Zassenhaus Splittings Beyond Bounded Operators

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Setting the stage

$$\partial_t u(t) = (A + B)u(t), \qquad u(0) = u_0, \qquad t \in [0, T].$$

- $A, B \colon \mathscr{H} \to \mathscr{H}$ bounded or unbounded linear operators.
- In general, $[A, B] = AB - BA \neq 0$.
- $u_0 \in \mathscr{H}$, and $T > 0$.

Example

$$\mathrm{i}\partial_t u = -\partial_x^2 u + V(x)u, \qquad x \in \mathbb{R}.$$

With $H = -\partial_x^2 + V$, the evolution equation is $\partial_t u = (A+B)u$, where

$$A = \mathrm{i}\partial_x^2, \qquad B = -\mathrm{i}V.$$

- A is unbounded on $\mathscr{H} = \mathrm{L}_2(\mathbb{R})$, with $\mathrm{dom}(A) = \mathrm{H}^2(\mathbb{R})$.
- If $V \in \mathrm{L}_\infty(\mathbb{R})$ is real-valued, then H is self-adjoint on $\mathrm{H}^2(\mathbb{R})$.
- $A + B = -\mathrm{i}H$ is skew-adjoint and generates a unitary group.

Bounded operators

Strang splitting

For a bounded operator X,

$$e^X := \exp(X) = \sum_{k=0}^{\infty} \frac{X^k}{k!}.$$

Define

$$U(\tau) := e^{\tau(A+B)}, \qquad S(\tau) := e^{\frac{1}{2}\tau A} e^{\tau B} e^{\frac{1}{2}\tau A}.$$

- The splitting is “useful” when the flows of A and B are simpler than those of $A + B$.
- For the TDSE, all three flows remain unitary.
- Question: **How accurately** does $S(\tau)$ approximate $U(\tau)$?

Symmetric BCH formula

Introduce $\mathrm{sBCH}(\tau A, \tau B)$ through

$$S(\tau) = \mathrm{e}^{\mathrm{sBCH}(\tau A, \tau B)}.$$

Expanding the exponentials shows

$$\mathrm{sBCH}(\tau A, \tau B) = \tau(A+B) - \frac{\tau^3}{24}[[B,A],A] - \frac{\tau^3}{12}[[B,A],B] + \mathscr{O}(\tau^5).$$

Hence, we identify **local order three**:

$$U(\tau) - S(\tau) = \frac{\tau^3}{24}\Big([[B,A],A] + 2[[B,A],B]\Big) + \mathscr{O}(\tau^4).$$

Bridging numerics and physics

The real line matters

The TDSE evolves on an **unbounded physical domain**.

A finite box introduces artificial boundaries: Dirichlet conditions may cause reflections, while periodic BCs make outgoing wave packets re-enter from the opposite boundary.

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Article

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Time-Sliced Thawed Gaussian Propagation Method for Simulations of Quantum Dynamics

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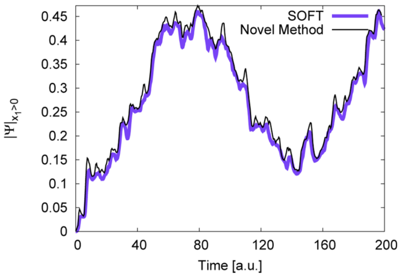

Motivation for higher-order splittings

$$\mathrm{i}\varepsilon\partial_t u = -\varepsilon^2\partial_x^2 u + V(x)u, \qquad 0 < \varepsilon \ll 1.$$

With $A = \mathrm{i}\varepsilon\partial_x^2$ and $B = -\mathrm{i}\varepsilon^{-1}V$,

$$[[A,B],B] = 2\varepsilon^{-1}(\partial_x V)^2.$$

Therefore, the leading Strang error scales as

$$\mathscr{O}(\tau^3\varepsilon^{-1}).$$

Effective order: $\tau \sim \varepsilon \Rightarrow \mathscr{O}(\tau^2)$, $\tau \sim \sqrt{\varepsilon} \Rightarrow \mathscr{O}(\tau)$.

Symmetric Zassenhaus splittings

Introduced for the TDSE by *Bader, Iserles, Kropielnicka and Singh* (2014); constructed so that

$$U(\tau) - Z_{2n-1}(\tau) = \mathscr{O}(\tau^{2n+1}), \qquad (n \geq 1).$$

The sZ splitting has the form (example on next slide)

$$Z_{2n-1}(\tau) := \prod_{\ell=0}^{n} \mathrm{e}^{\mathscr{R}_{2\ell-1}(\tau)} \prod_{\ell=0}^{n} \mathrm{e}^{\mathscr{R}_{2(n-\ell)-1}(\tau)} =: Z^{[-1,2n-1]}(\tau) Z^{[2n-1,-1]}(\tau),$$

with $\mathscr{R}_{-1}(\tau) = \frac{1}{2}\tau A$, $\mathscr{R}_{1}(\tau) = \frac{1}{2}\tau B$, and nested commutators $\mathscr{R}_{2\ell-1}$ of length $2\ell - 1$.

In particular, $S(\tau) = Z_1(\tau)$.

The **local order-five method** is

$$Z_3(\tau) = \mathrm{e}^{\frac{1}{2}\tau A}\mathrm{e}^{\frac{1}{2}\tau B}\mathrm{e}^{2\mathscr{R}_3(\tau)}\mathrm{e}^{\frac{1}{2}\tau B}\mathrm{e}^{\frac{1}{2}\tau A},$$

$$\mathscr{R}_3(\tau) = \frac{\tau^3}{48}\Big([[B,A],A] + 2[[B,A],B]\Big).$$

The higher exponents $\mathscr{R}_{2\ell-1}$ follow by repeatedly applying truncated sBCH formulas and separating the leading term at each stage.

For the TDSE, *Lasser and Lubich* (2020) showed (for bounded potentials) that:

- $\|U(\tau)\psi - Z_1(\tau)\psi\|_{L^2} \leq c\tau^3\|\psi\|_{H^2}$
- $\|U(\tau)\psi - Z_3(\tau)\psi\|_{L^2} \leq c\tau^5\|\psi\|_{H^4}$

The direct proof fails for unbounded operators

The Taylor remainder of $\tau \mapsto U(\tau)u_0$ contains

$$\mathrm{e}^{\xi(A+B)}(A+B)^{2n+1}u_0, \qquad \xi \in (0,\tau).$$

It therefore requires

$$u_0 \in \operatorname{dom}\left((A+B)^{2n+1}\right).$$

Directly expanding Z_{2n-1} creates a similar domain problem.

Integral representation of the local error

$$E_{2n-1}(\tau) = U(\tau) - Z_{2n-1}(\tau). \tag{1}$$

After differentiating (1), a Duhamel argument yields

$$E_{2n-1}(\tau) = \int_0^\tau U\left(\frac{\tau - s}{2}\right) N_{2n-1}(s) U\left(\frac{\tau - s}{2}\right) \mathrm{d}s.$$

The bounded analysis implies $E_{2n-1}(\tau) = \mathscr{O}(\tau^{2n+1})$. We therefore conclude

$$N_{2n-1}(s) = \mathscr{O}(s^{2n}).$$

The remainder function can be written as

$$N_{2n-1}(\tau) = \sum_{\ell=1}^{n} \Big(Z_{2n-1}(\tau) f_\ell(\tau) + f_\ell(-\tau) Z_{2n-1}(\tau) \Big) \tau^{2\ell-2},$$

with

$$f_1(\tau) := \frac{1}{2}B - \frac{1}{2}\mathrm{e}^{-\frac{1}{2}\tau A} B \mathrm{e}^{\frac{1}{2}\tau A},$$

$$f_\ell(\tau) := (1-2\ell) Z^{[-1,2\ell-3]}(-\tau) \mathscr{R}_{2\ell-1}(1) Z^{[2\ell-3,-1]}(\tau), \quad 2 \le \ell \le n.$$

We can see the appearance of **sandwich terms**.

Subspace restriction: $\mathrm{ad}_A^2(B) = [A,[A,B]]$ is controlled in H^2, $\mathrm{ad}_A^3(B)$ in H^4.

Infinite expansion for bounded operators

The identity we exploit is

$$\mathrm{e}^{tX} Y \mathrm{e}^{-tX} = \sum_{j=0}^{\infty} \frac{t^j}{j!} \operatorname{ad}_X^j(Y).$$

More generally, for

$$A(t) := \left(\mathrm{e}^{t^{k_q} X_q} \cdots \mathrm{e}^{t^{k_1} X_1}\right) Y \left(\mathrm{e}^{-t^{k_1} X_1} \cdots \mathrm{e}^{-t^{k_q} X_q}\right),$$

there are commutators B_p of length $p + \ell(Y)$ such that

$$A(t) = \sum_{p=0}^{\infty} B_p t^p.$$

Algebraic identities

Applying the expansions to the error representation gives

$$\mathscr{O}(s^{2n}) = N_{2n-1}(s) = \sum_{m=0}^{2n-1} \mathscr{N}_m(s)s^m + \mathscr{O}(s^{2n}).$$

Collecting equal powers of s yields

$$\sum_{m=0}^{2n-1} \mathscr{N}_m(s)s^m = \sum_{k=0}^{2n-1} s^k \sum_{(m,r)\in\Omega_k} [s^r]\mathscr{N}_m(s) + \mathscr{O}(s^{2n}).$$

$\Omega_k := \{(m,r) \in \mathbb{Z}^2_{\geq 0} : m + r = k\}$, $\forall m : \mathscr{N}_m(s)$ contains $Z_{2n-1}(s)$

Theorem (condensed version)

The symmetric Zassenhaus construction provides the **algebraic identities**

$$\sum_{(m,r)\in\Omega_k} [s^r]\mathscr{N}_m(s) = 0, \qquad 0 \le k \le 2n-1.$$

Example

$$[s^2]\mathscr{N}_0(s) + [s^1]\mathscr{N}_1(s) + [s^0]\mathscr{N}_2(s) = \frac{1}{4}\,[A+B,[A,B]] - \frac{2}{8}\,[A+B,[A,B]] = 0.$$

Unbounded operators

(From now on, the symbol e^{tX} denotes a strongly continuous group on $\mathscr{H}$.)

Finite expansions

$$h(t) := \mathrm{e}^{t^k X} Y \mathrm{e}^{-t^k X}, \qquad k = \ell(X).$$

Taylor's theorem gives

$$h(t) = \sum_{s=0}^{\nu} \frac{t^s}{s!} h^{(s)}(0) + \int_0^t \frac{(t-\tau)^\nu}{\nu!} h^{(\nu+1)}(\tau)\, \mathrm{d}\tau.$$

Moreover (via Faà di Bruno),

$$h^{(s)}(t) = \sum_m C_{m,s} \mathrm{e}^{t^k X} \mathrm{ad}_X^{|m|}(Y) \mathrm{e}^{-t^k X} t^{k|m|-s}.$$

Largest commutator: $\mathrm{ad}_X^{\nu+1}(Y)$, length $k(\nu+1)+\ell(Y)$. Remainder needs special treatment.

Theorem (condensed version)

Let $X_1, \dots, X_q$ and Y be commutators, with

$$\ell(X_j) = k_j, \qquad k_1 \geq \cdots \geq k_q \geq 1.$$

For a truncation order $P \geq 1$, set $P^* := P + \ell(Y) + k_1$.

Let $\mathscr{D}$ be densely and continuously embedded into $\mathscr{H}$ and assume that:

- commutators up to length P^* extend boundedly from $\mathscr{D}$ to $\mathscr{H}$,
- the Zassenhaus factors leave $\mathscr{D}$ invariant and satisfy local group bounds.

Then,

$$\left(\mathrm{e}^{t^{k_q}X_q}\cdots\mathrm{e}^{t^{k_1}X_1}\right)Y\left(\mathrm{e}^{-t^{k_1}X_1}\cdots\mathrm{e}^{-t^{k_q}X_q}\right)=\sum_{p=0}^{P}B_p t^p+R_{P+1}(t)$$

as an identity in $\mathscr{L}(\mathscr{D},\mathscr{H})$, where

$$R_{P+1}(t)=\mathscr{O}(t^{P+1}),\qquad \ell(B_p)=p+\ell(Y).$$

A formal truncation at order P suggests **commutators up to length** $P+\ell(Y)+1$.

Overshoots

The remainder estimate requires commutators up to

$$P^* = P + \ell(Y) + k_1.$$

Whenever $k_1 > 1$,

$$\underbrace{P + \ell(Y) + 1}_{\text{formal expectation}} \quad < \quad \underbrace{P + \ell(Y) + k_1}_{\text{remainder control}}.$$

We call this additional commutator depth an **overshoot**.

Local error for unbounded operators

Theorem (condensed version)

For $n \geq 1$, consider the symmetric Zassenhaus splitting Z_{2n-1} and let

$$L_n = \max\{2n+1, 4n-3\} = \begin{cases} 3, & n = 1, \\ 4n-3, & n \geq 2. \end{cases}$$

Assume that commutators up to length L_n extend boundedly from $\mathscr{D}$ to $\mathscr{H}$, and that there is a dense subset $\mathscr{D}_0 \subseteq \mathscr{D}$ on which the required commutator identities hold.

Then there exists $C > 0$ such that

$$\|U(\tau)\psi - Z_{2n-1}(\tau)\psi\|_{\mathscr{H}} \leq C\tau^{2n+1}\|\psi\|_{\mathscr{D}}, \qquad \psi \in \mathscr{D}.$$

Thank you