lecture3

April 30, 2019

1 Lecture Notes 3: Rounding, Overflow, Linear Algebra

1.1 Rounding

Let's start with a weird experiment:

```
In [1]: import numpy
        a = numpy.array([1,10,100,1000],dtype='float32')
        print(a)
```

```
[   1.    10.   100.  1000.]
```

```
In [2]: print((a + 1e9) - 1e9)
```

```
[   0.     0.   128.  1024.]
```

Now, let's repeat the experiment with higher precision (`float64`):

```
In [3]: a = numpy.array([1,10,100,1000],dtype='float64')
        print(a)
```

```
[   1.    10.   100.  1000.]
```

```
In [4]: print((a + 1e9) - 1e9)
```

```
[   1.    10.   100.  1000.]
```

We can also reach the limits of `float64`:

```
In [5]: print((a + 1e18) - 1e18)
```

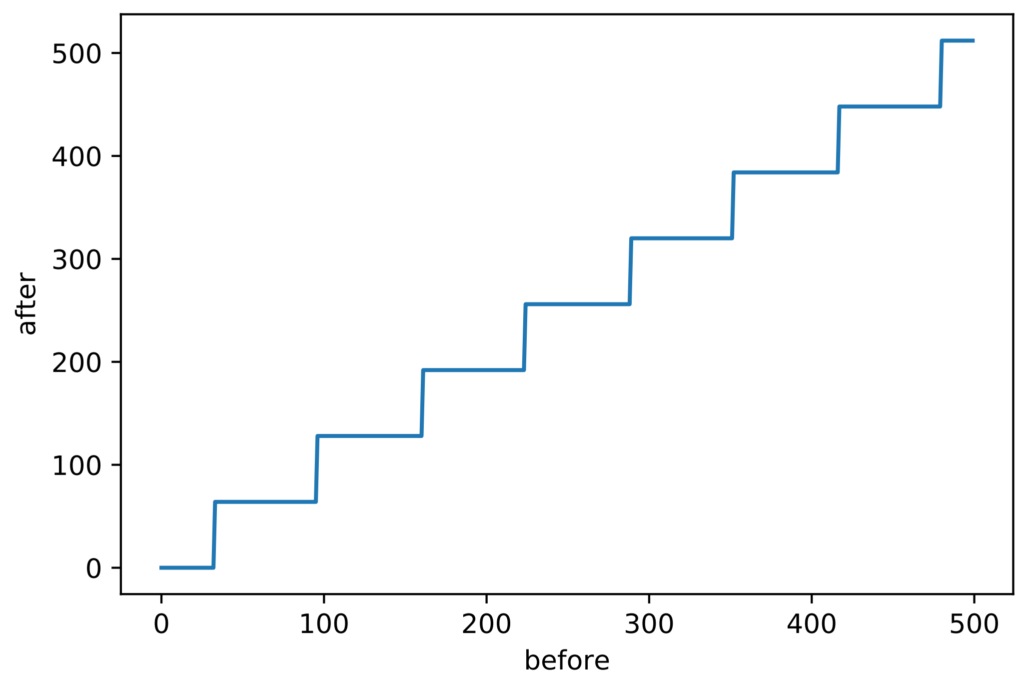
```
[   0.     0.   128.  1024.]
```

1.1.1 Understanding of rounding effect

```
In [6]: import matplotlib
        %matplotlib inline
        import matplotlib.pyplot as plt

        from IPython.display import set_matplotlib_formats
        set_matplotlib_formats('pdf','png')
        plt.rcParams['savefig.dpi'] = 90
```

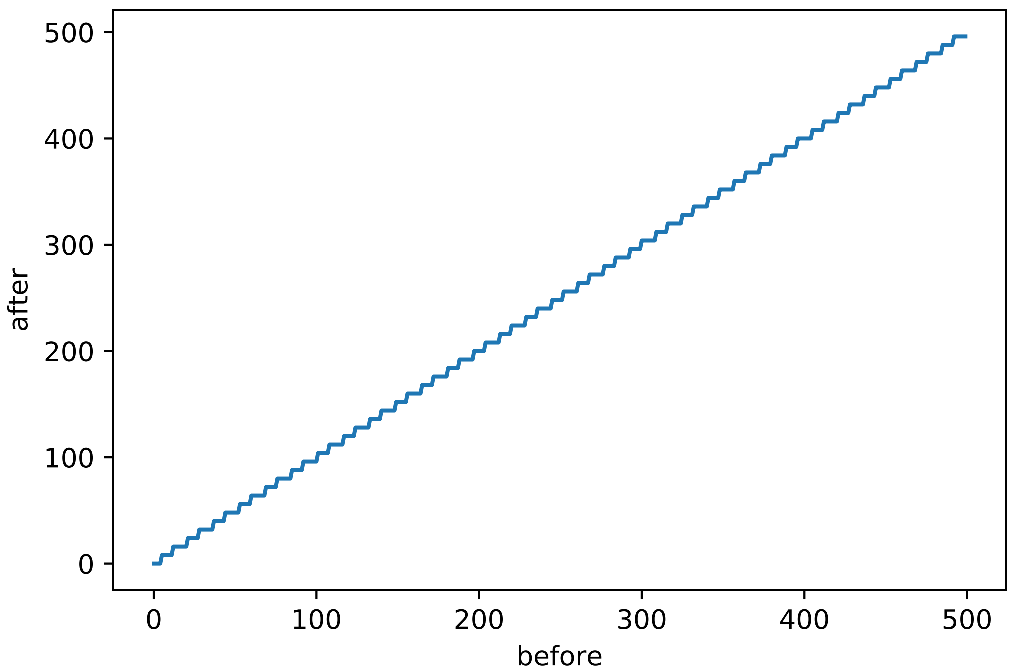
We plot all numbers before and after application of the addition and substraction:

```
In [7]: a = numpy.arange(500).astype('float32')
        b = (a + 1e9) - 1e9
        plt.plot(a, b)
        plt.xlabel('before')
        plt.ylabel('after')

Out[7]: Text(0,0.5,'after')
```




```
In [8]: a = numpy.arange(500).astype('float32')
        b = (a + 1e8) - 1e8
        plt.plot(a, b)
        plt.xlabel('before')
        plt.ylabel('after')
```

```
Out[8]: Text(0,0.5,'after')
```

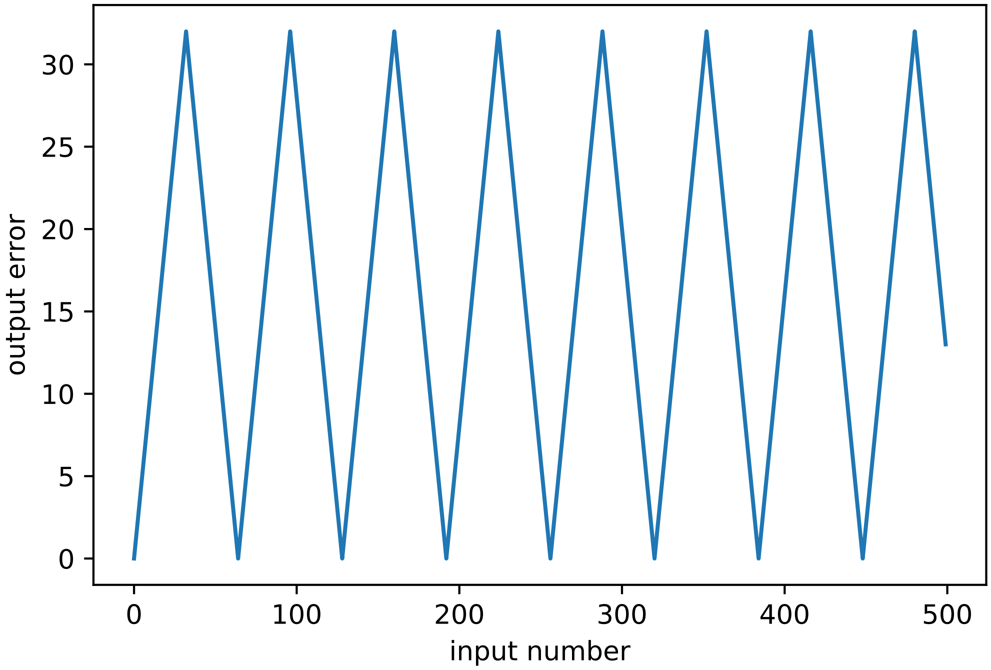


1.1.2 Comments

- The `float32` and `float64` number representations have a certain budget of bits to represent real numbers. Therefore, they allocate precision where it is important (e.g. for small numbers).
- The smaller the precision, the less memory is used and therefore the more efficient, but also the more careful we should be about potential loss of precision.
- Unlike typical observed data, error is not random-looking, but very structured:

```
In [9]: a = numpy.arange(500).astype('float32')
        error = numpy.abs(a - ((a + 1e9) - 1e9))
        plt.plot(a, error)
        plt.xlabel('input number')
        plt.ylabel('output error')
```

```
Out[9]: Text(0,0.5,'output error')
```



1.2 Overflow

Overflow is a frequently encountered problem when implementing machine learning algorithms.

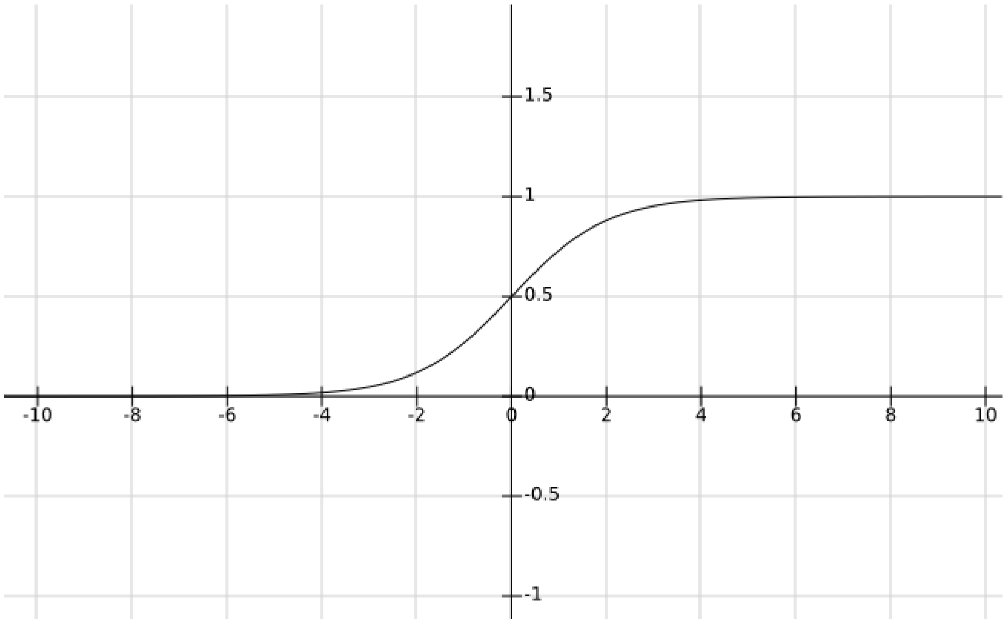
```
In [10]: a = numpy.array([1, 10, 100, 1000], dtype='float32')

         print(numpy.exp(a))
```

```
[2.7182817e+00 2.2026465e+04            inf            inf]


/home/sdogadov/anaconda/envs/pyML3/lib/python3.6/site-packages/ipykernel_launcher.py:3: Runtime
  This is separate from the ipykernel package so we can avoid doing imports until
```

1.2.1 The sigmoid function

$$\text{sigmoid}(x) = \frac{\exp(x)}{1 + \exp(x)}$$

```
In [11]: X = numpy.array([-1e9, -1e6, -1e3, -1e1, 2, 1, 0, 1, 2, 1e1, 1e3, 1e6, 1e9],dtype='fl

         def sigmoid(x):
             return numpy.exp(x) / (1 + numpy.exp(x))

         print(sigmoid(X))
```



plot generated by fooplot.com

```
[0.000000e+00 0.000000e+00 0.000000e+00 4.539787e-05 8.807971e-01
 7.310586e-01 5.000000e-01 7.310586e-01 8.807971e-01 9.999546e-01
          nan          nan          nan]
```

```
/home/sdogadov/anaconda/envs/pyML3/lib/python3.6/site-packages/ipykernel_launcher.py:4: Runtime
  after removing the cwd from sys.path.
/home/sdogadov/anaconda/envs/pyML3/lib/python3.6/site-packages/ipykernel_launcher.py:4: Runtime
  after removing the cwd from sys.path.
```

Where does the nan come from?

```
In [12]: print(numpy.exp(1000))
```

```
inf
```

```
/home/sdogadov/anaconda/envs/pyML3/lib/python3.6/site-packages/ipykernel_launcher.py:1: Runtime
  """Entry point for launching an IPython kernel.
```

```
In [13]: print(float('inf') / float('inf'))
```

```
nan
```

1.2.2 The sigmoid function (2)

Let's rewrite the sigmoid function in a different way

$$\text{sigmoid}(x) = \frac{\exp(x)}{1+\exp(x)} = \frac{\exp(-x)\exp(x)}{\exp(-x)(1+\exp(x))} = \frac{1}{1+\exp(-x)}$$

```
In [14]: def sigmoid(x):
             return 1 / (1 + numpy.exp(-x))

         print(sigmoid(X))
```

```
[0.0000000e+00 0.0000000e+00 0.0000000e+00 4.5397872e-05 8.8079703e-01
 7.3105860e-01 5.0000000e-01 7.3105860e-01 8.8079703e-01 9.9995458e-01
 1.0000000e+00 1.0000000e+00 1.0000000e+00]
```

```
/home/sdogadov/anaconda/envs/pyML3/lib/python3.6/site-packages/ipykernel_launcher.py:2: Runtime
```

Here, we still get an overflow. But this time, we are lucky since 1/inf = 0.0, which is the desired result for large negative inputs.

```
In [15]: 1.0 / float('inf')
```

```
Out[15]: 0.0
```

1.2.3 The sigmoid function (3)

The sigmoid function can be written in yet another way:

$$\text{sigmoid}(x) = \frac{\exp(x)}{1+\exp(x)} = \frac{1}{2}\left(\frac{2\exp(x)}{1+\exp(x)}\right) = \frac{1}{2}\left(\frac{\exp(x)-1+1+\exp(x)}{1+\exp(x)}\right) = \frac{1}{2}\left(\frac{\exp(x)-1}{\exp(x)+1}+1\right) = \frac{1}{2}\Big(\tanh($$

$$\tanh(x) = \frac{\exp(2x)-1}{\exp(2x)+1}$$

```
In [16]: def sigmoid(x):
             return 0.5 * ( numpy.tanh(0.5 * x) + 1 )

         print(sigmoid(X))
```

```
[0.0000000e+00 0.0000000e+00 0.0000000e+00 4.5388937e-05 8.8079709e-01
 7.3105860e-01 5.0000000e-01 7.3105860e-01 8.8079709e-01 9.9995458e-01
 1.0000000e+00 1.0000000e+00 1.0000000e+00]
```

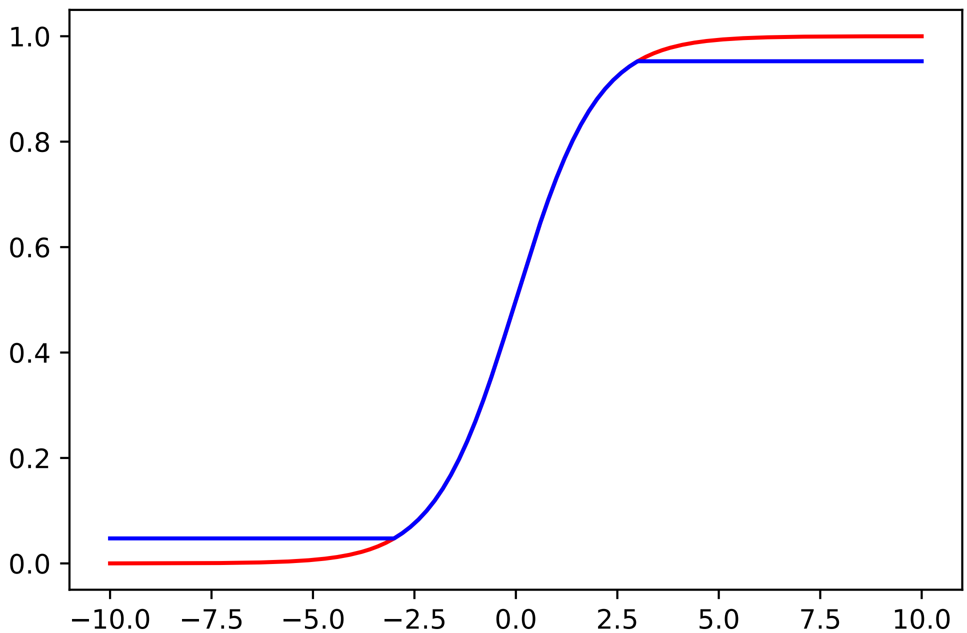
And there is no runtime warning this time.

1.2.4 The sigmoid function (4)

Suppose we cannot use the tanh function. The sigmoid function can alternatively be approximated to avoid the overflow:

```
In [17]: X = numpy.arange(-10, 10.01, 0.1)

         plt.plot(X, sigmoid(X), 'r')
         plt.plot(X, sigmoid(numpy.clip(X, -3, 3)), 'b')
```

```
Out[17]: [<matplotlib.lines.Line2D at 0x7f66656635c0>]
```



The numpy clip function prevents the input from going outside a certain interval. This effectively avoids overflow in the exponential, but also causes a small approximation error.

1.2.5 Another source of overflow: normalizing probability distributions

Many probability functions can be written this way:

$$p(x) = \frac{1}{Z} \exp(f(x))$$

- Example of such functions: Gaussian distribution, Gibbs distribution.
- Machine learning algorithms often use these distributions, because their parameters can be learned easily. For example, the mean parameter of a Gaussian distribution can be learned by computing the empirical mean of the data, and the scale parameter can be learned by computing the empirical standard deviation.

- On the other hand, these probability functions have a risk of overflow due to the exponential function.

```
In [18]: # Let p(x) be a discrete distribution with function values
         f = numpy.array([1.0, 8.0, 100.0, 0.1, 3.5, 2.3], dtype='float32')

         # The normalization factor is the sum of these function values
         # after application of the exponential function
         Z = numpy.exp(f).sum()

         print(Z)
```

```
inf
```

```
/home/sdogadov/anaconda/envs/pyML3/lib/python3.6/site-packages/ipykernel_launcher.py:6: Runtim
```

Even taking the logarithm of `Z` won't solve the overflow.

```
In [19]: print(numpy.log(Z))
```

```
inf
```

This problem will be studied in the homework.

1.3 Linear Algebra

Many machine learning techniques are based on linear algebra. Two important ones are linear regression and principal component analysis. These techniques can be implemented easily in Python and Numpy.

1.3.1 Linear regression

The model assumes that the data is generated as following:

$$y_n = \beta_1 x_n + \beta_2 + \epsilon_n, \quad n = \overline{1..N}, \quad \epsilon_n \sim \mathcal{N}(0, \sigma^2)$$

or

$$y = \beta_1 \hat{X} + \beta_2 \mathbb{1}_N + \mathcal{E}, \quad \text{where} \quad y, \hat{X}, \mathcal{E} \in \mathbb{R}^{(N)}$$

$$y = [\beta_1, \beta_2] \times [\hat{X}, \mathbb{1}_N]^\top + \mathcal{E}$$

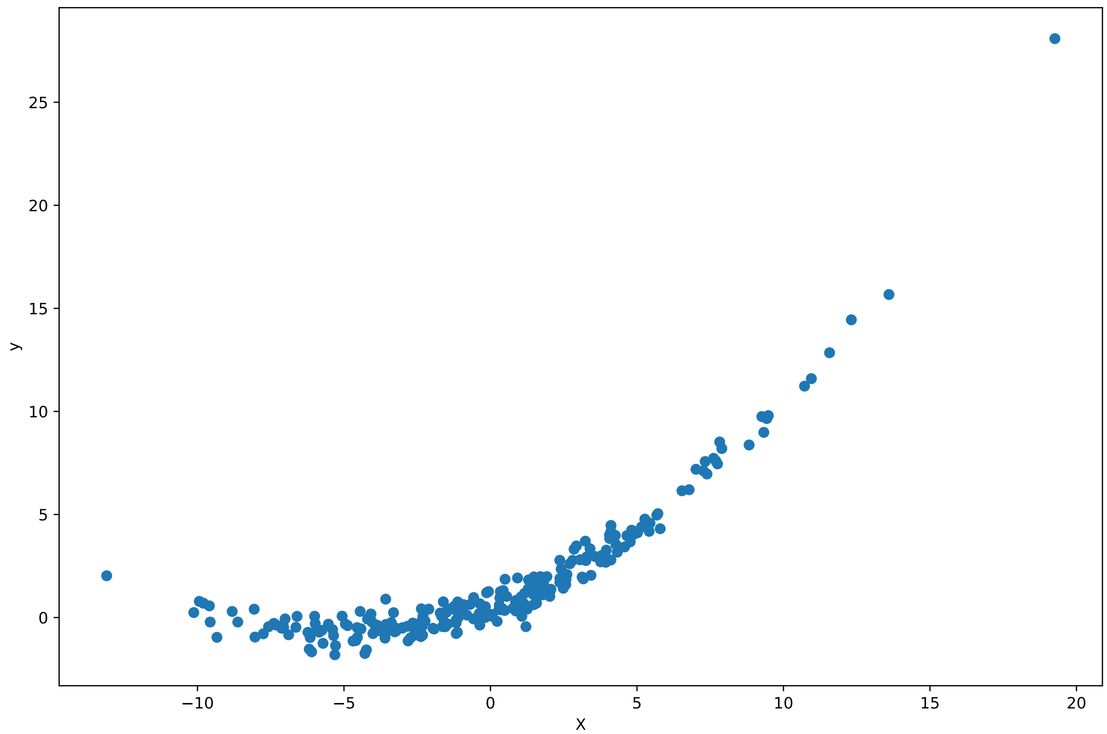
$$y = \beta \times X^\top + \mathcal{E}, \quad \text{where} \quad \beta = [\beta_1, \beta_2] \in \mathbb{R}^{(2)}, \quad \text{and} \quad X = [\hat{X}, \mathbb{1}_N] \in \mathbb{R}^{(N,2)}$$

Finding the best linear fit of a labeled dataset.

```
In [27]: # Create a dataset

         #Fix the random seed

         numpy.random.seed(42)

         N = 250 # number of data points

         X = numpy.random.normal(0, 5, size = (N, 1))
         X_ones = numpy.ones_like(X)

         X = numpy.concatenate((X, X_ones), axis=1)
         print(X.shape)

         plt.figure(figsize = (12,8))

         # Create targets (outputs) and make them depend on X in some way
         y = 0.5 * X[:, 0] + 0.05 * X[:, 0] ** 2 + 0.5

         sigma2 = 0.5

         Eps = numpy.random.normal(0, sigma2, (N)) # random noise

         y += Eps # add noise to the targets

         # Plot the labeled dataset
         plt.scatter(X[:, 0], y)
         plt.xlabel('X')
         plt.ylabel('y')
```

```
(250, 2)
```

```
Out[27]: Text(0,0.5,'y')
```



Split dataset randomly into *train* and *test* datasets

```
In [28]: # set split ratio
         split_ratio = 0.8 # 80 % for train and 20 % for test

         idx = numpy.arange(N) # create all indexes
         numpy.random.shuffle(idx) # shuffle them

         split_idx =int(split_ratio*N)
         # create train and test indexes
         tr_idx = idx[:split_idx]
         te_idx = idx[split_idx:]

         print((len(tr_idx), len(te_idx)))

         # create Train dataset
         X_tr = X[tr_idx]
         y_tr = y[tr_idx]

         # create Test dataset
         X_te = X[te_idx]
         y_te = y[te_idx]
```

```
(200, 50)
```

The parameter of the model is given by:

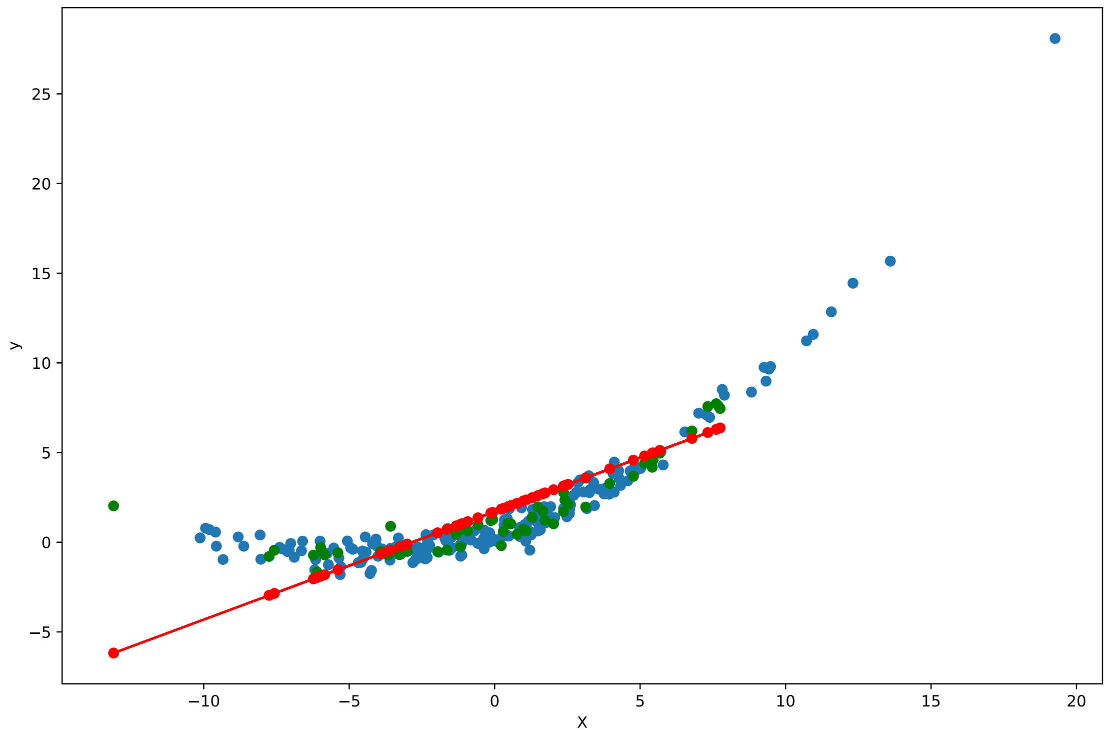
$$\beta = (X_{\text{tr}}^\top X_{\text{tr}})^{-1} X_{\text{tr}}^\top y_{\text{tr}}$$

And the prediction for new "test" points by:

$$\hat{y}_{\text{te}} = X_{\text{te}} \beta$$

In [29]:
```
import numpy.linalg

# Learn the model parameter
beta = numpy.dot(numpy.dot(numpy.linalg.inv(numpy.dot(X_tr.T, X_tr)), X_tr.T), y_tr)

# Equivalent expression
beta_short = numpy.linalg.inv(X_tr.T.dot(X_tr)).dot(X_tr.T.dot(y_tr))

# check if the results are numerically the same
assert numpy.allclose(beta, beta_short)

# Predict outputs for the test data
y_te_predict = numpy.dot(X_te, beta)

plt.figure(figsize = (12,8))

# Plot the data and the prediction
plt.scatter(X_tr[:, 0], y_tr)
plt.scatter(X_te[:, 0], y_te, color='g')
plt.xlabel('X')
plt.ylabel('y')

plt.plot(X_te[:, 0],y_te_predict, 'o-', color='r')
plt.xlabel('X')
plt.ylabel('y')
```

Out[29]:
```
Text(0,0.5,'y')
```



Compute the *root mean square error* (RMSE) for the predicted outputs: $\text{RMSE} = \sqrt{\frac{1}{N}\sum_{n=1}^{N}(\hat{y}_{\text{te}_n} - y_{\text{te}_n})^2}$

```
In [33]: rmse = numpy.sqrt(numpy.square(y_te_predict - y_te).mean())
         print("RMSE: {:0.3f} where y_tr variance: {:0.2f}".format(rmse, numpy.var(y_tr)))
```

```
RMSE: 1.619 where y_tr variance: 12.49
```

1.3.2 Principal component analysis (PCA)

PCA is a technique widely used for applications such as dimensionality reduction - lossy data compression - feature extraction - data visualization

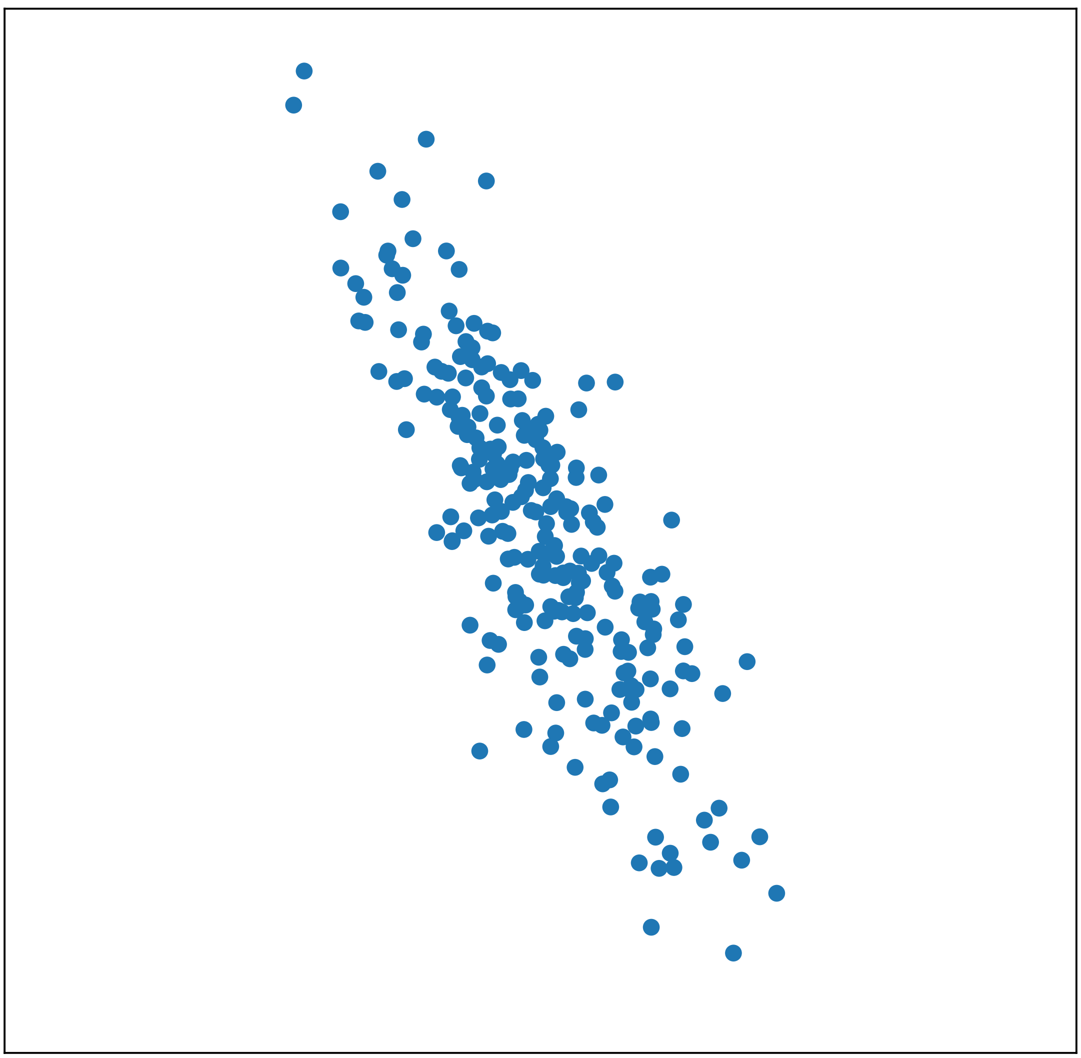
There are two commonly used definitions of PCA: - Orthogonal projection onto lower dimensional linear space such that the variance of projected data is maximized.

- Linear projection that minimizes the average projection cost, defined as the mean squared distance between the data and their projections.

```
In [31]: # create a random dataset
         N = 250
         M = numpy.random.normal(0, 5, (N, 2))

         # create some relation between dimensions
```

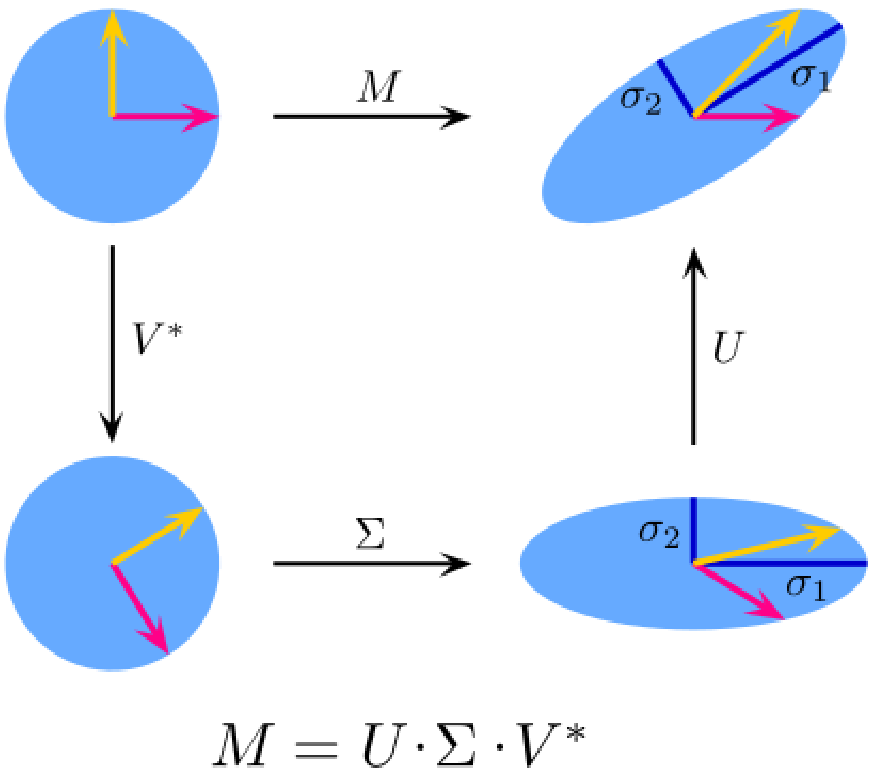
```
M[:, 1] -= 1.5 * M[:, 0]

# PCA only applies to centered data, so we center the data
M -= M.mean(axis=0)

# Plot the centered dataset
plt.figure(figsize=(8, 8))
plt.scatter(M.T[0], M.T[1])

# Turn off axis ticks
plt.xticks([])
plt.yticks([])

plt.axis([-30, 30, -30, 30])
```

Out[31]: [-30, 30, -30, 30]



1.4 Singular value decomposition (SVD)

The Singular-Value Decomposition, or SVD for short, is a matrix decomposition method for reducing a matrix to its constituent parts in order to make e.g. certain subsequent matrix calculations like matrix inversion simpler.




```
In [32]: # Find the principal components
         U, Sigma, V = numpy.linalg.svd(M , full_matrices = False)

         print("U shape: ", U.shape)
         print("Sigma shape:", Sigma.shape)
         print("V shape:", V.shape)

         X = U.dot(numpy.diag(Sigma).dot(V.T))

         assert numpy.allclose(numpy.sum(M - X) , numpy.zeros_like(M))

         HAT1 = numpy.outer(V[0], V[0]) # projection matrix to the axis representing the most

         HAT2 = numpy.outer(V[1], V[1]) # projection matrix to the axis representing the secon
```

```python
Mtest     = numpy.random.uniform(-20, 20, (500, 2))

# Project some test data onto the fisrt principal compenent
MtestPCA1 = numpy.dot(Mtest, HAT1)

# Project some test data onto the second principal compenent
MtestPCA2 = numpy.dot(Mtest, HAT2)

# Plot the original data and the projected test data
plt.figure(figsize=(8, 8))

plt.scatter(*M.T)  # equivalent to M.T[0], M.T[1]

plt.plot(*Mtest.T, 'o', color='g', ms=1)
plt.plot(*MtestPCA1.T, 'o-', color='r', ms=2)
plt.plot(*MtestPCA2.T, 'o-', color='k', ms=2)

plt.xticks([])
plt.yticks([])

plt.axis([-30, 30, -30, 30])
```

```
U shape:  (250, 2)
Sigma shape: (2,)
V shape: (2, 2)
```

```
Out[32]: [-30, 30, -30, 30]
```