StatLab Workshop

Principal Components Analysis with R

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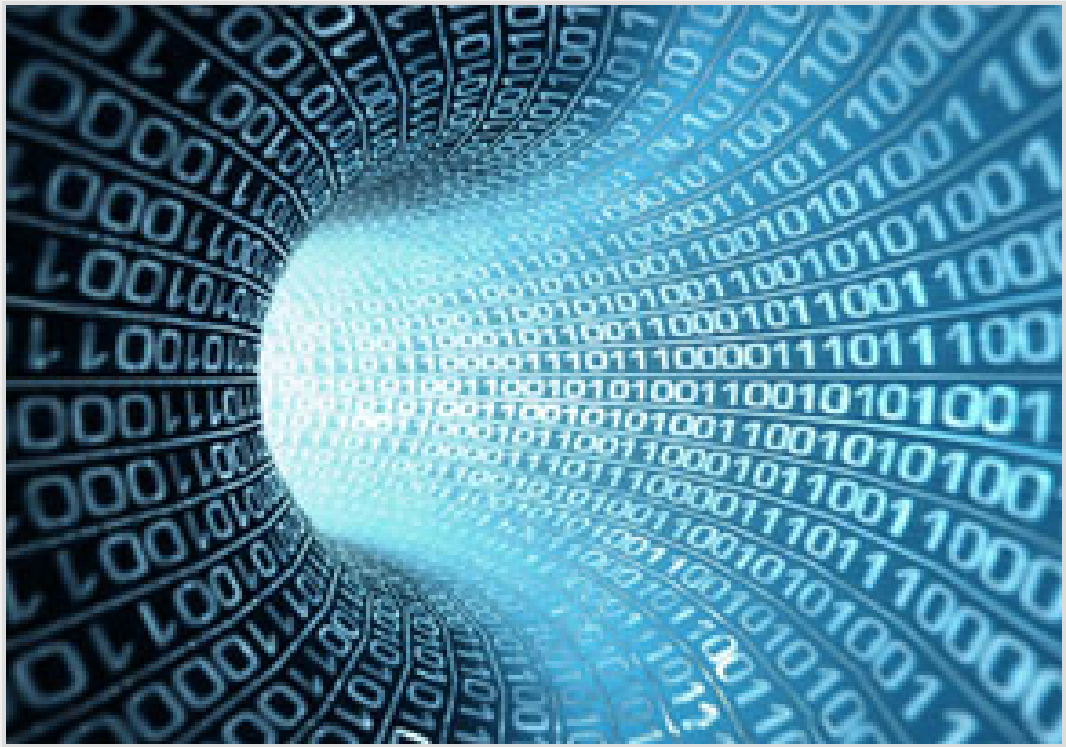

Outline

1 Theory
- Dimension reduction
- The PCA algorithm

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1. Theory
   - Dimension reduction
   - The PCA algorithm

2. Implementation in R
   - Running example code together
   - Exercises to try for yourself

Theory

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- Visualization, e.g. reduce many quantitative variables down to a few, then draw scatterplots
- Meaningful interpretations of relationships among variables
- Decreasing variance of estimation (while likely increasing bias)
- A technique that you want to use is computationally impossible or intractable in the data's original dimension

Bias-variance trade-off

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Dimension reduction techniques tend to increase squared bias and decrease variance.

Linear transformations for dim reduction

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- Principal components analysis (PCA) "spreads out the *points* as much as possible"
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PCA is our focus, but we'll also see LDA in one of the R code examples later.

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To be frank, it's probably more than you can process in a single sitting. Just do your best to follow along and see how much you can make sense of. Then, if you'd like to really understand the details, take your time looking over these notes again later.

Spreading out the data points

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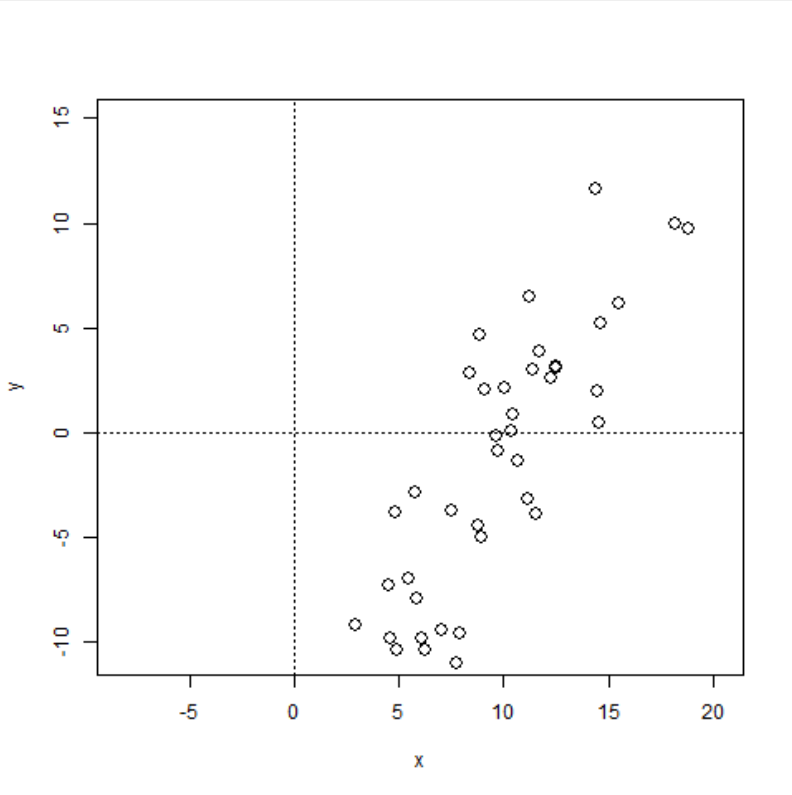
How about *variance*, the average squared difference from the mean. Each variable has a variance, and some variables will have larger variances than others.

A cloud of data point and their coordinates



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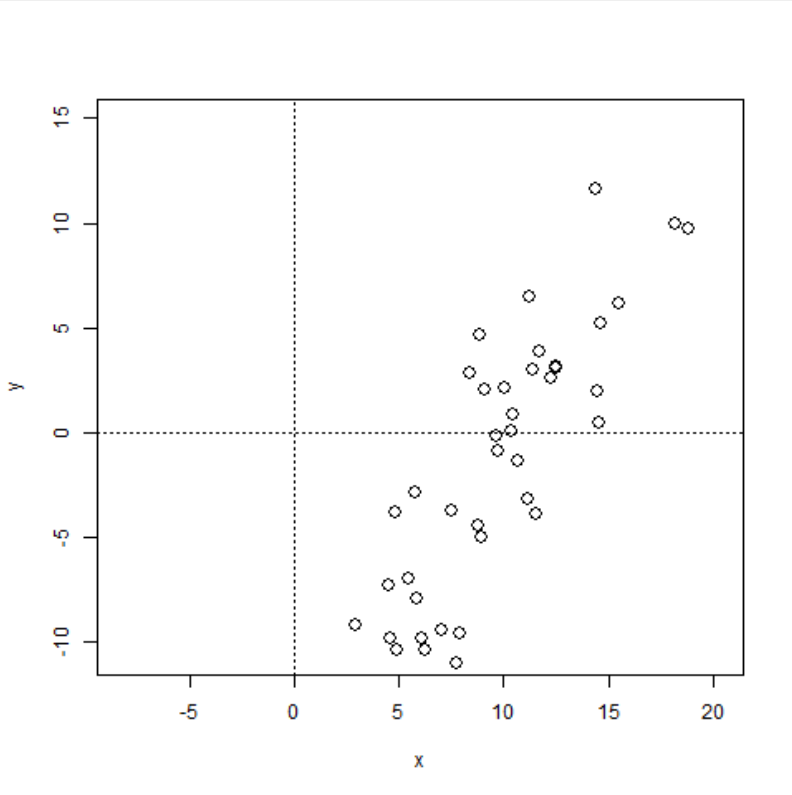

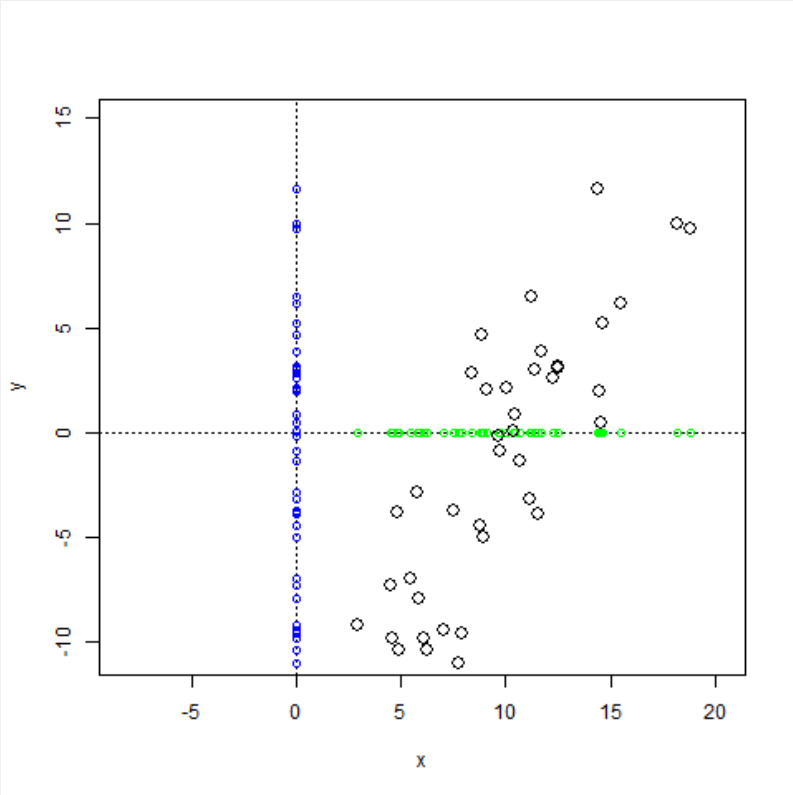

Alternative bases

Consider the first observation $\mathbf{x}_1 = (x_{i,1}, \ldots, x_{i,d})$. It's the sum of its orthogonal projections onto the coordinate axes:

$$\mathbf{x}_1 = x_{1,1}\mathbf{e}_1 + \ldots + x_{1,d}\mathbf{e}_d$$

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However, $\mathbf{x}_1$ is also the sum of its orthogonal projections onto *any* orthonormal basis $\mathbf{u}_1, \ldots, \mathbf{u}_d$. The general formula is simply

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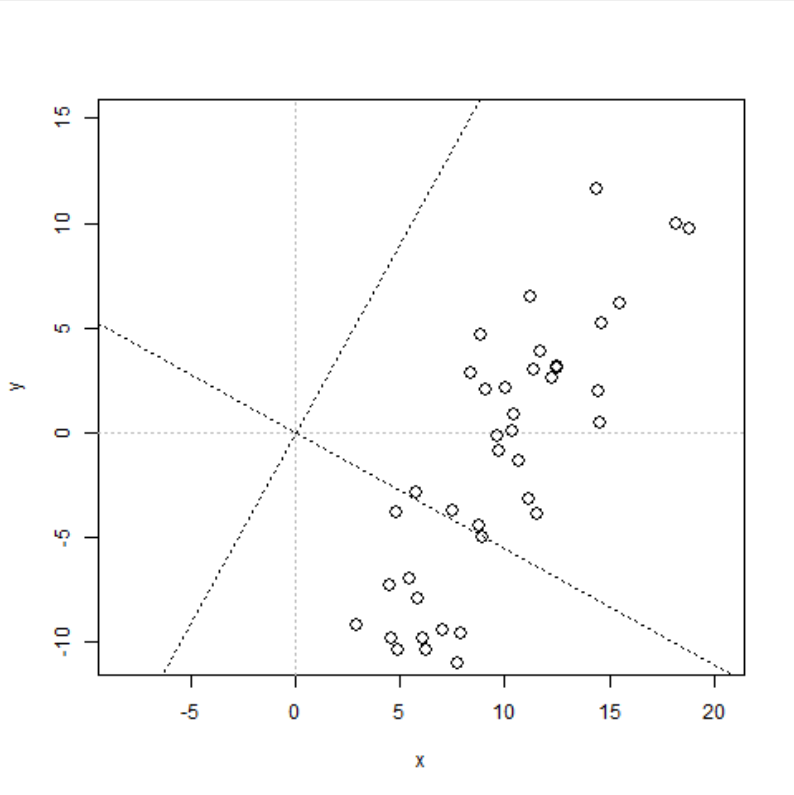
The other observations can be represented likewise. Thus, the *coordinates* of $\mathbf{x}_1, \ldots, \mathbf{x}_n$ *with respect to* a basis vector $\mathbf{u}$ are $\mathbf{x}_1^T\mathbf{u}, \ldots, \mathbf{x}_n^T\mathbf{u}$.

Alternative axes and coordinates



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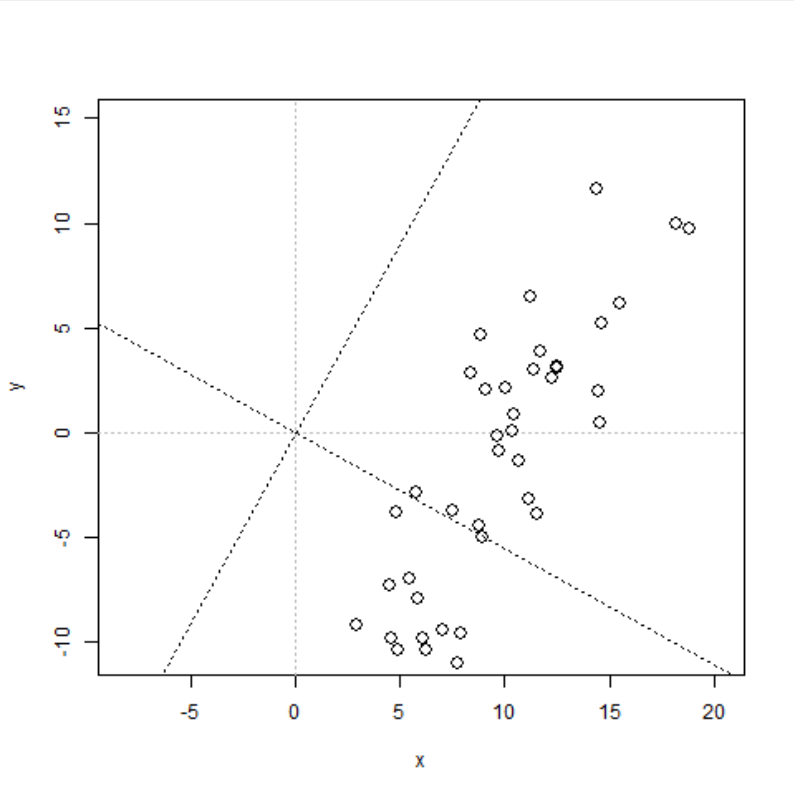

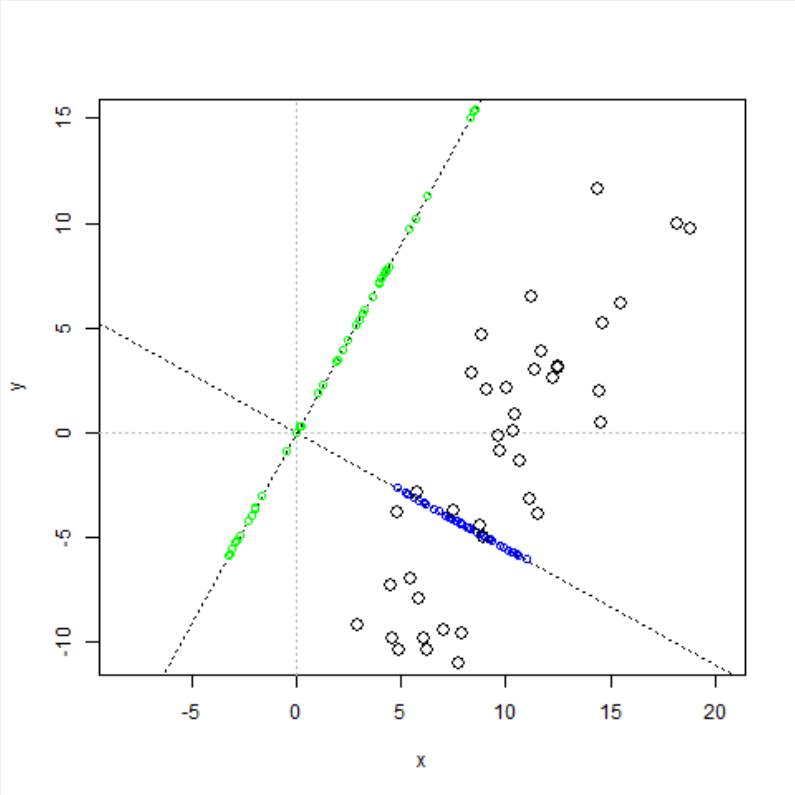

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- Let $\frac{1}{n}\mathbb{X}^T\mathbb{X}$ have eigenvalues $\lambda_1 \geq \ldots \geq \lambda_n$ with orthonormal eigenvectors $\mathbf{q}_1, \ldots, \mathbf{q}_n$. Spectral decomposition shows that the quadratic form $\mathbf{u}^T(\frac{1}{n}\mathbb{X}^T\mathbb{X})\mathbf{u}$ is maximized if $\mathbf{u}$ equals $\mathbf{q}_1$.

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The variance of the coordinates of $\mathbf{x}_1, \ldots, \mathbf{x}_n$ (with respect to any basis vector) is exactly the same as the variance of the coordinates of the *centered* vectors $\mathbf{x}_1 - \bar{\mathbf{x}}, \ldots, \mathbf{x}_n - \bar{\mathbf{x}}$.

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Let $\widetilde{\mathbb{X}}$ be the matrix whose rows are $\mathbf{x}_1 - \bar{\mathbf{x}}, \ldots, \mathbf{x}_n - \bar{\mathbf{x}}$, and let $\frac{1}{n}\widetilde{\mathbb{X}}^T\widetilde{\mathbb{X}}$ have eigenvalues $\lambda_1 \geq \ldots \geq \lambda_n$ with orthonormal eigenvectors $\mathbf{q}_1, \ldots, \mathbf{q}_n$. The variance of the coordinates of $\mathbf{x}_1, \ldots, \mathbf{x}_n$ is maximized by $\mathbf{q}_1$. Among all unit vectors that are orthogonal to $\mathbf{q}_1$, the variance of the coordinates of $\mathbf{x}_1, \ldots, \mathbf{x}_n$ is maximized by $\mathbf{q}_2$, and so on.

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Then the average of the coordinates of $\mathbf{x}_1, \ldots, \mathbf{x}_n$ with respect to a unit vector $\mathbf{u}$ is

$$\frac{1}{n}(\mathbf{x}_1^T\mathbf{u} + \ldots + \mathbf{x}_n^T\mathbf{u}) = \underbrace{\frac{1}{n}(\mathbf{x}_1 + \ldots + \mathbf{x}_n)^T}_{\mathbf{o}}\mathbf{u}$$
$$= 0$$

Variance of coordinates

If $\mathbf{x}_1, \ldots, \mathbf{x}_n$ have mean $\mathbf{o}$, then the variance of the coordinates of $\mathbf{x}_1, \ldots, \mathbf{x}_n$ with respect to a unit vector $\mathbf{u}$ is simply the average of the squared coordinates

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Let's derive a more useful representation of this quantity in terms of the matrix $\mathbb{X}$ whose rows are $\mathbf{x}_1, \ldots, \mathbf{x}_n$. The coordinates $\mathbf{x}_1^T\mathbf{u}, \ldots, \mathbf{x}_n^T\mathbf{u}$ are the entries of the vector

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Therefore, the variance of the coordinates can be represented

$$\frac{1}{n}\sum_i (\mathbf{x}_1^T\mathbf{u})^2 = \frac{1}{n}\|\mathbb{X}\mathbf{u}\|^2 = \frac{1}{n}(\mathbb{X}\mathbf{u})^T(\mathbb{X}\mathbf{u}) = \mathbf{u}^T(\frac{1}{n}\mathbb{X}^T\mathbb{X})\mathbf{u}.$$

Maximizing variance

Assuming $\mathbf{x}_1, \ldots, \mathbf{x}_n$ have mean $\mathbf{o}$, we've realized that the variance of their coordinates with respect to any unit vector $\mathbf{u}$ equals the *quadratic form* $\mathbf{u}^T(\frac{1}{n}\mathbb{X}^T\mathbb{X})\mathbf{u}$.

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It turns out that this is easy to maximize via a *spectral decomposition*. The symmetric matrix $\frac{1}{n}\mathbb{X}^T\mathbb{X}$ can be rewritten in terms of its eigenvalues $\lambda_1 \geq \ldots \geq \lambda_d$ and orthonormal eigenvectors $\mathbf{q}_1, \ldots, \mathbf{q}_d$:

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The numbers $\mathbf{u}^T\mathbf{q}_1, \ldots, \mathbf{u}^T\mathbf{q}_n$ are exactly the coordinates of $\mathbf{u}$ with respect to the orthonormal basis $\mathbf{q}_1, \ldots, \mathbf{q}_d$. Because $\mathbf{u}$ is a unit vector, their squares must sum to 1 (Parseval's identity). Therefore, $\mathbf{u}^T(\frac{1}{n}\mathbb{X}^T\mathbb{X})\mathbf{u}$ is a weighted average of the eigenvalues $\lambda_1, \ldots, \lambda_d$. Its maximum possible value of λ_1 is achieved if $\mathbf{u}$ equals $\mathbf{q}_1$.

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By similar reasoning, among all unit vectors that are orthogonal to $\mathbf{q}_1$, the variance of the coordinates of $\mathbf{x}_1, \ldots, \mathbf{x}_n$ is maximized by $\mathbf{q}_2$, and so on.

Centering

Define the *mean vector* $\bar{\mathbf{x}}$ to be the vector whose first entry is the average of the first entries of $\mathbf{x}_1, \ldots, \mathbf{x}_n$, and so on. The *centered* points $\mathbf{x}_1 - \bar{\mathbf{x}}, \ldots, \mathbf{x}_n - \bar{\mathbf{x}}$ have two key properties.

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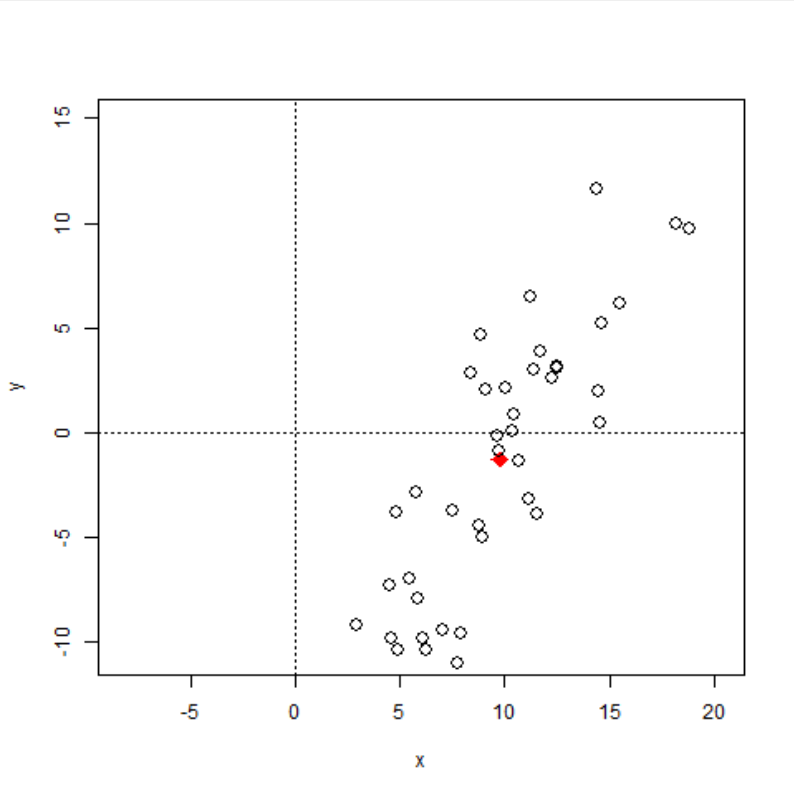
- The centered points have mean $\mathbf{o}$. $(\frac{1}{n}\sum_i(\mathbf{x}_i - \bar{\mathbf{x}}) = (\frac{1}{n}\sum_i \mathbf{x}_i) - \bar{\mathbf{x}} = \mathbf{o}.)$

Centering the data points



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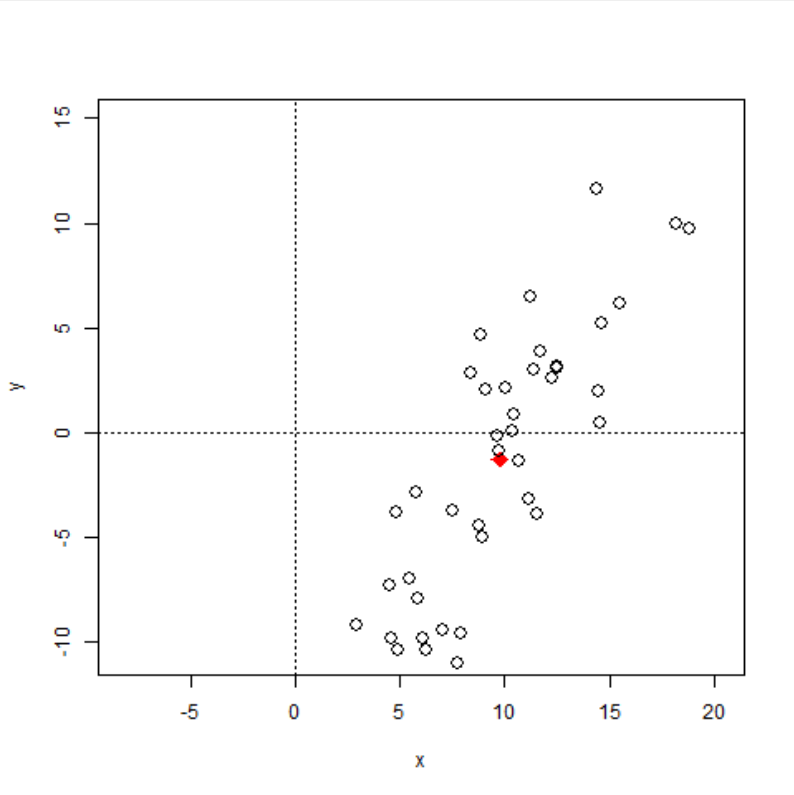

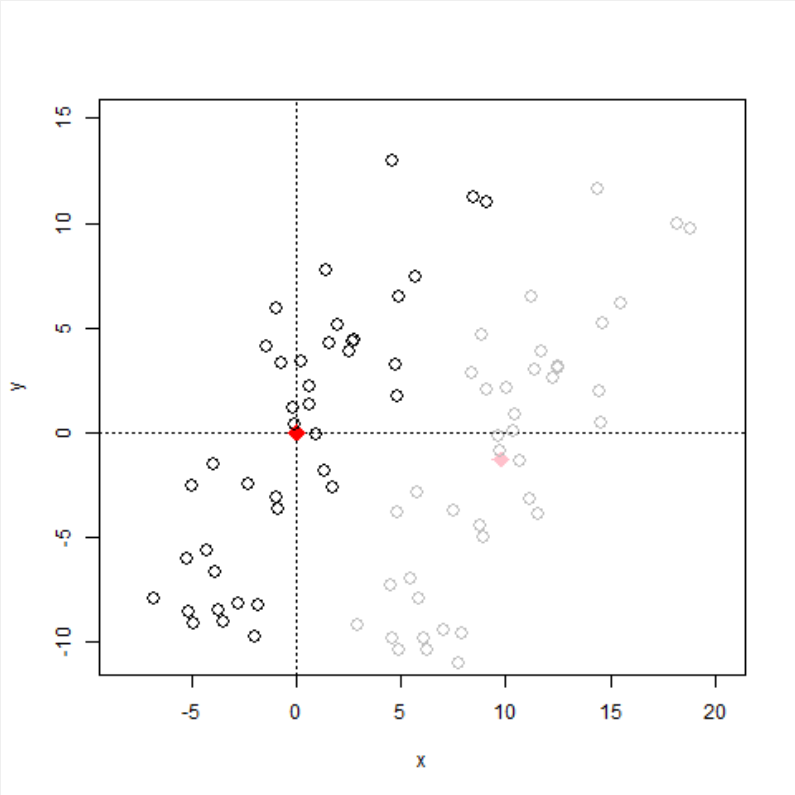

PCA algorithm

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Let $\widetilde{\mathbb{X}}$ be the matrix whose rows are $\mathbf{x}_1 - \bar{\mathbf{x}}, \ldots, \mathbf{x}_n - \bar{\mathbf{x}}$, and let $\frac{1}{n}\widetilde{\mathbb{X}}^T\widetilde{\mathbb{X}}$ have eigenvalues $\lambda_1 \geq \ldots \geq \lambda_d$ with orthonormal eigenvectors $\mathbf{q}_1, \ldots, \mathbf{q}_d$. The variance of the coordinates of $\mathbf{x}_1, \ldots, \mathbf{x}_n$ is maximized by $\mathbf{q}_1$. Among all unit vectors that are orthogonal to $\mathbf{q}_1$, the variance of the coordinates of $\mathbf{x}_1, \ldots, \mathbf{x}_n$ is maximized by $\mathbf{q}_2$, and so on.

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Notice that $\frac{1}{n}\widetilde{\mathbb{X}}^T\widetilde{\mathbb{X}}$ is the covariance matrix of the data points.

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The eigenvector basis coordinates

The spectral decomposition of the covariance matrix $\frac{1}{n}\widetilde{\mathbb{X}}^T\widetilde{\mathbb{X}}$ is usually expressed as $\mathbb{Q}\mathbb{\Lambda}\mathbb{Q}^T$ where $\mathbb{\Lambda}$ is a diagonal matrix of eigenvalues and the columns of $\mathbb{Q}$ are orthonormal unit eigenvectors.

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The coordinates of $\mathbf{x}_1$ with respect to the eigenvectors of the covariance matrix are precisely the entries of

$$\mathbb{Q}^T\mathbf{x}_1 = \begin{bmatrix} - & \mathbf{q}_1 & - \\ & \vdots & \\ - & \mathbf{q}_d & - \end{bmatrix} \begin{bmatrix} | \\ \mathbf{x}_1 \\ | \end{bmatrix} = \begin{bmatrix} \mathbf{q}_1^T\mathbf{x}_1 \\ \vdots \\ \mathbf{q}_d^T\mathbf{x}_1 \end{bmatrix}.$$

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Indeed, one can easily compute the coordinates of all the observations at once:

$$\mathbb{X}\mathbb{Q} = \begin{bmatrix} - & \mathbf{x}_1 & - \\ & \vdots & \\ - & \mathbf{x}_n & - \end{bmatrix} \begin{bmatrix} | & & | \\ \mathbf{q}_1 & \cdots & \mathbf{q}_d \\ | & & | \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1^T\mathbf{q}_1 & \cdots & \mathbf{x}_1^T\mathbf{q}_d \\ \vdots & \ddots & \vdots \\ \mathbf{x}_n^T\mathbf{q}_1 & \cdots & \mathbf{x}_n^T\mathbf{q}_d \end{bmatrix}.$$

The ith row contains the coordinates of $\mathbf{x}_i$ with respect to $\mathbf{q}_1, \ldots, \mathbf{q}_n$.

The principal components

An often more convenient matrix is $\widetilde{\mathbb{X}}\mathbb{Q}$ which contains the coordinates of the *centered* observations with respect to $\mathbf{q}_1, \ldots, \mathbf{q}_n$. In that case, the columns are orthogonal.

$$\begin{aligned}(\widetilde{\mathbb{X}}\mathbb{Q})^T(\widetilde{\mathbb{X}}\mathbb{Q}) &= \mathbb{Q}^T\widetilde{\mathbb{X}}^T\widetilde{\mathbb{X}}\mathbb{Q} \\ &= \mathbb{Q}^T(n\mathbb{Q}\Lambda\mathbb{Q}^T)\mathbb{Q} \\ &= n\Lambda\end{aligned}$$

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These columns that were called *principal components* of the dataset, though the terminology is used inconsistently. You may see the columns of $\mathbb{X}\mathbb{Q}$ called the principal components. Or you may see $\mathbf{q}_1, \ldots, \mathbf{q}_n$ called the principal components.

Singular value decomposition

The eigenvectors and eigenvalues of the covariance matrix can also be obtained directly from a *singular value decomposition* of $\frac{1}{\sqrt{n}}\widetilde{\mathbb{X}}$:

$$\frac{1}{\sqrt{n}}\widetilde{\mathbb{X}} = \mathbb{U}\mathbb{D}\mathbb{V}^T$$

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How does this relate to the spectral decomposition of the covariance matrix?

$$\begin{aligned}\frac{1}{n}\widetilde{\mathbb{X}}^T\widetilde{\mathbb{X}} &= (\frac{1}{\sqrt{n}}\widetilde{\mathbb{X}})^T(\frac{1}{\sqrt{n}}\widetilde{\mathbb{X}}) \\ &= (\mathbb{U}\mathbb{D}\mathbb{V}^T)^T(\mathbb{U}\mathbb{D}\mathbb{V}^T) \\ &= \mathbb{V}\mathbb{D}\mathbb{U}^T\mathbb{U}\mathbb{D}\mathbb{V}^T \\ &= \mathbb{V}\mathbb{D}^2\mathbb{V}^T\end{aligned}$$

reveals a spectral decomposition of the covariance matrix. The columns of $\mathbb{V}$ are unit eigenvectors while the squares of the diagonals in $\mathbb{D}$ are the corresponding eigenvalues.

Variances equal to eigenvalues

The variance of the coordinates with respect to $\mathbf{q}_1$ is

$$\begin{aligned}
\mathbf{q}_1^T\left(\tfrac{1}{n}\widetilde{\mathbb{X}}^T\widetilde{\mathbb{X}}\right)\mathbf{q}_1 &= \mathbf{q}_1^T(\lambda_1\mathbf{q}_1\mathbf{q}_1^T + \ldots + \lambda_d\mathbf{q}_d\mathbf{q}_d^T)\mathbf{q}_1 \\
&= \lambda_1(\underbrace{\mathbf{q}_1^T\mathbf{q}_1}_{1})^2 + \ldots + \lambda_d(\underbrace{\mathbf{q}_1^T\mathbf{q}_d}_{0})^2 \\
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Likewise the variance of the coordinates with respect to any eigenvector $\mathbf{q}_j$ is the corresponding eigenvalue λ_j. If only the first $k \leq d$ principal components are retained, then the sum of the variances in the lower-dimensional approximation is $\lambda_1 + \ldots + \lambda_k$.

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The sum of the variances of the eigenvector basis coordinates equals the sum of the variances of the original coordinates.

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$$\sum_{j=1}^{d} \frac{1}{n} \sum_{i=1}^{n} (\mathbf{q}_j^T \mathbf{x}_i)^2 = \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{d} (\mathbf{q}_j^T \mathbf{x}_i)^2 = \frac{1}{n} \sum_{i=1}^{n} \|\mathbf{x}_i\|^2 = \frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{d} x_{i,j}^2 = \sum_{j=1}^{d} \frac{1}{n} \sum_{i=1}^{n} x_{i,j}^2$$

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Let v equal the sum of the variances of the original coordinates. If only the first $k \leq d$ principal components are retained, then the proportion of the variance that is preserved is $\frac{\lambda_1 + \ldots + \lambda_k}{v}$.

Scale-dependence

Although variance doesn't depend on location, it does depend on *scale*. If a set of heights were measured in inches, they will have a much larger variances than they would if measured in feet. Likewise, the choice of units of measurement also affect which basis vectors are returned by the PCA algorithm.

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However, if all of the original variables are measured in the same units, you may want to preserve their differing variances rather than rescaling.

Implementation in R

Running example code together

See *PCA-examples.R* Exercises 1 - 3.

Exercises to try for yourself

Work through *PCA-examples.R* Exercise 4.