orthog - Orthogonalize variables and compute orthogonal polynomials

| Description | Quick start | Menu |
| :--- | :--- | :--- |
| Syntax | Options for orthog | Options for orthpoly |
| Remarks and examples | Methods and formulas | References |

## Description

orthog orthogonalizes a set of variables, creating a new set of orthogonal variables (all of type double), using a modified Gram-Schmidt procedure (Golub and Van Loan 2013). The order of the variables determines the orthogonalization; hence, the "most important" variables should be listed first.

Execution time is proportional to the square of the number of variables. With many ( $>10$ ) variables, orthog will be fairly slow.
orthpoly computes orthogonal polynomials for one variable.

## Quick start

Generate ox1, ox2, and ox3 containing orthogonalized versions of $x 1$, $x 2$, and $x 3$ orthog x1 x2 x3, generate (ox1 ox2 ox3)

Same as above

```
orthog x1 x2 x3, generate(ox*)
```

Generate op1, op2, and op3 containing degree 1, 2, and 3 orthogonal polynomials for x1 orthpoly x1, generate(op1 op2 op3) degree(3)

Same as above
orthpoly x1, generate(op1-op3) degree(3)
Same as above, and generate matrix op containing coefficients of the orthogonal polynomials

```
orthpoly x1, generate(op1-op3) degree(3) poly(op)
```


## Menu

## orthog

Data $>$ Create or change data $>$ Other variable-creation commands $>$ Orthogonalize variables
orthpoly
Data $>$ Create or change data $>$ Other variable-creation commands $>$ Orthogonal polynomials

## Syntax

Orthogonalize variables

$$
\text { orthog }[\text { varlist }][\text { if }][\text { in }][\text { weight }], \underline{g}{ }^{\text {generate(newvarlist) })}[\underline{\text { matrix }} \text { (matname) }]
$$

Compute orthogonal polynomial

$$
\begin{aligned}
& \text { orthpoly varname }[\text { if }][\text { in }][\text { weight }], \\
& \qquad\{\underline{g e n e r a t e(n e w v a r l i s t) ~} \mid \underline{\text { poly }} \text { (matname) }\}[\text { degree(\#) }]
\end{aligned}
$$

orthpoly requires that generate (newvarlist) or poly (matname), or both, be specified.
varlist may contain time-series operators; see [U] 11.4.4 Time-series varlists.
iweights, aweights, fweights, and pweights are allowed, see [U] 11.1.6 weight.

## Options for orthog

Main
generate (newvarlist) is required. generate() creates new orthogonal variables of type double. For orthog, newvarlist will contain the orthogonalized varlist. If varlist contains $d$ variables, then so will newvarlist. newvarlist can be specified by giving a list of exactly $d$ new variable names, or it can be abbreviated using the styles newvar1-newvard or newvar*. For these two styles of abbreviation, new variables newvar1, newvar2, ... newvard are generated.
matrix (matname) creates a $(d+1) \times(d+1)$ matrix containing the matrix $R$ defined by $X=Q R$, where $X$ is the $N \times(d+1)$ matrix representation of varlist plus a column of ones and $Q$ is the $N \times(d+1)$ matrix representation of newvarlist plus a column of ones ( $d=$ number of variables in varlist, and $N=$ number of observations).

## Options for orthpoly

$\qquad$ Main
generate (newvarlist) or poly(), or both, must be specified. generate() creates new orthogonal variables of type double. newvarlist will contain orthogonal polynomials of degree 1, 2, ..., $d$ evaluated at varname, where $d$ is as specified by degree $(d)$. newvarlist can be specified by giving a list of exactly $d$ new variable names, or it can be abbreviated using the styles newvar1newvard or newvar*. For these two styles of abbreviation, new variables newvar1, newvar $2, \ldots$, newvard are generated.
poly (matname) creates a $(d+1) \times(d+1)$ matrix called matname containing the coefficients of the orthogonal polynomials. The orthogonal polynomial of degree $i \leq d$ is

```
matname \([i, d+1]+\) matname \([i, 1] *\) varname + matname \([i, 2] *\) varname \(^{2}\)
    \(+\cdots+\) matname \([i, i] *\) varname \({ }^{i}\)
```

The coefficients corresponding to the constant term are placed in the last column of the matrix. The last row of the matrix is all zeros, except for the last column, which corresponds to the constant term.
degree(\#) specifies the highest-degree polynomial to include. Orthogonal polynomials of degree 1, $2, \ldots, d=\#$ are computed. The default is $d=1$.

## Remarks and examples

stata.com
Orthogonal variables are useful for two reasons. The first is numerical accuracy for highly collinear variables. Stata's regress and other estimation commands can face much collinearity and still produce accurate results. But, at some point, these commands will drop variables because of collinearity. If you know with certainty that the variables are not perfectly collinear, you may want to retain all their effects in the model. If you use orthog or orthpoly to produce a set of orthogonal variables, all variables will be present in the estimation results.

Users are more likely to find orthogonal variables useful for the second reason: ease of interpreting results. orthog and orthpoly create a set of variables such that the "effects" of all the preceding variables have been removed from each variable. For example, if we issue the command

```
. orthog x1 x2 x3, generate(q1 q2 q3)
```

the effect of the constant is removed from x 1 to produce q 1 ; the constant and x 1 are removed from $x 2$ to produce $q 2$; and finally the constant, $x 1$, and $x 2$ are removed from $x 3$ to produce $q 3$. Hence,

$$
\begin{aligned}
& \mathrm{q} 1=r_{01}+r_{11} \mathrm{x} 1 \\
& \mathrm{q} 2=r_{02}+r_{12} \times 1+r_{22} \times 2 \\
& \mathrm{q} 3=r_{03}+r_{13} \times 1+r_{23} \times 2+r_{33} \times 3
\end{aligned}
$$

This effect can be generalized and written in matrix notation as

$$
X=Q R
$$

where $X$ is the $N \times(d+1)$ matrix representation of varlist plus a column of ones, and $Q$ is the $N \times(d+1)$ matrix representation of newvarlist plus a column of ones ( $d=$ number of variables in varlist and $N=$ number of observations). The $(d+1) \times(d+1)$ matrix $R$ is a permuted uppertriangular matrix, that is, $R$ would be upper triangular if the constant were first, but the constant is last, so the first row/column has been permuted with the last row/column. Because Stata's estimation commands list the constant term last, this allows $R$, obtained via the matrix () option, to be used to transform estimation results.
> Example 1: orthog
Consider Stata's auto.dta dataset. Suppose that we postulate a model in which price depends on the car's length, weight, headroom, and trunk size (trunk). These predictors are collinear, but not extremely so-the correlations are not that close to 1 :

regress certainly has no trouble fitting this model:
. regress price length weight headroom trunk

| Source | SS | df | MS |
| ---: | :---: | ---: | ---: |
| Model | 236016580 | 4 | 59004145 |
| Residual | 399048816 | 69 | 5783316.17 |
| Total | 635065396 | 73 | 8699525.97 |


| Number of obs | $=$ | 74 |
| :--- | :--- | ---: |
| $\mathrm{~F}(4,69)$ | $=$ | 10.20 |
| Prob $>$ F | $=$ | 0.0000 |
| R-squared | $=$ | 0.3716 |
| Adj R-squared | $=$ | 0.3352 |
| Root MSE | $=$ | 2404.9 |


| price | Coefficient | Std. err. | $t$ | P>\|t| | [95\% conf. interval] |  |
| ---: | ---: | :--- | ---: | :--- | ---: | ---: |
| length | -101.7092 | 42.12534 | -2.41 | 0.018 | -185.747 | -17.67147 |
| weight | 4.753066 | 1.120054 | 4.24 | 0.000 | 2.518619 | 6.987512 |
| headroom | -711.5679 | 445.0204 | -1.60 | 0.114 | -1599.359 | 176.2236 |
| trunk | 114.0859 | 109.9488 | 1.04 | 0.303 | -105.2559 | 333.4277 |
| _cons | 11488.47 | 4543.902 | 2.53 | 0.014 | 2423.638 | 20553.31 |

However, we may believe a priori that length is the most important predictor, followed by weight, headroom, and trunk. We would like to remove the "effect" of length from all the other predictors, remove weight from headroom and trunk, and remove headroom from trunk. We can do this by running orthog, and then we fit the model again using the orthogonal variables:

```
. orthog length weight headroom trunk, gen(olength oweight oheadroom otrunk)
> matrix(R)
. regress price olength oweight oheadroom otrunk
```

| Source | SS | df | MS |
| ---: | :---: | ---: | ---: |
| Model | 236016580 | 4 | 59004145 |
| Residual | 399048816 | 69 | 5783316.17 |
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| Number of obs | $=$ | 74 |
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| F (4, 69) | $=$ | 10.20 |
| Prob > F | $=$ | 0.0000 |
| R-squared | $=$ | 0.3716 |
| Adj R-squared | $=$ | 0.3352 |
| Root MSE | $=$ | 2404.9 |


| price | Coefficient | Std. err. | t | P>\|t| | [95\% conf. interval] |  |
| ---: | ---: | :---: | :---: | :---: | ---: | ---: |
| olength | 1265.049 | 279.5584 | 4.53 | 0.000 | 707.3454 | 1822.753 |
| oweight | 1175.765 | 279.5584 | 4.21 | 0.000 | 618.0617 | 1733.469 |
| oheadroom | -349.9916 | 279.5584 | -1.25 | 0.215 | -907.6955 | 207.7122 |
| otrunk | 290.0776 | 279.5584 | 1.04 | 0.303 | -267.6262 | 847.7815 |
| _cons | 6165.257 | 279.5584 | 22.05 | 0.000 | 5607.553 | 6722.961 |

Using the matrix $R$, we can transform the results obtained using the orthogonal predictors back to the metric of original predictors:

```
. matrix b = e(b)*inv(R)'
. matrix list b
b [1,5]
\begin{tabular}{rrrrrr} 
& length & weight & headroom & trunk & -cons \\
y1 & -101.70924 & 4.7530659 & -711.56789 & 114.08591 & 11488.475
\end{tabular}
```


## Technical note

The matrix $R$ obtained using the matrix() option with orthog can also be used to recover $X$ (the original varlist) from $Q$ (the orthogonalized newvarlist), one variable at a time. Continuing with the previous example, we illustrate how to recover the trunk variable:

```
. matrix C = R[1...,"trunk"]'
```

. matrix score double rtrunk $=C$
. compare rtrunk trunk

|  |  |  | Count |  |  | Minimum | Difference <br> Average | Maximum |
| :--- | ---: | ---: | ---: | ---: | :---: | :---: | :---: | :---: |
| rtrunk>trunk | 74 | $8.88 \mathrm{e}-15$ | $1.91 \mathrm{e}-14$ | $3.55 \mathrm{e}-14$ |  |  |  |  |
|  |  | 74 | $8.88 \mathrm{e}-15$ | $1.91 \mathrm{e}-14$ |  |  |  |  |
| Jointly defined | 74 |  | $3.55 \mathrm{e}-14$ |  |  |  |  |  |
| Total |  |  |  |  |  |  |  |  |

Here the recovered variable rtrunk is almost exactly the same as the original trunk variable. When you are orthogonalizing many variables, this procedure can be performed to check the numerical soundness of the orthogonalization. Because of the ordering of the orthogonalization procedure, the last variable and the variables near the end of the varlist are the most important ones to check.

The orthpoly command effectively does for polynomial terms what the orthog command does for an arbitrary set of variables.

## > Example 2: orthpoly

Again consider the auto.dta dataset. Suppose that we wish to fit the model

$$
\operatorname{mpg}=\beta_{0}+\beta_{1} \text { weight }+\beta_{2} \text { weight }^{2}+\beta_{3} \text { weight }^{3}+\beta_{4} \text { weight }^{4}+\epsilon
$$

We will first compute the regression with natural polynomials:

```
. generate double w1 = weight
. generate double w2 = w1*w1
. generate double w3 = w2*w1
. generate double w4 = w3*w1
. correlate w1-w4
(obs=74)
```

|  | w1 | w2 | w3 | w4 |
| ---: | ---: | ---: | ---: | ---: |
| w1 | 1.0000 |  |  |  |
| w2 | 0.9915 | 1.0000 |  |  |
| w3 | 0.9665 | 0.9916 | 1.0000 |  |
| w4 | 0.9279 | 0.9679 | 0.9922 | 1.0000 |

. regress mpg w1-w4

| Source | SS | df | MS | Number of obs | = | 74 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  |  | F (4, 69) | = | 36.06 |
| Model | 1652.73666 | 4 | 413.184164 | Prob > F | = | 0.0000 |
| Residual | 790.722803 | 69 | 11.4597508 | R-squared | = | 0.6764 |
|  |  |  |  | Adj R-squared | = | 0.6576 |
| Total | 2443.45946 | 73 | 33.4720474 | Root MSE | = | 3.3852 |


| mpg | Coefficient | Std. err. | t | $\mathrm{P}>\|\mathrm{t}\|$ | [95\% conf. interval] |  |
| ---: | ---: | :---: | :---: | :---: | ---: | ---: |
| w1 | .0289302 | .1161939 | 0.25 | 0.804 | -.2028704 | .2607307 |
| w2 | -.0000229 | .0000566 | -0.40 | 0.687 | -.0001359 | .0000901 |
| w3 | $5.74 \mathrm{e}-09$ | $1.19 \mathrm{e}-08$ | 0.48 | 0.631 | $-1.80 \mathrm{e}-08$ | $2.95 \mathrm{e}-08$ |
| w4 | $-4.86 \mathrm{e}-13$ | $9.14 \mathrm{e}-13$ | -0.53 | 0.596 | $-2.31 \mathrm{e}-12$ | $1.34 \mathrm{e}-12$ |
| _cons | 23.94421 | 86.60667 | 0.28 | 0.783 | -148.8314 | 196.7198 |

Some of the correlations among the powers of weight are very large, but this does not create any problems for regress. However, we may wish to look at the quadratic trend with the constant removed, the cubic trend with the quadratic and constant removed, etc. orthpoly will generate polynomial terms with this property:

```
. orthpoly weight, generate(pw*) deg(4) poly(P)
```

. regress mpg pw1-pw4

| Source | SS | df | MS |
| ---: | :---: | ---: | :---: |
| Model | 1652.73666 | 4 | 413.184164 |
| Residual | 790.722803 | 69 | 11.4597508 |
| Total | 2443.45946 | 73 | 33.4720474 |


| Number of obs | $=$ | 74 |
| :--- | :--- | ---: |
| $\mathrm{~F}(4,69)$ | $=$ | 36.06 |
| Prob $>\mathrm{F}$ | $=$ | 0.0000 |
| R-squared | $=$ | 0.6764 |
| Adj R-squared | $=$ | 0.6576 |
| Root MSE | $=$ | 3.3852 |


| mpg | Coefficient | Std. err. | t | P>\|t| | [95\% conf. interval] |  |
| ---: | ---: | :---: | :---: | :---: | ---: | ---: |
| pw1 | -4.638252 | .3935245 | -11.79 | 0.000 | -5.423312 | -3.853192 |
| pw2 | .8263545 | .3935245 | 2.10 | 0.039 | .0412947 | 1.611414 |
| pw3 | -.3068616 | .3935245 | -0.78 | 0.438 | -1.091921 | .4781982 |
| pw4 | -.209457 | .3935245 | -0.53 | 0.596 | -.9945168 | .5756028 |
| _cons | 21.2973 | .3935245 | 54.12 | 0.000 | 20.51224 | 22.08236 |

Compare the $p$-values of the terms in the natural polynomial regression with those in the orthogonal polynomial regression. With orthogonal polynomials, it is easy to see that the pure cubic and quartic trends are not significant and that the constant, linear, and quadratic terms each have $p<0.05$.

The matrix P obtained with the poly () option can be used to transform coefficients for orthogonal polynomials to coefficients for natural polynomials:

```
. orthpoly weight, poly(P) deg(4)
. matrix b = e(b)*P
. matrix list b
b [1,5]
\begin{tabular}{lrrrrr} 
& deg 1 & deg 2 & deg 3 & deg 4 & - cons \\
y 1 & .02893016 & -.00002291 & \(5.745 \mathrm{e}-09\) & \(-4.862 \mathrm{e}-13\) & 23.944212
\end{tabular}
```


## Methods and formulas

orthog's orthogonalization can be written in matrix notation as

$$
X=Q R
$$

where $X$ is the $N \times(d+1)$ matrix representation of varlist plus a column of ones and $Q$ is the $N \times(d+1)$ matrix representation of newvarlist plus a column of ones ( $d=$ number of variables in varlist, and $N=$ number of observations). The $(d+1) \times(d+1)$ matrix $R$ is a permuted uppertriangular matrix; that is, $R$ would be upper triangular if the constant were first, but the constant is last, so the first row/column has been permuted with the last row/column.
$Q$ and $R$ are obtained using a modified Gram-Schmidt procedure; see Golub and Van Loan (2013, 254-255) for details. The traditional Gram-Schmidt procedure is notoriously unsound, but the modified procedure is good. orthog performs two passes of this procedure.
orthpoly uses the Christoffel-Darboux recurrence formula (Abramowitz and Stegun 1964).

Both orthog and orthpoly normalize the orthogonal variables such that

$$
Q^{\prime} W Q=M I
$$

where $W=\operatorname{diag}\left(w_{1}, w_{2}, \ldots, w_{N}\right)$ with weights $w_{1}, w_{2}, \ldots, w_{N}$ (all 1 if weights are not specified), and $M$ is the sum of the weights (the number of observations if weights are not specified).

## References

Abramowitz, M., and I. A. Stegun, ed. 1964. Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables. Washington, DC: National Bureau of Standards.

Golub, G. H., and C. F. Van Loan. 2013. Matrix Computations. 4th ed. Baltimore: Johns Hopkins University Press.

## Also see

$[\mathrm{R}]$ regress - Linear regression

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