Lab 2: Matrix Decompositions

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Introduction

In this lab you will be working with the functions svd() and eigen() to perform singular value decomposition, and eigenvalue decomposition, respectively.

In addition, you will have to write code in R to implement the Power Method, which is a basic procedure to obtain the dominant eigenvector (and related eigenvalue) of a square matrix.

The content of this lab will introduce you to a series of concepts and computations that will constantly emerge throughout the course. So it makes more sense to start learning first about these two fundamental decompositions (SVD & EVD) before tackling any of the statistical learning tasks (both supervised and unsupervised).

Data USArrests

In this lab we are going to use the data set USArrests that comes in R—see ?USArrests for more information. This data set is about "Violent Crime Rates by US State", and contains statistics, in arrests per 100,000 residents for assault, murder, and rape in each of the 50 US states in 1973. Also given is the percent of the population living in urban areas.

head(USArrests)

##		Murder	Assault	UrbanPop	Rape
##	Alabama	13.2	236	58	21.2
##	Alaska	10.0	263	48	44.5
##	Arizona	8.1	294	80	31.0
##	Arkansas	8.8	190	50	19.5
##	California	9.0	276	91	40.6
##	Colorado	7.9	204	78	38.7

The four variables are:

- Murder: numeric Murder arrests (per 100,000)
- Assault: numeric Assault arrests (per 100,000)
- UrbanPop: numeric Percent urban population
- Rape: numeric Rape arrests (per 100,000)

Singular Value Decomposition

Let **M** be an $n \times p$ matrix of full column-rank p (assume n > p). The singular value decomposition (SVD) of **M** is given by:

$$\mathbf{M} = \mathbf{U}\mathbf{D}\mathbf{V}^\mathsf{T}$$

where:

- U is an $n \times p$ matrix of left singular vectors
- **D** is a $p \times p$ diagonal matrix of singular values
- V is a $p \times p$ matrix of right singular vectors

Function svd()

R provides the function svd() that allows you to compute the SVD of any rectangular matrix. Here's a basic example with USArrests:

```
SVD <- svd(USArrests)
```

The default output of svd() is a list with three elements:

- u: matrix of left singular vectors
- v: matrix of right singular vectors
- d: vector of singular values

You can use the arguments nu and nv to have more control over the behavior of svd():

- nu: the number of left singular vectors to be computed.
- nv: the number of right singular vectors to be computed.

SVD on raw data

- Use svd() to compute the SVD of USArrests
- Take the output of svd() and create the matrices U, D, and V
- Confirm that the data of USArrests can be obtained as the product of: UDV

SVD and best Rank-one Approximations

As we saw in lecture, one of the most attractive uses of the SVD is that it allows you to decompose a matrix \mathbf{M} as a sum of rank-one matrices of the form: $l_k \mathbf{u_k} \mathbf{v_k}^\mathsf{T}$. This is the result of the famous Eckart-Young-Mirsky theorem, which says that the best rank r approximation to \mathbf{X} is given by:

$$\mathbf{X_r} = \sum_{k=1}^r l_k \mathbf{u_k} \mathbf{v_k}^\mathsf{T}$$

where l_k is the k-th singular vector, that is, the k-th diagonal element in **D**.

Consequently, the best r = 2 rank approximation to **X** is:

$$\mathbf{X_2} = l_1 \mathbf{u_1} \mathbf{v_1}^\mathsf{T} + l_2 \mathbf{u_2} \mathbf{v_2}^\mathsf{T}$$

In other words, $\mathbf{u_1}$, and $\mathbf{u_2}$ form the best 2-dimensional approximation of the objects in \mathbf{X} (living a p-dim space).

Your turn

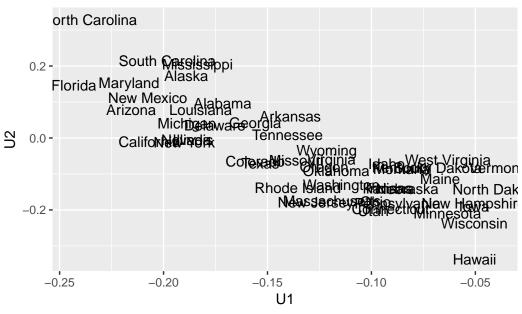
- Confirm that the sum: $\sum_{k=1}^4 l_h \mathbf{u_k} \mathbf{v_k^T}$ equals USArrests
- Create a new variable (vector) MA by adding Murder + Assault
- Create a new data.frame Arrests2 with the variables Murder, Assault, UrbanPop, Rape, and MA.
- Compute the SVD of Arrests2
- How does the singular values of USArrests compare to those of Arrests2?
- What is the rank of Arrests2?

Lab continues on next page

Using SVD output to visualize data

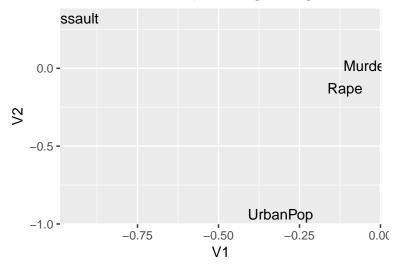
Knowing that we can approximate USArrests with $l_1\mathbf{u_1}\mathbf{v_1}^\mathsf{T} + l_2\mathbf{u_2}\mathbf{v_2}^\mathsf{T}$, use $\mathbf{u_1}$ and $\mathbf{u_2}$ to visualize the States with a simple scatterplot. Create your own scatterplot like the one below:

Plot of States (first 2 left singular vectors)



In the same way, use the first two right singular vectors of \mathbf{V} to graph a scatterplot (e.g. 2-dimensional representation) of the variables:

Plot of Variables (first 2 right singular vecto



Later in the course, we will see how to get—and interpret—better visualizations (based on some kind of SVD or EVD factorization).

Eigenvalue Decomposition

R provides the function eigen() to compute the spectral decomposition—better known as eigenvalue decomposition—of a square matrix.

For multivariate analysis and statistical learning techniques, the typical square matrices are some variation of the sum-of-squares and cross-products: $\mathbf{X}^\mathsf{T}\mathbf{X}$ and $\mathbf{X}\mathbf{X}^\mathsf{T}$. For instance, assuming that variables in \mathbf{X} are standardized (mean = 0, var = 1), the (sample) correlation matrix \mathbf{R} is based on the product $\mathbf{X}^\mathsf{T}\mathbf{X}$, that is: $\mathbf{R} = \frac{1}{n-1}\mathbf{X}^\mathsf{T}\mathbf{X}$,.

```
R <- cor(USArrests)
```

The output of eigen() is a list of two elements, values and vectors.

```
# EVD of correlation matrix
evd <- eigen(R)</pre>
```

You can be more specific and use the argument symmetric = TRUE to indicate that the input matrix is symmetric (and don't let R guess it by itself):

```
evd <- eigen(R, symmetric = TRUE)</pre>
```

If you need only the eigenvalues you can use the parameter only.values = TRUE:

```
eigenvalues <- eigen(R, symmetric = TRUE, only.values = TRUE)
eigenvalues</pre>
```

```
## $values
## [1] 2.4802416 0.9897652 0.3565632 0.1734301
##
## $vectors
## NULL
```

Inverse of covariance matrix

- Without using scale(), compute a matrix X as the mean-centered data of USArrests.
- Calculate the sum-of-squares and cross-products matrix $S = X^TX$
- **S** is proportional to the (sample) covariance matrix $\frac{1}{n-1}\mathbf{X}^{\mathsf{T}}\mathbf{X}$. Confirm that $\mathsf{cov}(\mathsf{X})$ is equal to $\frac{1}{n-1}\mathbf{X}^{\mathsf{T}}\mathbf{X}$.
- Use solve() to compute the inverse S^{-1}
- Use eigen() to compute the EVD of $S = V\Lambda V^{\mathsf{T}}$
- Confirm that \mathbf{S}^{-1} can also be obtained as: $\mathbf{V} \mathbf{\Lambda}^{-1} \mathbf{V}^{\mathsf{T}}$

```
# mean-centered matrix X
means <- colMeans(USArrests)
X <- as.matrix(sweep(USArrests, 2, means, FUN = "-"))</pre>
```

```
# minor product moment XtX
S \leftarrow t(X) \% \% X
# covariance matrix
n <- nrow(USArrests)</pre>
(1/(n-1)) * S
##
                Murder
                          Assault
                                    UrbanPop
                                                   Rape
## Murder
             18.970465
                        291.0624
                                    4.386204
                                              22.99141
## Assault
            291.062367 6945.1657 312.275102 519.26906
## UrbanPop
              4.386204
                        312.2751 209.518776
                                               55.76808
## Rape
             22.991412
                         519.2691
                                   55.768082
                                               87.72916
cov(USArrests)
##
                Murder
                                    UrbanPop
                          Assault
                                                   Rape
## Murder
             18.970465
                        291.0624
                                    4.386204
                                              22.99141
## Assault
            291.062367 6945.1657 312.275102 519.26906
## UrbanPop
              4.386204
                         312.2751 209.518776
                                               55.76808
                                  55.768082
## Rape
             22.991412
                         519.2691
                                              87.72916
# inverse of S via solve()
Sinv <- solve(S)
# inverse of S via EVD
S evd <- eigen(S)
Vs <- S evd$vectors
Ls <- diag(1/S_evd$values)
Vs %*% Ls %*% t(Vs)
##
                                [,2]
                  [,1]
                                               [,3]
                                                              [,4]
## [1,] 0.0032804923 -1.304887e-04
                                     1.794220e-04 -2.014203e-04
## [2,] -0.0001304887 1.046419e-05 -6.597122e-06 -2.354634e-05
## [3,] 0.0001794220 -6.597122e-06 1.271111e-04 -8.877578e-05
## [4,] -0.0002014203 -2.354634e-05 -8.877578e-05 4.812179e-04
```

Power Method

The **Power Method** is an iterative procedure for approximating eigenvalues.

First assume that the matrix **A** has a dominant eigenvalue with corresponding dominant eigenvector. Then choose an initial approximation \mathbf{w}_0 (must be a non-zero vector) of one of the dominant eigenvectors. This choice is arbitrary (and in theory should work with almost any vector). Then, form the sequence $\mathbf{w}_1, \mathbf{w}_2, \dots, \mathbf{w}_k$, given by:

$$\mathbf{w}_1 = \mathbf{A}\mathbf{w}_0$$

$$\mathbf{w}_2 = \mathbf{A}\mathbf{w}_1 = \mathbf{A}^2\mathbf{w}_0$$

$$\mathbf{w}_3 = \mathbf{A}\mathbf{w}_2 = \mathbf{A}^3\mathbf{w}_0$$

$$\vdots$$

$$\mathbf{w}_k = \mathbf{A}\mathbf{w}_{k-1} = \mathbf{A}^{k-1}\mathbf{w}_0$$

For large powers of k, and by **properly scaling** this sequence, you will see that you obtain a good approximation \mathbf{w}_k of the dominant eigenvector of \mathbf{A} .

Here's an example. Consider the following matrix

$$\mathbf{A} = \begin{pmatrix} 2 & -12 \\ 1 & -5 \end{pmatrix}$$

Let's start with an initial nonzero vector \mathbf{w}_0

$$\mathbf{w}_0 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

In R, we create **A** and \mathbf{w}_0

[,1]

[1,] -10

```
# square matrix
A <- matrix(c(2, 1, -12, -5), nrow = 2, ncol = 2)
# starting vector
w0 <- c(1, 1)</pre>
```

Let's see what happens in the first four iterations:

```
w_old <- w0

for (k in 1:4) {
    w_new <- A %*% w_old
    print(paste('iteration =', k))
    print(w_new)
    cat("\n")
    # update w_old
    w_old <- w_new
}

## [1] "iteration = 1"</pre>
```

```
## [2,]
           -4
##
  [1] "iteration = 2"
##
         [,1]
           28
## [1,]
## [2,]
           10
##
   [1] "iteration = 3"
         [,1]
##
   [1,]
          -64
##
## [2,]
         -22
##
## [1] "iteration = 4"
##
         [,1]
## [1,]
          136
## [2,]
           46
```

Note that the obtained vectors seem to be very different from one another. However, the difference is in the scale. This is why the part "properly scaling" is very important. How do you scale \mathbf{w}_k ? Well, there are different options, but probably the simplest one is by using the L_{∞} -norm.

Reminder of L_p -norms:

• L_1 -norm: $\sum_{i=1}^n |w_i|$

• L_2 -norm: $\sqrt{\sum_{i=1}^n (w_i)^2}$

• L_{∞} -norm: $max\{|w_1|,\ldots,|w_n|\}$

• L_p -norm: $(\sum_{i=1}^n |w_i|^p)^{1/p}$

Description of Power Method

Here is the procedure of the Power Method to find the largest eigenvalue and its corresponding eigenvector. Write code in R to implement such method.

- 1. Start with an arbitrary vector \mathbf{w}_0
- 2. Iteration for a series of steps $k = 0, 1, 2, \dots, n$ to form the series of \mathbf{w}_k vectors:

$$\mathbf{w}_{k+1} = \frac{\mathbf{A}\mathbf{w}_k}{s_{k+1}}$$

where s_{k+1} is the entry of $\mathbf{A}\mathbf{w}_k$ which has the largest absolute value (this is actually a scaling operation dividing by the L_{∞} -norm).

3. When the scaling factors s_k are not changing much, s_{k+1} will be close to the largest eigenvalue of \mathbf{A} , and \mathbf{w}_{k+1} will be close to the eigenvector associated to s_{k+1} .

4. You can also veirfy that s_{k+1} will be very close to the eigenvalue given by the Rayleigh quotient:

$$\lambda pprox rac{\mathbf{w}_{k+1}^\mathsf{T} \mathbf{A} \mathbf{w}_{k+1}}{\mathbf{w}_{k+1}^\mathsf{T} \mathbf{w}_{k+1}}$$

Your turn: Implement the power method to find the largest eigenvalue of the following matrix:

$$\mathbf{A} = \begin{pmatrix} 5 & -14 & 11 \\ -4 & 4 & -4 \\ 3 & 6 & -3 \end{pmatrix}$$

Compare your results with those provided by eigen(). Keep in mind that the eigenvectors of eigen() have unit Euclidean norm (i.e. L_2 -norm). Likewise, recall that the eigenvectors are only defined up to a constant: even when the length is specified they are still only defined up to a scalar.

Other scaling options

The scaling step in the power method:

$$\mathbf{w}_{k+1} = \frac{\mathbf{A}\mathbf{w}_k}{s_{k+1}}$$

involves choosing a value for s_{k+1} . One option for s_{k+1} is the entry of $\mathbf{A}\mathbf{w}_k$ with the largest absolute value (i.e. L_{∞} -norm). But you can actually use other scaling strategies. For instance, you can use the L_1 -norm or the L_2 -norm.

Modify your code to use any other L_p -norm in the power algorithm, and confirm that you get the same dominant eigenvectors and eigenvalues.

Deflation and more eigenvectors

In order to get more eigenvectors and eigenvalues, you need to apply the Power Method on the residual matrix obtained by **deflating A** with respect to the first eigenvector. This deflation operation is:

$$\mathbf{A}_1 = \mathbf{A} - \lambda_1 \mathbf{v}_1 \mathbf{v}_1^\mathsf{T}$$

where λ_1 is the first eigenvalue and \mathbf{v}_1 is the corresponding eigenvalue.

Deflate the matrix A and apply the power method on A_1 to obtain more eigenvalues and eigenvectors.

```
## @knitr matrix A2
# square matrix
A <- cbind(
  c(5, 1),
  c(1, 5)
## @knitr power method
# 1) dividing by L-max norm
set.seed(123)
w_old <- rnorm(2)</pre>
crit <- 1
iteration <- 1
while (crit > 1e-9 & iteration <= 50) {
  w new <- A %*% w old
  # scaling to L-max norm
  w norm <- max(abs(w new))</pre>
  w_new <- w_new / w_norm</pre>
  # check convergence
  w diff <- abs(w old) - abs(w new)
  crit <- max(abs(w_diff))</pre>
  # print
  print(paste('iteration', iteration))
  print(paste('crit =', crit))
  print(w new)
  cat("\n")
  # next iteration
  iteration <- iteration + 1
  w_old <- w_new
}
## [1] "iteration 1"
## [1] "crit = 0.439524353447787"
## [1,] -1.0000000
## [2,] -0.5643303
## [1] "iteration 2"
## [1] "crit = 0.12248218028062"
               [,1]
## [1,] -1.0000000
```

```
## [2,] -0.6868125
##
## [1] "iteration 3"
## [1] "crit = 0.0928971391706254"
##
             [,1]
## [1,] -1.0000000
## [2,] -0.7797096
##
## [1] "iteration 4"
## [1] "crit = 0.0678326296513324"
             [,1]
## [1,] -1.0000000
## [2,] -0.8475423
##
## [1] "iteration 5"
## [1] "crit = 0.0481693190480987"
              [,1]
## [1,] -1.000000
## [2,] -0.8957116
##
## [1] "iteration 6"
## [1] "crit = 0.0335329800806962"
              [,1]
## [1,] -1.000000
## [2,] -0.9292446
##
## [1] "iteration 7"
## [1] "crit = 0.0230222518427066"
              [,1]
## [1,] -1.0000000
## [2,] -0.9522668
## [1] "iteration 8"
## [1] "crit = 0.015655872977308"
              [,1]
##
## [1,] -1.000000
## [2,] -0.9679227
##
## [1] "iteration 9"
## [1] "crit = 0.0105774980352772"
              [,1]
##
## [1,] -1.000000
## [2,] -0.9785002
##
## [1] "iteration 10"
```

```
## [1] "crit = 0.00711506318363009"
## [1,] -1.0000000
## [2,] -0.9856152
##
## [1] "iteration 11"
## [1] "crit = 0.00477187391452161"
             [,1]
## [1,] -1.0000000
## [2,] -0.9903871
## [1] "iteration 12"
## [1] "crit = 0.00319401180338807"
              [,1]
## [1,] -1.0000000
## [2,] -0.9935811
## [1] "iteration 13"
## [1] "crit = 0.00213504229144956"
              [,1]
## [1,] -1.000000
## [2,] -0.9957162
##
## [1] "iteration 14"
## [1] "crit = 0.00142590394429798"
              [,1]
## [1,] -1.0000000
## [2,] -0.9971421
##
## [1] "iteration 15"
## [1] "crit = 0.000951735150284683"
              [,1]
## [1,] -1.000000
## [2,] -0.9980938
##
## [1] "iteration 16"
## [1] "crit = 0.000634994202567407"
##
              [,1]
## [1,] -1.0000000
## [2,] -0.9987288
##
## [1] "iteration 17"
## [1] "crit = 0.000423553739399063"
##
              [,1]
## [1,] -1.000000
```

```
## [2,] -0.9991524
##
## [1] "iteration 18"
## [1] "crit = 0.00028246890250605"
##
             [,1]
## [1,] -1.000000
## [2,] -0.9994348
##
## [1] "iteration 19"
## [1] "crit = 0.000188356951687951"
             [,1]
## [1,] -1.0000000
## [2,] -0.9996232
##
## [1] "iteration 20"
## [1] "crit = 0.000125591018124593"
              [,1]
## [1,] -1.000000
## [2,] -0.9997488
##
## [1] "iteration 21"
## [1] "crit = 8.37361102701273e-05"
              [,1]
## [1,] -1.000000
## [2,] -0.9998325
##
## [1] "iteration 22"
## [1] "crit = 5.58279695207498e-05"
              [,1]
## [1,] -1.0000000
## [2,] -0.9998883
## [1] "iteration 23"
## [1] "crit = 3.72203780588665e-05"
##
              [,1]
## [1,] -1.000000
## [2,] -0.9999256
##
## [1] "iteration 24"
## [1] "crit = 2.48143550675151e-05"
              [,1]
##
## [1,] -1.000000
## [2,] -0.9999504
##
## [1] "iteration 25"
```

```
## [1] "crit = 1.65432454786174e-05"
##
## [1,] -1.0000000
## [2,] -0.9999669
##
## [1] "iteration 26"
## [1] "crit = 1.10289823674892e-05"
             [,1]
## [1,] -1.0000000
## [2,] -0.9999779
##
## [1] "iteration 27"
## [1] "crit = 7.35272249008379e-06"
              [,1]
## [1,] -1.000000
## [2,] -0.9999853
## [1] "iteration 28"
## [1] "crit = 4.90184502843771e-06"
              [,1]
## [1,] -1.000000
## [2,] -0.9999902
##
## [1] "iteration 29"
## [1] "crit = 3.26791003457672e-06"
              [,1]
## [1,] -1.0000000
## [2,] -0.9999935
##
## [1] "iteration 30"
## [1] "crit = 2.17861262286068e-06"
              [,1]
## [1,] -1.000000
## [2,] -0.999956
##
## [1] "iteration 31"
## [1] "crit = 1.45241105198313e-06"
##
              [,1]
## [1,] -1.0000000
## [2,] -0.9999971
##
## [1] "iteration 32"
## [1] "crit = 9.68275206680858e-07"
##
              [,1]
## [1,] -1.000000
```

```
## [2,] -0.9999981
##
## [1] "iteration 33"
## [1] "crit = 6.45517325370548e-07"
##
             [,1]
## [1,] -1.000000
## [2,] -0.9999987
##
## [1] "iteration 34"
## [1] "crit = 4.30345114876829e-07"
             [,1]
## [1,] -1.0000000
## [2,] -0.9999991
##
## [1] "iteration 35"
## [1] "crit = 2.86896846168894e-07"
              [,1]
## [1,] -1.000000
## [2,] -0.9999994
##
## [1] "iteration 36"
## [1] "crit = 1.91264609927799e-07"
              [,1]
## [1,] -1.000000
## [2,] -0.9999996
##
## [1] "iteration 37"
## [1] "crit = 1.27509760305955e-07"
              [,1]
## [1,] -1.0000000
## [2,] -0.9999997
## [1] "iteration 38"
## [1] "crit = 8.50065158264357e-08"
##
              [,1]
## [1,] -1.000000
## [2,] -0.999998
##
## [1] "iteration 39"
## [1] "crit = 5.667101454776e-08"
              [,1]
##
## [1,] -1.000000
## [2,] -0.9999999
##
## [1] "iteration 40"
```

```
## [1] "crit = 3.77806781415302e-08"
## [1,] -1.0000000
## [2,] -0.9999999
##
## [1] "iteration 41"
## [1] "crit = 2.51871196121911e-08"
        [,1]
## [1,] -1.0000000
## [2,] -0.999999
##
## [1] "iteration 42"
## [1] "crit = 1.67914133708535e-08"
## [,1]
## [1,] -1
## [2,] -1
##
## [1] "iteration 43"
## [1] "crit = 1.11942758396211e-08"
## [,1]
## [1,] -1
## [2,] -1
##
## [1] "iteration 44"
## [1] "crit = 7.46285055974738e-09"
## [,1]
## [1,] -1
## [2,] -1
##
## [1] "iteration 45"
## [1] "crit = 4.97523378051312e-09"
## [,1]
## [1,] -1
## [2,] -1
##
## [1] "iteration 46"
## [1] "crit = 3.31682248333465e-09"
## [,1]
## [1,] -1
## [2,] -1
##
## [1] "iteration 47"
## [1] "crit = 2.21121498888976e-09"
## [,1]
## [1,] -1
```

```
## [2,] -1
##
## [1] "iteration 48"
## [1] "crit = 1.47414347395625e-09"
##
       [,1]
## [1,] -1
## [2,] -1
##
## [1] "iteration 49"
## [1] "crit = 9.82762315970831e-10"
        [,1]
## [1,] -1
## [2,] -1
## @knitr eigenvalue
# scaling factor(i.e. the norm) is close to eigenvalue
w_norm
## [1] 6
# eigenvalue with Rayleigh quotient
sum(w_new * (A %*% w_new)) / sum(w_new*w_new)
## [1] 6
w_1 <- w_new / sqrt(sum(w_new^2))</pre>
w_1
##
               [,1]
## [1,] -0.7071068
## [2,] -0.7071068
## @knitr deflation
A1 \leftarrow A - w_norm * (w_1 %*% t(w_1))
set.seed(123)
w_old <- rnorm(2)</pre>
crit <- 1
iteration <- 1
while (crit > 1e-9 & iteration <= 50) {
  w new <- A1 %*% w old
  # scaling to L-max norm
  w_norm <- max(abs(w_new))</pre>
  w_new <- w_new / w_norm</pre>
  # check convergence
```

```
w diff <- abs(w old) - abs(w new)</pre>
  crit <- max(abs(w diff))</pre>
  # print
  print(paste('iteration', iteration))
  print(paste('crit =', crit))
  print(w new)
  cat("\n")
  # next iteration
  iteration <- iteration + 1
  w_old <- w_new
}
## [1] "iteration 1"
## [1] "crit = 0.769822509936266"
## [,1]
## [1,] -1
## [2,] 1
##
## [1] "iteration 2"
## [1] "crit = 2.94828650382328e-09"
      [,1]
## [1,] -1
## [2,] 1
##
## [1] "iteration 3"
## [1] "crit = 0"
##
       [,1]
## [1,] -1
## [2,]
w new / sqrt(sum(w new^2))
              [,1]
##
## [1,] -0.7071068
## [2,] 0.7071068
eigen(A)
## eigen() decomposition
## $values
## [1] 6 4
##
## $vectors
##
             [,1]
                        [,2]
## [1,] 0.7071068 -0.7071068
## [2,] 0.7071068 0.7071068
```