Bad Honnef School

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Problem 3, Solution

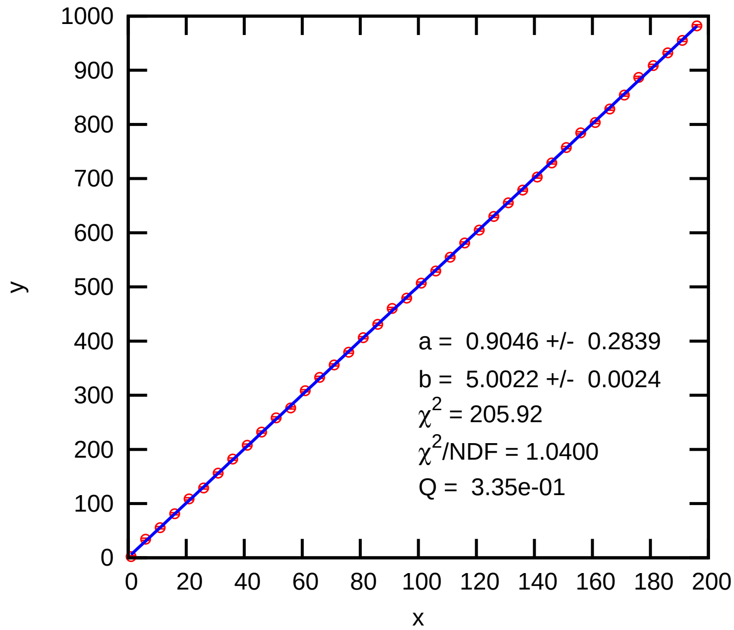
Least squares fit.

a. Source code is given in C, perl, and python at the bottom. (Thanks to Matt Wittmann for doing the python scripts.)

```
OUTPUT

slope     =      5.0022 +/-   0.0024
intercept =      0.9046 +/-   0.2839

chi squared / DOF =  1.0400

Note: The data actually corresponds to y = 1 + 5x (plus some random noise).
Hence the fit obtained the correct answer within the error bars.

The chi squared per degree of freedom is close to 1, as expected.
```

b. See the figure below which includes the fits.

The gnuplot script to do the fit (and procduce a figure) is at the bottom. Note how I present the fit parameters with error bars, the χ^2 and the goodness of fit parameter Q, *on the figure*. This is useful. All the fit parameters agree with what was found in part (a). Note too that I had to divide gnuplot's error bars by `FIT_STDFIT` $\equiv \sqrt{\chi^2/N_{\mathrm{DOF}}}$. The reason for this is discussed in the handout. The figure only shows every fifth point for clarity.



A python script, using fitting functions from the scipy package, is also shown at the bottom.

```
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Perl Code for part (a):
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```

```
#!/usr/bin/perl

$n = 0;
while(<>)
{
    @line = split;
    $x[$n] = $line[0];
    $y[$n] = $line[1];
    $err[$n] = $line[2];
    $err2 = $err[$n]**2;
    $s += 1 / $err2;
    $sumx  += $x[$n] / $err2 ;
    $sumy  += $y[$n] / $err2 ;
    $sumxx += $x[$n]*$x[$n] / $err2 ;
    $sumxy += $x[$n]*$y[$n] / $err2 ;
    $n++;
}

$delta = $s * $sumxx - $sumx * $sumx ;
$c = ($sumy * $sumxx - $sumx * $sumxy) / $delta ;
$m = ($s  *  $sumxy - $sumx * $sumy) / $delta ;
$errm = sqrt($s / $delta) ;
$errc = sqrt($sumxx / $delta) ;

printf ("slope     = %10.4f +/- %7.4f \n", $m, $errm);
printf ("intercept = %10.4f +/- %7.4f \n\n", $c, $errc);

$NDF = $n - 2; # the no. of degrees of freedom is n-no. of fit params
$chisq = 0;
for ($i = 0; $i < $n; $i++)
{
    $chisq += (($y[$i] - $m*$x[$i] - $c)/$err[$i])**2;
}
$chisq /= $NDF;
printf ("chi squared / NDF = %7.4lf \n", $chisq);

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C Code for part (a):
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#include "math.h";
#include "stdio.h";

main()
{
    double m, sumx, sumy, sumxx, sumxy, s, x[200], y[200], err[200], err2;
    double errc, errm, c, delta, chisq;
    int i, n;

    s = 0; sumx=0; sumy = 0; sumxx = 0; sumxy = 0;
    n = 200;

    for (i = 0; i < n; i++)
    {
```

```
        scanf("%lf %lf %lf", &x[i], &y[i], &err[i]);
        err2 = err[i]*err[i] ;
        s     += 1 / err2 ;
        sumx  += x[i] / err2 ;
        sumy  += y[i] / err2 ;
        sumxx += x[i]*x[i] / err2 ;
        sumxy += x[i]*y[i] / err2 ;
    }

    delta = s * sumxx - sumx * sumx ;
    c = (sumy * sumxx - sumx * sumxy) / delta ;
    m = (s  *  sumxy - sumx * sumy) / delta ;
    errm = sqrt(s / delta) ;
    errc = sqrt(sumxx / delta) ;

    printf ("slope     = %10.4f +/- %7.4f \n", m, errm);
    printf ("intercept = %10.4f +/- %7.4f \n\n", c, errc);

    chisq = 0;
    for (i = 0; i < n; i++)
    {
        chisq += pow((y[i] - m*x[i] - c)/err[i], 2);
    }
    chisq /= (n - 2); // the no. of degrees of freedom is n - no. of fit params
    printf ("chi squared / DOF = %7.4lf \n", chisq);

}
==========================
Python Code for part (a):
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import fileinput
from math import *

x = []
y = []
err = []
s = sumx = sumy = sumxx = sumxy = 0.

for line in fileinput.input():
    line = line.split()
    x_i = float(line[0]);   x.append(x_i)
    y_i = float(line[1]);   y.append(y_i)
    err_i = float(line[2]); err.append(err_i)
    err2 = err_i**2
    s += 1 / err2
    sumx    += x_i / err2
    sumy    += y_i / err2
    sumxx   += x_i*x_i / err2
    sumxy   += x_i*y_i / err2

n = len(x)
delta = s * sumxx - sumx * sumx
c = (sumy * sumxx - sumx * sumxy) / delta
```

```
m = (s * sumxy - sumx * sumy) / delta
errm = sqrt(s / delta)
errc = sqrt(sumxx / delta)

print "slope     = %10.4f +/- %7.4f " % (m, errm)
print "intercept = %10.4f +/- %7.4f \n" % (c, errc)

NDF = n - 2
chisq = 0.

for i in xrange(n):
    chisq += ((y[i] - m*x[i] - c)/err[i])**2;

chisq /= NDF
print "chi squared / NDF = %7.4lf " % chisq

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Gnuplot Code for part (b):
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set size 1.0, 0.6
set terminal postscript portrait enhanced font 'Helvetica,16'
set output "HW3b.eps"
set fit errorvariables
f(x) = a + b * x
fit f(x) "data.HW3" using 1:2:3 via a, b
set xlabel "x"
set ylabel "y"
ndf = FIT_NDF
chisq = FIT_STDFIT**2 * ndf
Q = 1 - igamma(0.5 * ndf, 0.5 * chisq)
set label sprintf("a = %7.4f +/- %7.4f", a, a_err/FIT_STDFIT) at 100, 400
set label sprintf("b = %7.4f +/- %7.4f", b, b_err/FIT_STDFIT) at 100, 330
set label sprintf("{/Symbol c}^2 = %6.2f", chisq) at 100, 270
set label sprintf("{/Symbol c}^2/NDF = %6.4f", FIT_STDFIT**2) at 100, 200
set label sprintf("Q = %9.2e", Q) at 100, 130
plot "data.HW3" using 1:2:3 every 5 with errorbars notitle pt 6 lc rgb "red" lw 2, \
f(x) notitle lc rgb "blue" lw 4 lt 1

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Python Code for part (b):
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from pylab import *
from scipy.optimize import leastsq

fname = sys.argv[1] if len(sys.argv) > 1 else 'data.txt'
x, y, err = np.loadtxt(fname, unpack=True)
n = len(x)

resids = lambda p: (p[0] + p[1]*x - y) / err
p0 = [5., 0.1]  # initial values of parameters

p, covm = leastsq(resids, p0, full_output=True)[:2]
```

```
c, m = p
errc, errm = sqrt(diag(covm))
chisq = sum(resids(p)**2)
chisq /= n - 2

print "slope     = %10.4f +/- %7.4f " % (m, errm)
print "intercept = %10.4f +/- %7.4f \n" % (c, errc)
print "chi squared / NDF = %7.4lf " % chisq
```