The Baker–Campbell–Hausdorff (BCH) Formula

Combining Exponentials of Non-commuting Operators

Graduate Physics Lecture

Outline

Motivation: Non-commuting Exponentials

- In quantum mechanics and Lie theory, we often encounter operators X and Y that do not commute ($[X, Y] \neq 0$).
- We want to find an effective operator Z such that: $\mathrm{e}^{X}\, e^{Y} = e^{Z}$, *for*X,Y*inaLiealgebra.If*X*and*Y*commute*, *thensimply*Z=X+Y.*Ifnot*,Z*ir* $= \log\left(e^{X} e^{Y}\right)$ is given by an infinite series in X, Y and their commutators. It provides a systematic expansion to combine exponentials of non-commuting operators .
- **Use Cases:** Combines two small transformations into one. Fundamental in connecting Lie group multiplication with Lie algebra addition, time-evolution with split Hamiltonians, etc.

Recall: Commutators and Lie Algebra

- The **commutator** of two operators is $[X, Y] = XY - YX$. It measures the failure to commute.
- For a Lie algebra (e.g. operators in quantum mechanics), commutators of algebra elements remain in the algebra.
- The BCH formula asserts Z can be expressed entirely in terms of X, Y, and nested commutators like $[X,[X,Y]]$, $[Y,[X,Y]]$, etc. – no other independent products appear .
- Notation: It's useful to denote $\mathrm{ad}_X(Y) := [X, Y]$. Then nested commutators are iterated adjoint actions (e.g. $\mathrm{ad}_X^2(Y) = [X,[X,Y]]$, etc.).
- We assume familiarity with basic Lie algebra identities (Jacobi identity: $[X,[Y,Z]] + [Y,[Z,X]] + [Z,[X,Y]] = 0$) which will simplify nested commutators.

BCH Expansion: First Terms

For $Z = \log(e^X e^Y)$, the expansion begins:

- The series alternates between symmetric and antisymmetric nested commutators at higher orders .
- All higher-order terms involve nested commutators of X and Y only. No ordinary products without commutators appear (ensuring Z lies in the same Lie algebra) .
- The coefficients $1/2, 1/12, 1/24, \ldots$ are fixed numerical values (involving Bernoulli numbers for higher terms). These were first worked out explicitly by Dynkin (1947) in general .

Series Characteristics

- The BCH series is generally infinite. In most cases, there is **no closed-form finite expression** for Z in terms of a finite number of terms .
- Each increasing order introduces more deeply nested commutators. For example:
  - 1st order: $X + Y$
  - 2nd order: $[X, Y]$
  - 3rd order: $[X, [X, Y]]$, $[Y, [X, Y]]$
  - 4th order: $[Y, [X, [X, Y]]]$, $[X, [Y, [Y, X]]]$, etc.
- The number of independent commutator terms grows rapidly with order. (All such terms up to 6th order are listed in the literature , but it becomes cumbersome beyond a few orders.)
- Fortunately, many practical scenarios require only the first few terms for approximation.
- If X and Y are "small" (e.g. small matrices or small time-step in evolution), the series converges and truncating after a few terms can give a good approximation .

Derivation: Outline (up to Third Order)

- **Method:** Compare power series of $e^X e^Y$ and e^Z and solve for Z order-by-order .
- Expand both sides: $e^X e^Y = I + X + Y + \frac{1}{2}(X^2 + XY + YX + Y^2) + \frac{1}{6}(X^3 + \cdots) + \cdots e^Z = I + Z + \frac{1}{2}Z^2 + \frac{1}{6}Z^3 + \cdots where \mathrm{Z} = \mathrm{X} + \mathrm{Y} + \mathrm{A}_2 + A_3 + \cdots$ (with A_n = terms of order n in X, Y).
- **First order:** Match linear terms: $Z^{(1)} = X + Y$. So far $Z = X + Y$.
- **Second order:** The $e^X e^Y$ expansion has $\frac{1}{2}(XY + YX)$ at order 2. Meanwhile e^Z gives $\frac{1}{2}(X + Y)^2 = \frac{1}{2}(X^2 + XY + YX + Y^2)$. The extra X^2 and Y^2 terms match on both sides, but $XY + YX$ vs $XY + YX$ is already present. However, note that $XY + YX$ cannot simplify to $2XY$ unless $XY = YX$. The discrepancy appears at this order .
- Thus, we postulate Z has a second-order correction $A_2 = \frac{1}{2}[X, Y]$ to account for the difference: $\mathrm{XY} + \mathrm{YX} = (\mathrm{X}{+}\mathrm{Y})^2 - X^2 - Y^2 = XY + YX, but including \mathrm{A}_2$ in Z yields new cross terms when squaring Z: $1 \frac{}{2(X+Y+A_2)^2 - \frac{1}{2}(X^2+XY+YX+Y^2+[X,Y]), which adds the}$ $\mathrm{[X,Y]} term we need. So \mathrm{A}_2$

Special Case: Commutator is Central

- If $[X, Y]$ commutes with both X and Y (i.e. $[X, Y] = c, I$, a scalar multiple of the identity), **all higher-order commutators vanish**. In this case the BCH series *terminates* after the second term .
- Then the exact result is: Z = X + Y + $1\frac{}{2[X,Y]\text{,andnofurthercorrectionsareneeded.Thisscenariooccursofteninquantummechanicswhe}}$ *number(forexample, ifXandYareoperatorsproportionaltocanonicalvariable*
- **Example:** Position and momentum operators satisfy $[x, p] = i\hbar I$. Thus, $\mathrm{e}^{\frac{i}{\hbar}ax}\, e^{\frac{i}{\hbar}bp} = \exp\Big(\frac{i}{\hbar}(ax + bp) + \frac{i}{2\hbar}ab[x, p]\Big) =$ $e^{\frac{i}{\hbar}(ax+bp+\frac{1}{2}ab\,i\hbar)}$ *,yieldingaphasefactor*$e$$\mathrm{e}^{-iab/2}$ times $e^{\frac{i}{\hbar}(ax+bp)}$. (This is the basis of the Weyl representation in quantum mechanics.)
- Another example: For harmonic oscillator ladder operators $[a, a^\dagger] = 1$, the displacement operator factorization $e^{\alpha a} e^{-\alpha^* a^\dagger} = e^{-|\alpha|^2/2} e^{-\alpha^* a^\dagger + \alpha a}$ follows from BCH truncation.

Application: Lie Groups and Lie Algebras

- The BCH formula formalizes how group multiplication near the identity corresponds to addition in the Lie algebra plus commutator corrections .
- If X and Y are infinitesimal generators (Lie algebra elements), e^X and e^Y are group elements. Their product $e^X e^Y$ can be expressed as e^Z with Z in the Lie algebra, ensuring closure of the group-law in algebra terms.
- This underpins the Lie group–Lie algebra correspondence: the complicated group law (when the group is nonabelian) is captured by a formal power series in the algebra.
- **Example:** In $SO(3)$ (rotations), let X and Y be two small rotation generators (non-commuting). $e^X e^Y$ is a rotation whose generator Z is given by BCH. Thus, the axis and angle of the combined rotation can be found by computing Z. (In practice, one can compute up to a certain order if X, Y are small.)
- The BCH formula is used to prove properties like $\mathrm{tr}(\log(e^X e^Y)) = \mathrm{tr}(X) + \mathrm{tr}(Y)$ (since commutator contributions have

Application: Quantum Time Evolution

- In quantum mechanics, if the Hamiltonian $H = H_1 + H_2$ (two parts that do not commute), the time-evolution operator is $U(t) = e^{-iHt}$. Directly computing $e^{-i(H_1+H_2)t}$ is hard if H_1 and H_2 don't commute.
- Using BCH, we can approximate: $\mathrm{e}^{-i(H_1+H_2)\Delta t} = \exp\Big(- iH_1\Delta t - iH_2\Delta t - \frac{1}{2}[H_1, H_2](\Delta t)^2 + \cdots \Big), sotofirstorderin\Delta t,$ $\mathrm{e}^{-i(H_1+H_2)\Delta t} \approx e^{-iH_1\Delta t}e^{-iH_2\Delta t}, withanerroroforder(\Delta t)^2$ governed by $\frac{-i}{2}[H_1, H_2](\Delta t)^2$.
- **Lie–Trotter Product Formula:** By taking n small time steps, $\Big(\mathrm{e}^{-iH_1t/n}e^{-iH_2t/n}\Big)^n = e^{-i(H_1+H_2)t+O(t^2/n)} \to e^{-i(H_1+H_2)t}$ as $n \to \infty. Inpractice, evenmodest\mathrm{n} yieldsagoodapproximation. Higher - ordersplittingschemes(e.g.$ **Suzuki–Trotter decompositions**$)useBCHter$ $ordererrors. Forexample: e^{-i(H_1+H_2)\Delta t} = e^{-iH_1\Delta t/2}e^{-iH_2\Delta t}e^{-iH_1\Delta t/2} + O((\Delta t)^3), whicheliminatesthe\mathrm{O}((\Delta t)^2)$ error by symmetry. BCH provides the systematic way to analyze these errors (they come from commutators $[H_1, H_2]$, $[H_1, [H_1, H_2]]$, etc.).

Application: Quantum Computing (Hamiltonian Simulation)

- In quantum algorithms, especially for Hamiltonian simulation, we need to implement $U(t) = e^{-i(H_1+H_2+\cdots)t}$ via a sequence of quantum gates.
- The BCH formula underlies the **Trotter-Suzuki product formula** approach: $\mathrm{e}^{-i(H_1+H_2)t} \approx \left(e^{-iH_1t/n}e^{-iH_2t/n}\right)^n, which becomes exact as \mathrm{n} \to \infty$. For finite n, one incurs a small error.
- The leading error term is $\sim \frac{t^2}{2n}[H_1, H_2]$ from the BCH expansion . By increasing n (more, smaller time slices), the error can be made arbitrarily small, at the cost of more gates.
- Quantum computing implementations often use higher-order BCH-based formulas to reduce error. For instance, the second-order formula above, or higher-order Suzuki expansions, include additional exponentials to cancel out commutator errors up to higher orders.
- **Example:** To simulate $H = H_x + H_y + H_z$ (say parts of a Hamiltonian along x, y, z axes), one can use: $\mathrm{U(t)} \approx \left(e^{-iH_xt/m}e^{-iH_yt/m}e^{-iH_zt/m}\right)^m and choose m large. BCH tells us the error scale$

Symbolic Computation with Sympy

Using Sympy, we can manipulate non-commuting symbols and verify the BCH expansion:

```
from sympy.physics.quantum import Commutator, Operator
from sympy import Rational, expand

X, Y = Operator('X'), Operator('Y')



BCH series up to third order:



Z = X + Y
+ Rational(1,2)Commutator(X, Y)
+ Rational(1,12)(Commutator(X, Commutator(X,Y))
+ Commutator(Y, Commutator(Y,X)))

print(Z.expand(commutator=True))
```

Numerical Verification with Numpy

We can also numerically test how including commutator terms improves the approximation. Consider two small 2×2 matrices A and B:

```
import numpy as np
from numpy.linalg import norm
from scipy.linalg import expm  # matrix exponential

A = np.array([[0, 0.1],
[0, 0   ]])
B = np.array([[0,   0 ],
[0.1, 0 ]])
```

```
Compute exponentials:
```

```
U = expm(A) @ expm(B)            # e^A e^B
U_direct = expm(A + B)           # e^{A+B}
```

Worked Example: SU(2) Rotations

As an example in a physics context, consider spin-$\frac{1}{2}$ operators (Pauli matrices). Let $X = i\theta\sigma_x$ and $Y = i\phi\sigma_y$, which generate rotations about the x- and y-axes by angles θ and ϕ.

- We know $[\sigma_x, \sigma_y] = 2i, \sigma_z$. Thus, $[X, Y] = i^2\theta\phi[\sigma_x, \sigma_y] = -2\theta\phi, \sigma_z$.
- Since σ_z does not commute with σ_x or σ_y, higher commutators will appear (the algebra is nonabelian but finite-dimensional).
- Using the BCH formula up to second order: $Z \approx X + Y + \frac{1}{2}[X, Y] = i\theta\sigma_x + i\phi\sigma_y - \theta\phi\,\sigma_z\,. Thissuggests e^X e^Y \approx \exp(i\theta\sigma_x + i\phi\sigma_y - \theta\phi, \sigma_z)$ for small angles.
- In fact, the exact combined rotation $e^{i\theta\sigma_x}e^{i\phi\sigma_y}$ equals a rotation about some axis in the xy-plane (at third order one would find adjustments to the axis angle). The BCH series can be resummed in this case to give a closed-form result (via $\mathrm{SO}(3)$ formulas for combining rotations).
- The key takeaway: BCH correctly identifies the σ_z component (proportional to $[X, Y]$) in the resultant rotation generator.

Exercises for Practice

1. Derive the BCH formula up to the third order term explicitly:
   1. Start from $\log\left(e^X e^Y\right) = Z = X + Y + A_2 + A_3 + \cdots$. Equate series coefficients to show $A_2 = \frac{1}{2}[X, Y]$ and $A_3 = \frac{1}{12}[X, [X, Y]] - \frac{1}{12}[Y, [X, Y]]$.
   2. (*Hint:* Use the expansion method or the identity $e^X Y e^{-X} = Y + [X, Y] + \frac{1}{2!}[X, [X, Y]] + \cdots$ to assist in the derivation.)
2. For operators A and B such that $[A, B] = cI$ (a central commutator), prove that $e^A e^B = \exp\left(A + B + \frac{1}{2}[A, B]\right)$ exactly. Verify this formula with a concrete example (e.g. 2×2 matrices or simple 2×2 block matrices).
3. Using the first-order Trotter approximation, show that $e^{(H_1+H_2)\Delta t} = e^{H_1 \Delta t} e^{H_2 \Delta t} + O((\Delta t)^2)$, *anddeterminetheformofthe*O(Δt^2) error term using the BCH expansion. What commutator appears?
4. Consider two 2×2 matrices (for example, Pauli matrices or random matrices) and numerically check the BCH formula:
   1. Compute $Z^{(n)}_{\mathrm{BCH}} = X + Y + \frac{1}{2}[X, Y] + \cdots$ up to nth order for your chosen X, Y.
   2. Compare $e^X e^Y$ with $\exp\left(Z^{(n)}_{\mathrm{BCH}}\right)$ for increasing n (e.g. using a Python

Summary

- The Baker–Campbell–Hausdorff formula provides a powerful tool to combine exponentials of non-commuting operators into a single exponential. It expresses the result as an infinite series of nested commutators .
- In general, the series is infinite and has no closed form, but truncations are extremely useful for approximate calculations .
- The first few terms ($X + Y$, $\frac{1}{2}[X, Y]$, $\frac{1}{12}[X, [X, Y]]$, $\dots$) often give insight into how non-commutativity affects combined operations.
- BCH is foundational in Lie theory (connecting local group structure to Lie algebra) and in practical computations in physics (quantum mechanics, quantum computing, optics, etc.) wherever splitting exponentials is needed .
- Through examples and exercises, we saw how BCH explains the error in splitting methods and how it can be checked with symbolic or numeric computation.
- Bottom line: Whenever you see $e^X e^Y$, remember the BCH formula allows you to rewrite it as e^Z with $Z = X + Y + \frac{1}{2}[X, Y] + \cdots$. This