is 1.

inertia [double, optional] Inertia used for the training the distributions.

pseudocount [double, optional] A pseudocount to add to the emission of each distribution. This effectively smoothes the states to prevent 0. probability symbols if they don't happen to occur in the data. Default is 0.

stop_threshold [double, optional, positive] The threshold at which EM will terminate for the improvement of the model. If the model does not improve its fit of the data by a log probability of 0.1 then terminate. Only required if doing semisupervised learning. Default is 0.1.

max_iterations [int, optional, positive] The maximum number of iterations to run EM for. If this limit is hit then it will terminate training, regardless of how well the model is improving per iteration. Only required if doing semisupervised learning. Default is 1e8.

verbose [bool, optional] Whether or not to print out improvement information over iterations. Only required if doing semisupervised learning. Default is False.

Returns

self [object] Returns the fitted model

freeze()

Freeze the distribution, preventing updates from occuring.

from_samples()

Create a mixture model directly from the given dataset.

First, k-means will be run using the given initializations, in order to define initial clusters for the points. These clusters are used to initialize the distributions used. Then, EM is run to refine the parameters of these distributions.

A homogenous mixture can be defined by passing in a single distribution callable as the first parameter and specifying the number of components, while a heterogeneous mixture can be defined by passing in a list of callables of the appropriate type.

Parameters

distributions [array-like, shape (n_components,) or callable]

The components of the model. If array, corresponds to the initial distributions of the components. If callable, must also pass in the number of components and kmeans++ will be used to initialize them.

n_components [int] If a callable is passed into distributions then this is the number of components to initialize using the kmeans++ algorithm.

X [array-like, shape (n_samples, n_dimensions)] This is the data to train on. Each row is a sample, and each column is a dimension to train on.

weights [array-like, shape (n_samples,), optional] The initial weights of each sample in the matrix. If nothing is passed in then each sample is assumed to be the same weight. Default is None.

pseudocount : double, optional, positive

A pseudocount to add to the emission of each distribution. This

effectively smoothes the states to prevent 0. probability symbols

if they don't happen to occur in the data. Only effects mixture

models defined over discrete distributions. Default is 0.

Returns

model [NaiveBayes] The fit naive Bayes model.

from_summaries()

Fit the model to the collected sufficient statistics.

Fit the parameters of the model to the sufficient statistics gathered during the summarize calls. This should return an exact update.

Parameters

inertia [double, optional] The weight of the previous parameters of the model. The new parameters will roughly be old_param*inertia + new_param*(1-inertia), so an inertia of 0 means ignore the old parameters, whereas an inertia of 1 means ignore the new parameters. Default is 0.0.

pseudocount [double, optional] A pseudocount to add to the emission of each distribution. This effectively smoothes the states to prevent 0. probability symbols if they don't happen to occur in the data. If discrete data, will smooth both the prior probabilities of each component and the emissions of each component. Otherwise, will only smooth the prior probabilities of each component. Default is 0.

Returns

None

log_probability()

Calculate the log probability of a point under the distribution.

The probability of a point is the sum of the probabilities of each distribution multiplied by the weights. Thus, the log probability is the sum of the log probability plus the log prior.

This is the python interface.

Parameters

X [numpy.ndarray, shape=(n, d) or (n, m, d)] The samples to calculate the log probability of. Each row is a sample and each column is a dimension. If emissions are HMMs then shape

is (n, m, d) where m is variable length for each obervation, and X becomes an array of n (m, d)-shaped arrays.

Returns

log_probability [double] The log probabiltiy of the point under the distribution.

predict()

Predict the most likely component which generated each sample.

Calculate the posterior P(M|D) for each sample and return the index of the component most likely to fit it. This corresponds to a simple argmax over the responsibility matrix.

This is a sklearn wrapper for the maximum_a_posteriori method.

Parameters

X [array-like, shape (n_samples, n_dimensions)] The samples to do the prediction on. Each sample is a row and each column corresponds to a dimension in that sample. For univariate distributions, a single array may be passed in.

Returns

y [array-like, shape (n_samples,)] The predicted component which fits the sample the best.

predict_log_proba()

Calculate the posterior log P(M|D) for data.

Calculate the log probability of each item having been generated from each component in the model. This returns normalized log probabilities such that the probabilities should sum to 1

This is a sklearn wrapper for the original posterior function.

Parameters

X [array-like, shape (n_samples, n_dimensions)] The samples to do the prediction on. Each sample is a row and each column corresponds to a dimension in that sample. For univariate distributions, a single array may be passed in.

Returns

y [array-like, shape (n_samples, n_components)] The normalized log probability log P(M|D) for each sample. This is the probability that the sample was generated from each component.

predict_proba()

Calculate the posterior P(M|D) for data.

Calculate the probability of each item having been generated from each component in the model. This returns normalized probabilities such that each row should sum to 1.

Since calculating the log probability is much faster, this is just a wrapper which exponentiates the log probability matrix.

Parameters

X [array-like, shape (n_samples, n_dimensions)] The samples to do the prediction on. Each sample is a row and each column corresponds to a dimension in that sample. For univariate distributions, a single array may be passed in.

Returns

probability [array-like, shape (n_samples, n_components)] The normalized probability P(M|D) for each sample. This is the probability that the sample was generated from each component.

probability()
Return the probability of the given symbol under this distribution.

Parameters

symbol [object] The symbol to calculate the probability of

Returns

probability [double] The probability of that point under the distribution.

sample()
Generate a sample from the model.

First, randomly select a component weighted by the prior probability, Then, use the sample method from that component to generate a sample.

Parameters

n [int, optional] The number of samples to generate. Defaults to 1.

Returns

sample [array-like or object] A randomly generated sample from the model of the type modelled by the emissions. An integer if using most distributions, or an array if using multivariate ones, or a string for most discrete distributions. If n=1 return an object, if n>1 return an array of the samples.

summarize()
Summarize data into stored sufficient statistics for out-of-core training.

Parameters

X [array-like, shape (n_samples, variable)] Array of the samples, which can be either fixed size or variable depending on the underlying components.

y [array-like, shape (n_samples,)] Array of the known labels as integers

weights [array-like, shape (n_samples,) optional] Array of the weight of each sample, a positive float

n_jobs [int] The number of jobs to use to parallelize, either the number of threads or the number of processes to use. Default is 1.

Returns

None

thaw()
Thaw the distribution, re-allowing updates to occur.

to_json()
Serialize the model to a JSON.

Parameters

separators [tuple, optional] The two separaters to pass to the json.dumps function for formatting. Default is (‘,’, ‘ : ‘).

indent [int, optional] The indentation to use at each level. Passed to json.dumps for formatting. Default is 4.

Returns

json [str] A properly formatted JSON object.

1.7 Markov Chains

IPython Notebook Tutorial

Markov chains are form of structured model over sequences. They represent the probability of each character in the sequence as a conditional probability of the last k symbols. For example, a 3rd order Markov chain would have each symbol depend on the last three symbols. A 0th order Markov chain is a naive predictor where each symbol is independent of all other symbols. Currently pomegranate only supports discrete emission Markov chains where each symbol is a discrete symbol versus a continuous number (like 'A' 'B' 'C' instead of 17.32 or 19.65).

1.7.1 Initialization

Markov chains can almost be represented by a single conditional probability table (CPT), except that the probability of the first k elements (for a k-th order Markov chain) cannot be appropriately represented except by using special characters. Due to this pomegranate takes in a series of k+1 distributions representing the first k elements. For example for a second order Markov chain:

```
from pomegranate import *
d1 = DiscreteDistribution({'A': 0.25, 'B': 0.75})
d2 = ConditionalProbabilityTable([['A', 'A', 0.1],
                                  ['A', 'B', 0.9],
                                  ['B', 'A', 0.6],
                                  ['B', 'B', 0.4]], [d1])
d3 = ConditionalProbabilityTable([['A', 'A', 'A', 0.4],
                                  ['A', 'A', 'B', 0.6],
                                  ['A', 'B', 'A', 0.8],
                                  ['A', 'B', 'B', 0.2],
                                  ['B', 'A', 'A', 0.9],
                                  ['B', 'A', 'B', 0.1],
                                  ['B', 'B', 'A', 0.2],
                                  ['B', 'B', 'B', 0.8]], [d1, d2])
model = MarkovChain([d1, d2, d3])
```

1.7.2 Probability

The probability of a sequence under the Markov chain is just the probabiliy of the first character under the first distribution times the probability of the second character under the second distribution and so forth until you go past the (k+1)th character, which remains evaluated under the (k+1)th distribution. We can calculate the probability or log probability in the same manner as any of the other models. Given the model shown before:

```
>>> model.log_probability(['A', 'B', 'B', 'B'])
-3.324236340526027
>>> model.log_probability(['A', 'A', 'A', 'A'])
-5.521460917862246
```

1.7.3 Fitting

Markov chains are not very complicated to chain. For each sequence the appropriate symbols are sent to the appropriate distributions and maximum likelihood estimates are used to update the parameters of the distributions. There are no latent factors to train and so no expectation maximization or iterative algorithms are needed to train anything.

1.7.4 API Reference

class pomegranate.MarkovChain.**MarkovChain**
A Markov Chain.

Implemented as a series of conditional distributions, the Markov chain models P(X_i | X_i-1... X_i-k) for a k-th order Markov network. The conditional dependencies are directly on the emissions, and not on a hidden state as in a hidden Markov model.

Parameters

distributions [list, shape (k+1)] A list of the conditional distributions which make up the markov chain. Begins with P(X_i), then P(X_i | X_i-1). For a k-th order markov chain you must put in k+1 distributions.

Examples

```
>>> from pomegranate import *
>>> d1 = DiscreteDistribution({'A': 0.25, 'B': 0.75})
>>> d2 = ConditionalProbabilityTable([['A', 'A', 0.33],
                                      ['B', 'A', 0.67],
                                      ['A', 'B', 0.82],
                                      ['B', 'B', 0.18]], [d1])
>>> mc = MarkovChain([d1, d2])
>>> mc.log_probability(list('ABBAABABABAABABA'))
-8.9119890701808213
```

Attributes

distributions [list, shape (k+1)] The distributions which make up the chain.

fit()
Fit the model to new data using MLE.

The underlying distributions are fed in their appropriate points and weights and are updated.

Parameters

sequences [array-like, shape (n_samples, variable)] This is the data to train on. Each row is a sample which contains a sequence of variable length

weights [array-like, shape (n_samples,), optional] The initial weights of each sample. If nothing is passed in then each sample is assumed to be the same weight. Default is None.

inertia [double, optional] The weight of the previous parameters of the model. The new parameters will roughly be old_param*inertia + new_param*(1-inertia), so an inertia of 0 means ignore the old parameters, whereas an inertia of 1 means ignore the new parameters. Default is 0.0.

Returns

None

from_json()
Read in a serialized model and return the appropriate classifier.

Parameters

s [str] A JSON formatted string containing the file.

Returns

model [object] A properly initialized and baked model.

from_samples()

Learn the Markov chain from data.

Takes in the memory of the chain (k) and learns the initial distribution and probability tables associated with the proper parameters.

Parameters

X [array-like, list or numpy.array] The data to fit the structure too as a list of sequences of variable length. Since the data will be of variable length, there is no set form

weights [array-like, shape (n_nodes), optional] The weight of each sample as a positive double. Default is None.

k [int, optional] The number of samples back to condition on in the model. Default is 1.

Returns

model [MarkovChain] The learned markov chain model.

from_summaries()

Fit the model to the collected sufficient statistics.

Fit the parameters of the model to the sufficient statistics gathered during the summarize calls. This should return an exact update.

Parameters

inertia [double, optional] The weight of the previous parameters of the model. The new parameters will roughly be old_param*inertia + new_param * (1-inertia), so an inertia of 0 means ignore the old parameters, whereas an inertia of 1 means ignore the new parameters. Default is 0.0.

Returns

None

log_probability()

Calculate the log probability of the sequence under the model.

This calculates the first slices of increasing size under the corresponding first few components of the model until size k is reached, at which all slices are evaluated under the final component.

Parameters

sequence [array-like] An array of observations

Returns

logp [double] The log probability of the sequence under the model.

sample()

Create a random sample from the model.

Parameters

length [int or Distribution] Give either the length of the sample you want to generate, or a distribution object which will be randomly sampled for the length. Continuous distributions will have their sample rounded to the nearest integer, minimum 1.

Returns

sequence [array-like, shape = (length,)] A sequence randomly generated from the markov chain.

summarize()
Summarize a batch of data and store sufficient statistics.

This will summarize the sequences into sufficient statistics stored in each distribution.

Parameters

sequences [array-like, shape (n_samples, variable)] This is the data to train on. Each row is a sample which contains a sequence of variable length

weights [array-like, shape (n_samples,), optional] The initial weights of each sample. If nothing is passed in then each sample is assumed to be the same weight. Default is None.

Returns

None

to_json()
Serialize the model to a JSON.

Parameters

separators [tuple, optional] The two separaters to pass to the json.dumps function for formatting. Default is (',', ' : ').

indent [int, optional] The indentation to use at each level. Passed to json.dumps for formatting. Default is 4.

Returns

json [str] A properly formatted JSON object.

1.8 Bayesian Networks

- IPython Notebook Tutorial
- IPython Notebook Structure Learning Tutorial

Bayesian networks are a probabilistic model that are especially good at inference given incomplete data. Much like a hidden Markov model, they consist of a directed graphical model (though Bayesian networks must also be acyclic) and a set of probability distributions. The edges encode dependency statements between the variables, where the lack of an edge between any pair of variables indicates a conditional independence. Each node encodes a probability distribution, where root nodes encode univariate probability distributions and inner/leaf nodes encode conditional probability distributions. Bayesian networks are exceptionally flexible when doing inference, as any subset of variables can be observed, and inference done over all other variables, without needing to define these groups in advance. In fact, the set of observed variables can change from one sample to the next without needing to modify the underlying algorithm at all.

Currently, pomegranate only supports discrete Bayesian networks, meaning that the values must be categories, i.e. 'apples' and 'oranges', or 1 and 2, where 1 and 2 refer to categories, not numbers, and so 2 is not explicitly 'bigger' than 1.

1.8.1 Initialization

Bayesian networks can be initialized in two ways, depending on whether the underlying graphical structure is known or not: (1) the graphical structure can be built one node at a time with pre-initialized distributions set for each node,

or (2) both the graphical structure and distributions can be learned directly from data. This mirrors the other models that are implemented in pomegranate. However, typically expectation maximization is used to fit the parameters of the distribution, and so initialization (such as through k-means) is typically fast whereas fitting is slow. For Bayesian networks, the opposite is the case. Fitting can be done quickly by just summing counts through the data, while initialization is hard as it requires an exponential time search through all possible DAGs to identify the optimal graph. More is discussed in the tutorials above and in the fitting section below.

Let's take a look at initializing a Bayesian network in the first manner by quickly implementing the Monty Hall problem. The Monty Hall problem arose from the gameshow *Let's Make a Deal*, where a guest had to choose which one of three doors had a prize behind it. The twist was that after the guest chose, the host, originally Monty Hall, would then open one of the doors the guest did not pick and ask if the guest wanted to switch which door they had picked. Initial inspection may lead you to believe that if there are only two doors left, there is a 50-50 chance of you picking the right one, and so there is no advantage one way or the other. However, it has been proven both through simulations and analytically that there is in fact a 66% chance of getting the prize if the guest switches their door, regardless of the door they initially went with.

Our network will have three nodes, one for the guest, one for the prize, and one for the door Monty chooses to open. The door the guest initially chooses and the door the prize is behind are uniform random processes across the three doors, but the door which Monty opens is dependent on both the door the guest chooses (it cannot be the door the guest chooses), and the door the prize is behind (it cannot be the door with the prize behind it).

```
from pomegranate import *

guest = DiscreteDistribution({'A': 1./3, 'B': 1./3, 'C': 1./3})
prize = DiscreteDistribution({'A': 1./3, 'B': 1./3, 'C': 1./3})
monty = ConditionalProbabilityTable(
        [['A', 'A', 'A', 0.0],
         ['A', 'A', 'B', 0.5],
         ['A', 'A', 'C', 0.5],
         ['A', 'B', 'A', 0.0],
         ['A', 'B', 'B', 0.0],
         ['A', 'B', 'C', 1.0],
         ['A', 'C', 'A', 0.0],
         ['A', 'C', 'B', 1.0],
         ['A', 'C', 'C', 0.0],
         ['B', 'A', 'A', 0.0],
         ['B', 'A', 'B', 0.0],
         ['B', 'A', 'C', 1.0],
         ['B', 'B', 'A', 0.5],
         ['B', 'B', 'B', 0.0],
         ['B', 'B', 'C', 0.5],
         ['B', 'C', 'A', 1.0],
         ['B', 'C', 'B', 0.0],
         ['B', 'C', 'C', 0.0],
         ['C', 'A', 'A', 0.0],
         ['C', 'A', 'B', 1.0],
         ['C', 'A', 'C', 0.0],
         ['C', 'B', 'A', 1.0],
         ['C', 'B', 'B', 0.0],
         ['C', 'B', 'C', 0.0],
         ['C', 'C', 'A', 0.5],
         ['C', 'C', 'B', 0.5],
         ['C', 'C', 'C', 0.0]], [guest, prize])

s1 = Node(guest, name="guest")
s2 = Node(prize, name="prize")
s3 = Node(monty, name="monty")
```

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```
model = BayesianNetwork("Monty Hall Problem")
model.add_states(s1, s2, s3)
model.add_edge(s1, s3)
model.add_edge(s2, s3)
model.bake()
```

Note: The objects 'state' and 'node' are really the same thing and can be used interchangable. The only difference is the name, as hidden Markov models use 'state' in the literature frequently whereas Bayesian networks use 'node' frequently.

The conditional distribution must be explicitly spelled out in this example, followed by a list of the parents in the same order as the columns take in the tabble that is provided (e.g. the columns in the table correspond to guest, prize, monty, probability.)

However, one can also initialize a Bayesian network based completely on data. As mentioned before, the exact version of this algorithm takes exponential time with the number of variables and typically can't be done on more than ~25 variables. This is because there are a super-exponential number of directed acyclic graphs that one could define over a set of variables, but fortunately one can use dynamic programming in order to reduce this complexity down to "simply exponential." The implementation of the exact algorithm actually goes further than the original dynamic programing algorithm by implementing an A* search to somewhat reduce computational time but drastically reduce required memory, sometimes by an order of magnitude.

```
from pomegranate import *
import numpy

X = numpy.load('data.npy')
model = BayesianNetwork.from_samples(X, algorithm='exact')
```

The exact algorithm is not the default, though. The default is a novel greedy algorithm that greedily chooses a topological ordering of the variables, but optimally identifies the best parents for each variable given this ordering. It is significantly faster and more memory efficient than the exact algorithm and produces far better estimates than using a Chow-Liu tree. This is set to the default to avoid locking up the computers of users that unintentionally tell their computers to do a near-impossible task.

1.8.2 Probability

You can calculate the probabiity of a sample under a Bayesian network as the product of the probability of each variable given its parents, if it has any. This can be expressed as $P = \prod_{i=1}^{d} P(D_i|Pa_i)$ for a sample with d dimensions. For example, in the Monty Hal problem, the probability of a show is the probability of the guest choosing the respective door, times the probability of the prize being behind a given door, times the probability of Monty opening a given door given the previous two values. For example, using the manually initialized network above:

```
>>> print model.probability([['A', 'A', 'A'],
                             ['A', 'A', 'B'],
                             ['C', 'C', 'B']])
[ 0.          0.05555556  0.05555556]
```

1.8.3 Prediction

Bayesian networks are frequently used to infer/impute the value of missing variables given the observed values. In other models, typically there is either a single or fixed set of missing variables, such as latent factors, that need to be imputed, and so returning a fixed vector or matrix as the predictions makes sense. However, in the case of Bayesian networks, we can make no such assumptions, and so when data is passed in for prediction it should be in the format as a matrix with `None` in the missing variables that need to be inferred. The return is thus a filled in matrix where the Nones have been replaced with the imputed values. For example:

```
>>> print model.predict([['A', 'B', None],
                         ['A', 'C', None],
                         ['C', 'B', None]])
[['A' 'B' 'C']
 ['A' 'C' 'B']
 ['C' 'B' 'A']]
```

In this example, the final column is the one that is always missing, but a more complex example is as follows:

```
>>> print model.predict([['A', 'B', None],
                 ['A', None, 'C'],
                 [None, 'B', 'A']])
[['A' 'B' 'C']
 ['A' 'B' 'C']
 ['C' 'B' 'A']]
```

1.8.4 Fitting

Fitting a Bayesian network to data is a fairly simple process. Essentially, for each variable, you need consider only that column of data and the columns corresponding to that variables parents. If it is a univariate distribution, then the maximum likelihood estimate is just the count of each symbol divided by the number of samples in the data. If it is a multivariate distribution, it ends up being the probability of each symbol in the variable of interest given the combination of symbols in the parents. For example, consider a binary dataset with two variables, X and Y, where X is a parent of Y. First, we would go through the dataset and calculate P(X=0) and P(X=1). Then, we would calculate P(Y=0|X=0), P(Y=1|X=0), P(Y=0|X=1), and P(Y=1|X=1). Those values encode all of the parameters of the Bayesian network.

1.8.5 API Reference

class pomegranate.BayesianNetwork.**BayesianNetwork**

A Bayesian Network Model.

A Bayesian network is a directed graph where nodes represent variables, edges represent conditional dependencies of the children on their parents, and the lack of an edge represents a conditional independence.

Parameters

name [str, optional] The name of the model. Default is None

Attributes

states [list, shape (n_states,)] A list of all the state objects in the model

graph [networkx.DiGraph] The underlying graph object.

add_edge()

Add a transition from state a to state b which indicates that B is dependent on A in ways specified by the distribution.

add_node()
Add a node to the graph.

add_nodes()
Add multiple states to the graph.

add_state()
Another name for a node.

add_states()
Another name for a node.

add_transition()
Transitions and edges are the same.

bake()
Finalize the topology of the model.

Assign a numerical index to every state and create the underlying arrays corresponding to the states and edges between the states. This method must be called before any of the probability-calculating methods. This includes converting conditional probability tables into joint probability tables and creating a list of both marginal and table nodes.

Parameters

None

Returns

None

clear_summaries()
Clear the summary statistics stored in the object.

copy()
Return a deep copy of this distribution object.

This object will not be tied to any other distribution or connected in any form.

Parameters

None

Returns

distribution [Distribution] A copy of the distribution with the same parameters.

dense_transition_matrix()
Returns the dense transition matrix. Useful if the transitions of somewhat small models need to be analyzed.

edge_count()
Returns the number of edges present in the model.

fit()
Fit the model to data using MLE estimates.

Fit the model to the data by updating each of the components of the model, which are univariate or multivariate distributions. This uses a simple MLE estimate to update the distributions according to their summarize or fit methods.

This is a wrapper for the summarize and from_summaries methods.

Parameters

items [array-like, shape (n_samples, n_nodes)] The data to train on, where each row is a sample and each column corresponds to the associated variable.

weights [array-like, shape (n_nodes), optional] The weight of each sample as a positive double. Default is None.

inertia [double, optional] The inertia for updating the distributions, passed along to the distribution method. Default is 0.0.

pseudocount [double, optional] A pseudocount to add to the emission of each distribution. This effectively smoothes the states to prevent 0. probability symbols if they don't happen to occur in the data. Only effects hidden Markov models defined over discrete distributions. Default is 0.

Returns

None

freeze()
Freeze the distribution, preventing updates from occuring.

from_json()
Read in a serialized Bayesian Network and return the appropriate object.

Parameters

s [str] A JSON formatted string containing the file.

Returns

model [object] A properly initialized and baked model.

from_samples()
Learn the structure of the network from data.

Find the structure of the network from data using a Bayesian structure learning score. This currently enumerates all the exponential number of structures and finds the best according to the score. This allows weights on the different samples as well. The score that is optimized is the minimum description length (MDL).

Parameters

X [array-like, shape (n_samples, n_nodes)] The data to fit the structure too, where each row is a sample and each column corresponds to the associated variable.

weights [array-like, shape (n_nodes), optional] The weight of each sample as a positive double. Default is None.

algorithm [str, one of 'chow-liu', 'greedy', 'exact', 'exact-dp' optional] The algorithm to use for learning the Bayesian network. Default is 'greedy' that greedily attempts to find the best structure, and frequently can identify the optimal structure. 'exact' uses DP/A* to find the optimal Bayesian network, and 'exact-dp' tries to find the shortest path on the entire order lattice, which is more memory and computationally expensive. 'exact' and 'exact-dp' should give identical results, with 'exact-dp' remaining an option mostly for debugging reasons. 'chow-liu' will return the optimal tree-like structure for the Bayesian network, which is a very fast approximation but not always the best network.

max_parents [int, optional] The maximum number of parents a node can have. If used, this means using the k-learn procedure. Can drastically speed up algorithms. If -1, no max on parents. Default is -1.

root [int, optional] For algorithms which require a single root ('chow-liu'), this is the root for which all edges point away from. User may specify which column to use as the root. Default is the first column.

constraint_graph [networkx.DiGraph or None, optional] A directed graph showing valid parent sets for each variable. Each node is a set of variables, and edges represent which variables can be valid parents of those variables. The naive structure learning task is just all variables in a single node with a self edge, meaning that you know nothing about

pseudocount [double, optional] A pseudocount to add to the emission of each distribution. This effectively smoothes the states to prevent 0. probability symbols if they don't happen to occur in the data. Default is 0.

state_names [array-like, shape (n_nodes), optional] A list of meaningful names to be applied to nodes

name [str, optional] The name of the model. Default is None.

n_jobs [int, optional] The number of threads to use when learning the structure of the network. If a constraint graph is provided, this will parallelize the tasks as directed by the constraint graph. If one is not provided it will parallelize the building of the parent graphs. Both cases will provide large speed gains.

Returns

model [BayesianNetwork] The learned BayesianNetwork.

from_structure()

Return a Bayesian network from a predefined structure.

Pass in the structure of the network as a tuple of tuples and get a fit network in return. The tuple should contain n tuples, with one for each node in the graph. Each inner tuple should be of the parents for that node. For example, a three node graph where both node 0 and 1 have node 2 as a parent would be specified as ((2,), (2,), ()).

Parameters

X [array-like, shape (n_samples, n_nodes)] The data to fit the structure too, where each row is a sample and each column corresponds to the associated variable.

structure [tuple of tuples] The parents for each node in the graph. If a node has no parents, then do not specify any parents.

weights [array-like, shape (n_nodes), optional] The weight of each sample as a positive double. Default is None.

pseudocount [double, optional] A pseudocount to add to the emission of each distribution. This effectively smoothes the states to prevent 0. probability symbols if they don't happen to occur in the data. Default is 0.

name [str, optional] The name of the model. Default is None.

state_names [array-like, shape (n_nodes), optional] A list of meaningful names to be applied to nodes

Returns

model [BayesianNetwoork] A Bayesian network with the specified structure.

from_summaries()

Use MLE on the stored sufficient statistics to train the model.

This uses MLE estimates on the stored sufficient statistics to train the model.

Parameters

inertia [double, optional] The inertia for updating the distributions, passed along to the distribution method. Default is 0.0.

pseudocount [double, optional] A pseudocount to add to the emission of each distribution. This effectively smoothes the states to prevent 0. probability symbols if they don't happen to occur in the data. Default is 0.

Returns

None

log_probability()

Return the log probability of samples under the Bayesian network.

The log probability is just the sum of the log probabilities under each of the components. The log probability of a sample under the graph A -> B is just P(A)*P(B|A). This will return a vector of log probabilities, one for each sample.

Parameters

X [array-like, shape (n_samples, n_dim)] The sample is a vector of points where each dimension represents the same variable as added to the graph originally. It doesn't matter what the connections between these variables are, just that they are all ordered the same.

Returns

logp [double] The log probability of that sample.

marginal()

Return the marginal probabilities of each variable in the graph.

This is equivalent to a pass of belief propogation on a graph where no data has been given. This will calculate the probability of each variable being in each possible emission when nothing is known.

Parameters

None

Returns

marginals [array-like, shape (n_nodes)] An array of univariate distribution objects showing the marginal probabilities of that variable.

node_count()

Returns the number of nodes/states in the model

plot()

Draw this model's graph using NetworkX and matplotlib.

Note that this relies on networkx's built-in graphing capabilities (and not Graphviz) and thus can't draw self-loops.

See networkx.draw_networkx() for the keywords you can pass in.

Parameters

****kwargs** [any] The arguments to pass into networkx.draw_networkx()

Returns

None

predict()

Predict missing values of a data matrix using MLE.

Impute the missing values of a data matrix using the maximally likely predictions according to the forward-backward algorithm. Run each sample through the algorithm (predict_proba) and replace missing values with the maximally likely predicted emission.

Parameters

items [array-like, shape (n_samples, n_nodes)] Data matrix to impute. Missing values must be either None (if lists) or np.nan (if numpy.ndarray). Will fill in these values with the maximally likely ones.

max_iterations [int, optional] Number of iterations to run loopy belief propogation for. Default is 100.

Returns

items [numpy.ndarray, shape (n_samples, n_nodes)] This is the data matrix with the missing values imputed.

predict_proba()

Returns the probabilities of each variable in the graph given evidence.

This calculates the marginal probability distributions for each state given the evidence provided through loopy belief propogation. Loopy belief propogation is an approximate algorithm which is exact for certain graph structures.

Parameters

data [dict or array-like, shape <= n_nodes, optional] The evidence supplied to the graph. This can either be a dictionary with keys being state names and values being the observed values (either the emissions or a distribution over the emissions) or an array with the values being ordered according to the nodes incorporation in the graph (the order fed into .add_states/add_nodes) and None for variables which are unknown. If nothing is fed in then calculate the marginal of the graph. Default is {}.

max_iterations [int, optional] The number of iterations with which to do loopy belief propogation. Usually requires only 1. Default is 100.

check_input [bool, optional] Check to make sure that the observed symbol is a valid symbol for that distribution to produce. Default is True.

Returns

probabilities [array-like, shape (n_nodes)] An array of univariate distribution objects showing the probabilities of each variable.

probability()

Return the probability of the given symbol under this distribution.

Parameters

symbol [object] The symbol to calculate the probability of

Returns

probability [double] The probability of that point under the distribution.

sample()

Return a random item sampled from this distribution.

Parameters

n [int or None, optional] The number of samples to return. Default is None, which is to generate a single sample.

Returns

sample [double or object] Returns a sample from the distribution of a type in the support of the distribution.

state_count()
Returns the number of states present in the model.

summarize()
Summarize a batch of data and store the sufficient statistics.

This will partition the dataset into columns which belong to their appropriate distribution. If the distribution has parents, then multiple columns are sent to the distribution. This relies mostly on the summarize function of the underlying distribution.

Parameters

items [array-like, shape (n_samples, n_nodes)] The data to train on, where each row is a sample and each column corresponds to the associated variable.

weights [array-like, shape (n_nodes), optional] The weight of each sample as a positive double. Default is None.

Returns

None

thaw()
Thaw the distribution, re-allowing updates to occur.

to_json()
Serialize the model to a JSON.

Parameters

separators [tuple, optional] The two separaters to pass to the json.dumps function for formatting.

indent [int, optional] The indentation to use at each level. Passed to json.dumps for formatting.

Returns

json [str] A properly formatted JSON object.

class pomegranate.BayesianNetwork.**ParentGraph**
Generate a parent graph for a single variable over its parents.

This will generate the parent graph for a single parents given the data. A parent graph is the dynamically generated best parent set and respective score for each combination of parent variables. For example, if we are generating a parent graph for x1 over x2, x3, and x4, we may calculate that having x2 as a parent is better than x2,x3 and so store the value of x2 in the node for x2,x3.

Parameters

X [numpy.ndarray, shape=(n, d)] The data to fit the structure too, where each row is a sample and each column corresponds to the associated variable.

weights [numpy.ndarray, shape=(n,)] The weight of each sample as a positive double. Default is None.

key_count [numpy.ndarray, shape=(d,)] The number of unique keys in each column.

pseudocount [double] A pseudocount to add to each possibility.

max_parents [int] The maximum number of parents a node can have. If used, this means using the k-learn procedure. Can drastically speed up algorithms. If -1, no max on parents. Default is -1.

parent_set [tuple, default ()] The variables which are possible parents for this variable. If nothing is passed in then it defaults to all other variables, as one would expect in the naive case. This allows for cases where we want to build a parent graph over only a subset of the variables.

Returns

structure [tuple, shape=(d,)] The parents for each variable in this SCC

pomegranate.BayesianNetwork.**discrete_exact_a_star**()

Find the optimal graph over a set of variables with no other knowledge.

This is the naive dynamic programming structure learning task where the optimal graph is identified from a set of variables using an order graph and parent graphs. This can be used either when no constraint graph is provided or for a SCC which is made up of a node containing a self-loop. It uses DP/A* in order to find the optimal graph without considering all possible topological sorts. A greedy version of the algorithm can be used that massively reduces both the computational and memory cost while frequently producing the optimal graph.

Parameters

X [numpy.ndarray, shape=(n, d)] The data to fit the structure too, where each row is a sample and each column corresponds to the associated variable.

weights [numpy.ndarray, shape=(n,)] The weight of each sample as a positive double. Default is None.

key_count [numpy.ndarray, shape=(d,)] The number of unique keys in each column.

pseudocount [double] A pseudocount to add to each possibility.

max_parents [int] The maximum number of parents a node can have. If used, this means using the k-learn procedure. Can drastically speed up algorithms. If -1, no max on parents. Default is -1.

n_jobs [int] The number of threads to use when learning the structure of the network. This parallelizes the creation of the parent graphs.

Returns

structure [tuple, shape=(d,)] The parents for each variable in this SCC

pomegranate.BayesianNetwork.**discrete_exact_component**()

Find the optimal graph over a multi-node component of the constaint graph.

The general algorithm in this case is to begin with each variable and add all possible single children for that entry recursively until completion. This will result in a far sparser order graph than before. In addition, one can eliminate entries from the parent graphs that contain invalid parents as they are a fast of computational time.

Parameters

X [numpy.ndarray, shape=(n, d)] The data to fit the structure too, where each row is a sample and each column corresponds to the associated variable.

weights [numpy.ndarray, shape=(n,)] The weight of each sample as a positive double. Default is None.

key_count [numpy.ndarray, shape=(d,)] The number of unique keys in each column.

pseudocount [double] A pseudocount to add to each possibility.

max_parents [int] The maximum number of parents a node can have. If used, this means using the k-learn procedure. Can drastically speed up algorithms. If -1, no max on parents. Default is -1.

n_jobs [int] The number of threads to use when learning the structure of the network. This parallelizes the creation of the parent graphs.

Returns

structure [tuple, shape=(d,)] The parents for each variable in this SCC

pomegranate.BayesianNetwork.**discrete_exact_dp**()

Find the optimal graph over a set of variables with no other knowledge.

This is the naive dynamic programming structure learning task where the optimal graph is identified from a set of variables using an order graph and parent graphs. This can be used either when no constraint graph is provided or for a SCC which is made up of a node containing a self-loop. This is a reference implementation that uses the naive shortest path algorithm over the entire order graph. The 'exact' option uses the A* path in order to avoid considering the full order graph.

Parameters

X [numpy.ndarray, shape=(n, d)] The data to fit the structure too, where each row is a sample and each column corresponds to the associated variable.

weights [numpy.ndarray, shape=(n,)] The weight of each sample as a positive double. Default is None.

key_count [numpy.ndarray, shape=(d,)] The number of unique keys in each column.

pseudocount [double] A pseudocount to add to each possibility.

max_parents [int] The maximum number of parents a node can have. If used, this means using the k-learn procedure. Can drastically speed up algorithms. If -1, no max on parents. Default is -1.

n_jobs [int] The number of threads to use when learning the structure of the network. This parallelizes the creation of the parent graphs.

Returns

structure [tuple, shape=(d,)] The parents for each variable in this SCC

pomegranate.BayesianNetwork.**discrete_exact_slap**()

Find the optimal graph in a node with a Self Loop And Parents (SLAP).

Instead of just performing exact BNSL over the set of all parents and removing the offending edges there are efficiencies that can be gained by considering the structure. In particular, parents not coming from the main node do not need to be considered in the order graph but simply added to each entry after creation of the order graph. This is because those variables occur earlier in the topological ordering but it doesn't matter how they occur otherwise. Parent graphs must be defined over all variables however.

Parameters

X [numpy.ndarray, shape=(n, d)] The data to fit the structure too, where each row is a sample and each column corresponds to the associated variable.

weights [numpy.ndarray, shape=(n,)] The weight of each sample as a positive double. Default is None.

key_count [numpy.ndarray, shape=(d,)] The number of unique keys in each column.

pseudocount [double] A pseudocount to add to each possibility.

max_parents [int] The maximum number of parents a node can have. If used, this means using the k-learn procedure. Can drastically speed up algorithms. If -1, no max on parents. Default is -1.

n_jobs [int] The number of threads to use when learning the structure of the network. This parallelizes the creation of the parent graphs.

Returns

structure [tuple, shape=(d,)] The parents for each variable in this SCC

pomegranate.BayesianNetwork.**discrete_exact_with_constraints**()

This returns the optimal Bayesian network given a set of constraints.

This function controls the process of learning the Bayesian network by taking in a constraint graph, identifying the strongly connected components (SCCs) and solving each one using the appropriate algorithm. This is mostly an internal function.

Parameters

X [numpy.ndarray, shape=(n, d)] The data to fit the structure too, where each row is a sample and each column corresponds to the associated variable.

weights [numpy.ndarray, shape=(n,)] The weight of each sample as a positive double. Default is None.

key_count [numpy.ndarray, shape=(d,)] The number of unique keys in each column.

pseudocount [double] A pseudocount to add to each possibility.

max_parents [int] The maximum number of parents a node can have. If used, this means using the k-learn procedure. Can drastically speed up algorithms. If -1, no max on parents. Default is -1.

constraint_graph [networkx.DiGraph] A directed graph showing valid parent sets for each variable. Each node is a set of variables, and edges represent which variables can be valid parents of those variables. The naive structure learning task is just all variables in a single node with a self edge, meaning that you know nothing about

n_jobs [int] The number of threads to use when learning the structure of the network. This parallelized both the creation of the parent graphs for each variable and the solving of the SCCs.

Returns

structure [tuple, shape=(d,)] The parents for each variable in the network.

pomegranate.BayesianNetwork.**discrete_exact_with_constraints_task**()

This is a wrapper for the function to be parallelzied by joblib.

This function takes in a single task as an id and a set of parents and children and calls the appropriate function. This is mostly a wrapper for joblib to parallelize.

Parameters

X [numpy.ndarray, shape=(n, d)] The data to fit the structure too, where each row is a sample and each column corresponds to the associated variable.

weights [numpy.ndarray, shape=(n,)] The weight of each sample as a positive double. Default is None.

key_count [numpy.ndarray, shape=(d,)] The number of unique keys in each column.

pseudocount [double] A pseudocount to add to each possibility.

max_parents [int] The maximum number of parents a node can have. If used, this means using the k-learn procedure. Can drastically speed up algorithms. If -1, no max on parents. Default is -1.

task [tuple] A 3-tuple containing the id, the set of parents and the set of children to learn a component of the Bayesian network over. The cases represent a SCC of the following:

0 - Self loop and no parents 1 - Self loop and parents 2 - Parents and no self loop 3 - Multiple nodes

n_jobs [int] The number of threads to use when learning the structure of the network. This parallelizes the creation of the parent graphs for each task or the finding of best parents in case 2.

Returns

structure [tuple, shape=(d,)] The parents for each variable in this SCC

pomegranate.BayesianNetwork.**discrete_greedy**()

Find the optimal graph over a set of variables with no other knowledge.

This is the naive dynamic programming structure learning task where the optimal graph is identified from a set of variables using an order graph and parent graphs. This can be used either when no constraint graph is provided or for a SCC which is made up of a node containing a self-loop. It uses DP/A* in order to find the optimal graph without considering all possible topological sorts. A greedy version of the algorithm can be used that massively reduces both the computational and memory cost while frequently producing the optimal graph.

Parameters

X [numpy.ndarray, shape=(n, d)] The data to fit the structure too, where each row is a sample and each column corresponds to the associated variable.

weights [numpy.ndarray, shape=(n,)] The weight of each sample as a positive double. Default is None.

key_count [numpy.ndarray, shape=(d,)] The number of unique keys in each column.

pseudocount [double] A pseudocount to add to each possibility.

max_parents [int] The maximum number of parents a node can have. If used, this means using the k-learn procedure. Can drastically speed up algorithms. If -1, no max on parents. Default is -1.

greedy [bool, default is True] Whether the use a heuristic in order to massive reduce computation and memory time, but without the guarantee of finding the best network.

n_jobs [int] The number of threads to use when learning the structure of the network. This parallelizes the creation of the parent graphs.

Returns

structure [tuple, shape=(d,)] The parents for each variable in this SCC

pomegranate.BayesianNetwork.**generate_parent_graph**()

Generate a parent graph for a single variable over its parents.

This will generate the parent graph for a single parents given the data. A parent graph is the dynamically generated best parent set and respective score for each combination of parent variables. For example, if we are generating a parent graph for x1 over x2, x3, and x4, we may calculate that having x2 as a parent is better than x2,x3 and so store the value of x2 in the node for x2,x3.

Parameters

X [numpy.ndarray, shape=(n, d)] The data to fit the structure too, where each row is a sample and each column corresponds to the associated variable.

weights [numpy.ndarray, shape=(n,)] The weight of each sample as a positive double. Default is None.

key_count [numpy.ndarray, shape=(d,)] The number of unique keys in each column.

pseudocount [double] A pseudocount to add to each possibility.

max_parents [int] The maximum number of parents a node can have. If used, this means using the k-learn procedure. Can drastically speed up algorithms. If -1, no max on parents. Default is -1.

parent_set [tuple, default ()] The variables which are possible parents for this variable. If nothing is passed in then it defaults to all other variables, as one would expect in the naive case. This allows for cases where we want to build a parent graph over only a subset of the variables.

Returns

structure [tuple, shape=(d,)] The parents for each variable in this SCC

1.9 Factor Graphs

1.9.1 API Reference

class pomegranate.FactorGraph.**FactorGraph**

A Factor Graph model.

A biparte graph where conditional probability tables are on one side, and marginals for each of the variables involved are on the other side.

Parameters

name [str, optional] The name of the model. Default is None.

bake()

Finalize the topology of the model.

Assign a numerical index to every state and create the underlying arrays corresponding to the states and edges between the states. This method must be called before any of the probability-calculating methods. This is the same as the HMM bake, except that at the end it sets current state information.

Parameters

None

Returns

None

marginal()

Return the marginal probabilities of each variable in the graph.

This is equivalent to a pass of belief propogation on a graph where no data has been given. This will calculate the probability of each variable being in each possible emission when nothing is known.

Parameters

None

Returns

marginals [array-like, shape (n_nodes)] An array of univariate distribution objects showing the marginal probabilities of that variable.

plot()

Draw this model's graph using NetworkX and matplotlib.

Note that this relies on networkx's built-in graphing capabilities (and not Graphviz) and thus can't draw self-loops.

See networkx.draw_networkx() for the keywords you can pass in.

Parameters

****kwargs** [any] The arguments to pass into networkx.draw_networkx()

Returns

None

predict_proba()

Returns the probabilities of each variable in the graph given evidence.

This calculates the marginal probability distributions for each state given the evidence provided through loopy belief propogation. Loopy belief propogation is an approximate algorithm which is exact for certain graph structures.

Parameters

data [dict or array-like, shape <= n_nodes, optional] The evidence supplied to the graph. This can either be a dictionary with keys being state names and values being the observed values (either the emissions or a distribution over the emissions) or an array with the values being ordered according to the nodes incorporation in the graph (the order fed into .add_states/add_nodes) and None for variables which are unknown. If nothing is fed in then calculate the marginal of the graph.

max_iterations [int, optional] The number of iterations with which to do loopy belief propogation. Usually requires only 1.

check_input [bool, optional] Check to make sure that the observed symbol is a valid symbol for that distribution to produce.

Returns

probabilities [array-like, shape (n_nodes)] An array of univariate distribution objects showing the probabilities of each variable.

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