
Subject: curve fitting: works badly?

Posted by [feil](#) on Mon, 06 Mar 1995 16:19:01 GMT

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I try to use CURVEFIT to get some simple data fitted to an harmonic oscillator.

Somehow things don't work very good.

these are the datapoints:

i	x(i)	y(i)
0 8	6.5550	-0.3052
1 8	6.6233	-0.3076
2 8	6.6915	-0.3088
3 8	6.7598	-0.3091
4 8	6.8281	-0.3086
5 8	6.8281	-0.3086
6 8	6.8964	-0.3074
7 8	6.9647	-0.3054

the calling sequence:

;;----- fit to harmonic oscillator -----

```
a = fltarr(3)
; start estimates
a(0) = etot(icnt/2)
dx = lattice(1)-lattice(0)
a(1) = (etot(2)+etot(0)-2*etot(1))/(dx*dx)
a(2) = lattice(icnt/2)
```

```
w = fltarr(icnt)
for i = 0,icnt-1 do begin
  w(i) = 1.
end
```

```
yfit = mod_curvefit(lattice,etot,w,a)
```

and the finction itself:

```
;
```

```
; the harmonic oscillator function
;
;
;
;
;
pro FUNCT,x,a,f,pder
```

```
f = a(0) + a(1)*(x-a(2))^2
```

```
PDER = FLTARR(N_ELEMENTS(X),3) ;YES, MAKE ARRAY.
```

```
PDER(*,0) = 1.0 ;COMPUTE PARTIALS
```

```
PDER(*,1) = (x-a(2))^2
```

```
PDER(*,2) = 2*a(1)*(x-a(2))
```

```
end
```

```
RETURN
```

```
end
```

Simple isn't it.

I never get a decent fit!!!!

HELP HELP

Hans

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