

The World's Largest Open Access Agricultural & Applied Economics Digital Library

# This document is discoverable and free to researchers across the globe due to the work of AgEcon Search.

Help ensure our sustainability.

Give to AgEcon Search

AgEcon Search
<a href="http://ageconsearch.umn.edu">http://ageconsearch.umn.edu</a>
<a href="mailto:aesearch@umn.edu">aesearch@umn.edu</a>

Papers downloaded from **AgEcon Search** may be used for non-commercial purposes and personal study only. No other use, including posting to another Internet site, is permitted without permission from the copyright owner (not AgEcon Search), or as allowed under the provisions of Fair Use, U.S. Copyright Act, Title 17 U.S.C.

## THE STATA JOURNAL

Editor

H. Joseph Newton Department of Statistics Texas A&M University College Station, Texas 77843 979-845-8817; fax 979-845-6077 jnewton@stata-journal.com

Associate Editors

Christopher F. Baum Boston College

Nathaniel Beck New York University

Rino Bellocco Karolinska Institutet, Sweden, and

Maarten L. Buis Tübingen University, Germany

A. Colin Cameron University of California—Davis

Mario A. Cleves Univ. of Arkansas for Medical Sciences

University of Milano-Bicocca, Italy

William D. Dupont Vanderbilt University

David Epstein Columbia University

Allan Gregory Queen's University

James Hardin University of South Carolina

Ben Jann University of Bern, Switzerland

Stephen Jenkins
London School of Economics and
Political Science

Ulrich Kohler WZB, Berlin

Frauke Kreuter University of Maryland-College Park

Stata Press Editorial Manager Stata Press Copy Editors Editor

Nicholas J. Cox Department of Geography Durham University South Road Durham DH1 3LE UK n.j.cox@stata-journal.com

Peter A. Lachenbruch Oregon State University

Jens Lauritsen Odense University Hospital

Stanley Lemeshow Ohio State University

J. Scott Long Indiana University

Roger Newson Imperial College, London

Austin Nichols Urban Institute, Washington DC

Marcello Pagano Harvard School of Public Health

Sophia Rabe-Hesketh University of California-Berkeley

J. Patrick Royston MRC Clinical Trials Unit, London

Philip Ryan University of Adelaide

Mark E. Schaffer Heriot-Watt University, Edinburgh

Jeroen Weesie Utrecht University

Nicholas J. G. Winter University of Virginia

Jeffrey Wooldridge Michigan State University

Lisa Gilmore Deirdre Skaggs

The Stata Journal publishes reviewed papers together with shorter notes or comments, regular columns, book reviews, and other material of interest to Stata users. Examples of the types of papers include 1) expository papers that link the use of Stata commands or programs to associated principles, such as those that will serve as tutorials for users first encountering a new field of statistics or a major new technique; 2) papers that go "beyond the Stata manual" in explaining key features or uses of Stata that are of interest to intermediate or advanced users of Stata; 3) papers that discuss new commands or Stata programs of interest either to a wide spectrum of users (e.g., in data management or graphics) or to some large segment of Stata users (e.g., in survey statistics, survival analysis, panel analysis, or limited dependent variable modeling); 4) papers analyzing the statistical properties of new or existing estimators and tests in Stata; 5) papers that could be of interest or usefulness to researchers, especially in fields that are of practical importance but are not often included in texts or other journals, such as the use of Stata in managing datasets, especially large datasets, with advice from hard-won experience; and 6) papers of interest to those who teach, including Stata with topics such as extended examples of techniques and interpretation of results, simulations of statistical concepts, and overviews of subject areas.

For more information on the  $Stata\ Journal$ , including information for authors, see the webpage

#### http://www.stata-journal.com

The Stata Journal is indexed and abstracted in the following:

- CompuMath Citation Index®
- Current Contents/Social and Behavioral Sciences®
- RePEc: Research Papers in Economics
- Science Citation Index Expanded (also known as SciSearch®)
- $\bullet$  Scopus
- Social Sciences Citation Index®

Copyright Statement: The Stata Journal and the contents of the supporting files (programs, datasets, and help files) are copyright © by StataCorp LP. The contents of the supporting files (programs, datasets, and help files) may be copied or reproduced by any means whatsoever, in whole or in part, as long as any copy or reproduction includes attribution to both (1) the author and (2) the Stata Journal.

The articles appearing in the *Stata Journal* may be copied or reproduced as printed copies, in whole or in part, as long as any copy or reproduction includes attribution to both (1) the author and (2) the *Stata Journal*.

Written permission must be obtained from StataCorp if you wish to make electronic copies of the insertions. This precludes placing electronic copies of the *Stata Journal*, in whole or in part, on publicly accessible websites, fileservers, or other locations where the copy may be accessed by anyone other than the subscriber.

Users of any of the software, ideas, data, or other materials published in the *Stata Journal* or the supporting files understand that such use is made without warranty of any kind, by either the *Stata Journal*, the author, or StataCorp. In particular, there is no warranty of fitness of purpose or merchantability, nor for special, incidental, or consequential damages such as loss of profits. The purpose of the *Stata Journal* is to promote free communication among Stata users.

The Stata Journal, electronic version (ISSN 1536-8734) is a publication of Stata Press. Stata, Mata, NetCourse, and Stata Press are registered trademarks of StataCorp LP.

#### tt: Treelet transform with Stata

Anders Gorst-Rasmussen
Department of Mathematical Sciences
Alborg University
Alborg, Denmark
agorstras@gmail.com

Abstract. The treelet transform is a recent data reduction technique from the field of machine learning. Sharing many similarities with principal component analysis, the treelet transform can reduce a multidimensional dataset to the projections on a small number of directions or components that account for much of the variation in the original data. However, in contrast to principal component analysis, the treelet transform produces sparse components. This can greatly simplify interpretation. I describe the tt Stata add-on for performing the treelet transform. The add-on includes a Mata implementation of the treelet transform algorithm alongside other functionality to aid in the practical application of the treelet transform. I demonstrate an example of a basic exploratory data analysis using the tt add-on.

**Keywords:** st0249, tt, ttcv, ttscree, ttdendro, ttloading, ttpredict, ttstab, treelet, principal component analysis, dimension reduction, factor analysis

#### 1 Introduction

A common task in data analysis is to summarize a multidimensional dataset. One popular and convenient approach is to find a few interesting directions in the data and use the corresponding linear projections of data as representatives of the original data in plots, regression models, and so forth. This is known as dimension reduction. Principal component analysis (PCA) is a standard dimension reduction method that works by calculating the first few eigenvectors (components) of a covariance or correlation matrix and reducing the dataset to a collection of component scores—the projection of data onto components. This strategy has the optimality property of explaining as much variation as possible in the original data using as few dimensions as possible.

Entries of the components (loadings) are often subject to interpretation. Variables corresponding to "large" loadings are interpreted as being important for describing the original data; variables corresponding to "small" loadings can be discarded. Such interpretation is complicated by the fact that all component loadings are nonzero. Various cutoff rules, component rotation strategies, and other procedures have been developed to simplify interpretation (Jolliffe 2002), but these largely ad hoc procedures do not contribute to the transparency or objectivity of PCA.

In the machine learning community, there has been a growing interest in developing alternatives to PCA that offer more-interpretable components by forcing loading patterns where many loadings are exactly zero (that is, by forcing sparse components). For

example, Zou, Hastie, and Tibshirani (2006) developed a variant of PCA where sparse components are estimated via penalized regression with automatic variable selection.

The treelet transform (TT) proposed by Lee, Nadler, and Wasserman (2008) is a similar recent alternative to PCA. The TT introduces sparsity among component loadings in an elegant and simple fashion by combining ideas from hierarchical clustering analysis with ideas from PCA. This leads to sparse components that, similarly to PCA components, account for a large part of the variation in the original data and can be used analogously. In addition, it leads to an associated cluster tree that provides a concise visual representation of loading sparsity patterns and the general dependency structure of the data.

I describe in this article the Stata add-on tt, which contains a Mata implementation of the TT algorithm. In addition to the TT algorithm itself, tt includes several other functions to aid in model selection and output analysis in practice. Using the auto.dta dataset that comes with Stata, I provide a small demonstration of how the various functions work together and how a complete TT analysis using tt might look.

## 2 The TT algorithm

This section provides a brief, nontechnical review of the TT algorithm. For a more formal derivation of the TT algorithm and its properties, see the original article by Lee, Nadler, and Wasserman (2008).

Given a collection of p variables, the TT algorithm proceeds as follows:

Variable pairing. Locate the two variables with the largest correlation coefficient.

**Local PCA.** Merge these two variables by performing PCA on them. Keep the new variable whose score has the largest variance (the "sum" variable); discard the other new variable (the "residual" variable).

This process yields a new collection of p-1 variables, namely, the sum variable and the remaining p-2 original variables, on which we then repeat the above two steps. The "variable pairing" and "local PCA" scheme is repeated for a total of p-1 times until only a single sum variable is left. This in turn defines a basic hierarchical clustering algorithm, the output of which is conveniently represented as a binary tree with p levels (a cluster tree or cluster dendrogram). Variables that are "close" in this cluster tree and that are merged early represent groups of more highly correlated variables.

Hierarchical clustering is itself a well-known technique. The novelty of the TT is its use of PCA to merge variables because it enables us to construct, at each level of the TT cluster tree, a complete coordinate system for the data. Specifically, viewing the TT in terms of its action on components rather than on variables, let us begin with a coordinate system consisting of the trivial, one-variable components (the standard coordinate system of  $\mathbb{R}^p$ ). Each local PCA of two variables corresponds to performing an orthogonal rotation of two components. It follows that a coordinate system for the data at a given level of the TT cluster tree is given by the collection of

- 1. the components corresponding to sum variables available at the current level;
- 2. components corresponding to all previously calculated residual variables; and
- 3. "trivial" components for variables that have not yet joined the cluster tree.

The level-specific and data-specific coordinate system thus comprises "sum" components that encode coarse-grained, low-resolution information about the dependency relationships between all variables included so far alongside "residual" components that encode information about the more local relationships between variables at an increasingly greater resolution. It can be shown that if a TT is applied to a collection of variables with a covariance matrix featuring high intrablock correlation and low interblock correlation, then the loadings of sum components will be constant on variables within blocks in large samples (Lee, Nadler, and Wasserman 2008). Hence, the TT can help identify groups of correlated variables.

#### 2.1 Selecting a cut-level

Application of the TT to a dataset yields, as its basic output, a cluster tree alongside a coordinate system for the data at each level of the cluster tree. As described above, the coordinate system combines coarse components (similar to components obtained from PCA) with higher-resolution components that reflect local dependency relationships. We seek to use this collection of coordinate systems for dimension reduction purposes.

If we knew which cluster tree level (cut-level) to use, we could calculate variances of the level-specific component scores and retain components corresponding to the highest-variance scores. This is the approach used in PCA with one difference: TT component scores are generally correlated and do not lead to a true decomposition of variance. This is a known issue in dimension reduction (Gervini and Rousson 2004) because PCA is the only method yielding both orthogonal components and uncorrelated scores.

Selecting a cut-level for the TT cluster tree amounts to deciding the level of detail desired in the dimension reduction (the amount of regularization). A coordinate system close to the leaves of the cluster tree mostly contains highly sparse components and may not be useful for dimension reduction in the sense that the high-resolution components are not much more informative than the original one-variable components. Conversely, a coordinate system close to the root includes coarse-grained, low-resolution components more suitable for dimension reduction, but it may be harder to interpret because of a lack of sparsity. We usually prefer a data-driven choice of cut-level.

Choosing a cut-level from data is not trivial because coordinate systems at different cut-levels are equally capable of describing the data so long as we use a sufficiently large number of components. However, cross-validation methods can be used to find a cut-level at which we can describe the data using only a few components. Suppose that we wish to describe the data using exactly m components. Then we determine an appropriate cut-level by using the following K-fold cross-validation strategy (Lee, Nadler, and Wasserman 2008):

1. Split the data randomly into K roughly equal-sized subsets. For each of these subsets, do the following:

- For each cut-level  $1, \ldots, p-1$ , calculate the m highest-variance components using all subsets of data except the current one. Next calculate the sum of variances of scores based on these components using only the current subset.
- 2. For each cut-level  $1, \ldots, p-1$ , calculate a cross-validation score by averaging the K sums of component variances obtained in step 1.

A flowchart visualizing step 1 of the cross-validation strategy is shown in figure 1.

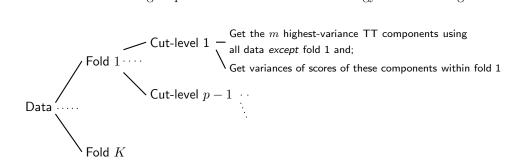


Figure 1. Flow chart of the cross-validation strategy for deciding an optimal cut-level

Once cross-validation scores have been obtained, a suitable cut-level can be found by locating a "knee" in the graph of cross-validation scores against cut-level (a "knee" is a point at which increasing the cut-level does not substantially increase the cross-validation score). In other words, we select the cut-level at which we can explain almost as much variation as possible, using as low a cut-level as possible to simplify interpretation of components.

Note that the cross-validation strategy requires us to specify the number of components m to use. This is not much different from the corresponding problem of selecting the number of components to retain in PCA, or selecting the number of clusters in a cluster analysis. In section 4, we propose a simple data-driven strategy for selecting both the cut-level and the number of components.

#### 2.2 Stability assessment

A data analyst may wish to know how much trust to place in a collection of components obtained using the TT. Because a key feature of the TT is its ability to produce sparse components, it is of particular interest to assess the stability of loading sparsity patterns. This can be done by using a subsampling approach inspired by Ben-Hur, Elisseeff, and Guyon (2002).

We first specify a cut-level k and a number m of TT components to retain. Then we repeat the following subsampling scheme 100 times:

- 1. Randomly sample 80% of the data.
- 2. Within this subsample, calculate the m highest-variance TT components at cutlevel k of the cluster tree. For each of these m components, do the following:
  - Calculate the sign pattern of the component. For example, a component whose loadings in the original variables are (-0.1, 0.2, 0, 0.1) corresponds to the sign pattern (-, +, 0, +).
  - Calculate the variance explained by the corresponding component.
  - Calculate the rank according to the variance explained by the corresponding component.

The collection of all  $100 \times m$  sign patterns, alongside their variances and ranks, carries information about the stability and the importance of different sign patterns appearing in the subsampled TT analyses. As a measure of stability, we count the number of times we see a particular sign pattern among all  $100 \times m$  patterns while using the average rank and average variance of the sign pattern as measures of importance. The final output of the stability analysis is the relative frequency, average variance, and average rank of each sign pattern occurring in more than 10 out of the 100 subsampled TT analyses. Note that this number is generally different from m.

#### 3 The tt add-on

#### 3.1 Syntax

The main function tt is implemented as a Mata function run via a Stata wrapper. It is loosely based on the R-code by Liu (2011) and has the following syntax:

```
tt varlist [if] [in] [weight], cut(#) [components(#) [correlation|covariance] noblanks]
```

After running tt, the user will typically run ttcv, which uses the cross-validation strategy of section 2.1 to select a cut-level for the TT cluster tree. ttcv has the following syntax:

```
ttcv varlist \ [if] \ [in] \ [weight], \ \underline{components}(\#) \ [\underline{f}olds(\#) \ \underline{r}eps(\#) \ \underline{percent}(\#) \ [\underline{correlation} \ | \underline{covariance}] \ force]
```

A range of different postestimation commands is also available. As usual with postestimation commands, they require an initial run of tt.

Stability assessment as described in section 2.2 is available through the command ttstab, which has the following syntax:

```
ttstab [, \underline{r}eps(\#) \underline{s}ubsample(\#) \underline{k}eep(\#) force]
```

The TT cluster tree can be plotted by using the following command:

```
ttdendro [ , dendro\_options]
```

Scree plots of variances and "skyscraper plots" of component loadings are implemented in the commands ttscree and ttloading, respectively, with these syntaxes:

```
ttscree [, scatter_options neigen(#)]
ttloading [, scatter_options components(numlist)]
```

Finally, ttpredict implements prediction of component scores. As previously described, these are the projections of the original data onto the relevant TT component and can be informally interpreted as the degree of "adherence" of a given observation vector to the given component. The ttpredict syntax is

```
\texttt{ttpredict} \ [\textit{if}\ ] \ [\textit{in}\ ] \ \{\textit{stub*} \mid \textit{newvarlist}\}
```

#### 3.2 tt options

- cut(#) is required and specifies the cut-level of the TT cluster tree at which to extract components. The cut-level influences both the sparsity and the composition of components. See ttcv for a cross-validation method to determine a cut-level.
- components (#) sets the maximum number of components to be retained. tt displays the full set of components variances but displays loadings only for retained components. The default is the number of variables in varlist.
- correlation or covariance specifies that TT cross-validation be calculated using the correlation matrix or the covariance matrix, respectively. Choose only one of these two options; the default is correlation. Usually, TT cross-validation using the covariance matrix will be meaningful only if variables are expressed in the same units.
- noblanks displays zero loadings as 0s instead of as blanks. This option is included for readability.

#### 3.3 ttcv options

- components(#) is required and sets the number of components to be retained. In practice, this number may not be known in advance, in which case one should investigate the output of ttcv for a range of different choices of #.
- folds (#) specifies the number of folds (test samples) to use in cross-validation. The default is folds (10).
- reps(#) specifies the number of Monte Carlo repetitions of cross-validation. The default is reps(5). Monte Carlo repetitions reduce the sampling variation inherent in cross-validation. Increase # if the output of ttcv appears unstable over different runs.
- percent(#) specifies that a "knee" on the graph of cross-validation scores should be sought among cut-levels for which the score is within # percent of the crossvalidation score associated with the maximal cut-level. The default is percent(10).
- correlation or covariance specifies that TT cross-validation use the correlation matrix or the covariance matrix, respectively. Use only one of these two options; the default is correlation. Usually, TT cross-validation using the covariance matrix will be meaningful only if variables are expressed in the same units.
- force tries to force cross-validation even when zero-variance variables are found in training samples. This is usually an indication that there is something wrong; use this option with caution.

#### 3.4 ttstab options

- reps(#) specifies the number of subsamples. The default is reps(100).
- subsample(#) specifies the subsample size as a percentage of the original sample size.
  The default is subsample(80).
- keep(#) specifies to keep sign patterns appearing in more than # percent of replications. The default is keep(20).
- force tries to force subsampling even when zero-variance variables are found in subsamples. This is usually an indication that there is something wrong; use this option with caution.

#### 3.5 ttdendro options

dendro\_options are any of the options allowed by the cluster dendrogram command; see [MV] cluster dendrogram.

#### 3.6 ttscree and ttloading options

scatter\_options are any of the options allowed by the graph twoway scatter command; see [G-2] graph twoway scatter.

The following option applies only to ttscree:

neigen(#) plots only the largest # component variances. The default is to plot all component variances.

The following option applies only to ttloading:

components (numlist) plots components in numlist. The default is components (1 2 3).

## 4 A data example

As a simple illustration of the proposed workflow when using the tt add-on, let us consider the 1978 automobile dataset that comes with Stata. This dataset describes various characteristics of 74 vehicles. We will use the 10 variables described below for the analysis; 69 vehicles have complete observations for these variables.

- . sysuse auto (1978 Automobile Data)
- . describe price-gear\_ratio

variable name	storage type	display format	value label	variable label	
price	int	%8.0gc		Price	
mpg	int	%8.0g		Mileage (mpg)	
rep78	int	%8.0g		Repair Record 1978	
headroom	float	%6.1f		Headroom (in.)	
trunk	int	%8.0g		Trunk space (cu. ft.)	
weight	int	%8.0gc		Weight (lbs.)	
length	int	%8.0g		Length (in.)	
turn	int	%8.0g		Turn Circle (ft.)	
displacement	int	%8.0g		Displacement (cu. in.)	
gear_ratio	float	%6.2f		Gear Ratio	

## 4.1 Step 1: Running tt

To familiarize ourselves with the dataset, we first make two preliminary runs of tt and the tt postestimation plotting routines.

. tt price-gear\_ratio, cut(3) correlation components(3)

Treelet transform/correlation Number of obs = 69 Number of comp. = 3 Cut-level = 3

Component	Variance	Proportion	Cumulative	Adj. proportion
TC1	3.6404	0.3640	0.3640	0.3640
TC2	1.0000	0.1000	0.4640	0.0360
TC3	1.0000	0.1000	0.5640	0.0746
TC4	1.0000	0.1000	0.6640	0.0344
TC5	1.0000	0.1000	0.7640	0.0787
TC6	1.0000	0.1000	0.8640	0.0371
TC7		0.1000	0.9640	0.0652
TC8	0.1875	0.0187	0.9828	0.0143
TC9	0.1199	0.0120	0.9948	0.0086
TC10	0.1199	0.0120	1.0000	0.0086

#### Components

Variable	TC1	TC2	TC3
price mpg rep78 headroom trunk weight length turn displacement gear_ratio	0.5080 0.5080 0.4851 0.4985	1.0000	1.0000

. tt price-gear\_ratio, cut(6) correlation components(3)

-	•	-			
Treelet	transform/correlation		Number of ob	s =	69
			Number of co	mp. =	3
			Cut-level	=	6

Component	Variance	Proportion	Cumulative	Adj. proportion
TC1	4.5497	0.4550	0.4550	0.4550
TC2	1.6565	0.1657	0.6206	0.0432
TC3	1.0000	0.1000	0.7206	0.0800
TC4	1.0000	0.1000	0.8206	0.0717
TC5	0.6353	0.0635	0.8842	0.0515
TC6	0.4555	0.0455	0.9297	0.0328
TC7	0.3435	0.0343	0.9640	0.0335
TC8	0.1875	0.0187	0.9828	0.0143
TC9	0.1199	0.0120	0.9948	0.0086
TC10	0.0522	0.0052	1.0000	0.0031

#### Components

Varia	ıble	TC1	TC2	TC3
re headr tr wei ler	runk ght igth urn	0.3052 0.3639 0.4471 0.4471 0.4269		1.0000
displacem gear_ra		0.4367	0.7071	

- . ttdendro
- . ttscree

In both runs of tt, we retain three components, but we use different cut-levels 3 and 6, respectively. The relatively low cut-level of 3 in the first analysis yields components that are more sparse. In fact, components 2 and 3 in this first analysis are somewhat uninteresting for the purpose of dimension reduction because they contain only one variable. The second analysis uses the cut-level 6 and yields components that are less sparse.

Running tt returns both the "raw" variances explained by components and the variances adjusted for correlation between scores using the conservative method of Gervini and Rousson (2004). For this dataset, the first TT component explains the majority of the variation for both cut-level 3 and cut-level 6, irrespective of the method used for variance calculation. In both analyses, this first component can be informally interpreted as measuring the overall "size" of a vehicle.

Our output of ttdendro is shown in figure 2. The TT cluster tree shows that trunk, weight, length, displacement, and turn form a tight cluster. With the addition of the variable headroom, it is this particular cluster that is reflected by the first TT component

in the second run of tt above. It is a general feature of the TT algorithm that cluster membership in the cluster tree translates to nonzero loadings in some TT component. In other words, the cluster tree provides a concise visual representation of the possible TT components.

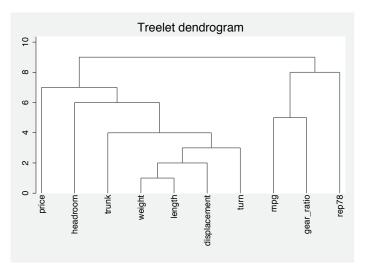


Figure 2. Cluster tree produced by ttdendro

Figure 3 is obtained by ttscree. It is a graphical representation, similar to PCA scree plots, of the (unadjusted) variance explained by components. It is clear from this plot that a single component suffices to capture much of the variation in the data.

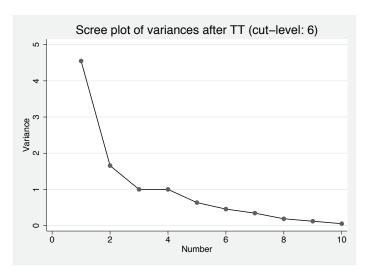


Figure 3. Scree plot of variances of TT component scores when cut-level 6 is used

The first TT component in the second run of tt above is very similar to the first component obtained from the corresponding PCA, as seen in the numerical loadings and Pearson correlation between scores calculated below. However, the first TT component is potentially simpler to interpret because of its sparsity.

- . ttpredict tt1score
  (9 components skipped)
- . pca price-gear\_ratio, correlation components(2)

Principal components/correlation

Number of obs = 69

Number of comp. = 2

Trace = 10

Rotation: (unrotated = principal)

Rho = 0.7389

Compo	nent	Eigenvalue	Difference	Proportion	Cumulative
C	omp1	6.31248	5.23618	0.6312	0.6312
C	omp2	1.0763	.0622654	0.1076	0.7389
C	omp3	1.01403	.583752	0.1014	0.8403
C	omp4	.430283	.0343745	0.0430	0.8833
C	omp5	.395908	.116712	0.0396	0.9229
C	omp6	.279196	.0229213	0.0279	0.9508
C	omp7	.256275	.130573	0.0256	0.9764
C	omp8	.125701	.0442338	0.0126	0.9890
C	omp9	.0814675	.0531123	0.0081	0.9972
Co	mp10	.0283551		0.0028	1.0000
	-				

Principal components (eigenvectors)

Variable	Comp1	Comp2	Unexplained
price	0.2074	0.3876	.5668
mpg	-0.3394	0.0520	. 2699
rep78	-0.1830	0.7639	.1606
headroom	0.2304	0.3049	.565
trunk	0.3003	0.3401	.3061
weight	0.3848	0.0095	.06535
length	0.3771	0.0432	.1003
turn	0.3542	-0.1831	.1719
displacement	0.3742	-0.0121	.1157
gear_ratio	-0.3306	0.1388	. 2895

- . predict pc1score
   (output omitted)
- . correlate tt1score pc1score
  (obs=69)

	tt1score	pc1score
tt1score	1.0000	
pc1score	0.9842	1.0000

#### 4.2 Step 2: Running ttcv

From the analysis in step 1, we found evidence that a single TT component suffices to describe the majority of variation in the data. It turns out that the optimal cut-level

for a single-component solution is 9 (the maximal possible) and that the single retained component has all nonzero loadings for this cut-level.

To illustrate, suppose instead that we decide to keep three components. We then find a suitable cut-level by running ttcv, as follows:

#### Cross-validation scores

Cut-level	Score	Proportion
1	5.3090	0.6464
2	6.1245	0.7457
3	6.8463	0.8336
4	7.1436	0.8698
5	7.4875	0.9116
6	7.7642	0.9453
7	7.8010	0.9498
8	7.9786	0.9715
9	8.2131	1.0000

Estimated optimal cut-level = 6 (optimal cut-level sought within 10% of highest cut-level score)

Figure 4 shows a plot of the cross-validation scores generated when running ttcv. Although not entirely convincing, a "knee" in the graph seems to be located around level 6, indicating that increasing the cut-level beyond this level may not substantially improve the amount of variance explained by the three components. Thus for a three-component solution, a cut-level of 6 appears adequate.

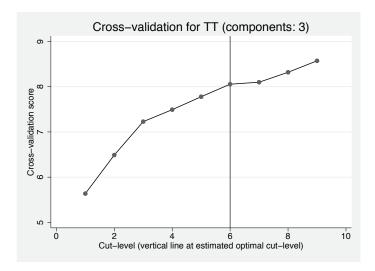


Figure 4. Graph of cross-validation scores for the TT when three components are retained; the graph suggests that a "knee" in the graph is located at cut-level 6

Choosing simultaneously the number of components to retain and a cut-level is easy for this dataset because a single-component solution seems to be preferable at most nontrivial cut-levels. In situations where it is unclear how many components to retain, the choice can be more difficult. The following strategy is recommended:

- 1. Decide on a range of different sensible values of components() for tt via, for example, an investigation of scree plots.
- 2. Perform ttcv for each of these choices of components().

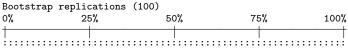
In our experience, there will often be a reasonably small range of cut-levels that are universally preferable for the selected range of components(). A parsimonious solution is then to use the smallest acceptable cut-level among these.

#### 4.3 Step 3: Running ttstab

For the choice cut(6) and components(3) in running tt, we conclude our analysis by investigating the stability of the obtained solution via ttstab.

. tt price-gear\_ratio, cut(6) correlation components(3)  $(output\ omitted)$ 

. ttstab



Stability of TT/correlation	Number of obs	=	69
	Number of comp.	=	3
	Cut-level	=	6
	Bootstrap rep.	=	100
	Subsample frac.	=	0.80
	Subsample size	=	55

Average rank (by amount of variance explained) and frequency of sign patterns Displaying results for patterns with frequency >= 10%

Sign pattern	Avg. rank	Frequency	Avg. variance
1 2 3	1.000 2.000 3.000	0.900 0.990 0.470	4.557 1.656 1.000
4	3.000	0.510	1.000

Structure of sign patterns

Variable	1	2	3	4
	_	_	_	
price	0	0	0	+
mpg	0	+	0	0
rep78	0	0	+	0
headroom	+	0	0	0
trunk	+	0	0	0
weight	+	0	0	0
length	+	0	0	0
turn	+	0	0	0
displacement	+	0	0	0
gear_ratio	0	+	0	0

ttstab performs 100 subsampling repetitions of the TT, keeping the three highest-variance components in each subsampled analysis (at cut-level 6). It then transforms these into their corresponding sign patterns. Note that ttstab is set to return all sign patterns seen in more than 10% of the subsampling repetitions, here corresponding to four sign patterns. In the output, Avg. rank is the rank (according to explained variance of the corresponding component) averaged over the 100 subsamples. Frequency is the relative frequency of the sign pattern among all  $3 \times 100$  sign patterns returned. Finally, Avg. variance is the variance explained by the component corresponding to the sign pattern, averaged over the 100 subsamples.

We can see that sign patterns similar to those of the first two components from the original TT analysis with components(3) and cut(6) appear in almost all subsampling repetitions. If the first type of sign pattern appears, it corresponds to a component with rank 1. Moreover, the first component remains by far the most important in terms of variance explained. Sign patterns 3 and 4, however, do not appear to be very stable. Increasing the number of retained components to 4 (not shown) leads to greater stability in terms of frequency of inclusion but does not improve stability of the rank of the last two components.

## 5 Concluding remarks

The TT can be viewed as an amalgamation of PCA and cluster analysis. It leads to components that are sparse, and they can be easier to interpret than their PCA counterparts. I described the tt add-on for Stata, which contains all the basic functionality needed to apply the TT in practice, including a Mata implementation of the TT algorithm. For a more advanced application example and a detailed comparison with the output produced by PCA, I recommend the article by Gorst-Rasmussen et al. (2011).

## 6 Acknowledgments

I thank Søren Lundbye-Christensen and Christina C. Dahm for their helpful comments and suggestions when preparing this article.

Some of the work on the tt add-on was completed while I was employed at the Center for Cardiovascular Research, Aalborg Hospital, Aarhus University Hospital in Aalborg, Denmark.

#### 7 References

Ben-Hur, A., A. Elisseeff, and I. Guyon. 2002. A stability based method for discovering structure in clustered data. *Pacific Symposium on Biocomputing* 7: 6–17.

Gervini, D., and V. Rousson. 2004. Criteria for evaluating dimension-reducing components for multivariate data. *American Statistician* 58: 72–76.

- Gorst-Rasmussen, A., C. C. Dahm, C. Dethlefsen, T. Scheike, and K. Overvad. 2011. Exploring dietary patterns by using the treelet transform. American Journal of Epidemiology 173: 1097–1104.
- Jolliffe, I. T. 2002. Principal Component Analysis. 2nd ed. New York: Springer.
- Lee, A. B., B. Nadler, and L. Wasserman. 2008. Treelets—an adaptive multi-scale basis for sparse unordered data. *Annals of Applied Statistics* 2: 435–471.
- Liu, D. 2011. treelet: Treelet. R package version 0.3-0. http://cran.r-project.org/package=treelet.
- Zou, H., T. Hastie, and R. Tibshirani. 2006. Sparse principal component analysis. Journal of Computational and Graphical Statistics 15: 265–286.

#### About the author

Anders Gorst-Rasmussen is a biostatistician at the Center for Cardiovascular Research, Aalborg Hospital, Aarhus University Hospital in Aalborg, Denmark. This article was completed in connection with the author's PhD studies in the Department of Mathematical Sciences at Aalborg University in Aalborg, Denmark.