曲线拟合

导入基础包:

In [1]:
```
import numpy as np
import matplotlib as mpl
import matplotlib.pyplot as plt
```

多项式拟合

导入线多项式拟合工具:

In [2]:
```
from numpy import polyfit, poly1d
```

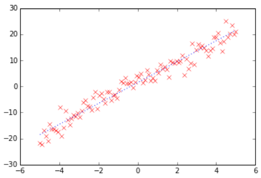
产生数据:

In [3]:
```
x = np.linspace(-5, 5, 100)
y = 4 * x + 1.5
noise_y = y + np.random.randn(y.shape[-1]) * 2.5
```

画出数据:

In [4]:
```
%matplotlib inline

p = plt.plot(x, noise_y, 'rx')
p = plt.plot(x, y, 'b:')
```



进行线性拟合，polyfit 是多项式拟合函数，线性拟合即一阶多项式:

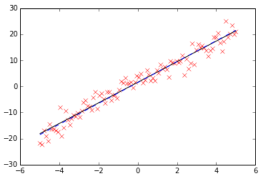
In [5]:
```
coeff = polyfit(x, noise_y, 1)
print coeff
```

```
[ 3.93921315  1.59379469]
```

一阶多项式 $y = a_1 x + a_0$ 拟合，返回两个系数 $[a_1, a_0]$。

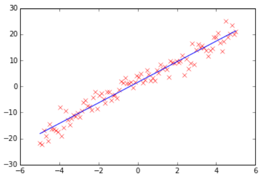
画出拟合曲线:

In [6]:
```
p = plt.plot(x, noise_y, 'rx')
p = plt.plot(x, coeff[0] * x + coeff[1], 'k-')
p = plt.plot(x, y, 'b--')
```



还可以用 poly1d 生成一个以传入的 coeff 为参数的多项式函数:

In [7]:
```
f = poly1d(coeff)
p = plt.plot(x, noise_y, 'rx')
p = plt.plot(x, f(x))
```



In [8]:
```
f
```

Out[8]:
```
poly1d([ 3.93921315,  1.59379469])
```

显示 f:

In [9]:
```
print f
```

```
3.939 x + 1.594
```

还可以对它进行数学操作生成新的多项式:

In [10]:
```
print f + 2 * f ** 2
```

```
       2
31.03 x + 29.05 x + 6.674
```

多项式拟合正弦函数

正弦函数:

In [11]:
```
x = np.linspace(-np.pi,np.pi,100)
y = np.sin(x)
```

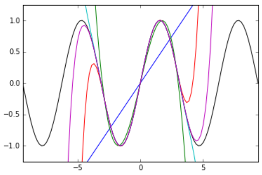
用一阶到九阶多项式拟合，类似泰勒展开:

In [12]:
```
y1 = poly1d(polyfit(x,y,1))
y3 = poly1d(polyfit(x,y,3))
y5 = poly1d(polyfit(x,y,5))
y7 = poly1d(polyfit(x,y,7))
y9 = poly1d(polyfit(x,y,9))
```

In [13]:
```
x = np.linspace(-3 * np.pi,3 * np.pi,100)

p = plt.plot(x, np.sin(x), 'k')
p = plt.plot(x, y1(x))
p = plt.plot(x, y3(x))
p = plt.plot(x, y5(x))
p = plt.plot(x, y7(x))
p = plt.plot(x, y9(x))

a = plt.axis([-3 * np.pi, 3 * np.pi, -1.25, 1.25])
```



黑色为原始的图形，可以看到，随着多项式拟合的阶数的增加，曲线与拟合数据的吻合程度在逐渐增大。

最小二乘拟合

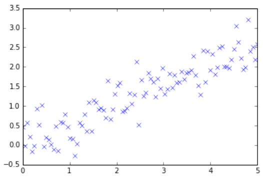
导入相关的模块：

In [14]:
```
from scipy.linalg import lstsq
from scipy.stats import linregress
```

In [15]:
```
x = np.linspace(0,5,100)
y = 0.5 * x + np.random.randn(x.shape[-1]) * 0.35

plt.plot(x,y,'x')
```

Out[15]: [<matplotlib.lines.Line2D at 0xbc98518>]



一般来书，当我们使用一个 N-1 阶的多项式拟合这 M 个点时，有这样的关系存在：

$$XC = Y$$

即

$$\begin{bmatrix} x_0^{N-1} & \dots & x_0 & 1 \\ x_1^{N-1} & \dots & x_1 & 1 \\ \dots & \dots & \dots & \dots \\ x_M^{N-1} & \dots & x_M & 1 \end{bmatrix} \begin{bmatrix} C_{N-1} \\ \dots \\ C_1 \\ C_0 \end{bmatrix} = \begin{bmatrix} y_0 \\ y_1 \\ \dots \\ y_M \end{bmatrix}$$

Scipy.linalg.lstsq 最小二乘解

要得到 C ，可以使用 `scipy.linalg.lstsq` 求最小二乘解。

这里，我们使用 1 阶多项式即 `N = 2`，先将 x 扩展成 X：

In [16]:
```
X = np.hstack((x[:,np.newaxis], np.ones((x.shape[-1],1))))
X[1:5]
```

Out[16]:
```
array([[ 0.05050505,  1.        ],
       [ 0.1010101 ,  1.        ],
       [ 0.15151515,  1.        ],
       [ 0.2020202 ,  1.        ]])
```

求解：

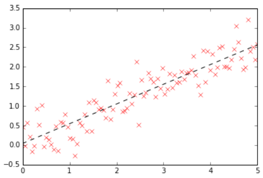
In [17]:
```
C, resid, rank, s = lstsq(X, y)
C, resid, rank, s
```

Out[17]:
```
(array([ 0.50432002,  0.0415695 ]),
 12.182942535066523,
 2,
 array([ 30.23732043,   4.82146667]))
```

画图：

In [18]:
```
p = plt.plot(x, y, 'rx')
p = plt.plot(x, C[0] * x + C[1], 'k--')
print "sum squared residual = {:.3f}".format(resid)
print "rank of the X matrix = {}".format(rank)
print "singular values of X = {}".format(s)
```

```
sum squared residual = 12.183
rank of the X matrix = 2
singular values of X = [ 30.23732043   4.82146667]
```



Scipy.stats.linregress 线性回归

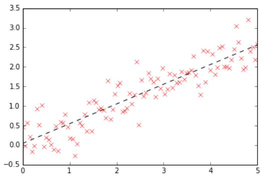
对于上面的问题，还可以使用线性回归进行求解：

In [19]:
```
slope, intercept, r_value, p_value, stderr = linregress(x, y)
slope, intercept
```

Out[19]: (0.50432001884393252, 0.041569499438028901)

In [20]:
```
p = plt.plot(x, y, 'rx')
p = plt.plot(x, slope * x + intercept, 'k--')
print "R-value = {:.3f}".format(r_value)
print "p-value (probability there is no correlation) = {:.3e}".format(p_value)
print "Root mean squared error of the fit = {:.3f}".format(np.sqrt(stderr))
```

```
R-value = 0.903
p-value (probability there is no correlation) = 8.225e-38
Root mean squared error of the fit = 0.156
```



可以看到，两者求解的结果是一致的，但是出发的角度是不同的。

更高级的拟合

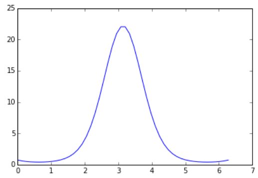
In [21]:
```
from scipy.optimize import leastsq
```

先定义这个非线性函数：$y = ae^{-b\sin(fx+\phi)}$

In [22]:
```
def function(x, a , b, f, phi):
    """a function of x with four parameters"""
    result = a * np.exp(-b * np.sin(f * x + phi))
    return result
```

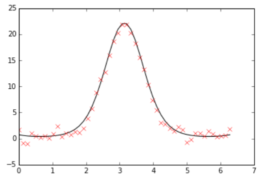
画出原始曲线：

In [23]:
```
x = np.linspace(0, 2 * np.pi, 50)
actual_parameters = [3, 2, 1.25, np.pi / 4]
y = function(x, *actual_parameters)
p = plt.plot(x,y)
```



加入噪声：

In [24]:
```
from scipy.stats import norm
y_noisy = y + 0.8 * norm.rvs(size=len(x))
p = plt.plot(x, y, 'k-')
p = plt.plot(x, y_noisy, 'rx')
```



Scipy.optimize.leastsq

定义误差函数，将要优化的参数放在前面：

In [25]:
```
def f_err(p, y, x):
    return y - function(x, *p)
```

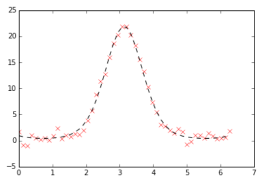
将这个函数作为参数传入 `leastsq` 函数，第二个参数为初始值：

In [26]:
```
c, ret_val = leastsq(f_err, [1, 1, 1, 1], args=(y_noisy, x))
c, ret_val
```

Out[26]:
```
(array([ 3.03199715,  1.97689384,  1.30083191,  0.6393337 ]), 1)
```

`ret_val` 是 1~4 时，表示成功找到最小二乘解：

In [27]:
```
p = plt.plot(x, y_noisy, 'rx')
p = plt.plot(x, function(x, *c), 'k--')
```



Scipy.optimize.curve_fit

更高级的做法：

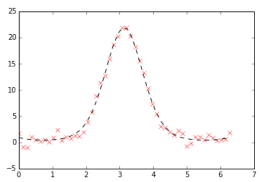
In [28]:
```
from scipy.optimize import curve_fit
```

不需要定义误差函数，直接传入 `function` 作为参数：

In [29]:
```
p_est, err_est = curve_fit(function, x, y_noisy)
```

In [30]:
```
print p_est
p = plt.plot(x, y_noisy, "rx")
p = plt.plot(x, function(x, *p_est), "k--")
```

```
[ 3.03199711  1.97689385  1.3008319   0.63933373]
```



这里第一个返回的是函数的参数，第二个返回值为各个参数的协方差矩阵：

In [31]:
```
print err_est
```

```
[[ 0.08483704 -0.02782318  0.00967093 -0.03029038]
 [-0.02782318  0.00933216 -0.00305158  0.00955794]
 [ 0.00967093 -0.00305158  0.0014972  -0.00468919]
 [-0.03029038  0.00955794 -0.00468919  0.01484297]]
```

协方差矩阵的对角线为各个参数的方差：

In [32]:
```
print "normalized relative errors for each parameter"
print "   a\t  b\t f\tphi"
print np.sqrt(err_est.diagonal()) / p_est
```

```
normalized relative errors for each parameter
   a       b       f      phi
[ 0.09606473  0.0488661   0.02974528  0.19056043]
```