how to plot and annotate hierarchical clustering dendrograms in scipy/matplotlib

Ask Question

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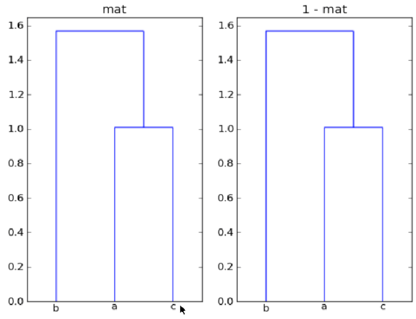
I'm using `dendrogram` from `scipy` to plot hierarchical clustering using `matplotlib` as follows:

```
mat = array([[1, 0.5, 0.9],
             [0.5, 1, -0.5],
             [0.9, -0.5, 1]])
plt.subplot(1,2,1)
plt.title("mat")
dist_mat = mat
linkage_matrix = linkage(dist_mat,
                         "single")
print "linkage2:"
print linkage(1-dist_mat, "single")
dendrogram(linkage_matrix,
           color_threshold=1,
           labels=["a", "b", "c"],
           show_leaf_counts=True)
plt.subplot(1,2,2)
plt.title("1 - mat")
dist_mat = 1 - mat
linkage_matrix = linkage(dist_mat,
                         "single")
dendrogram(linkage_matrix,
           color_threshold=1,
           labels=["a", "b", "c"],
           show_leaf_counts=True)
```

My questions are: first, why does `mat` and `1-mat` give identical clusterings here? and second, how can I annotate the distance along each branch of the tree using `dendrogram` so that the distances between pairs of nodes can be compared?

finally it seems that `show_leaf_counts` flag is ignored, is there a way to turn it on so that the number of objects in each class is shown? thanks.



python numpy matplotlib scipy dendrogram

1,485 14 14

asked Aug 11 '12 at 21:24

user248237dfsf

25.9k 113 270 411

2 Answers

67

+250

The input to `linkage()` is either an n x m array, representing n points in m-dimensional space, or a one-dimensional array containing the [*condensed* distance matrix](). In your example, `mat` is 3 x 3, so you are clustering three 3-d points. Clustering is based on the distance between these points.

Why does mat and 1-mat give identical clusterings here?

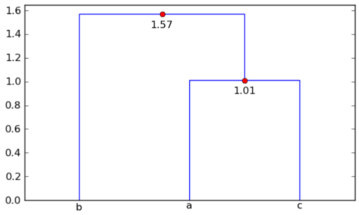
The arrays `mat` and `1-mat` produce the same clustering because the clustering is based on distances between the points, and neither a reflection (`-mat`) nor a translation (`mat + offset`) of the entire data set change the relative distances between the points.

How can I annotate the distance along each branch of the tree using dendrogram so that the distances between pairs of nodes can be compared?

In the code below, I show how you can use the data returned by dendrogram to label the horizontal segments of the diagram with the corresponding distance. The values associated with the keys `icoord` and `dcoord` give the x and y coordinates of each three-segment inverted-U of the figure. In `augmented_dendrogram` this data is used to add a label of the distance (i.e. y value) of each horizontal line segment in dendrogram.

```
from scipy.cluster.hierarchy impo
import matplotlib.pyplot as plt


def augmented_dendrogram(*args, *

    ddata = dendrogram(*args, **kw

    if not kwargs.get('no_plot',
        for i, d in zip(ddata['ic
            x = 0.5 * sum(i[1:3])
    return ddata
```

For your `mat` array, the augmented dendrogram is



So point 'a' and 'c' are 1.01 units apart, and point 'b' is 1.57 units from the cluster ['a', 'c'].

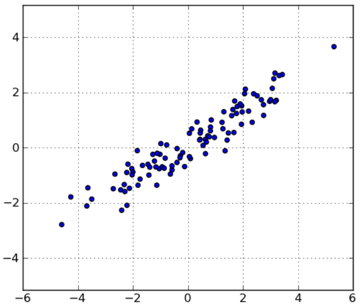
It seems that `show_leaf_counts` flag is ignored, is there a way to turn it on so that the number of objects in each class is shown?

The flag `show_leaf_counts` only applies when not all the original data points are shown as leaves. For example, when `trunc_mode = "lastp"`, only the last `p` nodes are show.

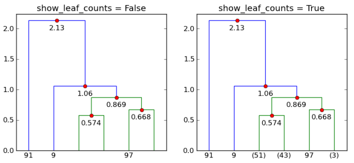
Here's an example with 100 points:

```
import numpy as np
from scipy.cluster.hierarchy impo
import matplotlib.pyplot as plt
from augmented_dendrogram import a


# Generate a random sample of `n`
np.random.seed(12312)
n = 100
x = np.random.multivariate_normal


plt.figure(1, figsize=(6, 5))
plt.clf()
plt.scatter(x[:, 0], x[:, 1])
plt.axis('equal')
plt.grid(True)

linkage_matrix = linkage(x, "sing

plt.figure(2, figsize=(10, 4))
plt.clf()

plt.subplot(1, 2, 1)
show_leaf_counts = False
ddata = augmented_dendrogram(linka
               color_threshold=1,
               p=6,
               truncate_mode='las
               show_leaf_counts=s
               )
plt.title("show_leaf_counts = %s"

plt.subplot(1, 2, 2)
show_leaf_counts = True
ddata = augmented_dendrogram(linka
plt.title("show_leaf_counts = %s"

plt.show()
```

These are the points in the data set:



With `p=6` and `trunc_mode="lastp"`, `dendrogram` only shows the "top" of the dendrogram. The following shows the effect of `show_leaf_counts`.



edited May 23 '17 at 12:25

Community ♦
1 1

answered Sep 7 '12 at 4:34

Warren Weckesser
71.7k 7 101 137

The first part of your response is correct, but incomplete. The input to linkage can also be "A condensed or redundant distance matrix. A condensed distance matrix is a flat array containing the upper triangular of the distance matrix. This is the form that pdist returns" From: docs.scipy.org/doc/scipy-0.18.0/reference/generated/… – Featherlegs Aug 25 '16 at 15:11

@Featherlegs Thanks for pointing that out. Actually, the docstring for linkage was recently corrected to reflect the reality of the code. The corrected docstring is not yet in a release. `linkage` accepts either a 1-d array containing the condensed distance matrix, or a 2-d array of points. It does not accept a dense distance matrix. I'll update my answer to reflect this. – Warren Weckesser Aug 25 '16 at 15:46

Here's the development version of the `linkage` documentation:

is it possible to use 2 different colors for parts of the same label? I mean, suppose instead of 'a' we want 'faa (foo)' but 'faa' in red and 'foo' in blue, everything together as label for the same leaf. – Sigur Aug 23 '17 at 20:02

1 @Sigur, I don't think that would be easy--it would probably require quite a bit of matplotlib hacking. – Warren Weckesser Aug 24 '17 at 11:15

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I think there's a couple misunderstandings as to the use of the functions that you are trying to use. Here's a fully working code snippet to illustrate my points:

```
import matplotlib.pyplot as plt
from scipy.cluster.hierarchy impor
from numpy import array
import numpy as np


mat = array([184, 222, 177, 216, 2
             45, 123, 128, 200,
             129, 121, 203,
             46, 83,
             83])

dist_mat = mat

linkage_matrix = linkage(dist_mat,
print linkage_matrix

plt.figure(101)
plt.subplot(1, 2, 1)
plt.title("ascending")
dendrogram(linkage_matrix,
           color_threshold=1,
           truncate_mode='lastp',
           labels=array(['a', 'b',
           distance_sort='ascendin

plt.subplot(1, 2, 2)
plt.title("descending")
dendrogram(linkage_matrix,
           color_threshold=1,
           truncate_mode='lastp',
           labels=array(['a', 'b',
           distance_sort='descendi


def make_fake_data():
    amp = 1000.
    x = []
    y = []
    for i in range(0, 10):
        s = 20
        x.append(np.random.normal(
        y.append(np.random.normal(
    for i in range(0, 20):
        s = 2
        x.append(np.random.normal(
        y.append(np.random.normal(
    for i in range(0, 10):
        s = 5
        x.append(np.random.normal(
        y.append(np.random.normal(
    d = []
    for i in range(len(x) - 1):
        for j in range(i+1, len(x)
            d.append(np.sqrt(((x[i
    return d

mat = make_fake_data()


plt.figure(102)
plt.title("Three Clusters")

linkage_matrix = linkage(mat, 'sin
print "three clusters"
print linkage_matrix

dendrogram(linkage_matrix,
           truncate_mode='lastp',
           color_threshold=1,
           show_leaf_counts=True)

plt.show()
```

First of all, the computation m -> m - 1 didn't really change your result since the distance matrix, which basically describes the relative distances between all unique pairs, didn't change in your specific case. (In my example code above, all distances are Euclidean so all are positive and consistent from points on a 2d plane.)

For your second question, you probably need to roll out your own annotation routine to do what you want, since I don't think dendromgram natively supports it...

For the last question, show_leaf_counts seems to work only when you try to display non-singleton leaf nodes with truncate_mode='lastp' option. Basically a leaves are bunched up so close together that they are not easy to see. So you have an option of just displaying a leaf but have an option of showing (in parenthesis) how many are bunched up in that leaf.

Hope this helps.

answered Sep 7 '12 at 4:13

Taro Sato
1,191 12 18

Taro, your answer appeared just as I was finishing mine. No answers in almost a month, and then two within a few minutes. I wonder how common that is... – Warren Weckesser Sep 7 '12 at 4:37

@WarrenWeckesser Haha, nice and

answers are mostly consistent.
Taro Sato Sep 7 '12 at 4:47