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Optimal control design of pulse shapes as analytic functions

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ABSTRACT

Representing NMR pulse shapes by analytic functions is widely employed in procedures for optimizing performance. Insights concerning pulse dynamics can be applied to the choice of appropriate functions that target specific performance criteria, focusing the solution search and reducing the space of possible pulse shapes that must be considered to a manageable level. Optimal control theory can accommodate significantly larger parameter spaces and has been able to tackle problems of much larger scope than more traditional optimization methods. However, its numerically generated pulses, as currently constructed, do not readily incorporate the capabilities of particular functional forms, and the pulses are not guaranteed to vary smoothly in time, which can be a problem for faithful implementation on older hardware. An optimal control methodology is derived for generating pulse shapes as simple parameterized functions. It combines the benefits of analytic and numerical protocols in a single powerful algorithm that both complements and enhances existing optimization strategies.

1. Introduction

A fundamental goal of pulse engineering is optimal pulse performance. The primary impediment to successful pulse optimization is the enormous space of possible pulse shapes that must be considered. One widely employed solution to this difficulty is to represent pulse waveforms by analytic functions [1–20]. Functions can be chosen for their suitability to a given problem using physical intuition and analytical insights, focusing the solution search. In addition, the space of possible pulse shapes is restricted to particular pulse families characterized by a relatively small set of parameters, making the optimization problem more tractable. An ancillary, but not insignificant, benefit is the smooth variation of the resulting pulses, enabling implementation with the necessary fidelity using basic (rather than more sophisticated) NMR hardware. However, this approach effectively scales the problem down to accommodate the limitations of a given optimization procedure. Pulse design problems of larger scope requiring more parameters are simply not accessible.

Another approach is to utilize more efficient optimization to identify the smaller subset of pulse shapes containing the solution to a desired problem. We have previously shown that optimal control theory is a powerful method that can be applied to a wide range of pulse design problems (see, e.g. [21], and references therein). It utilizes an efficiently calculated gradient towards better performing pulse parameters to narrow the solution search. Optimal control provides the flexibility to introduce important constraints, such as relaxation and compensation for RF inhomogeneity, enabling it to obtain solutions for large-scale problems that were previously deemed to be computationally impractical. Its fast convergence has allowed the optimization of as many as 300,000 independent parameters [22]. Thus, restricting the scale of the problem is less of an issue for optimal control. But insights into the performance of its numerically generated pulses are less evident, and the resulting pulses are not guaranteed to be smooth.

The topic of the present work is a method for incorporating the benefits of both approaches discussed so far. We derive an optimal control algorithm to generate pulse shapes expressed as simple parameterized functions. Examples follow illustrating the capabilities of this optimized parameterization for pulse design, which we designate as OP and pronounce "Opie". The resulting pulses are guaranteed to have the smooth variation of the underlying functions.

2. Optimal control algorithm

Optimal control algorithms relevant to the present treatment have been described previously [22–25], with specific details related to incorporating relaxation and phase slope given in [26,27]. A synopsis of the standard optimal control formulation underlying the new approach is provided in the next section. We then derive the modifications necessary to optimize the performance of pulses constrained to be analytic functions.

2.1. Standard formulation

Optimal control theory is a generalization (e.g. [28]) of the classical Euler–Lagrange formalism, with the Lagrangian replaced by a

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cost function L chosen to impose some desired measure of performance on the state variable for the system of interest. Given a dynamical equation for the time evolution of state $\boldsymbol{x}(t)$ that depends on controls $\boldsymbol{u}(t)$, the goal is to find the path or trajectory $\boldsymbol{x}_{\text{opt}}(t)$ producing an extremal value of the functional

$$J[\boldsymbol{x}] = \int_{t_0}^{t_f} L[t, \boldsymbol{x}(t), \boldsymbol{u}(t)]\, dt \tag{1}$$

over a specified time interval $[t_0, t_f]$. Often, L is chosen with no explicit dependence on $\boldsymbol{x}$ or t. A final cost term $\Phi[\boldsymbol{x}(t_f)]$ evaluated at the end of the time interval is also generally included.

Additional constraints on the optimizing curve, of the form $g(\boldsymbol{x}) = c$, can be included in the formalism by the standard method of introducing Lagrange multipliers λ_j for each constraint equation g_j, which defines the "hamiltonian" for the system in terms of the inner product between $\boldsymbol{\lambda}$ and $\boldsymbol{g}$ (components λ_j and g_j, respectively) as

$$h = L - \langle \boldsymbol{\lambda} | \boldsymbol{g} \rangle. \tag{2}$$

The necessary condition for an optimizing trajectory is that the variation δJ at all points of the path be equal to zero. Imposing the system evolution equation as a constraint in the form $\dot{\boldsymbol{x}}(t) = g(\boldsymbol{x}(t))$ results in the following requirements to optimize the cost, given an initial starting point $\boldsymbol{x}_0$ for the trajectory:

$$\dot{\boldsymbol{x}} = \frac{\partial h}{\partial \boldsymbol{\lambda}}, \qquad \boldsymbol{x}(t_0) = \boldsymbol{x}_0 \tag{3}$$

$$\dot{\boldsymbol{\lambda}} = -\frac{\partial h}{\partial \boldsymbol{x}}, \qquad \boldsymbol{\lambda}(t_f) = \partial \Phi / \partial \boldsymbol{x} \tag{4}$$

$$\frac{\partial h}{\partial \boldsymbol{u}} = 0 \tag{5}$$

If $\partial h / \partial \boldsymbol{u}$ is *not* equal to zero, it represents a gradient giving the proportional adjustment to make in the controls for a more optimal solution.

To be more specific, consider a system of noninteracting spins evolving according to the Bloch equation. The state variable is the magnetization $\boldsymbol{M}(t)$. In units of angular frequency (radians/s), the effective RF field in the rotating frame is

$$\begin{aligned} \boldsymbol{\omega}_e(t) &= \omega_{AM}(t)[\cos\phi(t)\hat{\boldsymbol{x}} + \sin\phi(t)\hat{\boldsymbol{y}}] + [\omega_3(t) + \delta\omega]\hat{\boldsymbol{z}} \\ &= \omega_1(t)\hat{\boldsymbol{x}} + \omega_2(t)\hat{\boldsymbol{y}} + [\omega_3(t) + \delta\omega]\hat{\boldsymbol{z}} \end{aligned} \tag{6}$$

which encompasses any desired modulation of the amplitude ω_{AM} and phase ϕ of the pulse, or, equivalently, the real and imaginary components ω_1, ω_2, and frequency modulation ω_3 with respect to chemical-shift $\delta\omega$. The inner product of Eq. (2) is the dot product between the vectors $\boldsymbol{\lambda}$ and $\boldsymbol{g} = \boldsymbol{\omega}_e \times \boldsymbol{M}$, giving

$$h = L - \boldsymbol{\lambda} \cdot (\boldsymbol{\omega}_e \times \boldsymbol{M}) = L - \boldsymbol{\omega}_e \cdot (\boldsymbol{M} \times \boldsymbol{\lambda}) \tag{7}$$

The controls $\boldsymbol{u}(t)$ in the standard formulation of optimal control theory are thus the RF pulses $\boldsymbol{\omega}(t)$ applied to the sample at each time t. At each pulse time increment $t_j = j\Delta t$, there is an independent control $\omega_i(t_j)$. The gradient $G_i(t_j)$ giving the adjustment to make in the control $\omega_i(t_j)$ at each iteration of the algorithm is

$$G_i(t_j) = \partial h / \partial \omega_i(t_j) = \partial L / \partial \omega_i(t_j) - [\boldsymbol{M}(t_j) \times \boldsymbol{\lambda}(t_j)]_i. \tag{8}$$

Often, the only performance measure of interest is the final cost, and the "running" cost L is set equal to zero.

2.2. The OP variation

If we now represent each pulse component ω_i by a given function f_i parameterized by constants c_n^i (designating the n^{th} constant comprising a vector $\boldsymbol{c}^i$), then

$$\omega_i(t) = f_i(\boldsymbol{c}^i, t), \tag{9}$$

and the controls become the c_n^i. Defining operations with the vector $\boldsymbol{c}^i$ as operations with each of the c_n^i, Eq. (5) for the gradient $\boldsymbol{G}^i$ with components G_n^i becomes

$$\begin{aligned} \frac{\partial h}{\partial \boldsymbol{c}^i} = \boldsymbol{G}^i &= \frac{\partial h}{\partial \omega_i} \cdot \frac{\partial \omega_i}{\partial \boldsymbol{c}^i} = \sum_j \partial h / \partial \omega_i(t_j)\, \partial \omega_i(t_j) / \partial \boldsymbol{c}^i \\ &= \sum_j G_i(t_j)\, \partial \omega_i(t_j) / \partial \boldsymbol{c}^i \end{aligned} \tag{10}$$

Thus, the new gradient G_n^i for adjusting the parameter c_n^i is effectively a time average of the gradients $G_i(t_j)$ from the standard formulation of the NMR optimal control problem for the $\omega_i(t_j)$ (Eq. (8)), weighted by the $\partial \omega_i(t_j) / \partial c_n^i$ derived from the dependence of ω_i on c_n^i at each time t_j. The rest of the OP algorithm proceeds according to standard gradient ascent methods, as described previously [23,29]:

(i) Choose an initial RF sequence $\omega_i(t) = f_i(\boldsymbol{c}^i, t)$.
(ii) Evolve $\boldsymbol{M}$ forward in time from the initial state $\boldsymbol{x}(t_0)$.
(iii) Evolve $\boldsymbol{\lambda}$ backwards in time from the target state $\boldsymbol{\lambda}(t_f)$.
(iv) $\boldsymbol{c}^i \to \boldsymbol{c}^i + \epsilon \boldsymbol{G}^i$.
(v) $\omega_i(t) = f_i(\boldsymbol{c}^i + \epsilon \boldsymbol{G}^i, t)$.
(vi) Repeat steps (ii)–(iv) until a desired convergence of Φ is reached.

In addition, if the optimization is performed over a range of chemical-shift offsets and/or variations in the peak RF calibration, the gradient $\boldsymbol{G}^i$ is averaged over the entire range. If f_i is linear in the sense that $f_i(\boldsymbol{c}^i + \epsilon \boldsymbol{G}^i, t) = f_i(\boldsymbol{c}^i, t) + \epsilon f_i(\boldsymbol{G}^i, t)$, then $\omega_i(t) \to \omega_i(t) + \epsilon f_i(\boldsymbol{G}^i, t)$ in step (v), which can be compared to the standard formulation $\omega_i(t) \to \omega_i(t) + \epsilon G_i(t)$.

Most generally, the c_n^i can be time dependent, and the sum in Eq. (10) is over those times for which the parameter is piecewise constant. We are most interested in the case where these controls are constant over the entire time interval of the pulse, since this provides the simplest parameterization of the pulse.

The results for alternative systems and evolution equations are similar, with simple, straightforward modifications. There is a control for each RF channel applied to a given spin species. For the Liouville equation, the density matrix, ρ, gives the state of the system, and the inner product in this representation is the trace of the matrix product $\lambda^\dagger g$, with $g = -i/\hbar[H, \rho]$ from the evolution equation. The inner product for a state $|\Psi>$ that evolves according to the Schrödinger equation is a generalization of the dot product that incorporates vectors with complex components.

3. Results and discussion

OP tailored pulses are presented to demonstrate the capabilities of the new algorithm. Unless noted otherwise, the cost function employed is the projection of the transformed magnetization onto the desired target state: the x-axis for excitation and the $-z$-axis for inversion. In all the cases presented, the "running" cost $L = 0$, giving $G_i(t_j) = [\boldsymbol{M}(t_j) \times \boldsymbol{\lambda}(t_j)]_i$.

3.1. Fourier series

Some of the earliest pulse optimizations in NMR employed Fourier series representations [6,7,11–13,16–18]. It continues to be a productive strategy for pulse design in contemporary work [20]. Motivations and insights regarding this approach are discussed in the examples which follow.

3.1.1. Excitation

As a first example, consider broadband polychromatic pulses [18] designed using the cosine Fourier series