FOUNDATION OF SCIENTIFIC COMMUNICATION:
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Operator-valued Taylor Expansion

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1. The setup

The goal of this exposition is to consider a strongly continuous one-parameter unitary group of operators and derive conditions for when such operators will admit a Taylor expansion. This result is directly related to the time and space evolution operators, since they are a class of operators that falls under the definition above.

The structure of this paper will rely on post-hoc assumptions since do not already know the required structures to imply analyticity and must derive them as we progress.

We will begin by first deriving conditions for analyticity for scalar-valued functions as a warm-up, the following chapter on Banach spaces is geared more towards highlighting how and why a topological notion of convergence is required when moving up to infinite dimensions, since of course our operators are defined to act on such spaces.

The fourth chapter on the operator valued Taylor expansion is half dedicated to setting up the topology required on operators to carry out further analysis which holds for a general one-parameter family of operators, and then we restrict ourselves to the case we're interested in by the (semi-)group properties of the operator family to greatly simplify derivatives and find constraints regarding the domain of the operators involved.

The fifth chapter introduces unitarity as an additional assumption and computes the anti self-adjointness (or self-adjointness if modified) of the generator as well as the quantitative upper bound on the growth of the norm of under n-fold applications of the generator.

We believe it will be fruitful to the reader if they first opt to skim the paper lightly to see the major differences in each chapter and then thoroughly read the material to find subtle nuances in the definitions, which we have done our absolute best to highlight.

2. The Scalar-valued Taylor expansion

The purpose of this section is two-fold, one is to serve as a review of the Taylor expansion in the familiar scalar valued case, the second is to carry out a bit of analysis in the 'post-hoc' style so that the reader can have a better understanding of how we intend to present things.

We consider $f(x) \in C^\infty(\mathbb{R})$ to be an infinitely differentiable real-valued function. The Taylor expansion with the integral form of the remainder is given by[1]

[1] The derivation of this is left as an exercise.

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(a)}{k!}(x-a)^k + \int_a^x \frac{f^{(n+1)}(t)}{n!}(x-t)^n \, dt$$

Where

$$R_n(x) = \int_a^x \frac{f^{(n+1)}(t)}{n!}(x-t)^n \, dt$$

Is the remainder term for the Taylor expansion upto the n-th order. Then as we add more and more terms into the expansion (make n larger) we expect the remainder term to go to zero as the polynomials should approximate the function better and better. To accomplish this we first estimate an upper bound on the remainder term

$$\begin{aligned} |R_n(x)| &\leq \left| \int_a^x \frac{f^{(n+1)}(t)}{n!}(x-t)^n \, dt \right| \\ &\leq \int_a^x \left| \frac{f^{(n+1)}(t)}{n!}(x-t)^n \right| \, dt \\ &= \frac{1}{n!} \int_a^x \left| f^{(n+1)}(t) \right| |(x-t)^n| \, dt \end{aligned}$$

The first observation is that we're only considering the Taylor expansion over a bounded set K, let the interval length (or more accurately, the Lebesgue measure) of K be ϵ. Then we have an upper bound on $(x-t)$, namely $|x-t| \leq \epsilon$, and so

$$|R_n(x)| \leq \frac{\epsilon^n}{n!} \int_a^x \left| f^{(n+1)}(t) \right| \, dt$$

Since we assumed that f was infinitely differentiable, all derivatives of f are continuous. Since K is a compact set, the extreme value theorem guarantees

$$\left| f^{(n+1)} \right|_\infty = \sup_{x \in K} \left| f^{(n+1)} \right|$$

exists and is finite. Furthermore, the integral $\int_a^x dt$ can also be bounded once again by ϵ and so

$$\begin{aligned} |R_n(x)| &\leq \frac{\epsilon^n}{n!} \left| f^{(n+1)} \right|_\infty \int_a^x dt \\ &\leq \frac{\epsilon^{(n+1)}}{n!} \left| f^{(n+1)} \right|_\infty \end{aligned}$$

We have simplified the upper bound as much as possible and are left with a condition, namely that the derivatives of f must grow at most factorially with an exponential rate strictly less than $\frac{1}{\epsilon}$, i.e.

$$\left| f^{(n+1)} \right|_\infty \leq C \frac{n!}{\epsilon'^{(n+1)}}$$

Where $\epsilon' > \epsilon$ Since then this will give

$$\begin{aligned} |R_n(x)| &\leq \frac{\epsilon^{(n+1)}}{n!} \cdot C \frac{n!}{\epsilon'^{(n+1)}} \\ &= C \left(\frac{\epsilon}{\epsilon'}\right)^{(n+1)} \end{aligned}$$

And this will tend to zero, this implies that smoothness alone is not enough for the remainder term to vanish and the Taylor expansion to be valid. It is necessary that the growth of the derivatives of the function must satisfy a quantitive growth condition, and this is precisely the condition for a function to be real-analytic over a compact set.

The summary of our results in then is as follows

A smooth function $f \in C^\infty(\mathbb{R})$ is real-analytic (admits a Taylor expansion that converges uniformly to f) on a compact set K with interval length ϵ if there exists a constant C and an $\epsilon' > \epsilon$ such that for all n

$$\left| f^{(n+1)} \right|_\infty \leq C \frac{n!}{\epsilon'^{(n+1)}}$$

3. The Banach-valued Taylor expansion

In the last section, we discussed a smooth single parametric scalar-valued function, i.e. $f : \mathbb{R} \to \mathbb{R}$. Now we generalize slightly to a smooth vector valued function $g : \mathbb{R} \to \mathbb{R}^p$. Fortunately, the generalization will not be too much of a hassle, as recall that a vector-valued function such as g can be written as

$$\begin{aligned} g &: \mathbb{R} \to \mathbb{R}^p \\ x &\mapsto \big(g_1(x), g_2(x), ...g_p(x)\big) \end{aligned}$$

We can then write out the Taylor expansion in two ways, the straightforward way is to consider each component g_l of g and write out its Taylor expansion

$$g_l(x) = \sum_{k=0}^{n} \frac{g_l^{(k)}(a)}{k!}(x-a)^k + \int_a^x \frac{g_l^{(n+1)}(t)}{n!}(x-t)^n \, dt$$

and then reach a very natural conclusion, if each component-function admits a Taylor expansion over some compact interval K, then g as a whole admits a Taylor expansion over K, formally

A smooth single-parametric vector-valued g function is analytic if, and only if, all of its component functions $g_l \in C^\infty(\mathbb{R})$ are real-analytic.

This, although a useful lemma in its own right, isn't easily applicable in the territory of infinite-dimensional vector spaces where we're headed since we'd have to check the analyticity of every one of the infinite component functions. Bearing this in mind, we are forced to develop a notion of convergence of vector-valued functions directly without considering component vectors.

From here on out, we will consider $g : \mathbb{R} \to \mathcal{B}$ to be a single-parametric function from $\mathbb{R}$ to a possibly infinite dimensional Banach space $\mathcal{B}$. The reason for choosing a Banach space is that it is a normed vector space, and so it is equipped with the following map

$$|\cdot| : \mathcal{B} \to \mathbb{R}$$

Which assigns a notion of 'length' to every vector in the vector space. Convergence is then straightforward to define, consider a sequence of vectors v_n, we say that v_n converges to a vector w if, and only if

$$\lim_{n\to\infty} |v_n - w| = 0$$

and the second reason is that a Banach space is complete, in particular, every sequence of vectors v_n that converges, converges to a vector inside the space $\mathcal{B}$, so we do not have any pathological edge cases in the following analysis. Now let us write out the Taylor expansion of g, not as components but as the entire function

$$g(x) = \sum_{k=0}^{n} \frac{g^{(k)}(a)}{k!}(x-a)^k + \int_a^x \frac{g^{(n+1)}(t)}{n!}(x-t)^n \, dt$$

Note that expressions on both sides evaluate to a vector. Recall that in the case of the scalar-valued expansion, we required that the remainder term tend to zero for larger and larger n. Here we will impose an almost identical condition, that is, that the remainder term tend to the zero vector. Recall however that a norm has the property

$$|v| = 0 \iff v = 0$$

So we impose the condition

$$\lim_{n\to\infty} \left| \int_a^x \frac{g^{(n+1)}(t)}{n!}(x-t)^n \, dt \right| \to 0$$

Assuming a compact K of interval length ϵ for which we want this Taylor expansion to be valid, the remainder term can be bounded above by

$$|R_n(x)| \leq \frac{\epsilon^n}{n!} \int_a^x \left| g^{(n+1)}(t) \right| \, dt$$

Now, very similarly to how the supremum norm of the scalar-valued function was defined, we can define a supremum norm of Banach valued functions over a compact interval as

$$\left| g^{(n+1)} \right|_\infty := \sup_{x\in K} \left| g^{(n+1)}(x) \right|$$

and then we arrive at the very familiar upper bound

$$|R_n(x)| \leq \frac{\epsilon^{(n+1)}}{n!} \left| g^{(n+1)}(t) \right|_\infty$$

which yields a quantitive bound on the growth rate of derivatives of g

$$\left| g^{(n+1)} \right|_\infty \leq C \frac{n!}{\epsilon'^{(n+1)}}$$

Where $\epsilon' > \epsilon$. One may ask after arriving at this conclusion that what exactly is the difference here and in the case of scalar valued expansions since they look exactly identical. The difference lies in definition of how $|\cdot|_\infty$ was defined, in the first case it was the absolute value of the output of f, in the Banach-valued case here it was the norm of the output of g, apart from that and the fact that they are maps into different spaces, the techniques used were identical. Whether or not this is an elegant difference or a curse of mathematics is up to the reader's interpretation.

4. The Operator-valued Taylor expansion

We have covered the case $g : \mathbb{R} \to \mathcal{B}$, now we consider operator valued functions $\hat{A} : \mathbb{R}^+ \to L(\mathcal{H})$ with domain $t \geq 0$ and the composition property $\hat{A}(t+s) = \hat{A}(t)\hat{A}(s)$ and $\hat{A}(0) = \hat{1}$. These two properties turn the family of operators in the image of $\hat{A}$ into a semi-group and then we will additionally assume continuity with respect to a notion of convergence which will enable us to define the derivative of such a function.

We can attempt to write out a formal Taylor series for $\hat{A}$ analogous to the previous cases

$$\hat{A}(x) = \sum_{k=0}^{n} \frac{\hat{A}^{(k)}(a)}{k!}(x-a)^k + \int_a^x \frac{\hat{A}^{(n+1)}(t)}{n!}(x-t)^n \, dt$$

But it is not immediately obvious how we can give meaning to such an expression. We can however take inspiration from Banach-valued expansions, recall there we had defined convergence using a norm and then it was relatively straightforward to ask for a condition for the convergence of the Taylor expansion. In a similar vein, we can attempt to define a notion of convergence on operators and under such a notion assert that the remainder term vanishes so that in the limit for large n the formal Taylor expansion becomes equal to the original operator valued function.

The natural choice of convergence for our purpose is the Strong operator topology which is defined as follows, let ϕ be an arbitrary vector in $\mathcal{H}$, let $\hat{A}_n$ be a sequence of operators, then $\hat{A}_n$ converges to $\hat{A}$ in the seminorm induced by ϕ if, and only if

$$\lim_{n\to\infty} |\hat{A}_n(\phi) - \hat{A}(\phi)| = 0$$

Essentially, two operators are equivalent in the seminorm induced by ϕ if their action on ϕ is identical. And then we can assert that two operators are identical if, and only if they are equivalent in the seminorms induced by every ϕ in the space $\mathcal{H}$.

With this, we now fix an arbitrary vector ϕ for our operators to act on and the Taylor expansion now reads

$$\left(\hat{A}(x)\right)(\phi) = \sum_{k=0}^{n} \frac{\left(\hat{A}^{(k)}(a)\right)(\phi)}{k!}(x-a)^k + \int_a^x \frac{\left(\hat{A}^{(n+1)}(t)\right)(\phi)}{n!}(x-t)^n \, dt$$

And upon closer inspection, we observe that the expression on either side evaluates ultimately to a vector and we have reduced back to the Banach-valued case. Up until this point everything that was said was true for arbitrary single-parametrized operator valued functions, however our main interest is in the class of operator valued functions that satisfy the semi-group properties stated above, and so we restrict our analysis to them.

The operator-valued function $\hat{A}$ is continuous at $t = 0$ with respect to the seminorm induced by $\phi \in \mathcal{H}$ if

$$\lim_{t \to 0} \left| \left(\hat{A}(t)\right)(\phi) - \hat{1}(\phi) \right| = 0$$

This defines continuity simply only at the point $t = 0$, however, combined the semigroup properties of $\hat{A}$ continuity at one point implies continuity everywhere since, assume WLOG $t > s$

$$\begin{aligned}
\lim_{t \to s} \left| \left(\hat{A}(t) - \hat{A}(s)\right)(\phi) \right| &= \lim_{t' \to 0} \left| \left(\hat{A}(t'+s) - \hat{A}(s)\right)(\phi) \right| \\
&= \lim_{t' \to 0} \left| \left(\hat{A}(t')\hat{A}(s) - \hat{A}(s)\right)(\phi) \right| \\
&= \lim_{t' \to 0} \left| \left[\left(\hat{A}(t') - \hat{1}\right)\hat{A}(s)\right](\phi) \right| \\
&= 0
\end{aligned}$$

And so, assuming continuity the derivative of $\hat{A}$ at $t = 0$

$$\hat{H} := \lim_{t \to 0} \frac{\left(\hat{A}(t)\right)(\phi) - \hat{1}(\phi)}{t}$$

And this is well-defined whenever limit exists, and whether or not it exists depends also on the fixed vector ϕ under consideration. It is also easy to see that differentiability at one point implies differentiability everywhere since

$$\begin{aligned}
\lim_{t \to s} \frac{\left(\hat{A}(t)\right)(\phi) - \left(\hat{A}(s)\right)(\phi)}{t-s} &= \lim_{t' \to 0} \frac{\left(\hat{A}(t'+s)\right)(\phi) - \left(\hat{A}(s)\right)(\phi)}{t'} \\
&= \lim_{t' \to 0} \frac{\left(\hat{A}(t')\hat{A}(s)\right)(\phi) - \left(\hat{A}(s)\right)(\phi)}{t'} \\
&= \lim_{t' \to 0} \left(\left[\frac{\hat{A}(t') - \hat{1}}{t'}\right]\hat{A}(s)\right)(\phi) \\
&= \left(\hat{H}\hat{A}(s)\right)(\phi)
\end{aligned}$$

$\hat{H}$ is called the generator of the operator $\hat{A}$. From here we have another constraint, namely that $\left(\hat{A}(s)\right)(\phi) \in D(\hat{H})$. For higher order derivatives, we have

$$\left(\hat{A}^{(n)}(s)\right)(\phi) = \left(\hat{H}^n \hat{A}(s)\right)(\phi)$$

Which implies that if we wish to have a well-defined Taylor expansion then

$$\left(\hat{A}(s)\right)(\phi) \in \bigcap_{n}^{\infty} D(\hat{H}^n)$$

must hold. It is very important to note here that what we just described is one constraint on ϕ required for *analyticity* of the operator, in the case of Schrödinger's equation and the time evolution operator the dynamics of the system are well defined so long as the state vector ϕ satisfies $\left(\hat{\mathcal{U}}(s)\right)(\phi) \in D(\hat{H})$. We may now write out the Taylor expansion as follows, however we postpone the derivation of the quantitative bound on the growth of $\left(\hat{H}^{(n+1)}\hat{A}(t)\right)(\phi)$ until the next chapter as well.

$$\left(\hat{A}(x)\right)(\phi) = \sum_{k=0}^{n} \frac{\left(\hat{H}^k\hat{A}(a)\right)(\phi)}{k!}(x-a)^k + \int_a^x \frac{\left(\hat{H}^{(n+1)}\hat{A}(t)\right)(\phi)}{n!}(x-t)^n \, dt$$

5. Analyticity of the Time-evolution operator

Consider the time-evolution operator $\hat{\mathcal{U}}(t)$, in physics this an operator on the Hilbert space of physical states $\mathcal{H}$ that takes a state vector depending on position x and time t_0 $\alpha(x, t_0)$ to $\alpha(x, t_0 + t)$. The family of these operators generated by the operator-valued function $\mathcal{U} : \mathbb{R} \to L(\mathcal{H})$ is a group[2] since $\hat{\mathcal{U}}(0)$ must leave the vector unaltered and $\hat{\mathcal{U}}(t+s)$ should correspond to first evolving the vector by s then t or vice versa. Additionally, this family of operators is unitary simply for the fact that all state vectors are normalized to have a length of one and time evolution must preserve this property otherwise there would be pathological implications regarding the probability amplitude of the state vector.

Unitarity of $\hat{\mathcal{U}}$ has direct implications on its generator $\hat{H}$ since

$$\begin{aligned}
\hat{\mathcal{U}}(t)^\dagger\hat{\mathcal{U}}(t) &= \hat{1} \\
\left(\hat{H}\hat{\mathcal{U}}(t)\right)^\dagger \hat{\mathcal{U}}(t) + \hat{\mathcal{U}}(t)^\dagger \left(\hat{H}\hat{\mathcal{U}}(t)\right) &= 0 \\
\hat{\mathcal{U}}(t)^\dagger\hat{H}^\dagger\hat{\mathcal{U}}(t) &= -\hat{\mathcal{U}}(t)^\dagger\hat{H}\hat{\mathcal{U}}(t) \\
\left(\hat{\mathcal{U}}(t)^\dagger\hat{H}\hat{\mathcal{U}}(t)\right)^\dagger &= -\hat{\mathcal{U}}(t)^\dagger\hat{H}\hat{\mathcal{U}}(t)
\end{aligned}$$

We see that the adjoint picks up a negative sign, since $\hat{\mathcal{U}}$ is self-adjoint by assumption the only possibility is that $\hat{H}$ is anti self-adjoint. In physics, it is preferable to keep all operators self-adjoint so that their spectra are real and the operator itself can correspond to some observable. In the case of an anti self-adjoint operator this is easily accomplished

$$H := -i\hat{H}$$

However this we will simply continue with $\hat{H}$ as we have done so far. We will now derive the quantitative growth bound on the remainder term of the Taylor expansion

[2] See remarks

from the last section

$$|R_n(x)| \leq \left| \int_a^x \frac{\left(\hat{H}^{(n+1)}\hat{A}(t)\right)(\phi)}{n!}(x-t)^n \, dt \right|$$

Recall that for a compact set K with interval length ϵ, we have an upper bound $(x-t) \leq |x-t| \leq \epsilon$

$$|R_n(x)| \leq \frac{\epsilon^n}{n!} \int_a^x \left| \left(\hat{H}^{(n+1)}\hat{A}(t)\right)(\phi) \right| \, dt$$

Since the expression $\left(\hat{H}^{(n+1)}\hat{A}(t)\right)(\phi)$ is a vector in our space of states $\mathcal{H}$ for each t, we can define using the inner product on $\mathcal{H}$

$$\left| \left(\hat{H}^{(n+1)}\hat{A}\right)(\phi) \right|_\infty = \sup_{x \in K} \left| \left(\hat{H}^{(n+1)}\hat{A}(t)\right)(\phi) \right|$$

However, since $\hat{A}$ is unitary, it preserves the inner product, so instead we write

$$\begin{aligned} \left| \hat{H}^{(n+1)}(\phi) \right|_\infty &= \sup_{t \in K} \left| \hat{H}^{(n+1)}(\phi) \right| \\ &= \left| \hat{H}^{(n+1)}(\phi) \right| \end{aligned}$$

And so we can simplify the supremum norm $|\cdot|_\infty$ to just the simple norm $|\cdot|$ since $\hat{H}$ is independent of t. Lastly, since $\left|\int_a^x dt\right| \leq \epsilon$ the upper bound on the remainder term is given by

$$|R_n(x)| \leq \frac{\epsilon^{(n+1)}}{n!} \left| \hat{H}^{(n+1)}(\phi) \right|$$

And once again, we have arrived for the third time at this expression, however this one does have an important difference from the previous two, in those cases the bound was on the growth of derivatives of the function over some compact interval and that was the condition of analyticity, in this case, the derivatives portion of the definition carries over, however this bound is with respect to a fixed vector $\phi \in \mathcal{H}$, and so it corresponds the analyticity of $\hat{\mathcal{U}}$ only in the seminorm induced by ϕ (or stated another way, only with respect to the vector ϕ) moreover, all the vectors for which $\hat{\mathcal{U}}$ is analytic are called the analytic vectors of $\hat{\mathcal{U}}$.

And now we can formally write out our results

A one-parameter family of strongly continuous unitary group of operators $\left\{\hat{T}(t)\right\}_{t\in\mathbb{R}}$ on $\mathcal{H}$ is analytic on a compact parameter domain K in the semi-norm induced by $\phi \in \mathcal{H}$ if

1. $\hat{T}$ is strongly differentiable wrt. the seminorm induced by ϕ so that the limit

$$\hat{H} := \lim_{x\to 0} \frac{\left(\hat{T}(x)\right)(\phi) - \hat{1}(\phi)}{x}$$

exists, where $\hat{H}$ is called the generator of the family of operators $\hat{T}$

2. The vector ϕ satisfies

$$\left(\hat{T}(t)\right)(\phi) \in \bigcap_{n}^{\infty} D(\hat{H}^n)$$

3. The quantitative growth constraint

$$\left|\hat{H}^{(n+1)}(\phi)\right| \leq C\frac{n!}{\epsilon'^{(n+1)}}$$

is satisfied, where $\epsilon' > \epsilon$ and $\epsilon = |K|$, the interval length of K

In addition, for all vectors ϕ for which the above conditions are satisfied are called analytic vectors of $\hat{T}$

Remarks

The last theorem in the document is a list of the necessary conditions for a family of operators to be analytic, however, as earlier stated in the text, the dynamics of a physical system do not require such strong conditions to be well defined, in particular condition (2) can be simplified to

$$\left(\hat{T}(t)\right)(\phi) \in D(\hat{H})$$

And condition (3) can be dropped entirely. For more information, the reader is encouraged to see Stone's theorem on strongly continuous one parameter unitary groups.

What was recovered in this text was the time evolution operator for the time-independent hamiltonian operator. For a time-dependent hamiltonian operator one would have to consider a family of two-parameter operators

$$\hat{\mathcal{U}}(t, t_0)$$

The reason for this is as follows, for dynamical systems exhibiting symmetry in time-translations it is sufficient to have a generator at any one point in time and the same generator defines time evolution over all of time. For systems where translations in time is not independent, at each time t the generator defining the time evolution will be different, the second parameter captures exactly this behaviour and the Taylor expansion in such a case will instead become what is referred to as a Dyson series.

In chapter four we assumed the one-parameter family to only have semi-group properties and that was sufficient for the derivations in listed there. In chapter five, by assuming unitarity of the family of operators, the semi-group becomes a group due to the additional structure lent by unitarity, in particular, it guarantees that each operator $\hat{T}(t)$ is invertible, which allows us to define

$$\hat{T}(-t) := \hat{T}(t)^{-1} = \hat{T}(t)^{\dagger}$$
$$\hat{T}(t)\hat{T}(-t) = \hat{T}(t)\hat{T}(t)^{\dagger} = \hat{1}$$

The reason why they are not a group from the start is because the one-parameter family is parametrized by $t \geq 0$, this definition is standard since other dynamical systems e.g. modelling heat, diffusion or other dissipative systems are not necessarily reversible. In quantum dynamical systems ideally the information contained within the state vector is entirely preserved, this is why unitarity is a postulate and reversibility is a possibility.

The reason why it is the Hamiltonian that is the generator of the time-evolution, to my knowledge, cannot be derived from mathematical principles alone, instead one must look to symmetries and the conservation laws of physics and postulate that if the one-parameter family in question is parametrized by time, and since symmetry in time corresponds to conservation of energy, the operator family must be generated by something associated to the energy of the dynamical system, which is indeed the Hamiltonian itself.