

## Lecture Notes 3: Rounding, Overflow, Linear Algebra

### 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.]
```

### Understanding of rounding effect

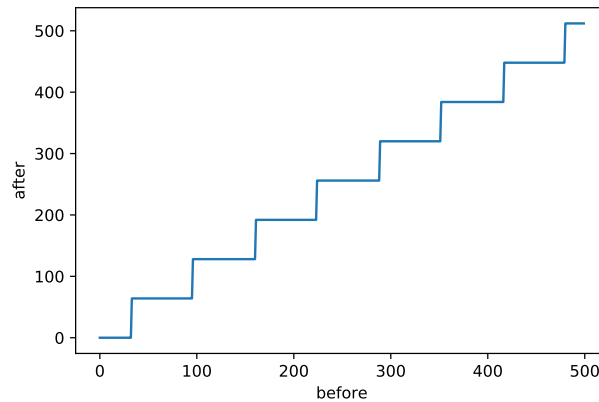
```
In [6]: import matplotlib
        %matplotlib inline
        import matplotlib.pyplot as plt

        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 subtraction:

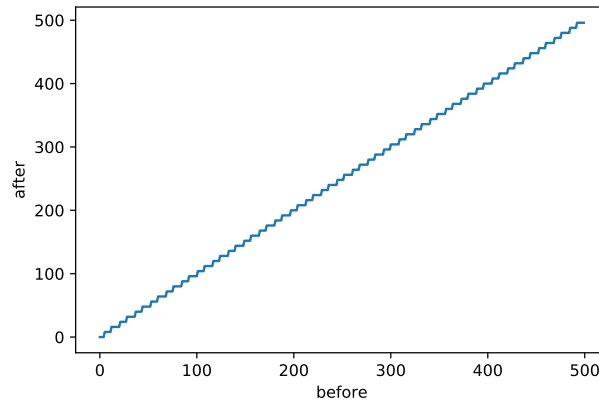
```
In [7]: a = numpy.arange(500).astype('float32')
        b = (a + 1e9) - 1e9
        plt.plot(a, b)
        plt.xlabel('before')
        plt.ylabel('after')
```

Out[7]: <matplotlib.text.Text at 0x7f4002c48860>



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

Out[8]: <matplotlib.text.Text at 0x7f4002b79be0>

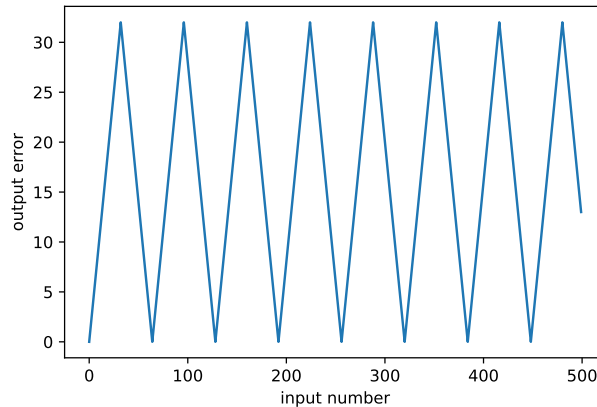


## Comments

- 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]: <matplotlib.text.Text at 0x7f40028fef60>
```



## 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))
```

```
[ 2.71828175e+00  2.20264648e+04          inf          inf]
```

```
/home/postskript/anaconda3/envs/pym1/lib/python3.6/site-packages/ipykernel_launcher.py:3: RuntimeWarning:
  This is separate from the ipykernel package so we can avoid doing imports until
```

## The sigmoid function

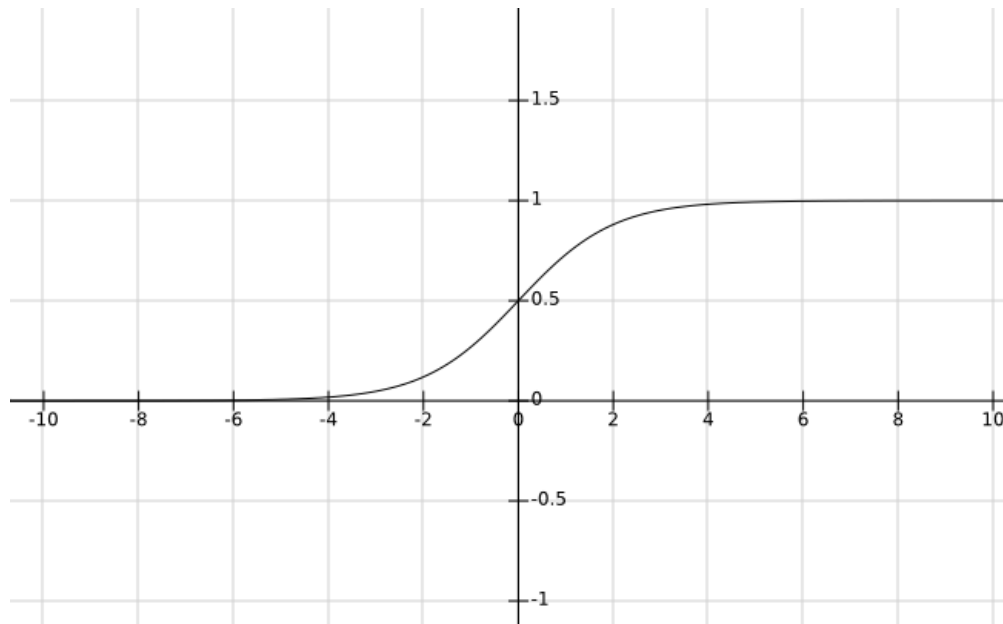
$$\text{sigmoid}(x) = \frac{\exp(x)}{1 + \exp(x)}$$

```
In [11]: X = numpy.array([-1e9, -1e6, -1e3, -1e1, 2, 1, 0, 1, 2, 1e1, 1e3, 1e6, 1e9], dtype='float32')
```

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

```
        print(sigmoid(X))
```

```
[ 0.00000000e+00  0.00000000e+00  0.00000000e+00  4.53978682e-05
 8.80797088e-01  7.31058598e-01  5.00000000e-01  7.31058598e-01
 8.80797088e-01  9.99954581e-01          nan          nan
          nan]
```



plot generated by fooplots.com

```
/home/postskript/anaconda3/envs/pym1/lib/python3.6/site-packages/ipykernel_launcher.py:4: RuntimeWarning:
  after removing the cwd from sys.path.
/home/postskript/anaconda3/envs/pym1/lib/python3.6/site-packages/ipykernel_launcher.py:4: RuntimeWarning:
  after removing the cwd from sys.path.
```

Where does the nan come from?

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

```
/home/postskript/anaconda3/envs/pym1/lib/python3.6/site-packages/ipykernel_launcher.py:1: RuntimeWarning:
  """Entry point for launching an IPython kernel.
```

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

## 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))
```

```
[ 0.00000000e+00  0.00000000e+00  0.00000000e+00  4.53978719e-05
 8.80797029e-01  7.31058598e-01  5.00000000e-01  7.31058598e-01
 8.80797029e-01  9.99954581e-01  1.00000000e+00  1.00000000e+00
 1.00000000e+00]
```

/home/postskript/anaconda3/envs/pyml/lib/python3.6/site-packages/ipykernel\_launcher.py:2: RuntimeWarning:

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

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

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

### The sigmoid function (3)

The sigmoid function can be written in yet another way:

$$\text{sigmoid}(x) = \frac{\exp(x)}{1 + \exp(x)} = 0.5 \tanh(0.5x) + 0.5$$

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

```
         print(sigmoid(X))
```

```
[ 0.00000000e+00  0.00000000e+00  0.00000000e+00  4.53889370e-05
 8.80797088e-01  7.31058598e-01  5.00000000e-01  7.31058598e-01
 8.80797088e-01  9.99954581e-01  1.00000000e+00  1.00000000e+00
 1.00000000e+00]
```

And there is no runtime warning this time.

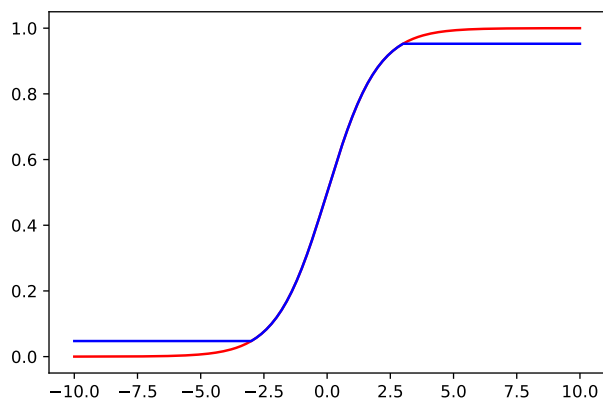
### The sigmoid function (4)

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 0x7f4002867240>]
```



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.

### 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/postskript/anaconda3/envs/pym1/lib/python3.6/site-packages/ipykernel\_launcher.py:6: RuntimeWarning: overflow encountered in exp

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.

## 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.

### Linear regression

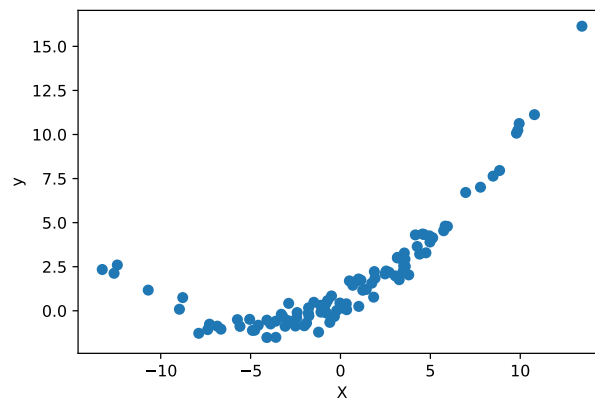
Finding the best linear fit of a labeled dataset.

```
In [20]: # Create a dataset
X = numpy.concatenate((numpy.random.normal(0, 5, (100, 1)), numpy.ones((100, 1))), axis=1)

# Create outputs and make them depend on X in some way
y = 0.5 * X[:, 0] + 0.05 * X[:, 0] ** 2 + 0.5 + numpy.random.normal(0, 0.5, (100))

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

Out[20]: <matplotlib.text.Text at 0x7f400289a668>



The parameter of the model is given by:

$$\beta = (X^T X)^{-1} X^T y$$

And the prediction for new “test” points by:

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

```
In [21]: import numpy.linalg

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

# Predict some test data
Xtest = numpy.arange(-15, 15, 0.1)
Xtest = numpy.array([Xtest, numpy.ones_like(Xtest)]).T
ytest = numpy.dot(Xtest, beta)
```

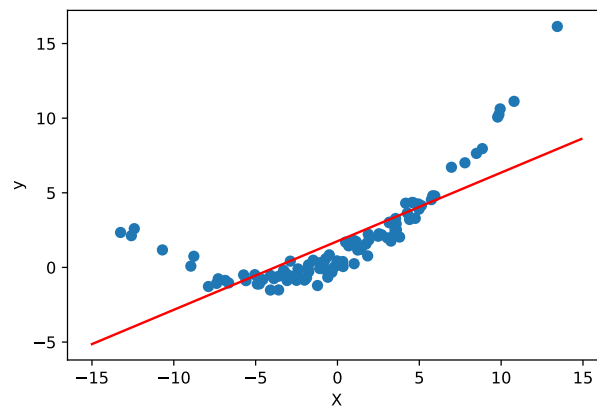
```

# Plot the data and the prediction
plt.figure()
plt.scatter(X[:, 0], y)
plt.xlabel('X')
plt.ylabel('y')

plt.plot(Xtest[:, 0], ytest, color='red')
plt.xlabel('X')
plt.ylabel('y')

```

Out[21]: <matplotlib.text.Text at 0x7f400275f7f0>



## Principal component analysis (PCA)

Find the most salient direction in a multidimensional unlabeled dataset.

```

In [22]: # create a random dataset
X = numpy.random.normal(0, 5, (100, 2))

# create some relation between dimensions
X[:, 1] -= 1.5 * X[:, 0]

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

# Plot the centered dataset
plt.figure(figsize=(5, 5))
plt.scatter(X.T[0], X.T[1])

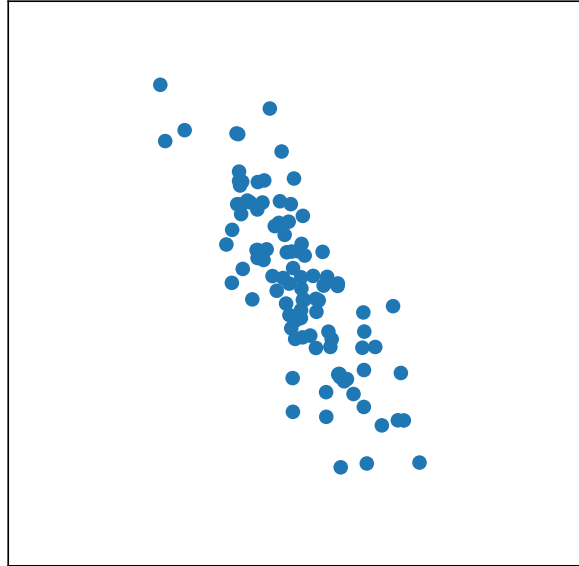
# Turn off axis ticks
plt.xticks([])
plt.yticks([])

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

```

Out[22]: [-30, 30, -30, 30]





```
In [23]: # Find the principal components
         U, W, V = numpy.linalg.svd(X)
         HAT = numpy.outer(V[0], V[0])

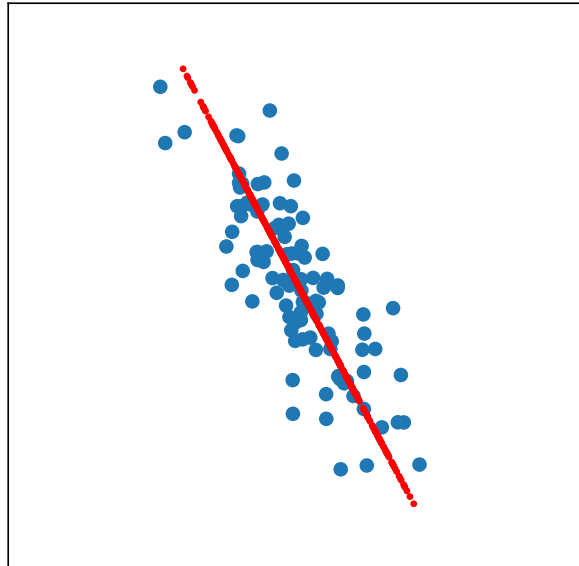
         # Project some test data on the principal component
         Xtest = numpy.random.uniform(-20, 20, (500, 2))
         XtestPCA = numpy.dot(Xtest, HAT)

         # Plot the original data and the projected test data
         plt.figure(figsize=(5, 5))
         plt.scatter(*X.T) # equivalent to X.T[0], X.T[1]
         plt.scatter(*XtestPCA.T, color='red', s=5)

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

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

```
Out[23]: [-30, 30, -30, 30]
```



In [ ]: