Statistical Operations and Matrices (II)

Predictive Modeling & Statistical Learning

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Data Matrix Perspectives

Motivation

I want to discuss how we can use vector-matrix notation to represent some basic statistical operations and summaries.

First we need to quickly review some concepts around inner products.

Geometry of the Data Matrix

Matrix Structure

Data

The analyzed data can be expressed in matrix format $\mathbf{X}$:

$$\underset{n \times p}{\mathbf{X}} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix}$$

- n objects in the rows
- p quantitative variables in the columns

Looking at Rows and Columns

Data Concerns

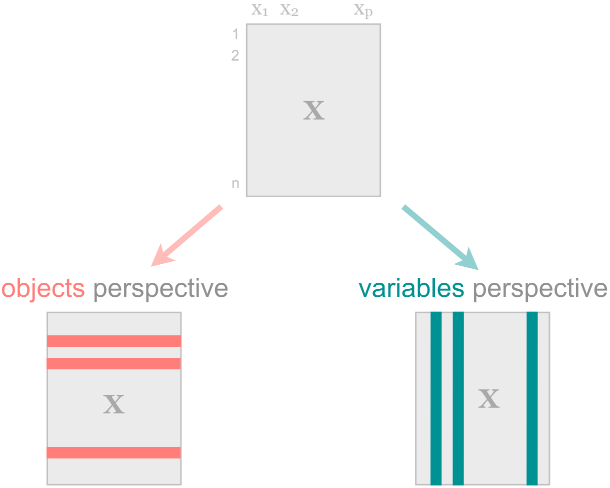
Two sides of the same coin

When the analyzed data can be expressed as a matrix with objects in rows, and variables in columns, we commonly care for two issues:

- Study the resemblance between objects
- Study the relationships among variables

Data Perspectives

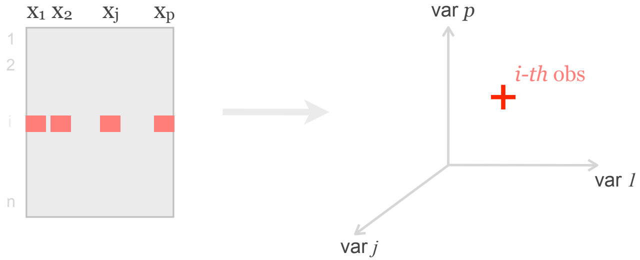
looking at a data matrix from two perspectives



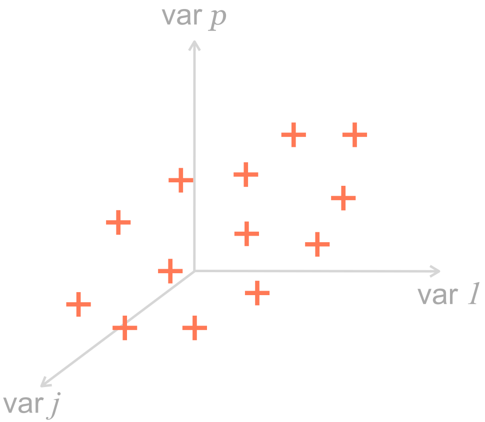
Objects Perspective

each object described
by p variables

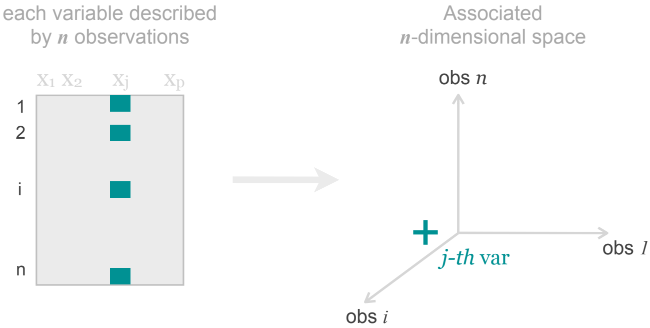
Associated
p-dimensional space



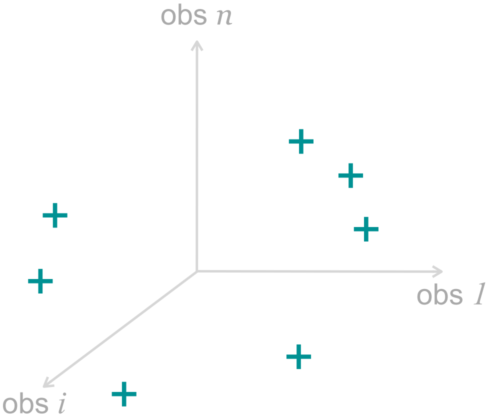
Objects as points in a p-dimensional space



Variables Perspective



Variables as points in a n-dimensional space



Raw Data

Raw Data Matrix

The analyzed data can be expressed in matrix format $\mathbf{X}$:

$$\underset{n \times p}{\mathbf{X}} = \begin{bmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{n2} & \cdots & x_{np} \end{bmatrix}$$

- n objects in the rows
- p quantitative variables in the columns

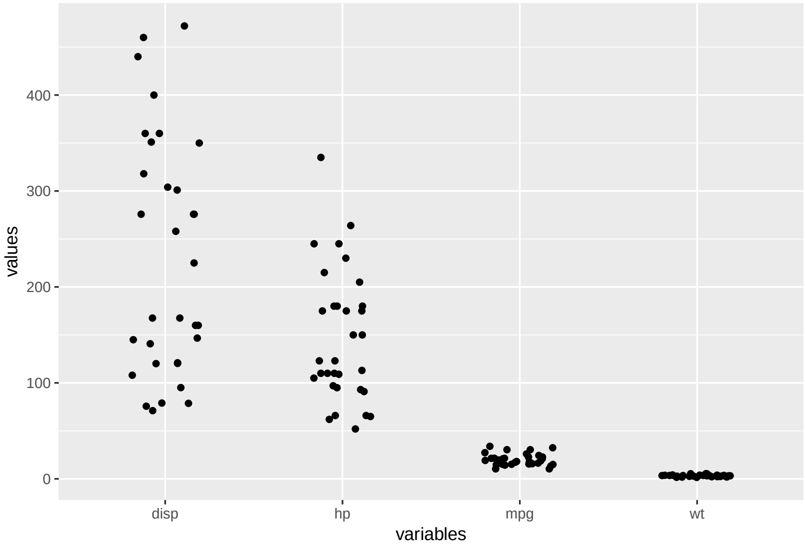
Data set `mtcars`

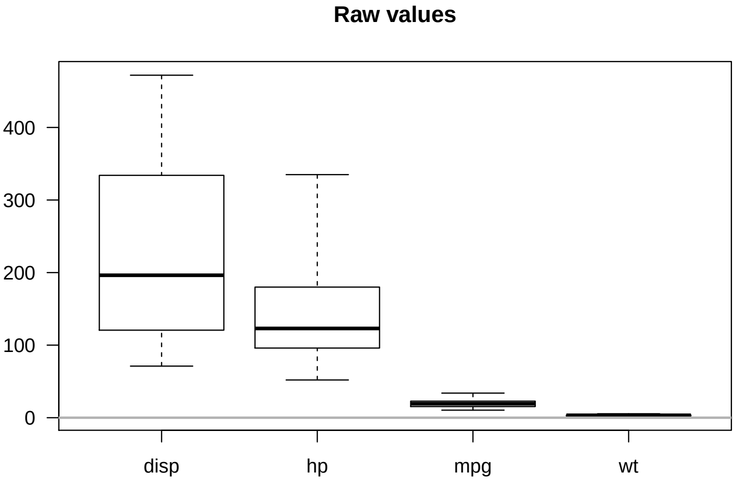
First 10 rows:

```
                   mpg cyl  disp  hp drat    wt  qsec vs am gear carb
Mazda RX4         21.0   6 160.0 110 3.90 2.620 16.46  0  1    4    4
Mazda RX4 Wag     21.0   6 160.0 110 3.90 2.875 17.02  0  1    4    4
Datsun 710        22.8   4 108.0  93 3.85 2.320 18.61  1  1    4    1
Hornet 4 Drive    21.4   6 258.0 110 3.08 3.215 19.44  1  0    3    1
Hornet Sportabout 18.7   8 360.0 175 3.15 3.440 17.02  0  0    3    2
Valiant           18.1   6 225.0 105 2.76 3.460 20.22  1  0    3    1
Duster 360        14.3   8 360.0 245 3.21 3.570 15.84  0  0    3    4
Merc 240D         24.4   4 146.7  62 3.69 3.190 20.00  1  0    4    2
Merc 230          22.8   4 140.8  95 3.92 3.150 22.90  1  0    4    2
Merc 280          19.2   6 167.6 123 3.92 3.440 18.30  1  0    4    4
```

Let's use variables: `mpg`, `disp`, `hp`, and `wt`.

Raw values: different means, different std−devs




Raw values
400
300
200
100
0
disp
hp
mpg
wt

Centering Data Matrix

Mean-Centered Data Matrix

A common operation consists of **centering** the data, which involves mean-centering the variables so that they all have mean zero.

Mean-Centered Data Matrix

The mean-centered (a.k.a. column centered) matrix $\mathbf{X_C}$:

$$\underset{n\times p}{\mathbf{X_C}} = \begin{bmatrix} x_{11}-\bar{x}_1 & x_{12}-\bar{x}_2 & \cdots & x_{1p}-\bar{x}_p \\ x_{21}-\bar{x}_1 & x_{22}-\bar{x}_2 & \cdots & x_{2p}-\bar{x}_p \\ \vdots & \vdots & \ddots & \vdots \\ x_{n1}-\bar{x}_1 & x_{n2}-\bar{x}_2 & \cdots & x_{np}-\bar{x}_p \end{bmatrix}$$

where $\bar{x}_j$ is the mean of the j-th variable $(j = 1, \ldots, p)$

Mean-Centered Data Matrix

Using matrix notation, the centering operation is expressed as:

$$\mathbf{X_C} = (\mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^\mathsf{T})\mathbf{X}$$

- $\mathbf{I}$ is the $n \times n$ identity matrix
- $\mathbf{1}$ is an $n \times 1$ vector of ones

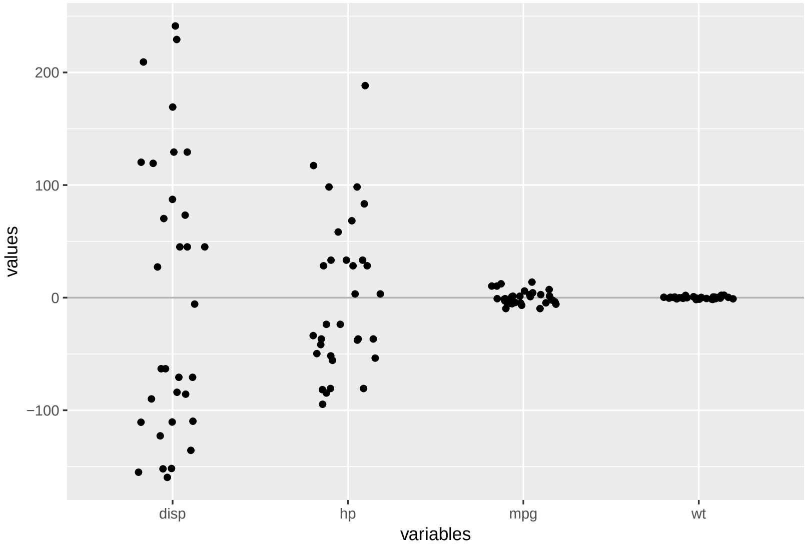
$\mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^\mathsf{T}$ is sometimes called the *centering* operator

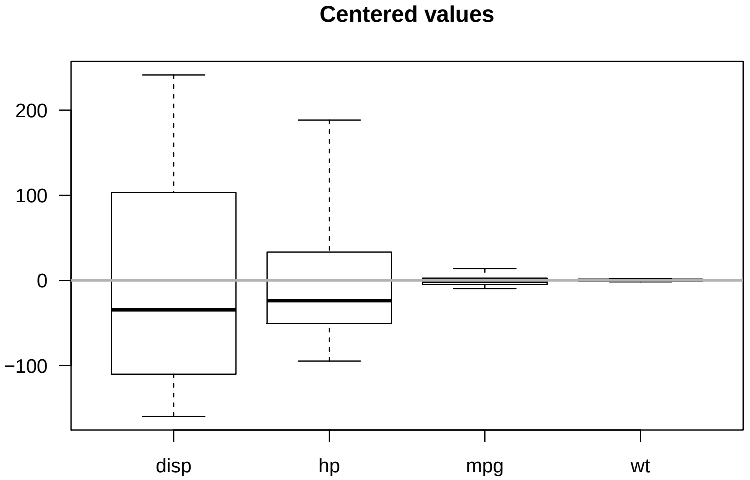
Centering Effects

What does mean-centering do to the cloud of points?

What does column-centering do in general?

Centered: mean = 0, different std−devs




Centered values
200
100
0
−100
disp
hp
mpg
wt

Centering Matrices in R

Centering with `scale()`

```
X_centered <- scale(X, center = TRUE, scale = FALSE)
```

Or also like this:

```
centroid <- colMeans(X)
X_centered <- sweep(X, 2, centroid, FUN = "-")
```

Scaled Data Matrix

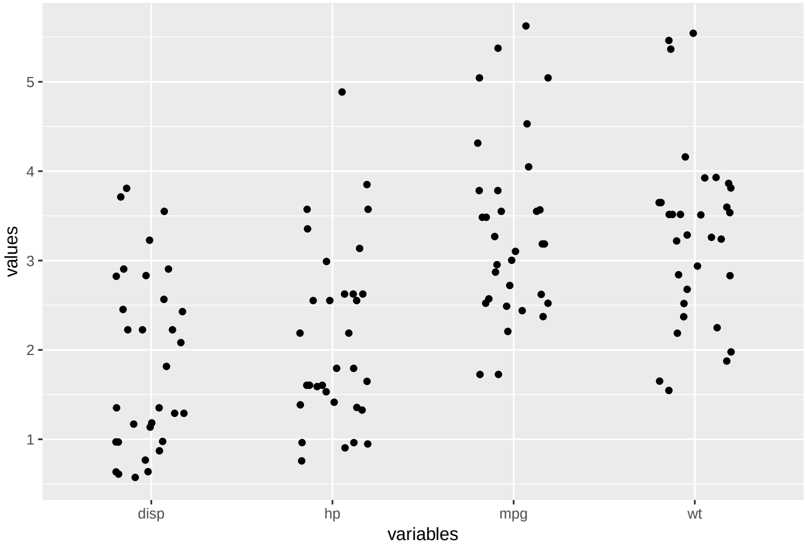
Scaled or Normalized Data Matrix

The scaled or *Normalized* matrix $\mathbf{X_N}$:

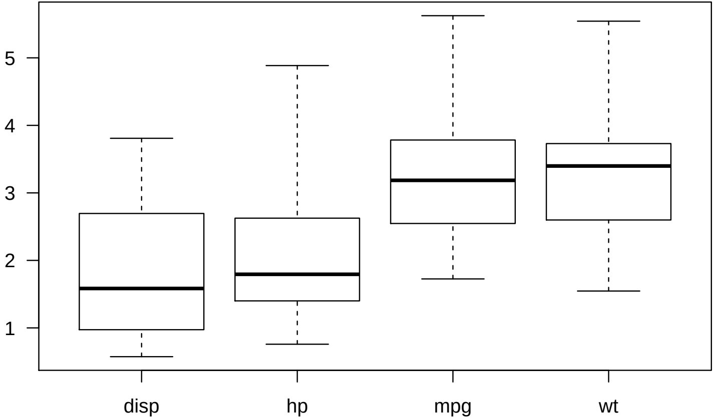
$$\underset{n\times p}{\mathbf{X_N}} = \begin{bmatrix} a_1x_{11} & a_2x_{12} & \cdots & a_px_{1p} \\ a_1x_{21} & a_2x_{22} & \cdots & a_px_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ a_1x_{n1} & a_2x_{n2} & \cdots & a_px_{np} \end{bmatrix}$$

where a_j is a scaling factor for the j-th column

Scaled: different means, scale with std−dev = 1



Scaled values



Some Scaling Options

- Standard Deviation: $a_j = sd_j = \frac{1}{n}\sum_{i=1}^{n}(x_{ij} - \bar{x}_j)^2$
- L_1-norm: $a_j = \sum_{i=1}^{n} |x_{ij}|$
- L_2-norm: $a_j = \sqrt{\sum_{i=1}^{n}(x_{ij})^2}$
- L_∞-norm: $a_j = max\{|x_{i1}|, \ldots, |x_{ip}|\}$
- L_p-norm: $a_j = \left(\sum_{i=1}^{n} |x_{ij}|^p\right)^{1/p}$

Scaled or Normalized Data Matrix

The scaling factors a_j can be put in a diagonal matrix $\mathbf{D_a}$

$$\underset{p\times p}{\mathbf{D_a}} = \begin{bmatrix} a_1 & 0 & \cdots & 0 \\ 0 & a_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_p \end{bmatrix}$$

then

$$\mathbf{X_N} = \mathbf{X}\mathbf{D_a}$$

Normalizing Effects

What does normalizing (i.e. scaling) do to the cloud of points?

Scaling Matrices in R

Scaling with standard deviation

```
scaling <- apply(X, 2, sd)

X_scaled <- scale(X, center = FALSE, scale = TRUE)
```

Scaling Matrices in R

Scaling with L_1-norm

```
# L-1 norm
one_norms <- apply(X, 2, function(u) max(abs(u)))

X_scaled <- scale(X, center = FALSE, scale = one_norms)
```

Scaling in R examples

Scaling with L_2-norm

```
# L-2 norm
two_norms <- apply(X, 2, function(u) sqrt(sum(u*u)))

X_scaled <- scale(X, center = FALSE, scale = two_norms)
```

Scaling Matrices in R

Scaling with L_∞-norm

```
# L-inf norm
inf_norms <- apply(X, 2, function(u) max(abs(u)))

X_scaled <- scale(X, center = FALSE, scale = inf_norms)
```

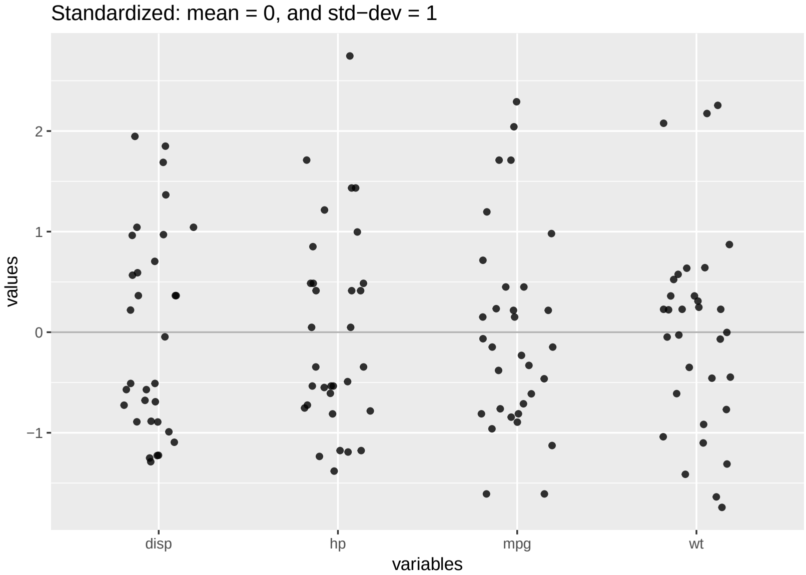
Standardized Data Matrix

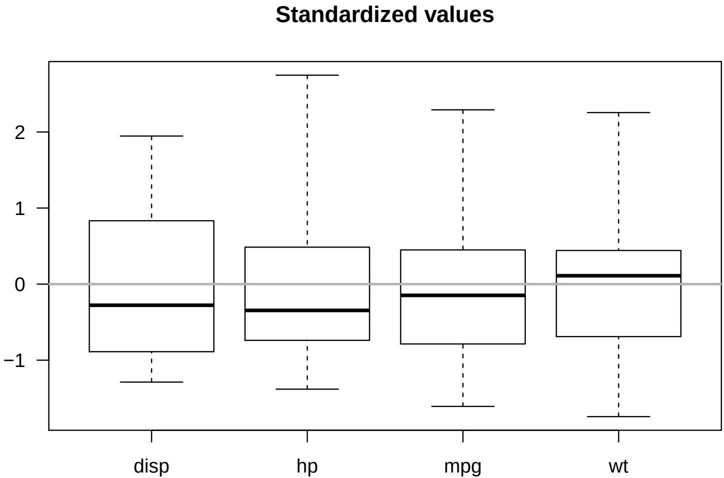
Standardized Data Matrix

The standardized matrix $\mathbf{X_S}$ is the mean-centered and scaled (by the standard deviation) matrix:

$$\underset{n\times p}{\mathbf{X_S}} = \begin{bmatrix} \frac{x_{11}-\bar{x}_1}{sd_1} & \frac{x_{12}-\bar{x}_2}{sd_2} & \cdots & \frac{x_{1p}-\bar{x}_p}{sd_p} \\ \frac{x_{21}-\bar{x}_1}{sd_1} & \frac{x_{22}-\bar{x}_2}{sd_2} & \cdots & \frac{x_{2p}-\bar{x}_p}{sd_p} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{x_{n1}-\bar{x}_1}{sd_1} & \frac{x_{n2}-\bar{x}_2}{sd_2} & \cdots & \frac{x_{np}-\bar{x}_p}{sd_p} \end{bmatrix}$$

- $\bar{x}_j$ is the mean of the j-th variable
- sd_j is the standard deviation of the j-th variable


Standardized: mean = 0, and std−dev = 1
values
2
1
0
−1
disp
hp
mpg
wt
variables


Standardized values
2
1
0
−1
disp
hp
mpg
wt

Standardized Data Matrix

When the scaling factors a_j are the standard deviations sd_j, the scaling matrix $\mathbf{D}_{\frac{1}{sd}}$ is:

$$\underset{p\times p}{\mathbf{D}_{\frac{1}{sd}}} = \begin{bmatrix} \frac{1}{sd_1} & 0 & \cdots & 0 \\ 0 & \frac{1}{sd_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \frac{1}{sd_p} \end{bmatrix}$$

then the standardized data matrix $\mathbf{X_S}$

$$\mathbf{X_S} = \mathbf{X_C}\mathbf{D}_{\frac{1}{sd}} = (\mathbf{I} - \frac{1}{n}\mathbf{1}\mathbf{1}^\mathsf{T})\mathbf{X}\mathbf{D}_{\frac{1}{sd}}$$

Standardizing Matrices in R

Standardizing with `scale()`

```
X_std <- scale(X, center = TRUE, scale = TRUE)

# equivalent to
X_std <- scale(X)
```

Objects and their weights

Weights of Objects

- We can assume that each object is associated to a **weight**
- Think of a weight as the "importance" of an observation
- Usually, we assume equal weights $1/n$ (i.e. equal importance)
- If we assume that objects come from a random sample, then the n objects have the same chance $1/n$ of being selected
- Sometimes, however, it is convenient to assume that each object has a general weight $w_i > 0$, such that $\sum_{i=1}^{n} w_i = 1$

Weights of Objects

We can consider a diagonal matrix of object weights $\mathbf{D}$:

$$\underset{n\times p}{\mathbf{D}} = \begin{bmatrix} w_1 & 0 & \cdots & 0 \\ 0 & w_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & w_n \end{bmatrix}$$

In the more common case that all weights are equal, we have $\mathbf{D} = \frac{1}{n}\mathbf{I}$

Weights of Objects

The vector $\mathbf{g}$ containing the means $\bar{X}_1, \bar{X}_2, \ldots, \bar{X}_p$ of all variables can be written as:

$$\mathbf{g} = \mathbf{X}^{\mathsf{T}}\mathbf{D}\mathbf{1_n}$$

where $\mathbf{1_n}$ is an $n \times 1$ vector of ones.

The vector $\mathbf{g}$ is also known as the **centroid** of the objects.

Centered Data Matrix

Using $\mathbf{D}$ and $\mathbf{g}$ we can write an expression to get a centered data matrix $\tilde{\mathbf{X}}$

$$\tilde{\mathbf{X}} = \mathbf{X} - \mathbf{1}\mathbf{g}^{\mathsf{T}} = (\mathbf{I} - \mathbf{1}\mathbf{1}^{\mathsf{T}}\mathbf{D})\mathbf{X}$$

Cross-Products

Data Matrix Products

Matrix Products

There are two fundamental matrix products that play a crucial role when the data is in an $n \times p$ matrix X with objects in rows, and variables in columns (typically assuming that $n > p$):

- $\mathbf{X}^\mathsf{T}\mathbf{X}$ association matrix for the variables
  a.k.a. "minor product" because is of size $p \times p$
- $\mathbf{X}\mathbf{X}^\mathsf{T}$ association matrix for the objects
  a.k.a. "major product" because is of size $n \times n$

(keep in mind we are assuming centered data)

Covariance Matrix

If $\mathbf{X}$ is mean-centered, then

$$\frac{1}{n}\mathbf{X}^\top\mathbf{X} \qquad \text{and} \qquad \frac{1}{n-1}\mathbf{X}^\top\mathbf{X}$$

are the covariance matrices (population and sample flavors)

Correlation Matrix

If $\mathbf{X}$ is standardized, then

$$\frac{1}{n}\mathbf{X}^\mathsf{T}\mathbf{X} \qquad \text{and} \qquad \frac{1}{n-1}\mathbf{X}^\mathsf{T}\mathbf{X}$$

are the correlation matrices (population and sample flavors)