

Matrices in R

Predictive Modeling & Statistical Learning

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Why Matrix Algebra?

Data Matrix

Data

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

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

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

Motivation

- ▶ Multivariate data is commonly represented in tabular format (rows and columns)
- ▶ Mathematically, a data table can be treated as a matrix
- ▶ Matrix algebra provides the analytical machinery and tools to manipulate and exploit values, information, and patterns of variability in data

In these slides I will cover key concepts about matrix operations with R.

Vector-Matrix Notation

- ▶ upper-case italics for variables: X, Y
- ▶ bold upper-case for matrices: \mathbf{A}, \mathbf{B}
- ▶ bold lower-case letters for vectors: \mathbf{x}, \mathbf{y}
- ▶ lower-case italics are used to represent scalars: a, b
- ▶ x_i is the i -th element of \mathbf{x}
- ▶ A_{ij} is the element in the i -th row and j -th column of \mathbf{A}
- ▶ By default, we'll consider a vector \mathbf{x} to be a one-column matrix
- ▶ \mathbf{x}^T to be a one-row matrix
- ▶ Occasionally I'll be using some greek letters too

Two Assumptions

I'm assuming 2 things about you:

Matrix Algebra & R basics

Matrix Algebra

You should have been exposed to concepts such as:

- ▶ Vector Spaces
- ▶ Inner Products
- ▶ Matrix Multiplication
- ▶ Linear Dependency
- ▶ Rank
- ▶ Trace, Determinant
- ▶ Inverse
- ▶ *etc*

R Basics

You should have been exposed to:

- ▶ R vector's, list's, data.frame's
- ▶ Subscripting and indexing (i.e. bracket notation)
- ▶ Writing functions: `function() {...}`
- ▶ Conditionals: `if {...} else {...}`
- ▶ Loops: `for`, `while`, `repeat`
- ▶ Graphics: `base`, `ggplot2`, etc
- ▶ Familiarity with RStudio

Same but different

Math Objects

- ▶ vector
- ▶ matrix

Same but different

Math Objects

- ▶ vector
- ▶ matrix

R objects

- ▶ vector
- ▶ matrix

Back to the (R) Basics

R Vectors

- ▶ A vector is the most basic data structure in R
- ▶ Vectors are contiguous cells containing data
- ▶ Can be of any length (including zero)
- ▶ There are really no scalars, just one-element vectors

Vectors

The most simple type of vectors are “scalars” or single values:

```
# integer
x <- 1L
# double (real)
y <- 5
# complex
z <- 3 + 5i
# logical
a <- TRUE
# character
b <- "yosemite"
```

although keep in mind that R does NOT really have scalars

Data modes (i.e. types)

- ▶ A **double** vector stores regular (i.e. real) numbers
- ▶ An **integer** vector stores integers (no decimal component)
- ▶ A **character** vector stores text
- ▶ A **logical** vector stores TRUE's and FALSE's values
- ▶ A **complex** vector stores complex numbers

Special Values

There are some special values

- ▶ NULL is the null object (it has length zero)
- ▶ Missing values are referred to by the symbol NA
(there are different modes of NA: logical, integer, etc)
- ▶ Inf indicates positive infinite
- ▶ -Inf indicates negative infinite
- ▶ NaN indicates Not a Number
(don't confuse NaN with NA)

Vectors

The function to create a vector from individual values is `c()`, short for *concatenate* or *combine*:

```
# some vectors
x <- c(1, 2, 3, 4, 5)

y <- c("one", "two", "three")

z <- c(TRUE, FALSE, FALSE)
```

Separate each element by a comma

Atomic Vectors

- ▶ vectors are **atomic** structures
- ▶ the values in a vector must be **ALL** of the same type
- ▶ either all integers, or reals, or complex, or characters, or logicals
- ▶ you cannot have a vector of different data types

Atomic Vectors

If you mix different data values, R will **implicitly coerce** them so they are all of the same type

```
# mixing numbers and characters
```

```
x <- c(1, 2, 3, "four", "five")
```

```
x
```

```
## [1] "1"      "2"      "3"      "four" "five"
```

```
# mixing numbers and logical values
```

```
y <- c(TRUE, FALSE, 3, 4)
```

```
y
```

```
## [1] 1 0 3 4
```

How does R coerce data types?

R follows two basic rules of implicit coercion

If a character is present, R will coerce everything else to characters

How does R coerce data types?

R follows two basic rules of implicit coercion

If a character is present, R will coerce everything else to characters

If a vector contains logicals and numbers, R will convert the logicals to numbers (TRUE to 1, FALSE to 0)

Properties of Vectors

- ▶ all vectors have a length
- ▶ vector elements can have associated names
- ▶ vectors are objects of class "vector"
- ▶ vectors have a mode (storage mode)

Vectorization

A vectorized computation is any computation that when applied to a vector operates on all of its elements

```
c(1, 2, 3) + c(3, 2, 1)
```

```
## [1] 4 4 4
```

```
c(1, 2, 3) * c(3, 2, 1)
```

```
## [1] 3 4 3
```

Recycling

When vectorized computations are applied, some problems may occur when dealing with two vectors of different length

```
c(1, 2, 3, 4) + c(1, 2)
```

```
## [1] 2 4 4 6
```

```
c(2, 1) + c(1, 2, 3)
```

```
## Warning in c(2, 1) + c(1, 2, 3): longer object length  
is not a multiple of shorter object length
```

```
## [1] 3 3 5
```

Recycling

The recycling rule can be very useful, like when operating between a vector and a “scalar”

```
x <- c(2, 4, 6, 8)
x + 3

## [1] 5 7 9 11
```


R Matrices and Arrays

From Vectors to Arrays

We can transform a vector in an **n-dimensional** array by giving it a dimensions attribute `dim`

```
# positive: from 1 to 8
```

```
x <- 1:8
```

```
# adding 'dim' attribute
```

```
dim(x) <- c(2, 4)
```

```
x
```

```
##      [,1] [,2] [,3] [,4]  
## [1,]    1    3    5    7  
## [2,]    2    4    6    8
```

From Vectors to Arrays

- ▶ a vector can be given a `dim` attribute (dimensions)
- ▶ a `dim` attribute is a numeric vector of length `n`
- ▶ R will reorganize the elements of the vector into `n` dimensions
- ▶ each dimension will have as many rows (or columns, etc.) as the `n`-th value of the `dim` vector

From Vectors to Arrays

```
# dim attribute with 3 dimensions
```

```
dim(x) <- c(2, 2, 2)
```

```
x
```

```
## , , 1
```

```
##
```

```
##      [,1] [,2]
```

```
## [1,]    1    3
```

```
## [2,]    2    4
```

```
##
```

```
## , , 2
```

```
##
```

```
##      [,1] [,2]
```

```
## [1,]    5    7
```

```
## [2,]    6    8
```

From Vector to Matrix

A dim attribute of length 2 will convert a vector into a matrix

```
# vector to matrix  
A <- 1:8  
class(A)  
  
## [1] "integer"  
  
dim(A) <- c(2, 4)  
class(A)  
  
## [1] "matrix" "array"
```

When using `dim()`, R always fills up each matrix by columns.

From Vector to Matrix

To have more control about how a matrix is filled, we use the `matrix()` function:

```
# vector to matrix (by rows)
a <- 1:8

A <- matrix(a, nrow = 2, ncol = 4)
A

##      [,1] [,2] [,3] [,4]
## [1,]    1    3    5    7
## [2,]    2    4    6    8
```

From Vector to Matrix

If you want to fill a matrix by rows use `byrow = TRUE`

```
# vector to matrix (by rows)
b <- 1:8

B <- matrix(b, nrow = 2, ncol = 4, byrow = TRUE)
B
```

##		[,1]	[,2]	[,3]	[,4]
##	[1,]	1	2	3	4
##	[2,]	5	6	7	8

More about R Matrices

- ▶ R stores matrices (and arrays in general) as vectors.
- ▶ Which means that matrices are also **atomic** structures.
- ▶ Matrices in R are stored column-major (i.e. by columns).
- ▶ This is like Fortran, Matlab, and Julia, but not like C or Python (e.g. numpy).

Matrix: Column-major

```
as.vector(A)
```

```
## [1] 1 2 3 4 5 6 7 8
```

```
as.vector(B)
```

```
## [1] 1 5 2 6 3 7 4 8
```

Matrices and Vectors in R

It is important to distinguish vectors and matrices, especially in R:

- ▶ In matrix algebra we use the convention that vectors are column vectors (i.e. they are $n \times 1$ matrices).
- ▶ In R, a vector with n elements is not the same as an $n \times 1$ matrix.
- ▶ Vectors in R behave more like “row vectors” (especially when displayed).
- ▶ However, depending on the type of functions you apply to vectors, sometimes R will handle vectors like if they were column vectors.

R common data structures

single data type

multiple data types

Vector

List

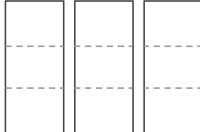
1D



Matrix

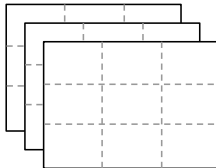
Data Frame

2D



Array

nD



Matrices vs Dataframes in R

It's also important to distinguish between matrices and `data.frames`:

- ▶ Both objects allow us to store data in a 2-dimensional object.
- ▶ In many cases, both R matrices and `data.frames` have similar behaviors.
- ▶ This is mostly the case when they are displayed on the screen.
- ▶ And sometimes it is hard to distinguish between a matrix and a `data.frame` by just looking at the displayed content on the screen.

Matrices vs Dataframes in R

- ▶ Dataframes are actually lists.
- ▶ Internally, a `data.frame` is stored as an R list (typically a list of vectors).
- ▶ This provides a very flexible way to manipulate `data.frames`, using the `$` operator, double brackets `[[]]`, and the regular `[,]`
- ▶ An R matrix is internally stored as a vector (with a `dim` attribute).
- ▶ Which means that you use the `[,]` operator.

Matrices vs Dataframes in R

Both matrices and data.frames have common methods

- ▶ bracket notation: `[,]`
- ▶ dimensions: `dim()`
- ▶ number of rows: `nrow()`
- ▶ number of columns: `ncol()`
- ▶ dim names: `dimnames()`
- ▶ names of columns: `colnames()`
- ▶ names of rows: `rownames()`
- ▶ apply functions: `apply()`

Notation System

Notation system to extract values from R objects

- ▶ to extract values use brackets: `[]`
- ▶ inside the brackets specify indices
- ▶ use as many indices as dimensions in the object
- ▶ each index is separated by comma
- ▶ indices can be numbers, logicals, or names

Elements-Extraction Notation System

object	notation	example
vector	[]	v[1:5]
factor	[]	g[1:5]
matrix	[,]	m[1:5, 1:3]
array	[, ,]	arr[1, 2, 3]
	[, , ,]	arr[1, 2, 3, 4]
list	[]	lst[3]
	[[]]	lst[[3]]
	\$	lst\$name
data frame	[,]	df[1, 2]
	\$	df\$name

Brackets, Parentheses, and Braces in R

Symbol	Use
[] brackets	Objects
() parentheses	Functions
{ } braces	Expressions

Basic Matrix Operations

Matrix Operations in R

We first quickly go through the basic matrix operations in R

- ▶ transpose
- ▶ addition
- ▶ scalar multiplication
- ▶ matrix-vector multiplication
- ▶ matrix-matrix multiplication

Matrix Transpose

The transpose of a $n \times p$ matrix \mathbf{X} is the $p \times n$ matrix \mathbf{X}^T . In R the transpose is given by the function `t()`

```
# matrix X
X <- matrix(1:6, 2, 3)
X
```

```
##      [,1] [,2] [,3]
## [1,]    1    3    5
## [2,]    2    4    6
```

```
# transpose of X
t(X)
```

```
##      [,1] [,2]
## [1,]    1    2
## [2,]    3    4
## [3,]    5    6
```

Matrix Addition

Matrix addition of two matrices $\mathbf{A} + \mathbf{B}$ is defined when \mathbf{A} and \mathbf{B} have the same dimensions:

```
A <- matrix(1:6, 2, 3)
```

```
B <- matrix(7:9, 2, 3)
```

```
A + B
```

```
##      [,1] [,2] [,3]  
## [1,]    8   12   13  
## [2,]   10   11   15
```

Scalar Multiplication

We can multiply a matrix by a scalar using the usual product operator `*`, moreover it doesn't matter if we pre-multiply or post-multiply:

```
X <- matrix(1:3, 3, 4)

# (pre)multiply X by 0.5
(1/2) * X

##      [,1] [,2] [,3] [,4]
## [1,]  0.5  0.5  0.5  0.5
## [2,]  1.0  1.0  1.0  1.0
## [3,]  1.5  1.5  1.5  1.5
```

Scalar Multiplication

You can also postmultiply by a scalar (although this is not recommended because may confuse readers):

```
X <- matrix(1:3, 3, 4)

# (post)multiply X by 0.5
X * (1/2)

##      [,1] [,2] [,3] [,4]
## [1,]  0.5  0.5  0.5  0.5
## [2,]  1.0  1.0  1.0  1.0
## [3,]  1.5  1.5  1.5  1.5
```

Matrix-Matrix Multiplication

The matrix product operator in R is `%*%`. We can multiply matrices **A** and **B** if the number of columns of **A** is equal to the number of rows of **B**

```
A <- matrix(1:6, 2, 3)
```

```
B <- matrix(7:9, 3, 2)
```

```
A %*% B
```

```
##      [,1] [,2]
```

```
## [1,]   76   76
```

```
## [2,]  100  100
```


Matrix-Matrix Multiplication

We can multiply matrices **A** and **B** if the number of columns of **A** is equal to the number of rows of **B**

```
A <- matrix(1:6, 2, 3)
```

```
B <- matrix(7:9, 3, 2)
```

```
B %*% A
```

```
##      [,1] [,2] [,3]  
## [1,]   21  49  77  
## [2,]   24  56  88  
## [3,]   27  63  99
```

Cross-Products

A very common type of products in multivariate data analysis are $\mathbf{X}^T\mathbf{X}$ and $\mathbf{X}\mathbf{X}^T$, sometimes known as cross-products:

```
# output with return()
# cross-product
t(A) %*% A
```

```
##      [,1] [,2] [,3]
## [1,]    5  11  17
## [2,]   11  25  39
## [3,]   17  39  61
```

```
# cross-product
A %*% t(A)
```

```
##      [,1] [,2]
## [1,]   35  44
## [2,]   44  56
```

Cross-Products

R provides functions `crossprod()` and `tcrossprod()` which are formally equivalent to:

- ▶ $\text{crossprod}(X, X) \equiv t(X) \%*\% X$

- ▶ $\text{tcrossprod}(X, X) \equiv X \%*\% t(X)$

However, `crossprod()` and `tcrossprod()` are usually faster than using `t()` and `%*%`

Matrix-Vector Multiplication

We can post-multiply an $n \times p$ matrix \mathbf{X} with a vector \mathbf{b} with p elements. This means making linear combinations (weighted sums) of the columns of \mathbf{X} :

```
X <- matrix(1:12, 3, 4)
b <- seq(0.25, 1, by = 0.25)
X %*% b
```

```
##      [,1]
## [1,] 17.5
## [2,] 20.0
## [3,] 22.5
```

Vector-Matrix Multiplication

In R we can pre-multiply a vector \mathbf{a} (with n elements) with an $n \times p$ matrix \mathbf{X} . This means making linear combinations (weighted sums) of the rows of \mathbf{X} :

```
X <- matrix(1:12, 3, 4)
a <- 1:3
a %*% X

##      [,1] [,2] [,3] [,4]
## [1,]   14   32   50   68
```

Note about `%*%`

Notice that when we use the product operator `%*%`, R is smart enough to use the convention that vectors are $n \times 1$ matrices. Notice also that if we ask for a vector-matrix multiplication, we can use both formulas:

- ▶ `a %*% X`
- ▶ `t(a) %*% X`

R will reformat the n vector as an $n \times 1$ matrix first.

Other Functions

Here are some other interesting functions for matrices

- ▶ `det()`: determinant
- ▶ `diag()`: extract or replace the diagonal elements
- ▶ `solve()`: solve system of equations
- ▶ `svd()`: singular value decomposition
- ▶ `eigen()`: eigen-decomposition
- ▶ `qr()`: QR decomposition