Introduction to the GRAPE Algorithm

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Optimal control of coupled spin dynamics: design of NMR pulse sequences by gradient ascent algorithms

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Acronym

GRAPE: **Gr**adient **A**scent **P**ulse **E**ngineering

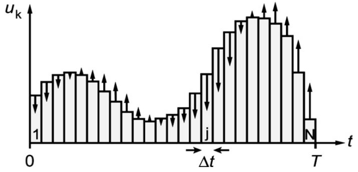
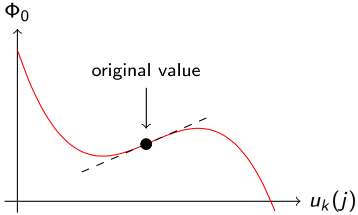


Fig. 1. Schematic representation of a control amplitude $u_k(t)$, consisting of N steps of duration $\Delta t = T/N$. During each step j, the control amplitude $u_k(j)$ is constant. The vertical arrows represent gradients $\delta\Phi_0/\delta u_k(j)$, indicating how each amplitude $u_k(j)$ should be modified in the next iteration to improve the performance function Φ_0.



at time index j: go in direction of gradient

Pulse Update

$$u_k(j) \longrightarrow u_k(j) + \epsilon \frac{\partial \Phi_0}{\partial u_k(j)}$$

Density Matrix

$$|\Psi\rangle \longrightarrow \rho = |\Psi\rangle\langle\Psi|$$

Liouville-von Neumann Equation

$$\dot{\rho}(t) = -i\,[H, \rho(t)]_{-} = -i\left[\left(H_0 + \sum_{k=1}^{m} u_k(t) H_k\right), \rho\right]_{-}$$

Time Propagation

$$U_j = \exp\left\{-i\Delta t\left(H_0 + \sum_{k=1}^{m} u_k(j) H_k\right)\right\}$$

$$\begin{aligned}\rho(T) &= U_N \dots U_1\, \rho(0)\, U_1^\dagger \dots U_N^\dagger \\ &= |\Psi(T)\rangle\langle\Psi(T)| \quad \text{with} \quad \Psi(T) = U_n \dots U_1 \Psi(0)\end{aligned}$$

Definition of Fidelity

Fidelity in Liouville space is defined in analogy to fidelity in Hilbert space: as the overlap between the propagated state with the optimal state.

Fidelity

$$\Phi_0 = \langle\langle C|\rho(T)\rangle\rangle \equiv \operatorname{tr}\left(C^\dagger \rho(T)\right)$$

$$C = O\,|\Psi(0)\rangle\langle\Psi(0)|\,O^\dagger \qquad \rho(T) = U\,|\Psi(0)\rangle\langle\Psi(0)|\,U^\dagger$$

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$$C = O \left|\Psi(0)\right\rangle\!\left\langle\Psi(0)\right| O^\dagger \qquad \rho(T) = U \left|\Psi(0)\right\rangle\!\left\langle\Psi(0)\right| U^\dagger$$

Equivalence to “normal” fidelity

$$\begin{aligned}
\operatorname{tr}\left(C^\dagger \rho(T) \right) &= \sum_n \left\langle n \middle| O \middle| \Psi(0) \right\rangle \left\langle \Psi(0) \middle| O^\dagger U \middle| \Psi(0) \right\rangle \left\langle \Psi(0) \middle| U^\dagger \middle| n \right\rangle \\
&= \left\langle \Psi(0) \middle| U^\dagger \sum \middle| n \right\rangle \left\langle n \middle| O \middle| \Psi(0) \right\rangle \left\langle \Psi(0) \middle| O^\dagger U \middle| \Psi(0) \right\rangle \\
&= \left\langle \Psi(0) \middle| U^\dagger O \middle| \Psi(0) \right\rangle \left\langle \Psi(0) \middle| O^\dagger U \middle| \Psi(0) \right\rangle \\
&= \left| \left\langle \Psi(0) \middle| O^\dagger U \middle| \Psi(0) \right\rangle \right|^2
\end{aligned}$$

A trace is invariant under cyclic permutation of its factors!

Fidelity at T

$$\begin{aligned}\Phi_0 = \langle C|\rho(T)\rangle &= \left\langle C|U_N \dots U_1 \rho(0) U_1^\dagger \dots U_N^\dagger \right\rangle \\ &= \left\langle U_{j+1}^\dagger \dots U_N^\dagger C U_N \dots U_{j+1} | U_j \dots U_1 \rho(0) U_1^\dagger \dots U_j^\dagger \right\rangle\end{aligned}$$

Propagated States → Fidelity at t_j

$$\lambda_j \equiv U_{j+1}^\dagger \dots U_N^\dagger C U_N \dots U_{j+1} \quad \text{bw. propagated optimal state}$$

$$\rho_j \equiv U_j \dots U_1 \rho(0) U_1^\dagger \dots U_j^\dagger \quad \text{fw. propagated initial state}$$

$$\Phi_0 = \langle C|\rho(T)\rangle = \langle \lambda_j | \rho_j \rangle$$

Note: all propagations with guess pulse!

Pulse Update

$$u_k(j) \longrightarrow u_k(j) + \epsilon \frac{\partial \Phi_0}{\partial u_k(j)} \qquad \text{We need to calculate } \frac{\partial \Phi_0}{\partial u_k(j)}$$

Two steps:

- For a variation $\delta u_k(j)$, calculate δU_j
- Use δU_j to calculate $\frac{\partial \Phi_0}{\partial u_k(j)}$

Calculations are not completely trivial.

Solution:

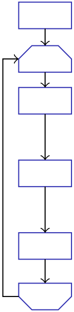
Gradient

$$\frac{\partial \Phi_0}{\partial u_k(j)} = -\left\langle \lambda_j \middle| i \Delta t [H_k, \rho_j]_- \right\rangle$$

Grape Algorithm

Pulse Update

$$u_k(j) \longrightarrow u_k(j) + \epsilon \frac{\partial \Phi_0}{\partial u_k(j)}; \qquad \frac{\partial \Phi_0}{\partial u_k(j)} = -\left\langle \lambda_j \middle| i \Delta t [H_k, \rho_j]_- \right\rangle$$



Guess initial controls $u_k(j)$

Update pulse according to gradient:

Forward propagation of $\rho(0)$: calculate and store all $\rho_j = U_j \dots U_1 \rho(0) U_1^\dagger \dots U_j^\dagger$ for $j \in [1, N]$

Backward propagation of C: calculate and store all $\lambda_j = U_{j+1}^\dagger \dots U_N^\dagger C U_N \dots U_{j+1}$ for $j \in [1, N]$

Evaluate $\frac{\partial \Phi_0}{\partial u_k(j)}$ and update the $m \times N$ control amplitudes $u_k(j)$

Done if fidelity converges

Non-Hermitian Operators

$$\Phi_1 = \Re[\Phi_0]; \quad \frac{\partial \Phi_1}{\partial u_k(j)} = -\left\langle \lambda_j^x | i\Delta t[H_k, \rho_j^x \right\rangle - \left\langle \lambda_j^y | i\Delta t[H_k, \rho_j^y \right\rangle$$

$$\Phi_2 = |\Phi_0|^2; \quad \frac{\partial \Phi_2}{\partial u_k(j)} = -2\Re\left\{ \langle \lambda_j | i\Delta t[H_k, \rho_j \rangle \langle \rho_N^y | C \rangle \right\}$$

Unitary Transformations

$$\Phi_3 = \Re \langle U_F | U(T) \rangle = \Re \left\langle U_{j+1}^\dagger \dots U_N^\dagger U_F | U_j \dots U_1 \right\rangle = \Re \langle P_j | X_j \rangle$$

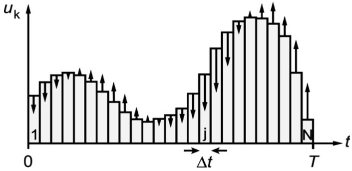
$$\frac{\partial \Phi_3}{\partial u_k(j)} = -\Re \langle P_j | i\Delta t H_k X_j \rangle$$

$$\Phi_4 = |\langle U_F | U(T) \rangle|^2 = \langle P_j | X_j \rangle \langle X_j | P_j \rangle$$

$$\frac{\partial \Phi_4}{\partial u_k(j)} = -2\Re\left\{ \langle P_j | i\Delta t H_k X_j \rangle \langle X_j | P_j \rangle \right\}$$

Also works with Lindbladt-Operators. Additional energy constraints are possible.

Comparison with OCT



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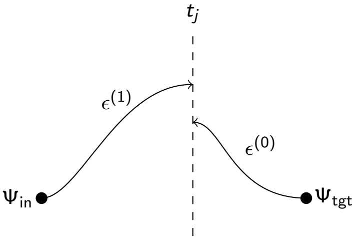

$$\Delta u(j) \sim \left\langle \Psi_{bw}(t_j) \left| \mu \right| \Psi_{fw}(t_j) \right\rangle$$

- GRAPE also needs forward- and backward-propagation, but only with old pulse. Propagated states also need to be stored.
- Pulse update at point j in the current iteration does *not* depend on other updated pulse values (non-sequential update)
- All updates in GRAPE can in principle be calculated in parallel.
- Convergence tends to be pretty lousy (so I'm told)
- What about the choice of ϵ?

Thank You!