Multinomial Classification: from binary to many classes

What if our targets come from a class C with more than two discrete values ?

$$C = \{c_1, \ldots, c_{\#\mathrm{C}}\}$$

where $||C|| > 2$

This is called *Multinomial Classification*

Some models (e.g. Decision Trees) can handle Multinomial classification directly.

For those that don't, we adapt the approach used for Binary Classification.

Since the target for Classification is Categorical

- we turned the Binary Classification task
- into the task of *predicting the probability* that the example's target is Positive

When the number of classes is greater than 2

- we convert Multinomial Classification into the task of constructing
- turn the task into computing a *probability vector*
$$\hat{\mathbf{y}}^{\mathbf{(i)}}_j = \text{Probability that example } i \text{ is in class } C_j$$
  for each C_j in C
- $\hat{\mathbf{y}}^{\mathbf{(i)}}_j$ is the probability that example i is in class c_j

Aside

In Logistic Regression

- we used a Linear Model for the *score* (logit)
$$s = \Theta^T \mathbf{x}$$
- and used the sigmoid to convert it into a probability
$$\hat{p} = \sigma(\Theta^T \mathbf{x})$$

Our approach for Multinomial Classification will be similar

- predict a *vector* of scores/logits
    - s_j is the score for class c_j
- convert the vector of scores into a *probability vector* $\hat{\mathbf{y}}$
$$\sum_{j=1}^{\#\text{C}} \hat{\mathbf{y}}_j = 1$$

Note that *true* target/label $\mathbf{y}^{(\mathbf{i})}$

- has all the probability mass concentrated at a single class

But *predicted* probability vector $\hat{\mathbf{y}}^{(\mathbf{i})}$

- may have non-zero probabilities at more than one class

So the final step of Multinomial Classification

- usually chooses *one* class c_j as the predicted target/label
- choice is often either of
  - c_k where $\hat{\mathbf{y}}_k$ is largest
$$\underset{k}{\operatorname{argmax}}\, \hat{\mathbf{y}}_k$$
  - sample k from distribution $\hat{\mathbf{y}}$

Multinomial classification using multiple binary classifiers

One versus all

The One versus All (OvA) method creates $||C||$ binary classifiers

- One for each $c \in C$
- The classifier for class c identifies
    - Positive examples as those having target c
    - Negative examples as those having targets other than c

For the binary classifier for class c, let

- $\hat{p}^c(\mathbf{x})$ denote the prediction of example $\mathbf{x}$ being Positive (i.e., class c) made by this binary classifier

We can combine the individual binary predictions into a single probability vector $\hat{\mathbf{y}}$

Note that the sum of probabilities across independent binary classifiers may not equal 1.

We need to normalize the individual probabilities to create the OvA prediction vector

$$\hat{\mathbf{y}}_c(\mathbf{x}) = \frac{\hat{p}^c(\mathbf{x})}{\sum_{c' \in C} \hat{p}^{c'}(\mathbf{x})}$$

That is: it normalizes the probabilities so that they sum to 1 for each example.

Note

We have abused notation by using class c as a subscript of $\hat{\mathbf{y}}, \hat{p}$ rather than the integer j, where c is the j^{th} class in C.

Note that the **binary classifier for each class c has it's own parameters $\mathbf{\Theta}_c$**.

- So the number of parameters in the Θ for the OvA classifier is $||C||$ times as big as the number of parameters for a single classifier.

Let's be clear on the number of coefficients estimated in One versus All:

For the digit classification problem where there are $C = 10$ classes the number of of parameters is *10 times* that of a binary classifier.

Fortunately, `sklearn` hides all of this from you.

What you *should* realize is that $||C||$ models are being fit, each with it's own parameters.

One versus one

The One versus One (OvO) method creates $\frac{||C|| * (||C|| - 1)}{2}$ binary classifiers

- one for each pair c, c' of distinct values in C
- the classifier for pair c, c' identifies
    - Positive examples as those having target c
    - Negative examples as those having targets c'

Essentially, OvO creates a "competition" between pairs of classes for a given example $\mathbf{x}$

- the class that "wins" most often is chosen as the predicted class for the OvO classifier on example $\mathbf{x}$

Softmax

As an alternative to normalizing the individual probabilities of the per-class Binary Classifiers

- we can produce a vector of scores/logits
- normalize the score vector

The Multinomial generalization of Sigmoid is the *Softmax* function

$$\hat{\mathbf{y}}_c(\mathbf{x}) = \frac{\exp(s^c(\mathbf{x}))}{\sum_{c \in C} \exp(s^c(\mathbf{x}))}$$

where $s^c(\mathbf{x})$ is the score predicted by the Binary classifier for class c

By exponentiating the score, the softmax magnifies small differences in scores into larger difference in probability.

To illustrate: suppose we have two relatively close scores s^c, $s^{c'}$ such that

$$\frac{s^c}{s^{c'}} = M \approx 1$$

- If we normalize scores by dividing a score by the sum (across all scores)
    - $\frac{\hat{\mathbf{y}}_c}{\hat{\mathbf{y}}_{c'}} = M$
- If we normalize by softmax
    - $\frac{\hat{\mathbf{y}}_c}{\hat{\mathbf{y}}_{c'}} = \frac{\exp(M \hat{s}_{c'})}{\exp(\hat{s}^{c'})} = \exp(\hat{s}_{c'}(M-1))$

Multinomial classification by generalizing the loss function

We will deal with the loss functions, both for Binary and Multinomial Classification in a separate module.

- For Binary Classification: the loss function is called Binary Cross Entropy
- The generalization of the loss function to Multinomial Classification is called *Cross Entropy*

Multinomial classification example: MNIST digit classifier

Remember the digit classifier using KNN from our introductory lecture ?

We criticized the model as being one of excessive template matching: one template per training example.

We can now use Logistic Regression to obtain a classifier with *many* fewer parameters.

It will also have the benefit of helping us *interpret* **how** the classifier is making its predictions.

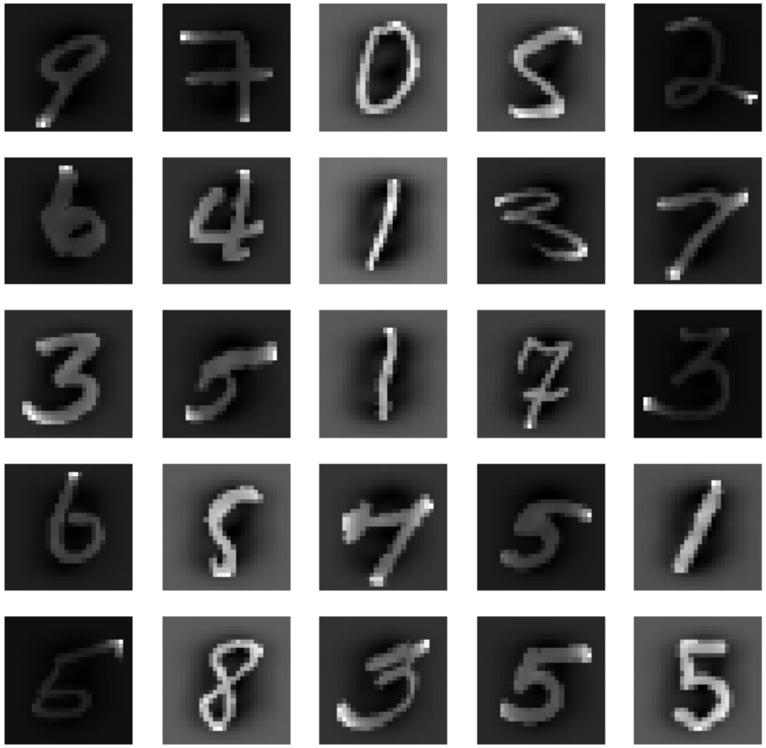
We won't go into interpretation until a later lecture, but for now: a preview of coming attractions.

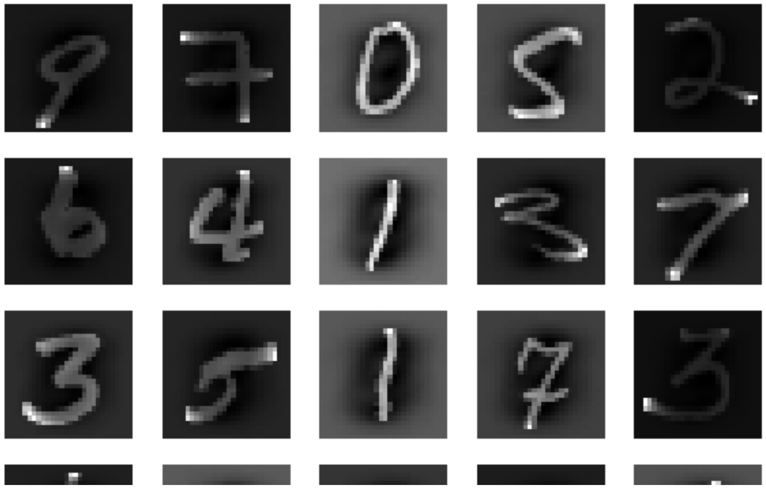
Let's fetch the data and visualize it.

In [5]:
```
mnh.setup()
mnh.visualize()
```

```
Retrieving MNIST_784 from cache
```

Out[5]:





In [6]:

```
print("Training set: X shape={xs}, y shape: {ys}".format(xs=mnh.X_train.shape, ys=mnh.y_train.shape) )
print("Training labels: y is of type {t}".format(t=type(mnh.y_train[0]) ) )
```

```
Training set: X shape=(5000, 784), y shape: (5000,)
Training labels: y is of type <class 'str'>
```

The training set $\mathbf{X}$ consists of 5000 examples, each having 784 features.

The 784 features are pixel intensity values (1=white, 0=black), visualized as a (28×28) image.

Importantly, the labels (targets) are strings, i.e, string "0" rather than integer 0.

$$C = \{" 0 "," 1 ", \ldots ," 9 "\}$$

Let's fit a Logistic Regression model.

In [7]:

```
mnist_lr = mnh.fit()
```

How did we do, i.e., what was the Performance Metric ?

In [8]:

```
clf = mnh.clf
score = clf.score(mnh.X_test, mnh.y_test)

# How many zero coefficients were forced by the penalty ?
sparsity = np.mean(clf.coef_ == 0) * 100

print("Test score with {p} penalty:{s:.2f}".format(p=clf.penalty, s=score) )
print("Sparsity with {p} penalty: {s:.2f}.".format(p=clf.penalty, s=sparsity) )
```

```
Test score with l2 penalty:0.87
Sparsity with l2 penalty: 16.07.
```

We achieved an accuracy on the Test set of about 88%.

Is this good ? We'll probe that question in a later lecture.

For now: it sounds pretty good, but

- In a Test set with equal quantities of each digit
- We could get *all* instances of a single digit wrong and still achieve 90% accuracy !
- **Lesson**: absolute numbers are misleading

Also notice that `LogisticRegression` used an L2 penalty (Ridge Regression)

- That caused about 16% of the parameters to become 0.

How many parameters did we fit (i.e., what is the size of Θ) ?

In [9]:

```
print("The classifier non-intercept parameters shape: {nc};  intercept parameter
s shape: {ni}".format(
    nc=mnh.clf.coef_.shape,
    ni=mnh.clf.intercept_.shape
)
     )
```

```
The classifier non-intercept parameters shape: (10, 784);  intercept parameter
s shape: (10,)
```

`sklearn` separately stores

- the intercept (`clf.intercept_`): the parameter associated with the `const` column in $\mathbf{X}'$)
- all other parameters (`clf.coef_`)

As you can see from the leading dimension (10) there are essentially $||C||$ binary classifiers

- One parameter per element of the feature vector
- Plus one intercept/constant parameter

In total Θ has $10 * (784 + 1) = 7850$ parameters.

More precisely

- The target vector $\mathbf{y}$ is of length $||C|| = 10$, i.e., OHE target
    - We have previously only seen scalar targets
- `LogisticRegression` is performing One versus All (OvA) classification
- Because $||\mathbf{y^{(i)}}|| > 1$, it is using a Cross Entropy Loss in the Loss function

Compare this to the KNN classifier from the first lecture

- one template per example, at $(28 \times 28) = 784$ parameters per example
- times $m = 5000$ examples

So the Logistic Classifier uses about $m = 5000$ times fewer parameters.

What do the 784 non-intercept parameters look like ?

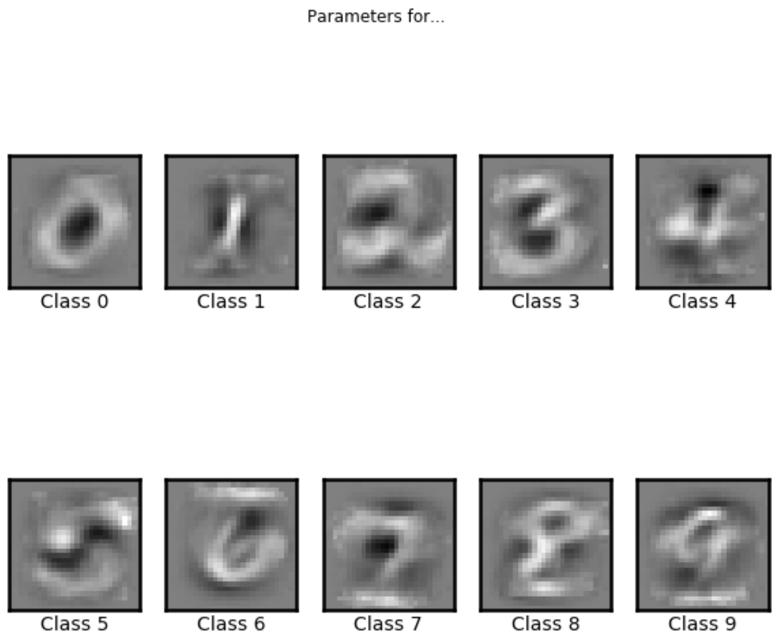
That is: what is the "template" for each class (digit) ?

Since there is one parameter per pixel, ordered in the same way as the input image pixels

- We can display the 784 parameters as a (28×28) image.

Remember: there is one parameter vector (template) for each of the $||C|| = 10$ classes.

In [10]:
```
mnist_fig, mnist_ax = mnh.plot_coeff()
```



Our model learned a template, per digit, which hopefully captures the "essence" of the digit

- Fuzzy, since it needs to match many possible examples of the digit, each written differently

We will "interpret" these coefficients in a subsequent lecture but, for now:

- Dark colored parameters indicate the template for the pixel best matches dark input pixels
- Bright colored parameters indicate the template for the pixel best matches bright input pixels

So the "essence" of an image representing the "1" digit is a vertical band of bright pixels.

TIP The `fetch_mnist_784` routine in the module takes a **long** time to execute. Caching results makes you more productive.

In [11]:
```
print("Done")
```

```
Done
```