lpoly — Kernel-weighted local polynomial smoothing

Description

lpoly performs a kernel-weighted local polynomial regression of \textit{yvar} on \textit{xvar} and displays a graph of the smoothed values with (optional) confidence bands.

Quick start

Kernel-weighted local polynomial regression of \textit{y} on \textit{x}

\begin{verbatim}
lpoly y x
\end{verbatim}

As above, but specify a bandwidth of 2

\begin{verbatim}
lpoly y x, bwidth(2)
\end{verbatim}

As above, but specify a degree of 1

\begin{verbatim}
lpoly y x, bwidth(2) degree(1)
\end{verbatim}

As above, but use the alternative Epanechnikov kernel

\begin{verbatim}
lpoly y x, bwidth(2) degree(1) kernel(epan2)
\end{verbatim}

As above, but create a new variable for the smoothing grid \textit{g} and smoothed values \textit{s}

\begin{verbatim}
lpoly y x, bwidth(2) degree(1) kernel(epan2) generate(g s)
\end{verbatim}

With 95\% confidence bands

\begin{verbatim}
lpoly y x, ci
\end{verbatim}

Use \texttt{twoway} to graph multiple local polynomial fits

\begin{verbatim}
twoway scatter y x ||
\end{verbatim}

\begin{verbatim}
lpoly y x, degree(1) kernel(epan2) ||
\end{verbatim}

\begin{verbatim}
lpoly y x, degree(1) kernel(epan2) bwidth(1) ||
\end{verbatim}

\begin{verbatim}
lpoly y x, degree(1) kernel(epan2) bwidth(7) ||
\end{verbatim}

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**Options**

- **kernel (kernel)** specifies the kernel function for use in calculating the weighted local polynomial estimate. The default is `kernel(epanechnikov)`.

- **bwidth (# | varname)** specifies the half-width of the kernel—the width of the smoothing window around each point. If `bwidth()` is not specified, a rule-of-thumb (ROT) bandwidth estimator is calculated and used. A local variable bandwidth may be specified in `varname`, in conjunction with an explicit smoothing grid using the `at()` option.

- **degree (#)** specifies the degree of the polynomial to be used in the smoothing. The default is `degree(0)`, meaning local-mean smoothing.

- **generate ([newvar_x] newvar_s)** stores the smoothing grid in `newvar_x` and the smoothed values in `newvar_s`. If `at()` is not specified, then both `newvar_x` and `newvar_s` must be specified. Otherwise, only `newvar_s` is to be specified.

- **n (#)** specifies the number of points at which the smooth is to be calculated. The default is `min(N, 50)`, where `N` is the number of observations.

- **at (varname)** specifies a variable that contains the values at which the smooth should be calculated. By default, the smoothing is done on an equally spaced grid, but you can use `at()` to instead perform the smoothing at the observed `x`’s, for example. This option also allows you to more easily obtain smooths for different variables or different subsamples of a variable and then overlay the estimates for comparison.

- **nograph** suppresses drawing the graph of the estimated smooth. This option is often used with the `generate()` option.

- **nosscatter** suppresses superimposing a scatterplot of the observed data over the smooth. This option is useful when the number of resulting points would be so large as to clutter the graph.

- **ci** plots confidence bands, using the confidence level specified in `level()`.

- **level (#)** specifies the confidence level, as a percentage, for confidence intervals. The default is `level(95)` or as set by `set level`; see [U] 20.8 Specifying the width of confidence intervals.

- **se (newvar)** stores the estimates of the standard errors in `newvar`. This option requires specifying `generate()` or `at()`.
`pwidth(#)` specifies the pilot bandwidth to be used for standard-error computations. The default is chosen to be 1.5 times the value of the `ROT` bandwidth selector. If you specify `pwidth()` without specifying `se()` or `ci`, then the `ci` option is assumed.

`var(# | varname)` specifies an estimate of a constant residual variance or a variable containing estimates of the residual variances at each grid point required for standard-error computation. By default, the residual variance at each smoothing point is estimated by the normalized weighted residual sum of squares obtained from locally fitting a polynomial of order $p + 2$, where $p$ is the degree specified in `degree()`. `var(varname)` is allowed only if `at()` is specified. If you specify `var()` without specifying `se()` or `ci`, then the `ci` option is assumed.

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**Remarks and examples**

Remarks are presented under the following headings:

- **Introduction**
- **Local polynomial smoothing**
- **Choice of a bandwidth**
- **Confidence bands**

**Introduction**

The last 25 years or so has seen a significant outgrowth in the literature on scatterplot smoothing, otherwise known as univariate nonparametric regression. Of most appeal is the idea of making no assumptions about the functional form for the expected value of a response given a regressor, but instead allowing the data to “speak for themselves”. Various methods and estimators fall into the category of nonparametric regression, including local mean smoothing as described independently by Nadaraya (1964) and Watson (1964), the Gasser and Müller (1979) estimator, locally weighted scatterplot smoothing (LOWESS) as described by Cleveland (1979), wavelets (for example, Donoho...
and splines (Eubank 1999), to name a few. Much of the vast literature focuses on automating the amount of smoothing to be performed and dealing with the bias/variance tradeoff inherent to this type of estimation. For example, for Nadaraya–Watson the amount of smoothing is controlled by choosing a bandwidth.

Smoothing via local polynomials is by no means a new idea but instead one that has been rediscovered in recent years in articles such as Fan (1992). A natural extension of the local mean smoothing of Nadaraya–Watson, local polynomial regression involves fitting the response to a polynomial form of the regressor via locally weighted least squares. Higher-order polynomials have better bias properties than the zero-degree local polynomials of the Nadaraya–Watson estimator; in general, higher-order polynomials do not require bias adjustment at the boundary of the regression space. For a definitive reference on local polynomial smoothing, see Fan and Gijbels (1996).

Local polynomial smoothing

Consider a set of scatterplot data \( \{(x_1, y_1), \ldots, (x_n, y_n)\} \) from the model

\[
y_i = m(x_i) + \sigma(x_i)\epsilon_i
\]

for some unknown mean and variance functions \( m(\cdot) \) and \( \sigma^2(\cdot) \), and symmetric errors \( \epsilon_i \) with \( E(\epsilon_i) = 0 \) and \( \text{Var}(\epsilon_i) = 1 \). The goal is to estimate \( m(x_0) = E[Y|X = x_0] \), making no assumption about the functional form of \( m(\cdot) \).

Ipoly estimates \( m(x_0) \) as the constant term (intercept) of a regression, weighted by the kernel function specified in kernel(), of yvar on the polynomial terms \( (xvar - x_0), (xvar - x_0)^2, \ldots, (xvar - x_0)^p \) for each smoothing point \( x_0 \). The degree of the polynomial, \( p \), is specified in degree(), the amount of smoothing is controlled by the bandwidth specified in bwidth(), and the chosen kernel function is specified in kernel().

Example 1

Consider the motorcycle data as examined (among other places) in Fan and Gijbels (1996). The data consist of 133 observations and measure the acceleration (accel measured in grams [g]) of a dummy’s head during impact over time (time measured in milliseconds). For these data, we use ipoly to fit a local cubic polynomial with the default bandwidth (obtained using the ROT method) and the default Epanechnikov kernel.
. use https://www.stata-press.com/data/r16/motorcycle
(Motorcycle data from Fan & Gijbels (1996))
. lpoly accel time, degree(3)

The default bandwidth and kernel settings do not provide a satisfactory fit in this example. To improve the fit, we can either supply a different bandwidth by using the `bwidth()` option or specify a different kernel by using the `kernel()` option. For example, using the alternative Epanechnikov kernel, `kernel(epan2)`, below provides a better fit for these data.

. lpoly accel time, degree(3) kernel(epan2)

Technical note

lpoly allows specifying in `degree()` both odd and even orders of the polynomial to be used for the smoothing. However, the odd-order, $2k + 1$, polynomial approximations are preferable. They have
an extra parameter compared with the even-order, $2k$, approximations, which leads to a significant bias reduction and there is no increase of variability associated with adding this extra parameter. Using an odd order when estimating the regression function is therefore usually sufficient. For a more thorough discussion, see Fan and Gijbels (1996).

Choice of a bandwidth

The choice of a bandwidth is crucial for many smoothing techniques, including local polynomial smoothing. In general, using a large bandwidth gives smooths with a large bias, whereas a small bandwidth may result in highly variable smoothed values. Various techniques exist for optimal bandwidth selection. By default, `lpoly` uses the ROT method to estimate the bandwidth used for the smoothing; see `Methods and formulas` for details.

Example 2

Using the `motorcycle` data, we demonstrate how a local linear polynomial fit changes using different bandwidths.

```
. lpoly accel time, degree(1) kernel(epan2) bwidth(1) generate(at smooth1)
> nograph
. lpoly accel time, degree(1) kernel(epan2) bwidth(7) at(at) generate(smooth2)
> nograph
. label variable smooth1 "smooth: width = 1"
. label variable smooth2 "smooth: width = 7"
. lpoly accel time, degree(1) kernel(epan2) at(at) addplot(line smooth* at)
> legend(label(2 "smooth: width = 3.42 (ROT)")) note("kernel = epan2, degree = 1")
```

From this graph, we can see that the local linear polynomial fit with larger bandwidth (`width = 7`) corresponds to a smoother line but fails to fit the curvature of the scatterplot data. The smooth obtained using the width equal to one seems to fit most data points, but the corresponding line has several spikes indicating larger variability. The smooth obtained using the ROT bandwidth estimator seems to have a good tradeoff between the fit and variability in this example.
In the above, we also demonstrated how the `generate()` and `addplot()` options may be used to produce overlaid plots obtained from `lpoly` with different options. The `nograph` option saves time when you need to save only results with `generate()`.

However, to avoid generating variables manually, one can use `twoway lpoly` instead; see [G-2] `graph twoway lpoly` for more details.

```
. twoway scatter accel time ||
>    lpoly accel time, degree(1) kernel(epan2) lpattern(solid) ||
>    lpoly accel time, degree(1) kernel(epan2) bwidth(1) ||
>    lpoly accel time, degree(1) kernel(epan2) bwidth(7) ||
>    , legend(label(2 "smooth: width = 3.42 (ROT)" label(3 "smooth: width = 1")
>             label(4 "smooth: width = 7")
>    title("Local polynomial smooth") note("kernel = epan2, degree = 1")
>    xtitle("time (msec)") ytitle("acceleration (g)"")
```

The ROT estimate is commonly used as an initial guess for the amount of smoothing; this approach may be sufficient when the choice of a bandwidth is less important. In other cases, you can pick your own bandwidth.

When the shape of the regression function has a combination of peaked and flat regions, a variable bandwidth may be preferable over the constant bandwidth to allow for different degrees of smoothness in different regions. The `bwidth()` option allows you to specify the values of the local variable bandwidths as those stored in a variable in your data.

Similar issues with bias and variability arise when choosing a pilot bandwidth (the `pwidth()` option) used to compute standard errors of the local polynomial smoother. The default value is chosen to be $1.5 \times \text{ROT}$. For a review of methods for pilot bandwidth selection, see Fan and Gijbels (1996).

**Confidence bands**

The established asymptotic normality of the local polynomial estimators under certain conditions allows the construction of approximate confidence bands. `lpoly` offers the `ci` option to plot these bands.
Example 3

Let us plot the confidence bands for the local polynomial fit from example 1.

```
.lpoly accel time, degree(3) kernel(epan2) ci
```

You can obtain graphs with overlaid confidence bands by using `twoway lpolyci`; see [G-2] `graph twoway lpolyci` for examples.

Constructing the confidence intervals involves computing standard errors obtained by taking a square root of the estimate of the conditional variance of the local polynomial estimator at each grid point $x_0$. Estimating the conditional variance requires fitting a polynomial of a higher order locally by using a different bandwidth, the pilot bandwidth. The value of the pilot bandwidth may be supplied by using `pwidth()`. By default, the value of $1.5 \times \text{ROT}$ is used. Also, estimates of the residual variance $\sigma^2(x_0)$ at each grid point, $x_0$, are required to obtain the estimates of the conditional variances. These estimates may be supplied by using the `var()` option. By default, they are computed using the normalized weighted residual sum of squares from a local polynomial fit of a higher order. See `Methods and formulas` for details. The standard errors may be saved by using `se()`.

Stored results

`lpoly` stores the following in `r()`:

Scalars

- `r(degree)`: smoothing polynomial degree
- `r(ngrid)`: number of successful regressions
- `r(N)`: sample size
- `r(bwidth)`: bandwidth of the smooth
- `r(pwidth)`: pilot bandwidth

Macros

- `r(kernel)`: name of kernel
Methods and formulas

Consider model (1), written in matrix notation,

\[ y = m(x) + \epsilon \]

where \( y \) and \( x \) are the \( n \times 1 \) vectors of scatterplot values, \( \epsilon \) is the \( n \times 1 \) vector of errors with zero mean and covariance matrix \( \Sigma = \text{diag}(\sigma(x_i))I_n \), and \( m() \) and \( \sigma() \) are some unknown functions. Define \( m(x_0) = E[Y|X = x_0] \) and \( \sigma^2(x_0) = \text{Var}[Y|X = x_0] \) to be the conditional mean and conditional variance of random variable \( Y \) (residual variance), respectively, for some realization \( x_0 \) of random variable \( X \).

The method of local polynomial smoothing is based on the approximation of \( m(x) \) locally by a \( p \)th order polynomial in \((x - x_0)\) for some \( x \) in the neighborhood of \( x_0 \). For the scatterplot data \( \{(x_1, y_1), \ldots, (x_n, y_n)\} \), the \( p \)th-order local polynomial smooth \( \hat{m}(x_0) \) is equal to \( \hat{\beta}_0 \), an estimate of the intercept of the weighted linear regression,

\[ \hat{\beta} = (X^T WX)^{-1}X^T Wy \quad (2) \]

where \( \hat{\beta} = (\hat{\beta}_0, \hat{\beta}_1, \ldots, \hat{\beta}_p)^T \) is the vector of estimated regression coefficients (with \( \{\hat{\beta}_j = (j!)^{-1}\hat{m}(j)(x)|x = x_0, j = 0, \ldots, p\} \) also representing estimated coefficients from a corresponding Taylor expansion; \( X = \{(x_i - x_0)^j\}^{n,p}_{i,j=1,0} \) is a design matrix; and \( W = \text{diag}\{K_h(x_i - x_0)\}^{n \times n} \) is a weighting matrix with weights \( K_h(\cdot) \) defined as \( K_h(x) = h^{-1}K(x/h) \), with \( K(\cdot) \) being a kernel function and \( h \) defining a bandwidth. The kernels are defined in Methods and formulas of \textit{R} \texttt{kdensity}.

The default bandwidth is obtained using the ROT method of bandwidth selection. The ROT bandwidth is the plugin estimator of the asymptotically optimal constant bandwidth. This is the bandwidth that minimizes the conditional weighted mean integrated squared error. The ROT plugin bandwidth selector for the smoothing bandwidth \( h \) is defined as follows; assuming constant residual variance \( \sigma^2(x_0) = \sigma^2 \) and odd degree \( p \):

\[ \hat{h} = C_{0,p}(K) \left[ \frac{\hat{\sigma}^2 \int w_0(x)dx}{n \int \{\hat{m}(p+1)(x)\}^2 w_0(x)f(x)dx} \right]^{1/(2p+3)} \quad (3) \]

where \( C_{0,p}(K) \) is a constant, as defined in Fan and Gijbels (1996), that depends on the kernel function \( K(\cdot) \), and the degree of a polynomial \( p \) and \( w_0 \) is chosen to be an indicator function on the interval \( [\min_x + 0.05 \times \text{range}_x, \max_x - 0.05 \times \text{range}_x] \) with \( \min_x \), \( \max_x \), and \( \text{range}_x \) being, respectively, the minimum, maximum, and the range of \( x \). To obtain the estimates of a constant residual variance, \( \hat{\sigma}^2 \), and \( (p + 1) \)th order derivative of \( m(x) \), denoted as \( \hat{m}(p+1)(x) \), a polynomial in \( x \) of order \( (p + 3) \) is fit globally to \( y \). \( \hat{\sigma}^2 \) is estimated as a standardized residual sum of squares from this fit.

The expression for the asymptotically optimal constant bandwidth used in constructing the ROT bandwidth estimator is derived for the odd-order polynomial approximations. For even-order polynomial fits the expression would depend not only on \( m^{(p+1)}(x) \) but also on \( m^{(p+2)}(x) \) and the design density and its derivative, \( f(x) \) and \( f'(x) \). Therefore, the ROT bandwidth selector would require estimation of these additional quantities. Instead, for an even-degree \( p \) of the local polynomial, 1poly uses the value of the ROT estimator (3) computed using degree \( p + 1 \). As such, for even degrees this is not a plugin estimator of the asymptotically optimal constant bandwidth.

The estimates of the conditional variance of local polynomial estimators are obtained using

\[ \text{Var}\{\hat{m}(x_0)|X = x_0\} = \hat{\sigma}^2_{m}(x_0) = (X^T WX)^{-1}(X^T W^2 X)(X^T WX)^{-1} \hat{\sigma}^2(x_0) \quad (4) \]
where \( \hat{\sigma}^2(x_0) \) is estimated by the normalized weighted residual sum of squares from the \((p + 2)\)th order polynomial fit using pilot bandwidth \( h^* \).

When the bias is negligible the normal-approximation method yields a \((1 - \alpha) \times 100\%\) confidence interval for \( m(x_0) \),

\[
\left\{ \hat{m}(x_0) - z_{(1-\alpha/2)} \hat{\sigma}_m(x_0), \hat{m}(x_0) + z_{(1-\alpha/2)} \hat{\sigma}_m(x_0) \right\}
\]

where \( z_{(1-\alpha/2)} \) is the \((1 - \alpha/2)\)th quantile of the standard Gaussian distribution, and \( \hat{m}(x_0) \) and \( \hat{\sigma}_m(x_0) \) are as defined in (2) and (4), respectively.

References


Also see

[R] *kdensity* — Univariate kernel density estimation

[R] *lowess* — Lowess smoothing

[R] *npregress intro* — Introduction to nonparametric regression

[R] *smooth* — Robust nonlinear smoother

[G-2] *graph twoway lpoly* — Local polynomial smooth plots

[G-2] *graph twoway lpolyci* — Local polynomial smooth plots with CIs