The adjoint method and the trace objective function

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The state equation

The state equation for $\Psi_j^\alpha \in \mathbb{C}^N$ is

$$\dot{\Psi}_j^\alpha + iH(t,\alpha)\Psi_j^\alpha = 0, \quad 0 \le t \le T, \quad \Psi_j^\alpha(0) = \mathbf{e}_j,$$

where the Hamiltonian matrix is $H(t,\boldsymbol{\alpha}) = H_0 + p(t,\boldsymbol{\alpha})H_1 = H^*$ and $\mathbf{e}_j$ is the j^{th} unit base vector.
The real-valued function $p(t,\boldsymbol{\alpha})$ depends on the control parameters

$$\boldsymbol{\alpha} = [\alpha_1, \alpha_2, \ldots, \alpha_D]^T.$$

The quantity $\Phi_{jk}^\alpha = \partial\Psi_j^\alpha/\partial\alpha_k$ satisfies

$$\dot{\Phi}_{jk}^\alpha + iH(t,\boldsymbol{\alpha})\Phi_{jk}^\alpha = -i\frac{\partial H(t,\boldsymbol{\alpha})}{\partial\alpha_k}\Psi_j^\alpha, \quad \Phi_{jk}^\alpha(0) = 0,$$

for $0 \le t \le T$.

The objective functional

Desired target gate after time T,

$$\mathbf{\Psi}^t(T) := [\mathbf{d}_1, \mathbf{d}_2, \ldots, \mathbf{d}_N] =: G_t, \;\; G_t^* G_t = I.$$

The control parameters $\boldsymbol{\alpha}$ result in the state

$$\mathbf{\Psi}^\alpha(t) = [\Psi_1^\alpha(t), \Psi_2^\alpha(t), \ldots, \Psi_N^\alpha(t)] = G_\alpha(t).$$

The distance between $G_\alpha(t)$ and G_t, in a weighted norm, with a weight function $0 \leq w(t) \leq 1$, $w(0) = 0$, $w(T) = 1$,

$$g_2(\mathbf{\Psi}^\alpha) = \int_0^T w(\tau) \left(1 - \frac{1}{N^2} S(\tau) \bar{S}(\tau) \right) \, d\tau.$$

The gate fidelity is measured using the Frobenius matrix scalar product,

$$S(\tau) = \sum_{j=1}^N \langle \Psi_j^\alpha(\tau), \mathbf{d}_j \rangle.$$

The gradient of the objective functional

$$
\begin{aligned}
\frac{\partial g_2}{\partial \alpha_k} &= -\frac{2}{N^2}\mathrm{Re}\int_0^T w(\tau)\frac{\partial S(\tau)}{\partial \alpha_k}\bar{S}(\tau)\,d\tau \\
&= -\frac{2}{N^2}\mathrm{Re}\int_0^T w(\tau)\sum_{j=1}^{N}\left\langle \frac{\partial \Psi_j^{\alpha}(\tau)}{\partial \alpha_k}, \mathbf{d}_j \right\rangle \bar{S}(\tau)\,d\tau \\
&= -\frac{2}{N^2}\mathrm{Re}\sum_{j=1}^{N}\int_0^T w(\tau)\left\langle \frac{\partial \Psi_j^{\alpha}(\tau)}{\partial \alpha_k}, \bar{S}(\tau)\mathbf{d}_j \right\rangle\,d\tau \\
&= -\frac{2}{N^2}\mathrm{Re}\sum_{j=1}^{N}\int_0^T \left\langle \Phi_{jk}(\tau), w(\tau)\bar{S}(\tau)\mathbf{d}_j \right\rangle\,d\tau
\end{aligned}
$$

where $\Phi_{jk} = \partial \Psi_j^{\alpha}/\partial \alpha_k$ and $k = 1, 2, \ldots, D$.

The state and adjoint equations

Let $\Phi_{jk} = \partial \Psi_j^\alpha / \partial \alpha_k$. It satisfies the state equation

$$\dot{\Phi}_{jk} + iH\Phi_{jk} = \mathbf{f}_{jk}(t), \quad \Phi_{jk}(0) = 0,$$

where $\mathbf{f}_{jk}(t) = -i(\partial H/\partial \alpha_k)\Psi_j^\alpha$. The adjoint equation is

$$-\dot{\boldsymbol{\lambda}}_j - iH\boldsymbol{\lambda}_j = \mathbf{h}_j(t), \quad \boldsymbol{\lambda}_j(T) = 0.$$

where we choose

$$\mathbf{h}_j(t) = w(t)\bar{S}(t)\mathbf{d}_j, \quad j = 1, 2, \ldots, N.$$

Note that the adjoint equation satisfies terminal conditions and is solved backwards in time, $T \geq t \geq 0$.

The adjoint relation

By integration by parts in time and using the initial and terminal conditions, it is straighforward to derive the adjoint relation,

$$\int_0^T \langle \Phi_{jk}(\tau), \mathbf{h}_j(\tau) \rangle \, d\tau = \int_0^T \langle \mathbf{f}_{jk}(\tau), \boldsymbol{\lambda}_j(\tau) \rangle \, d\tau.$$

By combining the above results,

$$\begin{aligned} \frac{\partial g_2}{\partial \alpha_k} &= -\frac{2}{N^2} \mathrm{Re} \sum_{j=1}^{N} \int_0^T \langle \Phi_{jk}(\tau), \mathbf{h}_j(\tau) \rangle \; d\tau \\ &= +\frac{2}{N^2} \mathrm{Re} \sum_{j=1}^{N} \int_0^T \left\langle i \left(\frac{\partial H}{\partial \alpha_k} \right) \Psi_j^{\alpha}(\tau), \boldsymbol{\lambda}_j(\tau) \right\rangle \; d\tau. \end{aligned}$$

Without adjoint: solve N state equations for Ψ_j^{α} and ND state equations for Φ_{jk}; total solves: $= (D+1)N$
With adjoint: solve N state equations for Ψ_j^{α} and N adjoint equations for $\boldsymbol{\lambda}_j$; ; total solves: $= 2N$