Jacobi Diagonalization Algorithm

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We want to diagonalize a real symmetric matrix $A \in \mathbb{R}^{n \times n}$:

$$A = A^\top, \quad Av_i = \lambda_i v_i,$$

where λ_i are the eigenvalues and v_i the corresponding eigenvectors.

Step 1: Find Largest Off-Diagonal Element

At each iteration, choose indices (p, q) such that

$$|a_{pq}| = \max_{i \neq j} |a_{ij}|,$$

i.e., the largest off-diagonal element.

Step 2: Compute Rotation Angle

We define a Jacobi rotation in the (p, q)-plane with angle θ:

$$R = I + \begin{bmatrix} \ddots & & & & \\ & \cos\theta & & \sin\theta & \\ & & \ddots & & \\ & -\sin\theta & & \cos\theta & \\ & & & & \ddots \end{bmatrix},$$

where the 2×2 block acts on rows/columns p, q.

The rotation angle θ is chosen such that it eliminates a_{pq}:

$$\tan(2\theta) = \frac{2a_{pq}}{a_{qq} - a_{pp}}.$$

Equivalently, one often defines

$$\tau = \frac{a_{qq} - a_{pp}}{2a_{pq}}, \quad t = \frac{\operatorname{sgn}(\tau)}{|\tau| + \sqrt{1 + \tau^2}}, \quad \theta = \arctan(t),$$

with

$$c = \cos\theta, \quad s = \sin\theta.$$

Step 3: Update the Matrix

We perform a similarity transformation:

$$A' = R^\top A R,$$

which preserves eigenvalues but reduces off-diagonal elements.

The updated entries are:

$$a'_{pp} = c^2 a_{pp} - 2sc\, a_{pq} + s^2 a_{qq},$$

$$a'_{qq} = s^2 a_{pp} + 2sc\, a_{pq} + c^2 a_{qq},$$

$$a'_{pq} = a'_{qp} = 0,$$

$$a'_{kp} = a'_{pk} = c\, a_{kp} - s\, a_{kq}, \quad k \neq p, q,$$

$$a'_{kq} = a'_{qk} = s\, a_{kp} + c\, a_{kq}, \quad k \neq p, q.$$

Step 4: Update Eigenvectors

The eigenvector matrix V is updated at each step:

$$V' = VR.$$

Initially, $V = I$, and after convergence the columns of V are the eigenvectors of A.

Step 5: Convergence

Repeat steps 1–4 until the off-diagonal elements satisfy

$$|a_{ij}| < \varepsilon \quad \forall i \neq j.$$

At convergence:

$$A \approx \operatorname{diag}(\lambda_1, \lambda_2, \dots, \lambda_n),$$

where $\lambda_i = a_{ii}$ are the eigenvalues, and the eigenvectors are the columns of V.

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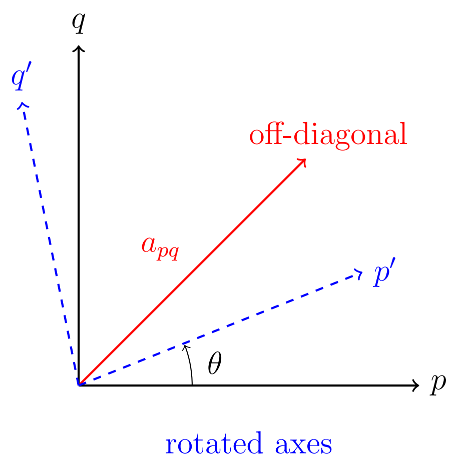
Jacobi Rotation in the (p, q) Plane

We visualize the Jacobi rotation applied to the 2x2 submatrix:

$$\begin{bmatrix} a_{pp} & a_{pq} \\ a_{pq} & a_{qq} \end{bmatrix}.$$



Explanation: - The solid axes (p, q) represent the original coordinates. - The red vector represents the off-diagonal contribution a_{pq}. - The dashed axes (p', q') are rotated by the Jacobi angle θ. - In the rotated basis, the off-diagonal term along $p'q'$ is zero, effectively diagonalizing this 2x2 submatrix.

Jacobi Rotation: 3x3 Matrix in Terms of $\cos\theta$ and $\sin\theta$

Consider a general symmetric 3×3 matrix:

$$A = \begin{bmatrix} a_{00} & a_{01} & a_{02} \\ a_{01} & a_{11} & a_{12} \\ a_{02} & a_{12} & a_{22} \end{bmatrix}.$$

We perform a Jacobi rotation in the $(1, 2)$ plane:

$$R = \begin{bmatrix} 1 & 0 & 0 \\ 0 & c & s \\ 0 & -s & c \end{bmatrix}, \quad c = \cos\theta,\ s = \sin\theta.$$

The rotated matrix is obtained by the similarity transformation:

$$A' = R^\top A R$$

After simplification, the elements of A' are:

$$\begin{bmatrix} a'_{00} & a'_{01} & a'_{02} \\ a'_{10} & a'_{11} & a'_{12} \\ a'_{20} & a'_{21} & a'_{22} \end{bmatrix} = \begin{bmatrix} a_{00} & ca_{01} - sa_{02} & sa_{01} + ca_{02} \\ ca_{01} - sa_{02} & c^2 a_{11} - 2sca_{12} + s^2 a_{22} & 0 \\ sa_{01} + ca_{02} & 0 & s^2 a_{11} + 2sca_{12} + c^2 a_{22} \end{bmatrix}.$$

Notes:

- The off-diagonal element in the pivot submatrix, a'_{12}, is zero.
- The first row and column are mixed with the pivot elements using c and s.
- Symmetry is preserved: $a'_{ij} = a'_{ji}$.

Jacobi Rotation: 4x4 Matrix in the $(2,3)$ Plane

Consider a symmetric 4×4 matrix:

$$A = \begin{bmatrix} a_{00} & a_{01} & a_{02} & a_{03} \\ a_{01} & a_{11} & a_{12} & a_{13} \\ a_{02} & a_{12} & a_{22} & a_{23} \\ a_{03} & a_{13} & a_{23} & a_{33} \end{bmatrix}.$$

We perform a Jacobi rotation in the $(2,3)$ plane:

$$R = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & c & s \\ 0 & 0 & -s & c \end{bmatrix}, \quad c = \cos\theta,\ s = \sin\theta$$

The rotated matrix is:

$$A' = R^\top A R = \begin{bmatrix} a_{00} & a_{01} & ca_{02} - sa_{03} & sa_{02} + ca_{03} \\ a_{01} & a_{11} & ca_{12} - sa_{13} & sa_{12} + ca_{13} \\ ca_{02} - sa_{03} & ca_{12} - sa_{13} & c^2 a_{22} - 2sc\, a_{23} + s^2 a_{33} & 0 \\ sa_{02} + ca_{03} & sa_{12} + ca_{13} & 0 & s^2 a_{22} + 2sc\, a_{23} + c^2 a_{33} \end{bmatrix}.$$

Notes:

- The pivot element a_{23} is eliminated: $a'_{23} = a'_{32} = 0$.
- Rows and columns 0 and 1 are mixed with the rotation using c and s.
- Symmetry is preserved: $a'_{ij} = a'_{ji}$.

Worked Example: First Iteration

Consider the matrix

$$A = \begin{bmatrix} 4 & -2 & 2 \\ -2 & 2 & -4 \\ 2 & -4 & 3 \end{bmatrix}.$$

Step 1: Choose Pivot

Largest off-diagonal element:

$$|a_{12}| = |-4| = 4 \quad \Rightarrow \quad p = 1, q = 2.$$

Step 2: Compute Rotation Parameters

$$a_{pp} = a_{11} = 2, \quad a_{qq} = a_{22} = 3, \quad a_{pq} = -4$$

$$\tau = \frac{a_{qq} - a_{pp}}{2a_{pq}} = \frac{3-2}{-8} = -0.125$$

$$t = \frac{\operatorname{sign}(\tau)}{|\tau| + \sqrt{1+\tau^2}} \approx -0.88278$$

$$\theta = \arctan(t) \approx -0.72322 \text{ rad}$$

$$c = \cos\theta \approx 0.74968, \quad s = \sin\theta \approx -0.66180$$

Step 3: Update Matrix A

$$a'_{pp} = c^2 a_{pp} - 2sca_{pq} + s^2 a_{qq} \approx -1.53113$$

$$a'_{qq} = s^2 a_{pp} + 2sca_{pq} + c^2 a_{qq} \approx 6.53113$$

$$a'_{pq} = 0$$

Other affected entries (row/column $k = 0$):

$$a'_{0p} = ca_{0p} - sa_{0q} \approx -0.17575, \quad a'_{0q} = sa_{0p} + ca_{0q} \approx 2.82296$$

Updated matrix:

$$A' \approx \begin{bmatrix} 4 & -0.17575 & 2.82296 \\ -0.17575 & -1.53113 & 0 \\ 2.82296 & 0 & 6.53113 \end{bmatrix}$$

Step 4: Update Eigenvectors

Starting with $V = I$:

$$V' \approx \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0.74968 & -0.66180 \\ 0 & 0.66180 & 0.74968 \end{bmatrix}.$$