Easy going estimates for variational approximation

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(work in progress with Chunmei Su)

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References

C. Lubich 2005:
numerical analysis of time-dependent variational methods

I. Burghardt, R. Martinazzo 2020:
applicable error estimates

Schrödinger equation

$$i\partial_t \psi = H\psi$$

$H : D(H) \to \mathcal{H}$ is a self-adjoint linear operator.

$\mathcal{H}$ is a Hilbert space.

Given an approximation manifold $\mathcal{M} \subseteq \mathcal{H}$.

$\triangleright$ Seek $u(t) \in \mathcal{M}$ with $u(t) \approx \psi(t)$.

Bilinear forms

The Hilbert space $\mathcal{H}$ is equipped with a complex inner product

$$\mathcal{H} \times \mathcal{H} \to \mathbb{C}, \quad (\varphi, \psi) \mapsto \langle \varphi \mid \psi \rangle$$

▷ $\mathcal{H} \times \mathcal{H} \to \mathbb{R}$, $(\varphi, \psi) \mapsto \mathrm{Re}\,\langle \varphi \mid \psi \rangle$ is a real inner product (bilinear, symmetric, positive definite)

▷ $\mathcal{H} \times \mathcal{H} \to \mathbb{R}$, $(\varphi, \psi) \mapsto \mathrm{Im}\,\langle \varphi \mid \psi \rangle$ is a symplectic form (bilinear, alternating, non-degenerate)

Complex tangent spaces cf. Lubich, 2005

Assume that $\mathcal{T}_u\mathcal{M}$ is a complex subspace of $\mathcal{H}$ for all $u \in \mathcal{M}$.

Time-dependent Dirac–Frenkel variational principle:
Seek $u(t) \in \mathcal{M}$ such that

1) $\partial_t u(t) \in \mathcal{T}_{u(t)}\mathcal{M}$

2) $\langle v \mid i\partial_t u(t) - Hu(t) \rangle = 0$ for all $v \in \mathcal{T}_{u(t)}\mathcal{M}$

Assume that $\mathcal{T}_u\mathcal{M}$ is a complex subspace of $\mathcal{H}$ for all $u \in \mathcal{M}$.

Time-dependent Dirac–Frenkel variational principle:
Seek $u(t) \in \mathcal{M}$ such that

$$i\partial_t u(t) = P_{u(t)} H u(t),$$

where

$$P_{u(t)} : \mathcal{H} \to \mathcal{T}_{u(t)}\mathcal{M}$$

is the orthogonal projection on the tangent space.

Assume that $u(t) \in \mathcal{T}_{u(t)}\mathcal{M}$. Then,

$$\begin{aligned} \frac{d}{dt}\|u(t)\|^2 &= 2\,\mathrm{Re}\,\langle u(t) \mid \partial_t u(t)\rangle \\ &= 2\,\mathrm{Re}\,\langle u(t) \mid \tfrac{1}{i} H u(t)\rangle \\ &= 0 \end{aligned}$$

Assume nothing. Then,

$$\begin{aligned}
\frac{d}{dt}\langle u(t) \mid Hu(t)\rangle &= 2\,\mathrm{Re}\,\langle \partial_t u(t) \mid Hu(t)\rangle \\
&= 2\,\mathrm{Re}\,\langle \partial_t u(t) \mid i\partial_t u(t)\rangle \\
&= 0
\end{aligned}$$

Towards error estimates

$$i\partial_t \left(\psi(t) - u(t)\right) = H\psi(t) - P_{u(t)} H u(t)$$

$$\overset{\text{a posteriori}}{=} \quad H\left(\psi(t) - u(t)\right) + \Big(H - P_{u(t)} H\Big)\, u(t)$$

$$\overset{\text{a priori}}{=} \quad P_{u(t)} H\left(\psi(t) - u(t)\right) + \Big(H - P_{u(t)} H\Big)\, \psi(t)$$

Towards error estimates

$$i\partial_t\left(\psi(t)-u(t)\right)=H\psi(t)-P_{u(t)}Hu(t)$$

$$\overset{\text{a posteriori}}{=} \quad H\left(\psi(t)-u(t)\right)+P^{\perp}_{u(t)}Hu(t)$$

$$\overset{\text{a priori}}{=} \quad P_{u(t)}H\left(\psi(t)-u(t)\right)+P^{\perp}_{u(t)}H\psi(t)$$

A posteriori error estimate

$$i\partial_t \left(\psi(t) - u(t)\right) = H\left(\psi(t) - u(t)\right) + P^{\perp}_{u(t)} H u(t)$$

Variations of constants/Duhamel formula:

$$\psi(t) - u(t) = \frac{1}{i} \int_0^t \mathrm{e}^{-iH(t-s)} P^{\perp}_{u(s)} H u(s) \, \mathrm{d}s$$

implies

$$\|\psi(t) - u(t)\| \leq \int_0^t \|P^{\perp}_{u(s)} H u(s)\| \, \mathrm{d}s$$

$$\|\psi(t) - u(t)\| \leq \int_0^t \|P^{\perp}_{u(s)} H u(s)\| \, \mathrm{d}s$$

$$\|P^{\perp}_{u(s)} H u(s)\| \;=\; \mathrm{dist}\left(Hu(s), \mathcal{T}_{u(s)}\mathcal{M}\right)$$

R. Coalson, M. Karplus 1990:
variational Gaussian wave packets

E. Faou, C. Lubich 2006:
Poisson integrator for Gaussian wave packets

Gaussian wave packets $d = 1$

$$H = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$$

$$\mathcal{M} = \Big\{ \exp(-\tfrac{\gamma}{2}|x-q|^2 + ip(x-q) + \zeta) \mid \mathrm{Re}(\gamma) > 0,\ (q,p) \in \mathbb{R}^2,\ \zeta \in \mathbb{C} \Big\}$$

For all $u \in \mathcal{M}$,

$$\mathcal{T}_u\mathcal{M} = \Big\{ \pi u \mid \pi \text{ complex polynomial of degree } \leq 2 \Big\}.$$

Gaussian wave packets $\quad d = 1$

For all $u \in \mathcal{M}$,

$$\mathcal{T}_u\mathcal{M} = \Big\{ \pi u \mid \pi \text{ complex polynomial of degree } \le 2 \Big\}.$$

Observe:

1) $\mathcal{T}_u\mathcal{M}$ is complex linear.

2) $u \in \mathcal{T}_u\mathcal{M}$ $\quad \to$ mass conservation

3) $-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2}u \in \mathcal{T}_u\mathcal{M}$

4) If V is a polynomial of degree ≤ 2, then $Hu \in \mathcal{T}_u\mathcal{M}$.
$\to$ exact solution for harmonic oscillators

$$\|\psi(t) - u(t)\| \leq \int_0^t \|P^{\perp}_{u(s)} H u(s)\| \, \mathrm{d}s$$

For

$$H = -\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)$$

with smooth potential V, the error is governed by $\|\partial^{\alpha} V u(s)\|$ with $|\alpha| \geq 3$.

$$\|\psi(t) - u(t)\| \leq \int_0^t \|P_{u(s)}^{\perp} H u(s)\| \, \mathrm{d}s$$

with

$$\begin{aligned} \|P_{u(s)}^{\perp} H u(s)\|^2 &= \mathrm{dist}\Big(Hu(s), \mathcal{T}_{u(s)}\mathcal{M}\Big)^2 \\ &= \min_{w \in \mathcal{T}_{u(s)}\mathcal{M}} \|w - Hu(s)\|^2 \\ &= \|Hu(s)\|^2 - \|\partial_s u(s)\|^2 \end{aligned}$$

Indeed,

$$
\begin{aligned}
\min_{w\in\mathcal{T}_{u(s)}\mathcal{M}} \|w - Hu(s)\|^2 &= \|i\partial_s u(s) - Hu(s)\|^2 \\
&= \|\partial_s u(s)\|^2 - 2\,\mathrm{Re}\,\langle i\partial_s u(s) \mid Hu(s)\rangle + \|Hu(s)\|^2 \\
&= \|\partial_s u(s)\|^2 - 2\,\mathrm{Re}\,\langle i\partial_s u(s) \mid i\partial_s u(s)\rangle + \|Hu(s)\|^2 \\
&= \|Hu(s)\|^2 - \|\partial_s u(s)\|^2,
\end{aligned}
$$

since $\partial_s u(s) \in \mathcal{T}_{u(s)}\mathcal{M}$.

Expectation and standard deviation: For $\varphi \neq 0$ set

$$E(H,\varphi) = \frac{\langle \varphi \mid H\varphi \rangle}{\|\varphi\|^2}, \qquad \mathcal{E}(H,\varphi) = \|(H - E(H,\varphi))\varphi\|.$$

Note that

$$\mathcal{E}(H,\varphi)^2 = \|H\varphi\|^2 - E(H,\varphi)^2\|\varphi\|^2.$$

$$\|\psi(t) - u(t)\| \leq \int_0^t \|P^{\perp}_{u(s)} H u(s)\| \, \mathsf{d}s$$

with

$$\begin{aligned} \|P^{\perp}_{u(s)} H u(s)\|^2 &= \mathsf{dist}\left(Hu(s), \mathcal{T}_{u(s)}\mathcal{M}\right)^2 \\ &= \|Hu(s)\|^2 - \|\partial_s u(s)\|^2 \\ &= \mathcal{E}(H, u(s)) - \mathcal{E}(P_{u(s)} H P_{u(s)}, u(s)), \end{aligned}$$

where we **assume** that $u(s) \in \mathcal{T}_{u(s)}\mathcal{M}$.

Indeed,

$$\begin{aligned} \min_{w \in \mathcal{T}_{u(s)}\mathcal{M}} \|w - Hu(s)\|^2 &= \|Hu(s)\|^2 - \|\partial_s u(s)\|^2 \\ &= \|Hu(s)\|^2 - \|P_{u(s)} H P_{u(s)} u(s)\|^2 \end{aligned}$$

and

$$\begin{aligned} E(P_{u(s)} H P_{u(s)}, u(s)) &= \frac{\langle u(s) \mid i\partial_s u(s) \rangle}{\|u(s)\|^2} \\ &= \frac{\langle u(s) \mid Hu(s) \rangle}{\|u(s)\|^2} = E(H, u(s)). \end{aligned}$$

$$\mathcal{M} = \Big\{ \exp(-\tfrac{\gamma}{2}|x-q|^2 + ip(x-q) + \zeta) \mid \mathrm{Re}(\gamma) > 0,\, (q,p) \in \mathbb{R}^2,\ \zeta \in \mathbb{C} \Big\}$$

is generalized to

$$\mathcal{M} = \Big\{ a(\sqrt{\gamma}(x-q))\, \mathrm{e}^{ip(x-q)+\zeta} \mid \gamma > 0,\, (q,p) \in \mathbb{R}^2,\ \zeta \in \mathbb{C} \Big\}$$

for some smooth, decaying function $a : \mathbb{R} \to \mathbb{C}$.

The tangent spaces of

$$\mathcal{M} = \Big\{ u(x_1, x_2) = \varphi_1(x_1)\varphi_2(x_2) \;\;|\;\; \varphi_j \in L^2(\mathbb{R}),\;\; \|\varphi_j\| = 1 \Big\}$$

are **not** complex subspaces of $L^2(\mathbb{R}^2)$.

Assume that $\mathcal{T}_u\mathcal{M}$ is a complex subspace of $\mathcal{H}$ for all $u \in \mathcal{M}$.

Time-dependent Dirac–Frenkel variational principle:
Seek $u(t) \in \mathcal{M}$ such that

1) $\partial_t u(t) \in \mathcal{T}_{u(t)}\mathcal{M}$

2) $\langle v \mid i\partial_t u(t) - Hu(t) \rangle = 0$ for all $v \in \mathcal{T}_{u(t)}\mathcal{M}$

McLachlan variational principle:
Seek $u(t) \in \mathcal{M}$ such that

1) $\partial_t u(t) \in \mathcal{T}_{u(t)}\mathcal{M}$

2) $\|i\partial_t u(t) - Hu(t)\| = \min_{w \in \mathcal{T}_{u(t)}\mathcal{M}} \|iw - Hu(t)\|$

McLachlan variational principle:
Seek $u(t) \in \mathcal{M}$ such that

1) $\partial_t u(t) \in \mathcal{T}_{u(t)}\mathcal{M}$

2) $\operatorname{Im} \langle v \mid i\partial_t u(t) - Hu(t) \rangle = 0$ for all $v \in \mathcal{T}_{u(t)}\mathcal{M}$

(Dirac) **Frenkel 1934:** book on wave mechanics

McLachlan, 1964: paper on Schrödinger equation

Kramer, Saraceno 1981: Springer lecture notes on the time-dependent variational principle

McLachlan variational principle:

Seek $u(t) \in \mathcal{M}$ such that

$$\partial_t u(t) = P_{u(t)} \frac{1}{i} H u(t),$$

where

$$P_{u(t)} : \mathcal{H} \to \mathcal{T}_{u(t)}\mathcal{M}$$

is the orth. projection with respect to the real inner product.

Time-dependent variational principle:

Seek $u(t) \in \mathcal{M}$ such that

1) $\partial_t u(t) \in \mathcal{T}_{u(t)}\mathcal{M}$

2) $\mathrm{Re}\,\langle v \mid i\partial_t u(t) - Hu(t)\rangle = 0$ for all $v \in \mathcal{T}_{u(t)}\mathcal{M}$

Time-dependent variational principle:
Seek $u(t) \in \mathcal{M}$ such that

$$i\partial_t u(t) = P_{u(t)} H u(t),$$

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is the orth. projection with respect to the real inner product.

Conservation properties

- ▷ The imaginary part variational principle conserves norm if $u \in \mathcal{T}_u\mathcal{M}$ for all $u \in \mathcal{M}$.

- ▷ The real part variational principle conserves energy.

Current agenda — with Chunmei Su

▷ Work out the error estimates for explicit examples (Hartree, wave packets, multi-configuration Hartree)

▷ Use the error estimates for adaptivity

Thank you.