Tools for General Parametric Splines

gsp

k_1 k_2 k_3

‘spida’ package in R developed for
the Summer Program In Data Analysis (SPIDA)
at York University

0th
1st
2nd

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Flexible tools to explore general parametric splines:

- Splines are conceptually simple but generally awkward to use in statistical analyses
- Goal: make splines as easy to use in regression as categorical variables
- "General parametric spline:"
  - Polynomials of different degrees in each interval
  - Different degrees of smoothness at each knot – including possible discontinuity
- Natural parametrization with interpretable coefficients:
  can use regular expression to test groups of coefficients
- Can estimate and test features of spline: slope, curvature, salti.
- Can interact with other variables (numerical or categorical), other splines, etc.
- Limitation: need to centre and scale variable

Installation

1) Install R http://cran.r-project.org/

   Only once: Install '**`car`**' and '**`spida`**'. After starting R:

```
>[1] install.packages('car')
> install.packages('spida',
        repos = 'http://r-forge.r-project.org')
```

2) Each time you run R: load spida

```
> library(spida)
```

[1] The '>' sign is the prompt in R. Type only what comes after the '>'.

Main Functions:

`gsp`	Creates general parametric splines
`wald`	Uses regular expressions or hypothesis matrices to estimate coefficients and test hypotheses
`Lmat`	Generates hypothesis matrices
`sc`	Operates on spline functions to generate hypothesis matrices for spline derivatives: slope, curvature, salti at knots
`smsp`	Non-parametric splines using mixed models

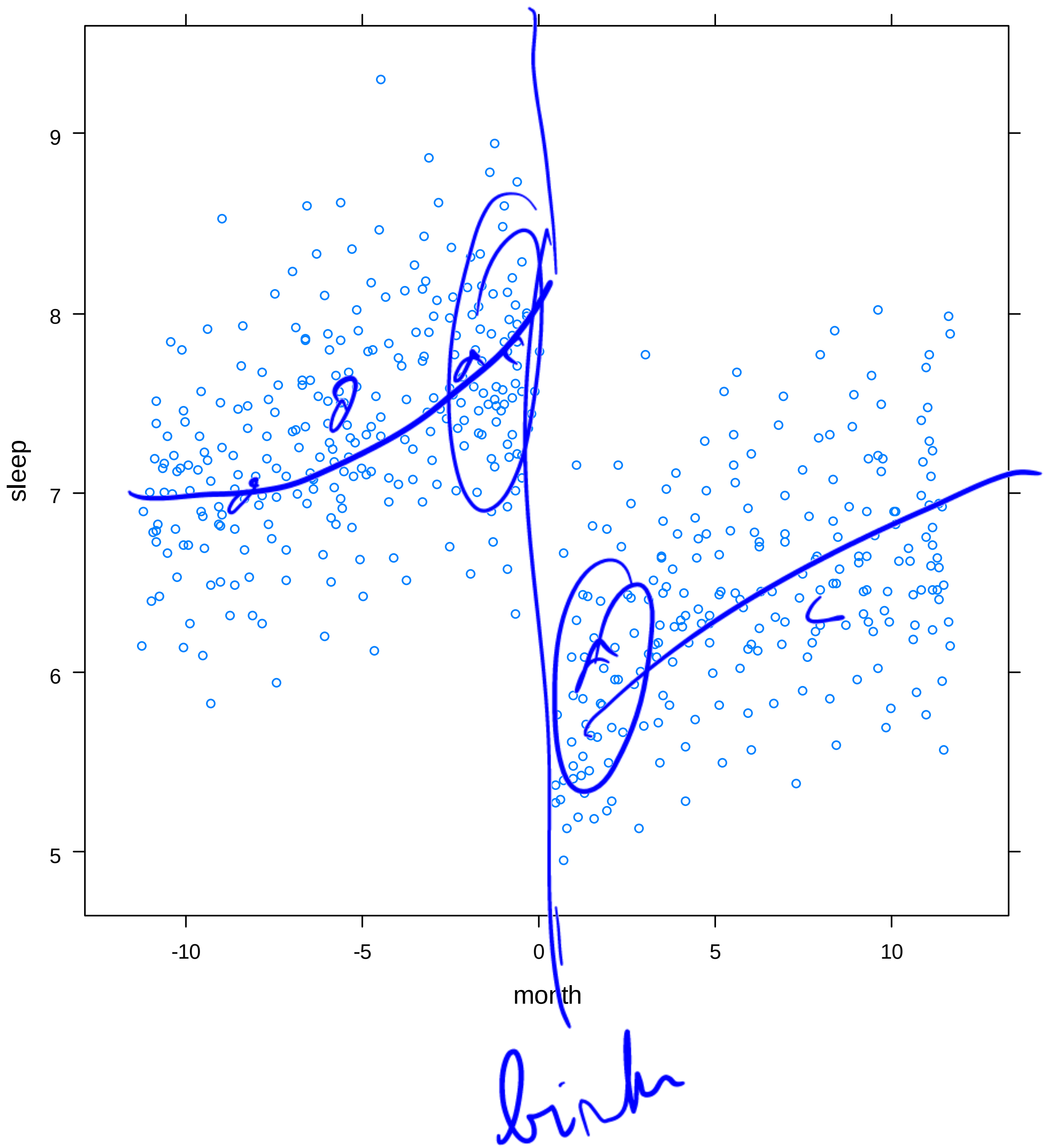
Example:

Simulated sleep data before and after birth.
Inspired by Kunkel, Reitav, Monette (2010)

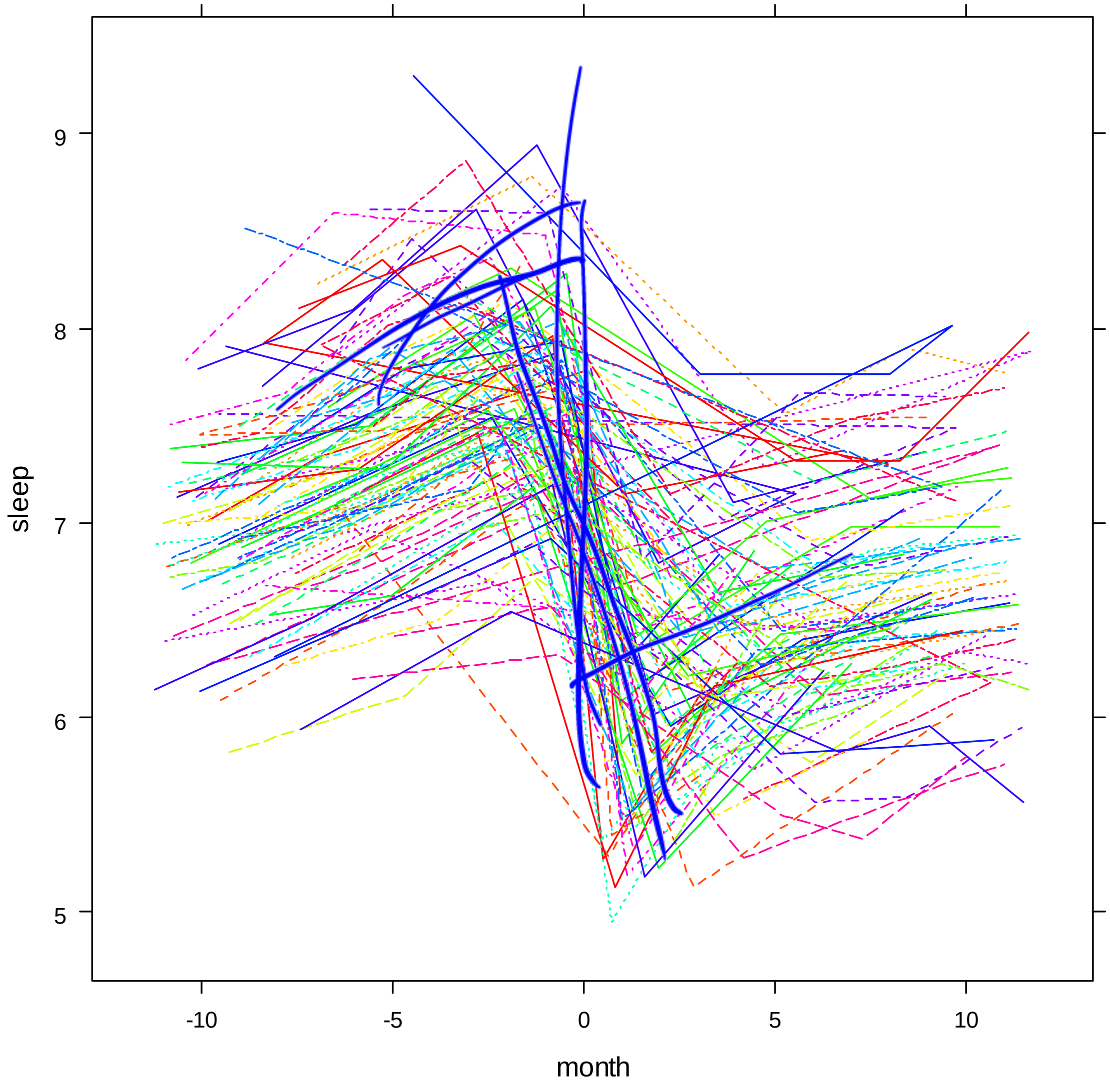
100 women each observed 5 times:

```
> sim.data <- read.csv(
'http://www.math.yorku.ca/~georges/Data/sim.data.csv')
> dim(sim.data)
[1] 500   4
> head( sim.data)
  X       month id    sleep
1 1 -9.86370968  1 7.008448
2 2 -6.95388563  1 7.336828
3 3 -2.11407625  1 7.642227
4 4  0.05344575  1 7.778133
5 5  0.97390029  1 5.609873
6 6 -7.66649560  2 7.184266
```

```
> xyplot( sleep ~ month, sim.data)
```



```
> td( col = rainbow(20))
> xyplot( sleep ~ month, sim.data,
     groups = id, type = 'l')
```



Defining a spline function:

Create your own spline function

```
> sp <- function( x ) gsp( x,
       knots  =  c(-5, 0, 5),      # position of knots
       degree =  c(2, 2, 2, 2),    # quad in each interval
       smooth =   c(1, -1, 1))     # smoothness at knot
```

`degree` parameter:

1,2,3,…	linear, quadratic, cubic, etc.
0	flat
-1	equal to 0

`smooth` parameter:

1	'smooth': same slope on both sides of knot	
2	same curvature on both sides	
0	continuous (no gap)	
-1	discontinuous	

What `sp` does:

Generates a portion of a model matrix:

```
> sp( c(-5,0,5) )

      D1(0) D2(0) C(0).0 C(0).1 C(0).2 C(5).2 C(-5).2
f(-5)    -5  12.5      0      0    0.0      0       0
f(0)      0   0.0      0      0    0.0      0       0
f(5)      5  12.5      1      5   12.5      0       0
```

linear term

saltus in level at 0

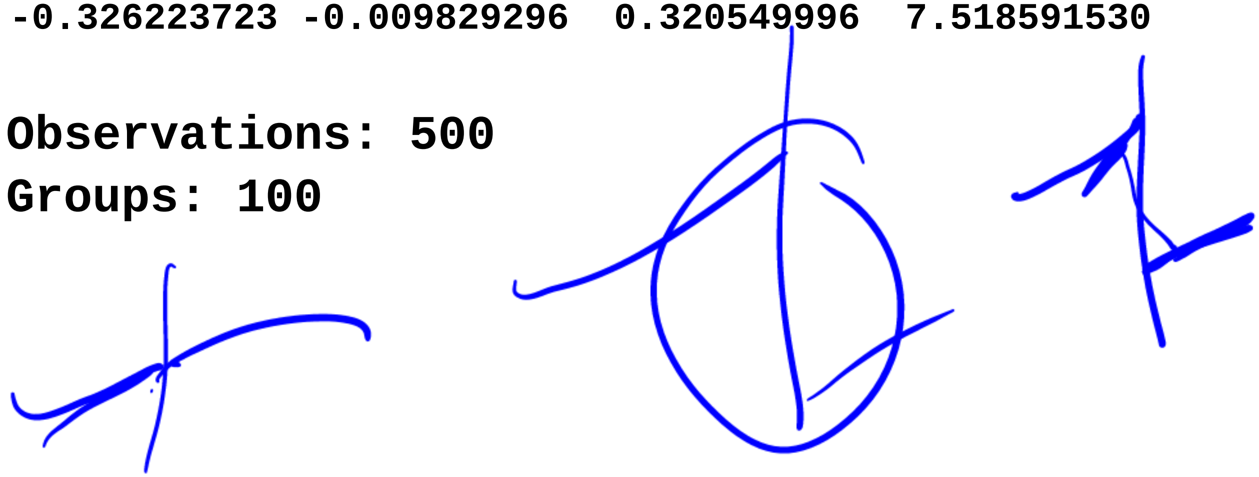
change in quad. term at 5

Using your **sp** in a linear multilevel mixed model:

```
> library( nlme )
> fit <- lme( sleep ~ sp(month), sim.data,
              random = ~ 1 | id )
> summary( fit )
Linear mixed-effects model fit by REML
 Data: sim.data
       AIC      BIC    logLik
  384.8794 426.8642 -182.4397

Random effects:
 Formula: ~1 | id
        (Intercept)  Residual
StdDev:   0.4922676 0.2439248

. . . .
```

```
Fixed effects: sleep ~ sp(month)

                       Value  Std.Error  DF   t-value p-value
(Intercept)         7.770252 0.07562772 393 102.74344  0.0000
sp(month)D1(0)      0.007316 0.04231428 393   0.17289  0.8628
sp(month)D2(0)     -0.027195 0.01204080 393  -2.25853  0.0245
sp(month)C(0).0    -2.284334 0.10143225 393 -22.52078  0.0000
sp(month)C(0).1     0.295341 0.06867966 393   4.30027  0.0000
sp(month)C(0).2    -0.015195 0.01850084 393  -0.82130  0.4120
sp(month)C(5).2     0.027771 0.02041699 393   1.36018  0.1746
sp(month)C(-5).2   -0.048239 0.01943028 393  -2.48267  0.0135

Standardized Within-Group Residuals:
         Min           Q1          Med           Q3          Max
-6.955982485 -0.326223723 -0.009829296  0.320549996  7.518591530

Number of Observations: 500
Number of Groups: 100
```

1



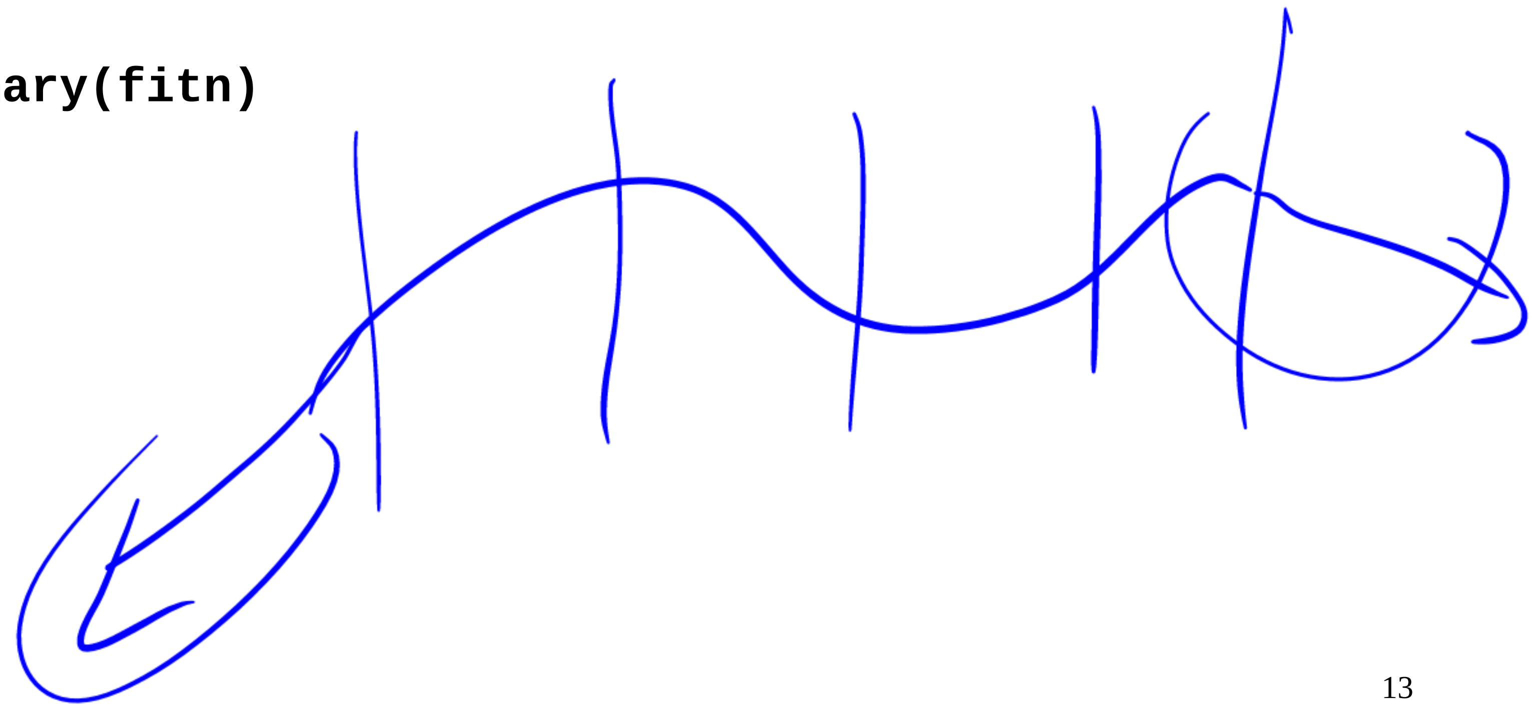
```
> round(model.matrix(fit) [1:5,],4)
  (Intercept) sp(month)D1(0) sp(month)D2(0) sp(month)C(0).0
1           1        -9.8637        48.6464               0
2           1        -6.9539        24.1783               0
3           1        -2.1141         2.2347               0
4           1         0.0534         0.0014               1
5           1         0.9739         0.4742               1
  sp(month)C(0).1 sp(month)C(0).2 sp(month)C(5).2 sp(month)C(-5).2
1          0.0000          0.0000               0         -11.8278
2          0.0000          0.0000               0          -1.9088
3          0.0000          0.0000               0           0.0000
4          0.0534          0.0014               0           0.0000
5          0.9739          0.4742               0           0.0000
```

Natural spline

You can create almost every kind of spline used in regression

Linear in the extreme intervals

```
> spn <- function( x ) gsp( x,
          knots   = c(-10,-5, 0, 5,10),
          degree =  c(1, 2, 2, 2, 2, 1),
          smooth =   c( 1, 1,-1, 1, 1))

> fitn <- lme( sleep ~ spn(month),
            sim.data, random = ~ 1 | id )

> summary(fitn)

. . .
```



```
Fixed effects: sleep ~ spn(month)
                        Value  Std.Error  DF   t-value p-value
(Intercept)          7.770115 0.07572201 393 102.61369  0.0000
spn(month)D1(0)      0.007163 0.04256467 393   0.16829  0.8664
spn(month)D2(0)     -0.027267 0.01214689 393  -2.24475  0.0253
spn(month)C(0).0    -2.278971 0.10190952 393 -22.36269  0.0000
spn(month)C(0).1     0.290233 0.06946431 393   4.17816  0.0000
spn(month)C(0).2    -0.013372 0.01882470 393  -0.71035  0.4779
spn(month)C(5).2     0.024200 0.02135186 393   1.13338  0.2577
spn(month)C(-5).2   -0.048604 0.01975742 393  -2.46003  0.0143
```

Note: Although the estimable coefficients have the same interpretation for both splines, the natural spline matrix is necessarily different. There are no estimable coefficients attached to the boundary knots.

Viewing the fitted model:

Create a data frame of values of functional predictors – here just months:

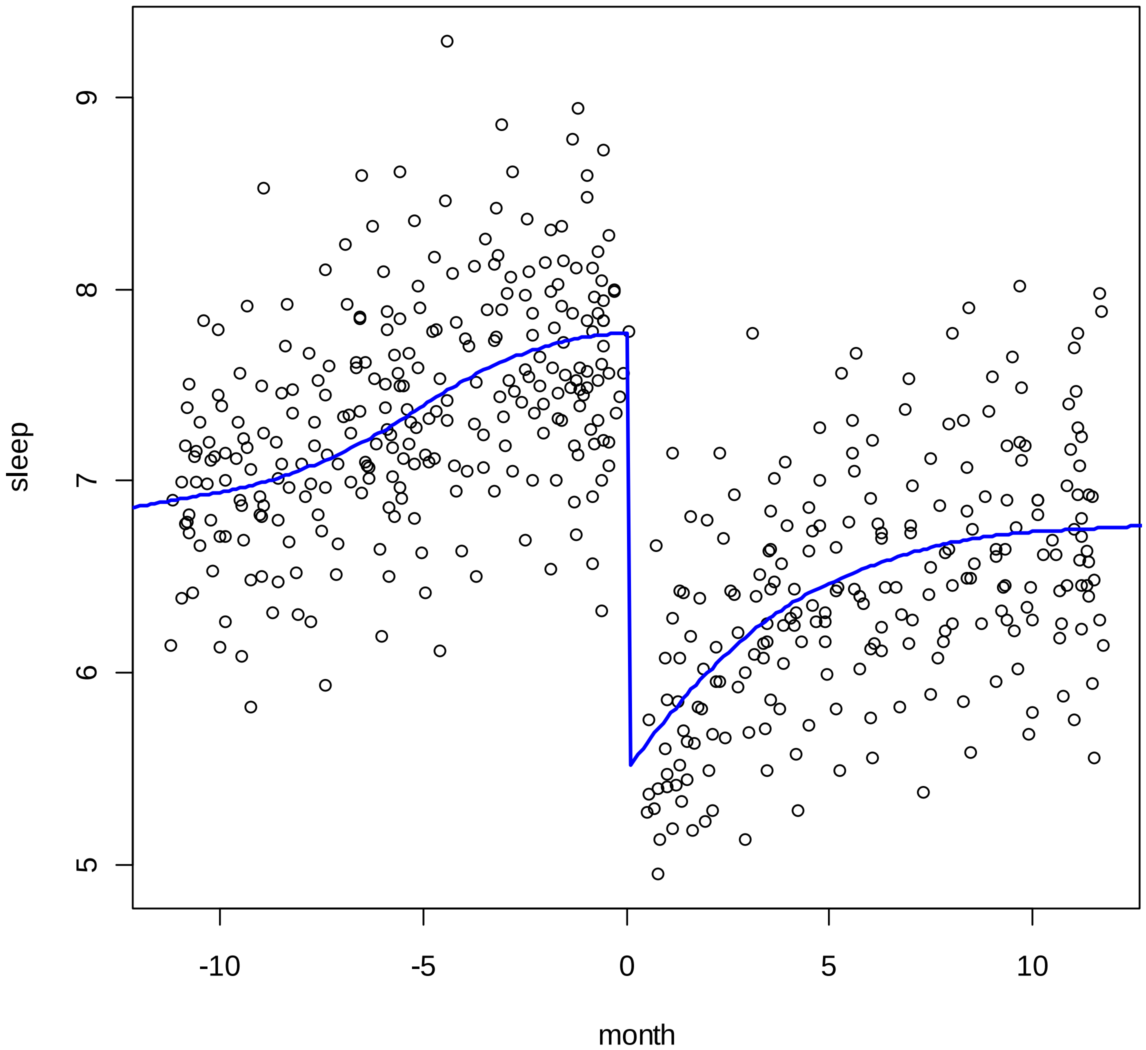
```
> pred <- expand.grid( month = seq(-13,13,.1))
> pred$sleep <- predict( fitn, pred, level =0)
      # Add predicted sleep to the 'pred' data frame
> head( pred )
  month    sleep
1 -13.0 6.832263
2 -12.9 6.835944
3 -12.8 6.839625
4 -12.7 6.843306
5 -12.6 6.846987
6 -12.5 6.850669
```

[2]

*adding predicted sleep in the the data frame '**pred**'*

[2] I used expand.grid although it is really needed only for multiple functional predictors

```
> plot( sleep ~ month, sim.data)
> lines( sleep ~ month, pred, col = 'blue', lwd = 2)
```



Estimation and testing:

Overall test for effect of time:

```
> wald( fitn, 'month')
```

'month' is a "regular expression" matching names of coefficients

```
      numDF denDF  F.value p.value
month     7   393 366.2914 <.00001

Coefficients          Estimate Std.Error  DF    t-value p-value
  spn(month)D1(0)     0.007163  0.042565 393   0.168293 0.86644
  spn(month)D2(0)    -0.027267  0.012147 393  -2.244749 0.02534
  spn(month)C(0).0   -2.278971  0.101910 393 -22.362687 <.00001
  spn(month)C(0).1    0.290233  0.069464 393   4.178156 0.00004
  spn(month)C(0).2   -0.013372  0.018825 393  -0.710346 0.47791
  spn(month)C(5).2    0.024200  0.021352 393   1.133384 0.25774
  spn(month)C(-5).2  -0.048604  0.019757 393  -2.460034 0.01432
```

Can we get rid of knots and just use a quadratic?

```
> wald( fitn, 'C')
  numDF denDF   F.value p.value
C     5   393 402.4999 <.00001
```

No

```
Coefficients              Estimate Std.Error  DF    t-value p-value
  spn(month)C(0).0   -2.278971  0.101910 393 -22.362687 <.00001
  spn(month)C(0).1    0.290233  0.069464 393   4.178156 0.00004
  spn(month)C(0).2   -0.013372  0.018825 393  -0.710346 0.47791
  spn(month)C(5).2    0.024200  0.021352 393   1.133384 0.25774
  spn(month)C(-5).2  -0.048604  0.019757 393  -2.460034 0.01432
```

Can we get rid of non-zero knots?

```
> wald( fitn, 'C\\(5|C\\(-5')
      # '(' is a special character and needs to be 'escaped' to
      # have its literal meaning
      # '|' means 'or'
             numDF denDF  F.value p.value
C\\(5|C\\(-5     2   393 3.646731 0.02696

Coefficients         Estimate Std.Error  DF   t-value p-value
  spn(month)C(5).2   0.024200  0.021352 393  1.133384 0.25774
  spn(month)C(-5).2 -0.048604  0.019757 393 -2.460034 0.01432
```

Using a hypothesis matrix:

```
> Lm <- rbind("at 5 mos" = c(0,0,0,0,0,0,1,0),
              "at -5 mos" = c(0,0,0,0,0,0,0,1))
> Lm
          [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8]
at 5 mos     0    0    0    0    0    0    1    0
at -5 mos    0    0    0    0    0    0    0    1

> wald( fitn, Lm)
  numDF denDF  F.value p.value
1     2   393 3.646731 0.02696

             Estimate Std.Error  DF   t-value p-value
  at 5 mos   0.024200  0.021352 393  1.133384 0.25774
  at -5 mos -0.048604  0.019757 393 -2.460034 0.01432
```

Generating Standard Errors

Wald tests generate estimated standard errors for coefficients, we need to capture them for plotting

Example: plotting the estimated response

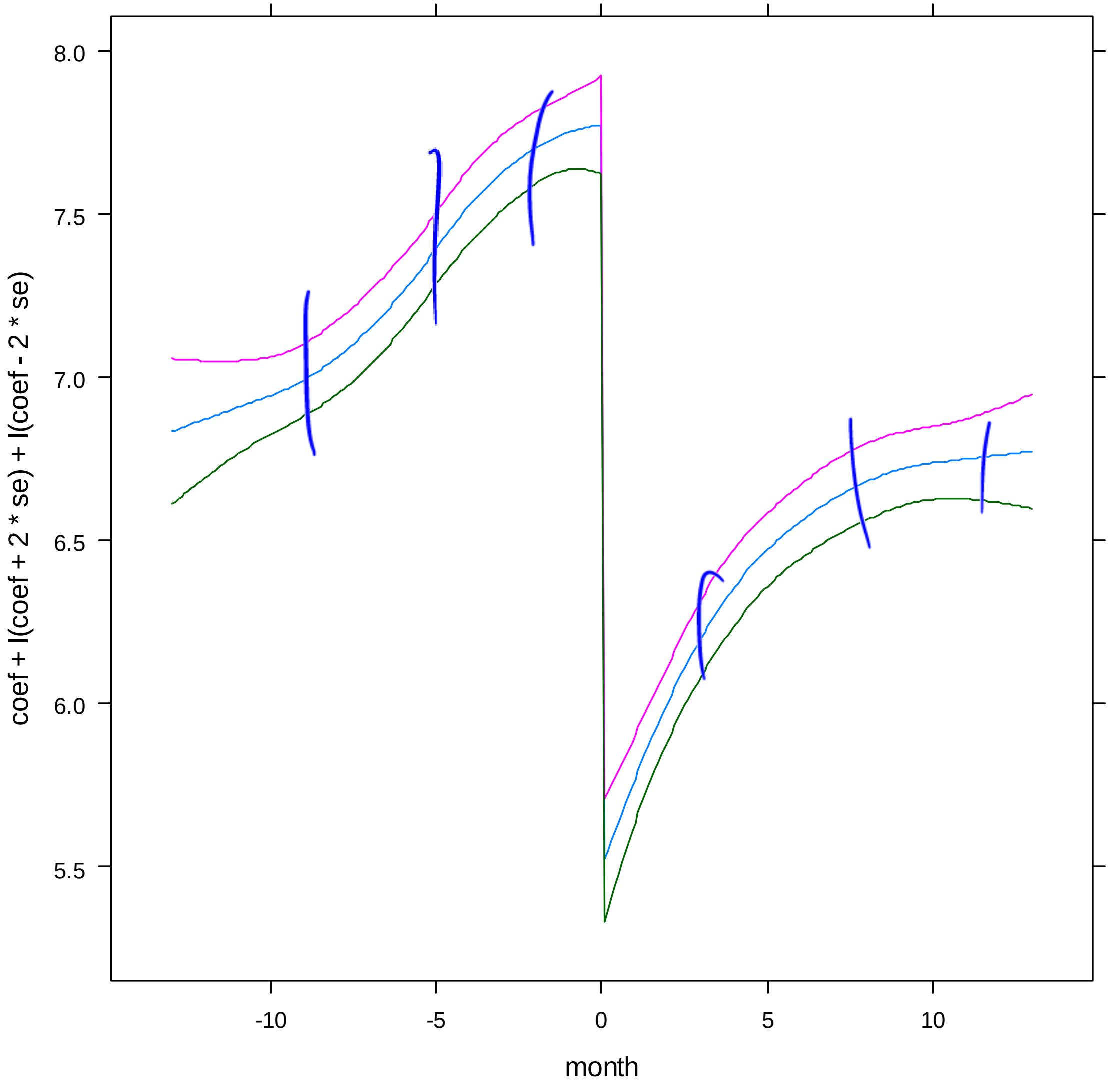
L matrix as model matrix evaluated over a range of predictors

```
> Lest <- with( pred, cbind( 1, spn(month)))
> dim(Lest)
[1] 261   8
> head(Lest)
            D1(0) D2(0) C(0).0 C(0).1 C(0).2 C(5).2 C(-5).2
f(-13)    1 -13.0    80      0      0      0      0   -27.5
f(-12.9) 1 -12.9    79      0      0      0      0   -27.0
f(-12.8) 1 -12.8    78      0      0      0      0   -26.5
f(-12.7) 1 -12.7    77      0      0      0      0   -26.0
f(-12.6) 1 -12.6    76      0      0      0      0   -25.5
f(-12.5) 1 -12.5    75      0      0      0      0   -25.0
```

```
> head( pred )
  month    sleep
1 -13.0 6.832263
2 -12.9 6.835944
3 -12.8 6.839625
4 -12.7 6.843306
5 -12.6 6.846987
6 -12.5 6.850669

> ww <- as.data.frame(wald(fitn, Lest))
          # capture estimates and SEs
> ww <- cbind( ww, pred)
          # combine back with pred
> head( ww )
              coef        se month    sleep
f(-13)    6.832263 0.1111460 -13.0 6.832263
f(-12.9) 6.835944 0.1089242 -12.9 6.835944
f(-12.8) 6.839625 0.1067182 -12.8 6.839625
f(-12.7) 6.843306 0.1045293 -12.7 6.843306
f(-12.6) 6.846987 0.1023583 -12.6 6.846987
f(-12.5) 6.850669 0.1002066 -12.5 6.850669
```

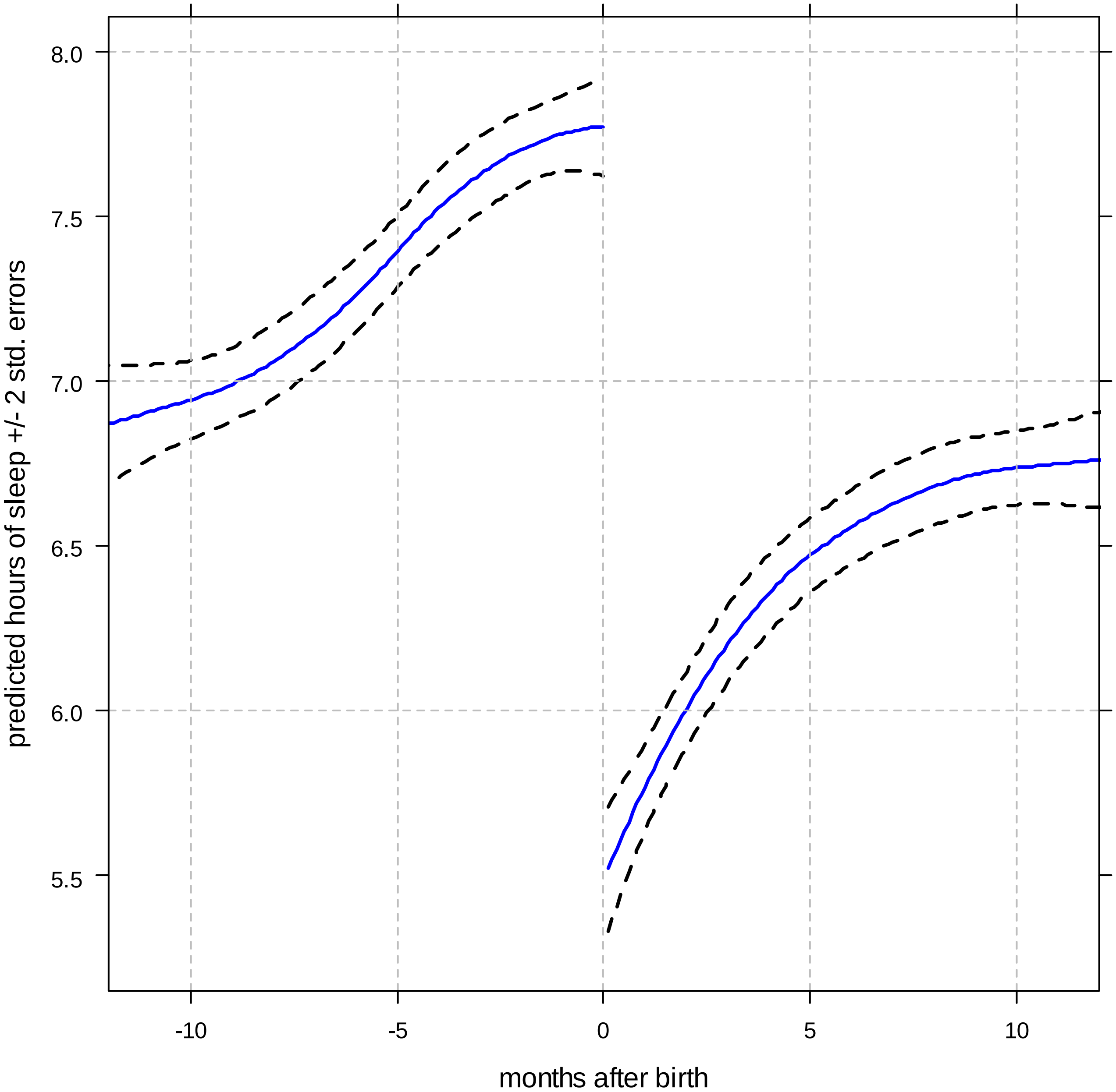
Easy plotting:

```
> xyplot(coef + I(coef + 2*se) + I(coef - 2*se) ~
month, ww, type = 'l')
```



Fancier plotting:

```
> td( col = c('blue','black','black'),
            lty = c( 1,2,2), lwd = 2)

> xyplot( coef + I(coef + 2*se) + I(coef - 2*se) ~
              month,
       rbind(ww[1:131,],NA,ww[132:261,]),
       type = 'l',
       panel = function(x,y,...) {
           panel.xyplot( x, y, ...)
           panel.abline( v = c(-10,-5,0,5,10),
               col = 'gray', lty = 2)
           panel.abline( h = seq(0,10,1),
               col = 'gray', lty = 2)
       },
       xlim = c(-12,12),
       ylab =
         'predicted hours of sleep +/- 2 std. errors',
       xlab = "months after birth")
```



8.0
7.5
7.0
6.5
6.0
5.5
-10
-5
0
5
10
predicted hours of sleep +/- 2 std. errors
months after birth

Inference concerning a spline

All fixed effects coefficients:

```
> wald( fitn )
 numDF denDF  F.value p.value
     8   393 2688.578 <.00001
Coefficients         Estimate Std.Error  DF    t-value p-value
  (Intercept)        7.770115  0.075722 393 102.613693 <.00001
  spn(month)D1(0)    0.007163  0.042565 393   0.168293 0.86644
  spn(month)D2(0)   -0.027267  0.012147 393  -2.244749 0.02534
  spn(month)C(0).0  -2.278971  0.101910 393 -22.362687 <.00001
  spn(month)C(0).1   0.290233  0.069464 393   4.178156 0.00004
  spn(month)C(0).2  -0.013372  0.018825 393  -0.710346 0.47791
  spn(month)C(5).2   0.024200  0.021352 393   1.133384 0.25774
  spn(month)C(-5).2 -0.048604  0.019757 393  -2.460034 0.01432
```

Test saltus at birth (month = 0):

```
> wald( fitn , "C\\(0.*0$")
           numDF denDF  F.value p.value
C\\(0.*0$     1   393 500.0898 <.00001

Coefficients         Estimate Std.Error  DF   t-value p-value
  spn(month)C(0).0 -2.278971   0.10191 393 -22.36269 <.00001
```

Better labelled:

```
> wald( fitn , list("discontinuity at 0" = "C\\(0.*0$"))
                   numDF denDF  F.value p.value
discontinuity at 0     1   393 500.0898 <.00001
```

Operating on splines: `sc` function

`sc( spn, x, D, type)`

generates a hypothesis matrix to estimate the D^th^ power coefficient of the spline **`spn`** at the points given by **`x`**. '**`type`**' only has an effect when the value of **`x`** corresponds to a knot. In that case, **`type`** determines whether the evaluation is to the left, to the right or across the knot.

sc parameters:		
D	0	value of spline
	1	first derivative
	2,...	quadratic,... terms
type	0	limit from the left of knot
	1	limit from the right of knot
	2	saltus: limit from the right minus limit from the left

Example:

Estimate value, slope and quadratic component at -1 months:

```
> sc(spn, c(-1,-1,-1), D = c(1,2,3) )
       D1(0) D2(0) C(0).0 C(0).1 C(0).2 C(5).2 C(-5).2
D1(-1)     1    -1      0      0      0      0       0
D2(-1)     0     1      0      0      0      0       0
D3(-1)     0     0      0      0      0      0       0

> wald( fitn, cbind(c(1,0,0,0),
+       sc(spn, c(-1,-1,-1,-1), D = c(0,1,2,3) )))

  numDF denDF  F.value p.value
1     3   393 6937.729 <.00001

         Estimate Std.Error  DF    t-value p-value
  g(-1)   7.749318  0.057332 393 135.165234 <.00001
  D1(-1)  0.034430  0.030741 393   1.120008 0.26339
  D2(-1) -0.027267  0.012147 393  -2.244749 0.02534
  D3(-1)  0.000000  0.000000 Inf        NaN     NaN
```

Using the sc function to test a saltus (type = 2):

```
> Lm <- cbind( 0, sc( spn, 0, D = 0, type = 2))
> Lm
              D1(0) D2(0) C(0).0 C(0).1 C(0).2 C(5).2 C(-5).2
g(0+)-g(0-) 0     0     0      1      0      0      0       0

> wald( fitn, Lm )
  numDF denDF  F.value p.value
1     1   393 500.0898 <.00001


               Estimate   Std.Error  DF   t-value p-value
  g(0+)-g(0-) -2.278971     0.10191 393 -22.36269 <.00001


> head( model.matrix( fitn))
  (Intercept) spn(month)D1(0) spn(month)D2(0) spn(month)C(0).0
1           1     -9.86370968    48.646384300                0
2           1     -6.95388563    24.178262681                0
3           1     -2.11407625     2.234659188                0
4           1      0.05344575     0.001428224                1
5           1      0.97390029     0.474240891                1
6           1     -7.66649560    29.387577401                0
```

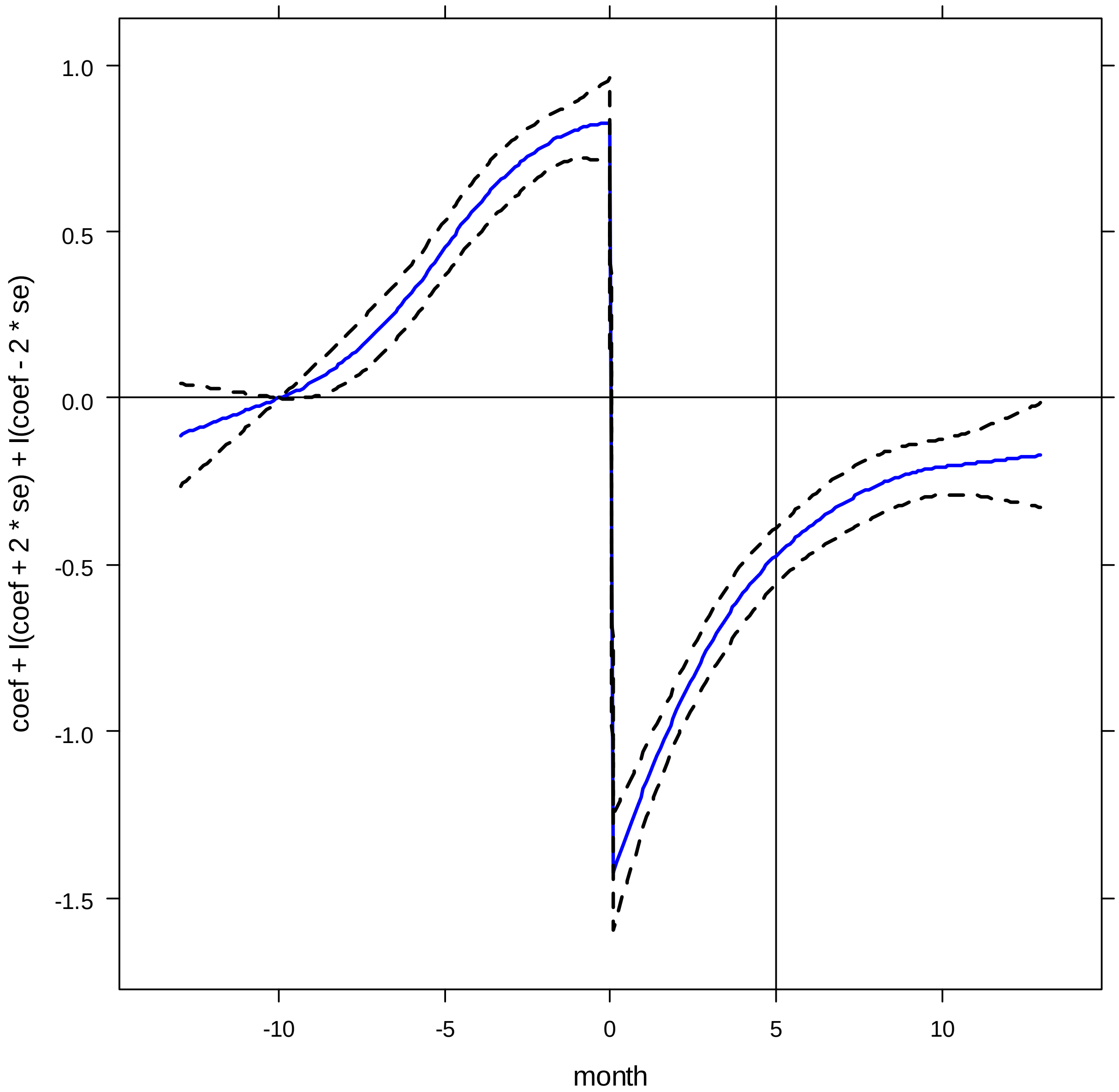
```
  spn(month)C(0).1 spn(month)C(0).2 spn(month)C(5).2 spn(month)C(-5).2
1       0.00000000      0.000000000     0.000000e+00        -11.827836
2       0.00000000      0.000000000     0.000000e+00         -1.908835
3       0.00000000      0.000000000     0.000000e+00          0.000000
4       0.05344575      0.001428224    -1.441111e-18          0.000000
5       0.97390029      0.474240891     1.717766e-16          0.000000
6       0.00000000      0.000000000     0.000000e+00         -3.555099
```

```
> L.level <- cbind( 1, spn( c(-10, 10)))
> L.level
          D1(0) D2(0) C(0).0 C(0).1 C(0).2 C(5).2 C(-5).2
f(-10) 1   -10    50      0      0      0    0.0   -12.5
f(10)  1    10    50      1     10     50   12.5     0.0
```

```
> wald( fitn, L.level )
  numDF denDF  F.value p.value
1     2   393 8216.843 <.00001

         Estimate Std.Error  DF  t-value p-value Lower 0.95 Upper 0.95
  f(-10) 6.942695  0.058820 393 118.0330 <.00001   6.827054   7.058337
  f(10)  6.735666  0.055838 393 120.6283 <.00001   6.625887   6.845445
```

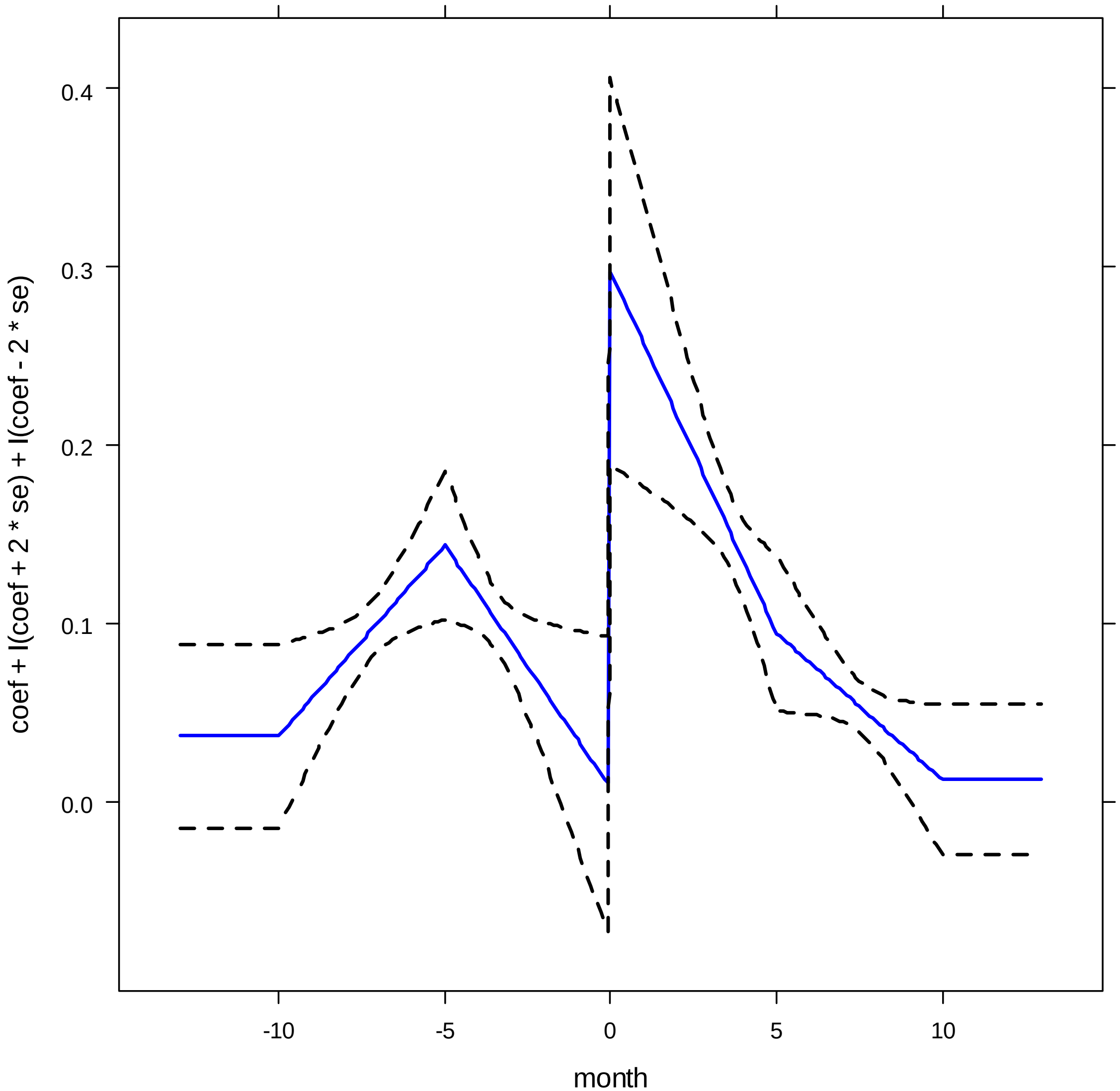
```
> wald( fitn, L.level[2,] - L.level[1,] )
  numDF denDF F.value p.value
1     1   393 24.4368 <.00001

       Estimate Std.Error  DF   t-value p-value Lower 0.95 Upper 0.95
  Larg -0.20703   0.04188 393 -4.943359 <.00001  -0.289367  -0.124692

> ?sc
> Lslope <- with( pred, cbind( 0 , sc( spn, month, D = 1)))
> ws <- as.data.frame(wald(fitn,Lslope))
> head(ws)
                  coef         se
D1(-13)   0.03681075 0.02576518
D1(-12.9) 0.03681075 0.02576518
D1(-12.8) 0.03681075 0.02576518
D1(-12.7) 0.03681075 0.02576518
D1(-12.6) 0.03681075 0.02576518
D1(-12.5) 0.03681075 0.02576518
> ws <- cbind(ws, pred)
```

```
> xyplot( coef + I(coef + 2*se)+I(coef - 2*se) ~ month,
     ws, type = 'l')
```

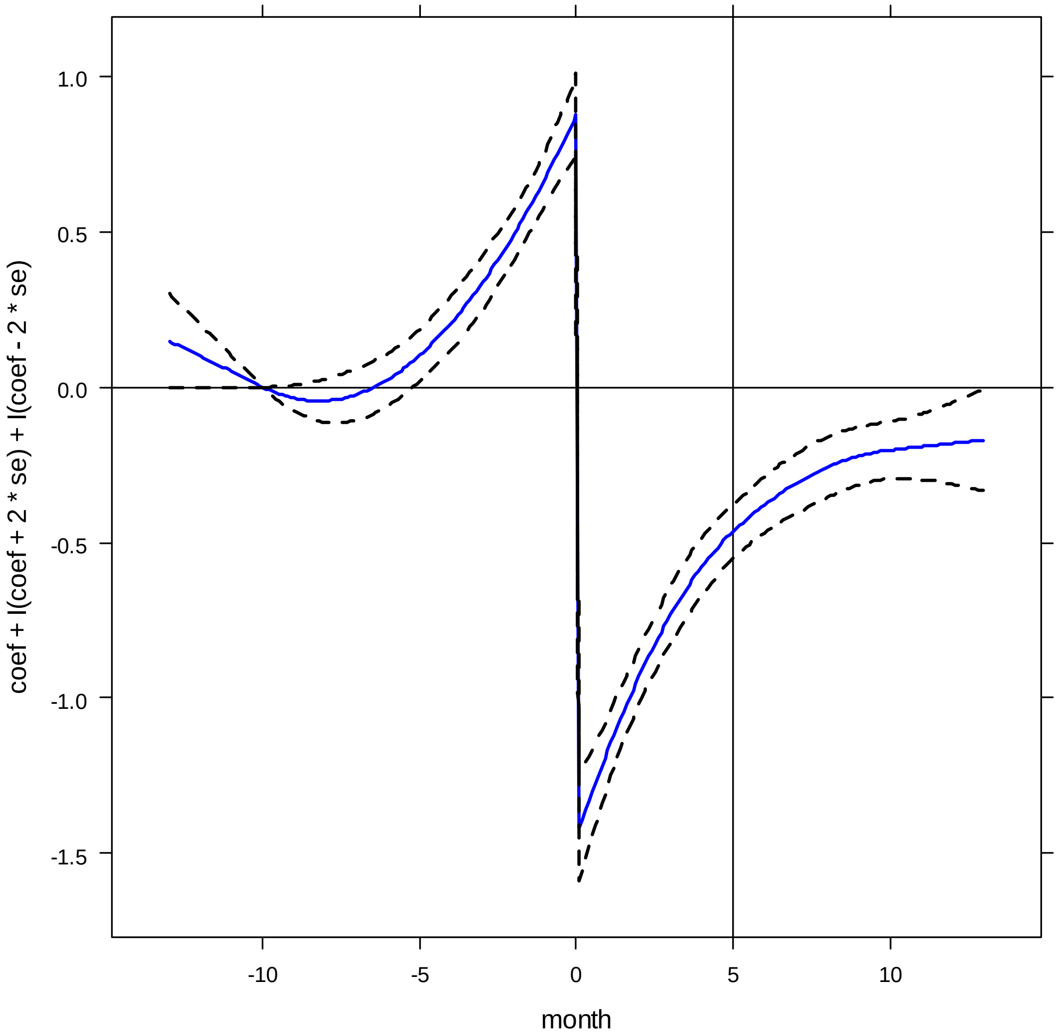


```
> head( Lest )
          D1(0) D2(0) C(0).0 C(0).1 C(0).2 C(5).2 C(-5).2
f(-13)    1 -13.0    80      0      0      0      0   -27.5
f(-12.9) 1 -12.9    79      0      0      0      0   -27.0
f(-12.8) 1 -12.8    78      0      0      0      0   -26.5
f(-12.7) 1 -12.7    77      0      0      0      0   -26.0
f(-12.6) 1 -12.6    76      0      0      0      0   -25.5
f(-12.5) 1 -12.5    75      0      0      0      0   -25.0
> L.m10 <- cbind( 1, spn(-10))
> L.m10
        D1(0) D2(0) C(0).0 C(0).1 C(0).2 C(5).2 C(-5).2
f(-10) 1   -10    50      0      0      0      0   -12.5
> Ldiff.m10 <- Lest - L.m10[rep(1,nrow(Lpred)),]
> wd <- as.data.frame( wald( fitn, Ldiff.m10))
> wd <- cbind(wd, pred)
> wdr <- as.data.frame( wald( fitnr, Ldiff.m10))
> wdr <- cbind(wdr, pred)
```

```
> xyplot(  coef + I(coef + 2*se)+I(coef - 2*se)
        ~ month, wd, type = 'l',
        abline = list(h=0,v=5))
```



```
> xyplot(  coef + I(coef + 2*se)+I(coef - 2*se) ~
       month, wdr, type = 'l',
       abline = list(h=0, v=5))
```



Caution:

Since gsp uses raw parametrization (in contrasts with b-splines, for example), you should center and rescale the predictor. A range within -10 to 10 for a spline with no power higher than cubic should be adequate.