# Math for Machine Learning

### Machine Learning Workshop @ MPSTME

### Instructor: Santosh Chapaneri

## Linear Algebra; Probability; Statistics; Optimization

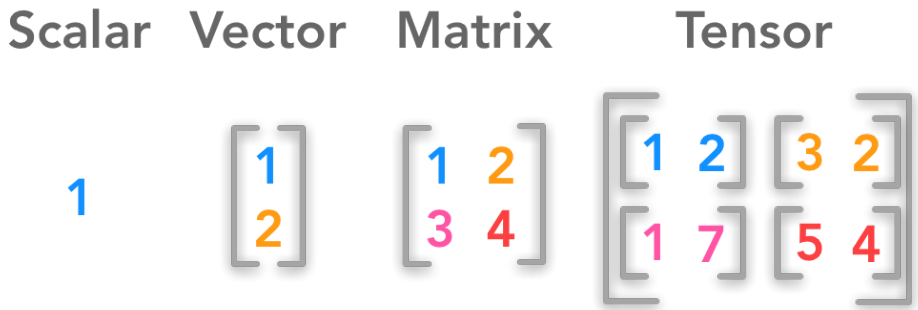
**Recommended Textbooks**:

- G. Strang, *Linear Algebra and Its Applications*, Academic Press 1980
- I. Goodfellow, Y. Bengio and A. Courville, *Deep Learning*, MIR Press 2016
- S. Boyd, *Convex Optimization*, Cambridge University Press 2004

# I. Linear Algebra

In [1]:
```
from IPython.display import Image
Image('Images/SVMT.png', width=600)
```

Out[1]:




# 1. Matrices Fundamentals

A matrix is a two-dimensional table. Here is an example of a $3 \times 3$ matrix

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

A vector is a $n \times 1$ vector (there are **row** and **column** vectors).

## Distances and Norms

- Norm is a **qualitative measure of length of a vector** and is typically denoted as $||x||$.

- The norm should satisfy certain properties:
  - $||\alpha x|| = |\alpha| ||x||$,
  - $||x + y|| \leq ||x|| + ||y||$ (triangle inequality),
  - If $||x|| = 0$ then $x = 0$.

- The **distance** between two vectors is then defined as

$$d(x, y) = ||x - y||$$

## Standard norms

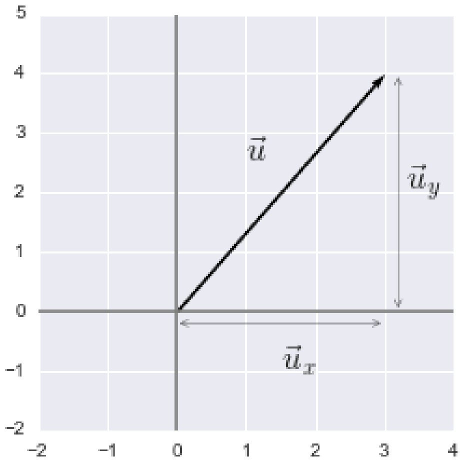
The most well-known and widely used norm is **Euclidean norm**:

$$\|x\|_2 = \sqrt{\sum_{i=1}^n |x_i|^2},$$

which corresponds to the distance in our real life (the vectors might have complex elements, thus is the modulus here).

In [2]:
```
from IPython.display import Image
Image('Images/L2Norm.png', width=300)
```

Out[2]:




## $p$-norm

Euclidean norm, or $2$-norm, is a subclass of an important class of $p$-norms:

$$\|x\|_p = \Big(\sum_{i=1}^n |x_i|^p\Big)^{1/p}.$$

There are two very important special cases:

- Infinity norm, or Chebyshev norm which is defined as the maximal element: $\|x\|_{\infty} = \max_i |x_i|$
- $L_1$ norm (or **Manhattan distance**) which is defined as the sum of modules of the elements of $x$: $\|x\|_1 = \sum_i |x_i|$

## Computing Norms

The `numpy` package has all we need for computing norms (`np.linalg.norm` function)

In [3]:
```
import numpy as np

n = 100
a = np.ones(n)

print(a)
print(np.linalg.norm(a, 1)) # L1 norm
print(np.linalg.norm(a, 2)) # L2 norm
print(np.linalg.norm(a, np.inf))

b = a + 1e-3 * np.random.randn(n)
print(b)
print()
print('Relative error:',
      np.linalg.norm(a - b, np.inf) / np.linalg.norm(b, np.inf))
```

```
[1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.
 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.
 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.
 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.
 1. 1. 1. 1.]
100.0
10.0
1.0
[1.00037435 0.99953124 0.99992333 1.0014888  1.00032329 1.00050046
 1.00078602 0.99924418 0.99969855 1.00210667 1.00094794 1.00080644
 0.9995451  0.9973272  0.99983952 1.00145786 1.00006065 1.00228847
 1.00024384 0.99927576 1.00074415 1.00052594 1.00042917 1.00072768
 0.99929429 1.00141766 1.00173564 0.99915889 1.00009986 0.99906971
 0.99996623 0.99950146 0.99925539 1.00130413 1.00083764 0.99949217
 0.99928815 0.99995427 1.00000749 0.9989179  0.99995726 0.99777181
 1.00036878 1.00070422 0.99823925 1.00020147 0.99977514 0.99915426
 0.99980286 1.00108473 0.99983239 1.00131403 1.00066266 1.00175787
 0.99936652 1.00029688 1.0008256  1.00069293 0.99890104 1.00069938
 1.00032954 0.9997104  1.00069634 1.0006385  0.9987517  0.99944188
 0.99896297 1.00068079 0.99903867 1.00045222 1.00141346 1.00191724
 0.99962728 0.99963954 0.99829915 1.00199422 1.00041936 1.0002962
 0.9986163  1.00145062 1.00210623 0.99923621 1.0001467  1.00030778
 1.00013833 0.9994478  0.99868239 1.00042074 0.99946207 0.99804034
 0.99985559 1.00228056 1.00085015 1.00133834 0.99957209 1.00028839
 1.0024329  1.00053665 1.00051172 1.00138696]

Relative error: 0.002666316967426874
```

## Matrix Norms

How to measure distances between matrices?

**Frobenius** norm of the matrix:

$$\|A\|_F = \left( \sum_{i=1}^{n} \sum_{j=1}^{m} |a_{ij}|^2 \right)^{1/2}$$

> Useful for computing objective function in machine learning for optimization

In [4]:
```
n = 100
a = np.random.randn(n, n) # Random n x n matrix

norm_a = np.linalg.norm(a, 'fro') # Frobenius

print('Frobenius:', norm_a)
```

```
Frobenius: 98.98238763060469
```

# 2. Operations on Matrices

The **Inner Product** is defined as

$$< x, y >= x^T y = \sum_{i=1}^{n} \overline{x}_i y_i,$$

where $\overline{x}$ denotes the *complex conjugate* of $x$.

The Euclidean norm is then

$$\|x\|^2 =< x, x >$$

=> the norm is **induced** by scalar product.

The **Outer Product** of vectors $x$ and $y$ is $xy^T$ (matrix with rank 1).

**Remarks**: The **angle** between two vectors is defined as

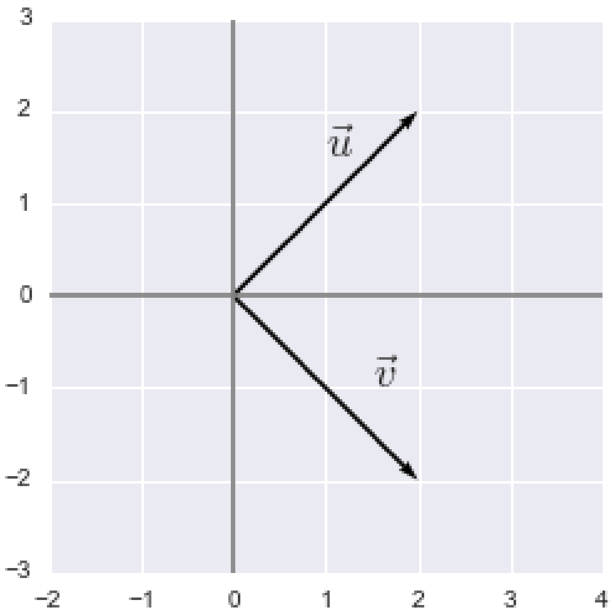
$$\cos\phi = \frac{< x, y >}{\|x\|\|y\|}$$

Two vectors $x$ and $y$ are **Orthogonal** if $< x, y >= 0$.

**Orthonormal vectors**: Vectors that satsify following condition are orthonormal $x_i^T x_j = 0$ when $i \neq j$ and $x_i^T x_i = 1$

In [5]:
```
Image('Images/Orthogonal.png', width = 400)
```

Out[5]:




In [6]:
```
x = np.array([1, 4, 0], float)
y = np.array([2, 2, 1], float)
print("x:", x)
print("y:", y)

print("Dot product of x and y:",   np.dot(x, y))
print("Inner product of x and y:", np.inner(x, y))
print("Outer product of x and y:", np.outer(x, y))
print("Cross product of x and y:", np.cross(x, y))
# The Cross Product of two vectors is another vector that is
# at right angles to both
```

```
x: [1. 4. 0.]
y: [2. 2. 1.]
Dot product of x and y: 10.0
Inner product of x and y: 10.0
Outer product of x and y: [[2. 2. 1.]
 [8. 8. 4.]
 [0. 0. 0.]]
Cross product of x and y: [ 4. -1. -6.]
```

## Matrix Inverse and Transpose

In [7]:
```
# Determinant of Matrix
n = 6
M = np.random.randint(100,size=(n,n))
print(M)
print('Determinant:',np.linalg.det(M))
```

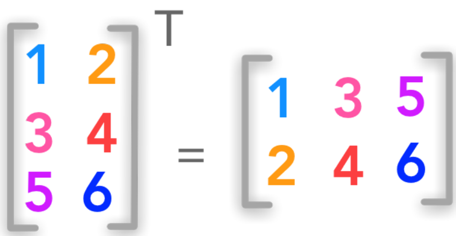
```
[[49 88 77 40 78 76]
 [35 80 40 85 13 29]
 [ 7 74 69 35 61  8]
 [96 80 42 16 87 65]
 [24 47  1 57 93 26]
 [36 14 49 35 85 42]]
Determinant: 107531492377.00043
```

In [8]:
```
# Inverse
A = np.random.randint(100,size=(5,5))
print(A)
print()
Ainv = np.linalg.inv(A)
print(Ainv)
```

```
[[61  6  0 64 58]
 [78 20 81 95 35]
 [57 41 32 29 49]
 [ 3 92 23 69 63]
 [14 25 70 47 70]]

[[ 0.00103756  0.00243244  0.01537544 -0.00524171 -0.00812118]
 [-0.00892033  0.00038418  0.01056552  0.00888594 -0.00819417]
 [-0.01106113  0.00544282  0.00261387 -0.00381301  0.00804552]
 [ 0.00702165  0.00802861 -0.01805784  0.00672609 -0.00324523]
 [ 0.00932492 -0.01145715  0.00266219 -0.00282829  0.01296986]]
```

In [9]:
```
from IPython.display import Image
Image('Images/Transpose.png', width=300)
```

Out[9]:



In [10]:
```
# Matrix Transpose

A = np.array([[1,2,0], [3,5,9]])
print(A)
print()
print(A.T)
```

```
[[1 2 0]
 [3 5 9]]

[[1 3]
 [2 5]
 [0 9]]
```

## Moore-Penrose Pseudo-Inverse of a Matrix

$$A^{+} = (A^{H}A)^{-1}A^{H}$$

In [11]:
```
# Moore-Penrose pseudo-inverse of a non-square matrix
A = np.random.randn(5, 3)
B = np.linalg.pinv(A)

print(A)
print()
print(B)

# Verify
np.allclose(A, np.dot(A, np.dot(B, A)))
```

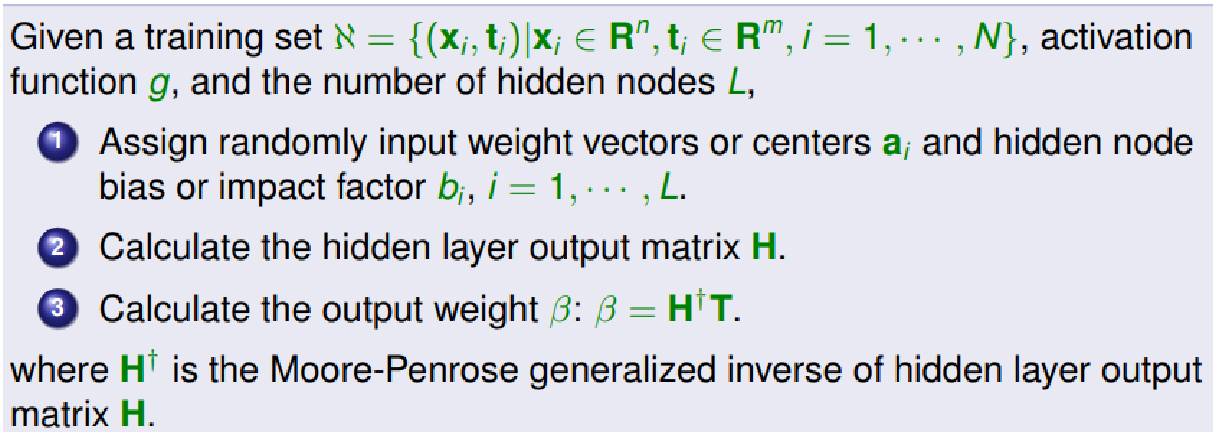
```
[[-0.05657874  1.38117289  0.10198001]
 [ 0.30139228 -2.18349837 -0.13083042]
 [ 0.09115627  0.01090333 -1.96365142]
 [ 0.98339875  0.13906339  0.48230502]
 [ 0.90294366 -0.11074621 -1.18896585]]

[[ 0.04931736  0.04872002 -0.1058513   0.62305502  0.42643188]
 [ 0.21081634 -0.32217067  0.02423116  0.07010307  0.04195099]
 [ 0.00276491  0.01877736 -0.37351909  0.17234944 -0.15609228]]
```

Out[11]: `True`

Used extensively in Machine Learning, for example, Extreme Learning Machine

In [12]:
```
from IPython.display import Image
Image('Images/ELM.png')
```

Out[12]:




## Matrix Multiplication

Consider composition of two linear operators:

1. $y = Bx$
2. $z = Ay$

Then, $z = Ay = ABx = Cx$, where $C$ is the **matrix-by-matrix product**.

A product of an $n \times k$ matrix $A$ and a $k \times m$ matrix $B$ is a $n \times m$ matrix $C$ with the elements

$$c_{ij} = \sum_{s=1}^{k} a_{is} b_{sj}, \quad i = 1, \dots, n, \quad j = 1, \dots, m$$

In [13]:
```
import numpy as np
def matmul(a, b):
    n = a.shape[0]
    k = a.shape[1]
    m = b.shape[1]
    c = np.zeros((n, m))
    for i in range(n):
        for j in range(m):
            for s in range(k):
                c[i, j] += a[i, s] * b[s, j]
```

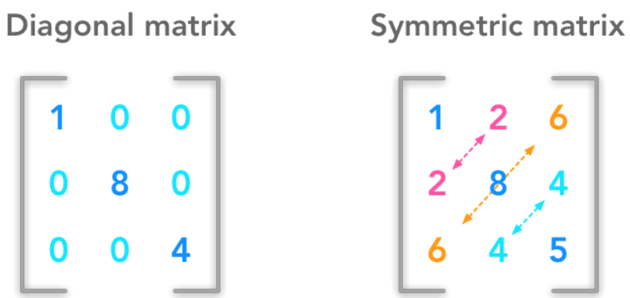
In [14]:
```
n = 100
a = np.random.randn(n, n)
b = np.random.randn(n, n)

%timeit c = matmul(a, b)

%timeit c = np.dot(a, b)
```

```
724 ms ± 27.4 ms per loop (mean ± std. dev. of 7 runs, 1 loop each)
77.3 µs ± 6.39 µs per loop (mean ± std. dev. of 7 runs, 10000 loops each)
```

# 3. Special Matrices

In [15]:
```
from IPython.display import Image
Image('Images/DiagSymm.png', width=400)
```

Out[15]:




## Diagonal Matrix

- Widely useful, eg. SVD

In [16]:
```
import numpy as np
v = np.array([2, 4, 3, 1])
np.diag(v)
```

Out[16]:
```
array([[2, 0, 0, 0],
       [0, 4, 0, 0],
       [0, 0, 3, 0],
       [0, 0, 0, 1]])
```

## Identity Matrix

In [17]:
```
np.identity(3)
```

Out[17]:
```
array([[1., 0., 0.],
       [0., 1., 0.],
       [0., 0., 1.]])
```

In [18]:
```
np.identity(3, dtype=int)
```

Out[18]:
```
array([[1, 0, 0],
       [0, 1, 0],
       [0, 0, 1]])
```

Show that for any matrix $A$, $AI = IA = A$

In [19]:
```
A = np.array([[4,2,1],[4,8,3],[1,1,0]])
I = np.identity(3, dtype=int)
np.dot(A,I)
```

Out[19]:
```
array([[4, 2, 1],
       [4, 8, 3],
       [1, 1, 0]])
```

In [20]:
```
np.dot(A,I) == np.dot(I,A)
```

Out[20]:
```
array([[ True,  True,  True],
       [ True,  True,  True],
       [ True,  True,  True]])
```

## Unitary / Orthogonal Matrices

A **Unitary** matrix is a matrix that when multiplied by its complex conjugate transpose matrix, equals the identity matrix.

$$U^H U = U U^H = I$$

When $U^H = U^\top$, the matrix is called **Orthogonal**.

**Product of two unitary matrices is a unitary matrix:**

$$(UV)^H UV = V^H (U^H U) V = V^H V = I$$

In [21]:
```
a = 0.7
b = (1-a**2)**0.5

U = np.array([[a,b], [-b,a]])
print(U)
print()
print(U.dot(U.conj().T))
```

```
[[ 0.7         0.71414284]
 [-0.71414284  0.7       ]]

[[1.00000000e+00 1.59237766e-18]
 [1.59237766e-18 1.00000000e+00]]
```

# 4. Matrix Rank

- The maximum number of linearly independent rows in a matrix $A$ is called the **row rank** of $A$, and the maximum number of linearly independent columns in $A$ is called **column rank** of $A$.

In [22]:
```
# Computing matrix rank
import numpy as np

n = 50
a1 = np.ones((n, n))
a2 = np.array([[1, 0, -1], [0, 1, 0], [1, 0, 1]])

print('Rank of the matrix:', np.linalg.matrix_rank(a1))
print('Rank of the matrix:', np.linalg.matrix_rank(a2))

b = a1 + 1e-6 * np.random.randn(n, n) # adding very small Gaussian noise
print('Rank of the matrix:', np.linalg.matrix_rank(b, tol=1e-8) )
# Boom!
```

```
Rank of the matrix: 1
Rank of the matrix: 3
Rank of the matrix: 49
```

### Stability and Condition Number

Example:

$$\begin{pmatrix} 8 & 6 & 4 & 1 \\ 1 & 4 & 5 & 1 \\ 8 & 4 & 1 & 1 \\ 1 & 4 & 3 & 6 \end{pmatrix} x = \begin{pmatrix} 19 \\ 11 \\ 14 \\ 14 \end{pmatrix}$$

In [23]:
```
import numpy.linalg as LA

A = np.array([[8,6,4,1],[1,4,5,1],[8,4,1,1],[1,4,3,6]])
b = np.array([19,11,14,14])
LA.solve(A,b)
```

Out[23]: `array([1., 1., 1., 1.])`

In [24]:
```
# Introduce tiny perturbations
b = np.array([19.01,11.05,14.07,14.05])

LA.solve(A,b)
```

Out[24]: `array([-2.34 ,  9.745, -4.85 , -1.34 ])`

Note that the *tiny* perturbations in the outcome vector $b$ cause large differences in the solution! When this happens, we say that the matrix $A$ is **ill-conditioned**.

This happens when a matrix is close to being **singular** (i.e. non-invertible).

- The **Condition Number** is defined as:

$$cond(A) = ||A|| \cdot ||A^{-1}||$$

- Also, defined as

$$cond(A) = \frac{\lambda_1}{\lambda_n}$$

  where $\lambda_1$ is the maximum singular value of $A$ and $\lambda_n$ is the smallest.
- The **higher the condition number, the more unstable the system**.

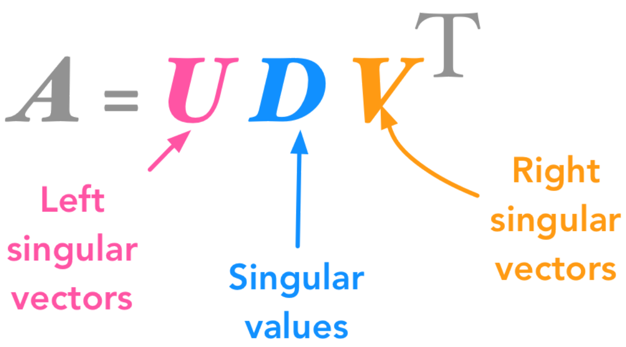
In [25]:
```
U, s, Vt = np.linalg.svd(A)
print('Condition number of A: ', max(s)/min(s))
```

```
Condition number of A:  3198.6725811994825
```

# 5. SVD (Singular Value Decomposition) of Matrix

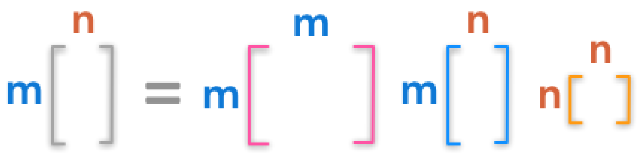
In [26]:
```
Image('Images/SVDEq.png', width=400)
```

Out[26]:



In [27]:
```
Image('Images/SVDMatDim.png', width=400)
```

Out[27]:




- The SVD decomposition is a factorization of a matrix, with many useful **applications in computer vision, signal processing and deep learning**.
- The SVD decomposition of a matrix $A$ is of the form
$$A = U\Sigma V^T$$
- Since $U$ and $V$ are orthogonal (this means that $U^T \times U = I$ and $V^T \times V = I$) we can write the inverse of $A$ as
$$A^{-1} = V\Sigma^{-1}U^T$$

In [28]:
```
A = np.floor(np.random.rand(4,4)*20-10) # generating a random matrix
b = np.floor(np.random.rand(4,1)*20-10) # system Ax = b

print(A)
print(b)
```

```
[[  2.  -6.  -4.  -2.]
 [  2.  -8. -10.   4.]
 [  2.  -8.  -8.   4.]
 [ -9.  -3.   4.   5.]]
[[-9.]
 [ 4.]
 [ 3.]
 [-3.]]
```

In [29]:
```
U,s,Vt = np.linalg.svd(A) # SVD decomposition of A

# computing the inverse using pinv
pinv = np.linalg.pinv(A)

# computing the inverse using the SVD decomposition
pinv_svd = np.dot(np.dot(Vt.T, np.linalg.inv(np.diag(s))), U.T)

print("Inverse computed by lingal.pinv()\n",pinv)
print("Inverse computed using SVD\n",pinv_svd)
```

```
Inverse computed by lingal.pinv()
 [[-7.44680851e-02 -4.46808511e-01  5.42553191e-01 -1.06382979e-01]
 [-1.22340426e-01  2.65957447e-01 -2.87234043e-01 -3.19148936e-02]
 [-2.33724540e-16 -5.00000000e-01  5.00000000e-01 -7.10485506e-17]
 [-2.07446809e-01 -2.44680851e-01  4.04255319e-01 -1.06382979e-02]]
Inverse computed using SVD
 [[-7.44680851e-02 -4.46808511e-01  5.42553191e-01 -1.06382979e-01]
 [-1.22340426e-01  2.65957447e-01 -2.87234043e-01 -3.19148936e-02]
 [-2.34235608e-16 -5.00000000e-01  5.00000000e-01 -7.49112654e-17]
 [-2.07446809e-01 -2.44680851e-01  4.04255319e-01 -1.06382979e-02]]
```

Now, we can solve $Ax = b$ using the inverse:
$$Ax = b \implies x = A^{-1}b$$

In [30]:
```
x = np.linalg.solve(A, b) # solve Ax=b using linalg.solve

xPinv = np.dot(pinv_svd, b) # solving Ax=b computing x = A^(-1)*b

print(x)
print(xPinv)
```

```
[[ 0.82978723]
 [ 1.39893617]
 [-0.5       ]
 [ 2.13297872]]
[[ 0.82978723]
 [ 1.39893617]
 [-0.5       ]
 [ 2.13297872]]
```

In [31]:
```
# How much FAST is SVD for finding inverses?

n = 30

A = np.floor(np.random.rand(n,n)*20-10) # generating a random matrix
U, s, Vt = np.linalg.svd(A) # SVD decomposition of A

# computing the inverse using pinv
%timeit np.linalg.pinv(A)

# computing the inverse using the SVD decomposition
%timeit np.dot(np.dot(Vt.T, np.linalg.inv(np.diag(s))), U.T)
```

```
324 µs ± 3.12 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
187 µs ± 5.26 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
```

# Exercise

### Write a function in Python to solve a system $Ax = b$ using SVD decomposition.

- Your function should take $A$ and $b$ as input and return $x$.
- Your function should include the following:
  - First, check that $A$ is invertible - return error message if it is not (*Hint*: product of singular values should be non-zero for invertibility)
  - Invert $A$ using SVD and solve (Remember: $A^{-1} = V\Sigma^{-1}U^T$)
  - return $x$

In [32]:
```
def svdsolver(A, b):
    U, s, Vt = np.linalg.svd(A)
    if np.prod(s) == 0:
       print('Matrix is singular')
    else:
       return np.dot(np.dot((Vt.T).dot(np.diag(s**(-1))), U.T),b)

A = np.array([[1,1],[1,2]])
b = np.array([3,1])
print(np.linalg.solve(A,b))
print(svdsolver(A,b))
```

```
[ 5. -2.]
[ 5. -2.]
```

# 6. Eigen-things

## What is an eigenvector

An vector $x \neq 0$ is called an **eigenvector** of a square matrix $A$ if there exists a number $\lambda$ such that

$$Ax = \lambda x.$$

The number $\lambda$ is called an **eigenvalue**.

In [33]:
```
from IPython.display import Image
Image('Images/Eigen.png', width=300)
```

Out[33]:

$$\begin{bmatrix} 2 & 3 \\ 2 & 1 \end{bmatrix} \times \begin{bmatrix} 3 \\ 2 \end{bmatrix} = \begin{bmatrix} 12 \\ 8 \end{bmatrix} = 4 \times \begin{bmatrix} 3 \\ 2 \end{bmatrix}$$

$$\mathbf{A} \;.\; \mathbf{v} \qquad = \lambda \;.\; \mathbf{v}$$

In [1]:
```
import numpy as np
import numpy.linalg as LA
A = np.diag((1, 2, 3))
print(A)

w, v = LA.eig(A)
print('Eigen Values:', w)
print('Eigen Vectors:')
print(v)
```

```
[[1 0 0]
 [0 2 0]
 [0 0 3]]
Eigen Values: [1. 2. 3.]
Eigen Vectors:
[[1. 0. 0.]
 [0. 1. 0.]
 [0. 0. 1.]]
```

In [2]:
```
# Eigen-decomposition of Covariance matrix
mu = [0,0]
sigma = [[0.6,0.2], [0.2,0.2]]
n = 1000
x = np.random.multivariate_normal(mu, sigma, n).T

A = np.cov(x)
print(A)
```

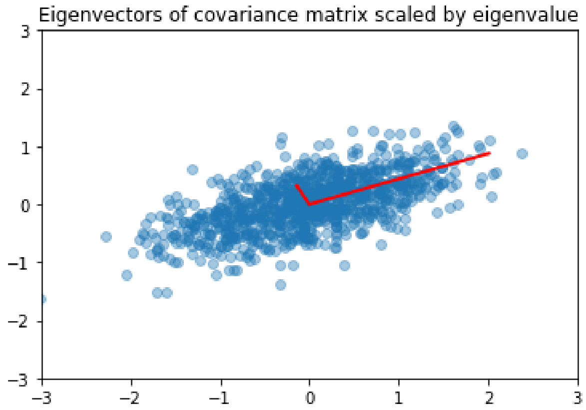
```
[[0.63301579 0.22564912]
 [0.22564912 0.21385278]]
```

In [3]:
```
w, v = LA.eig(A)
print(w)
print(v)
```

```
[0.73139846 0.11547011]
[[ 0.91666204 -0.39966324]
 [ 0.39966324  0.91666204]]
```

In [37]:
```
?zip
```

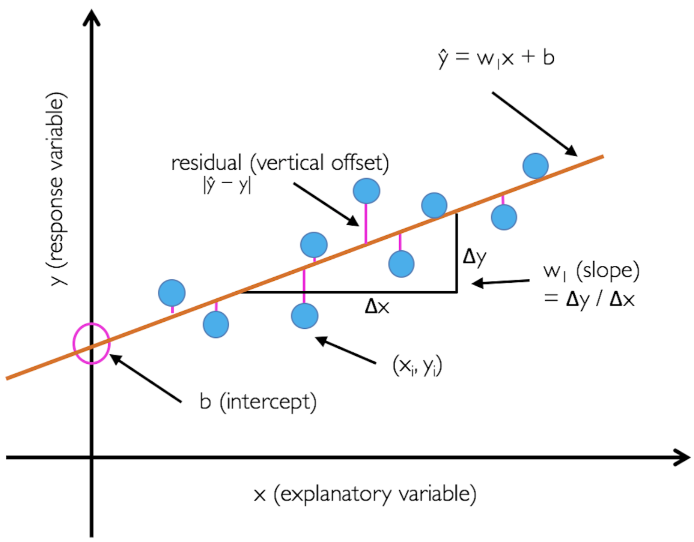
In [5]:
```
import matplotlib.pyplot as plt

plt.scatter(x[0,:], x[1,:], alpha=0.4)

for evals, evecs in zip(w, v.T):
    plt.plot([0, 3*evals*evecs[0]], [0, 3*evals*evecs[1]], 'r-', lw=2)

plt.axis([-3, 3, -3, 3])
plt.title('Eigenvectors of covariance matrix scaled by eigenvalue')
plt.show()
```



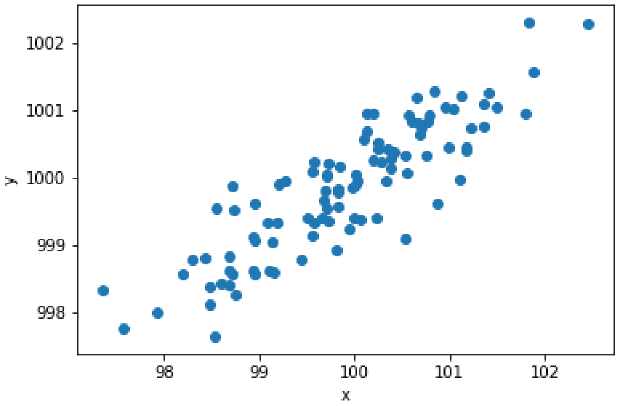

# 7. Application: Least-Squares Linear Regression

In [39]:
```
import scipy.stats
import matplotlib.pyplot as plt
%matplotlib inline
```

- Fit slope and intercept so that the linear regression fit minimizes the sum of the residuals (vertical offsets or distances)



In [40]:
```
rng = np.random.RandomState(123)
mean = [100, 1000]
cov = [[1, 0.9], [0.9, 1]]
sample = rng.multivariate_normal(mean, cov, size=100)
x, y = sample[:, 0], sample[:, 1]

plt.scatter(x, y)
plt.xlabel('x')
plt.ylabel('y')
plt.show()
```




- Closed-form (analytical) solution:

$$L = \frac{1}{2}\sum_{i=1}^{N}(y_i - x_i^\intercal w)^2 = \frac{1}{2}\|y - Xw\|^2 = \frac{1}{2}(y - Xw)^\intercal(y - Xw)$$

$$\frac{\partial L}{\partial w} = -y^\intercal X + w^\intercal X^\intercal X = 0$$

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

In [41]:
```
# x.shape => (100,)
# newaxis: increase the dimension of existing array by one more dimension
X = x[:, np.newaxis]
# X.shape => (100,1)
print(X.shape[0])
```

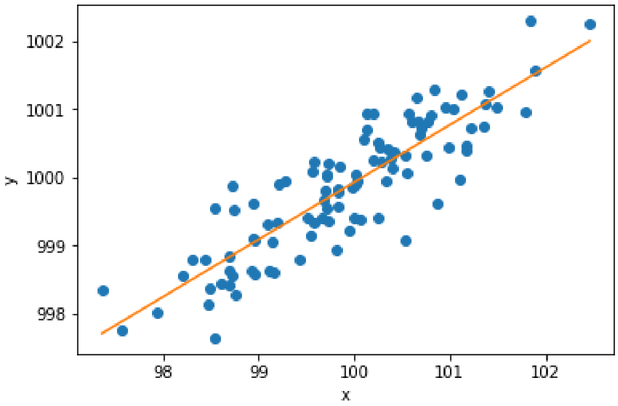
```
100
```

In [42]:
```
# adding a column vector of "ones"
# hstack: stack arrays in sequence horizontally (column wise)
Xb = np.hstack((np.ones((X.shape[0], 1)), X))
# Xb.shape => (100, 2); first column for bias, second column for X
w = np.zeros(X.shape[1])

# Closed-form solution
z = np.linalg.inv(np.dot(Xb.T, Xb))
w = np.dot(z, np.dot(Xb.T, y))

b, w1 = w[0], w[1]

print('slope: %.2f' % w1)
print('y-intercept: %.2f' % b)
```

```
slope: 0.84
y-intercept: 915.59
```

### Show line fit

In [43]:
```
extremes = np.array([np.min(x), np.max(x)])
predict = extremes*w1 + b

plt.plot(x, y, marker='o', linestyle='')
plt.plot(extremes, predict)
plt.xlabel('x')
plt.ylabel('y')
plt.show()
```




### Evaluate

#### Mean squared error (MSE)

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

In [44]:
```
y_predicted = x*w1 + b

mse = np.mean((y - y_predicted)**2)
mse
```

Out[44]: 0.21920128791623675

In [45]:
```
rmse = np.sqrt(mse)
rmse
```

Out[45]: 0.46818937185313886

# II. Probability

In [46]:
```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
from scipy import stats
```

## Probability Mass Functions

- Goal of probability and uncertainty computations is to estimate population parameters from samples

## Bernoulli Trial

Bernoulli trial (or binomial trial): random experiment with 2 possible outcomes

In [47]:
```
rng = np.random.RandomState(123)

coin_flips = rng.randint(0, 2, size=1000)
heads = np.sum(coin_flips)
heads
```

Out[47]: 520

In [48]:
```
tails = coin_flips.shape[0] - heads
tails
```

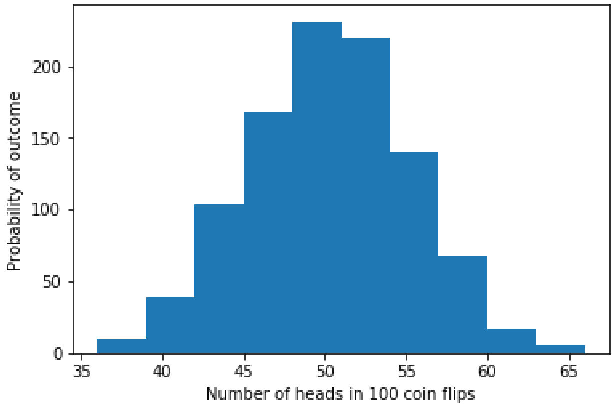
Out[48]: 480

In [49]:
```
rng = np.random.RandomState(123)

for i in range(7):
    num = 10**i
    coin_flips = rng.randint(0, 2, size=num)
    heads_proba = np.mean(coin_flips)
    print('Heads chance: %.2f' % (heads_proba*100))
```

```
Heads chance: 0.00
Heads chance: 40.00
Heads chance: 47.00
Heads chance: 53.70
Heads chance: 49.53
Heads chance: 49.80
Heads chance: 50.03
```

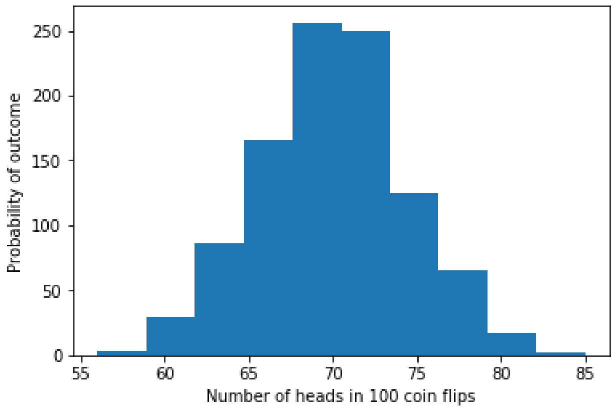
### Do 100 coin flips 1000 times:

In [50]:
```
n_experiments = 1000
n_bernoulli_trials = 100

rng = np.random.RandomState(123)
outcomes = np.empty(n_experiments, dtype=np.float)

for i in range(n_experiments):
    coin_flips = rng.randint(0, 2, size=n_bernoulli_trials)
    head_counts = np.sum(coin_flips)
    outcomes[i] = head_counts

plt.hist(outcomes)
plt.xlabel('Number of heads in 100 coin flips')
plt.ylabel('Probability of outcome')
plt.show()
```



### Repeat with biased coin

In [51]:
```
p = 0.7
n_experiments = 1000
n_bernoulli_trials = 100

rng = np.random.RandomState(123)
outcomes = np.empty(n_experiments, dtype=np.float)

for i in range(n_experiments):
    coin_flips = rng.rand(n_bernoulli_trials)
    head_counts = np.sum(coin_flips < p)
    outcomes[i] = head_counts

plt.hist(outcomes)
plt.xlabel('Number of heads in 100 coin flips')
plt.ylabel('Probability of outcome')
plt.show()
```




## Binomial Distribution

- Bernoulli trial (or binomial trial): random experiment with 2 possible outcomes
- a binomial distribution describes a binomial variable $B(n, p)$ of *n* of Bernoulli trials (which are statistically independent); *p* is the probability of success (and *q* is the probability of failure, 1-*p*)
- Probability of *k* successes:

$$P(k) = \binom{n}{k} p^k q^{n-k}$$

where $\binom{n}{k}$ ("*n choose k*") is the binomial coefficient

$$\binom{n}{k} = \frac{n!}{k!(n-k)!}$$

### Compute probability of 50 heads in 100 Bernoulli trials flipping a fair coin:

In [52]:
```
def factorial(n):
    if n == 0:
        return 1
    else:
        return n * factorial(n-1)

def combin(n, k): # "n choose k*
    return factorial(n) / factorial(k) / factorial(n - k)
```

In [53]:
```
p = 0.5 # probability of success
n = 100 # n_trials
k = 50 # k_successes

proba = combin(n, k) * p**k * (1 - p)**(n - k)
proba
```

Out[53]: 0.07958923738717877

In [54]:
```
# Direct method
rv = stats.binom(n, p)
rv.pmf(50)
```

Out[54]: 0.07958923738717888

# Probability Density Functions (PDFs)

- for working with continuous variables (vs. probability mass functions for discrete variables)
- here, the area under the curve give the probability (in contrast to probability mass functions where we have probabilities for every single value)
- the area under the whole curve is 1

# Normal Distribution (Gaussian Distribution)

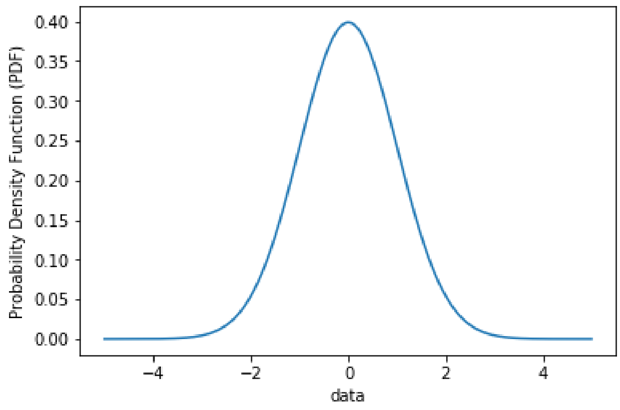
## Probability Density Function of the Normal Distribution

- unimodal and symmetric
- many algorithms in machine learning & statistics have normality assumptions
- two parameters: mean (center of the peak) and standard deviation (spread); $\mu, \sigma$
- we can estimate parameters of $\mathcal{N}(\mu, \sigma^2)$ by sample mean ($\bar{x}$) and sample variance ($s^2$)
- univariate Normal distribution:

$$f(x \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left( - \frac{(x-\mu)^2}{2\sigma^2} \right)$$

- standard normal distribution with zero mean and unit variance, $\mathcal{N}(0, 1)$

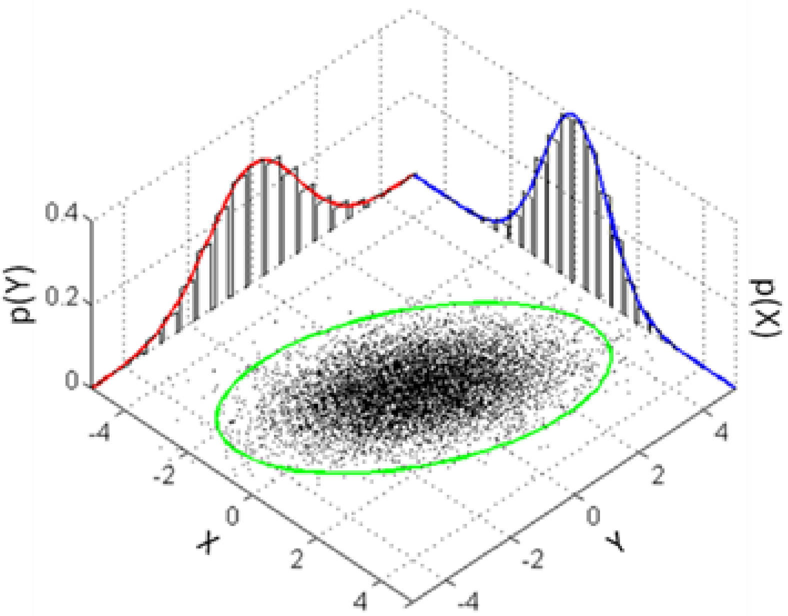
In [55]:
```
def univariate_gaussian_pdf(x, mean, variance):
    return (1. / np.sqrt(2*np.pi*variance) *
            np.exp(- ((x - mean)**2 / 2.*variance)))

mean = 0
stddev = 1
x = np.arange(-5, 5, 0.01)
y = univariate_gaussian_pdf(x, mean, stddev**2)
plt.plot(x, y)
plt.xlabel('data')
plt.ylabel('Probability Density Function (PDF)')
plt.show()
```




# Application: Anomaly Detection

In [6]:
```
from IPython.display import Image
Image('Images/MVN.png', width=500)
```

Out[6]:

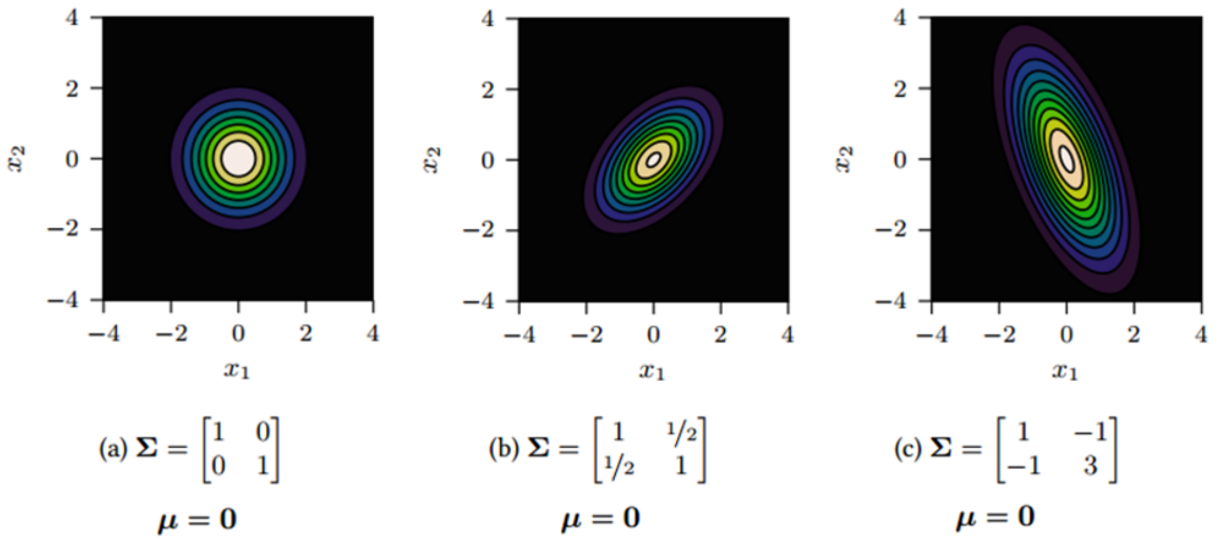



### Multi-variate Normal (MVN)

$$\mathcal{N}(x|\mu,\Sigma) = \frac{1}{\sqrt{(2\pi)^D}}\frac{1}{\sqrt{|\Sigma|}}\exp\left(-\frac{1}{2}(x-\mu)^\intercal\Sigma^{-1}(x-\mu)\right)$$

In [7]:
```
Image('Images/MVNCov.png', width=800)
```

Out[7]:



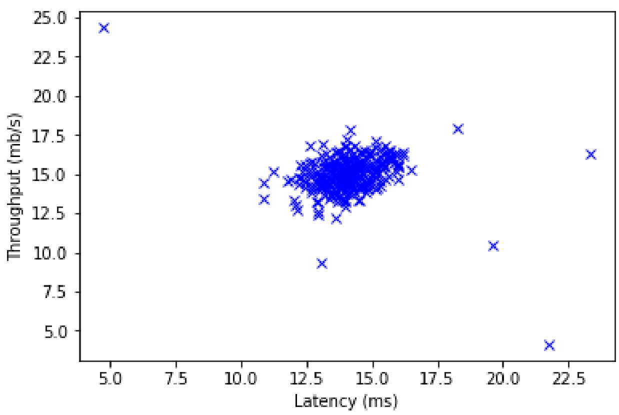

In [56]:
```
import matplotlib.pyplot as plt
import numpy as np
from numpy import genfromtxt
from scipy.stats import multivariate_normal
```

In [57]:
```
def read_dataset(filePath,delimiter=','):
    return genfromtxt(filePath, delimiter=delimiter)

tr_data = read_dataset('Data/anomaly_detect_data.csv')
```

In [58]:
```
n_training_samples = tr_data.shape[0]
n_dim = tr_data.shape[1]

print('Number of datapoints in training set: %d' % n_training_samples)
print('Number of dimensions/features: %d' % n_dim)
print(tr_data[1:5,:])
```

```
Number of datapoints in training set: 307
Number of dimensions/features: 2
[[13.409 13.763]
 [14.196 15.853]
 [14.915 16.174]
 [13.577 14.043]]
```

In [59]:
```
plt.xlabel('Latency (ms)')
plt.ylabel('Throughput (mb/s)')
plt.plot(tr_data[:,0],tr_data[:,1],'bx')
plt.show()
```



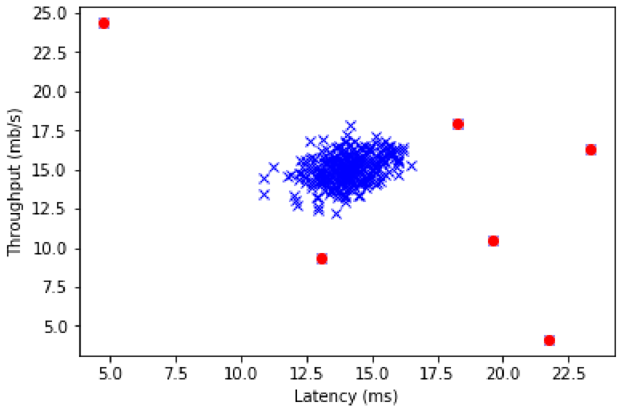
In [60]:
```
def estimateGaussian(dataset):
    mu = np.mean(dataset, axis=0) # mean along each dimension / column
    sigma = np.cov(dataset.T)
    return mu, sigma

def multivariateGaussian(dataset,mu,sigma):
    p = multivariate_normal(mean=mu, cov=sigma)
    return p.pdf(dataset)
```

In [61]:
```
mu, sigma = estimateGaussian(tr_data)
p = multivariateGaussian(tr_data,mu,sigma)
```

In [62]:
```
thresh = 9e-05
# determining outliers/anomalies
outliers = np.asarray(np.where(p < thresh))
outliers
```

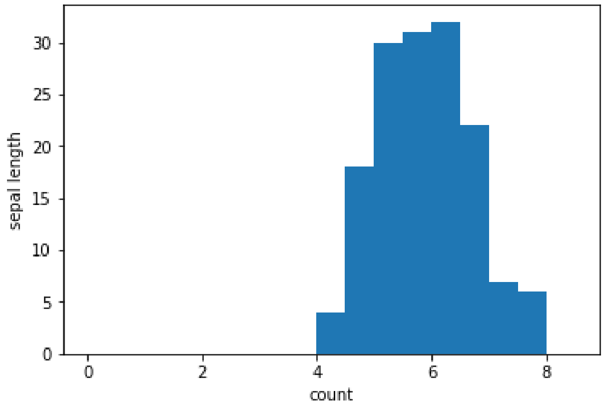
Out[62]:
```
array([[300, 301, 303, 304, 305, 306]], dtype=int64)
```

In [63]:
```
plt.figure()
plt.xlabel('Latency (ms)')
plt.ylabel('Throughput (mb/s)')
plt.plot(tr_data[:,0],tr_data[:,1],'bx')
plt.plot(tr_data[outliers,0],tr_data[outliers,1],'ro')
plt.show()
```




# III. Statistics

In [64]:
```
import pandas as pd
import numpy as np
from scipy import stats
import matplotlib.pyplot as plt
%matplotlib inline

# read dataset
df = pd.read_csv('Data/iris.csv')

def histo():
    # create histogram
    bin_edges = np.arange(0, df['sepal_length'].max() + 1, 0.5)
    fig = plt.hist(df['sepal_length'], bins=bin_edges)

    # add plot labels
    plt.xlabel('count')
    plt.ylabel('sepal length')


histo()
plt.show()
```




### Sample Mean:

$$\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$$

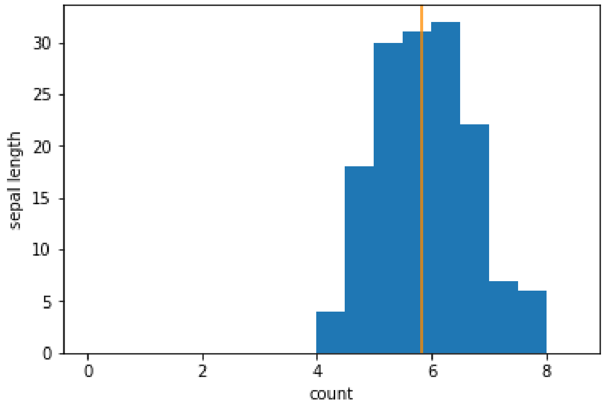
In [65]:
```
x = df['sepal_length'].values
sum(i for i in x) / len(x)
```

Out[65]: 5.843333333333335

In [66]:
```
x_mean = np.mean(x)
x_mean
```

Out[66]: 5.843333333333334

In [67]:
```
histo()
plt.axvline(x_mean, color='darkorange')
plt.show()
```




### Sample Variance:

$$Var_x = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$$

- Bessel's correction to correct the bias of the population variance estimate
- Note the $unit$ of the variable is now $unit^2$

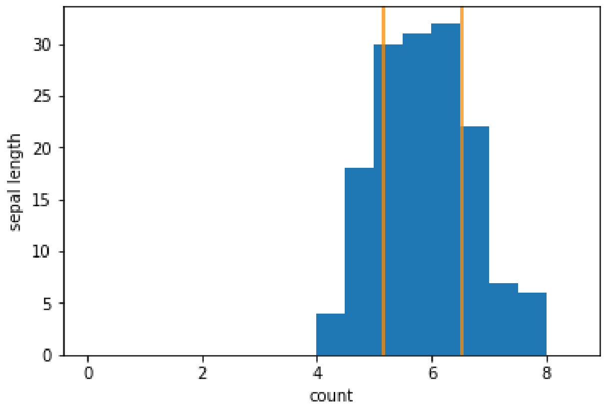
In [68]:
```
sum([(i - x_mean)**2 for i in x]) / (len(x) - 1)
```

Out[68]: 0.6856935123042504

In [69]:
```
var = np.var(x, ddof=1)
var
```

Out[69]: 0.6856935123042507

In [70]:
```
histo()
plt.axvline(x_mean + var, color='darkorange')
plt.axvline(x_mean - var, color='darkorange')
plt.show()
```




### Sample Standard Deviation:

$$Std_x = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2}$$

In [71]:
```
np.sqrt(np.var(x, ddof=1))
```

Out[71]: 0.828066127977863

In [72]:
```
std = np.std(x, ddof=1)
std
```

Out[72]: 0.828066127977863

### Min/Max:

In [73]:
```
print(np.min(x))
print(np.max(x))
```

```
4.3
7.9
```

### 25th and 75th Percentile:

In [74]:
```
np.percentile(x, q=[25, 75], interpolation='lower')
```

Out[74]: array([5.1, 6.4])

### Median (50th Percentile):

In [75]:
```
np.median(x)
```

Out[75]: 5.8

## Covariance and Correlation

In [76]:
```
# read dataset
df = pd.read_csv('Data\iris.csv')
X = df[df.columns[:-1]].values
X.shape
```

Out[76]: (150, 4)

## Sample Covariance

- Measures how two variables differ from their mean
- Positive Covariance: that the two variables are both above or both below their respective means
    - variables are positively "correlated" -- they go up or down together
- Negative Covariance: valuables from one variable tends to be above the mean and the other below their mean
    - negative covariance means that if one variable goes up, the other variable goes down

$$\sigma_{x,y} = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})$$

- note that similar to variance, the dimension of the covariance is $unit^2$

In [77]:
```
# Compute covariance between 2nd and 3rd feature:

x_mean, y_mean = np.mean(X[:, 2:4], axis=0)

sum([(x - x_mean) * (y - y_mean)
     for x, y in zip(X[:, 2], X[:, 3])]) / (X.shape[0] - 1)
```

Out[77]: 1.2956093959731545

Covariance matrix for the 4-feature dataset:

$$\Sigma = \begin{bmatrix} \sigma_1^2 & \sigma_{1,2} & \sigma_{1,3} & \sigma_{1,4} \\ \sigma_{2,1} & \sigma_2^2 & \sigma_{2,3} & \sigma_{2,4} \\ \sigma_{3,1} & \sigma_{3,2} & \sigma_3^2 & \sigma_{4,3} \\ \sigma_{4,1} & \sigma_{4,2} & \sigma_{4,3} & \sigma_4^2 \end{bmatrix}$$

- Notice the variance along the diagonal
- Remember, the sample variance is computed as follows:

$$\sigma_x^2 = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2$$

In [78]:
```
np.cov(X.T)
```

Out[78]:
```
array([[ 0.68569351, -0.042434  ,  1.27431544,  0.51627069],
       [-0.042434  ,  0.18997942, -0.32965638, -0.12163937],
       [ 1.27431544, -0.32965638,  3.11627785,  1.2956094 ],
       [ 0.51627069, -0.12163937,  1.2956094 ,  0.58100626]])
```

## Pearson Correlation Coefficient

- Pearson correlation is "dimensionless" version of the covariance, achieved by dividing by the standard deviation
- Pearson correlation coefficient:

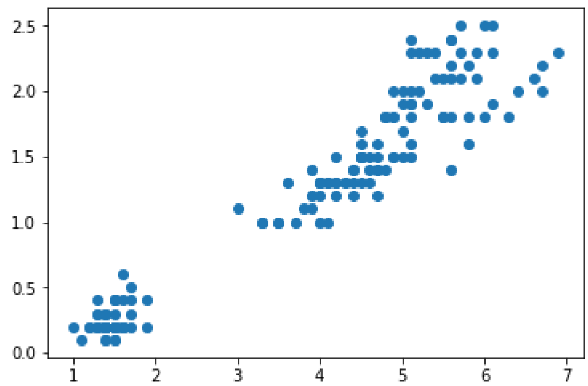
$$\rho_{x,y} = \frac{\frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(x_i - \bar{x})^2}\sqrt{\frac{1}{n-1}\sum_{i=1}^{n}(y_i - \bar{y})^2}}$$

$$= \frac{\sigma_{x,y}}{\sigma_x \sigma_y}$$

- Measures degree of a linear relationship between variables, assuming the variables follow a normal distribution
  - $\rho = 1$: perfect positive correlation
  - $\rho = -1$: perfect negative correlation
  - $\rho = 0$: no correlation

In [79]:
```
plt.scatter(X[:, 2], X[:, 3])
```

Out[79]: <matplotlib.collections.PathCollection at 0x1c77ec6f390>




In [80]:
```
(np.cov(X[:, 2:4].T)[0, 1] /
 (np.std(X[:, 2], ddof=1) * np.std(X[:, 3], ddof=1)))
```

Out[80]: 0.9628654314027963

In [81]:
```
np.corrcoef(X[:, 2:4].T)
```

Out[81]:
```
array([[1.        , 0.96286543],
       [0.96286543, 1.        ]])
```

In [82]:
```
stats.pearsonr(X[:, 2], X[:, 3])
```

Out[82]:
```
(0.9628654314027961, 4.675003907327543e-86)
```

> The p-value roughly indicates the probability of an uncorrelated system producing datasets that have a Pearson correlation at least as extreme as the one computed from these datasets. The p-values are not entirely reliable but are probably reasonable for datasets larger than 500 or so. (https://docs.scipy.org/doc/scipy-0.19.0/reference/generated/scipy.stats.pearsonr.html (https://docs.scipy.org/doc/scipy-0.19.0/reference/generated/scipy.stats.pearsonr.html))

# Scaled Variables

## Standardization

$$Z = \frac{X - \mu}{\sigma}$$

In [83]:
```
from sklearn import preprocessing
import numpy as np
X_train = np.array([[ 1., -1.,  2.],[ 2.,  0.,  0.],[ 0.,  1., -1.]])
print(X_train)
X_scaled = preprocessing.scale(X_train)
print(X_scaled)
```

```
[[ 1. -1.  2.]
 [ 2.  0.  0.]
 [ 0.  1. -1.]]
[[ 0.         -1.22474487  1.33630621]
 [ 1.22474487  0.         -0.26726124]
 [-1.22474487  1.22474487 -1.06904497]]
```

- Scaled data has zero mean and unit variance:

In [84]:
```
X_scaled.mean(axis=0)
```

Out[84]:
```
array([0., 0., 0.])
```

In [85]:
```
X_scaled.std(axis=0)
```

Out[85]:
```
array([1., 1., 1.])
```

## Min-Max Scaler aka Normalization

$$Z = \frac{X - \min(X)}{\max(X) - \min(X)}$$

In [86]:
```
X_train = np.array([[ 1., -1.,  2.],
...                 [ 2.,  0.,  0.],
...                 [ 0.,  1., -1.]])
...
min_max_scaler = preprocessing.MinMaxScaler()
X_train_minmax = min_max_scaler.fit_transform(X_train)
X_train_minmax
```

Out[86]:
```
array([[0.5       , 0.        , 1.        ],
       [1.        , 0.5       , 0.33333333],
       [0.        , 1.        , 0.        ]])
```

The same instance of the transformer can then be applied to some new test data unseen during the fit call: the same scaling and shifting operations will be applied to be consistent with the transformation performed on the train data:

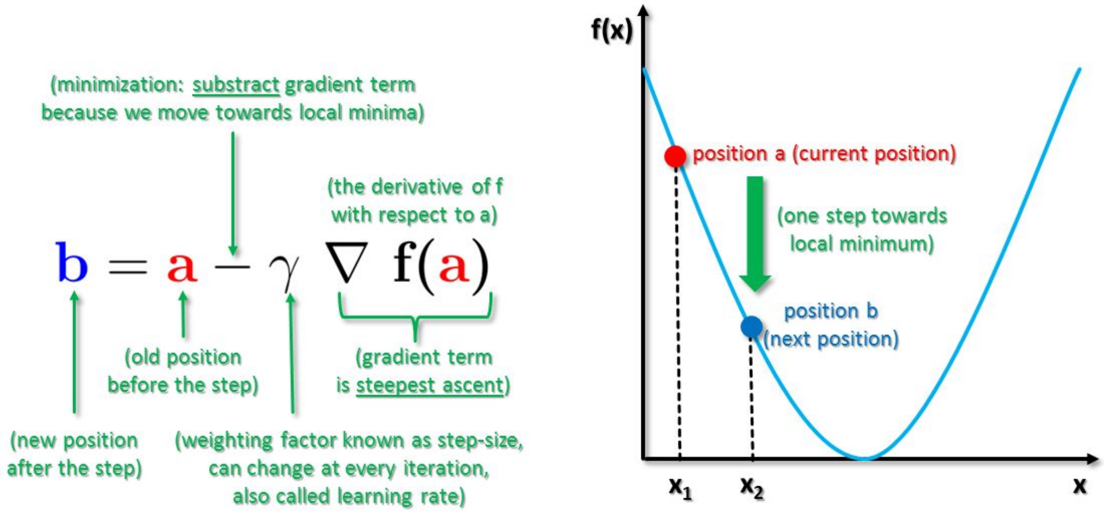
In [87]:
```
X_test = np.array([[ -3., -1.,  4.]])
X_test_minmax = min_max_scaler.transform(X_test)
X_test_minmax
```

Out[87]:
```
array([[-1.5       ,  0.        ,  1.66666667]])
```

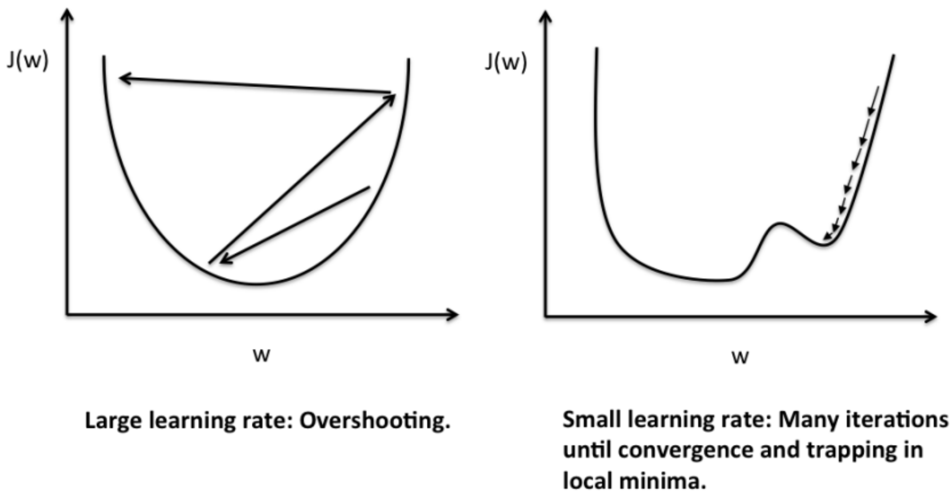
# IV. Optimization

## Gradient Descent

In [89]:
```
from IPython.display import Image, display
display(Image(filename='Images/GradDescent.jpg', width=700))
```




In [90]:
```
from IPython.display import Image, display
display(Image(filename='Images/learningrate.png', width=600))
```



## Batch Gradient Descent

Assume that we have a vector of parameters $\theta$ and a cost function $J(\theta)$ which is the variable we want to minimize (our objective function). Typically, the objective function has the form:

$$J(\theta) = \sum_{i=1}^{m} J_i(\theta)$$

where $J_i$ is associated with the $i$-th observation in our data set.

- The batch gradient descent algorithm, starts with some initial feasible $\theta$ (which we can either fix or assign randomly) and then repeatedly performs the update:

$$\theta := \theta - \eta \nabla_\theta J(\theta) = \theta - \eta \sum_{i=1}^{m} \nabla J_i(\theta)$$

where $\eta$ is a constant controlling step-size and is called the learning rate.

- Note that in order to make a single update, we need to calculate the gradient using the **entire dataset**. This can be very **inefficient for large datasets**.
- In code, batch gradient descent looks like this:

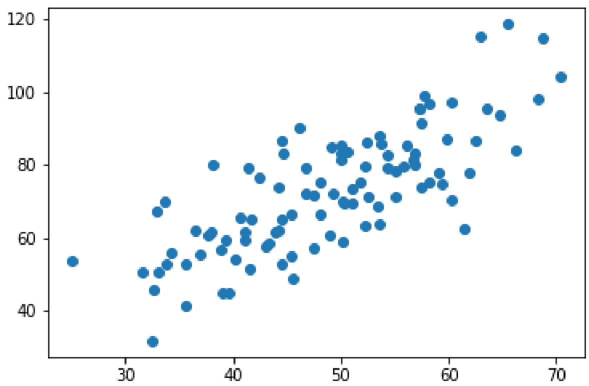
```
for i in range(n_epochs):
  params_grad = evaluate_gradient(loss_function, data, params)
  params = params - learning_rate * params_grad
```

- For a given number of epochs $n_{epochs}$, we first evaluate the gradient vector of the loss function using **ALL** examples in the data set, and then we update the parameters with a given learning rate.
- Batch gradient descent is guaranteed to converge to the global minimum for convex error surfaces and to a local minimum for non-convex surfaces.

In [91]:
```
import numpy as np
points = np.genfromtxt("Data/gd_data.csv", delimiter=",")
```

In [92]:
```
import matplotlib.pyplot as plt
%matplotlib inline

plt.scatter(points[:,0],points[:,1])
```

Out[92]: `<matplotlib.collections.PathCollection at 0x1c70792b6a0>`



- Let's suppose we want to model the above set of points with a line.
- To do this we'll use the standard $y = mx + b$ line equation where $m$ is the line's slope and $b$ is the line's $y$-intercept.
- To find the best line for our data, we need to find the best set of slope $m$ and $y$-intercept $b$ values.
- The error function is given by:

$$E = \frac{1}{N}\sum_{i=1}^{N}(y_i - (mx_i + b))^2$$

- The partial derivatives are given by:

$$\frac{\partial E}{\partial m} = \frac{2}{N}\sum_{i=1}^{N} -x_i(y_i - (mx_i + b))$$

$$\frac{\partial E}{\partial b} = \frac{2}{N}\sum_{i=1}^{N} -(y_i - (mx_i + b))$$

In [93]:
```
%run gradient_descent.py
```

```
Starting gradient descent at b = 0, m = 0, error = 5565.107834483211
Running...
After 1000 iterations b = 0.08893651993741346, m = 1.4777440851894448, error = 112.61481011613473

<Figure size 432x288 with 0 Axes>
```

## Stochastic Gradient Descent (SGD)

- When we have very large data sets, the calculation of $\nabla(J(\theta))$ can be costly as we must process every data point before making a single step (hence the name "batch").
- An alternative approach, the stochastic gradient descent method, is to update $\theta$ sequentially with every observation. The updates then take the form:

$$\theta := \theta - \alpha\nabla_\theta J_i(\theta)$$

- This allows us to start making progress on the minimization problem right away. It is **computationally cheaper**, but it results in a **larger variance** of the loss function in comparison with GD.
- In code, the algorithm should look something like this:

```
for i in range(nb_epochs):
  np.random.shuffle(data)
  for example in data:
    params_grad = evaluate_gradient(loss_function, example, params)
    params = params - learning_rate * params_grad
```

- For a given epoch, we first reshuffle the data (to avoid bias from a particular order), and then for a single example, we evaluate the gradient of the loss function and then update the params with the chosen learning rate.

## Mini-batch SGD

- What if instead of single example from the dataset, we use a batch of data examples with a given size every time we calculate the gradient:

$$\theta = \theta - \eta \nabla_\theta J(\theta; x^{(i:i+n)}; y^{(i:i+n)})$$

- Using mini-batches has the advantage that the **variance in the loss function is reduced**, while the **computational burden is still reasonable**, since we do not use the full dataset.

- The size of the mini-batches becomes another hyper-parameter of the problem. In standard implementations it ranges from 50 to 256.

- In code, mini-batch gradient descent looks like this:

```
for i in range(nb_epochs):
  np.random.shuffle(data)
  for batch in get_batches(data, batch_size=50):
    params_grad = evaluate_gradient(loss_function, batch, params)
    params = params - learning_rate * params_grad
```

- The difference with SGD is that for each update we use a batch of few examples (eg. 100) to estimate the gradient.