Workshop: A Quantum Engineer's Guide to the Quantum Optimal Control Suite (QuOCS)

Ressa Said & Hendry Lim

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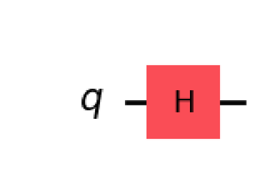
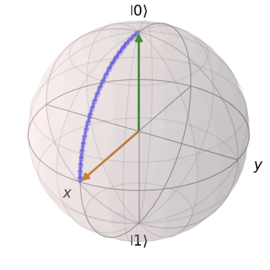
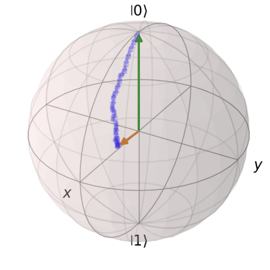
What we theoretically want:



What we ideally expect:



What we will most likely get:



Quantum Optimal Control

Loose definition: Tuning variables in the system dynamics to achieve a certain goal.

The control landscape:

- System dynamics.
- Cost function or figure of merit.
- Control space restriction.

Traversing the control landscape: QOC search methods

Type 1: **Gradient-based**

- Gradient Ascent Pulse Engineering (GRAPE).
- Krotov's method.
- Gradient Optimization Using Parameterization (GROUP).
- Gradient Optimization of Analytic Controls (GOAT).

Type 2: **Gradient-free**

- Chopped Random Basis (CRAB).
- **Dressed Chopped Random Basis (dCRAB).**

[Rembold et al., AVS Quantum Sci. 2, 024701 (2020).]

The Dressed Chopped Random Basis (dCRAB) Algorithm

- Set **superiteration** $s = 1$.
- Expand control using a **chopped basis** $\{f_k^s\}$ with **randomized basis parameters** β_k^s:

$$f^s(t) = \sum_{k=1}^{N_c} a_k^s f_k^s(\beta_k^s; t)$$

- Numerically optimize a_k^s using algorithms such as the **Nelder-Mead (NM) simplex** or **Covariance Matrix Adaptation Evolution Strategy (CMA-ES)**.
- Carry the optimized pulse in superiteration $s = 1$ over to superiteration $s = 2$. Repeat optimization.

$$f^s(t) = a_0^s f^{s-1}(t) + \sum_{k=1}^{N_c} a_k^s f_k^s(\beta_k^s; t)$$

- Rinse and repeat.

Scaling function

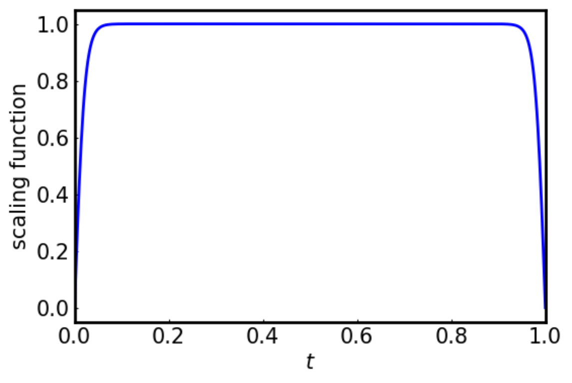
Multiplies the pulse; useful to hold the end-values at zero.

$$\Lambda(t) = \tanh\left[\sigma \sin\left(\frac{\pi t}{2T}\right)\right] \tanh\left[-\sigma \sin\left(\frac{\pi(t-T)}{2T}\right)\right]$$

where

σ : ramp steepness.

T : pulse duration.



Optimization hyperparameters

General:

- Initial guess.
- Stopping criteria and tolerances of search methods.

dCRAB-specific:

$$f^s(t) = a_0^s f^{s-1}(t) + \sum_{k=1}^{N_c} a_k^s f_k^s(\beta_k^s; t)$$

- Number N_c of basis per superiteration.
- Variation of amplitude a_k^s between iterations.
- The basis $\{f_k^s\}$ used.
- Sampling interval $[\beta_{\min}, \beta_{\max}]$ of the randomized basis parameters β_k^s.

Experiments:

- Drift compensation.
- Pulse re-evaluation.

The Quantum Optimal Control Suite (QuOCS)

Why use QuOCS?

- Open source and actively maintained.
- Informative logging.
- Provides popular QOC algorithms (dCRAB, GRAPE, etc.).
- Easy to use with simple syntax.
- Highly modular and customizable, even allowing users to add customized algorithms and bases.

Using QuOCS

1. Set up the optimization parameters in the **optimization dictionary.**
2. Create the appropriate **Figure of Merit** object.
3. Create the optimizer object and run the optimization.

Example problem: The Ising Chain

System dynamics:

$$\hat{H} = -J\sum_{k=0}^{N-1}\hat{\sigma}_k^z\hat{\sigma}_{k+1}^z + u(t)\cdot\sum_{k=0}^{N-1}\hat{\sigma}_k^x, \qquad \hat{\sigma}_{N-1}^z = \hat{\sigma}_0^z$$

Cost function:

$$|\psi_i\rangle = \bigotimes_{k=0}^{N-1}|0\rangle_k\,, \qquad |\psi_{\mathrm{target}}\rangle = \bigotimes_{k=0}^{N-1}|1\rangle_k$$

$$J = 1 - F\left(|\psi_f\rangle\,, |\psi_{\mathrm{target}}\rangle\right) = 1 - |\langle\psi_f|\psi_{\mathrm{target}}\rangle|$$

Control space restrictions:

$$|u(t)| \leq 10$$

Further reading

- QuOCS' article: 10.1016/j.cpc.2023.108782 or arXiv:2212.11144
- QuOCS' repository on GitHub
- A review on QOC for NV center systems by Rembold et al.: 10.1116/5.0006785
- A great textbook on QOC theory by D'Alessandro: 10.1201/9781003051268