Linear Regression with PyTorch

In this section we'll use PyTorch's machine learning model to progressively develop a best-fit line for a given set of data points. Like most linear regression algorithms, we're seeking to minimize the error between our model and the actual data, using a *loss function* like mean-squared-error.

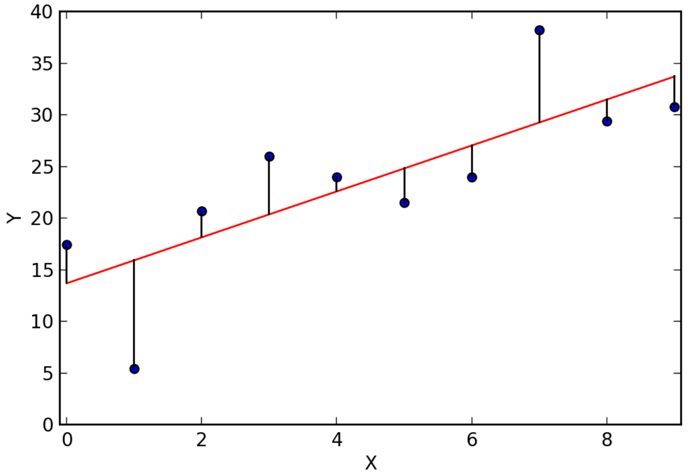


Image source: [https://commons.wikimedia.org/wiki/File:Residuals_for_Linear_Regression_Fit.png (https://commons.wikimedia.org/wiki/File:Residuals_for_Linear_Regression_Fit.png)](https://commons.wikimedia.org/wiki/File:Residuals_for_Linear_Regression_Fit.png)

To start, we'll develop a collection of data points that appear random, but that fit a known linear equation $y = 2x + 1$

Perform standard imports

In [1]:

```
import torch
import torch.nn as nn  # we'll use this a lot going forward!

import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
```

Create a column matrix of X values

We can create tensors right away rather than convert from NumPy arrays.

In [2]:

```
X = torch.linspace(1,50,50).reshape(-1,1)

# Equivalent to
# X = torch.unsqueeze(torch.linspace(1,50,50), dim=1)
```

Create a "random" array of error values

We want 50 random integer values that collectively cancel each other out.

In [3]:

```
torch.manual_seed(71) # to obtain reproducible results
e = torch.randint(-8,9,(50,1),dtype=torch.float)
print(e.sum())
```

```
tensor(0.)
```

Create a column matrix of y values

Here we'll set our own parameters of $\text{weight} = 2, \ \text{bias} = 1$, plus the error amount.
y will have the same shape as **X** and **e**

In [4]:

```
y = 2*X + 1 + e
print(y.shape)
```

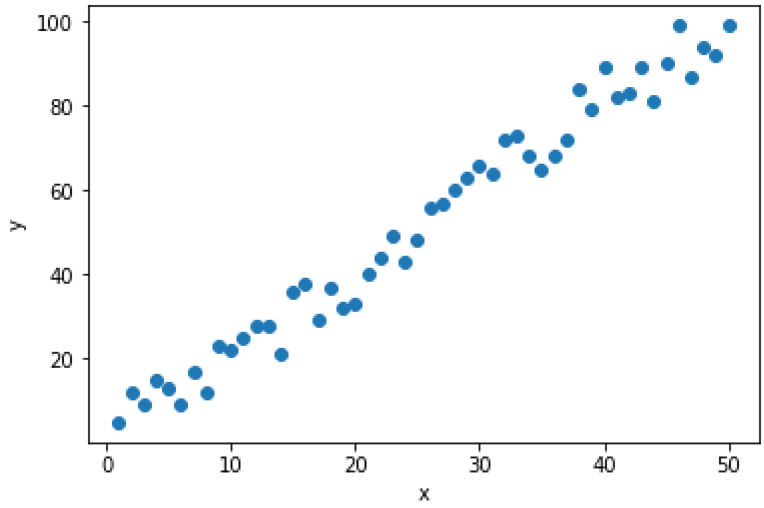
```
torch.Size([50, 1])
```

Plot the results

We have to convert tensors to NumPy arrays just for plotting.

In [5]:

```
plt.scatter(X.numpy(), y.numpy())
plt.ylabel('y')
plt.xlabel('x');
```



Note that when we created tensor X, we did *not* pass `requires_grad=True`. This means that y doesn't have a gradient function, and `y.backward()` won't work. Since PyTorch is not tracking operations, it doesn't know the relationship between X and y.

Simple linear model

As a quick demonstration we'll show how the built-in `nn.Linear()` model preselects weight and bias values at random.

In [6]:

```
torch.manual_seed(59)

model = nn.Linear(in_features=1, out_features=1)
print(model.weight)
print(model.bias)
```

```
Parameter containing:
tensor([[0.1060]], requires_grad=True)
Parameter containing:
tensor([0.9638], requires_grad=True)
```

Without seeing any data, the model sets a random weight of 0.1060 and a bias of 0.9638.

Model classes

PyTorch lets us define models as object classes that can store multiple model layers. In upcoming sections we'll set up several neural network layers, and determine how each layer should perform its forward pass to the next layer. For now, though, we only need a single `linear` layer.

In [7]:

```
class Model(nn.Module):
    def __init__(self, in_features, out_features):
        super().__init__()
        self.linear = nn.Linear(in_features, out_features)

    def forward(self, x):
        y_pred = self.linear(x)
        return y_pred
```

NOTE: The "Linear" model layer used here doesn't really refer to linear regression. Instead, it describes the type of neural network layer employed. Linear layers are also called "fully connected" or "dense" layers. Going forward our models may contain linear layers, convolutional layers, and more.

When `Model` is instantiated, we need to pass in the size (dimensions) of the incoming and outgoing features.
For our purposes we'll use (1,1).
As above, we can see the initial hyperparameters.

In [8]:

```
torch.manual_seed(59)
model = Model(1, 1)
print(model)
print('Weight:', model.linear.weight.item())
print('Bias:  ', model.linear.bias.item())
```

```
Model(
  (linear): Linear(in_features=1, out_features=1, bias=True)
)
Weight: 0.10597813129425049
Bias:   0.9637961387634277
```

As models become more complex, it may be better to iterate over all the model parameters:

In [9]:

```
for name, param in model.named_parameters():
    print(name, '\t', param.item())
```

```
linear.weight    0.10597813129425049
linear.bias      0.9637961387634277
```

NOTE: In the above example we had our Model class accept arguments for the number of input and output features.
For simplicity we can hardcode them into the Model:

```
class Model(torch.nn.Module):
    def __init__(self):
        super().__init__()
        self.linear = Linear(1,1)
```

```
model = Model()
```

Alternatively we can use default arguments:

```
class Model(torch.nn.Module):
    def __init__(self, in_dim=1, out_dim=1):
        super().__init__()
        self.linear = Linear(in_dim,out_dim)

model = Model()
# or
model = Model(i,o)
```

Now let's see the result when we pass a tensor into the model.

In [10]:

```
x = torch.tensor([2.0])
print(model.forward(x))   # equivalent to print(model(x))
```

```
tensor([1.1758], grad_fn=<AddBackward0>)
```

which is confirmed with $f(x) = (0.1060)(2.0) + (0.9638) = 1.1758$

Plot the initial model

We can plot the untrained model against our dataset to get an idea of our starting point.

In [11]:

```
x1 = np.array([X.min(),X.max()])
print(x1)
```

```
[ 1. 50.]
```

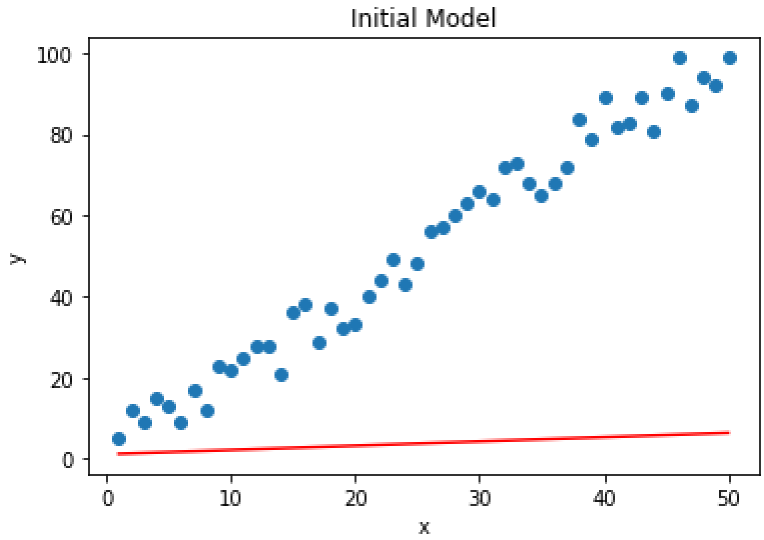
In [12]:

```
w1,b1 = model.linear.weight.item(), model.linear.bias.item()
print(f'Initial weight: {w1:.8f}, Initial bias: {b1:.8f}')
print()

y1 = x1*w1 + b1
print(y1)
```

```
Initial weight: 0.10597813, Initial bias: 0.96379614

[1.0697743 6.2627025]
```

In [13]:

```
plt.scatter(X.numpy(), y.numpy())
plt.plot(x1,y1,'r')
plt.title('Initial Model')
plt.ylabel('y')
plt.xlabel('x');
```



Set the loss function

We could write our own function to apply a Mean Squared Error (MSE) that follows

$$\begin{split}MSE &= \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \\ &= \frac{1}{n}\sum_{i=1}^{n}(y_i - (wx_i + b))^2\end{split}$$

Fortunately PyTorch has it built in.
By convention, you'll see the variable name "criterion" used, but feel free to use something like "linear_loss_func" if that's clearer.

In [14]:

```
criterion = nn.MSELoss()
```

Set the optimization

Here we'll use [Stochastic Gradient Descent (https://en.wikipedia.org/wiki/Stochastic_gradient_descent)](https://en.wikipedia.org/wiki/Stochastic_gradient_descent) (SGD) with an applied [learning rate (https://en.wikipedia.org/wiki/Learning_rate)](https://en.wikipedia.org/wiki/Learning_rate) (lr) of 0.001. Recall that the learning rate tells the optimizer how much to adjust each parameter on the next round of calculations. Too large a step and we run the risk of overshooting the minimum, causing the algorithm to diverge. Too small and it will take a long time to converge.

For more complicated (multivariate) data, you might also consider passing optional [`momentum` (https://en.wikipedia.org/wiki/Stochastic_gradient_descent#Momentum)](https://en.wikipedia.org/wiki/Stochastic_gradient_descent#Momentum) and [`weight_decay` (https://en.wikipedia.org/wiki/Tikhonov_regularization)](https://en.wikipedia.org/wiki/Tikhonov_regularization) arguments. Momentum allows the algorithm to "roll over" small bumps to avoid local minima that can cause convergence too soon. Weight decay (also called an L2 penalty) applies to biases.

For more information, see **`torch.optim`** (https://pytorch.org/docs/stable/optim.html)

In [15]:

```
optimizer = torch.optim.SGD(model.parameters(), lr = 0.001)

# You'll sometimes see this as
# optimizer = torch.optim.SGD(model.parameters(), lr = 1e-3)
```

Train the model

An *epoch* is a single pass through the entire dataset. We want to pick a sufficiently large number of epochs to reach a plateau close to our known parameters of $\mathrm{weight} = 2,\ \mathrm{bias} = 1$

Let's walk through the steps we're about to take:

1. Set a reasonably large number of passes
   `epochs = 50`
2. Create a list to store loss values. This will let us view our progress afterward.
   `losses = []`
   `for i in range(epochs):`
3. Bump "i" so that the printed report starts at 1
   `i+=1`
4. Create a prediction set by running "X" through the current model parameters
   `y_pred = model.forward(X)`
5. Calculate the loss
   `loss = criterion(y_pred, y)`
6. Add the loss value to our tracking list
   `losses.append(loss)`
7. Print the current line of results
   `print(f'epoch: {i:2} loss: {loss.item():10.8f}')`
8. Gradients accumulate with every backprop. To prevent compounding we need to reset the stored gradient for each new epoch.
   `optimizer.zero_grad()`
9. Now we can backprop
   `loss.backward()`
10. Finally, we can update the hyperparameters of our model
   `optimizer.step()`

In [16]:

```
epochs = 50
losses = []

for i in range(epochs):
    i+=1
    y_pred = model.forward(X)
    loss = criterion(y_pred, y)
    losses.append(loss)
    print(f'epoch: {i:2}  loss: {loss.item():10.8f}  weight: {model.linear.weight.i
bias: {model.linear.bias.item():10.8f}')
    optimizer.zero_grad()
    loss.backward()
    optimizer.step()
```

```
epoch:  1  loss: 3057.21679688  weight: 0.10597813  bias: 0.96379614
epoch:  2  loss: 1588.53100586  weight: 3.33490038  bias: 1.06046367
epoch:  3  loss: 830.30010986  weight: 1.01483274  bias: 0.99226278
epoch:  4  loss: 438.85241699  weight: 2.68179965  bias: 1.04252183
epoch:  5  loss: 236.76152039  weight: 1.48402119  bias: 1.00766504
epoch:  6  loss: 132.42912292  weight: 2.34460592  bias: 1.03396463
epoch:  7  loss: 78.56572723  weight: 1.72622538  bias: 1.01632178
epoch:  8  loss: 50.75775909  weight: 2.17050409  bias: 1.03025162
epoch:  9  loss: 36.40123367  weight: 1.85124576  bias: 1.02149546
epoch: 10  loss: 28.98922729  weight: 2.08060074  bias: 1.02903891
epoch: 11  loss: 25.16238213  weight: 1.91576838  bias: 1.02487016
epoch: 12  loss: 23.18647385  weight: 2.03416562  bias: 1.02911627
epoch: 13  loss: 22.16612816  weight: 1.94905841  bias: 1.02731562
epoch: 14  loss: 21.63911057  weight: 2.01017213  bias: 1.02985907
epoch: 15  loss: 21.36677170  weight: 1.96622372  bias: 1.02928054
epoch: 16  loss: 21.22591782  weight: 1.99776423  bias: 1.03094459
epoch: 17  loss: 21.15294647  weight: 1.97506487  bias: 1.03099668
epoch: 18  loss: 21.11501122  weight: 1.99133754  bias: 1.03220642
epoch: 19  loss: 21.09517670  weight: 1.97960854  bias: 1.03258383
epoch: 20  loss: 21.08468437  weight: 1.98799884  bias: 1.03355861
epoch: 21  loss: 21.07901382  weight: 1.98193336  bias: 1.03410351
epoch: 22  loss: 21.07583046  weight: 1.98625445  bias: 1.03495669
epoch: 23  loss: 21.07393837  weight: 1.98311269  bias: 1.03558779
epoch: 24  loss: 21.07269859  weight: 1.98533309  bias: 1.03637791
epoch: 25  loss: 21.07181931  weight: 1.98370099  bias: 1.03705311
epoch: 26  loss: 21.07110596  weight: 1.98483658  bias: 1.03781021
epoch: 27  loss: 21.07048416  weight: 1.98398376  bias: 1.03850794
epoch: 28  loss: 21.06991386  weight: 1.98455977  bias: 1.03924775
epoch: 29  loss: 21.06936646  weight: 1.98410904  bias: 1.03995669
epoch: 30  loss: 21.06883621  weight: 1.98439610  bias: 1.04068720
epoch: 31  loss: 21.06830788  weight: 1.98415291  bias: 1.04140162
epoch: 32  loss: 21.06778145  weight: 1.98429084  bias: 1.04212701
epoch: 33  loss: 21.06726265  weight: 1.98415494  bias: 1.04284394
epoch: 34  loss: 21.06674004  weight: 1.98421574  bias: 1.04356635
epoch: 35  loss: 21.06622314  weight: 1.98413551  bias: 1.04428422
epoch: 36  loss: 21.06570625  weight: 1.98415649  bias: 1.04500473
epoch: 37  loss: 21.06518936  weight: 1.98410451  bias: 1.04572272
epoch: 38  loss: 21.06466866  weight: 1.98410523  bias: 1.04644191
epoch: 39  loss: 21.06415749  weight: 1.98406804  bias: 1.04715967
epoch: 40  loss: 21.06363869  weight: 1.98405814  bias: 1.04787791
epoch: 41  loss: 21.06312370  weight: 1.98402870  bias: 1.04859519
epoch: 42  loss: 21.06260681  weight: 1.98401320  bias: 1.04931259
epoch: 43  loss: 21.06209564  weight: 1.98398757  bias: 1.05002928
epoch: 44  loss: 21.06157875  weight: 1.98396957  bias: 1.05074584
```

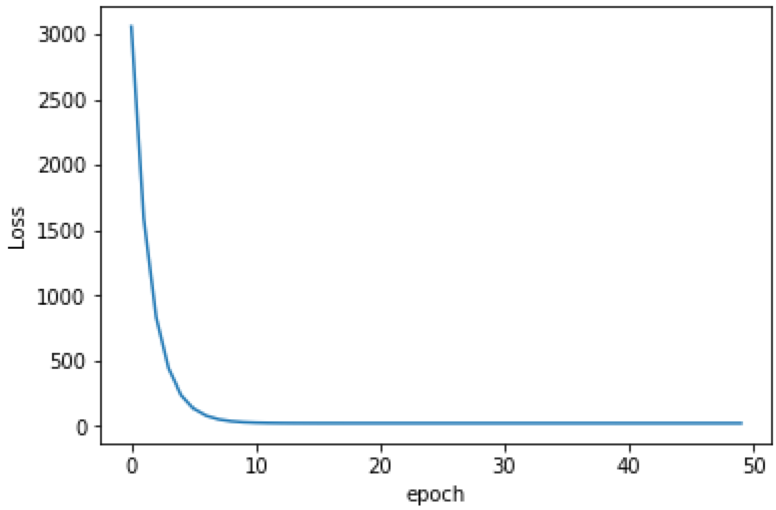
```
epoch: 45  loss: 21.06106949  weight: 1.98394585  bias: 1.05146194
epoch: 46  loss: 21.06055450  weight: 1.98392630  bias: 1.05217779
epoch: 47  loss: 21.06004143  weight: 1.98390377  bias: 1.05289316
epoch: 48  loss: 21.05953217  weight: 1.98388338  bias: 1.05360830
epoch: 49  loss: 21.05901527  weight: 1.98386145  bias: 1.05432308
epoch: 50  loss: 21.05850983  weight: 1.98384094  bias: 1.05503750
```

Plot the loss values

Let's see how loss changed over time

In [17]:

```
plt.plot(range(epochs), losses)
plt.ylabel('Loss')
plt.xlabel('epoch');
```



Plot the result

Now we'll derive y1 from the new model to plot the most recent best-fit line.

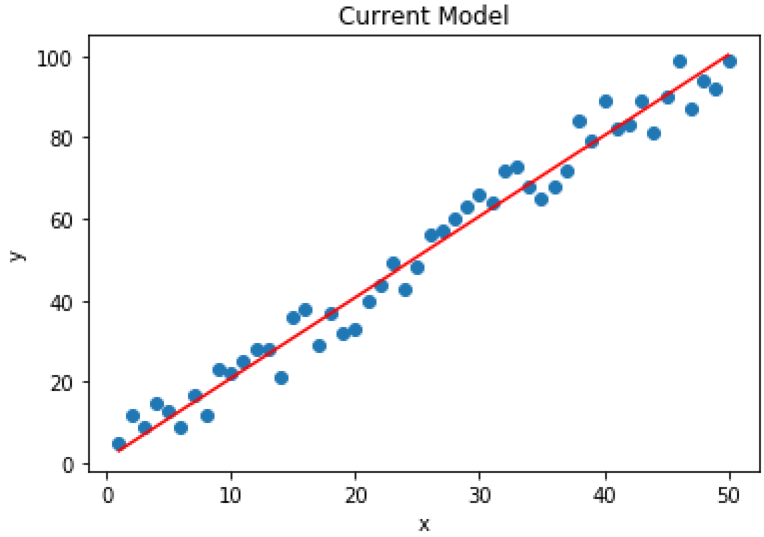
In [18]:

```
w1,b1 = model.linear.weight.item(), model.linear.bias.item()
print(f'Current weight: {w1:.8f}, Current bias: {b1:.8f}')
print()

y1 = x1*w1 + b1
print(x1)
print(y1)
```

```
Current weight: 1.98381913, Current bias: 1.05575156

[ 1. 50.]
[  3.0395708 100.246704 ]
```

In [19]:

```
plt.scatter(X.numpy(), y.numpy())
plt.plot(x1,y1,'r')
plt.title('Current Model')
plt.ylabel('y')
plt.xlabel('x');
```



Great job!