

```

*chi2=0.0;                                Calculate  $\chi^2$ .
if (mwt == 0) {
  for (i=1;i<=ndata;i++)
    *chi2 += SQR(y[i]-(*a)-(*b)*x[i]);
  *q=1.0;
  sigdat=sqrt((*chi2)/(ndata-2));          For unweighted data evaluate typical sig using chi2, and adjust the standard deviations.
  *sig_a *= sigdat;
  *sig_b *= sigdat;
} else {
  for (i=1;i<=ndata;i++)
    *chi2 += SQR((y[i]-(*a)-(*b)*x[i])/sig[i]);
  *q=gammq(0.5*(ndata-2),0.5*(chi2));      Equation (15.2.12).
}
}

```

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### 15.3 Straight-Line Data with Errors in Both Coordinates

If experimental data are subject to measurement error not only in the  $y_i$ 's, but also in the  $x_i$ 's, then the task of fitting a straight-line model

$$y(x) = a + bx \quad (15.3.1)$$

is considerably harder. It is straightforward to write down the  $\chi^2$  merit function for this case,

$$\chi^2(a, b) = \sum_{i=1}^N \frac{(y_i - a - bx_i)^2}{\sigma_{y_i}^2 + b^2 \sigma_{x_i}^2} \quad (15.3.2)$$

where  $\sigma_{x_i}$  and  $\sigma_{y_i}$  are, respectively, the  $x$  and  $y$  standard deviations for the  $i$ th point. The weighted sum of variances in the denominator of equation (15.3.2) can be understood both as the variance in the direction of the smallest  $\chi^2$  between each data point and the line with slope  $b$ , and also as the variance of the linear combination  $y_i - a - bx_i$  of two random variables  $x_i$  and  $y_i$ ,

$$\text{Var}(y_i - a - bx_i) = \text{Var}(y_i) + b^2 \text{Var}(x_i) = \sigma_{y_i}^2 + b^2 \sigma_{x_i}^2 \equiv 1/w_i \quad (15.3.3)$$

The sum of the square of  $N$  random variables, each normalized by its variance, is thus  $\chi^2$ -distributed.

We want to minimize equation (15.3.2) with respect to  $a$  and  $b$ . Unfortunately, the occurrence of  $b$  in the denominator of equation (15.3.2) makes the resulting equation for the slope  $\partial\chi^2/\partial b = 0$  nonlinear. However, the corresponding condition for the intercept,  $\partial\chi^2/\partial a = 0$ , is still linear and yields

$$a = \left[ \sum_i w_i (y_i - bx_i) \right] / \sum_i w_i \quad (15.3.4)$$

where the  $w_i$ 's are defined by equation (15.3.3). A reasonable strategy, now, is to use the machinery of Chapter 10 (e.g., the routine `brent`) for minimizing a general one-dimensional function to minimize with respect to  $b$ , while using equation (15.3.4) at each stage to ensure that the minimum with respect to  $b$  is also minimized with respect to  $a$ .

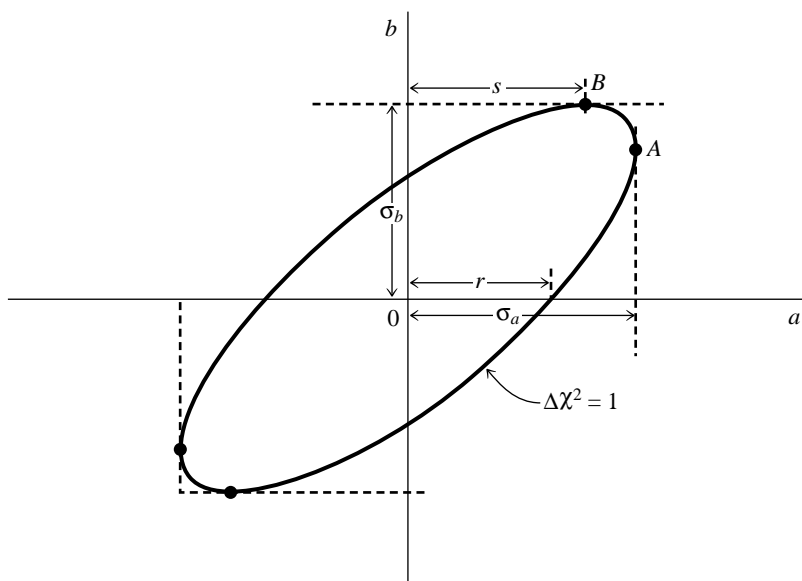


Figure 15.3.1. Standard errors for the parameters  $a$  and  $b$ . The point  $B$  can be found by varying the slope  $b$  while simultaneously minimizing the intercept  $a$ . This gives the standard error  $\sigma_b$ , and also the value  $s$ . The standard error  $\sigma_a$  can then be found by the geometric relation  $\sigma_a^2 = s^2 + r^2$ .

Because of the finite error bars on the  $x_i$ 's, the minimum  $\chi^2$  as a function of  $b$  will be finite, though usually large, when  $b$  equals infinity (line of infinite slope). The angle  $\theta \equiv \arctan b$  is thus more suitable as a parametrization of slope than  $b$  itself. The value of  $\chi^2$  will then be periodic in  $\theta$  with period  $\pi$  (not  $2\pi$ !). If any data points have very small  $\sigma_y$ 's but moderate or large  $\sigma_x$ 's, then it is also possible to have a maximum in  $\chi^2$  near zero slope,  $\theta \approx 0$ . In that case, there can sometimes be two  $\chi^2$  minima, one at positive slope and the other at negative. Only one of these is the correct global minimum. It is therefore important to have a good starting guess for  $b$  (or  $\theta$ ). Our strategy, implemented below, is to scale the  $y_i$ 's so as to have variance equal to the  $x_i$ 's, then to do a conventional (as in §15.2) linear fit with weights derived from the (scaled) sum  $\sigma_{y_i}^2 + \sigma_{x_i}^2$ . This yields a good starting guess for  $b$  if the data are even *plausibly* related to a straight-line model.

Finding the standard errors  $\sigma_a$  and  $\sigma_b$  on the parameters  $a$  and  $b$  is more complicated. We will see in §15.6 that, in appropriate circumstances, the standard errors in  $a$  and  $b$  are the respective projections onto the  $a$  and  $b$  axes of the “confidence region boundary” where  $\chi^2$  takes on a value one greater than its minimum,  $\Delta\chi^2 = 1$ . In the linear case of §15.2, these projections follow from the Taylor series expansion

$$\Delta\chi^2 \approx \frac{1}{2} \left[ \frac{\partial^2 \chi^2}{\partial a^2} (\Delta a)^2 + \frac{\partial^2 \chi^2}{\partial b^2} (\Delta b)^2 \right] + \frac{\partial^2 \chi^2}{\partial a \partial b} \Delta a \Delta b \quad (15.3.5)$$

Because of the present nonlinearity in  $b$ , however, analytic formulas for the second derivatives are quite unwieldy; more important, the lowest-order term frequently gives a poor approximation to  $\Delta\chi^2$ . Our strategy is therefore to find the roots of  $\Delta\chi^2 = 1$  numerically, by adjusting the value of the slope  $b$  away from the minimum. In the program below the general root finder `zbrout` is used. It may occur that there are no roots at all — for example, if all error bars are so large that all the data points are compatible with each other. It is important, therefore, to make some effort at bracketing a putative root before refining it (cf. §9.1).

Because  $a$  is minimized at each stage of varying  $b$ , successful numerical root-finding leads to a value of  $\Delta a$  that minimizes  $\chi^2$  for the value of  $\Delta b$  that gives  $\Delta\chi^2 = 1$ . This (see Figure 15.3.1) directly gives the tangent projection of the confidence region onto the  $b$  axis, and thus  $\sigma_b$ . It does not, however, give the tangent projection of the confidence region onto the  $a$  axis. In the figure, we have found the point labeled  $B$ ; to find  $\sigma_a$  we need to find the

point  $A$ . Geometry to the rescue: To the extent that the confidence region is approximated by an ellipse, then you can prove (see figure) that  $\sigma_a^2 = r^2 + s^2$ . The value of  $s$  is known from having found the point  $B$ . The value of  $r$  follows from equations (15.3.2) and (15.3.3) applied at the  $\chi^2$  minimum (point  $O$  in the figure), giving

$$r^2 = 1 / \sum_i w_i \quad (15.3.6)$$

Actually, since  $b$  can go through infinity, this whole procedure makes more sense in  $(a, \theta)$  space than in  $(a, b)$  space. That is in fact how the following program works. Since it is conventional, however, to return standard errors for  $a$  and  $b$ , not  $a$  and  $\theta$ , we finally use the relation

$$\sigma_b = \sigma_\theta / \cos^2 \theta \quad (15.3.7)$$

We caution that if  $b$  and its standard error are both large, so that the confidence region actually includes infinite slope, then the standard error  $\sigma_b$  is not very meaningful. The function `chixy` is normally called only by the routine `fitexy`. However, if you want, you can yourself explore the confidence region by making repeated calls to `chixy` (whose argument is an angle  $\theta$ , not a slope  $b$ ), after a single initializing call to `fitexy`.

A final caution, repeated from §15.0, is that if the goodness-of-fit is not acceptable (returned probability is too small), the standard errors  $\sigma_a$  and  $\sigma_b$  are surely not believable. In dire circumstances, you might try scaling all your  $x$  and  $y$  error bars by a constant factor until the probability is acceptable (0.5, say), to get more plausible values for  $\sigma_a$  and  $\sigma_b$ .

```
#include <math.h>
#include "nrutil.h"
#define POTN 1.571000
#define BIG 1.0e30
#define PI 3.14159265
#define ACC 1.0e-3

int nn;
float *xx,*yy,*sx,*sy,*ww,aa,offs;

void fitexy(float x[], float y[], int ndat, float sigx[], float sigy[],
            float *a, float *b, float *siga, float *sigb, float *chi2, float *q)
Straight-line fit to input data x[1..ndat] and y[1..ndat] with errors in both x and y, the
respective standard deviations being the input quantities sigx[1..ndat] and sigy[1..ndat].
Output quantities are a and b such that y = a + bx minimizes chi^2, whose value is returned
as chi2. The chi^2 probability is returned as q, a small value indicating a poor fit (sometimes
indicating underestimated errors). Standard errors on a and b are returned as siga and sigb.
These are not meaningful if either (i) the fit is poor, or (ii) b is so large that the data are
consistent with a vertical (infinite b) line. If siga and sigb are returned as BIG, then the data
are consistent with all values of b.
{
    void avevar(float data[], unsigned long n, float *ave, float *var);
    float brent(float ax, float bx, float cx,
                float (*f)(float), float tol, float *xmin);
    float chixy(float bang);
    void fit(float x[], float y[], int ndata, float sig[], int mwt,
            float *a, float *b, float *siga, float *sigb, float *chi2, float *q);
    float gammq(float a, float x);
    void mnbrak(float *ax, float *bx, float *cx, float *fa, float *fb,
                float *fc, float (*func)(float));
    float zbrent(float (*func)(float), float x1, float x2, float tol);
    int j;
    float swap, amx, amn, varx, vary, ang[7], ch[7], scale, bmm, bmx, d1, d2, r2,
            dum1, dum2, dum3, dum4, dum5;

    xx=vector(1,ndat);
    yy=vector(1,ndat);
```

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```

sx=vector(1,ndat);
sy=vector(1,ndat);
ww=vector(1,ndat);
avevar(x,ndat,&dum1,&varx);
avevar(y,ndat,&dum1,&vary);
scale=sqrt(varx/vary);
nn=ndat;
for (j=1;j<=ndat;j++) {
  xx[j]=x[j];
  yy[j]=y[j]*scale;
  sx[j]=sigx[j];
  sy[j]=sigy[j]*scale;
  ww[j]=sqrt(SQR(sx[j])+SQR(sy[j]));
}
fit(xx,yy,nn,ww,1,&dum1,b,&dum2,&dum3,&dum4,&dum5);
offs=ang[1]=0.0;
ang[2]=atan(*b);
ang[4]=0.0;
ang[5]=ang[2];
ang[6]=POTN;
for (j=4;j<=6;j++) ch[j]=chixy(ang[j]);
mnbrak(&ang[1],&ang[2],&ang[3],&ch[1],&ch[2],&ch[3],chixy);
Bracket the  $\chi^2$  minimum and then locate it with brent.
*chi2=brent(ang[1],ang[2],ang[3],chixy,ACC,b);
*chi2=chixy(*b);
*a=aa;
*q=gammq(0.5*(nn-2),*chi2*0.5);
for (r2=0.0,j=1;j<=nn;j++) r2 += ww[j];
r2=1.0/r2;
bmx=BIG;
bmn=BIG;
offs=(*chi2)+1.0;
for (j=1;j<=6;j++) {
  if (ch[j] > offs) {
    d1=fabs(ang[j]-(*b));
    while (d1 >= PI) d1 -= PI;
    d2=PI-d1;
    if (ang[j] < *b) {
      swap=d1;
      d1=d2;
      d2=swap;
    }
    if (d1 < bmx) bmx=d1;
    if (d2 < bmn) bmn=d2;
  }
}
if (bmx < BIG) {
  bmx=zbrent(chixy,*b,*b+bmx,ACC)-(*b);
  amx=aa-(*a);
  bmn=zbrent(chixy,*b,*b-bmn,ACC)-(*b);
  amn=aa-(*a);
  *sigb=sqrt(0.5*(bmx*bmx+bmn*bmn))/(scale*SQR(cos(*b)));
  *siga=sqrt(0.5*(amx*amx+amn*amn)+r2)/scale;
} else (*sigb)=(*siga)=BIG;
*a /= scale;
*b=tan(*b)/scale;
free_vector(ww,1,ndat);
free_vector(sy,1,ndat);
free_vector(sx,1,ndat);
free_vector(yy,1,ndat);
free_vector(xx,1,ndat);
}

```

Find the  $x$  and  $y$  variances, and scale the data into the global variables for communication with the function `chixy`.

Use both  $x$  and  $y$  weights in first trial fit.

Trial fit for  $b$ . Construct several angles for reference points, and make  $b$  an angle.

Compute  $\chi^2$  probability. Save the inverse sum of weights at the minimum. Now, find standard errors for  $b$  as points where  $\Delta\chi^2 = 1$ .

Go through saved values to bracket the desired roots. Note periodicity in slope angles.

Call `zbrent` to find the roots.

Error in  $a$  has additional piece  $r2$ . Unscale the answers.

```

#include <math.h>
#include "nrutil.h"
#define BIG 1.0e30

extern int nn;
extern float *xx,*yy,*sx,*sy,*ww,aa,offs;

float chixy(float bang)
Captive function of fitexy, returns the value of  $(\chi^2 - \text{offs})$  for the slope  $b=\tan(\text{bang})$ .
Scaled data and offs are communicated via the global variables.
{
    int j;
    float ans,avex=0.0,avey=0.0,sumw=0.0,b;

    b=tan(bang);
    for (j=1;j<=nn;j++) {
        ww[j] = SQR(b*sx[j])+SQR(sy[j]);
        sumw += (ww[j] = (ww[j] < 1.0/BIG ? BIG : 1.0/ww[j]));
        avex += ww[j]*xx[j];
        avey += ww[j]*yy[j];
    }
    avex /= sumw;
    avey /= sumw;
    aa=avey-b*avex;
    for (ans = -offs,j=1;j<=nn;j++)
        ans += ww[j]*SQR(yy[j]-aa-b*xx[j]);
    return ans;
}

```

Be aware that the literature on the seemingly straightforward subject of this section is generally confusing and sometimes plain wrong. Deming's [1] early treatment is sound, but its reliance on Taylor expansions gives inaccurate error estimates. References [2-4] are reliable, more recent, general treatments with critiques of earlier work. York [5] and Reed [6] usefully discuss the simple case of a straight line as treated here, but the latter paper has some errors, corrected in [7]. All this commotion has attracted the Bayesians [8-10], who have still different points of view.

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## 15.4 General Linear Least Squares

An immediate generalization of §15.2 is to fit a set of data points  $(x_i, y_i)$  to a model that is not just a linear combination of 1 and  $x$  (namely  $a + bx$ ), but rather a linear combination of *any*  $M$  specified functions of  $x$ . For example, the functions could be  $1, x, x^2, \dots, x^{M-1}$ , in which case their general linear combination,

$$y(x) = a_1 + a_2x + a_3x^2 + \dots + a_Mx^{M-1} \quad (15.4.1)$$

is a polynomial of degree  $M - 1$ . Or, the functions could be sines and cosines, in which case their general linear combination is a harmonic series.

The general form of this kind of model is

$$y(x) = \sum_{k=1}^M a_k X_k(x) \quad (15.4.2)$$

where  $X_1(x), \dots, X_M(x)$  are arbitrary fixed functions of  $x$ , called the *basis functions*.

Note that the functions  $X_k(x)$  can be wildly nonlinear functions of  $x$ . In this discussion “linear” refers only to the model’s dependence on its *parameters*  $a_k$ .

For these linear models we generalize the discussion of the previous section by defining a merit function

$$\chi^2 = \sum_{i=1}^N \left[ \frac{y_i - \sum_{k=1}^M a_k X_k(x_i)}{\sigma_i} \right]^2 \quad (15.4.3)$$

As before,  $\sigma_i$  is the measurement error (standard deviation) of the  $i$ th data point, presumed to be known. If the measurement errors are not known, they may all (as discussed at the end of §15.1) be set to the constant value  $\sigma = 1$ .

Once again, we will pick as best parameters those that minimize  $\chi^2$ . There are several different techniques available for finding this minimum. Two are particularly useful, and we will discuss both in this section. To introduce them and elucidate their relationship, we need some notation.

Let  $\mathbf{A}$  be a matrix whose  $N \times M$  components are constructed from the  $M$  basis functions evaluated at the  $N$  abscissas  $x_i$ , and from the  $N$  measurement errors  $\sigma_i$ , by the prescription

$$A_{ij} = \frac{X_j(x_i)}{\sigma_i} \quad (15.4.4)$$

The matrix  $\mathbf{A}$  is called the *design matrix* of the fitting problem. Notice that in general  $\mathbf{A}$  has more rows than columns,  $N \geq M$ , since there must be more data points than model parameters to be solved for. (You can fit a straight line to two points, but not a very meaningful quintic!) The design matrix is shown schematically in Figure 15.4.1.

Also define a vector  $\mathbf{b}$  of length  $N$  by

$$b_i = \frac{y_i}{\sigma_i} \quad (15.4.5)$$

and denote the  $M$  vector whose components are the parameters to be fitted,  $a_1, \dots, a_M$ , by  $\mathbf{a}$ .