Welcome to the DeBaCl tutorial. This IPython Notebook closely follows the script gauss_demo.py in the bin/ folder. DeBaCl is a library for estimating level set trees for interactive data visualization and clustering. It is based on the premise that a good, statistically principled way to define clusters is to associate them with modes of a probability density function. Level set trees are particularly useful with complex and high-dimensional data when there is reason to believe the data exhibit multi-scale clustering behavior.

This document demonstrates some of the basic uses of the DeBaCl package. The accompanying user manual and paper give much greater detail. The first example is data from a mixture of 3 Gaussian distributions in 1-dimension. First, we import the required libraries and set some plotting parameters. The geom_tree module is the workhorse of the library, while utils contains useful utility functions.

```
## Set up
import sys
sys.path.append('..') # shouldn't need this once installed from PyPI

from debacl import geom_tree as gtree
from debacl import utils as utl

import numpy as np
import matplotlib.pyplot as plt


## Output parameters
utl.setPlotParams(axes_labelsize=24, xtick_labelsize=18, ytick_labelsize=18, figsize
    =(6,6))
```

1,500 observations are drawn from the Gaussian mixture distribution, and the data are illustrated with a histogram. p_k is a smoothness parameter; for each data point, it is the fraction of observations to consider as neighbors. p_gamma indicates the size threshold (again as a fraction of n) for tree leaves; nodes with fewer observations will be pruned from the tree.

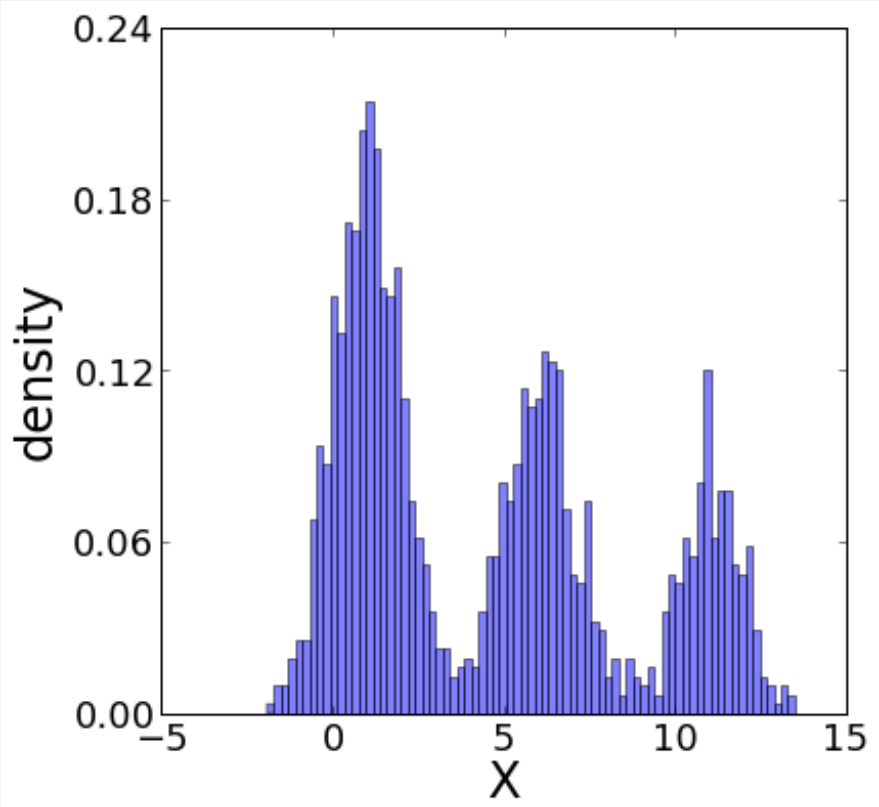
```
## Data parameters
n = 1500
ctr = ((1,), (6,), (11,))
sdev = (np.eye(1),) * 3
mix = (0.5, 0.3, 0.2)

## Generate data
membership = np.random.multinomial(n, pvals=mix)
p = len(ctr[0])
X = np.zeros((n, p), dtype=np.float)
g = np.zeros((n, ), dtype=np.int)
b = np.cumsum((0,) + tuple(membership))

for i, (size, mu, sigma) in enumerate(zip(membership, ctr, sdev)):
        ix = range(b[i], b[i+1])
        X[ix, :] = np.random.multivariate_normal(mu, sigma, size)
        g[ix] = i
```

```
X = np.sort(X, axis=0) # sort the points for prettier downstream plotting


## Plot a histogram of the data to show the simulation worked
fig, ax = plt.subplots()
ax.hist(X, bins=n/20, normed=1, alpha=0.5)
ax.set_xlabel('X')
ax.set_ylabel('density')
fig.show()
```



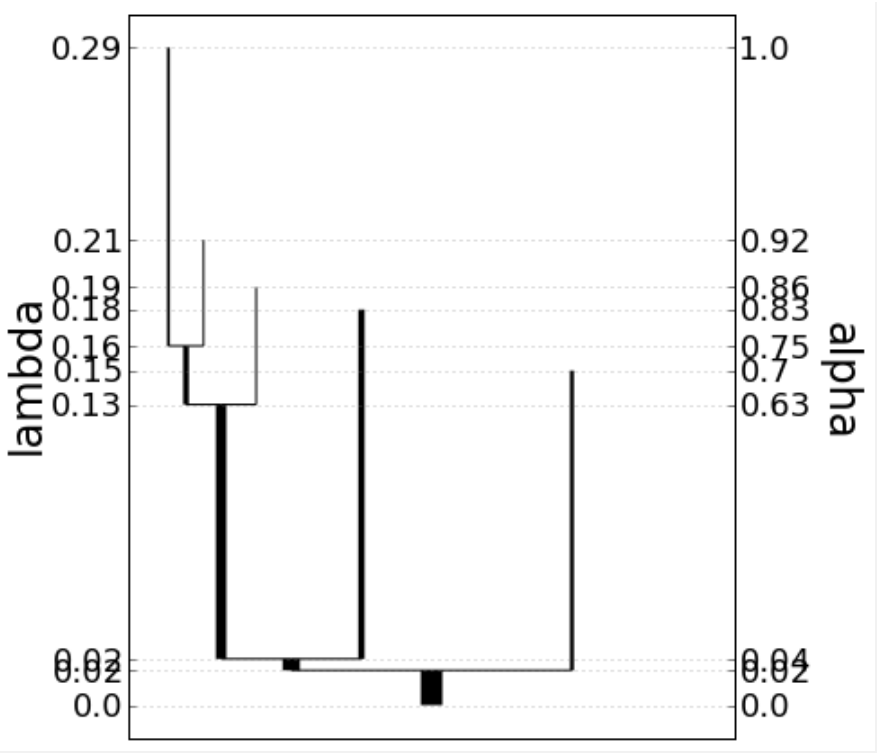
Estimating a level set tree involves four main steps: estimating the probability density function, constructing a similarity graph, finding connected components over successively smaller subgraphs, and pruning the tree. The geomTree method does all of these steps, and for most applications is the easiest way to use DeBaCl. We can see what's in a level set tree with the print function, although it's much easier to use level set trees with the dendrogram visualization, available through the plot method. Note that the plot method returns a tuple with several objects; only the first is useful unless you want to modify the figure.

```
## Estimate the level set tree - the easy way
p_k = 0.02
k = int(p_k * n)
p_gamma = 0.05
gamma = int(p_gamma * n)
```

```
tree = gtree.geomTree(X, k, gamma, n_grid=None, verbose=True)
print tree

fig = tree.plot(form='lambda', width='uniform')[0]
fig.show()
```

```
iteration 0
iteration 100
iteration 200
iteration 300
iteration 400
iteration 500
iteration 600
iteration 700
iteration 800
iteration 900
iteration 1000
iteration 1100
iteration 1200
iteration 1300
iteration 1400
       alpha1    alpha2  children   lambda1   lambda2 parent  size
key
0    0.000000  0.018000    [1, 2]  0.000000  0.015621   None  1500
1    0.018000  0.041333    [3, 4]  0.015621  0.020742      0  1197
2    0.018000  0.699333        []  0.015621  0.150048      0   276
3    0.041333  0.627333  [27, 28]  0.020742  0.134807      1   731
4    0.041333  0.827333        []  0.020742  0.177435      1   439
27   0.627333  0.750667  [31, 32]  0.134807  0.161119      3   399
28   0.627333  0.863333        []  0.134807  0.187444      3    88
31   0.750667  0.916667        []  0.161119  0.208673     27    77
32   0.750667  1.000000        []  0.161119  0.294931     27   204
```



While the level set tree plot offers a great deal of information about the structure of the dataset, often the task is to assign a single cluster label to each observation. DeBaCl offers several ways to retrieve labels from a level set tree, through the getClusterLabels function. Our preference is the 'all-mode' method, which designates each tree leaf as a cluster. The first-k option is appropriate if a specific number of clusters is desired or known in advance, and the upper-set option allows us to find clusters in a fraction of the data with highest density.

```
## Retrieve cluster assignments from the tree
uc, leaves = tree.getClusterLabels(method='all-mode')
print "cluster counts:", np.bincount(uc[:, 1])
print "leaf indices:", leaves
```

```
cluster counts: [276 439  88  77 204]
leaf indices: [2, 4, 28, 31, 32]
```

Generally speaking, retrieving clusters from a level set tree does not assign every point to a cluster. In particular, once high-density "foreground" clusters are obtained, observations with low density must be assigned to a group. This can be done with any classification method, and DeBaCl includes a handful of options, including a k-nearest neighbors classifier.

```
## Assign background points
fc = utl.assignBackgroundPoints(X.reshape((n, -1)), uc, method='knn', k=9)
print "final cluster counts:", np.bincount(fc[:, 1])
```

```
final cluster counts: [294 475 203 282 246]
```

The four main phases of level set tree estimation can be done individually for greater control of the methods and parameters. In this example we use a kernel density estimator instead of the default k-nearest neighbor estimator. For the sake of variety, the data are now in $\mathbb{R}^2$, and the smoothness and pruning parameters are tweaked to produce a reasonable tree. The scipy.stats package is loaded for the kernel density estimate.

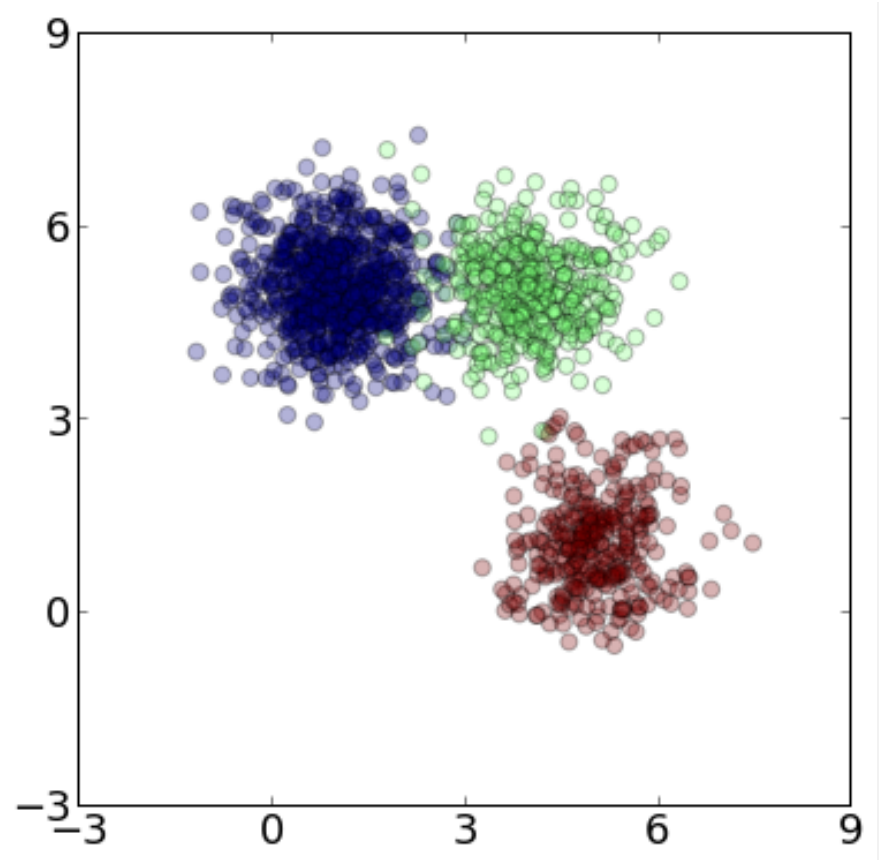
```
## Add the stats package for kernel density estimation
import scipy.stats as spstat

## Re-set data parameters
n = 1500
ctr = ((1, 5), (4, 5), (5, 1))
sdev = (0.5*np.eye(2),) * 3
mix = (0.5, 0.3, 0.2)


## Generate data
membership = np.random.multinomial(n, pvals=mix)
p = len(ctr[0])
X = np.zeros((n, p), dtype=np.float)
g = np.zeros((n, ), dtype=np.int)
b = np.cumsum((0,) + tuple(membership))

for i, (size, mu, sigma) in enumerate(zip(membership, ctr, sdev)):
        ix = range(b[i], b[i+1])
        X[ix, :] = np.random.multivariate_normal(mu, sigma, size)
        g[ix] = i


## Scatterplot, to show the simulation worked
fig, ax = plt.subplots()
ax.scatter(X[:,0], X[:,1], s=50, c=g, alpha=0.3)
fig.show()
```



The utils package (shortened to 'utl' here for brevity) contains functions to construct k-nearest neighbor and ϵ-neighborhood similarity graphs, although any similarity graph will work. Once the similarity graph and density estimate are computed, the constructDensityGrid method defines the relevant density levels and finds the graph vertices removed from the similarity graph at each level (called bg_sets here). The program can be accelerated by using a grid of density levels; here we use 300. The mode argument of this function specifies if the grid should be built on density level values or blocks of data points of equal size. The latter is specified by the 'mass' option. Finally, the constructTree method builds the level set tree. Because our ordering function here is a density, we set the mode argument to density. If the ordering function does not have a natural floor of 0 (like a density or pseudo-density function), we set mode to 'general'.

```
## Construct the similarity graph and density estimate
p_k = 0.005
k = int(p_k * n)

W, k_radius = utl.knnGraph(X, k, self_edge=False)
kernel = spstat.gaussian_kde(X.T)
fhat = kernel(X.T)


## Construct the level set tree
bg_sets, levels = utl.constructDensityGrid(fhat, mode='mass', n_grid=300)
```

```
tree = gtree.constructTree(W, levels, bg_sets, mode='density', verbose=True)
print tree
```

```
iteration 0
iteration 100
iteration 200
       alpha1    alpha2 children   lambda1   lambda2 parent  size
key
0    0.000000  0.013333   [1, 2]  0.000000  0.004890   None  1500
1    0.013333  0.173333   [3, 4]  0.004890  0.022043      0  1167
2    0.013333  0.528000       []  0.004890  0.044852      0   313
3    0.173333  0.183333   [5, 6]  0.022043  0.022945      1  1040
4    0.173333  0.196667       []  0.022043  0.023848      1     1
5    0.183333  0.347333   [7, 8]  0.022945  0.034565      3  1028
6    0.183333  0.217333       []  0.022945  0.025501      3     2
7    0.347333  0.919333  [9, 10]  0.034565  0.097013      5   630
8    0.347333  0.698667       []  0.034565  0.059618      5   241
9    0.919333  1.000000       []  0.097013  0.109606      7   119
10   0.919333  0.936000       []  0.097013  0.099801      7     2
```

Trees can be saved and loaded as MATLAB objects. This is shown here for demonstration purposes, but is not necessary for this small dataset. Pruning on the other hand, is necessary given that nodes with 1 or 2 members are likely due to random noise and should be removed.

```
## Save and/or load a tree (obviously redundant in this tutorial)
tree.save('test_tree')
tree = gtree.loadTree('test_tree')


## Prune the tree
p_gamma = 0.01
gamma = int(p_gamma * n)
tree.mergeBySize(gamma)
print tree
```

```
       alpha1    alpha2 children   lambda1   lambda2 parent  size
key
0    0.000000  0.013333   [1, 2]  0.000000  0.004890   None  1500
1    0.013333  0.347333   [7, 8]  0.004890  0.034565      0  1167
2    0.013333  0.528000       []  0.004890  0.044852      0   313
8    0.347333  0.698667       []  0.034565  0.059618      1   241
7    0.347333  1.000000       []  0.034565  0.109606      1   630
```

The level set tree plot can act as very useful scaffold for exploring spatially coherent subsets of data and the progression of high-density clusters. The commands don't work well in an Ipython Notebook, but can be uncommented and used at a regular Python or IPython command line.

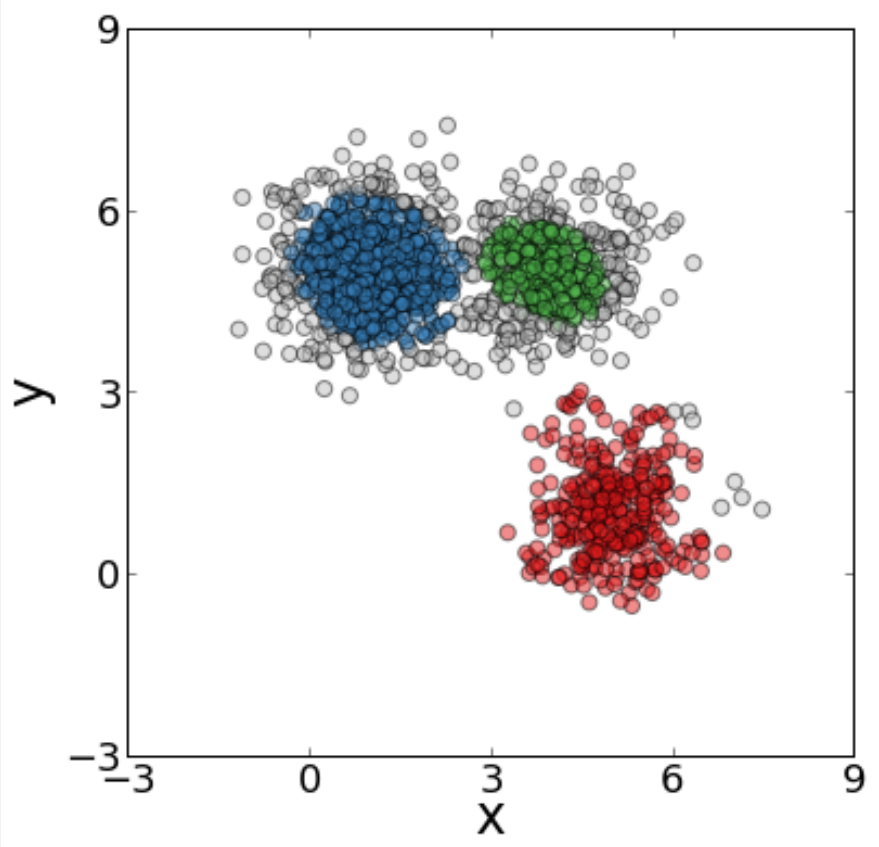
```
## Interactive tools
#tool = gtree.ComponentGUI(tree, X, form='alpha', width='mass', output=['scatter'])
```

```
#tool = gtree.ClusterGUI(tree, X, form='alpha', width='mass', output=['scatter'])
#tool.show()
```

Again we retrieve foreground cluter labels, although for this example we suppose we know there are three clusters and use the first-K method. The DeBaCl utils library includes the function plotForeground, for visualizing foreground clusters in a 1-, 2- or 3-dimensional feature space.

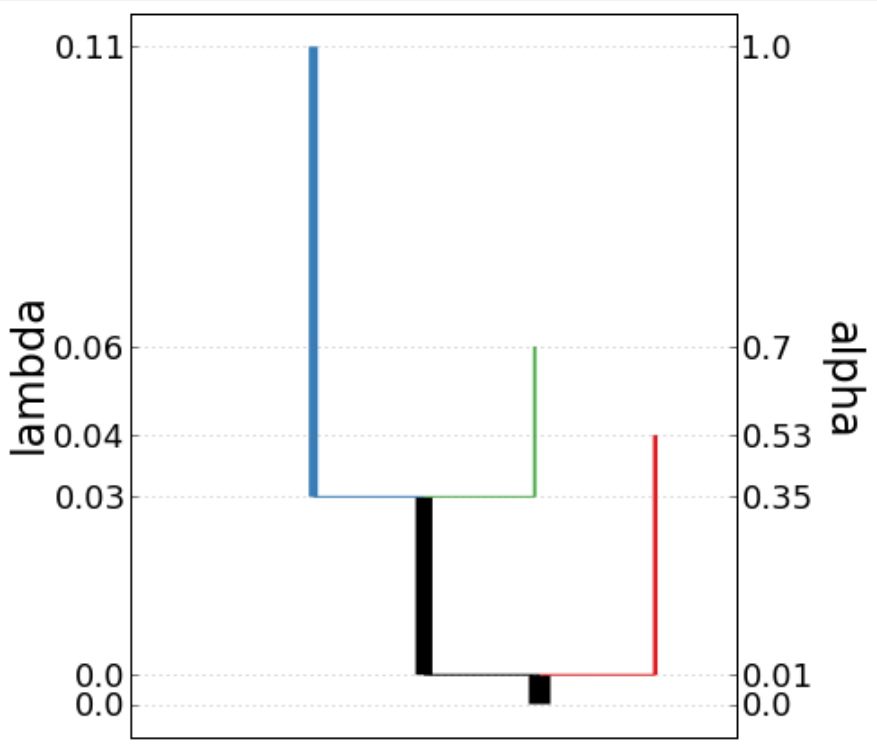
```
## Get foreground clusters and plot them
uc, nodes = tree.getClusterLabels(method='first-k', k=3)

fig, ax = utl.plotForeground(X, uc, s=50, alpha=0.5)
fig.show()
```



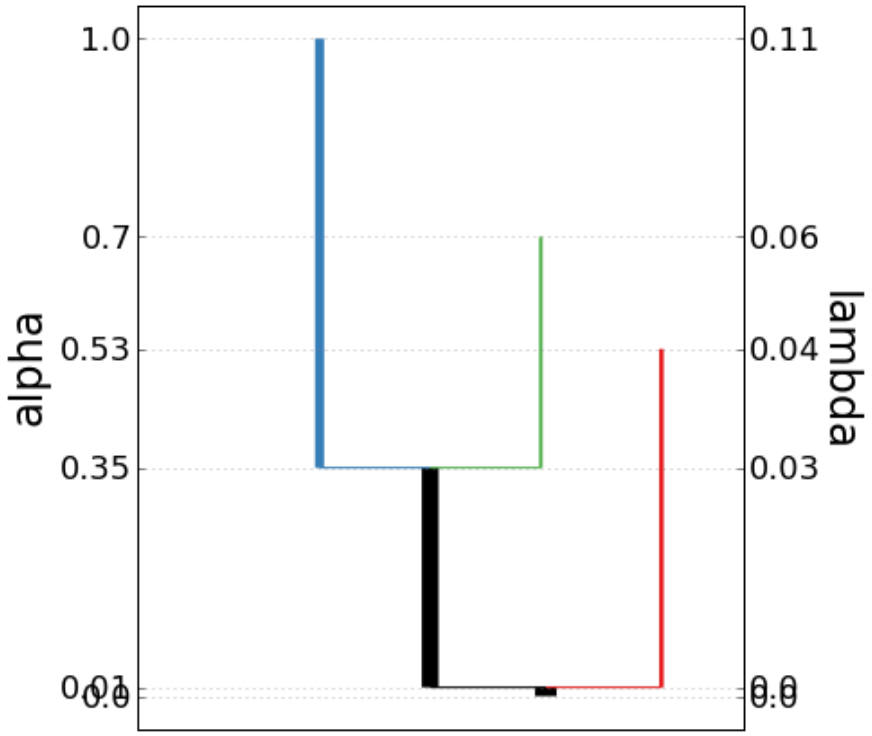
Finally, the level set tree is plotted. The most basic form uses the density scale (i.e. λ) as the dominant vertical axis, and spaces the branches according to their mass (i.e. fraction of data contained in the maximal cluster of the branch). The nodes are colored to match the foreground clusters above.

```
## Plot the basic level set tree with mass-based spacing
fig = tree.plot(form='lambda', width='mass', color_nodes=nodes)[0]
fig.show()
```



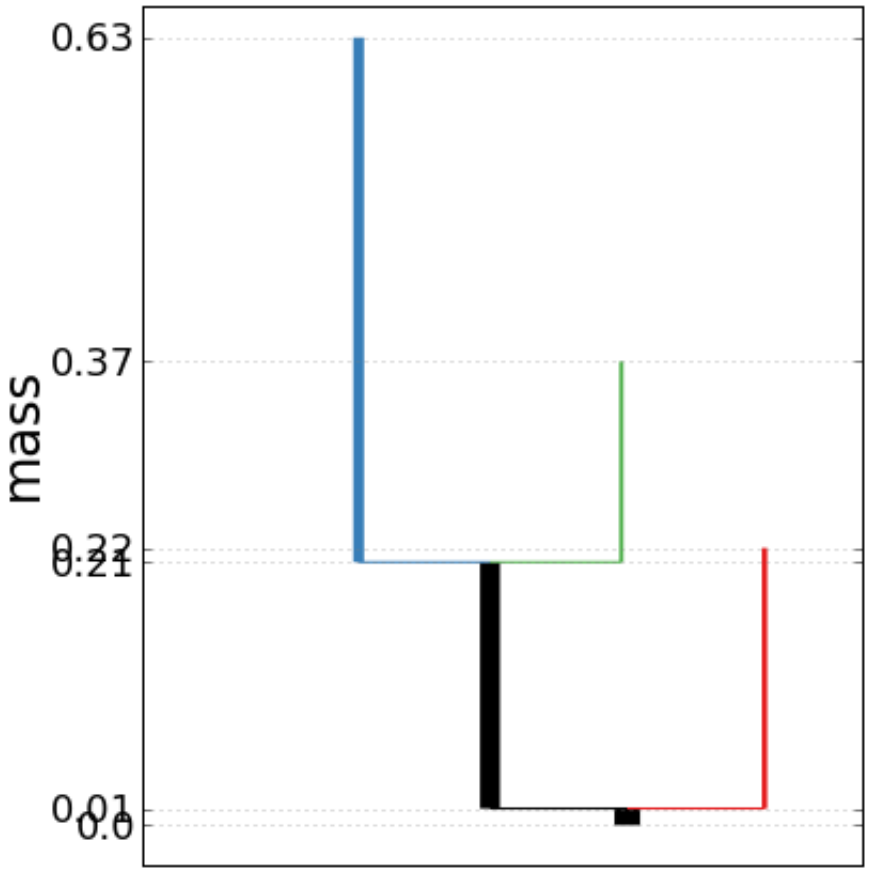
The α scale shows the fraction of data excluded from the upper level set for each value of λ. To use this more interpretable scale, we change the form argument to 'alpha'.

```
## Plot the level set tree with alpha scale
fig = tree.plot(form='alpha', width='mass', color_nodes=nodes)[0]
fig.show()
```



The α scale improves interpetability in several ways. Because it is based on mass, it is tempting to intuit that long vertical branches in an α tree plot contain a lot of mass, but this intuition is incorrect. To facilitate reading a plot this way, we use the κ form of the tree, where each branch's height is proportional to its salient mass. For leaf nodes, the salient mass is the fraction of points in the cluster, and for internal nodes the salient mass is the mass of the boundary region. In this example it does not look very different from the α and λ trees.

```
## Plot the level set tree with kappa scale
fig = tree.plot(form='kappa', width='mass', color_nodes=nodes)[0]
fig.show()
```


0.63
0.37
0.22
0.21
0.01
0.0
mass