

Overview

The purpose of this notebook is two-fold

- to introduce a systematic approach to problem solving in Machine Learning
- to introduce our first model for Supervised Machine Learning: Linear Regression

We will

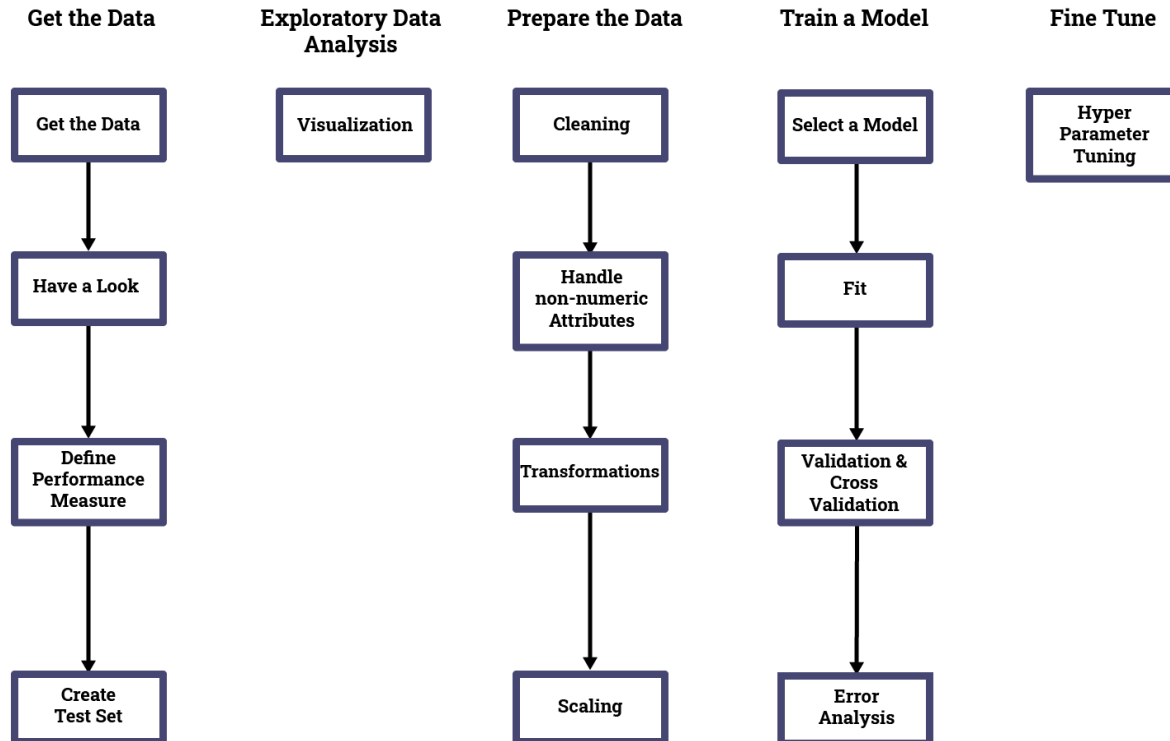
- introduce our systematic approach
- and illustrate it using Linear Regression as the chosen model

What is the "Recipe" for Machine Learning

We will define a methodical approach to solve problems using Machine Learning.

This is the *Recipe for Machine Learning*

Recipe for Machine Learning



There are no short-cuts !

Each step in the Recipe both prepares you for the next and, crucially, gives you *deeper insight* which improves the result.

Plan

We will illustrate *some* of the major steps in the Recipe.

The prediction problem we are solving is relatively simple

- so some steps of the Recipe won't be applicable

Disclaimer:

The purpose of this lecture is **not** to make you an expert in sklearn.

It is to introduce you to concepts that you can apply no matter what toolkit you use in the future.

Recipe step A: Get the data

Frame the problem

The first step in the Recipe is

- to define the problem !
- Why is it important ?
- Define terms

We are going to define a "toy" problem (probably unrealistic, but it will illustrate concepts)

We are in the real-estate business.

Our task: given a house/apartment for sale: predict the selling price (to advise the seller/buyer)

Our goal is *informed* prediction.

So our first step is

- to *hypothesize* one or more features that is predictive of Price
- using your intuition (or conducting research) as to what may drive apartment/house prices
 - size
 - location
 - amenities (kitchen, bath, pool)

Once we decide on the features we perform the **Get the data** step

- gather *labeled* examples
 - pairs of: $\langle \mathbf{x}, \mathbf{y} \rangle$
 - vector of features \mathbf{x} , target (Price) \mathbf{y}
- which we will use to train a model for prediction

The difficulty of this step may be under-appreciated

- *finding* data is not always easy
- Interesting data is scattered: requires collection, merging
- Supervised Learning requires labeled data;
 - where do the labels come from ?
- *extracting* data from its source (e.g., a web page) may involve specialized skills (*web-scraping*)

Get the data

As a gross over-simplification

- we will use a single feature: Size
- and we will give you the $\langle \text{Size}, \text{Price} \rangle$ pairs via a method within a helper class

```
In [5]: lr_demo = lrh.LinReg()

# Some options to configure the data
rho, sigma_mult = 0, 20

# Generate the data
df = lr_demo.gen_data(samples=300, rho=rho, sigma_mult=sigma_mult)

# Restrict the view to features used in the first experiment
df_initial = df[ ["x_1", "y"] ]
```

For illustration

- the full dataset (DataFrame `df`) has all the features (including the ones we only use in the future)
- for now: we will only look at the relevant features (DataFrame `df_initial`)

Column

- "x_1" is our first feature: Size
- "y" is our target: Price

Look at the data

Always put your eyes on the data !

- You will learn about its "shape":
 - tabular ? What are the attribute names ?
 - What are the types of the attributes ? Numeric ? Text ?

Let's look at the first few examples.

In [6]: `df_initial.head()`

Out[6]:

	x_1	y
0	0.000000	104.242391
1	0.033445	96.073816
2	0.066890	112.187158
3	0.100334	124.460065
4	0.133779	96.855848

- You will learn about potential data problems
 - missing data
 - strange values

Don't even try to do anything with your data until you have at least the most basic understanding by performing an inspection.

We can get some summary information:

In [7]: `df_initial.info()`

```
<class 'pandas.core.frame.DataFrame'>  
RangeIndex: 300 entries, 0 to 299  
Data columns (total 2 columns):  
x_1      300 non-null float64  
y        300 non-null float64  
dtypes: float64(2)  
memory usage: 4.8 KB
```

From the above

- we see the number of examples
- that the feature and target are both numeric (float)
- **no** missing data
 - number of non-null equals number of examples

We can also calculate statistics of the columns:

In [8]: `df_initial.describe()`

Out[8]:

	x_1	y
count	300.000000	300.000000
mean	5.000000	210.010372
std	2.901229	97.074015
min	0.000000	76.624519
25%	2.500000	126.719483
50%	5.000000	189.308862
75%	7.500000	282.030633
max	10.000000	430.461341

We see a statistical summary above ?

What "units" are the features/targets denominated in ?

- "x_1" (Size): range 0 to 10
 - clearly not Area
 - some scale from smallest (0) to largest (10)
 - unimportant for our illustration
 - but **important** in order to interpret
 - the feature
 - its associated parameter
 - increment in Price for a unit change in feature

- "y" (Price)
 - Units
 - "hundreds of thousands" of currency
 - number of Bitcoin ?

Again: unimportant for our illustration

- but important for the end-user

Define a Performance Measure

Our model "learns" from training data, so we might expect it to predict well on training examples

- the training examples are *in sample*: used by the model to learn \ominus

How well should I expect the model to predict on examples not encountered during training?

- "test" examples never seen during training, called *out of sample* examples

We define a *Performance Measure* to measure how well the model performs out of sample.

A Performance Measure can be thought of as the promise you make

- to a client/customer/boss
- on how well your model will perform on arbitrary, yet to be seen examples (non-training, out-of-sample)

In order for you to have confidence in your promise

- you evaluate the Performance Measure on *out of sample* examples
- using the out of sample examples *once* so that your model doesn't learn from them (i.e., become in-sample)

Root Mean Square Error: an absolute performance metric

Our problem is to predict continuous values (Regression task).

- A common performance measure for Regression is the Root Mean Square Error (RMSE):

$$\text{RMSE}(\mathbf{y}, \hat{\mathbf{y}}) = \sqrt{\frac{1}{m} \times \sum_{i=1}^m (\mathbf{y}^{(i)} - \hat{\mathbf{y}}^{(i)})^2}$$

Our goal is to minimize the RMSE by making each prediction $\hat{\mathbf{y}}^{(i)}$ close to the true value $\mathbf{y}^{(i)}$.

n.b., we will sometimes ignore the square root

$$\text{MSE}(\mathbf{y}, \hat{\mathbf{y}}) = \text{RMSE}(\mathbf{y}, \hat{\mathbf{y}})^2$$

Performance Measure versus Loss Function

There may some confusion between the Performance Measure and Loss functions

- they are both evaluated over a set of examples
- they both measure performance of some sort

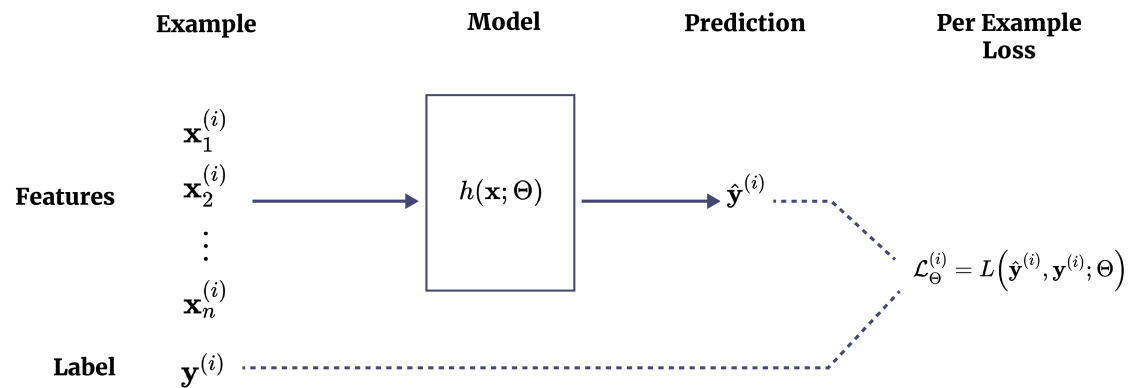
To be clear

- the Loss function is evaluated over the *training* examples
 - it is the objective that we try to minimize
 - by finding optimal Θ
- the Performance Measure is evaluated over the *test* examples
 - a prediction of out of sample performance
 - using test examples as a proxy for examples to be seen in the future

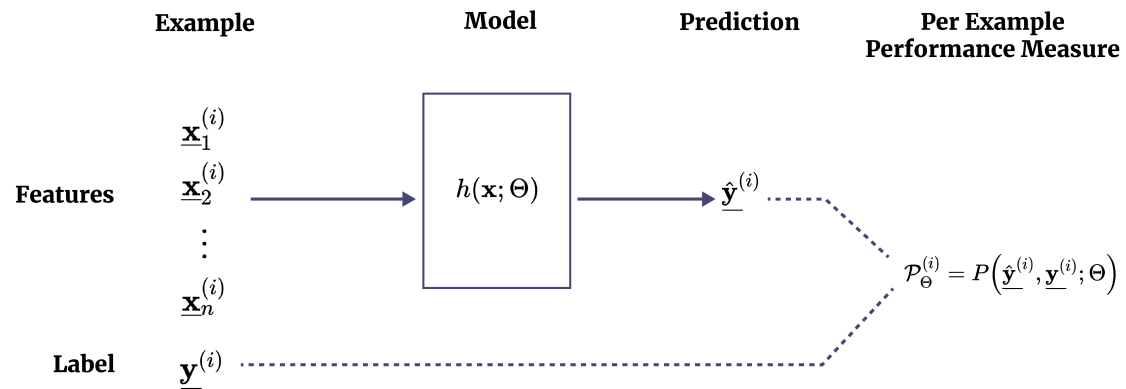
To illustrate, let

- \mathbf{X} denote our set of training examples, $\mathbf{x}^{(i)} \in \mathbf{X}$
- $\underline{\mathbf{X}}$ denote a set of test examples (out of sample: not used in training), $\underline{\mathbf{x}}^{(i)} \in \underline{\mathbf{X}}$

Loss on Training example



Performance on Test example



- A Performance Measure
 - is a property of the *problem* (not the model used to solve the problem)
 - you may have more than one Performance Measure
 - each expressing some desired quality of the prediction
 - is evaluated *out of sample*, that is, on non-training examples

- The Loss Function
 - is a property of a *model*: it guides a particular model's search for the best Θ
 - different models may have different Loss Functions
 - but the *problem's* Performance Metric is the same
 - is evaluated *in sample*, that is, on training data

Create a test set

Our Performance Metric is evaluated

- on a test dataset
- derived from our complete dataset
- but **used only once**

We split our complete dataset into

- train dataset
- test dataset

[illegible]

```
In [10]: X.shape, y.shape
```

```
Out[10]: ((300, 2), (300,))
```

```
In [11]: print("Train: ", X_train.shape, y_train.shape, X_train[:, [0]].shape,  
              "\n",  
              "Test:", X_test.shape, y_test.shape, X_test[:, [0]].shape)
```

```
Train: (240, 2) (240,) (240, 1)  
Test: (60, 2) (60,) (60, 1)
```

In the above

- you can see the number of examples in the train and test datasets
- in the initial model: we will only access the *first* feature

Note

- the single feature is a **two**-dimensional ndarray
 - singleton second dimension
- the target is a **one** dimensional ndarray
 - `sklearn` is sensitive (different behavior) when target is 2D with a singleton dimension

Note

In the above

- we included a second feature (x_2) to be used in the future
- in real life: you would only be accessing x_1 at this point

Exploratory Data Analysis

This is one of the key steps of a good Data Scientist.

Besides "seeing" the data, we need to hear it: what is it telling us that may aid prediction

- Any problems with the data that would inhibit learning ?
- Any obviously useful predictive features ?
 - relationship between target and a single feature ?
 - relationship between target and combinations of features ?

Any more complex relationships that may be useful ?

- Relationship *between* features ?
- Relative magnitudes of features ?

Often, understanding the data intimately can lead to

- transformations of the features that will aid prediction
- improved models

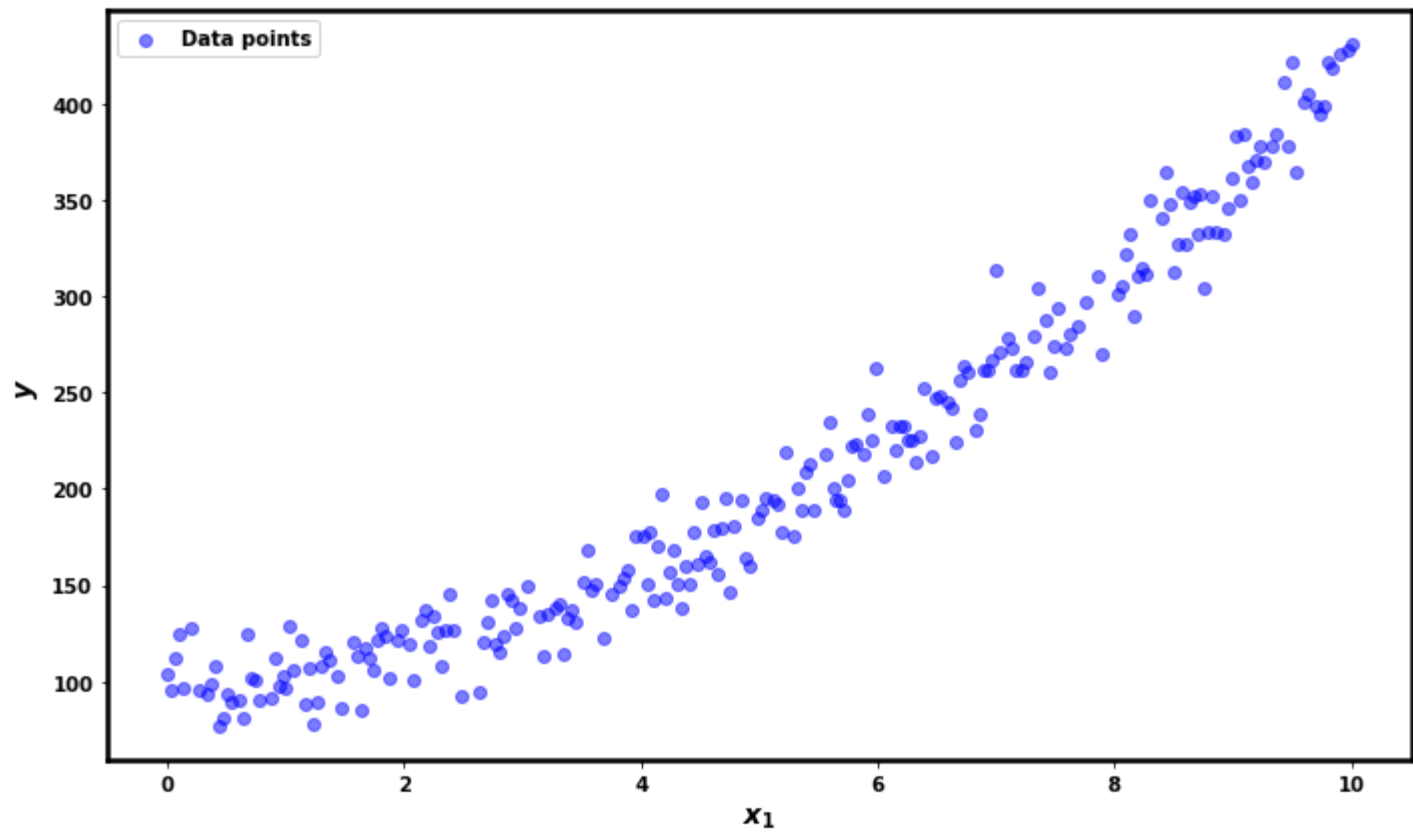
Given a single feature

- at this point, we can only really explore the relationship between feature and target
- in the presence of more than one feature we can examine
 - the feature/target relationship for each feature
 - the feature/feature relationships

```
In [12]: # Create the plot
_ = plt.figure(figsize=(10, 6))
_ = plt.scatter(X_train[:,0], y_train, color='blue', alpha=0.5, label='Data point
s')

# Set labels and title
_ = plt.xlabel('$x_1$')
_ = plt.ylabel('$y$')
_ = plt.legend()

# Show the plot
_ = plt.tight_layout()
_ = plt.show()
```



At first glance

- the relationship may not be exactly linear
- **but**
 - take small steps
 - start with a simple model
 - try to improve it

We will start with the hypothesis

- that a linear relationship between target and feature will suffice
- this suggest Linear Regression as the model to use

Prepare the data

It is not always the case that the data in "raw" form is adequate for modeling

- Cleanliness
 - dealing with missing data or anomalous values
- Numericalization
 - Converting non-numeric/categorical data into appropriate numbers
- Scaling, normalization
 - putting features on compatible scales

A key part of the Prepare the Data step is *feature engineering* or *transformations*

- Creating new, synthetic features from the "raw" features
- Knowing when/how to do this is what separates a good Data Scientist from an average one

In our toy example

- there is no missing data
- no "unclean" data: outliers

We won't perform any *feature engineering* in our first pass at the model

- in our second pass:
 - we will create a second feature
 - derived from x_1

Train a model

The model is our "predictor": the machine that takes features and produces predictions.

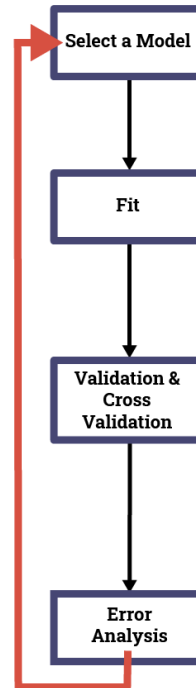
All the prior steps of the recipe were "prep-work": preparing the ingredients (data) for cooking (modeling)

Unlike actual cooking, this step is *iterative*

- Try a simple model, fit it to the data and evaluate the results
- Perform Error Analysis: Examine the results critically
 - Have our changes improved the Loss ? Is the Loss value acceptable ?
 - Is there some commonality among the examples with "bad" predictions ?
 - Can we change the model or perform Feature Engineering to compensate for common errors ?
 - Perform Feature Engineering, modify the model.
- Repeat !

Iterative training

Train a Model



The iterative nature is often overlooked in the rush to learn as many models as possible.

As we shall see

- The lessons learned from the Error Analysis is how we systematically progress from
 - Simple but poor models
 - To better models of increasing complexity

Select a model: Linear Regression

Based on our Exploratory Data Analysis

- we hypothesize a linear relationship between Price and Size
- we select the *Linear Regression* model as the *prediction function*

Linear Regression says that our prediction $\hat{\mathbf{y}}$ is a *linear* function of the features \mathbf{x}

$$\hat{\mathbf{y}} = \Theta \cdot \mathbf{x}$$

Remember: the dot product is nothing more than the sum of the pair-wise products

- of each feature \mathbf{x}_j with its corresponding parameters Θ_j

For our problem

- predicted target (Price) is a linear function of \mathbf{x}_1 (Size)

Fit the model

To create the prediction function

- we *fit* the model
- to the training examples

That is

- we minimize the Loss Function that is associated with Linear Regression
- over the set of training examples: (Size, Price) pairs

The definition of the Loss Function for Linear Regression will be presented shortly.

Here is code for our single-feature model

```
In [13]: # Create and fit the linear regression model  
model = LinearRegression()  
  
# Note: we access the single feature as X_train[:, [9]] rather than X_train[:,  
0] to ensure the result is 2D  
# - with a singleton final dimension, as required by sklearn  
_ = model.fit(X_train[:,[0] ], y_train)
```


Easy enough !

- sklearn API: all models respond to a method `fit`
 - takes training data
 - sets weights
 - internal variables of the model object

Validation

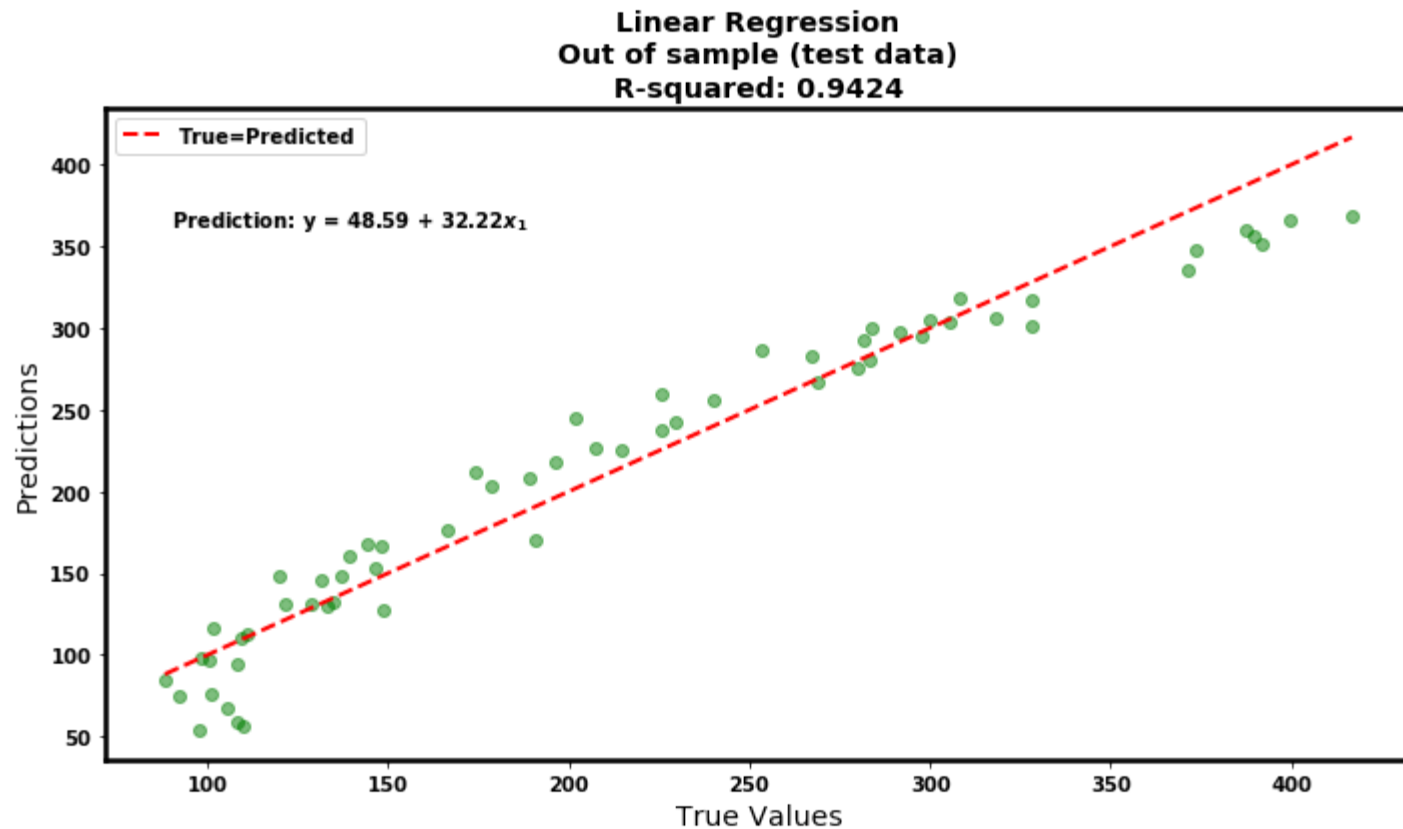
The proof is in the pudding

- How does our fitted model perform out of sample?
- That is
 - compute the Performance Metric (out of sample)

We show the Performance Metric as part of a plot

- of Predicted values vs True Value
- the 45 degree line is the imaginary line where Predicted and True values are identical

```
In [14]: fig, ax = lr_demo.plot_pred_vs_true(model, y_test, X_test[:,[0] ], feature_name
s=["$x_1$"],
title="Linear Regression\nOut of sample (te
st data)\n")
```



The Performance Metric is close to 100 %

- Technically
 - our Performance Metric is RMSE
 - we show R^2 , a related quantity

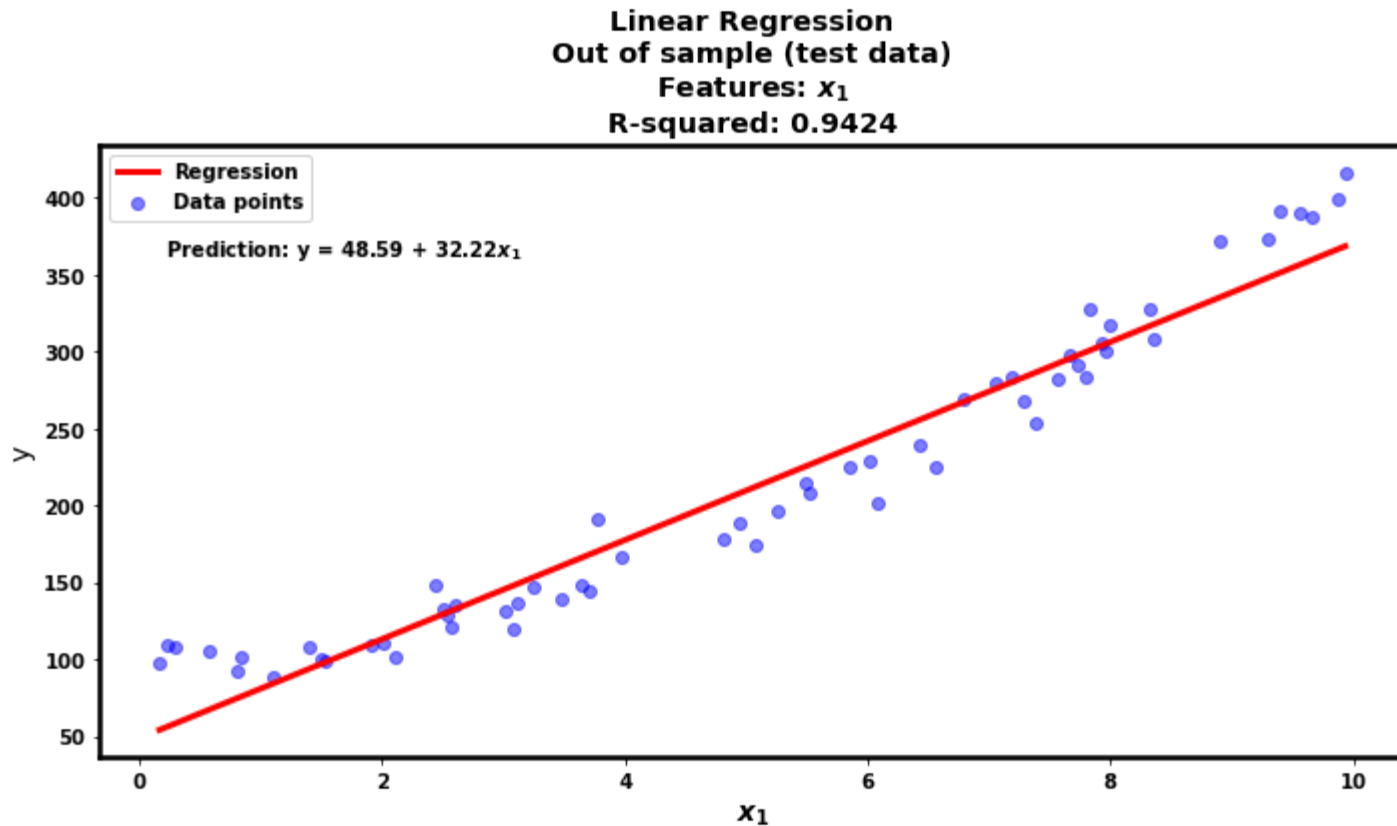
But observe a systematic mis-estimation

- For extreme values of True y (horizontal axis)
 - our predictions *under-estimate* the True
- For mid-range values of y
 - our predictions *over-estimate* the True

Since there is only a single feature

- we can also visual the mis-estimation as a function of x_1

```
In [15]: fig, ax = lr_demo.plot(model, y_test, X_test[:,[0] ], feature_names=["$x_1$"],
                                title="Linear Regression\nOut of sample (test data)\n",
                                showTrue=False)
```



Observe

- low and high values of x_1 result in *under-estimates* (red fitted line below true target)
- mid-range values of x_1 result in *over estimation* (red fitted line above true target)

This is probably not good for business !

- Arbitrage opportunity ?
 - Buy very small and very large homes from the user of the model (under-priced); re-sell to others at higher, true value
 - Buy mid-size homes from others at True value; sell to user of model (over-priced) at higher price

Error Analysis

How good is our model ?

Our ultimate measure

- evaluate the Performance Metric on out of sample data

We observed a systematic mis-estimation.

How do we remove this systematic estimation bias ?

In general

- the Loss Function and Performance Metric are distinct
 - identical in the case of Linear Regression
- changing the model
 - only *directly* affects the Loss Function

But we can also perform **Error Analysis**

- examine the success of the model
- on each *training* example
- comparing prediction to target

We can hope that removing the systematic estimation bias from the Loss (in sample)

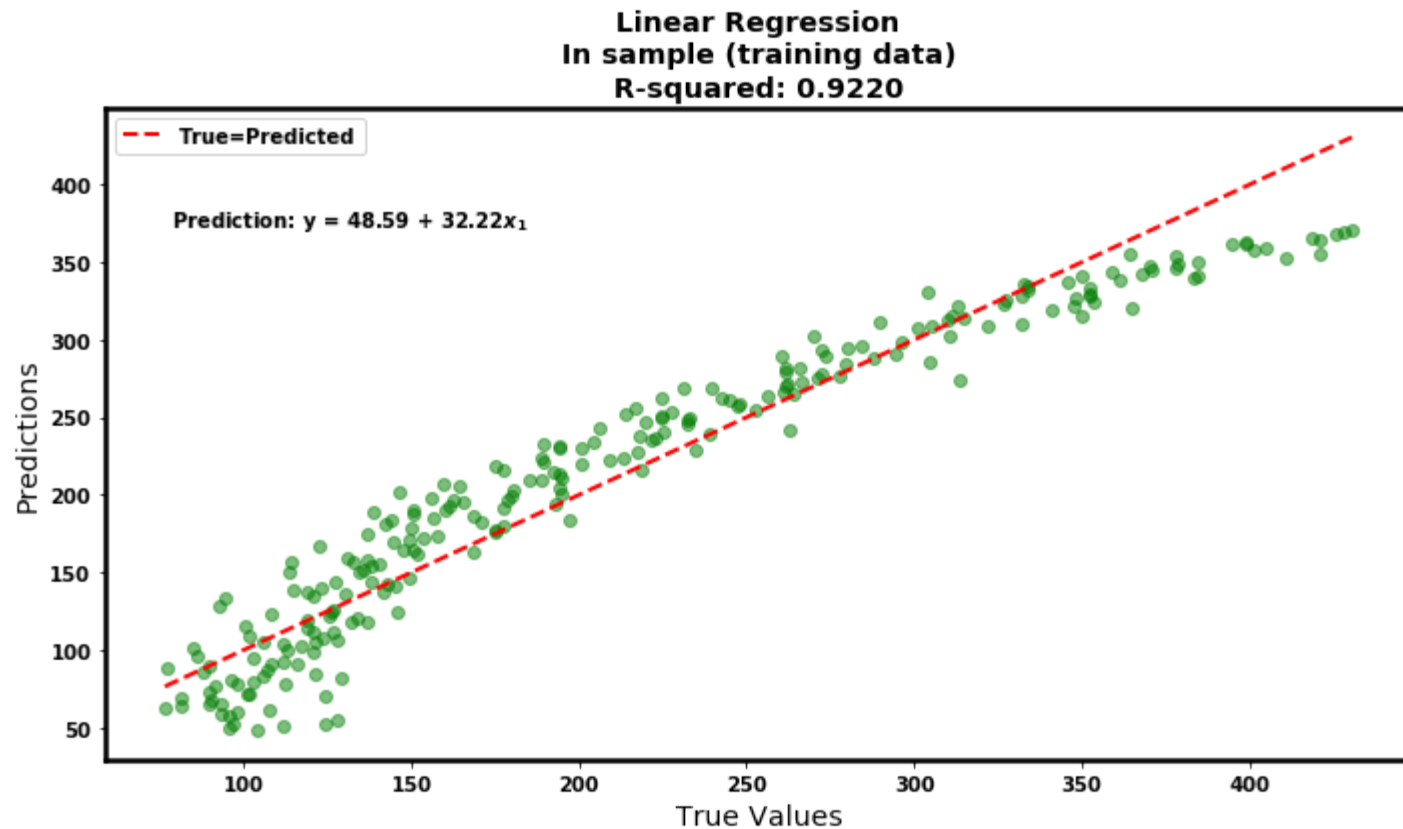
- will lead to it being removed from the Performance Metric (out of sample)

Here is a visualization that may be helpful for Error Analysis

It is nearly identical to the plot we used for the Performance Metric

- Red line: the ideal, where Predicted = True
- True value (green points)
- **But** here we are using the **training** examples
 - our previous plot used **test** examples

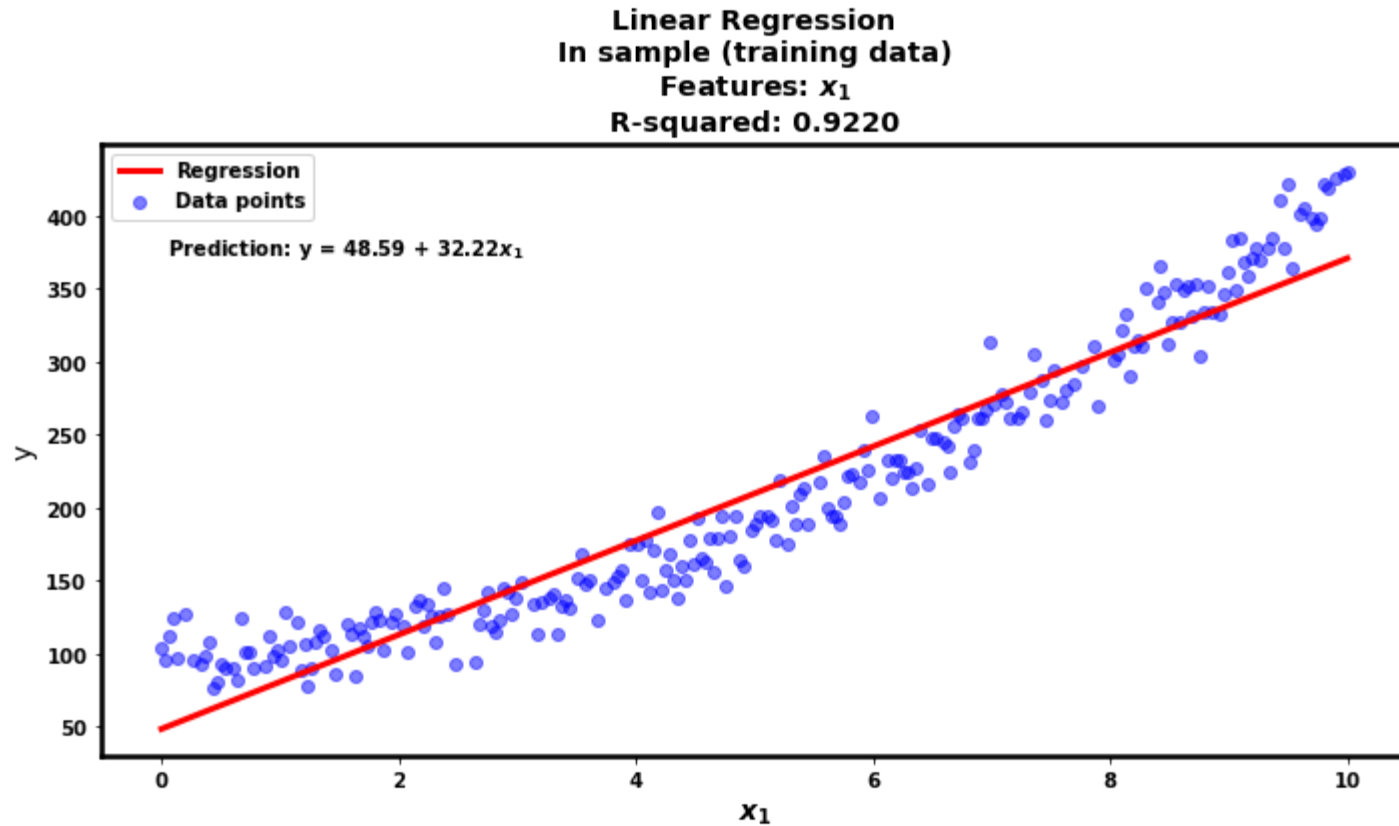
```
In [16]: fig, ax = lr_demo.plot_pred_vs_true(model, y_train, X_train[:,[0] ], feature_names=["$x_1$"],
                                             title="Linear Regression\nIn sample (training data)\n")
```



We can see a similar pattern of mis-estimation in the training dataset as we saw in the test dataset.

- to be expected if the two *empirical* datasets are derived from the same underlying distribution

```
In [17]: fig, ax = lr_demo.plot(model, y_train, X_train[:,[0] ], feature_names=["$x_1$"],  
                                title="Linear Regression\nIn sample (training data)\n",  
                                showTrue=False)
```



Don't be confused

Linear Regression is a special case where

- the Loss Function (re-expressed as R^2)
- the Performance Metric (re-expressed as R^2)

are the same !

This is not always the case

- Loss function is evaluated on **training** dataset (in sample)
- Performance Metric is evaluated on **test** dataset (out of sample)

What is the Error Analysis telling us ?

The R^2 (Loss Function proxy) is quite good

- almost 100%

But this is only a **summary** measure

- good on average
- but perhaps bad in a systematic way !

The Error Analysis reveals a potentially dangerous flaw in our hypothesis

- Price (y)
 - is *under-estimated* for
 - low Sizes (x_1)
 - high Sizes (x_1)
 - is *over-estimated* for
 - intermediate values of Size

Never be satisfied with just a summary measure

- examine per-example losses

The systematic pattern of errors suggest a need to refine our hypothesis

- of a single feature, linear relationship between Price and Size

Iterate: Linear Regression with higher order features

The Error Analysis we performed on our first model (single non-constant feature) suggested a need for improvement.

Two types of improvement come to mind

- Hypothesis iteration: try a different model
 - different *functional form* for the prediction: non-linear model
 - models without functional forms (Decision Tree)
- Feature iteration: change/add to the features of the current model
 - adding a previously discarded feature
 - creating a synthetic feature

We go back to our Exploratory Data Analysis

- which suggested some curvature in the relationship between y and x_1

Rather than changing to a non-linear model

- we will use *feature engineering* (feature iteration)
- to add a *feature* capturing curvature
- while keeping the functional form linear !

How can this be achieved ?

Answer

Add a second feature: x_1^2

Our (first-order) linear model was

$$\mathbf{y} = \Theta_0 * 1 + \Theta_1 \mathbf{x}_1$$

We can create a *second order* linear model by adding a feature x_1^2 :

$$\mathbf{y} = \Theta_0 * 1 + \Theta_1 \mathbf{x}_1 + \Theta_2 \mathbf{x}_1^2$$

The model is still linear in x_1 and x_1^2

- can be expressed as a dot product

$$y = \Theta \cdot \mathbf{x}$$

It is

- a linear model
 - so can use Linear Regression as the model
- whose terms are polynomial in a common feature

```
In [18]: # Add an  $x_1^2$  column to  $X_{train}$  AND  $X_{test}$   
X_train_with_sq = np.column_stack( (X_train[:, 0], X_train[:, 0]**2) )  
X_test_with_sq = np.column_stack( (X_test[:, 0], X_test[:, 0]**2) )  
  
# Fit the model  
model = LinearRegression()  
_ = model.fit(X_train_with_sq, y_train)
```

In the above

- the first feature is `X_train[:, 0]`
- we added a second feature `X_train[:, 0]**2`
 - the square of the first feature

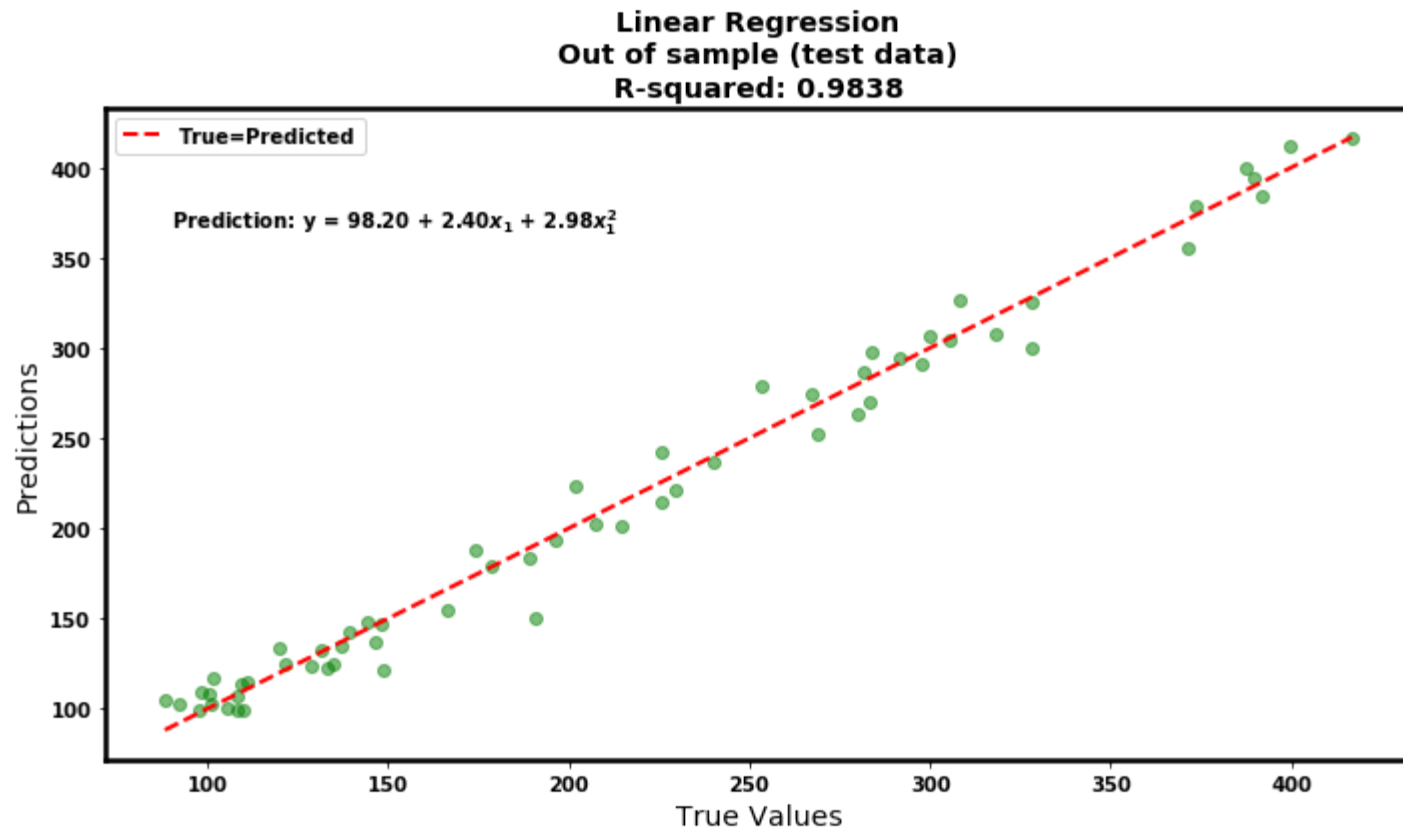
Also notice

- We have performed *feature engineering*
 - Added a feature
- Feature engineering is applied
 - to **both** training and test examples
 - if we trained on two features
 - the model expects these same two feature in test (out of sample) examples

Validation on the new model:

- how is our new out of sample Performance ?

```
In [19]: fig, ax = lr_demo.plot_pred_vs_true(model, y_test, X_test_with_sq, feature_names=["$x_1$", "$x_1^2$"],
                                             title="Linear Regression\nOut of sample (test data)\n")
```



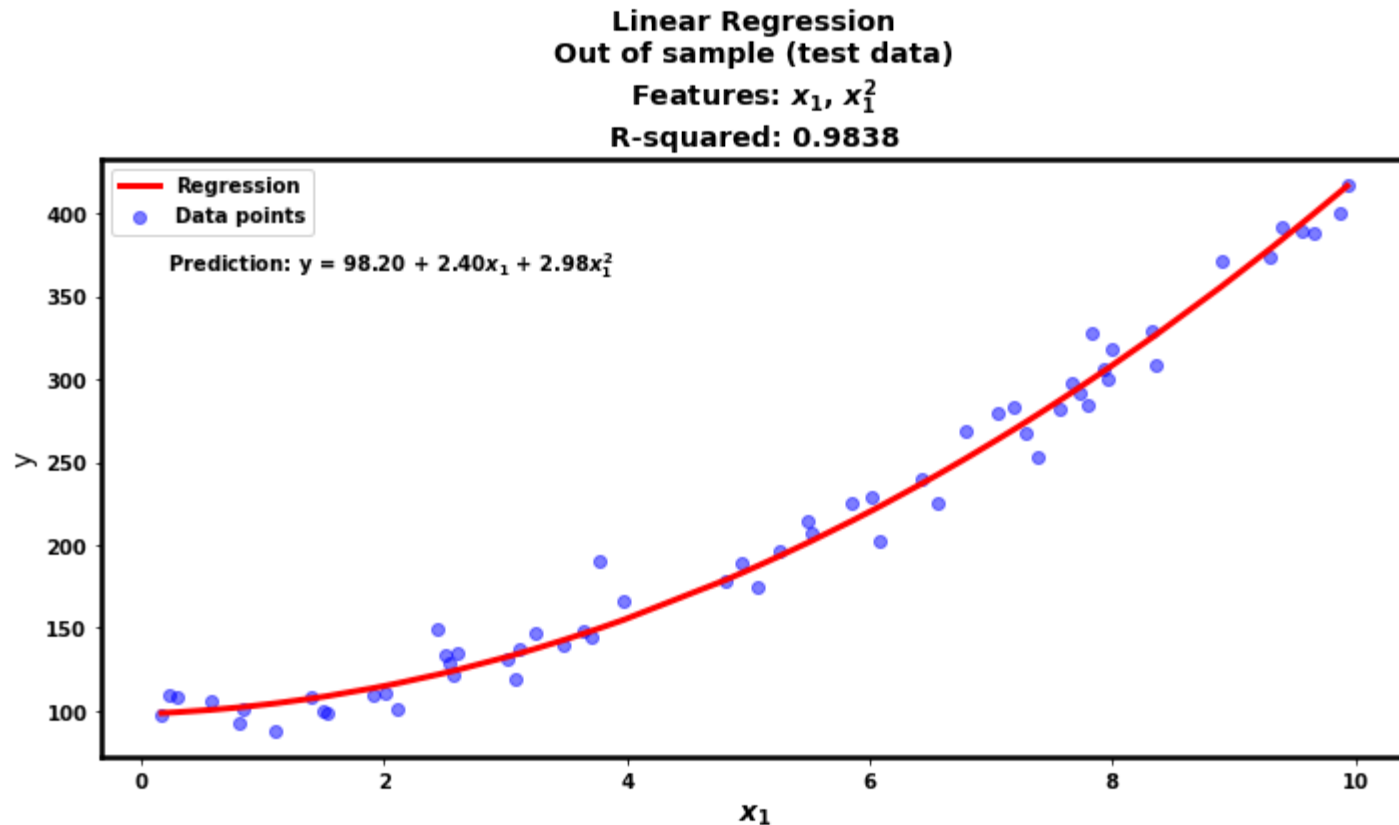
The Performance Metric has increased !

- adding the new feature helped

We also no longer see the systematic mis-estimation.

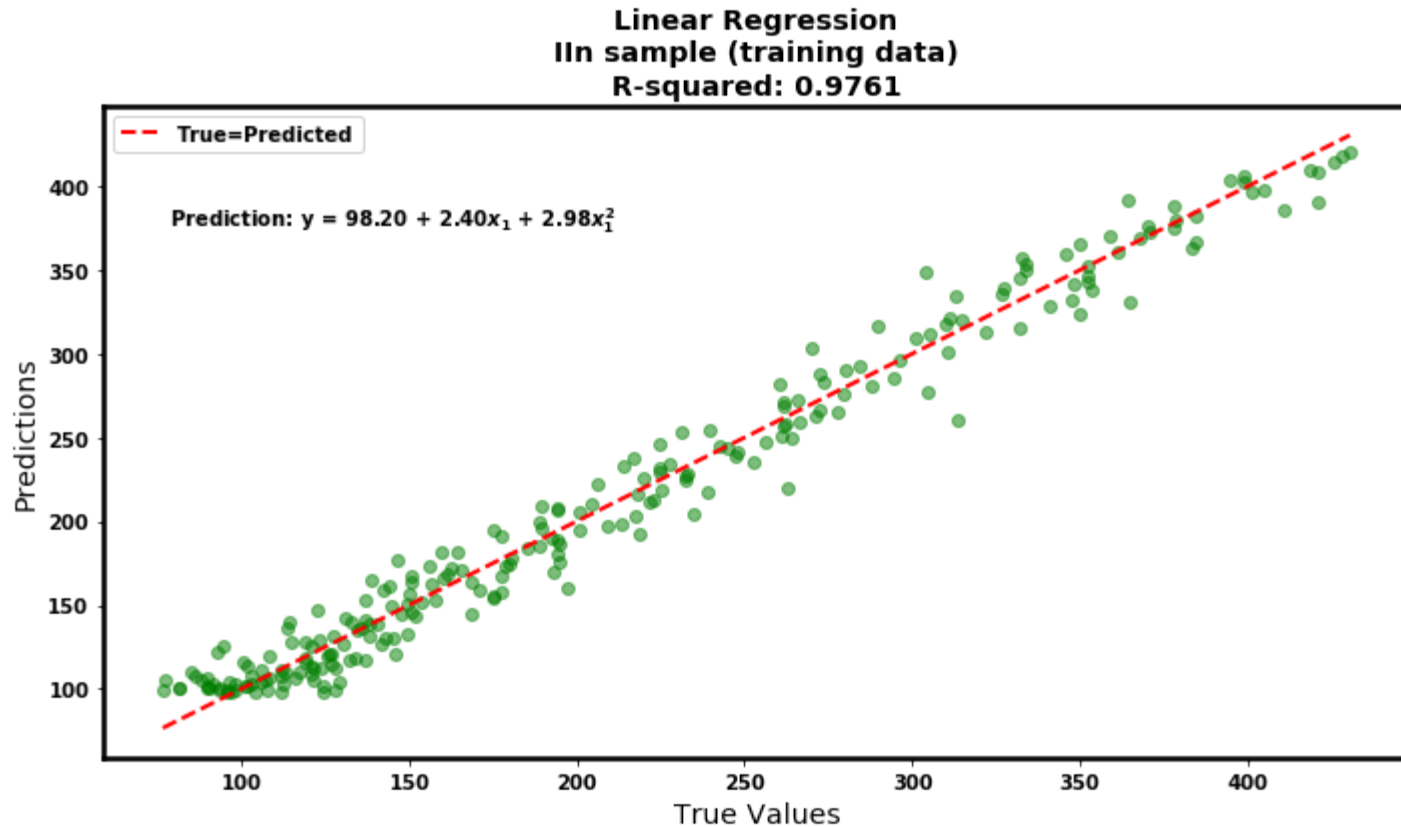
We can also visualize this as a function of one feature (x_1)

```
In [20]: fig, ax = lr_demo.plot(model, y_test, X_test_with_sq, feature_names=["$x_1$",
"$x_1^2$"],
                                title="Linear Regression\nOut of sample (test data)\n",
                                showTrue=False)
```

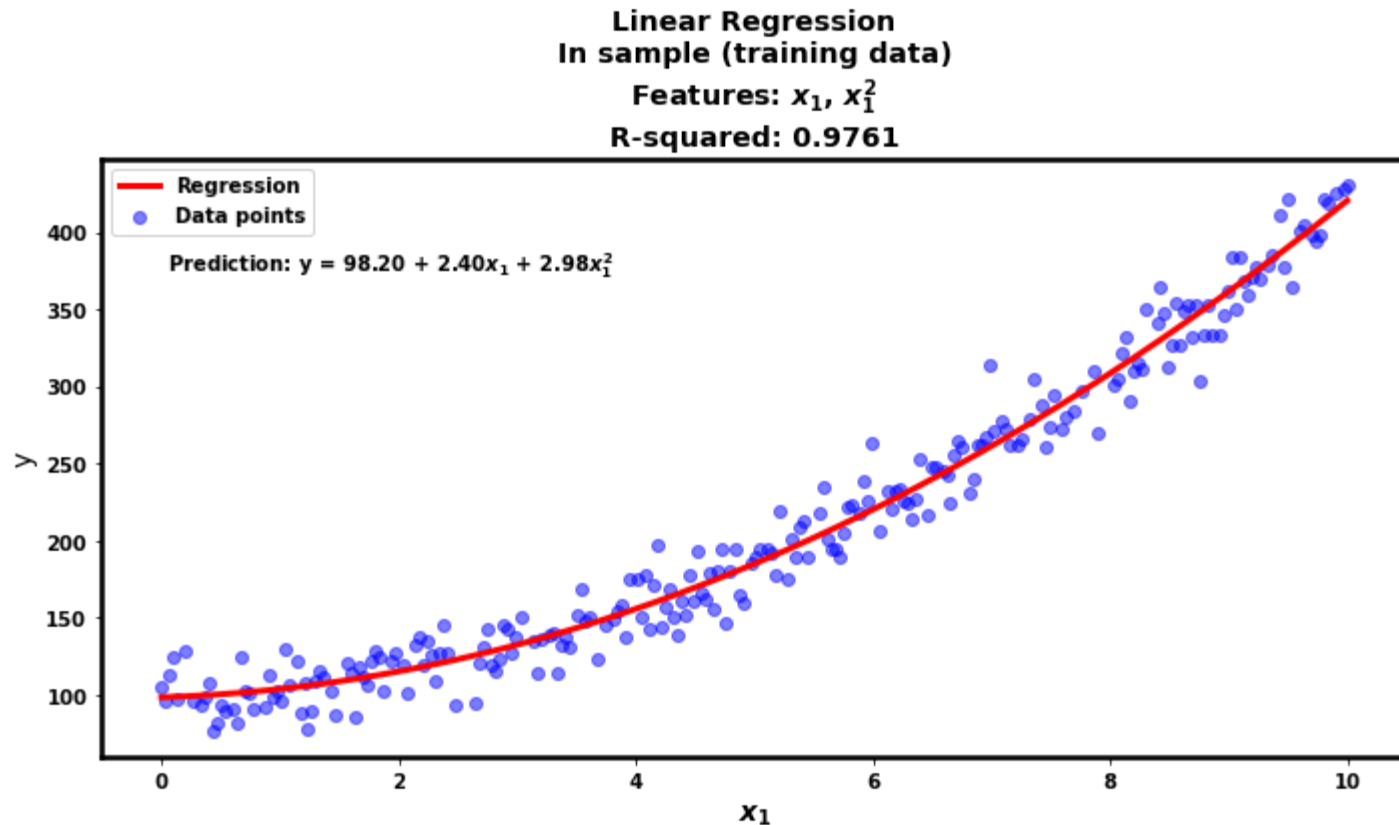


Let's perform Error Analysis on this revised model

```
In [21]: fig, ax = lr_demo.plot_pred_vs_true(model, y_train, X_train_with_sq, feature_names=["$x_1$", "$x_1^2$"],
                                              title="Linear Regression\nIn sample (training data)\n")
```



```
In [22]: fig, ax = lr_demo.plot(model, y_train, X_train_with_sq, feature_names=["$x_1$",  
"$x_1^2$"],  
                                title="Linear Regression\nIn sample (training data)\n",  
                                showTrue=False)
```



Notice

- the decrease in the Loss Function
 - expressed as increase in R^2
- compared to the first model

There is no obvious systematic pattern in the errors.

How is our model linear when the plot is curved ?

You may be uncomfortable seeing a curve when we call our model "linear".

It is *linear* in the features x_1 and x_1^2

- That is: it can be written as a dot product linear in
 - $y = \Theta \cdot \mathbf{x}$

The fact that one feature (x_1^2) depends on another (x_1) does not alter the fact that the form is linear

You see a curve because

- because we are plotting \hat{y} against **only one** of the features
 - it is **not** linear in x_1 alone

Let's plot the fitted surface against both features.


```
In [23]: import numpy as np
import matplotlib.pyplot as plt
from mpl_toolkits.mplot3d import Axes3D
from sklearn.linear_model import LinearRegression
from sklearn.metrics import r2_score

# Calculate R-squared
y_pred = model.predict(X_train_with_sq)
r_squared = r2_score(y_train, y_pred)

# Create a mesh grid for plotting
xx, xx_squared = np.meshgrid(np.linspace(X_train_with_sq[:, 0].min(), X_train_with_sq[:, 0].max(), 50),
                             np.linspace(X_train[:, 1].min(), X_train[:, 1].max(), 50))

# Predict using the model
Z = model.predict(np.column_stack((xx.ravel(), xx_squared.ravel()))).reshape(xx.shape)

# Plotting
fig = plt.figure(figsize=(12, 8))
ax = fig.add_subplot(111, projection='3d')

# Plot the original data points
scatter = ax.scatter(X_train_with_sq[:, 0], X_train_with_sq[:, 1], y_train, c=y_train, cmap='viridis', s=50, alpha=0.6)

# Plot the regression plane
surf = ax.plot_surface(xx, xx_squared, Z, alpha=0.3, cmap='viridis')

# Set labels and title
_ = ax.set_xlabel('$x_1$')
_ = ax.set_ylabel('$x_1^2$')
```

```
_ = ax.set_zlabel('y')
_ = ax.set_title(f'Linear Regression in 3D with Features  $x_1$  and  $x_1^2$ \nR-squared: {r_squared:.4f}')

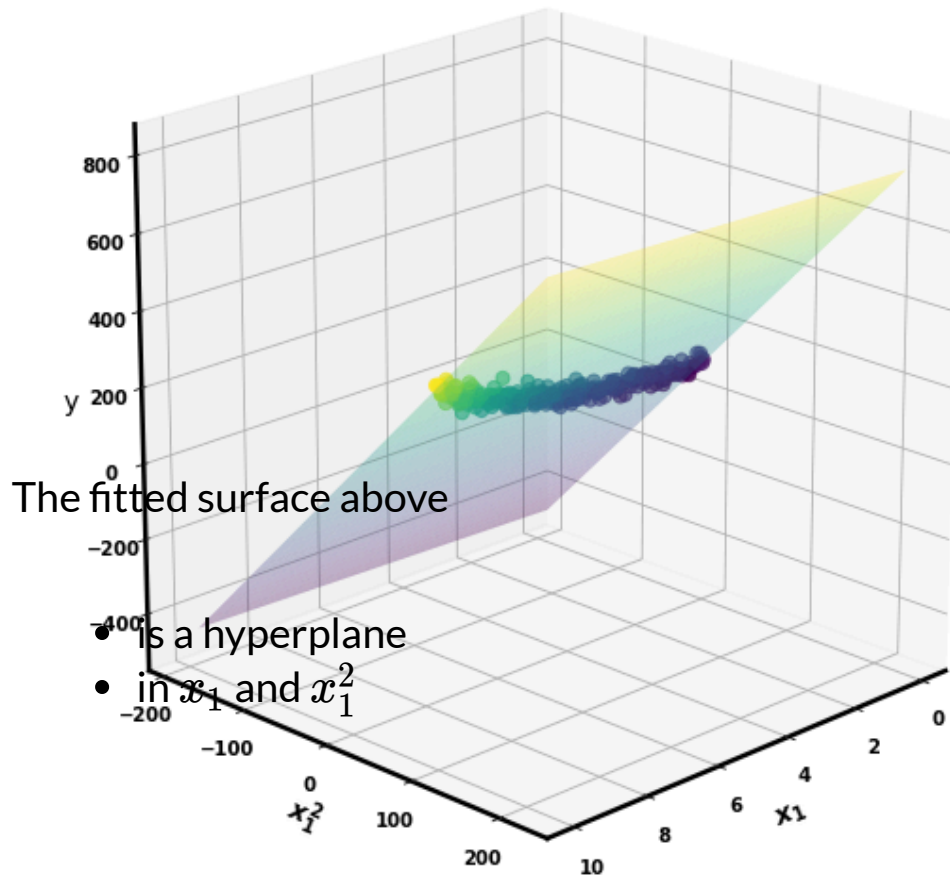
# Adjust the viewing angle
_ = ax.view_init(elev=20, azim=45)

# Add colorbars
_ = fig.colorbar(scatter, ax=ax, shrink=0.5, aspect=5, label='Actual y values')
_ = fig.colorbar(surf, ax=ax, shrink=0.5, aspect=5, label='Predicted y values')

_ = plt.tight_layout()
_ = plt.show()

# Print model coefficients
print(f"Intercept: {model.intercept_:.4f}")
print(f"Coefficient for x: {model.coef_[0]:.4f}")
print(f"Coefficient for  $x^2$ : {model.coef_[1]:.4f}")
```

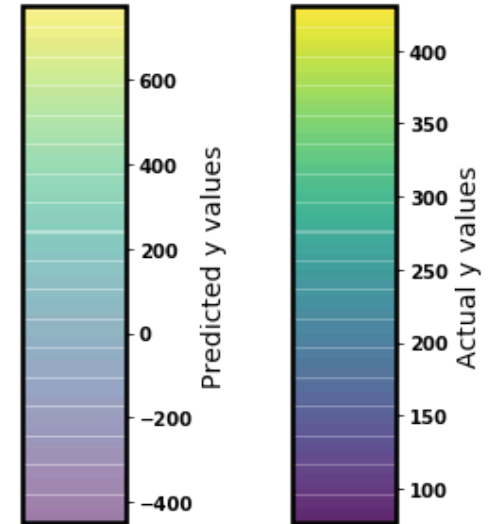
Linear Regression in 3D with Features x_1 and x_1^2
R-squared: 0.9761



The fitted surface above

- Is a hyperplane
- in x_1 and x_1^2

Intercept: 98.2032
Coefficient for x : 2.4046
Coefficient for x^2 : 2.9834



When to stop iterating

Adding second order features resulted in a much better model

- both in sample
- and out of sample

So our "fix" to the first (single feature) model was successful.

But this will not always be the case

- perhaps our hypothesis of a Linear functional form is wrong
- perhaps more features are needed

We should consider ourselves Scientists conducting experiments

- Propose a theory
 - gather data
 - test the theory
- Revise/Improve the current theory **OR** discard it and start with a different theory

Considering our success at adding the second features

- At this point
- we may ask whether further improvement is needed
 - continue iterating
- or is the model sufficient for our purposes
 - stop iterating

We encourage you to do a Deeper Dive by examining the topic of [Bias and Variance](#)
([Bias and Variance.ipynb](#)).

Continue iterating: the case of a missing feature

You may be disappointed that our fit is not perfect.

- we could try adding higher order polynomial features

Sometimes, this is because

- our model is **missing a feature**
 - we need to improve our hypothesis
 - gather data for this new feature

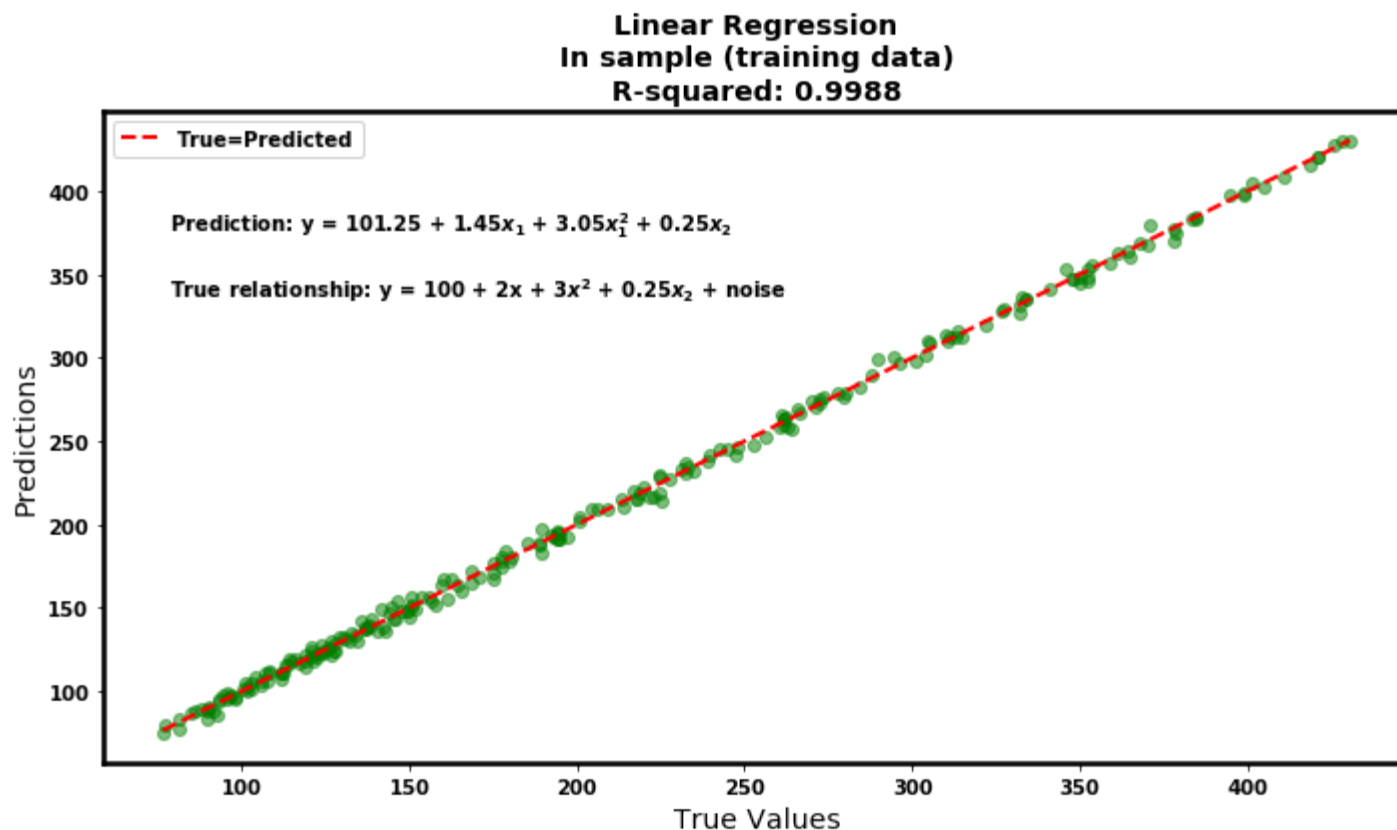
In our "Get the data" step

- we indicated the presence of a second feature x_2
 - which we hid from view until now

Let's imagine that we hypothesized that this was a useful feature and added it to our model.

```
In [24]: # Add an  $x_1^2$  column to  $X_{train}$  and  $X_{test}$   
X_train_full = np.column_stack( (X_train[:, 0], X_train[:, 0]**2, X_train[:,1])  
)  
X_test_full  = np.column_stack( (X_test[:, 0], X_test[:, 0]**2 , X_test[:,1])  
)  
  
# Fit the model  
model = LinearRegression()  
_ = model.fit(X_train_full, y_train)
```

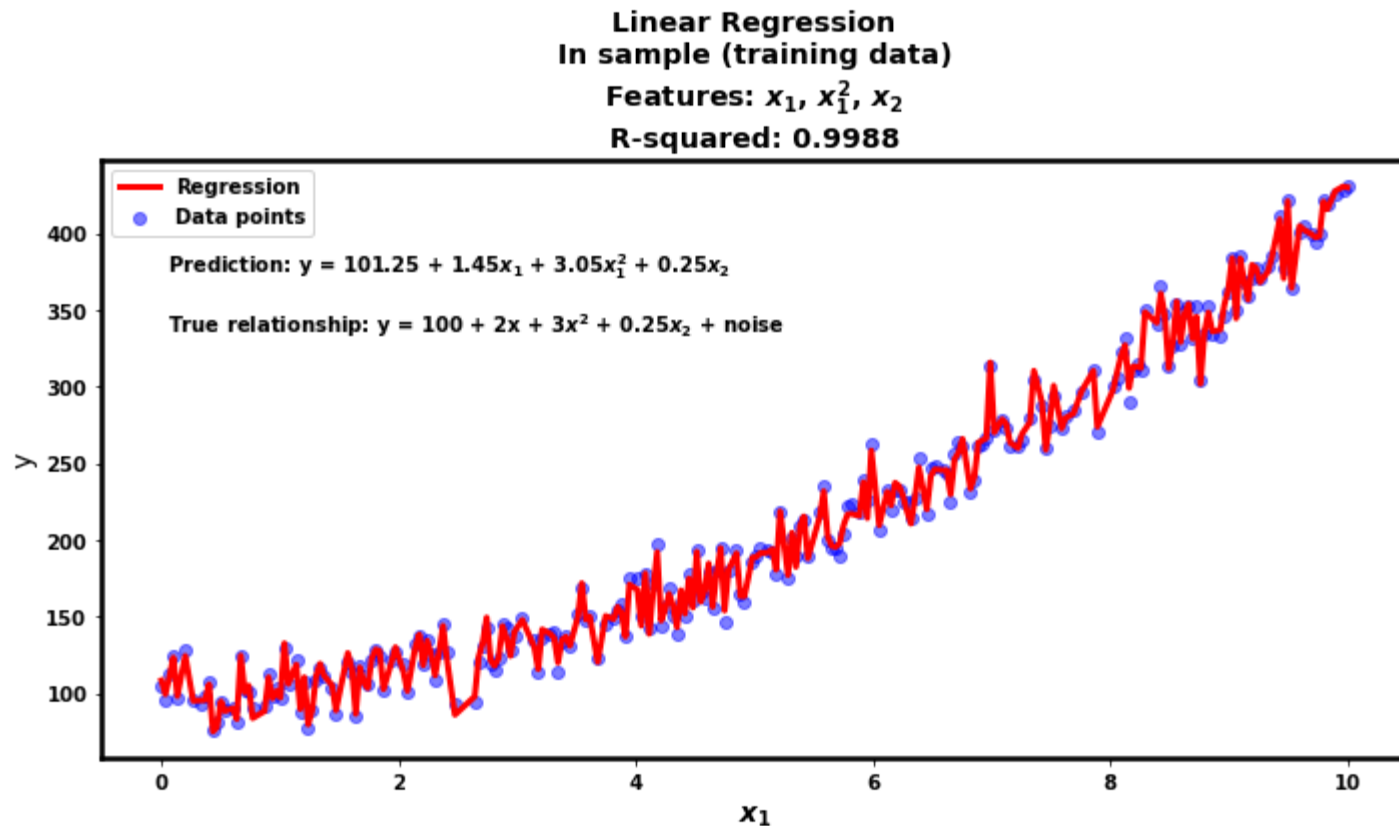
```
In [25]: fig, ax = lr_demo.plot_pred_vs_true(model, y_train, X_train_full, feature_names
=["$x_1$", "$x_1^2$", "$x_2$"], showTrue=True,
                                     title="Linear Regression\nIn sample (training
ng data)\n")
```



Since there is a second feature (x_2)

- we really need to plot with 2 (or 3) feature dimensions
- we take the liberty of plotting against just the x_1 feature
 - so we no longer see a straight line

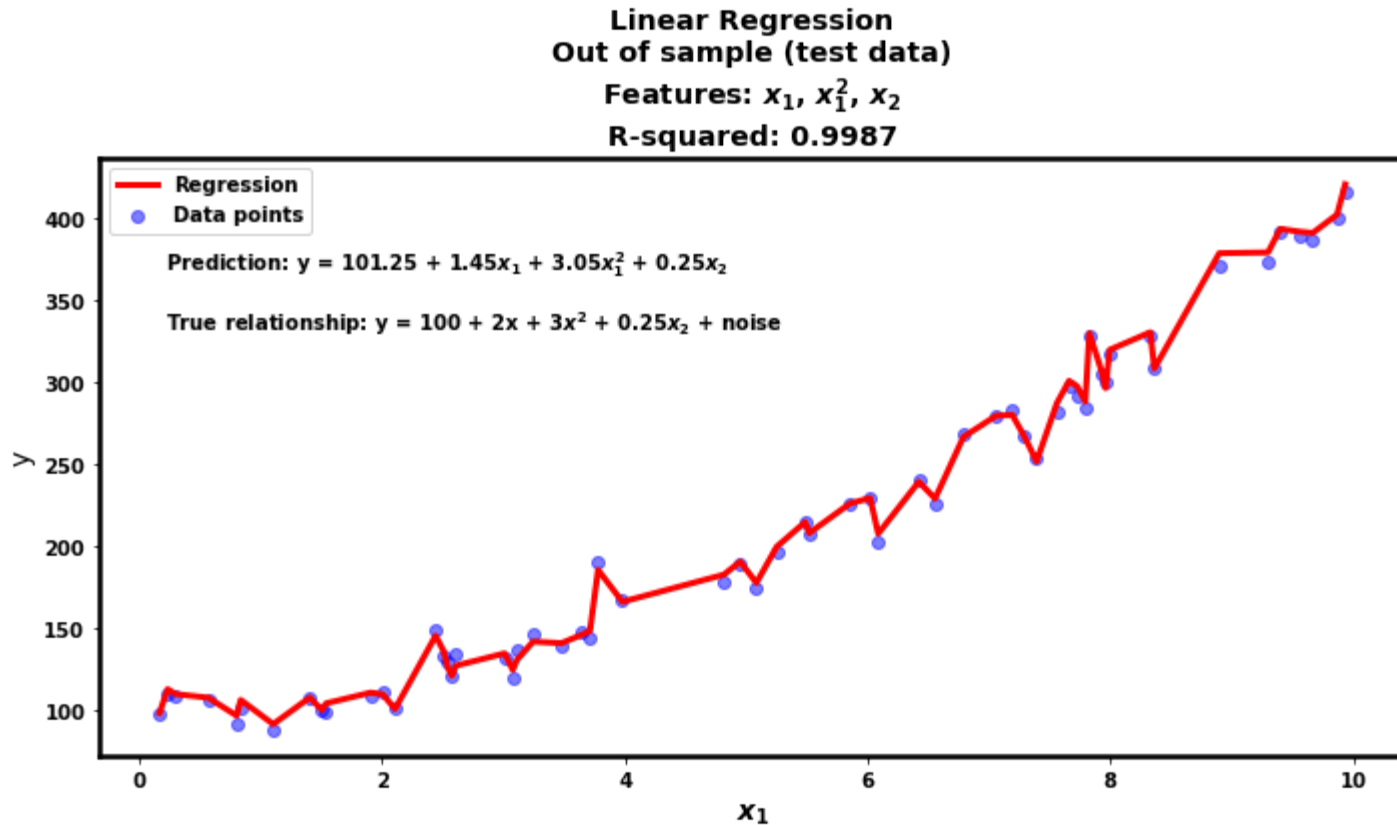

```
In [26]: fig, ax = lr_demo.plot(model, y_train, X_train_full, feature_names=["$x_1$", "$x_1^2$", "$x_2$"],
                                title="Linear Regression\nIn sample (training data)\n",
                                showTrue=True)
```



Almost perfect R^2 !

Similar results out of sample:

```
In [27]: fig, ax = lr_demo.plot(model, y_test, X_test_full, feature_names=["$x_1$", "$x_1$^2$", "$x_2$"],
                                title="Linear Regression\nOut of sample (test data)\n",
                                showTrue=True)
```



Aside: Near perfect fit but our weight estimates don't match true values

In the plots above, we show both

- the predicted relationship between target and features
- the *true* relationship
 - known to us because we created the artificial dataset

Although the R^2 is almost perfect

- the weights (true equation coefficients) of the predicted and true models are not exactly equal

This is a function of a small training sample size.

We repeat with a much larger number of samples, and get much closer estimates for the weights

```
In [28]: lr_big_demo = lrh.LinReg()

df_big = lr_big_demo.gen_data(samples=3000, rho=rho, sigma_mult=sigma_mult)

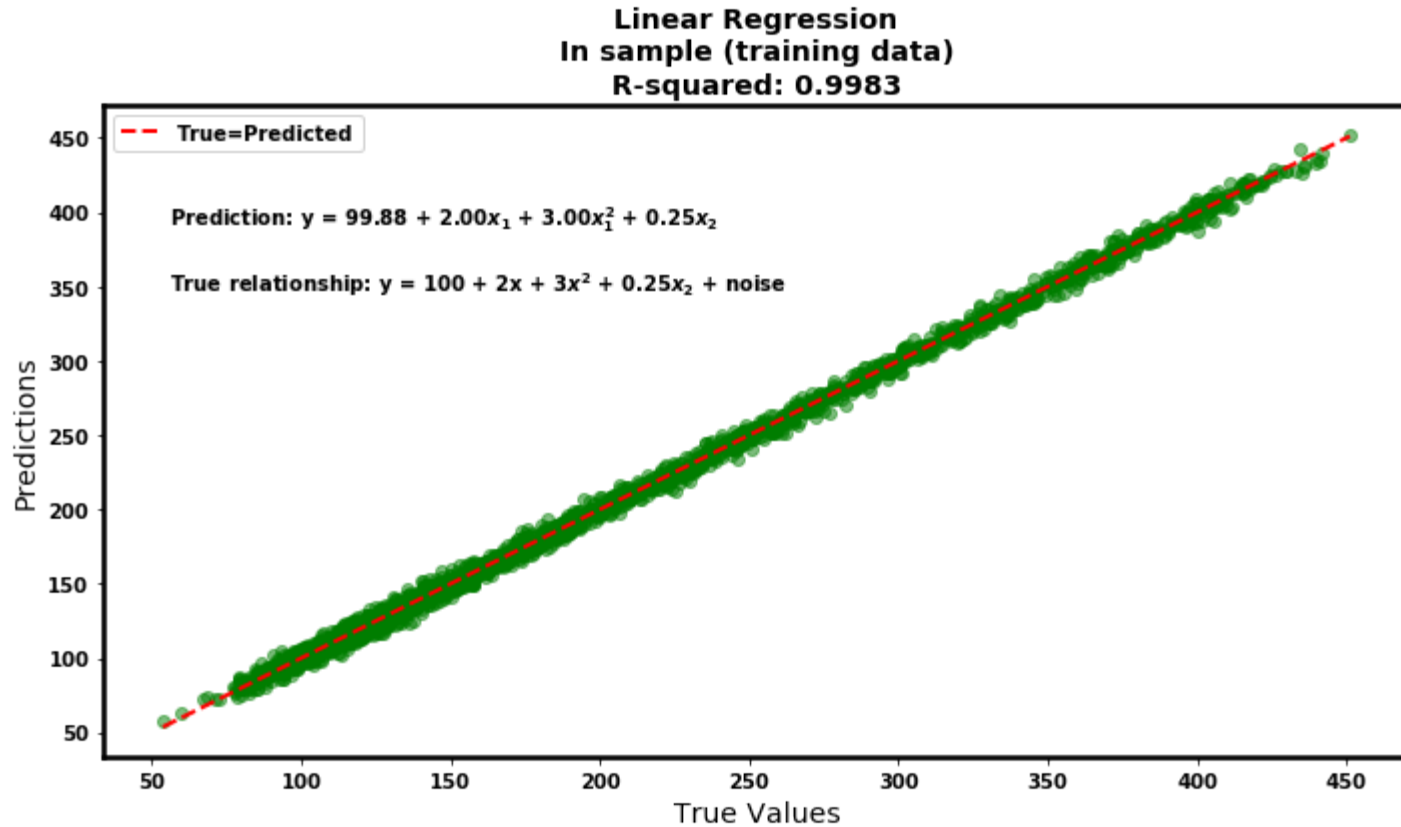
# Separate the features from the target
X = df_big[ ["x_1", "x_2"]].to_numpy()
y = df_big[ "y"].to_numpy()
```

[illegible]

```
In [30]: # Create feature matrix
X_train_full = np.column_stack( (X_train[:, 0], X_train[:, 0]**2, X_train[:,1])
)
X_test_full  = np.column_stack( (X_test[:, 0],  X_test[:, 0]**2,  X_test[:,1])
)

# Fit the model
model = LinearRegression()
_ = model.fit(X_train_full, y_train)
```

```
In [31]: fig, ax = lr_big_demo.plot_pred_vs_true(model, y_train, X_train_full, feature_names=["$x_1$", "$x_1^2$", "$x_2$"],
                                                showTrue=True,
                                                title="Linear Regression\nIn sample (training data)\n")
```



The weights of the

- prediction equation
- true relationship

are now much closer than with the smaller training dataset.

Validation and Cross Validation

In our Validation step in the model development above

- we used our test dataset

But

- after you use the test dataset
- you are not "allowed" to continue refining the model !
 - the test dataset is a proxy for the future (out of sample)
 - you cannot use future knowledge

This creates a dilemma

- we need to examine out of sample performance while developing a model
- but we are not allowed to use the test dataset as a proxy

Validation

[Geron notebook on validation](#)

[\(external/PythonDataScienceHandbook/notebooks/05.03-Hyperparameters-and-Model-Validation.ipynb#Thinking-about-Model-Validation\)](#)

So how can we perform out of sample prediction to evaluate our model ?

- Answer: Split the *training set* into two pieces
 - a smaller training set
 - a *hold-out* piece called the *validation set*
 - the validation set serves a similar role to the test set; it's out of sample
 - it is used to see how well the model generalizes
 - you can use the validation set *many* times (sort of) during your iterative process
 - unlike the test set, which you may look at only once, at the end

Train/Validation/Test split

Train/Validation/Test Split



Train/Test



Train/Validation/Test

Cross-Validation

Splitting into a smaller training set, and a validation set

- is a step in the right direction
 - it allows you to evaluate out of sample predictions without peeking into the test set.

You might still be uncomfortable with the idea of a validation set that is used many times.

Rightly so.

- We can wind up over-fitting to the validation set. Isn't that cheating too ?
- The validation set is just *one* sample.
 - How do we know the Performance Measure on this one sample is representative ?
 - Where are the error bars or confidence intervals for this statistic ?

Cross-Validation to the rescue !

K-fold cross-validation

- Split the training data into K pieces (called *folds*. so K-fold means K pieces).
- Select one fold as the validation set, and use the other $(K - 1)$ folds as the smaller training set
 - Fit the model on the smaller training set
 - Evaluate the Performance measure on the fold selected as the validation set
- Repeat the above $(K - 1)$ times, using a different fold as the validation set each time.

Cross Validation/Test split

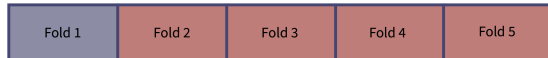


Train/Test

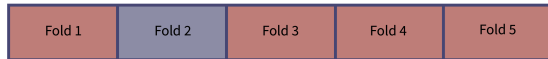


Train/Validation/Test

Cross Validation



Split 1



Split 2



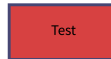
Split 3



Split 4



Split 5



Cross validation creates k proxies for the out of sample dataset

- one for each split

This means we don't over fit to a single validation dataset.

But it also gives us a *distribution* of the Performance Metric

- one for each split
- the distribution may be more informative of out of sample performance than a single validation dataset

We can *summarize* the distribution with a single value, if needed (or convenient)

- mean
- 95% confidence
 - This is akin to the statistical confidence interval for in-sample estimators

The cost of this advantage

- we need to fit the model k times
 - one for each split
- we need to summarize the distribution

This sounds like a lot of work.

Fear not !

sklearn has a function to do this for us: `cross_val_score`

```
from sklearn.cross_validation import cross_val_score  
  
scores = cross_val_score(model, X, y, cv=5)
```

This will

- create $k = 5$ splits
- train k models
- return an array `score`
 - length k
 - one Performance Metric per split

Note

`cross_val_score` trains a model on a *subset* ($k - 1$ folds) of the training dataset

The state of `model` after this method is called

- is *probably* the model fit on the *last* split

It is used **only** to compute the (distribution) of the Performance Metric !

As a final step:

- fit the model on the *complete* training dataset
- this is the model that you will use for out of sample prediction

The typical work-flow

```
scores = cross_val_score(model, X, y, cv=5)
```

```
# Train the model using the training sets  
_ = model.fit(X, y)
```

In general you should be using Cross Validation in Classical ML in the absence of a good reason not to !

- helps you determine stability of your model's predictions
- once we get to Deep Learning:
 - training may be so expensive as to preclude the use of Cross Validation

Remember: you still have the Test set as the "gold standard"

Fine tune

There are often "tweaks" that can be applied to a near-final model in order to squeeze out increase performance.

For example: many models have *hyper parameters*.

These are values that are *chosen* at model construction, rather than *discovered* by fitting during training (Θ)

- the degree d of the polynomial when constructing higher order features \mathbf{x}^d
- whether to include/exclude the intercept Θ_0 in a Linear Regression
- strength of the regularization penalty (coming attraction: to be discussed together with the Loss function)
- the k in K Nearest Neighbors

Perhaps a different choice of a hyper-parameter would improve the model ?

We can try many choices before settling on the one giving the best Performance Metric.

Hyper parameters search is another reason for using Cross Validation

- we can't use the Test set more than once
- with a single Validation set: we might overfit to the validation set
 - that is, choose a value for the hyper parameter that is best for this *single* validation set

We encourage you to do a Deeper Dive by examining the topic of [Fine Tuning](#)
[\(Fine_tuning.ipynb\)](#).

Recap

- We have briefly detailed the multi-step process for Machine Learning
- This should be a model for you (and your assignments !)
- We will explore some of the steps in greater depth in future modules.

In [32]: `print("Done !")`

Done !

