On Averaging of One-Parameter Semigroups and Their Generators

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Outline

1. History of the problem
2. Preliminaries
3. Generalized averages for unbounded operators
4. Examples and obtained result
5. Possible applications and future works

Key idea

Let $\hat{U}$ be a random strongly continuous semigroup.

The mathematical expectation (averaging) $\mathbb{E}\hat{U}(t)$, in general, is not a semigroup.

Consider the sequence of Feynman-Chernoff averagings:

$$\left\{ \mathbb{E}\left(\hat{U}_n\left(\frac{t}{n}\right) \circ \ldots \circ \hat{U}_1\left(\frac{t}{n}\right)\right)\right\}_{n=1}^{\infty}, \ t \in \mathbb{R}_+. \tag{1}$$

Under certain sufficient conditions, this sequence converges to the semigroup $e^{(\mathbb{E}\hat{U}(t))'_0 t}$.

The seminal works

The formulas representing solutions to evolutionary equations in the form of limits of multiple integrals as the multiplicity tends to infinity were first published by Feynman:

- **Feynman R.P. Space-time approach to nonrelativistic quantum mechanics // Rev. Mod. Phys. (1948)**
- **Feynman R.P. An operation calculus having applications in quantum electrodynamics // Phys. Rev. (1951.)**

The theoretical foundation was provided in:

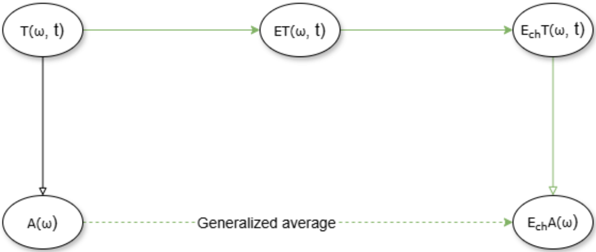
- **Nelson E. Feynman Integrals and the Schroedinger Equation // J. Math. Phys. (1964)**
- **Smolyanov O.G., Tokarev A.G., Truman A. Hamiltonian Feynman path integrals via the Chernoff formula // J. Math. Phys. (2002)**

In the paper

Yu. N. Orlov, V. Zh. Sakbaev, O. G. Smolyanov, Unbounded random operators and Feynman formulae// Izvestiya: Mathematics (2016)

the method for finding the expectation of random unbounded operators that are generators of strongly continuous one-parameter semigroups in a separable Hilbert space was proposed. The method is based on Feynman-Chernoff iterations of averaging the corresponding semigroups.

Generalized expectation of a random generator



$T(\omega, T)$ – random semigroup
$A(\omega)$ – random generator

Random bounded operators in $\mathcal{H}$

Let $\mathcal{H}$ be a separable Hilbert space with inner product $(\cdot, \cdot)$.
Let $(\Omega, \mathcal{A}, \mu)$ be a probability space.

Definition

The mapping $\hat{U} : \Omega \to B(\mathcal{H})$ is called a random operator in $\mathcal{H}$ if the functions $(\hat{U}u, v) : \Omega \to \mathbb{C}$ are $(\Omega, \mathcal{A})$-measurable (i.e., they are random variables) for all $u, v \in \mathcal{H}$.

Definition

The mathematical expectation (or averaging) of the random operator $\hat{U}$ is an operator $\mathbb{E}\hat{U} \in B(\mathcal{H})$ such that

$$(\mathbb{E}\hat{U}u, v) = \mathbb{E}(\hat{U}u, v), \quad \forall u, v \in \mathcal{H}. \tag{2}$$

Let $C_s(\mathbb{R}_+, B(\mathcal{H}))$ be a topological vector space of strongly continuous operator-valued functions $U(t) : \mathbb{R}_+ \to B(\mathcal{H})$.

The topology τ_s in $C_s(\mathbb{R}_+, B(\mathcal{H}))$ is generated by a family of seminorms.

$$\Phi_{T,u}(U) = \sup_{t\in[0,T]} \|U(t)u\|_{\mathcal{H}}, \quad \forall T > 0, \forall u \in \mathcal{H}. \tag{3}$$

For $U, \{U_n\}_{n=0}^{\infty} \in C_s(\mathbb{R}_+, B(\mathcal{H}))$ the convergence $U_n \xrightarrow{\tau_s} U$ as $n \to \infty$ means

$$\lim_{n\to\infty} \sup_{t\in[0,T]} \|U_n(t)u - U(t)u\|_{\mathcal{H}} = 0, \qquad \forall T > 0, \forall u \in \mathcal{H}. \tag{4}$$

Definition

The mapping $\hat{U} : \Omega \to C_s(\mathbb{R}_+, B(\mathcal{H}))$ with values $U_\omega(\cdot) \in C_s(\mathbb{R}_+, B(\mathcal{H})), \omega \in \Omega$, is called a random operator-valued function if $U_{(\cdot)}(t)$ is a random operator for all $t \in \mathbb{R}_+$.

Definition

For a sequence of independent identically distributed (iid) random operator-valued functions $\hat{U}_k(t)$, $k \in \mathbb{N}$, and an arbitrary non-negative t, the sequence of Feynman-Chernoff iterations is defined as the sequence of operator compositions:

$$\left\{ \hat{U}_n\left(\frac{t}{n}\right) \circ \ldots \circ \hat{U}_1\left(\frac{t}{n}\right) \right\}_{n=1}^{\infty}. \tag{5}$$

Let $\hat{U} : \Omega \to C_s(\mathbb{R}_+, B(\mathcal{H}))$ be a random operator-valued strongly continuous function (or a random C_0-semigroup)..

The mathematical expectation (averaging) $\mathbb{E}\hat{U}(t)$, in general, is not a semigroup.

For a sequence of iid random functions $\{\hat{U}_n\}_{n=1}^{\infty}$, consider the sequence of Feynman-Chernoff averagings:

$$\left\{\mathbb{E}\left(\hat{U}_n\left(\frac{t}{n}\right)\circ \ldots \circ \hat{U}_1\left(\frac{t}{n}\right)\right)\right\}_{n=1}^{\infty},\ t\in\mathbb{R}_+. \qquad (6)$$

Under certain sufficient conditions, this sequence converges in the topology of the space $C_s(\mathbb{R}_+, B(\mathcal{H}))$ to the semigroup $e^{(\mathbb{E}\hat{U}(t))'_0 t}$.

Generalized average

Definition

A semigroup $(T_U(t))_{t\geqslant 0}$ is called a generalized expectation of a random semigroup $U(\omega, t), \omega \in \Omega, t \geqslant 0$, if it is Chernoff equivalent to the expectation $\mathbb{E}U(t)$.

Automatically, we define the expectation of a random generator uniquely corresponding to a random semigroup.

Definition

The generator of semigroup $(T_U(t))_{t\geqslant 0}$ is called a generalized expectation of a random generator of random semigroup $U \in C_s(\mathbb{R}_+, B(\mathcal{H}))$ if the expectation $\mathbb{E}U$ is Chernoff equivalent to T_U.

Transport Equation and (semi)group of Shifts

For $a \in \mathbb{R}$, consider the Cauchy problem for the transport equation

$$\frac{\partial u}{\partial t} = a\frac{\partial u}{\partial x}, \quad u|_{t=0} = f \in L_2(\mathbb{R}). \tag{7}$$

C_0-semigroup $T[a] : \mathbb{R}_+ \to B(L_2(\mathbb{R}))$:

$$T[a](t)f(x) = f(x + at), \; t \in \mathbb{R}_+, \tag{8}$$

is called the **shift semigroup**, and formula (8) gives the solution to the Cauchy problem (7) for arbitrary initial conditions.

The generator of the semigroup $T[a]$ is the operator A:

$$\begin{aligned} &Af = af', \\ &D(A) = \{f \in L_2(\mathbb{R}) : f \text{ is absolutely continuous and } f' \in L_2(\mathbb{R}\}. \end{aligned} \tag{9}$$

Engel K.-J., Nagel R., One-Parameter Semigroups for Linear Evolution Equations// Springer New York, NY (1999).

Heat Equation

Consider the Cauchy problem for the heat equation

$$\frac{\partial u}{\partial t} = \frac{1}{2}\frac{\partial^2 u}{\partial x^2}, \quad u|_{t=0} = f \in L_2(\mathbb{R}). \tag{10}$$

C_0-semigroup $H : \mathbb{R}_+ \to B(L_2(\mathbb{R}))$:

$$H(t)f(x) = \frac{1}{\sqrt{\pi t}} \int_{\mathbb{R}} e^{\frac{-(y-x)^2}{t}} f(y)dy, \quad t \in \mathbb{R}_+, \tag{11}$$

gives the solution to the Cauchy problem (10) for arbitrary initial conditions.

The generator of the semigroup $H(t)$ is the closure of the Laplace operator:

$$\begin{aligned} Af &= \frac{1}{2}f'', \\ D(A) &= S(\mathbb{R}), \end{aligned} \tag{12}$$

where $S(\mathbb{R})$ is the Schwartz space.

Engel K.-J., Nagel R., One-Parameter Semigroups for Linear Evolution Equations// Springer New York, NY (1999).

Averaging of Shift Semigroups

Let $a : \Omega \to \mathbb{R}$ be a real random variable with zero mean and unit variance.

Then $\hat{T}[a] : \Omega \to C_s(\mathbb{R}_+, B(L_2(\mathbb{R})))$ is a random C_0-semigroup.

The following holds[1]:

$$\mathbb{E}\left(\hat{T}_n[a]\left(\sqrt{\frac{t}{n}}\right) \circ \ldots \circ \hat{T}_1[a]\left(\sqrt{\frac{t}{n}}\right)\right) \xrightarrow{\tau_s} \hat{H}(t) \quad \text{as } n \to \infty, \tag{13}$$

where $\{\hat{T}_i[a]\}_{i=1}^{\infty}$ is a sequence of iid random C_0-shift semigroups.

[1] R.Sh. Kalmetev, Yu.N. Orlov, V.Zh. Sakbaev *Chernoff Iterations as a Method for Averaging Random Affine Transformations* // Comput. Math. and Math. Phys. **62**:6, 1030-1041 (2022).

Example 1

$\mathbf{A} = -\frac{d^2}{dx^2}$, $D(\mathbf{A}) = W_2^2(\mathbb{R})$,
$\mathbf{B} = -\frac{d}{dx}\left(g\frac{d}{dx}\right)$, $D(\mathbf{B}) = \{u \in W_2^1(\mathbb{R}) : g\frac{d}{dx}u \in W_2^1(\mathbb{R})\}$.

The function $g \in L_\infty(\mathbb{R})$ satisfies the inequalities $1 \le g(x) \le 2$ for all $x \in \mathbb{R}$, and is defined by the following rule.
Let $\{r_k\}$ be a sequence enumerating the rational numbers. Then the function is given by:

$$g(x) = 1 + \sum_{r_k \in [-\infty, x]} 2^{-k}.$$

The half-sum of the operators $\mathbf{A}$ and $\mathbf{B}$ in the sense of quadratic forms coincides with their half-sum in the sense of Definition 6 and is a self-adjoint operator with the domain
$D = \{u \in W_2(\mathbb{R}) : (1+g)\hat{u}_a[u] \in W_2(\mathbb{R})\}$.

Yu. N. Orlov, V. Zh. Sakbaev, O. G. Smolyanov, Unbounded random operators and Feynman formulae// Izvestiya: Mathematics (2016).

Theorem

Let $A(\omega), \omega \in \Omega$ *be a random generator of a random strongly continuous semigroup and*

$$||e^{A(\omega)t}|| \leq Me^{\alpha t}, \forall \omega \in \Omega,$$

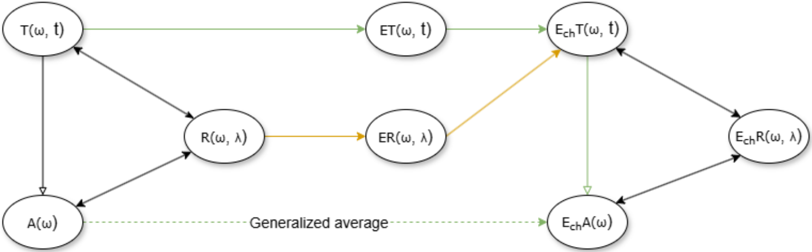
for some constants $M \geqslant 1$ *and* $\alpha \in \mathbb{R}$*. Assume that the operator-valued functions* $\mathbb{E}e^{At}$ *and* $\mathbb{E}(\frac{1}{t}R(\omega, \frac{1}{t}))$ *satisfy the conditions of the Chernoff theorem. Then*

$$\lim_{n\to\infty} \sup_{t\in[0,T]} \left\| \left(\mathbb{E}e^{A(\omega)t/n}\right)^n u - \left(\mathbb{E}\left(\frac{n}{t}R\left(\omega, \frac{n}{t}\right)\right)\right)^n u \right\| = 0,$$

$$\forall T > 0, \forall u \in \mathcal{H}.$$

R. Sh. Kalmetev, "Random One-Parameter Semigroups: On the Equivalence of Semigroup and Resolvent Averaging, "Lobachevskii Journal of Mathematics (in press, 2025).

Resolvent Averaging



Example 2

Let a be a real-valued random variable with $\rho(a) = 2/a^3,\ a \in (1, +\infty)$. Consider the random semigroup $e^{(a+i)t}$ in $\mathcal{H} = \mathbb{C}$.

We have:

- $\mathbb{E}a = 2 + i$,
- $\mathbb{E}e^{at} = \int_1^{+\infty} \frac{e^{(a+i)t}}{a^3} da$ diverges,
- $\mathbb{E}\left(\frac{1}{t} R\left(\omega, \frac{1}{t}\right)\right) = \frac{1}{t}\int_1^{+\infty} \frac{1}{(1/t-a-i)a^3} da,\ t \leqslant 1$, and for operator-valued function $V(t) = \mathbb{E}\left(\frac{1}{t} R\left(\omega, \frac{1}{t}\right)\right)$ satisfies:

$$\lim_{t \downarrow 0} \frac{V(t)x - x}{t} = (2+i)x.$$

Thus, in this example, the ordinary expectation and the one defined via resolvent averaging coincide, whereas semigroup averaging does not exist.

Example 3

Let a be a real-valued random variable with $\rho(a) = e^{-a},\ a \in (0, +\infty)$ in $\mathcal{H} = \mathbb{C}$. Consider the random semigroup e^{at}.

We have

- $\mathbb{E}a = 1$,
- $\mathbb{E}e^{at} = \int_0^{+\infty} e^{a(t-1)} da \frac{1}{1-t}, \quad t \leqslant 1$, and for operator-valued function $\mathbb{E}e^{at}$ satisfies:
$$\lim_{t \downarrow 0} \frac{V(t)x - x}{t} = x,$$
- $\mathbb{E}\left(\frac{1}{t} R\left(\omega, \frac{1}{t}\right)\right) = \frac{1}{t} \int_0^{+\infty} \frac{1}{(1/t-a)} e^{-a} da$ diverges for $t > 0$.

In this example, we observe the opposite situation: the conventional mathematical expectation and the one defined via semigroup averaging coincide, whereas resolvent averaging does not exist.

Canonical commutation relation

Let $\mathcal{H}$ be a separable Hilbert space.
Consider linear operators $\hat{a}$ (annihilation), $\hat{a}^\dagger$ (creation) and $\hat{n}$ (particle number) in $\mathcal{H}$ with

- $\hat{n}$ is a self-adjoint operator;
- the operators $a, \hat{a}^\dagger$ are Hermitian conjugate to each other;
- the commutation relations holds:

$$[\hat{a}, \hat{a}^\dagger] = I, \; [\hat{n}, \hat{a}] = -\hat{a}, \; [\hat{n}, \hat{a}^\dagger] = \hat{a}^\dagger. \qquad (14)$$

The Fock space representation for these operators in the standard orthonormal basis $\{|n\rangle\}_{n=0}^{\infty}$ has the form:

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle, \; \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle, \; \hat{n}|n\rangle = n|n\rangle. \qquad (15)$$

Coherent states

A **coherent state** $|z\rangle, z \in \mathbb{C}$ is the state corresponding to the eigenvector of the annihilation operator:

$$\hat{a} |z\rangle = z |z\rangle . \tag{16}$$

Some properties of coherent states:

- the vacuum state $|0\rangle$ is coherent: $\hat{a} |0\rangle = 0 |0\rangle$;
- the resolution of the identity holds:

$$\frac{1}{\pi} \int |z\rangle\langle z| \, d^2 z = I. \tag{17}$$

Displacement operator

The displacement operator (operator-valued function $\mathbb{C} \to B(\mathcal{H})$)

$$\hat{D}(z) = \exp\left(z\hat{a}^{\dagger} - \overline{z}\hat{a}\right), \; z \in \mathbb{C} \tag{18}$$

when acting on the vacuum state $|0\rangle$ generates a coherent state $|z\rangle$:

$$\hat{D}(z)\,|0\rangle = |z\rangle\,. \tag{19}$$

- Displacement operators are unitary: $\hat{D}^{*}(z)\hat{D}(z) = \hat{D}(z)\hat{D}^{*}(z) = Id$;
- $\hat{D}(\alpha)\hat{D}(\beta) = e^{(\alpha\beta^{*} - \alpha^{*}\beta)/2}\hat{D}(\alpha+\beta), \; \alpha, \beta \in \mathbb{C}$ - the semigroup property doesn't hold;
- the semigroup property holds for restriction to any line in the complex plane passing through the origin $(\alpha\beta^{*} - \alpha^{*}\beta = 0)$: $\hat{D}(\alpha)\hat{D}(\beta) = \hat{D}(\alpha+\beta)$.

Random displacement operators

Let $z = z(\omega)$, $\omega \in \Omega$ be a complex random variable, where $(\Omega, \mathcal{A}, \mu)$ is some probability space.
Then $\hat{D}(\omega, t) = \hat{D}(z(\omega)t) = exp\big(z\omega t\hat{a}^+ - \overline{z\omega t}\hat{a}\big), \forall t \in \mathbb{R}_+$, is a random C_0-semigroup.

Theorem

If the complex random variable z has a finite mathematical expectation, then the operator $\mathbb{E}\hat{D}(zt)$ is Chernoff-equivalent to the operator $\hat{D}(\mathbb{E}zt)$, meaning that:

$$\lim_{n\to\infty} \sup_{t\in[0,T]} \left\| \left(\left(\mathbb{E}\hat{D}\left(zt/n\right)\right)^n - \hat{D}(\mathbb{E}zt) \right) |\psi\rangle \right\| = 0, \ \forall T > 0, \forall |\psi\rangle \in \mathcal{H}. \tag{20}$$

Borisov L.A., Orlov Yu.N., Sakbaev V.Zh. «Chernoff Equivalence for Shift Operators, Generating Coherent States in Quantum Optics» Lobachevskii J Math 39 (2018).

Noncanonical commutation relations

Consider non-negative non-decreasing sequence of real numbers

$$\{A_n\}_{n=0}^{\infty} : A_0 = 0, \;\; A_{n+1} \geq A_n. \tag{21}$$

and the Fock space representation of noncanonical ladder operators:

$$\hat{a}|n\rangle = \sqrt{A_n}|n-1\rangle, \;\; \hat{a}^\dagger|n\rangle = \sqrt{A_{n+1}}|n+1\rangle, \;\; \hat{n}|n\rangle = n|n\rangle, \tag{22}$$

The commutation relations hold:

$$[\hat{a}, \hat{a}^\dagger]\,|n\rangle = (A_{n+1} - A_n)\,|n\rangle\,, \tag{23}$$

$$[\hat{n}, \hat{a}] = -\hat{a}, \;\; [\hat{n}, \hat{a}^\dagger] = \hat{a}^\dagger. \tag{24}$$

Generalized coherent states

A generalized **coherent state**[2] [3] $|z\rangle, z \in \mathbb{C}$ is the state corresponding to the eigenvector of the annihilation operator:

$$\hat{a}\,|z\rangle = z\,|z\rangle\,. \tag{25}$$

The analogue of the classical displacement operator $\hat{D}(z) = \exp\big(z\hat{a}^\dagger - \overline{z}\hat{a}\big)$ does not generate a coherent state from the vacuum state:

$$\hat{D}(z)|0\rangle \neq |z\rangle. \tag{26}$$

Main problem: the possibility of defining a unitary semigroup of displacement operators and the possibility of generalizing the result on the convergence of Feynman–Chernoff iterations for the corresponding random semigroups.

[2] Barut A.O., Girardello L. *New «Coherent» States associated with non-compact groups*// Communications in Mathematical Physics. 21(1), (1971).

[3] Aniello P. et al. *On the coherent states, displacement operators and quasidistributions associated with deformed quantum oscillators*// J.Opt.B 2(6), (2000).

Displacement duality

Let

$$\hat{a}|n\rangle = \sqrt{A_n}|n-1\rangle, \quad \hat{a}^\dagger|n\rangle = \sqrt{A_{n+1}}|n+1\rangle. \tag{27}$$

Displacement dual ladder operators are:

$$\hat{b}|n\rangle = \sqrt{B_n}|n-1\rangle = \frac{n}{\sqrt{A_n}}|n-1\rangle, \tag{28}$$

$$\hat{b}^\dagger|n\rangle = \sqrt{B_{n+1}}|n+1\rangle = \frac{n+1}{\sqrt{A_{n+1}}}|n+1\rangle. \tag{29}$$

Displacement duality

Theorem

The action of the operator $\tilde{D}_a(z) = \exp\left(z\hat{b}^\dagger\right), \ \ z \in M_a = \{|z| < \lim_{n\to+\infty} \sqrt{A_n}\}$ *on the vacuum state* $|0\rangle$ *generates an eigenvector* $|z\rangle_a$ *of the annihilation operator* $\hat{a}$.

The action of the operator $\tilde{D}_b(z) = \exp\left(z\hat{a}^\dagger\right), \ \ z \in M_b = \{|z| < \lim_{n\to+\infty} \frac{n}{\sqrt{A_n}}\}$ *on the vacuum state* $|0\rangle$ *generates an eigenvector* $|z\rangle_b$ *of the annihilation operator* $\hat{b}$.

$\tilde{D}_a(z)$ and $\tilde{D}_b(z)$ are not unitary!

Theorem

Let the ladder operators have the form

$$\hat{a}|n\rangle = \sqrt{\frac{n}{(1-\alpha)+\alpha n}}|n-1\rangle,\ \hat{a}^{\dagger}|n\rangle = \sqrt{\frac{n+1}{1+\alpha n}}|n+1\rangle, \tag{30}$$

for some $\alpha \geq 0$, than the displacement operator

$$\hat{D}_a(z) = \exp\left(z\hat{b}^{\dagger} - \overline{z}\hat{b}\right),\ \forall z \in \mathbb{C},$$

where $\hat{b}, b^{+}$ are displacement dual ladder operators:

$$\hat{b}|n\rangle = \sqrt{n((1-\alpha)+\alpha n)}|n-1\rangle,\ \hat{b}^{+}|n\rangle = \sqrt{(n+1)(1+\alpha n)}|n+1\rangle,$$

1. *generates the coherent state $|\tilde{z}\rangle_a = |\frac{-1+\sqrt{1+4\alpha|z|^2}}{2\alpha|z|^2}z\rangle_a$ of the annihilation operator $\hat{a}$,*
2. *is unitary and satisfies the semigroup property on lines passing through the origin.*

Let $z = z(\omega)$, $\omega \in \Omega$ be a complex random variable, where $(\Omega, \mathcal{A}, \mu)$ is some probability space.
Then $\hat{D}_a(\omega, t) = \hat{D}_a(z(\omega)t) = exp\Big(z\omega t\hat{b}^{+} - \overline{z\omega t}\hat{b}\Big), \forall t \in \mathbb{R}_{+}$, is a random C_0-semigroup.

Theorem

Let the ladder operators be given by relations (30) for some $\alpha \geq 0$, and let the complex random variable z has a finite mathematical expectation, then the operator $\mathbb{E}\hat{D}_a(zt)$ is Chernoff-equivalent to the operator $\hat{D}_a(\mathbb{E}zt)$, meaning that:

$$\lim_{n\to\infty} \sup_{t\in[0,T]} \left\| \left(\left(\mathbb{E}\hat{D}_a\left(zt/n\right) \right)^n - \hat{D}_a(\mathbb{E}zt) \right) |\psi\rangle \right\| = 0,\ \forall T > 0, \forall |\psi\rangle \in \mathcal{H}. \tag{31}$$

Finite dimensional approximations

Consider the problem of approximating displacement operators in the truncated Hilbert space in the case of arbitrary commutation relations. The problem is divided into two cases.

1. If the ladder operators are of the form (30), then the displacement operators $\hat{D}_a(zt) = \exp\left\{\left(z\hat{b}^\dagger - \overline{z}\hat{b}\right) t\right\}$ are unitary, satisfies the semigroup property in t, and their generators $\left(z\hat{b}^\dagger - \overline{z}\hat{b}\right)$ are tridiagonal and anti-Hermitian.
2. For the general case of commutation relations, we will construct approximations of nonunitary dispalcement operators $\exp\left(zt\hat{b}^\dagger\right)$ or $\exp\left\{(z\hat{b}^\dagger - \overline{z}\hat{a})t\right\}$. In this case, the displacement operators also satisfy the property $\hat{D}_a(z) = \hat{D}_a(zt) \circ \hat{D}_a(z(1-t))$ for $t \in (0,1)$, the generators are tridiagonal, but are no longer anti-Hermitian.

Approximation methods for displacement operators

1. **expm** – matrix exponent approximation method from 'scipy' package [1,2];
2. **QuTiP** – method for approximation the classical displacement operator from a fairly popular package for quantum computing QuTiP (QuTiP uses methods from 'scipy' to compute the displacement operator, so it's essentially the same method, just with extra "syntactic sugar"for quantum computing, https://qutip.org/);
3. **Pade** – own implementation of the matrix exponential approximation based on the method using Padé approximants and the principle of scaling and squaring [1];

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[1] Al-Mohy A.H., Higham N.J. A New Scaling and Squaring Algorithm for the Matrix Exponential // SIAM J. Matrix Anal. Appl. — 2009. — Vol. 31, no. 3. — Pp. 970–989.

[2] Higham N.J., Tisseur F. A Block Algorithm for Matrix 1-Norm Estimation, with an Application to 1-Norm Pseudospectra // S SIAM J. Matrix Anal. Appl. — 2000. — Vol. 21, no. 4. — Pp. 1185–1201.

Approximation methods for displacement operators

4. **eig** – finding matrix exponent using diagonalization (can only be used for diagonalizable operators) based on 'scipy' package;
5. **triag** – finding the matrix exponent using the efficient diagonalization algorithm for a tridiagonal Hermitian matrix from the 'scipy' package (can only be used for Hermitian matrices);
6. **triag_precalc** – an optimized version of the **triag** method, where part of the precomputation is done in advance and is not taken into account in the execution time calculation;
7. **Chernoff** – approximation algorithm using Chernoff iterations.

Main groups of algorithms

Scaling and squaring	Decomposition	Chernoff approximation
$D \approx \left(R\left(\frac{A\Delta t}{T}\right)\right)^{2^{\log_2 T}}$ Complexity: $O(N^{2.4}\ln T)$	$D \approx S\exp(B)S^{-1}$ Complexity: $O(N^2 + N\ln T)$	$Dx \approx \underbrace{(I + \frac{A\Delta t}{T})\ldots(I + \frac{A\Delta t}{T})}_{T}x$ Complexity: $O(NT)$

N – #dim, T - number of «timesteps».

A – generator matrix, $R(\cdot)$ – Pade approximation of matrix exponential.

Running times of the algorithms in seconds for the case (1) and low accuracy approximation, depending on the dimension #dim of the truncated Hilbert space:

#dim	QuTiP	expm	Pade	eig	tridiag	tridiag_precalc	Chernoff
100	0.007	0.007	0.003	0.015	0.002	0.000	0.003
500	1.667	1.637	1.113	0.685	0.037	0.024	0.050
1000	11.77	12.38	6.75	3.49	0.19	0.15	0.18
2000	71.17	71.04	36.18	20.74	1.24	0.85	1.03

Conclusions:

1. **triag_precalc** algorithm is optimal for approximation of unitary displacement operators.
2. In nonunitary case: 'Scaling and squaring' (**expm**, **QuTiP**, **Pade**) algorithms is optimal for high accuracy approximation and **Chernoff** algorithm for low accuracy.

Approximation of Solutions to Multidimensional Kolmogorov Equation

Consider the Cauchy problem

$$\partial_t u = Lu, \qquad t \in (0, T] \tag{32}$$

$$u|_{t=0} = u_0, \tag{33}$$

where $u_0 \in L_2(\mathbb{R}^d) \cap C^2(\mathbb{R}^d)$ is some initial condition, and

$$L = \mu^i(x)\partial_i + \frac{1}{2}D^{ij}(x)\partial_i\partial_j \tag{34}$$

is a differential operator defined by drift coefficients $\mu : \mathbb{R}^d \to \mathbb{R}^d$ and diffusion $D = \sigma\sigma^T : \mathbb{R}^d \to \mathbb{R}^{d\times d}$.

Consider also the corresponding stochastic differential equation in Ito form

$$dX = \mu dt + \sigma dW, \tag{35}$$

where W is a standard Wiener process.

When the following sufficient conditions are satisfied:

1. $\exists C_1 > 0 : \|\mu(x)\| + \|\sigma(x)\| \leq C_1(1 + \|x\|),\ \forall x \in \mathbb{R}^d,$
2. $\exists C_2 > 0 : \|\mu(x_1) - \mu(x_2)\| + \|\sigma(x_1) - \sigma(x_2)\| \leq C_2(\|x_1 - x_2\|),$ $\forall x_1, x_2 \in \mathbb{R}^d,$
3. $\exists C_3 > 0 : (\eta, \sigma\sigma^T(x)\eta) \geq C_3\|\eta\|,\ \forall x \in \mathbb{R}^d, \forall \eta \in T_x\mathbb{R}^d,$

the Cauchy problem (32)-(33) has for arbitrary $u_0 \in L_2(\mathbb{R}^d) \cap C^2(\mathbb{R}^d)$ a unique strong solution $u(x,t) \in C^{2,1}(\mathbb{R}^d \times [0,T])$, and the equation (35) with initial condition $X(0) = x_0 \in \mathbb{R}^d$ has a strongly unique strong solution $X(t)$.

The Feynman-Kac formula connects these two solutions as follows:

$$u(x,t) = \mathbb{E}(u_0(X(t))|X(0) = x). \quad (36)$$

Karatzas I., Shreve S.E. Brownian Motion and Stochastic Calculus// Springer New York, New York (1998).

If the differential operator L (34) is the generator of a strongly continuous semigroup $e^{Lt} : \mathbb{R}_+ \to L_2(\mathbb{R}^d)$, then for any initial condition $u_0 \in L_2(\mathbb{R}^d)$ the weak solution of the Cauchy problem (32)-(33) can be represented as:

$$u(x,t) = e^{Lt} u_0(x), \quad t \in [0,T]. \tag{37}$$

Let $\{F_k(t)\}, k \in \mathbb{N}$ be a sequence of independent identically distributed random strongly continuous operator-valued functions $\Omega \to C_s(\mathbb{R}_+, B(X))$, defined on a probability space $(\Omega, \mathcal{A}, \mu)$. Suppose also that the expectations $\mathbb{E}F_k(t) : \mathbb{R}_+ \to B(X)$ are Chernoff equivalent to the semigroup e^{Lt}.
Then by the Chernoff theorem, the finite composition of operators

$$\prod_{i=1}^{N} \mathbb{E}F_i\left(\frac{t}{N}\right) = \mathbb{E}\left(\prod_{i=1}^{N} F_i\left(\frac{t}{N}\right)\right) \tag{38}$$

for sufficiently large N can be used as an approximation of the operator e^{Lt}.

Approximation of Solutions for Kolmogorov Equation

$$\frac{\partial u}{\partial t} = (b^i(x)\partial_i + \frac{1}{2}(\sigma(x)\sigma^T(x))^{ij}\partial_i\partial_j)u, \qquad u|_{t=0} = u_0 \tag{39}$$

Monte Carlo method using Feynman-Kac formula:

$$u(\xi, t) = \mathbb{E}\left[u(x_t, 0)|(\xi, 0)\right]$$

where x_t is the solution of SDE

$$dx = b(x)dt + \sigma(x)dW$$

approximated by Euler-Maruyama method.

- Meshless method;
- Computational complexity $O(NM)$;
- Lower variance for L_1, L_2 norms.

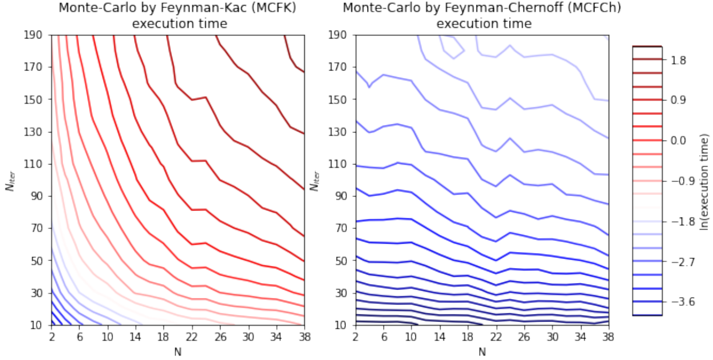
Monte Carlo method using Feynman-Chernoff iterations:

$$u(t) = \mathbb{E}\left[\prod_{i=1}^{n} S_i\left(\frac{t}{n}\right)\right]u(0)$$

where S_i are corresponding i.i.d. operator-valued random functions.

- Meshless method;
- Computational complexity $O(N+M)$ for affine S_i;
- Lower RMSE for L_∞, C_1, C_2 norms;
- Preserves smoothness.

Logarithmic execution times of MCFK and MCFCh algorithms as functions of the number of Monte Carlo iterations and evaluation points.



Computational complexity of MCFK algorithm: $O(NN_{iter})$
Computational complexity of MCFCh algorithm: $O(N + N_{iter})$.

R.Sh. Kalmetev, "Approximation of Solutions to Multidimensional Kolmogorov Equation Using Feynman-Chernoff Iterations"// Keldysh Institute Preprints, 15 pp. (2023).

Appications to quantum theory:

Theoretical:

- Orlov, Y.N., Sakbaev, V.Z. Feynman–Kac Formulas for Solutions of Nonstationarily Perturbed Evolution Equations// Comput. Math. and Math. Phys. (2025).
- N. Drago, S. Mazzucchi, A. Pinamonti Chernoff solutions of the heat and the Schrödinger equation in the Heisenberg group// arXiv:2503.18481

Numerical approximations:

- P.T. Grochowski, H. Pichler, C.A. Regal, O. Romero-Isart, Quantum control of continuous systems via nonharmonic potential modulation// arXiv:2311.16819
- O.E. Galkin, I.D. Remizov, Upper and lower estimates for rate of convergence in the Chernoff product formula for semigroups of operators. Isr. J. Math. (2025).

Thanks!

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