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 [5]:

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

```
Retrieving MNIST_784 from cache
```

Out[5]:

```
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)
```

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=0.87

Sparsity with l2 penalty: 16.20.
```

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

For simplicity: let's begin with a Classification task with only two classes (Positive and Negative).

We can divide overall Accuracy into 4 subsets:

- the row labels correspond to the predicted class
- the column labels correspond to the target (actual) 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 test examples predicted as Positive that were in fact Positive
- True Positives (TN) are test examples predicted as Negative that were in fact Negative

The incorrect predictions

- False Positives (FP) are test examples predicted as Positive that were in fact Negative
- False Positives (FN) are test 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 Survive than Not Survive

Metrics based on unconditional accuracy favor the dominant category (the one with most examples).

- They are more numerous and hence have greater cumulative influence

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

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

Recall

- Conditioned on Positive test examples

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

- The fraction of Positive examples that were correctly classified
- You can achieve 100% Recall by always predicting positive, but Unconditional Accuracy will suffer.
- Also goes by the names: True Positive Rate (TPR), Sensitivity

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.

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

There is a degenerate case of perfect precision:

- predict "Positive" for only a single, known actual positive
- 100% precision, but you fail to correctly predict most actual positives

False Positive Rate

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

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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) have hyperparameters that compare numerical "scores" to a threshold in order to make a prediction.

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 "score" that our example is in each of the target classes
- Construct a probability distribution (over the target classes) from the scores
  - convert the per class score into a probability via the sigmoid/softmax function
- Compare the probability to a threshhold

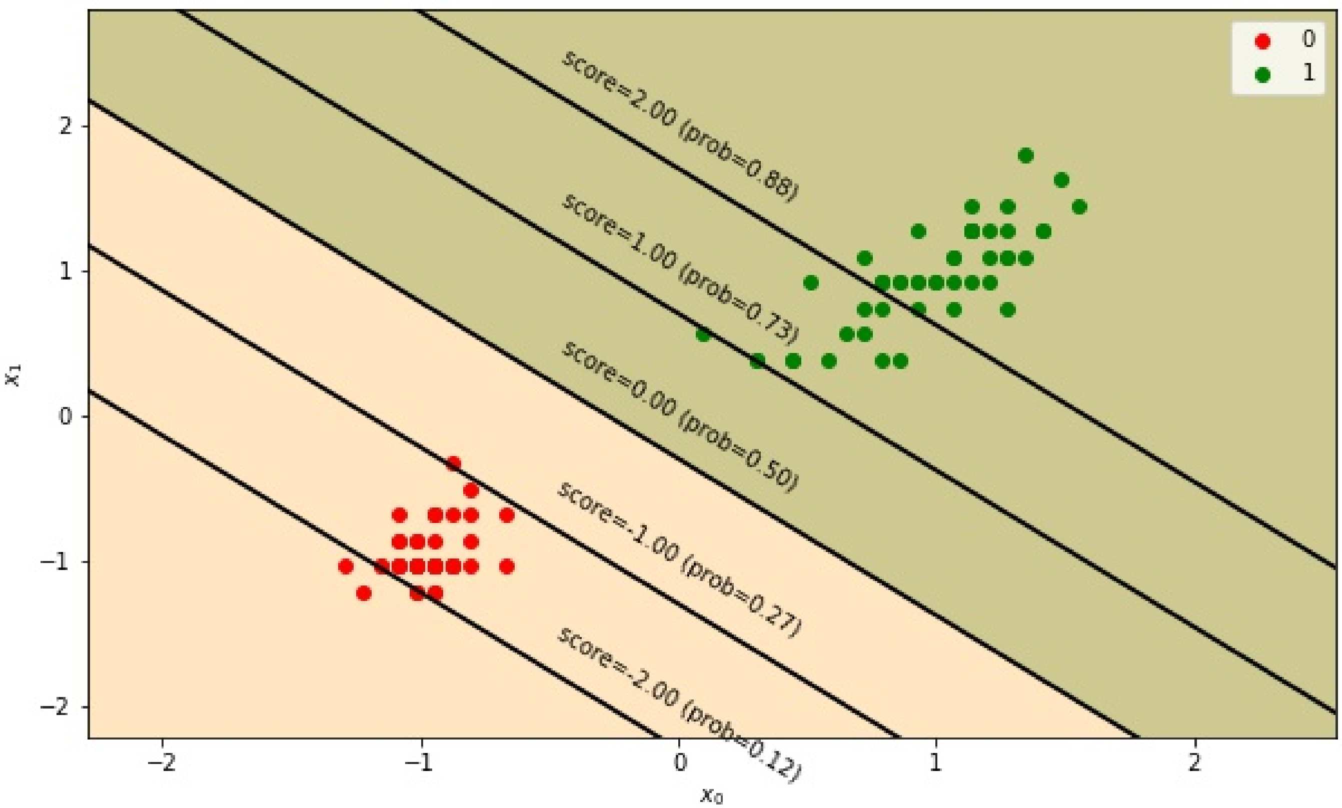
$$\hat{p} = \sigma(\Theta^T \mathbf{x})$$

where σ, the *logistic function*, is:

Convert $\hat{p}^{(\mathbf{i})}$ into Classification prediction $\hat{y}^{(\mathbf{i})}$

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

Separation bounday as function of probability threshold



We can affect the prediction of Positive/Negative by varying the choice of Threshhold.

We can increase the number of Positive predictions by lowering the threshhold

- this will increase TP
    - increase Recall by increasing numerator
    - degenerate case: *always* predict Positive !
- but also increase FP
    - no effect on Recall (FP *does not* appear in denominator)
    - which decreases Precision (where FP *does* appear in the denominator)

So there is a tradeoff between Recall and Precision that is determine by our choice of threshold.

Precision vs Recall: which one to favor ?

- Depending on the context, you may favor Precision over Recall, or vice-versa:
    - Favor Precision when a False Positive is undesirable
        - FP: mistakenly tell someone they are in trouble
    - Favor Recall when False Negative is undesirable
        - FN: mistakenly fail to identify a highly-communicable disease

Why would we want to increase Recall (at the potential cost of decreased unconditional Accuracy) ?

It depends on your task.

Consider a diagnostic test for an extremely dangerous, infectious disease

- It might very important to have high Recall (catch truly infected patients)
- Even at the expense of incorrectly labelling some healthy patients as infected

By *decreasing* the threshold we increase the number of Positive predictions

- Recall increases (by increasing TP)
- Precision decreases (by increasing FP)

By *raising* the threshhold, we can decrease the number of Positive predictions.

- Potentially decrease Recall (by decreasing TP)
- Increase Precision (by decreasing FP)

Decreasing the number of Positive predictions increases the number of Negatives

- Complementary effect on the Negative counterparts of the Positive metrics (Recall:Specificity)
- Increase Specificity (by decreasing FP, we increase TN)

Why would we want to increase Specificity (potentially decreasing unconditional Accuracy) ?

- decrease Unconditional Accuracy by increasing the False Negatives (FN)

Consider a diagnostic test for a mild, non-infectious disease

- A Positive prediction might entail an expensive/painful remedy, which we want to avoid
- Even at the expense of incorrectly labelling some non-healthy patients as healthy

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]:

```python
# Fetch the MNIST data into object

mnh_d = mnist_helper.MNIST_Helper()
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="accuracy")

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, method="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

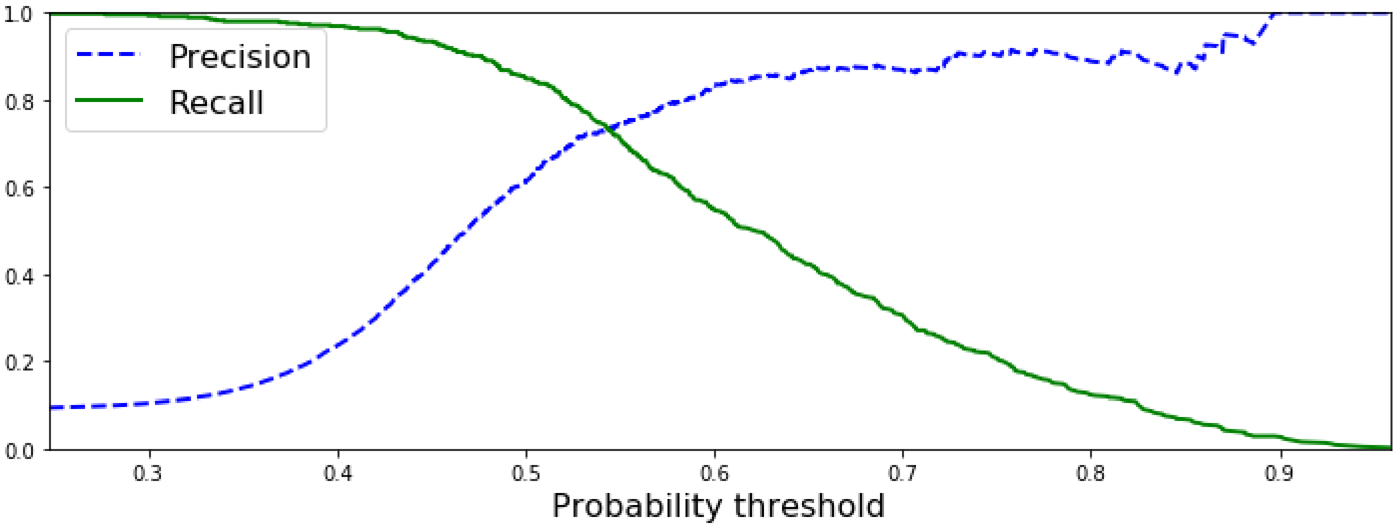
In [8]:

```
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]:



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

You can see how varying the threshold (units is log odds ?) affects Recall and Precision

- one at the expense of the other

ROC/AUC: Evaluating the Precision/Recall tradeoff

The **ROC** plots the True Positive Rate (TPR) versus the False Positive Rate (FPR).

The resulting curve helps us choose a threshold.

Our goal is to get a high TPR with a low FPR.

This corresponds to the Area Under the Curve being as high as possible, as we will see in the plots.

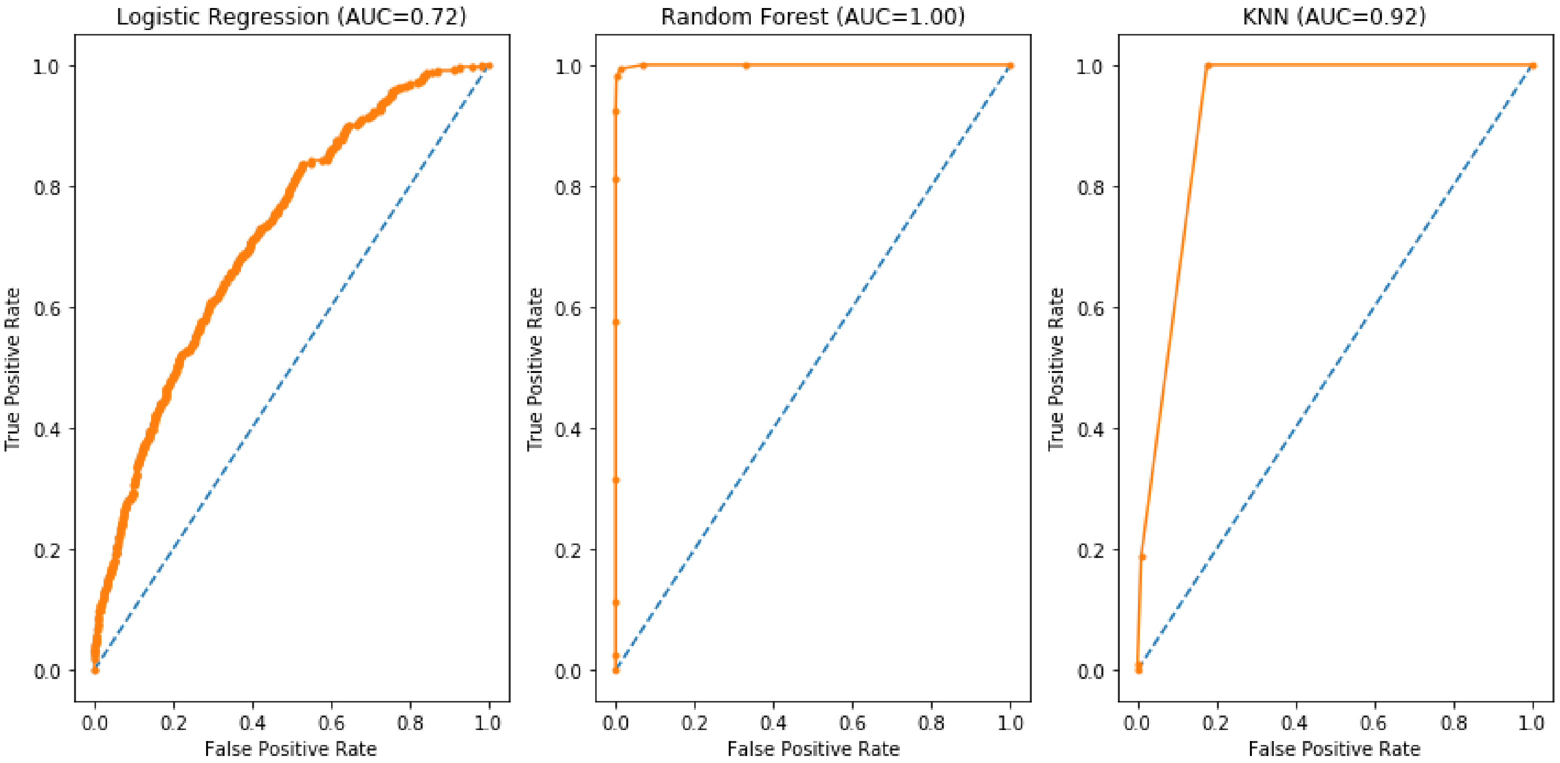
Here's how it works

- fit a binary classifier
- predict on a dataset (e.g., test)
    - this gives a vector of probabilities for each example
    - classifier predicts Positive if corresponding probability exceeds a threshold
- vary the threshold between 0 and 1
    - each threshold value gives a TPR and FPR

We illustrate with a couple of classifiers for the binary MNIST digit classification problem.

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)
```



You can see the results of

- Logistic Regression
- KNN
- Random Forests

$\boldsymbol{F_1}$: Another way to combine Precision and Recall

There is a simple metric to combine Precision and Recall into 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

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

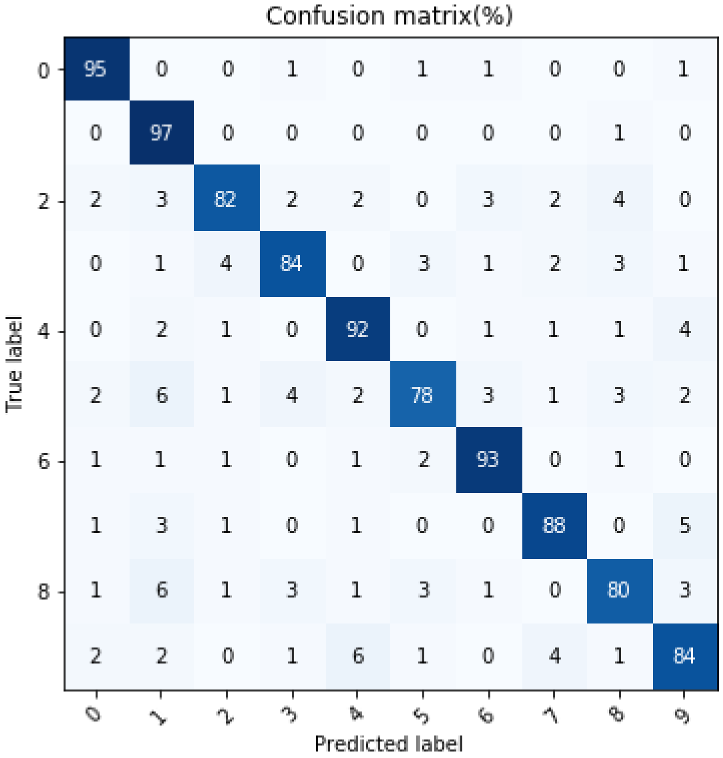
was sufficient.

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

```
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	95	0	0	1	0	1	1	0	0	1
	0	97	0	0	0	0	0	0	1	0
2	2	3	82	2	2	0	3	2	4	0
	0	1	4	84	0	3	1	2	3	1
4	0	2	1	0	92	0	1	1	1	4
	2	6	1	4	2	78	3	1	3	2
6	1	1	1	0	1	2	93	0	1	0
	1	3	1	0	1	0	0	88	0	5
8	1	6	1	3	1	3	1	0	80	3
	2	2	0	1	6	1	0	4	1	84

- The row labels are the (correct) targets
- The column labels are the predictions

The entry in the matrix for row i, column j

- fraction of test examples for class i that were predicted as class 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

By analyzing the non-diagnonal elements of a row, we may be able to diagnose (and correct) defficiencies in our model.

From the confusion matrix:

- our classifier is doing a great job recognizing the digit 0
- our classifier is struggling to recognize the digit 5
    - most often confusing it with the digit 3
- our classifier is struggling to recognize the digit 8
    - most often confusing it with the digits 5 and 1

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Regression: beyond RMSE/R^2

We just spent time developing methods to study errors of classification.

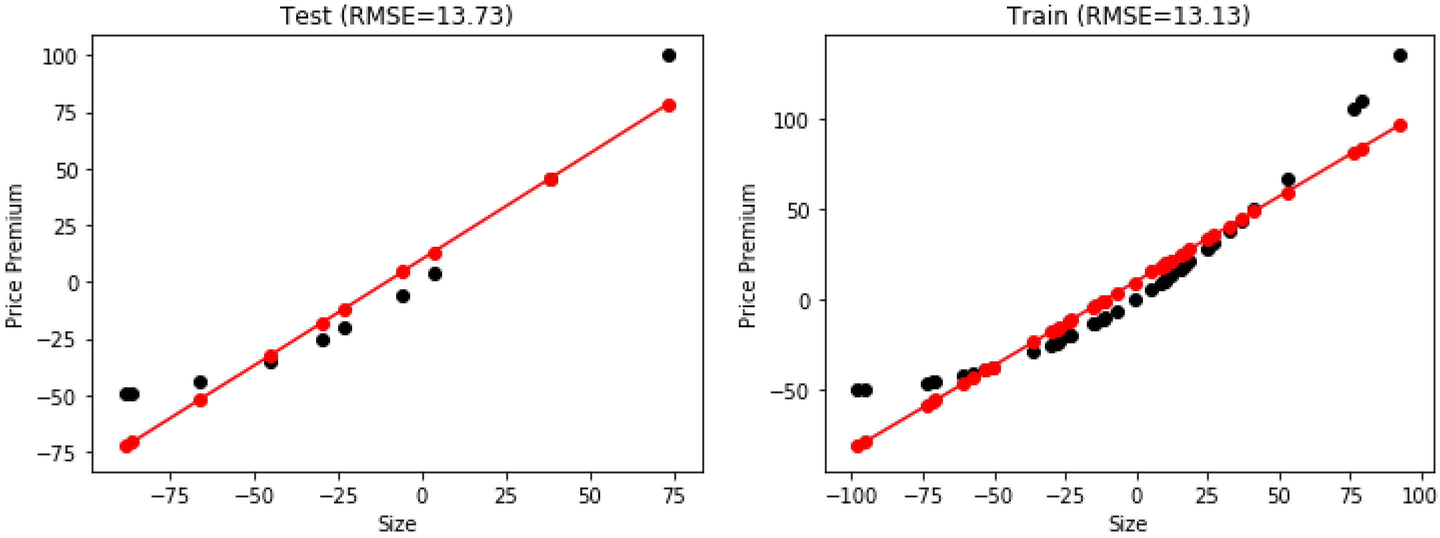
What is the analog for Regression ?

Examining the residuals.

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
```



Test (RMSE=13.73)

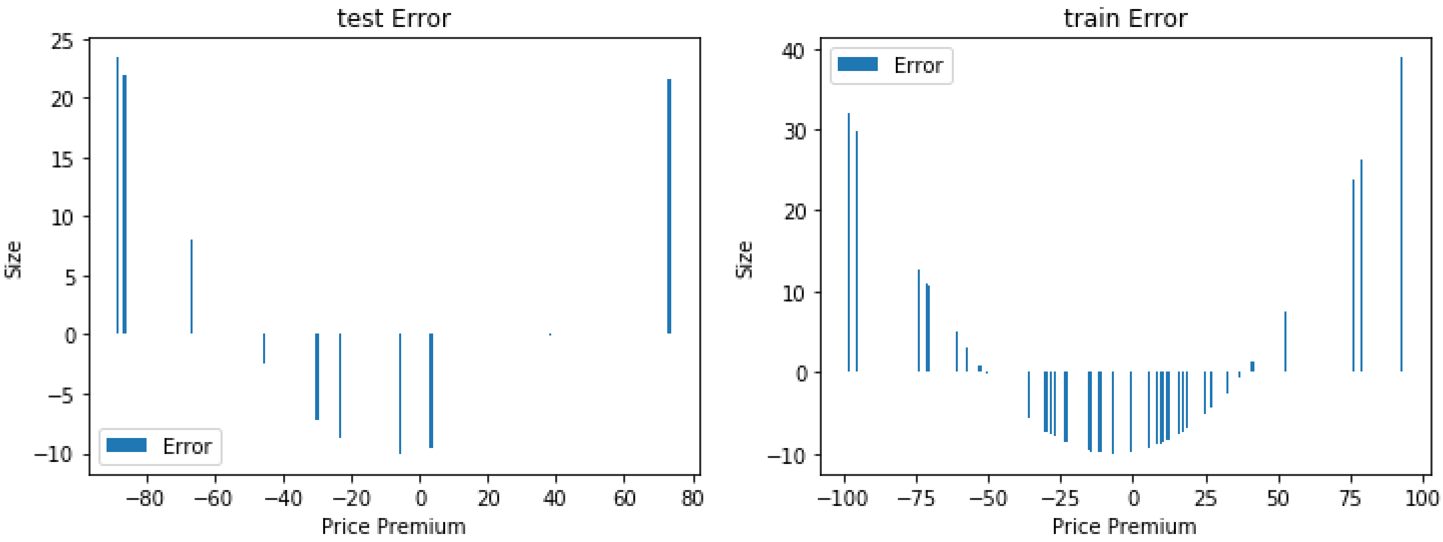
Train (RMSE=13.13)

Let's focus on the errors.

In [13]:

```
fig
```

Out[13]:



Not good !

- clear pattern: errors increase in the tails
- not constant variance

Recall that our conclusion was that there was a missing feature: a higher order x^2 term.

Once we added that term, the target became linear in

$$\Theta^T \cdot X = \beta_1 * x + \beta_2 * x^2$$

In [14]:

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

```
Done
```