Displays for Statistics 5401/8401

Lecture 25

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Class Web Page

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Scale Dependence

The SVD $\mathbf{X} = \mathbf{LTR}'$, PC's $\mathbf{Z}_j = t_j\mathbf{L}_j = \mathbf{X}\mathbf{r}_j$ and the rank m approximation $\mathbf{X}^{(m)} = \sum_{1\le j\le m}\mathbf{Z}_j\mathbf{r}_j'$, are very dependent the scales of the columns of $\mathbf{X}$.

Suppose $\mathbf{D} = \text{diag}[d_1,\ldots,d_p]$ is diagonal. Then

$$\mathbf{X}^* = [\mathbf{X}_1/d_1, \mathbf{X}_2/d_2, \ldots, \mathbf{X}_p/d_p] = \mathbf{X}\mathbf{D}^{-1}$$

is a *scaled version* of $\mathbf{X}$, for example by changing measurement units.

- Except when $d_1 = d_2 = \ldots = d_p$, there is *no* simple relationship between the SVD $\mathbf{L}^*\mathbf{T}^*\mathbf{R}^{*\prime}$ for $\mathbf{X}^*$ and the SVD for $\mathbf{X}$. It's true that $\mathbf{X}^* = \mathbf{LT}\tilde{\mathbf{R}}' = \sum_{1\le j\le p} t_j\mathbf{L}_j\tilde{\mathbf{r}}_j'$, $\tilde{\mathbf{R}} = [\tilde{\mathbf{r}}_1, \ldots, \tilde{\mathbf{r}}_p] \equiv [\mathbf{D}^{-1}\mathbf{r}_1, \ldots, \mathbf{D}^{-1}\mathbf{r}_p]$ but $\mathbf{LT}\tilde{\mathbf{R}}'$ is not the SVD of $\mathbf{X}^*$ ($\tilde{\mathbf{R}}'\tilde{\mathbf{R}} \ne \mathbf{I}_p$).
- And, $\mathbf{X}^{(m)}\mathbf{D}^{-1} = \sum_{1\le j\le m} t_j\mathbf{L}_j\tilde{\mathbf{r}}_j'$, $\tilde{\mathbf{r}}_j = \mathbf{D}^{-1}\mathbf{r}_j$ is *not* the best rank m approximation to $\mathbf{X}^*$ in the least squares sense.

Example from Monday continued

Compute and print approximations to x of ranks 1, 2, 3, and 4 using original scaling.

```
Cmd> x <- run(10)^run(0,3)' # powers of run(10)

Cmd> setlabels(x,\
       structure("@",vector("i^0","i^1","i^2","i^3")))

Cmd> x # 10 ny 4 matrix
            i^0         i^1         i^2         i^3
(1)           1           1           1           1
(2)           1           2           4           8
(3)           1           3           9          27
(4)           1           4          16          64
(5)           1           5          25         125
(6)           1           6          36         216
(7)           1           7          49         343
(8)           1           8          64         512
(9)           1           9          81         729
(10)          1          10         100        1000

Cmd> svdresults  <- svd(x,all:T)

Cmd> svdresults$values #just Sing values
(1)      1415.4       27.14      2.2961     0.41587
```

Because the two smallest singular values are so much smaller than the largest, one might say x is "almost of rank 2".

The for loop in the following MacAnova command computes and prints successively rank m approximations using m = 1, ..., 4 singular values and vectors.

```
Cmd> for(i,run(4)){
       left    <- svdresults$leftvectors[,run(i)]
       right   <- svdresults$rightvectors[,run(i)]
       tmatrix <- dmat(svdresults$values[run(i)])
       approx  <- left %*% tmatrix %*% right'
       print(approx, name:paste("Rank",i,"approximation"))
     }
Rank 1 approximation:
             i^0         i^1         i^2         i^3
(1)    0.0017032    0.014251     0.12416       1.112
(2)     0.012818     0.10725     0.93436      8.3681
(3)     0.042422     0.35494      3.0923      27.695
(4)     0.099592     0.83328      7.2597      65.018
(5)       0.1934      1.6182      14.098      126.26
(6)      0.33293      2.7856      24.269      217.35
(7)      0.52725      4.4115      38.434      344.21
(8)      0.78544      6.5718      57.255      512.77
(9)       1.1166      9.3424      81.393      728.95
(10)      1.5297      12.799      111.51      998.68
```

Last column is fit pretty well, others quite poorly.

```
Rank 2 approximation:    Better fit
             i^0         i^1         i^2         i^3
(1)     0.082063     0.34448      1.2546     0.98138
(2)      0.25314      1.0948      4.3149      7.9776
(3)      0.48224      2.1623      9.2793       26.98
(4)       0.7338      3.4394      16.181      63.987
(5)      0.97227      4.8188      25.054         125
(6)       1.1621      6.1929      35.933         216
(7)       1.2677      7.4541       48.85      343.01
(8)       1.2535      8.4951      63.839      512.01
(9)        1.084      9.2083      80.934         729
(10)     0.72351      9.4862      100.17      999.99
```

```
Rank 3 approximation:    Still better fit
            i^0         i^1         i^2         i^3
(1)       0.74505     1.1878     0.96351      1.0021
(2)       0.97771     2.0164      3.9968      8.0002
(3)        1.0892     2.9343      9.0128      26.999
(4)        1.1105     3.9186      16.016      63.999
(5)        1.0727     4.9465       25.01         125
(6)        1.0066     5.9951      36.001         216
(7)       0.94342     7.0417      48.992         343
(8)       0.91403     8.0633      63.988         512
(9)       0.94946     9.0372      80.993         729
(10)       1.0807     9.9406      100.01        1000
Rank 4 approximation:    = LTR' = x
            i^0         i^1         i^2         i^3
(1)           1           1           1           1
(2)           1           2           4           8
(3)           1           3           9          27
(4)           1           4          16          64
(5)           1           5          25         125
(6)           1           6          36         216
(7)           1           7          49         343
(8)           1           8          64         512
(9)           1           9          81         729
(10)          1          10         100        1000
```

The last is an exact reconstruction of x.

Rescale columns so that their sums of squares = 10, dividing column ℓ by $d_\ell = \sqrt{\{\sum x_{i\ell}^2\}}/\sqrt{10}$, and do the same.

```
Cmd> x # original matrix
            i^0         i^1         i^2         i^3
(1)           1           1           1           1
(2)           1           2           4           8
(3)           1           3           9          27
(4)           1           4          16          64
(5)           1           5          25         125
(6)           1           6          36         216
(7)           1           7          49         343
(8)           1           8          64         512
(9)           1           9          81         729
(10)          1          10         100        1000

Cmd> d <- sqrt(sum(x^2))/sqrt(10)

Cmd> scaledx <- x / d #divide each row by d

Cmd> scaledx # scaled matrix
            (1)         (2)         (3)         (4)
(1)           1     0.16116    0.019868   0.0022482
(2)           1     0.32233    0.079472    0.017986
(3)           1     0.48349     0.17881    0.060702
(4)           1     0.64466     0.31789     0.14389
(5)           1     0.80582      0.4967     0.28103
(6)           1     0.96699     0.71525     0.48562
(7)           1      1.1282     0.97354     0.77115
(8)           1      1.2893      1.2716      1.1511
(9)           1      1.4505      1.6093       1.639
(10)          1      1.6116      1.9868      2.2482

Cmd> sum(scaledx^2) # Column SS are all 10 as promised
            i^0         i^1         i^2         i^3
(1)          10          10          10          10

Cmd> svdresults1 <- svd(scaledx,all:T) # SVD of rescaled x

Cmd> svdresults1$values # singular values of scaled x
(1)      6.0089      1.9225     0.44084    0.051852

Cmd> svdresults$values # singular values of unscaled x
(1)      1415.4       27.14      2.2961     0.41587
```


This computes approximations to scaled x and then "unscales" by multiplying by d, so they should be close to x:

```
Cmd> for(i,run(4)){
       left    <- svdresults1$leftvectors[,run(i)]
       right   <- svdresults1$rightvectors[,run(i)]
       tmatrix <- dmat(svdresults1$values[run(i)])
       approx  <- (left %*% tmatrix %*% right') * d
       print(approx,labels:F,\
             name:paste("Rank",i,"approximation"))}
Rank 1 approximation:    Not good at all
     0.25452      1.7995      14.429      123.02
     0.31094      2.1985      17.628      150.29
     0.38296      2.7077      21.711      185.11
     0.47367       3.349      26.853      228.95
     0.58615      4.1444       33.23      283.32
      0.7235      5.1155      41.016      349.71
      0.8888      6.2842      50.387      429.61
      1.0851      7.6724      61.518      524.51
      1.3156      9.3019      74.583      635.91
      1.5833      11.194      89.758      765.29
Rank 2 approximation:    A little better
     0.90039      2.2239      2.0124     -59.496
     0.94675      2.6162      5.4043     -29.382
       0.988      3.1052      10.079      14.125
      1.0217      3.7091      16.316      74.068
      1.0456      4.4462      24.398      153.49
      1.0571      5.3346      34.603      255.44
      1.0539      6.3927      47.214      382.96
      1.0336      7.6385       62.51      539.09
     0.99369      9.0904      80.772      726.88
      0.9319      10.767      102.28      949.36
Rank 3 approximation:    Close except for column 4
     0.99753      1.0804      -0.109      6.1239
      1.0005      1.9833      4.2302      6.9364
      1.0017      2.9435      9.7789      23.401
      1.0017      3.9453      16.755      60.514
      1.0008      4.9728      25.375      123.27
     0.99968      6.0104      35.857      216.66
     0.99871      7.0421      48.419      345.69
     0.99839      8.0524      63.278      515.34
     0.99922      9.0253      80.651      730.61
      1.0017      9.9451      100.76       996.5
```



```
Rank 4 approximation:    Perfect fit with all 4
          1           1           1           1
          1           2           4           8
          1           3           9          27
          1           4          16          64
          1           5          25         125
          1           6          36         216
          1           7          49         343
          1           8          64         512
          1           9          81         729
          1          10         100        1000
```

MacAnova note:
In the loop, * d multiplies each row of the approximation by the elements of row vector d. This restores the original scaling of x.

With m = 3, x[,1] and x[,2] are fit reasonably well, but not x[,3] and x[,4].

In any event, the approximations from the SVD of scaledx are different from the approximations from the SVD of x.

SVD of $\tilde{\mathbf{X}} = \mathbf{X} - \mathbf{1}_N\overline{\mathbf{x}}'$ (resids from mean) is related to eigenvalues $\hat{\lambda}_1, \hat{\lambda}_2, \ldots, \hat{\lambda}_p$ and eigenvectors $[\hat{\mathbf{v}}_1, \ldots, \hat{\mathbf{v}}_p]$ of the sample variance matrix $\mathbf{S} = (1/f_e)\tilde{\mathbf{X}}'\tilde{\mathbf{X}}$, $f_e = N-1$.

- Singular values of $\tilde{\mathbf{X}}$ are $t_j = \sqrt{\{f_e\hat{\lambda}_j\}}$ The eigenvalues of $\mathbf{S}$ are $\hat{\lambda}_j = t_j^2/f_e$
- The right singular vector $\mathbf{r}_j = \hat{\mathbf{v}}_j$, where $\hat{\mathbf{v}}_j$ is an eigenvector of $\mathbf{S}$
- The left singular vectors $\mathbf{L}_j$ are eigenvectors $\hat{\boldsymbol{\ell}}_j$ of $\tilde{\mathbf{X}}\tilde{\mathbf{X}}'$ with eigenvalues $f_e\hat{\lambda}_1 = t_1^2, \ldots, f_e\hat{\lambda}_p = t_p^2$, 0, ..., 0 (N-p 0's)

$-\mathbf{L}_j$ and $-\mathbf{r}_j$ (changing signs of both) are equally valid singular vectors. The choice of signs may differ between programs.

Similarly, $\mathbf{L}_j = \pm\hat{\boldsymbol{\ell}}_j$, $\mathbf{r}_j = \pm\hat{\mathbf{v}}_j$.

Continuing with PC's from the point of view of finding a low rank approximation to $\tilde{\mathbf{X}} = \mathbf{X} - \mathbf{1}_N\overline{\mathbf{x}}' = \sum_{1\le j\le p}(t_j\mathbf{L}_j)\mathbf{r}_j' = \sum_{1\le j\le p} t_j\hat{\boldsymbol{\ell}}_j\hat{\mathbf{v}}_j'$

$\hat{\boldsymbol{\ell}}_j$ and $\hat{\mathbf{v}}_j$ are eigenvectors of $\tilde{\mathbf{X}}'\tilde{\mathbf{X}}$ and $\tilde{\mathbf{X}}\tilde{\mathbf{X}}'$

Because $t_j = \sqrt{\{f_e\hat{\lambda}_j\}}$, $\hat{\lambda}_j$ eigenvalue of $\mathbf{S}$

- $\tilde{\mathbf{X}} = \sum_{1\le j\le p}(\sqrt{\{f_e\hat{\lambda}_j\}}\mathbf{L}_j)\mathbf{r}_j' = \sum_{1\le j\le p}\tilde{\mathbf{Z}}_j\mathbf{r}_j'$ where $\tilde{\mathbf{Z}}_j \equiv t_j\mathbf{L}_j = \sqrt{\{f_e\hat{\lambda}_j\}}\times\mathbf{L}_j = \tilde{\mathbf{X}}\mathbf{r}_j = \tilde{\mathbf{X}}\hat{\mathbf{v}}_j$.
- $\overline{\tilde{\mathbf{Z}}_j} = (1/N)\mathbf{1}_N'\tilde{\mathbf{Z}}_j = 0$ (because $\mathbf{1}_N'\tilde{\mathbf{X}} = \mathbf{0}$)
- The best rank m approximation to $\tilde{\mathbf{X}}$ is

$$\tilde{\mathbf{X}}^{(m)} = \sum_{1\le j\le m}\tilde{\mathbf{Z}}_j\mathbf{r}_j' = \tilde{\mathbf{X}}\sum_{1\le j\le m}\mathbf{r}_j\mathbf{r}_j'$$

Reminder: $\pm\mathbf{r}_j = \hat{\mathbf{v}}_j$ is the j^{th} eigenvector of $\mathbf{S}$ and satisfies $\mathbf{S}\mathbf{r}_j = \hat{\lambda}_j\mathbf{r}_j$, so you can compute PCs by either using the SVD to find $\mathbf{r}_j$ or by computing eigenvectors of $\mathbf{S}$.

MacAnova: Compute all PCs by

```
Z <- (X - xbar') %*% eigen(s)$vectors
```


Here's how to think about this.

- Each N×1 principal component vector

$$\tilde{\mathbf{Z}}_j = \tilde{\mathbf{X}}\mathbf{r}_j = \sum_{1\le\ell\le p} r_{\ell j}\tilde{\mathbf{X}}_\ell$$

  is a new variable, a linear combination of the columns $\tilde{\mathbf{X}}_\ell$ of $\tilde{\mathbf{X}}$. The coefficients in the linear combination come from $\mathbf{r}_j$, the j^{th} eigenvector of $\mathbf{S}$.
- Each column $\tilde{\mathbf{X}}_\ell^{(m)}$ of the rank m approximation $\tilde{\mathbf{X}}^{(m)}$ is a linear combination of the first m PC's

$$\tilde{\mathbf{X}}_\ell^{(m)} = \sum_{1\le j\le m}\tilde{\mathbf{Z}}_j r_{\ell j}$$
$$= \text{column } \ell \text{ of } \tilde{\mathbf{X}}^{(m)} = \sum_{1\le j\le m}\tilde{\mathbf{Z}}_j\mathbf{r}_j'.$$

  The coefficients of $\tilde{\mathbf{Z}}_j$ $\{r_{\ell j}\}_{1\le j\le m}$ are from row ℓ of $\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_m$

So the elements of $[\mathbf{r}_1\ \mathbf{r}_2\ \ldots\ \mathbf{r}_m]$ play a role in defining principal components and in approximating $\tilde{\mathbf{X}}$ by $\tilde{\mathbf{X}}^{(m)}$.

- The "total sum of squares" is

$$\|\tilde{\mathbf{X}}\|^2 = \sum_{1\le\ell\le p}\{\sum_{1\le i\le N}(x_{i\ell} - \overline{x_\ell})^2\}$$
$$= f_e\sum_{1\le\ell\le p}s_{\ell\ell} = f_e\,\text{trace}(\mathbf{S})$$
$$= f_e\sum_{1\le j\le p}\hat{\lambda}_j = \sum_{1\le j\le p}t_j^2.$$

  Here $s_{\ell\ell} = s_\ell^2 = \sum_{1\le i\le N}(x_{i\ell} - \overline{x_{j\ell}})^2/f_e$ are the sample variances for each column of $\mathbf{X}$.
- The "residual sum of squares" is $\|\tilde{\mathbf{X}} - \tilde{\mathbf{X}}^{(m)}\|^2 = f_e\sum_{m+1\le j\le p}\hat{\lambda}_j = \sum_{m+1\le j\le p}t_j^2$
- Relative RSS (analogous to $1 - R^2$) is

$$\|\tilde{\mathbf{X}} - \tilde{\mathbf{X}}^{(m)}\|^2/\|\tilde{\mathbf{X}}\|^2$$
$$= \sum_{m+1\le j\le p}t_j^2/\sum_{1\le j\le p}t_j^2 = \sum_{m+1\le j\le p}\hat{\lambda}_j/\sum_{1\le j\le p}\hat{\lambda}_j$$
$$= \sum_{m+1\le j\le p}\hat{\lambda}_j/\sum_{1\le\ell\le p}s_{\ell\ell} = 1-(\sum_{1\le j\le m}\hat{\lambda}_j/\sum_{1\le j\le p}\hat{\lambda}_j)$$
$$= 1 - (\sum_{1\le j\le m}\hat{\lambda}_j/\sum_{1\le\ell\le p}s_{\ell\ell})$$

Thus $\sum_{1\le j\le m}\hat{\lambda}_j/\sum_{1\le j\le p}\hat{\lambda}_j = \sum_{1\le j\le m}\hat{\lambda}_j/\sum_{1\le\ell\le p}s_{\ell\ell}$ is the proportion of the total SS "explained" by $\tilde{\mathbf{Z}}_1, \ldots \tilde{\mathbf{Z}}_m$.

$\tilde{\mathbf{X}}^{(m)}$ should be a good rank-m approximation to $\tilde{\mathbf{X}}$ when the *"trailing" eigenvalues* $\hat{\lambda}_{m+1}, \ldots, \hat{\lambda}_p$ are small compared to $\sum_{1\le j\le p}\hat{\lambda}_j$, so that $\sum_{1\le j\le m}\hat{\lambda}_j / \sum_{1\le j\le p}\hat{\lambda}_j \approx 1$.

You can add back the mean $\overline{\mathbf{x}}$ to get a rank m+1 approximation $\mathbf{X}^{(m)*}$ for $\mathbf{X}$:

$$\mathbf{X}^{(m)*} = 1_N\overline{\mathbf{x}}' + \tilde{\mathbf{X}}^{(m)} = (1_N\overline{\mathbf{x}}') + \sum_{1\le j\le m}\tilde{\mathbf{Z}}_j\mathbf{r}_j'$$

Since $\|\tilde{\mathbf{X}} - \tilde{\mathbf{X}}^{(m)}\|^2 = \|\mathbf{X} - \mathbf{X}^{(m)*}\|^2$, $\mathbf{X}^{(m)*}$ is a good approximation to $\mathbf{X}$ whenever $\tilde{\mathbf{X}}^{(m)}$ is a good approximation to $\tilde{\mathbf{X}}$.

$\mathbf{X}^{(m)*}$ is a rank m+1 approximation, but not the *best* rank m+1 approximation $\mathbf{X}^{(m+1)}$. We prefer $\mathbf{X}^{(m)*}$ to $\mathbf{X}^{(m+1)}$ because one of the outer products $(1_N\overline{\mathbf{x}}')$ has an immediate interpretation as a matrix all of whose rows are $\overline{\mathbf{x}}'$.

You can generalize this to a linear model situation when $\mathbf{X} = \mathbf{UB} + \boldsymbol{\varepsilon}$, where

- the k+1 columns $\mathbf{U}_0, \mathbf{U}_1, \ldots, \mathbf{U}_k$ of $\mathbf{U}$ are predictor (independent) variables, possibly dummy variables
- $\mathbf{B} = [\boldsymbol{\beta}_0, \boldsymbol{\beta}_1, \ldots, \boldsymbol{\beta}_k]'$ is a matrix of coefficients (not the same as J&W use of $\mathbf{B}$ as "between" groups matrix).

The estimate $\hat{\mathbf{B}}$ has rows $\hat{\boldsymbol{\beta}}_0', \hat{\boldsymbol{\beta}}_1', \ldots, \hat{\boldsymbol{\beta}}_k'$ and the "fitted values" are

$$\hat{\mathbf{X}} = \mathbf{U}\hat{\mathbf{B}} = \sum_{0\le j\le k}\mathbf{U}_j\hat{\boldsymbol{\beta}}_j'$$

$\hat{\mathbf{X}}$ is a rank k+1 approximation to $\mathbf{X}$, just as $1_N\overline{\mathbf{x}}'$ is a rank 1 approximation to $\mathbf{X}$.

$\hat{\mathbf{X}}$ is not the best rank k+1 since it is not constructed from the SVD of $\mathbf{X}$.

Consider $\tilde{\mathbf{X}} \equiv \mathbf{X} - \mathbf{U}\hat{\mathbf{B}}$, the matrix of residuals from the linear model.

To understand the structure of $\tilde{\mathbf{X}}$ it is natural to look at the rank m approximation $\tilde{\mathbf{X}}^{(m)} = \sum_{1\le j\le m}\tilde{\mathbf{Z}}_j\mathbf{r}_j'$ for $\tilde{\mathbf{X}}$. The PC's $\tilde{\mathbf{Z}}_j = \tilde{\mathbf{X}}\mathbf{r}_j = t_j\mathbf{L}_j$ computed from the matrix $\tilde{\mathbf{X}}$ of residuals are multiples of $\tilde{\mathbf{X}}$'s left singular vectors $\mathbf{L}_j$. $\mathbf{r}_j$ is an eigenvector of $\mathbf{S} = f_e^{-1}\mathbf{E}$.

Then

$$\mathbf{U}\hat{\mathbf{B}} + \tilde{\mathbf{X}}^{(m)} = \sum_{0\le j\le k}\mathbf{U}_j\hat{\boldsymbol{\beta}}_j' + \sum_{1\le j\le m}\tilde{\mathbf{Z}}_j\mathbf{r}_j'$$

is a rank k+m+1 approximation to $\mathbf{X}$ with the first k+1 components having an interpretation as predictors. It is not the "best" rank k+m+1 approximation to $\mathbf{X}$. That would be $\mathbf{X}^{(k+m+1)}$ computed from the SVD of $\mathbf{X}$.


```
Cmd> irisdata <- read("","t11_05",silent:T)

Cmd> x <- irisdata[,-1]; xbar <- describe(x,mean:T) #col vector

Cmd> svdstuff <- svd(x - xbar',all:T) # resids from mean

Cmd> svals <- svdstuff$values; leftvecs <- svdstuff$leftvectors

Cmd> svals # Singular values
(1)        25.1       6.0131       3.4137       1.8845

Cmd> rightvecs <- svdstuff$rightvectors

Cmd> xhat_2 <- svals[1]*leftvecs[,1] %*% rightvecs[,1]' +\
     svals[2]*leftvecs[,2] %*% rightvecs[,2]' + xbar'
```

xhat_2 = $\tilde{\mathbf{X}}^{(2)} + 1_N\overline{\mathbf{x}}'$ = approximation to $\mathbf{X}$

```
Cmd> sum(vector(x - xhat_2)^2) # residual SS
(1)      15.205

Cmd> sum(svals[-run(2)]^2) # t_3^2 + t_4^2 (trailing sing vals)
(1)      15.205

Cmd> sum(svals[run(2)]^2)/sum(svals^2)
(1)     0.97769      97.8% of variability "explained"

Cmd> head(x,8) # first 8 rows of x
        SepLen      SepWid      PetLen      PetWid
(1)        5.1         3.5         1.4         0.2 Original
(2)        4.9           3         1.4         0.2 values of
(3)        4.7         3.2         1.3         0.2 x_ij
(4)        4.6         3.1         1.5         0.2
(5)          5         3.6         1.4         0.2
(6)        5.4         3.9         1.7         0.4
(7)        4.6         3.4         1.4         0.3
(8)          5         3.4         1.5         0.2

Cmd> print(head(xhat_2,8),format:".2f") #first 8 rows of xhat_2
MATRIX:     Pretty good match of rank 2 approximation
      SepLen    SepWid    PetLen    PetWid
(1)     5.08      3.52      1.40      0.21  These are the
(2)     4.75      3.16      1.46      0.24  approximate
(3)     4.70      3.20      1.31      0.18  values of x_ij
(4)     4.64      3.06      1.46      0.24  computed using
(5)     5.07      3.53      1.36      0.20  the first two
(6)     5.51      3.79      1.68      0.33  principal com-
(7)     4.77      3.23      1.36      0.20  ponents
(8)     5.00      3.40      1.48      0.25
```

MacAnova Notes:

- `head(x)` gets the first 10 rows of x.
- `head(x,n)` gets the first n rows of x.
- `tail(x)` gets the last 10 rows of x.
- `tail(x,n)` gets the last n rows of x.

There is some ambiguity as to how the principal components associated with a N×p data matrix $\mathbf{X}$ are defined:

- Linear combinations $\mathbf{Z}_j = \mathbf{X}\mathbf{r}_j$ of the data themselves

or, as I have defined them,

- Linear combinations $\tilde{\mathbf{Z}}_j = \tilde{\mathbf{X}}\mathbf{r}_j$ of residuals in $\tilde{\mathbf{X}} = \mathbf{X} - \mathbf{1}_N\overline{\mathbf{x}}'$.

They are closely related:

$$\mathbf{Z}_j = \mathbf{X}\mathbf{r}_j = \mathbf{1}_N\overline{\mathbf{x}}'\mathbf{r}_j + \tilde{\mathbf{X}}\mathbf{r}_j = \overline{z}_j\mathbf{1}_N + \tilde{\mathbf{Z}}_j$$

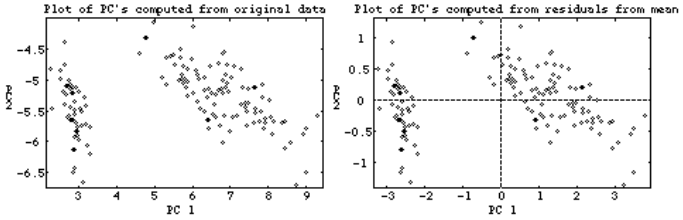
This means that $\mathbf{Z}_j - \tilde{\mathbf{Z}}_j = \overline{z}_j\mathbf{1}_N$ is a constant vector. Scatter plots of $\mathbf{Z}_j$ vs $\mathbf{Z}_k$ will look like plots of $\tilde{\mathbf{Z}}_j$ vs $\tilde{\mathbf{Z}}_k$.


```
Cmd> z_a <- x %*% rightvecs # PC's computed from X
Cmd> z_b <- (x - xbar') %*% rightvecs#PC's computed from resids
```

Columns of z_a are $\mathbf{Z}_j = \mathbf{X}\mathbf{r}_j$.

Columns of z_b are $\tilde{\mathbf{Z}}_j = \tilde{\mathbf{X}}\mathbf{r}_j$.

```
Cmd> head(z_a - z_b,3) #difference is constant
            (1)         (2)         (3)         (4)
(1)      5.5024      -5.327     0.63185    0.033352
(2)      5.5024      -5.327     0.63185    0.033352
(3)      5.5024      -5.327     0.63185    0.033352

Cmd> plot(z_a[,1], z_a[,2],xlab:"PC 1",ylab:"PC2", \
title:"Plot of PC's computed from original data",symbols:"\11")

Cmd> plot(z_b[,1], z_b[,2],xlab:"PC 1",ylab:"PC2", \
     title:"Plot of PC's computed from residuals from mean",\
     symbols:"\11")
```



Here is another way to view the best rank m approximation $\tilde{\mathbf{X}}^{(m)} = \sum_{1\le j\le m}\tilde{\mathbf{Z}}_j\mathbf{r}_j'$:

$$\begin{aligned}\mathbf{X} &= \mathbf{1}_N\overline{\mathbf{x}}' + \tilde{\mathbf{X}} = (\text{mean} + \text{residuals})\\ &= \mathbf{1}_N\overline{\mathbf{x}}' + \sum_{1\le j\le m}\tilde{\mathbf{Z}}_j\mathbf{r}_j' + \left(\sum_{m+1\le j\le p}\tilde{\mathbf{Z}}_j\mathbf{r}_j'\right)\\ &= \mathbf{1}_N\overline{\mathbf{x}}' + \tilde{\mathbf{X}}^{(m)} + \mathbf{e},\end{aligned}$$

where $\mathbf{e} \equiv \tilde{\mathbf{X}} - \sum_{1\le j\le m}\mathbf{Z}_j\mathbf{r}_j' = \sum_{m+1\le j\le p}\tilde{\mathbf{Z}}_j\mathbf{r}_j'$ is the "error" made when you approximate $\tilde{\mathbf{X}}$ by $\tilde{\mathbf{X}}^{(m)}$.

This decomposes the data into

- a part coming from the *means* in $\overline{\mathbf{x}}$
- the *best rank m approximation* $\tilde{\mathbf{X}}^{(m)}$ to the residuals from $\overline{\mathbf{x}}$
- an *"error"* $\mathbf{e} = \tilde{\mathbf{X}} - \tilde{\mathbf{X}}^{(m)}$, the residuals from the approximation.

In the more complex linear model case

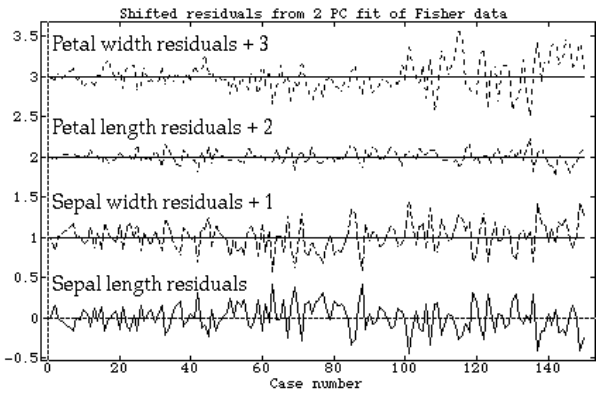
$$\mathbf{X} = \mathbf{U}\hat{\mathbf{B}} + \tilde{\mathbf{X}}^{(m)} + \mathbf{e}$$

where $\mathbf{e} = \tilde{\mathbf{X}} - \tilde{\mathbf{X}}^{(m)}$, $\tilde{\mathbf{X}} = \mathbf{X} - \mathbf{U}\hat{\mathbf{B}}$.

What might the elements of $\mathbf{e}$ look like?

Computation of $\mathbf{e}$ for Fisher data.

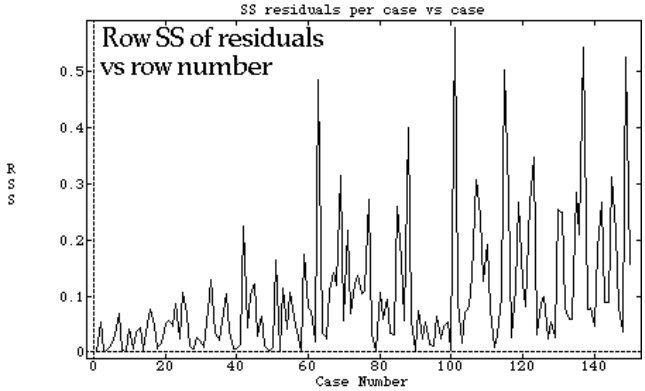
```
Cmd> e <- x - xhat_2 # Fisher residuals, 150 by 4 matrix

Cmd> sum(e) # column sums and hence means are 0
        SepLen       SepWid       PetLen       PetWid
(1)  5.7732e-14 -6.2617e-14 -3.1308e-14  4.8628e-14

Cmd> sum(describe(e,var:T))/sum(describe(x,var:T))
(1)    0.022315   Like 1 - R^2

Cmd> sum(svals[-run(2)]^2)/sum(svals^2) # trailing sing vals
(1)    0.022315

Cmd> lineplot(1,e + run(0,3)',xlab:"Case number",\
 title:"Shifted residuals from 2 PC fit of Fisher data",show:F)

Cmd> addlines(vector(0,150,?,0,150,?,0,150),\
          vector(1,1,?,2,2,?,3,3)) # add 0 lines
```



It looks cases 1-50 may have slightly smaller residuals than cases 51-150

The row sums of squares $\sum_{1 \le \ell \le p} e_{i\ell}^2$, i = 1, ..., N measure the lack of fit to each case:

```
Cmd> rowss <- vector(sum(e'^2)) # Note the transpose
Cmd> lineplot(1,rowss,xlab:"Case Number",ylab:"RSS",\
               title:"SS residuals per case vs case")
```



For reasons that might be explored further, the rank 2 fit seems to do better for variety 1 (cases 1-50) than for the other two varieties as appeared might be the case from the earlier plot.