Inverse design of dissipative quantum steady-states with implicit differentiation

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Abstract

Inverse design of a property that depends on the steady-state (SS) of an open quantum system (OQS) is commonly done by grid-search type of methods. **In this paper we present a new methodology that allows us to compute the gradient of the steady-state of an open quantum system with respect to any parameter of the Hamiltonian using the implicit differentiation theorem.** As an example, we present a simulation of a spin-boson model where the steady-state solution is obtained using Redfield theory.

Background: Steady-state

- For many open quantum systems the properties of interest are related to the steady-state, ρ^{ss}, $\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = 0$.
  1. Energy transfer efficiency in biological systems excited by natural incoherent light.
  2. Performance of quantum heat engines or refrigerators.
- What if we could learn how ρ^{ss} changes with respect to any parameters of the Hamiltonian (θ_i)? $\rightarrow \frac{\partial \rho^{ss}}{\partial \theta_i}$.

Implicit Differentiation of the steady-state (1/2)

- **Goal**: Compute the gradient of the steady state with respect to the Hamiltonian parameters, $\frac{\partial \rho^{ss}}{\partial \theta_i}$.
- We solve for the SS using an ODE solver for a sufficiently long period of time.

Problem: To differentiate through the internals of the ODE solver requires,

1. Store the entire trajectory of $\rho(t)$ $\rightarrow$ memory demanding
2. Solving $\rho(t)$ in reverse time $\rightarrow$ impossible for ρ^{ss}

Solution:

- ρ^{ss} is the solution of a **fixed point problem**.
- The Jacobian $\frac{d\rho^{ss}}{d\boldsymbol{\theta}}$ can be expressed using the implicit function theorem,

$$\frac{d\rho^{ss}}{d\boldsymbol{\theta}} = -\left(\frac{df(\rho^{ss},\boldsymbol{\theta})}{d\rho}\right)^{-1}\left[\frac{df(\rho^{ss},\boldsymbol{\theta})}{d\boldsymbol{\theta}}\right]. \quad (1)$$

Implicit Differentiation of the steady-state (2/2)

Advantages:

- Constant memory cost
- Does not require how ρ^{ss} is computed as long as it satisfies the steady-state criterion, $f(\rho^{ss},\boldsymbol{\theta}) = 0$.

Scalar loss function $\mathcal{L}(\boldsymbol{\theta},\rho^{ss})$:

- Gradient with respect to parameters can be factored with the chain rule $\frac{d\mathcal{L}}{d\rho^{ss}}\frac{d\rho^{ss}}{d\boldsymbol{\theta}}$.
- All gradients were computed using JAX[I].

Background: Spin-Boson model

- The spin-boson (SB) model is commonly used to describe a wide variety of physical phenomena[II],
  - Electron/Energy transfer or Heat transport

The total Hamiltonian is,

$$H_S = \frac{\epsilon}{2}\sigma_z + \frac{\Delta}{2}\sigma_x, \quad H_B = \sum_k \omega_k b_k^\dagger b_k, \quad H_{SB} = \sigma_z \sum_k \lambda_k (b_k^\dagger + b_k), \quad (2)$$

where $b_k^\dagger$ (b_k) is the creation (annihilation) operator of mode k in the bath, σ_z and σ_x are Pauli matrices, and $\{\lambda_k\}$ are the coupling strength parameters, and ϵ and Δ are system parameters. • In the Redfield theory (RT), equations of motions are[III],

$$\frac{\partial \rho_{\mu,\nu}(t)}{\partial t} = -i\omega_{\mu,\nu}\rho_{\mu,\nu}(t) + \sum_{\kappa,\lambda} R_{\mu,\nu,\kappa,\lambda}\, \rho_{\kappa,\lambda}(t), \quad (3)$$

$R_{\mu,\nu,\kappa,\lambda}$ are the Redfield tensors which describe the interaction of the system and bath and are given by,

$$R_{\mu,\nu,\kappa,\lambda} = \Gamma^+_{\lambda,\nu,\mu,\kappa} + \Gamma^-_{\lambda,\nu,\mu,\kappa} - \delta_{\nu,\lambda}\sum_\alpha \Gamma^+_{\mu,\alpha,\alpha,\kappa} - \delta_{\mu,\kappa}\sum_\alpha \Gamma^+_{\lambda,\alpha,\alpha,\nu}, \quad (4)$$

which contain the transition rates,

$$\Gamma^+_{\lambda,\nu,\mu,\kappa} = \langle\lambda|\sigma_z|\nu\rangle\langle\mu|\sigma_z|\kappa\rangle \int_0^\infty \mathrm{d}\tau F(\tau) e^{-i\omega_{\mu,\kappa}\tau}, \quad \Gamma^-_{\lambda,\nu,\mu,\kappa} = \langle\lambda|\sigma_z|\nu\rangle\langle\mu|\sigma_z|\kappa\rangle \int_0^\infty \mathrm{d}\tau F^*(\tau) e^{-i\omega_{\lambda,\nu}\tau},$$

that are in turn comprised of the bath correlation function,

$$F(\tau) = \int_0^\infty \mathrm{d}\omega\, g(\omega)\left[\coth(\beta\omega/2)\cos(\omega\tau) - i\sin(\omega\tau)\right]. \quad (5)$$

where $[\mu,\nu,\kappa,\lambda]$ are eigenstates of H_S. $g(\omega)$ is the super Ohmic spectral density function, and η is the bath friction parameter that is on the order of λ_k^2 and β is the inverse temperature.

Results: Sensitivity analysis

- **Loss**: Population difference at equilibrium for the SB model, $\langle\sigma_z\rangle = \mathrm{Tr}[\sigma_z\rho^{ss}]$.

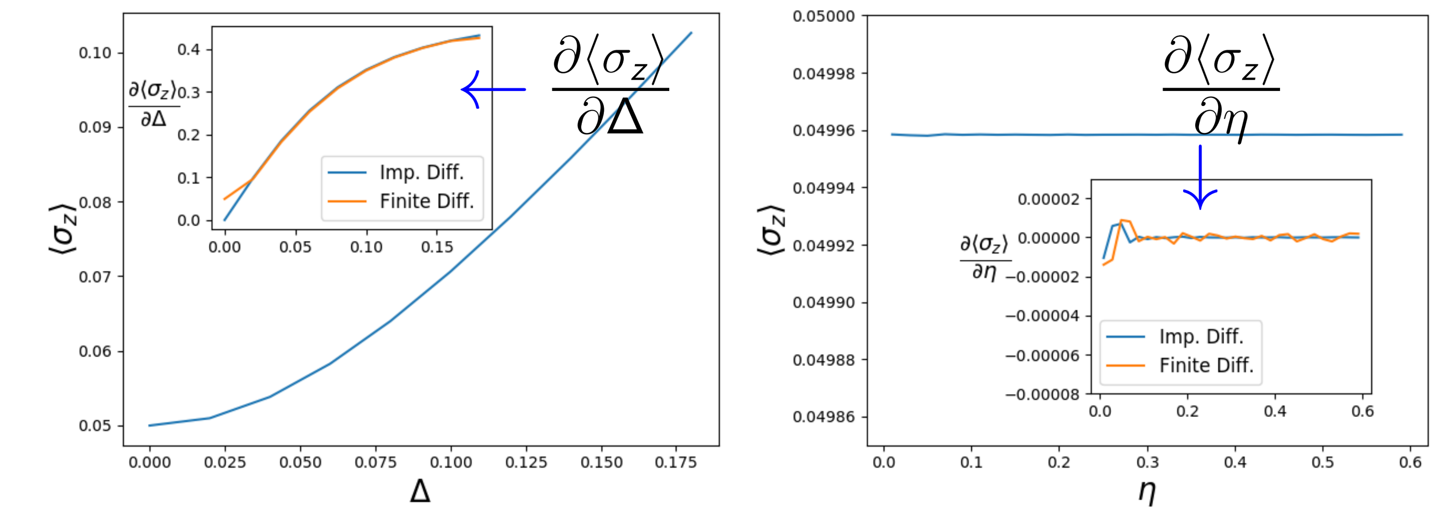

Figure: The inset of each figure compares the gradient computed with Eq. (1) (blue solid curve) and finite differences (orange solid curve). For all calculations, except for the parameter in play, we used $\beta = 0.1$, $\eta = 0.01$, $w_c = 1$, $\epsilon = 0.1$, and $\Delta = 0$. The initial density matrix used was $\rho_S(t_0) = [3/4, -i\frac{\sqrt{3}}{4}, i\frac{\sqrt{3}}{4}, 1/4]$.

Results: Inverse design

- **Goal**: Inverse design of the system parameters (ϵ,Δ) to reproduce a target $\hat{\langle\sigma_z\rangle}$; $\mathcal{L}(\epsilon,\Delta) = \left\|\langle\sigma_z\rangle - \hat{\langle\sigma_z\rangle}\right\|_2$.

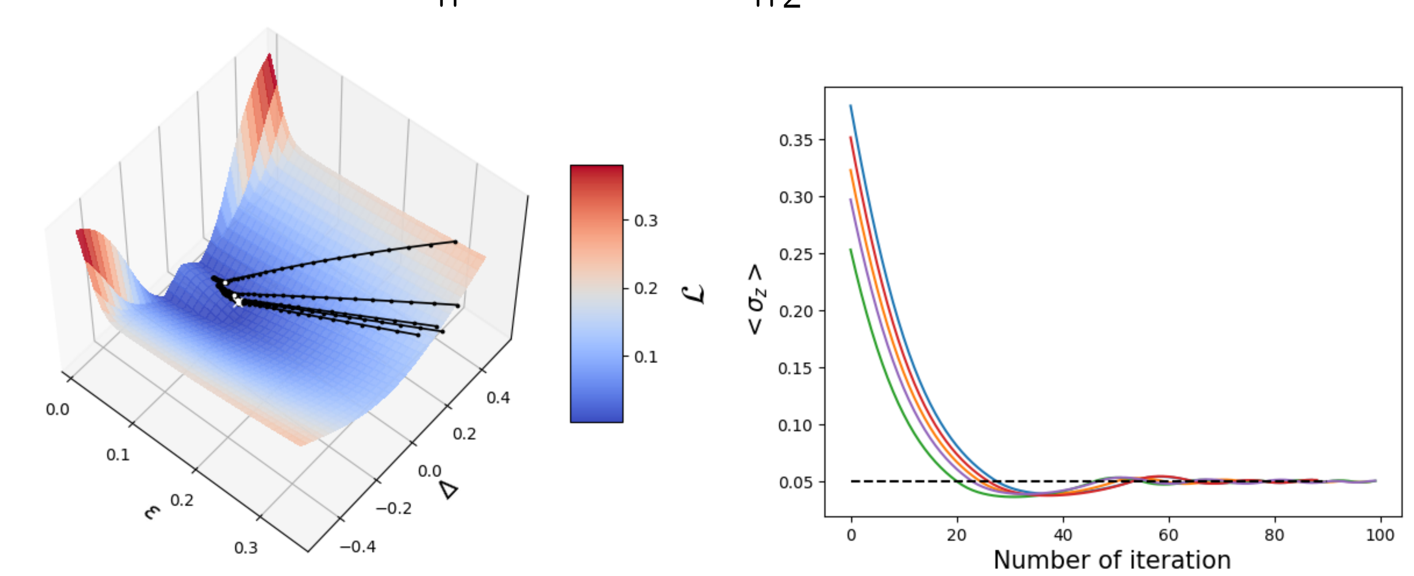

Figure: The iterations of the optimization procedure in the parameter space for different random initialization. $\frac{\partial\mathcal{L}}{\partial\epsilon}$ and $\frac{\partial\mathcal{L}}{\partial\Delta}$ used in the Adam optimizer were computed with Eq. (1); the learning rate was set to 0.1. For all calculations, we used $\beta = 0.1$, $\eta = 0.10$, $w_c = 1.$ and $\hat{\langle\sigma_z\rangle} = 0.04996$.

References

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