Finding the Number of Principal Components

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1 Getting Started

In this section, we describe how to select significant number of PCs using the **PCDimension** R package. The latest version of the package is always available from the R-Forge webpage (`http://r-forge.r-project.org/R/?group_id=1900`); the latest stable version can be found on CRAN. We illustrate the methods by exploring a small simulated data set.

First, we load all of the R library packages that we need for this analysis. Note that **PCDimension** implements the Broken-Stick model, the randomization-based procedure of ter Brack [1,2], and the Auer-Gervini model [3], while **nFactors** (developed by Raiche and Magis) is used to run Bartlett's test and its variants.

```
> library(PCDimension)
> library(nFactors) # implements Bartlett's test
> library(MASS) # for mvrnorm to simulate data
```

2 Testing on Unstructured Data

Next, we simulate an unstructured data set with random noise. That is, the variation of the data is isotropic and the number of significant PCs is 0. The data is generated via the command:

```
> set.seed(12345)
> NC <- 15
> NS <- 200
> ranData <- matrix(rnorm(NS*NC, 6), ncol=NC)
```

2.1 Bartlett's Test

Now, we apply Bartlett's test to the simulated data. The required input includes the raw data and the number of subjects (rows).

```
> nBartlett(data.frame(ranData), nrow(ranData))
```

```
$detail
    v    values  bartlett bartlett.chi bartlett.df bartlett.p anderson.chi
1   1 1.4646022 0.5811268  104.8482325         105  0.4858195  108.5572726
2   2 1.3301697 0.6364281   86.9876297          91  0.5995868   90.3767582
3   3 1.2587707 0.6773467   74.7328956          78  0.5838392   77.9144003
```

```
4   4 1.2303421 0.7138211   64.4466584          66  0.5311236   67.4245772
5   5 1.1537568 0.7543483   53.7021487          55  0.5243156   56.3802086
6   6 1.1204785 0.7881762   45.1867156          45  0.4641529   47.6067241
7   7 1.0644224 0.8245035   36.5042393          36  0.4452273   38.5947904
8   8 1.0357668 0.8581814   28.8291453          28  0.4212319   30.5879526
9   9 0.9636934 0.8968358   20.4517639          21  0.4928295   21.7765010
10 10 0.8806406 0.9291664   13.7506548          15  0.5445180   14.6934869
11 11 0.8216507 0.9510221    9.3656543          10  0.4977885   10.0435971
12 12 0.7727787 0.9679198    6.0592821           6  0.4165822    6.5212004
13 13 0.7216466 0.9826413    3.2424724           3  0.3557300    3.5022204
14 14 0.6272634 0.9961553    0.7107126           1  0.3992073    0.7704202
15 15 0.5540174 1.0000000    0.0000000           0  1.0000000    0.0000000
   anderson.df anderson.p lawley.chi lawley.df  lawley.p
1          119  0.7435170 104.848232       105 0.4858195
2          104  0.8270435  87.059078        91 0.5974780
3           90  0.8144247  74.799593        78 0.5816965
4           77  0.7739155  64.506178        66 0.5290321
5           65  0.7682480  53.751380        55 0.5224186
6           54  0.7178408  45.229911        45 0.4623519
7           44  0.7018560  36.539032        36 0.4436253
8           35  0.6810483  28.857191        28 0.4197981
9           27  0.7486461  20.471358        21 0.4916057
10          20  0.7936695  13.764296        15 0.5434754
11          14  0.7589891   9.375495        10 0.4968766
12           9  0.6868314   6.065849         6 0.4158543
13           5  0.6230517   3.246031         3 0.3552250
14           2  0.6803077   0.711493         1 0.3989486
15           0  1.0000000   0.000000         0 1.0000000

$nFactors
bartlett anderson   lawley
      15       15        0

attr(,"class")
[1] "nFactors" "list"
```

The original version of Bartlett's test, and the Anderson variant, fail to return the correct number of components. The Lawley variant does yield the correct value, 0.

2.2 Randomization-Based Methods

The **PCDimension** package implements both of the randomization-based statistics that were identified as successful in a previous study [4]. The number of permutations (default, $B = 1000$) and the significance level (default, $\alpha = 0.05$) are optional input arguments in addition to the required data set. The estimated number of PCs is the last point at which the p-value of the statistic of interest greater than the observed one is at least the threshold significance level.

```
> rndLambdaF(ranData) # input argument is data
```

```
rndLambda      rndF
        0         0
```

The randomization-based procedure successfully recovers the true number of PCs.

2.3 Broken-Stick

The **PCDimension** package also implements the Broken-Stick model. Both this model and the Auer-Gervini model require the eigenvalues from the singular value decomposition of the data matrix used to compute the principal components. We compute the decomposition using the `SamplePCA` function from the **ClassDiscovery** package, and then extract the variances.

```
> spca <- SamplePCA(t(ranData))
> lambda <- spca@variances[1:(NC-1)]
> bsDimension(lambda)
```

```
[1] 0
```

In the Broken-Stick model, the individual percentages of variance of the components are compared with the values expected from the "broken stick" distribution. The two distributions are compared element-by-element, and first value $d + 1$ where the expected value is larger than the observed value determines the dimension. The Broken-Stick model also correctly finds that there are zero significant PCs.

Note: In our implementation of tbhe `bsDimension` function, we add an extra parameter (`FUZZ`, with default value 0.005) for this comparison to deal with numerical errors in the estimates of the eigenvalues.

2.4 Auer-Gervini

We now use the `SamplePCA` object to construct an Auer-Gervini object.

```
> ag.obj <- AuerGervini(spca)
> agDimension(ag.obj)

[1] 0
```

The `agDimension` function takes an optional argument, `agfun` that specifies the method used to automate the computation of the number of PCs. The default value uses the **TwiceMean** method, which correctly concludes that there are zero significant PCs. We can also compare the results of multiple algorithms to automate the procedure.

```
> f <- makeAgCpmFun("Exponential")
> agfuns <- list(twice=agDimTwiceMean, specc=agDimSpectral,
+                km=agDimKmeans, km3=agDimKmeans3,
+                tt=agDimTtest, tt2=agDimTtest2,
+                cpt=agDimCPT, cpm=f)
> compareAgDimMethods(ag.obj, agfuns) # compare the list of all criteria

twice specc    km   km3    tt   tt2   cpt   cpm
    0     0     0     0     1     0     0     0
```

Overall, the Auer-Gervini model does an excellent job in selecting the actual number of components since 7 criteria out of 8 return 0 while only the "Ttest" procedure yields 1. If the majority rule is applied, that is, the estimated number of PCs is the one selected in more than 4 criteria in Auer-Gervini model, then we will definitely have 0 as the estimated number of components.

To get a more comprehensive understanding of the Broken-Stick method and the Auer-Gervini model, we use the command to generate the plots of these two models in Figures 1 and 2:

```
> bs <- brokenStick(1:NC, NC)
> bs0 <- brokenStick(1:(NC-1), (NC-1))
```

Figure 1 shows the broken stick distributions and the relative proportions of the variation that are explained by all the components in the simulated data set. The blue dotted line reprensents the broken stick distributions under the condition that p equals the number

```
> pts <- screeplot(spca, ylim=c(0, 0.2))
> lines(pts, bs, type='b', col='blue', lwd=2, pch=16)
> lines(pts[-NC], bs0, type='b', col='red', lwd=2, pch=16)
```

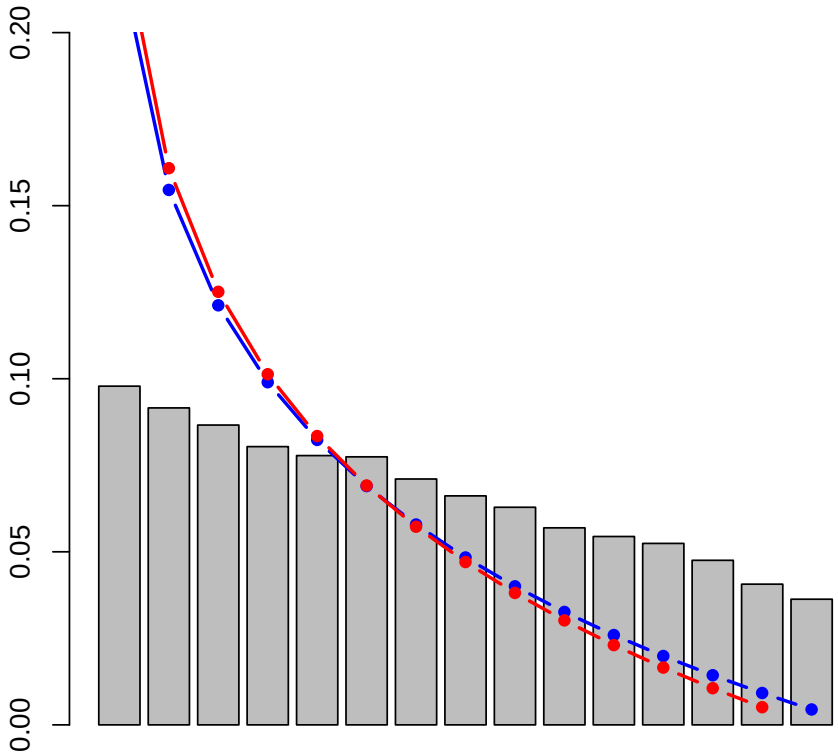

Figure 1: Screeplot of the data and the Broken-Stick model.

```
> plot(ag.obj, agfuns)
```

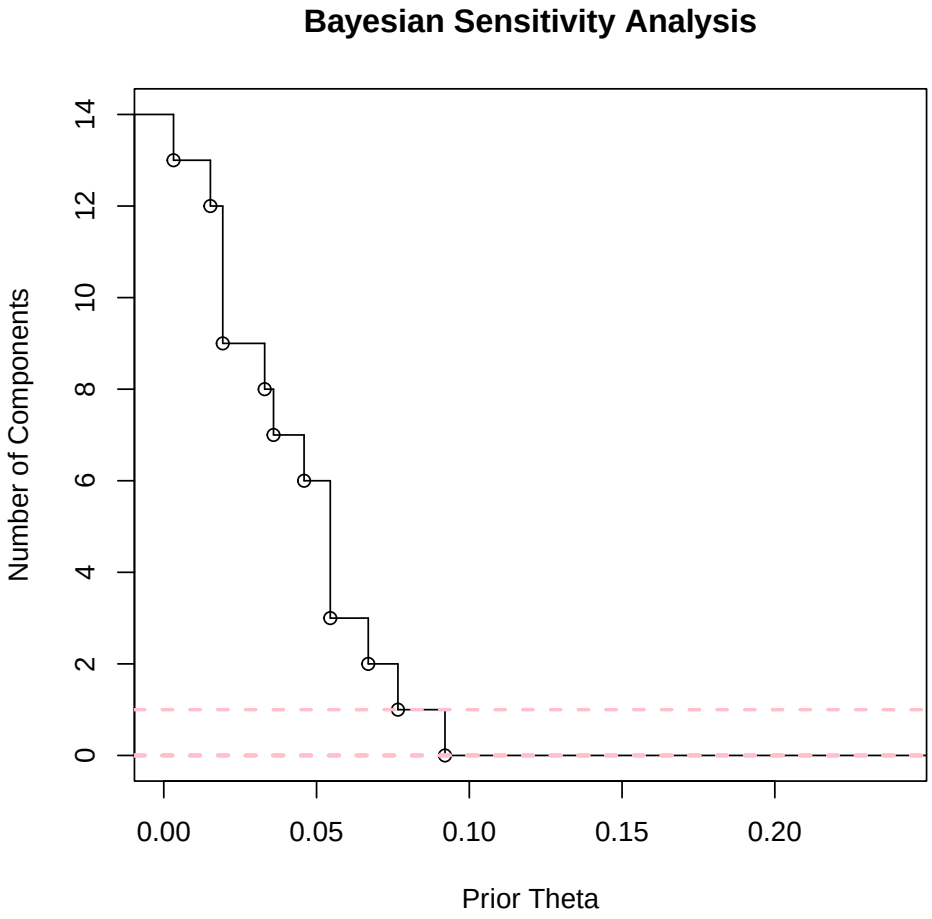

Figure 2: Auer-Gervini step function relating the prior hyperparameter θ to the maximum posterior estimate of the number K of significant principal components.

of features, while the red one means the broken stick distributions after removing the 0 eigenvalue with p equating with the number of features minus one. And there is almost no difference after removing the effect of eigenvalue 0. The grey rectangles are the relative proportions of the variation explained by all PCs. This figure provides a clear illustration on how the relative proportions are compared with the broken stick distributions and how the estimated number of PCs is chosen from the Broken-Stick model. Figure 2 illustrates how the Auer-Gervini model works. For the simulated data set, there are $NC = 15$ features, so the possible models $\mathcal{M}_d$ range from $\mathcal{M}_0$ to $\mathcal{M}_{14}$. The values $d = 0, 3, 4, 6, 7, 8, 11, 12, 13$ and 14 should be retained since the step functions are flat on those vertical coordinates. From the plot, we can see that the highest dimension d for which the step is significantly large is at $d = 0$. So $\mathcal{M}_0$ is a reasonable model.

3 Testing on Data with Structure

Now we simulate another dataset, with two groups of correlated samples.

```
> mu <- rep(0, 15)
> sigma <- matrix(0, 15, 15)
> sigma[1:8, 1:8] <- 0.7
> sigma[9:15, 9:15] <- 0.3
> diag(sigma) <- 1
> struct <- mvrnorm(200, mu, sigma)
```

3.1 Bartlett's Test

As before, we start by applying Bartlett's test to the simulated data.

```
> nBartlett(data.frame(struct), nrow(struct))
```

```
$detail
    v    values     bartlett bartlett.chi bartlett.df    bartlett.p
1   1 6.0810120 0.0001832254 1662.1592934         105 2.561146e-278
2   2 2.6210352 0.0166105559  788.8105014         104 9.426647e-106
3   3 1.0094725 0.1419738398  374.4802412          90  2.285714e-36
4   4 0.7866754 0.2121517991  296.3949752          77  1.751407e-27
5   5 0.7411964 0.2683570789  250.5907107          65  1.343425e-23
6   6 0.7038556 0.3452489339  201.8857709          54  6.149201e-19
7   7 0.6553115 0.4613915368  146.3219822          44  6.484416e-13
```

```
8   8 0.5446527 0.6422826664   83.4539984          35  7.780985e-06
9   9 0.3880309 0.8414173931   32.4327001          27  2.164379e-01
10 10 0.2990730 0.9311136612   13.3588195          20  8.614634e-01
11 11 0.2860686 0.9561475369    8.3632289          14  8.695576e-01
12 12 0.2473571 0.9834091489    3.1089955           9  9.598163e-01
13 13 0.2319970 0.9923990427    1.4128201           5  9.229058e-01
14 14 0.2091488 0.9987945770    0.2225347           2  8.946995e-01
15 15 0.1951131 1.0000000000    0.0000000           0  1.000000e+00
   anderson.chi anderson.df    anderson.p   lawley.chi lawley.df      lawley.p
1   1720.958716         119 5.698231e-282 1662.1592934       105 2.561146e-278
2    819.543378         104 1.396252e-111  788.8473505        91 1.062088e-111
3    390.422493          90  4.881417e-39  374.5277480        78  2.540012e-40
4    310.090645          77  9.971799e-30  296.5381658        66  5.828867e-31
5    263.087360          65  1.184840e-25  250.7447552        55  8.639871e-27
6    212.697915          54  1.053760e-20  202.0062587        45  8.985241e-22
7    154.701655          44  3.098939e-14  146.4039267        36  2.931901e-15
8     88.545356          35  1.568219e-06   83.4976948        28  1.988980e-07
9     34.533487          27  1.510814e-01   32.4512213        21  5.266764e-02
10    14.274785          20  8.162948e-01   13.3694995        15  5.737813e-01
11     8.968610          14  8.330561e-01    8.3718671        10  5.925628e-01
12     3.346004           9  9.489850e-01    3.1121719         6  7.946422e-01
13     1.525998           5  9.100503e-01    1.4144460         3  7.021520e-01
14     0.241230           2  8.863751e-01    0.2227962         1  6.369176e-01
15     0.000000           0  1.000000e+00    0.0000000         0  1.000000e+00

$nFactors
bartlett anderson   lawley
       8        8        8

attr(,"class")
[1] "nFactors" "list"
```

All three variants grossly overestimate the dimension.

3.2 Randomization-Based Methods

Next, we apply ter Braak's randomization procedures. Here we again use the defaulkt values of the parametes, but include them explicitly to illustrate the function.

```
> rndLambdaF(struct, B = 1000, alpha = 0.05) # input argument is data
```

```
rndLambda      rndF
        2         9
```

The randomization-based procedure `rndLambda` successfully recovers the true number of PCs, but the `rndF` procedure overestimates it. These results are consistent with a larger set of simulations that we have performed..

3.3 Broken-Stick

Next, we apply the broken-stick model. As before, we first compute the singular value decomposition using the `SamplePCA` function from the **ClassDiscovery** package.

```
> spca <- SamplePCA(t(struct))
> lambda <- spca@variances[1:(NC-1)]
> bsDimension(lambda)
```

```
[1] 2
```

The scree-plot (Figure 3) explains how the broken-stick model gets the correct answer.

```
> bs <- brokenStick(1:NC, NC)
> bs0 <- brokenStick(1:(NC-1), (NC-1))
```

3.4 Auer-Gervini

We now use the `SamplePCA` object to construct an Auer-Gervini object.

```
> ag.obj <- AuerGervini(spca)
> agDimension(ag.obj)
```

```
[1] 2
```

The `agDimension` function takes an optional argument, `agfun` that specifies the method used to automate the computation of the number of PCs. The default value uses the **TwiceMean** method, which correctly concludes that there are zero significant PCs. We can also compare the results of multiple algorithms to automate the procedure.

```
> pts <- screeplot(spca)
> lines(pts, bs, type='b', col='blue', lwd=2, pch=16)
> lines(pts[-NC], bs0, type='b', col='red', lwd=2, pch=16)
```

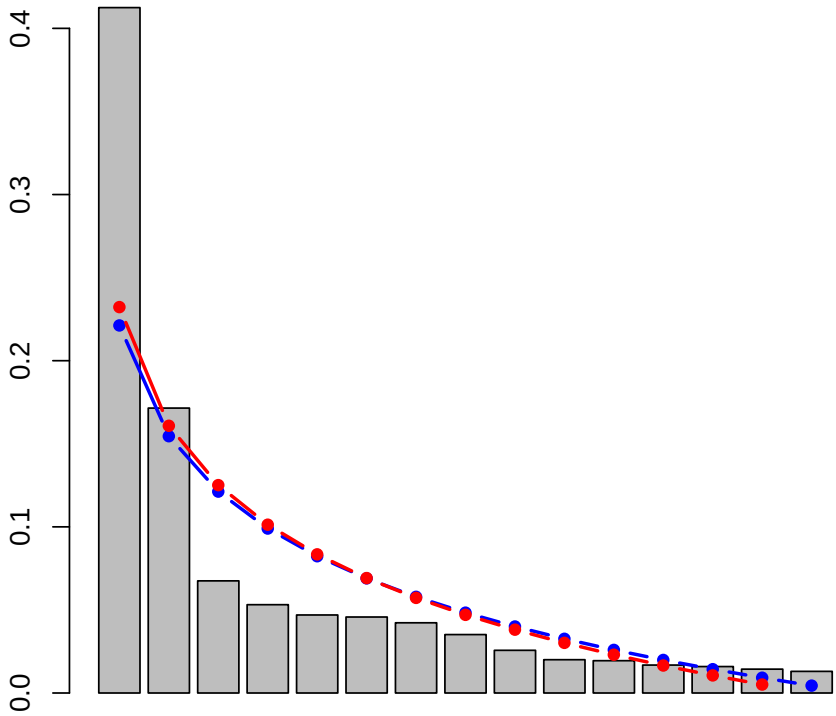

Figure 3: Screeplot of the structured data and the Broken-Stick model.

```
> f <- makeAgCpmFun("Exponential")
> agfuns <- list(twice=agDimTwiceMean, specc=agDimSpectral,
+                km=agDimKmeans, km3=agDimKmeans3,
+                tt=agDimTtest, tt2=agDimTtest2,
+                cpt=agDimCPT, cpm=f)
> compareAgDimMethods(ag.obj, agfuns) # compare the list of all criteria

twice specc    km   km3    tt   tt2   cpt   cpm
    2     2     2     2     3     2     1     2
```

Again, most of the criteria used to automate the Auer-Gervni method get te right answer. Two of them (`Ttest` and `CPM`), however, grossly overestimate it. Figure 4 shows the Auer-Gervini plot.

```
> plot(ag.obj, agfuns)
```

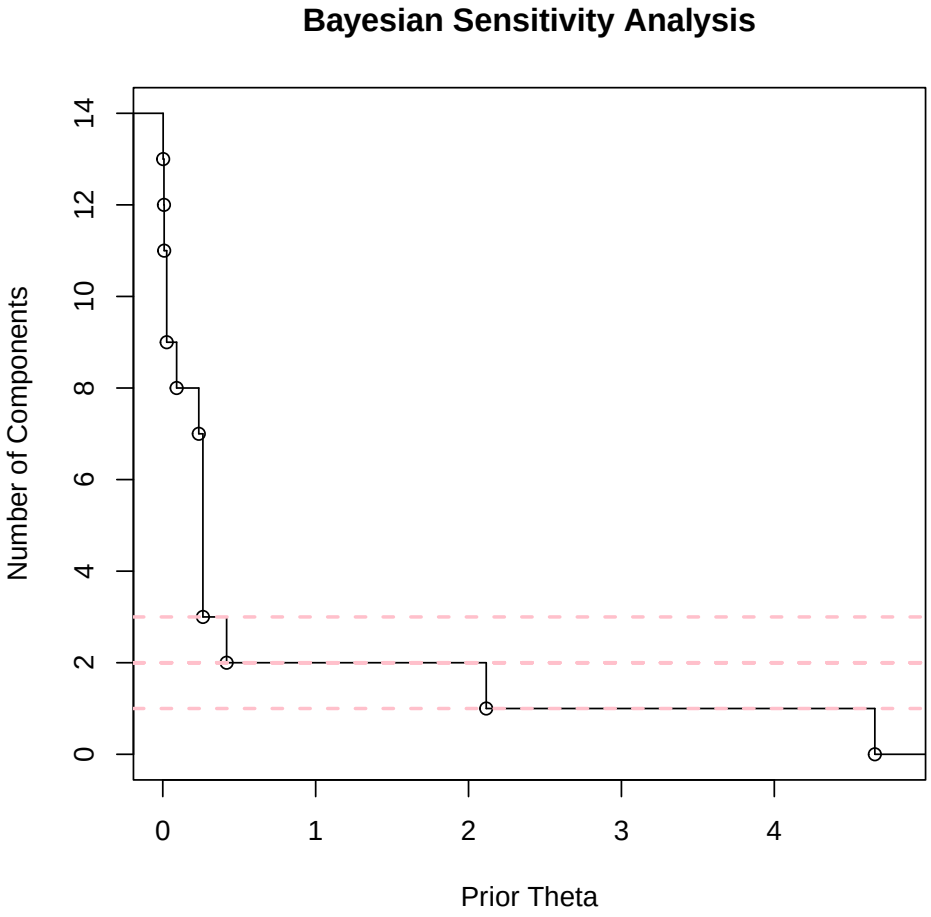

Figure 4: Auer-Gervini step function relating the prior hyperparameter θ to the maximum posterior estimate of the number K of significant principal components in the example with structured data.

4 References

[1] ter Braak CFJ. *CANOCO – a Fortran program for canonical community ordination by [partial] [detrended] [canonical] correspondence analysis, principal component analysis and redundancy analysis (version 2.1).* Agricultural Mathematics Group, Report LWA-88-02, Wageningen, 1988.

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[3] Auer P and Gervini D. Choosing principal components: A new graphical method based on Bayesian model selection. *Communications in Statistics - Simulation and Computation* 2008; 37: 962–977.

[4] Peres-Neto PR, Jackson DA and Somers KM. How many principal components? Stopping rules for determining the number of non-trivial axes revisited. *Computational Statistics and Data Analysis* 2005; 49: 974–997.