OLS with Gradient Descent

Prerequisites

- Tensorflow
- Linear models
- Gradient Descent

Outcomes

- Understand how gradient descent can be applied to machine learning models
- See how to use gradient descent to find parameters of OLS model
- Be introduced to `tf.keras` high level API

In [3]:

```
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
import seaborn as sns
sns.set()

import tensorflow as tf
from tensorflow.keras.layers.experimental import preprocessing
```

Gradient Descent

- First order method for local non-linear optimization
- Given a domain $X \subseteq \mathbb{R}^D$ and a function $f : X \to \mathbb{R}$
- Iterative updates according to gradient (∇f) and learning rate (α):

$$x' = x - \alpha \nabla f(x)$$

- Can be applied for arbitrary non-linear optimization problems

Application to ML

- Ingredients to supervised learning:
  1. Cleaned/transformed data $(x_i, y_i)_{i=1}^N$
  2. Choice of model $\hat{y} = f(x; \theta)$
  3. Choice of loss function $\ell(y, \hat{y})$
  4. Strategy/algorithm for updating parameters θ to minimize $\ell(y, \hat{y})$
- We will use gradient descent as part 4

Dataset

- We'll use a dataset presented in a tensorflow tutorial
- Label: miles per gallon for car
- Features: car/engine characteristics

In [4]:

```
url = 'http://archive.ics.uci.edu/ml/machine-learning-databases/auto-mpg/auto-mpg.data'
column_names = ['MPG', 'Cylinders', 'Displacement', 'Horsepower', 'Weight',
                'Acceleration', 'Model Year', 'Origin']

raw_dataset = pd.read_csv(url, names=column_names,
                          na_values='?', comment='\t',
                          sep=' ', skipinitialspace=True)

dataset = raw_dataset.copy().dropna()
dataset.tail()
```

Out[4]:

	MPG	Cylinders	Displacement	Horsepower	Weight	Acceleration	Model Year	Origin
393	27.0	4	140.0	86.0	2790.0	15.6	82	1
394	44.0	4	97.0	52.0	2130.0	24.6	82	2
395	32.0	4	135.0	84.0	2295.0	11.6	82	1
396	28.0	4	120.0	79.0	2625.0	18.6	82	1
397	31.0	4	119.0	82.0	2720.0	19.4	82	1

Split and Plot Data

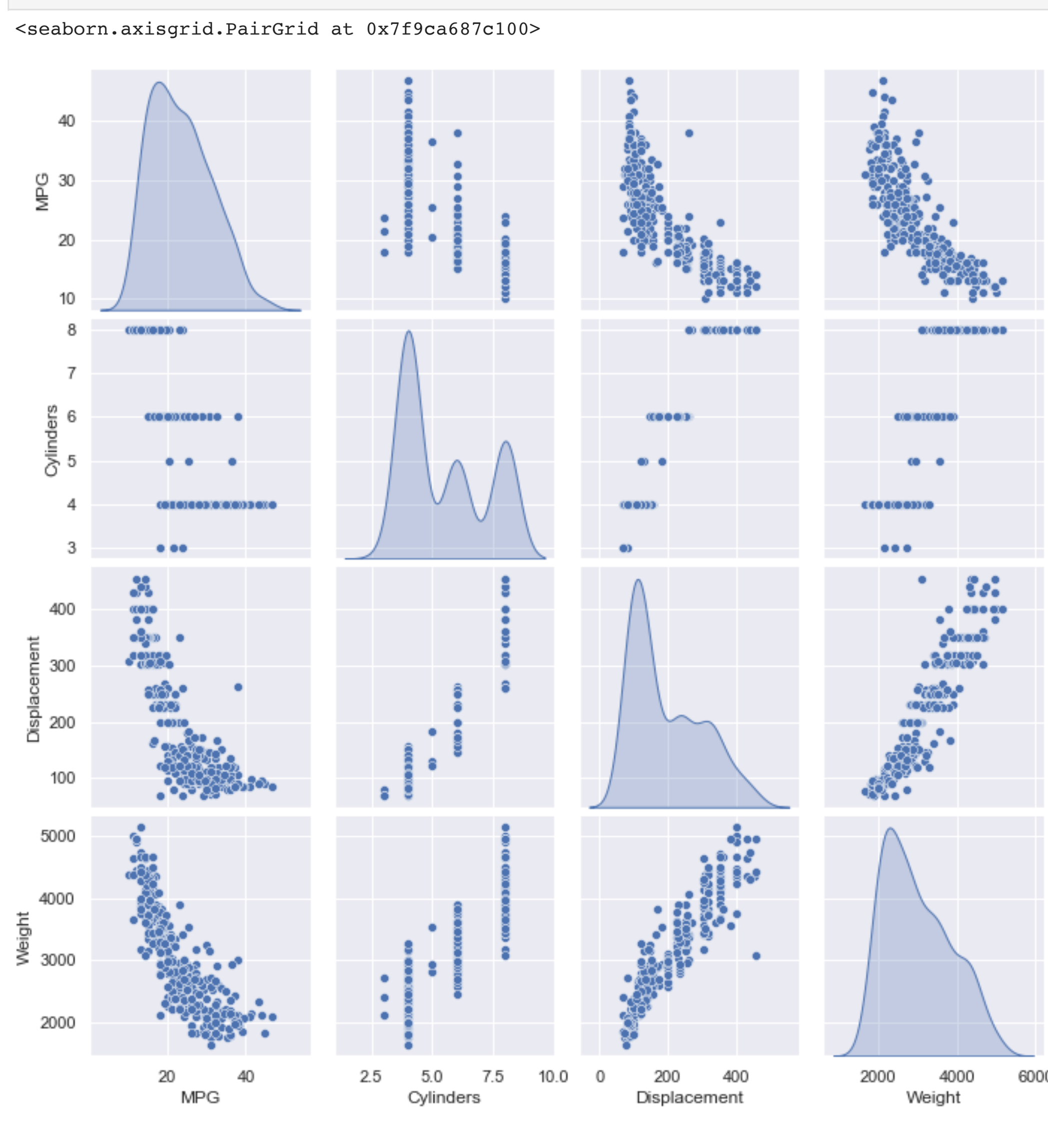
In [5]:

```
train_dataset = dataset.sample(frac=0.8, random_state=0)
test_dataset = dataset.drop(train_dataset.index)
```

In [6]:

```
sns.pairplot(train_dataset[['MPG', 'Cylinders', 'Displacement', 'Weight']], diag_kind='kde')
```

Out[6]: <seaborn.axisgrid.PairGrid at 0x7f9ca687c100>



Separate Features and Targets

- We'll try to predict MPG using the other features

In [7]:

```
train_features = train_dataset.copy()
test_features = test_dataset.copy()

train_labels = train_features.pop('MPG')
test_labels = test_features.pop('MPG')
```

Normalization

- We now need to normalize the features X to have mean 0 std 1
- We'll also convert the targets to `Tensor` s

In [8]:

```
normalizer = preprocessing.Normalization()
normalizer.adapt(train_features)
X = normalizer(train_features)
X_test = normalizer(test_features)

# convert y
y = tf.convert_to_tensor(train_labels, dtype="float32")
y_test = tf.convert_to_tensor(test_labels, dtype="float32")
```

OLS as Optimization Problem

- Let's use least squares on `df` in order to predict the MPG of a car
- In doing this, we'll transition to a notation used throughout the ML/DL literature
- The model will be:

$$\hat{y}_i = W x_i + b$$

  - W is a parameter vector (matrix) called *weights*
  - b is a parameter vector called *bias*
  - W and b together are the parameters we've been calling θ
- Loss function is MSE

OLS via gradient descent

- We are now ready to apply gradient descent to the OLS model

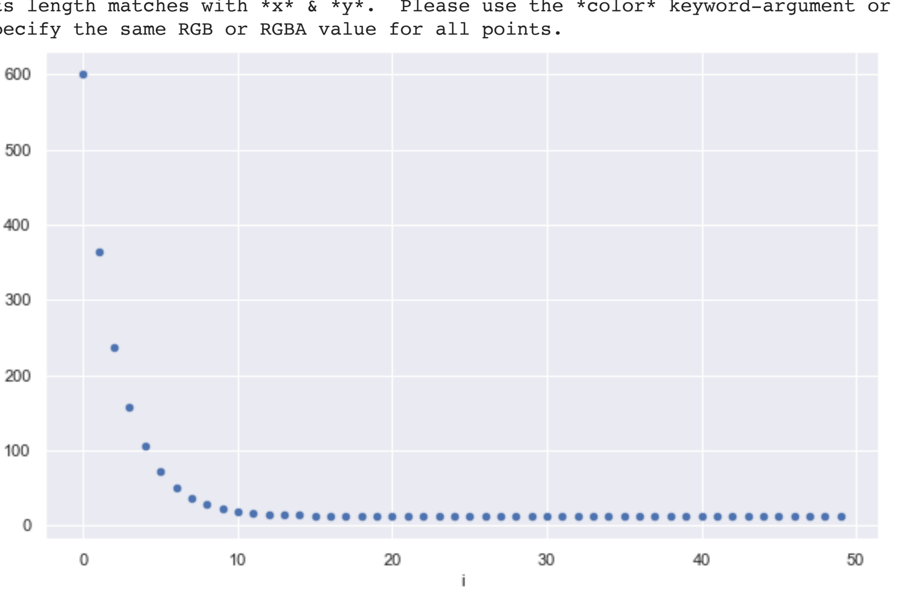
In [9]:

```
def grad_desc_tf_ols(X, y, T=200, alpha=0.1):

    # initialize weights and biases
    W = tf.Variable(np.random.randn(X.shape[1]).astype("float32"))
    b = tf.Variable([0.0])

    trace = []
    for i in range(T):
        # compute loss function
        with tf.GradientTape() as tape:
            yhat = tf.linalg.matvec(X, W) + b
            loss = tf.losses.mse(y, yhat)

        # compute gradients
        dW, db = tape.gradient(loss, [W, b])

        # apply update to each parameter using its gradient
        Wp = W - alpha * dW
        bp = b - alpha * db

        # book keeping
        err_theta = max(abs(bp - b), max(abs(Wp - W)))
        err = max(abs(db), max(abs(dW)))
        status = dict(
            i=i,
            loss=loss.numpy(),
            dW=dW.numpy(),
            db=db.numpy(),
            err=err.numpy(),
            err_theta=err_theta.numpy(),
            W=W.numpy(),
            b=b.numpy(),
        )
        trace.append(status)

        # update weights and biases for next iteration
        W = tf.Variable(Wp)
        b = tf.Variable(bp)

    return trace
```

In [10]:

```
trace = grad_desc_tf_ols(X, y, T=50)
pd.DataFrame(trace).plot.scatter(x="i", y="loss", figsize=(10,6));
```

```
*c* argument looks like a single numeric RGB or RGBA sequence, which should be avoided as value-mapping will have precedence in case its length matches with *x* & *y*.  Please use the *color* keyword-argument or provide a 2-D array with a single row if you intend to specify the same RGB or RGBA value for all points.
```



Using Keras

- Above we implemented OLS via gradient descent using lower level tensorflow primitives like `tf.linalg.matvec` and `tf.GradientTape()`
- This allowed us to build up the algorithm from first principles and control all the computations
- Sometimes this level of flexibility is needed, most of the time it isn't
- Tensorflow has a built in high-level API called `keras` that provides common modeling building blocks

Keras Sequential Models

- sklearn pipelines: data processing + modeling steps $\Rightarrow$ single "model"
- Separates responsibilities:
  - Library (sklearn): apply data transformations, parameters/variables
  - Us: describing data flow and model
- Keras (and its `Sequential` model) plays a similar role for tensorflow

OLS in Keras

- To see how keras works, we'll replicate our OLS example

Model

- Recall we used the OLS model $y = Wx + b$
- This is built into keras as the `Dense` layer
- We can combine our `normalizer` and a `Dense` layer into a `Sequential` model

In [11]:

```
model = tf.keras.Sequential([
    normalizer,
    tf.keras.layers.Dense(1)
])

model.summary()
```

```
Model: "sequential"
_________________________________________________________________
 Layer (type)                Output Shape              Param #
=================================================================
 normalization (Normalizatio  (None, 7)                15
 n)

 dense (Dense)               (None, 1)                 8

=================================================================
Total params: 23
Trainable params: 8
Non-trainable params: 15
_________________________________________________________________
```

Optimizer and Loss

- Optimizer
  - Keras has a number of gradient descent variants in the `tf.keras.optimizers` package
    - We learn about these variants in SGD video!
  - Can use `tf.keras.optimizers.SGD` for gradient descent
- `.compile`
  - The `.compile` method allows us to specifiy an optimizer and a loss
  - We'll use SGD and MSE

In [12]:

```
model.compile(
    optimizer=tf.optimizers.SGD(learning_rate=0.1),
    loss='mean_squared_error'
)
```

Training

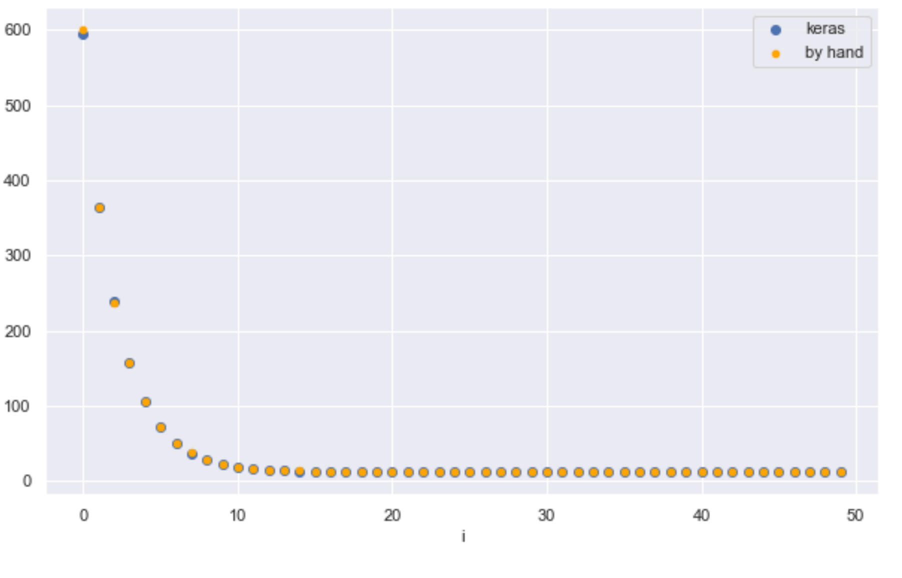
- Now that the model has been compiled (linked to loss and optimizer), we are ready to train
- We use the `.fit` method, which will produce a trace

In [13]:

```
trace_tf = model.fit(
    train_features, train_labels,
    batch_size=train_features.shape[0],  # for normal gradient descent
    epochs=50,
    # suppress logging
    verbose=0,
    # Calculate validation results on 20% of the training data
    validation_data=(test_features, test_labels),
)
```

In [14]:

```
fig, ax = plt.subplots(figsize=(10, 6))
ax.scatter(np.arange(len(trace_tf.history["loss"])), trace_tf.history["loss"]);
pd.DataFrame(trace).plot.scatter(x="i", y="loss", ax=ax, c="orange");
ax.legend(["keras", "by hand"]);
```



Review: full code

- The keras version allowed us to abstract away many of the details
- Below we have reproduced all the keras code to see how easy it was:

```
# define model
model = tf.keras.Sequential([
    normalizer,
    tf.keras.layers.Dense(1)
])

# compile: link model to loss and optimizer
model.compile(
    optimizer=tf.optimizers.SGD(learning_rate=0.1),
    loss='mean_squared_error'
)

# fit model
trace_tf = model.fit(
    train_features, train_labels,
    batch_size=train_features.shape[0],  # for normal gradient descent
    epochs=50,
    # suppress logging
    verbose=0,
    # Calculate validation results on 20% of the training data
    validation_data=(test_features, test_labels),
)
```

- The benefits we get from using keras will compound as we fit more involved models and/or use more extensive optimization algorithms