Becoming a successful Data Scientist: Error Analysis

As of now, you should know

- how to construct models (the "recipe")
- how to use them for prediction
- some simple metrics on how they perform

In this module, the topics to be covered provide answers:

- model diagnostics

In other words: the importance of Error Analysis in diagnosing and improving models.

Classification: Beyond accuracy

Let's re-run the MNIST problem and examine measures of error more detailed than accuracy

In [5]:

```
mnh = mnist_helper.MNIST_Helper(random_seed=42)
mnh.setup()
_= mnh.fit()
```

```
Retrieving MNIST_784 from cache
```

Examine the score (n.b., ran with L2 penalty)

In [6]:

```
clf = mnh.clf

 # Cross validation
scores = cross_val_score(clf, mnh.X_train, mnh.y_train, cv=10)
print("Avg cross val score={s:3.2f}\n".format( s=scores.mean()) )

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

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

```
Avg cross val score=0.88

Sparsity with l2 penalty: 16.07.
```

We achieved an out of sample accuracy of about 87%

That sounds good, but is it really ?

If each of the 10 labels occurs with equal frequency among the training examples

- We could mis-predict *every* occurrence of a single digit (i.e., 10% of the training examples)
- And still achieve an Accuracy of 90% if we perfectly predict all other digits

Would that be satisfactory ?

This motivates the need to measure *Conditional Performance* or *Conditional Loss*

- Performance/Loss conditioned on meaningful subsets of training examples

We will examine some conditional metrics for the Classification task.

Binary classification: Conditional accuracy

An ideal model would have perfect Accuracy.

In the absence of perfection

- we want to measure accuracy *conditional* on subsets of examples.

For a Binary Classification task, we can partition the examples into a two dimensions

- Row labels: the *predicted* class
- Column labels: the *true* class

	P	**N**
P	TP	FP
N	FN	TN

The correct predictions

- True Positives (TP) are examples predicted as Positive that were in fact Positive
- True Positives (TN) are examples predicted as Negative that were in fact Negative

The incorrect predictions

- False Positives (FP) are examples predicted as Positive that were in fact Negative
- False Positives (FN) are examples predicted as Negative that were in fact Positive

Unconditional Accuracy can thus be written as

$$\mathrm{Accuracy} = \frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \mathrm{FP} + \mathrm{TN} + \mathrm{FN}}$$

We can also define some conditional Accuracy measures

Imbalanced data: the case for conditional accuracy

Conditional Accuracy becomes particularly important

- when the number of Positive and Negative examples in a dataset are quite different
    - Titanic example: many fewer examples with `Survived` than `Not Survived`

This is called *imbalanced* data.

When this occurs, unconditional measures are highly influenced by success on the dominant category

- Titanic example: The Negative examples are almost twice as numerous as the Positive
$$\mathrm{TP} + \mathrm{FN} << \mathrm{TN} + \mathrm{FP}$$

Conditional metrics are one way of placing focus on success in the non-dominant category.

Recall (Sensitivity, True Positive Rate: TPR)

Regardless of whether the Positive class is dominant, we may be interested in how well our model identifies Positive examples.

Recall is a metric Conditioned on Positive examples.

$$\text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

- The fraction of Positive examples (denominator) that were correctly classified
- Also goes by the names: True Positive Rate (TPR), Sensitivity

FN (mis-classified Positive examples) detract from Recall

Why is Recall important ?

Consider a diagnostic test for Covid

- we want to correctly identify Covid positive patients
- even though they are a small fraction of the population
    - hence have a smaller contribution to Unconditional Accuracy than the Negative class

But be careful ! It is easy to achieve 100% Recall.

Degenerate case:

- Always predicting Positive, ignoring all features of the example
    - lots of FP
- Unconditional Accuracy will suffer.
- And FP (Negative patients incorrectly classified as infected) may bear a cost

Specificity

Similarly: we may be interested in knowing how well our model identifies (or mis-identifies) Negative examples.

For example

- we *don't want to mis-label* as Positive, a patient who is truly Covid Negative.

Specificity is a metric conditioned on Negative examples

$$\text{Specificity} = \frac{\text{TN}}{\text{TN} + \text{FP}}$$

- The fraction of Negative examples that were correctly classified
- Also goes by the name: True Negative Rate (TNR)

FP (mis-classified Negative examples) detract from Specificity

A good model (e.g., Covid test) has

- high Recall
    - correctly identifies a large fraction of Positive patients
- high Specificity
    - does not have too many FP (mis-diagnosed Negative patients)
        - who may bear a cost of being mis-diagnosed

False Positive Rate (FPR)

The fraction of Negative examples misclassified as Positive.

$$\begin{aligned}\mathrm{FPR} &= \tfrac{\mathrm{FP}}{\mathrm{FP}+\mathrm{TN}} \\ &= 1 - \mathrm{Specificity}\end{aligned}$$

Precision

Recall seeks to correctly label Positive examples

- degenerate case: label all examples as Positive; achieve 100% Recall

But we would also like to have confidence that our Positive predictions are accurate.

Precision is a metric to tell you the fraction of your Positive predictions that were correct.

$$\text{Precision} = \frac{\text{TP}}{\text{TP} + \text{FP}}$$

FP (mis-classified Negative examples) detract from Precision.

Just like with Recall, it is easy to achieve 100% Precision.

Degenerate case:

- Predict Positive for only a *single example* that is actually Positive
    - Lots of FN
    - Recall will suffer

Precison/Recall Tradeoff

We showed (via degenerate cases) that it was easy to have **either**

- Perfect Recall
- **OR** Perfect Precision

But it may not be possible to have both.

We will

- Show how to trade off one measure for the other
- Discuss when to favor one type of error over another

Some Classification models (e.g., Logistic Regression)

- Use hyper-parameters (e.g., threshold)
- To convert a numerical "score" to a Categorical predicted value

By varying the threshold, we can change predictions to favor a particular Conditional Performance metric.

We will show how this happens and demonstrate ways to evaluate the trade-off between metrics.

Recall our methodology for Classification via Logistic Regression:

- Compute a numerical "score" for our example based on its features
$$\hat{s}^{(\mathbf{i})} = \Theta \cdot \mathbf{x}^{(\mathbf{i})}$$
- Construct a probability distribution (over the target classes) from the scores
$$\hat{\mathbf{p}}^{(\mathbf{i})} = \sigma(\hat{s}^{(\mathbf{i})})$$
- Predict by comparing the probability to a threshold

$$\hat{\mathbf{y}}^{(\mathbf{i})} = \begin{cases} 0 & \text{if } \hat{\mathbf{p}}^{(\mathbf{i})} < 0.5 & \text{Negative} \\ 1 & \text{if } \hat{\mathbf{p}}^{(\mathbf{i})} \geq 0.5 & \text{Positive} \end{cases}$$

We can visualize the step of converting probabilities to predicted class by plotting lines (hyper-planes) of constant score/probability

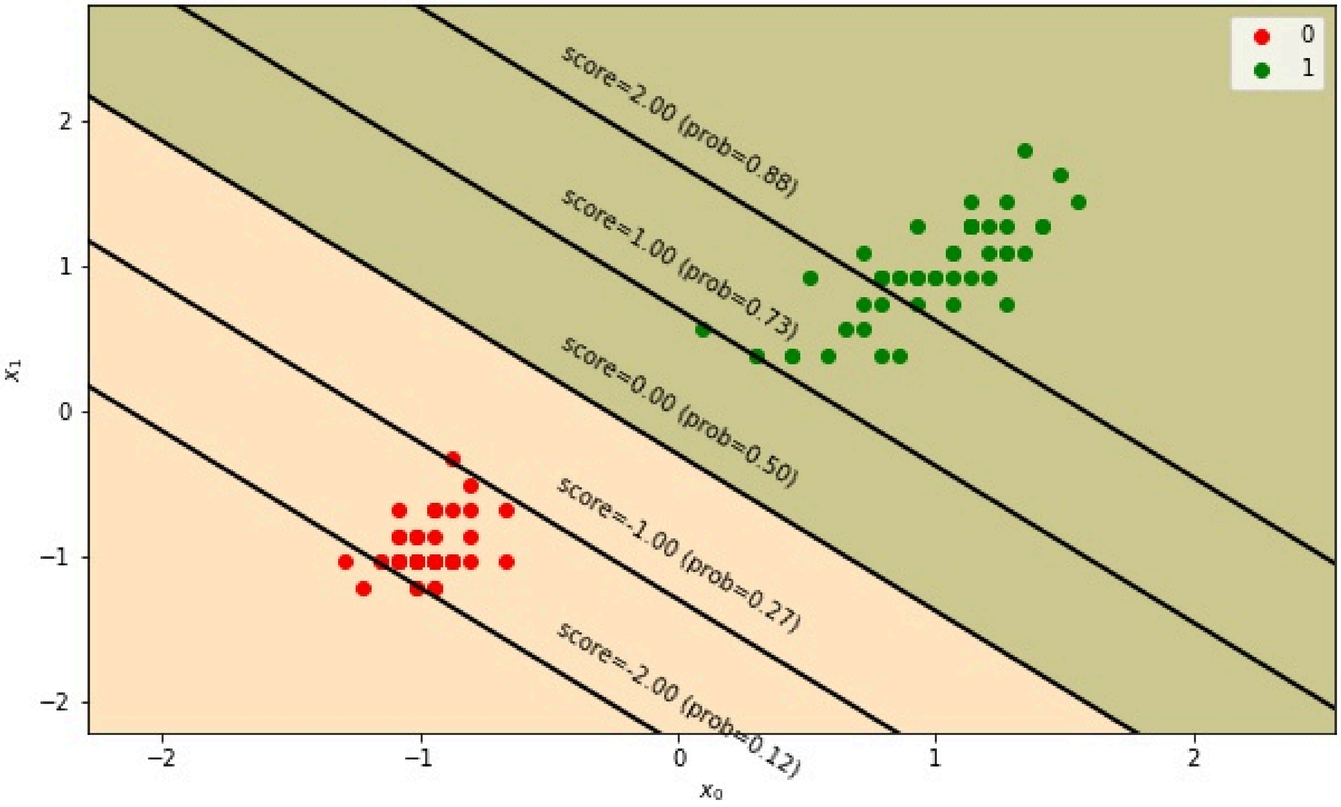
For a given constant value of score or probability:

- Examples above the line are classified as Positive
- Examples below the line are classified as Negative

We can choose **any score/probability** as our decision boundary for prediction.

Let's see what happens as we vary the boundary.

Separation bounday as function of probability threshold



- By choosing the boundary
  $\Theta^T \mathbf{x} = -1 \ \ (\text{resp., prob} = 0.27)$
- Rather than the boundary
  $\Theta^T \mathbf{x} = 0 \ \ (\text{resp., prob} = 0.50)$

we potentially **increase** the number of examples classified as Positive

- Increasing the number of TP $\rightsquigarrow$ Increasing Recall
- But also potentially increasing the number of FP $\rightsquigarrow$ Decreasing Precision

Thus, by varying threshold, we can choose the **trade-off between Recall and Precision**.

For models that rely on a Threshold

- the threshold is a **hyper-parameter**
- that **you can choose**
- in order to achieve some externally-specified objective
    - e.g., high Recall

Precision vs Recall: which one to favor ?

What factors might lead us to favor one metric over the other ?

Consider a diagnostic test whose goal is to classify highly infectious patients as Positive

- High Recall: catch most infected patients
- Low Precision: frighten patients that are misclassified as Positive

You might favor Recall

- When a False Negative has very bad consequences (e.g., lead to an increase in infections in population)

You might favor Precision

- When a False Positive has very bad consequences (e.g., cause a non-infected patient to isolate)

Moving the boundary to increase Positives will naturally decrease Negative predictions.

So we also affect metrics conditioned on Negative (FN, TN), with similar trade-offs.

Precision/Recall trade-off: plot

To be concrete: let's examine the trade-off between Recall and Precision in the context of a binary classifier

- Using MNIST examples: classify an example as being a **single** chosen digit versus the 9 other digits
- Create a binary classifier for a single MNIST digit

In [7]:

```
# Fetch the MNIST data into object

mnh_d = mnist_helper.MNIST_Helper(random_seed=42)
mnh_d.setup()

# Turn the 10 class training set into a binary training set
# - Same examples, different targets
# - targets are now "is 'digit'" or "is not 'digit'" for a single digit
digit = '5'
y_train_d, y_test_d = mnh_d.make_binary(digit)

# Fit a binary model: Is digit/Is not digit
mnh_d.fit(y_train=y_train_d)
scores = cross_val_score(mnh_d.clf, mnh_d.X_train, y_train_d, cv=3, scoring="acc
uracy")

from sklearn.model_selection import cross_val_predict

y_train_pred = cross_val_predict(mnh_d.clf, mnh_d.X_train, y_train_d, cv=5, meth
od="decision_function")
```

```
Retrieving MNIST_784 from cache
```

Out[7]:

▾ LogisticRegression ⓘ ?

(https://scikit-learn.org/1.5/modules/generate

```
LogisticRegression(C=0.01, solver='saga', tol=0.1)
```

Let's plot the trade-off

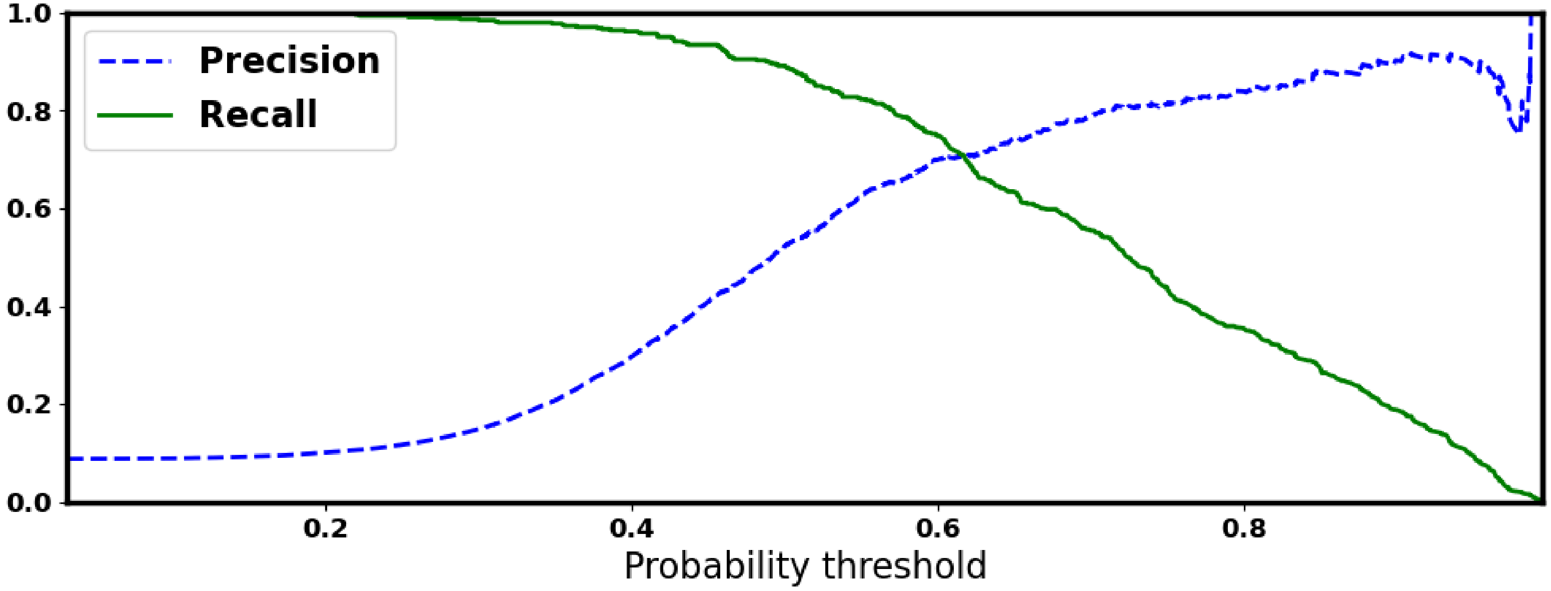
In [8]:

```
from sklearn.metrics import precision_recall_curve

precisions, recalls, thresholds = precision_recall_curve(y_train_d, y_train_pred)

# Convert thresholds (log odds) to probability
probs = np.exp(thresholds)/(1+np.exp(thresholds))

def plot_precision_recall_vs_threshold(precisions, recalls, thresholds, probs=None):
    fig, ax = plt.subplots(1,1, figsize=(12,4))

    if probs is None:
        horiz = thresholds
        label = "Threshold"
    else:
        horiz = probs
        label = "Probability threshold"
    _ = ax.plot(horiz, precisions[:-1], "b--", label="Precision", linewidth=2)
    _ = ax.plot(horiz, recalls[:-1], "g-", label="Recall", linewidth=2)
    _ = ax.set_xlabel(label, fontsize=16)
    _ = ax.legend(loc="upper left", fontsize=16)
    _ = ax.set_ylim([0, 1])

    _ = ax.set_xlim([ horiz.min(), horiz.max()])

    return fig, ax

fig, ax = plot_precision_recall_vs_threshold(precisions, recalls, thresholds, probs=probs)
plt.close(fig)
```

In [9]:

```
fig
```

Out[9]:


1.0
0.8
0.6
0.4
0.2
0.0
0.2
0.4
0.6
0.8
Probability threshold
Precision
Recall

You can see how varying the threshold affects Recall and Precision

- One at the expense of the other

ROC/AUC: Evaluating the Precision/Recall tradeoff

There is another common tool used to evaluate the trade-off between competing metrics.

The **ROC** is a plot of True Positive Rate (TPR) versus the False Positive Rate (FPR) as we vary the threshold.

- each point in the plot corresponds to a particular threshold
- the TPR and FPR is measured for that threshold

Our goal is to choose a threshold (corresponding to a point on the curve)

- With the highest True Positive Rate (TPR)
    - i.e., Recall
    - fraction of correctly classified Positives
- With the smallest *acceptable* False Positive Rate (FPR)
    - fraction of negatives that are misclassified as Positive
    - larger FPR means *worse* Precision

We illustrate by showing the ROC/AUC curve for three different classifiers on the MNIST digit recognition problem.

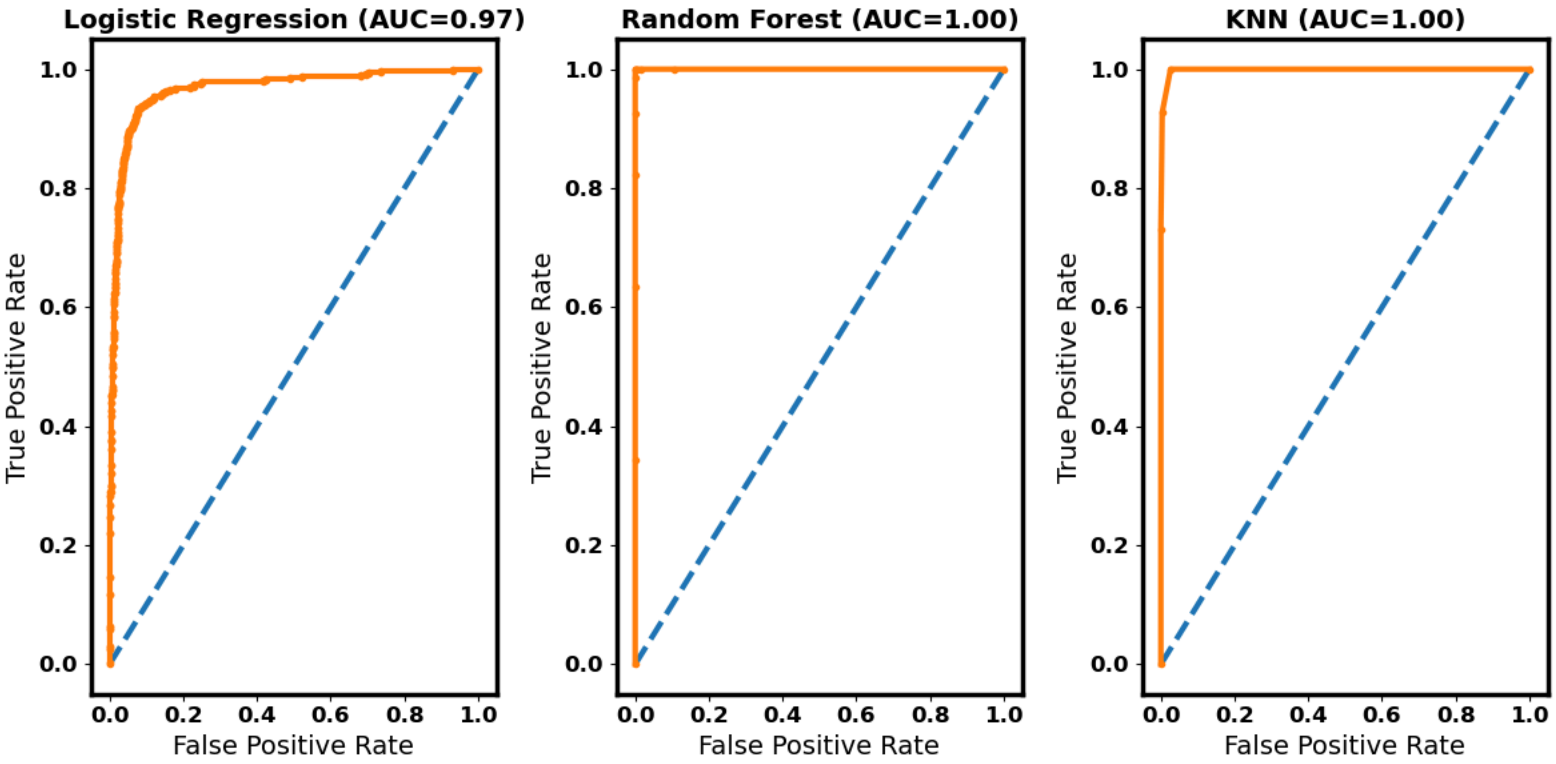
- Logistic Regression
- KNN
- Random Forests

We vary the threshold

- translate the result into TPR and FPR
    - plot
- a point on the curve corresponds to one value of the threshold

In [10]:

```
# ROC curves for binary classifier: Is Digit/Is not Digit
clh.AUC_plot(X_train=mnh.X_train, y_train=y_train_d, X_test=mnh.X_train, y_test=
y_train_d)
```



The "ideal" curve would resemble an inverted "L"

- With a top, horizontal line near a TPR of 1
- That rises vertically from a FPR of near 0

That would imply that there is a choice of threshold with low FPR and high TPR.

You decide which threshold produces an acceptable trade-off

But you can also compare the curves across models

- A model whose curve is closer to the inverted "L" shape has a better trade-off
- We can measure this by the *Area Under the Curve* (AUC) of the model
    - Higher AUC gets us closer to the ideal
- The model whose curve has highest AUC might be the model of choice.

Note on the mechanics of plotting the ROC/AUC

To produce the ROC/AUC curve

- Fit a binary classifier
- For each possible value of the threshold
    - Predict using this threshold
    - Evaluate the TPR and FPR
    - This gives a single point on the curve

Fortunately: most ML toolkits will implement this process for you

- But the principle of "there is no magic" means that you should always understand what is happening

F_1: Another way to combine Precision and Recall

There another metric call the F_1 which expresses the trade-off between Precision and Recall as a single number:

$$\mathrm{F}_1 = \frac{\mathrm{TP}}{\mathrm{TP} + \frac{\mathrm{FN}+\mathrm{FP}}{2}}$$

Multinomial classification: Confusion matrix

So far we have been dealing with a classifier with only two classes.

So the simple grid

$$\begin{array}{lll} & \mathbf{P} & \mathbf{N} \\ \mathbf{P} & \mathrm{TP} & \mathrm{FP} \\ \mathbf{N} & \mathrm{FN} & \mathrm{TN} \end{array}$$

was sufficient.

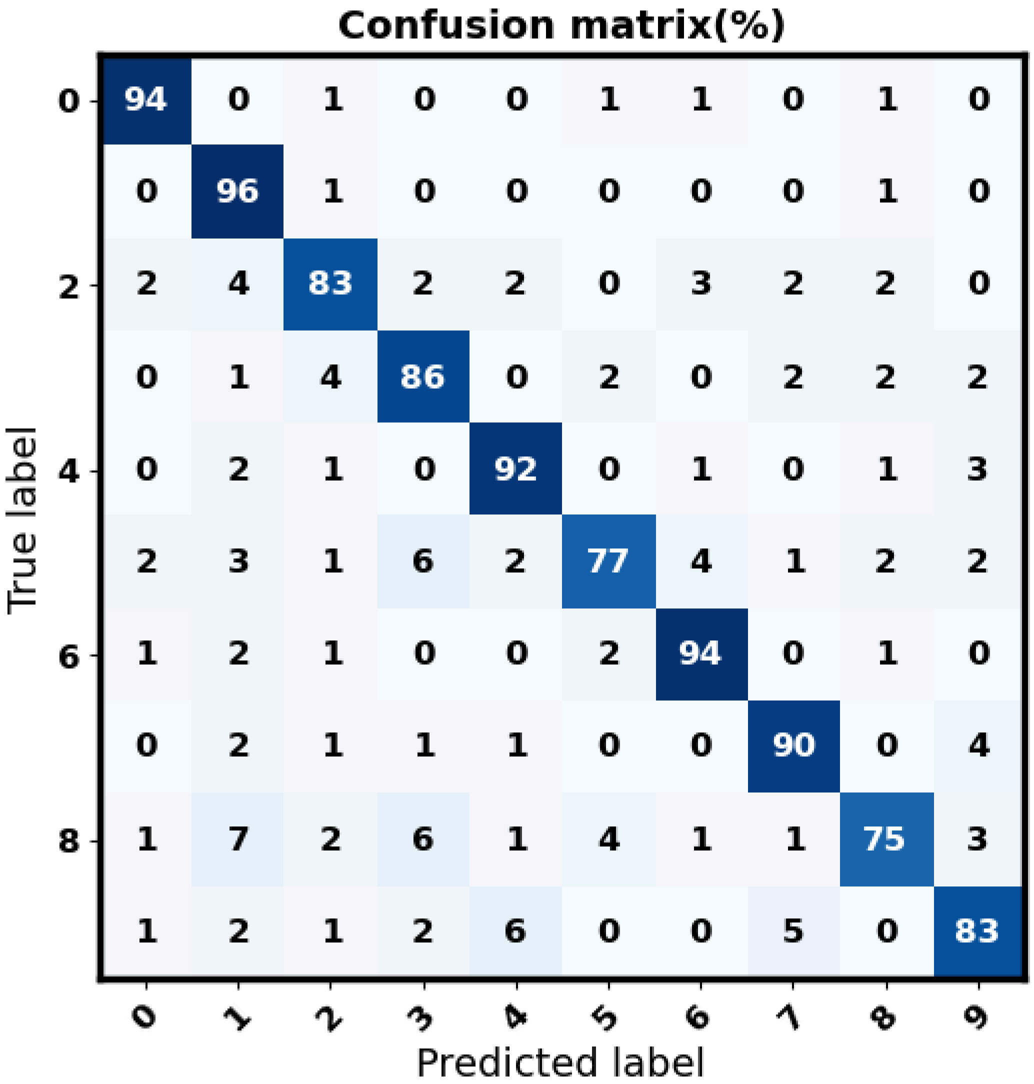
The generalization of the grid to multiple classes is called the *Confusion Matrix*

Here is the Confusion Matrix for a classifier on the task of predicting which of 10 digits is represented by an image (MNIST digit recognition)

In [11]:

```
# Now predict the value of the digit on the second half:
fig, ax = plt.subplots(figsize=(12,6))
confusion_mat = mnh.create_confusion_matrix()

digits = range(0,10)
_= clh.plot_confusion_matrix(confusion_mat, digits, ax=ax, normalize=True)
```

```
Normalized confusion matrix
```



	0	1	2	3	4	5	6	7	8	9
0	94	0	1	0	0	1	1	0	1	0
	0	96	1	0	0	0	0	0	1	0
2	2	4	83	2	2	0	3	2	2	0
	0	1	4	86	0	2	0	2	2	2
4	0	2	1	0	92	0	1	0	1	3
	2	3	1	6	2	77	4	1	2	2
6	1	2	1	0	0	2	94	0	1	0
	0	2	1	1	1	0	0	90	0	4
8	1	7	2	6	1	4	1	1	75	3
	1	2	1	2	6	0	0	5	0	83

The entry in the matrix for row i, column j

- **Percentage** of examples for true digit i that were predicted as digit j.

The diagonal of the Confusion Matrix is the Recall for each digit/

The non-diagonal elements of a row show how often a given digit was mistaken for another.

Confusion warning

Our Binary Confusion matrix has True label and Predicted label axes swapped

- Predicted label as row label
- our plot is consistent with `sklearn`'s `ConfusionMatrixDisplay`
- Row labels: the *true* class
- Column labels: the *predicted* class

The confusion matrix for MNIST digit recognition tells us that our classifier

- Does a great job (90+% correct) on images corresponding to digits 0,1,6
- Is struggling ($< 80\%$ correct) on images of the digits 5, 8
    - Mis-classifying them as "3" most often

Studying the Confusion Matrix in depth can help you

- Diagnose the weaknesses in your model
- And *perhaps take steps to compensate* for them (improve the model)
- By analyzing the examples belonging to the subset corresponding to non-diagonal entries

This is the true power of Error Analysis !

- Having a process and the tools to diagnose mis-prediction will make you more successful !
- That is why we emphasize the importance of the Error Analysis step of the Recipe

We will perform this analysis *in code* for the MNIST digit classifier shortly.

Return to parent notebook

Regression: beyond RMSE/R^2

What is the process of diagnosing errors for the Regression task ?

Answer: Examining the residuals.

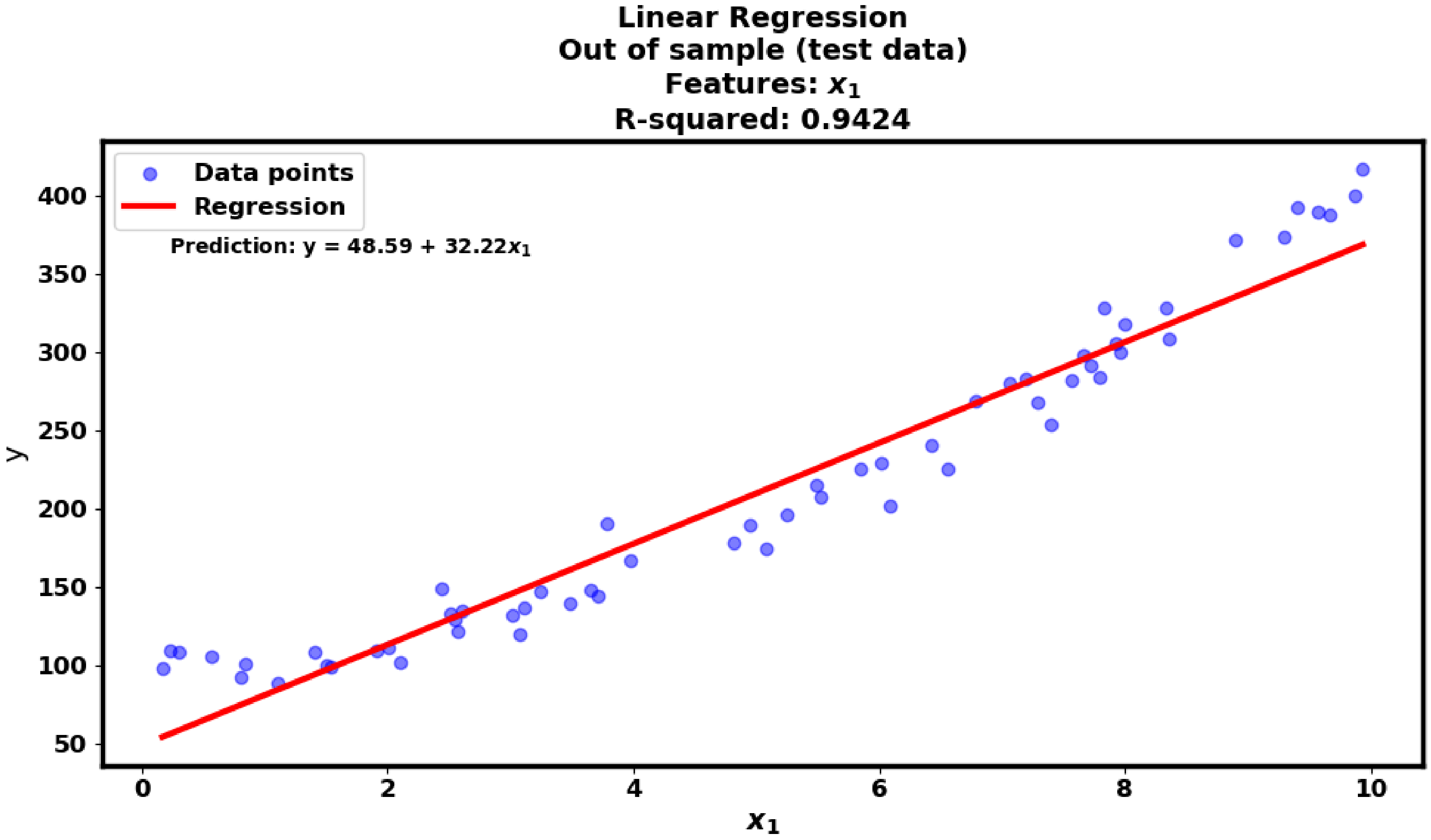
- the difference $\mathbf{y}^{(\mathbf{i})} - \hat{\mathbf{y}}^{(\mathbf{i})}$

Recall our first attempt at Linear Regression

- where we systematically *under-predicted* (positive residuals) the Target
- for low and high values of the single feature $\mathbf{x}_1$

```
In [14]: fig_x1
```

```
Out[14]:
```



Our Error Analysis

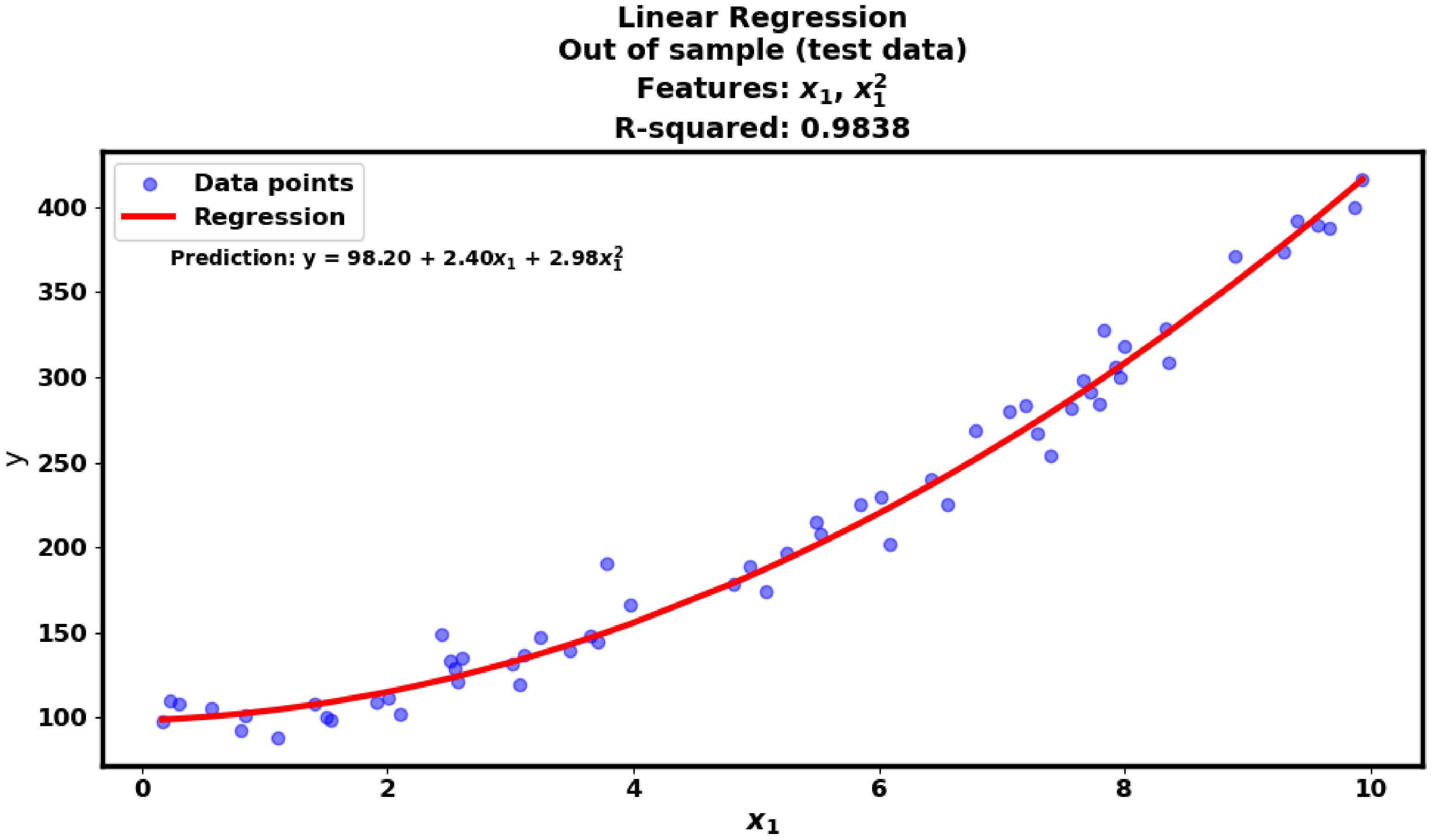
- observing the systematic mispricing

led us to improve the model

- by adding a second feature $\mathbf{x}_1^2$

```
In [15]: fig_x1_x1sq
```

```
Out[15]:
```



Linear Regression
Out of sample (test data)
Features: x_1, x_1^2
R-squared: 0.9838

In [16]:

```
print("Done")
```

```
Done
```