Spectral Theorem & Applications

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Statement of the Spectral Theorem

For finite-dimensional vector spaces:

- Over the reals: A real symmetric matrix $A = A^T$ is diagonalizable by an orthogonal matrix Q:

  $$A = QDQ^T$$

  where D is diagonal with real eigenvalues, and Q has orthonormal eigenvectors as columns.

- Over the complex numbers: A complex Hermitian matrix $A = A^*$ is diagonalizable by a unitary matrix U:

  $$A = UDU^*$$

  with D real diagonal; eigenvalues are real and eigenvectors can be chosen orthonormal.

Consequences

- Eigenvectors corresponding to distinct eigenvalues are orthogonal.
- All eigenvalues of Hermitian/symmetric matrices are real.
- Quadratic form $x^T Ax$ (or $x^* Ax$) can be analyzed via eigenvalues.

Hermitian/Symmetric Matrices

- Real symmetric: $A = A^T$.
- Complex Hermitian: $A = A^*$ (conjugate transpose).
- Positive semidefinite (PSD): $x^* Ax \geq 0$ for all x; equivalent to all eigenvalues ≥ 0.
- Positive definite (PD): $x^* Ax > 0$ for all $x \neq 0$; eigenvalues > 0.

QC connection: Observables (e.g., spin, energy) are represented by Hermitian operators; measurement outcomes are the real eigenvalues.

ML connection: Sample covariance matrices are symmetric PSD; their eigen-decomposition underpins PCA.

Orthogonal/Unitary Diagonalization

If A is symmetric/Hermitian, there exists orthonormal eigenbasis $\{q_i\}_{i=1}^n$ and real eigenvalues $\{\lambda_i\}$ such that:

$$A = \sum_{i=1}^{n} \lambda_i q_i q_i^T \quad \text{(real)}, \qquad A = \sum_{i=1}^{n} \lambda_i q_i q_i^* \quad \text{(complex)}$$

This expansion is called the spectral decomposition.

Rayleigh Quotient and Variational Characterization

For unit vector x:

$$R_A(x) = \frac{x^* A x}{x^* x}$$

- $\lambda_{\max} = \max_{\|x\|=1} R_A(x)$ - $\lambda_{\min} = \min_{\|x\|=1} R_A(x)$

Applications in QC/ML/Applied Math

- QC: Any state can be expanded in an observable's orthonormal eigenbasis; time evolution under a Hamiltonian uses eigen-decomposition.
- ML: PCA = eigen-decomposition of covariance $\Sigma = \frac{1}{m} X^T X$; principal directions are eigenvectors with largest eigenvalues.
- Stability: For linear dynamical system $x_{k+1} = Ax_k$, eigenvalues determine growth/decay/oscillation.
- Quadratic optimization: Optimize $x^T A x$ under constraints via eigenvalues and eigenvectors.

Animation: Animation: Use "Eigenvalues & Eigenvectors" demo in `interactive-visualizations.py` to see invariant directions and scaling.

Worked Examples

Example 1: Diagonalization of a Symmetric Matrix

Let

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

Characteristic polynomial: $\det(A - \lambda I) = (2-\lambda)^2 - 1 = \lambda^2 - 4\lambda + 3$. Eigenvalues: $\lambda_1 = 1, \lambda_2 = 3$. Eigenvectors: for $\lambda_1 = 1$, $v_1 = (1, -1)^T$; for $\lambda_2 = 3$, $v_2 = (1, 1)^T$. Orthonormal basis: $q_1 = \frac{1}{\sqrt{2}}(1, -1)^T$, $q_2 = \frac{1}{\sqrt{2}}(1, 1)^T$. Then $Q = [q_1\, q_2]$, $D = \text{diag}(1, 3)$, and $A = QDQ^T$.

Example 2: PCA via Spectral Decomposition

Given centered data matrix $X \in \mathbb{R}^{m \times n}$, covariance $\Sigma = \frac{1}{m} X^T X$. Eigen-decompose $\Sigma = Q \Lambda Q^T$. The top-k principal components are the first k columns of Q. Projected data: $Y = XQ_k$. Explained variance ratio: $\lambda_i / \sum_j \lambda_j$.

Practice Problems

1. Prove that a real symmetric matrix has orthogonal eigenvectors corresponding to distinct eigenvalues.
2. Let A be PSD. Show $\lambda_{\min} \geq 0$ using the Rayleigh quotient.
3. Diagonalize $\begin{pmatrix} 4 & 0 & 0 \\ 0 & 2 & 1 \\ 0 & 1 & 2 \end{pmatrix}$ and classify as PD/PSD/indefinite.
4. For a covariance matrix Σ, explain why all eigenvalues are nonnegative and how PCA selects directions.
5. QC: For a Hermitian operator H, explain why measurement outcomes are real and relate eigenbasis to measurement probabilities.

Solutions

Solution to Problem 1

If A is real symmetric, there exists an orthonormal basis of eigenvectors; let x, y be eigenvectors with $Ax = \lambda x$, $Ay = \mu y$, $\lambda \neq \mu$. Then

$$\lambda\langle x, y\rangle = \langle Ax, y\rangle = \langle x, Ay\rangle = \mu\langle x, y\rangle,$$

so $(\lambda - \mu)\langle x, y\rangle = 0$ and hence $\langle x, y\rangle = 0$.

Solution to Problem 2

For unit x, $R_A(x) = x^T Ax$. Since A is PSD, $x^T Ax \geq 0$ for all x, so the extremal values of R_A (which equal eigenvalues) satisfy $\lambda_{\min} \geq 0$.

Solution to Problem 3

Compute the characteristic polynomial, find eigenvalues/eigenvectors, and orthonormalize. One finds eigenvalues $\{4, 3, 1\}$ with orthonormal eigenvectors; the matrix is PD because all eigenvalues are > 0.

Solution to Problem 4

Covariance matrices are symmetric and for any z, $z^T \Sigma z = \mathrm{Var}(z^T X) \geq 0$, so eigenvalues are ≥ 0. PCA selects eigenvectors with largest eigenvalues (directions of maximal variance).

Solution to Problem 5

Hermitian H has real eigenvalues and an orthonormal eigenbasis. Measurement outcomes are eigenvalues (real). If $|\psi\rangle = \sum_i c_i |h_i\rangle$ in the eigenbasis, probability of outcome λ_i is $|c_i|^2$.