#### Generalized Regression Splines in R

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  - Traditional regression-spline bases, such as B-splines, are selected for numerical stability rather than for interpretability.
  - Although the emphasis on graphical interpretation makes sense, it also represents a missed opportunity.

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  - Further thoughts on implementing generalized regression splines in R.
- To install the carEx package:

install.packages("carEx", repos="http://R-Forge.R-project.org").

• To provide a point of reference, we randomly generate *n* = 200 observations according to the simple nonlinear regression model

$$x \sim unif(0, 10)$$
  

$$\varepsilon \sim N(0, 0.5^2)$$
  

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- The broken line on the graph shows  $E(y|x) = \cos(1.25(x+1)) + x/5.$
- We introduce a succession of increasingly complex segmented polynomial regression models, culminating in traditional cubic regression splines.



Monette & Fox (York & McMaster)

Piecewise polynomials begin by dividing the range of x into non-overlapping intervals at k ordered x-values t<sub>j</sub> called knots: (-∞, t<sub>1</sub>], (t<sub>1</sub>, t<sub>2</sub>], ..., (t<sub>k</sub>, ∞).

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- Then a degree-*p* polynomial is fit by least-squares regression to the data in each interval.

**Piecewise Polynomials** 

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- The simplest case is a degree-0 polynomial, which generates a *piecewise-constant* fit by computing the mean y-value in each interval.
- For the example, we set k = 2 knots at t<sub>1</sub> = 10/3 and t<sub>2</sub> = 2 × 10/3, which are the 1/3 and 2/3 quantiles of the uniform[0, 10] distribution from which the x-values were generated.



**Piecewise Polynomials** 

• A next step is to generalize the model to a *piecewise-linear* fit (that is, a piecewise degree-1 polynomial).



Linear Regression Spline

• We convert the piecewise-linear fit into a *linear regression spline* by constraining the regression lines on the two sides of each knot to be equal at the knot.



Linear Regression Spline

• We can do this by fitting the linear model

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \beta_3 x_{i3} + \varepsilon_i$$

where  $x_{i1} = x_i$ ,

$$x_{i2} = \begin{cases} 0 & \text{for } x_i \leq t_1 \\ x_i - t_1 & \text{for } x_i > t_1 \end{cases}$$

and

$$x_{i3} = \begin{cases} 0 & \text{for } x_i \le t_2 \\ x_i - t_2 & \text{for } x_i > t_2 \end{cases}$$





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Residual SD = 0.694 on 196 df, R-squared = 0.643

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c  $\sim$ 0 0 7 tっ 0 2 6 10 8 х

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- Our goal is to maintain interpretability even in much more complex spline models.





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- This approach generalizes readily to higher-degree polyomials, the most common of which is the third-degree or *cubic regression spline*.
- Removing both the linear terms  $(\beta_{21}x_{i2})$ and  $\beta_{31}x_{i3}$  and the quadratic terms  $(\beta_{22}x_{i2}^2)$  and  $\beta_{32}x_{i3}^2$  from the the model forces the slope and curvature to be equal on both sides of each knot, producing *order-2 smoothess* and a traditional cubic regression spline:

$$y_{i} = \beta_{0} + \beta_{11}x_{i1} + \beta_{12}x_{i1}^{2} + \beta_{13}x_{i1}^{3} + \beta_{23}x_{i2}^{3} + \beta_{33}x_{i3}^{3} + \varepsilon_{i}$$

#### Cubic Regression Spline, Order-2 Smoothness


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  - The function returned by gspline() can also be used to generate hypothesis matrices, a topic we don't pursue here.

Monette & Fox (York & McMaster)

Here are all of the preceding examples (and more) fit via gspline(); in each case, we'd use the generated spline function in a call of the form lm(y ~ sp(x)), and the knots are in the vector t <- c(10/3, 20/3):</li>

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  - cubic regression spline with matching slopes, sp <- gspline(knots=t, degree=3, smoothness=1)</li>
  - cubic regression spline with matching slopes and curvature, sp <- gspline(knots=t, degree=3, smoothness=2) or just sp <- gspline(knots=t)</li>

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- gspline() doesn't treat boundary knots specially, but using the knots, degree, and smoothness arguments it's simple to specify the equivalent of a natural spline: e.g., gspline(knots=c(0, 10/3, 20/3, 10),

```
degree=c(1, 3, 3, 3, 1),
smoothness=c(2, 2, 2, 2))
```

→

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  - 2) a vector of polynomial *degrees*,  $d_1, d_2, ..., d_{k+1}$ , of length k + 1,
  - a vector of orders of continuity or smoothness, c<sub>1</sub>, c<sub>2</sub>, ..., c<sub>k</sub>, of length k, the highest order for which the derivatives on each side of a knot t<sub>i</sub> match.

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- The linear space for the model is  $\mathcal{M} = \{\eta = X_f \phi : \phi \in \mathbb{R}^q, C\phi = 0\}.$
- We wish to construct an  $n \times p$  model matrix X with p = q c so that  $\mathcal{M} = \{\eta = X\beta : \beta \in \mathbb{R}^p\}.$

- Let  $X_f$  be an  $n \times q$  matrix for a model whose coefficients are subject to c linearly independent constraints given by a  $c \times q$  matrix C.
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• Then the  $q \times q$  partitioned matrix  $\begin{bmatrix} C \\ E \end{bmatrix}$  has linearly independent rows and is invertible with a conformably partitioned inverse  $\begin{bmatrix} F & G \end{bmatrix} = \begin{bmatrix} C \\ E \end{bmatrix}^{-1}$ .

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- Consider the model matrix  $X = X_f G$ .
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- Given the least-squares estimator  $\hat{\beta}$  of  $\beta$ , We can estimate any linear function  $\psi = L\phi$  of  $\phi$  under the constraint  $C\phi = 0$  with the estimator  $\hat{\psi} = A\hat{\beta}$  with A = LG.
### Generalized Regression Splines: Theory General Principles

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  - Thus, G serves as a post-multiplier to transform  $X_f$  into a model matrix  $X = X_f G$  that can be used in a linear model.

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  - Thus, G serves as a post-multiplier to transform  $X_f$  into a model matrix  $X = X_f G$  that can be used in a linear model.
  - G also serves as a post-multiplier to transform any general linear hypothesis matrix expressed in terms of  $\phi$  into a general linear hypothesis matrix in terms of of  $\beta$ .

• Our goal is to generate model matrices for splines that produces interpretable coefficients and simple estimates and tests of properties of the spline that are linear functions of parameters: slope, curvature, discontinuities, etc.

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- Generating model matrices in more general situations, for example with degrees that are not monotone, nor monotone increasing as the index radiates from a central value, is more challenging.
- The approach described here works for any pattern of degrees, *d<sub>i</sub>* and smoothness constraints, *c<sub>i</sub>*.
- We start by constucting a matrix,  $X_f$ , for a spline in which the polynomial degree in each interval is the maximal value,  $\max(d_i)$ , and then construct constraints for the coefficients of this model to produce the desired spline.

• Extending our earlier examples, consider a spline, S, with knots at t = (10/3, 20/3), polynomial degrees, d = (2, 3, 2), and smoothness, c = (1, 2).

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- Columns of the full matrix  $X_f$  contain the intercept, and linear, quadratic, and cubic terms in each interval of the spline.
- To create an instance of  $X_f$  we need to specify the values over which the matrix is evaluated, say at x = 0, 1, ..., 10 (where the function Xf(), used to generate the matrix, is local to the gspline() function in the **carEx** package and thus not normally called by the user):

> Xf(0:10, knots=c(10/3, 20/3), degree = 3)

	XO	X1	Х2	ΧЗ	XO	X1	Х2	ΧЗ	ХО	X1	X2	XЗ	
f(0)	1	0	0	0	0	0	0	0	0	0	0	0	
f(1)	1	1	1	1	0	0	0	0	0	0	0	0	
f(2)	1	2	4	8	0	0	0	0	0	0	0	0	
f(3)	1	3	9	27	0	0	0	0	0	0	0	0	
f(4)	0	0	0	0	1	4	16	64	0	0	0	0	
f(5)	0	0	0	0	1	5	25	125	0	0	0	0	
f(6)	0	0	0	0	1	6	36	216	0	0	0	0	
f(7)	0	0	0	0	0	0	0	0	1	7	49	343	
f(8)	0	0	0	0	0	0	0	0	1	8	64	512	
f(9)	0	0	0	0	0	0	0	0	1	9	81	729	
f(10)	0	0	0	0	0	0	0	0	1	10	100	1000	

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• The model for the unconstrained maximal polynomial is  $X_f \phi : \phi \in \mathbb{R}^{12}$ .

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- We impose three types of constraints on  $\phi$ .
  - $X_f \phi$  should evaluate to 0 at x = 0 so an intercept term in the model will have the correct interpretation.
  - The limits of the value and of the first derivative of the spline must be the same when approaching the first knot from the right or from the left, and the limits of the value, the first and second derivatives should be the same when approaching the second knot from the right or from the left.

- The model for the unconstrained maximal polynomial is  $X_f \phi : \phi \in \mathbb{R}^{12}$ .
- We impose three types of constraints on  $\phi$ .
  - $X_f \phi$  should evaluate to 0 at x = 0 so an intercept term in the model will have the correct interpretation.
  - The limits of the value and of the first derivative of the spline must be the same when approaching the first knot from the right or from the left, and the limits of the value, the first and second derivatives should be the same when approaching the second knot from the right or from the left.
  - Solution The degree of the polynomial in the first and third intervals must be reduced to 2.

• The constraint matrix, C, is created by the (internal) Cmat() function:

> Cmat(knots=c(10/3, 20/3), degree=c(2, 3, 2), smooth=c(1, 2))

	XO	X1	X2	хз	XO	X1	X2	XЗ	XO	X1	X2	XЗ	
f(0)	1	0.0000	0.0000	0.000	0	0.0000	0.0000	0.000	0	0.0000	0.000	0.00	
C0 3.33	-1	-3.3333	-11.1111	-37.037	1	3.3333	11.1111	37.037	0	0.0000	0.000	0.00	
C1 3.33	0	-1.0000	-6.6667	-33.333	0	1.0000	6.6667	33.333	0	0.0000	0.000	0.00	
C0 6.67	0	0.0000	0.0000	0.000	-1	-6.6667	-44.4444	-296.296	1	6.6667	44.444	296.30	
C1 6.67	0	0.0000	0.0000	0.000	0	-1.0000	-13.3333	-133.333	0	1.0000	13.333	133.33	
C2 6.67	0	0.0000	0.0000	0.000	0	0.0000	-2.0000	-40.000	0	0.0000	2.000	40.00	
I.1.3	0	0.0000	0.0000	1.000	0	0.0000	0.0000	0.000	0	0.0000	0.000	0.00	
I.3.3	0	0.0000	0.0000	0.000	0	0.0000	0.0000	0.000	0	0.0000	0.000	1.00	
attr(,"	ranl	ks")											
npar.	ful	1	C.n	C.rank	sp	line.rank	:						
	12	2	8	8		4							
attr(,"	d")												
[1] 469	.012	2615 63	.081291	10.48923	Э	3.528970	0.9822	249 0.8	1684	18 0.3	375998	0.0700	72

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> Cmat(knots=c(10/3, 20/3), degree=c(2, 3, 2), smooth=c(1, 2))

	XO	X1	X2	XЗ	XO	X1	X2	XЗ	XO	X1	X2	XЗ	
f(0)	1	0.0000	0.0000	0.000	0	0.0000	0.0000	0.000	0	0.0000	0.000	0.00	
C0 3.33	-1	-3.3333	-11.1111	-37.037	1	3.3333	11.1111	37.037	0	0.0000	0.000	0.00	
C1 3.33	0	-1.0000	-6.6667	-33.333	0	1.0000	6.6667	33.333	0	0.0000	0.000	0.00	
C0 6.67	0	0.0000	0.0000	0.000	-1	-6.6667	-44.4444	-296.296	1	6.6667	44.444	296.30	
C1 6.67	0	0.0000	0.0000	0.000	0	-1.0000	-13.3333	-133.333	0	1.0000	13.333	133.33	
C2 6.67	0	0.0000	0.0000	0.000	0	0.0000	-2.0000	-40.000	0	0.0000	2.000	40.00	
I.1.3	0	0.0000	0.0000	1.000	0	0.0000	0.0000	0.000	0	0.0000	0.000	0.00	
I.3.3	0	0.0000	0.0000	0.000	0	0.0000	0.0000	0.000	0	0.0000	0.000	1.00	
attr(,"1	ank	ks")											
npar.f	ull	L	C.n	C.rank	sp]	line.rank	:						
	12	2	8	8		4							
attr(,"d	i")												
[1] 469.	012	2615 63	.081291	10.489239	9	3.528970	0.9822	249 0.8	1684	48 0.3	375998	0.0700	72

• The row labels of the constraint matrix show the role of each row.

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f(0)	1	0.0000	0.0000	0.000	0	0.0000	0.0000	0.000	0	0.0000	0.000	0.00	
C0 3.33	-1	-3.3333	-11.1111	-37.037	1	3.3333	11.1111	37.037	0	0.0000	0.000	0.00	
C1 3.33	0	-1.0000	-6.6667	-33.333	0	1.0000	6.6667	33.333	0	0.0000	0.000	0.00	
C0 6.67	0	0.0000	0.0000	0.000	-1	-6.6667	-44.4444	-296.296	1	6.6667	44.444	296.30	
C1 6.67	0	0.0000	0.0000	0.000	0	-1.0000	-13.3333	-133.333	0	1.0000	13.333	133.33	
C2 6.67	0	0.0000	0.0000	0.000	0	0.0000	-2.0000	-40.000	0	0.0000	2.000	40.00	
I.1.3	0	0.0000	0.0000	1.000	0	0.0000	0.0000	0.000	0	0.0000	0.000	0.00	
I.3.3	0	0.0000	0.0000	0.000	0	0.0000	0.0000	0.000	0	0.0000	0.000	1.00	
attr(,"1	cank	("s											
npar.f	full	L	C.n	C.rank	sp]	line.rank	:						
	12	2	8	8		4							
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- The row labels of the constraint matrix show the role of each row.
- The d attribute contains the vector of singular values of the constraint matrix.

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- The matrix *E* of estimable functions is created by the (internal) Emat() function:
  - > Emat(knots=c(10/3, 20/3), degree=c(2, 3, 2), smooth=c(1, 2))

	XO	X1	Х2	ΧЗ	XO	X1	Х2	ΧЗ	XO	X1	Х2	ΧЗ
D1 0	0	1	0	0	0	0	0	0	0	0	0	0
D2 0	0	0	2	0	0	0	0	0	0	0	0	0
C2 3.33	0	0	-2	-20	0	0	2	20	0	0	0	0
C3 3.33	0	0	0	-6	0	0	0	6	0	0	0	0

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  - > Emat(knots=c(10/3, 20/3), degree=c(2, 3, 2), smooth=c(1, 2))

 X0
 X1
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• The row labels signify the first derivative at x = 0, D1(0), the second derivative at x = 0, D2(0), the change in the second derivative at x = 10/3, C(3.33).2, and the change in the third derivative at x = 10/3, C(3.33).3.

## Generalized Regression Splines: Theory

Application to Splines

• The full-rank model matrix  $X = X_f G$  for the spline parametrized by linear estimable coefficients is generated as previously described, as a closure produced by the gspline() function:

```
> sp <- gspline(knots=c(10/3, 20/3), degree=c(2, 3, 2), smooth=c(1, 2))
> sp(0:10)
```

	D1 0	D2 0	C2 3.33	C3 3.33
f(0)	0	0.0	0.000	0.000
f(1)	1	0.5	0.000	0.000
f(2)	2	2.0	0.000	0.000
f(3)	3	4.5	0.000	0.000
f(4)	4	8.0	0.222	0.049
f(5)	5	12.5	1.389	0.772
f(6)	6	18.0	3.556	3.160
f(7)	7	24.5	6.722	8.210
f(8)	8	32.0	10.889	16.543
f(9)	9	40.5	16.056	28.210
f(10)	10	50.0	22.222	43.210

----

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f(4)	4	8.0	0.222	0.049
f(5)	5	12.5	1.389	0.772
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f(7)	7	24.5	6.722	8.210
f(8)	8	32.0	10.889	16.543
f(9)	9	40.5	16.056	28.210
f(10)	10	50.0	22.222	43.210

• The closure sp() created by gspline() can be used in a linear or similar model formula.

## Example: Canadian Unemployment and the 2008 Crash Data

• We use the monthly Canadian unemployment rates from January 1995 to February 2019 to illustrate a model with a discontinuity and, subsequently, a periodic spline component for annual seasonal patterns.

## Example: Canadian Unemployment and the 2008 Crash $$\mathsf{D}_{\mathsf{ata}}$$

- We use the monthly Canadian unemployment rates from January 1995 to February 2019 to illustrate a model with a discontinuity and, subsequently, a periodic spline component for annual seasonal patterns.
- The data are in the Unemployment data set in the carEx package:

```
> brief(Unemployment)
```

290	x 2 data.frame	(285 rows	omitted)
	date unem	nployment	
	[D]	[n]	
1	1995-01-01	10.6	
2	1995-02-01	10.4	
3	1995-03-01	10.7	
289	2019-01-01	6.2	
290	2019-02-01	6.1	

## Example: Canadian Unemployment and the 2008 Crash $$_{\text{Data}}$$

• For convenience, we add year and month variables to the data:

```
> toyear <- function(x) (as.numeric(x) -
+ as.numeric(as.Date("2000-01-01")))/365.25
> Unemp <- within(
+ Unemployment,
+ {
+ year <- toyear(date)
+ month <- as.numeric(format(date, "%m"))
+ })
</pre>
```



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```
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> Unemp <- within(
+ Unemployment,
+ {
+ year <- toyear(date)
+ month <- as.numeric(format(date, "%m"))
</pre>
```

 Graphing the data, marking the date of the crash, which we take as mid-December:

```
> plot(unemployment ~ date, data=Unemp,
+ col=gray(0.60), type="b")
> abline(v=as.Date("2008-12-15"), lty=2)
```



- We create knots at the quintiles of year, and add a knot for the date of the crash:
  - > knots <- quantile(Unemp\$year, (1:4)/5)</pre>
  - > knots.d <- sort(c(knots, toyear(as.Date("2008-12-15"))))</pre>

- We create knots at the quintiles of year, and add a knot for the date of the crash:
  - > knots <- quantile(Unemp\$year, (1:4)/5)</pre>
  - > knots.d <- sort(c(knots, toyear(as.Date("2008-12-15"))))</pre>
- We proceed to fit several quadratic and cubic regression spline models to the data, with and without a discontinuity at the date of the crash:
  - > sp2 <- gspline(knots=knots, degree=2, smoothness=1)</pre>
  - > sp3 <- gspline(knots=knots, degree=3, smoothness=2)</pre>
  - > sp2.d <- gspline(knots=knots.d, degree=2, smoothness=c(1,1,-1,1,1))</pre>
  - > sp3.d <- gspline(knots=knots.d, degree=3, smoothness=c(2,2,-1,2,2))</pre>
  - > fit2 <- lm(unemployment ~ sp2(year), data=Unemp)</pre>
  - > fit3 <- lm(unemployment ~ sp3(year), data=Unemp)</pre>
  - > fit2.d <- lm(unemployment ~ sp2.d(year), data=Unemp)</pre>
  - > fit3.d <- lm(unemployment ~ sp3.d(year), data=Unemp)</pre>

- Graphing the various fits:
  - Quadratic regression spline:
    - > plot(unemployment ~ date, data=Unemp,
    - + col=gray(0.60), type="b",
    - + main="Quadratic Regression Spline")
    - > abline(v=as.Date("2008-12-15"), lty=2)
    - > lines(Unemp\$date, predict(fit2), lwd=3,
    - + col="magenta")





- Graphing the various fits:
  - Cubic regression spline:
    - > plot(unemployment ~ date, data=Unemp,
    - + col=gray(0.60), type="b",
    - + main="Cubic Regression Spline")
    - > abline(v=as.Date("2008-12-15"), lty=2)
    - > lines(Unemp\$date, predict(fit3), lwd=3,
    - + col="magenta")



**Cubic Regression Spline** 

- Graphing the various fits:
  - Quadratic regression spline with discontinuity:
- > plot(unemployment ~ date, data=Unemp,
- + col=gray(0.60), type="b",
- + main="Discontinuous Quadratic Regression Spline")
- > abline(v=as.Date("2008-12-15"), lty=2)
- > lines(Unemp\$date, predict(fit2.d), lwd=3,
- + col="magenta")

#### **Discontinuous Quadratic Regression Spline**



- Graphing the various fits:
  - Cubic regression spline with discontinuity:
- > plot(unemployment ~ date, data=Unemp,
- + col=gray(0.60), type="b",
- + main="Discontinuous Cubic Regression Spline")
- > abline(v=as.Date("2008-12-15"), lty=2)
- > lines(Unemp\$date, predict(fit3.d), lwd=3,
- + col="magenta")





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- To model this pattern, we add a periodic spline component as a function of months, using a cubic spline with period 12 and 4 internal knots at  $12 \times (1/5, 2/5, 3/5, 4/5)$  plus a boundary knot at 12.
- The derivatives parametrizing the periodic spline are derivatives from the left at the maximum knot, which are identified with the same derivatives from the left at 0.

> per.3 <- gspline(knots=12\*(1:5)/5, degree=3, smoothness=2, periodic=TRUE)

> fit3.d.p <- lm(unemployment ~ sp3.d(year) + per.3(month), data=Unemp)</pre>
## Example: Canadian Unemployment and the 2008 Crash

Adding a Periodic Regression Spline to the Model

• Graphing the fit:



Discontinuous and Periodic Cubic Regression Splines



## Example: Canadian Unemployment and the 2008 Crash Adding a Periodic Regression Spline to the Model

• Some model comparisons:

> AIC(fit2, fit3, fit2.d, fit3.d, fit3.d.p)

dfAICfit28633.55fit39657.07fit2.d11525.27fit3.d13469.35fit3.d.p17239.01

## Example: Canadian Unemployment and the 2008 Crash Adding a Periodic Regression Spline to the Model

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• The AIC strongly favours the cubic model with both discontinuity and a periodic component.

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  - We have a plan, tested but not fully implemented, to accomplish this while still maintaining an interpretable parametrization of the regression splines.
- We'd also like to make the wald() function (which is useful for testing hypotheses about regression splines but is not illustrated in this presentation) more intelligent in how it deals with spline models whose linear predictors have terms related by marginality, e.g., of the form generated by sp(numeric.predictor)\*factor.

- Fox, J. (2016). Applied Regression Analysis and Generalized Linear Models. Sage, Thousand Oaks, CA, 3rd edition.
- Harrell, Jr., F. E. (2015). Regression Modeling Strategies, With Applications to Linear Models, Logistic Regression, and Survival Analysis. Springer, New York, second edition.