
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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Subject: Re: curve fitting: works badly?

Posted by [thompson](#) on Mon, 06 Mar 1995 23:49:09 GMT

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feil@prl.philips.nl (Hans Feil) writes:

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

> Somehow things don't work very good.

(stuff deleted)

```
> 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
```

I think that your problem is here. I believe that the sign of this partial derivative should be negative.

I've often had this problem with this technique. If the partial derivatives are calculated wrong, you can compute till doomsday and it'll never converge. I often just don't bother to try to figure it out anymore, and just do the derivatives numerically.

Bill Thompson

Subject: Re: curve fitting: works badly?

Posted by [swalton](#) on Tue, 14 Mar 1995 19:16:03 GMT

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I just peeked in here and saw a discussion of one of my recent favorite topics, nonlinear least squares. (We have IDL, but I haven't learned it yet; my brain is full :-).).

I've been using the routine variously known as NL2SOL or N2G. It is described in ACM Trans. Math. Software, Vol. 9, PP. 369-383 (An Adaptive Nonlinear Least-Squares Algorithm, By J.E. Dennis, D.M. Gay, and R.E. Welsch). They are available by anonymous FTP from netlib.att.com in the freely distributable subset of the AT&T PORT library. It comes in several versions, including one which can bound the fit parameters and versions which calculate the derivatives numerically. The precise details of the algorithm escape me at the

moment, but I'm using it to fit an 11-parameter (!) model to some solar data. Highly recommended.

As to errors: a recent article in Computers in Physics compared a couple of different techniques for estimating the errors in a fit, and concluded that Monte Carlo techniques give the best estimate.

--

Stephen Walton, California State University, Northridge

"Be careful what you wish for; you might get it." swalton@csun.edu
