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 Aanalysis 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 [15]:

```
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]:

```python
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.

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Binary classification: Conditional accuracy

To review:

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

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

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

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

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

We can also define some conditional Accuracy measures

Imbalanced data: the case for conditional accuracy

It is quite possible that the number of Positive and Negative examples in a dataset are quite different

- Titanic example: many fewer examples with `Survived` than `Not Survived`

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

$$\text{TP} + \text{FN} << \text{TN} + \text{FP}$$

Conditional metrics are one way of placing focus on success in the minority category.

Recall

Conditioned on Positive examples.

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

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

Degenerate case:

- You can achieve 100% Recall by always predicting Positive
- But Unconditional Accuracy will suffer.

Specificity

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)

Precision

A metric to tell you the fraction of your Positive predictions that were correct.

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

Degenerate case:

- You can achieve 100% Precision: Predict Positive for only a *single example* that is actually Positive
- But you fail to correctly predict all other Positive examples

False Positive Rate (FPR)

The fraction of Negative examples misclassified as Positive.

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

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Precison/Recall Tradeoff

Ideally, we would like our model to have both

- High Recall: correctly identify a large fraction of Positive examples
- High Precision: do not mis-identify too many Negative examples as positive

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 hyperparamters (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 tradeoff between metrics.

Recall our methodology for Classification via Logistic Regression:

- Compute a numerical "score" for our example based on its features
$$\hat{s}^{(\mathbf{i})} = \mathbf{\Theta} \cdot \mathbf{x}^{(\mathbf{i})}$$

- Construct a probability distribution (over the target classes) from the scores
$$\hat{p}^{(\mathbf{i})} = \sigma(\hat{s}^{(\mathbf{i})})$$

- Predict by comparing the probability to a threshhold

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

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

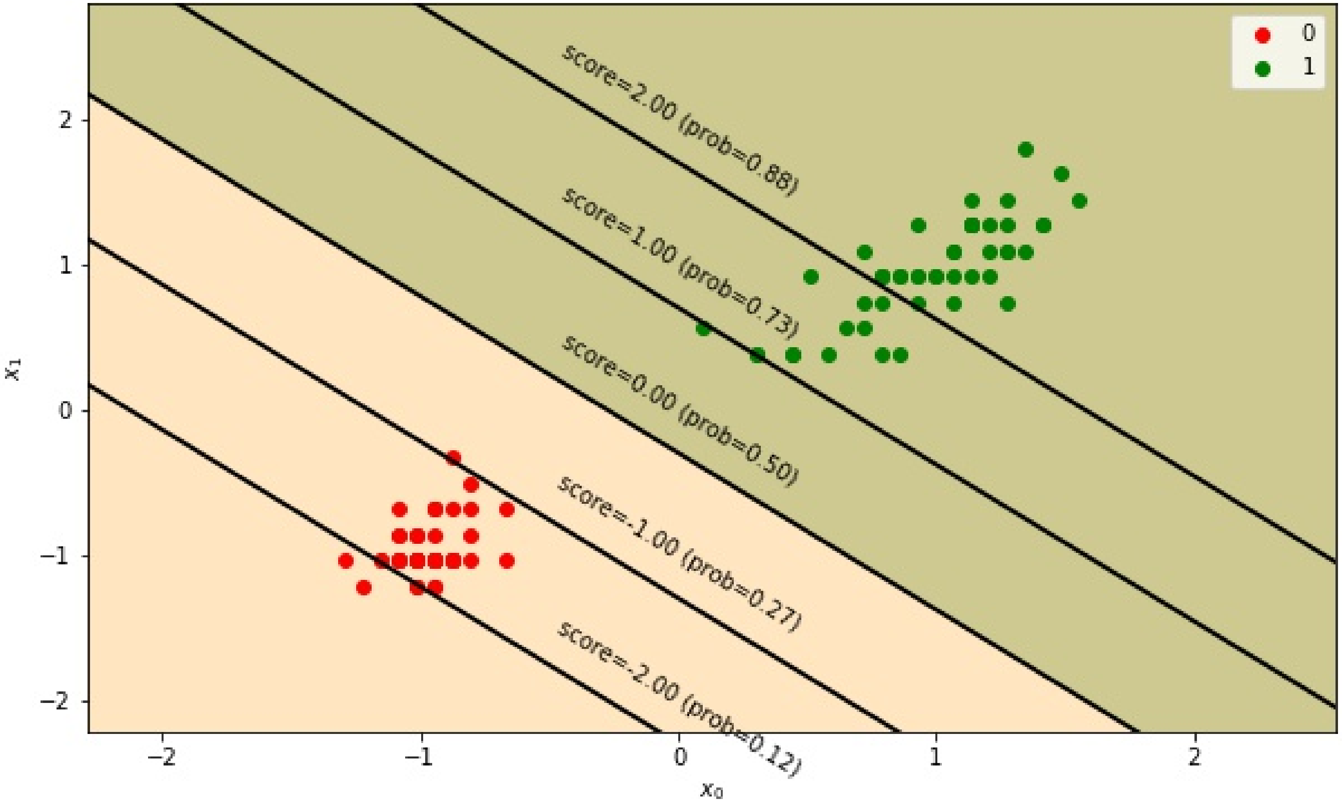
For a given constant value of score or probability:

- 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/center>



- 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 **tradeoff between Recall and Precision**.

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 tradeoffs.

Precision/Recall tradeoff: plot

To be concrete: let's examine the tradeoff 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(C=0.01, class_weight=None, dual=False, fit_intercept=True,
                   intercept_scaling=1, l1_ratio=None, max_iter=100,
                   multi_class='multinomial', n_jobs=None, penalty='l2',
                   random_state=None, solver='saga', tol=0.1, verbose=0,
                   warm_start=False)
```

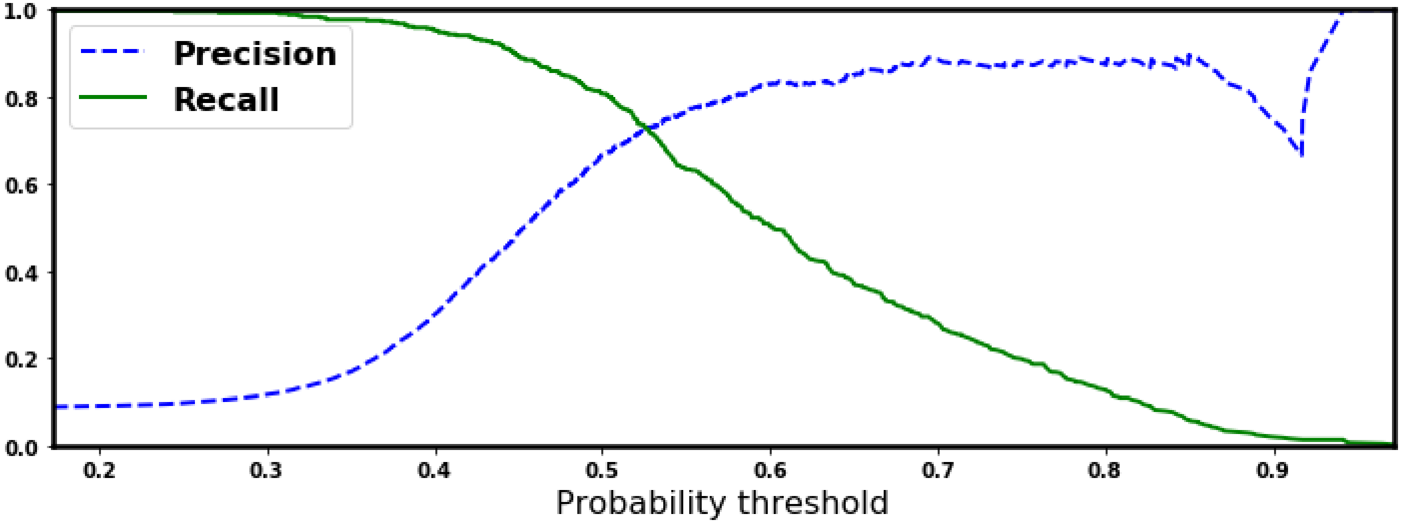
Let's plot the tradeoff

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=No
ne):
    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, pr
obs=probs)
plt.close(fig)
```

In [9]:
```
fig
```

Out[9]:


Precision
Recall
1.0
0.8
0.6
0.4
0.2
0.0
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
Probability threshold

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 tradeoff between competing metrics.

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

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

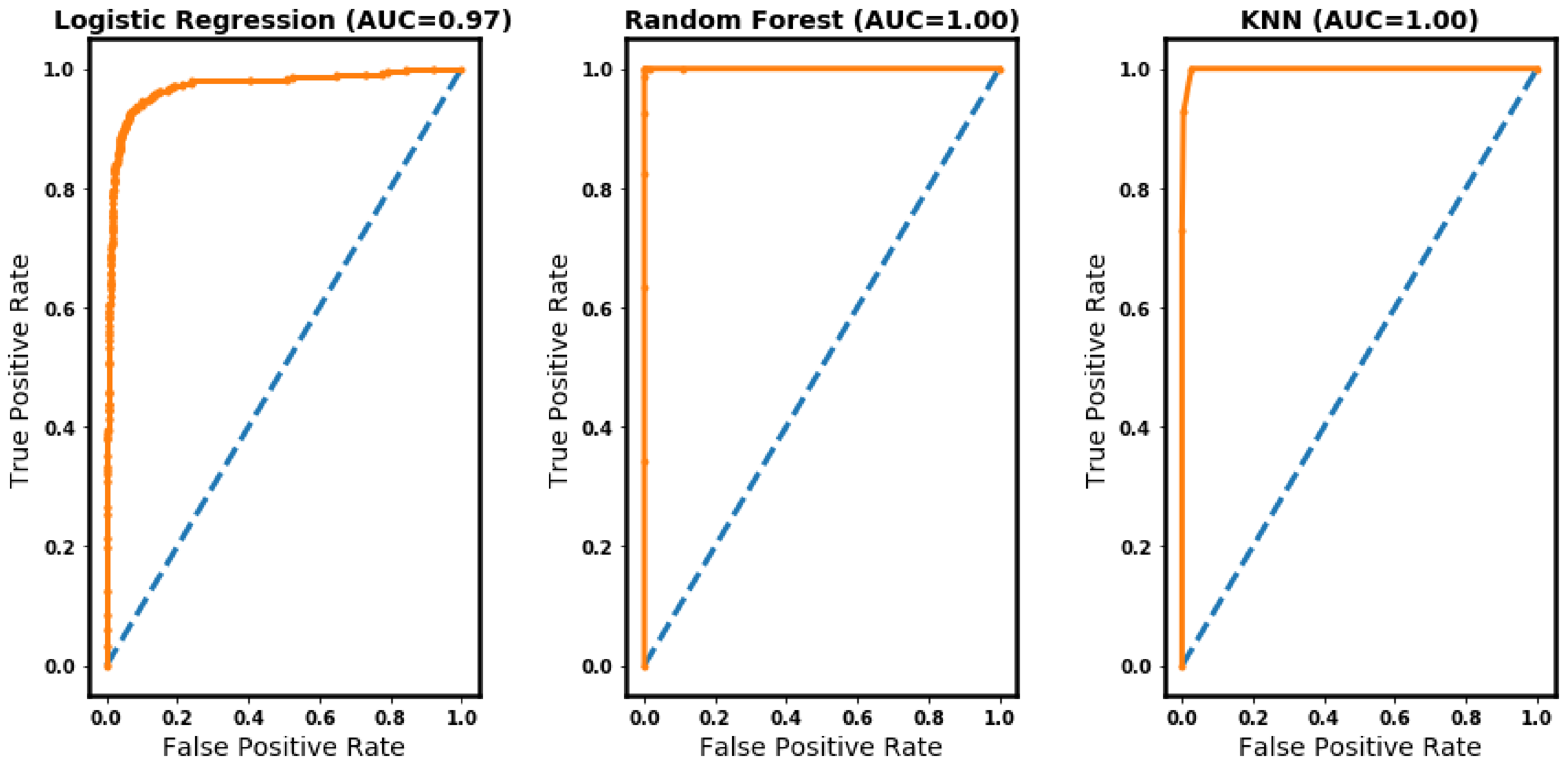
- With the highest True Positive Rate (TPR): fraction of correctly classified Positives
- With the smallest *acceptable* False Positive Rate (FPR): fraction of negatives that are misclassified as Positve

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

- Logistic Regression
- KNN
- Random Forests

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 tradeoff

But you can also compare the curves across models

- A model whose curve is closer to the inverted "L" shape has a better tradeoff
- 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 tradeoff between Precision and Recall as a single number:

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

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Multinomial classification: Confusion matrix

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

So the simple grid

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

was sufficient.

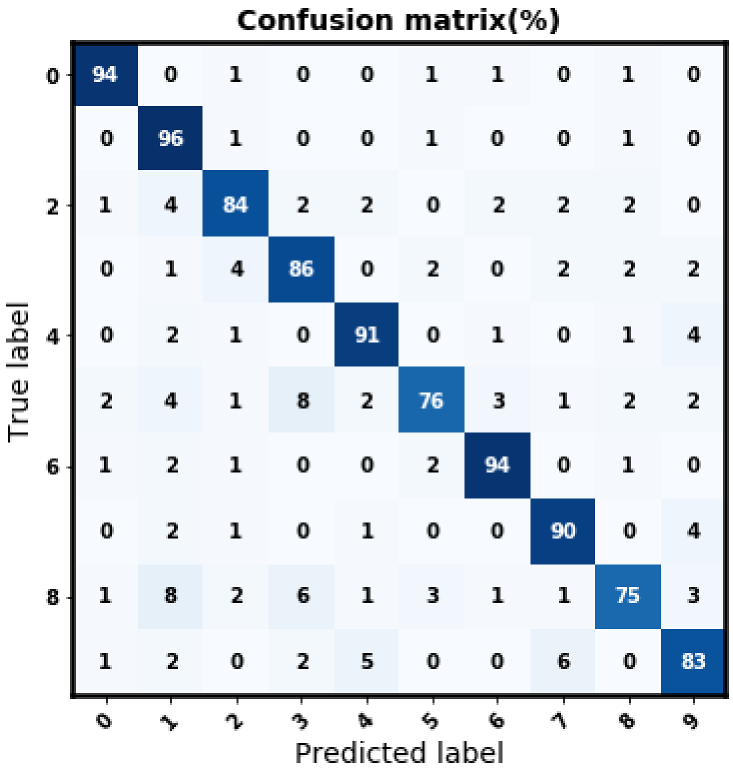
The generalization of the grid to multiple classes is called the *Confusion Matrix*

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 [18]:
```python
# 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
```



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

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.

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

- Does a great job (97% correct) on images corresponding to digits 0,1
- 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.

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Regression: beyond RMSE/R^2

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

Answer: Examining the residuals.

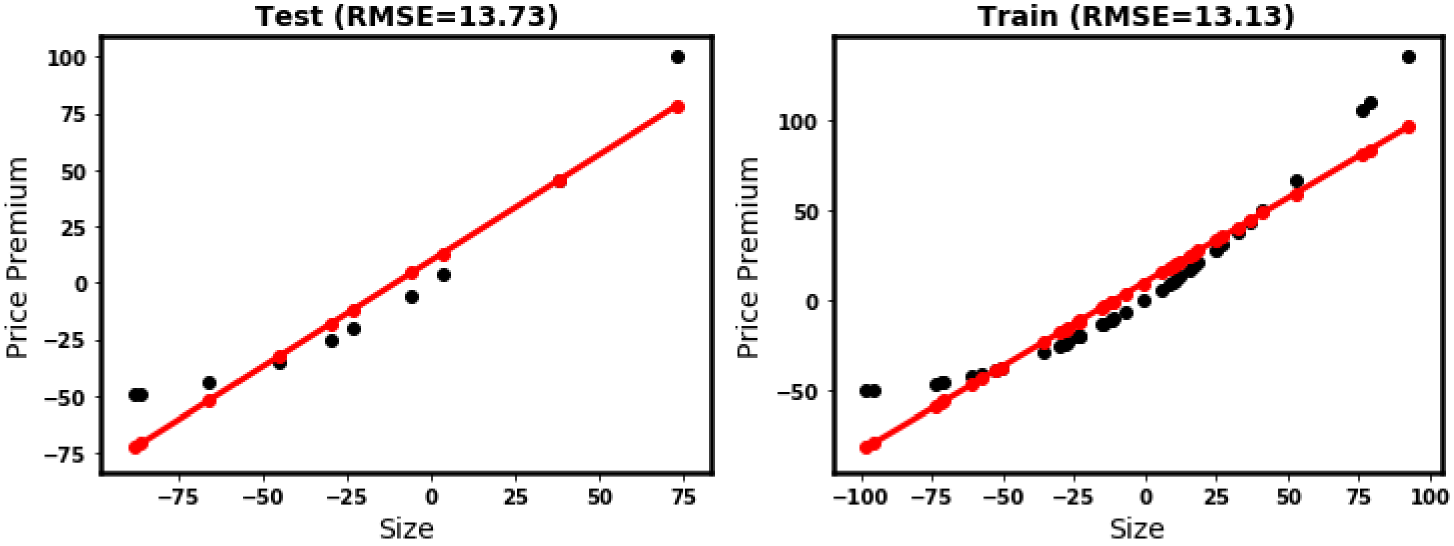
We illustrate that by examining the errors for one of our first models

- Using Linear Regression with the single, raw feature (Size) to fit the "curvy" dataset of Price Premium

In [12]:
```
v1, a1 = 1, .005
v2, a2 = v1, a1*2
curv = recipe_helper.Recipe_Helper(v = v2, a = a2)
X_curve, y_curve = curv.gen_data(num=50)

(xlabel, ylabel) = ("Size", "Price Premium")

figp, axp = curv.gen_plot(X_curve,y_curve, xlabel, ylabel)

fig, axs = curv.regress_with_error(X_curve, y_curve, xlabel=xlabel, ylabel=ylabe
l)
plt.close(fig)
```

```
Coefficients:
 [9.86448852] [[0.93673892]]


R-squared (test): 0.91
Root Mean squared error (test): 13.73


R-squared (train): 0.91
Root Mean squared error (train): 13.13
```

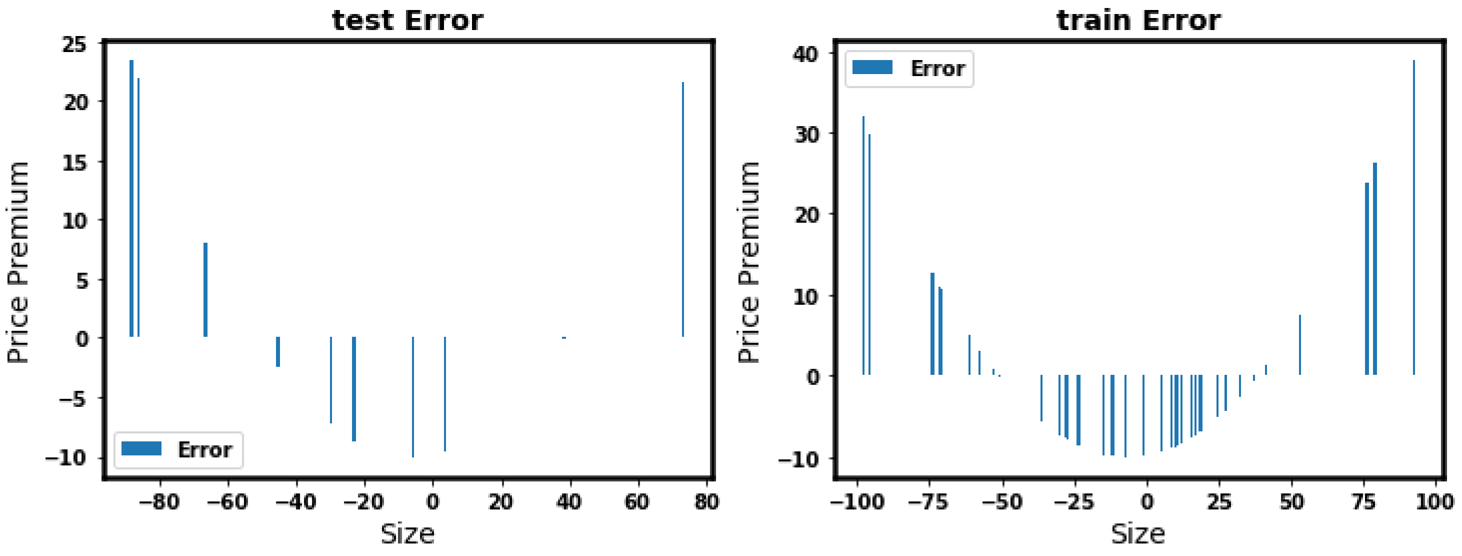

125


Test (RMSE=13.73)
Train (RMSE=13.13)
Price Premium
Size

Let's focus on the Test errors (which are the *residuals*: difference between predicted and true targets)

```
In [13]: fig
```

Out[13]:



Not good !

- There is a clear pattern to the errors:
    - Positive mis-prediction for extreme values of the single feature (Size)
    - Negative mis-prediction for central values of the single feature
- Non-constant variance
    - Absolute value of the errors at the extremes are larger

Let's consider the business implication of this pattern

- We *overprice* extremely large and extremely small homes
- We *underprice* homes of a more common size

This systematic mispricing may drive away customers !

A new feature (Size squared)

- Is large for extreme values of the Size feature
- Is small for central values of the feature

That is: it has the same pattern as the residuals of the single-feature model.

So adding it as a new synthetic feature "predicts" the residuals and thus result in a two-feature model with *smaller* residuals

Once we added that term, we saw that the target was fit well by the model

$$\hat{\mathbf{y}} = \beta_0 + \beta_1 * \mathbf{x} + \beta_2 * \mathbf{x}^2$$

In [14]:

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

Done