

# pomegranate

fast and flexible probabilistic modelling in python

Jacob Schreiber

Paul G. Allen School of Computer Science  
University of Washington



jmschreiber91



@jmschrei



@jmschreiber91



# 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

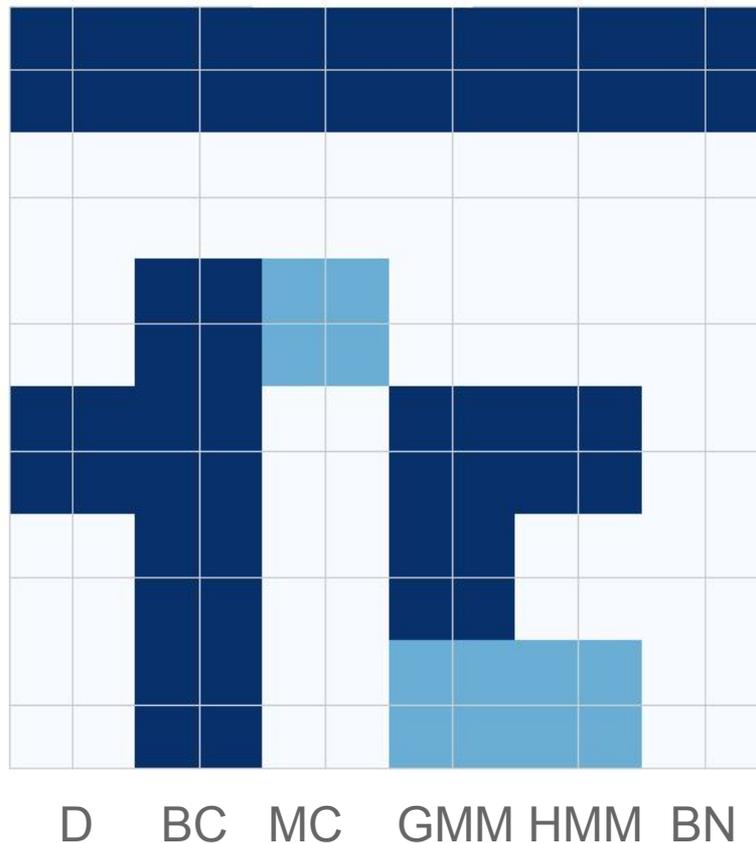
Bayes Classifiers

Markov Chains

General Mixture Models

Hidden Markov Models

Bayesian Networks





# Overview: model stacking in pomegranate

Distributions

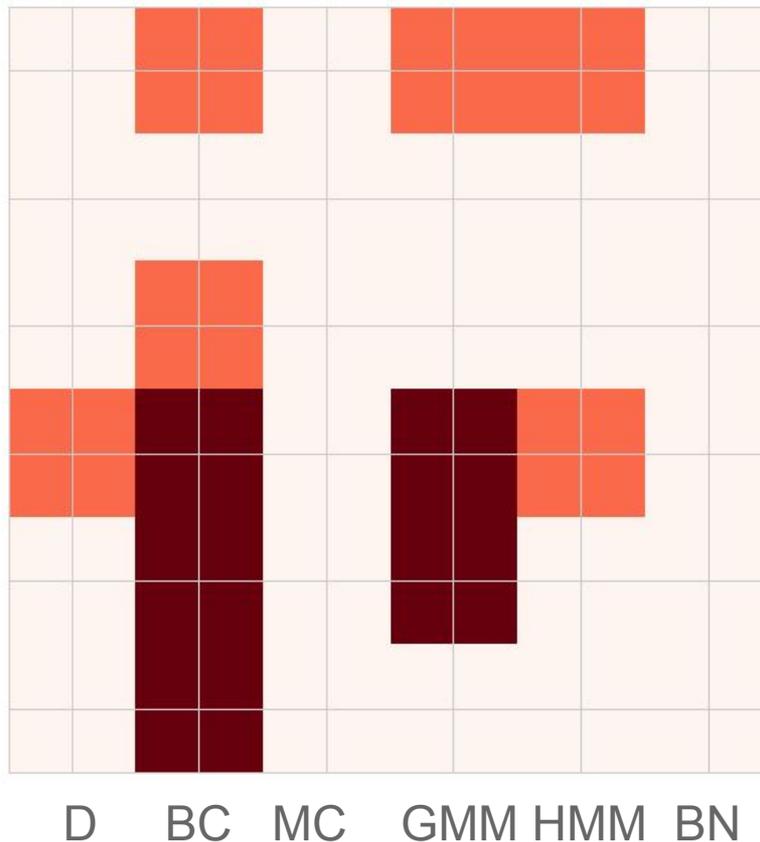
Bayes Classifiers

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)`

`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 have these methods!

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

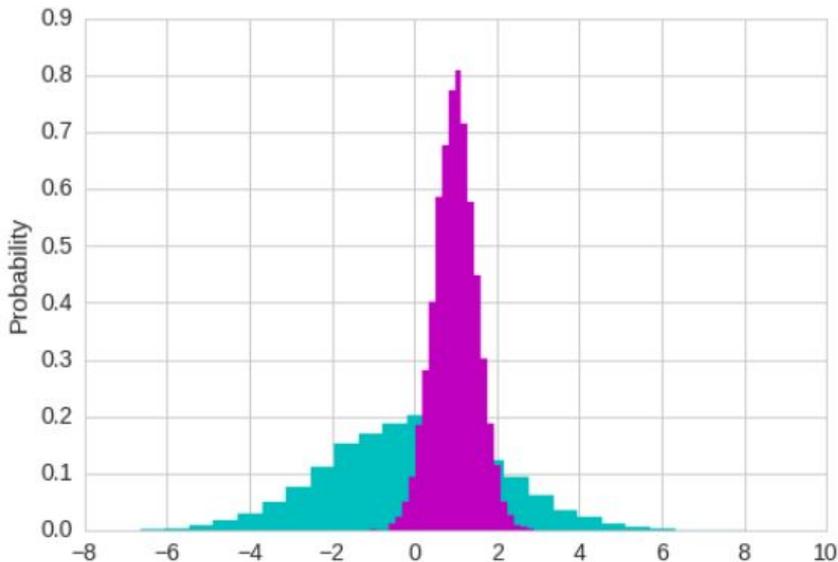
1. IndependentComponentsDistribution
2. MultivariateGaussianDistribution
3. DirichletDistribution
4. ConditionalProbabilityTable
5. JointProbabilityTable



# Models can be created from known values

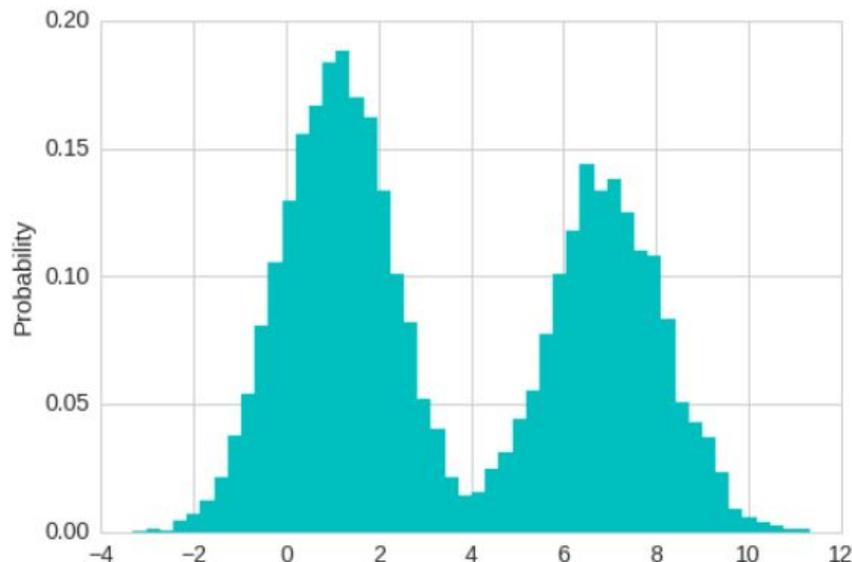
$\mu, \text{sig} = 0, 2$

`a = NormalDistribution(mu, sig)`



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

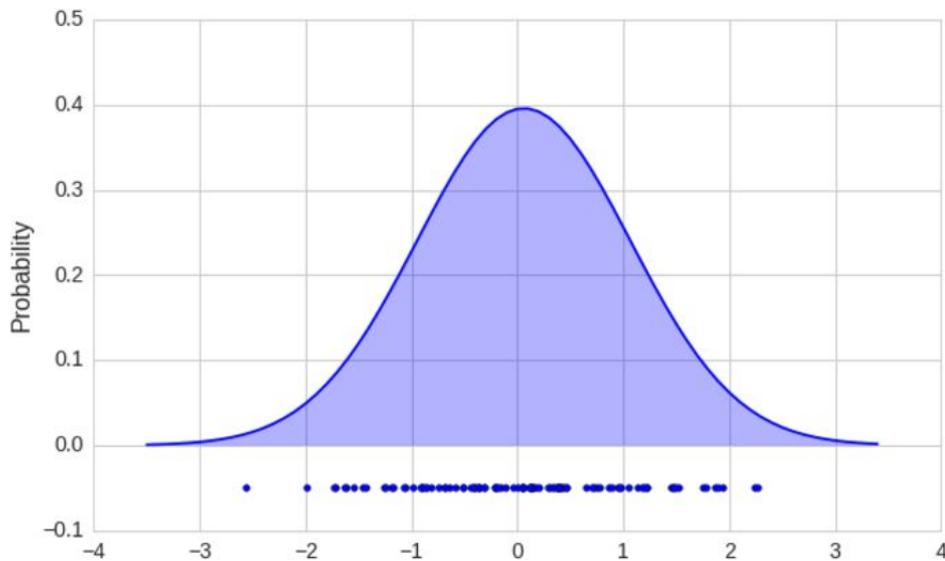
`a = GaussianKernelDensity(X)`





# 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  $\mu$ s per loop

pomegranate time:  
100 loops, best of 3: 22.2  $\mu$ 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)
```

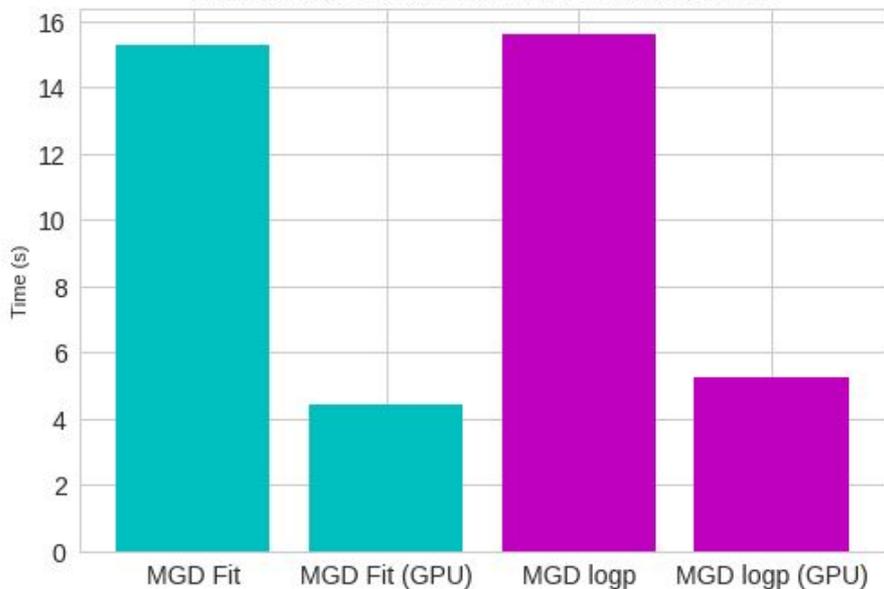
numpy time:  
10 loops, best of 3: 1.02 s per loop

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

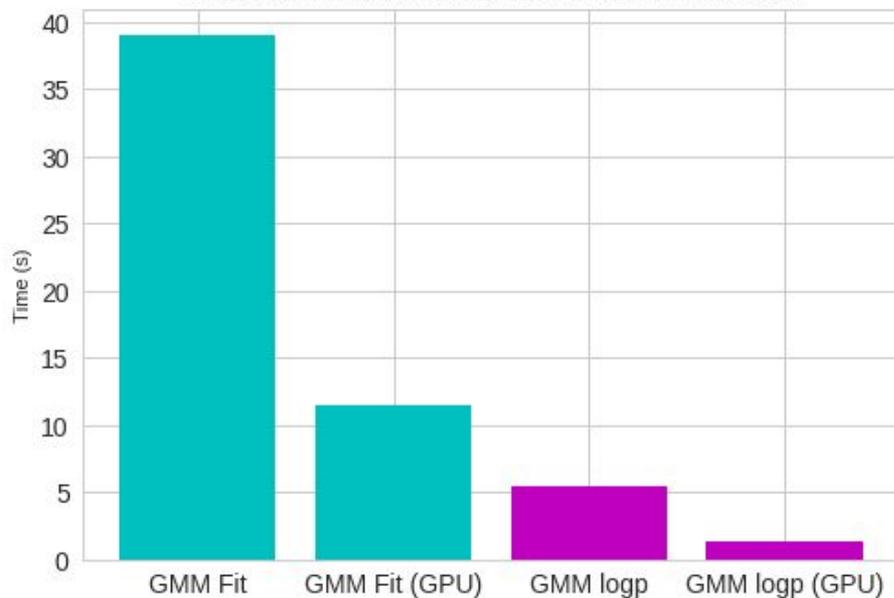


# pomegranate just merged GPU support

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

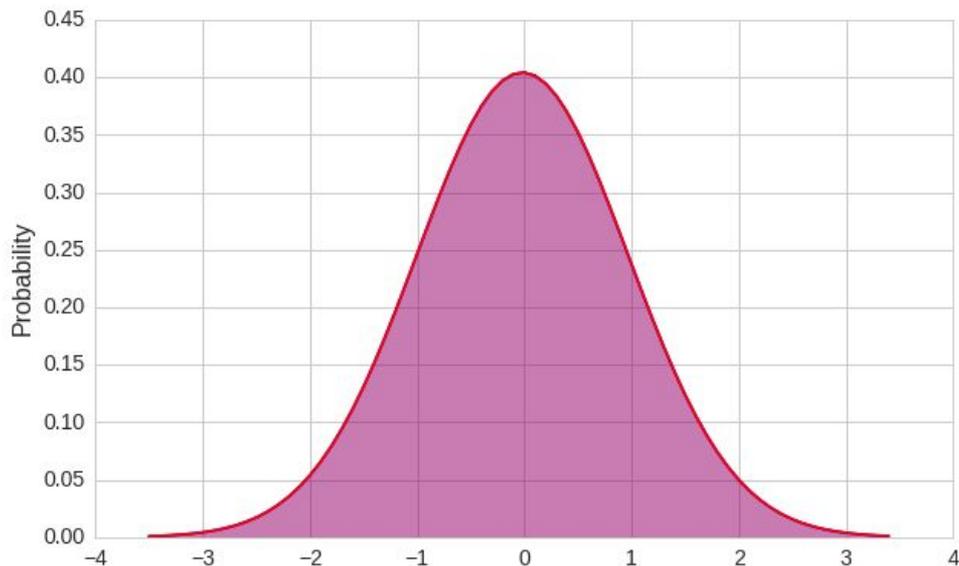
$$\sum_{i=1}^n w_i \quad \sum_{i=1}^n w_i x_i \quad \sum_{i=1}^n w_i x_i^2 \quad \longrightarrow \quad \begin{aligned} \mu &= \frac{\sum_{i=1}^n w_i x_i}{\sum_{i=1}^n w_i} \\ \sigma^2 &= \frac{\sum_{i=1}^n w_i x_i^2}{\sum_{i=1}^n w_i} - \frac{\left(\sum_{i=1}^n w_i x_i\right)^2}{\left(\sum_{i=1}^n w_i\right)^2}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



# 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.

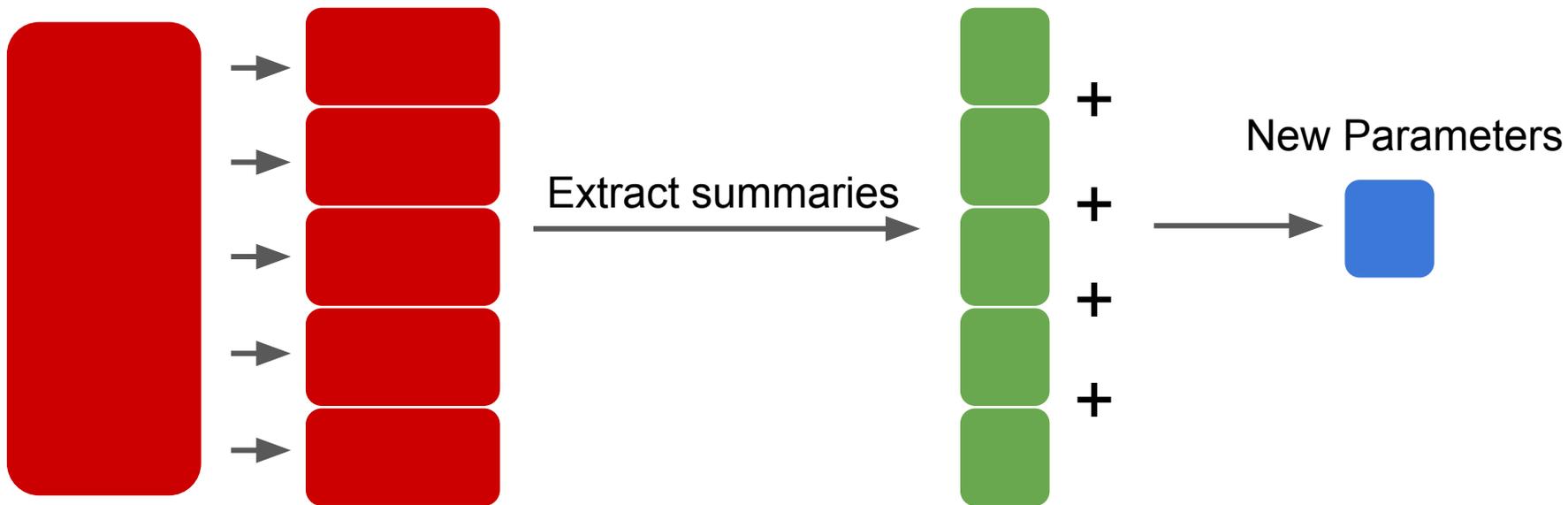
```
a.fit(data)
b.summarize(data[:1000])
b.summarize(data[1000:2000])
b.summarize(data[2000:3000])
b.summarize(data[3000:4000])
b.summarize(data[4000:])
b.from_summaries()
```



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



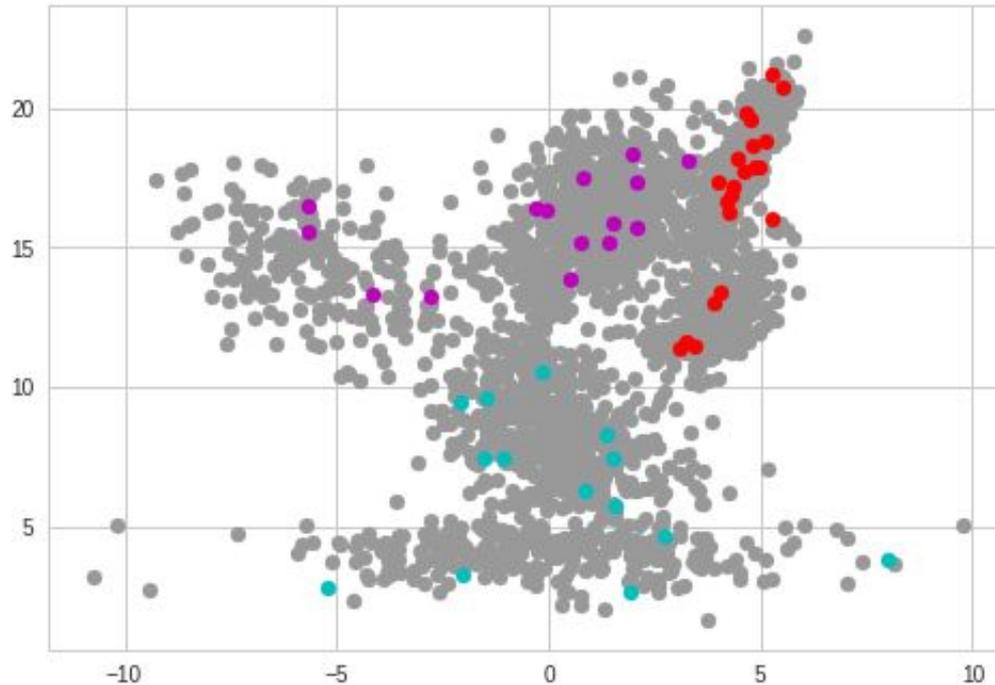
# Parallelization exploits additive summaries





# 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.

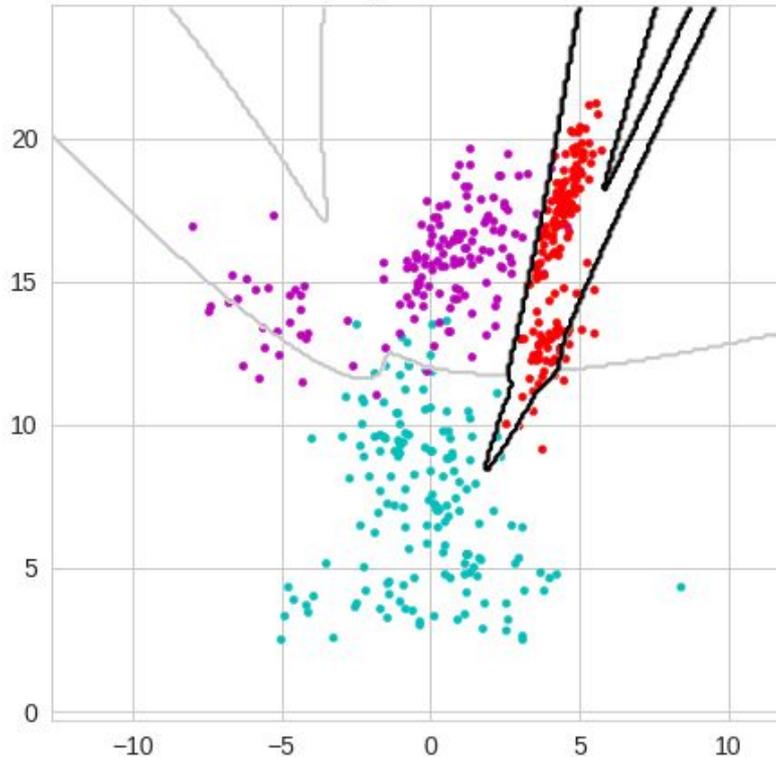




# pomegranate supports semisupervised learning

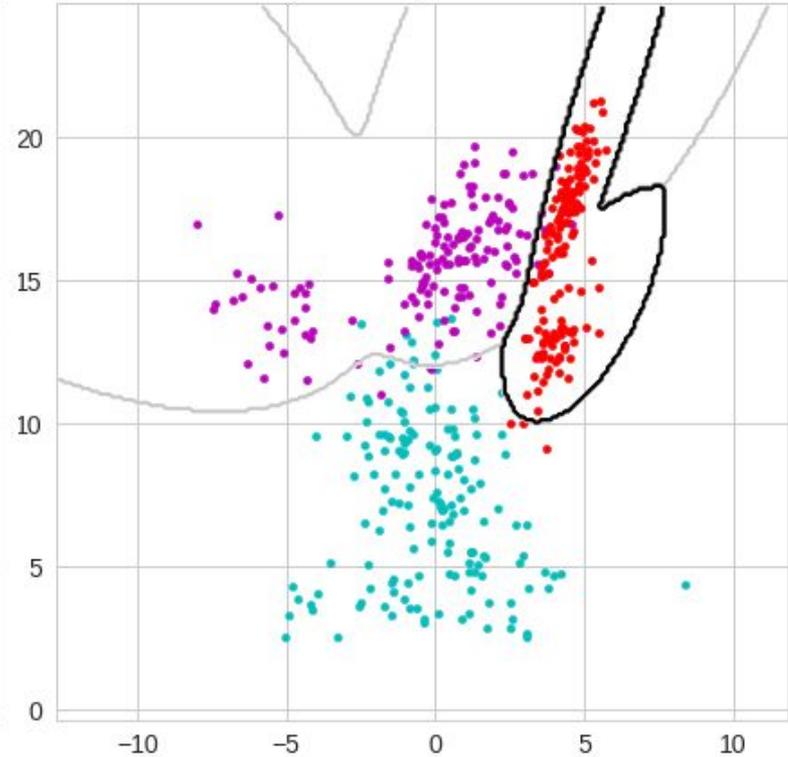
Supervised Accuracy: 0.93

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

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

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

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



# GOSSIP GIRL



## 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

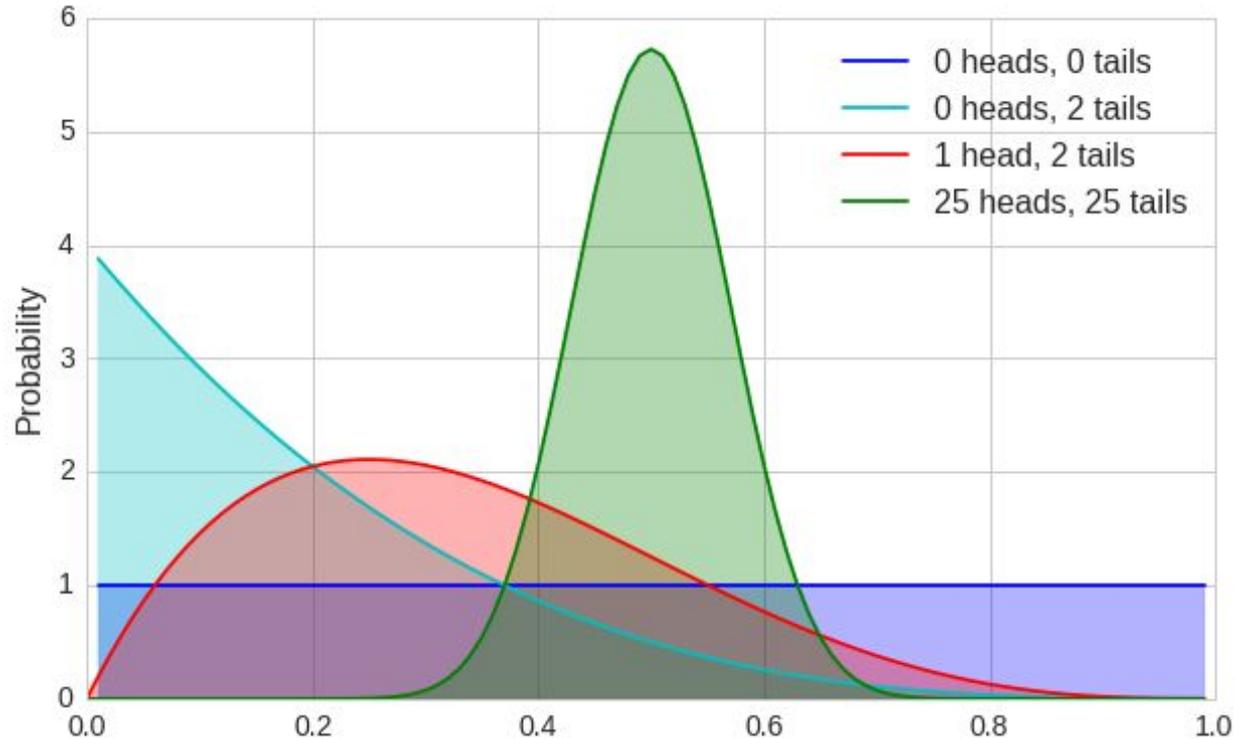


# Simple summations don't work well



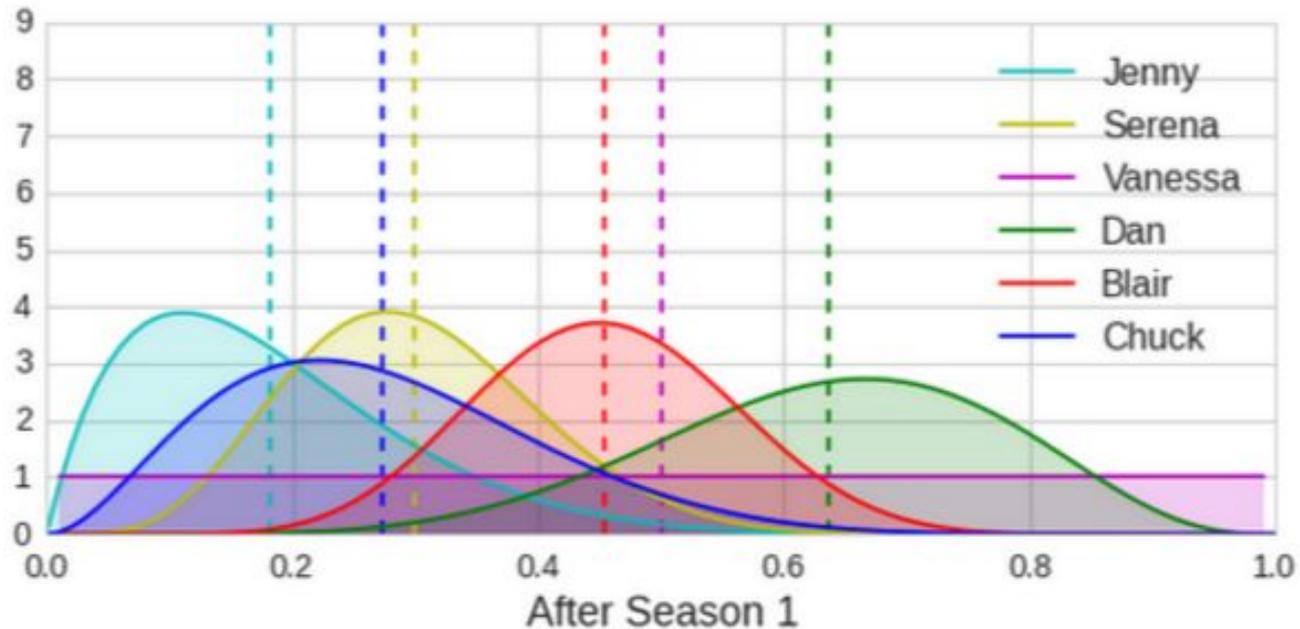


# Beta distributions can model uncertainty



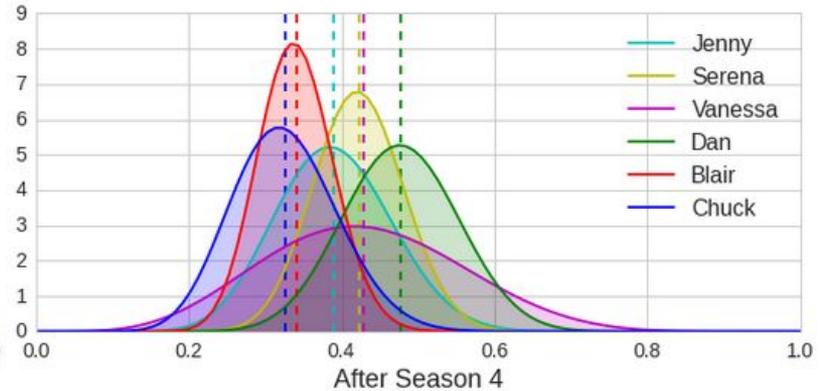
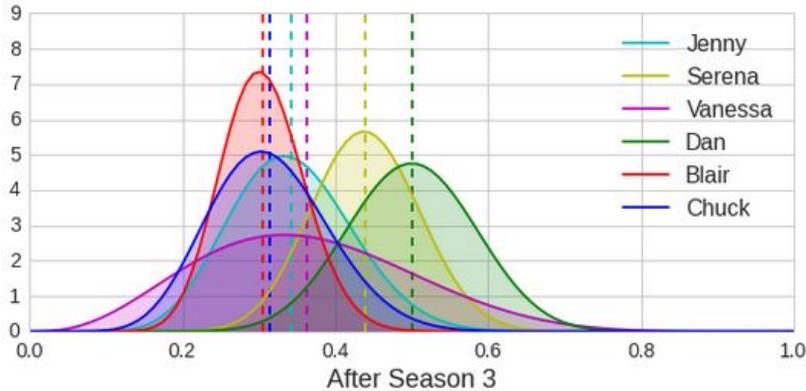
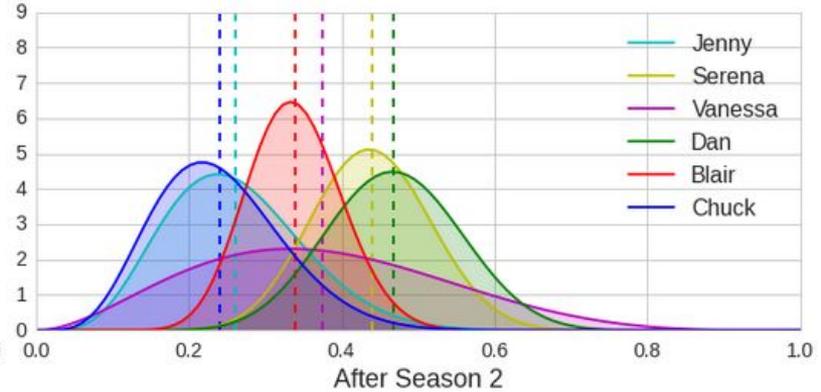
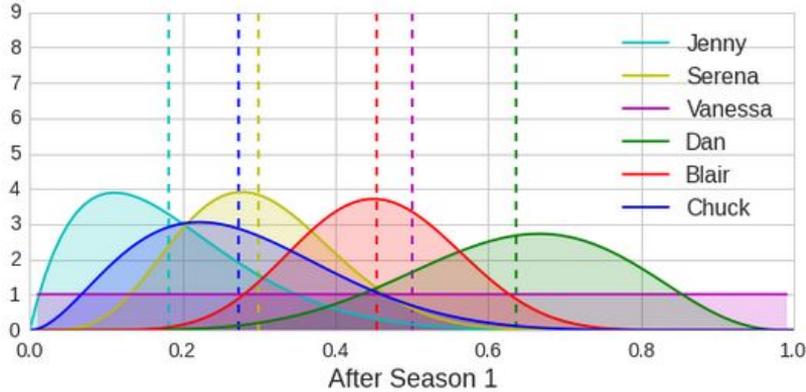


# Beta distributions can model uncertainty





# Beta distributions can model uncertainty





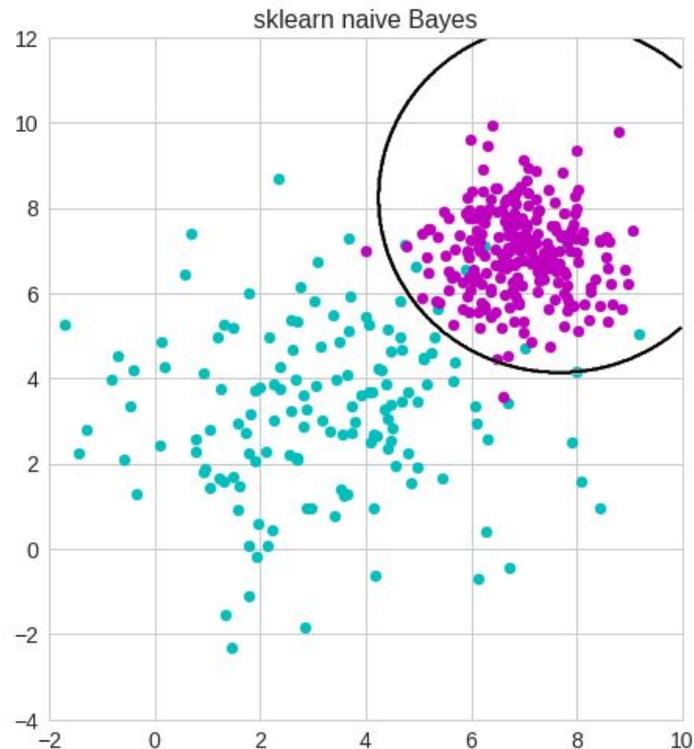
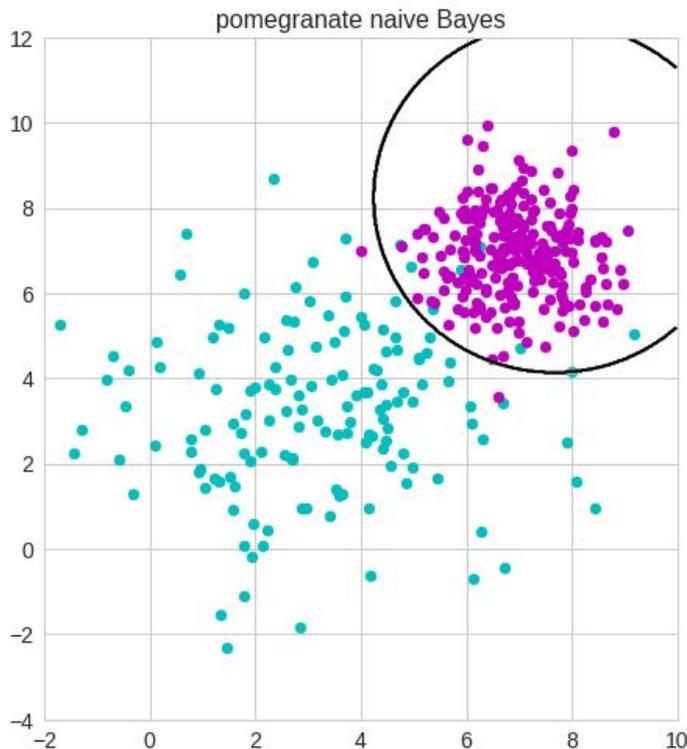
# Naive Bayes assumes independent features

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

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



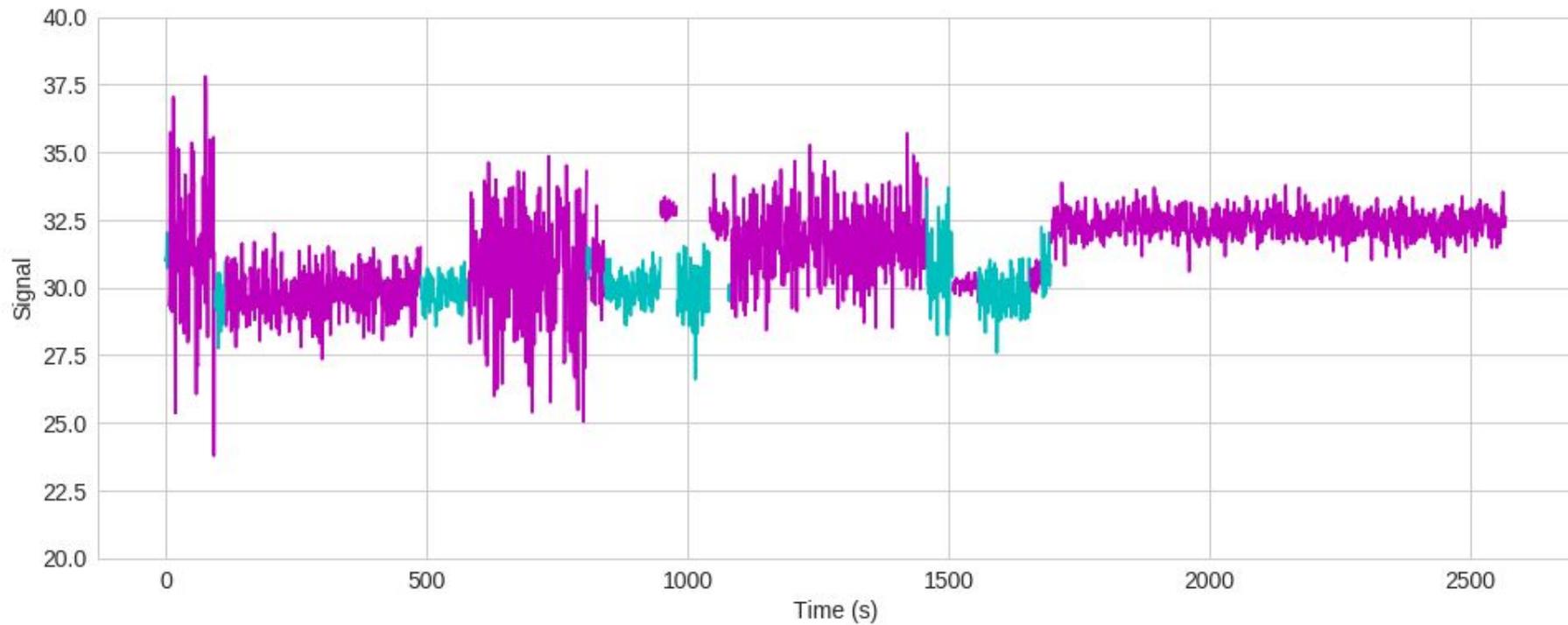
# Naive Bayes produces ellipsoid boundaries



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



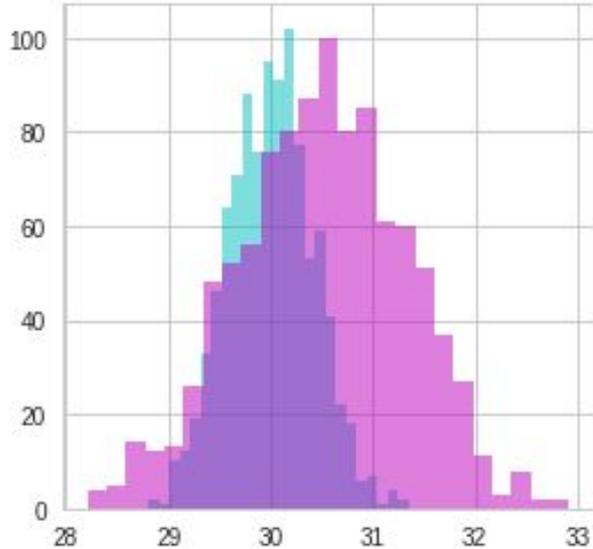
# Naive Bayes can be heterogeneous



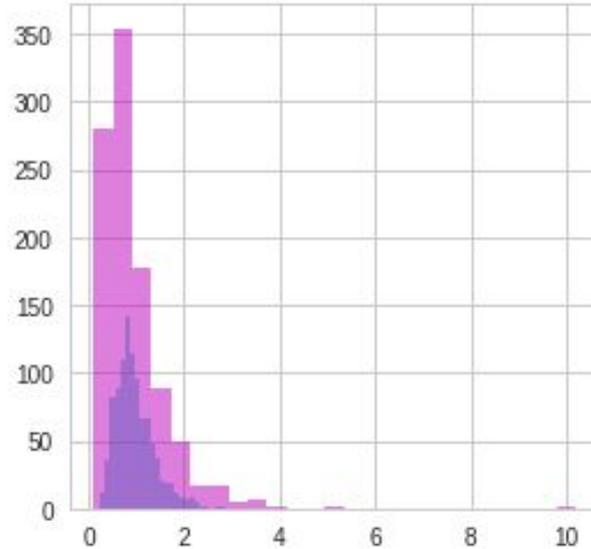


# Data can fall under different distributions

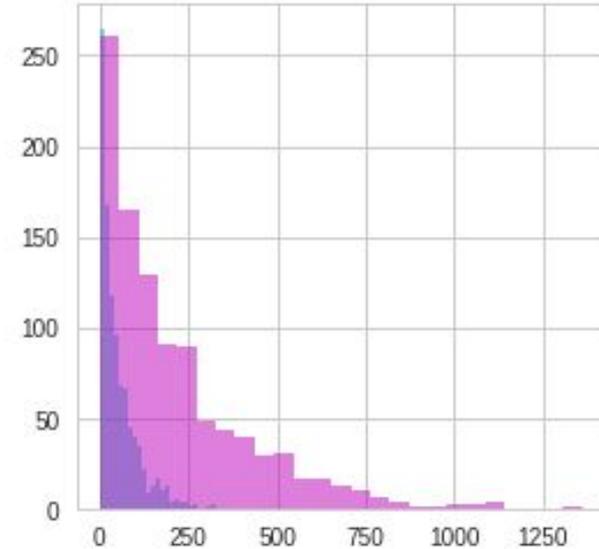
Mean



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()
```

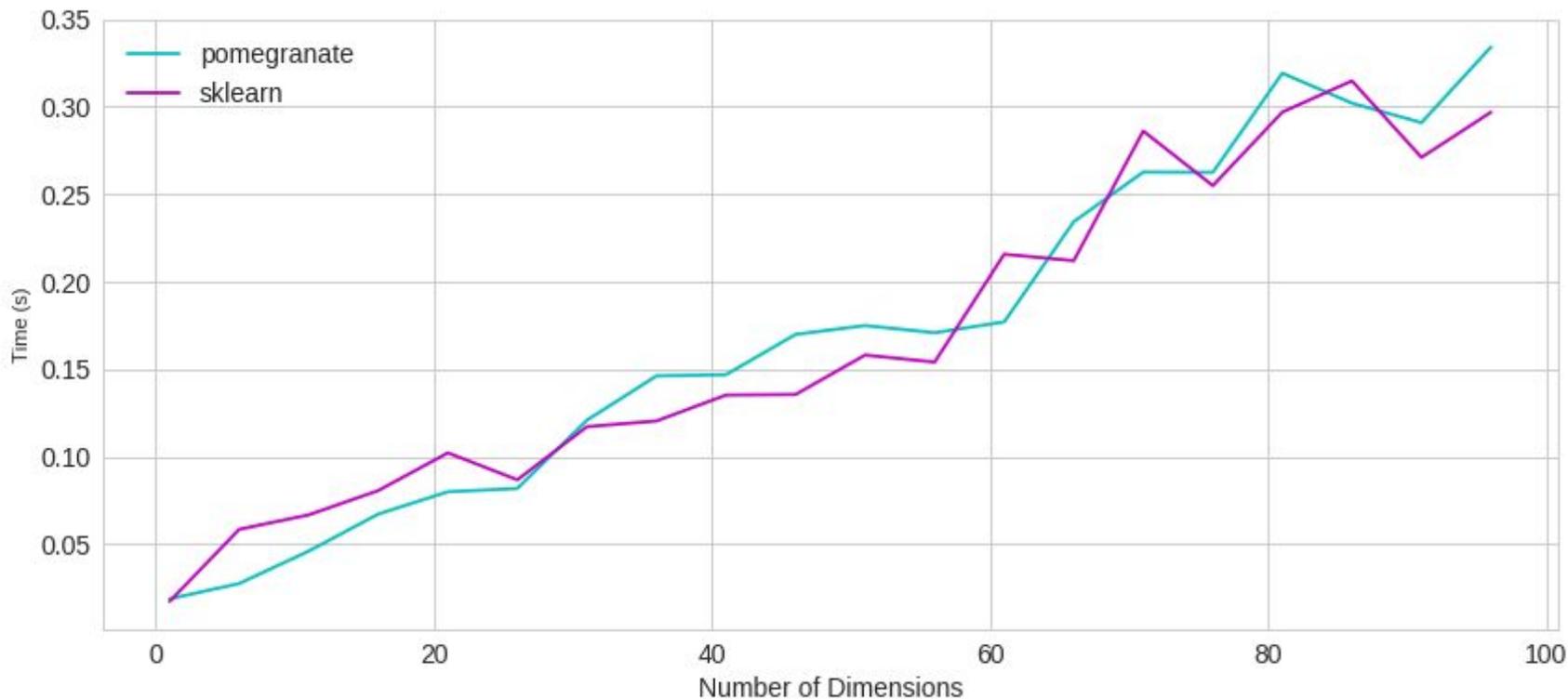
Gaussian Naive Bayes: 0.798

sklearn Gaussian Naive Bayes: 0.798

Heterogeneous Naive Bayes: 0.844



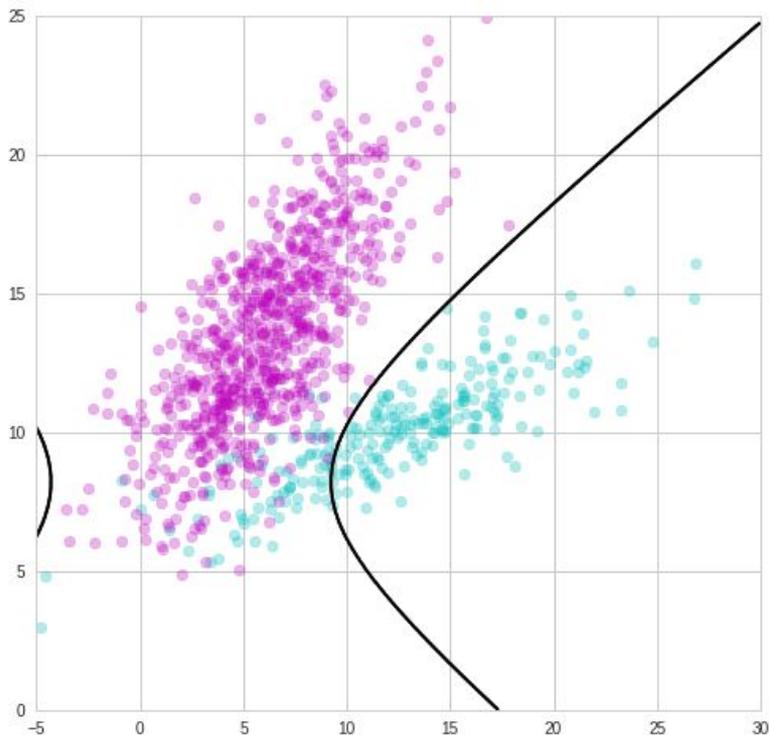
# This additional flexibility is just as fast



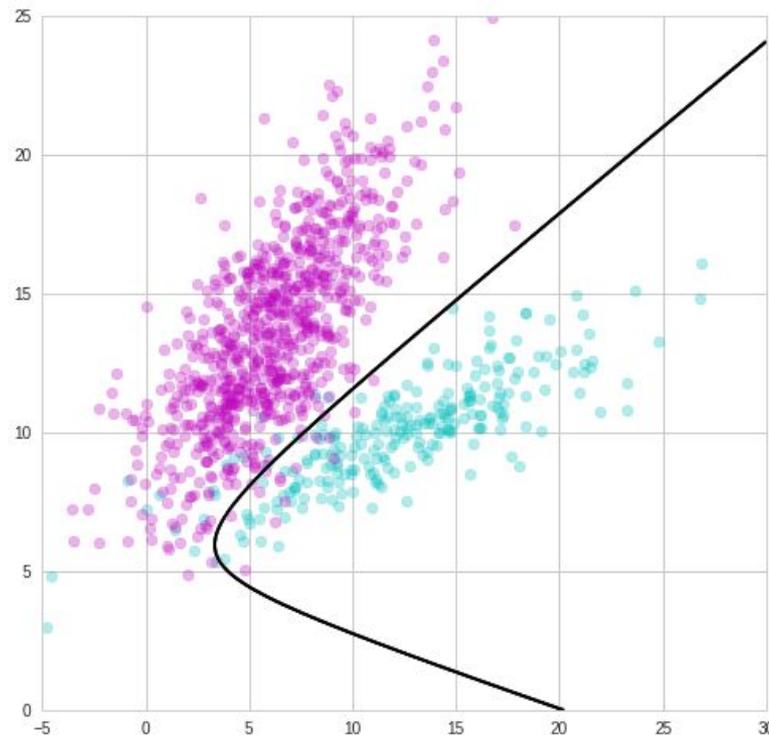


# Bayes classifiers don't require independence

naive accuracy: 0.929

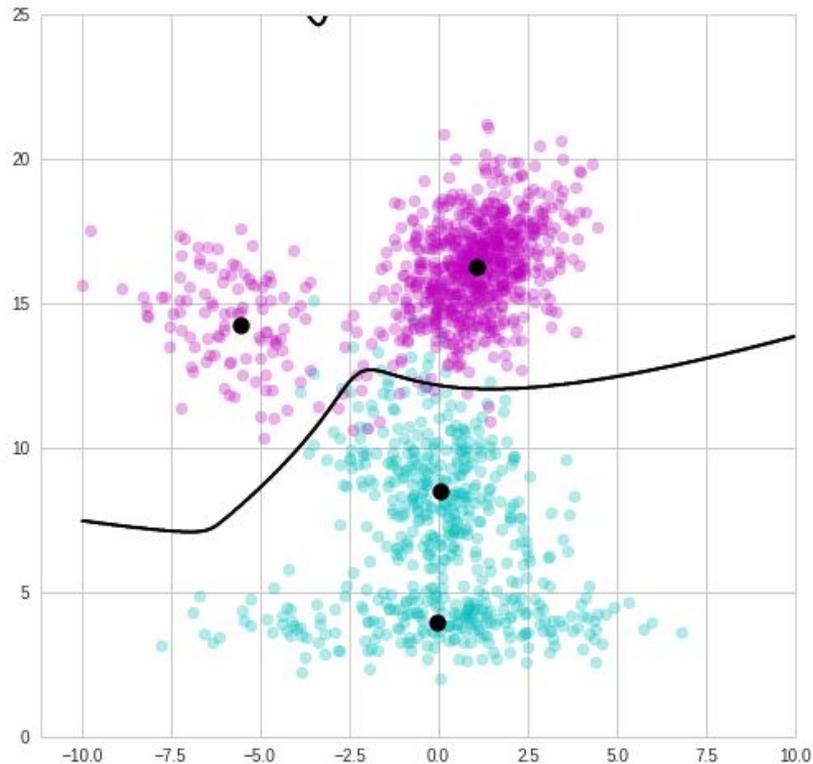
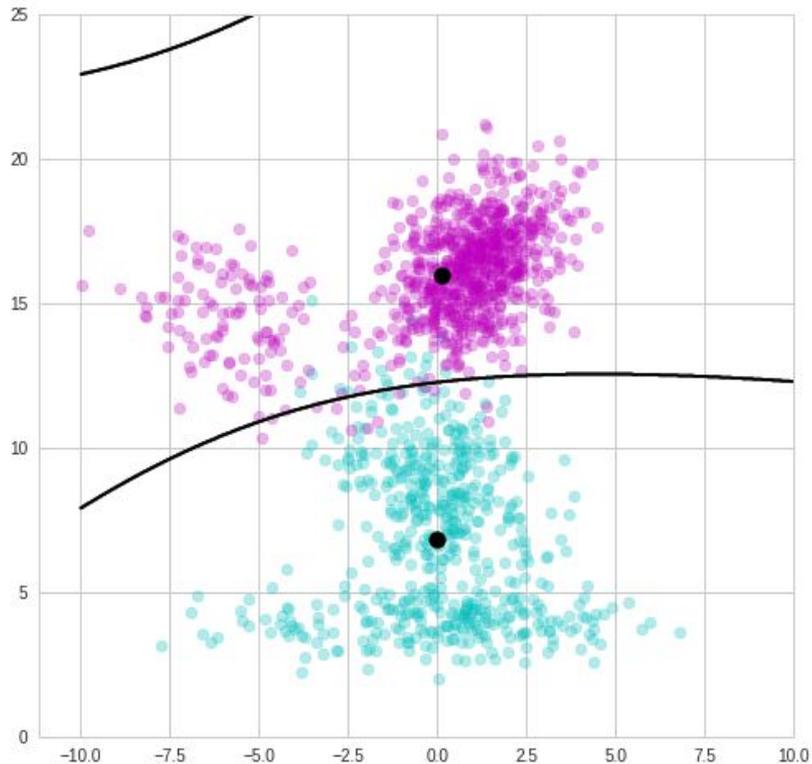


bayes classifier accuracy: 0.966





# 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

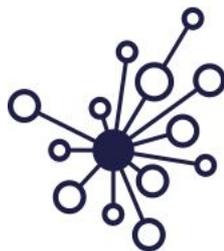
Branch: master ▾ pomegranate / tutorials / Create new file Upload files Find file History

jmschrei ADD bayes backend	Latest commit 724510d 10 hours ago
..	
GGBlasts.xlsx	PyData Chicago 2016 8 months ago
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 3 months ago
Tutorial_1_Distributions.ipynb	ENH tutorials 2 years ago
Tutorial_2_General_Mixture_Models.ipynb	FIX hmm dimensionality 11 months ago
Tutorial_3_Hidden_Markov_Models.ipynb	edit tutorial 3 to remove deprecated bake 7 months ago
Tutorial_4_Bayesian_Networks.ipynb	ENH pomegranate vs libpgm tutorial 7 months ago
Tutorial_4b_Bayesian_Network_Structure_Learning.i...	ENH a* search 28 days ago
Tutorial_5_Bayes_Classifiers.ipynb	ADD bayes backend 10 hours ago
Tutorial_6_Markov_Chain.ipynb	FIX markov chain notebooks 3 months ago
Tutorial_7_Parallelization.ipynb	ADD tutorial 7 parallelization 8 months ago

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



# Acknowledgements



UNIVERSITY of WASHINGTON  
**eScience Institute**  
ADVANCING DATA-INTENSIVE DISCOVERY IN ALL FIELDS