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Subject: Fast linear least squares fitting beta test  
Posted by [dudley](#) on Sat, 28 May 1994 06:58:15 GMT  
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The following is a translation from Fortran 90 of the fast fitting program given in a new Rybicki and Press preprint. Please let me know if you find any bugs.

Chris

```
;+
; NAME:
;
;Fastfit
;
; PURPOSE:
;
;Linear least squares type fitting of basis to data with arbitrary
;absissa.
;
; CATEGORY:
;
;New numerical recipies based on Ribicki and Press 5/94 preprint "A
;Class of Fast Methods for Processing Irregularly Samples or Otherwise
;Inhomogenous One-Dimentional Data". The preprint can be obtained by sending
;mail to comp-gas@xyz.lanl.gov with the subject line 'get 9405004'.
;
; CALLING SEQUENCE:
;
; fit=fast_fitting(x,y,sig,psig,pw,xel,el,q,chisq)
;
; INPUTS:
;
; x,y,sig: data x,y, and yerror bars.
; psig: estimated population sigma
; pw: estimated inverse decorrelation distance.
; xel: xvalues for basis matrix el
; el: basis matrix
;
; OPTIONAL INPUTS:
;
;
;
;
; KEYWORD PARAMETERS:
;
;
; /usesvd specifies the use of sigular value decomposition and back
; substitution rather than Gauss-Jordan elimination.
;
```

```
; OUTPUTS:  
;  
; fit: y values of fit at xel  
; q: solution vector (fit=el#q)  
; chisq: fit chi^2  
;  
; OPTIONAL OUTPUTS:  
;  
;  
;  
;  
; COMMON BLOCKS:  
;  
;  
;  
;  
; SIDE EFFECTS:  
;  
;  
;  
;  
;  
; RESTRICTIONS:  
;  
; You are responsible to see that x and xel are unique and that the  
; basis of el are independent. This is a beta test. Please let me  
; know if other problems arise.  
;  
; PROCEDURE:  
;  
; Suppose you have an irregularly sampled spectrum with an SRF FWHM of  
; .2 microns. guess psig=<sig> and pw=5.  
;  
; EXAMPLE:  
;  
; s=23  
; a=findgen(1000)+randomu(s,1000)-.5  
; c=randomu(s,1000)  
; d=randomu(s,20)*5  
; d=rebin(abs(d-2.5),1000)  
; b=smooth(sin(a/30.)+(c-.5)*d,4.)  
;  
; el=fltarr(1000,4)  
; el(*,0)=1.  
; el(*,1)=sin(findgen(1000)/25.)  
; el(*,2)=sin(findgen(1000)/30.)  
; el(*,3)=sin(findgen(1000)/35.)  
; fit=fastfit(a,b,d,.25,findgen(1000),el,q,chisq)  
; plot,a,b  
; oplot,fit  
;  
; MODIFICATION HISTORY:
```

```
; adapted from Rybicki and Press preprint May 23 1994 by C. dudley
; dudley@galileo.ifa.hawaii.edu
;-
```

```
PRO Gaussj, a, b
```

```
n = size(a)
```

```
m = size(b)
```

```
indx = indgen(n(1))
```

```
indx = indgen(n(1))
```

```
ipiv = intarr(n(1))
```

```
FOR i = 0, n(1)-1 DO BEGIN
```

```
    big = 0.
```

```
    FOR j = 0, n(1)-1 DO BEGIN
```

```
        IF ipiv(j) NE 1 THEN BEGIN
```

```
            FOR k = 0, n(1)-1 DO BEGIN
```

```
                IF ipiv(k) EQ 0 THEN BEGIN
```

```
                    IF abs(a(j, k)) GE big THEN BEGIN
```

```
                        big = abs(a(j, k))
```

```
                        irow = j
```

```
                        icol = k
```

```
                ENDIF
```

```
            ENDIF ELSE IF ipiv(k) GT 1 THEN BEGIN
```

```
                print, 'singular matrix-1'
```

```
                return
```

```
            ENDIF
```

```
        ENDFOR
```

```
    ENDIF
```

```
ENDFOR
```

```
ipiv(icol) = ipiv(icol)+1
```

```
IF irow NE icol THEN BEGIN
```

```
    dumm = a(irow, *)
```

```
    a(irow, *) = a(icol, *)
```

```
    a(icol, *) = dumm
```

```
    dumm = b(irow, *)
```

```
    b(irow, *) = b(icol, *)
```

```
    b(icol, *) = dumm
```

```
ENDIF
```

```
pivinv = 1./a(icol, icol)
```

```
a(icol, icol) = 1.
```

```
a(icol, *) = a(icol, *) * pivinv
```

```
b(icol, *) = b(icol, *) * pivinv
```

```

FOR ll = 0, n(1)-1 DO BEGIN
  IF ll NE icol THEN BEGIN
    dum = a(ll, icol)
    a(ll, icol) = 0.0
    a(ll, *) = a(ll, *) - a(icol, *) * dum
    b(ll, *) = b(ll, *) - b(icol, *) * dum
  ENDIF
ENDFOR
ENDFOR

```

```

FOR l = n(1)-1, 0, -1 DO BEGIN
  IF indxr(l) NE indxc(l) THEN BEGIN
    dumm = a(*, indxr(l))
    a(*, indxr(l)) = a(*, indxc(l))
    a(*, indxc(l)) = dumm
  ENDIF
ENDFOR

```

END

FUNCTION Tridiag, a, b, c, r

```

n = n_elements(b)

bet = b(0)
IF bet EQ 0. THEN BEGIN
  print, 'error 1 in tridiag'
  return, -1
ENDIF ELSE BEGIN
  gam = fltarr(n)
  u = fltarr(n)
  u(0) = r(0)/bet
  eflag = 0
  FOR j = 1, n-1 DO BEGIN
    gam(j) = c(j-1)/bet
    bet = b(j)-a(j-1)*gam(j)
    IF bet EQ 0. THEN eflag = 1 ELSE u(j) = (r(j)-a(j-1)*u(j-1))/bet
  ENDFOR
  IF eflag eq 1 THEN BEGIN
    print, 'error 2 in tridiag'
    return, -1
  ENDIF
  FOR j = n-2, 0, -1 DO u(j) = u(j)-gam(j+1)*u(j+1)
  return, u

```

```
ENDELSE  
END ;tridiag
```

```
FUNCTION symtrimul, a, b, u
```

```
n = n_elements(u)
```

```
result = fltarr(n)
```

```
result(0) = b(0)*u(0)+a(0)*u(1)
```

```
result(1:n-2) = a(0:n-3)*u(0:n-3)+b(1:n-2)*u(1:n-2)+a(1:n-2)*u(2:n-1)
```

```
result(n-1) = a(n-2)*u(n-2)+b(n-1)*u(n-1)
```

```
return, result
```

```
END ;symtrimul
```

```
FUNCTION Apply_cinv, x, y, sig, psig, pw
```

```
n = n_elements(x)
```

```
m = size(y)
```

```
tmp = sig^2
```

```
b = fltarr(n)
```

```
r = exp(-abs(pw*(x(1:n-1)-x(0:n-2))))
```

```
g = where(1./r-r GT 1e-4)
```

```
ng = where(1./r-r LE 1e-4, count)
```

```
a = r*0
```

```
a(g) = -1./(1./r(g)-r(g))
```

```
IF count NE 0 THEN a(ng) = -1./1e-4
```

```
r = r*a
```

```
b(0) = 1.-r(0)
```

```
b(1:n-2) = 1.-r(1:n-2)-r(0:n-3)
```

```
b(n-1) = 1.-r(n-2)
```

```
a = a/psig^2
```

```
b = b/psig^2
```

```
;stop
```

```
aa = a*tmp(1:n-1)
```

```
bb = b*tmp+1.
```

```
cc = a*tmp(0:n-2)
```

```
result = y*0.
```

```
FOR j = 0, m(2)-1 DO BEGIN
```

```
    temp = tridiag(aa, bb, cc, y(*, j))
```

```
;tridiag, [[0], aa], bb, [cc, [0]], y(*, j), temp
```

```
    result(*, j) = symtrimul(a, b, temp)
```

```
ENDFOR
```

```
return, result
```

```
END ;apply_cinv
```

```
FUNCTION Fastfit, x, y, sig, psig, pw, xel, el, q, chisq, usesvd=usesvd
```

```
n = n_elements(x)  
nl = n_elements(xel)  
m = size(el)
```

```
IF (n_elements(y) NE n OR n_elements(sig) NE n OR m(1) NE nl ) THEN BEGIN  
print, 'size errors', n,nl, m  
return, -1  
ENDIF
```

```
y = y(sort(x))  
sig = sig(sort(x))  
x = x(sort(x))  
el = el(sort(xel), *)  
xel = xel(sort(xel))  
nt = n+nl  
fl = bytarr(nt)  
fl(0:n-1) = 1  
xx = [x, xel]  
order = sort(xx)  
xx = xx(order)  
ell = fltarr(nt, m(2)+1)  
ell(0:n-1, m(2)) = y  
ell(n:*, 0:m(2)-1) = el  
ell(*, *) = ell(order, *)  
sigg = [sig, fltarr(nl)]  
sigg = sigg(order)
```

```
cil = apply_cinv(xx, ell, sigg, psig, pw)  
qq = fltarr(m(2), 1)  
qq(*, 0) = transpose(ell(*, 0:m(2)-1))#cil(*, m(2))  
;stop  
IF keyword_set(usesvd) THEN BEGIN
```

```
    svd, transpose(ell(*, 0:m(2)-1))#cil(*, 0:m(2)-1), w, u, v
```

```
    small = where(w LT max(w)*1e-6, count)  
    IF count NE 0 THEN w(small) = 0.  
    svbksb, u, w, v, -qq, q  
ENDIF ELSE BEGIN  
    gaussj, transpose(ell(*, 0:m(2)-1))#cil(*, 0:m(2)-1), qq  
    q = -qq(*, 0)  
ENDELSE
```

```
ell(*, 0) = ell(*, m(2))+ell(*, 0:m(2)-1)#q
```

```
cil(*, 0) = cil(*, m(2))+cil(*, 0:m(2)-1)#q  
chisq = total(ell(*, 0)*cil(*, 0))  
return, el#q  
END
```

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