Eigenvalues and eigenvectors

Eigenvector, v_λ, and **eigenvalue**, λ, of matrix A are defined by

$$A \cdot v_\lambda = \lambda v_\lambda \quad \text{or} \quad (A - \lambda\delta) \cdot v_\lambda = 0$$

The second equation can hold (for nonzero vector v_λ) only if matrix $A-\lambda\delta$ is singular, i.e:

$$\det(A - \lambda\delta) = 0$$

⇒ algebraic equation of the n-th degree, with n roots (incl. multiplicity).

Examples: weighted matrix of 2nd derivatives of a potential in a calculation of fundamental frequencies, heat (conduction) equation, wave equation, Schrödinger equation, stochastic matrix, system of linear differential equations, . . .

Example. Calculate eigenvalues and eigenvectors of matrix

$$\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$

$1+i,\ 1-i;\ \begin{pmatrix} i \\ 1 \end{pmatrix}, \begin{pmatrix} -i \\ 1 \end{pmatrix}$

Eigenvalues

A **symmetric** matrix (in $\mathbb{R}$): $A = A^\mathrm{T}$

A **self-adjoint** (Hermitean) matrix (in $\mathbb{C}$): $A = A^\dagger$, $A^\dagger \equiv (A^*)^\mathrm{T}$

Eigenvalues of a self-adjoint (symmetric in $\mathbb{R}$) matrix are real.

Proof: Left-multiply $A \cdot v = \lambda v$ by $v^\dagger$:

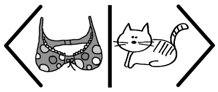
$$v^\dagger \cdot A \cdot v = \sum_{ij} v_i^* A_{ij} v_j = \sum_i v_i^* \lambda v_i = \lambda |v|^2$$

$$= \sum_{ij} v_i^* A_{ji}^* v_j = \sum_{ij} v_j A_{ji}^* v_i^* = \left(\sum_{ij} v_j^* A_{ji} v_i \right)^* = \lambda^* |v|^2$$

$\Rightarrow \lambda = \lambda^* \Rightarrow \lambda \in \mathbb{R}$.

- The proof for symmetric matrices in $\mathbb{R}$ uses a (richer) complex Hilbert space
- Matrices in $\mathbb{R}$ have real eigenvalues or pairs of complex conjugate ones

Bra-ket notation



Vector = “ket” = $|v\rangle$, $|v\rangle_i = v_i$ (“column vector”)

Co-vector = “bra” = Hermitean conjugate:
$|v\rangle^\dagger = \langle v|$, $\langle v|_i = v_i^*$ (“row vector”)

Scalar product: $\langle u|v\rangle = \sum_i u_i^* v_i = \sum_i \langle u|_i |v\rangle_i = \sum_i |u\rangle_i^* \langle v|_i^* = \sum_i \langle v|_i^* |u\rangle_i^* = \langle v|u\rangle^*$

Operator: A or $\hat{A}$: $|Av\rangle$, in some context also $A|v\rangle$ or $|A|v\rangle$; $|Av\rangle_i = \sum_j A_{ij} v_j$

Operator acting on a bra: $\langle uA|$ = bra such that $\langle uA|v\rangle = \langle u|Av\rangle\ \forall v$;

Hence, we can write a matrix element as: $\langle u|A|v\rangle = \sum_{ij} u_i^* A_{ij} v_j$

In coordinates: $\langle uA|_j = \sum_i u_i^* A_{ij} = (\sum_i u_i A_{ij}^*)^* = (\sum_i A_{ij}^* u_i)^* = (\sum_i A_{ji}^\dagger u_i)^* = (|A^\dagger u\rangle)_j^*$

Any matrix: $\langle u|A^\dagger|v\rangle = \langle v|A|u\rangle^*$

Distinguish: $\langle Au|$ and $\langle uA|$: $\langle Au|_j = \sum_i A_{ji}^* u_i^*$

For a Hermitean (self-adjoint) matrix: $A^\dagger = A \Rightarrow \langle u|A|v\rangle = \langle v|A|u\rangle^*$

Proving $\lambda \in \mathbb{R}$ again: $\langle v|A|v\rangle = \langle v|\lambda v\rangle = \lambda\langle v|v\rangle \stackrel{!}{=} \langle v|A|v\rangle^* = \lambda^*\langle v|v\rangle$

credit: http://backreaction.blogspot.cz/2006/07/bra-cat.html

Orthogonality of eigenvectors

Eigenvectors (of different eigenvalues) of a self-adjoint matrix are perpendicular.
Proof:

$$\langle v^{(2)}|A|v^{(1)}\rangle = \langle v^{(2)}|Av^{(1)}\rangle = \langle v^{(2)}|\lambda_1 v^{(1)}\rangle = \lambda_1 \langle v^{(2)}|v^{(1)}\rangle$$

$$\langle v^{(2)}|A|v^{(1)}\rangle = \langle v^{(1)}|A|v^{(2)}\rangle^* = [\lambda_2 \langle v^{(1)}|v^{(2)}\rangle]^* = \lambda_2^* \langle v^{(2)}|v^{(1)}\rangle = \lambda_2 \langle v^{(2)}|v^{(1)}\rangle$$

which can hold (for $\lambda_1 \neq \lambda_2$), only if $\langle v^{(1)}|v^{(2)}\rangle = 0$. We can always orthonormalize a subspace of degenerate eigenvalues, hence **a self-adjoint matrix generates an orthonormal basis**.

In coordinates:

$$\sum_{ij} v_i^{(2)*} A_{ij} v_j^{(1)} = \sum_i v_i^{(2)*} \sum_j A_{ij} v_j^{(1)} = \sum_i v_i^{(2)*} \lambda_1 v_i^{(1)} = \lambda_1 \sum_i v_i^{(2)*} v_i^{(1)}$$

$$\sum_{ij} v_i^{(2)*} A_{ij} v_j^{(1)} = \sum_{ij} v_j^{(1)} A_{ji}^* v_i^{(2)*} = \sum_j v_j^{(1)} \lambda_2^* v_j^{(2)*} = \lambda_2^* \sum_i v_i^{(1)} v_i^{(2)*}$$

$$= \lambda_2 \sum_i v_i^{(2)*} v_i^{(1)}$$

Examples see `mmpc2.mw`

Spectral theorem

A similar statement (“spectral theorem”) holds for **compact** self-adjoint operators in ∞-dimensional Hilbert spaces. Various generalizations exist.

Hermitean in physics = self-adjoint, in mathematics there are subtleties: the generated basis may not span the entire Hilbert space.

Compact operator:
A map of a sequence in a 1-ball contains a Cauchy subsequence (which converges).
Loosely: An image of a 1-ball shrinks enough (“in higher dimensions”).

An operator is compact if it is bounded and it maps a compact (= closed + bounded) set to a set whose closure space is compact (closure = set + boundary).

Compact set X:
Every sequence in X has a convergent subsequence whose limit is in X.
Loosely (Peter Lax): A compact city can be guarded by finitely many near-sighted policemen.

Every open cover of X has a finite subcover.

Examples:

- $\mathrm{diag}\{1, 1/4, 1/9, \dots\}$ is compact self-adjoint
- Identity $\delta = \mathrm{diag}\{1, 1, 1, \dots\}$ in ∞-dimensional space is not compact
- $\hat{p}_x = -i\hbar\frac{\partial}{\partial x}$ is self-adjoint but not compact

Diagonalization of a quadratic form

Let $A \in \mathbb{R}^n \times \mathbb{R}^n$ be a symmetric matrix and $b^{(j)}$ be its eigenvectors, $|b^{(j)}| = 1$.
Let matrix U be composed of column vectors $b^{(j)}$, i.e., $U_{ij} = b_i^{(j)}$.
Then $b^{(j)} \cdot b^{(k)} = \delta_{jk} \Rightarrow U$ is orthogonal, $U^\mathrm{T} \cdot U = \delta$.
The eigenvector condition becomes:

$$b^{(i)\mathrm{T}} \cdot A \cdot b^{(j)} = b^{(i)\mathrm{T}} \cdot \lambda_j b^{(j)} = \lambda_j \delta_{ij} \quad \Rightarrow \quad U^\mathrm{T} \cdot A \cdot U = \Lambda$$

where $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \dots)$, $\Lambda_{ij} = \lambda_j \delta_{ij} = \lambda_i \delta_{ij}$ is a diagonal matrix with eigenvalues at the diagonal.

The transformed **quadratic form** is

$$x^\mathrm{T} \cdot A \cdot x = u^\mathrm{T} \cdot U^\mathrm{T} \cdot A \cdot U \cdot u = u^\mathrm{T} \cdot \Lambda \cdot u = \sum_i \lambda_i u_i^2$$

where

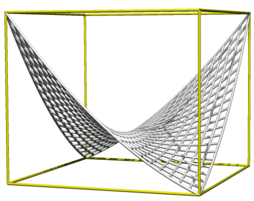
$$x = U \cdot u \quad \text{or} \quad u = U^{-1} \cdot x \equiv U^\mathrm{T} \cdot x$$

Similarly in $\mathbb{C}$ for self-adjoint matrices ($^\mathrm{T}$ replaced by †)

The unitary transformation U (e.g., a rotation in $\mathbb{R}^n$) transforms a symmetric (in $\mathbb{R}$) or self-adjoint matrix (in $\mathbb{C}$) to a diagonal one. Thus “diagonalization = calculating eigenvectors and eigenvalues”.

Example – quadratic form

$$x^2 - 4xy + y^2$$



Matrix:

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

Characteristic equation:

$$\det \begin{pmatrix} 1-\lambda & -2 \\ -2 & 1-\lambda \end{pmatrix} = \lambda^2 - 2\lambda - 3$$

roots: $\lambda_1 = -1, \lambda_2 = 3$. Equations for the eigenvectors:

$$Av_1 = -v_1 \quad \Rightarrow \quad v_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$Av_2 = 3v_2 \quad \Rightarrow \quad v_2 = \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

And normalized eigenvectors → basis:

$$v = \begin{pmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{pmatrix}$$

rotation by 45°

Signature of a quadratic form

The signature = number of (positive,negative,zero) eigenvalues.

Example: the signature of $x^2 - 4xy + y^2$ is $(+, -)$[a].

For $f(x_i)$ “countinuous enough”, the condition for an extreme is:

$$\frac{\partial f}{\partial x_i} = 0, \ i = 1, \dots, n$$

If this holds true for x^0, the Taylor expansion at the minimum is:

$$f(x) = f(x^0) + \frac{1}{2}\sum_{ij}(x_i - x_i^0) A_{ij} (x_j - x_j^0), \quad A_{ij} = \frac{\partial f^2}{\partial x_i \partial x_j}\Big|_{x_i = x_i^0, x_j = x_j^0}$$

- If the signature of A is $(n, 0, 0) = (++++\dots)$, the form is **positive definite** and f has a local minimum at x^0.
- If the signature of A is $(0, n, 0) = (----\dots)$, then the form is **negative definite**, and f has a local maximum at x^0.
- If the signature contains pluses and minuses, it is **indefinite**, and f has a saddle point at x^0.

[a] Often written in form $(n_+, n_-, n_0) = (1, -1, 0)$

Sylvestr criterion

We calculate the subdeterminants:

$$\det|A_{ij}|_{i,j=1}$$

$$\det|A_{ij}|_{i,j=1..2}$$

$$\det|A_{ij}|_{i,j=1..3}$$

- All are positive at point x^0: minimum.
- Alternating signs at point x^0 $(-,+,-,\ldots)$: maximum.

The proof uses the spectral theorem and the Cholesky decomposition of a Hermitean matrix $A = L^* \cdot L$, where L is a triangular matrix.

Fundamental vibrations

Let PES be $U_{\rm pot}(\boldsymbol\tau)$, $\boldsymbol\tau = \{\vec r_1, \ldots, \vec r_N,\}$, with a (local) minimum at $\boldsymbol\tau_{\rm min}$, deviation from the minimum: $\Delta\boldsymbol\tau = \boldsymbol\tau - \boldsymbol\tau_{\rm min}$.

Taylor expansion to the 2nd order:

$$U_{\rm pot}(\boldsymbol\tau) = U_{\rm pot}(\boldsymbol\tau_{\rm min}) + \underbrace{\sum_i \frac{\partial U_{\rm pot}}{\partial \vec r_i}(\boldsymbol\tau_{\rm min})}_{=0} \cdot \Delta\vec r_i + \frac{1}{2}\sum_{i,j}\Delta\vec r_i \cdot \frac{\partial^2 U_{\rm pot}}{\partial \vec r_i \partial \vec r_j}(\boldsymbol\tau)\cdot\Delta\vec r_j$$

Newton equations of motion:

$$m_i \Delta\ddot{\vec r}_i \equiv m_i \frac{\partial^2 \Delta\vec r_i}{\partial t^2} = \vec f_j = -\sum_j A_{ij}\Delta\vec r_j$$

where the so called Hessian matrix is

$$A_{ij} = \frac{\partial^2 U_{\rm pot}}{\partial \vec r_i \partial \vec r_j}(\boldsymbol\tau_{\rm min}),\quad \Delta\vec r_i = \vec r_i - \vec r_{i,\rm min}$$

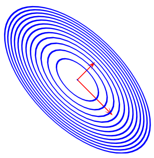
In the matrix form (vector = $3N$ numbers, matrix = $3N \times 3N$):

$$\boldsymbol M \cdot \Delta\ddot{\boldsymbol\tau} = -\boldsymbol A \cdot \Delta\boldsymbol\tau,\ \text{ where } \boldsymbol M = \mathrm{diag}(m_1, m_1, m_1, \ldots, m_N, m_N, m_N)$$

Fundamental vibrations

$$\boldsymbol M \cdot \Delta\ddot{\boldsymbol\tau} = -\boldsymbol A \cdot \Delta\boldsymbol\tau,\ \text{ where } \boldsymbol M = \mathrm{diag}(m_1, m_1, m_1, \ldots, m_N, m_N, m_N)$$

We are looking for a transformation (basis) in the form



$$\Delta\boldsymbol\tau = \boldsymbol M^{-1/2}\cdot \boldsymbol U \cdot \boldsymbol u$$

where $\boldsymbol U$ is orthogonal. By inserting:

$$\boldsymbol M \cdot \boldsymbol M^{-1/2}\cdot \boldsymbol U \cdot \ddot{\boldsymbol u} = -\boldsymbol A \cdot \boldsymbol M^{-1/2}\cdot \boldsymbol U \cdot \boldsymbol u$$

Left-multiplied by $\boldsymbol U^{-1}\cdot \boldsymbol M^{-1/2}\cdot$:

$$\ddot{\boldsymbol u} = -\boldsymbol\Lambda \cdot \boldsymbol u,\quad \boldsymbol\Lambda = \boldsymbol U^{-1}\cdot \boldsymbol M^{-1/2}\cdot \boldsymbol A \cdot \boldsymbol M^{-1/2}\cdot \boldsymbol U$$

There exists an orthogonal matrix $\boldsymbol U$ so that $\boldsymbol\Lambda = \boldsymbol U^{-1}\cdot \boldsymbol M^{-1/2}\cdot \boldsymbol A \cdot \boldsymbol M^{-1/2}\cdot \boldsymbol U$ is diagonal, in other words, we diagonalize the symmetric matrix $\boldsymbol A'$:

$$\boldsymbol A' = \boldsymbol M^{-1/2}\cdot \boldsymbol A \cdot \boldsymbol M^{-1/2}$$

The Newton equations separate into $3N$ independent harmonic oscillators:

$$\ddot u_\alpha = -\Lambda_{\alpha\alpha} u_\alpha,\quad \alpha = 1, \ldots, 3N$$

The frequences are

$$\nu_\alpha = \frac{\sqrt{\Lambda_{\alpha\alpha}}}{2\pi}$$

6 are zero for a general molecule, 5 for linear molecules

Fundamental vibrations – diatomic molecule

Two atoms connected by a spring:

$$U_{\rm pot} = \frac{K}{2}(x-y)^2 \ \Rightarrow\ \boldsymbol A' = \begin{pmatrix} K/m & -K/m \\ -K/m & K/m \end{pmatrix} \ \Rightarrow\ \boldsymbol B = \mathrm{diag}(2K/m, 0)$$

The frequences are

$$\nu_1 = \frac{\sqrt{2K/m}}{2\pi}\ \text{(sym. stretch)},\quad \nu_2 = 0\ \text{(translation)}$$

Unnormalized eigenvectors:

$$\psi_1 = \begin{pmatrix} 1 \\ -1 \end{pmatrix},\quad \psi_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

→← →→

Homogeneous linear differential equations of the 1st order

The system of homogeneous linear differential equations of the 1st order:

$$\left.\begin{array}{rcl} \dot x_1 &=& A_{11}x_1 + A_{12}x_2 + \cdots + A_{1n}x_n \\ \vdots && \\ \dot x_n &=& A_{n1}x_1 + A_{n2}x_2 + \cdots + A_{nn}x_n \end{array}\right\} \quad \dot x = A \cdot x$$

One of n linearly independent solutions:

$$x = e^{\lambda t} v \ \Rightarrow\ A \cdot v = \lambda v$$

For real A, λ are real or complex conjugate pairs.

General solution if all λ's are diferent:

$$x = \sum_\lambda C_\lambda e^{\lambda t} v_\lambda$$

where C_λ's are determined from the initial conditions.

If there are multiple eigenvalues (roots of the characteristic equation), we have $e^{\lambda t}$, $te^{\lambda t}$, $t^2 e^{\lambda t}$, etc.

The set is always equivalent to one homogeneous linear differential equations of the n-th order.

see `mmpc2.mw`

Example

$$\dot x = y,\ \dot y = -x$$

$$A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \ \Rightarrow\ \lambda = \pm i,\quad v_i = \begin{pmatrix} i \\ 1 \end{pmatrix}, v_{-i} = \begin{pmatrix} 1 \\ i \end{pmatrix}$$

$$v_i = \begin{pmatrix} i \\ 1 \end{pmatrix}, v_{-i} = \begin{pmatrix} 1 \\ i \end{pmatrix}$$

General solution:

$$C_i v_i e^{it} + C_{-i} v_{-i} e^{-it} \quad \left\{ \begin{array}{rcl} x &=& iC_i e^{it} + C_{-i}e^{-it} \\ y &=& C_i e^{it} + iC_{-i}e^{-it} \end{array}\right.$$

With initial conditions $x(0) = 1, y(0) = 0$: $iC_i = C_{-i} = 1/2$, so that

$$x = \cos(t),\ y = -\sin(t)$$

Equivalent differential equation of the 2nd order:

$$\ddot x = -x\ \ \text{(harmonic oscillator)}$$

see `mmpc2.mw`