QCB 508 – Week 12

John D. Storey Spring 2017

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EDA of HD Data

Rationale

Exploratory data analysis (EDA) of high-dimensional data adds the additional challenge that many variables must be examined simultaneously. Therefore, in addition to the EDA methods we discussed earlier, methods are often employed to organize, visualize, or numerically capture high-dimensional data into lower dimensions.

Examples of EDA approaches applied to HD data include:

- Traditional EDA methods covered earlier
- Cluster analysis
- Dimensionality reduction

Cluster Analysis

An overview of common cluster analysis methods can be found here:

http://sml201.github.io/lectures/week12/week12.html

These slides include:

- Distance measures
- Hierarchical clustering
- K-means clustering

Example: Cancer Subtypes

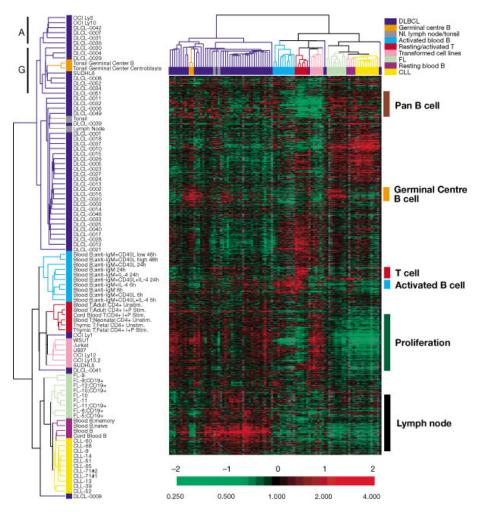


Figure from Alizadeh et al. (2000) Nature.

Dimensionality Reduction

The goal of **dimensionality reduction** is to extract low dimensional representations of high dimensional data that are useful for visualization, exploration, inference, or prediction.

The low dimensional representations should capture key sources of variation in the data.

Some Methods

- Principal component analysis
- Singular value decomposition
- Latent variable modeling
- Vector quantization
- Self-organizing maps
- Multidimensional scaling

Example: Weather Data

These daily temperature data (in tenths of degrees C) come from meteorogical observations for weather stations in the US for the year 2012 provided by NOAA (National Oceanic and Atmospheric Administration).:

```
> load("../data/weather_data.RData")
> dim(weather data)
[1] 2811
          50
> weather_data[1:5, 1:7]
                  11
                           16 18
                                        19
                                            27
                                                30
                                                         31
AG000060611 138.0000 175.0000 173 164.0000 218 160 163.0000
AGM00060369 158.0000 162.0000 154 159.0000 165 125 171.0000
AGM00060425 272.7619 272.7619 152 163.0000 163 108 158.0000
AGM00060444 128.0000 102.0000 100 111.0000 125
                                               33 125.0000
AGM00060468 105.0000 122.0000 97 263.5714 155 52 263.5714
```

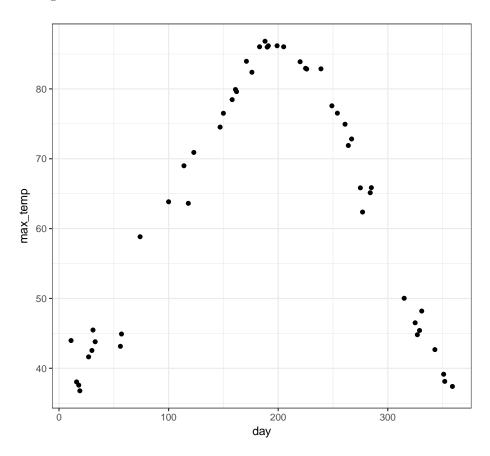
This matrix contains temperature data on 50 days and 2811 stations that were randomly selected.

Convert temperatures to Fahrenheit:

```
> weather data <- 0.18*weather data + 32
> weather_data[1:5, 1:6]
                  11
                           16
                                  18
                                           19
                                                 27
                                                       30
AG000060611 56.84000 63.50000 63.14 61.52000 71.24 60.80
AGM00060369 60.44000 61.16000 59.72 60.62000 61.70 54.50
AGM00060425 81.09714 81.09714 59.36 61.34000 61.34 51.44
AGM00060444 55.04000 50.36000 50.00 51.98000 54.50 37.94
AGM00060468 50.90000 53.96000 49.46 79.44286 59.90 41.36
> apply(weather_data, 1, median) %>%
    quantile(probs=seq(0,1,0.1))
        0%
                             20%
                                         30%
                                                    40%
                  10%
  8.886744
            49.010000
                       54.500000
                                  58.460000
                                              62.150000
       50%
                  60%
                             70%
                                         80%
                                                    90%
 65.930000 69.679318 73.490000
                                  77.990000
                                              82.940000
```

100**%** 140.000000

Here are the 2811 rows converted to a single row that captures the most variation among the rows:



Principal Component Analysis

Goal

For a given set of variables, **principal component analysis** (PCA) finds (constrained) weighted sums of the variables to produce variables (called principal components) that capture consectuive maximum levels of variation in the data.

Specifically, the first principal component is the weighted sum of the variables that results in a component with the highest variation.

This component is then "removed" from the data, and the second principal component is obtained on the resulting residuals.

This process is repeated until there is no variation left in the data.

Population PCA

Suppose we have m random variables X_1, X_2, \ldots, X_m . We wish to identify a set of weights w_1, w_2, \ldots, w_m that maximizes

$$\operatorname{Var}(w_1 X_1 + w_2 X_2 + \dots + w_m X_m).$$

However, this is unbounded, so we need to constrain the weights. It turns out that constraining the weights so that

$$\|\boldsymbol{w}\|_{2}^{2} = \sum_{i=1}^{m} w_{i}^{2} = 1$$

is both interpretable and mathematically tractable.

Therefore we wish to maximize

$$\operatorname{Var}\left(w_1X_1 + w_2X_2 + \dots + w_mX_m\right)$$

subject to $\|\boldsymbol{w}\|_2^2 = 1$. Let Σ be the $m \times m$ population covariance matrix of the random variables X_1, X_2, \dots, X_m . It follows that

$$\operatorname{Var}(w_1X_1 + w_2X_2 + \cdots + w_mX_m) = \boldsymbol{w}^T\boldsymbol{\Sigma}\boldsymbol{w}.$$

Using a Lagrange multiplier, we wish to maximize

$$\boldsymbol{w}^T \boldsymbol{\Sigma} \boldsymbol{w} + \lambda (\boldsymbol{w}^T \boldsymbol{w} - 1).$$

Differentiating with respect to w and setting to $\mathbf{0}$, we get $\Sigma w - \lambda w = 0$ or

$$\Sigma w = \lambda w$$
.

For any such \boldsymbol{w} and λ where this holds, note that

$$Var(w_1X_1 + w_2X_2 + \cdots + w_mX_m) = \boldsymbol{w}^T\boldsymbol{\Sigma}\boldsymbol{w} = \lambda$$

so the variance is λ .

The eigendecomposition of a matrix identifies all such solutions to $\Sigma w = \lambda w$. Specifically, it calculates the decompositon

$$\Sigma = W \Lambda W^T$$

where W is an $m \times m$ orthogonal matrix and Λ is a diagonal matrix with entries $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m$.

The fact that W is orthogonal means $WW^T = W^TW = I$.

The following therefore hold:

- For each column j of \boldsymbol{W} , say \boldsymbol{w}_j , it follows that $\boldsymbol{\Sigma}\boldsymbol{w}_j = \lambda_j \boldsymbol{w}_j$
- $\|\boldsymbol{w}_j\|_2^2 = 1$ and $\boldsymbol{w}_j^T \boldsymbol{w}_k = \mathbf{0}$ for $\lambda_j \neq \lambda_k$
- $\operatorname{Var}(\boldsymbol{w}_{i}^{T}\boldsymbol{X}) = \lambda_{i}$
- $\operatorname{Var}(\boldsymbol{w}_{1}^{T}\boldsymbol{X}) \geq \operatorname{Var}(\boldsymbol{w}_{2}^{T}\boldsymbol{X}) \geq \cdots \geq \operatorname{Var}(\boldsymbol{w}_{m}^{T}\boldsymbol{X})$ $\boldsymbol{\Sigma} = \sum_{j=1}^{m} \lambda_{j} \boldsymbol{w}^{j} \boldsymbol{w}_{j}^{T}$ For $\lambda_{j} \neq \lambda_{k}$,

$$\operatorname{Cov}(\boldsymbol{w}_{i}^{T}\boldsymbol{X}, \boldsymbol{w}_{k}^{T}\boldsymbol{X}) = \boldsymbol{w}_{i}^{T}\boldsymbol{\Sigma}\boldsymbol{w}_{k} = \lambda_{k}\boldsymbol{w}_{i}^{T}\boldsymbol{w}_{k} = \boldsymbol{0}$$

Population PCs

The jth population principal component (PC) of X_1, X_2, \dots, X_m is

$$\mathbf{w}_{i}^{T}\mathbf{X} = w_{1j}X_{1} + w_{2j}X_{2} + \dots + w_{mj}X_{m}$$

where $\mathbf{w}_j = (w_{1j}, w_{2j}, \dots, w_{mj})^T$ is column j of \mathbf{W} from the eigendecomposition

$$\Sigma = W \Lambda W^T$$
.

The column w_i are called the **loadings** of the jth principal component. The variance explained by the jth PC is λ_j , which is diagonal element j of Λ .

Sample PCA

Suppose we have m variables, each with n observations:

$$x_1 = (x_{11}, x_{12}, \dots, x_{1n})$$

 $x_2 = (x_{21}, x_{22}, \dots, x_{2n})$
 \vdots
 $x_m = (x_{m1}, x_{m2}, \dots, x_{mn})$

We can organize these variables into an $m \times n$ matrix X where row i is x_i .

PCA can be extended from the population scenario applied to rv's to the sample scenario applied to the observed data X.

Consider all possible weighted sums of these variables

$$\tilde{\boldsymbol{x}} = \sum_{i=1}^m u_i \boldsymbol{x_i}$$

where we constrain $\sum_{i=1}^{m} u_i^2 = 1$.

The first principal component of \boldsymbol{X} is the results $\tilde{\boldsymbol{x}}$ with maximum sample variance

$$s_{\tilde{x}}^{2} = \frac{\sum_{j=1}^{n} \left(\tilde{x}_{j} - \frac{1}{n} \sum_{k=1}^{n} \tilde{x}_{k} \right)^{2}}{n-1}.$$

This first sample principal component (PC) is then "removed" from the data, and the procedure is repeated until $\min(m, n-1)$ sample PCs are constructed.

The sample PCs are found in a manner analogous to the population PCs. First, we construct the $m \times m$ sample covariance matrix S with (i, j) entry

$$s_{ij} = \frac{\sum_{k=1}^{n} (x_{ik} - \bar{x}_{i \cdot})(x_{jk} - \bar{x}_{j \cdot})}{n-1}.$$

Identifying \boldsymbol{u} that maximizes $s_{\tilde{\boldsymbol{x}}}^2$ also maximizes

$$\boldsymbol{u}^T \boldsymbol{S} \boldsymbol{u}$$
.

Following the steps from before, we want to identify u and λ where

$$Su = \lambda u$$
.

which is accomplished with the eigendecomposition

$$S = U \Lambda U^T$$

where again $\boldsymbol{U}^T\boldsymbol{U} = \boldsymbol{U}\boldsymbol{U}^T = \boldsymbol{I}$ and $\boldsymbol{\Lambda}$ is a diagonal matrix so that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_m \geq 0$.

Sample PCs

Let $x_{ij}^* = x_{ij} - \bar{x}_i$ be the row-wise mean-centered values of X, and let X^* be the matrix composed of these values. Also, let u_j be column j of U from $S = U\Lambda U^T$.

Sample PC j is then

$$\tilde{oldsymbol{x}}_j = oldsymbol{u}_j^T oldsymbol{X}^* = \sum_{i=1}^m u_{ij} oldsymbol{x}_i^*$$

for $j = 1, 2, ..., \min(m, n - 1)$.

The loadings corresponding to PC j are u_j .

Note that the mean of PC j is zero, i.e., that

$$\frac{1}{n}\sum_{k=1}^{n}\tilde{x}_{jk}=0.$$

It can be calculated that the variance of PC j is

$$s_{\tilde{x}_j}^2 = \frac{\sum_{k=1}^n \tilde{x}_{jk}^2}{n-1} = \lambda_j.$$

Proportion of Variance Explained

The proportion of variance explained by PC j is

$$PVE_j = \frac{\lambda_j}{\sum_{k=1}^m \lambda_k}.$$

Singular Value Decomposition

One way in which PCA is performed is to carry out a **singular value decomposition** (SVD) of the data matrix \boldsymbol{X} . Let $q = \min(m, n-1)$. Recalling that \boldsymbol{X}^* is the row-wise mean centered \boldsymbol{X} , we can take the SVD of $\boldsymbol{X}^*/\sqrt{n-1}$ to obtain

$$\frac{1}{\sqrt{n-1}}\boldsymbol{X}^* = \boldsymbol{U}\boldsymbol{D}\boldsymbol{V}^T$$

where $U_{m\times q}$, $V_{n\times q}$, and diagonal $D_{q\times q}$. Also, we have the orthogonality properties $V^TV = U^TU = I_q$. Finally, D is composed of diagonal elements $d_1 \geq d_2 \geq \cdots \geq d_q \geq 0$ where $d_q = 0$ if q = n - 1.

Note that

$$S = \frac{1}{n-1} X^* X^{*T} = UDV^T \left(UDV^T \right)^T = UD^2 U^T.$$

Therefore:

- The variance of PC j is $\lambda_j = d_j^2$
- The loadings of PC j are contained in the columns of the left-hand matrix from the decomposition of S or X^*
- PC j is row j of DV^T

My PCA Function

```
> pca <- function(x, space=c("rows", "columns"),</pre>
                    center=TRUE, scale=FALSE) {
    space <- match.arg(space)</pre>
    if(space=="columns") \{x \leftarrow t(x)\}
    x <- t(scale(t(x), center=center, scale=scale))</pre>
    x \leftarrow x/sqrt(nrow(x)-1)
    s \leftarrow svd(x)
    loading <- s$u
    colnames(loading) <- paste0("Loading", 1:ncol(loading))</pre>
    rownames(loading) <- rownames(x)</pre>
    pc <- diag(s$d) %*% t(s$v)
   rownames(pc) <- paste0("PC", 1:nrow(pc))</pre>
    colnames(pc) <- colnames(x)</pre>
    pve <- s$d^2 / sum(s$d^2)
   if(space=="columns") {pc <- t(pc); loading <- t(loading)}</pre>
    return(list(pc=pc, loading=loading, pve=pve))
```

How It Works

Input is as follows:

- x: a matrix of numerical values
- space: either "rows" or "columns", denoting which dimension contains the variables
- \bullet center: if TRUE then the variables are mean centered before calculating PCs

 $\bullet\,$ scale: if TRUE then the variables are std dev scaled before calculating PCs

Output is a list with the following items:

- pc: a matrix of all possible PCs
- loading: the weights or "loadings" that determined each PC
- pve: the proportion of variation explained by each PC

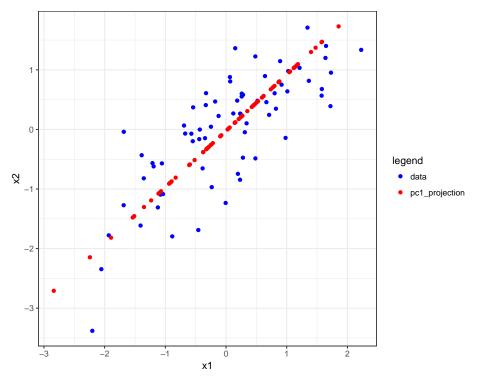
Note that the rows or columns of pc and loading have names to let you know on which dimension the values are organized.

The Ubiquitous Example

Here's an example very frequently encountered to explain PCA, but it's slightly complicated.

```
> set.seed(508)
> n <- 70
> z <- sqrt(0.8) * rnorm(n)
> x1 <- z + sqrt(0.2) * rnorm(n)
> x2 <- z + sqrt(0.2) * rnorm(n)
> X <- rbind(x1, x2)
> p <- pca(x=X, space="rows")</pre>
```

"The first PC finds the direction of maximal variance in the data..."



The above figure was made with the following code:

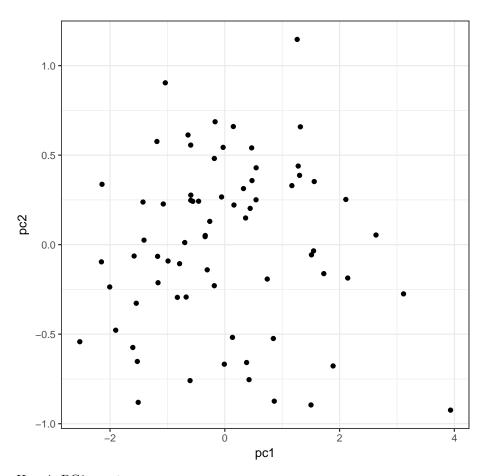
The red dots are therefore the projection of x1 and x2 onto the first PC, so they are neither the loadings nor the PC.

Note that

```
outer(p$loading[,1], p$pc[1,])[1,] + mean(x1)
# yields the same as
lm(x1 ~ p$pc[1,])$fit # and
outer(p$loading[,1], p$pc[1,])[2,] + mean(x2)
# yields the same as
lm(x2 ~ p$pc[1,])$fit
```

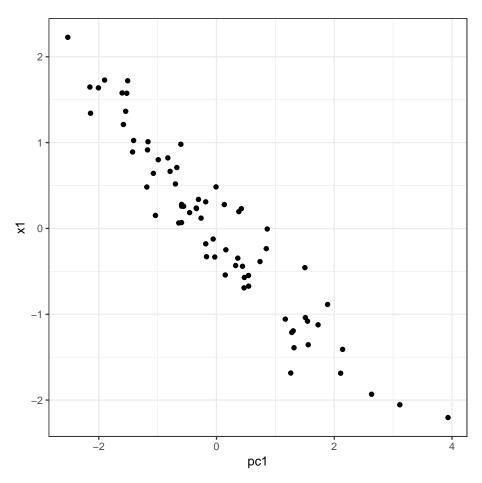
```
Here is PC1 vs PC2:
```

```
> data.frame(pc1=p$pc[1,], pc2=p$pc[2,]) %>%
+ ggplot() + geom_point(aes(x=pc1,y=pc2)) +
+ theme(aspect.ratio=1)
```



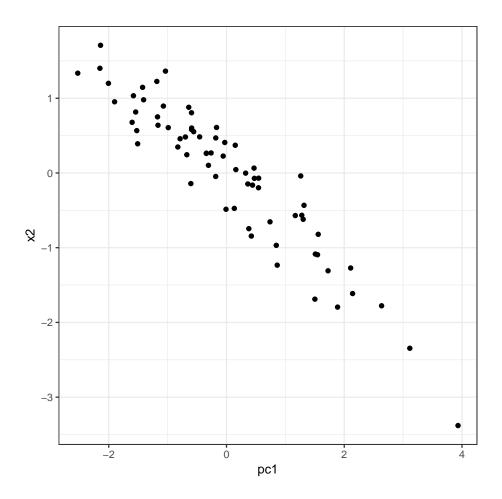
Here is PC1 vs x1:

```
> data.frame(pc1=p$pc[1,], x1=x1) %>%
+ ggplot() + geom_point(aes(x=pc1,y=x1)) +
+ theme(aspect.ratio=1)
```



Here is PC1 vs x2:

```
> data.frame(pc1=p$pc[1,], x2=x2) %>%
+ ggplot() + geom_point(aes(x=pc1,y=x2)) +
+ theme(aspect.ratio=1)
```

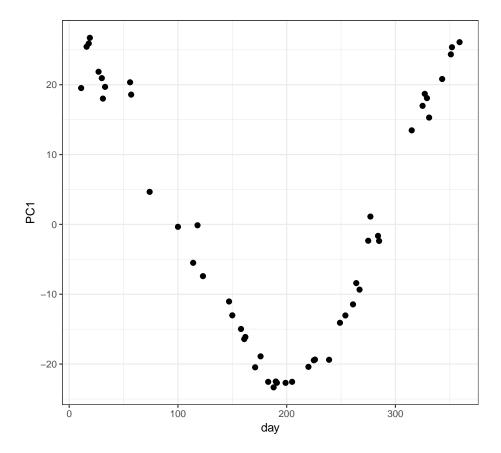


PCA Examples

Weather Data

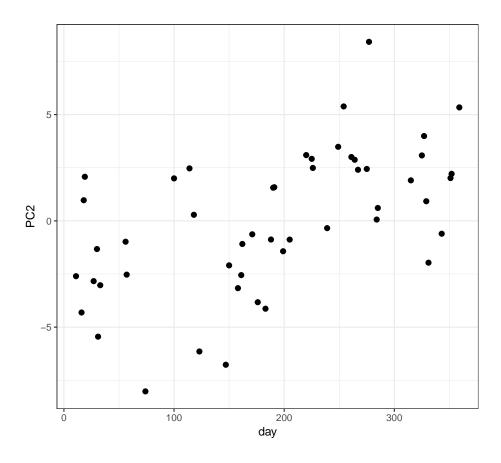
PC1 vs Time

```
> day_of_the_year <- as.numeric(colnames(weather_data))
> data.frame(day=day_of_the_year, PC1=mypca$pc[1,]) %>%
+ ggplot() + geom_point(aes(x=day, y=PC1), size=2)
```



PC2 vs Time

```
> data.frame(day=day_of_the_year, PC2=mypca$pc[2,]) %>%
+ ggplot() + geom_point(aes(x=day, y=PC2), size=2)
```



PC Biplots

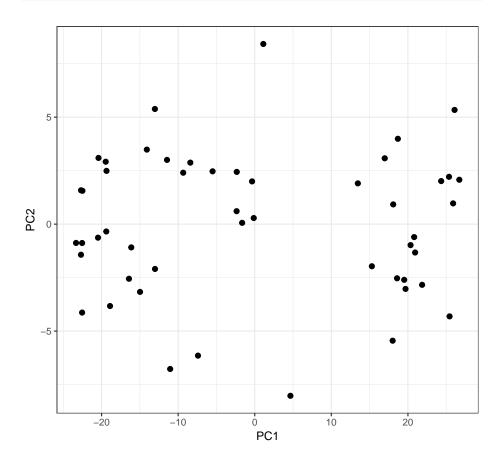
Sometimes it is really informative to plot a PC versus another PC (as in the previous slide). This is called a $PC\ biplot$.

It is possible that interesting subgroups or clusters of observations will emerge.

This does not appear to be the case in the weather data set, however, due to what we observe in the next two plots.

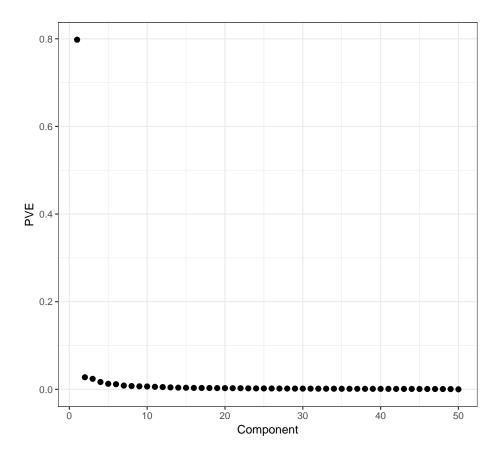
PC1 vs PC2 Biplot

```
> data.frame(PC1=mypca$pc[1,], PC2=mypca$pc[2,]) %>%
+ ggplot() + geom_point(aes(x=PC1, y=PC2), size=2)
```



Proportion of Variance Explained

```
> data.frame(Component=1:length(mypca$pve), PVE=mypca$pve) %>%
+ ggplot() + geom_point(aes(x=Component, y=PVE), size=2)
```



PCs Reproduce the Data

We can multiple the loadings matrix by the PCs matrix to reproduce the data:

Loadings

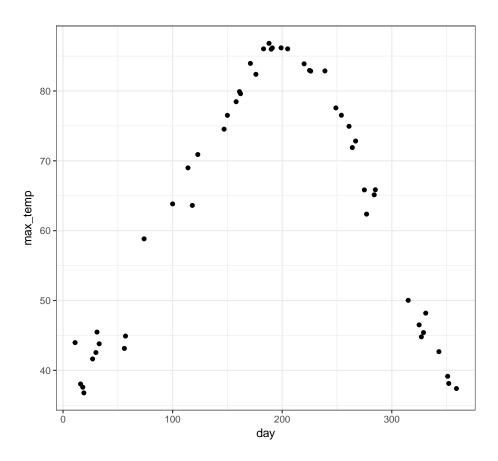
The sum of squared weights - i.e., loadings - equals one for each component:

```
> sum(mypca$loading[,1]^2)
[1] 1
> apply(mypca$loading, 2, function(x) {sum(x^2)})
Loading1 Loading2 Loading3 Loading4 Loading5 Loading6
             1
                     1
Loading7 Loading8 Loading9 Loading10 Loading11 Loading12
             1
                     1
Loading13 Loading14 Loading15 Loading16 Loading17 Loading18
         1
                    1 1 1
Loading19 Loading20 Loading21 Loading22 Loading23 Loading24
      1 1 1 1 1
Loading25 Loading26 Loading27 Loading28 Loading29 Loading30
                    1 1 1
Loading31 Loading32 Loading33 Loading34 Loading35 Loading36
      1 1 1 1 1
Loading37 Loading38 Loading39 Loading40 Loading41 Loading42
          1 1 1 1
Loading43 Loading44 Loading45 Loading46 Loading47 Loading48
      1
             1
                     1
                        1
Loading49 Loading50
```

Pairs of PCs Have Correlaton Zero

PCs by contruction have sample correlation equal to zero:

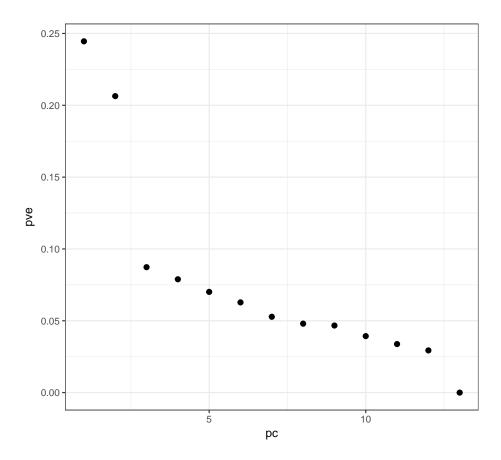
```
> cor(mypca$pc[1,], mypca$pc[2,])
[1] 3.135149e-17
> cor(mypca$pc[1,], mypca$pc[3,])
[1] 2.273613e-16
> cor(mypca$pc[1,], mypca$pc[12,])
[1] -1.231339e-16
> cor(mypca$pc[5,], mypca$pc[27,])
[1] -2.099516e-17
> # etc...
> day_of_the_year <- as.numeric(colnames(weather_data))
> y <- -mypca$pc[1,] + mean(weather_data)
> data.frame(day=day_of_the_year, max_temp=y) %>%
+ ggplot() + geom_point(aes(x=day, y=max_temp))
```



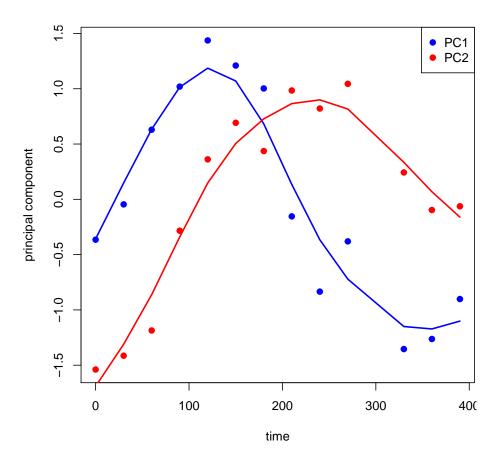
Yeast Gene Expression

Yeast cells were synchronized so that they were on the same approximate cell cycle timing. The goal was to understand how gene expression varies over the cell cycle from a genome-wide perspective.

Proportion Variance Explained



PCs vs Time (with Smoothers)



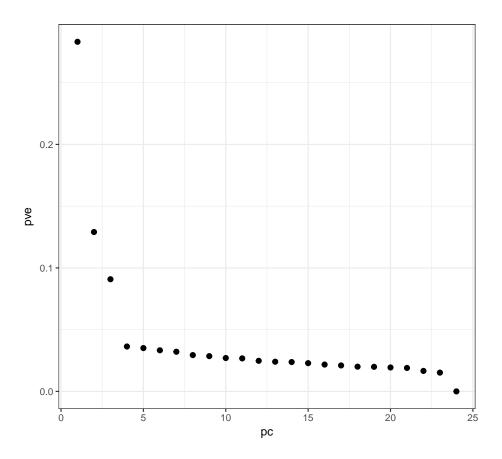
HapMap Genotypes

Recall the example of HapMap data used to demonstrate the MCMC algorithm for estimating structure. We curated a small data set that cleanly separated human subpopulations.

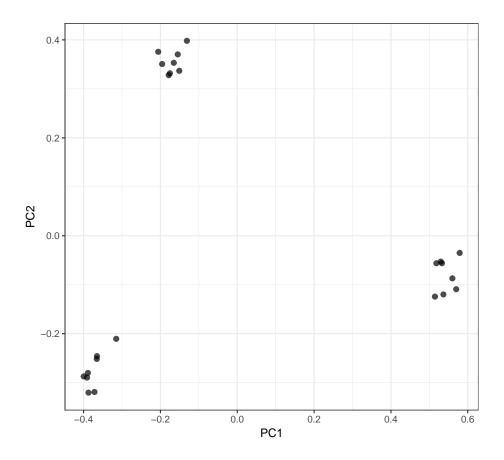
```
> hapmap <- read.table("../data/hapmap_sample.txt")</pre>
> dim(hapmap)
[1] 400 24
> hapmap[1:6,1:6]
            NA18516 NA19138 NA19137 NA19223 NA19200 NA19131
                                    2
rs2051075
                  0
                                             1
                                                      1
                            1
                                                               1
                                     0
                                             0
rs765546
                   2
                            2
                                                      0
                                                               0
rs10019399
                   2
                            2
                                     2
                                             1
                                                      1
                                                               2
rs7055827
                   2
                            2
                                     1
                                             2
                                                      0
                                                               2
                                             0
                            0
                                    2
                                                               0
rs6943479
                  0
                                                       1
rs2095381
                            2
                                             2
                                                               1
```

Proportion Variance Explained

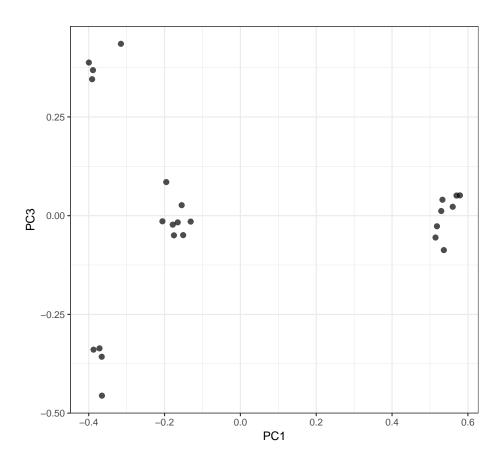
```
> p <- pca(hapmap, space="rows")
> ggplot(data.frame(pc=(1:ncol(hapmap)), pve=p$pve)) +
+ geom_point(aes(x=pc,y=pve), size=2)
```



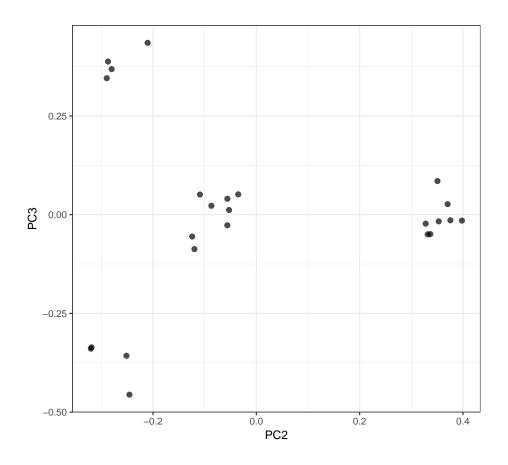
PC1 vs PC2 Biplot



PC1 vs PC3 Biplot



PC2 vs PC3 Biplot



HD Latent Variable Models

Jackstraw

Surrogate Variable Analysis

Regression Herding

Extras

Source

License

Session Information

```
> sessionInfo()
R version 3.3.2 (2016-10-31)
Platform: x86_64-apple-darwin13.4.0 (64-bit)
Running under: macOS Sierra 10.12.4
locale:
[1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8
attached base packages:
[1] stats
             graphics grDevices utils
                                          datasets methods
[7] base
other attached packages:
 [1] MASS_7.3-47
                    broom_0.4.2
                                    dplyr_0.5.0
                    readr_1.1.0
 [4] purrr_0.2.2
                                   tidyr 0.6.1
 [7] tibble_1.3.0
                    ggplot2_2.2.1 tidyverse_1.1.1
[10] knitr_1.15.1
                    magrittr_1.5
                                   devtools_1.12.0
loaded via a namespace (and not attached):
                                     cellranger_1.1.0
 [1] Rcpp_0.12.10
                    highr_0.6
 [4] plyr_1.8.4
                     forcats_0.2.0
                                     tools_3.3.2
 [7] digest_0.6.12
                     lubridate_1.6.0 jsonlite_1.4
[10] evaluate_0.10
                     memoise_1.1.0
                                     nlme_3.1-131
[13] gtable_0.2.0
                     lattice_0.20-35 psych_1.7.3.21
[16] DBI_0.6-1
                     yaml_2.1.14
                                     parallel_3.3.2
[19] haven_1.0.0
                     xml2_1.1.1
                                     withr_1.0.2
[22] stringr_1.2.0
                     httr_1.2.1
                                     hms_0.3
[25] rprojroot_1.2
                     grid_3.3.2
                                     R6_2.2.0
                     foreign_0.8-68
[28] readxl_1.0.0
                                     rmarkdown_1.5
[31] modelr_0.1.0
                     reshape2_1.4.2
                                     backports_1.0.5
[34] scales_0.4.1
                     htmltools_0.3.6 rvest_0.3.2
[37] assertthat_0.2.0 mnormt_1.5-5
                                      colorspace_1.3-2
[40] labeling 0.3
                     stringi_1.1.5
                                     lazyeval_0.2.0
[43] munsell_0.4.3
```