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

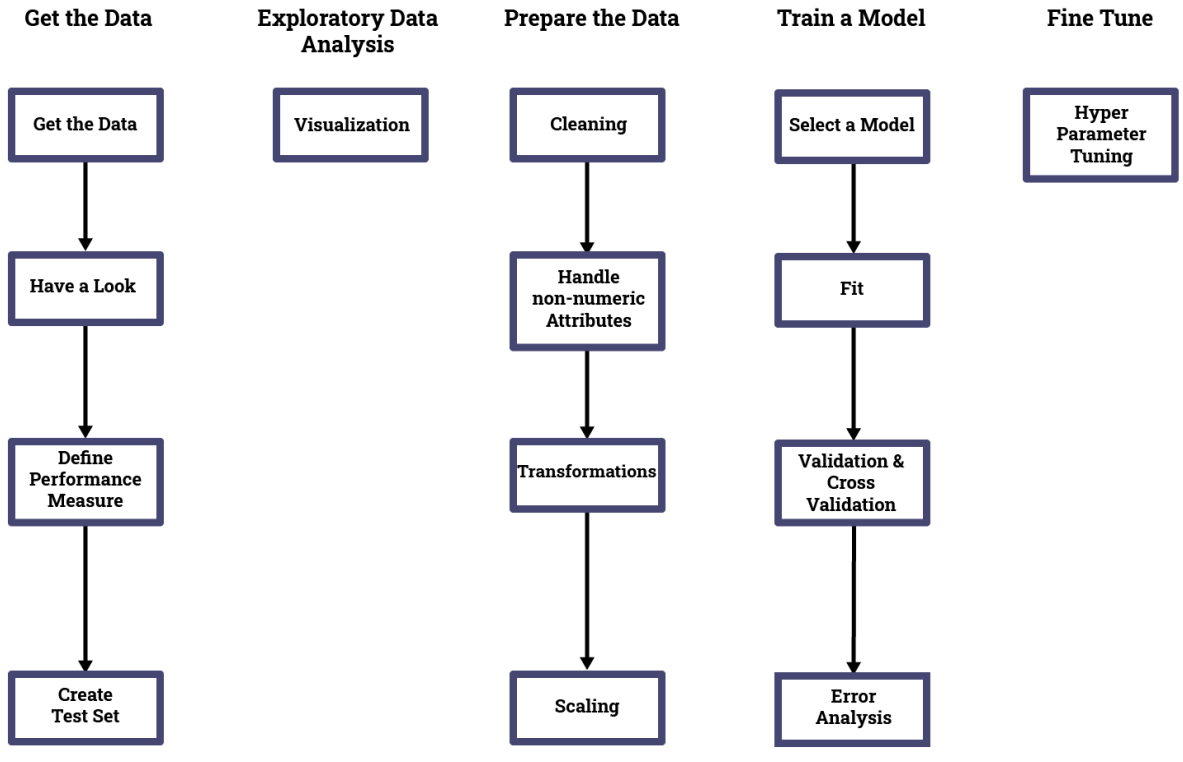
- introduce our systematic approach
- and illustrate it using Linear Regression as the chosen model

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 $\langle \mathrm{Size}, \mathrm{Price} \rangle$ 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 Θ

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):

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

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

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

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

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

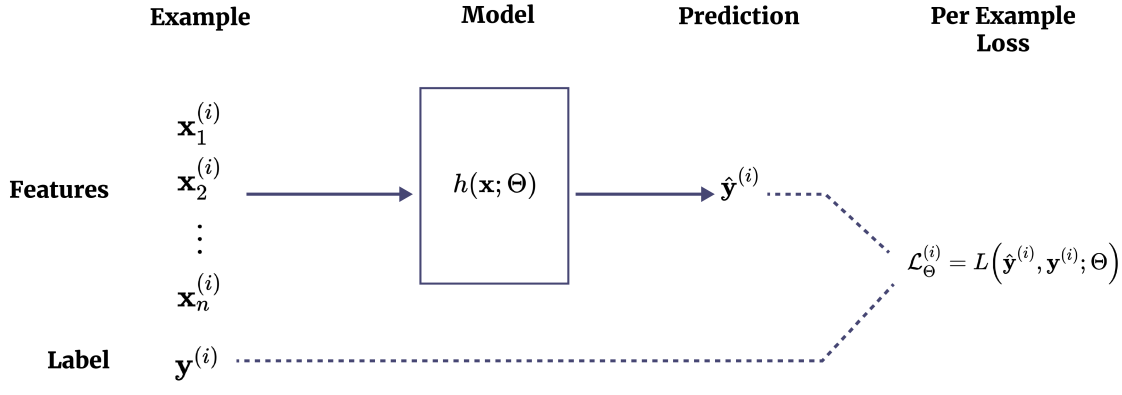
To be clear

- 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

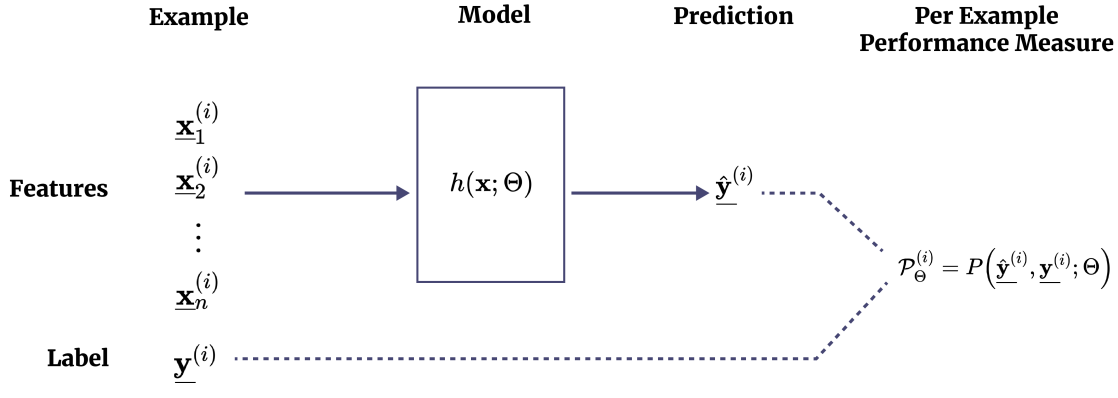
To illustrate, let

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

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

In [9]:

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

X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                    random_state=lr_demo.seed,
                                                    test_size=0.2,
                                                    shuffle=True)
```

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

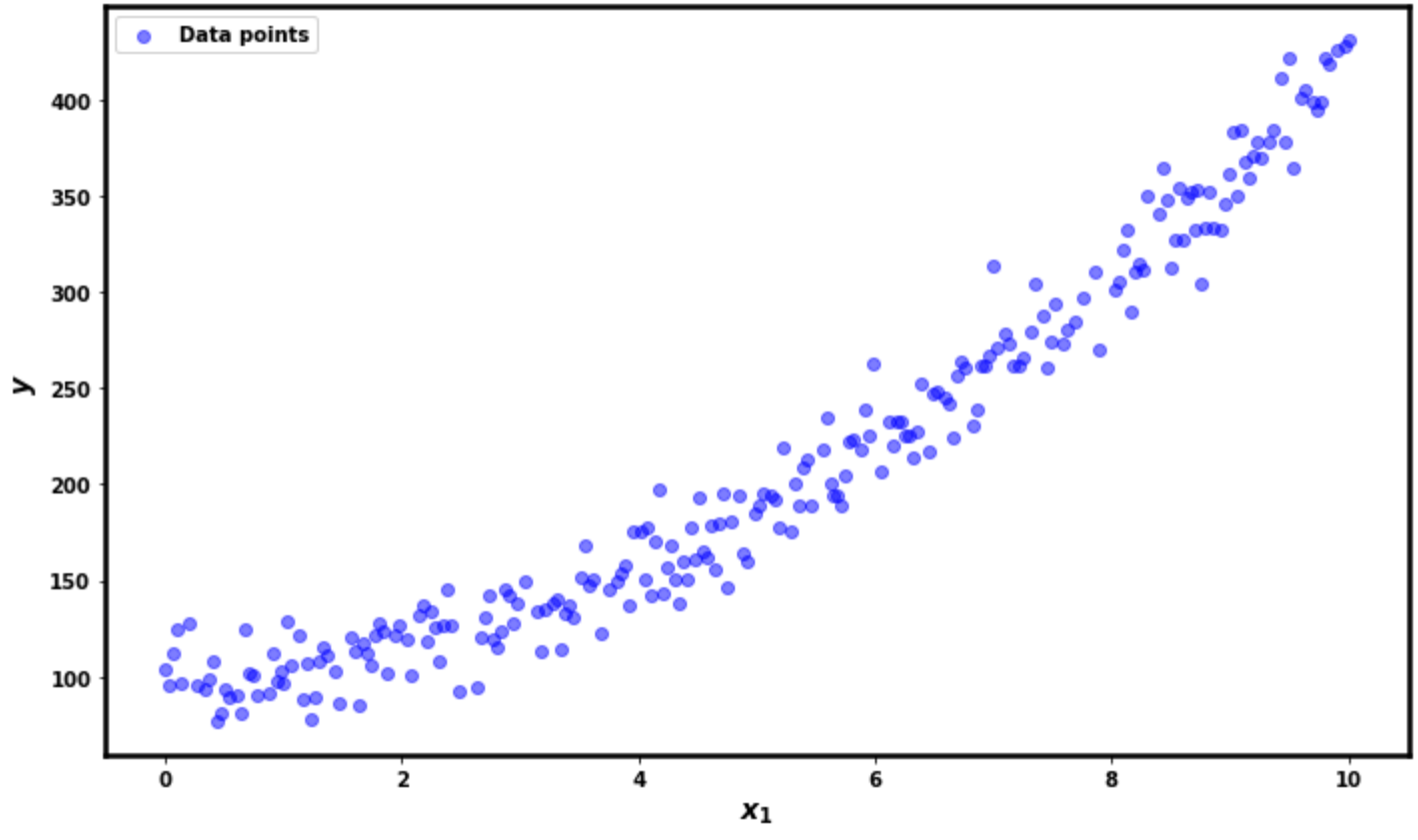
In [12]:

```
# 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()
```


Data points
400
350
300
250
200
150
100
y
0
2
4
6
8
10
x_1

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

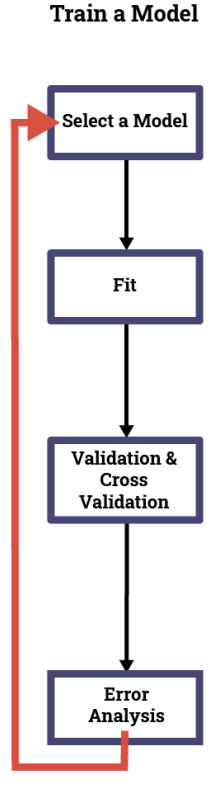
Train a model

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 !


Train a Model
Select a Model
Fit
Validation & Cross Validation
Error Analysis

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 noting 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: $(\mathrm{Size}, \mathrm{Price})$ 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[:, [0]] rather than X_train[:,
0] to ensure the result is 2D
# - with a singlteon 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

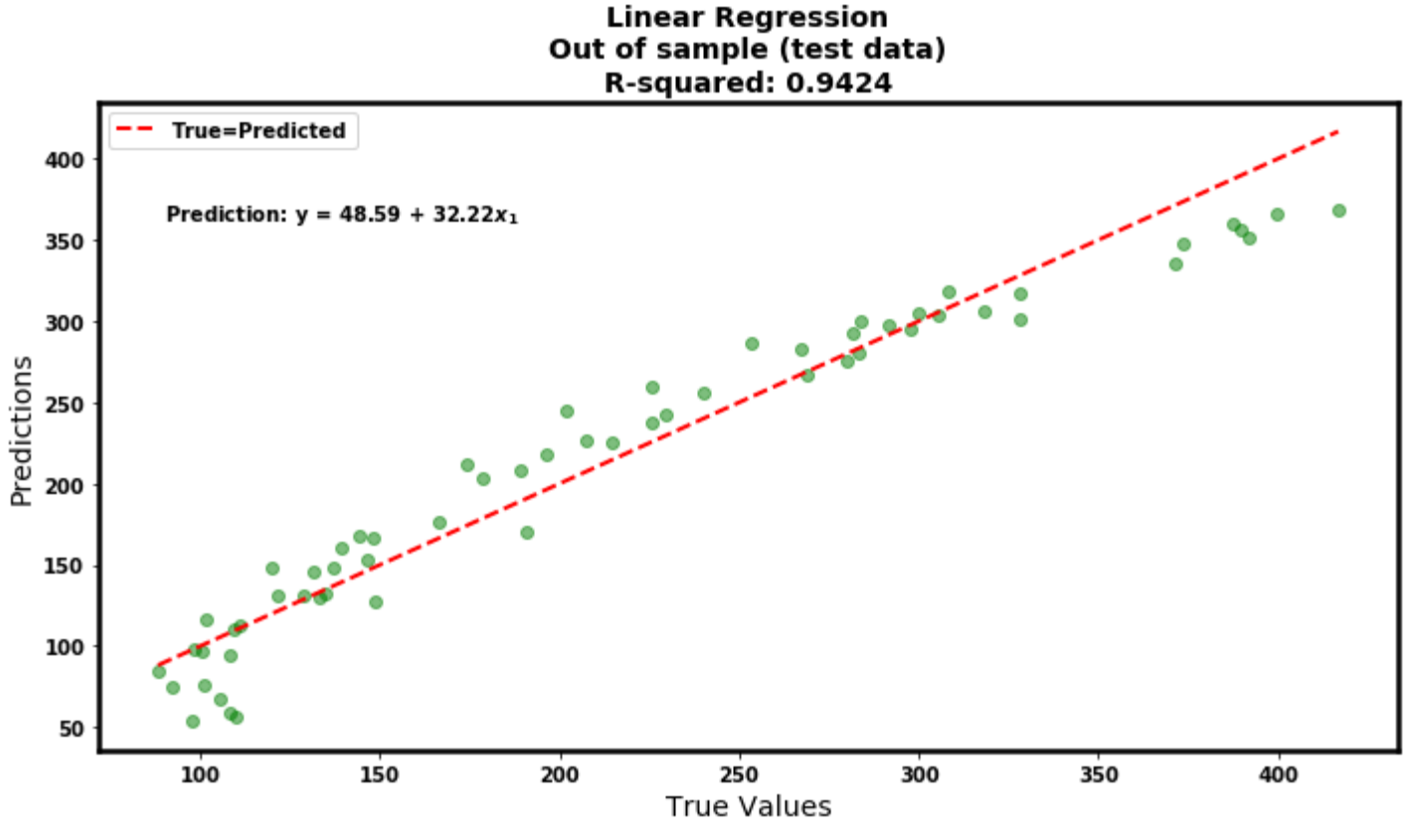
- How does our fitted model perform out of sample ?
- That is
    - compute the Performance Metric (out of sample)

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

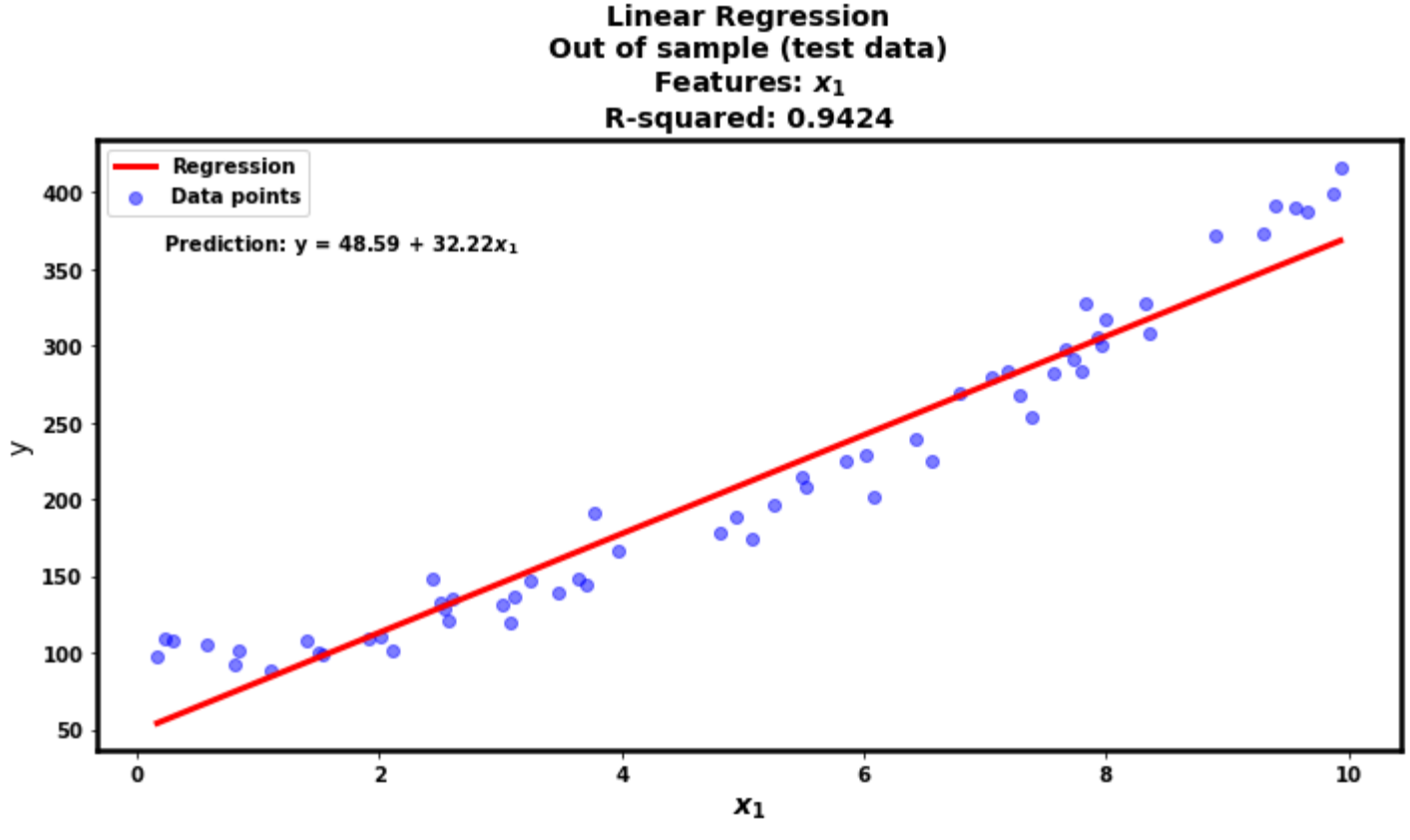
But observe a systematic mis-estimation

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

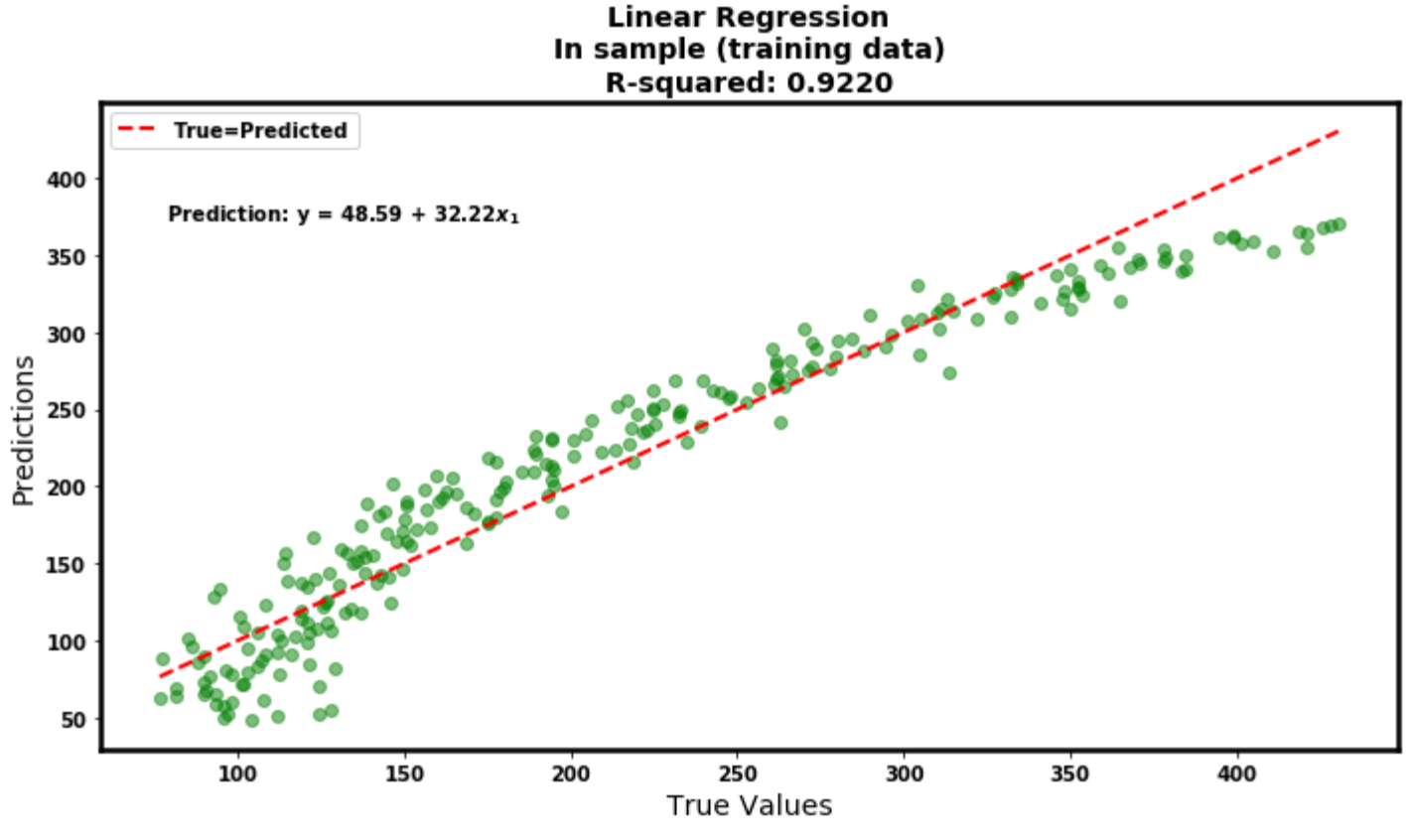
- will lead to it being removed from the Performance Metric (out of sample)

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_na
mes=["$x_1$"],
                                     title="Linear Regression\nIn sample (traini
ng data)\n")
```

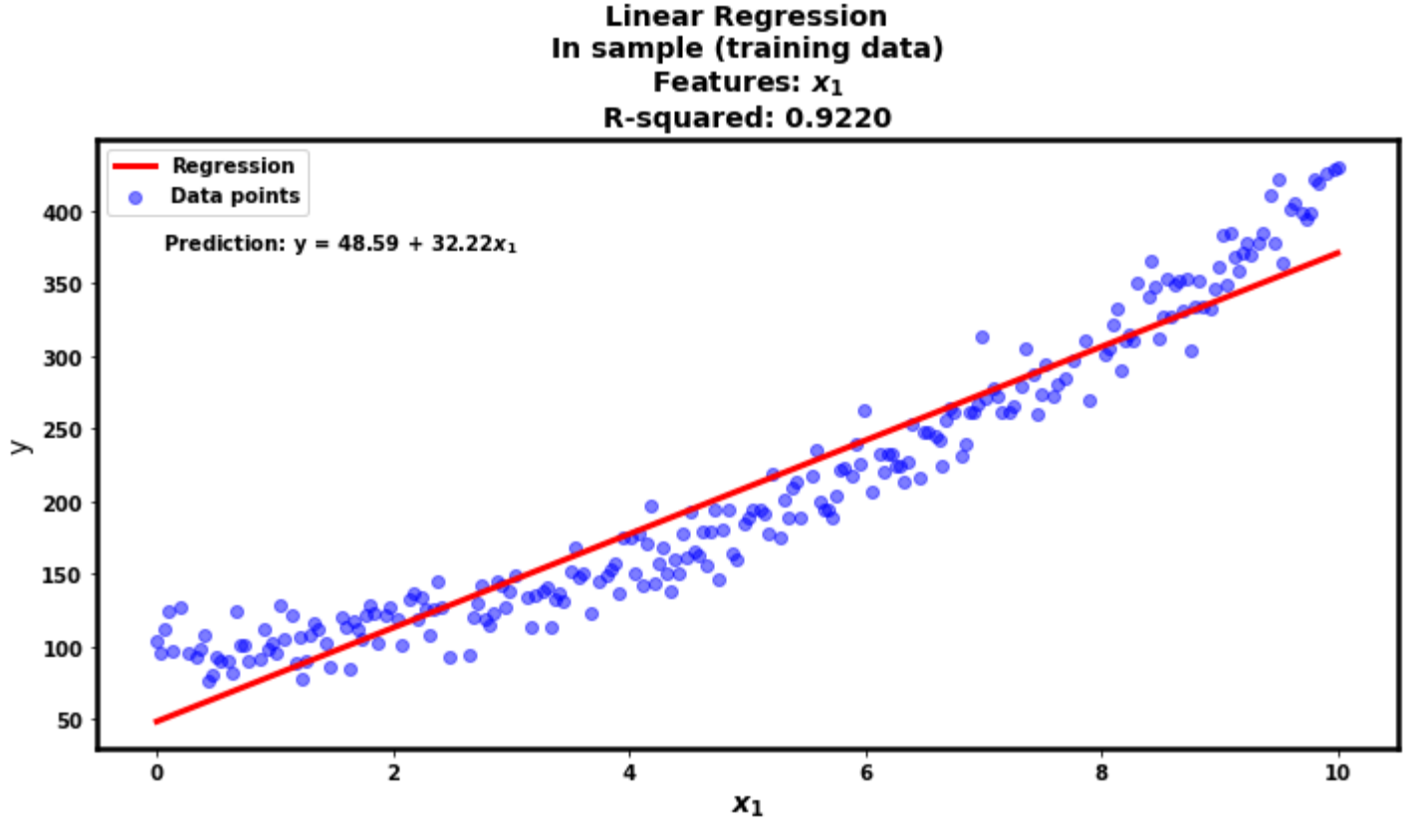


We can see a similar pattern of mis-estimation in the training dataset as we saw in the test dataset.

- 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

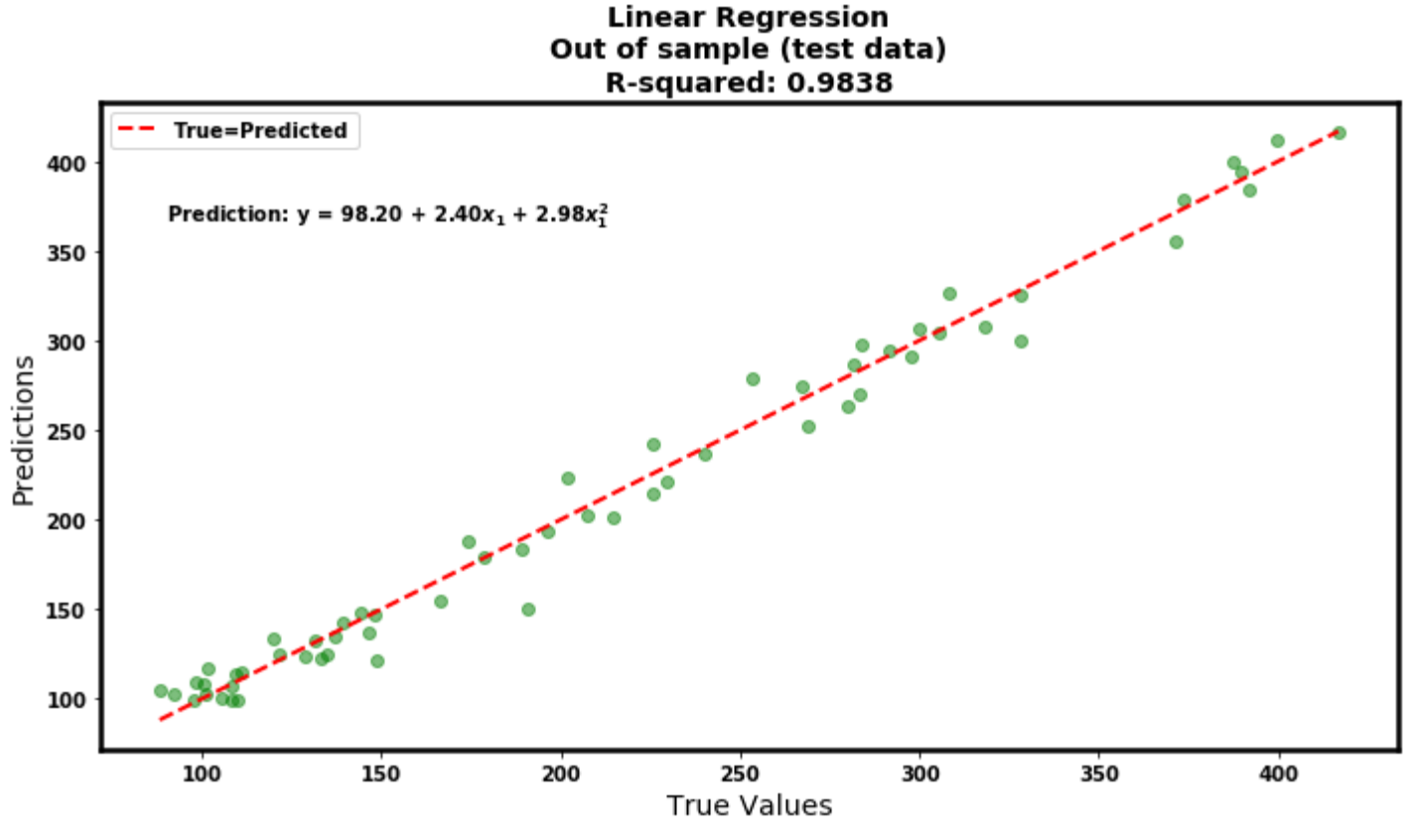
Also notice

- 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")
```



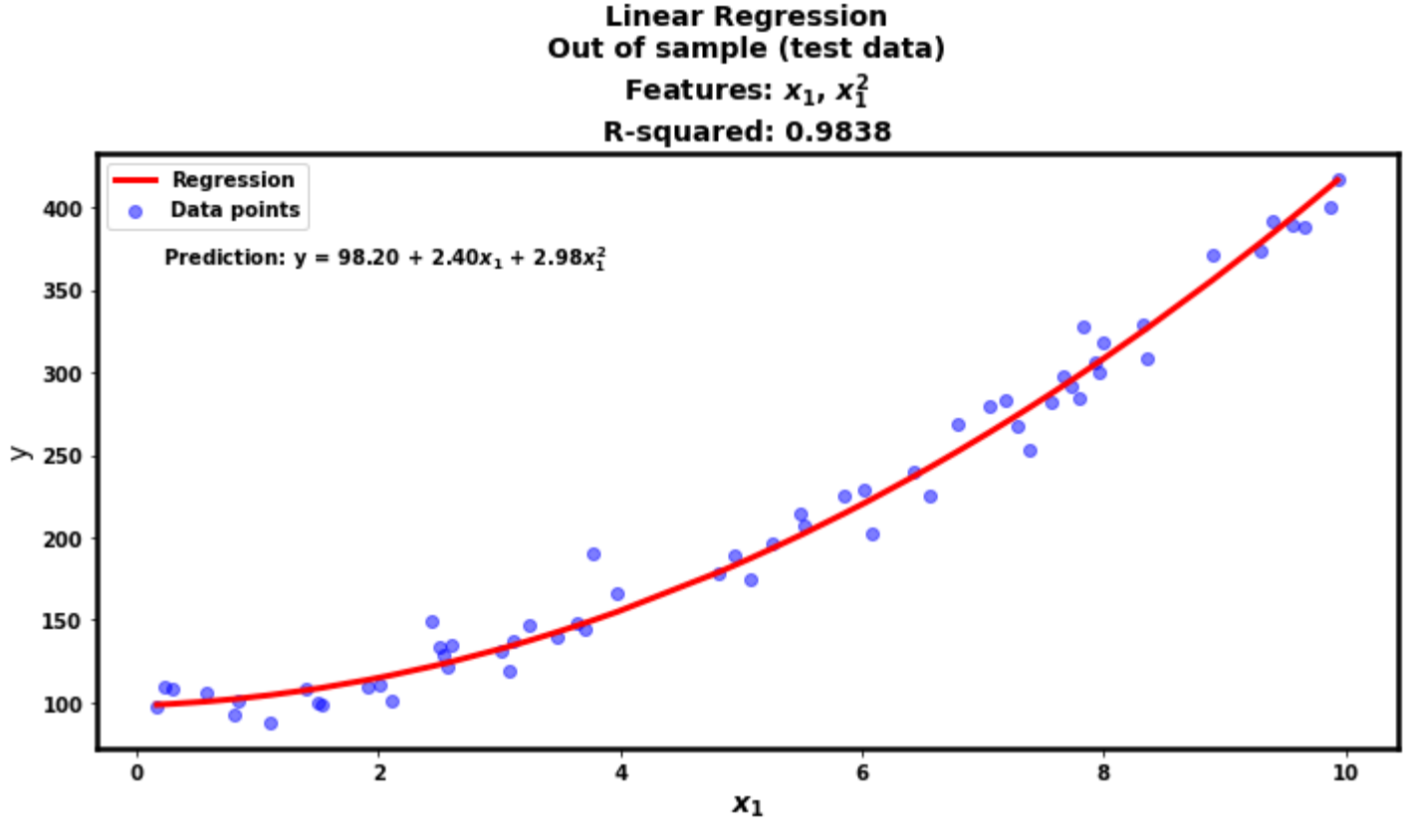
The Performance Metric has increased !

- adding the new feature helped

We also no longer see the systematic mis-estimation.

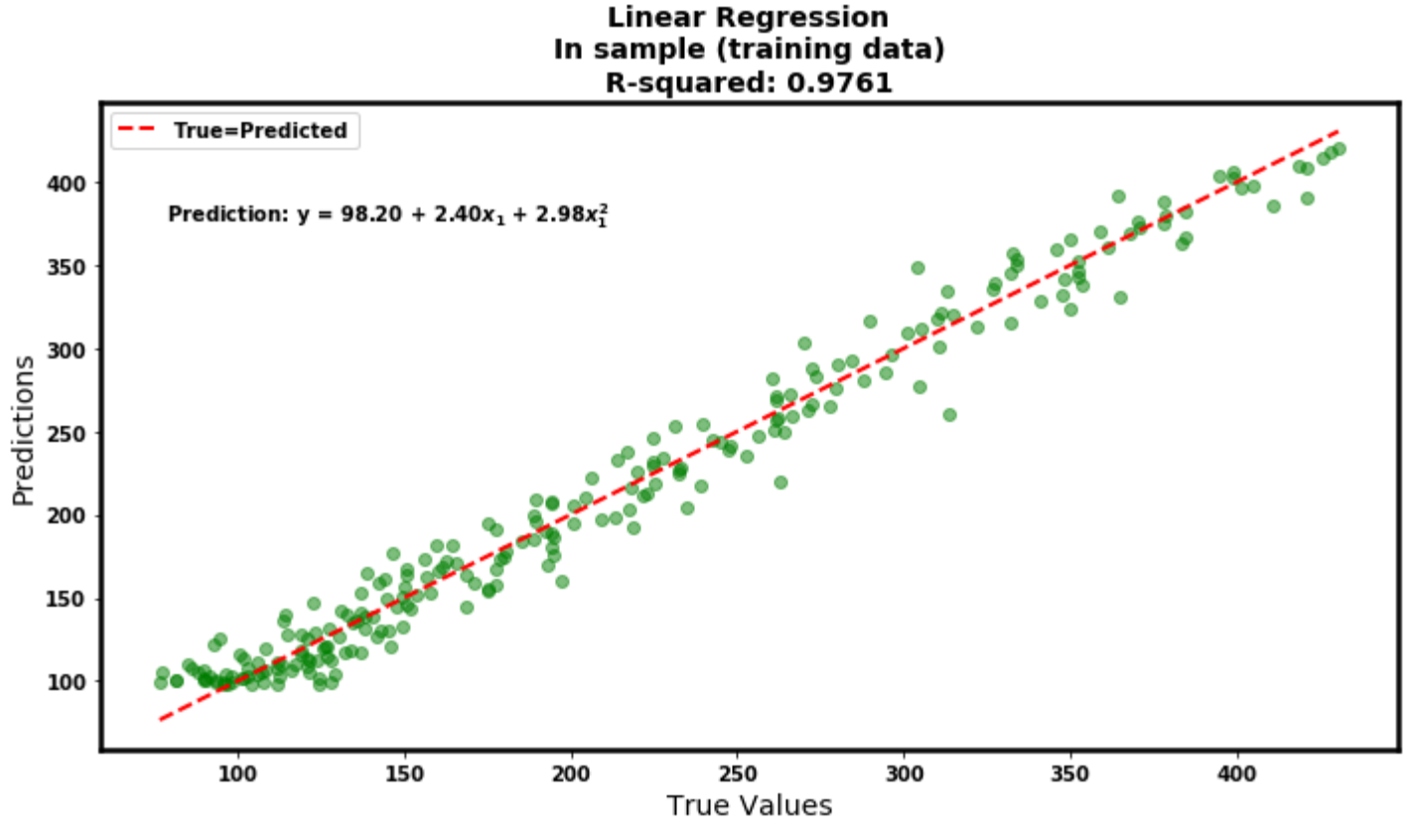
We can also visualize this as a function of one feature (x_1)

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)
```



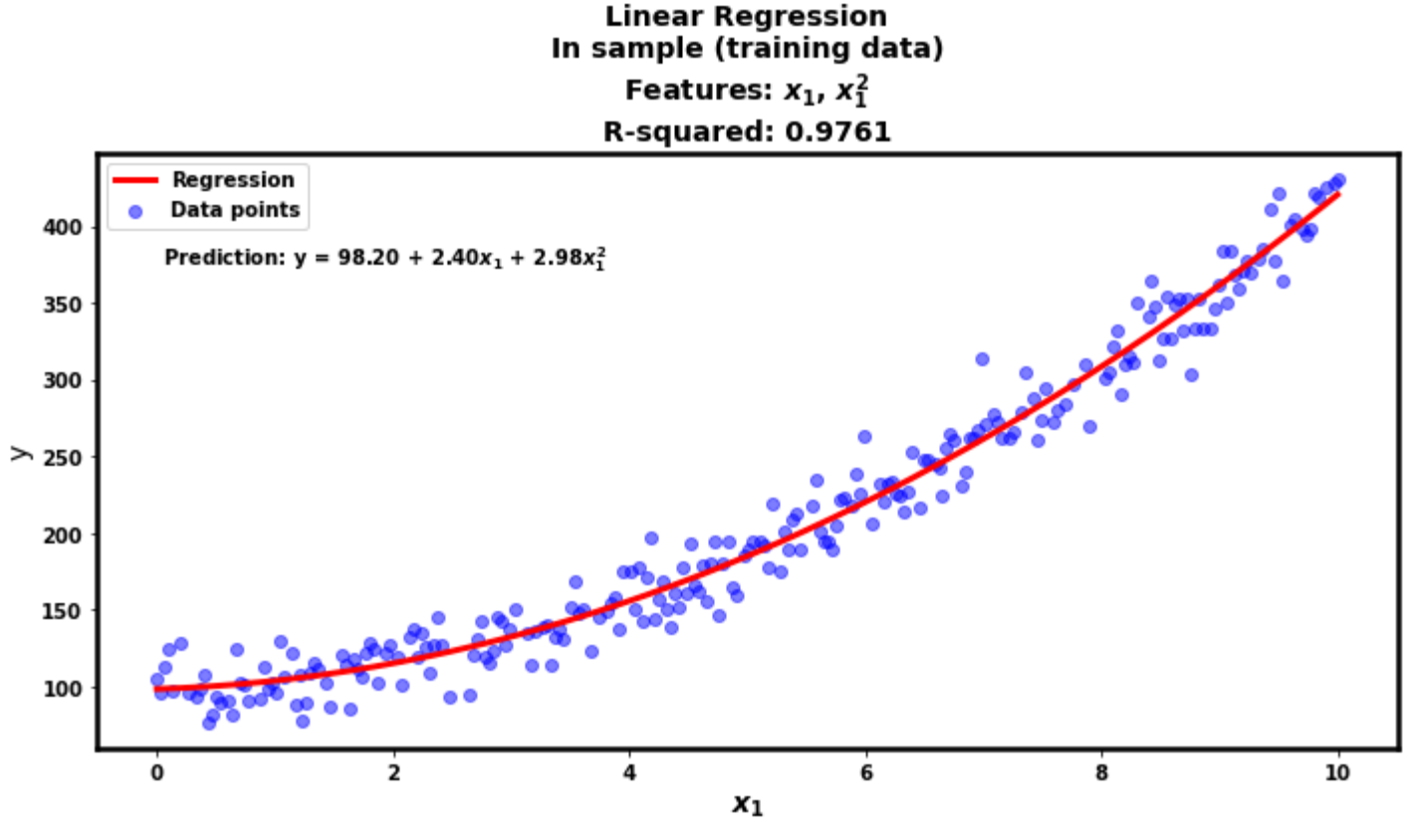
Let's perform Error Analysis on this revised model

In [21]:
```
fig, ax =  lr_demo.plot_pred_vs_true(model, y_train, X_train_with_sq, feature_na
mes=["$x_1$", "$x_1^2$"],
                                     title="Linear Regression\nIn sample (traini
ng 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 $\hat{\mathbf{y}}$ 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_wi
th_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('$x_1^2$')
```

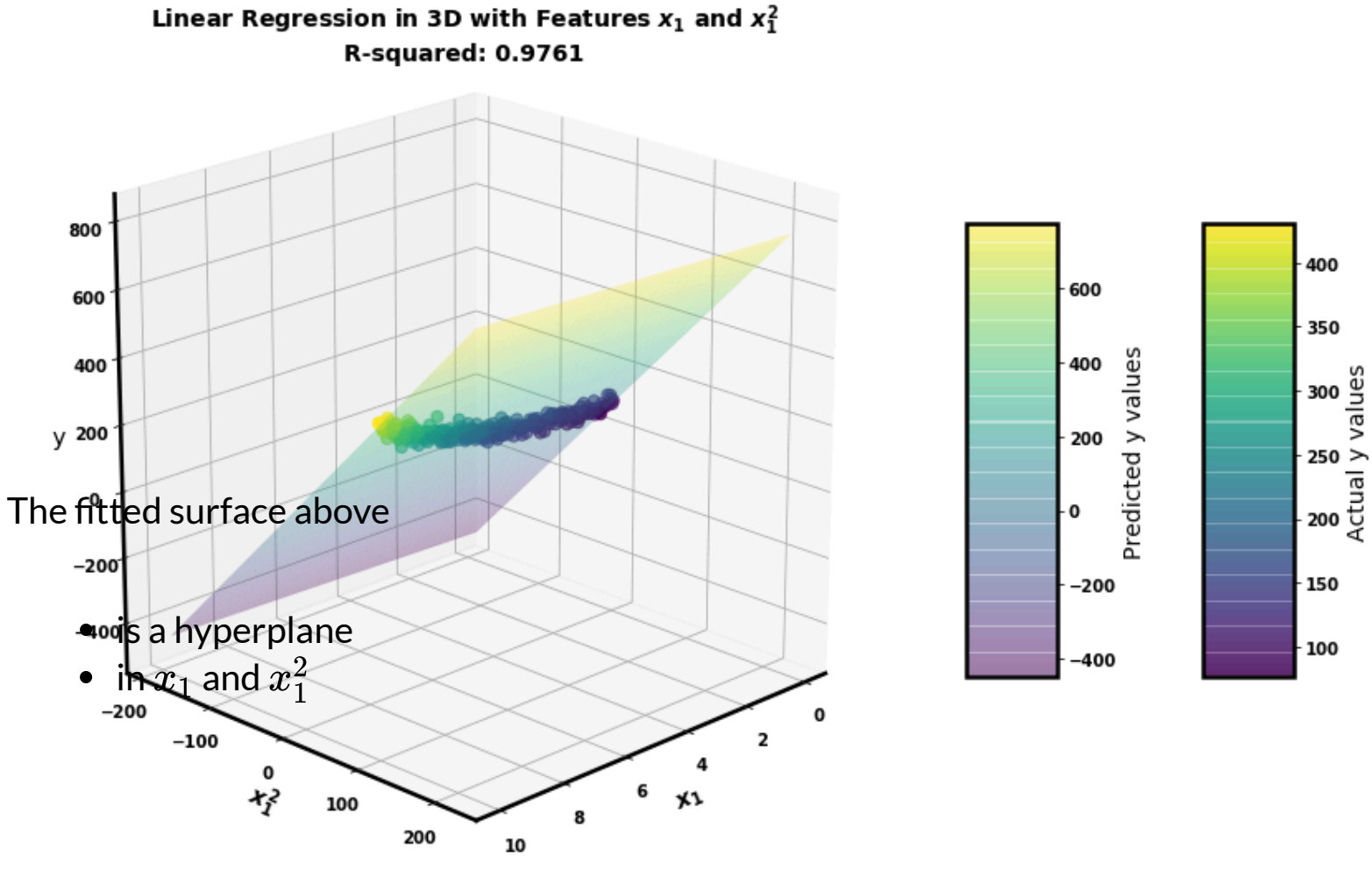
```
_= ax.set_zlabel('y')
_= ax.set_title(f'Linear Regression in 3D with Features $x_1$ and $x_1^2$\nR-squ
ared: {r_squared:.4f}')

# 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}")
```



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

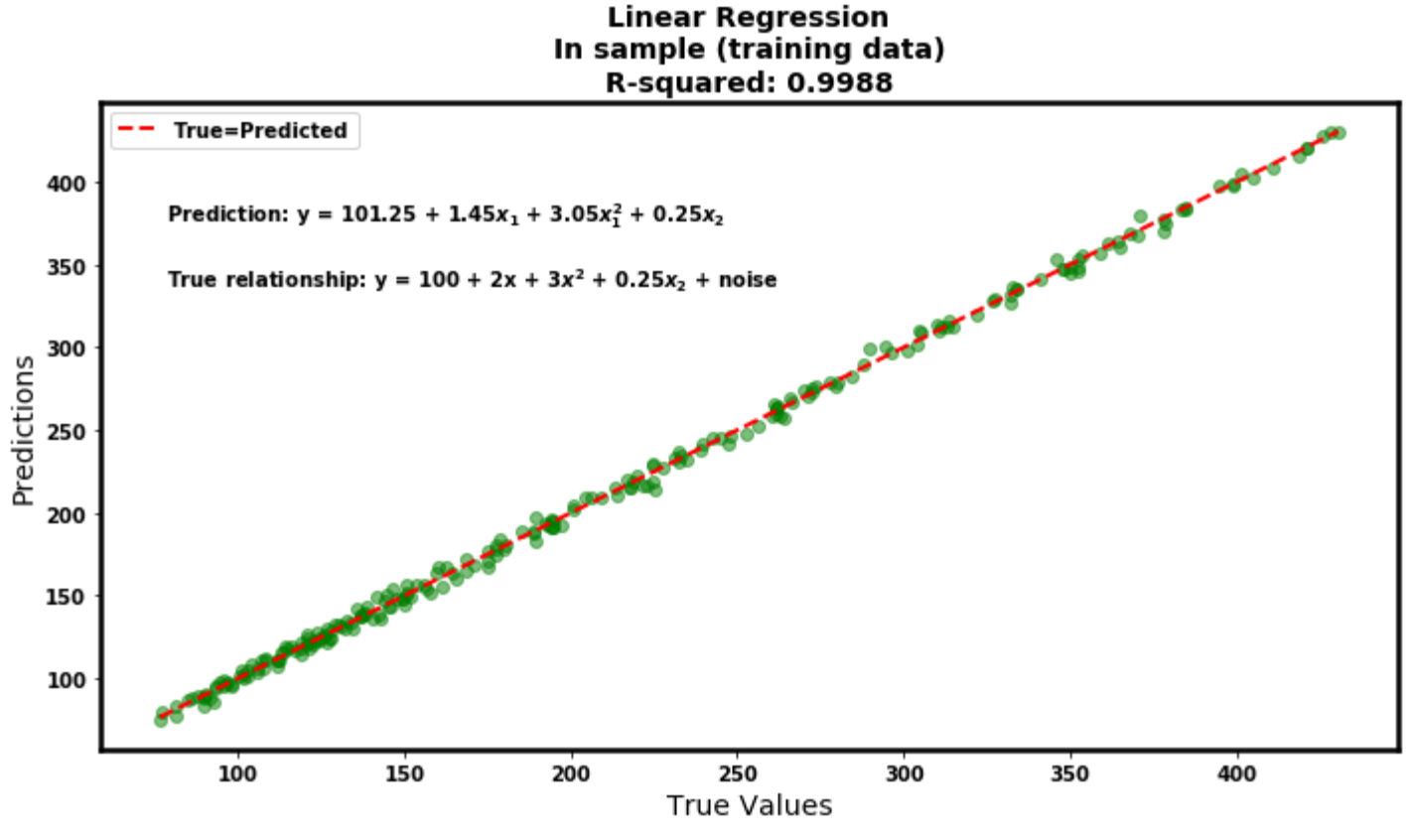
Let's imagine that we hypothesized that this was a useful feature and added it to our model.

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)
```

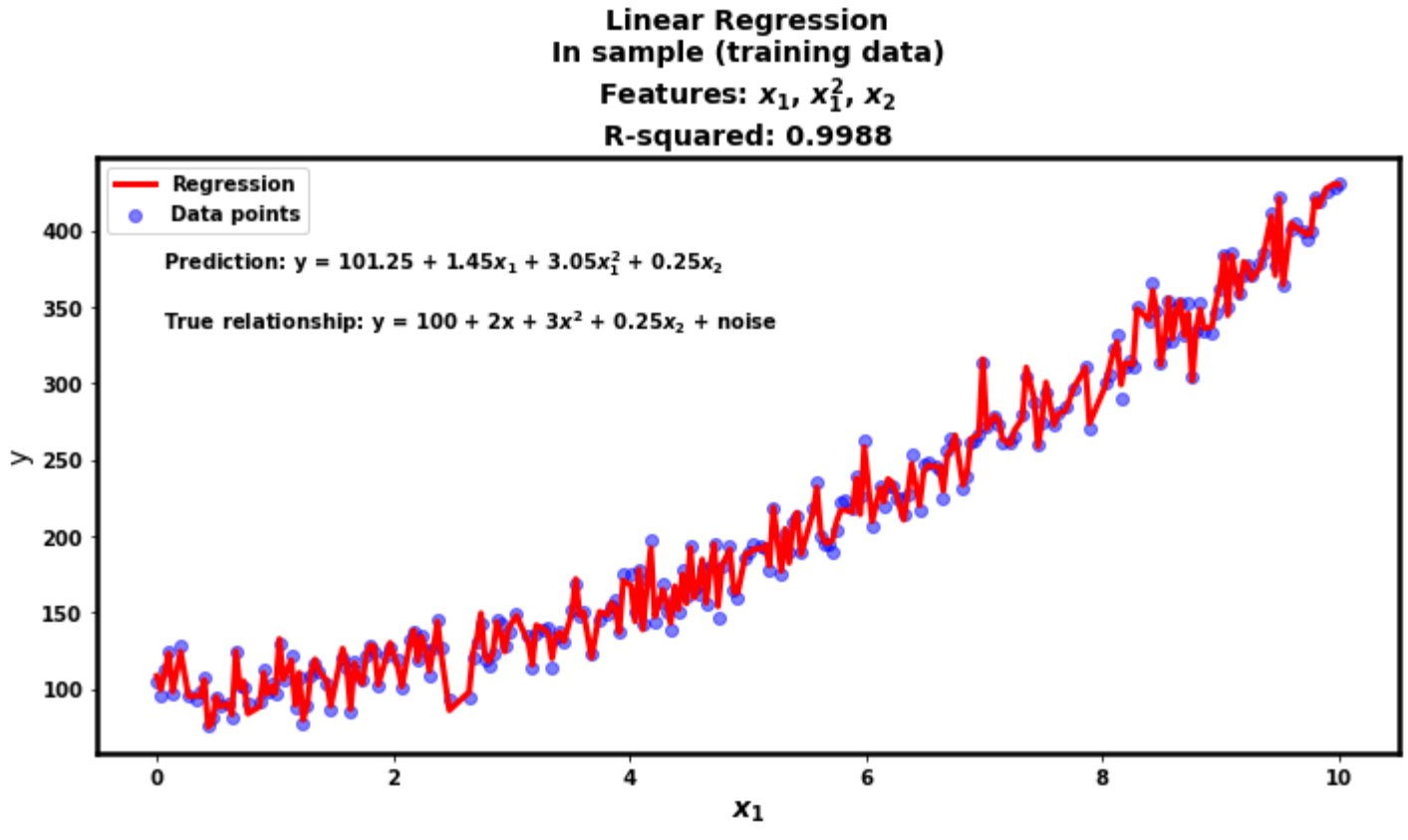
In [25]:
```
fig, ax =  lr_demo.plot_pred_vs_true(model, y_train, X_train_full, feature_names
=["$x_1$", "$x_1^2$", "$x_2$"], showTrue=True,
                                     title="Linear Regression\nIn sample (traini
ng data)\n")
```



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

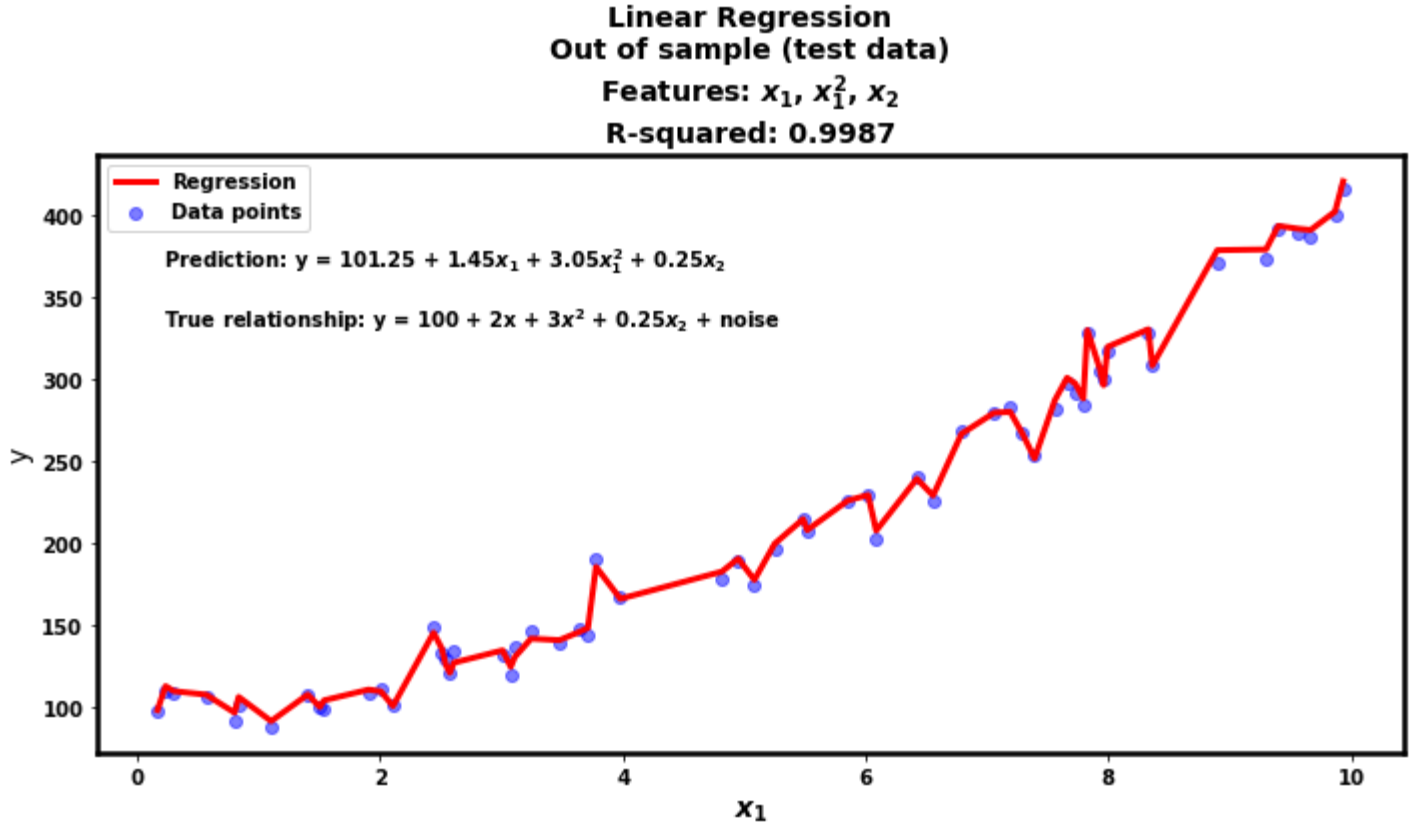
In [26]:
```
fig, ax = lr_demo.plot(model, y_train, X_train_full, feature_names=["$x_1$", "$x_1^2$", "$x_2$"],
                       title="Linear Regression\nIn sample (training data)\n",
                       showTrue=True)
```



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()
```

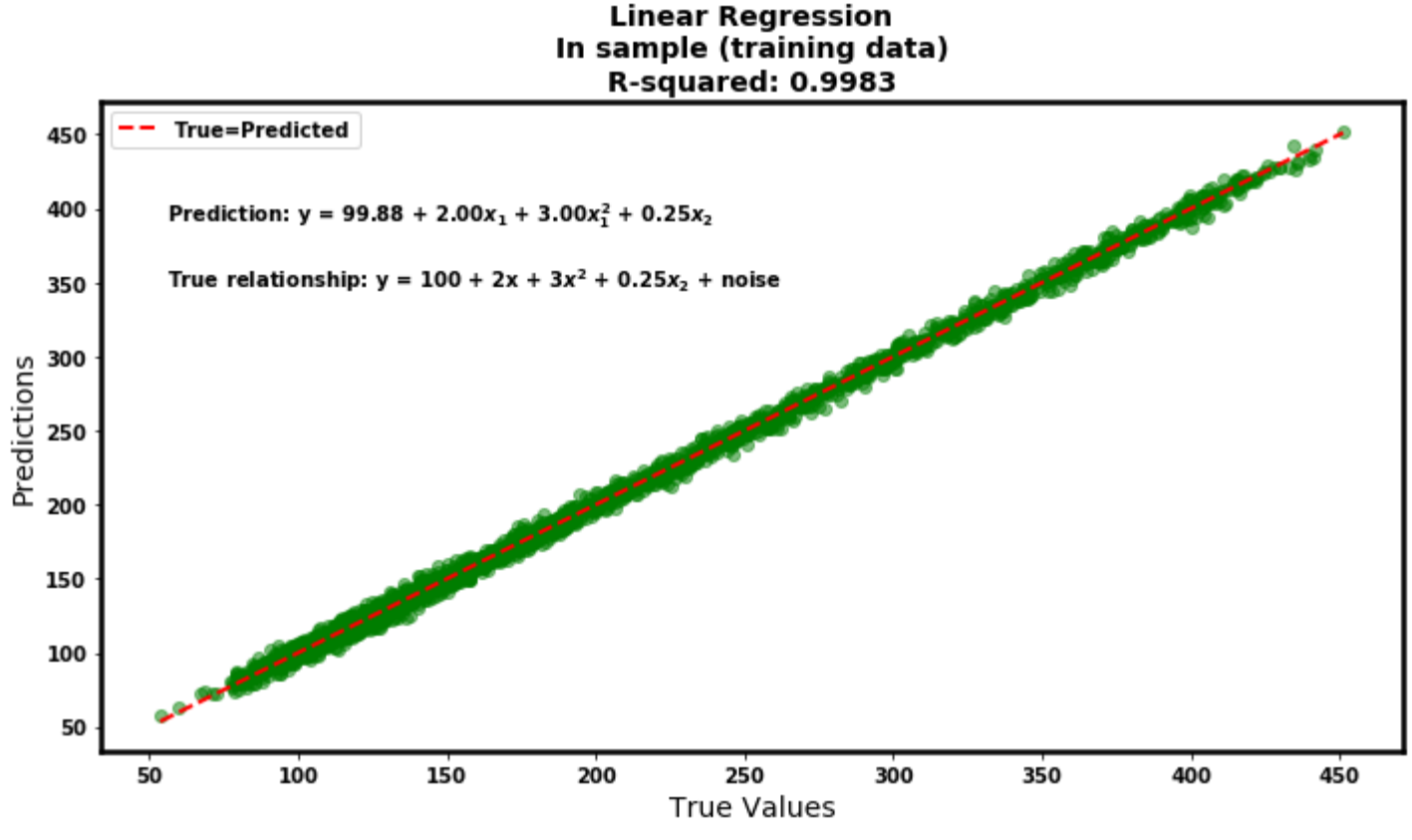
In [29]:
```
X_train, X_test, y_train, y_test = train_test_split(X, y,
                                                    random_state=lr_demo.seed,
                                                    test_size=0.2,
                                                    shuffle=True)
```

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_n
ames=["$x_1$", "$x_1^2$", "$x_2$"],
                                         showTrue=True,
                                         title="Linear Regression\nIn sample (tr
aining 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/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

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 predicto

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 !
```