Pertubation theory for linear operators

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Introduction and motivation

Linear operators are fundamental in describing a multitude of physical systems via quantum mechanics and differential equations, yet in many applications their behaviour can be highly non-trivial to determine analytically. Perturbation theory takes a simpler, analytically solvable system and studies how its solution space changes as it is perturbed towards the operator of interest. This can be done rigorously, producing an exact result in the form of a power series, which can then be truncated to the required accuracy with known bounds on the error. This poster presents the theory used to rigorously justify commonly used equations in quantum mechanics such as $E_n^{(1)} = \langle \psi_n^{(0)} | H' | \psi_n^{(0)} \rangle$.

The resolvent

Consider a linear operator T in a vector space X. The **resolvent** of T is defined as the operator-valued function

$$R(\zeta) = (T - \zeta)^{-1}$$

The resolvent is singular wherever $det(T - \zeta) = 0$, i.e. ζ is an eigenvalue of T. This enables the study of operators and their eigenvalues via complex analysis.

For instance, the resolvent can be used to define functions on an operator via the Dunford-Taylor integral

$$\phi(T) = \frac{-1}{2\pi i} \int_{\Gamma} \phi(\zeta) R(\zeta) \, d\zeta$$

where Γ is a simple closed curve in the complex plane containing all the eigenvalues λ_h of T in its interior, and $\phi(\zeta)$ is holomorphic on the interior of Γ . This is equivalent to the Cauchy integral formula for complex-valued functions.

Also of note is the resolvent equation

$$R(\zeta_1) - R(\zeta_2) = (\zeta_1 - \zeta_2)R(\zeta_1)R(\zeta_2)$$

which can be verified by expanding the left side as $R(\zeta_1)(T - \zeta_2)R(\zeta_2) - R(\zeta_1)(T - \zeta_1)R(\zeta_2)$.

Eigenprojections and eigennilpotents

The behaviour of the resolvent is best understood via its Laurent series around some eigenvalue λ_h of T. Use of the resolvent equation alongside the integral formula for Laurent coefficients results in the series

$$R(\zeta) = -(\zeta - \lambda_h)^{-1} P_h - \sum_{n=1}^{m_h - 1} (\zeta - \lambda_h)^{-n - 1} D_h^n + \sum_{n=0}^{\infty} (\zeta - \lambda_h)^n S_h^{n+1}.$$

Eigenvalue splitting

A key aspect of perturbation theory is that not all operators in the family T(x) may have the same number of eigenvalues. It is therefore crucial to understand when and how the splitting of eigenvalues occurs.

We know that the eigenvalues $\lambda_h(x)$ of T(x) satisfy the characteristic equation $\det(T(x) - \lambda_h(x)) = 0$. It is clear from the matrix expression of T(x) that this gives a polynomial in $\lambda_h(x)$ of degree $N = \dim X$ with coefficients that are holomorphic functions of x. Therefore, the number of eigenvalues is a constant s except at finitely many so-called **exceptional points**, and the eigenvalue functions $\lambda_h(x)$ are holomorphic for $x \in D_0$ except potentially at these exceptional points where they may have algebraic singularites.



Figure 1. Path of the eigenvalues of $T_1(x)$ in the ζ -plane.

Pictured above are the paths in the ζ -plane that the eigenvalues of

$$T_1(x) = \begin{bmatrix} 1 & x & 0 \\ x^2 & -1 & 1 \\ x^2 & 1 & x \end{bmatrix}$$

trace as x rotates around the unit circle, with the corresponding phase of x denoted by the hue in standard ROYGBIV order.

1d quantum anharmonic oscillator

Recall that for a quantum harmonic oscillator in one dimension we have a quadratic potential and thus the Hamiltonian

$$H_0 = \frac{-\hbar^2}{2m}\nabla^2 + \frac{m\omega^2}{2}x^2$$

with (unnormalised) eigenfunctions and eigenvalues

$$\psi_n(x) = H_n(\sqrt{\frac{m\omega}{\hbar}}x) \exp \frac{-1}{2}\sqrt{\frac{m\omega}{\hbar}}x^2$$
$$E = (n + \frac{1}{2})\hbar\omega$$

where $H_n(x)$ are Hermite polynomials. Applying the below perturbation gives the quantum anharmonic oscillator. The perturbation series gives a good approximation to the true energy levels for small perturbations, even when truncated to third order.



Figure 3. Energy levels derived to third order via perturbation theory of the 1d quantum anharmonic oscillator (solid) vs reference energy levels (dashed)

2d quantum harmonic oscillator

In two dimensions we have the Hamiltonian

$$H_0 = \frac{-\hbar^2}{2m} \nabla^2 + \frac{m\omega^2}{2} (x^2 + y^2).$$

with (unnormalised) eigenfunctions and eigenvalues

$$n=1$$
 $n=0$

where P_h is a projection and D_h is nilpotent. Furthermore, we get the relation $P_hD_h = D_hP_h = D_h$, $P_hS_h = S_hP_h = 0$. Thus, the Laurent series around λ_h naturally provides a decomposition of $R(\zeta)$ according to $X = M_h \oplus M'_h$ where $M_h = P_hX$ and $M'_h = (1 - P_h)X$. The part of $R(\zeta)$ in M_h has only one singularity, $\zeta = \lambda_h$, and therefore M_h is the algebraic eigenspace of T with eigenvalue λ_h .

Expanding the resolvent as a Laurent series around each eigenvalue in this way allows us to extract its part in each of the algebraic eigenspaces M_h . The algebraic eigenspaces are in direct sum $X = M_1 \oplus \cdots \oplus M_s$ and thus the resolvent can be expressed as the sum of its parts in each algebraic eigenspace

$$R(\zeta) = -\sum_{k=1}^{s} \left[(\zeta - \lambda_h)^{-1} P_h + \sum_{n=1}^{m_h - 1} (\zeta - \lambda_h)^{-n - 1} D_h^n \right].$$

Since $TP_h = \lambda_h P_h + D_h$, there is a corresponding decomposition of T given by

 $T = \sum_{h} \lambda_h P_h + D_h.$

Perturbation series

We are particularly interested in perturbations T(x) which are holomorphic functions of x in some domain of the complex plane, ensuring they can be expressed as a power series $T(x) = \sum_{n=0}^{\infty} x^n T_n$. This allows us to derive power series (and the associated radii of convergence) for the resolvent and eigenprojections of this perturbed operator, which determine its eigenvalues and eigenvectors and therefore ultimately its behaviour. These series are given by $R(\zeta, x) =$ $R(\zeta) + \sum_{n=1}^{\infty} x^n R_n(\zeta)$ and $P(x) = P + \sum_{n=1}^{\infty} x^n P_n$, where

$$R_{n}(\zeta) = \sum_{\substack{v_{1} + \dots + v_{p} = n \\ 1 \le v_{j}, \ 1 \le p \le n}} (-1)^{p} R(\zeta) T_{v_{1}} R(\zeta) T_{v_{2}} \dots T_{v_{p}} R(\zeta)$$

$$P_n = -\sum_{p=1}^n (-1)^p \sum_{\substack{v_1 + \dots + v_p = n \\ k_1 + \dots + k_{p+1} = p \\ v_j \ge 1, \ k_j \ge -m+1}} R(\zeta) T_{v_1} R(\zeta) T_{v_2} \dots T_{v_p} R(\zeta) \ d\zeta.$$

Note the sums for each coefficient are finite and computable.

We can observe that as x makes one rotation around the origin, the left eigenvalue returns to its initial position. However the two eigenvalues on the right swap places, forming a so-called λ -group of order 2.



Figure 2. Path of the eigenvalues of $T_2(x)$ in the ζ -plane.

Figure 2 provides an example of eigenvalue splitting. x varies along the real interval [0, 1], with corresponding eigenvalues given a hue accordingly in ROYGBIV order.

$$T_2(x) = \begin{bmatrix} 0 & x & 0 \\ -x & 0 & 1 \\ 0 & 1 & x \end{bmatrix}$$

Hilbert spaces and quantum mechanics

Quantum mechanics takes place in the Hilbert space $L_2(-\infty,\infty)$, the space of all square-integrable functions on the real line f(x) such that $\int_{-\infty}^{\infty} |f(x)|^2 dx$ exists. Quantum states are elements of this Hilbert space, and observables are represented by self-adjoint operators. An observable, when observed, may only take values in its spectrum. Thus the study of the spectrum of operators can be applied to find the allowed states of a quantum system. The previously discussed results generalise from finite-dimensional vector spaces to Hilbert spaces (being aware of some technicalities such as operators now being able to have continuous spectra).

$$\psi_{n_x,n_y}(x,y) = H_{n_x}(\sqrt{\frac{m\omega}{\hbar}}x)H_{n_y}(\sqrt{\frac{m\omega}{\hbar}}y)\exp\frac{-1}{2}\sqrt{\frac{m\omega}{\hbar}}(x^2+y^2)$$
$$E = (n_x + n_y + 1)\hbar\omega$$

where $H_n(x)$ are Hermite polynomials, derived by separation of variables. Clearly, for $E \ge 2\hbar\omega$, there are multiple combinations of n_x and n_y resulting in the same energy level. Such states are called degenerate, and applying a perturbation will cause the eigenvalues to split. The perturbation series describes this splitting, pictured below with all series truncated to second order, when we apply the perturbation

$$H(g) = H_0 + gm\omega^2 xy.$$



Figure 4. Energy levels of the perturbed system derived to second order via perturbation theory (left) vs reference energy levels (right).

Note that here, and in the previous example, the reference energy levels have been produced to sufficient precision numerically in Mathematica using spatial discretisation with the finite element method.

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References

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