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npregress series — Nonparametric series regression

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Description

npregress series performs nonparametric series estimation using a B-spline, piecewise polynomial spline, or polynomial basis. Like linear regression, nonparametric regression models the mean of the outcome conditional on the covariates, but unlike linear regression, it makes no assumptions about the functional form of the relationship between the outcome and the covariates. npregress series may be used to model the mean of a continuous, count, or binary outcome.

Quick start

Nonparametric regression of y on x and discrete covariate a using the default B-spline basis npregress series y x i.a

Same as above, but use a polynomial basis

npregress series y x i.a, polynomial

Same as above, but use a piecewise polynomial spline basis npregress series y x i.a, spline

Same as above, but use AIC to find the optimal basis function npregress series y x i.a, criterion(aic) spline

Interpolate using three knots

npregress series y x i.a, knots(3)

Specify values of knots in matrix K

npregress series y x i.a, knotsmat(K)

Menu

Statistics > Nonparametric analysis > Nonparametric series regression

Syntax

```
npregress series depvar\ indepvars_{
m series}\ \left[\it{if}\ \right]\ \left[\it{in}\ \right]\ \left[\it{weight}\ \right]\ \left[\it{,\ options}\ \right]
```

indepvars_{series} is the list of independent variables for which a basis function will be formed.

nird-order B-spline basis; the default B-spline basis of order # nird-order piecewise polynomial spline basis iecewise polynomial spline basis of order # olynomial basis olynomial basis of order # varlist in model as specified; do not use in basis iesvarlist in basis without interactions in to use; crittype may be cv, gcv, aic, bic, or mallows iecewise polynomial spline or B-spline basis function # knots ots in matrix matname for piecewise polynomial spline -spline estimation um number of distinct values allowed in continuous
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knots tots in matrix matname for piecewise polynomial spline spline estimation
knots ots in matrix <i>matname</i> for piecewise polynomial spline -spline estimation
-spline estimation
m number of distinct values allowed in continuous
riates; default is distinct(10)
ements of piecewise polynomial spline or B-spline basis ion using <i>stub</i>
escaled values of covariates using stub
may be robust, ols, or <u>boot</u> strap
fidence level; default is level(95)
auxiliary regression coefficients
columns and column formats, row spacing, line width, ay of omitted variables and base and empty cells, and r-variable labeling
the maximization process
legend instead of statistics
1

Weights are not allowed with the bootstrap prefix; see [R] bootstrap.

fweights and iweights are allowed; see [U] 11.1.6 weight.

coeflegend does not appear in the dialog box.

See [U] 20 Estimation and postestimation commands for more capabilities of estimation commands.

Options

Model

- bspline specifies that a third-order B-spline be selected. It is the default basis.
- bspline(#) specifies that a B-spline of order # be used as the basis. The order may be 1, 2, or 3. spline specifies that a third-order piecewise polynomial spline be selected as the basis.
- spline (#) specifies that a piecewise polynomial spline of order # be used as the basis. The order may be 1, 2, or 3.
- polynomial specifies that a polynomial be selected as the basis.
- polynomial(#) specifies that a polynomial of order # be used as the basis. The order may be an integer between 1 and 16.
- asis(varlist) specifies that variables in varlist be included as independent variables in the model without any transformation. No B-spline, piecewise polynomial spline, or polynomial basis function will be formed from these variables. Variables in varlist may not be specified in indepvars_{series}.
- nointeract(seriesvarlist) specifies that the terms in the basis function formed from variables in seriesvarlist not be interacted with the terms of the basis function formed from other variables in indepvars_{series}. Covariates specified in seriesvarlist must be in indepvars_{series}.
- criterion(crittype) specifies that crittype be used to select the optimal number of terms in the basis function. crittype may be one of the following: cv (cross-validation), gcv (generalized cross-validation), aic (Akaike's information criterion), bic (Schwarz's Bayesian information criterion), or mallows (Mallows's C_p). The default is criterion(cv).
- knots(#) specifies that a piecewise polynomial spline or B-spline basis function with # knots be used. The minimum number of knots must be an integer greater than or equal to 1. The maximum number of knots is either 4,096 or two-thirds of the sample size, whichever is smaller.
- knotsmat(matname) specifies that the knots for each continuous covariate be the values in each row of matname. The number of knots should be the same for each covariate, and there must be as many rows as there are continuous covariates. If rows of matname are not labeled with varnames, then rows are assumed to be in the order of indepvars_{series}.
- distinct(#) specifies the minimum number of distinct values allowed in continuous variables. By default, continuous variables that enter the basis through either *indepvars*_{series} or *seriesvarlist* are required to have at least 10 distinct values. Continuous variables with few distinct values provide little information for determining an appropriate basis function and may produce unreliable estimates.
- basis(stub [, replace]) specifies that the elements of the basis function generated by npregress series be stored with the specified names.
 - The option argument *stub* is the prefix used to generate enumerated variables for each element of the basis.
 - When replace is used, existing variables named with *stub* are replaced by those from the new computation.
- $rescale(stub\ [$, $replace\])$ specifies that the rescaled covariates used to generate the basis function be stored with the specified names.
 - The option argument *stub* is the prefix used to generate enumerated variable names for the covariates.
 - When replace is used, existing covariates named with *stub* are replaced by those from the new computation.

SF

vce(*vcetype*) specifies the type of standard error reported, which includes types that are robust to some kinds of misspecification (robust), that assume homoskedasticity (ols), and that use bootstrap methods (bootstrap); see [R] *vce_option*.

Reporting

level(#); see [R] Estimation options.

aequations specifies that the auxiliary regression coefficients be reported. By default, only the average marginal effects of the covariates on the outcome are reported.

display_options: noci, nopvalues, noomitted, vsquish, noemptycells, baselevels, allbaselevels, nofvlabel, fvwrap(#), fvwrapon(style), cformat(%fmt), pformat(%fmt), sformat(%fmt), and nolstretch; see [R] Estimation options.

[Maximization]

maximize_options: <u>iter</u>ate(#), [no]log, <u>tol</u>erance(#); see [R] Maximize. These options are seldom used

The following option is available with npregress series but is not shown in the dialog box: coeflegend; see [R] Estimation options.

Remarks and examples

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This entry assumes that you are already familiar with nonparametric regression. Below, we discuss nonparametric series estimation; see [R] **npregress intro** for an overview of nonparametric regression and the models fit by npregress series and npregress kernel.

Remarks are presented under the following headings:

Overview
Estimation and effects

Overview

npregress series implements nonparametric series estimation using a B-spline, piecewise polynomial spline, or polynomial basis. The covariates may be continuous or discrete. npregress series allows you to estimate covariate effects and other counterfactuals related to the unknown mean function after estimation.

The word "nonparametric" refers to the fact that the parameter of interest—the mean as a function of the covariates—is given by the unknown function $g(\mathbf{x}_i)$, which is an element of an infinite-dimensional space of functions. In contrast, in a parametric model, the mean for a given value of the covariates, $E(y_i|\mathbf{x}_i) = f(\mathbf{x}_i, \boldsymbol{\beta})$, is a known function that is fully characterized by the parameter of interest, $\boldsymbol{\beta}$, which is a finite-dimensional real vector (Shao 2003).

The nonparametric regression model of outcome y_i given the k-dimensional vector of covariates \mathbf{x}_i is given by

$$y_i = g\left(\mathbf{x}_i\right) + \varepsilon_i \tag{1}$$

$$E\left(\varepsilon_{i}|\mathbf{x}_{i}\right) = 0\tag{2}$$

where ε_i is the error term. Equations (1) and (2) imply that

$$E\left(y_i|\mathbf{x}_i\right) = g\left(\mathbf{x}_i\right)$$

Once we account for the information in the covariates, the error term provides no information about the mean of our outcome. The conditional mean function is therefore given by $g(\mathbf{x}_i)$.

The mean estimate we obtain using nonparametric series estimation has the same form of the mean function estimate we obtain using linear regression. The regressors, however, are not variables in the data but functions of the variables. An example would be a kth-order polynomial. Suppose we have one covariate. The elements of the polynomial in this case would be $(x_i, x_i^2, \ldots, x_i^k)$. If we define \mathbf{z}_i as a vector with elements $(x_i, x_i^2, \ldots, x_i^k)$, we may write the estimate of the mean function as

$$\mathbf{z}_i' \hat{\boldsymbol{\beta}}$$

where $\widehat{\beta}$ has the form of an ordinary least-squares estimate.

npregress series allows us to specify other functional forms for \mathbf{z}_i depending on the basis we select: B-spline, piecewise polynomial spline, or polynomial. See *Methods and formulas* for the formulas for each basis.

Although the estimate of the mean function has the form of a linear regression, the individual coefficients are not easily interpretable. For instance, in our kth-order polynomial example, if x_i is continuous, the marginal effect of x_i is not a single coefficient but rather is a function of k elements of β and the covariate x_i .

In the example above, we had only one covariate, x_i . If we have more than one covariate, we approximate the mean function by using interactions of the terms in the basis function for each covariate. For instance, a polynomial of x_i and w_i would have terms $(x_i, w_i, x_i w_i, x_i^2, w_i^2, \dots, w_i^k x_i^k)$. As the number of covariates increases, the number of terms in the basis function increases exponentially. This is referred to in the literature as the curse of dimensionality.

npregress series allows us to reduce the dimensionality by using the nointeract() option to request that some covariates not be interacted with others. For the example above, this is equivalent to specifying a model of the form

$$y_i = g_1(x_i) + g_2(w_i) + \varepsilon_i \tag{3}$$

In (3), $g_1(x_i)$ and $g_2(w_i)$ are unknown functions, but there are no interactions between x_i and w_i . This ameliorates the curse of dimensionality but imposes more structure to the model.

You may also want to reduce the curse of dimensionality by requesting a parametric component, by using the asis() option, to fit models like this:

$$y_i = g(x_i) + w_i \beta + \varepsilon_i \tag{4}$$

In (4), $g(x_i)$ is unknown but we assume that w_i enters the model linearly.

As mentioned above, the regression coefficients are not easily interpretable. We can, however, estimate marginal effects, as reported in the npregress series output, and use margins to answer specific questions about the effects of covariates on the conditional mean, $g(\mathbf{x}_i)$. We demonstrate this in the examples below.

For detailed introductions to series estimators and the methods implemented by npregress series, see de Boor (2001), Schumaker (2007), Eubank (1999), Schoenberg (1969), Newey (1997), and Chen (2007).

Estimation and effects

Example 1: Nonparametric series regression estimation

dui.dta contains information about the number of monthly drunk driving citations in a local jurisdiction (citations). Suppose we want to know the effect of increasing fines on the number of citations. Because citations is a count variable, we could consider fitting the model with poisson or nbreg. However, both of these estimators make assumptions about the distribution of the data. If these assumptions are not true, we will obtain inconsistent estimates.

By using npregress series, we do not have to make any assumptions about how citations is distributed. We use npregress series to estimate the average marginal effect of drunk driving penalties (fines) on citations.

. use https://www.stata-press.com/data/r18/dui (Fictional data on monthly drunk driving citations)

. npregress series citations fines

Computing approximating function

Minimizing cross-validation criterion

Iteration 0: Cross-validation criterion = 55.15697
Iteration 1: Cross-validation criterion = 55.11413

Computing average derivatives

Cubic B-spline estimation Number of obs = 500 Criterion: cross-validation Number of knots = 3

citations	Effect	Robust std. err.	z	P> z	[95% conf.	interval]
fines	-8.020769	.464836	-17.26	0.000	-8.931831	-7.109707

Note: Effect estimates are averages of derivatives.

The iteration log first tells us that the approximating function is being computed. At this stage, the number of knots of the cubic B-spline is selected using cross-validation. Three knots were selected.

After the approximating function is computed, average marginal effects are computed. This second step is computationally expensive. The computation time increases with the number of elements in the basis function, which in turn increases with the complexity of the mean function we are trying to compute.

The table reports that the average marginal effect of fines on the mean number of citations is -8.02. Increasing fines, on average, reduces the number of citations.

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npregress series generates a system variable for each element of the basis function. Additionally, variables are generated with the rescaled values of the continuous covariates used to construct the basis function. To see the variables that npregress series generated for example 1, we type

. describe *_*, fullnames

Variable name	Storage type	Display format	Value label	Variable label
x1rs	double	%10.0g		fines rescaled to [0,1]
_x1b1	double	%10.0g		Basis term 1 for fines
_x1b2	double	%10.0g		Basis term 2 for fines
_x1b3	double	%10.0g		Basis term 3 for fines
_x1b4	double	%10.0g		Basis term 4 for fines
_x1b5	double	%10.0g		Basis term 5 for fines
_x1b6	double	%10.0g		Basis term 6 for fines
_x1b7	double	%10.0g		Basis term 7 for fines

To specify a name for each of the elements of the basis function, we can use the basis() option with a stub.

. npregress series citations fines, basis(basis) (output omitted)

We get the following set of names for the elements of the basis function:

. describe basis*. fullnames

Variable name	Storage type	Display format	Value label	Variable label	
basis1	double	%10.0g		Basis term 1 for fines	
basis2	double	%10.0g		Basis term 2 for fines	
basis3	double	%10.0g		Basis term 3 for fines	
basis4	double	%10.0g		Basis term 4 for fines	
basis5	double	%10.0g		Basis term 5 for fines	
basis6	double	%10.0g		Basis term 6 for fines	
basis7	double	%10.0g		Basis term 7 for fines	

We may also modify the name of the rescaled variable by using the rescale() option.

. npregress series citations fines, rescale(rescaled) (output omitted)

This will give us

. describe rescaled*, fullnames

variable name	storage type	display format	value label	variable label
rescaled1	double	%10.0g		fines rescaled to [0,1]

Example 2: Estimation with more than one regressor

We now extend example 1. In addition to fines, we model citations as a function of whether the jurisdiction is small, medium, or large (csize) and whether there is a college in the jurisdiction (college).

. npregress series citations fines i.csize i.college

Computing approximating function

Minimizing cross-validation criterion

Iteration 0: Cross-validation criterion = 30.26251

Computing average derivatives

Cubic B-spline estimation Number of obs = 500 Criterion: cross-validation Number of knots = 1

citations	Effect	Robust std. err.	z	P> z	[95% conf.	interval]
fines	-7.787386	.2917941	-26.69	0.000	-8.359292	-7.215481
csize (Medium vs						
Small) (Large	4.732592	.5087968	9.30	0.000	3.735368	5.729815
vs Small)	10.91757	.5350892	20.40	0.000	9.868813	11.96632
college (College vs						
Not coll)	6.514286	.5958949	10.93	0.000	5.346353	7.682218

Note: Effect estimates are averages of derivatives for continuous covariates and averages of contrasts for factor covariates.

The average marginal effect of fines is -7.79, slightly less in magnitude than the -8.02 that we estimated in example 1. The output also shows effects for the variables csize and college. In these categorical variables, the effects are differences instead of derivatives. For example, if every jurisdiction in the population were a college town, we would expect 6.51 more citations than if none were college towns.

Example 3: Expected citations for different levels of fines

The npregress series command reported that the average marginal effect of fines on number of citations is negative. We can use margins to further explore the relationship between level of fines and expected number of citations. What would we expect if all jurisdictions set fines to \$8,000? What if they all set fines to \$9,000? \$10,000? \$11,000? We use the at(fines=(8 9 10 11)) option with margins to estimate these expected values.

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. margins, at(fines=(8 9 10 11))

Predictive margins Number of obs = 500

Model VCE: Robust

Expression: Mean function, predict()

1._at: fines = 8 2._at: fines = 9 3._at: fines = 10 4._at: fines = 11

	Margin	Delta-method std. err.	z	P> z	[95% conf.	interval]
_at						
1	49.58234	1.47392	33.64	0.000	46.69351	52.47117
2	28.35154	.5730302	49.48	0.000	27.22842	29.47466
3	20.40163	.3320855	61.43	0.000	19.75075	21.0525
4	14.78085	.4297201	34.40	0.000	13.93862	15.62309

There appears to be a dramatic drop in the expected number of citations as fines increase from \$8,000 to \$9,000. We can visualize these results if we type marginsplot.

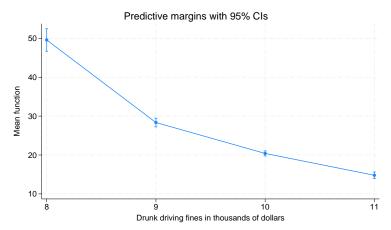


Figure 1.

Are there significant differences in the expected number of citations as we increase fines in increments of \$1,000? If we use the reverse-adjacent contrast operator, ar., with margins, we can estimate these differences and perform tests.

. margins, at(fines=(8 9 10 11)) contrast(atcontrast(ar._at) nowald effects) Contrasts of predictive margins Number of obs = 500

Model VCE: Robust

Expression: Mean function, predict()

1._at: fines = 8 $2._at: fines = 9$ $3._at: fines = 10$ $4._at: fines = 11$

Expression: Mean function, predict()

1._at: fines = 8 2._at: fines = 9 3._at: fines = 10 4._at: fines = 11

	Contrast	Delta-method std. err.	Z	P> z	[95% conf	. interval]
_at (2 vs 1) (3 vs 2) (4 vs 3)	-21.2308	1.610261	-13.18	0.000	-24.38685	-18.07475
	-7.94991	.7085254	-11.22	0.000	-9.338595	-6.561226
	-5.620773	.5683614	-9.89	0.000	-6.734741	-4.506806

When fines are increased from \$8,000 to \$9,000, we expect a decrease of 21.23 in the number of citations. Smaller but still statistically significant decreases in the number of citations are expected as fines are increased from \$9,000 to \$10,000 and from \$10,000 to \$11,000.

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Example 4: Estimating the effect for different levels of jurisdiction size

Now, we estimate the effect of increasing fines for different jurisdiction sizes.

. margins csize, dydx(fines)

Average marginal effects Number of obs = 500

Model VCE: Robust

Expression: Mean function, predict()

dy/dx wrt: fines

	dy/dx	Delta-method std. err.	z	P> z	[95% conf.	interval]
fines						
csize						
Small	-5.992484	.4491224	-13.34	0.000	-6.872747	-5.11222
Medium	-7.740284	.4366709	-17.73	0.000	-8.596144	-6.884425
Large	-10.20492	.564166	-18.09	0.000	-11.31067	-9.099178

If all jurisdictions were small but other characteristics were as they are observed, then we expect that the marginal effect of fines would be -5.99. We see that the effect is more extreme as the size of the jurisdiction increases. If all jurisdictions were large, we expect that the average marginal effect of fines would be -10.20.

We can further explore the effects of fines for different jurisdiction sizes by estimating the expected number of citations with fines at specific levels.

. margins csize, at(fines=(8(1)11)) (output omitted)

To visualize the effect, we type marginsplot.

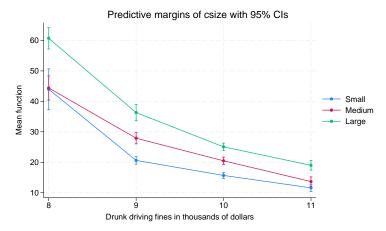


Figure 2.

For each jurisdiction size, we see that on average higher fines result in fewer citations. We also see that the effect of changing fine levels is nonlinear and differs across the counterfactual jurisdiction size. For instance, as fines increase from \$8,000 to \$9,000, the expected number of citations decreases faster for small jurisdictions than for medium ones.

Stored results

npregress series stores the following in e():

```
Scalars
    e(N)
                             number of observations
                             R^2
    e(r2)
    e(r2_a)
                             adjusted R^2
                             1 if converged, 0 otherwise
    e(converged)
                             order of basis function
    e(order)
    e(rank)
                             rank of e(V)
Macros
    e(cmd)
                             npregress
    e(cmdline)
                             command as typed
    e(depvar)
                             name of dependent variable
    e(basis)
                             bsplines, splines, or polynomials
    e(wtype)
                             weight type
    e(wexp)
                             weight expression
                             title in estimation output
    e(title)
    e(vce)
                             vcetype specified in vce()
    e(vcetype)
                             title used to label Std. err.
    e(knots)
                             number of knots selected
                             variables used in calculation of checksum
    e(datasignaturevars)
                             the checksum
    e(datasignature)
    e(estat_cmd)
                             program used to implement estat
                             program used to implement predict
    e(predict)
    e(properties)
                             predictions allowed by margins
    e(marginsok)
    e(marginsprop)
                             signals to the margins command
    e(marginsnotok)
                             predictions disallowed by margins
```

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In addition to the above, the following is stored in r():

Matrices

r(table) matrix containing the coefficients with their standard errors, test statistics, p-values, and confidence intervals

Note that results stored in r() are updated when the command is replayed and will be replaced when any r-class command is run after the estimation command.

Methods and formulas

Methods and formulas are presented under the following headings:

Overview
Polynomials
Piecewise polynomial splines
B-splines
Model selection
Cross-validation
Generalized cross-validation
Mallows's Cp
AIC and BIC

Overview

The regression model of outcome y_i given the k-dimensional vector of covariates \mathbf{x}_i was defined in (1) and (2) of *Remarks and examples* and is repeated here:

$$y_i = g\left(\mathbf{x}_i\right) + \varepsilon_i \tag{1}$$

$$E\left(\varepsilon_{i}|\mathbf{x}_{i}\right) = 0\tag{2}$$

where ε_i is the error term. The covariates may include discrete and continuous variables. Equations (1) and (2) imply that

$$E\left(y_i|\mathbf{x}_i\right) = g\left(\mathbf{x}_i\right)$$

As discussed in *Remarks and examples*, series estimators have the form of ordinary least squares. Thus, we can write the estimate of the mean function as

$$\widehat{E}(y_i|\mathbf{x}_i) = \mathbf{z}(\mathbf{x}_i)\widehat{\boldsymbol{\beta}} \tag{5}$$

where $\mathbf{z}(\mathbf{x}_i)$ is a known q-dimensional vector for which every one of the q terms is a function of the k-dimensional vector of covariates \mathbf{x}_i . Let n be the sample size. If we define \mathbf{Z} as the $n \times q$ matrix formed by the $\mathbf{z}(\mathbf{x}_i)$ for each individual i, then the q-dimensional coefficient vector $\widehat{\boldsymbol{\beta}}$ is the ordinary least-squares vector that comes from regressing the $n \times 1$ outcome vector \mathbf{y} on \mathbf{Z} and has the known form

$$\widehat{\boldsymbol{\beta}} = (\mathbf{Z}'\mathbf{Z})^{-1} (\mathbf{Z}'\mathbf{y}) \tag{6}$$

Each one of the series estimators has a different form for $\mathbf{z}(\mathbf{x}_i)$. Below, we define $\mathbf{z}(\mathbf{x}_i)$ for polynomials, piecewise polynomial splines, and B-splines.

Polynomials

For a polynomial of order 1 with k continuous covariates, $\mathbf{x}_i \equiv (x_{i1}, x_{i2}, \dots, x_{ik}), \mathbf{z}(\mathbf{x}_i)$ is

$$\mathbf{z}\left(\mathbf{x}_{i}\right) = \left(x_{i1}, x_{i2}, \dots, x_{ik}\right) \tag{P1}$$

For notational convenience, we will refer to the polynomial above as P1, which also corresponds to the name we gave to the equation. More formally, we could have written $(x_{i1}, x_{i2}, \dots, x_{ik}) \equiv P1$. We will maintain this notational convention below.

A polynomial of order 2 with k continuous covariates includes P1 and second-order terms:

$$\mathbf{z}(\mathbf{x}_i) = (P1, x_{i1}^2, x_{i1}x_{i2}, \dots, x_{i1}x_{ik}, x_{i2}x_{i3}, \dots, x_{ik}^2)$$
(P2)

A third-order polynomial with k continuous covariates includes the terms in P2 (which already includes P1) and third-order terms:

$$\mathbf{z}(\mathbf{x}_i) = (P2, x_{i1}^3, x_{i1}^2 x_{i2}, \dots, x_{i1}^2 x_{ik}, x_{i1} x_{i2} x_{i3}, \dots, x_{ik}^3)$$
(P3)

This recursive relationship continues. Thus, fourth-order polynomials includes the terms in P3 (which already includes P1 and P2) plus fourth-order terms.

For the polynomials above and all series estimators below, discrete covariates enter the model in levels, and each level is interacted with all other covariates in the model.

Piecewise polynomial splines

Piecewise polynomial splines are formed by a polynomial and functions of the form

$$\max(x_{ik} - t_{1k}, 0)$$

In the expression above, t_{1k} is a constant that is called a knot. The subscript of t_{1k} indicates that it is the first knot of the continuous covariate x_k . The max(·) function is 0 when $x_{ik} < t_{1k}$ and is $x_{ik}-t_{1k}$ otherwise. npregress series selects a set of knots for each one of the continuous covariates.

The regressors for npregress series using a piecewise polynomial spline of order 3 with one continuous covariate, \mathbf{x}_1 , and k knots, $t_{11} < t_{21} < \cdots < t_{k1}$, are given by

$$\mathbf{z}(x_{i1}) = \left\{ x_{i1}, x_{i1}^{2}, x_{i1}^{3}, \max(x_{i1} - t_{11}, 0)^{3}, \max(x_{i1} - t_{21}, 0)^{3}, \dots, \max(x_{i1} - t_{k1}, 0)^{3} \right\}$$
(S1)

Equivalently, for another continuous covariate, \mathbf{x}_2 , and k knots, $t_{12} < t_{22} < \cdots < t_{k2}$, we have

$$\mathbf{z}(x_{i2}) = \left\{ x_{i2}, x_{i2}^2, x_{i2}^3, \max(x_{i2} - t_{12}, 0)^3, \max(x_{i2} - t_{22}, 0)^3, \dots, \max(x_{i2} - t_{k2}, 0)^3 \right\}$$
(S2)

To get $\mathbf{z}(x_{i1}, x_{i2})$ for \mathbf{x}_1 and \mathbf{x}_2 and k knots, we include all terms in S1 and S2 as well as all the terms that result from the interaction of their terms. We write it succinctly as

$$\mathbf{z}(x_{i1}, x_{i2}) = \{S1, S2, (S1)(S2)\} \tag{S12}$$

The description above refers to the default third-order piecewise polynomial spline. Below, we describe the cases for piecewise polynomial splines of order 1 and order 2. Going back to the one covariate case, if we want a piecewise polynomial spline of order 1 with k knots, we have

$$\mathbf{z}(x_{i1}) = \{x_{i1}, \max(x_{i1} - t_{11}, 0), \max(x_{i1} - t_{21}, 0), \dots, \max(x_{i1} - t_{k1}, 0)\}\$$

And for order 2 with k knots and one covariate, we have

$$\mathbf{z}\left(x_{i1}\right) = \left\{x_{i1}, x_{i1}^{2}, \max\left(x_{i1} - t_{11}, 0\right)^{2}, \max\left(x_{i1} - t_{21}, 0\right)^{2}, \dots, \max\left(x_{i1} - t_{k1}, 0\right)^{2}\right\}$$

If we have more than one covariate, the logic of interacting the expressions for each covariate is the same as the logic we used for the third-order piecewise polynomial spline in (S12).

To construct $\mathbf{z}(\mathbf{x}_i)$, continuous covariates are rescaled to be between 0 and 1 with the expression

$$\left\{\mathbf{x}_i - \min(\mathbf{x}_i)\right\} \left\{ \frac{1}{\max(\mathbf{x}_i) - \min(\mathbf{x}_i)} \right\}$$

This rescaling is used to construct the piecewise polynomial spline and B-spline bases.

B-splines

To construct a B-spline basis, we need to define knots that are on the interior of the range of the covariates and knots that are at the upper and lower limits of the range or outside the range. The number of knots that are not in the interior differs depending on the order of the B-spline. For a B-spline of order 1 with k interior knots, t_1, t_2, \ldots, t_k , we need 4 additional knots. The set of knots for a first-order B-spline is therefore

$$t_{-1}, t_0, t_1, \dots, t_k, t_{k+1}, t_{k+2}$$

We added t_{-1}, t_0, t_{k+1} , and t_{k+2} to the interior knots. By convention, $t_{-1} = t_0$ and $t_{k+1} = t_{k+2}$. For a B-spline of order 2 with k interior knots, we need 6 additional knots. The set of knots is

$$t_{-2}, t_{-1}, t_0, t_1, \dots, t_k, t_{k+1}, t_{k+2}, t_{k+3}$$

For a B-spline of order 3, the set of knots is

$$t_{-3}, t_{-2}, t_{-1}, t_0, t_1, \dots, t_k, t_{k+1}, t_{k+2}, t_{k+3}, t_{k+4}$$

We first define a first-order B-spline for one continuous covariate \mathbf{x} with k interior knots. Let \mathbf{t}_j denote an $n \times 1$ vector for which all elements take the value of the jth knot t_j . The B-spline basis is formed by k+2 functions of the form

$$B_{j,1} = \frac{(\mathbf{x} - t_j)}{t_{j+1} - t_j} \mathbf{1} \left(\mathbf{t}_j \le \mathbf{x} < \mathbf{t}_{j+1} \right) + \frac{(t_{j+2} - \mathbf{x})}{t_{j+2} - t_{j+1}} \mathbf{1} \left(\mathbf{t}_{j+1} \le \mathbf{x} < \mathbf{t}_{j+2} \right)$$

$$j = -1, 0, 1, 2, \dots, k$$
(7)

Above, we use the indicator function $\mathbf{1}(\cdot)$, which is 1 when the condition inside the parentheses is satisfied and is 0 otherwise. Also, any term for which $t_{j+1}=t_j$ or $t_{j+2}=t_{j+1}$ is considered to be a vector of 0s.

The function $\mathbf{z}(\mathbf{x})$ used to estimate $g(\mathbf{x})$ is given by

$$\mathbf{z}(\mathbf{x}) = (B_{-1,1}, B_{0,1}, B_{1,1}, \dots, B_{k,1})$$

We now define a second-order B-spline for one continuous covariate x with k interior knots. The basis is constructed using the relationship given by

$$B_{j,2} = \frac{(\mathbf{x} - t_j)}{t_{j+2} - t_j} B_{j,1} + \frac{(t_{j+3} - \mathbf{x})}{t_{j+3} - t_{j+1}} B_{j+1,1}$$
$$j = -2, -1, 0, 1, 2, \dots, k$$

where $B_{j,1}$ and $B_{j+1,1}$ come from (7) above. Thus, second-order B-splines are a function of first-order B-splines, and as we will see below, third-order B-splines are a function of second-order B-splines. This recursion continues into higher orders, but npregress series stops at B-splines of order 3.

The function $\mathbf{z}(\mathbf{x})$ for the second-order B-spline is given by

$$\mathbf{z}(\mathbf{x}) = (B_{-2,2}, B_{-1,2}, B_{0,2}, B_{1,2}, \dots, B_{k,2})$$

The terms of the basis for a third-order B-spline are given by

$$B_{j,3} = \frac{(\mathbf{x} - t_j)}{t_{j+3} - t_j} B_{j,2} + \frac{(t_{j+4} - \mathbf{x})}{t_{j+4} - t_{j+1}} B_{j+1,2}$$
$$j = -3, -2, -1, 0, 1, 2, \dots, k$$

and the function z(x) for the third-order B-spline is

$$\mathbf{z}(\mathbf{x}) = (B_{-3,3}, B_{-2,3}, B_{-1,3}, B_{0,3}, B_{1,3}, \dots, B_{k,3})$$
(B1)

As was the case with piecewise polynomial splines, when there is more than one covariate, you include all functions of the form (B1) and their interactions to form expressions like the one in (S12).

Model selection

Below, we define the criteria used for model selection. In the case of B-splines and piecewise polynomial splines, npregress series selects the number of knots to be used for estimation. In the case of a polynomial basis, npregress series selects the order of the polynomial.

Let us first define the squared residuals, e_i^2 , where $e_i = y_i - \widehat{g}(\mathbf{x}_i)$ and $\widehat{g}(\cdot)$ is the mean function estimate defined in (5). We denote the residuals for the regressions below as $e_i(\mathbf{t}_k)$ instead of e_i to signal that the estimates we obtain are a function of the set of knots, \mathbf{t}_k , used. In the case of polynomials, \mathbf{t}_k will refer to the degree of the polynomial instead of knots.

Cross-validation

The cross-validation criterion, $CV(\mathbf{t}_k)$, is defined by

$$\operatorname{cv}(\mathbf{t}_{k}) = \frac{1}{n} \sum_{i=1}^{n} \frac{e_{i}(\mathbf{t}_{k})^{2}}{(1 - h_{ii})^{2}}$$
 (8)

In (8), h_{ii} are the diagonal elements of the matrix $\mathbf{Z}(\mathbf{Z}'\mathbf{Z})\mathbf{Z}'$, where Z is defined in (6) above and n is the size of the estimation sample.

npregress series computes $CV(\mathbf{t}_k)$ for different sets of knots, $\mathbf{t}_1, \mathbf{t}_2, \dots, \mathbf{t}_k, \dots$, where $\mathbf{t}_1 \subset \mathbf{t}_2 \subset \dots \subset \mathbf{t}_k \subset \dots$, and then selects the model with the smallest value for the cross-validation criterion.

Generalized cross-validation

The generalized cross-validation criterion, GCV (\mathbf{t}_k) , is given by

$$\operatorname{GCV}\left(\mathbf{t}_{k}\right) = \frac{1}{n} \sum_{i=1}^{n} \frac{e_{i}\left(\mathbf{t}_{k}\right)^{2}}{\left\{1 - \left(K/n\right)\right\}^{2}}$$

where K is the number of estimated parameters and the other arguments are equivalent to those defined in (8). As with cross-validation, GCV (\mathbf{t}_k) is computed for a set of models with an increasing number of nested knots, in the case of piecewise polynomial splines and B-splines, and of polynomial order in the case of polynomials. The minimum of the sequence is the selected model.

Mallows's \mathbf{C}_p

$$\operatorname{Mallows}\left(\mathbf{t}_{k}\right) = \frac{1}{n} \sum_{i=1}^{n} e_{i} \left(\mathbf{t}_{k}\right)^{2} \left(1 + \frac{2K}{n}\right)$$

As with cross-validation, Mallows (\mathbf{t}_k) is computed for a set of models with an increasing number of nested knots, and the minimum of the sequence is the selected model.

AIC and BIC

See Methods and formulas in [R] estat ic.

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Also see

- [R] **npregress series postestimation** Postestimation tools for npregress series
- [R] **npregress intro** Introduction to nonparametric regression
- [R] **kdensity** Univariate kernel density estimation
- [R] **lpoly** Kernel-weighted local polynomial smoothing
- [R] makespline Spline generation
- [U] 20 Estimation and postestimation commands

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