Linear Perturbation Series

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Abstract

The perturbation series for the eigenvalues of a linear perturbation (Rayleigh-Schrödinger series) is derived in the context of bounded operators on a Banach space. The Haskell code implementation to compute the coefficients in the linear perturbation series is briefly described.

1 Introduction to the Main Result

Let X be a complex Banach space. For example $X = \mathbb{C}^n$. Denote by $\mathscr{B}(X)$ the space of all bounded linear operators $X \to X$. So $\mathscr{B}(X) \cong \mathbb{C}^{n\times n}$ in the case $X = \mathbb{C}^n$. Let $T_0,\ T_1 \in \mathscr{B}(X)$. Define $T : \mathbb{C} \to \mathscr{B}(X)$ by $T(x) = T_0 + x \cdot T_1$. Then T is called a linear perturbation of T_0 by T_1. Let λ_0 be a semi-simple eigenvalue of T_0 that is isolated in T_0's spectrum. Let $m < \infty$ be the dimension of the eigenspace of T_0 to eigenvalue λ_0.

Then there exists a sequence $(\alpha_n)_{n\in\mathbb{N}}$ of complex numbers such that the following is true: The sum $\alpha(x)$ of the eigenvalues of $T(x)$, where each eigenvalue is counted according to the dimension of the corresponding generalized eigenspace, is given by

$$\boxed{\alpha(x) = m \cdot \lambda_0 + \sum_{n=1}^{\infty} \alpha_n x^n} \tag{1.0.1}$$

for x in some disk $D \subset \mathbb{C}$ centered at 0. The most interesting case is of course when $m = 1$. Then $\alpha(x)$ is an eigenvalue of $T(x)$ with $\lim_{x\to 0} \alpha(x) = \lambda_0$.

Let $n \in \mathbb{N}$. Then the coefficient α_n can be obtained as follows: Define

$$S_n := \{(j_1, \ldots, j_n) \in \mathbb{N}^n : j_1 + \cdots + j_n = n - 1\}. \tag{1.0.2}$$

Then the cyclic group of n elements, C_n, acts on S_n by circularly shifting the index of the tuple. Let $O_n \subset S_n$ be such that O_n contains exactly one element of every orbit of the action of C_n on S_n. Then

$$\boxed{\alpha_n = \sum_{o\in O_n} \operatorname{tr}(T_1 \cdot V_{o_1 - 1} \cdots T_1 \cdot V_{o_n - 1}),} \tag{1.0.3}$$

where V_j is the j-th coefficient in the Laurent expansion of the resolvent of T_0 around λ_0.

The code computes α_n in the case $X = \mathbb{C}^n$. The function pertCoeff in app/PerturbationSeries.hs returns a list of the coefficients α_n up to a given order. The algorithm to compute O_n (as a list of lists instead of a set of tuples) is implemented in app/Combinatorics.hs. for mathematical and implementation details on the computation of O_n see my blog post [**blog**].

2 Perturbation Series

In this section the main result is derived. The main source is Katos book [**kato_perturbation**].

2.1 Laurent-Expansion of the Resolvent

Let X be a complex Banach space and $T_0 : X \to X$ a bounded linear operator and R the resolvent of T_0. Let $\lambda_0 \in \sigma(T_0)$ be an isolated point of the spectrum of T_0. Let P be the spectral projection associated to λ_0 and $Q := I - P$ the complementary projection. Then the Laurent-expansion of R around λ_0 is:

$$\begin{aligned} R(\lambda) = &\sum_{n=1}^{\infty} (\lambda - \lambda_0)^{-n} \cdot (T_0 - \lambda_0 I)^{n-1} P \\ &+ \sum_{n=0}^{\infty} (\lambda - \lambda_0)^{n} \cdot (-1)^n \cdot S^{n+1} Q, \end{aligned} \tag{2.1.1}$$

where S is the inverse of $(\lambda_0 I - T_0)|_{Q(X)} : Q(X) \to Q(X)$. S is called the reduced resolvent of T_0 at λ_0. The inner radius of convergence of the Laurent-series is 0 and the outer $d(\lambda_0, \sigma(T))$.

2.2 Perturbation-series for the Resolvent

Let $(T_n)_{n\in\mathbb{N}}$ be a sequence in $\mathscr{B}(X)$ (bounded linear operators on X). Let $T : D \to \mathscr{B}(X)$ defined by

$$T(x) := \sum_{n=0}^{\infty} T_n x^n, \tag{2.2.1}$$

where D is the open disk centered at 0 whose radius is the radius of convergence of the power series (assumed > 0).

Let $U := \{(\lambda, x) \in \mathbb{C}^2 : \lambda I - T(x) \text{ invertible}\}$ and define $R : U \to \mathscr{B}(X)$ by

$$R(\lambda, x) := (\lambda I - T(x))^{-1}. \tag{2.2.2}$$

Let $A(x) := T(x) - T_1$. Now

$$\lambda I - T(x) = \lambda I - T_0 - A(x) = (I - A(x)R(\lambda, 0))(\lambda I - T_0) \tag{2.2.3}$$

and so by using the geometric series:

$$R(\lambda, x) = R(\lambda, 0)(I - A(x)R(\lambda, 0))^{-1} = R(\lambda, 0)\sum_{n=0}^{\infty}(A(x)R(\lambda, 0))^n \tag{2.2.4}$$

with a > 0 radius of convergence. From this it follows, by collecting the terms that have the same power of x, that $R(\lambda, x)$ is analytic in x at 0. Similarly one can show that R is bi-analytic on U as well.

2.3 Eigenvalue Perturbation-series

Let λ_0 be an isolated element of $\sigma(T_0)$ with finite dimensional generalized eigenspace (which is equivalent to the Laurent-expansion having only finitely many non-zero coefficients to negative power). Let m be the dimension of the generalized eigenspace. Let γ be a circular path surrounding λ_0 once in the positiv sense. It follows from abstract properties of the holomorphic functional calculus, that for $x \in \mathbb{C}$ "small enough"

$$P(x) = \frac{1}{2\pi i}\int_\gamma R(\lambda, x)d\lambda \tag{2.3.1}$$

is the projection onto sum of all the generalized eigenspaces to the eigenvalues that have split from λ_0 ("split eigenvalues"). Therefore

$$\alpha(x) := \operatorname{tr} T(x)P(x) \tag{2.3.2}$$

is the weighted (by the dimension of the generalized eigenspaces) sum of all the split eigenvalues.

Therefore

$$\alpha(x) - m\lambda_0 = \operatorname{tr}(T(x) - \lambda_0 I)P(x) = \frac{1}{2\pi i}\operatorname{tr}\int_\gamma(\lambda - \lambda_0)R(\lambda, x)d\lambda \tag{2.3.3}$$

Inserting the expansion for R (equation 2.2.4):

$$\begin{aligned}
\alpha(x) - m\lambda_0 &= \frac{1}{2\pi i}\operatorname{tr}\int_\gamma(\lambda - \lambda_0)R(\lambda, 0)\sum_{n=1}^{\infty}(A(x)R(\lambda, 0))^n d\lambda \\
&= -\frac{1}{2\pi i}\operatorname{tr}\int_\gamma(\lambda - \lambda_0)\sum_{n=1}^{\infty}\frac{1}{n}\left(\frac{\partial}{\partial z}(A(x)R(z, 0))^n\right)(\lambda)d\lambda \\
&= \frac{1}{2\pi i}\operatorname{tr}\int_\gamma\sum_{n=1}^{\infty}\frac{1}{n}(A(x)R(\lambda, 0))^n d\lambda.
\end{aligned} \tag{2.3.4}$$

In the first equality the $n = 0$ term vanishes. For the second the cyclicity of the trace and the derivative of the resolvent are used. For the third partial integration is used. Collecting powers of x in the above:

$$\alpha(x) - m\lambda_0 = \sum_{n=1}^{\infty} \alpha_n x^n \tag{2.3.5}$$

with

$$\alpha_n := \sum_{k=1}^{n} \sum_{\substack{(i_1,\dots,i_k)\in(\mathbb{N}\setminus\{0\})^k \\ i_1+\cdots+i_k=n}} \frac{1}{2\pi k i} \operatorname{tr} \int_\gamma T_{i_1} R(\lambda, 0) \cdots T_{i_k} R(\lambda, 0) d\lambda. \tag{2.3.6}$$

For $n \in \mathbb{Z}$ let $V_n \in \mathscr{B}(X)$ be the coefficient of $(\lambda - \lambda_0)^n$ in the Laurent expansion of T_0 around λ_0, then using the residue theorem and the Laurent expansion of the Resolvent (equation 2.1.1) around λ_0 to evaluate the integral:

$$\alpha_n = \sum_{k=1}^{n} \sum_{\substack{(i_1,\dots,i_k)\in(\mathbb{N}\setminus\{0\})^k \\ i_1+\cdots+i_k=n}} \frac{1}{k} \sum_{\substack{(j_1,\dots,j_k)\in\mathbb{Z}^k \\ j_1+\cdots+j_k=-1}} \operatorname{tr} T_{i_1} V_{j_1} \cdots T_{i_k} V_{j_k}. \tag{2.3.7}$$

2.4 Eigenvalue Perturbation-series for Linear Perturbation and Semi-simple Eigenvalue

In the special case of a linear perturbation ($T_n = 0$ for all $n \in \mathbb{N}$ with $n \geq 2$) and a semi simple eigenvalue (meaning that $(T_0 - \lambda_0 I)P = 0$) we obtain

$$\begin{aligned} \alpha_n &= \frac{1}{n} \sum_{\substack{(j_1,\dots,j_n)\in\mathbb{Z}^n \\ j_1+\cdots+j_n=-1}} \operatorname{tr} T_1 V_{j_1} \cdots T_1 V_{j_n} \\ &= \frac{1}{n} \sum_{\substack{(j_1,\dots,j_n)\in\mathbb{N}^n \\ j_1+\cdots+j_n=n-1}} \operatorname{tr} T_1 V_{j_1-1} \cdots T_1 V_{j_n-1}. \end{aligned} \tag{2.4.1}$$

To reduce the computational complexity we want to find all $(j_1, \dots, j_n) \in \mathbb{N}^n$ with $j_1 + \cdots + j_n = n - 1$ that are the same up to cyclic permutations. It turns out, that every orbit under the cyclic group action on these indices has n elements. For $n \in \mathbb{N}$ let O_n be a set of indices so that each element is a representant of each distinct orbit of the cyclic group acting on the the indices $(j_1, \dots, j_n) \in \mathbb{N}^n$ with $j_1 + \cdots + j_n = n - 1$. Then

$$\alpha_n = \sum_{o\in O_n} \operatorname{tr} T_1 V_{o_1-1} \cdots T_1 V_{o_n-1}. \tag{2.4.2}$$

3 Exact Solution of 2×2 Case

In this section the linear perturbations series for a special toy case will be solved by hand. This allows to compare the results generated by the code to the analytic result. Namely the coefficients of the powers of x in equation 3.0.4 can be compared to the ones calculated using the code. This comparison is implemented in app/test.hs. For $E_1, E_2, a \in \mathbb{R}$ let

$$H := \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}$$

and

$$V := \begin{pmatrix} 0 & a \\ a & 0 \end{pmatrix}.$$

Define $T : \mathbb{C} \to \mathbb{C}^{2\times 2}$ by $T\ x = H + x \cdot V$. Assume that $E_1 \neq E_2$, then the two eigenvalues $E_\pm$ of $T\ x$ (the roots of the characteristic polynomial) can be found as

$$E_\pm(x) = \frac{E_1 + E_2}{2} \pm \frac{|E_1 - E_2|}{2} \sqrt{1 + \left(\frac{2ax}{E_1 - E_2}\right)^2}. \tag{3.0.1}$$

Now upon potentially relabeling $E_\pm$ we obtain

$$E_\pm(x) = \frac{E_1 + E_2}{2} \pm \frac{E_1 - E_2}{2} \sqrt{1 + \left(\frac{2ax}{E_1 - E_2}\right)^2}. \tag{3.0.2}$$

Now the binomial series says that for $x \in \mathbb{C}$ with $|x| < 1$:

$$(1 + x)^{1/2} = \sum_{k=0}^{\infty} \binom{1/2}{k} x^k, \tag{3.0.3}$$

where the radius of convergence of the power series is 1. Therefore

$$\begin{aligned} E_\pm(x) &= \frac{E_1 + E_2}{2} \pm \frac{E_1 - E_2}{2} \sum_{k=0}^{\infty} \binom{1/2}{k} \left(\frac{2ax}{E_1 - E_2}\right)^{2k} \\ &= E_{1/2} \pm \frac{1}{2} \sum_{k=1}^{\infty} \binom{1/2}{k} \frac{(2a)^{2k}}{(E_1 - E_2)^{2k-1}} x^{2k} \end{aligned} \tag{3.0.4}$$

where the radius of convergence r of the power series is

$$r = \frac{|E_1 - E_2|}{2|a|}. \tag{3.0.5}$$