

## **Principal Component Analysis Lab**

This lab delves into exploratory analysis of neuroscience data, specifically using principal component analysis (PCA) and feature-based aggregation. We will use a dataset of light-sheet imaging recorded by the <a href="http://www.janelia.org/lab/ahrens-lab">Ahrens Lab</a> (<a href="http://www.janelia.org/lab/ahrens-lab">http://www.janelia.org/lab/ahrens-lab</a>) at Janelia Research Campus, and hosted on the CodeNeuro <a href="http://datasets.codeneuro.org">data repository (http://datasets.codeneuro.org</a>).

Our dataset is generated by studying the movement of a larval <u>zebrafish</u> (<a href="http://en.wikipedia.org/wiki/Zebrafish">http://en.wikipedia.org/wiki/Zebrafish</a>), an animal that is especially useful in neuroscience because it is transparent, making it possible to record activity over its entire brain using a technique called <a href="light-sheet\_microscopy">light-sheet\_microscopy</a> (<a href="http://en.wikipedia.org/wiki/Light\_sheet\_fluorescence\_microscopy">http://en.wikipedia.org/wiki/Light\_sheet\_fluorescence\_microscopy</a>). Specifically, we'll work with time-varying images containing patterns of the zebrafish's neural activity as it is presented with a moving visual pattern. Different stimuli induce different patterns across the brain, and we can use exploratory analyses to identify these patterns. Read <a href="mailto:"Mapping brain activity at scale with cluster computing" (http://thefreemanlab.com/work/papers/freeman-2014-nature-methods.pdf">http://thefreemanlab.com/work/papers/freeman-2014-nature-methods.pdf</a>) for more information about these kinds of analyses.

During this lab you will learn about PCA, and then compare and contrast different exploratory analyses of the same data set to identify which neural patterns they best highlight.

### This lab will cover:

- Part 1: Work through the steps of PCA on a sample dataset
  - Visualization 1: Two-dimensional Gaussians
- Part 2: Write a PCA function and evaluate PCA on sample datasets
  - Visualization 2: PCA projection
  - Visualization 3: Three-dimensional data

- Visualization 4: 2D representation of 3D data
- Part 3: Parse, inspect, and preprocess neuroscience data then perform PCA
  - Visualization 5: Pixel intensity
  - Visualization 6: Normalized data
  - Visualization 7: Top two components as images
  - Visualization 8: Top two components as one image
- Part 4: Perform feature-based aggregation followed by PCA
  - Visualization 9: Top two components by time
  - Visualization 10: Top two components by direction

Note that, for reference, you can look up the details of the relevant Spark methods in Spark's Python API (https://spark.apache.org/docs/latest/api/python/pyspark.html#pyspark.RDD) and the relevant NumPy methods in the NumPy Reference (http://docs.scipy.org/doc/numpy/reference/index.html)

In [1]:

labVersion = 'cs190\_week5\_v\_1\_2'

## Part 1: Work through the steps of PCA on a sample dataset

## Visualization 1: Two-dimensional Gaussians

Principal Component Analysis, or PCA, is a strategy for dimensionality reduction. To better understand PCA, we'll work with synthetic data generated by sampling from the <a href="two-dimensional Gaussian distribution">two-dimensional Gaussian distribution</a> (<a href="http://en.wikipedia.org/wiki/Multivariate\_normal\_distribution">http://en.wikipedia.org/wiki/Multivariate\_normal\_distribution</a>). This distribution takes as input the mean and variance of each dimension, as well as the covariance between the two dimensions.

In our visualizations below, we will specify the mean of each dimension to be 50 and the variance along each dimension to be 1. We will explore two different

values for the covariance: 0 and 0.9. When the covariance is zero, the two dimensions are uncorrelated, and hence the data looks spherical. In contrast, when the covariance is 0.9, the two dimensions are strongly (positively) correlated and thus the data is non-spherical. As we'll see in Parts 1 and 2, the non-spherical data is amenable to dimensionality reduction via PCA, while the spherical data is not.

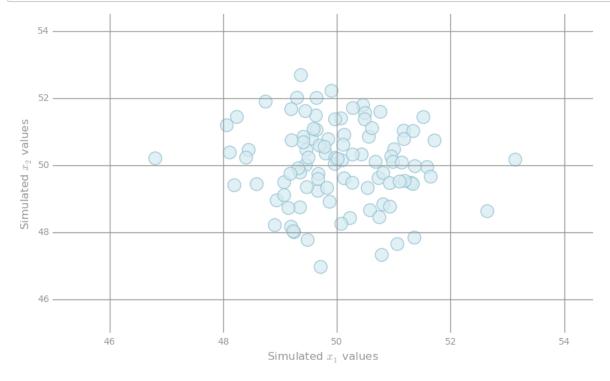
#### In [2]:

```
import matplotlib.pyplot as plt
import numpy as np
def preparePlot(xticks, yticks, figsize=(10.5, 6), hideLabels=False, gridColor='#9999
                gridWidth=1.0):
    """Template for generating the plot layout."""
    plt.close()
    fig, ax = plt.subplots(figsize=figsize, facecolor='white', edgecolor='white')
    ax.axes.tick_params(labelcolor='#999999', labelsize='10')
    for axis, ticks in [(ax.get_xaxis(), xticks), (ax.get_yaxis(), yticks)]:
        axis.set ticks position('none')
        axis.set ticks(ticks)
        axis.label.set color('#999999')
        if hideLabels: axis.set_ticklabels([])
    plt.grid(color=gridColor, linewidth=gridWidth, linestyle='-')
    map(lambda position: ax.spines[position].set visible(False), ['bottom', 'top', 'l
    return fig, ax
def create2DGaussian(mn, sigma, cov, n):
    """Randomly sample points from a two-dimensional Gaussian distribution"""
    np.random.seed(142)
    return np.random.multivariate_normal(np.array([mn, mn]), np.array([[sigma, cov],
```

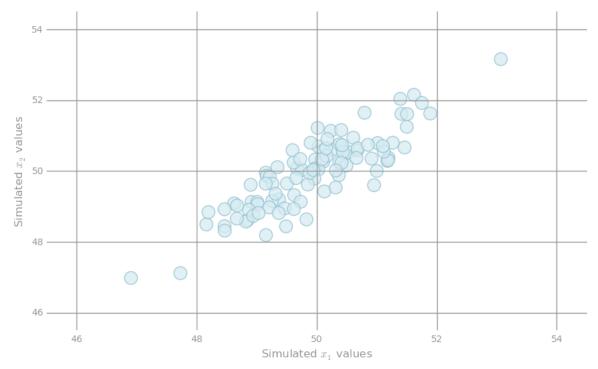
### In [3]:

```
dataRandom = create2DGaussian(mn=50, sigma=1, cov=0, n=100)

# generate Layout and plot data
fig, ax = preparePlot(np.arange(46, 55, 2), np.arange(46, 55, 2))
ax.set_xlabel(r'Simulated $x_1$ values'), ax.set_ylabel(r'Simulated $x_2$ values')
ax.set_xlim(45, 54.5), ax.set_ylim(45, 54.5)
plt.scatter(dataRandom[:,0], dataRandom[:,1], s=14**2, c='#d6ebf2', edgecolors='#8cbf
pass
```



#### In [4]:



## (1a) Interpreting PCA

PCA can be interpreted as identifying the "directions" along which the data vary the most. In the first step of PCA, we must first center our data. Working with our correlated dataset, first compute the mean of each feature (column) in the dataset. Then for each observation, modify the features by subtracting their corresponding mean, to create a zero mean dataset.

Note that correlatedData is an RDD of NumPy arrays. This allows us to perform certain operations more succinctly. For example, we can sum the columns of our dataset using correlatedData.sum().

#### In [5]:

```
# TODO: Replace <FILL IN> with appropriate code
correlatedData = sc.parallelize(dataCorrelated)

meanCorrelated = correlatedData.mean()
correlatedDataZeroMean = correlatedData.map(lambda x: x - meanCorrelated)

print meanCorrelated
print correlatedData.take(1)
print correlatedDataZeroMean.take(1)
```

```
[ 49.95739037 49.97180477]
[array([ 49.6717712 , 50.07531969])]
[array([-0.28561917, 0.10351492])]
```

#### In [6]:

- 1 test passed.
- 1 test passed.

## (1b) Sample covariance matrix

We are now ready to compute the sample covariance matrix. If we define  $\mathbf{X} \in \mathbb{R}^{n \times d}$  as the zero mean data matrix, then the sample covariance matrix is defined as:

$$\mathbf{C}_{\mathbf{X}} = \frac{1}{n} \mathbf{X}^{\top} \mathbf{X}$$
 .

To compute this matrix, compute the outer product of each data point, add together these outer products, and divide by the number of data points. The data are two dimensional, so the resulting covariance matrix should be a 2x2 matrix.

## Note that np.outer()

(http://docs.scipy.org/doc/numpy/reference/generated/numpy.outer.html) can be used to calculate the outer product of two NumPy arrays.

#### In [19]:

Test.assertTrue(np.allclose(covResult, correlatedCov), 'incorrect value for correlate

1 test passed.

## (1c) Covariance Function

Next, use the expressions above to write a function to compute the sample covariance matrix for an arbitrary data RDD.

#### In [28]:

```
# TODO: Replace <FILL IN> with appropriate code
def estimateCovariance(data):
    """Compute the covariance matrix for a given rdd.
    Note:
        The multi-dimensional covariance array should be calculated using outer produ
        forget to normalize the data by first subtracting the mean.
        data (RDD of np.ndarray): An `RDD` consisting of NumPy arrays.
    Returns:
        np.ndarray: A multi-dimensional array where the number of rows and columns bo
            length of the arrays in the input `RDD`.
    mean, n = data.mean(), data.count()
    dataZeroMean = data.map(lambda x: x - mean)
    outer = dataZeroMean.map(lambda x: np.outer(x, x))
    cov = outer.reduce(lambda a, b: np.add(a, b)) / n
correlatedCovAuto= estimateCovariance(correlatedData)
print correlatedCovAuto
```

```
[[ 0.99558386  0.90148989]  [ 0.90148989  1.08607497]]
```

In [29]:

1 test passed.

## (1d) Eigendecomposition

Now that we've computed the sample covariance matrix, we can use it to find directions of maximal variance in the data. Specifically, we can perform an eigendecomposition of this matrix to find its eigenvalues and eigenvectors. The d eigenvectors of the covariance matrix give us the directions of maximal variance, and are often called the "principal components." The associated eigenvalues are the variances in these directions. In particular, the eigenvector corresponding to the largest eigenvalue is the direction of maximal variance (this is sometimes called the "top" eigenvector). Eigendecomposition of a  $d \times d$  covariance matrix has a (roughly) cubic runtime complexity with respect to d. Whenever d is relatively small (e.g., less than a few thousand) we can quickly perform this eigendecomposition locally.

Use a function from numpy.linalg called eigh

(http://docs.scipy.org/doc/numpy/reference/generated/numpy.linalg.eigh.html) to perform the eigendecomposition. Next, sort the eigenvectors based on their corresponding eigenvalues (from high to low), yielding a matrix where the columns are the eigenvectors (and the first column is the top eigenvector). Note that np.argsort

(http://docs.scipy.org/doc/numpy/reference/generated/numpy.argsort.html#numpy-argsort) can be used to obtain the indices of the eigenvalues that correspond to the ascending order of eigenvalues. Finally, set the topComponent variable equal to the top eigenvector or prinicipal component, which is a 2-dimensional vector (array with two values).

Note that the eigenvectors returned by eigh appear in the columns and not the rows. For example, the first eigenvector of eigVecs would be found in the first column and could be accessed using eigVecs[:,0].

#### In [81]:

```
# TODO: Replace <FILL IN> with appropriate code
from numpy.linalg import eigh
# Calculate the eigenvalues and eigenvectors from correlatedCovAuto
eigVals, eigVecs = eigh(correlatedCovAuto)
print 'eigenvalues: {0}'.format(eigVals)
print '\neigenvectors: \n{0}'.format(eigVecs)
# Use np.argsort to find the top eigenvector based on the largest eigenvalue
inds = np.argsort(eigVals)
#print inds
topComponent = eigVecs[:,inds[-1]]
print '\ntop principal component: {0}'.format(topComponent)
eigenvalues: [ 0.13820481  1.94345403]
eigenvectors:
[[-0.72461254 0.68915649]
[ 0.68915649  0.72461254]]
top principal component: [ 0.68915649 0.72461254]
In [82]:
# TEST Eigendecomposition (1d)
def checkBasis(vectors, correct):
    return np.allclose(vectors, correct) or np.allclose(np.negative(vectors), correct
Test.assertTrue(checkBasis(topComponent, [0.68915649, 0.72461254]),
```

1 test passed.

## (1e) PCA scores

We just computed the top principal component for a 2-dimensional non-spherical dataset. Now let's use this principal component to derive a one-dimensional representation for the original data. To compute these compact representations, which are sometimes called PCA "scores", calculate the dot product between each data point in the raw data and the top principal component.

'incorrect value for topComponent')

```
In [83]:
```

```
# TODO: Replace <FILL IN> with appropriate code
# Use the topComponent and the data from correlatedData to generate PCA scores
correlatedDataScores = correlatedData.map(lambda x: x.dot(topComponent))
print 'one-dimensional data (first three):\n{0}'.format(np.asarray(correlatedDataScor
one-dimensional data (first three):
[ 70.51682806 69.30622356 71.13588168]
```

### In [84]:

1 test passed.

## Part 2: Write a PCA function and evaluate PCA on sample datasets

## (2a) PCA function

We now have all the ingredients to write a general PCA function. Instead of working with just the top principal component, our function will compute the top k principal components and principal scores for a given dataset. Write this general function pca, and run it with correlatedData and k = 2. Hint: Use results from Part (1c), Part (1d), and Part (1e).

Note: As discussed in lecture, our implementation is a reasonable strategy when  $\it d$  is small, though more efficient distributed algorithms exist when  $\it d$  is large.

```
# TODO: Replace <FILL IN> with appropriate code
def pca(data, k=2):
    """Computes the top `k` principal components, corresponding scores, and all eigen
    Note:
        All eigenvalues should be returned in sorted order (largest to smallest). `ei
        each eigenvectors as a column. This function should also return eigenvectors
    Args:
        data (RDD of np.ndarray): An `RDD` consisting of NumPy arrays.
        k (int): The number of principal components to return.
    Returns:
        tuple of (np.ndarray, RDD of np.ndarray, np.ndarray): A tuple of (eigenvector
            scores, eigenvalues). Eigenvectors is a multi-dimensional array where th
            rows equals the length of the arrays in the input `RDD` and the number of
                 The `RDD` of scores has the same number of rows as `data` and consi
            of length `k`. Eigenvalues is an array of length d (the number of featur
    .....
    covAuto = estimateCovariance(data)
    eigVals, eigVecs = eigh(covAuto)
    inds = np.argsort(eigVals)[::-1]
    # Return the `k` principal components, `k` scores, and all eigenvalues
    #eigVecs = eigVecs.T
    eigVals = eigVals[inds]
    topComponents = eigVecs[:, inds[:k]] #eigVecs[inds[-k:]]
    dataScores = data.map(lambda x: [x.dot(topComponents[:,i]) for i in range(k)])
    return topComponents, dataScores, eigVals
# Run pca on correlatedData with k = 2
topComponentsCorrelated, correlatedDataScoresAuto, eigenvaluesCorrelated = pca(correl
# Note that the 1st principal component is in the first column
print 'topComponentsCorrelated: \n{0}'.format(topComponentsCorrelated)
print ('\ncorrelatedDataScoresAuto (first three): \n{0}'
       .format('\n'.join(map(str, correlatedDataScoresAuto.take(3)))))
print '\neigenvaluesCorrelated: \n{0}'.format(eigenvaluesCorrelated)
# Create a higher dimensional test set
pcaTestData = sc.parallelize([np.arange(x, x + 4) for x in np.arange(0, 20, 4)])
componentsTest, testScores, eigenvaluesTest = pca(pcaTestData, 3)
print '\npcaTestData: \n{0}'.format(np.array(pcaTestData.collect()))
print '\ncomponentsTest: \n{0}'.format(componentsTest)
print ('\ntestScores (first three): \n{0}'
       .format('\n'.join(map(str, testScores.take(3)))))
print '\neigenvaluesTest: \n{0}'.format(eigenvaluesTest)
pcaTestData:
[[ 0 1 2 3]
 [4 5 6 7]
 [8 9 10 11]
 [12 13 14 15]
[16 17 18 19]]
componentsTest:
   5.00000000e-01 6.89413646e-02 -4.41317416e-19]
    5.00000000e-01
                   -8.36885766e-01 -6.39585002e-17]
```

```
5.00000000e-01
                     3.83972201e-01 -7.07106781e-01]
    5.00000000e-01
                     3.83972201e-01
                                      7.07106781e-01]]
testScores (first three):
[3.0, 1.0829752381861808, 0.70710678118654768]
[11.0, 1.0829752381861804, 0.70710678118654791]
[19.0, 1.0829752381861797, 0.70710678118654813]
eigenvaluesTest:
                                                       1 /21116/0~ 1/1
  1 200000000102
                    1 517570250 15
                                     2 1/7/11000 22
In [86]:
# TEST PCA Function (2a)
Test.assertTrue(checkBasis(topComponentsCorrelated.T,
                           [[0.68915649, 0.72461254], [-0.72461254, 0.68915649]]),
                'incorrect value for topComponentsCorrelated')
firstThreeCorrelated = [[70.51682806, 69.30622356, 71.13588168], [1.48305648, 1.58886
Test.assertTrue(np.allclose(firstThreeCorrelated,
                            np.vstack(np.abs(correlatedDataScoresAuto.take(3))).T),
                'incorrect value for firstThreeCorrelated')
Test.assertTrue(np.allclose(eigenvaluesCorrelated, [1.94345403, 0.13820481]),
                           'incorrect values for eigenvaluesCorrelated')
topComponentsCorrelatedK1, correlatedDataScoresK1, eigenvaluesCorrelatedK1 = pca(corr
Test.assertTrue(checkBasis(topComponentsCorrelatedK1.T, [0.68915649, 0.72461254]),
                incorrect value for components when k=1')
Test.assertTrue(np.allclose([70.51682806, 69.30622356, 71.13588168],
                            np.vstack(np.abs(correlatedDataScoresK1.take(3))).T),
                'incorrect value for scores when k=1')
Test.assertTrue(np.allclose(eigenvaluesCorrelatedK1, [1.94345403, 0.13820481]),
                            'incorrect values for eigenvalues when k=1')
Test.assertTrue(checkBasis(componentsTest.T[0], [ .5, .5, .5]),
                 'incorrect value for componentsTest')
Test.assertTrue(np.allclose(np.abs(testScores.first()[0]), 3.),
                'incorrect value for testScores')
Test.assertTrue(np.allclose(eigenvaluesTest, [ 128, 0, 0, 0 ]), 'incorrect value for
1 test passed.
```

## (2b) PCA on dataRandom

Next, use the PCA function we just developed to find the top two principal components of the spherical dataRandom we created in Visualization 1.

```
In [89]:
```

```
# TODO: Replace <FILL IN> with appropriate code
randomData = sc.parallelize(dataRandom)
# Use pca on randomData
topComponentsRandom, randomDataScoresAuto, eigenvaluesRandom = pca(randomData)
print 'topComponentsRandom: \n{0}'.format(topComponentsRandom)
print ('\nrandomDataScoresAuto (first three): \n{0}'
       .format('\n'.join(map(str, randomDataScoresAuto.take(3)))))
print '\neigenvaluesRandom: \n{0}'.format(eigenvaluesRandom)
topComponentsRandom:
[[-0.2522559 -0.96766056]
 [ 0.96766056 -0.2522559 ]]
randomDataScoresAuto (first three):
[36.610685715878752, -61.348992904346971]
[35.973142953442306, -62.088136714613611]
[35.59836628262682, -60.613904149581764]
eigenvaluesRandom:
[ 1.4204546
             0.99521397]
In [90]:
# TEST PCA on `dataRandom` (2b)
Test.assertTrue(checkBasis(topComponentsRandom.T,
                           [[-0.2522559]
                                           0.96766056], [-0.96766056,
                                                                       -0.2522559]]),
                'incorrect value for topComponentsRandom')
firstThreeRandom = [[36.61068572, 35.97314295,
                                                 35.59836628],
                    [61.3489929 , 62.08813671,
                                                 60.61390415]]
Test.assertTrue(np.allclose(firstThreeRandom, np.vstack(np.abs(randomDataScoresAuto.t
                'incorrect value for randomDataScoresAuto')
Test.assertTrue(np.allclose(eigenvaluesRandom, [1.4204546, 0.99521397]),
                            'incorrect value for eigenvaluesRandom')
1 test passed.
```

- 1 test passed.
- 1 test passed.

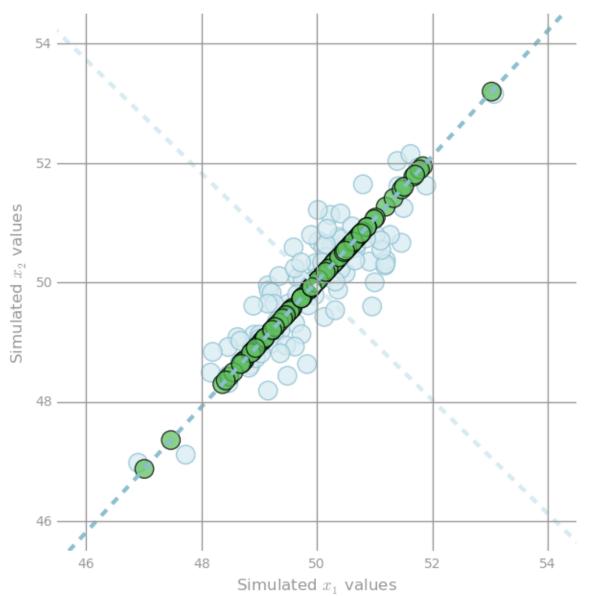
## Visualization 2: PCA projection

Plot the original data and the 1-dimensional reconstruction using the top principal component to see how the PCA solution looks. The original data is plotted as before; however, the 1-dimensional reconstruction (projection) is plotted in green on top of the original data and the vectors (lines) representing the two principal components are shown as dotted lines.

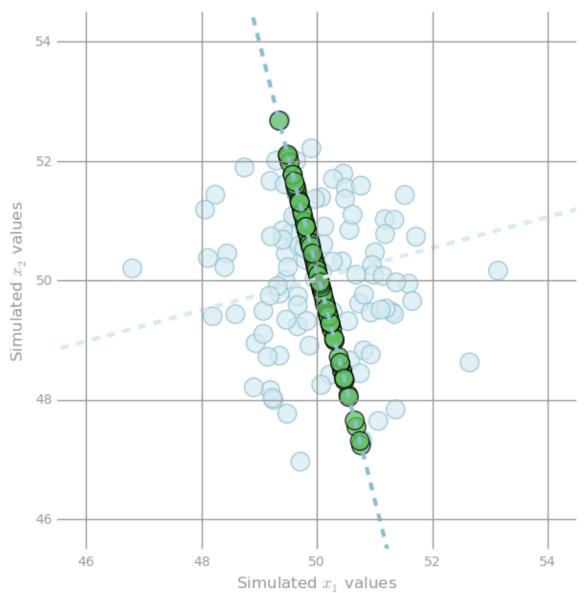
#### In [91]:

```
def projectPointsAndGetLines(data, components, xRange):
    """Project original data onto first component and get line details for top two co
    topComponent= components[:, 0]
    slope1, slope2 = components[1, :2] / components[0, :2]
    means = data.mean()[:2]
    demeaned = data.map(lambda v: v - means)
    projected = demeaned.map(lambda v: (v.dot(topComponent) /
                                        topComponent.dot(topComponent)) * topComponen
    remeaned = projected.map(lambda v: v + means)
    x1,x2 = zip(*remeaned.collect())
    lineStartP1X1, lineStartP1X2 = means - np.asarray([xRange, xRange * slope1])
    lineEndP1X1, lineEndP1X2 = means + np.asarray([xRange, xRange * slope1])
    lineStartP2X1, lineStartP2X2 = means - np.asarray([xRange, xRange * slope2])
    lineEndP2X1, lineEndP2X2 = means + np.asarray([xRange, xRange * slope2])
    return ((x1, x2), ([lineStartP1X1, lineEndP1X1], [lineStartP1X2, lineEndP1X2]),
            ([lineStartP2X1, lineEndP2X1], [lineStartP2X2, lineEndP2X2]))
```

#### In [92]:



#### In [93]:



### Visualization 3: Three-dimensional data

So far we have worked with two-dimensional data. Now let's generate three-dimensional data with highly correlated features. As in Visualization 1, we'll

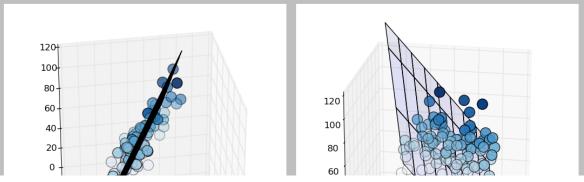
In [94]:

create samples from a multivariate Gaussian distribution, which in three dimensions requires us to specify three means, three variances, and three covariances.

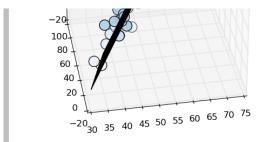
In the 3D graphs below, we have included the 2D plane that corresponds to the top two principal components, i.e. the plane with the smallest euclidean distance between the points and itself. Notice that the data points, despite living in threedimensions, are found near a two-dimensional plane: the left graph shows how most points are close to the plane when it is viewed from its side, while the right graph shows that the plane covers most of the variance in the data. Note that darker blues correspond to points with higher values for the third dimension.

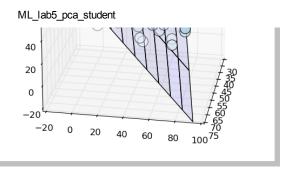
	'
ttp://localhost:8001/notebooks/ML_lab5_pca_student.ipynb#	17/4

```
from mpl toolkits.mplot3d import Axes3D
m = 100
mu = np.array([50, 50, 50])
r1 2 = 0.9
r1 3 = 0.7
r2_3 = 0.1
sigma1 = 5
sigma2 = 20
sigma3 = 20
c = np.array([[sigma1 ** 2, r1_2 * sigma1 * sigma2, r1_3 * sigma1 * sigma3],
             [r1_2 * sigma1 * sigma2, sigma2 ** 2, r2_3 * sigma2 * sigma3],
             [r1_3 * sigma1 * sigma3, r2_3 * sigma2 * sigma3, sigma3 ** 2]])
np.random.seed(142)
dataThreeD = np.random.multivariate normal(mu, c, m)
from matplotlib.colors import ListedColormap, Normalize
from matplotlib.cm import get cmap
norm = Normalize()
cmap = get_cmap("Blues")
clrs = cmap(np.array(norm(dataThreeD[:,2])))[:,0:3]
fig = plt.figure(figsize=(11, 6))
ax = fig.add subplot(121, projection='3d')
ax.azim=-100
ax.scatter(dataThreeD[:,0], dataThreeD[:,1], dataThreeD[:,2], c=clrs, s=14**2)
xx, yy = np.meshgrid(np.arange(-15, 10, 1), np.arange(-50, 30, 1))
normal = np.array([0.96981815, -0.188338, -0.15485978])
z = (-normal[0] * xx - normal[1] * yy) * 1. / normal[2]
xx = xx + 50
yy = yy + 50
z = z + 50
ax.set_zlim((-20, 120)), ax.set_ylim((-20, 100)), ax.set_xlim((30, 75))
ax.plot_surface(xx, yy, z, alpha=.10)
ax = fig.add_subplot(122, projection='3d')
ax.azim=10
ax.elev=20
#ax.dist=8
ax.scatter(dataThreeD[:,0], dataThreeD[:,1], dataThreeD[:,2], c=clrs, s=14**2)
ax.set_zlim((-20, 120)), ax.set_ylim((-20, 100)), ax.set_xlim((30, 75))
ax.plot_surface(xx, yy, z, alpha=.1)
plt.tight_layout()
pass
```



7/21/2015





## (2c) 3D to 2D

We will now use PCA to see if we can recover the 2-dimensional plane on which the data live. Parallelize the data, and use our PCA function from above, with k = 2 components.

```
In [95]:
```

```
# TODO: Replace <FILL IN> with appropriate code
threeDData = sc.parallelize(dataThreeD)
componentsThreeD, threeDScores, eigenvaluesThreeD = pca(threeDData)
print 'componentsThreeD: \n{0}'.format(componentsThreeD)
print ('\nthreeDScores (first three): \n{0}'
       .format('\n'.join(map(str, threeDScores.take(3)))))
print '\neigenvaluesThreeD: \n{0}'.format(eigenvaluesThreeD)
componentsThreeD:
[[ 0.23952078  0.045635
[ 0.61699931  0.76409466]
[ 0.74962768 -0.64348799]]
threeDScores (first three):
[85.257986059926651, -8.296944069807779]
[89.663379110884833, 15.733815169845593]
[75.926168718966551, -20.501570898232295]
eigenvaluesThreeD:
[ 614.46863537 349.47737219
                                5.85043581]
In [96]:
# TEST 3D to 2D (2c)
```

Test.assertEquals(componentsThreeD.shape, (3, 2), 'incorrect shape for componentsThre

'incorrect value for componentsThreeD')

- 1 test passed.
  1 test passed.
- 1 test passed.
- 1 test passed.

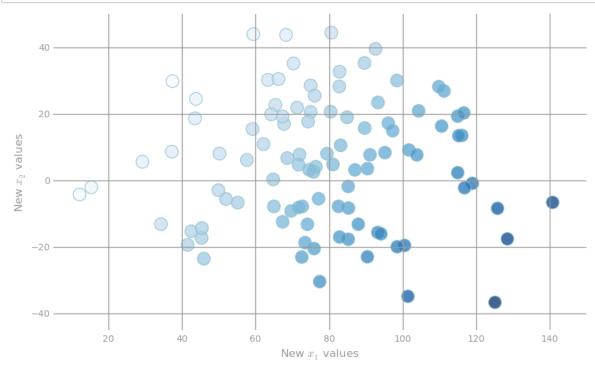
## Visualization 4: 2D representation of 3D data

See the 2D version of the data that captures most of its original structure. Note that darker blues correspond to points with higher values for the original data's third dimension.

#### In [97]:

```
scoresThreeD = np.asarray(threeDScores.collect())

# generate Layout and plot data
fig, ax = preparePlot(np.arange(20, 150, 20), np.arange(-40, 110, 20))
ax.set_xlabel(r'New $x_1$ values'), ax.set_ylabel(r'New $x_2$ values')
ax.set_xlim(5, 150), ax.set_ylim(-45, 50)
plt.scatter(scoresThreeD[:,0], scoresThreeD[:,1], s=14**2, c=clrs, edgecolors='#8cbfd
pass
```



## (2d) Variance explained

Finally, let's quantify how much of the variance is being captured by PCA in each of the three synthetic datasets we've analyzed. To do this, we'll compute the fraction of retained variance by the top principal components. Recall that the eigenvalue corresponding to each principal component captures the variance along this direction. If our initial data is d-dimensional, then the total variance in our data equals:  $\sum_{i=1}^{d} \lambda_i$ , where  $\lambda_i$  is the eigenvalue corresponding to the ith principal component. Moreover, if we use PCA with some k < d, then we can compute the variance retained by these principal components by adding the top k eigenvalues. The fraction of retained variance equals the sum of the top k

eigenvalues divided by the sum of all of the eigenvalues.

#### In [98]:

```
# TODO: Replace <FILL IN> with appropriate code
def varianceExplained(data, k=1):
    """Calculate the fraction of variance explained by the top `k` eigenvectors.
    Args:
        data (RDD of np.ndarray): An RDD that contains NumPy arrays which store the
            features for an observation.
        k: The number of principal components to consider.
    Returns:
        float: A number between 0 and 1 representing the percentage of variance expla
            by the top `k` eigenvectors.
    components, scores, eigenvalues = pca(data)
    eigenvalues = sorted(eigenvalues, reverse=True)
    return sum(eigenvalues[:k]) / sum(eigenvalues)
varianceRandom1 = varianceExplained(randomData, 1)
varianceCorrelated1 = varianceExplained(correlatedData, 1)
varianceRandom2 = varianceExplained(randomData, 2)
varianceCorrelated2 = varianceExplained(correlatedData, 2)
varianceThreeD2 = varianceExplained(threeDData, 2)
print ('Percentage of variance explained by the first component of randomData: {0:.1f
       .format(varianceRandom1 * 100))
print ('Percentage of variance explained by both components of randomData: {0:.1f}%'
       .format(varianceRandom2 * 100))
print ('\nPercentage of variance explained by the first component of correlatedData:
       format(varianceCorrelated1 * 100))
print ('Percentage of variance explained by both components of correlatedData: {0:.1f
       .format(varianceCorrelated2 * 100))
print ('\nPercentage of variance explained by the first two components of threeDData:
       .format(varianceThreeD2 * 100))
Percentage of variance explained by the first component of randomData:
Percentage of variance explained by both components of randomData: 10
0.0%
```

Percentage of variance explained by both components of randomData: 10 0.0%

Percentage of variance explained by the first component of correlatedData: 93.4%

Percentage of variance explained by both components of correlatedData: 100.0%

Percentage of variance explained by the first two components of threeDD ata: 99.4%

#### In [99]:

- 1 test passed.

# Part 3: Parse, inspect, and preprocess neuroscience data then perform PCA

## **Data introduction**

A central challenge in neuroscience is understanding the organization and function of neurons, the cells responsible for processing and representing information in the brain. New technologies make it possible to monitor the responses of large populations of neurons in awake animals. In general, neurons communicate through electrical impulses that must be recorded with electrodes, which is a challenging process. As an alternative, we can genetically engineer animals so that their neurons express special proteins that flouresce or light up when active, and then use microscopy to record neural activity as images. A recently developed method called light-sheet microscopy lets us do this in a special, transparent animal, the larval zebrafish, over nearly its entire brain. The resulting data are time-varying images containing the activity of hundreds of thousands of neurons. Given the raw data, which is enormous, we want to find compact spatial and temporal patterns: Which groups of neurons are active together? What is the time course of their activity? Are those patterns specific to particular events happening during the experiment (e.g. a stimulus that we might present). PCA is a powerful technique for finding spatial and temporal patterns in these kinds of data, and that's what we'll explore here!

## (3a) Load neuroscience data

In the next sections we will use PCA to capture structure in neural datasets. Before doing the analysis, we will load and do some basic inspection of the data. The raw data are currently stored as a text file. Every line in the file contains the

time series of image intensity for a single pixel in a time-varying image (i.e. a movie). The first two numbers in each line are the spatial coordinates of the pixel, and the remaining numbers are the time series. We'll use first() to inspect a single row, and print just the first 100 characters.

## In [100]:

```
import os
baseDir = os.path.join('data')
inputPath = os.path.join('cs190', 'neuro.txt')

inputFile = os.path.join(baseDir, inputPath)

lines = sc.textFile(inputFile)
print lines.first()[0:100]

# Check that everything loaded properly
assert len(lines.first()) == 1397
assert lines.count() == 46460
```

0 0 103 103.7 103.2 102.7 103.8 102.8 103 103.3 103.8 103.2 102.1 103.5 103.2 102.7 103.1 102.2 102.

## (3b) Parse the data

Parse the data into a key-value representation. We want each key to be a tuple of two-dimensional spatial coordinates and each value to be a NumPy array storing the associated time series. Write a function that converts a line of text into a (tuple, np.ndarray) pair. Then apply this function to each record in the RDD, and inspect the first entry of the new parsed data set. Now would be a good time to cache the data, and force a computation by calling count, to ensure the data are cached.

#### In [101]:

```
# TODO: Replace <FILL IN> with appropriate code
def parse(line):
    """Parse the raw data into a (`tuple`, `np.ndarray`) pair.
    Note:
        You should store the pixel coordinates as a tuple of two ints and the element
        time series as an np.ndarray of floats.
    Args:
        line (str): A string representing an observation. Elements are separated by
            first two elements represent the coordinates of the pixel, and the rest o
            represent the pixel intensity over time.
    Returns:
        tuple of tuple, np.ndarray: A (coordinate, pixel intensity array) `tuple` whe
            a `tuple` containing two values and the pixel intensity is stored in an N
            which contains 240 values.
    line = line.split()
    return ((int(line[0]), int(line[1])), np.array(map(float, line[2:])))
rawData = lines.map(parse)
rawData.cache()
entry = rawData.first()
print 'Length of movie is {0} seconds'.format(len(entry[1]))
print 'Number of pixels in movie is {0:,}'.format(rawData.count())
print ('\nFirst entry of rawData (with only the first five values of the NumPy array)
       .format(entry[0], entry[1][:5]))
Length of movie is 240 seconds
Number of pixels in movie is 46,460
First entry of rawData (with only the first five values of the NumPy ar
ray):
((0, 0), [103. 103.7 103.2 102.7 103.8])
```

#### In [102]:

```
# TEST Parse the data (3b)
Test.assertTrue(isinstance(entry[0], tuple), "entry's key should be a tuple")
Test.assertEquals(len(entry), 2, 'entry should have a key and a value')
Test.assertTrue(isinstance(entry[0][1], int), 'coordinate tuple should contain ints')
Test.assertEquals(len(entry[0]), 2, "entry's key should have two values")
Test.assertTrue(isinstance(entry[1], np.ndarray), "entry's value should be an np.ndar
Test.assertTrue(isinstance(entry[1][0], np.float), 'the np.ndarray should consist of
Test.assertEquals(entry[0], (0, 0), 'incorrect key for entry')
Test.assertEquals(entry[1].size, 240, 'incorrect length of entry array')
Test.assertTrue(np.allclose(np.sum(entry[1]), 24683.5), 'incorrect values in entry ar
1 test passed.
```

## (3c) Min and max flouresence

Next we'll do some basic preprocessing on the data. The raw time-series data are in units of image flouresence, and baseline flouresence varies somewhat arbitrarily from pixel to pixel. First, compute the minimum and maximum values across all pixels.

```
In [105]:
```

```
# TODO: Replace <FILL IN> with appropriate code
mn = rawData.map(lambda x: min(x[1])).min()
mx = rawData.map(lambda x: max(x[1])).max()

print mn, mx

100.6 940.8

In [106]:
# TEST Min and max flouresence (3c)
Test.assertTrue(np.allclose(mn, 100.6), 'incorrect value for mn')
Test.assertTrue(np.allclose(mx, 940.8), 'incorrect value for mx')

1 test passed.
1 test passed.
```

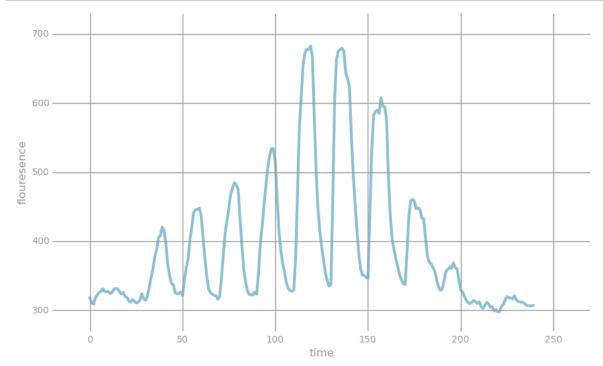
## **Visualization 5: Pixel intensity**

Let's now see how a random pixel varies in value over the course of the time series. We'll visualize a pixel that exhibits a standard deviation of over 100.

### In [107]:

```
example = rawData.filter(lambda (k, v): np.std(v) > 100).values().first()

# generate Layout and plot data
fig, ax = preparePlot(np.arange(0, 300, 50), np.arange(300, 800, 100))
ax.set_xlabel(r'time'), ax.set_ylabel(r'flouresence')
ax.set_xlim(-20, 270), ax.set_ylim(270, 730)
plt.plot(range(len(example)), example, c='#8cbfd0', linewidth='3.0')
pass
```



## (3d) Fractional signal change

To convert from these raw flouresence units to more intuitive units of fractional signal change, write a function that takes a time series for a particular pixel and subtracts and divides by the mean. Then apply this function to all the pixels. Confirm that this changes the maximum and minimum values.

## In [109]:

```
# TODO: Replace <FILL IN> with appropriate code
def rescale(ts):
    """Take a np.ndarray and return the standardized array by subtracting and dividin

Note:
    You should first subtract the mean and then divide by the mean.

Args:
    ts (np.ndarray): Time series data (`np.float`) representing pixel intensity.

Returns:
    np.ndarray: The times series adjusted by subtracting the mean and dividing by
    """

return ts * len(ts) / sum(ts) - 1

scaledData = rawData.mapValues(lambda v: rescale(v))
mnScaled = scaledData.map(lambda (k, v): v).map(lambda v: min(v)).min()
mxScaled = scaledData.map(lambda (k, v): v).map(lambda v: max(v)).max()
print mnScaled, mxScaled
```

-0.271512880125 0.905448764348

#### In [110]:

```
# TEST Fractional signal change (3d)
Test.assertTrue(isinstance(scaledData.first()[1], np.ndarray), 'incorrect type return
Test.assertTrue(np.allclose(mnScaled, -0.27151288), 'incorrect value for mnScaled')
Test.assertTrue(np.allclose(mxScaled, 0.90544876), 'incorrect value for mxScaled')
```

```
1 test passed.
```

## Visualization 6: Normalized data

Now that we've normalized our data, let's once again see how a random pixel varies in value over the course of the time series. We'll visualize a pixel that exhibits a standard deviation of over 0.1. Note the change in scale on the y-axis compared to the previous visualization.

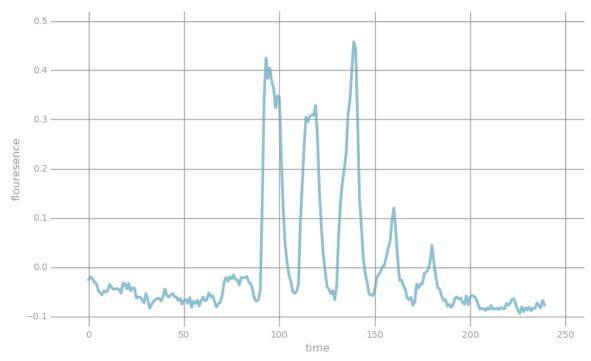
<sup>1</sup> test passed.

<sup>1</sup> test passed.

#### In [111]:

```
example = scaledData.filter(lambda (k, v): np.std(v) > 0.1).values().first()

# generate Layout and plot data
fig, ax = preparePlot(np.arange(0, 300, 50), np.arange(-.1, .6, .1))
ax.set_xlabel(r'time'), ax.set_ylabel(r'flouresence')
ax.set_xlim(-20, 260), ax.set_ylim(-.12, .52)
plt.plot(range(len(example)), example, c='#8cbfd0', linewidth='3.0')
pass
```



## (3e) PCA on the scaled data

We now have a preprocessed dataset with n=46460 pixels and d=240 seconds of time series data for each pixel. We can interpret the pixels as our observations and each pixel value in the time series as a feature. We would like to find patterns in brain activity during this time series, and we expect to find correlations over time. We can thus use PCA to find a more compact representation of our data and allow us to visualize it.

Use the pca function from Part (2a) to perform PCA on the preprocessed neuroscience data with k=3, resulting in a new low-dimensional 46460 by 3 dataset. The pca function takes an RDD of arrays, but data is an RDD of key-value pairs, so you'll need to extract the values.

#### In [118]:

```
# TODO: Replace <FILL IN> with appropriate code
# Run pca using scaledData
#print scaledData.take(1)
componentsScaled, scaledScores, eigenvaluesScaled = pca(scaledData.map(lambda x: x[1])
```

#### In [120]:

- 1 test passed.
- 1 test passed.
- 1 test passed.
- 1 test passed.

## Visualization 7: Top two components as images

Now, we'll view the scores for the top two component as images. Note that we reshape the vectors by the dimensions of the original image, 230 x 202.

These graphs map the values for the single component to a grayscale image. This provides us with a visual representation which we can use to see the overall structure of the zebrafish brain and to identify where high and low values occur. However, using this representation, there is a substantial amount of useful information that is difficult to interpret. In the next visualization, we'll see how we can improve interpretability by combining the two principal components into a single image using a color mapping.

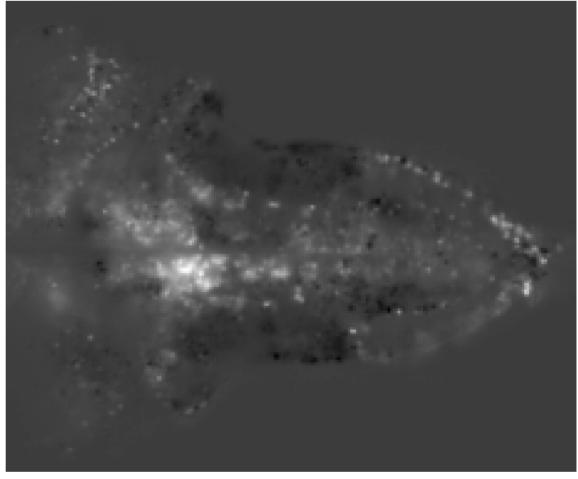
## In [121]:

```
import matplotlib.cm as cm

scoresScaled = np.vstack(scaledScores.collect())
imageOneScaled = scoresScaled[:,0].reshape(230, 202).T

# generate Layout and plot data
fig, ax = preparePlot(np.arange(0, 10, 1), np.arange(0, 10, 1), figsize=(9.0, 7.2), h
ax.grid(False)
ax.set_title('Top Principal Component', color='#888888')
image = plt.imshow(imageOneScaled,interpolation='nearest', aspect='auto', cmap=cm.gra
pass
```

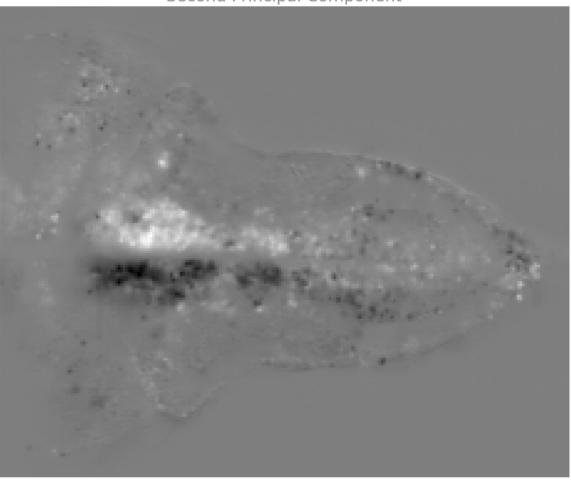
Top Principal Component



#### In [122]:

```
imageTwoScaled = scoresScaled[:,1].reshape(230, 202).T
# generate layout and plot data
fig, ax = preparePlot(np.arange(0, 10, 1), np.arange(0, 10, 1), figsize=(9.0, 7.2), h
ax.grid(False)
ax.set title('Second Principal Component', color='#888888')
image = plt.imshow(imageTwoScaled,interpolation='nearest', aspect='auto', cmap=cm.gra
pass
```





## Visualization 8: Top two components as one image

When we perform PCA and color neurons based on their location in the lowdimensional space, we can interpret areas with similar colors as exhibiting similar responses (at least in terms of the simple representation we recover with PCA). Below, the first graph shows how low-dimensional representations, which correspond to the first two principal components, are mapped to colors. The second graph shows the result of this color mapping using the zebrafish neural data.

The second graph clearly exhibits patterns of neural similarity throughout

different regions of the brain. However, when performing PCA on the full dataset, there are multiple reasons why neurons might have similar responses. The neurons might respond similarly to different stimulus directions, their responses might have similar temporal dynamics, or their response similarity could be influenced by both temporal and stimulus-specific factors. However, with our initial PCA analysis, we cannot pin down the underlying factors, and hence it is hard to interpret what "similarity" really means.

Optional Details: Note that we use <u>polar coordinates</u> (<a href="https://en.wikipedia.org/wiki/Polar\_coordinate\_system">https://en.wikipedia.org/wiki/Polar\_coordinate\_system</a>) to map our low-dimensional points to colors. Using polar coordinates provides us with an angle ( $\phi$ ) and magnitude ( $\rho$ ). We then use the well-known polar color space, <u>hue-saturation-value</u> (<a href="https://en.wikipedia.org/wiki/HSL\_and\_HSV">https://en.wikipedia.org/wiki/HSL\_and\_HSV</a>) (HSV), and map the angle to hue and the magnitude to value (brightness). This maps low magnitude points to black while allowing larger magnitude points to be differentiated by their angle. Additionally, the function polarTransform that maps low-dimensional representations to colors has an input parameter called scale, which we set to 2.0, and you can try lower values for the two graphs to see more nuanced mappings -- values near 1.0 are particularly interesting.

#### In [123]:

```
# Adapted from python-thunder's Colorize.transform where cmap='polar'.
# Checkout the library at: https://github.com/thunder-project/thunder and
# http://thunder-project.org/

def polarTransform(scale, img):
    """Convert points from cartesian to polar coordinates and map to colors."""
    from matplotlib.colors import hsv_to_rgb

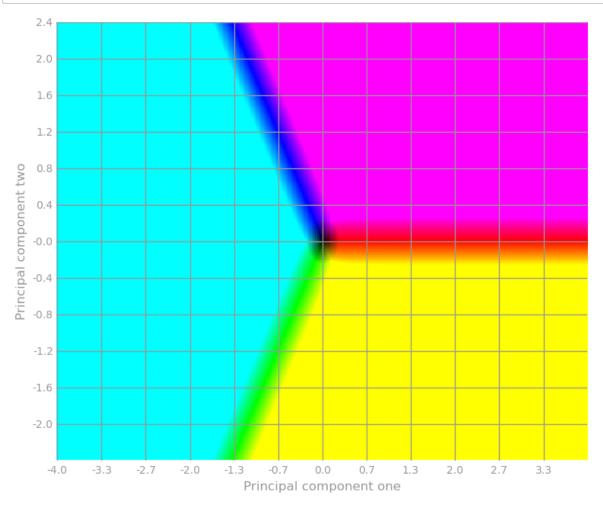
img = np.asarray(img)
dims = img.shape

phi = ((np.arctan2(-img[0], -img[1]) + np.pi/2) % (np.pi*2)) / (2 * np.pi)
rho = np.sqrt(img[0]**2 + img[1]**2)
saturation = np.ones((dims[1], dims[2]))

out = hsv_to_rgb(np.dstack((phi, saturation, scale * rho)))
return np.clip(out * scale, 0, 1)
```

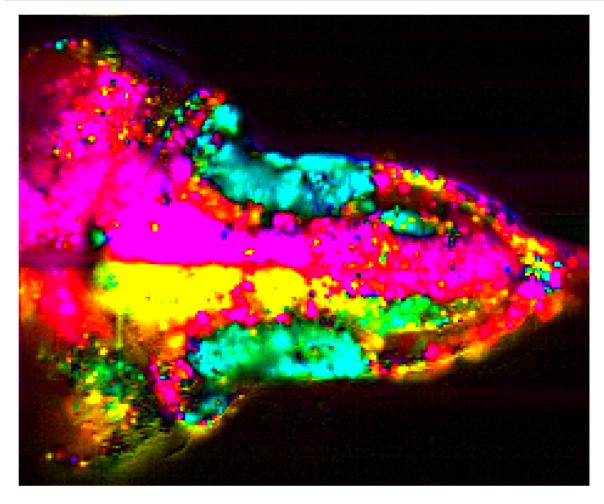
## In [124]:

```
# Show the polar mapping from principal component coordinates to colors.
x1AbsMax = np.max(np.abs(imageOneScaled))
x2AbsMax = np.max(np.abs(imageTwoScaled))
numOfPixels = 300
x1Vals = np.arange(-x1AbsMax, x1AbsMax, (2 * x1AbsMax) / numOfPixels)
x2Vals = np.arange(x2AbsMax, -x2AbsMax, -(2 * x2AbsMax) / numOfPixels)
x2Vals.shape = (numOfPixels, 1)
x1Data = np.tile(x1Vals, (numOfPixels, 1))
x2Data = np.tile(x2Vals, (1, numOfPixels))
# Try changing the first parameter to lower values
polarMap = polarTransform(2.0, [x1Data, x2Data])
gridRange = np.arange(0, numOfPixels + 25, 25)
fig, ax = preparePlot(gridRange, gridRange, figsize=(9.0, 7.2), hideLabels=True)
image = plt.imshow(polarMap, interpolation='nearest', aspect='auto')
ax.set_xlabel('Principal component one'), ax.set_ylabel('Principal component two')
gridMarks = (2 * gridRange / float(numOfPixels) - 1.0)
x1Marks = x1AbsMax * gridMarks
x2Marks = -x2AbsMax * gridMarks
ax.get_xaxis().set_ticklabels(map(lambda x: '{0:.1f}'.format(x), x1Marks))
ax.get yaxis().set ticklabels(map(lambda x: '{0:.1f}'.format(x), x2Marks))
pass
```



#### In [125]:

```
# Use the same transformation on the image data
# Try changing the first parameter to lower values
brainmap = polarTransform(2.0, [imageOneScaled, imageTwoScaled])
# generate layout and plot data
fig, ax = preparePlot(np.arange(0, 10, 1), np.arange(0, 10, 1), figsize=(9.0, 7.2), h
ax.grid(False)
image = plt.imshow(brainmap,interpolation='nearest', aspect='auto')
pass
```



Part 4: Feature-based aggregation and PCA

## (4a) Aggregation using arrays

In the analysis in Part 3, we performed PCA on the full time series data, trying to find global patterns across all 240 seconds of the time series. However, our analysis doesn't use the fact that different events happened during those 240 seconds. Specifically, during those 240 seconds, the zebrafish was presented with 12 different direction-specific visual patterns, with each one lasting for 20 seconds, for a total of  $12 \times 20 = 240$  features. Stronger patterns are likely to emerge if we incorporate knowledge of our experimental setup into our analysis.

As we'll see, we can isolate the impact of temporal response or direction-specific impact by appropriately aggregating our features.

In order to aggregate the features we will use basic ideas from matrix multiplication. First, note that if we use np.dot with a two-dimensional array, then NumPy performs the equivalent matrix-multiply calculation. For example, np.array([[1, 2, 3], [4, 5, 6]]).dot(np.array([2, 0, 1])) produces np.array([5, 14]).

$$\left[egin{array}{ccc} 1 & 2 & 3 \ 4 & 5 & 6 \end{array}
ight] \left[egin{array}{ccc} 2 \ 0 \ 1 \end{array}
ight] = \left[egin{array}{ccc} 5 \ 14 \end{array}
ight]$$

By setting up our multi-dimensional array properly we can multiply it by a vector to perform certain aggregation operations. For example, imagine we had a 3 dimensional vector,  $\begin{bmatrix} 1 & 2 & 3 \end{bmatrix}^T$  and we wanted to create a 2 dimensional vector containing the sum of its first and last elements as one value and three times its second value as another value, i.e.,  $\begin{bmatrix} 4 & 6 \end{bmatrix}^T$ . We can generate this result via matrix multiplication as follows: np.array([[1, 0, 1], [0, 3, 0]]).dot(np.array([1, 2, 3]) which produces np.array([4, 6].

$$\left[egin{array}{ccc} 1 & 0 & 1 \ 0 & 3 & 0 \end{array}
ight] \left[egin{array}{ccc} 1 \ 2 \ 3 \end{array}
ight] = \left[egin{array}{ccc} 4 \ 6 \end{array}
ight]$$

For this exercise, you'll create several arrays that perform different types of aggregation. The aggregation is specified in the comments before each array. You should fill in the array values by hand. We'll automate array creation in the next two exercises.

## In [127]:

```
# TODO: Replace <FILL IN> with appropriate code
vector = np.array([0., 1., 2., 3., 4., 5.])
# Create a multi-dimensional array that when multiplied (using .dot) against vector,
# a two element array where the first element is the sum of the 0, 2, and 4 indexed e
# vector and the second element is the sum of the 1, 3, and 5 indexed elements of vec
# This should be a 2 row by 6 column array
sumEveryOther = np.array([[1,0]*3, [0,1]*3])
# Create a multi-dimensional array that when multiplied (using .dot) against vector,
# three element array where the first element is the sum of the 0 and 3 indexed eleme
# the second element is the sum of the 1 and 4 indexed elements of vector, and the th
# the sum of the 2 and 5 indexed elements of vector.
# This should be a 3 row by 6 column array
sumEveryThird = np.array([[1,0,0,1,0,0], [0,1,0,0,1,0], [0,0,1,0,0,1]])
# Create a multi-dimensional array that can be used to sum the first three elements o
# the last three elements of vector, which returns a two element array with those val
# with vector.
# This should be a 2 row by 6 column array
sumByThree = np.array([[1]*3+[0]*3,[0]*3+[1]*3])
# Create a multi-dimensional array that sums the first two elements, second two eleme
# last two elements of vector, which returns a three element array with those values
# with vector.
# This should be a 3 row by 6 column array
sumByTwo = np.array([[1]*2+[0]*4,[0]*2+[1]*2+[0]*2,[0]*4+[1]*2])
print 'sumEveryOther.dot(vector):\t{0}'.format(sumEveryOther.dot(vector))
print 'sumEveryThird.dot(vector):\t{0}'.format(sumEveryThird.dot(vector))
print '\nsumByThree.dot(vector):\t{0}'.format(sumByThree.dot(vector))
print 'sumByTwo.dot(vector): \t{0}'.format(sumByTwo.dot(vector))
sumEveryOther.dot(vector):
                                [ 6.
sumEveryThird.dot(vector):
                                [ 3. 5. 7.]
sumByThree.dot(vector): [ 3. 12.]
sumByTwo.dot(vector): [ 1. 5. 9.]
```

#### In [128]:

```
1 test passed.
```

- 1 test passed.

## (4b) Recreate with np.tile and np.eye

np.tile (http://docs.scipy.org/doc/numpy/reference/generated/numpy.tile.html) is useful for repeating arrays in one or more dimensions. For example, np.tile(np.array([[1, 2], [3, 4]]), 2) produces np.array([[1, 2, 1, 2], [3, 4, 3, 4]])).

$$np.\ tile(\left[egin{array}{ccc}1&2\3&4\end{array}
ight],2)
ightarrow\left[egin{array}{cccc}1&2&1&2\3&4&3&4\end{array}
ight]$$

## Recall that np.eye

(http://docs.scipy.org/doc/numpy/reference/generated/numpy.eye.html) can be used to create an identity array  $(\mathbf{I_n})$ . For example, np.eye(3) produces np.array([[1, 0, 0], [0, 1, 0], [0, 0, 1]]).

$$np.\,eye(3) 
ightarrow egin{bmatrix} 1 & 0 & 0 \ 0 & 1 & 0 \ 0 & 0 & 1 \end{bmatrix}$$

In this exercise, recreate sumEveryOther and sumEveryThird using np.tile

```
and np.eye.
```

```
In [ ]:
# Reference for what to recreate
print 'sumEveryOther: \n{0}'.format(sumEveryOther)
print '\nsumEveryThird: \n{0}'.format(sumEveryThird)
```

```
In [129]:
```

```
# TODO: Replace <FILL IN> with appropriate code
# Use np.tile and np.eye to recreate the arrays
sumEveryOtherTile = np.tile(np.eye(2), 3)
sumEveryThirdTile = np.tile(np.eye(3), 2)
print sumEveryOtherTile
print 'sumEveryOtherTile.dot(vector): {0}'.format(sumEveryOtherTile.dot(vector))
print '\n', sumEveryThirdTile
print 'sumEveryThirdTile.dot(vector): {0}'.format(sumEveryThirdTile.dot(vector))
              0.
[[ 1.
      0.
          1.
                   1.
                      0.1
[ 0.
      1.
          0.
               1.
                   0.
                      1.]]
sumEveryOtherTile.dot(vector): [ 6. 9.]
[[ 1. 0.
          0.
              1.
                  0.
                      0.1
              0.
[ 0. 1.
          0.
                  1.
                      0.1
[ 0.
          1.
              0.
                   0.
                      1.]]
      0.
sumEveryThirdTile.dot(vector): [ 3. 5. 7.]
In [130]:
# TEST Recreate with `np.tile` and `np.eye` (4b)
Test.assertEquals(sumEveryOtherTile.shape, (2, 6), 'incorrect shape for sumEveryOther
Test.assertEquals(sumEveryThirdTile.shape, (3, 6), 'incorrect shape for sumEveryThird
Test.assertTrue(np.allclose(sumEveryOtherTile.dot(vector), [6, 9]),
                'incorrect value for sumEveryOtherTile')
```

```
1 test passed.
```

- 1 test passed.
- 1 test passed.
- 1 test passed.

## (4c) Recreate with np.kron

The Kronecker product is the generalization of outer products involving matrices, and we've included some examples below to illustrate the idea. Please refer to the Wikipedia page (https://en.wikipedia.org/wiki/Kronecker\_product) for a detailed definition. We can use <a href="np.kron">np.kron</a> (http://docs.scipy.org/doc/numpy/reference/generated/numpy.kron.html) to compute Kronecker products and recreate the sumBy arrays. Note that  $\otimes$  indicates a Kronecker product.

$$\left[\begin{array}{cccc} 1 & 2 \\ 3 & 4 \end{array}\right] \otimes \left[\begin{array}{cccccc} 1 & 2 \end{array}\right] = \left[\begin{array}{ccccc} 1 \cdot 1 & 1 \cdot 2 & 2 \cdot 1 & 2 \cdot 2 \\ 3 \cdot 1 & 3 \cdot 2 & 4 \cdot 1 & 4 \cdot 2 \end{array}\right] = \left[\begin{array}{ccccc} 1 & 2 & 2 & 4 \\ 3 & 6 & 4 & 8 \end{array}\right]$$

We can see how the Kronecker product continues to expand if we add another row to the second array.

For this exercise, you'll recreate the sumByThree and sumByTwo arrays using np.kron, np.eye, and np.ones. Note that np.ones creates an array of all ones.

```
In [ ]:
```

```
# Reference for what to recreate
print 'sumByThree: \n{0}'.format(sumByThree)
print '\nsumByTwo: \n{0}'.format(sumByTwo)
```

#### In [131]:

```
# TODO: Replace <FILL IN> with appropriate code
# Use np.kron, np.eye, and np.ones to recreate the arrays
sumByThreeKron = np.kron(np.eye(2), np.ones(3))
sumByTwoKron = np.kron(np.eye(3), np.ones(2))

print sumByThreeKron
print 'sumByThreeKron.dot(vector): {0}'.format(sumByThreeKron.dot(vector))
print '\n', sumByTwoKron
print 'sumByTwoKron.dot(vector): {0}'.format(sumByTwoKron.dot(vector))
[[ 1.  1.  1.  0.  0.  0. ]
```

```
[ 0. 0. 0. 1. 1. 1.]]
sumByThreeKron.dot(vector): [ 3. 12.]

[[ 1. 1. 0. 0. 0. 0.]
  [ 0. 0. 1. 1. 0. 0.]
  [ 0. 0. 0. 0. 1. 1.]]
sumByTwoKron.dot(vector): [ 1. 5. 9.]
```

#### In [132]:

- 1 test passed.
- 1 test passed.
- 1 test passed.
- 1 test passed.

(4d) Aggregate by time As we discussed in Part (4a), we would like to incorporate knowledge of our experimental setup into our analysis. To do this, we'll first study the temporal aspects of neural response, by aggregating our features by time. In other words, we want to see how different pixels (and the underlying neurons captured in these pixels) react in each of the 20 seconds after a new visual pattern is displayed, regardless of what the pattern is. Hence, instead of working with the 240 features individually, we'll aggregate the original features into 20 new features, where the first new feature captures the pixel response one second after a visual pattern appears, the second new feature is the response after two seconds, and so on.

We can perform this aggregation using a map operation. First, build a multi-dimensional array  $\mathbf{T}$  that, when dotted with a 240-dimensional vector, sums every 20-th component of this vector and returns a 20-dimensional vector. Note that this exercise is similar to (4b). Once you have created your multi-dimensional array  $\mathbf{T}$ , use a map operation with that array and each time series to generate a transformed dataset. We'll cache and count the output, as we'll be using it again.

## In [147]:

```
# TODO: Replace <FILL IN> with appropriate code
# Create a multi-dimensional array to perform the aggregation
T = np.tile(np.eye(20), 12)
#print T, T.shape
#print scaledData.take(1)
# Transform scaledData using T. Make sure to retain the keys.
timeData = scaledData.map(lambda x: (x[0], x[1].dot(T.T)))
timeData.cache()
print timeData.count()
print timeData.first()
46460
((0, 0), array([0.00802155, 0.00607693, -0.0075354, 0.00121539,
0.02163388,
       0.00121539, -0.03087082, 0.00510462, 0.01191079, 0.02455081,
       -0.0182308 , 0.00802155, -0.00948002, -0.00948002,
                                                            0.02163388,
       -0.02212004,
                   0.00704924, 0.00121539, -0.01142464, -0.0085077
1]))
In [148]:
# TEST Aggregate by time (4d)
Test.assertEquals(T.shape, (20, 240), 'incorrect shape for T')
timeDataFirst = timeData.values().first()
timeDataFifth = timeData.values().take(5)[4]
Test.assertEquals(timeData.count(), 46460, 'incorrect length of timeData')
Test.assertEquals(timeDataFirst.size, 20, 'incorrect value length of timeData')
Test.assertEquals(timeData.keys().first(), (0, 0), 'incorrect keys in timeData')
Test.assertTrue(np.allclose(timeDataFirst[:2], [0.00802155, 0.00607693]),
                'incorrect values in timeData')
Test.assertTrue(np.allclose(timeDataFifth[-2:],[-0.00636676, -0.0179427]),
                'incorrect values in timeData')
1 test passed.
```

- 1 test passed.

## (4e) Obtain a compact representation

We now have a time-aggregated dataset with n=46460 pixels and d=20 aggregated time features, and we want to use PCA to find a more compact representation. Use the pca function from Part (2a) to perform PCA on the this data with k=3, resulting in a new low-dimensional 46,460 by 3 dataset. As before, you'll need to extract the values from timeData since it is an RDD of key-value pairs.

```
In [150]:
```

```
# TODO: Replace <FILL IN> with appropriate code
componentsTime, timeScores, eigenvaluesTime = pca(timeData.map(lambda x: x[1]), k=3)
print 'componentsTime: (first five) \n{0}'.format(componentsTime[:5,:])
print ('\ntimeScores (first three): \n{0}'
       .format('\n'.join(map(str, timeScores.take(3)))))
print '\neigenvaluesTime: (first five) \n{0}'.format(eigenvaluesTime[:5])
componentsTime: (first five)
[[ 0.27392702 -0.16152431 0.01388556]
[ 0.09941893 -0.31968127 -0.34738824]
[-0.03376505 -0.32933108 -0.35606954]
[-0.12092744 -0.2845482 -0.27232364]
[-0.18219248 -0.22998061 -0.12248985]]
timeScores (first three):
[-0.0072061686153766635, -0.0029297857382522374, -0.002236448549428035]
[0.023530759500869941, -0.001974574148106905, 0.0036209435448801715]
[0.013106233925334951, 0.0012306897550586988, -0.0058297382592386827]
eigenvaluesTime: (first five)
[ 0.77528991  0.05038881  0.01173423  0.0059711
                                                  0.00138073]
In [151]:
# TEST Obtain a compact representation (4e)
Test.assertEquals(componentsTime.shape, (20, 3), 'incorrect shape for componentsTime'
Test.assertTrue(np.allclose(np.abs(np.sum(componentsTime[:5, :])), 2.37299020),
                'incorrect value for componentsTime')
Test.assertTrue(np.allclose(np.abs(np.sum(timeScores.take(3))), 0.0213119114),
                'incorrect value for timeScores')
Test.assertTrue(np.allclose(np.sum(eigenvaluesTime[:5]), 0.844764792),
                'incorrect value for eigenvaluesTime')
1 test passed.
1 test passed.
1 test passed.
```

1 test passed.

## Visualization 9: Top two components by time

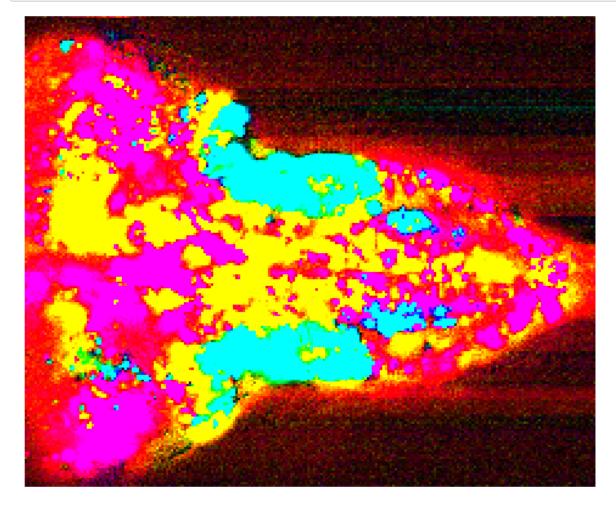
Let's view the scores from the first two PCs as a composite image. When we preprocess by aggregating by time and then perform PCA, we are only looking at variability related to temporal dynamics. As a result, if neurons appear similar -- have similar colors -- in the resulting image, it means that their responses vary similarly over time, regardless of how they might be encoding direction. In the image below, we can define the midline as the horizontal line across the middle of the brain. We see clear patterns of neural activity in different parts of the brain, and crucially note that the regions on either side of the midline are similar, which suggests that temporal dynamics do not differ across the two sides of the

brain.

#### In [152]:

```
scoresTime = np.vstack(timeScores.collect())
imageOneTime = scoresTime[:,0].reshape(230, 202).T
imageTwoTime = scoresTime[:,1].reshape(230, 202).T
brainmap = polarTransform(3, [imageOneTime, imageTwoTime])

# generate layout and plot data
fig, ax = preparePlot(np.arange(0, 10, 1), np.arange(0, 10, 1), figsize=(9.0, 7.2), h
ax.grid(False)
image = plt.imshow(brainmap,interpolation='nearest', aspect='auto')
pass
```



## (4f) Aggregate by direction

Next, let's perform a second type of feature aggregation so that we can study the direction-specific aspects of neural response, by aggregating our features by direction. In other words, we want to see how different pixels (and the underlying neurons captured in these pixels) react when the zebrafish is presented with 12 direction-specific patterns, ignoring the temporal aspect of the reaction. Hence, instead of working with the 240 features individually, we'll aggregate the original features into 12 new features, where the first new feature captures the average pixel response to the first direction-specific visual pattern, the second new feature

is the response to the second direction-specific visual pattern, and so on.

As in Part (4c), we'll design a multi-dimensional array D that, when multiplied by a 240-dimensional vector, sums the first 20 components, then the second 20 components, and so on. Note that this is similar to exercise (4c). First create D. then use a map operation with that array and each time series to generate a transformed dataset. We'll cache and count the output, as we'll be using it again.

```
In [154]:
```

```
# TODO: Replace <FILL IN> with appropriate code
# Create a multi-dimensional array to perform the aggregation
D = np.kron(np.eye(12), np.ones(20))
#print D, D.shape
# Transform scaledData using D. Make sure to retain the keys.
directionData = scaledData.map(lambda x: (x[0], x[1].dot(D.T)))
directionData.cache()
print directionData.count()
print directionData.first()
[[ 1.
      1. 1. ...,
                   0.
                       0. 0.1
      0. 0. ..., 0.
                           0.1
[ 0.
                       0.
 Γ0.
          0. ..., 0.
      0.
                       0.
                           0.]
 . . . ,
  0. 0. 0. ..., 0. 0.
                          0.]
 [ 0. 0. 0. ...,
                   0.
                       0. 0.1
                       1. 1.]] (12, 240)
 [ 0.
          0. ..., 1.
46460
((0, 0), array([0.03346365, 0.03638058, -0.02195799, -0.02487492,
0.00721129,
        0.00332206, -0.02098568, 0.00915591, -0.00542873, -0.01029027,
        0.0081836 , -0.01417951]))
In [ ]:
# TEST Aggregate by direction (4f)
Test.assertEquals(D.shape, (12, 240), 'incorrect shape for D')
directionDataFirst = directionData.values().first()
directionDataFifth = directionData.values().take(5)[4]
Test.assertEquals(directionData.count(), 46460, 'incorrect length of directionData')
Test.assertEquals(directionDataFirst.size, 12, 'incorrect value length of directionDa
Test.assertEquals(directionData.keys().first(), (0, 0), 'incorrect keys in directionD
Test.assertTrue(np.allclose(directionDataFirst[:2], [ 0.03346365,
                'incorrect values in directionData')
Test.assertTrue(np.allclose(directionDataFifth[:2], [ 0.01479147, -0.02090099]),
```

## (4g) Compact representation of direction data

'incorrect values in directionData')

We now have a direction-aggregated dataset with n=46460 pixels and d=12 aggregated direction features, and we want to use PCA to find a more compact representation. Use the pca function from Part (2a) to perform PCA on the this data with k=3, resulting in a new low-dimensional 46460 by 3 dataset. As before, you'll need to extract the values from directionData since it is an RDD of key-value pairs.

```
In [155]:
```

```
# TODO: Replace <FILL IN> with appropriate code
componentsDirection, directionScores, eigenvaluesDirection = pca(directionData.map(la
print 'componentsDirection: (first five) \n{0}'.format(componentsDirection[:5,:])
print ('\ndirectionScores (first three): \n{0}'
       .format('\n'.join(map(str, directionScores.take(3)))))
print '\neigenvaluesDirection: (first five) \n{0}'.format(eigenvaluesDirection[:5])
componentsDirection: (first five)
[[-0.25952179 0.16201941 0.24947433]
[-0.31369506 -0.09185175 0.29464223]
[-0.21716693 -0.35944645 0.35296454]
[-0.11517273 -0.37356905 0.07169062]
 [ 0.02996577 -0.36272623 -0.14783897]]
directionScores (first three):
[-0.016225126032969651, 0.013229977105146977, 0.013222036913440299]
[0.0099948176483919716, 0.065236703268025956, -0.045247583658719233]
[0.0046459956551536084, 0.057510966666728495, 0.0075638332761037977]
eigenvaluesDirection: (first five)
[ 0.96411048  0.77613553  0.12762987  0.09775924  0.04333691]
In [156]:
# TEST Compact representation of direction data (4g)
Test.assertEquals(componentsDirection.shape, (12, 3), 'incorrect shape for components
Test.assertTrue(np.allclose(np.abs(np.sum(componentsDirection[:5, :])), 1.080232069),
                'incorrect value for componentsDirection')
Test.assertTrue(np.allclose(np.abs(np.sum(directionScores.take(3))), 0.10993162084),
                'incorrect value for directionScores')
Test.assertTrue(np.allclose(np.sum(eigenvaluesDirection[:5]), 2.0089720377),
                'incorrect value for eigenvaluesDirection')
1 test passed.
1 test passed.
1 test passed.
```

## Visualization 10: Top two components by direction

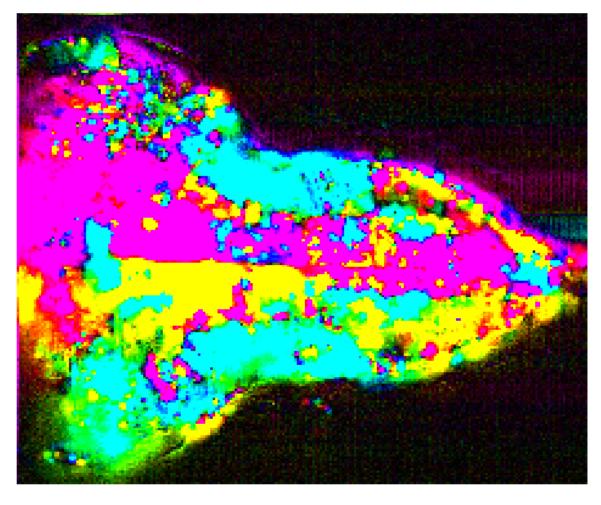
Again, let's view the scores from the first two PCs as a composite image. When we preprocess by averaging across time (group by direction), and then perform PCA, we are only looking at variability related to stimulus direction. As a result, if

1 test passed.

neurons appear similar -- have similar colors -- in the image, it means that their responses vary similarly across directions, regardless of how they evolve over time. In the image below, we see a different pattern of similarity across regions of the brain. Moreover, regions on either side of the midline are colored differently, which suggests that we are looking at a property, direction selectivity, that has a different representation across the two sides of the brain.

#### In [157]:

```
scoresDirection = np.vstack(directionScores.collect())
imageOneDirection = scoresDirection[:,0].reshape(230, 202).T
imageTwoDirection = scoresDirection[:,1].reshape(230, 202).T
brainmap = polarTransform(2, [imageOneDirection, imageTwoDirection])
# with thunder: Colorize(cmap='polar', scale=2).transform([imageOneDirection, imageTw
# generate layout and plot data
fig, ax = preparePlot(np.arange(0, 10, 1), np.arange(0, 10, 1), figsize=(9.0, 7.2), h
ax.grid(False)
image = plt.imshow(brainmap, interpolation='nearest', aspect='auto')
pass
```



## (4h) Next steps

In the analyses above we have successfully identified regions of the brain that encode particular properties, e.g., a particular temporal pattern or selectivity to a

stimulus. However, this is only the first step! These exploratory analyses are typically followed with more targeted investigation, both through analysis and experiment. For example, we might find all neurons that prefer one stimulus direction, and then do an experiment in which we stimulate or inactivate only those neurons and look at the effect on the animal's behavior. Alternatively, we might subdivide neurons into groups based on simple forms of stimulus selectivity like the ones analyzed here, and then estimate coupling across different neuronal populations, i.e. can we predict one population's response as a function of another. This can be framed as a massive pair-wise regression problem, related to techniques you learned earlier in the course, and demanding large-scale implementations.