sg151.y	B-splines and splines parameterized by their values at reference points
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# Abstract

A package of 3 programs is presented for generating a basis of splines in an X-variable, to be input to regression programs to fit spline models. The first, **bspline**, generates a basis of Schoenberg *B*-splines, which avoid the stability problems associated with plus-functions. The second, **frencurv**, generates a basis of reference splines, whose parameters in the regression model are simply values of the spline at reference points on the X-axis. The third, **flexcurv**, is an easy-to-use version of **frencurv**, which generates reference splines with sensibly-spaced knots. **frencurv** and **flexcurv** have the additional option of generating an incomplete basis of reference splines, with the reference spline for one reference point omitted. This incomplete basis can be completed by adding the standard constant vector to the design matrix, and can then be used to estimate differences between values of the spline at the remaining reference points and the value of the spline at the omitted reference point.

# Key phrases

Spline; B-spline; interpolation; quadratic; cubic.

# $\mathbf{Syntax}$

bspline [ newvarlist ] [ if exp ] [ in range ], xvar(varname) [ power(#) knots(numlist) noexknot generate(prefix) type(type) labfmt(format) labprefix(string) ] frencurv [ newvarlist ] [ if exp ] [ in range ], xvar(varname) [ power(#) refpts(numlist) noexref omit(#) base(#) knots(numlist) noexknot generate(prefix) type(type) labfmt(format) labprefix(string) ] flexcurv [ newvarlist ] [ if exp ] [ in range ], xvar(varname) [ power(#) refpts(numlist) omit(#) base(#) include(numlist) krule(knot\_rule) generate(prefix) type(type) labfmt(format) labprefix(string) ]

where *knot\_rule* is

<u>r</u>egular | <u>i</u>nterpolate

# Description

The bspline package contains 3 commands, bspline, frencurv and flexcurv. bspline generates a basis of B-splines in the X-variate based on a list of knots, for use in the design matrix of a regression model. frencurv generates a basis of reference splines, for use in the design matrix of a regression model, with the property that the parameters fitted will be values of the spline at a list of reference points. flexcurv is an easy-to-use version of frencurv, and generates reference splines with regularly-spaced knots, or with knots interpolated between the reference points. frencurv and flexcurv have the additional option of generating an incomplete basis of reference splines, which can be completed by the addition of the standard constant variable used in regression models. The splines are either given the names in the *newvarlist* (if present), or (more usually) generated as a list of numbered variables, prefixed by the generate() option. Usually (but not always), the regression command is called using the noconst option.

## Options for use with bspline and frencurv

xvar(varname) specifies the X-variable on which the splines are based.

- knots(numlist) specifies a list of at least 2 knots, on which the splines are based. If knots() is absent, then bspline
  will initialize the list to the minimum and maximum of the xvar() variable, and frencurv will create a list
  of knots equal to the reference points (in the case of odd-degree splines such as a linear, cubic or quintic) or
  midpoints between reference points (in the case of even-degree splines such as constant, quadratic or quartic).
  flexcurv does not have the knots() option, as it automatically generates a list of knots, containing the required
  number of knots "sensibly" spaced on the xvar() scale.
- noexknot specifies that the original knot list is not to be extended. If noexknot is not specified, then the knot list is extended on the left and right by a number of extra knots on each side specified by power(), spaced by the

distance between the first and last 2 original knots, respectively. flexcurv does not have the noexknot option, as it specifies the knots automatically.

- generate(*prefix*) specifies a prefix for the names of the generated splines, which (if there is no *newvarlist*) will be named as *prefix*1...*prefix*N, where N is the number of splines.
- type(*type*) specifies the storage type of the splines generated (float or double). If type() is given as anything else (or not given), then it is set to float.
- labfmt(format) specifies the format to be used in the variable labels for the generated splines. If absent, then it is set to the format of the xvar() variable.
- labprefix(string) specifies the prefix to be used in the variable labels for the generated splines. If absent, then it
  is set to "Spline at " for flexcurv and frencurv, and to "B-spline on " for bspline.

## Options for use with frencurv

- refpts(numlist) specifies a list of at least 2 reference points, with the property that, if the splines are used in a regression model, then the fitted parameters will be values of the spline at those points. If refpts() is absent, then the list is initialized to two points, equal to the minimum and maximum of the xvar() variable. If the omit() option is specified with flexcurv or frencurv, and the spline corresponding to the omitted reference point is replaced with a standard constant term in the regression model, then the fitted parameters will be relative values of the spline (differences or ratios), compared to the value of the spline at the omitted reference point.
- noexref specifies that the original reference list is not to be extended. If noexref is not specified, then the reference list is extended on the left and right by int(power/2) extra reference points on each side, where power is the value specified by power(), spaced by the distance between the first and last 2 original reference points, respectively. If noexref and noexknot are both specified, then the number of knots must be equal to the number of reference points plus power + 1. flexcurv does not have the noexref option, as it automatically chooses the knots and does not extend the reference points.
- omit(#) specifies a reference point, which must be present in the refpts() list (after any extension requested by frencurv), and whose corresponding reference spline will be omitted from the set of generated splines. If the user specifies omit(), then the set of generated splines will not be a complete basis of the set of splines with the specified power and knots, but can be completed by the addition of a constant variable, equal to 1 in all observations. If the user then uses the generated splines as predictor variables for a regression command, such as regress or glm, then the noconst option should usually not be used, and, if the omitted reference point is in the completeness region of the basis, then the intercept parameter \_cons will be the value of the spline at the omitted reference point, and the model parameters corresponding to the generated splines will be differences between the values of the spline at the corresponding reference points and the value of the spline at the omitted reference point. If omit() is not specified, then the generated splines form a complete basis of the set of splines with the specified power and knots. If the user then uses the generated splines as predictor variables for a regression command, such as regress or glm, then the noconst option should be used, and the fitted model parameters corresponding to the generated splines as predictor variables for a regression command, such as regress or glm, then the noconst option should be used, and the fitted model parameters corresponding to the generated splines will be the values of the spline at the corresponding reference points.
- base(#) is an alternative to omit() for use in Stata Versions 11 or higher. It specifies a reference point, which must be present in the refpts() list (after any extension requested by frencurv), and whose corresponding reference spline will be set to zero. If the user specifies base(), then the set of generated splines will not be a complete basis of the set of splines with the specified power and knots, but can be completed by the addition of a constant variable, equal to 1 in all observations. The generated splines can then be used in the design matrix by an estimation command in Stata Versions 11 or higher.

# Options for use with flexcurv only

Note that flexcurv uses all the options available to frencurv, except for knots(), noexknot, and noexref.

include(numlist) specifies a list of additional numbers to be included within the boundaries of the completeness region of the spline basis, in addition to the available values of the xvar() variable and the refpts() values (if provided). This allows the user to specify a non-default infimum and/or supremum for the completeness region of the spline basis. If include() is not provided, then the completeness region will extend from the minimum to the maximum of the values either available in the xvar() variable or specified in the refpts() list.

krule(knot\_rule) specifies a rule for generating knots, based on the reference points, which may be regular (the

default) or interpolate. If regular is specified, then the knots are spaced regularly over the completeness region of the spline. If interpolate is specified, then the knots are interpolated between the reference points, in a way that produces the same knots as krule(regular) if the reference points are regularly spaced. Whichever krule() option is specified, any extra knots to the left of the completeness region are regularly spaced with a spacing equal to that between the first 2 knots of the completeness region, and any extra knots to the right of the completeness region. Therefore, krule(regular) specifies that all knots will be regularly spaced, whether or not the reference points are regularly spaced, whereas krule(interpolate) specifies that the knots will be interpolated between the reference points in a way that will cause reference splines to be definable, even if the reference points are not regularly spaced.

# Remarks

The options described above appear complicated, but imply simple defaults for most users, especially if flexcurv is used. Advanced users and programmers are given the power to specify a comprehensive choice of non-default splines. The splines are either given the names in the *newvarlist* (if present), or (more usually) generated as a list of numbered variables, prefixed by the generate() option. (The *newvarlist* is intended mainly for programmers, and allows them to store the splines in temporary variables with temporary names.)

#### Saved results

bspline, frencurv and flexcurv save the following results in r():

Scalars r(xsup) r(nincomp) r(nspline)	upper bound of completeness region number of $X$ -values out of completeness region number of splines	r(xinf) r(nknot) r(power)	lower bound of completeness region number of knots power (or degree) of splines
Macros r(knots) r(labfmt) r(type)	final list of knots format used in spline variable labels storage type of splines (float or double)	r(splist) r(labprefix) r(xvar)	varlist of generated splines prefix used in spline variable labels X-variable specified by xvar() option
Matrices r(knotv)	row vector of knots		

frencurv and flexcurv save all of the above results in r(), and also the following:

Scalars r(omit)	omitted reference point specified by <b>omit()</b>	r(base)	base reference point specified by <b>base()</b>
Macros r(refpts)	final list of reference points		
Matrices r(refv)	row vector of reference points		

The result r(nincomp) is the number of values of the xvar() variable outside the completeness region of the space of splines defined by the reference splines or *B*-splines. The number lists r(knots) and r(refpts) are the final lists after any left and right extensions carried out by bspline, frencurv or flexcurv, and the vectors r(knotv) and r(refv) contain the same values in double precision (mainly for programmers). The scalars r(xinf)and r(xsup) are knots, such that the completeness region is  $r(xinf) \le x \le r(xsup)$  for positive-degree splines and  $r(xinf) \le x < r(xsup)$  for zero-degree splines.

In addition, bspline, frencurv and flexcurv save variable characteristics for the output spline basis variables. The characteristic varname[xvar] is set by bspline, frencurv and flexcurv to be equal to the input X-variable name set by xvar(). The characteristics varname[xinf] and varname[xsup] are set by bspline to be equal to the infimum and supremum, respectively, of the interval of X-values for which the B-spline is non-zero. The characteristic varname[xvalue] is set by frencurv and flexcurv to be equal to the reference point on the X-axis corresponding to the reference spline. The characteristic varname[basestat] is set by frencurv and flexcurv to be 1 if the reference point on the X-axis corresponding to the reference spline is equal to the base() option, and to be 0 otherwise.

## Methods and Formulas for *B*-splines

The principles and definitions of B-splines are given in de Boor (1978) and Ziegler (1969). Practical applications in chemistry are described in Wold (1971 and 1974). They are used in signal processing, and are associated with a wavelet transformation (Unser, Aldroubi and Eden, 1992).

Splines are a method of defining models regressing a scalar Y-variate with respect to a scalar X-variate. By definition, a kth degree spline is defined with reference to a set of q knots  $s_1 < s_2 < \ldots < s_q$ , dividing the X-axis into intervals of the form  $[s_i, s_{i+1})$ . In each of those intervals, the regression is a kth degree polynomial in X (usually a different one in each interval), but the polynomials in any two contiguous intervals have the same *j*th derivatives at the knot separating the two intervals, for *j* from zero to k - 1. By convention, the 0th derivative is the function itself, so a 0th degree spline is simply a right-continuous step function, and a first-degree spline is a simple linear interpolation of values between the knots. (By convention, the intervals  $[s_i, s_{i+1})$  are closed on the left and open on the right, but this convention only matters for splines of degree zero, which, by convention, are right-continuous rather than left-continuous.)

Splines can be defined using plus–functions. For a power k and a knot s, the kth power plus–function at s is defined as

$$P_k(x;s) = \begin{cases} (x-s)^k, & x \ge s, \\ 0, & x < s. \end{cases}$$
(1)

The plus-functions are a basis for the space of splines. That is to say, for any kth degree spline  $S(\cdot)$ , with knots  $s_1 < s_2 < \ldots < s_q$ , there exists a q-vector  $\alpha$  such that, for any x,

$$S(x) = \sum_{j=1}^{q} \alpha_j P_k(x; s_j).$$

$$\tag{2}$$

It might seem that, to fit a spline in a covariate X to a Y-variate, all we have to do is to define a design matrix U, such that  $U_{ij} = P_k(x_i; s_j)$ , and fit  $\beta$  as a vector of regression coefficients. This is not a good idea, for two reasons. First, there are problems with stability, as  $P_k(x; s)$  will be very large for k > 1 and x much greater than s. Second, the  $\beta$ -parameters estimated will not be easy to explain in words to a non-mathematician. The first problem was solved with the introduction of B-splines by I. J. Schoenberg in the 1960s, and these are calculated by **bspline**. The second problem is solved using **frencurv** and **flexcurv**, which call **bspline**, and then transform the B-splines, so that the regression parameters will simply be relative or absolute values of the spline at reference points.

The *B*-splines define an alternative basis of the splines with a given set of knots. Ziegler (1969) defines the *B*-spline for a set of k + 2 knots  $s_1 < s_2 < ... < s_{k+2}$  as

$$B(x; s_1, \dots, s_{k+2}) = (k+1) \sum_{j=1}^{k+2} \left[ \prod_{1 \le h \le k+2, h \ne j} (s_h - s_j) \right]^{-1} P_k(x; s_j).$$
(3)

The *B*-spline (3) is positive for x in the open interval  $(s_1, s_{k+2})$ , and zero for other x. If the  $s_j$  are part of an extended set of knots extending forwards to  $+\infty$  and backwards to  $-\infty$ , then the set of *B*-splines based on sets of k+2 consecutive knots forms a basis of the set of all *k*th-degree splines defined on the full set of knots. Figure 1 shows the constant, linear, quadratic and cubic *B*-splines originating at zero and corresponding to unit knots.

For the purposes of **bspline** and **frencurv**, I have taken the liberty of redefining *B*-splines by scaling the  $B(x; s_1, \ldots, s_{k+2})$  of (3) by a factor equal to the mean distance between two consecutive knots, to arrive at the scale-invariant *B*-spline

$$A(x; s_1, \dots, s_{k+2}) = \frac{s_{k+2} - s_1}{k+1} B(x; s_1, \dots, s_{k+2}) = \begin{cases} \sum_{j=1}^{k+1} \prod_{h=1}^{k+2} \phi_{jh}(x), & \text{if } s_1 \le x < s_{k+2}, \\ 0, & \text{otherwise,} \end{cases}$$

where the functions  $\phi_{jh}(\cdot)$  are defined by

$$\phi_{jh}(x) = \begin{cases} 1, & \text{if } h = j, \\ (s_{k+2} - s_1)/(s_h - s_j), & \text{if } h = j+1, \\ P_1(x; s_j)/(s_h - s_j), & \text{otherwise.} \end{cases}$$
(4)

The scaled *B*-spline  $A(x; s_1, \ldots, s_{k+2})$  has the advantage that it is dimensionless, being a sum of products of the dimensionless quantities  $\phi_{hj}(x)$ . That is to say, it is unaffected by the scale of units of the *X*-axis, and therefore has the same values, whether *x* is time in millennia or time in nanoseconds. The original Ziegler *B*-spline  $B(x; s_1, \ldots, s_{k+2})$  is expressed in units of  $x^{-1}$ . Therefore, if the scaled *B*-spline  $A(x; s_1, \ldots, s_{k+2})$  appears in a design matrix, then its regression coefficient is expressed in units of the *Y*-variate, whereas, if the original *B*-spline  $B(x; s_1, \ldots, s_{k+2})$  appears

in a design matrix, then its regression coefficient is expressed in Y-units multiplied by X-units, and will be difficult to interpret, even for a mathematician. The B-splines computed by **bspline** are therefore the  $A(x; s_1, \ldots, s_{k+2})$ , and users who prefer the original Ziegler B-splines must scale them by  $(k+1)/(s_{k+2}-s_1)$ . (This factor happens to be one for splines with unit-spaced knots, such as those in Figure 1.)

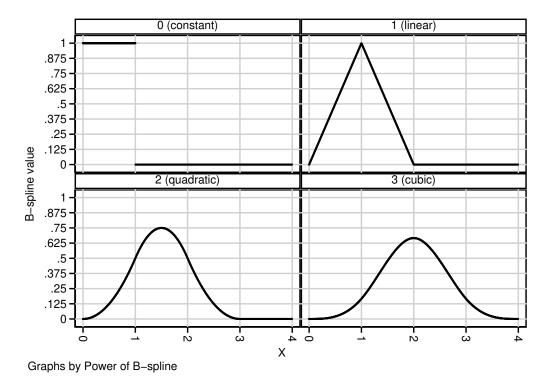


Figure 1. B-splines originating at zero with unit knots.

Given n data points, a Y-variate, an X-covariate, and a set of q + k + 1 consecutive knots  $s_h < \ldots < s_{h+q} < \ldots < s_{h+q+k}$ , we can regress the Y-variate with respect to a kth degree spline in X by defining a design matrix V, with one row for each of the n data points and one column for each of the first q knots, such that

$$V_{ij} = A(x_i; s_{h+j-1}, \dots, s_{h+j+k}).$$
(5)

We can then regress the Y-variate with respect to the design matrix V, and compute a vector  $\beta$  of regression coefficients, such that  $V\beta$  is the fitted spline. The parameter  $\beta_j$  measures the contribution to the fitted spline of the B-spline originating at the knot  $s_{h+j-1}$  and terminating at the knot  $s_{h+j+k}$ . There will be no stability problems such as we are likely to have with the original plus-function basis, as each B-spline is bounded, and localized in its effect.

It is important to define enough knots. If the sequence of knots  $\{s_j\}$  extends to  $+\infty$  on the right and to  $-\infty$  on the left, then the kth degree B-splines  $A(\cdot; s_{h+j-1}, \ldots, s_{h+j+k})$  on sets of k+2 consecutive knots are a basis for the full space of kth degree splines on the full set of knots. If  $S(\cdot)$  is one of these splines, and  $[s_j, s_{j+1})$  is an interval between consecutive knots, then the values of S(x) in the interval are affected by the k+1 B-splines originating at the knots  $s_{j-k}, \ldots, s_j$  and terminating at the knots  $s_{j+1}, \ldots, s_{j+k+1}$ . It follows that, if we start by specifying a sequence of knots  $s_0 < \ldots < s_m$ , and we want to fit a spline for values of x in the interval  $[s_0, s_m)$ , then we must also use k extra knots  $s_{-k} < \ldots < s_{-1}$  to the left of  $s_0$ , and k extra knots  $s_{m+1} < \ldots < s_{m+k}$  to the right of  $s_m$ , to define the m + k consecutive B-splines affecting S(x) for x in the interval  $[s_0, s_m)$ . These m + k B-splines originate at the knots  $s_{-k}, \ldots, s_{m-1}$ , and terminate at the knots  $s_1, \ldots, s_{m+k}$ , respectively. Any spline  $S(\cdot)$ , in the full space of kth degree splines defined using the full set of knots, is equal to a linear combination of these m + k B-splines in the interval  $[s_0, s_m]$  (in the case of positive-degree splines, which are continuous) or  $[s_0, s_m)$  (in the case of zero-degree splines, which are only right-continuous). We will refer to this interval as the *completeness region* for splines which are linear combinations of these m + k B-splines which are linear combinations of these m + k B-splines. These linear combinations are zero for  $x < s_{-k}$  and  $x \ge s_{m+k}$ , and "incomplete" in the outer regions  $(s_{-k}, s_0)$  and  $(s_m, s_{m+k})$ , in which the spline is "returning to zero".

bspline and frencurv assume, in default, that the knots() option specified by the user is only intended to span the completeness region, and that the specified knots correspond to the  $s_0, \ldots, s_m$ . (flexcurv has no knots()

option, as it defines its own "sensibly-spaced" knots, which are then input to **frencurv**.) In default, **bspline** and **frencurv** generate k extra knots on the left, with spacing equal to the difference between the first two knots, and k extra knots on the right, with spacing equal to the difference between the last two knots. If the user specifies the option **noexknot**, then **bspline** assumes that the user has specified the full set of knots, corresponding to  $s_{-k}, \ldots, s_{m+k}$ , and does not generate any new knots. This allows users to specify their own spacing for the outer knots if they wish, but makes the specification of knots() simpler in the default case, because users do not have to count the extra outer knots for themselves.

### Methods and formulas for reference splines

The *B*-spline regression parameters are expressed in units of the *Y*-variable, but they are not easy to interpret. If we have calculated the  $n \times q$  matrix *V* of *B*-splines as in (5), and we also have a set of *q* reference *X*-values  $r_1 < r_2 < \ldots < r_q$ , then we might prefer to re-parameterize the spline by its values at the  $r_j$ . To do this, we first calculate a  $q \times q$  square matrix *W*, defined such that

$$W_{ij} = A(r_i; s_{h+j-1}, \dots, s_{h+j+k}), \tag{6}$$

the value of the *j*th *B*-spline at the *i*th reference point. If  $\beta$  is the (column) *q*-vector of regression coefficients with respect to the *B*-splines in *V*, and  $\gamma$  is the (column) *q*-vector of values of the spline at the reference points, then

$$\gamma = W\beta. \tag{7}$$

If W is invertible, then the n-vector of values of the fitted spline at the data points is

$$V\beta = VW^{-1}W\beta = VW^{-1}\gamma = Z\gamma,\tag{8}$$

where  $Z = VW^{-1}$  is a transformed  $n \times q$  design matrix, whose columns contain values of a set of reference splines, for the estimation of the reference-point spline values  $\gamma$ .

The choice of reference points is open to the user, and constrained mainly by the requirement that the matrix W is invertible. This implies that each of the q B-splines must be positive for at least one of the q reference values, and that each reference value must have at least one positive B-spline value. A natural choice of reference values might be one in the mid-range of each B-spline, possibly the central knot for an odd-degree B-spline (such as a linear, cubic or quintic), or the mid-point between the two central knots for an even-degree B-spline (such as a constant, quadratic or quartic). This choice has the consequence that, for a spline of degree k, there will be int(k/2) reference points outside the spline's completeness region on the left, and another int(k/2) reference points outside the spline on the right, where  $int(\cdot)$  is the truncation (or "integer-part") function. The parameters corresponding to these "extra" reference points will not be easy to explain to non-mathematicians, as they describe the behaviour of the spline as it returns to zero outside its completeness region. However, for a quadratic or cubic spline, there is only one such external reference Y-value at each end of the completeness region.

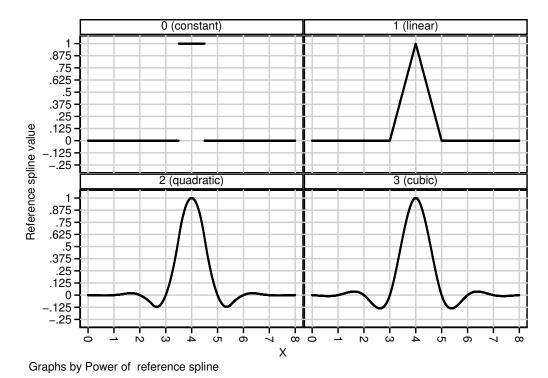
By default (if the user provides no knots() option), frencurv starts with the reference points originally provided (which default to the minimum and maximum of the xvar() variable if no refpts() option is provided), and chooses knots "appropriately". For an odd-degree spline (power() odd), the knots are initialized to the original reference points themselves. For an even-degree spline (power() even), the knots are initialized to mid-points corresponding to the original reference points. That is to say, if there are m original reference points  $r_1 < \ldots < r_m$ , and power() is even, then the original knots  $s_0 < \ldots < s_m$  are initialized to

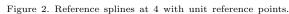
$$s_j = \begin{cases} r_1 - (r_2 - r_1)/2, & \text{if } j = 0, \\ (r_j + r_{j+1})/2, & \text{if } 1 \le j \le m - 1, \\ r_m + (r_m - r_{m-1})/2, & \text{if } j = m. \end{cases}$$
(9)

frencurv assumes, by default, that the reference points initially provided are all in the completeness region, and adds int(k/2) extra reference points to the left, spaced by the difference between the first two original reference points, and int(k/2) extra reference points to the right, spaced by the difference between the last two original reference points, where k is specified by the power() option. If noexref is specified, then the original refpts() list is assumed to be the complete list, and it is the user's responsibility to choose sensible ones. In either case, the original knots are extended on the left and right as described above, unless noexknot is specified. (These rules seem complicated, but lead to sensible defaults if the naive user specifies a list of reference points and naively expects

them to be in the completeness region of the spline, while preserving the ability of advanced users to specify exactly what they want at their own risk.)

Figure 2 shows the constant, linear, quadratic and cubic reference splines corresponding to a reference point at 4, assuming unit reference points and default knots (equal to reference points for odd degree and inter-reference midpoints for even degree). Note that each spline is one at its own reference point, and zero at all other reference points. (This is always the case for a basis of reference splines, at least for reference splines corresponding to reference points in the completeness region of the basis.) The reference splines are similar to (but not the same as) the B-spline wavelets of Unser *et al.* (1992).





flexcurv uses an alternative method to define knots from reference points, which guarantees that the reference points, the values of the X-variable specified by xvar(), and (optionally) a list of other X-values specified by the include() option will be in the completeness region of the generated spline basis. It also guarantees that the knots will be "sensibly" spaced, using a definition of sensibility specified by the krule() option. Suppose that there are q reference points  $r_1, \ldots, r_q$  provided by the user in the refpts() option. flexcurv first calculates the numbers  $x_{inf}$  and  $x_{sup}$  as the minimum and maximum, respectively, of all values present in the xvar() variable, the refpts() list or the include() list. The numbers  $x_{inf}$  and  $x_{sup}$  will be the infimum and the supremum, respectively, of the completeness region of the spline basis. The number of intervals between adjacent knots in and bordering the completeness region are  $s_0, \ldots, s_m$ .

If the user specifies krule(regular) (the default), then these  $s_j$  are spaced regularly, and defined by the simple formula

$$s_j = \frac{j}{m} x_{\sup} + \frac{m-j}{m} x_{\inf}.$$
 (10)

If the user specifies krule(interpolate), then these  $s_j$  are interpolated between the reference points, using a more complicated formula. If the spline power k is 0, we define  $s_0 = x_{inf}$ ,  $s_m = x_{sup}$ , and  $s_j = r_{j+1}$  for other j. Otherwise, we first define, for each j from 0 to m,

$$\sigma(j) = 1 + j(q-1)/m, \quad \pi(j) = \inf[\sigma(j)], \quad \rho(j) = \sigma(j) - \pi(j).$$
(11)

We then define the  $s_i$  as

$$s_{j} = \begin{cases} x_{\inf}, & j = 0, \\ x_{\sup}, & j = m, \\ [1 - \rho(j)] r_{\pi(j)} + \rho(j) r_{\pi(j)+1}, & \text{otherwise.} \end{cases}$$
(12)

\_\_\_\_\_

This formula ensures that the knots  $s_j$  are interpolated between the reference points in a way which will be regularly spaced, if the reference points themselves are regularly spaced from  $r_1 = x_{inf}$  to  $r_q = x_{sup}$ . However, if the reference points are not regularly spaced, then the user can specify krule(interpolate) to ensure that the reference splines will still be definable, which may possibly not be the case if the user specifies krule(regular) with irregularly-spaced reference points.

flexcurv then calls frencurv to generate the reference splines, with the reference points  $r_1, \ldots, r_q$  as the refpts() option, and the knots  $s_0, \ldots, s_m$  as the knots() option, with the noexref option but without the noexknot option. This implies that, whichever krule() option is specified, any extra knots to the left of the completeness region will be regularly spaced by the distance between the first 2 internal knots, and any extra knots to the right of the completeness region will be regularly spaced by the distance between the last 2 internal knots. Therefore, krule(regular) specifies that the knots inside and outside the completeness region are regularly spaced, so that any pair of adjacent knots inside or outside the completeness region is separated by  $(x_{sup} - x_{inf})/m$  X-axis units. Both krule() options result in the generation of a basis of q reference splines, corresponding to the respective reference points, with a completeness region  $x_{inf} \leq x \leq x_{sup}$  (for positive-degree splines) or  $x_{inf} \leq x < x_{sup}$  (for zero-degree splines). Note that, in the case of zero-degree splines, the user must specify  $x_{sup}$  in the include() option, as a number strictly greater than any reference points and xvar() values, because  $x_{sup}$  is outside the completeness region for a zero-degree spline, which is a right-continuous step function with discontinuities at its knots, which include  $x_{sup}$ .

If the user specifies one of the reference points as the omit() option for flexcurv or frencurv, then the corresponding reference spline is dropped, and the basis will be incomplete. If the omitted reference point is in the completeness region, then this incomplete basis can be completed by including a constant variable, equal to 1 in all observations. This is because, within the completeness region of the reference spline basis, a constant variable is equal to a linear combination of the reference splines, with all coordinates equal to the constant. Therefore, if we drop a reference spline corresponding to a reference point in the completeness region, and substitute a variable equal to 1 throughout the completeness region, then the resulting list of variables will be a basis of the same spline space, with the same completeness region. However, if we then use this new basis as the design matrix in a regression model, then the parameter corresponding to the constant variable will be the value of the spline at the omitted reference point, and the other parameters, corresponding to the remaining reference points, will be the differences between the values of the spline at these remaining reference points and the value of the spline at the omitted reference point. Therefore, if the user uses flexcurv or frencurv to generate a spline basis for input to a regression model, then the noconst option should be used if no omit() option is specified, but not if an omit() option is specified. In this respect, the basis (or incomplete basis) of reference splines generated by flexcurv or frencurv is a continuous version of a single-factor basis (or incomplete basis) of indicator functions generated by xi with (or without) the noomit option.

In Stata Versions 11 or higher, the user may use the base() option for flexcurv or frencurv, instead of the omit() option, to specify a reference point whose corresponding reference spline is set to zero. The reference spline basis will then be an incomplete "super-basis", augmented by a zero vector, and can be completed similarly by adding a unit vector. This allows the user to use the "super-basis" in the design matrix of a regression model, fitted by a Stata Version 11 estimation command, with an omitted parameter corresponding to the base reference spline.

## Example

In the auto data, we can use flexcurv and regress (with the noconst option) to fit a cubic spline for miles per gallon with respect to weight (in US pounds):

. describe cs*		t) refpts(17 display format	760(770)4840 value label	<pre>)) gen(cs) power(3) variable label</pre>			
cs1 cs2 cs3 cs4 cs5 . regress mpg	float float float float float float	%8.4f %8.4f %8.4f %8.4f %8.4f		Spline at 1,760 Spline at 2,530 Spline at 3,300 Spline at 4,070 Spline at 4,840			
Linear regress	sion			Number of F( 5, Prob > F R-squared Root MSE	69) 1	= = =	0.0000 0.9780

mpg	Coef.	Robust Std. Err.	t	P> t	[95% Conf.	Interval]
cs1	30.83764	1.79533	17.18	0.000	$\begin{array}{c} 27.25606\\ 22.03479\\ 17.70541\\ 14.20634\\ 10.77484\end{array}$	34.41923
cs2	23.56232	.7657011	30.77	0.000		25.08985
cs3	18.79659	.546976	34.36	0.000		19.88778
cs4	15.95229	.8751852	18.23	0.000		17.69824
cs5	12.15876	.6937123	17.53	0.000		13.54268

We have chosen the reference points (arbitrarily) to be equally spaced from the minimum of weight (1,760 pounds) to the maximum of weight (4,840 pounds). flexcurv ensures that the spline is complete in the interval of X-values spanned by the original reference points provided by the user. The describe command lists the reference splines, with their variable labels. The coefficients fitted by regress (with the noconst option) are simply the fitted values of mpg at the reference points. Figure 3 shows observed and fitted values of mpg, plotted against weight. The fitted curve is calculated using predict (see [R] predict), and is interpolated cubically between the reference points.

The flexcurv parameterization allows us to use lincom to calculate confidence intervals for differences (or other contrasts) between the values of the spline at different reference points. Here, we estimate the difference between expected mileage at weights of 3,300 and 4,840 pounds:

. lincom cs3-cs ( 1) cs3 - cs						
mpg	Coef.	Std. Err.	t	P> t	[95% Conf.	Interval]
(1)	6.637834	.7610751	8.72	0.000	5.119531	8.156137

We see that cars weighing 3,300 pounds are expected to travel 5.12 to 8.16 more miles per gallon than cars weighing 4,070 pounds.

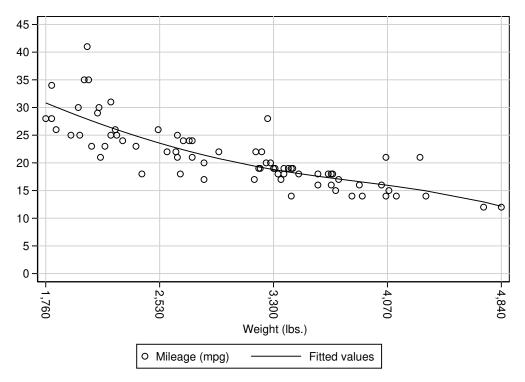


Figure 3. Mileage plotted against weight (points) with fitted cubic spline (line).

Alternatively, we might want to choose the lowest reference point (1,760) as the base level of weight, and estimate the difference in mileage between the other reference points and the base level. To do this, we use flexcurv with the omit() option, followed by regress without the noconst option. This time, only splines for reference points other than 1,760 pounds are generated. The regression model contains a parameter \_cons, equal to the expected

mileage for cars with the base weight of 1,760 US pounds. The other parameters are differences in mean mileage between cars with weights equal to the non-base reference weights and cars with weights equal to the base reference weight.

. flexcurv, xvar(weight) refpts(1760(770)4840) omit(1760) gen(ics) power(3) . describe ics*								
variable name	storage type				variable	label		
ics2 ics3 ics4 ics5 . regress mpg Linear regress		%8.4f			Spline a Spline a Spline a Spline a	t 3,300 t 4,070 t 4,840 Number of obs	= 42.19 = 0.0000 = 0.6754	
mpg	Co		obust d. Err.	tt	P> t	[95% Conf.	Interval]	
ics2 ics3 ics4 ics5 _cons		104 1. 534 2. 789 1.	000318 853056 069253 937786 795329	-3.64 -6.50 -7.19 -9.64 17.18	0.000 0.000	-11.26584 -15.73779 -19.01339 -22.54468 27.25606	-3.284787 -8.344299 -10.75729 -14.81312 34.41923	

Alternatively, we might want to fit the same model, with reference points equal to the knots of the spline in and around the completeness region of the spline, which are 1,760, 3,300 and 4,840 US pounds. This can be done using **frencurv**, which generates two extra reference points, equal to knots outside the completeness region. The variable labels of the reference splines at these reference points contain an indication that these reference points are outside the completeness region. The **regress** command is used with the **noconst** option, and estimates parameters for all the reference points, including the reference points outside the completeness region. These parameters are not easy to explain to non-mathematicians, and one of them even represents a negative mileage. However, in some applications, such as seasonal time series, the knots (or the between-knot midpoints) are typically placed where sudden change is likely to occur, and it might therefore be considered especially interesting to know the value of the spline at these knots (or midpoints).

. frencurv, xvar(weight) refpts(1760 3300 4840) gen(kcs) power(3)

variable name	storage	display format	value label	variabl	e label	
kcs1 float %8.4f kcs2 float %8.4f kcs3 float %8.4f kcs4 float %8.4f kcs5 float %8.4f . regress mpg kcs*, robust noconst Linear regression					at 220 (INCOMPL at 1,760 at 3,300 at 4,840 at 6,380 (INCOM Number of obs F( 5, 69) Prob > F R-squared Root MSE	PLETE) = 74 = 751.86 = 0.0000
mpg	Coe	Robu f. Std.		t P> t	[95% Conf.	Interval]
kcs1 kcs2 kcs3 kcs4 kcs5	18.796	64 1.79 59 .546 76 .6937	53317.97634.12217.	18 0.000 36 0.000 53 0.000	27.25606 17.70541 10.77484	

It is also possible to specify the omit() option with frencurv. If we add the options omit(1760) gen(ikcs) to the previous example, and use regress without the noconst option, then the parameter \_cons is the mileage at a weight of 1,760 US pounds, the parameters ikcs3 and ikcs4 are the differences between the mileages at 3,300 and 4,840 US pounds respectively, and the parameters ikcs1 and ikcs5 represent the behavior of the spline as it converges to zero outside its completeness region. (Note that the omitted reference point must be inside the completeness region for this interpretation to apply. frencurv issues a warning if the reference point specified by omit() is outside the completeness region.)

. frencurv, xvar(weight) refpts(1760 3300 4840) omit(1760) gen(ikcs) power(3) . describe ikcs*								
variable name	storage dis type for	play val mat lab		variable	label			
ikcs1 ikcs3 ikcs4 ikcs5 . regress mpg Linear regress		4f 4f 4f		Spline a Spline a		PLETE) = 74 = 42.19 = 0.0000		
mpg	Coef.	Robust Std. Err.	t	P> t	[95% Conf.	Interval]		
ikcs1 ikcs3 ikcs4 ikcs5 _cons	-18.6789	$\begin{array}{c} 12.47861 \\ 1.853056 \\ 1.937786 \\ 11.34446 \\ 1.795329 \end{array}$	1.07 -6.50 -9.64 -2.31 17.18	0.000 0.024	-11.5474 -15.73779 -22.54468 -48.83264 27.25606	38.24089 -8.344299 -14.81312 -3.569498 34.41923		

Finally, for the most technical people, we can fit the same model yet again, using **bspline** instead of **frencurv**. Here, the splines are B-splines rather than reference splines. The variable labels show the interval with positive values of each B-spline, delimited by knots, including the extra knots calculated by **bspline**. The parameters are expressed in miles per gallon, but none of them are easy for non-mathematicians to interpret.

. bspline,xvar . describe bs*	< _	knots(1760	3300 4840)	gen(bs) p	oower(3)		
variable name	storage type	display format	value label	variable	e label		
bs1 bs2 bs3 bs4 bs5 . regress mpg Linear regress		%8.4f %8.4f %8.4f %8.4f		B-spline B-spline B-spline	e on [-2,860,3, e on [-1,320,4, e on [220,6,380 e on [1,760,7,9 e on [3,300,9,4 Number of obs F( 5, 69) Prob > F R-squared Root MSE	840) ) 20) 60) = 74 = 751.86 = 0.0000 = 0.9780	
 mpg	Coe	Robus ef. Std. E		P> t	[95% Conf.	Interval]	
bs1   bs2   bs3   bs4   bs5	51.279 29.152 17.139 15.089 -4.5258	2914.49425222.87955794.9585	33     6.4       49     5.9       62     3.0	$\begin{array}{ccc} 9 & 0.000 \\ 5 & 0.000 \\ 4 & 0.003 \end{array}$	5.193726	93.75957 38.11866 22.87976 24.97785 32.13608	

# Technical note

There are other programs in Stata to generate splines. mkspline (see [R] mkspline) generates a basis of linear

splines to be used in a design matrix, as does frencurv, power(1), but the basis is slightly different, because the fitted parameters for frencurv are reference values, whereas the fitted parameters for mkspline are the local slopes of the spline in the inter-knot intervals. Patrick Royston and Gareth Ambler's splinegen (Royston and Sauerbrei, 2007), William Dupont's rc\_spline (downloadable from SSC), and Peter Sasieni's spline and spbase (Sasieni, 1994), from STB-22, are used for fitting the so-called "natural" cubic spline, which is constrained to be linear outside its completeness region, and is parameterized using the natural spline basis. (For more information about natural cubic splines, see Durrlemain and Simon, 1999, and/or Harrell, 2001.) The splines fitted using bspline, frencurv or flexcurv, on the other hand, are unconstrained, and parameterized using the *B*-spline or reference spline basis.

## Historical note

This document is a post–publication update of an article which appeared in the Stata Technical Bulletin (STB) as Newson (2000). A similar article, also updating the principles of reference splines, is Newson (2012).

## Acknowledgements

The idea for the name **frencurv** came from Nicholas J. Cox of Durham University, UK, who remarked that the method was like an updated French curve when I described it on Statalist.

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