A Candidate Framework for Structure-Preserving Discretizations

D. Tageddine (McGill)

joint work with J-C. Nave (McGill)

2024 SIAM Annual Meeting (AN24), July 10th 2024

Motivations:

Conference at the Foundations of Computational Mathematics in Paris (2023) at la Sorbonne.

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Berezin-Toeplitz quantization: $\mathfrak{g} = (C^\infty(\mathbb{S}^2, \mathbb{C}), \{\cdot,\cdot\})$ remplaced by $\mathfrak{g}_N = (\mathfrak{gl}(N,\mathbb{C}), [\cdot,\cdot]_N)$ as a discretization of Euler's equations,

$$\dot{\omega} = \{\psi, \omega\}, \quad \Delta\psi = \omega, \quad (\omega,\psi) \in C_0^\infty(\mathbb{S}^2,\mathbb{C}) \times C_0^\infty(\mathbb{S}^2,\mathbb{C})$$

$$\dot{W} = \frac{1}{\hbar}[P, W], \quad \Delta_\hbar P = W, \quad (W, P) \in \mathfrak{su}(N) \times \mathfrak{su}(N)$$

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Question: Is the quantization theory a theory of discretization ?

Axiomatization of the theory of discretization

Definition (Discretization method)

A *discretization* $\mathfrak{D}(C_1, f)$ of an arrow $(f : C_1 \to C_2)$ is a sequence of arrows $(f_n : C_1^n \to C_2^n)_{n\in\mathbb{N}}$ producing the following diagram

$$\begin{array}{ccc} C_1 & \xrightarrow{\mu} & C_2 \\ {\scriptstyle \pi_1^n}\downarrow & & \downarrow{\scriptstyle \pi_2^n} \\ C_1^n & \xrightarrow{\mu_n} & C_2^n \end{array}$$

1) $\pi_i^n : C_i \to C_i^n$ surjective, contractive linear maps.
2) $\lim_{n\to\infty} \|\pi_i^n x\|_{C_i^n} = \|x\|_{C_i}$

Structure preserving discretizations

A discretization $\mathfrak{D}(f)$ is faithful if:

$$(f \text{ is an invertible arrow}) \implies (f_n \in \mathfrak{D}(f) \text{ is invertible for all } n \in \mathbb{N}).$$

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Definition (Structure preserving discretization)

1) $(C_1^n, f_n) \in \mathrm{ob}(\mathcal{C})$ for all $n \in \mathbb{N}$.
2) the diagram commutes asymptotically:

$$\|f_n \circ \pi_1^n(x) - \pi_2^n \circ f(x)\| \longrightarrow 0 \quad \text{as } n \to \infty \text{ and for all } x \in C_1$$

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Definition (Strongly structure preserving discretization)

1) $(C_1^n, f_n) \in \mathrm{ob}(\mathcal{C})$ for all $n \in \mathbb{N}$.
2) the diagram commutes for all $n \in \mathbb{N}$;

Non-example: Euler's method

Consider the right-shift map on $\mathbb{C}^n$

$$S : \mathbb{C}^n \to \mathbb{C}^n \quad S(y_1, y_2, \ldots, y_n) = (y_n, y_1, y_2, \ldots, y_{n-1})$$

and define the family Euler operators by

$$E_n = \frac{n}{2\pi}(S - 1)$$

Moreover, we define the maps

$$\pi^n : C^\infty(\mathbb{S}^1) \to \mathrm{Hom}(X_n, \mathbb{C}^n) \qquad \pi^n(f) = (f(x_1), f(x_2), \cdots, f(x_n)).$$

Consider now the differential operator

$$\frac{d}{d\theta} : C^\infty(\mathbb{S}^1) \to C^\infty(\mathbb{S}^1) \qquad f \mapsto \frac{df}{d\theta}$$

such that $(C^\infty(\mathbb{S}^1), \frac{d}{d\theta})$ is an object of the category of differential algebra

Non-example: Euler's method

We can now look at the Euler discretization method of the pair $(C^\infty(\mathbb{S}^1), \frac{d}{d\theta})$ defined by the following diagram:

$$\begin{array}{ccc} C^\infty(\mathbb{S}^1) & \xrightarrow{\frac{d}{d\theta}} & C^\infty(\mathbb{S}^1) \\ \pi^n \downarrow & & \downarrow \pi^n \\ \mathrm{Hom}(X_n, \mathbb{C}^n) & \xrightarrow{E_n} & \mathrm{Hom}(X_n, \mathbb{C}^n) \end{array}$$

We readily verify

$$\lim_{n\to\infty} \|\pi^n(f)\|_\infty = \|f\|_\infty \quad \text{and} \quad \|E_n \circ \pi^n(f) - \pi^n \circ \frac{d}{d\theta}(f)\| \longrightarrow 0$$

and thus, the Euler method defines a discretization. However, this is not the case since the pair $(\mathrm{Hom}(X_n, \mathbb{C}^n), E_n)$ does not define a differential algebra since E_n does not satisfy the Leibniz rule.

Convergence

The graph of an arrow f, denoted $\mathrm{Gr}(f)$, is defined as the subset of $C_1 \times C_2$ such that

$$\mathrm{Gr}(f) = \{(x, y) \in C_1 \times C_2 : y = f(x)\}$$

We denote by $p_i : \mathrm{Gr}(f) \to C_i$ for $i = 1, 2$ the obvious coordinate projections.

Definition

Consider a discretization $\mathfrak{D}(f)$ of an arrow f. We say that $\mathfrak{D}(f)$ is *convergent* if to any of the projection maps $\pi_i^n : C_i \to C_i^n$, we can associate an injective contractive linear map $s_i^n : C_i^n \to C_i$ such that

$$\lim_{n \to +\infty} \|x - s_i^n \circ \pi_i^n(x)\| = 0, \quad \text{for all } x \in p_i(\mathrm{Gr}(f)), \text{ and for } i = 1, 2.$$

The maps s_i^n will be called *section* map.

Example: Finite Element Exterior Calculus

The framework of the finite element exterior calculus is given by the L^2-de Rham complex, represented by the following complex

$$0 \to \mathrm{H}\Lambda^0(\Omega) \xrightarrow{d} \mathrm{H}\Lambda^1(\Omega) \xrightarrow{d} \cdots \xrightarrow{d} \mathrm{H}\Lambda^n(\Omega) \to 0$$

where $\Omega \subseteq \mathbb{R}^n$ is a Lipschitz domain. In order to give a numerical approximation of a PDE, the method builds a finite-dimensional subcomplex

$$0 \to \Lambda^1_\hbar(\Omega) \xrightarrow{d} \cdots \xrightarrow{d} \Lambda^n_\hbar(\Omega) \to 0$$

of the de Rham complex.

Example: Finite Element Exterior Calculus

In order to construct this subcomplex, there exists morphism $\pi^{\hbar}$ projecting the de Rham complex down to the appropriate subcomplex; so that each map $\pi_k^{\hbar} : \mathrm{H}\Lambda^k \to \Lambda_{\hbar}^k$ is a projection onto the subspace $\Lambda_{\hbar}^k$. This morphism defines induces the following commuting diagram

$$\begin{array}{ccc} H\Lambda^k & \xrightarrow{d} & H\Lambda^{k+1} \\ \pi_k^{\hbar}\downarrow & & \downarrow\pi_k^{\hbar} \\ \Lambda_{\hbar}^k & \xrightarrow{d} & \Lambda_{\hbar}^{k+1} \end{array}$$

Theorem

The Finite Element Exterior Calculus is a strongly structure preserving discretization.

Example: Diffeomorphism groups

Fix a diffeomorphism ψ, in order to present a structure preserving discretization of the pair $(C^\infty(X), \widehat{\psi})$ (it as an object of the category of *-algebra dynamical system). Therefore, following the definition, a *faithful* structure preserving discretization is the following commuting diagram

$$\begin{array}{ccc} C^\infty(X) & \xrightarrow{\widehat{\psi}} & C^\infty(X) \\ \downarrow{\scriptstyle \pi^n} & & \downarrow{\scriptstyle \pi^n} \\ A_N & \xrightarrow{\widehat{\psi}_N} & A_N \end{array}$$

Theorem

For any diffeomorphism $\psi \in \mathrm{Diff}(X)$, there exists a faithful structure preserving discretization of $\mathfrak{D}(C^\infty(X), \widehat{\psi})$. In addition, the discretization does not depend on the choice of ψ.

Example: Diffeomorphism groups

Theorem

Let $(A_N, \widehat{\psi}_N)$ be a structure preserving discretization of $(C^\infty(X), \psi)$.

i) $\mathfrak{D}(\mathrm{Diff}(X)) = \mathrm{GL}_N(\mathbb{C})$.

ii) $\mathfrak{D}(\mathrm{Diff}_\omega(X)) = \mathrm{SL}_N(\mathbb{C})$.

iii) $\mathfrak{D}(\mathrm{Diff}_0^+(X)) = \mathrm{SO}_N(\mathbb{C})$.

iv) $\mathfrak{D}(\mathrm{Diff}_{\mathrm{m}}(X)) = \mathrm{GL}_N^{\mathrm{st}}(\mathbb{C})$.

The pullback representation

$$\mathrm{Diff}(X) \to \mathrm{Der}(C^\infty(X)) \quad \psi \mapsto \psi^*$$

can be thought as a Lie group anti-isomorphism. Differentiating it at the identity $\psi = \mathrm{id}$ gives a linear map

$$\mathrm{Vect}(X) \to \mathrm{Der}(C^\infty(X)) \quad X \mapsto \mathcal{L}_X$$

Example: Derivations

Consider a derivation $\delta : A \to A$ on a *-algebra. A structure preserving discretization is given by the following commuting diagram:

$$\begin{array}{ccc} A & \xrightarrow{\delta} & A \\ {\scriptstyle \pi^n}\downarrow & & \downarrow{\scriptstyle \pi^n} \\ A_n & \xrightarrow{\delta_n} & A_n \end{array}$$

Theorem

If A_n is isomorphic to a matrix algebra then there exists a self-adjoint element D_n such that

$$d_n(a) = [D_n, a]$$

In addition, if the discretization (A_n, d_n) is structure preserving, then

$$\lim_{n\to\infty} \|\pi^n \circ d(a) - [D_n, \pi^n(a)]\| = 0$$

Example: Derivations

Q: Existence of such discretization ?

Definition

A linear operator D on a Hilbert space H is called *block diagonal*, respectively *quasidiagonal*), if there exists an increasing sequence of finite rank projections, $P_1 \leq P_2 \leq P_3 \leq \cdots$ such $\|[D, P_n]\| = \|DP_n - P_nD\| = 0$, respectively $\to 0$ for all $n \in \mathbb{N}$ and $P_n \to 1_{\mathcal{H}}$ (in the strong operator topology) as $n \to \infty$.

The surjection maps are given by $\pi^n(a) := P_n a P_n$

$$\pi^n \delta(a) = \delta \pi^n(a) \iff P_n[D, a]P = [P_n D P_n, P_n a P_n]$$

An example of projectors P is given by the spectral projectors of $D = D^*$. The discrete geometry can then be summarized by the data: $(P_n A P_n, H_n, P_n D P_n)$

Example: The Berezin-Toeplitz Quantization

Let (M, ω) be a compact Kähler manifold.

$$\mathcal{H} = \bigoplus_m (\mathcal{H}^{(m)}, \langle \cdot, \cdot \rangle_m), \quad \mathcal{H}^{(m)} = \Gamma_{hol}(M, L^m), \quad \Pi^{(m)} : \mathcal{H} \to \mathcal{H}^{(m)}$$

For $f \in C^\infty(M)$ the Toeplitz operator $T_f^{(m)}$ (of level m) is defined by

$$T_f^{(m)} := \Pi^{(m)} f \Pi^{(m)} : \mathcal{H}^{(m)} \to \mathcal{H}^{(m)}$$

Theorem (Bordemann, Meinrenken, Schlichenmaier)

For all functions $f, g \in C^\infty(M)$, we have

$$(a) \quad \lim_{n \to \infty} \| T_f^{(m)} \| = \| f \|_\infty$$

$$(b) \quad \| im[T_f^{(m)}, T_g^{(m)}] - T_{\{f,g\}}^{(m)} \| = O(m^{-1})$$

Example: The Berezin-Toeplitz Quantization

Theorem

The Berezin-Toeplitz quantization induces a structure preserving discretization of the differential algebra $(C^\infty(M), \mathcal{D})$ *given by the following commuting diagram*

$$\begin{array}{ccc} C^\infty(M) & \xrightarrow{\mathcal{D}} & C^\infty(M) \\ T^{(m)}\downarrow & & \downarrow T^{(m)} \\ \mathrm{End}(\mathcal{H}_m) & \xrightarrow{d_m} & \mathrm{End}(\mathcal{H}_m) \end{array} \tag{1}$$

where the differential d_m *is given by the following commutator:*

$$A \mapsto d_m(A) = [D_m, A], \qquad D_m := \sum_{k=1}^{d} \partial_m^k := \sum_{k=1}^{d} \Pi^{(m)} X^k \Pi^{(m)} \tag{2}$$

Noncommutative Laplace operator

Assume that $X^1, \ldots, X^n$ are isometric embedding (Nash's embedding) coordinates of a compact Kähler M. The Bochner-Laplace operator can be writtenn as:

$$\Delta\varphi = \sum_{k=1}^{n} \{X^k, \{X^k, \varphi\}\}$$

After applying the Berezin-Toeplitz projection, we get:

$$T_m(\Delta\varphi) = -m^2[T_m(X^k), [T_m(X^k), T_m(\varphi)]] = \Delta_m \Phi_m$$

Theorem

The discrete Bochner-Laplace operator

$$\widetilde{\Delta}_m : C^\infty(M) \to C^\infty(M), \qquad \widetilde{\Delta}_m(f) = \sigma^{(m)} \circ \Delta_m \circ T^{(m)}$$

is a self-adjoint operator on $(\mathcal{H}_m, < \cdot, \cdot >_m)$ *with discrete spectrum.*

Convergence and Stability

Theorem

The discrete Bochner-Laplace operator $\widetilde{\Delta}_m$ *converges in the strong-graph limit sense to the Bochner-Lapalce operator* Δ*:*

$$\mathrm{sgr} - \lim \widetilde{\Delta}_m = \Delta \tag{3}$$

Theorem (No spurious eigenvalues)

Let A_n $(n \in \mathbb{N})$ *and* A *be (unbounded) self-adjoint operators and assume that* $D(A) = D(A_n)$*. Assume, furthermore, that there are null-sequences* (a_n) *and* (b_n) *from* $\mathbb{R}$ *for which*

$$\|(A - A_n)f\| \leq a_n\|f\| + b_n\|Af\| \quad \textit{for all } f \in D(A). \tag{4}$$

Then $\sigma(A) = \lim_{n\to\infty} \sigma(A_n)$*.*

Convergence and Stability

Proof.

On one hand, using structure preserving we have

$$\begin{aligned}
&\|\Delta(\varphi) - \sigma^{(m)} \circ \Delta_m \circ T^{(m)}(\varphi)\|_\infty \\
&\leq \|\Delta(\varphi) - \sigma^{(m)} \circ T^{(m)}(\Delta(\varphi))\|_\infty \\
&+ \|\sigma^{(m)} \circ T^{(m)}(\Delta(\varphi)) - \sigma^{(m)} \circ \Delta_m \circ T^{(m)}(\varphi)\|_\infty \leq a_m \|\Delta(\varphi)\|_\infty
\end{aligned}$$

and on the other hand, using Sobolev's embedding

$$\|\Delta(\varphi) - \sigma^{(m)} \circ \Delta_m \circ T^{(m)}(\varphi)\|_2 \leq a_m \|\varphi\|_{H^k}$$

□

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- Effective algorithm to construct such basis.

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Remaining open questions:

- Find a necessary and sufficient condition for the existence of (strongly) structure preserving projectors.
- Effective algorithm to construct such basis.
- Stability in all generality.

Thank You !

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