Nearest neighbor for handwritten digit recognition

In this notebook we will build a classifier that takes an image of a handwritten digit and outputs a label 0-9. We will look at a particularly simple strategy for this problem known as the **nearest neighbor classifier**.

To run this notebook you should have the following Python packages installed:

- `numpy`
- `matplotlib`
- `sklearn`

1. The MNIST dataset

`MNIST` is a classic dataset in machine learning, consisting of 28x28 gray-scale images handwritten digits. The original training set contains 60,000 examples and the test set contains 10,000 examples. In this notebook we will be working with a subset of this data: a training set of 7,500 examples and a test set of 1,000 examples.

In [18]:

```
%matplotlib inline
import numpy as np
import matplotlib.pyplot as plt
import time

## Load the training set
train_data = np.load('../data/MNIST/train_data.npy')
train_labels = np.load('../data/MNIST/train_labels.npy')

## Load the testing set
test_data = np.load('../data/MNIST/test_data.npy')
test_labels = np.load('../data/MNIST/test_labels.npy')
```

In [19]:

```
## Print out their dimensions
print("Training dataset dimensions: ", np.shape(train_data))
print("Number of training labels: ", len(train_labels))
print("Testing dataset dimensions: ", np.shape(test_data))
print("Number of testing labels: ", len(test_labels))
```

```
Training dataset dimensions:  (7500, 784)
Number of training labels:  7500
Testing dataset dimensions:  (1000, 784)
Number of testing labels:  1000
```

In [20]:

```
## Compute the number of examples of each digit
train_digits, train_counts = np.unique(train_labels, return_counts=True)
print("Training set distribution:")
print(dict(zip(train_digits, train_counts)))
```

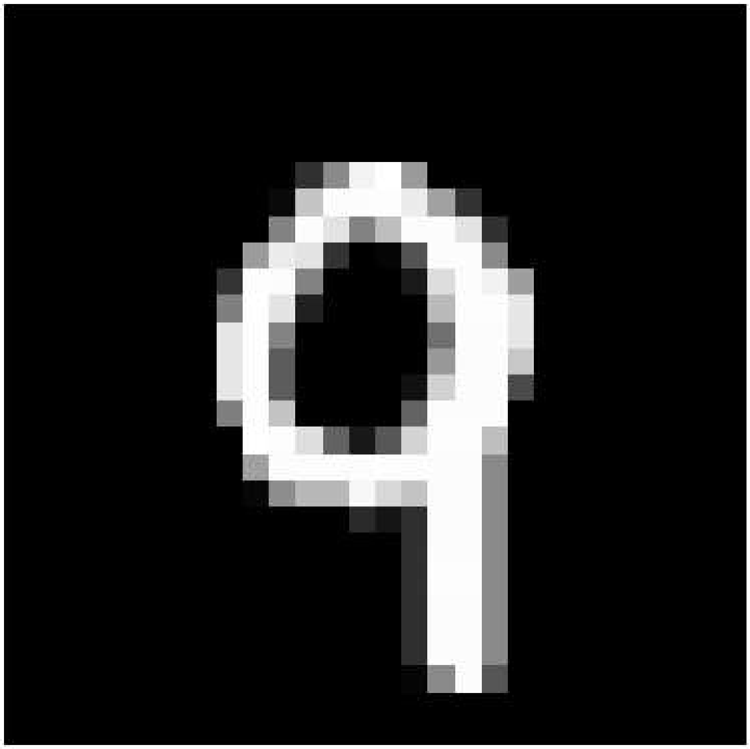
```python
test_digits, test_counts = np.unique(test_labels, return_counts=True)
print("Test set distribution:")
print(dict(zip(test_digits, test_counts)))
```

```
Training set distribution:
{0: 750, 1: 750, 2: 750, 3: 750, 4: 750, 5: 750, 6: 750, 7: 750, 8: 750, 9: 750}
Test set distribution:
{0: 100, 1: 100, 2: 100, 3: 100, 4: 100, 5: 100, 6: 100, 7: 100, 8: 100, 9: 100}
```

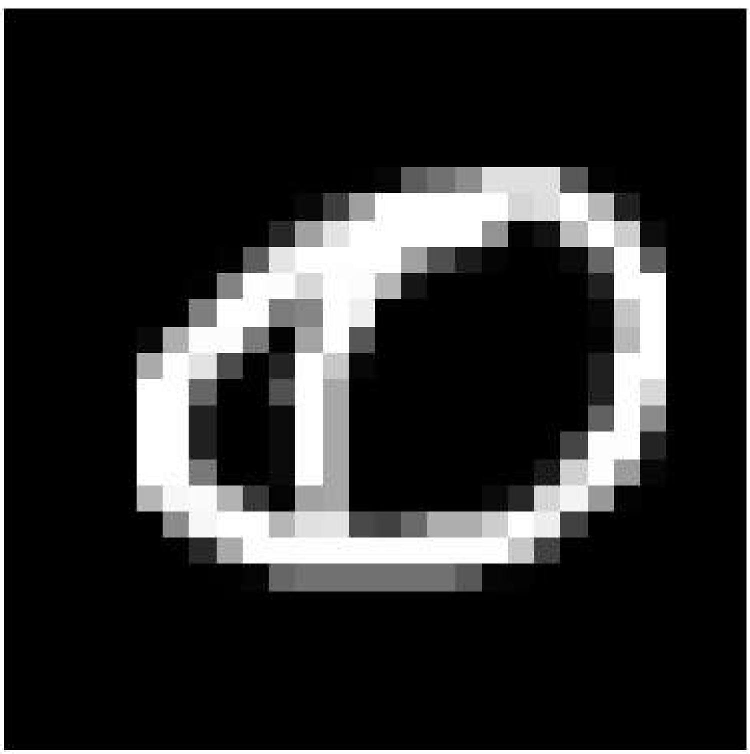
2. Visualizing the data

Each data point is stored as 784-dimensional vector. To visualize a data point, we first reshape it to a 28x28 image.

In [21]:
```python
## Define a function that displays a digit given its vector representation
def show_digit(x):
    plt.axis('off')
    plt.imshow(x.reshape((28,28)), cmap=plt.cm.gray)
    plt.show()
    return

## Define a function that takes an index into a particular data set ("train" or "test'
def vis_image(index, dataset="train"):
    if(dataset=="train"):
        show_digit(train_data[index,])
        label = train_labels[index]
    else:
        show_digit(test_data[index,])
        label = test_labels[index]
    print("Label " + str(label))
    return

## View the first data point in the training set
vis_image(0, "train")

## Now view the first data point in the test set
vis_image(0, "test")
```



```
Label 9
```



```
Label 0
```

3. Squared Euclidean distance

To compute nearest neighbors in our data set, we need to first be able to compute distances between data points. A natural distance function is *Euclidean distance*: for two vectors $x, y \in \mathbb{R}^d$
, their Euclidean distance is defined as

$$\|x - y\| = \sqrt{\sum_{i=1}^{d} (x_i - y_i)^2}.$$

Often we omit the square root, and simply compute *squared Euclidean distance*:

$$\|x - y\|^2 = \sum_{i=1}^{d} (x_i - y_i)^2.$$

For the purposes of nearest neighbor computations, the two are equivalent: for three vectors $x, y, z \in \mathbb{R}^d$, we have $\|x - y\| \leq \|x - z\|$ if and only if $\|x - y\|^2 \leq \|x - z\|^2$.

Now we just need to be able to compute squared Euclidean distance. The following function does so.

In [22]:
```
## Computes squared Euclidean distance between two vectors.
def squared_dist(x,y):
    return np.sum(np.square(x-y))

## Compute distance between a seven and a one in our training set.
print("Distance from 7 to 1: ", squared_dist(train_data[4,],train_data[5,]))

## Compute distance between a seven and a two in our training set.
print("Distance from 7 to 2: ", squared_dist(train_data[4,],train_data[1,]))

## Compute distance between two seven's in our training set.
print("Distance from 7 to 7: ", squared_dist(train_data[4,],train_data[7,]))
```

```
Distance from 7 to 1:  5357193.0
Distance from 7 to 2:  12451684.0
Distance from 7 to 7:  5223403.0
```

4. Computing nearest neighbors

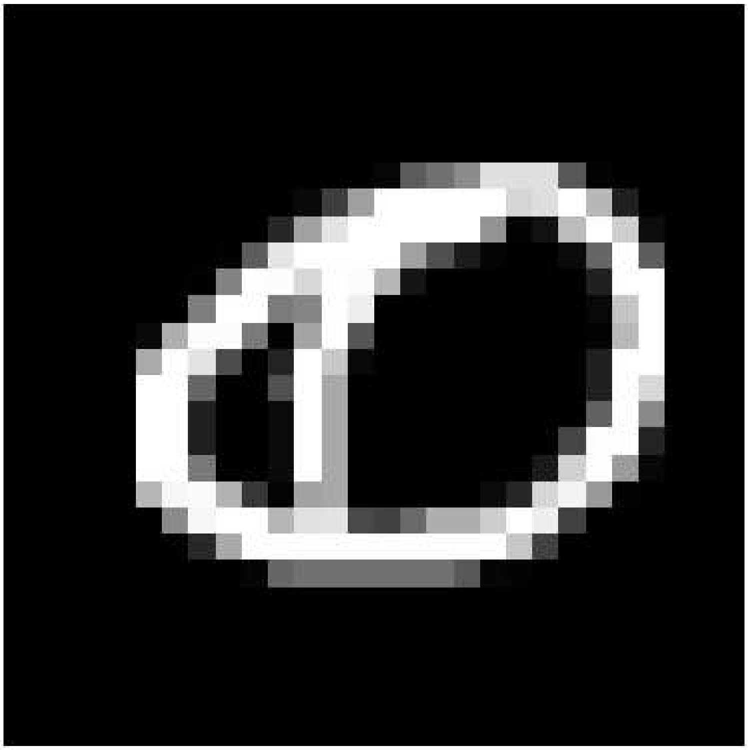
Now that we have a distance function defined, we can now turn to nearest neighbor classification.

In [23]:
```
## Takes a vector x and returns the index of its nearest neighbor in train_data
def find_NN(x):
    # Compute distances from x to every row in train_data
    distances = [squared_dist(x,train_data[i,]) for i in range(len(train_labels))]
    # Get the index of the smallest distance
    return np.argmin(distances)

## Takes a vector x and returns the class of its nearest neighbor in train_data
def NN_classifier(x):
    # Get the index of the the nearest neighbor
    index = find_NN(x)
    # Return its class
    return train_labels[index]
```

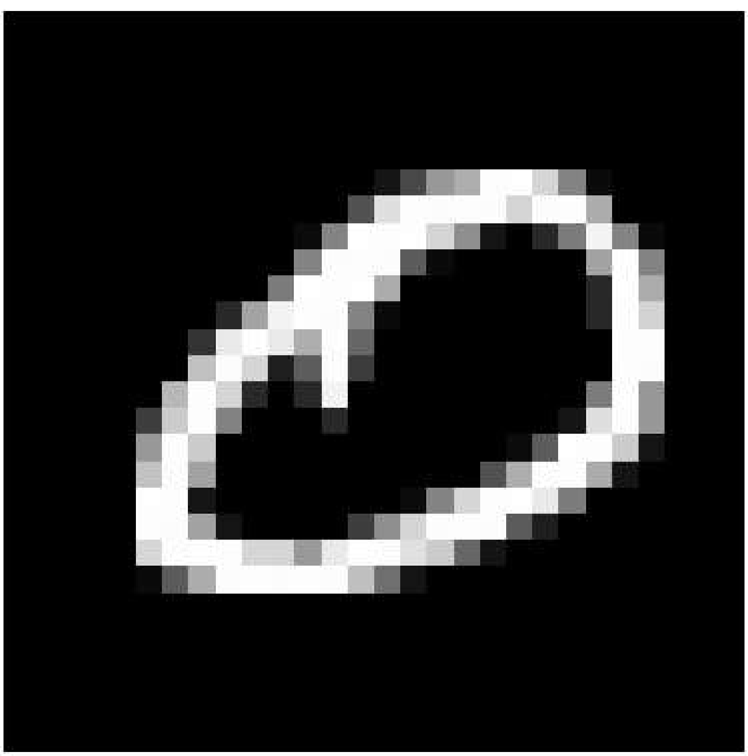
In [24]:
```
## A success case:
print("A success case:")
print("NN classification: ", NN_classifier(test_data[0,]))
```

```
print("True label: ", test_labels[0])
print("The test image:")
vis_image(0, "test")
print("The corresponding nearest neighbor image:")
vis_image(find_NN(test_data[0,]), "train")
```

```
A success case:
NN classification:  0
True label:  0
The test image:
```



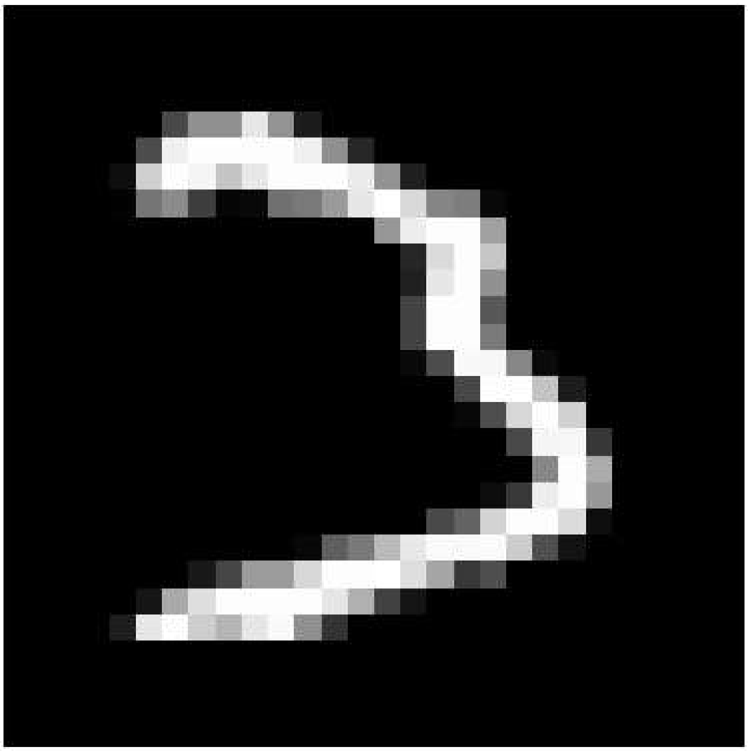
```
Label 0
The corresponding nearest neighbor image:
```



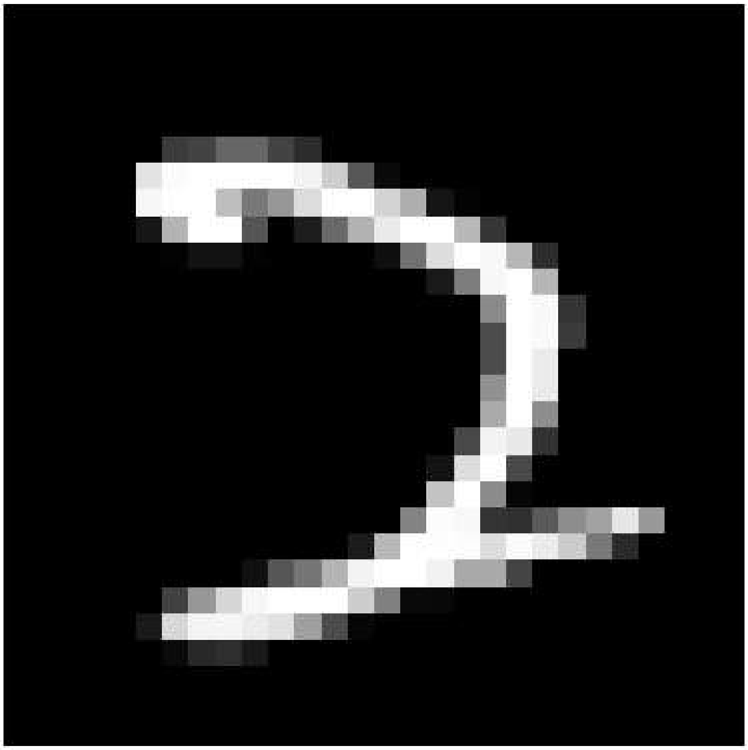
Label 0

In [25]:
```
## A failure case:
print("A failure case:")
print("NN classification: ", NN_classifier(test_data[39,]))
print("True label: ", test_labels[39])
print("The test image:")
vis_image(39, "test")
print("The corresponding nearest neighbor image:")
vis_image(find_NN(test_data[39,]), "train")
```

```
A failure case:
NN classification:  2
True label:  3
The test image:
```



```
Label 3
The corresponding nearest neighbor image:
```



```
Label 2
```

5. For you to try

The above two examples show the results of the NN classifier on test points number 0 and 39.

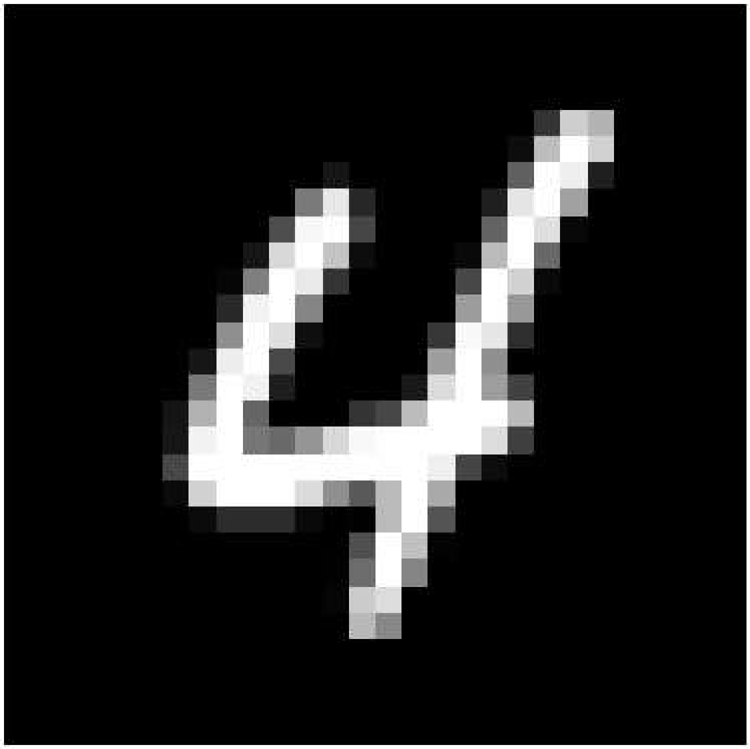
Now try test point number 100.

- What is the index of its nearest neighbor in the training set? *Record the answer: you will enter it as part of this week's assignment.*
- Display both the test point and its nearest neighbor.
- What label is predicted? Is this the correct label?

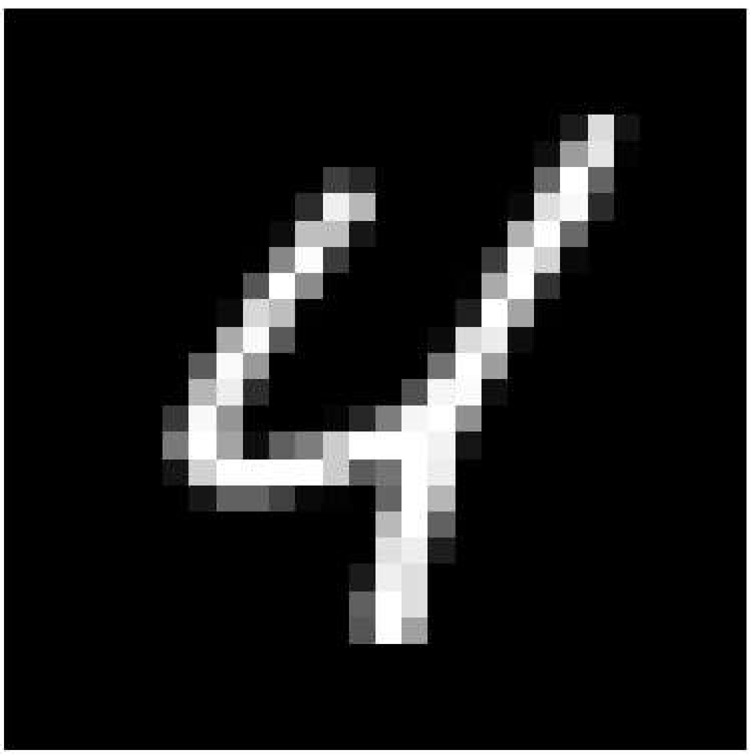
In [26]:

```
print("=== Sample test_id=100 ===")
vis_image(100, "test")
print(f"=== NN: train_id={find_NN(test_data[100])} ===")
vis_image(find_NN(test_data[100]), "train")
```

```
=== Sample test_id=100 ===
```



```
Label 4
=== NN: train_id=4711 ===
```



```
Label 4
```

6. Processing the full test set

Now let's apply our nearest neighbor classifier over the full data set.

Note that to classify each test point, our code takes a full pass over each of the 7500 training examples. Thus we should not expect testing to be very fast. The following code takes about 100-150 seconds on 2.6 GHz Intel Core i5.

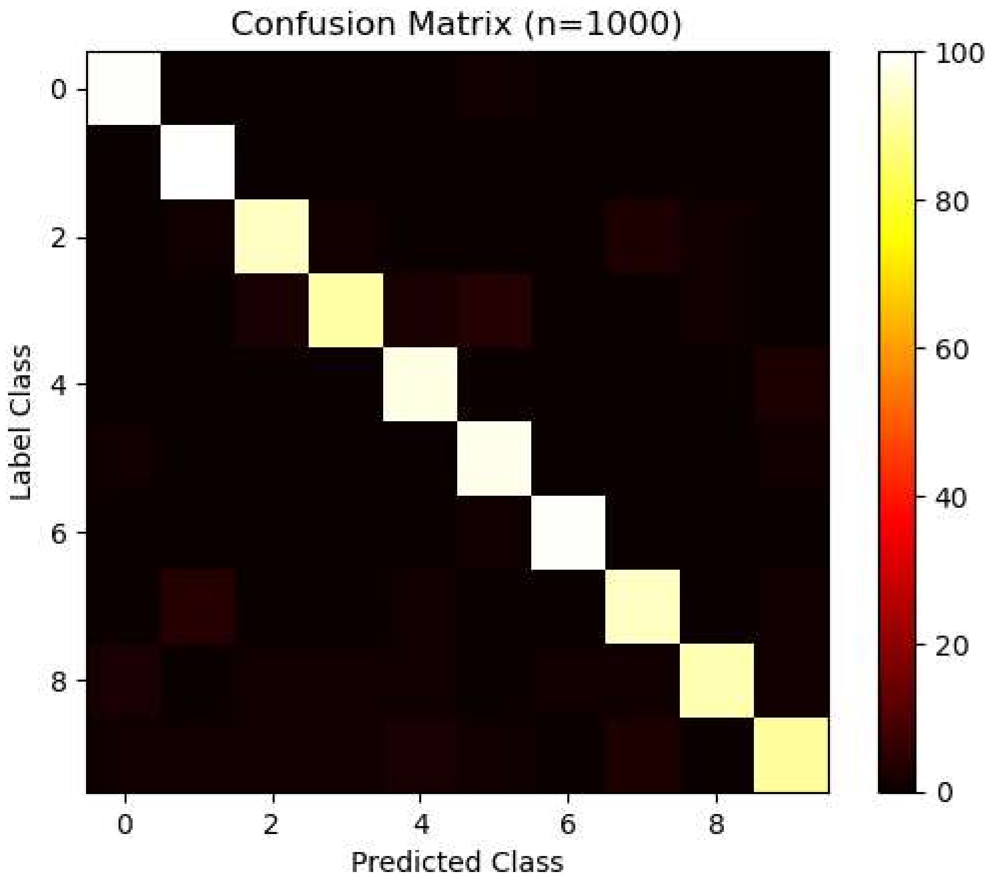
In [27]:
```
## Predict on each test data point (and time it!)
t_before = time.time()
test_predictions = [NN_classifier(test_data[i,]) for i in range(len(test_labels))]
t_after = time.time()

## Compute the error
err_positions = np.not_equal(test_predictions, test_labels)
error = float(np.sum(err_positions))/len(test_labels)

print("Error of nearest neighbor classifier: ", error)
print("Classification time (seconds): ", t_after - t_before)
```

```
Error of nearest neighbor classifier:  0.046
Classification time (seconds):  44.084826707839966
```

In [28]:
```
len(test_predictions)
mat = np.zeros((10, 10))
for lab, pred in zip(test_labels, test_predictions):
  mat[lab, pred] += 1
print(mat)
plt.imshow(mat, cmap="hot")
plt.xlabel("Predicted Class")
plt.ylabel("Label Class")
plt.title(f"Confusion Matrix (n={len(test_predictions)})")
plt.colorbar()
```

```
[[ 99.   0.   0.   0.   0.   1.   0.   0.   0.   0.]
 [  0. 100.   0.   0.   0.   0.   0.   0.   0.   0.]
 [  0.   1.  94.   1.   0.   0.   0.   3.   1.   0.]
 [  0.   0.   2.  91.   2.   4.   0.   0.   1.   0.]
 [  0.   0.   0.   0.  97.   0.   0.   0.   0.   3.]
 [  1.   0.   0.   0.   0.  98.   0.   0.   0.   1.]
 [  0.   0.   0.   0.   0.   1.  99.   0.   0.   0.]
 [  0.   4.   0.   0.   1.   0.   0.  94.   0.   1.]
 [  2.   0.   1.   1.   1.   0.   1.   1.  92.   1.]
 [  1.   1.   1.   1.   2.   1.   0.   3.   0.  90.]]
```

Out[28]:
```
<matplotlib.colorbar.Colorbar at 0x2daa16f33a0>
```



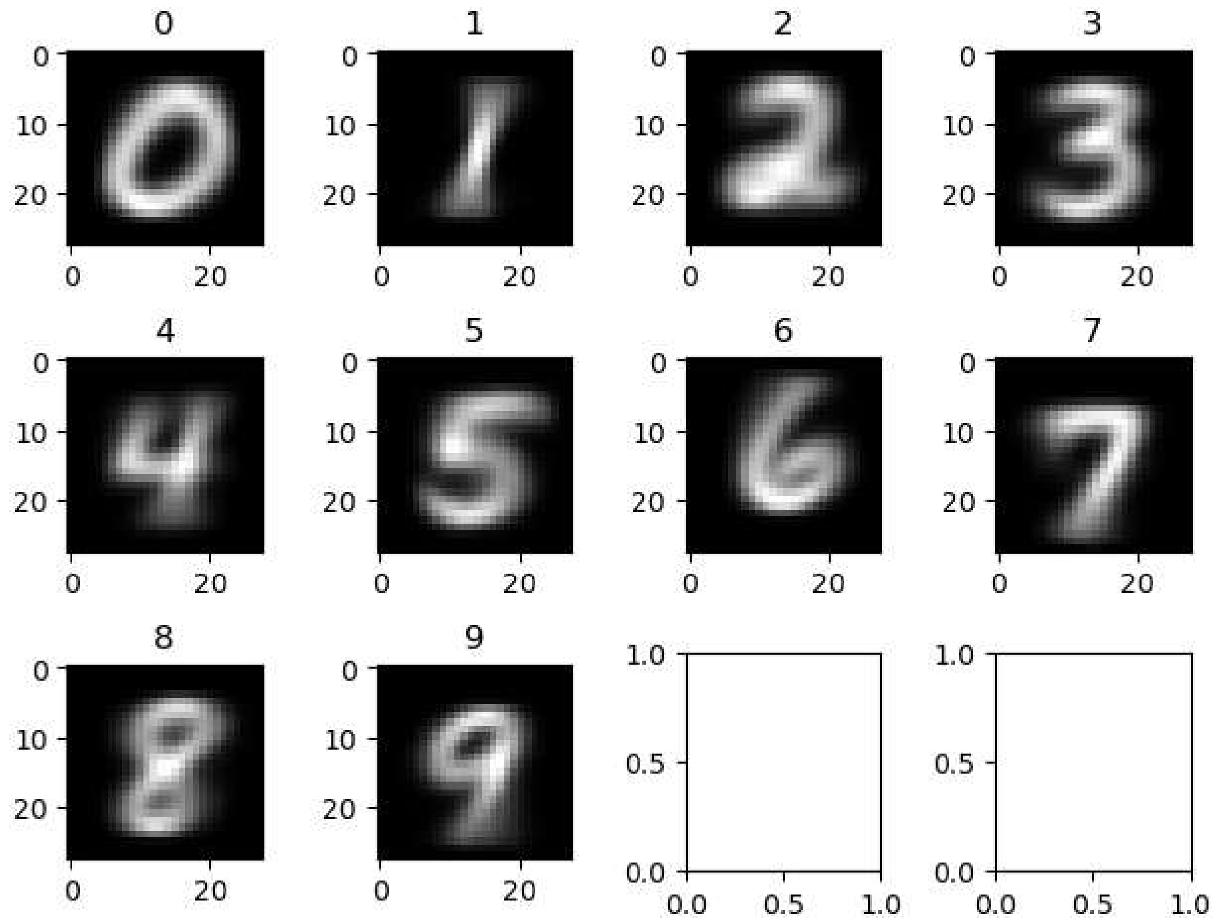
In [29]:

```
miscls_arr = np.zeros((10,))
ct_arr = np.zeros((10,))

for lab, pred in zip(test_labels, test_predictions):
  ct_arr[lab] += 1
  if lab != pred:
    miscls_arr[lab] += 1
print(miscls_arr)
print(ct_arr)
```

```
[ 1.   0.   6.   9.   3.   2.   1.   6.   8. 10.]
[100. 100. 100. 100. 100. 100. 100. 100. 100. 100.]
```

In [34]:

```
fig, axs = plt.subplots(nrows=3, ncols=4)
fig.tight_layout()
for i in range(10):
  ct, img = 0, np.zeros(784)
  for d, l in zip(train_data, train_labels):
    if l == i:
      img += d
      ct += 1
  mean_img = img / ct
  axs[i//4,i%4].imshow(mean_img.reshape((28, 28)), cmap="gray")
  axs[i//4,i%4].set_title(str(i))
  # show_digit(mean_img.reshape((28, 28)))
```



7. Faster nearest neighbor methods

Performing nearest neighbor classification in the way we have presented requires a full pass through the training set in order to classify a single point. If there are N training points in $\mathbb{R}^d$, this takes $O(Nd)$ time.

Fortunately, there are faster methods to perform nearest neighbor look up if we are willing to spend some time preprocessing the training set. `scikit-learn` has fast implementations of two useful nearest neighbor data structures: the *ball tree* and the *k-d tree*.

In [31]:
```
from sklearn.neighbors import BallTree

## Build nearest neighbor structure on training data
t_before = time.time()
ball_tree = BallTree(train_data)
t_after = time.time()

## Compute training time
t_training = t_after - t_before
print("Time to build data structure (seconds): ", t_training)

## Get nearest neighbor predictions on testing data
t_before = time.time()
test_neighbors = np.squeeze(ball_tree.query(test_data, k=1, return_distance=False))
ball_tree_predictions = train_labels[test_neighbors]
t_after = time.time()
```

```
## Compute testing time
t_testing = t_after - t_before
print("Time to classify test set (seconds): ", t_testing)

## Verify that the predictions are the same
print("Ball tree produces same predictions as above? ", np.array_equal(test_predictio
```

```
Time to build data structure (seconds):  0.6670012474060059
Time to classify test set (seconds):  5.663107872009277
Ball tree produces same predictions as above?  True
```

In [32]:

```
from sklearn.neighbors import KDTree

## Build nearest neighbor structure on training data
t_before = time.time()
kd_tree = KDTree(train_data)
t_after = time.time()

## Compute training time
t_training = t_after - t_before
print("Time to build data structure (seconds): ", t_training)

## Get nearest neighbor predictions on testing data
t_before = time.time()
test_neighbors = np.squeeze(kd_tree.query(test_data, k=1, return_distance=False))
kd_tree_predictions = train_labels[test_neighbors]
t_after = time.time()

## Compute testing time
t_testing = t_after - t_before
print("Time to classify test set (seconds): ", t_testing)

## Verify that the predictions are the same
print("KD tree produces same predictions as above? ", np.array_equal(test_predictions,
```

```
Time to build data structure (seconds):  1.1469993591308594
Time to classify test set (seconds):  6.542593240737915
KD tree produces same predictions as above?  True
```