Lecture 26:
PCA (cont.)

Big Data and Machine Learning for Applied Economics
Econ 4676

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Agenda

1. Factor Models

2. PCA: Theory
   - PC Computation

3. Factor Interpretation

4. Review & Next Steps

5. Further Readings

Factor Models

- Text is super high dimensional
- There is often abundant *unlabeled* text
- Some times unsupervized factor model is a popular and useful strategy with text data
- You can first fit a factor model to a giant corpus, get a few factors (reduce the dimensionality)
- Use these factors for supervised learning on a subset of labeled documents.
- The unsupervised dimension reduction facilitates the supervised learning

Topic Models: Example

- We have 6,166 reviews, with an average length of 90 words per review, we8there.com.

- A useful feature of these reviews is that they contain both text and a multidimensional rating on overall experience, atmosphere, food, service, and value.

- For example, one user submitted a glowing review for Waffle House #1258 in Bossier City, Louisiana:

  I normally would not revue a Waffle House but this one deserves it. The workers, Amanda, Amy, Cherry, James and J.D. were the most pleasant crew I have seen. While it was only lunch, B.L.T. and chili, it was great. The best thing was the 50′ s rock and roll music, not to loud not to soft. This is a rare exception to what you all think a Waffle House is. Keep up the good work.
  Overall: 5, Atmosphere: 5, Food: 5, Service: 5, Value: 5.

Topic Models: Example

- We can apply PCA to get a factor representation of the review text.
- PC1 looks like it will be big and positive for positive reviews,

```r
pca <- prcomp(x, scale=TRUE) # can take a long time

tail(sort(pca$rotation[,1]))
```

```
##     food great     staff veri     excel food high recommend     great food
##    0.007386860    0.007593374    0.007629771    0.007821171    0.008503594
##     food excel
##    0.008736181
```

- while PC4 will be big and negative

```r
tail(sort(pca$rotation[,4]))
```

```
##   order got after minut  never came   ask check readi order drink order
##  0.05918712  0.05958572  0.06099509  0.06184512  0.06776281  0.07980788
```

Factor Models

- Lets assume that we have a data matrix $X_{n \times p}$
- A factor model looks like

$$\begin{aligned} x_1 &= \phi_{11} f_1 + \cdots + \phi_{1k} f_k \\ x_2 &= \phi_{21} f_1 + \cdots + \phi_{2k} f_k \\ &\vdots \\ x_p &= \phi_{p1} f_1 + \cdots + \phi_{pk} f_k \end{aligned} \tag{1}$$

- where
  - x_j are the inputs of the regressions (independent vars)
  - The f_k $k = 1, \ldots K$ are the factors, unobserved, and that we want to estimate
  - ϕ_{jk} are called loadings or rotations
  - When you use a K that is much smaller than p, factor models provide a parsimonious representation for X.

Factor Models: PCA

- How do you estimate a Factor Model with PCA?
- We are trying to learn from high-dimensional X some low-dimensional summaries that contain the information necessary to make good decisions.

Factor Models: PCA

- How do you estimate a Factor Model with PCA?
- We are trying to learn from high-dimensional X some low-dimensional summaries that contain the information necessary to make good decisions.
- Suppose that there is only one underlying factor f_1

$$\begin{aligned} x_1 &= \phi_{11} f_1 \\ x_2 &= \phi_{21} f_1 \\ &\vdots \\ x_p &= \phi_{p1} f_1 \end{aligned} \tag{2}$$

Factor Models: PCA

- or in a more compact form form

$$X = \phi_1 f_1 \tag{3}$$

- and

$$f_1 = \phi_1^{-1} X \tag{4}$$

- so we don't have to deal with inverses (things do not change), let's call $\delta_1 = \phi_1^{-1}$

$$\begin{aligned} f_1 &= \delta_1 X && (5) \\ &= \delta_{11} x_1 + \delta_{12} x_2 + \cdots + \delta_{1k} x_k && (6) \end{aligned}$$

- This equation also illustrates the fact that the first principal component is a linear combination of the original variables.

Detour: Algebra Review

- Let $A_{m\times m}$. It exists
  - a scalar λ such that $Ap = \lambda p$ for a vector $p_{m\times 1}$,
  - if $p \neq 0$, then λ is an eigenvalue of A.
  - and p is an eigenvector of A corresponding to the eigenvalue λ.
- $A_{m\times m}$ with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_m$, then:

$$tr(A) = \sum_{i=1}^{m} \lambda_i \tag{7}$$

$$det(A) = \Pi_{i=1}^{m} \lambda_i \tag{8}$$

- If $A_{m\times m}$ has m different eigenvalues, then the associated eigenvectors are all linearly independent.

Detour: Algebra Review

- Spectral decomposition:

$$A = P\Lambda P \tag{9}$$

- where $\Lambda = diag(\lambda_1, \dots \lambda_m)$ and P is the matrix whose columns are the corresponding eigenvectors.

$$A = \begin{pmatrix} p_1 & p_2 & \dots & \dots & p_m \end{pmatrix} \begin{pmatrix} \lambda_1 & & & & 0 \\ & \lambda_2 & & & \\ & & \ddots & & \\ & & & \ddots & \\ 0 & & & & \lambda_m \end{pmatrix} \begin{pmatrix} p_1 \\ p_2 \\ \vdots \\ \vdots \\ p_m \end{pmatrix} \tag{10}$$

$$A = \sum_{i=1}^{m} \lambda_i p_i p_i' \tag{11}$$

Principal Component Analysis

$$
\begin{aligned}
f_1 &= \delta_1 X && (12)\\
&= \delta_{11}x_1 + \delta_{12}x_2 + \cdots + \delta_{1k}x_k && (13)
\end{aligned}
$$

- How are these components calculated in a way that preserves as much information as possible?
- The task is then finding the best linear combination of the original variables.
- What is best?

Principal Component Analysis

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- PCA response: the one that preserves the most information
- In other words, we are going to try to generate an index that reproduces (the best it can) the information (variability) of the original variables
- How we do that?

Principal Component Analysis

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- How we do that?
- Maximize the variance

Principal Component Analysis

- The problem then looks like

$$maxV(f_1) = maxV(\delta_1 X) \tag{14}$$

- where
  - $X = (x_1, \ldots, x_K)_{N \times K}$,
  - $S = V(X)$
  - $\delta_1 \in K$
- Let's set up the problem as

$$\underset{\delta}{max} \;\; \delta_1 X \delta_1' \tag{15}$$

- What is the solution to this problem?

Principal Component Analysis

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- What is the solution to this problem?
- Bring δ to infinity.

Principal Component Analysis

- Let's "fix" the problem by normalizing δ

$$\begin{aligned} \max_{\delta} \; \delta_1 S \delta_1' \\ \text{subject to} \\ \delta_1 \delta_1' = 1 \end{aligned} \tag{16}$$

- Let us call the solution to this problem δ_1^*.
- $f_1^* = \delta_1^* X$ is the 'best' linear combination of X.
- Intuition: X has K columns and $f_1^* = \delta_1^* X$ has only one. The factor built with the first principal component is the best way to represent the K variables of X using a single single variable.

Principal Component Analysis

- Solution to the problem of the first principal component
- Let's set the lagrangian

$$\mathcal{L} = \delta_1 S \delta_1' + \lambda_1 (1 - \delta_1 \delta_1') \tag{17}$$

- Rearranging

$$S\delta_1' = \lambda_1 \delta_1' \tag{18}$$

- At the optimum, δ is the eigenvector corresponding to the eigenvalue λ of S.
- Premultiplying by δ_1 and remembering that $\delta_1\delta_1' = 1$:

Principal Component Analysis

$$\delta_1 S \delta_1' = \lambda_1 \tag{19}$$

- In order to maximize $\delta S \delta$ we must choose λ equal to the maximum eigenvalue of S and δ is the corresponding eigenvalue.
- The problem of finding the best linear combination that reproduces the variability of X is finding the biggest eigenvalue of S and it's corresponding eigenvector

Principal Component Analysis

- The first main component? Are there others?
- Let's consider the following problem:

$$\max_{\delta_2} \delta_2 S \delta_2' \tag{20}$$

$$\text{st} \tag{21}$$

$$\delta_2\delta_2' = 1 \tag{22}$$

$$\delta_2\delta_1' = 0 \tag{23}$$

- $f_2^* = \delta_2^* X$ is the second principal component : the best linear combination which is orthogonal to the best initial linear combination.
- Recursively, using this logic you can form q main components.
- Note that algebraically we could construct $q = K$ factors, actually the number of PC are $min(n-1, K)$

q main components

- Let $\lambda_1, \dots, \lambda_K$ be the eigenvalues of $S = V(X)$, ordered from highest to lowest,
- $p_1, \dots, p_K$ the corresponding eigenvectors.
- Call P the matrix of eigenvectors.
- Then $\delta_j = p_j$, $\forall j$ ('loadings' of the principal components =ordered eigenvectors of S).

Relative importance of factors

- Now we want to know the relative importance of factors, to have a way of choosing them

- Let $f_j = X\delta_j$, $j = 1, \ldots, K$ be the j-th principal component.

$$V(f_j) = \delta_j S \delta_j' \tag{24}$$

$$= p_j P \Lambda P p_j' \tag{25}$$

$$= \lambda_j \tag{26}$$

  (the variance of the j-th principal component is the j-th ordered eigenvalue of S).

- We this result we can show that the total variance of X is the sum of the variances of x_j , $j = 1, ..., K$, that is $trace(S)$

Relative importance of factors

- We the above result we can show that the total variance of X is the sum of the variances of x_j , $j = 1, ..., K$, that is $trace(S)$
- Note the following:

$$trace(S) = trace(P\Lambda P') = trace(PP'\Lambda) = \sum_{j=1}^{K} \lambda_j = \sum_{j=1}^{K} V(F_j) \qquad (27)$$

- Then

$$\frac{\lambda_k}{\sum_{j=1}^{K} \lambda_j} \qquad (28)$$

- measures the relative importance of the jth principal component.

Selection of factors

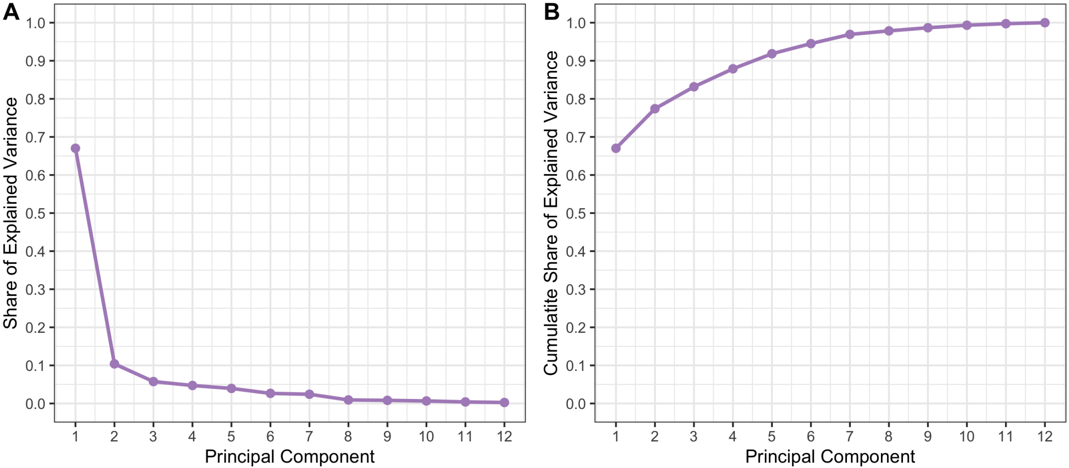
- Although a matrix X of dimension $n\ timesK$ generally has $min(n-1, K)$ different principal components.
- In practice, we are generally not interested in all the components, but rather stay with the first ones that allow us to visualize or interpret data.
- Indeed, we would like to keep the minimum number that allows us a good understanding of the data.
- The natural question that arises here is whether there is an established way to determine the number of principal components to use.
- Unfortunately, there is no accepted objective way in the literature to answer it.

Selection of factors

- However, there are three simple approaches that can guide you in deciding the number of relevant major components.
  - Visual examination of screeplot
  - Kaiser criterion.
  - Proportion of variance explained.

Selection of factors

Screeplot



Selection of factors

Kaiser criterion

- Let the columns of X be standardized, so that each variable has unit variance.
- In this case:

$$trace(S) = \sum_{j=1}^{K} V(F_j) = K \tag{29}$$

- and recall $\sum_{j=1}^{K} \lambda_j = \sum_{j=1}^{K} V(F_j)$ then

$$\sum_{j=1}^{K} \lambda_j = K \tag{30}$$

- On average, each factor contributes one unit. When $\lambda_j > 1$, that factor it explains the total variance more than the average. $\rightarrow$ Retain the factors with $\lambda_j > 1$

Selection of factors

Proportion of variance explained

- Another approach often used in practice is to impose a threshold a priori and choose the main components based on it.
  - For example, we could define a threshold of 90%, which in the previous example plot would result in 5 main components.
  - Whereas if it were 70% we would have 2 main components.
- The threshold to be defined will depend on the application, the context, and the data set. Thresholds between 70% and 90% are typically used.

PC Computation

- Befroe I mentioned that data was standardized, that is, re-centered to have zero mean and scaled to have variance one.
- From a strictly mathematical point of view, there is nothing inherently wrong with making linear combinations of variables with different units of measurement.
- However, when we use PCA we seek to maximize variance and the variance is affected by the units of measurement.
- This implies that the principal components based on the covariance matrix S will change if the units of measure of one or more variables change.

PC Computation

- To prevent this from happening, it is common practice to standardize the variables. That is, each X value is re-centered and divided by the standard deviation:

$$z_{ij} = \frac{x_{ij} - \bar{x}_j}{s_j} \tag{31}$$

- where $\bar{x}_j$ is the mean and s_j is the standard deviation of column j.
- Then the initial data matrix X is replaced by the standardized data matrix Z.
- Note also that when standardizing the data matrix, the covariance matrix S is simply the original data correlation matrix. This is sometimes referred to in the literature as the PCA correlation matrix.

PC Computation

Uniqueness of the main components

- It is necessary to warn that the "loadings" of the main components δ are unique except for a sign change.
- This implies that depending on the implementation we can obtain different results in two libraries.
- The "loadings" will be the same but the signs may differ.
- The signs may differ because each weight specifies a direction in k-dimensional space and the change of sign has no effect on the direction.

PC Computation

- As a practical aside, note that `prcomp` converts X here from sparse to dense matrix storage.

- For really big text DTMs, which will be very sparse, this will cause you to run out of memory.

- A big data strategy for PCA is to first calculate the covariance matrix for X and then obtain PC rotations as the eigenvalues of this covariance matrix.
  - The first step can be done using sparse matrix algebra.
  - The rotations are then available as

```
## eigen( xvar, symmetric = TRUE)$vec.
```

- There are also approximate PCA algorithms available for fast factorization on big data. See, for example, the `irlba` package for R.

Factor Interpretation

- $f_s = \delta_s X$: 'loadings' often suggest that a factor works as a 'index' of a group of variables.

- Idea: look at the 'loadings'

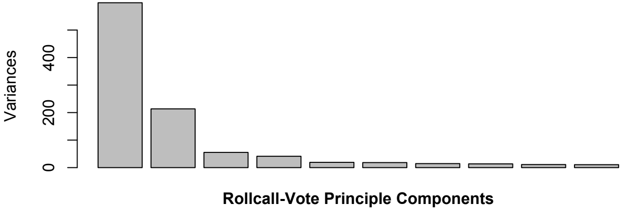
- Caution: factors via principal components are orthogonal recursively.

Factor Interpretation: Example

- **Congress and Roll Call Voting**
  - Votes in which names and positions are recorded are called ‘roll calls’.
  - The site `voteview.com` archives vote records and the R package `pscl` has tools for this data.
  - 445 members in the last US House (the 111^{th})
  - 1647 votes: nea = -1, yea=+1, missing = 0.
  - This leads to a large matrix of observations that can probably be reduced to simple factors (party).

Factor Interpretation

- Vote components in the **111**th house
- Each PC is $f_s = \delta_s X$



- Huge drop in variance from 1st to 2nd and 2nd to 3rd PC.
- Poli-Sci holds that PC1 is usually enough to explain congress.
  2nd component has been important twice: 1860's and 1960's.

Factor Interpretation

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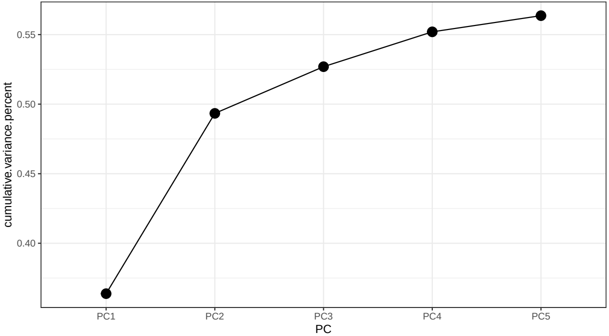

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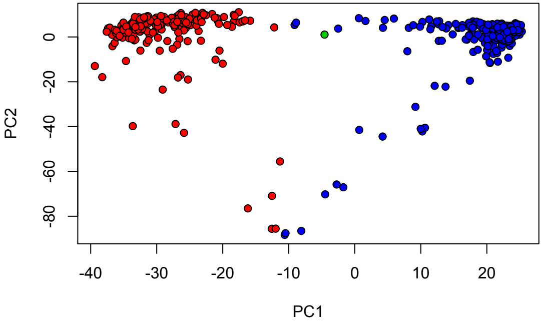
Factor Interpretation

- Top two PC directions in the **111**th house



- Republicans in red and Democrats in blue:
  - Clear separation on the first principal component.
  - The second component looks orthogonal to party.

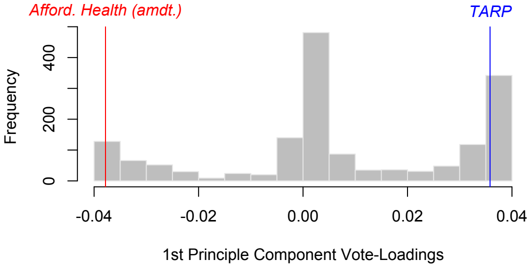
Factor Interpretation

```
## Far right (very conservative)
> sort(votepc[,1])
     BROUN (R GA-10)       FLAKE (R AZ-6)   HENSARLIN (R TX-5)
         -39.3739409          -38.2506713          -37.5870597

## Far left (very liberal)
> sort(votepc[,1], decreasing=TRUE)
    EDWARDS (D MD-4)   PRICE (D NC-4)    MATSUI (D CA-5)
         25.2915083        25.1591151         25.1248117

## social issues?  immigration?  no clear pattern
> sort(votepc[,2])
     SOLIS (D CA-32) GILLIBRAND (D NY-20)      PELOSI (D CA-8)
        -88.31350926         -87.58871687         -86.53585568
   STUTZMAN (R IN-3)       REED (R NY-29)      GRAVES (R GA-9)
        -85.59217310         -85.53636319         -76.49658108
```

- PC1 is easy to read, PC2 is ambiguous (is it even meaningful?)

Factor Interpretation

- **High PC1-loading votes are ideological battles.**
- These tend to have informative voting across party lines.



- A vote for Repulican amendments to 'Affordable Health Care for America' strongly indicates a negative PC1 (more conservative), while
  a vote for Troubled Asset Relief Program (TARP) indicates a positive PC1 (more progressive).

Factor Interpretation

- Look at the largest loadings in δ_2 to discern an interpretation.

```
> loadings[order(abs(loadings[,2]), decreasing=TRUE)[1:5],2]
 Vote.1146   Vote.658  Vote.1090  Vote.1104  Vote.1149
0.05605862 0.05461947 0.05300806 0.05168382 0.05155729
```

- These votes all correspond to near-unanimous symbolic action.

- For example, 429 legislators voted for resolution 1146:
  'Supporting the goals and ideals of a Cold War Veterans Day'
  If you didn't vote for this, you weren't in the house.

- Mystery Solved: the second PC is just attendance!

```
> sort(rowSums(votes==0), decreasing=TRUE)
    SOLIS (D CA-32) GILLIBRAND (D NY-20)       REED (R NY-29)
               1628                 1619                 1562
  STUTZMAN (R IN-3)      PELOSI (D CA-8)      GRAVES (R GA-9)
               1557                 1541                 1340
```

Principal Component Regression

- The concept is very simple: instead of regressing onto X, use a lower dimension set of principal components f_s as covariates.
- This works well for a few reasons:
  - PCA reduces dimension, which is always good.
  - Higher variance covariates are good in regression, and we choose the top PCs to have highest variance.
  - The PCs are independent: no multicollinearity.
- The 2-stage algorithm is straightforward. For example,

```
mypca = prcomp(X, scale=TRUE)
z = predict(mypca)[,1:K]
reg = glm(y˜., data=as.data.frame(z))
```

Review & Next Steps

- Factor Models
- PCA Theory
- PC Computation
- Factor Interpretation
- Next class: More on PC regression and LDA
- Questions? Questions about software?

Further Readings

- Ahumada, H. A., Gabrielli, M. F., Herrera Gomez, M. H., & Sosa Escudero, W. (2018). Una nueva econometría: Automatización, big data, econometría espacial y estructural.
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