Eigenvalues and Eigenvectors

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http://github.com/thsis/NIS18

Agenda

PCA

- ⊡ The iris dataset is already linearly separable.

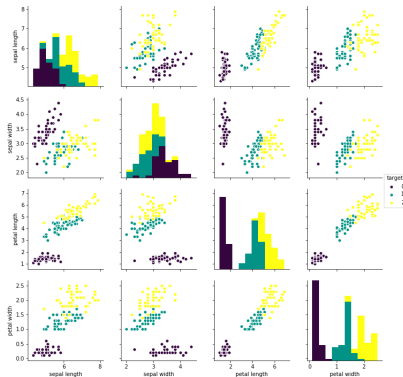- ⊡ With various techniques we can show this in even more detail.

Figure 1: Iris Pairplot

PCA

⊡ objective:

$$\max \ \delta' Var(X) \delta \ s.t. \ \sum \delta_i^2 = 1. \quad (1)$$

where $X \in \mathbb{R}^{n \times m}; m, n \in \mathbb{N}; \delta \in \mathbb{R}^m$

⊡ solution ▸Proof :

$$Y = \Gamma'(X - \mu) \quad (2)$$

where $Y \in \mathbb{R}^{n \times m}$ is the matrix of rotations, $\Gamma \in \mathbb{R}^{m \times m}$ is the matrix of eigenvectors, $\mu \in \mathbb{R}^m$ is the vector of sample means.
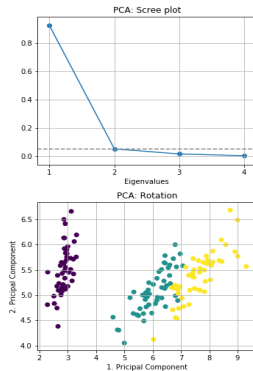

Figure 2: Iris PCA

LDA

⊡ objective:

$$max \ \frac{w' S_B w}{w' S_W w},$$ (3)

where

$$S_B = \sum_{c}^{C} (\mu_c - \mu)(\mu_c - \mu)',$$

$$S_W = \sum_{c}^{C} \sum_{i=1}^{n} (x_i - \mu_c)(x_i - \mu_c)'$$

and $x_i \in \mathbb{R}^m$, μ_c is the vector of class means.

LDA

▫ solution ▸Proof :

$$S_B^{-\frac{1}{2}} S_W^{-1} S_B^{-\frac{1}{2}} w = \lambda w \qquad (4)$$

where this is again an Eigenvalue
problem and it's solution will provide
the rotation that ensures the largest
possible (linear) separability.

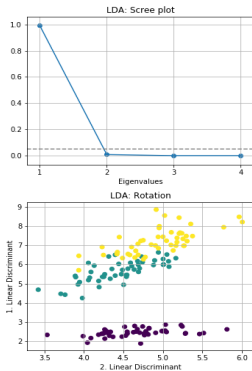▫ Now how do we get the Eigenvalues?

Figure 3: Iris LDA

Eigenvalue

If A is an $n \times n$ matrix, v is a non-zero vector and λ is a scalar, such that

$$Av = \lambda v \qquad (5)$$

then v is called an *eigenvector* and λ is called an *eigenvalue* of the matrix A. An eigenvalue of A is a root of the characteristic equation,

$$det\,(A - \lambda I) = 0 \qquad (6)$$

The characteristic polynomial

Consider the polynomial

$$f(\lambda) = \lambda^p + a_{p-1}\lambda^{p-1} + \cdots + a_1\lambda + a_0 \tag{7}$$

We now construct a matrix $A \in \mathbb{R}^{n \times n}$ such that the eigenvalues of A are the roots of the polynomial $f(\lambda)$ ▸ Example :

$$A = \begin{bmatrix} 0 & 1 & 0 & \ldots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ & & & \ddots & \\ 0 & 0 & 0 & \ldots & 1 \\ -a_0 & -a_1 & -a_2 & \ldots & -a_{p-1} \end{bmatrix} \tag{8}$$

General Idea

What are the eigenvalues of X_1 and X_2?

$$X_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 3 & 0 \\ 0 & 0 & 0 & 4 \end{bmatrix} \quad X_2 = \begin{bmatrix} 2.297 & -0.461 & -0.459 & 0.225 \\ -0.461 & 1.4 & -0.097 & -0.829 \\ -0.459 & -0.097 & 2.672 & 0.224 \\ 0.225 & -0.829 & 0.224 & 3.631 \end{bmatrix}$$

Similarity Transformations

Two $n \times n$ matrices A and B, are said to be *similar* if there exists a nonsingular matrix P such that

$$A = P^{-1}BP \tag{9}$$

If the two matrices A and B are similar, then they also share the same eigenvalues. ▶ Proof

Householder Reflections

Let u and v be orthonormal vectors and let x be a vector in the space spanned by u and v, such that

$$x = c_1 u + c_2 + v$$

for some scalars c_1 and c_2. The vector

$$\tilde{x} = -c_1 u + c_2 v$$

is a *reflection* of x through the line difined by the vector u. Now consider the matrix

$$Q = I - 2uu'. \tag{10}$$

Note that ▸Proof :

$$Qx = \tilde{x}$$

Householder Reflections

We will use Householder-Reflections to tranform a vector

$$a = (a_1, \ldots, a_n)$$

into

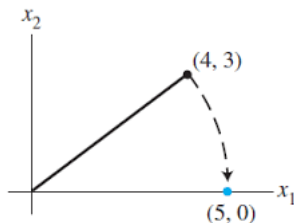$$\hat{a} = (\hat{a}_1, 0, \ldots, 0)$$

Givens Rotations

Using orthogonal transformations we can also rotate a vector in such a way that a specified element becomes 0 and only one other element in the vector is changed.

where the entries in the pth and q^{th} rows and columns are

$$\cos\theta = \frac{x_p}{||x||}$$

A Givens rotation in $\mathbb{R}^2$.

Givens Rotations

$$
V_{pq}(\theta) =
\begin{bmatrix}
1 & & & & & & & & \\
& \ddots & & & & & & & \\
& & 1 & & & & & & \\
& & & \cos\theta & & \sin\theta & & & \\
& & & & \ddots & & & & \\
& & & -\sin\theta & & \cos\theta & & & \\
& & & & & & 1 & & \\
& & & & & & & \ddots & \\
& & & & & & & & 1
\end{bmatrix}
\tag{11}
$$

Jacobi Method

The Jacobi method for determining the eigenvalues of a symmetric matrix A uses a sequence of orthogonal similarity transformations that result in the transformation:

$$A = P \Lambda P^{-1}$$

or rather:

$$\Lambda = P^{-1} A P$$

where we use Givens Rotations to obtain P. The Jacobi iteration is:

$$A^k = V_{p_k q_k}(\theta_k) A^{k-1} V_{p_k q_k}(\theta_k) \tag{12}$$

The Jacobi Method is of $O(n^3)$

Jacobi-Method

Algorithm 1 `jacobi`

Require: symmetric matrix A
Ensure: $0 < precision < 1$
  initialize: $L \leftarrow A$; $U \leftarrow I$; $L_{max} \leftarrow 1$
  while $L_{max} > precision$ **do**
    Find indices i, j of largest value in lower triangle of $abs(L)$
    $L_{max} \leftarrow L_{i,j}$
    $\alpha \leftarrow \frac{1}{2} \cdot \arctan(\frac{2A_{i,j}}{A_{i,i} - A_{j,j}})$
    $V \leftarrow I$
    $V_{i,i}, V_{j,j} \leftarrow \cos\alpha$; $V_{i,j}, V_{j,i} \leftarrow -\sin\alpha, \sin\alpha$
    $A \leftarrow V'AV$; $U \leftarrow UV$
  return $diag(A), U$

QR-Method

The QR-Method is the most common algorithm for obtaining
eigenvalues and eigenvectors of a matrix A. It relies on the so
called QR-Factorization:

$$A = QR, \tag{13}$$

where Q is orthogonal and R is upper triangular.
The QR iteration is:

$$A^k = Q'_{k-1} A_{k-1} Q_{k-1} = RQ \tag{14}$$

The QR Method is of $O(n^3)$

Basic QR-Method

Algorithm 2 QRM1

Require: square matrix A
  initialize: $conv \leftarrow False$
  while not $conv$ **do**
      $Q, R \leftarrow$ QR-Factorization of A
      $A \leftarrow RQ$
      if A is diagonal **then**
          $conv \leftarrow$ True

  return $diag\,(A)\,, Q$

Refined QR-Method

For faster convergence it is common to convert the matrix first into a so called upper Hessenberg form.

$$\begin{bmatrix} X & X & X & X & X & X & X \\ X & X & X & X & X & X & X \\ 0 & X & X & X & X & X & X \\ 0 & 0 & X & X & X & X & X \\ 0 & 0 & 0 & X & X & X & X \\ 0 & 0 & 0 & 0 & X & X & X \\ 0 & 0 & 0 & 0 & 0 & X & X \end{bmatrix}$$

Algorithm 3 QRM2
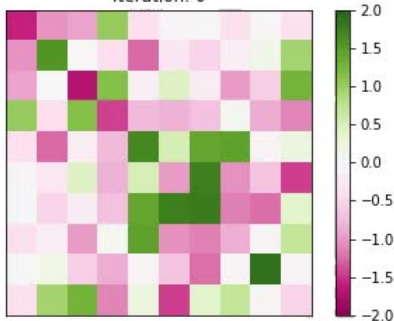

Require: square matrix A
  $A \leftarrow$ hessenberg(A)
  continue with: QRM1(A)

QRM2 Visualized

Demonstrate QR-Method on a 10x10 matrix
Iteration: 0

QR-Method

Accelerated QR-Method

We can accelerate the QR-Method by creating an artificial zero on
the main diagonal of A^ks Hessenberg form T at an iteration step k:

$$T^\star = T - t_{p-1,p-1}I$$
$$T^\star = QR$$
$$T = T^\star + t_{p-1,p-1}I$$

Accelerated QR-Method

Require: square matrix $A \in \mathbb{R}^{p \times p}$
  $T \leftarrow \texttt{hessenberg}(A)$, $conv \leftarrow False$
  while not $conv$ **do**
    $Q, R \leftarrow$ QR-Factorization of $T - t_{p-1,p-1}I$
    $T \leftarrow RQ + t_{p-1,p-1}I$
    if T is diagonal **then**
      $conv \leftarrow True$
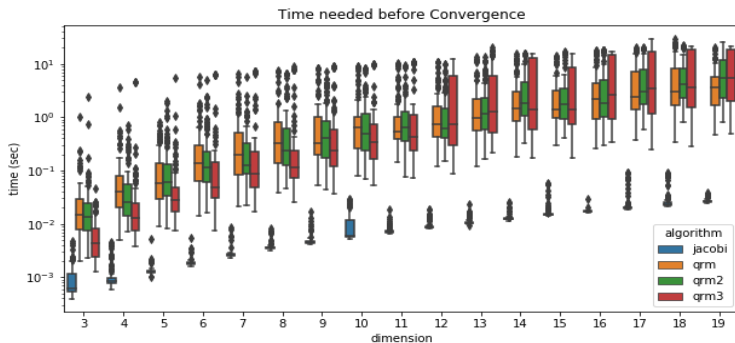 **return** $diag\,(T), Q$

Unit tests - Idea

1. Construct a $p \times p$ matrix, with known Eigenvalues $\lambda_{true} \in \mathbb{R}^p$. To do this we can invert the spectral decomposition.

2. Run the implemented algorithm on it, obtain the computed Eigenvalues $\lambda_{algo} \in \mathbb{R}^p$.

3. Assess L_1-Norm: $|\lambda_{true} - \lambda_{algo}|$, pass the test if it is smaller than a threshold ϵ
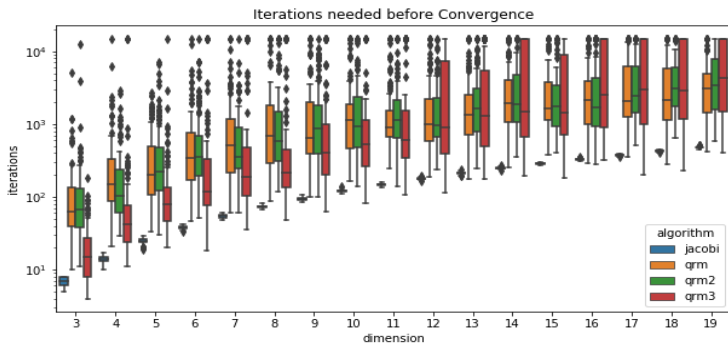
Repeat the procedure 1000 times.

Time taken

Figure 4: Unit-tests: Time

Iterations needed

Figure 5: Unit-tests: Iterations

Iterations needed before Convergence

PCA: proof

The objective of (▸ PCA):

$$max \ \delta' Var\left(X\right)\delta \ s.t. \ \sum \delta_i^2 = 1$$

Corresponding Lagrangean:

$$\mathcal{L}(Var\left(X\right), \delta, \lambda) = \delta' Var\left(X\right)\delta - \lambda\left(\delta'\delta - 1\right),$$

where $\lambda \in \mathbb{R}^m$

First order condition:

$$\frac{\partial \mathcal{L}}{\partial \delta} \overset{!}{=} 0$$

$$2Var(X)\delta - 2\lambda_k\delta \overset{!}{=} 0$$

$$Var(X)\delta = \lambda_k\delta$$

Which is now reduced to a common Eigenvalue problem.

LDA: proof

The objective of `▸ LDA`:

$$max \ \frac{w'S_B w}{w'S_W w},$$

Which we can reformulate to:

$$max \ w'S_B w \ s.t. w'S_W w = 1.$$

Corresponding Lagrangean:

$$\mathcal{L}(w, S_B, S_W, \lambda) = w'S_B w - \lambda \left(w'S_W w - 1 \right)$$

LDA: proof

First order condition:

$$\frac{\partial \mathcal{L}}{\partial w} \overset{!}{=} 0$$

$$2S_B w - 2\lambda S_W w \overset{!}{=} 0$$

$$S_W^{-1} S_B w = \lambda w,$$

which is known as a generalized Eigenvalue problem. We can also rewrite this as:

$$S_B^{-\frac{1}{2}} S_W^{-1} S_B^{-\frac{1}{2}} w = \lambda w$$

Which is a now just a normal Eigenvalue problem as before ▸ back.

Eigenvalues of similar matrices

From the definition in (9) it follows immediately that a matrix A with wigenvalues $\lambda_1, \ldots, \lambda_n$ is similar to the matrix $diag(\lambda_1, \ldots, \lambda_n)$.
If A and B are similar, as in (9), it holds:

$$B - \lambda I = P^{-1}BP - \lambda P^{-1}IP$$
$$= A - \lambda I.$$

Hence A and B have the same eigenvalues. Additionally, important transformations are based around orthogonal matrices. If Q is orthogonal and

$$A = Q'BQ,$$

A and B are said to be *orthogonally similar* ▸ back .

Companion-Matrix: Example

Demonstrate that the companion matrix ▸ back :

1. corresponds to a polynomial.
2. has eigenvalues equal to the roots of the polynomial.

$$A = \begin{bmatrix} 0 & 1 \\ -a_0 & -a_1 \end{bmatrix}$$

$$
\begin{aligned}
det\,(A - \lambda I) &= \begin{bmatrix} 0 - \lambda & 1 \\ -a_0 & -a_1 - \lambda \end{bmatrix} \\
&= -\lambda\,(-a_1 - \lambda) + a_0 \\
&= \lambda^2 + a_1\lambda + a_0
\end{aligned}
$$

Householder Reflections: proof

Remember:

- ⊡ $Q = I - 2uu'$.
- ⊡ u v are orthonormal.

$$
\begin{aligned}
Qx &= c_1 u + c_2 v - 2c_1 uuu' - 2c_2 vuu' \\
&= c_1 u + c_2 v - 2c_1 u'uu - 2c_2 u'vu \\
&= -c_1 u + c_2 v \qquad\qquad\qquad = \tilde{x}
\end{aligned}
$$

Sources

📄 Seffen Börm and Christian Mehl. Numerical Methods for Eigenvalue Problems. Walter de Gruyter GmbH & Co.KG, Berlin/Boston, 2012.

📄 James E. Gentle. Numerical Linear Algebra for Applications in Statistics. Springer Science + Business Media, New York, 2003.

📄 Wolfgang K. Härdle and Léopold Simar. Applied Multivariate Statistical Analysis. Springer-Verlag Gmbh, Berlin, Heidelberg, 2015.