

pomegranate

fast and flexible probabilistic modelling in python

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Overview

pomegranate is **more flexible** than other packages, **faster**, is **intuitive to use**, and can do it all **in parallel**



Overview: supported models

Six Main Models:

1. Probability Distributions
2. General Mixture Models
3. Markov Chains
4. Hidden Markov Models
5. Bayes Classifiers / Naive Bayes
6. Bayesian Networks

Two Helper Models:

1. k-means++/kmeans||
2. Factor Graphs



Overview: model stacking in pomegranate

Distributions

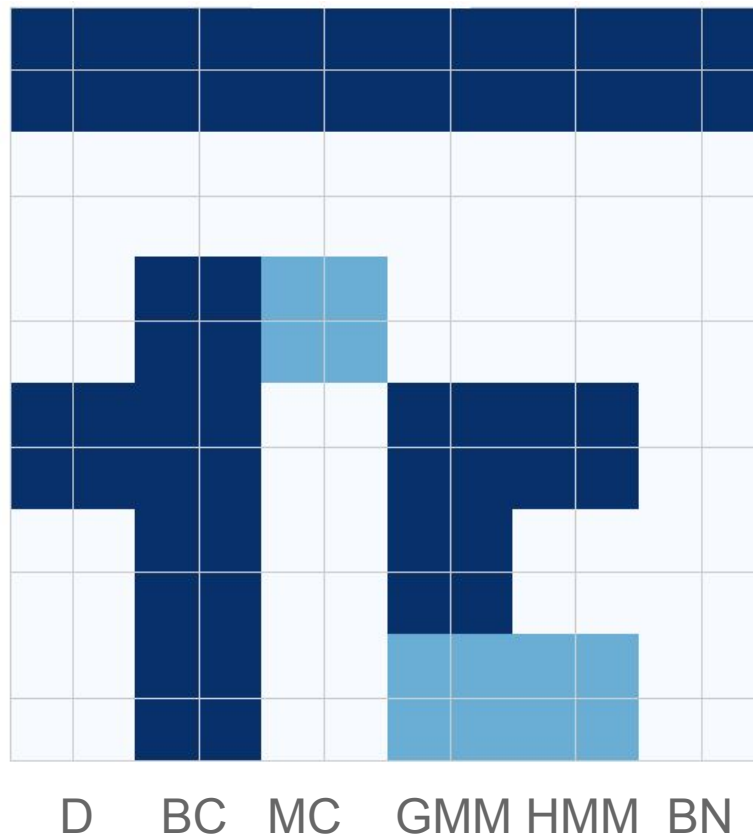
Bayes Classifiers

Markov Chains

General Mixture Models

Hidden Markov Models

Bayesian Networks





Overview: model stacking in pomegranate

Distributions

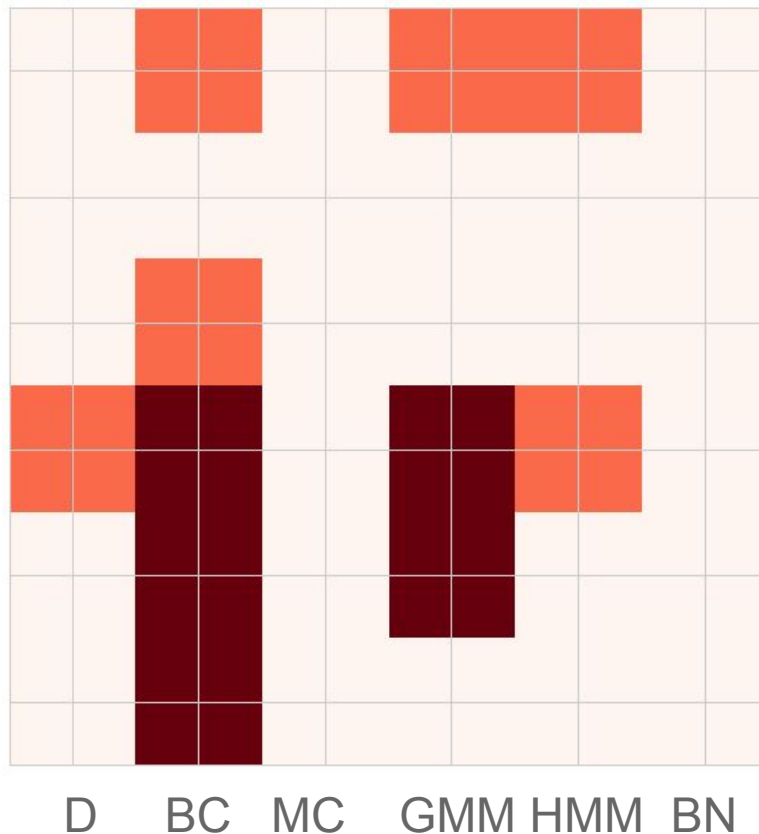
Bayes Classifiers

Markov Chains

General Mixture Models

Hidden Markov Models

Bayesian Networks





The API is common to all models

`model.log_probability(X) / model.probability(X)`

`model.sample()`

`model.fit(X, weights, inertia)`

All models have these methods!

`model.summarize(X, weights)`

`model.from_summaries(inertia)`

`model.predict(X)`

`model.predict_proba(X)`

`model.predict_log_proba(X)`

`Model.from_samples(X, weights)`

All models composed of distributions (like GMM, HMM...) have these methods too!



pomegranate supports many distributions

Univariate Distributions

1. UniformDistribution
2. BernoulliDistribution
3. NormalDistribution
4. LogNormalDistribution
5. ExponentialDistribution
6. BetaDistribution
7. GammaDistribution
8. DiscreteDistribution
9. PoissonDistribution

Kernel Densities

1. GaussianKernelDensity
2. UniformKernelDensity
3. TriangleKernelDensity

Multivariate Distributions

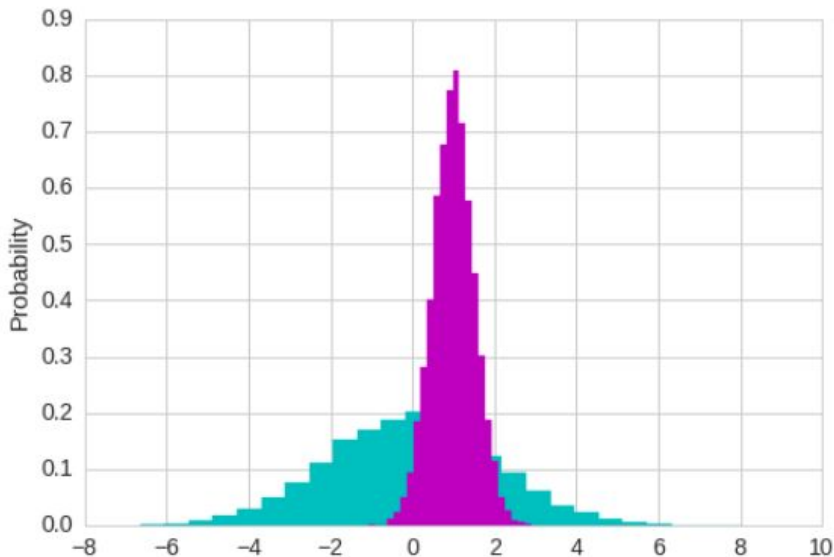
1. IndependentComponentsDistribution
2. MultivariateGaussianDistribution
3. DirichletDistribution
4. ConditionalProbabilityTable
5. JointProbabilityTable



Models can be created from known values

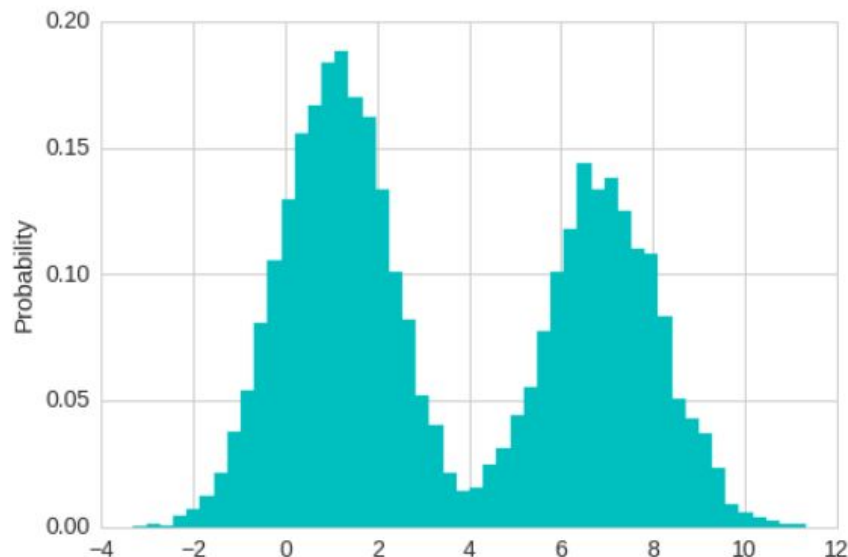
`mu, sig = 0, 2`

`a = NormalDistribution(mu, sig)`



`X = [0, 1, 1, 2, 1.5, 6, 7, 8, 7]`

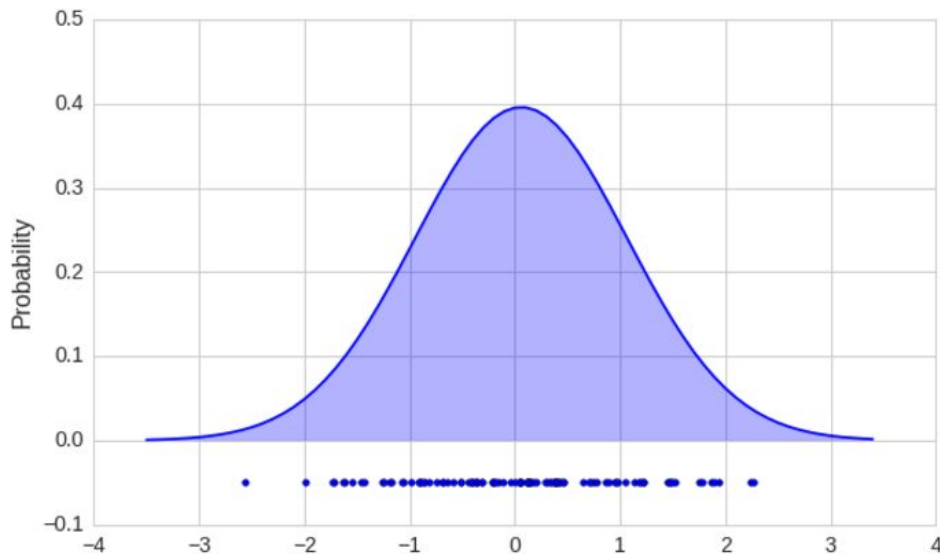
`a = GaussianKernelDensity(X)`





Models can be learned from data

```
X = numpy.random.normal(0, 1, 100)  
a = NormalDistribution.from_samples(X)
```





pomegranate can be faster than numpy

Fitting a Normal Distribution to 1,000 samples

```
data = numpy.random.randn(1000)

print "numpy time:"
%timeit -n 100 data.mean(), data.std()

print
print "pomegranate time:"
%timeit -n 100 NormalDistribution.from_samples(data)
```

numpy time:
100 loops, best of 3: 46.6 μ s per loop

pomegranate time:
100 loops, best of 3: 22.2 μ s per loop



pomegranate can be faster than numpy

Fitting Multivariate Gaussian to 10,000,000 samples of 10 dimensions

```
data = numpy.random.randn(10000000, 10)

print "numpy time:"
%timeit -n 10 data.mean(), numpy.cov(data.T)
print
print "pomegranate time:"
%timeit -n 10 MultivariateGaussianDistribution.from_samples(data)
```

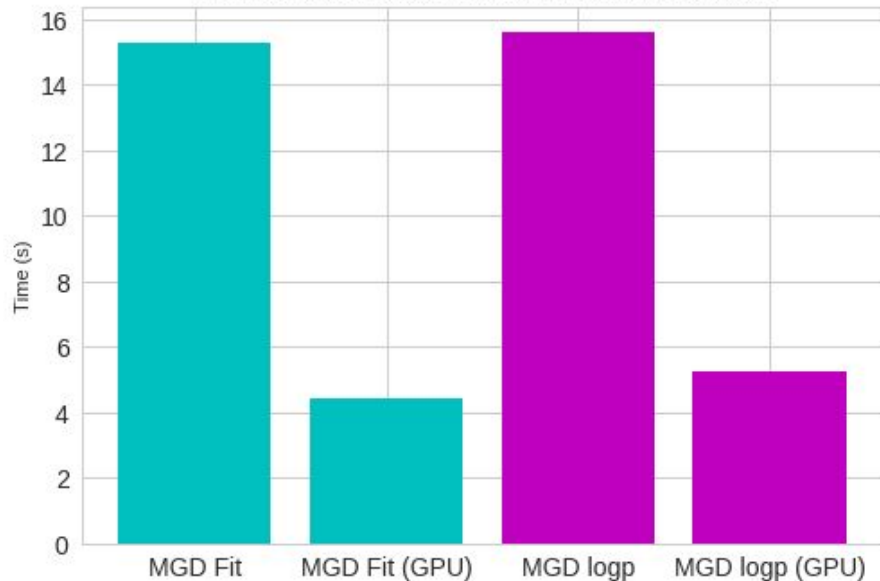
numpy time:
10 loops, best of 3: 1.02 s per loop

pomegranate time:
10 loops, best of 3: 799 ms per loop

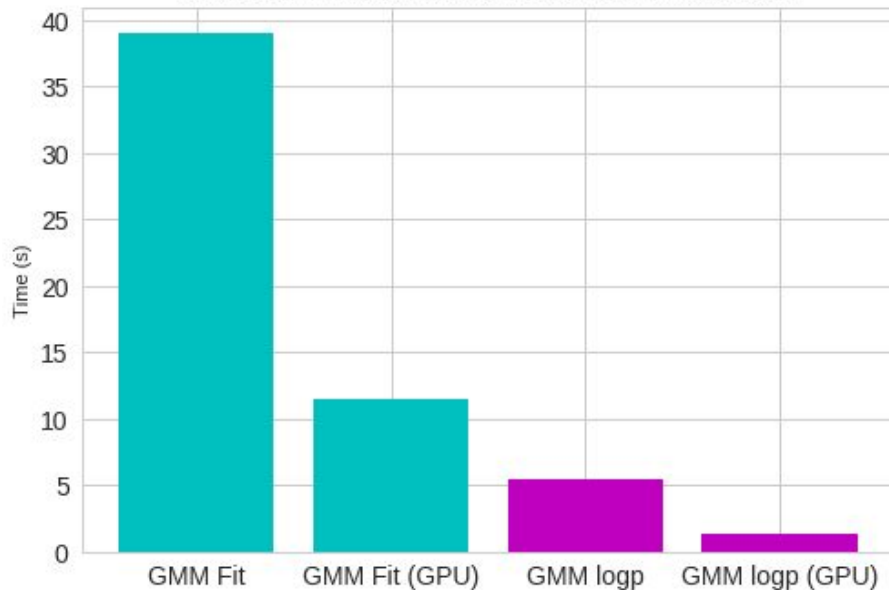


pomegranate just merged GPU support

Multivariate Gaussian with GPU Acceleration



Gaussian Mixture Model with GPU Acceleration





pomegranate uses additive summarization

pomegranate reduces data to sufficient statistics for updates and so only has to go datasets once (for all models).

Here is an example of the Normal Distribution sufficient statistics

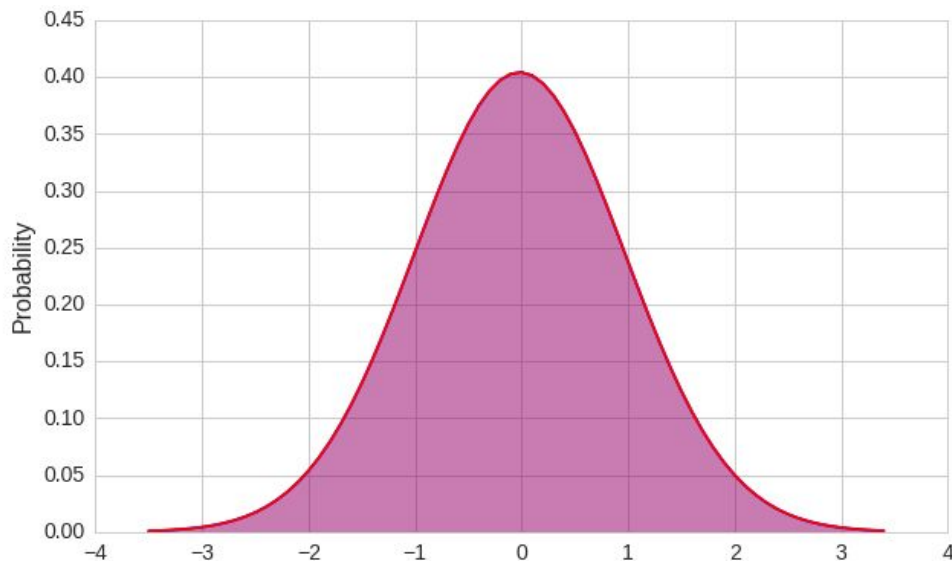
$$\sum_{i=1}^n w_i \quad \sum_{i=1}^n w_i x_i \quad \sum_{i=1}^n w_i x_i^2 \quad \longrightarrow \quad \begin{aligned} \mu &= \frac{\sum_{i=1}^n w_i x_i}{\sum_{i=1}^n w_i} \\ \sigma^2 &= \frac{\sum_{i=1}^n w_i x_i^2}{\sum_{i=1}^n w_i} - \frac{\left(\sum_{i=1}^n w_i x_i \right)^2}{\left(\sum_{i=1}^n w_i \right)^2} \end{aligned}$$



pomegranate supports out-of-core learning

Batches from a dataset can be reduced to additive summary statistics, enabling exact updates from data that can't fit in memory.

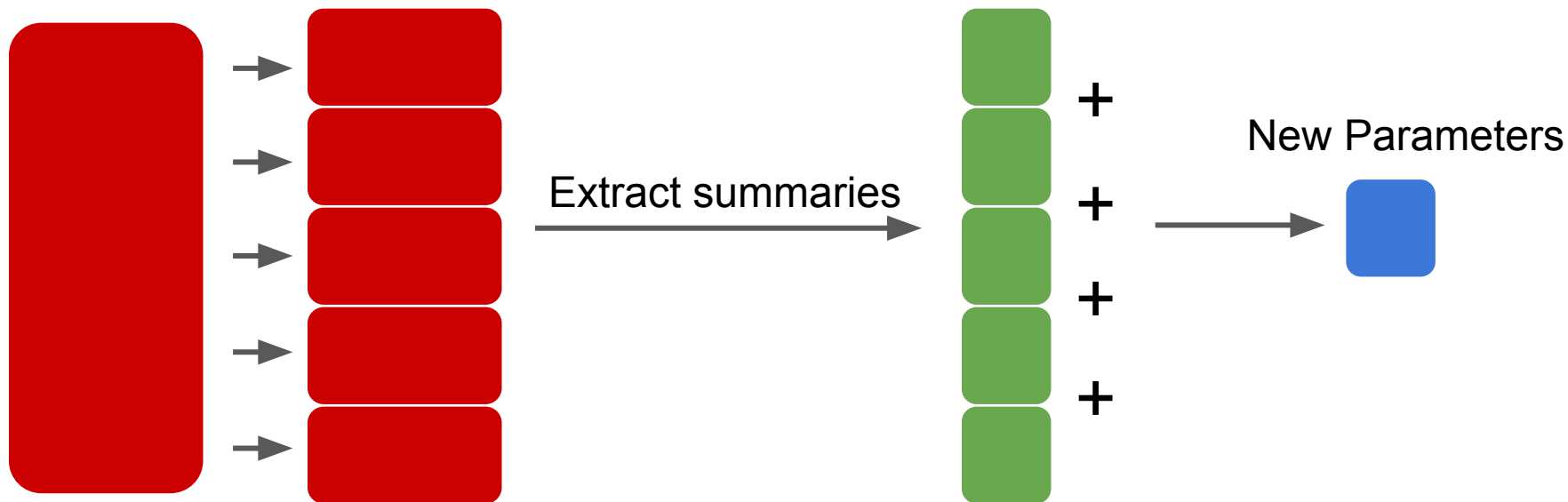
```
a.fit(data)
b.summarize(data[:1000])
b.summarize(data[1000:2000])
b.summarize(data[2000:3000])
b.summarize(data[3000:4000])
b.summarize(data[4000:])
b.from_summaries()
```



Fit Mean: -0.0174820965846, Fit STD: 0.986767322871
Summarize Mean: -0.0174820965846, Summarize STD: 0.986767322871



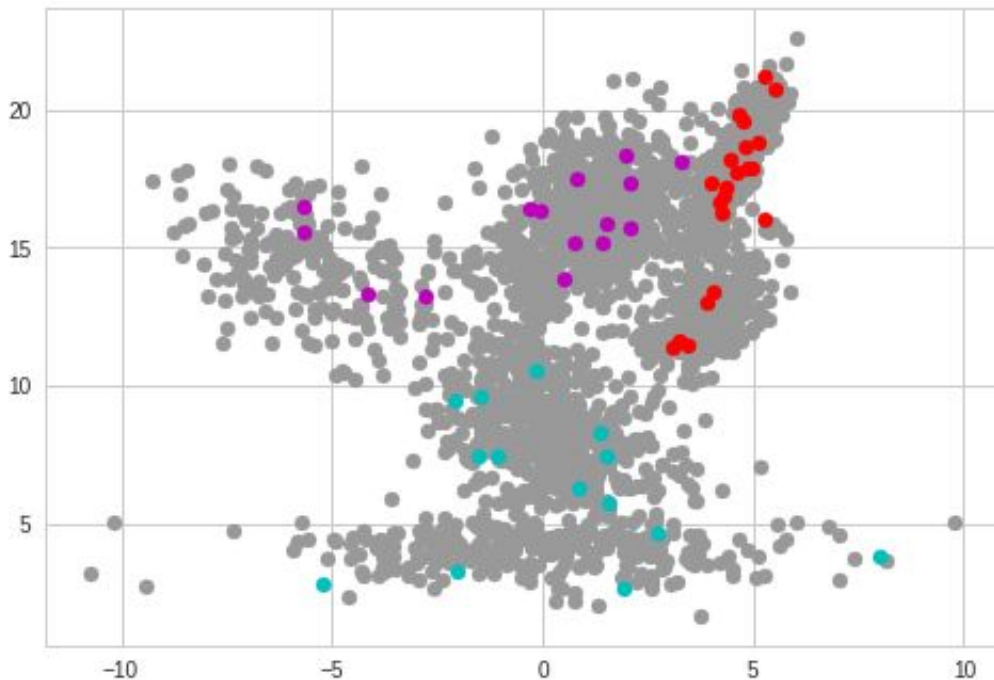
Parallelization exploits additive summaries





pomegranate supports semisupervised learning

Summary statistics from supervised models can be added to summary statistics from unsupervised models to train a single model on a mixture of labeled and unlabeled data.

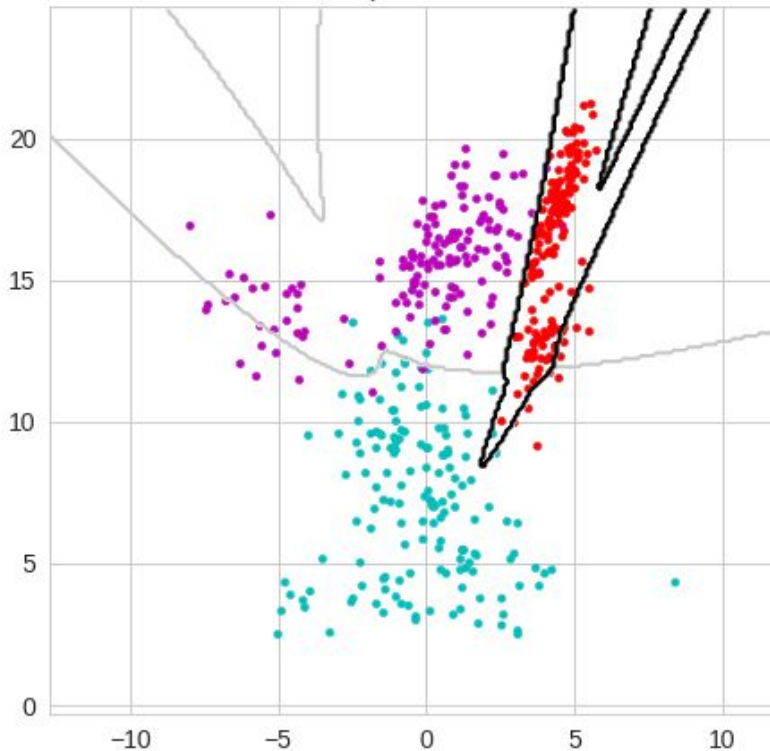




pomegranate supports semisupervised learning

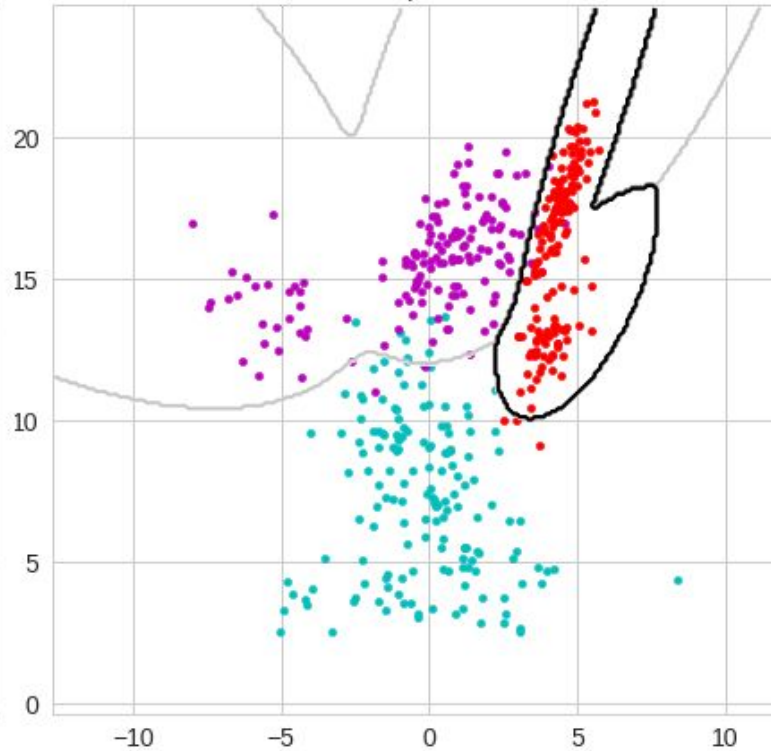
Supervised Accuracy: 0.93

Test Data, Supervised Boundaries



Semisupervised Accuracy: 0.96

Test Data, Semi-supervised Boundaries





pomegranate can be faster than scipy

```
mu, cov = numpy.random.randn(2000), numpy.eye(2000)
d = MultivariateGaussianDistribution(mu, cov)
X = numpy.random.randn(2000, 2000)
print "scipy time: ",
%timeit multivariate_normal.logpdf(X, mu, cov)
print "pomegranate time: ",
%timeit MultivariateGaussianDistribution(mu, cov).log_probability(X)
print "pomegranate time (w/ precreated object): ",
%timeit d.log_probability(X)
```

```
scipy time: 1 loop, best of 3: 1.67 s per loop
pomegranate time: 1 loop, best of 3: 801 ms per loop
pomegranate time (w/ precreated object): 1 loop, best of 3: 216 ms per loop
```



pomegranate uses aggressive caching

$$P(X|\mu, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x - \mu)^2}{2\sigma^2}\right)$$

$$\log P(X|\mu, \sigma) = -\log(\sqrt{2\pi}\sigma) - \frac{(x - \mu)^2}{2\sigma^2}$$

$$\log P(X|\mu, \sigma) = \alpha - \frac{(x - \mu)^2}{\beta}$$





Example 'blast' from Gossip Girl

Spotted: Lonely Boy. Can't believe the love of his life has returned. If only she knew who he was. But everyone knows Serena. And everyone is talking. Wonder what Blair Waldorf thinks. Sure, they're BFF's, but we always thought Blair's boyfriend Nate had a thing for Serena.



Example 'blast' from Gossip Girl

Why'd she leave? Why'd she return? Send me all the deets.
And who am I? That's the secret I'll never tell. The only one.
—XOXO. Gossip Girl.



How do we encode these 'blasts'?

Better lock it down with Nate, B. Clock's ticking.

+1 Nate

-1 Blair



How do we encode these 'blasts'?

This just in: S and B committing a crime of fashion. Who doesn't love a five-finger discount. Especially if it's the middle one.

-1 Blair

-1 Serena

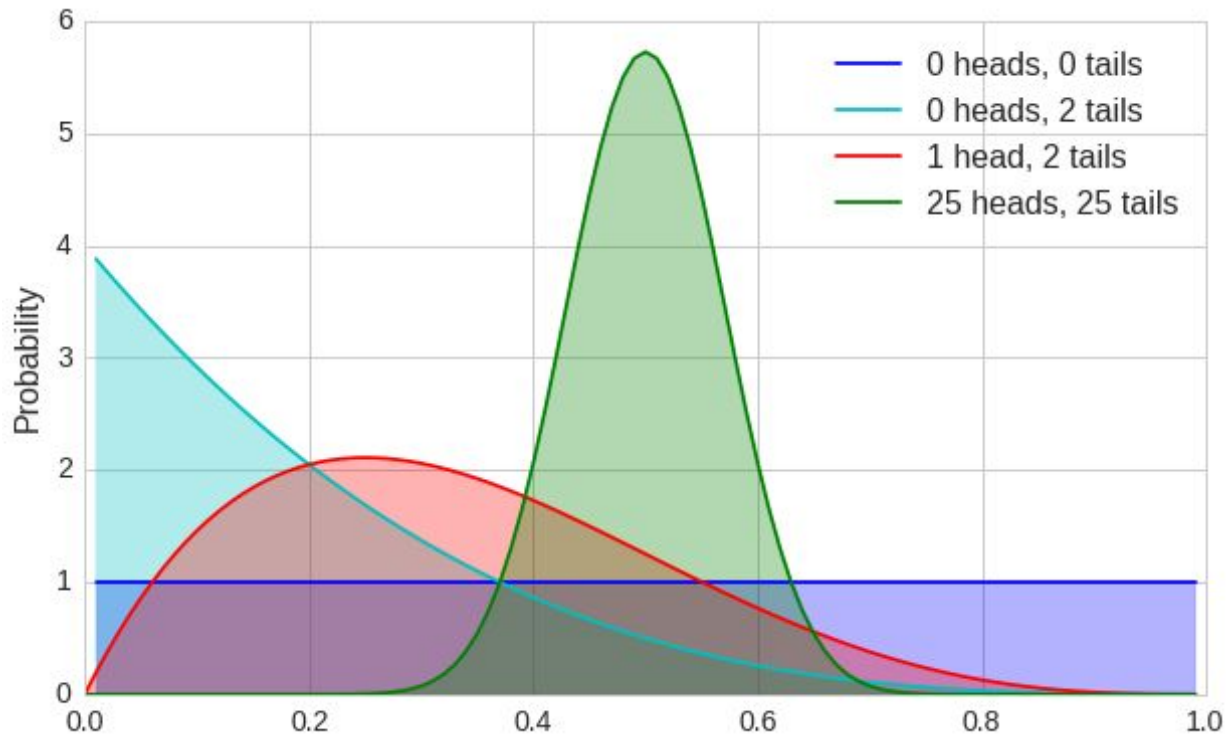


Simple summations don't work well



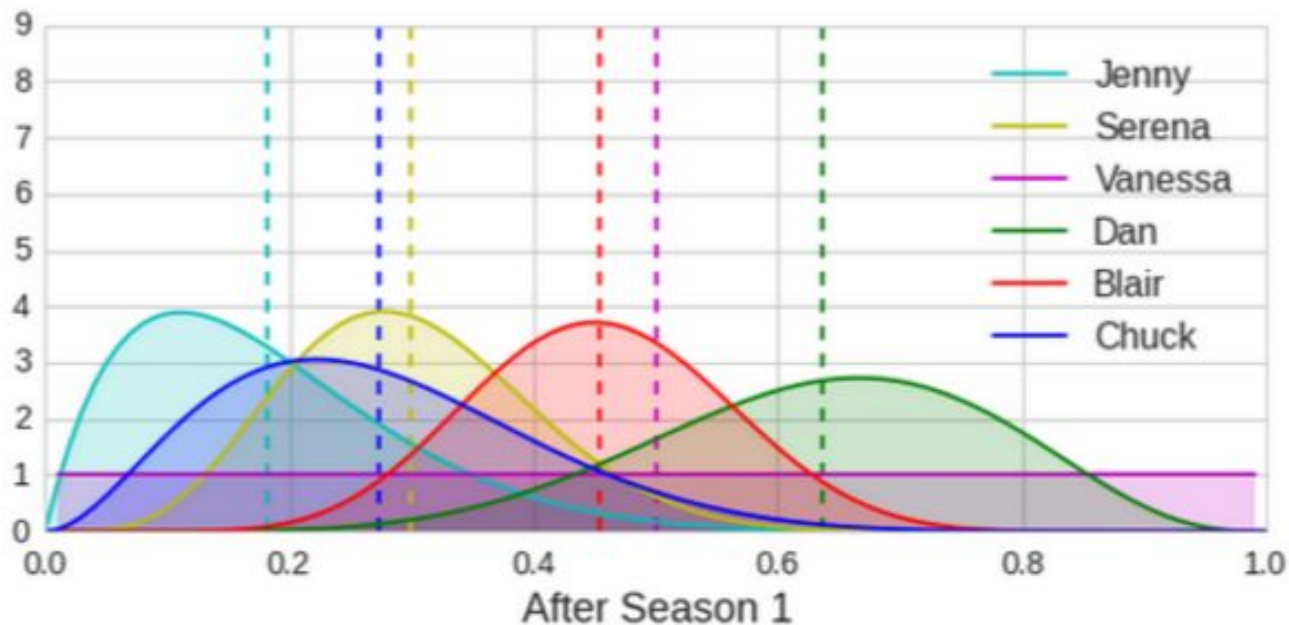


Beta distributions can model uncertainty



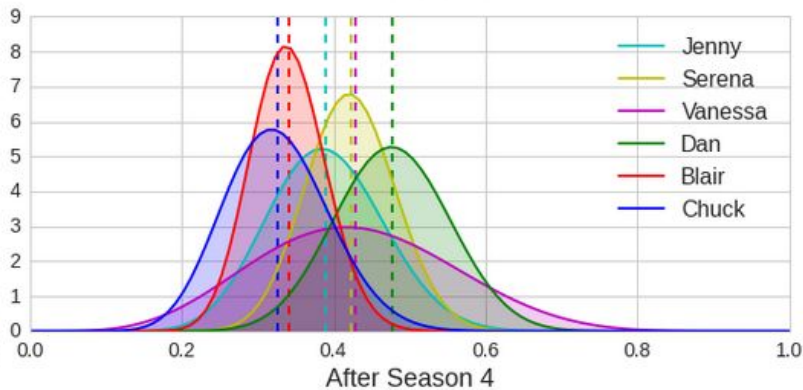
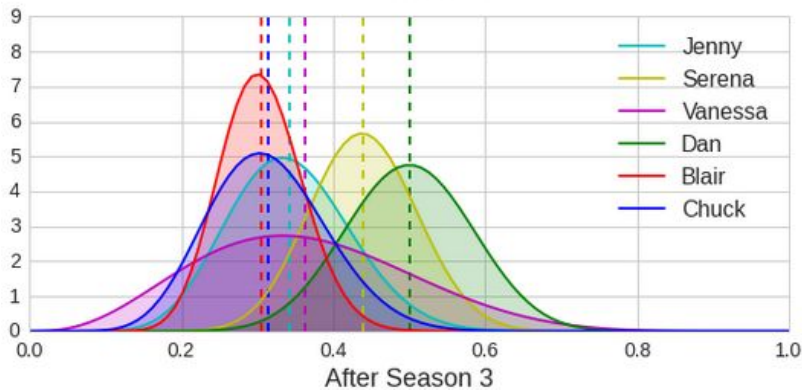
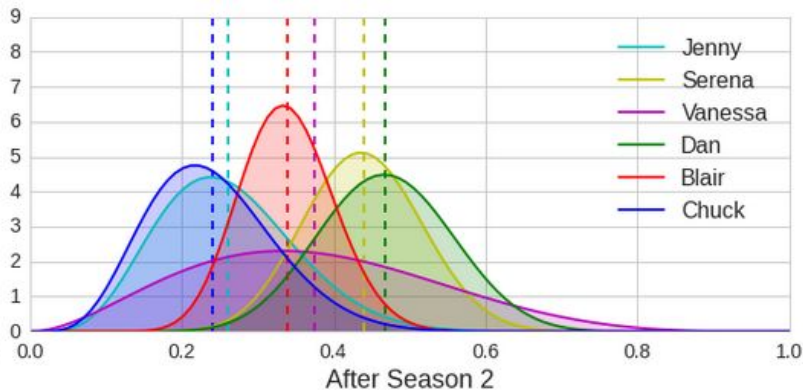
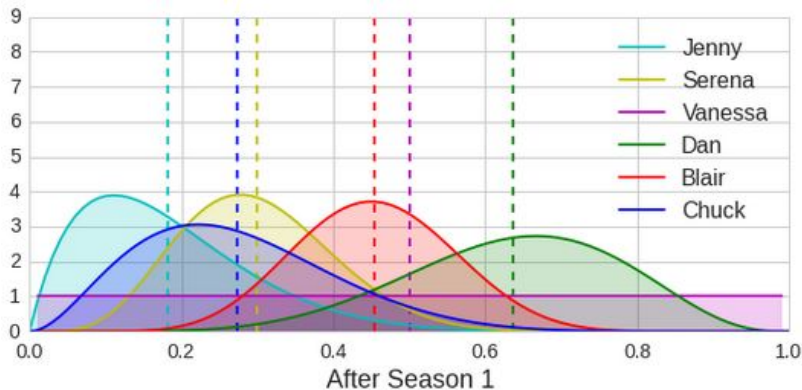


Beta distributions can model uncertainty





Beta distributions can model uncertainty





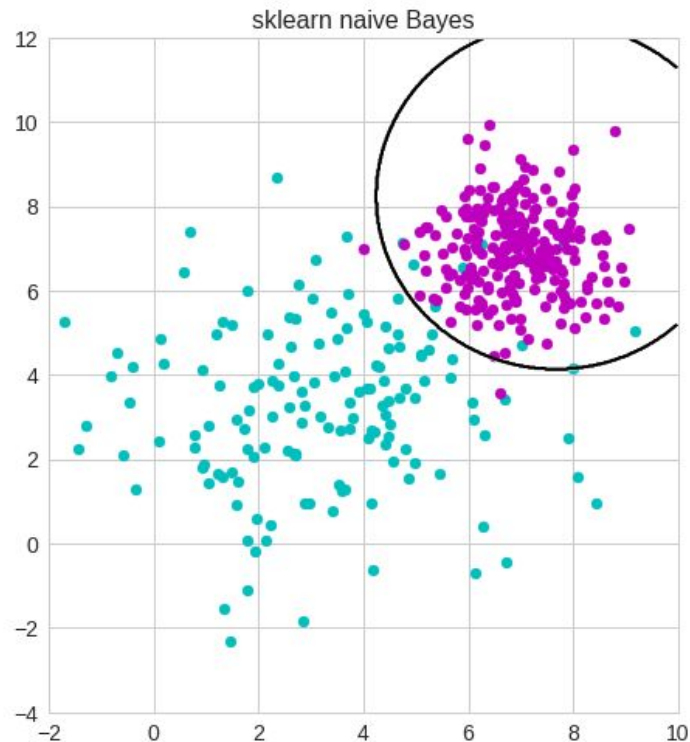
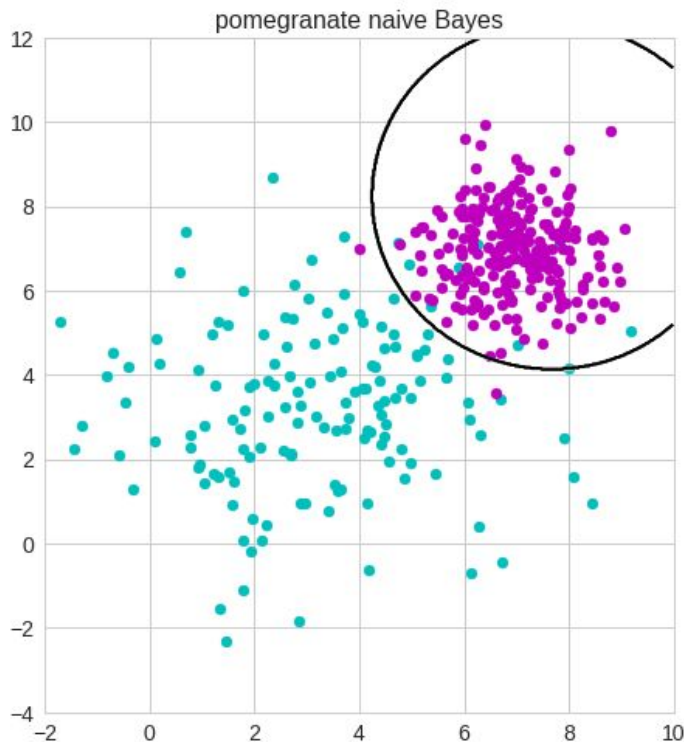
Naive Bayes assumes independent features

$$P(M|D) = \frac{\prod_{i=1}^d P(D_i|M)P(M)}{\sum_M \prod_{i=1}^d P(D_i|M)P(M)}$$

$$\textit{Posterior} = \frac{\textit{Likelihood} * \textit{Prior}}{\textit{Normalization}}$$



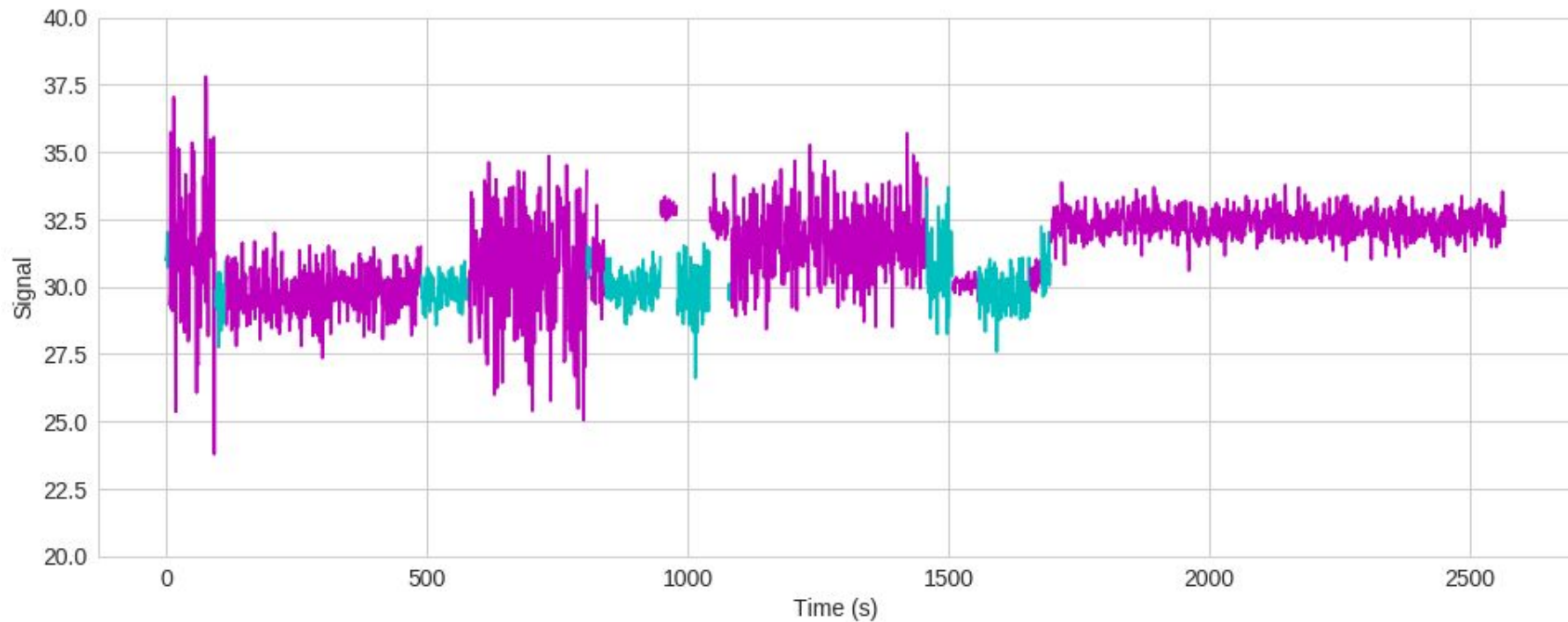
Naive Bayes produces ellipsoid boundaries



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



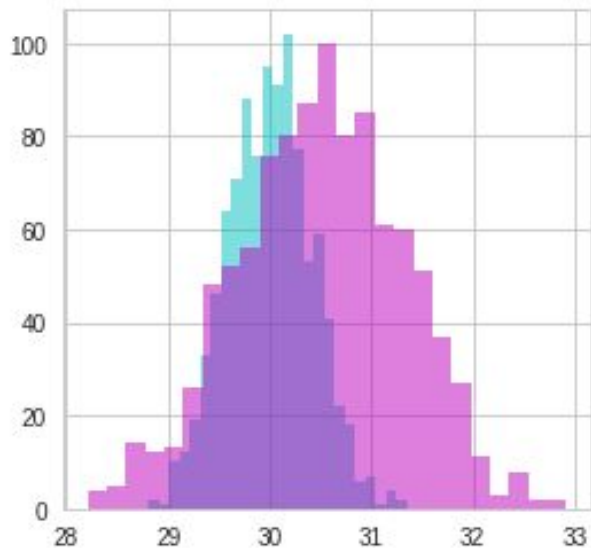
Naive Bayes can be heterogeneous



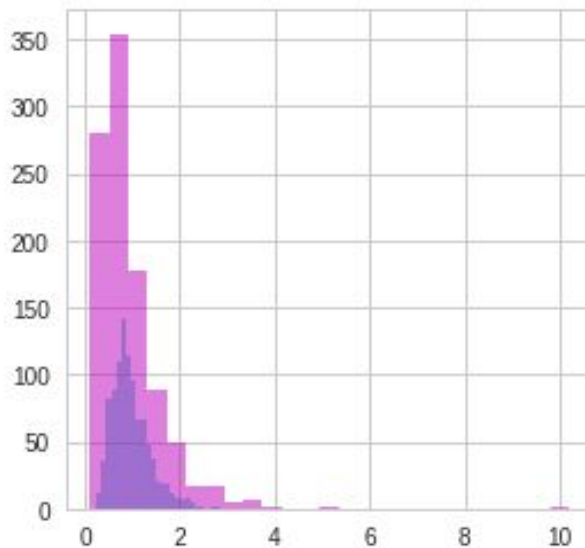


Data can fall under different distributions

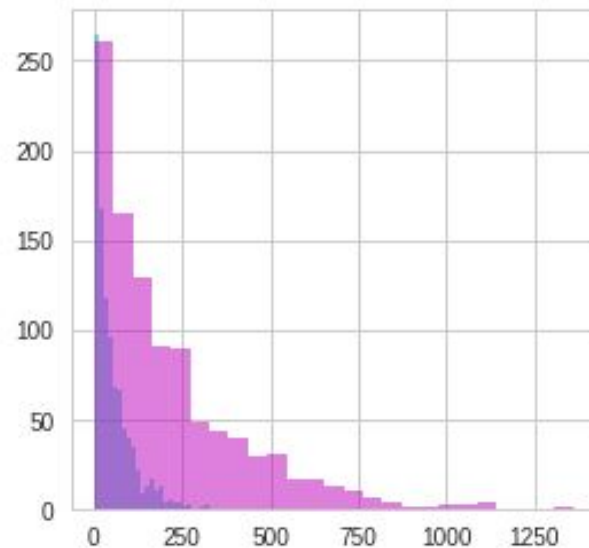
Mean



Standard Deviation



Duration





Using appropriate distributions is better

```
model = NaiveBayes.from_samples(NormalDistribution, X_train, y_train)
print "Gaussian Naive Bayes: ", (model.predict(X_test) == y_test).mean()
clf = GaussianNB().fit(X_train, y_train)
print "sklearn Gaussian Naive Bayes: ", (clf.predict(X_test) == y_test).mean()
model = NaiveBayes.from_samples([NormalDistribution, LogNormalDistribution,
ExponentialDistribution], X_train, y_train)
print "Heterogeneous Naive Bayes: ", (model.predict(X_test) == y_test).mean()
```

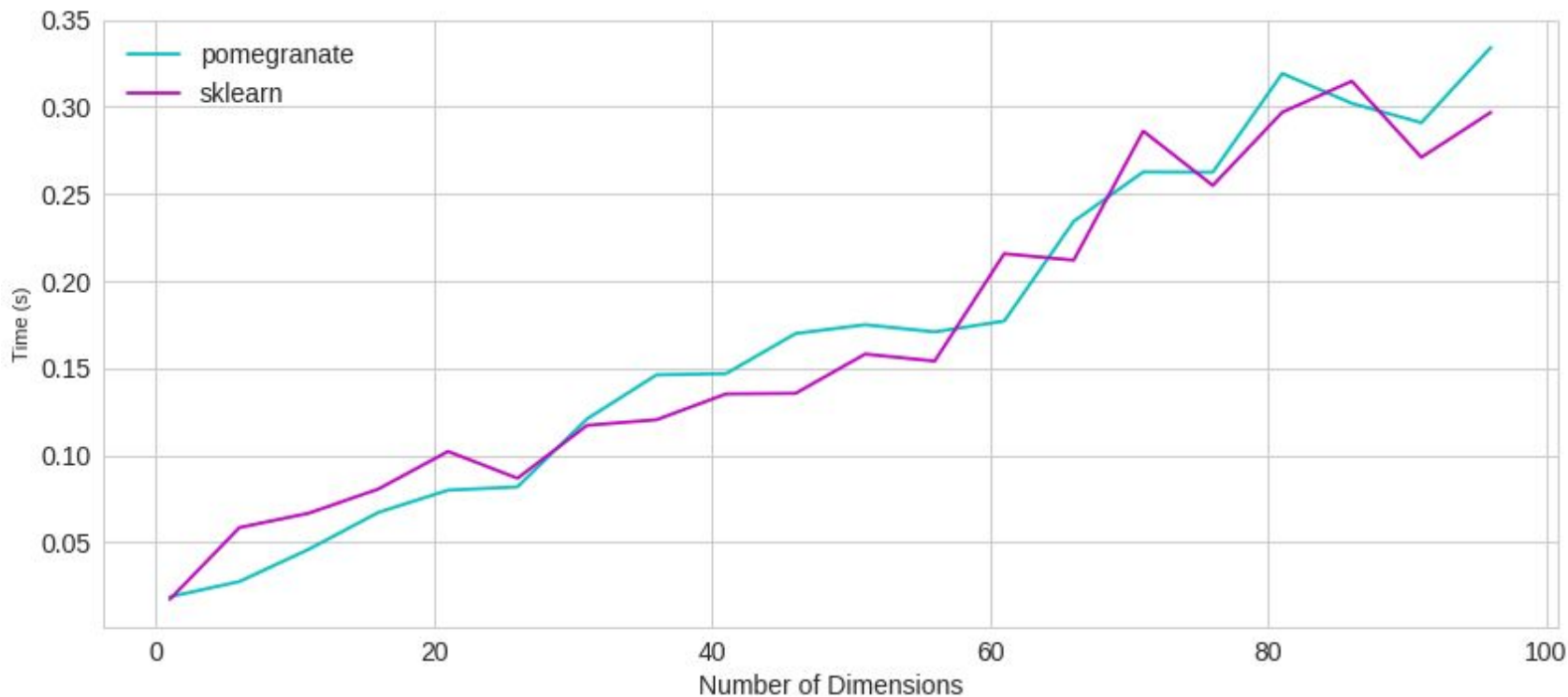
Gaussian Naive Bayes: 0.798

sklearn Gaussian Naive Bayes: 0.798

Heterogeneous Naive Bayes: 0.844



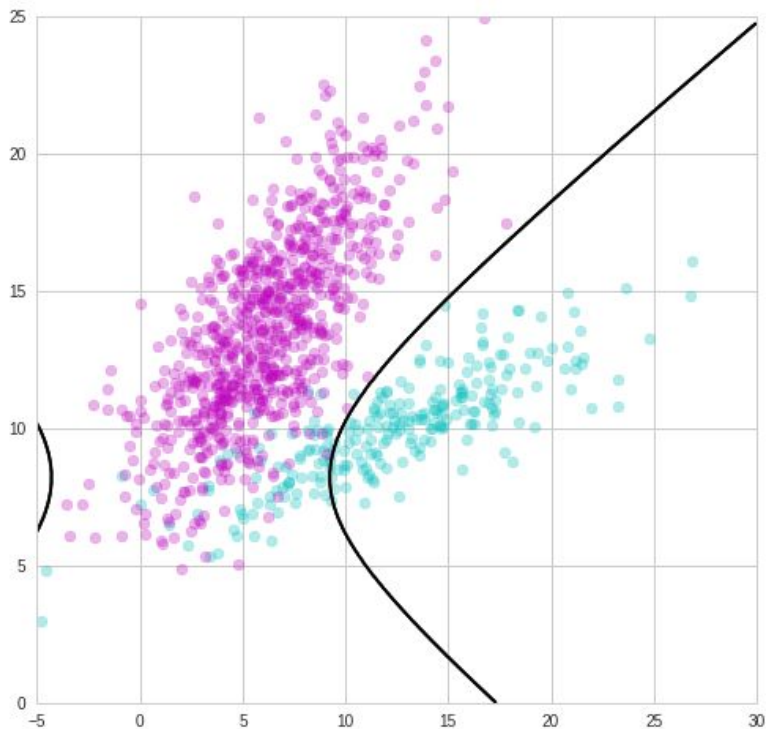
This additional flexibility is just as fast



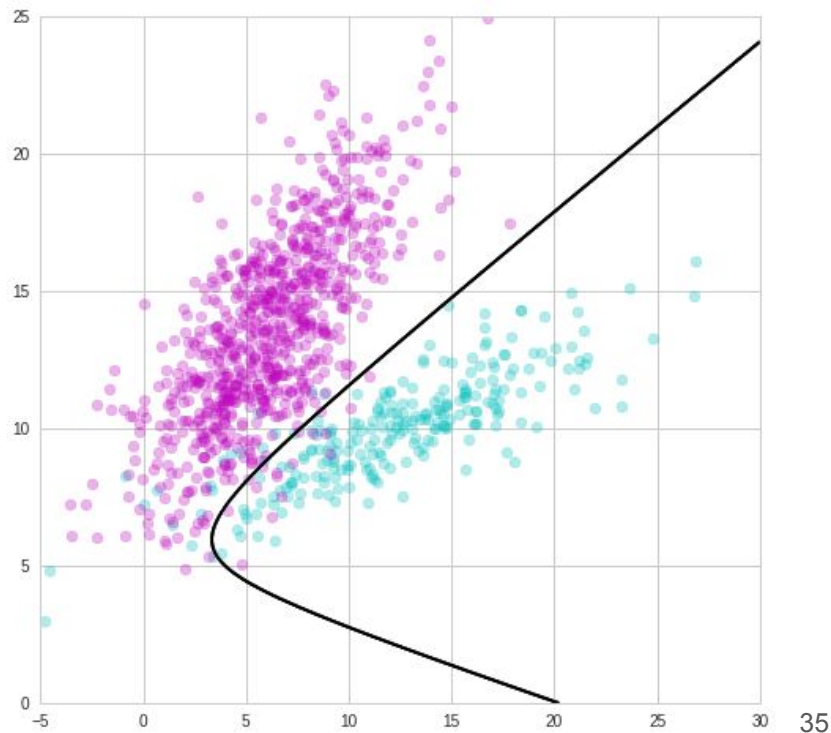


Bayes classifiers don't require independence

naive accuracy: 0.929

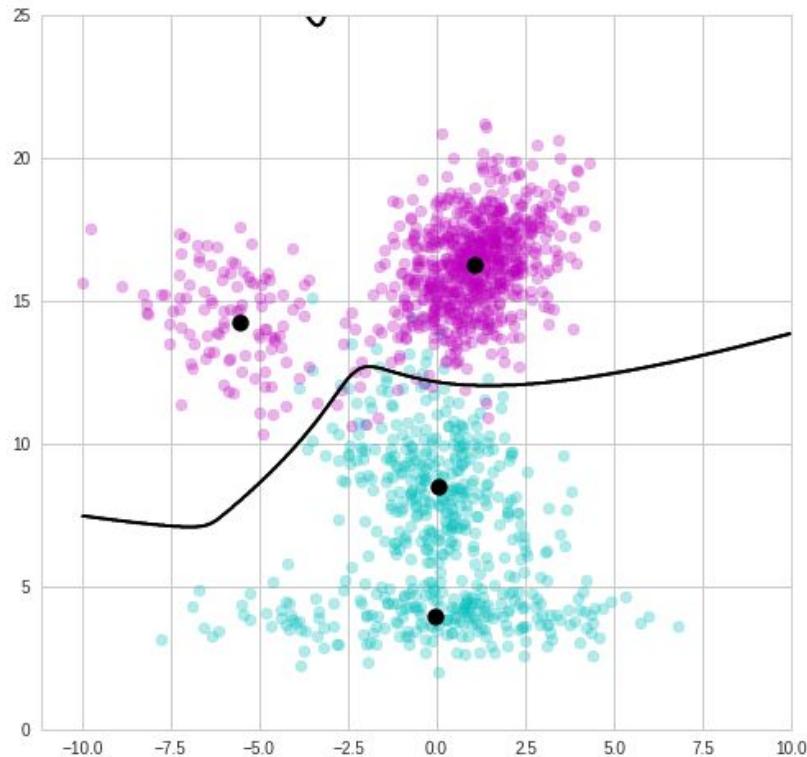
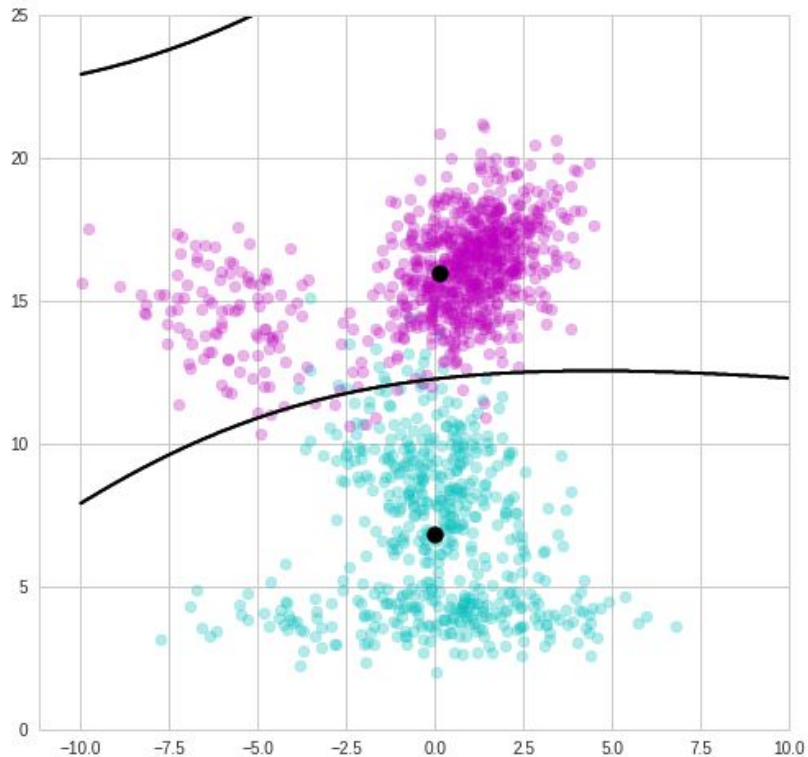


bayes classifier accuracy: 0.966





Gaussian mixture model Bayes classifier






Overview

pomegranate is **more flexible** than other packages, **faster**, is **intuitive to use**, and can do it all **in parallel**



Documentation available at Readthedocs

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Home

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.



Tutorials available on github

Branch: master ▾


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History

 jmschrei ADD bayes backend


Latest commit 724510d 10 hours ago

..

 GGBlasts.xlsx


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 PyData_2016_Chicago_Tutorial.ipynb


FIX markov chain notebooks

3 months ago

 README.md


Update README.md

2 years ago

 Tutorial_0_pomegranate_overview.ipynb


Minor typos

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 Tutorial_1_Distributions.ipynb


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FIX hmm dimensionality

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edit tutorial 3 to remove deprecated bake

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 Tutorial_4b_Bayesian_Network_Structure_Learning.i...


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 Tutorial_5_Bayes_Classifiers.ipynb


ADD bayes backend

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 Tutorial_6_Markov_Chain.ipynb

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3 months ago

 Tutorial_7_Parallelization.ipynb

ADD tutorial 7 parallelization

8 months ago

<https://github.com/jmschrei/pomegranate/tree/master/tutorials>



Acknowledgements



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ADVANCING DATA-INTENSIVE DISCOVERY IN ALL FIELDS