Principal Component Analysis

Statistics 407

ISU

Definition

Principal component analysis is concerned with summarizing the variance-covariance matrix. PCA involves computing the eigenvectors and eigenvalues of the variance-covariance matrix, S, or correlation matrix, R, as the first step. The eigenvectors are used to project the data from p dimensions down to a lower dimensional representation. The eigenvalues give the variance of the data in the direction of the eigenvector. The first eigenvector is the vector which defines the direction of maximum variance in the data.

Objectives

The objectives of principal component analysis are

- *To* ***reduce the dimensionality****. That is, if the data is plotted in p-dimensional space does it fill up all p dimensions. If not then the true dimensionality of the data may be less than p, and we can use a smaller number of variables to describe the data.*
- *Identify new meaningful underlying variables. The new variables are not always meaningful, but they may still be convenient.*

Common Uses

- ***Data screening:*** *finding outliers, finding strong association, finding clusters. Principal component analysis is badly affected by outliers, hence the practical usage for finding outliers.*
- ***Cluster analysis:*** *Find a low-dimensional projection of the data which reveals clusters.*
- *Discriminant analysis, Regression analysis: Removing multicollinearity among explanatory variables.*

Definition

- *Principal components are projections of the original variables. The first principal component is:*

$$\mathbf{Y}_1 = \mathbf{X}\mathbf{e}_1 = \begin{bmatrix} e_{11}X_{11} + e_{21}X_{12} + \ldots + e_{p1}X_{1p} \\ e_{11}X_{21} + e_{21}X_{22} + \ldots + e_{p1}X_{2p} \\ e_{11}X_{31} + e_{21}X_{32} + \ldots + e_{p1}X_{3p} \\ \vdots \\ e_{11}X_{n1} + e_{21}X_{n2} + \ldots + e_{p1}X_{np} \end{bmatrix} = \begin{bmatrix} Y_{11} \\ Y_{21} \\ Y_{31} \\ \vdots \\ Y_{n1} \end{bmatrix}$$

- *Where the projection,* $\mathbf{e}_1$ *, is found by finding the* ***direction*** *of maximum variance of the data in the multivariate space.*

Definition

- *The k'th principal component is:*

$$\mathbf{Y}_k = \mathbf{X}\mathbf{e}_k = \begin{bmatrix} e_{1k}X_{11} + e_{2k}X_{12} + \ldots + e_{pk}X_{1p} \\ e_{1k}X_{k2} + e_{2k}X_{22} + \ldots + e_{pk}X_{2p} \\ e_{1k}X_{31} + e_{2k}X_{32} + \ldots + e_{pk}X_{3p} \\ \vdots \\ e_{1k}X_{n1} + e_{2k}X_{n2} + \ldots + e_{pk}X_{np} \end{bmatrix} = \begin{bmatrix} Y_{11} \\ Y_{21} \\ Y_{31} \\ \vdots \\ Y_{n1} \end{bmatrix}$$

- *Where the projection, $\mathbf{e}_k$, is found by finding the* ***direction*** *of maximum variance of the data orthogonal to all the previous projections in the multivariate space.*

Eigen-decomposition

- *Mathematically, the directions of maximum variation can be solved using an eigen-decomposition of the variance-covariance (or correlation) matrix.*

$$\mathbf{S} = \mathbf{E}'\Lambda\mathbf{E}$$

where $\mathbf{E} = \begin{bmatrix} e_{11} & e_{12} & \cdots & e_{1p} \\ e_{21} & e_{22} & \cdots & e_{2p} \\ \vdots & \vdots & & \vdots \\ e_{p1} & e_{p2} & \cdots & e_{pp} \end{bmatrix} = [\mathbf{e}_1 \quad \mathbf{e}_2 \quad \ldots \quad \mathbf{e}_p]$ is the matrix of eigenvectors, and $\Lambda = \begin{bmatrix} \lambda_1 & 0 & \ldots & 0 \\ 0 & \lambda_2 & & \\ \vdots & & \ddots & \\ 0 & & & \lambda_p \end{bmatrix}$ is a diagonal matrix of eigenvalues.

The eigenvectors have length equal to 1 and are orthogonal ($\mathbf{e}_j'\mathbf{e}_k = 0, j \neq k$) to each other.

Principal Component Scores

- *The centered principal components are called the principal component scores:*

$$\mathbf{Y}_k = (\mathbf{X} - \bar{\mathbf{X}})\mathbf{e}_k, k = 1, \ldots p$$

- *These are the values that the cases take on the new set of variables.*

Total Variance

- *The total variance is the sum of the diagonal elements of the variance-covariance (or correlation) matrix:*

$$s_{11}+s_{22}+\ldots+s_{pp} = \sum_{i=1}^{p} Var(\mathbf{X}_i) = \lambda_1+\lambda_2+\ldots+\lambda_p = \sum_{i=1}^{p} Var(\mathbf{Y}_i).$$

- *It is equal to the sum of the eigenvalues.*
- *Total variance is used to decide how many principal components to keep. The proportion of variation explained by the first k PCs is:* $\dfrac{\lambda_1+\ldots+\lambda_k}{\lambda_1+\ldots+\lambda_p}$

Properties of PCs

- *The variance of the k'th principal component is equal to the value of the k'th eigenvalue,* λ_k .
- *Two principal components are uncorrelated.*
- *The total variance of the principal components is equal to the total variance of the original data, if all p principal components are used.*
- *The total variance is equal to p when the correlation matrix is used.*

Importance of Variables

- *The correlation between the i'th PC and the k'th variable is* $\frac{e_{ik}\sqrt{\lambda_i}}{s_k}, \quad i,k = 1,\ldots,p \cdot$
- *This helps to determine how much variable k contributes to PC i.*

Example: Track records

- *This data contains the women's national records for 100m, 200m, 400m, 800m, 1500m, 3000m and marathon, for 55 countries. We will look at the first two track events, 100m and 200m, for all the countries.*

country	m100 (sec)	m200 (sec)	m400 (sec)	m800 (min)	m1500 (min)	m3000 (min)	marathon (min)
argentin(SA)	11.61	22.94	54.50	2.15	4.43	9.79	178.52
australi(PC)	11.20	22.35	51.08	1.98	4.13	9.08	152.37
austria(EU)	11.43	23.09	50.62	1.99	4.22	9.34	159.37
...							

Results for S

$$\mathbf{S} = \begin{bmatrix} 0.204 & 0.479 \\ 0.479 & 1.234 \end{bmatrix}$$

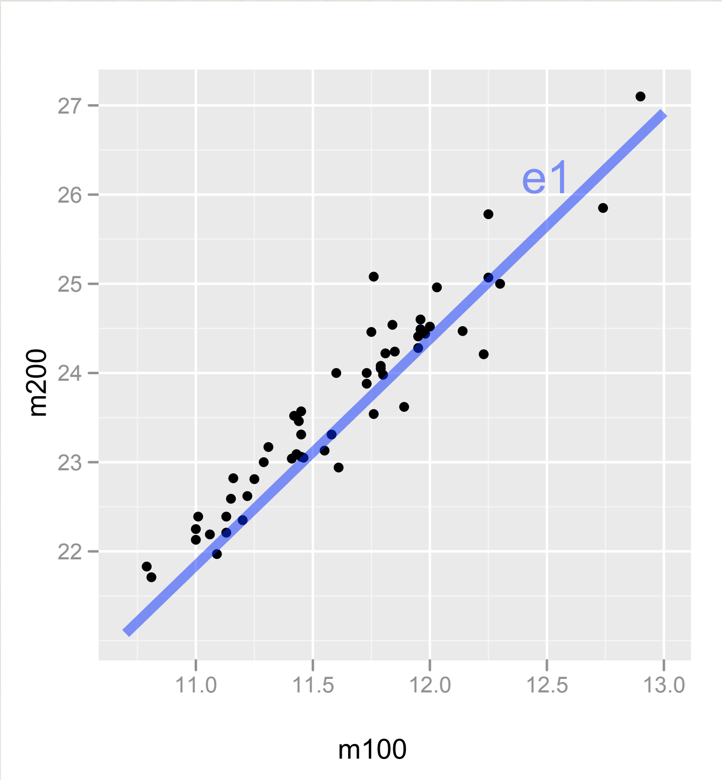
Variable	$\mathbf{e}_1$	$\mathbf{e}_2$
100m	0.366	0.931
200m	0.931	-0.366
Variance	1.423	0.016
% Tot Var	98.9	100.0

- *PC 1 explains 98.9% of the variation. This would suggest that 1 PC would be enough to summarize the variation in this data.*
- *The correlation between PC 1 and the 100m is 0.97, and with the 200m is 1.00, so both variables are important.*
- *The principal component scores for Argentina are:*

$$Y_{11} = 0.366 \times (11.61 - 11.62) + 0.931 \times (22.94 - 23.64) = -0.656,$$
$$Y_{12} = 0.931 \times (11.61 - 11.62) - 0.366 \times (22.94 - 23.64) = 0.266$$

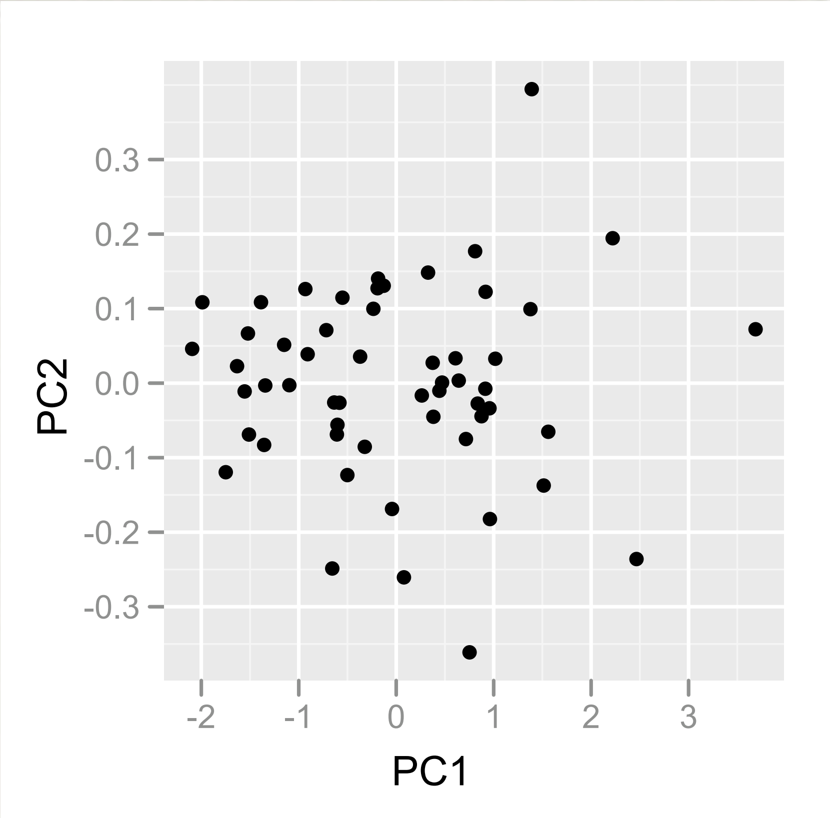
where the mean of 100m is 11.62, and for 200m is 23.64.

Results for S

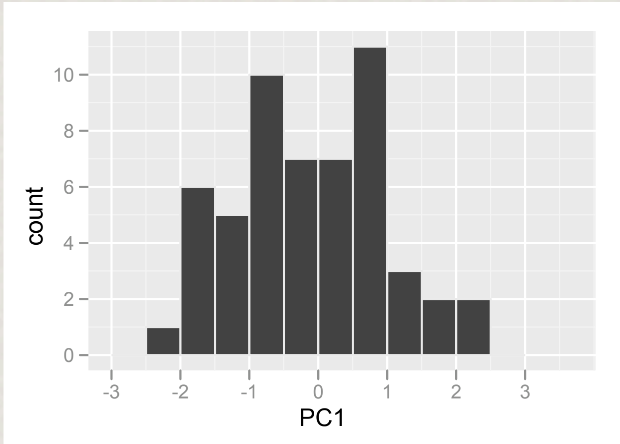


- *The first eigenvector is shown. This is the direction of maximum variance for this data. Its plotted here close to the data.*
- *First principal component scores are obtained by projecting the points onto this line.*
- *The second eigenvector is orthogonal to this one.*

Results for S



- *There should be NO obvious structure to the new variables, PCs.*
- *PC 1 should be unrelated to PC2.*



When to use R, not S?

- *PCA finds directions of maximum variance. If some variables have much larger variance than the other variables, the PCA will simply return these large variance variables as the first few PCs.*
- *Use the correlation matrix, if there are big differences in the variances. This is the same as first standardizing the variables.*

Results for R

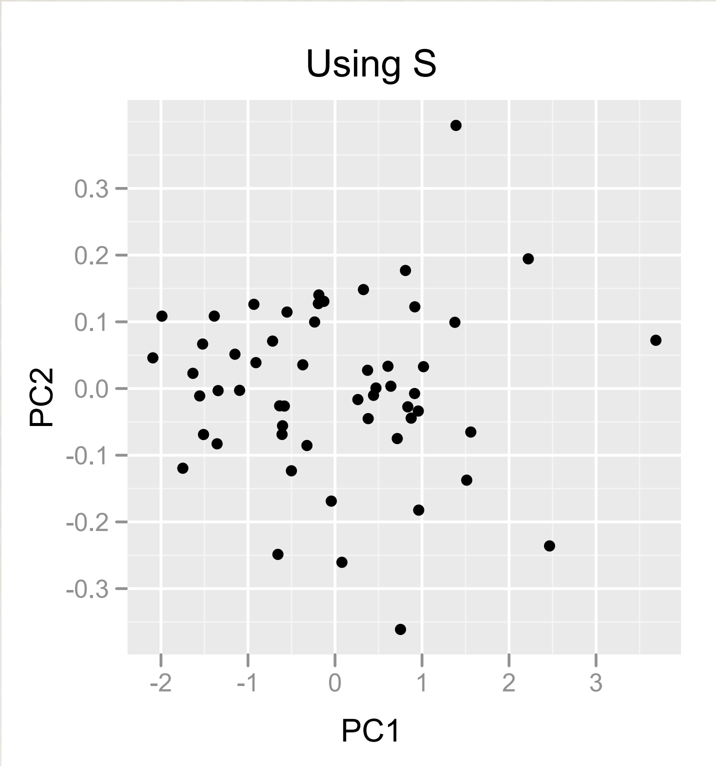
$$\mathbf{R} = \begin{bmatrix} 1.000 & 0.953 \\ 0.953 & 1.000 \end{bmatrix}$$

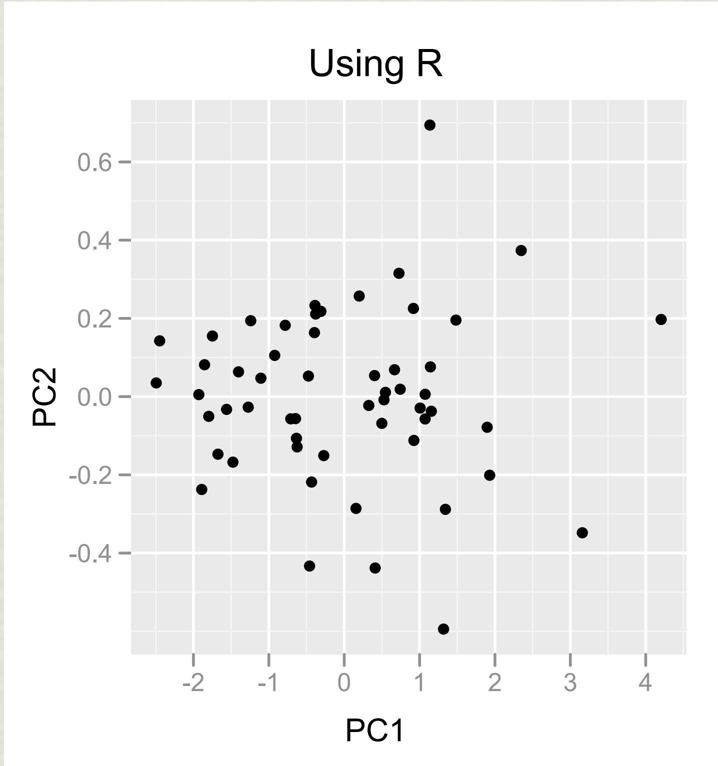
Variable	$\mathbf{e}_1$	$\mathbf{e}_2$
100m	0.707	0.707
200m	0.707	-0.707
Variance	1.95	0.0472
% Tot Var	97.6	100.0

- *Equal contribution from each variable. Why?*
- *PC 1 explains 97.6% of the variation. It drops, why?*
- *The correlation between PC 1 and the 100m is 0.97, and with the 200m is 1.00. Same as for S, why?*
- *Which analysis (on S or R) is more appropriate?*

S vs R

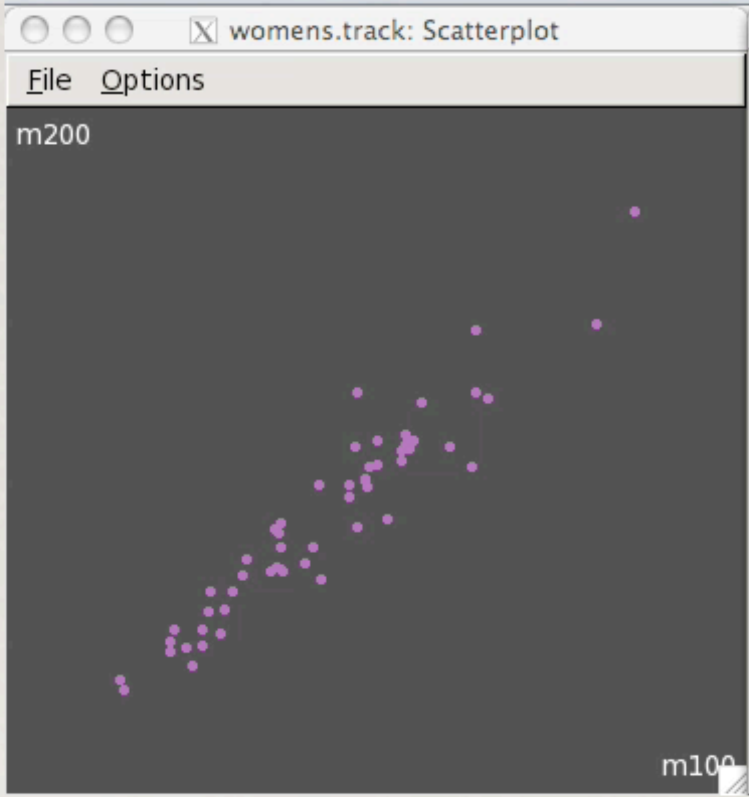
Are they the same?

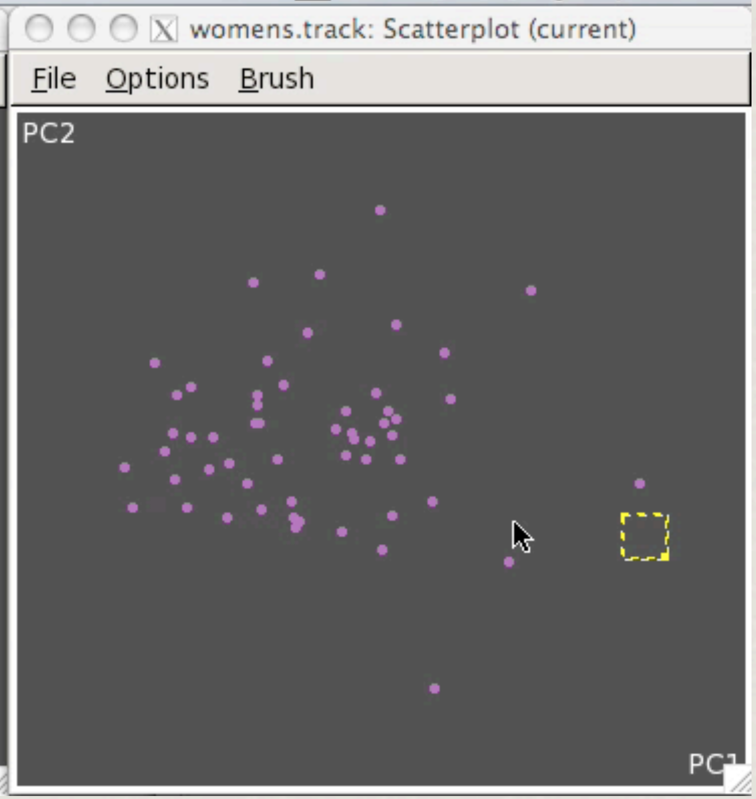




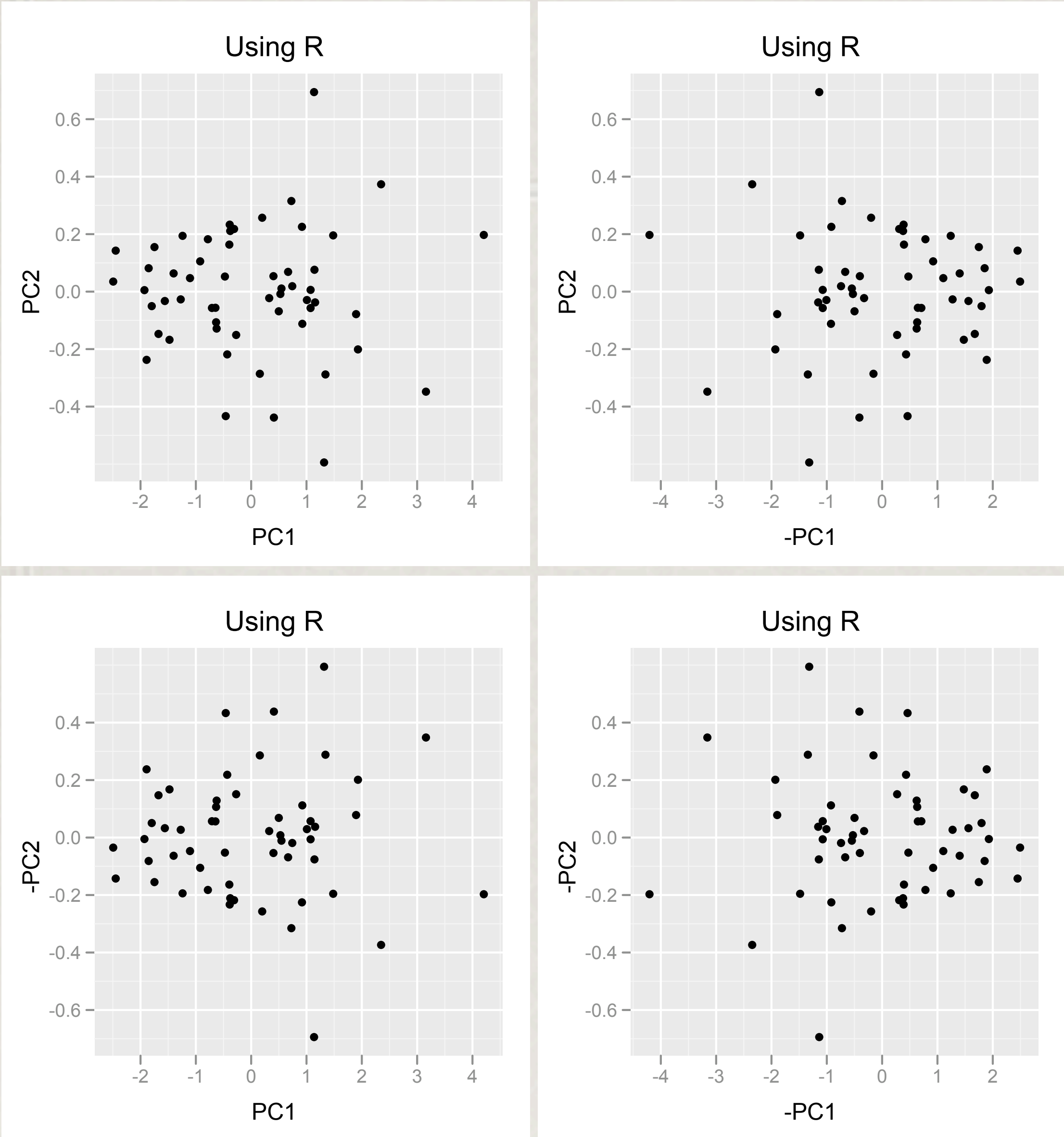
Exploring results

RAW *PCs*



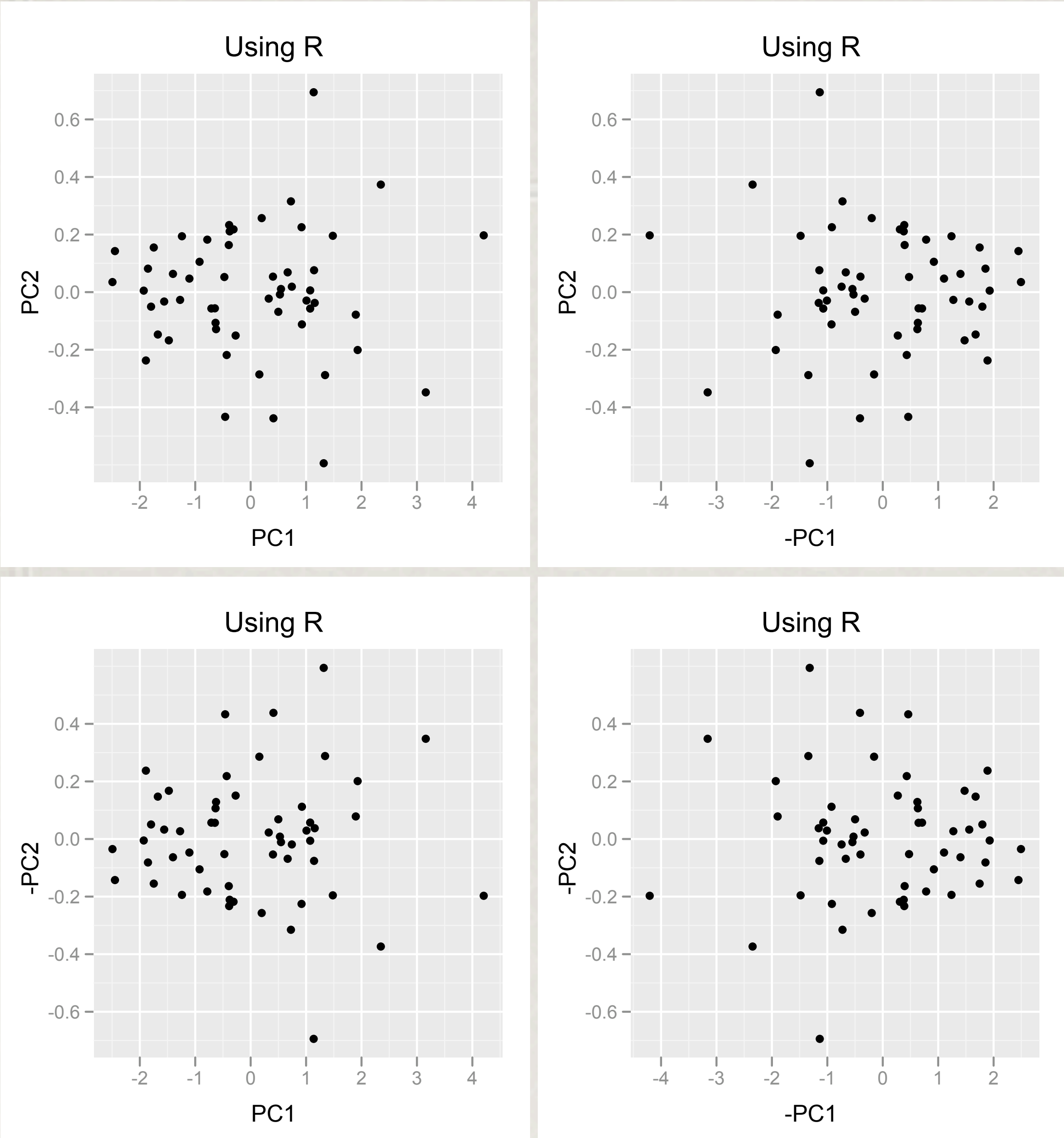


Geometry



- *Are these the same?*
- *Yes - coefficients x (-1) - direction of the vector is not important.*

Geometry



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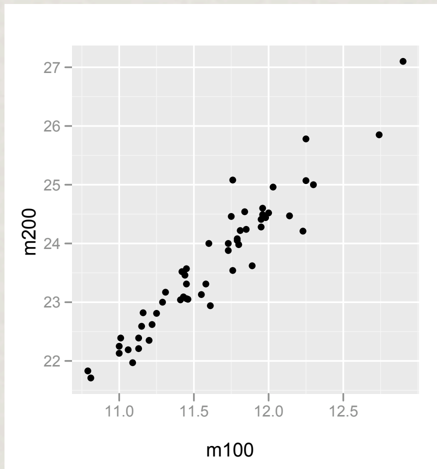

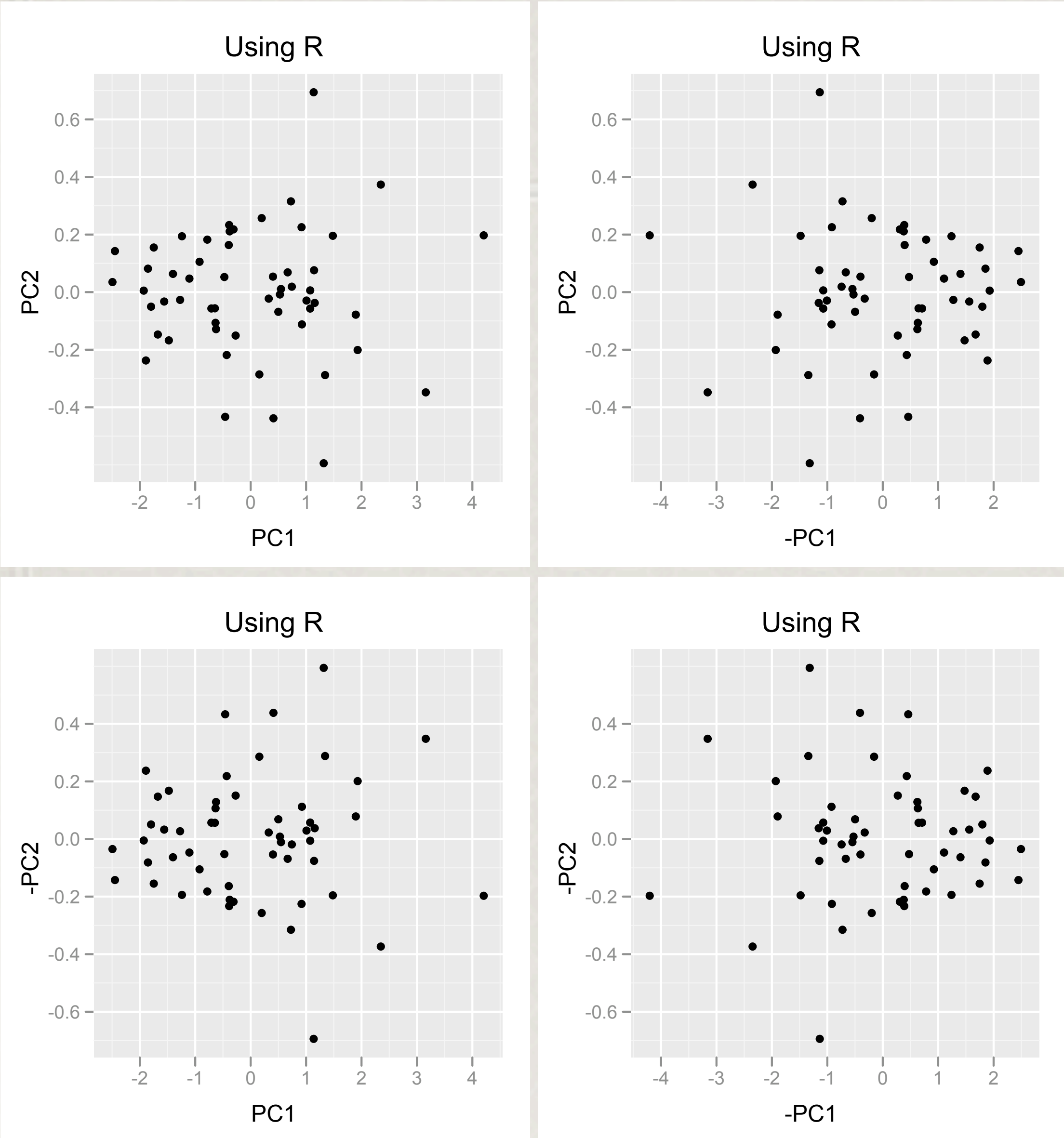

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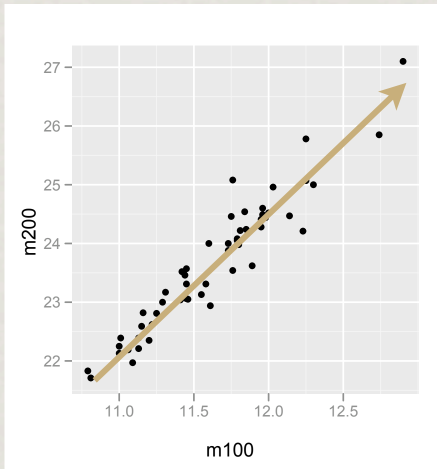

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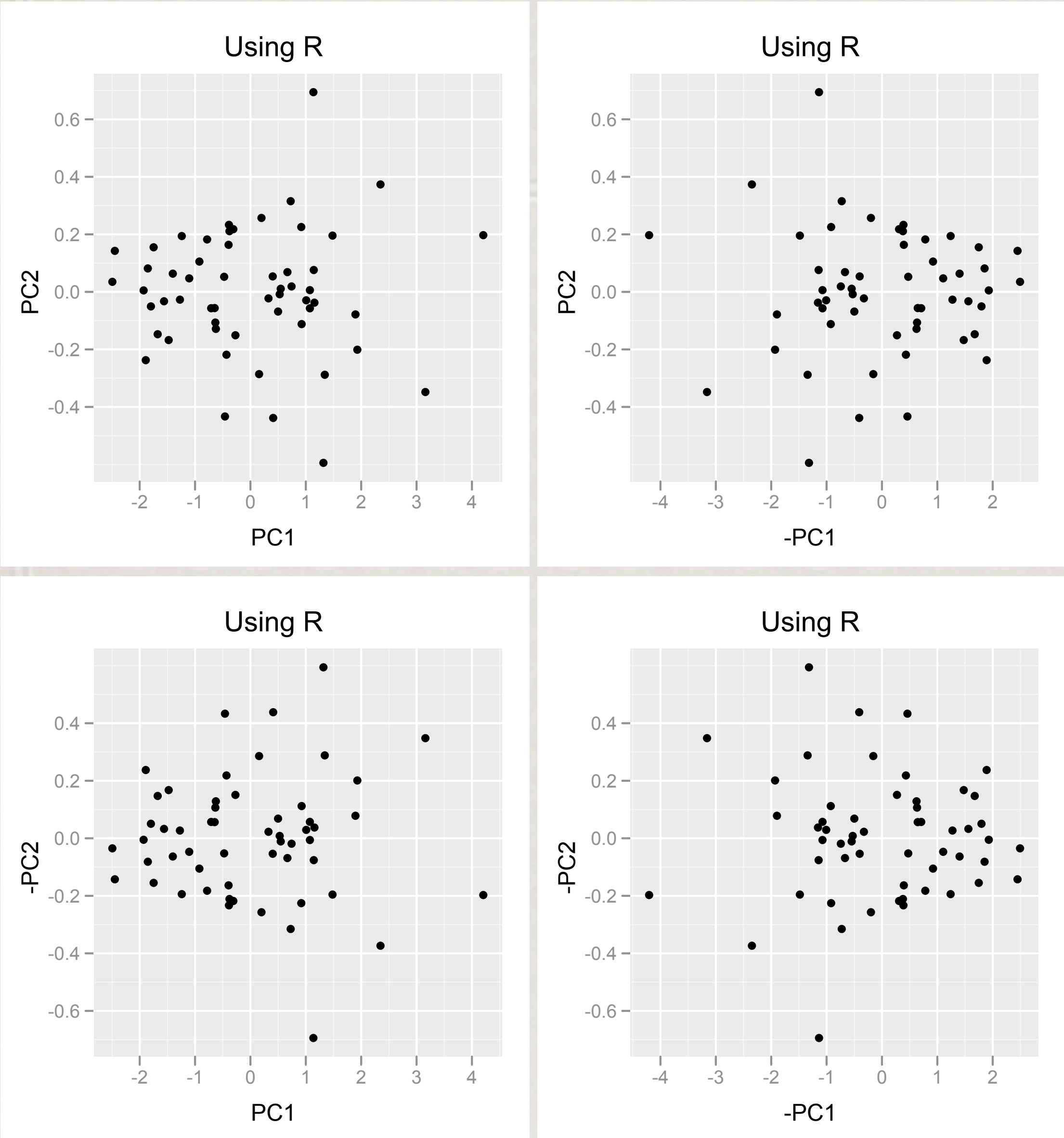

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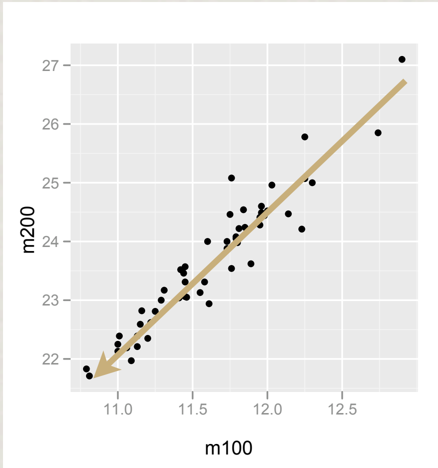

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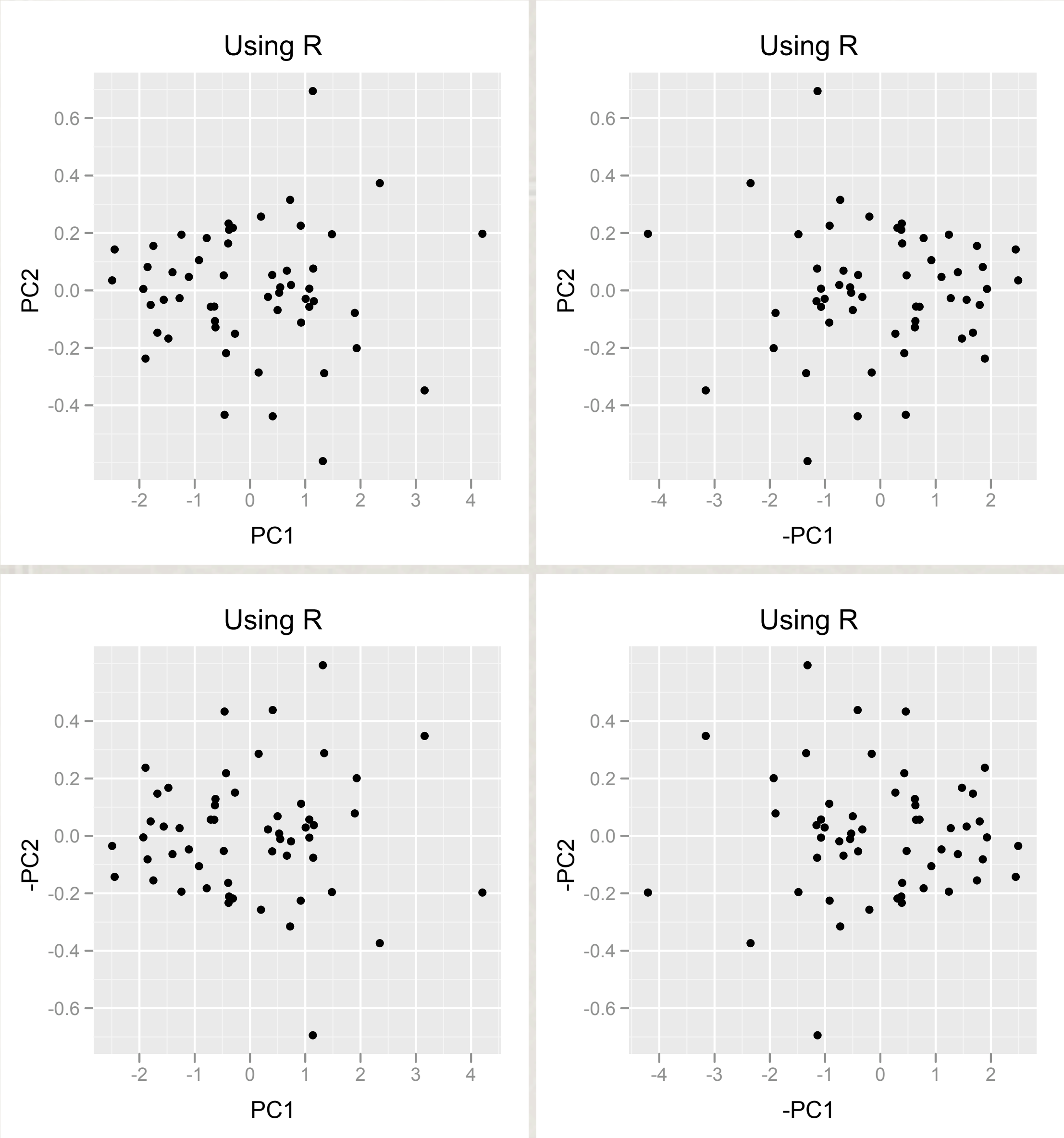
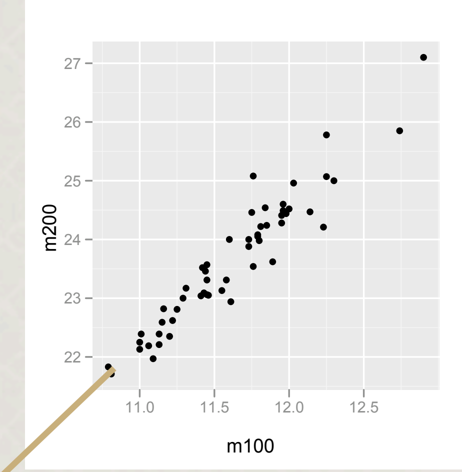
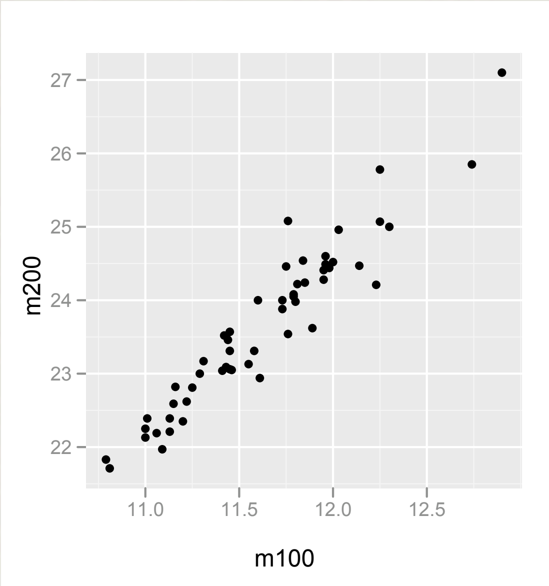
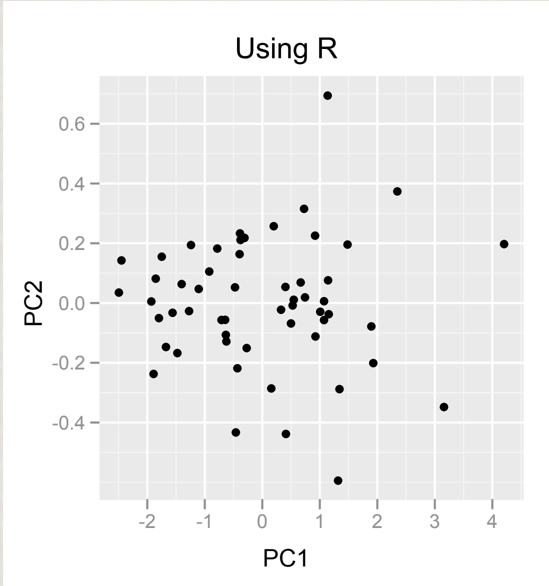




Geometry

Raw data is transformed by “sphering” to produce PCs.





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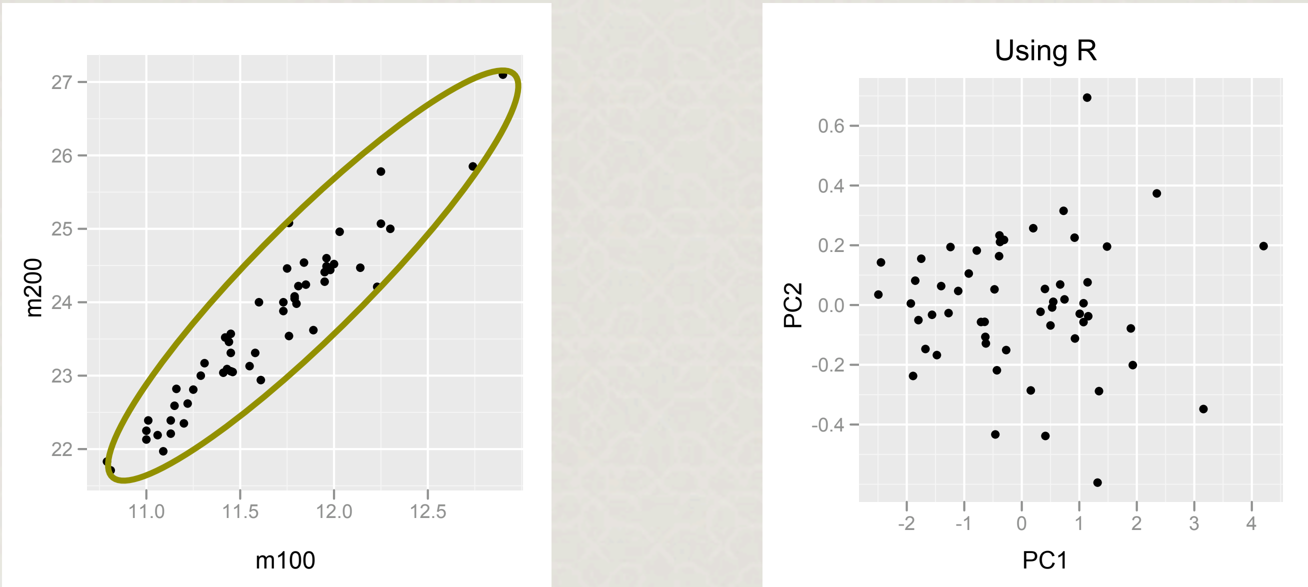

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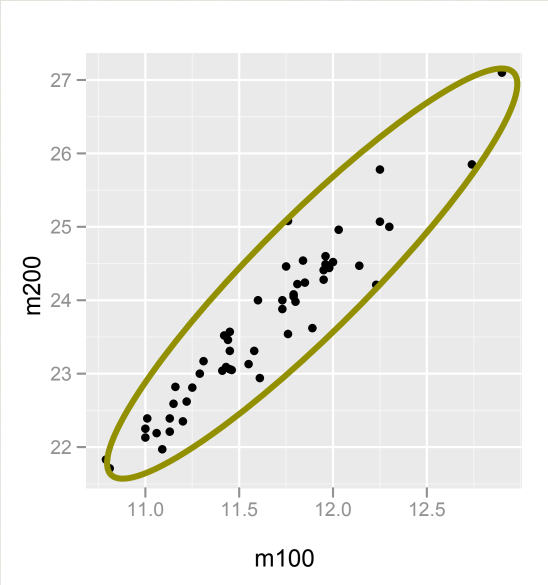

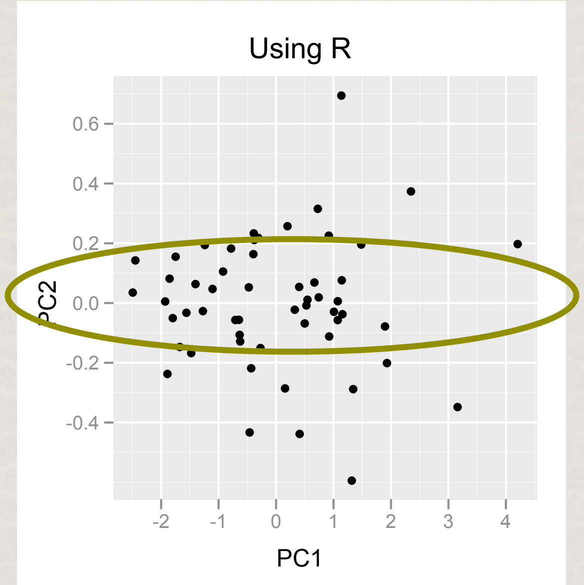

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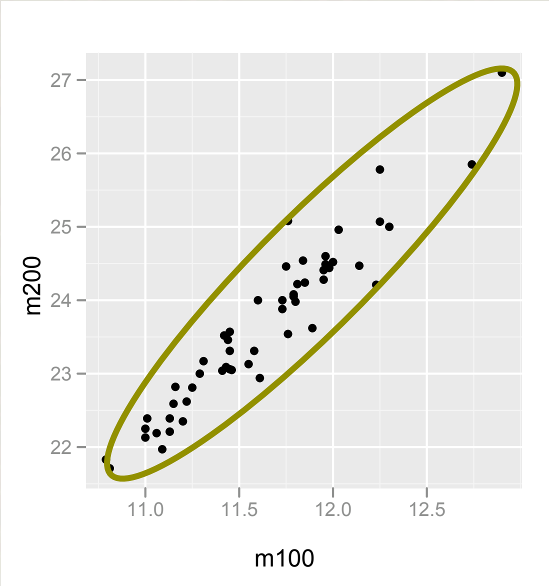

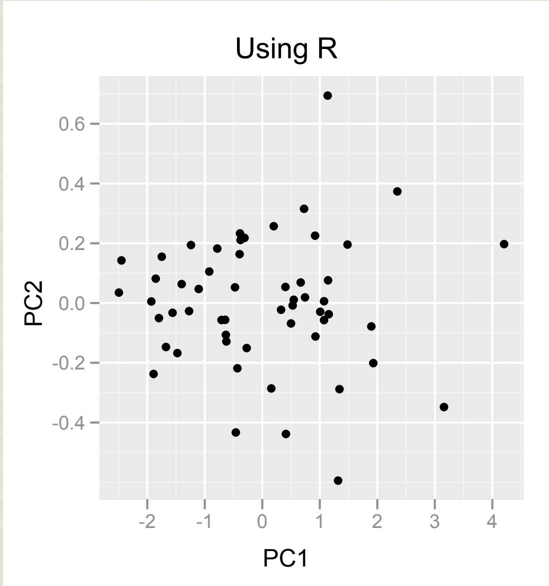

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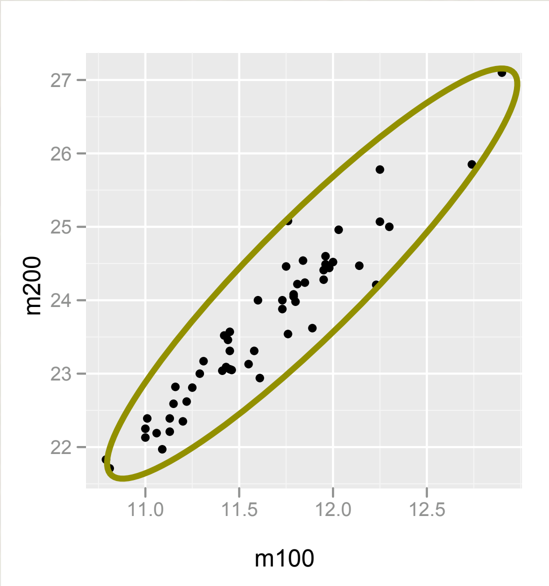

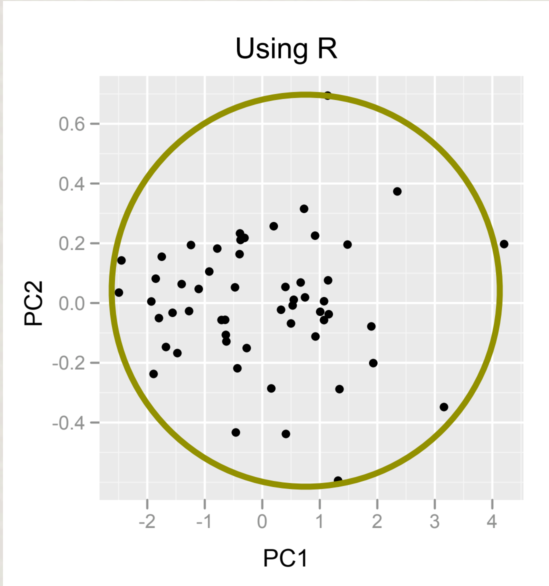

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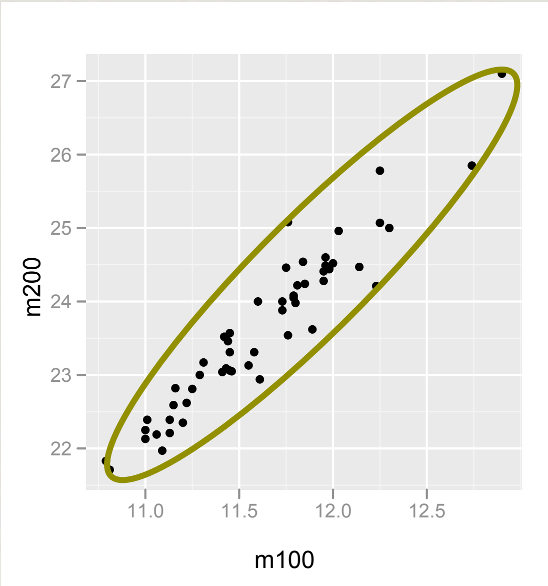
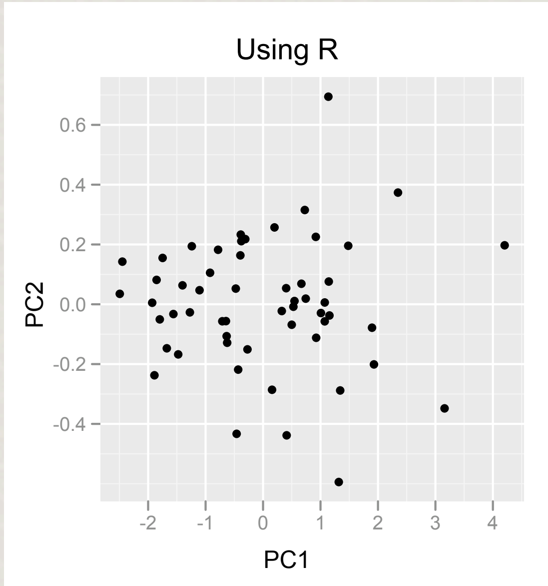
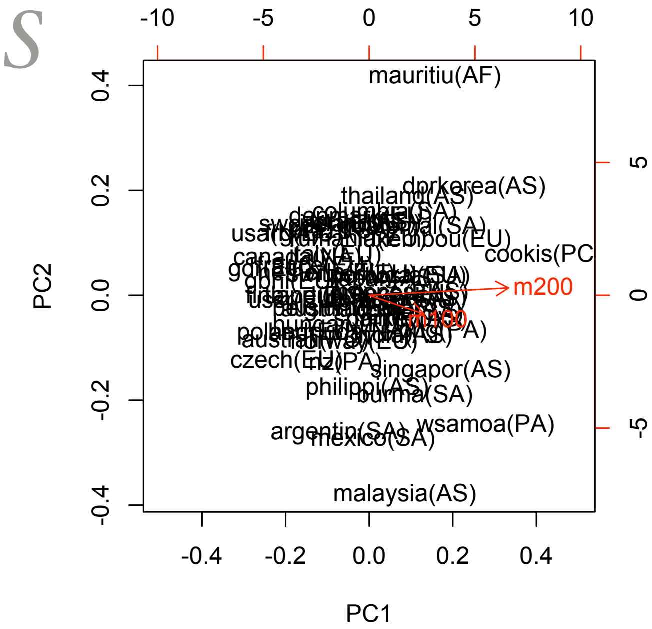
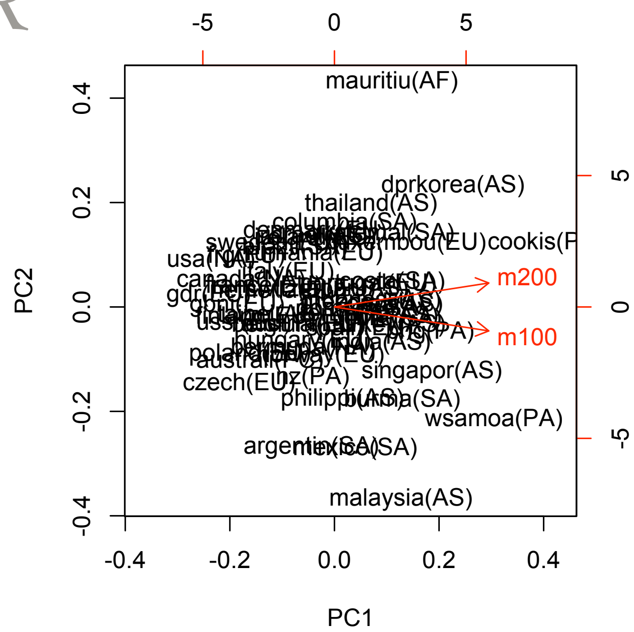




S



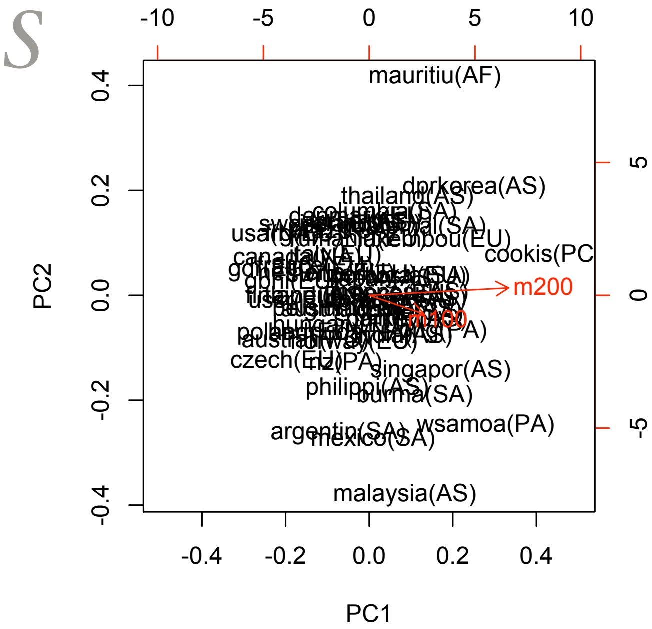
R



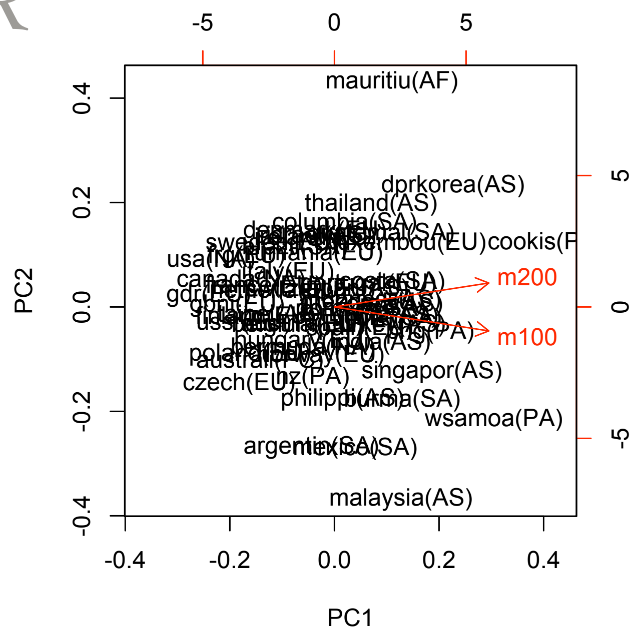
biplots

- *Original axes plotted on the plot of the principal components.*
- *Helps to interpret the new variables.*
- *Here we learn that PC1 is a combination of both the 100m and 200m, slightly different weights for PCA on S, equal for PCA on R*

S



R



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JUST LIKE TOUR AXES!!!!!

Example: Track records

- *This data contains the women's national records for 100m, 200m, 400m, 800m, 1500m, 3000m and marathon, for 55 countries.*

country	m100 (sec)	m200 (sec)	m400 (sec)	m800 (min)	m1500 (min)	m3000 (min)	marathon (min)
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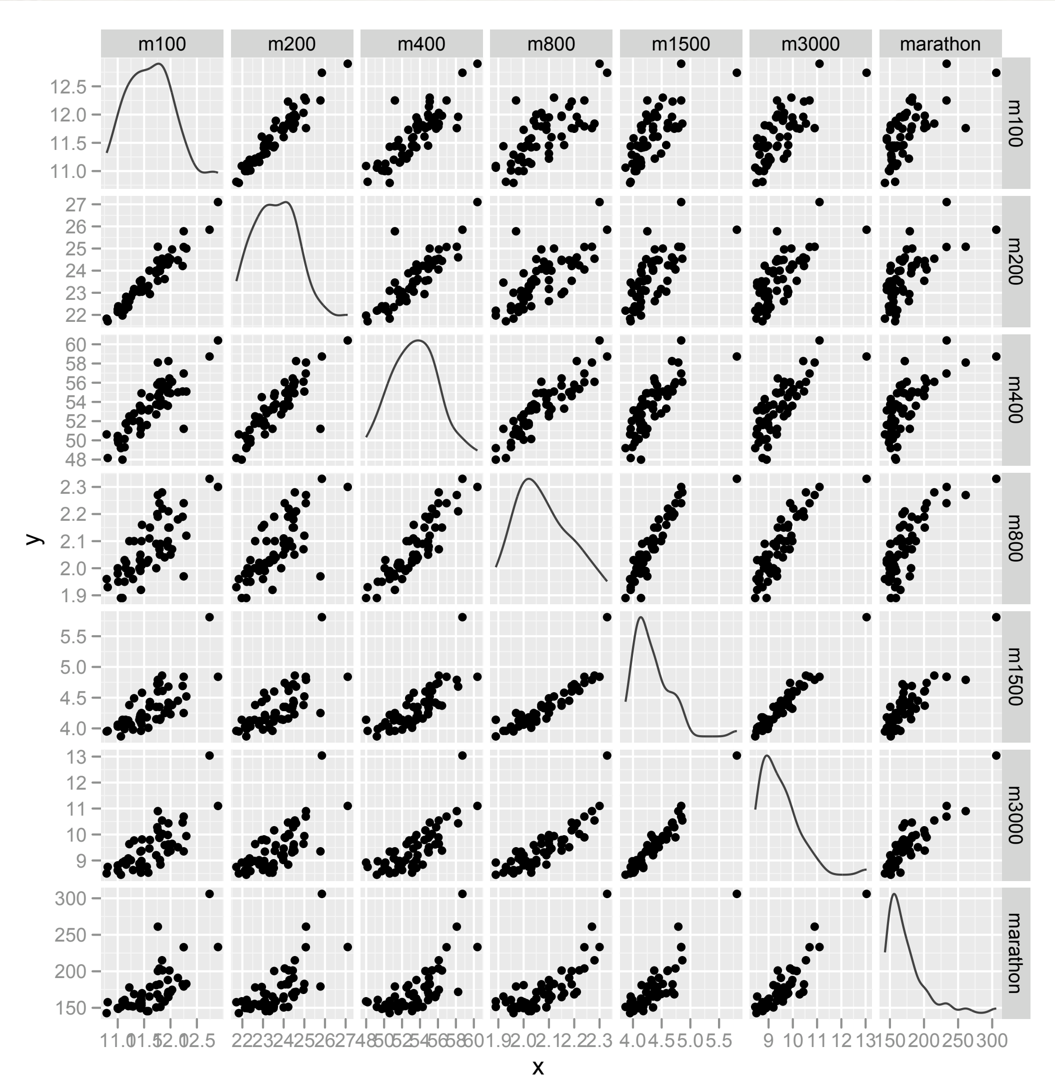
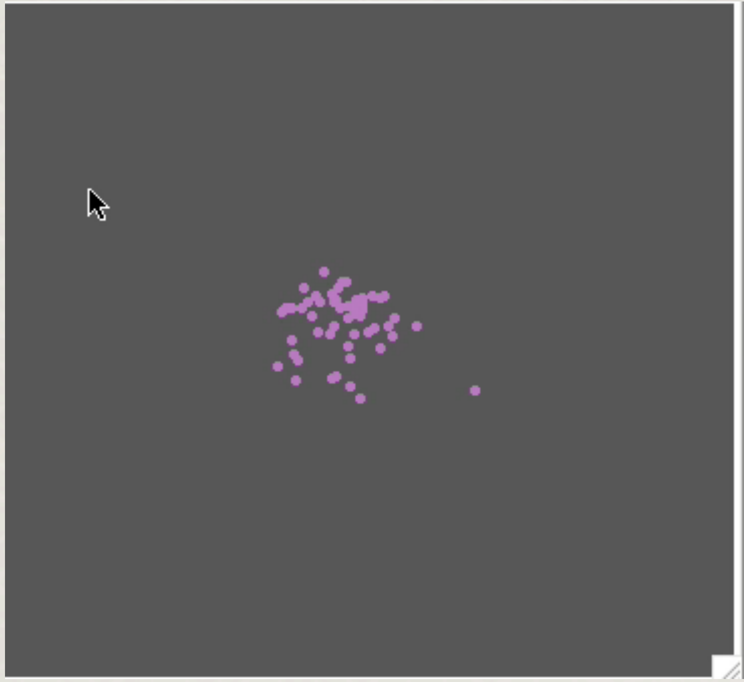
Pre-screening



- *What patterns do you see?*
- *Outliers, linear dependence, non-linear dependence.*



PCA on S or R?

S

	m100	m200	m400	m800	m1500	m3000	marathon
m100	0.204	0.479	1.01	0.036	0.109	0.276	9.4
m200	0.479	1.234	2.55	0.087	0.258	0.650	23.2
m400	1.011	2.550	7.17	0.260	0.701	1.717	57.5
m800	0.036	0.087	0.26	0.012	0.032	0.077	2.6
m1500	0.109	0.258	0.70	0.032	0.111	0.266	8.9
m3000	0.276	0.650	1.72	0.077	0.266	0.680	22.6
marathon	9.444	23.179	57.49	2.566	8.881	22.572	926.0

R

	m100	m200	m400	m800	m1500	m3000	marathon
m100	1.00	0.95	0.83	0.73	0.73	0.74	0.69
m200	0.95	1.00	0.86	0.72	0.70	0.71	0.69
m400	0.83	0.86	1.00	0.90	0.79	0.78	0.71
m800	0.73	0.72	0.90	1.00	0.90	0.86	0.78
m1500	0.73	0.70	0.79	0.90	1.00	0.97	0.88
m3000	0.74	0.71	0.78	0.86	0.97	1.00	0.90
marathon	0.69	0.69	0.71	0.78	0.88	0.90	1.00

- Variances very different between variables.
- Variables measure in different units.
- Should do PCA on R.

PCA on S

	$\mathbf{e}_1$	$\mathbf{e}_2$	$\mathbf{e}_3$	$\mathbf{e}_4$	$\mathbf{e}_5$	$\mathbf{e}_6$	$\mathbf{e}_7$
100	0.0102	0.120	0.326	0.150	0.925	-.00166	0.0168
200	0.025	0.315	0.880	0.0140	-.354	0.025	0.012
400	0.062	0.934	-.328	-.122	0.013	-.022	-.025
800	0.003	0.026	-.0371	0.049	-.015	0.262	0.963
1500	0.019	0.039	-.055	0.340	-.034	0.900	-.265
3000	0.024	0.082	-.088	0.919	-.130	-.349	0.041
mar	0.997	-.070	-.002	-.020	0.002	-.000	-.000
Var	930.9	4.05	0.319	0.115	0.014	0.006	0.001
Cum%	99.5	99.8	99.9	99.9	99.9	100.0	100.0

- *What's wrong with these results?*

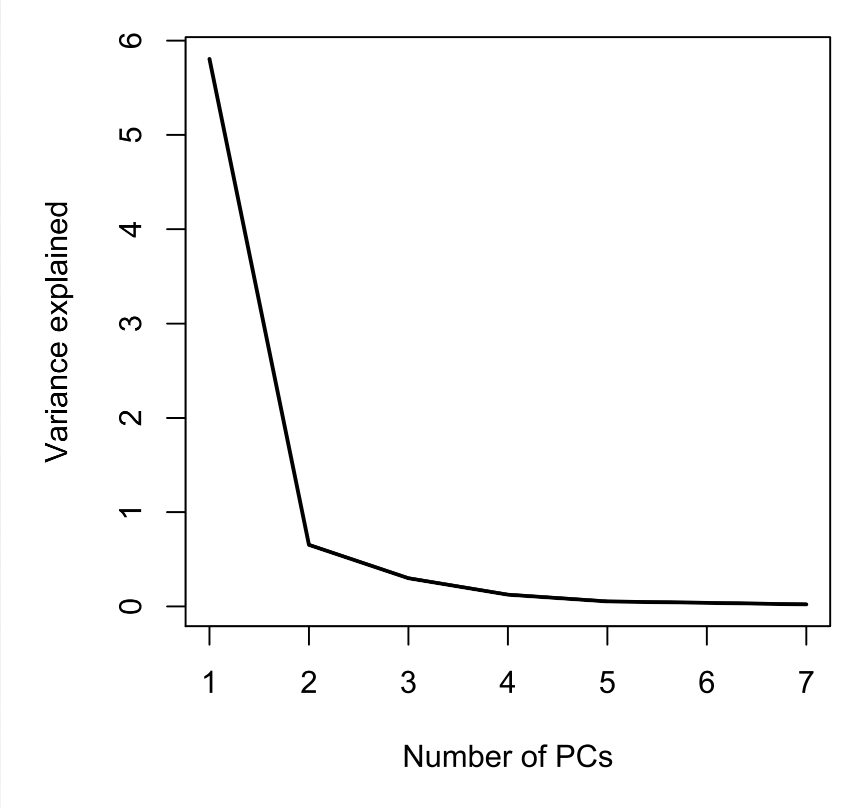
Marathon is the only variable contributing to PC1!

PCA on R

Variable	$\mathbf{e}_1$	$\mathbf{e}_2$	$\mathbf{e}_3$	$\mathbf{e}_4$	$\mathbf{e}_5$	$\mathbf{e}_6$	$\mathbf{e}_7$
100	0.368	0.490	0.286	-.319	0.231	0.620	0.052
200	0.365	0.537	0.230	0.083	0.042	-.711	-.109
400	0.382	0.247	-.515	0.348	-.572	0.191	0.208
800	0.385	-.155	-.585	0.0421	0.620	-.019	-.315
1500	0.389	-.360	-.013	-.430	0.030	-.231	0.693
3000	0.389	-.348	0.153	-.363	-.463	0.009	-.598
mar	0.367	-.369	0.484	0.672	0.130	0.142	0.070
Var	5.81	0.654	0.300	0.125	0.054	0.039	0.022
Cum%	83.0	92.3	96.6	98.4	99.2	99.7	100.0

- *First PC is a linear combination of all events, athletic prowess? It explains 83% of the variation.*
- *Second PC is a contrast between short and long distance events. Jointly explains 92.3%.*

How many PCs?



- *Scree plot: Eigenvalue vs Number of PCs*
- *Look for an "elbow".*
- *Scree plot suggests 2 PCs.*
- *Also consider neighbors (1 and 3), and proportion of total variance explained.*

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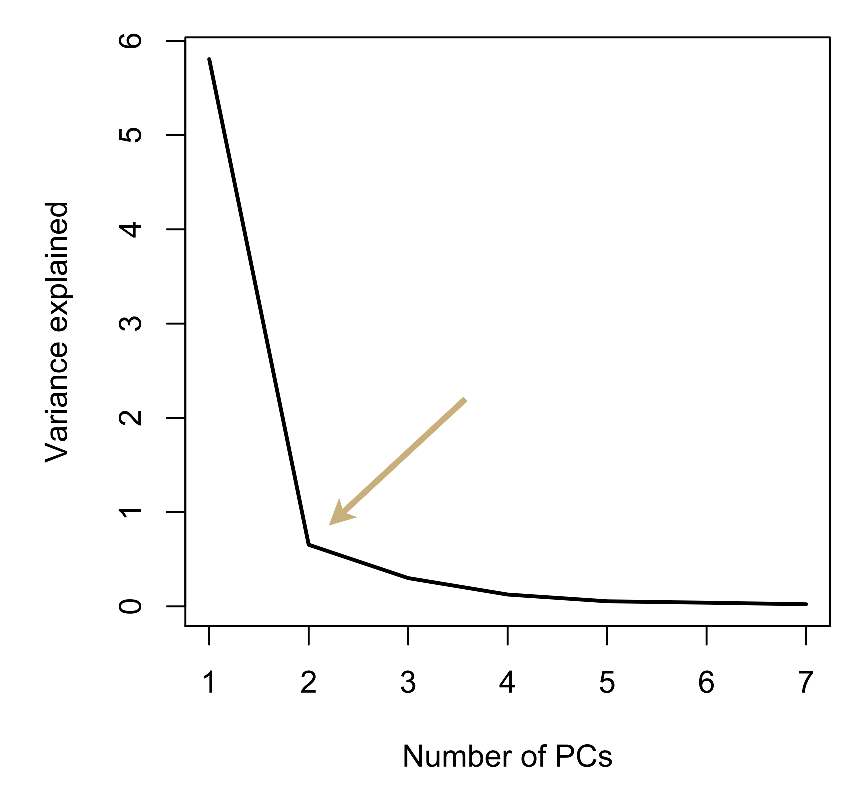

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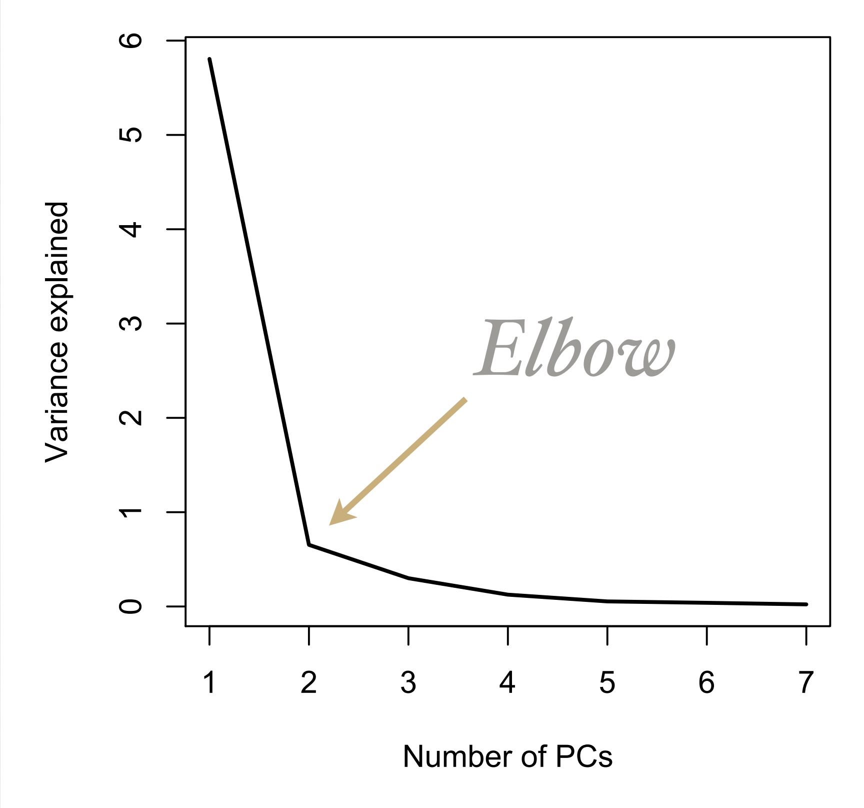
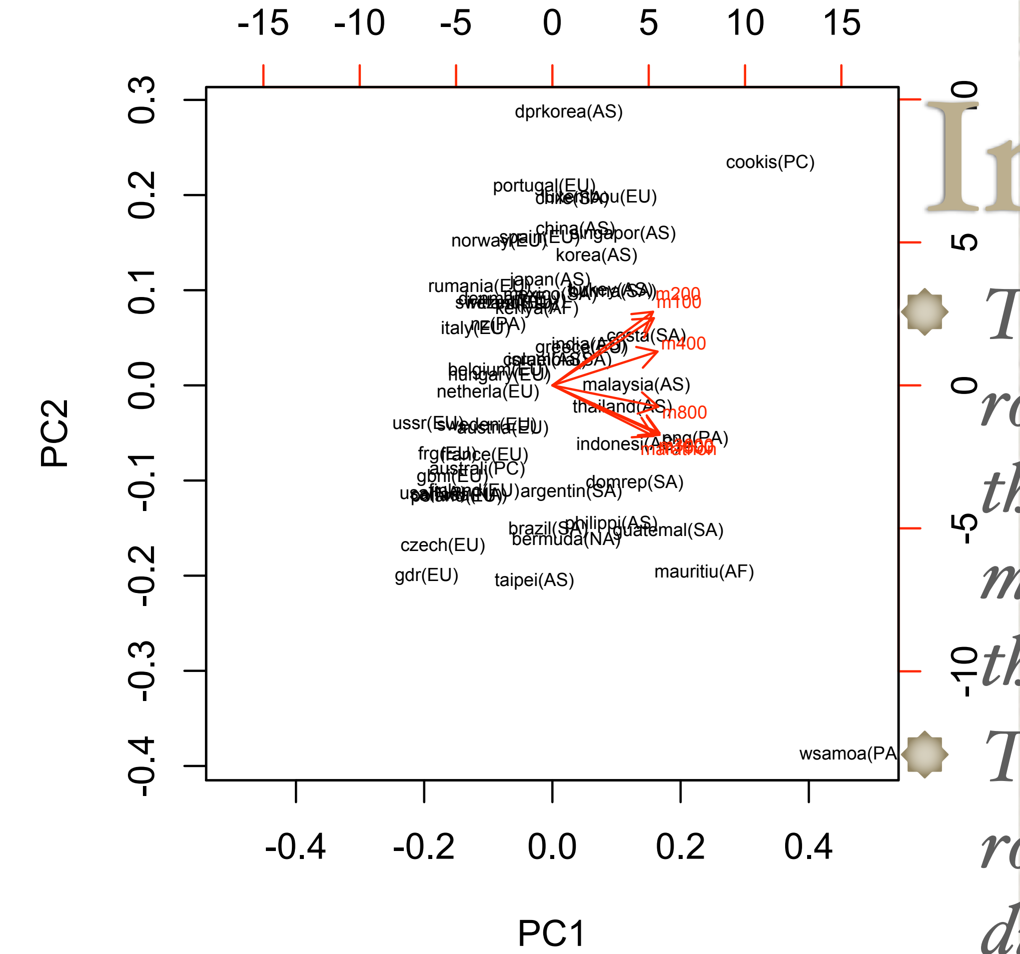
How many PCs?



- *Scree plot: Eigenvalue vs Number of PCs*
- *Look for an "elbow".*
- *Scree plot suggests 2 PCs.*
- *Also consider neighbors (1 and 3), and proportion of total variance explained.*

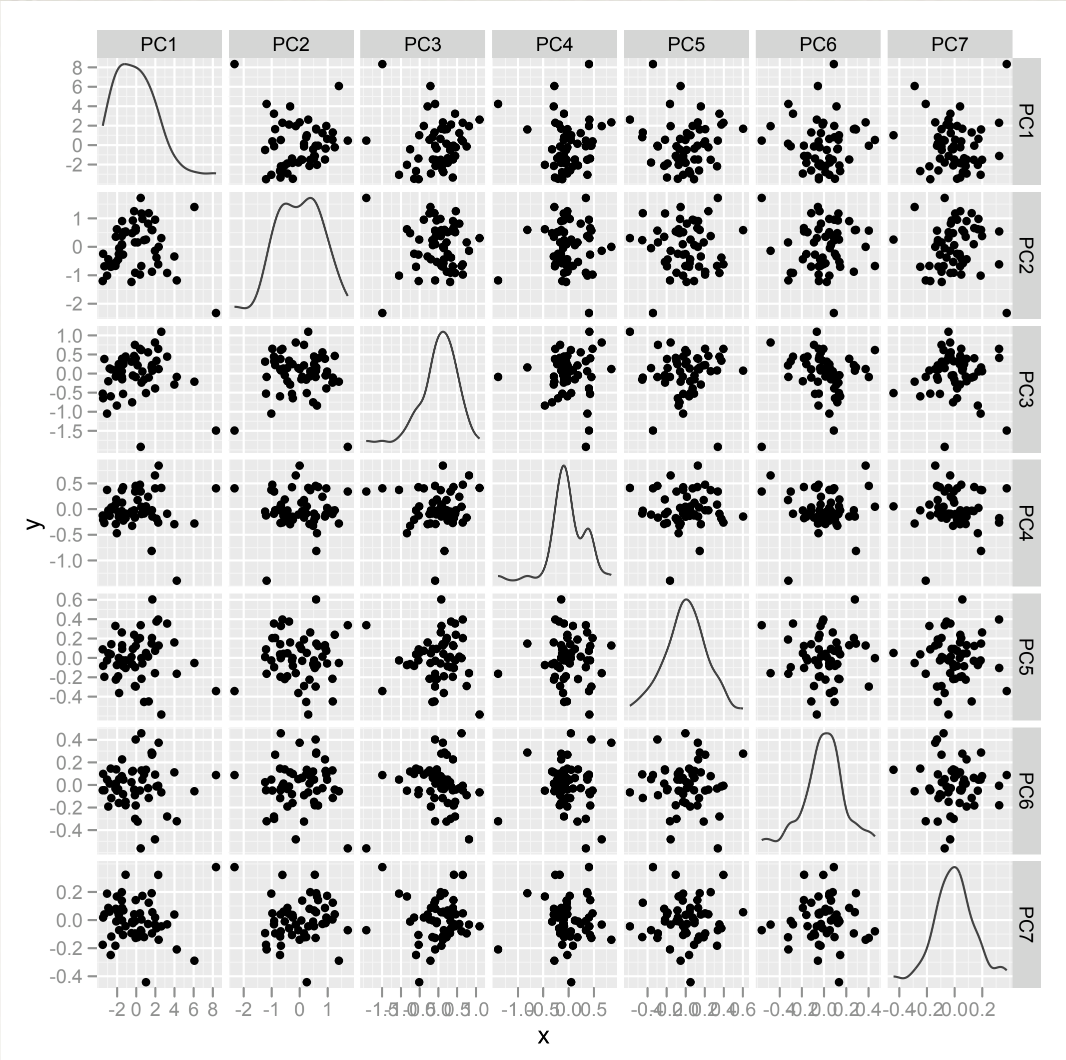


Interpretation

- *The first principal component is a roughly equal combination of all of the variables. Consider PC1 to be a measure the the overall strength of the athletic program.*
- *The second principal component is roughly a contrast between short distance and long distance events. Consider PC2 to be a measure of the countries skills in the different distance events.*

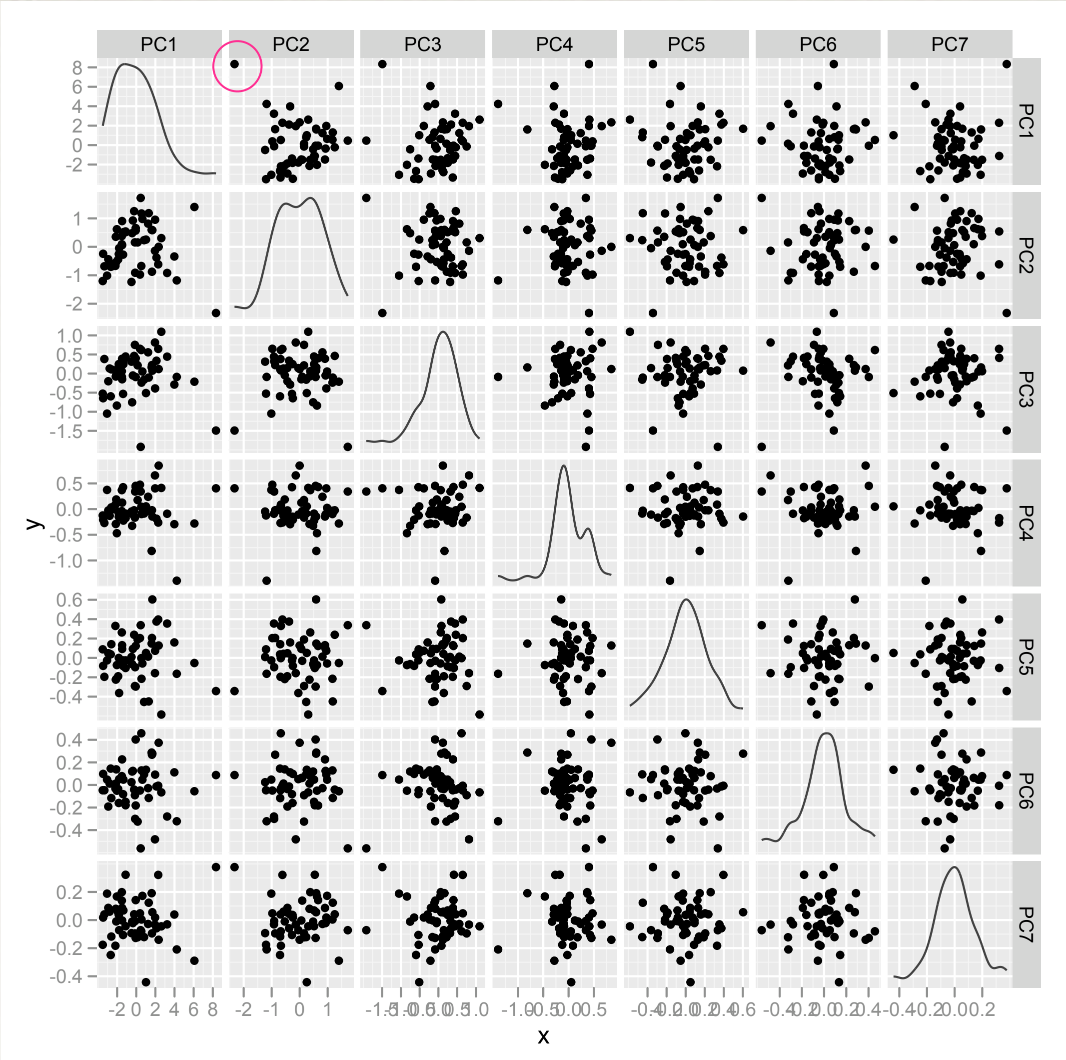
Which country has the best (worst) program? Short distance program?

Post-screening



- *Plot the PCs*
- *Should be NO structure*
- *What do you see here?*
- *Outliers*
- *SOLUTION: Remove outliers, and re-do PCA.*

Post-screening



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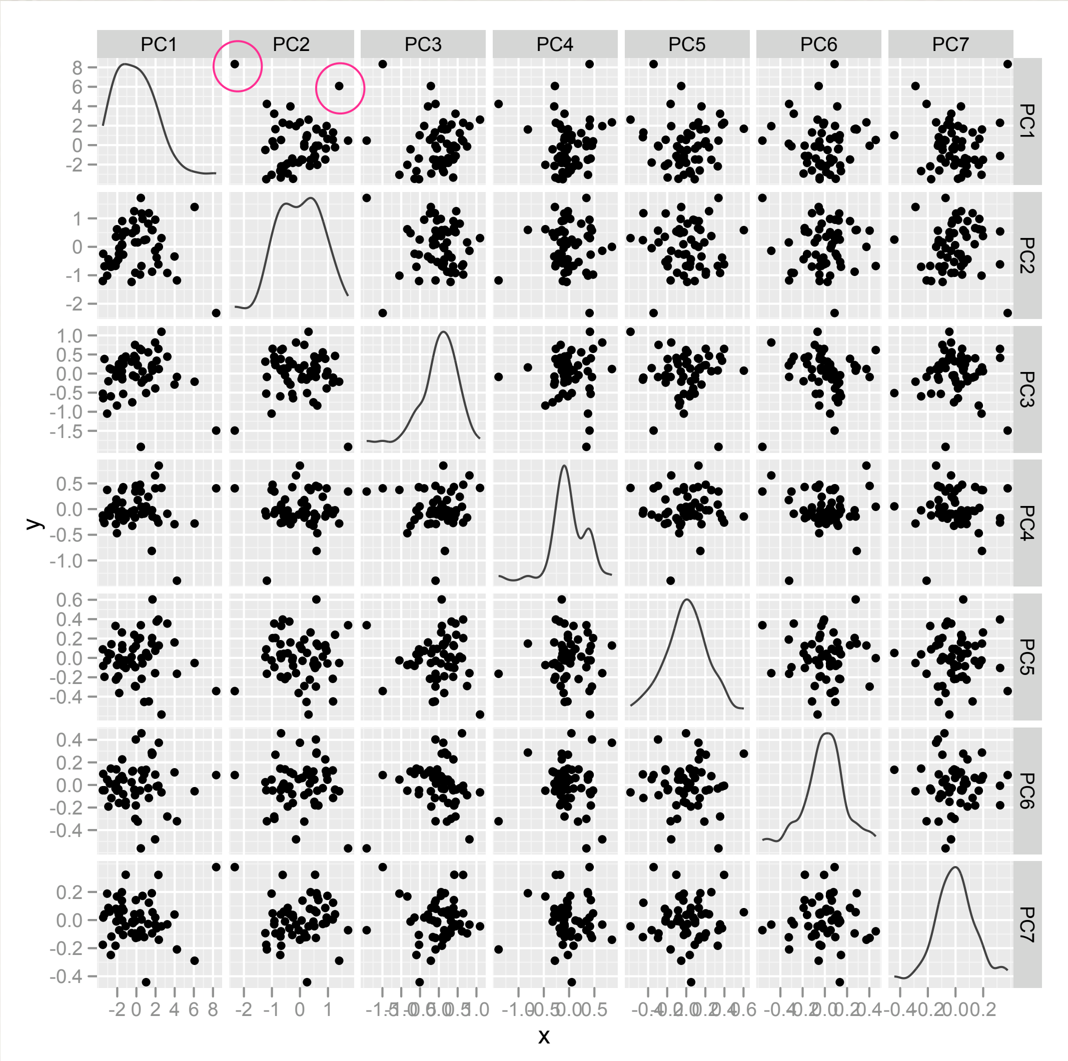

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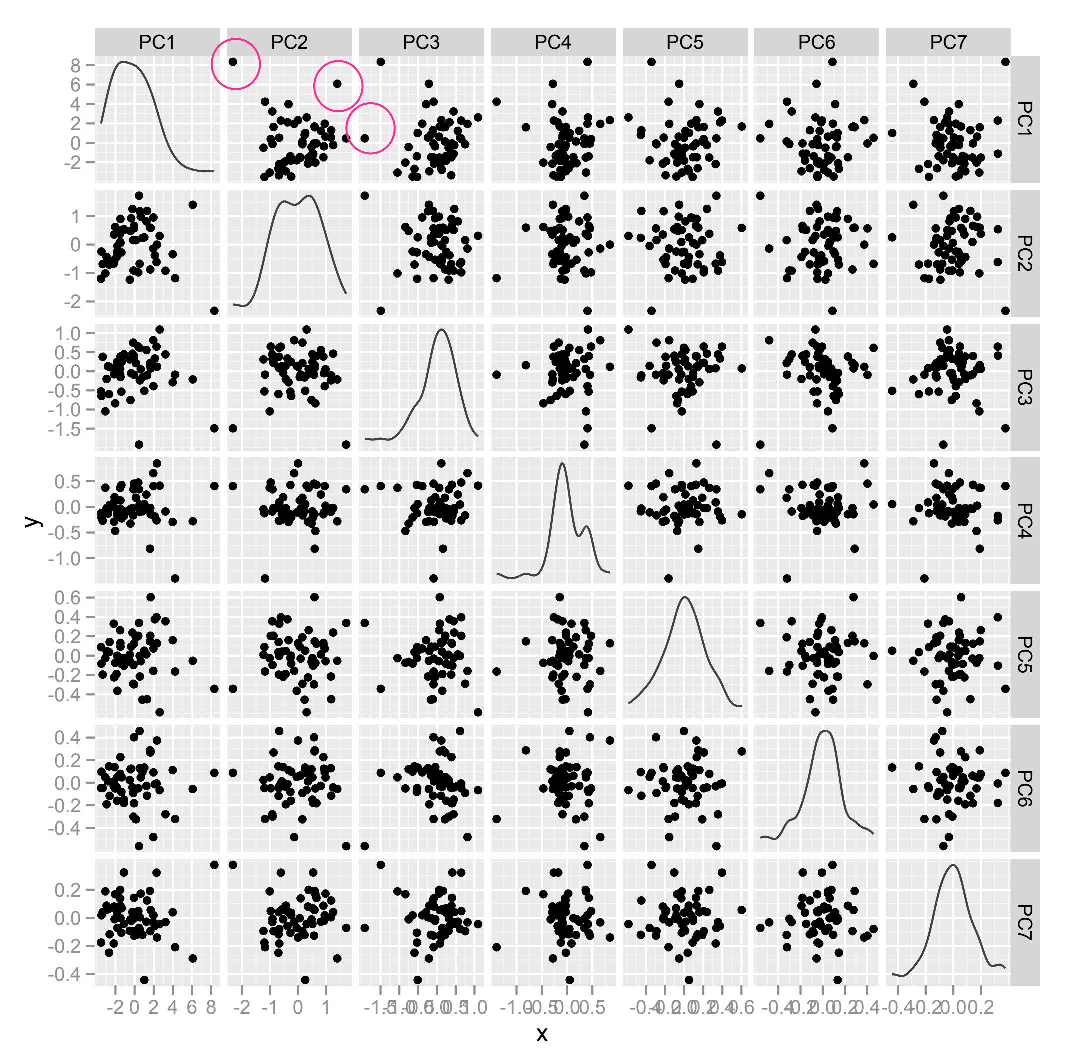

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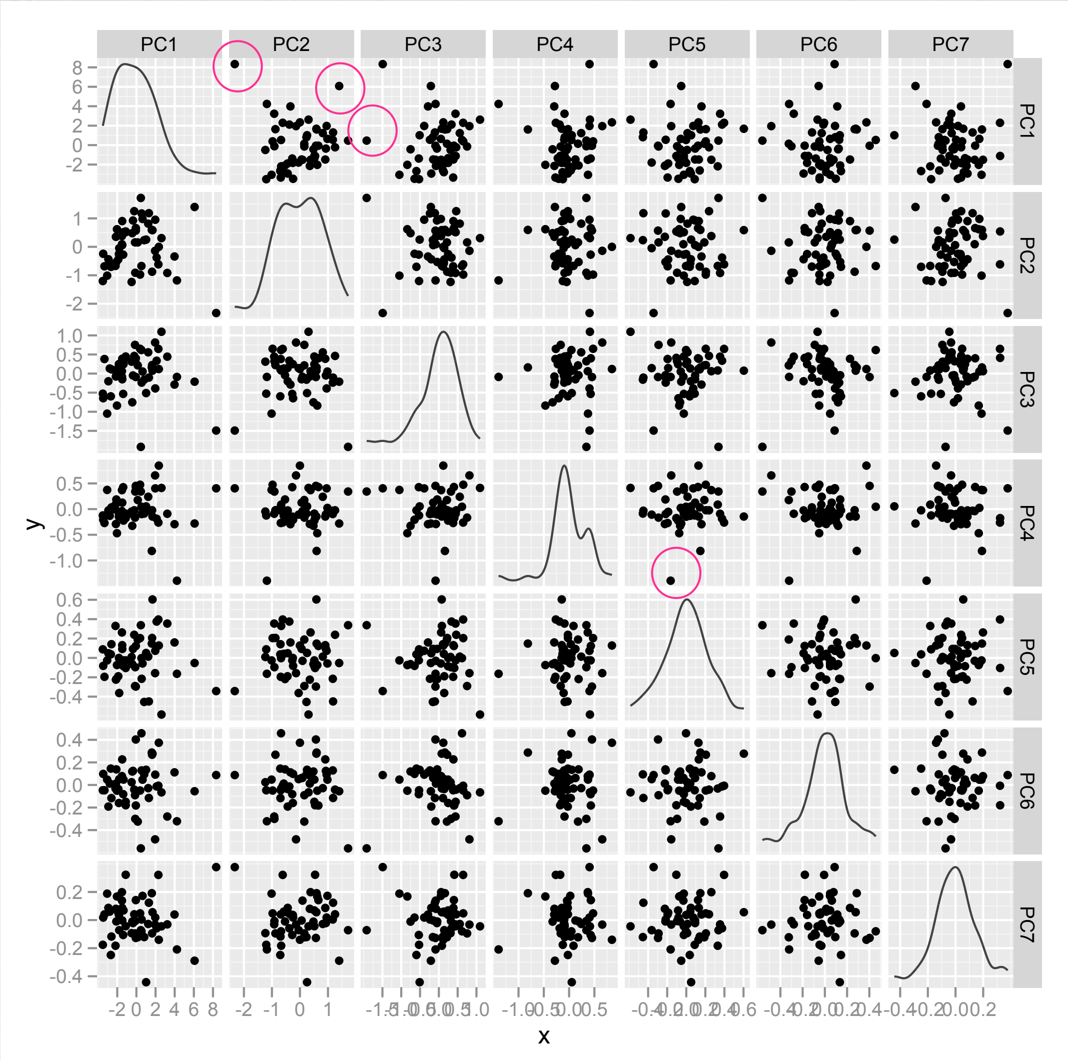

- *Plot the PCs*
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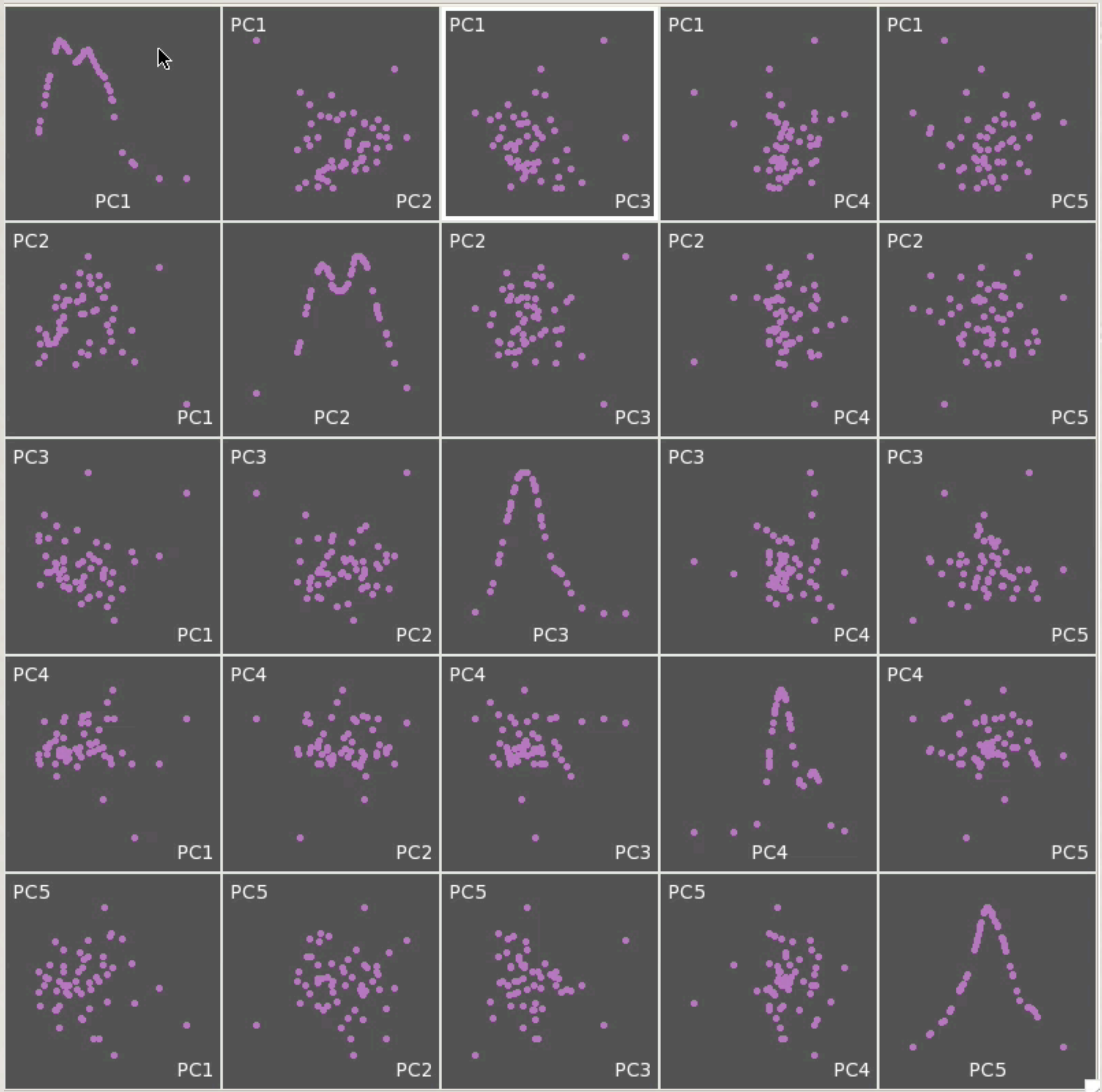
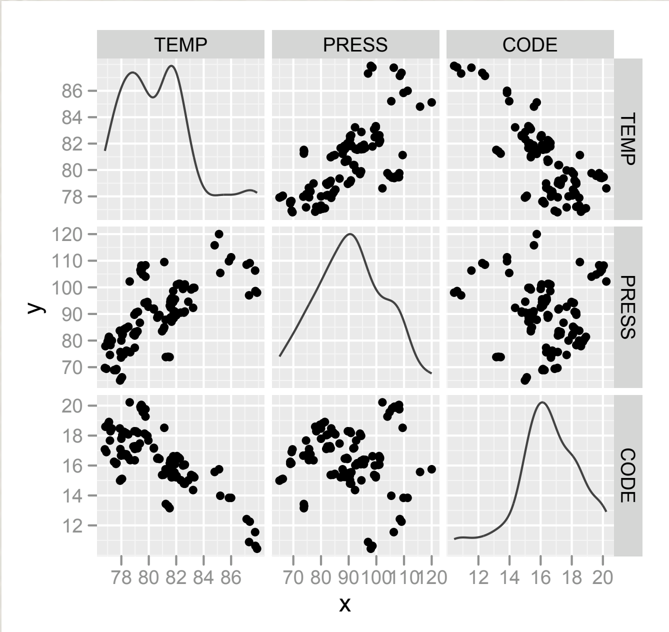


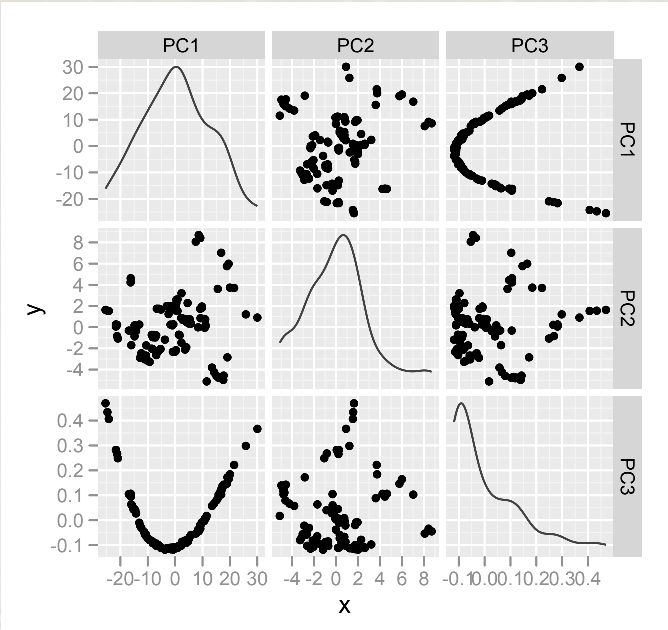
- *Outliers are: Samoa, Cook Islands, Mauritius, DPRKorea*

More examples

- *Flow through meters*

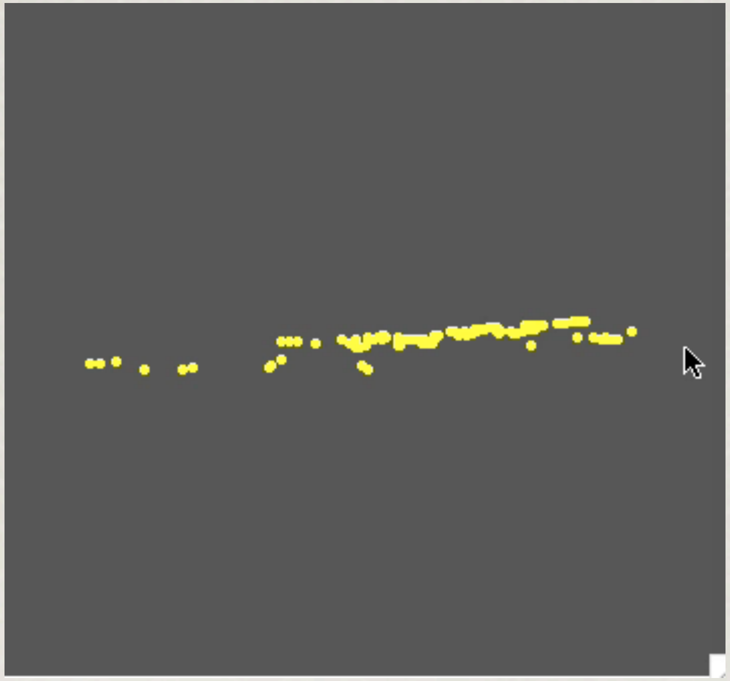


	Temp	Press	Code
Temp	1.00	0.63	-0.75
Press	0.63	1.00	0.04
Code	-0.75	0.04	1.00



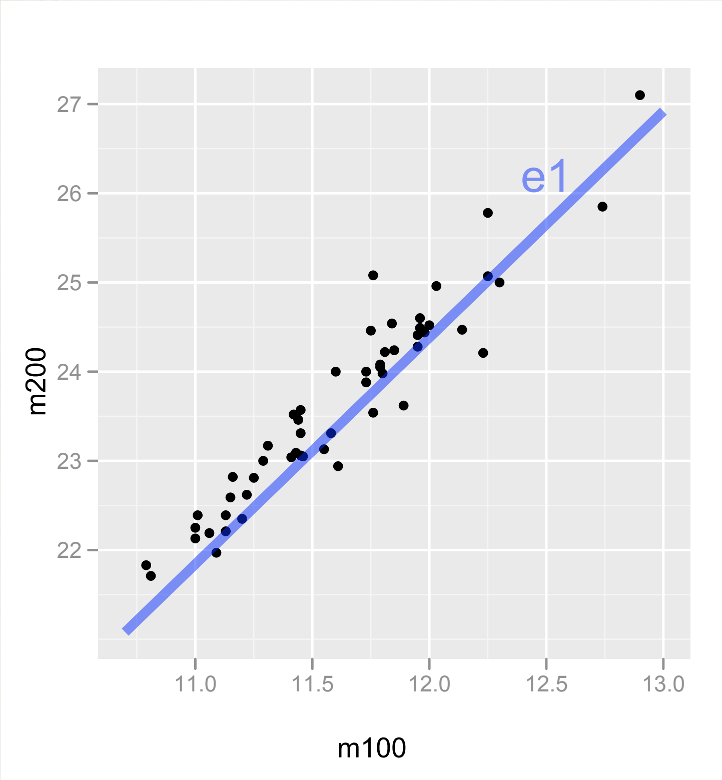
	PC1	PC2	PC3
Temp	1.00	0.63	-0.75
Press	0.63	1.00	0.04
Code	-0.75	0.04	1.00
Var	146.6	8.08	0.018
Prop	0.95	0.99	1.00

Flow meters



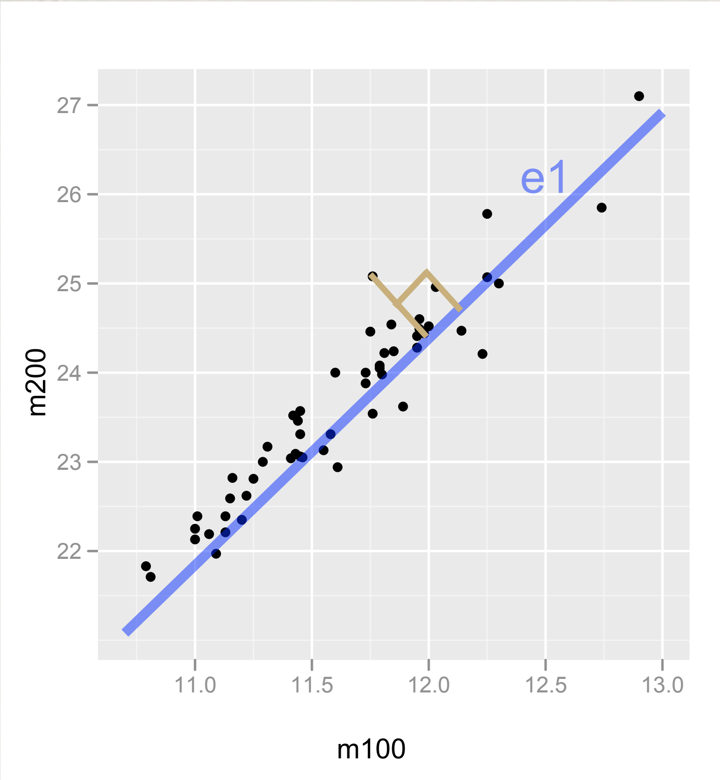
- *Classic example of multicollinearity: pairs of variables do not show extremely strong correlation.*
- *Relationship between the 3 variables is perfectly defined by an equation though.*
- *PCA: Detects the main pattern of linear association, removes this with PC1, PC2. The the non-linear association is captured in PC3.*

PCA vs Regression



- *PCA is VERY MUCH LIKE Regression.*
- *The first few PCs are like the linear model, and the lower PCs are like the residuals. If there is non-linear dependence you'll likely see it in the lower PCs.*
- *The linear model is fit by minimizing ORTHOGONAL distance, not vertical distance between points and lines.*

PCA vs Regression



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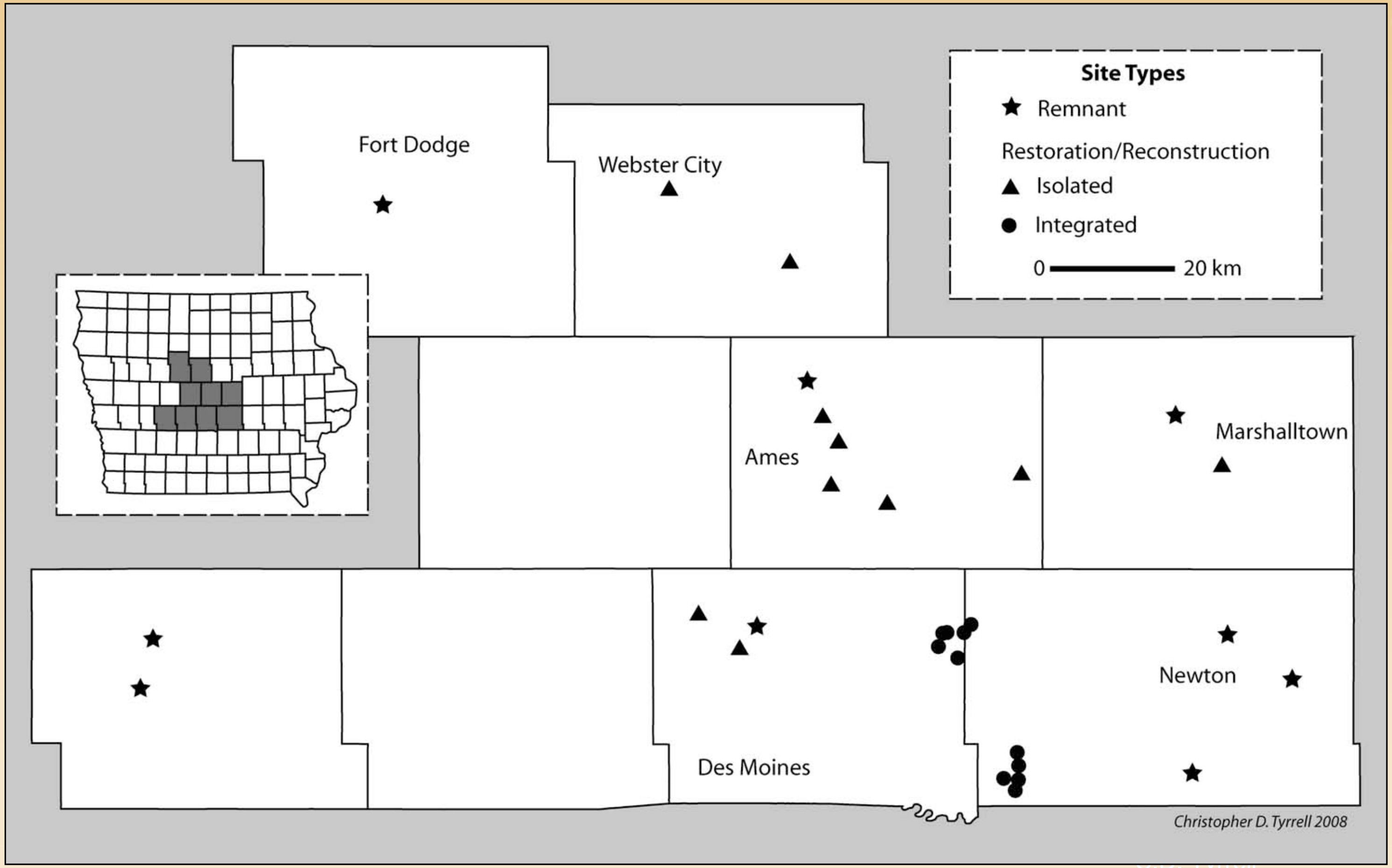
More Examples

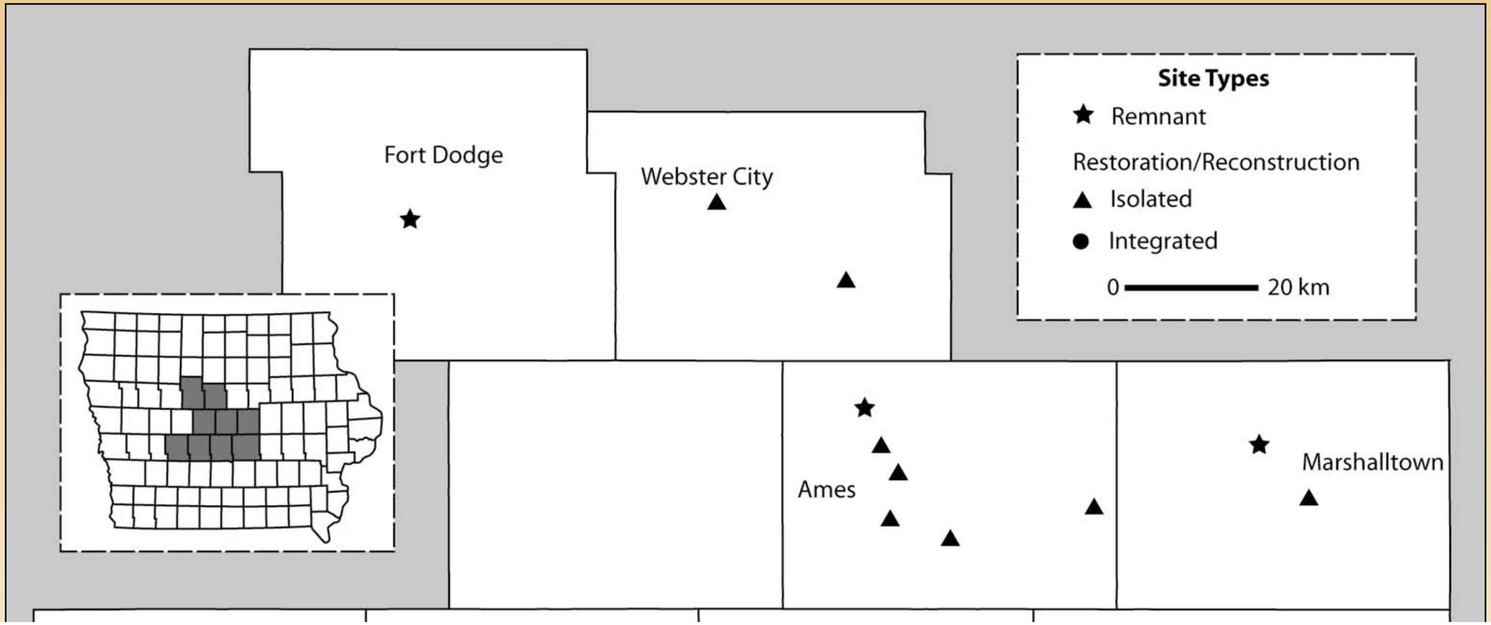
Prairies



- *Species diversity in Iowa prairies.*
- *Different types of prairies*
- *Data collected by Jessica Orlofske under the supervision of Diane Debinski, EEOB, ISU*

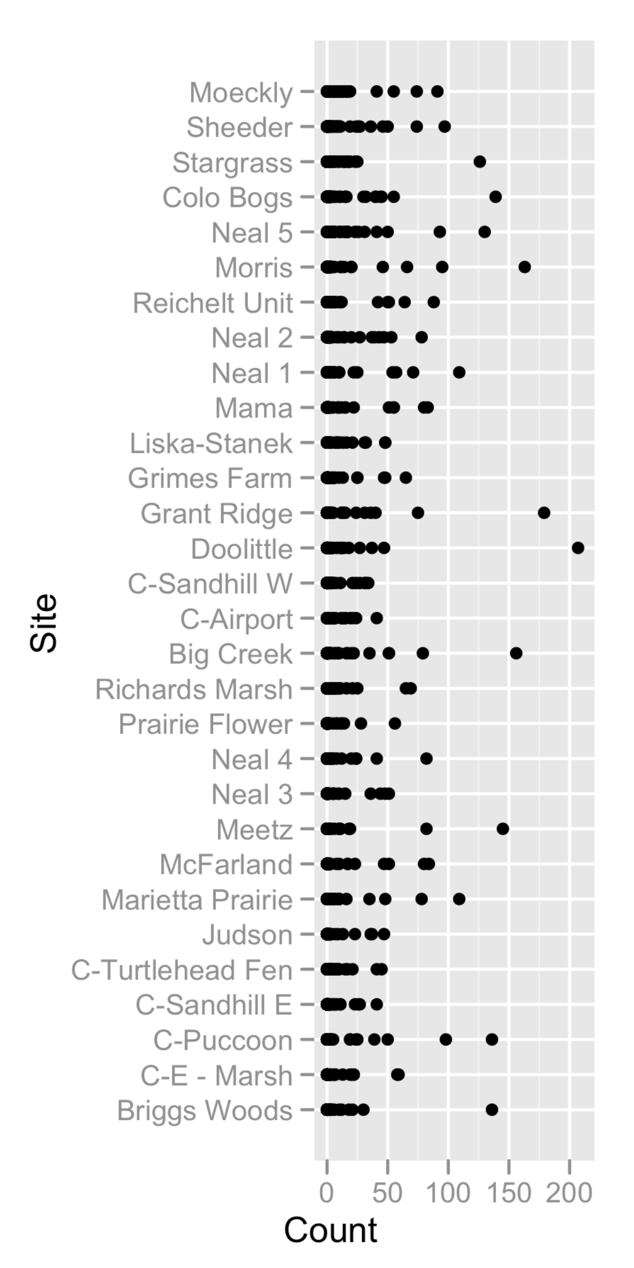
More Examples

Prairies



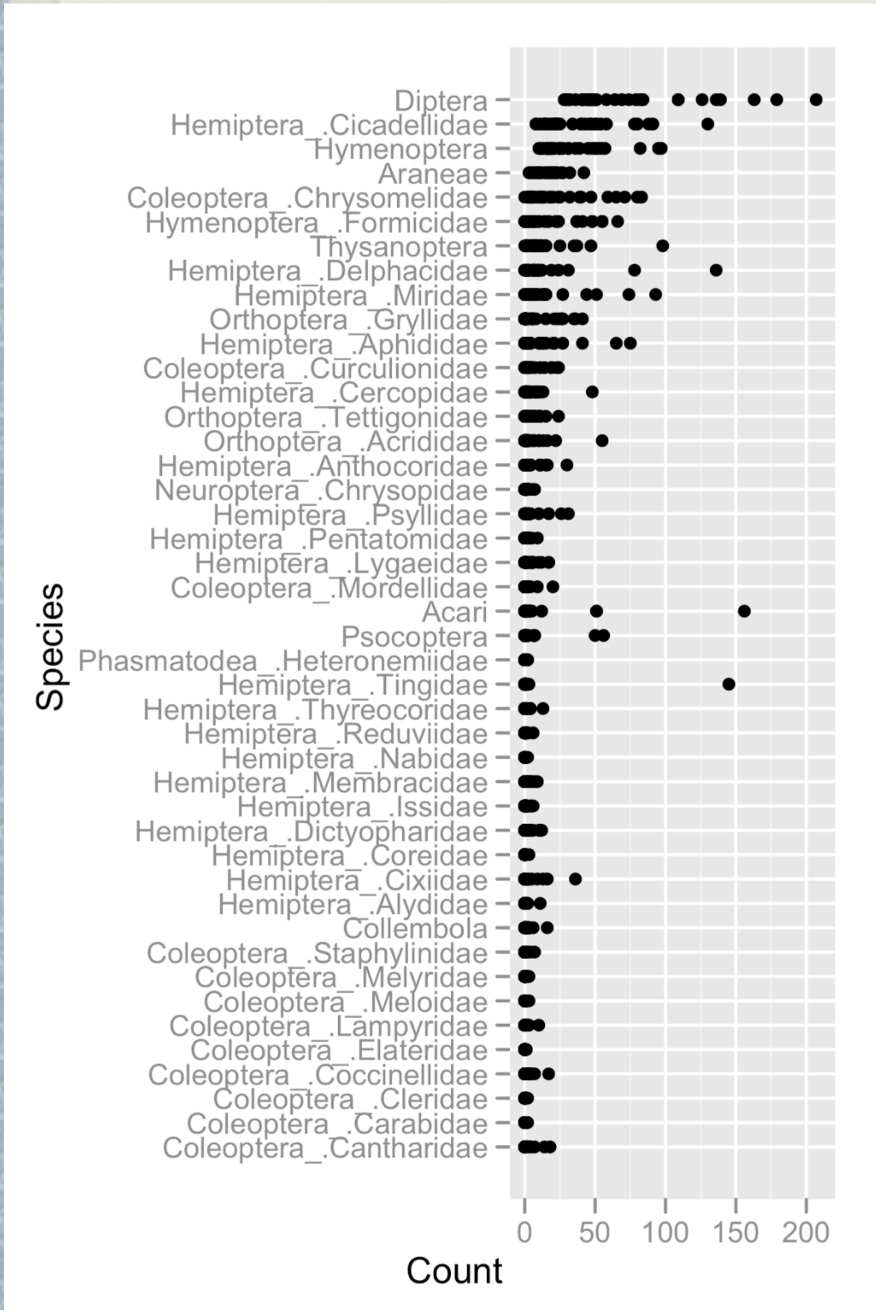
Site	Type	Araneae	Acari	Coleoptera_.Cantharidae	Coleoptera_.Carabidae
C-Turtlehead Fen	1	15	0	0	0
Doolittle	1	3	1	0	0
Judson	1	23	0	0	0
Liska-Stanek	1	9	0	0	0
Mama	1	22	1	0	0
Marietta Prairie	1	10	0	0	1

- *Species diversity in Iowa prairies.*
- *Different types of prairies*
- *Data collected by Jessica Orlofske under the supervision of Diane Debinski, EEOB, ISU*



Iowa Prairies

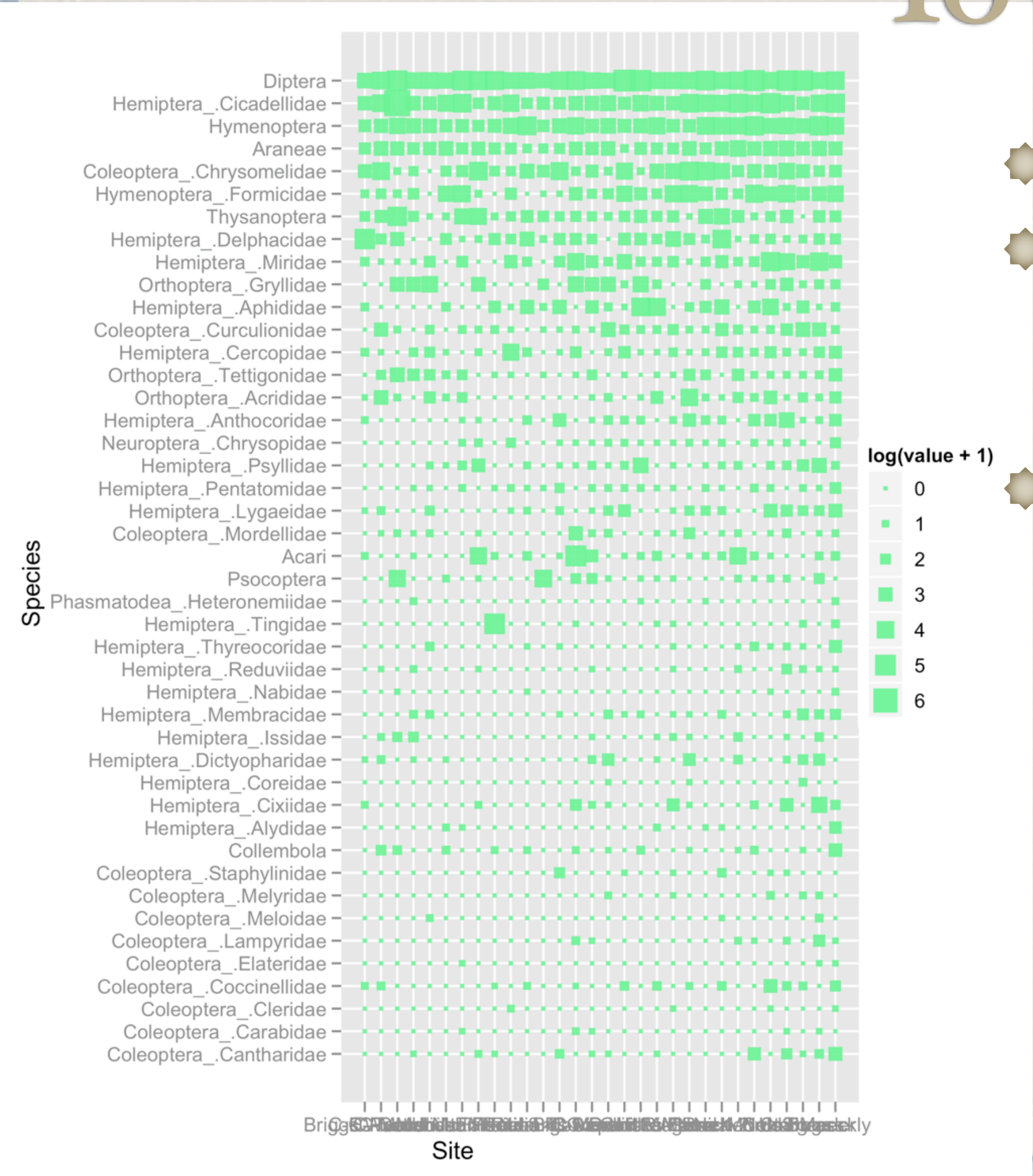
- *Each point is a count for one of the species, at that site.*
- *One observation outside domain of plot: C-Puccoon has 719 Hemiptera_.Cicadellidae.*
- *Is there a difference between sites?*



Iowa Prairies

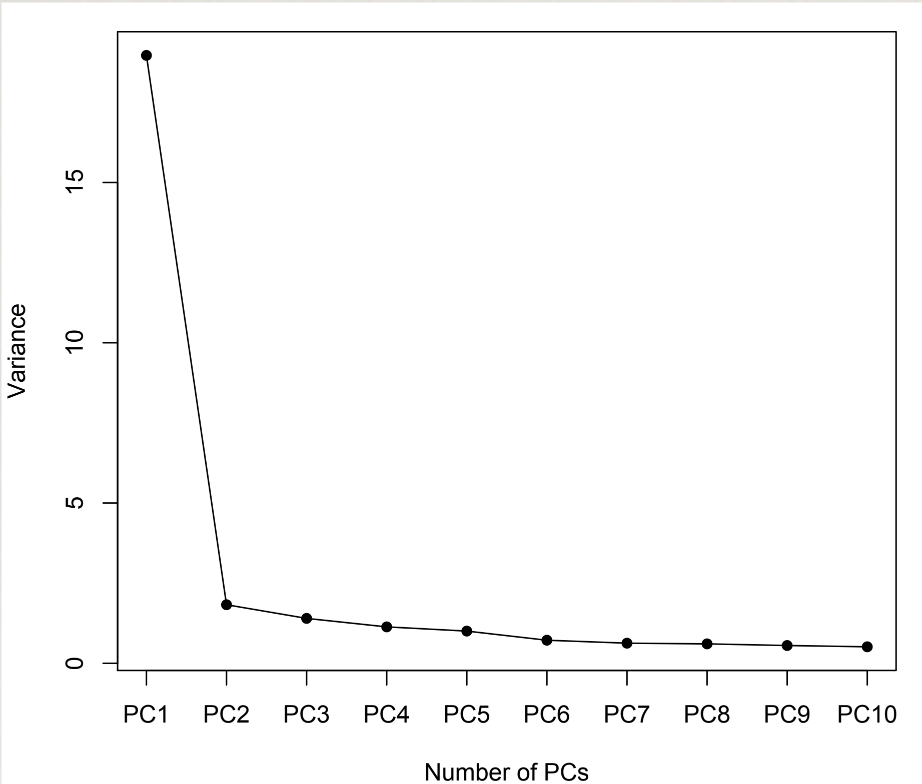
- *Each point is a count for one of the sites, for that species.*
- *One observation outside domain of plot: C-Puccoon has 719 Hemiptera_.Cicadellidae.*
- *What are the differences between species?*

Iowa Prairies



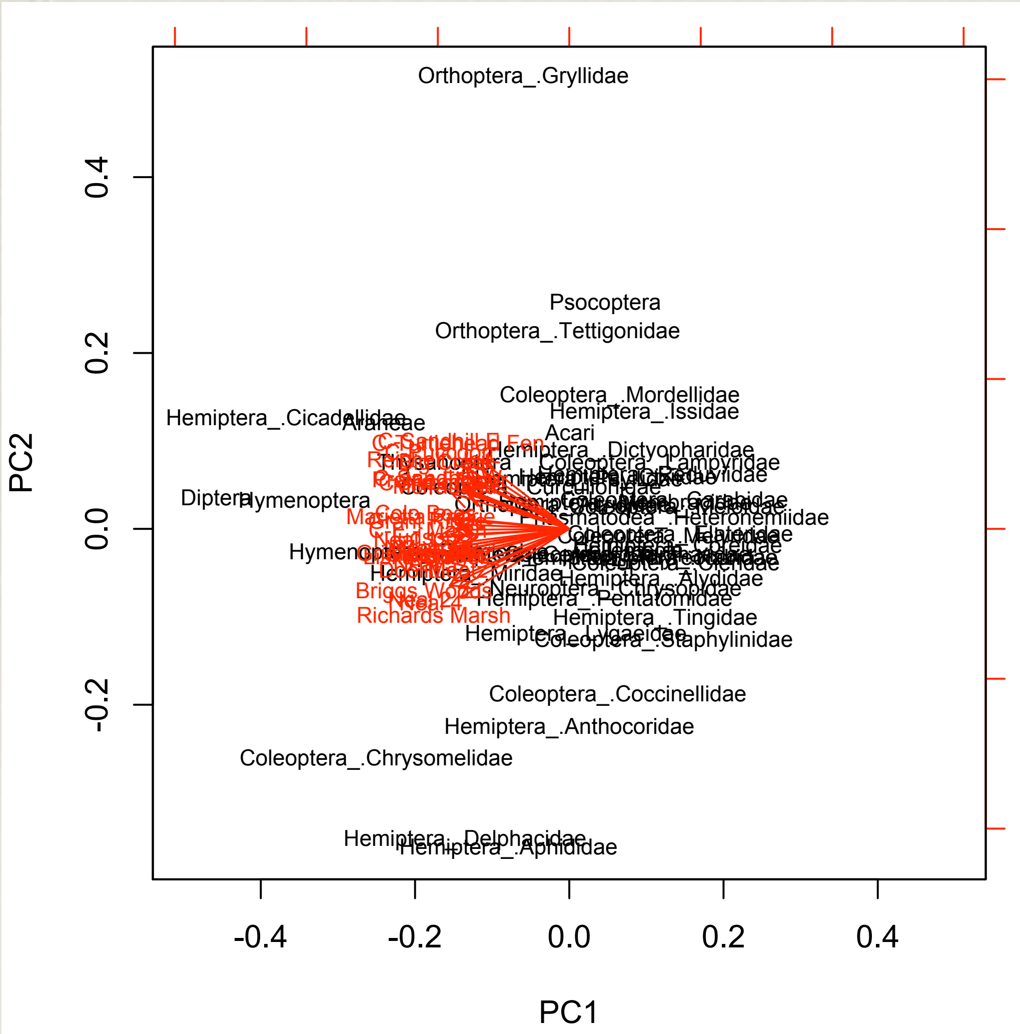
- *Full data set shown.*
- *Count represented by size of the square. (Log count used.)*
- *Some species prevalent everywhere. Some, eg Acari have large populations in just a few sites.*

Iowa Prairies - PCA



- *Two principal components suggested.*

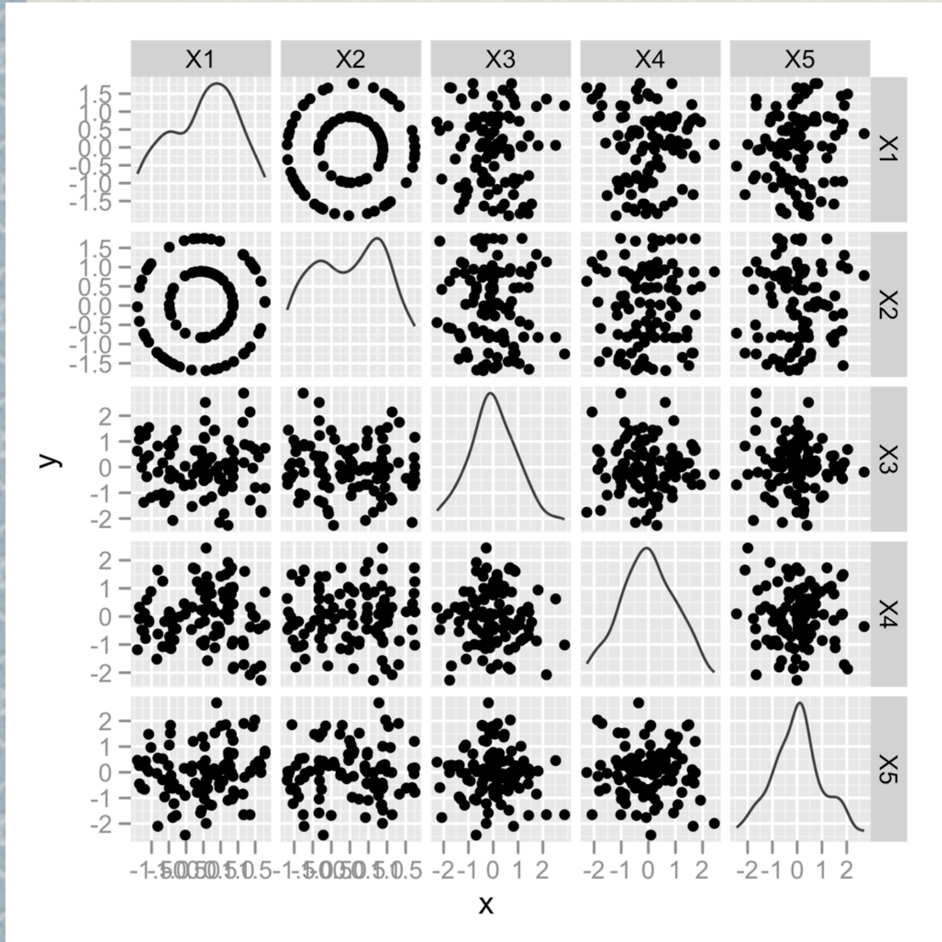
Iowa Prairies - PCA



- *First principal component is purely size of the population: Diptera highest counts.*
- *Second principal component is a contrast between sites revealing difference between populations, eg Orthoptera_.Gryllidae and Hemiptera_.Delphacidae*

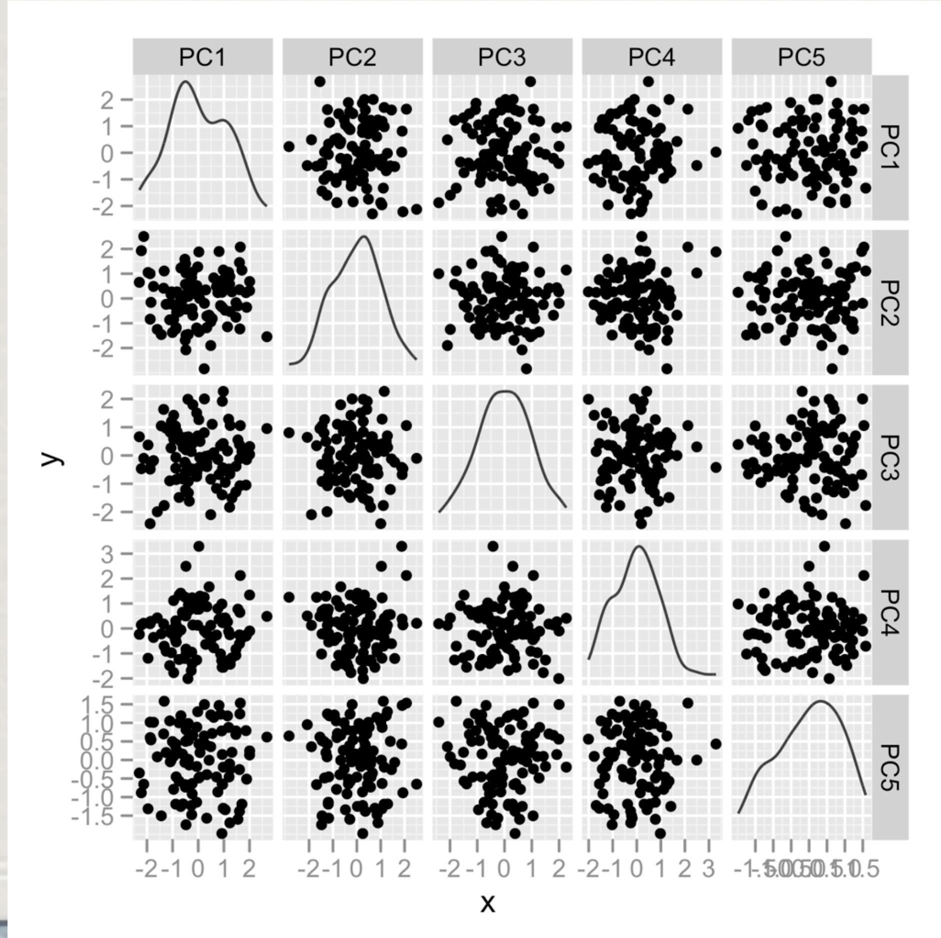
More examples

Raw

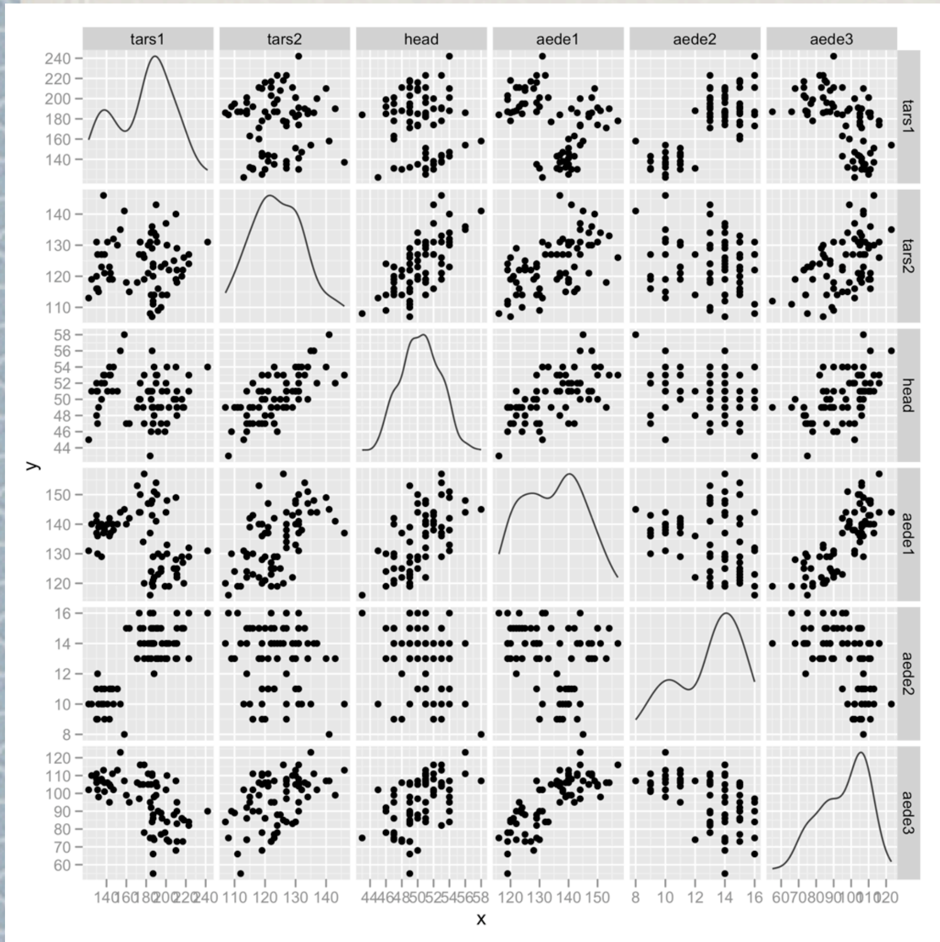


- *Non-linear structure is not recognized by PCA*

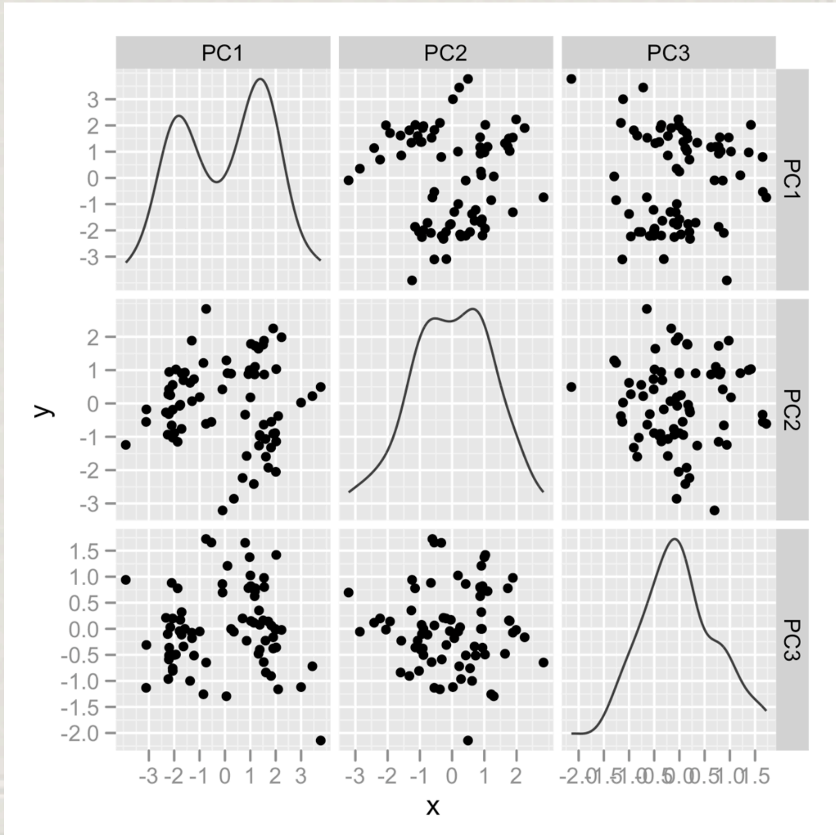
PCs



More examples

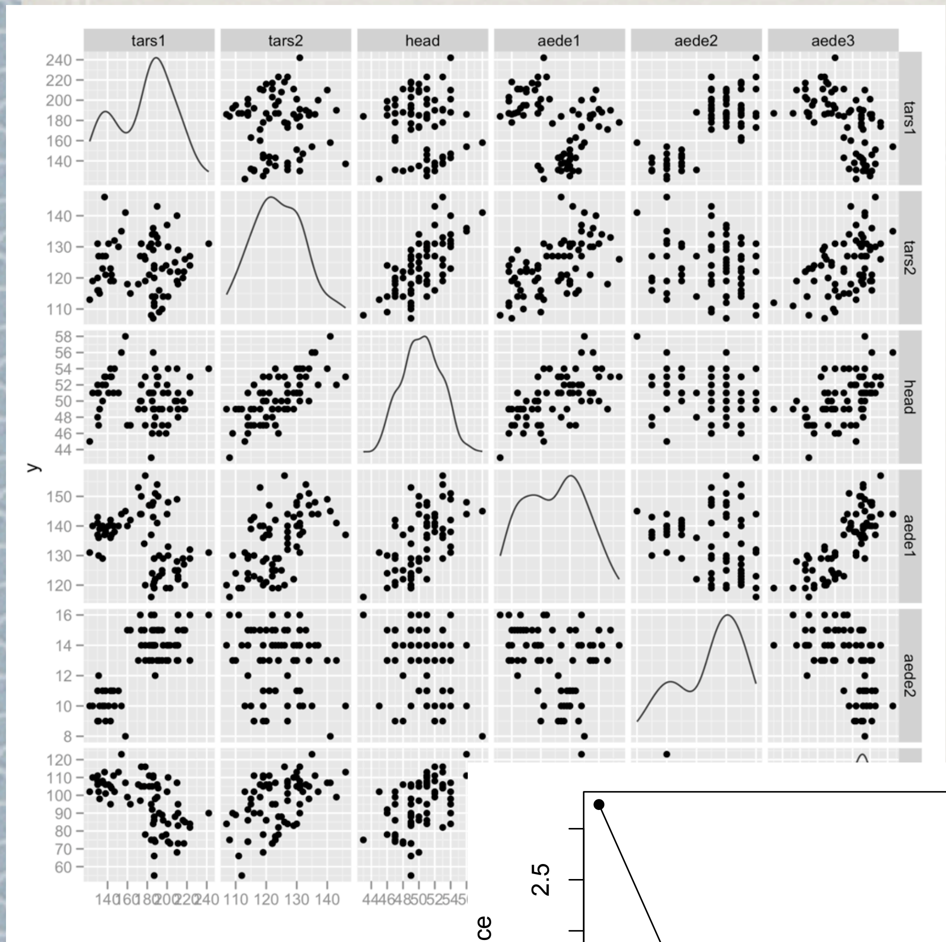


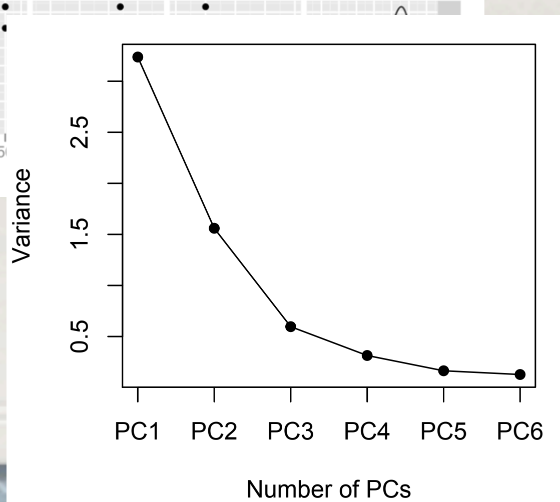
- *Flea beetles - clusters not revealed by PCA*

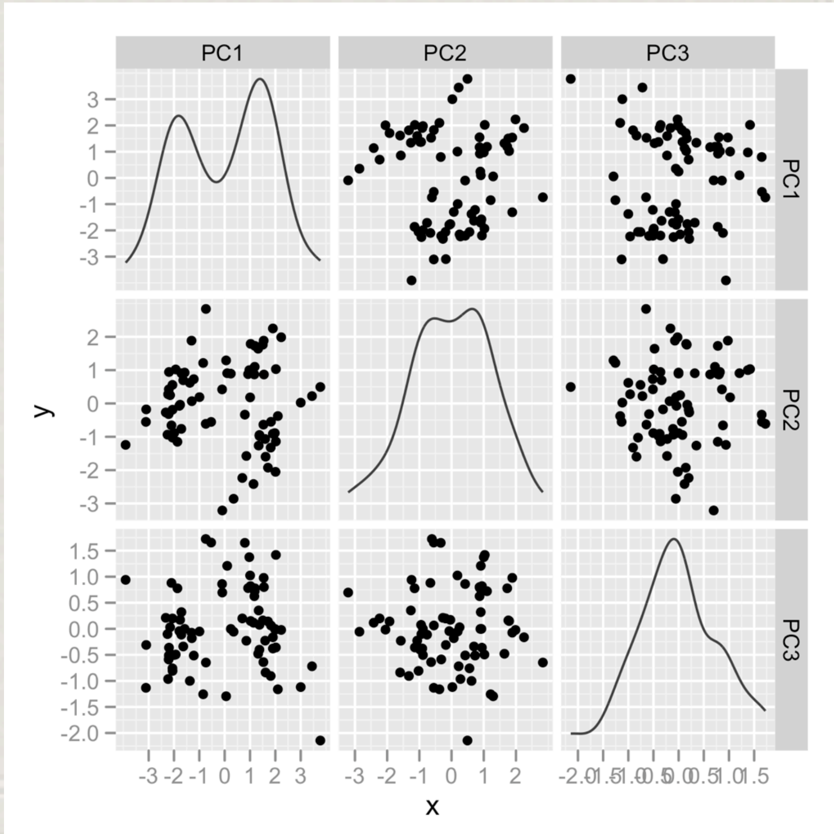


More examples

- *Flea beetles - clusters not revealed by PCA*





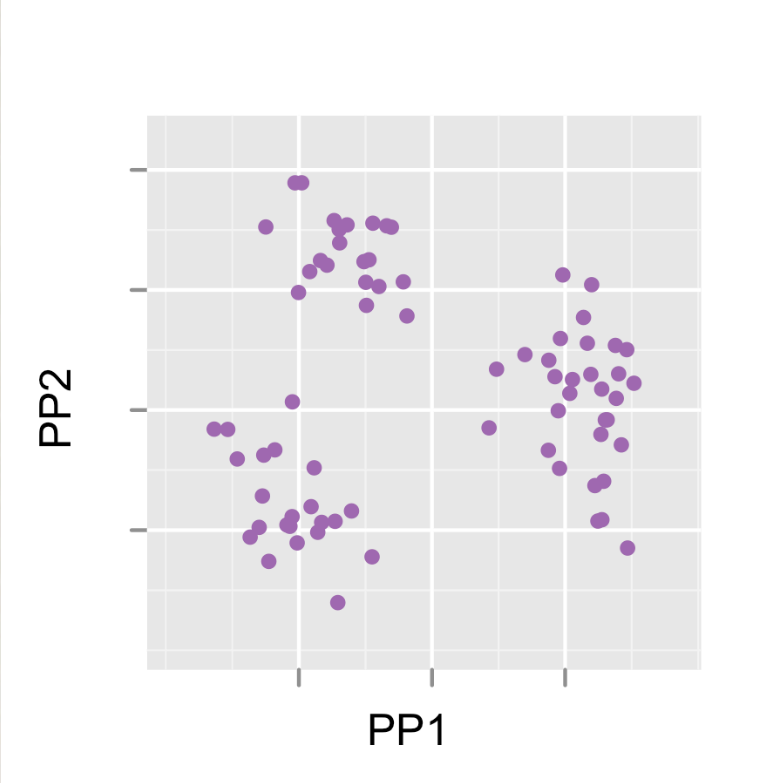


PP & PCA

- *Projection pursuit generalizes PCA. Any arbitrary function is optimized over all directions in the data.*
- *For PCA "f" is "variance"*

$$\max f(\mathbf{X}\mathbf{a}_1) \text{ subject to } \mathbf{a}_1'\mathbf{a}_1 = 1$$

PP & PCA



- *PP using the Holes index will find clusters that PCA misses.*

$$\mathbf{y} = \mathbf{X}\mathbf{A},$$

$$I_{\text{holes}}(\mathbf{A}) = \frac{1 - \frac{1}{n}\sum_{i=1}^{n} \exp(-\frac{1}{2}\mathbf{y}_i\mathbf{y}_i')}{1 - \exp(-\frac{p}{2})}$$

PCA & MDS

- *Multidimensional scaling (MDS) also generalizes PCA.*
- *MDS finds a low-dimensional representation of the data that preserves the interpoint distances, as closely as possible.*
- *PCA is MDS when Euclidean distance is used.*

Example: Womens track

Distances between all countries: variables standardized

	argentin(SA)	australi(PC)	austria(EU)	belgium(EU)	bermuda(NA)	brazil(SA)	burma(SA)
australi(PC)	2.738						
austria(EU)	2.357	0.983					
belgium(EU)	2.332	0.920	0.806				
bermuda(NA)	0.782	2.671	2.257	2.370			
brazil(SA)	1.112	2.100	1.673	1.846	0.736		
burma(SA)	1.916	4.041	3.372	3.305	2.257	2.571	
canada(NA)	3.231	0.737	1.510	1.412	3.095	2.547	4.525

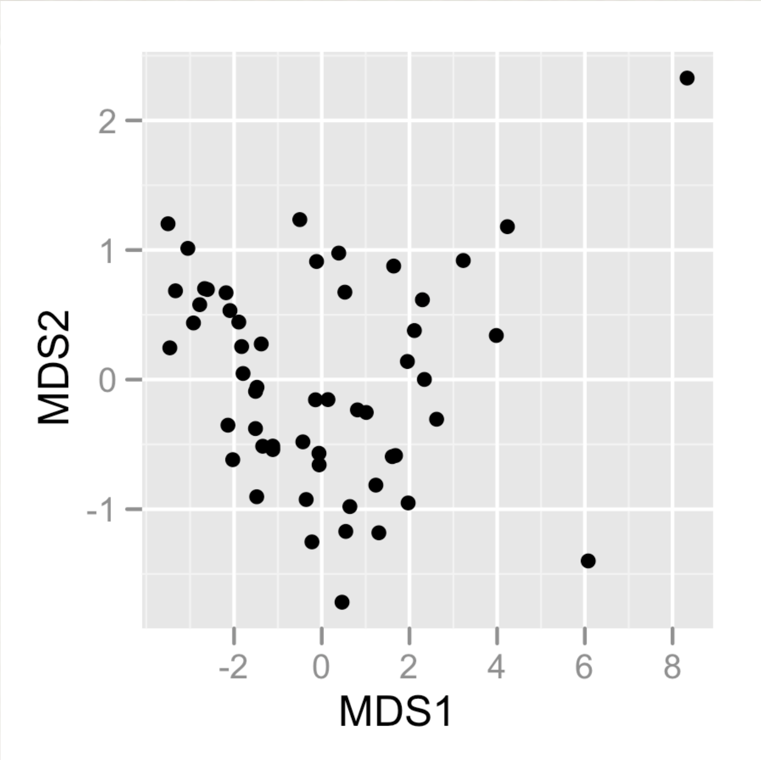
$D_{n \times n}$

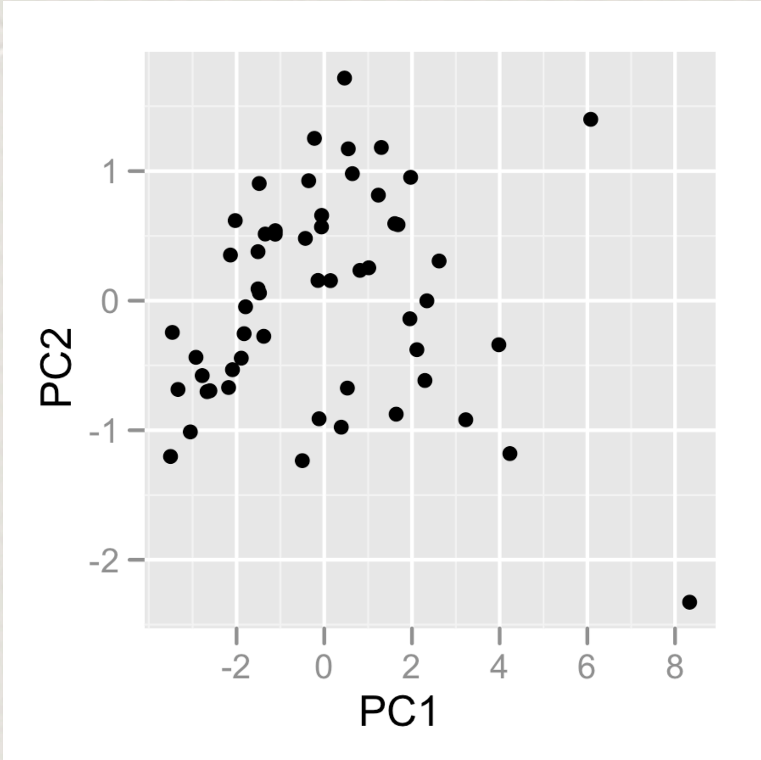
- *MDS minimizes the difference between these interpoint distances, and the distance between points in the low-dimensional representation.*

$$\text{Stress}_D(\mathbf{x}_1, \ldots \mathbf{x}_n) = \sqrt{\sum_{i \neq j} (D_{ij} - d_k(\mathbf{x}_i, \mathbf{x}_j))^2}$$

$d_k(\mathbf{x}_i, \mathbf{x}_j)$ is interpoint distance in k dimensions.

Example: Womens track





- *PCA is MDS when Euclidean distance is used.*
- *But different distance metrics can be used, and different stress functions can produce nonlinear mappings.*

Practicalities

- *Womens track example, PC1=0.368 100m+0.365 200m + 0.382 400m+0.385 800m+0.389 1500m+ 0.389 3000m+ 0.367 marathon, where all variables have been standardized.*
- *What does this tell you???*
- *Use an equal combination of all of the variables: PC1=0.378 100m+0.378 200m + 0.378 400m+0.378 800m +0.378 1500m+ 0.378 3000m+ 0.378 marathon*