Design of Optimal RF Pulses for NMR as a Discrete-Valued Control Problem [*]

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1. INTRODUCTION

Designing optimal radiofrequency (RF) pulses for nuclear magnetic resonance (NMR) imaging consists of driving a collection of spin systems using external electromagnetic fields of minimal energy to a desired spin state. However, in some cases the hardware only allows a discrete set of pulse phases and amplitudes. In contrast to methods based on quantization (Dridi et al., 2015), we aim to compute such pulses by solving a suitable optimal control problem.

A standard model for NMR is given by the Bloch equation in a rotating reference frame without relaxation, i.e.,

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{M}^{(\omega)}(t) = \mathbf{M}^{(\omega)}(t) \times \mathbf{B}^{(\omega)}(t), \quad \mathbf{M}^{(\omega)}(0) = \mathbf{M}_0,$$

which describes the temporally evolving magnetization $\mathbf{M}^{(\omega)} \in \mathbb{R}^3$ of an ensemble of spins rotating at the same resonance offset frequency ω (called *isochromat*), starting from a given equilibrium magnetization $\mathbf{M}_0 \in \mathbb{R}^3$ (e.g., aligned to a strong external field). The time-varying effective magnetic field $\mathbf{B}^{(\omega)}(t)$ is of the form

$$\mathbf{B}^{(\omega)}(t) = (\omega_x(t), \omega_y(t), \omega)^T,$$

where $u(t) := (\omega_x(t), \omega_y(t)) \in \mathbb{R}^2$ can be controlled. The aim is to achieve a magnetization $\mathbf{M}^{(\omega)}(T) = \mathbf{M}_d^{(\omega)}$ within the time interval $\Omega = [0, T]$ for a list of offset frequencies $\omega_1, \dots, \omega_J$ using control values $u(t)$ from a discrete set

$$\mathcal{M} = \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \omega_0 \cos\theta_1 \\ \omega_0 \sin\theta_1 \end{pmatrix}, \dots, \begin{pmatrix} \omega_0 \cos\theta_M \\ \omega_0 \sin\theta_M \end{pmatrix} \right\}$$

for a fixed amplitude $\omega_0 > 0$ and $M > 2$ equi-distributed phases $0 \le \theta_1 < \dots < \theta_M < 2\pi$.

Introducing the control space $U := L^2(0, T; \mathbb{R}^2)$, the control-to-state operator

$$S : U \to (\mathbb{R}^3)^J, \qquad u \mapsto \left[\mathbf{M}^{(\omega_1)}(T), \dots, \mathbf{M}^{(\omega_J)}(T) \right],$$

and the target vector $z := [\mathbf{M}_d^{(\omega_1)}, \dots, \mathbf{M}_d^{(\omega_J)}]^T \in (\mathbb{R}^3)^J$, this problem can be formulated as an optimal control problem

$$(1) \qquad \min_{u \in U} \frac{1}{2}\|S(u) - z\|_2^2 + \int_0^T g(u(t))\, \mathrm{d}t.$$

Here, $g : \mathbb{R}^2 \to [0, \infty]$ is a vector-valued version of the *multi-bang penalty* from Clason and Kunisch (2014, 2016) that can be motivated as the convex hull of the non-convex penalty $\frac{\alpha}{2}|\cdot|_2^2 + \delta_\mathcal{M}$, where $\delta_\mathcal{M}$ denotes the indicator function in the sense of convex analysis, and can thus be expected to promote controls with values only in $\mathcal{M}$. The main advantage of this formulation is that it leads to a convex optimization problem that can be efficiently solved using a semismooth Newton method (Clason et al., 2016).

2. CONVEX ANALYSIS FRAMEWORK

Standard arguments from convex analysis and on the continuity and differentiability of S yield the following results.

Theorem 2.1. There exists a solution $\bar{u} \in U$ to (1)

Theorem 2.2. Let $\bar{u} \in U$ be a local minimizer of (1). Then there exists a $\bar{p} \in U$ satisfying

$$(2) \qquad \begin{cases} -\bar{p} = S'(\bar{u})^*(S(\bar{u}) - z) =: \mathcal{F}'(\bar{u}), \\ \bar{u}(t) \in \partial g^*(\bar{p}(t)) \quad \text{a.e. } t \in [0, T]. \end{cases}$$

Here, $S'(u)^*$ denotes the adjoint of the Fréchet derivative of S, which can be computed as the solution of the adjoint Bloch equation, and ∂g^* denotes the convex subdifferential of the Fenchel conjugate of g, which will be specified below.

For the numerical solution, we also require the Moreau–Yosida regularization

$$(3) \qquad \begin{cases} -p_\gamma = S'(u_\gamma)^*(S(u_\gamma) - z) = \mathcal{F}'(u_\gamma), \\ u_\gamma(t) = h_\gamma(p_\gamma(t)) \quad \text{a.e. } t \in [0, 1], \end{cases}$$

where

$$h_\gamma := (\partial g^*)_\gamma = \frac{1}{\gamma}(\mathrm{Id} - \mathrm{prox}_{\gamma g^*})$$

and $\mathrm{prox}_{\gamma g^*} = (\mathrm{Id} - \gamma \partial g^*)^{-1}$ denotes the (single-valued and Lipschitz-continuous) proximal mapping of g^*.

3. MULTIBANG PENALTY

Letting $\bar{u}_i$, $i = 0, \ldots, M$, denote the admissible control values in $\mathcal{M}$ (with $\bar{u}_0 = 0$), we obtain from the definition of the Fenchel conjugate and the maximum rule for the subdifferential by straightforward if tedious computation the following explicit characterization for $q := p(t)$:

$$\partial g^*(q) = \begin{cases} \{\bar{u}_i\} & q \in Q_i, \\ \mathrm{co}\{\bar{u}_{i_1}, \ldots, \bar{u}_{i_k}\} & q \in Q_{i_1 \ldots i_k}. \end{cases}$$

Together with (2) this yields that apart from singular cases corresponding to the second line, the optimal control $\bar{u}$ will indeed take on values from the admissible set. The sets Q_i can be characterized using polar coordinates; here we only illustrate their distribution in Fig. 1a.

Similarly, we obtain for the Moreau–Yosida regularization

$$h_\gamma(q) = \begin{cases} 0 & q \in Q_0^\gamma, \\ \bar{u}_i & q \in Q_i^\gamma, \\ \left(\frac{\langle q, \bar{u}_i\rangle}{\gamma\omega_0^2} - \frac{\alpha}{2\gamma}\right)\bar{u}_i & q \in Q_{0,i}^\gamma, \\ \frac{\bar{u}_i + \bar{u}_{i+1}}{2} + \frac{\langle q, \bar{u}_i - \bar{u}_{i+1}\rangle(\bar{u}_i - \bar{u}_{i+1})}{\gamma|\bar{u}_i - \bar{u}_{i+1}|_2^2} & q \in Q_{i,i+1}^\gamma, \\ \frac{q}{\gamma} - \frac{\alpha}{\gamma}\left(\frac{\omega_0}{|\bar{u}_i + \bar{u}_{i+1}|_2}\right)^2(\bar{u}_i + \bar{u}_{i+1}) & q \in Q_{0,i,i+1}^\gamma, \end{cases}$$

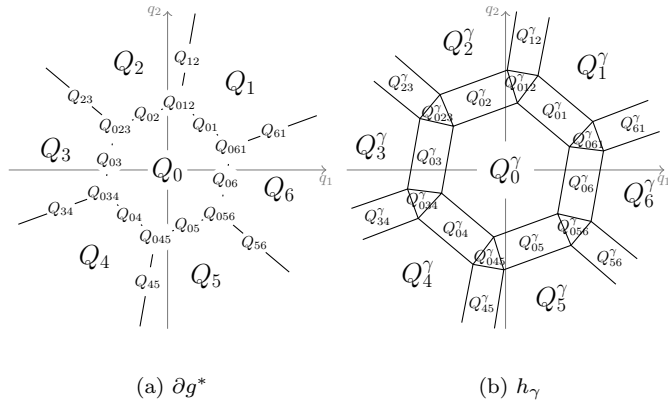with the subdomains Q_i^γ illustrated in Fig. 1b.

(a) ∂g^* (b) h_γ

Fig. 1. Subdomains for radially distributed $\mathcal{M}$, $M = 6$

4. NUMERICAL SOLUTION

Introducing the superposition operator $H_\gamma : U \to U$ via $[H_\gamma(p)](t) = h_\gamma(p(t))$, we can write (3) in reduced form as

$$u_\gamma - H_\gamma(\mathcal{F}'(u_\gamma)) = 0.$$

Since h_γ is Lipschitz continuous and piecewise differentiable and the range of $S'(u)^* \subset L^\infty(0, T; \mathbb{R}^2)$, this is a Newton-differentiable equation. Taking

$$D_N h_\gamma(q) = \begin{cases} 0 & q \in Q_i^\gamma, \\ \frac{\bar{u}_i \bar{u}_i^T 1}{\gamma\omega_0^2} & q \in Q_{0,i}^\gamma, \\ \frac{(\bar{u}_i - \bar{u}_{i+1})(\bar{u}_i - \bar{u}_{i+1})^T}{\gamma|\bar{u}_i - \bar{u}_{i+1}|_2^2} & q \in Q_{i,i+1}^\gamma, \\ \frac{1}{\gamma}\,\mathrm{Id} & q \in Q_{0,i,i+1}^\gamma, \end{cases}$$

the corresponding superposition operator $D_N H_\gamma(p)$ leads to a superlinearly convergent semismooth Newton method

$$\left(\mathrm{Id} - D_N H_\gamma(\mathcal{F}'(u^k))\mathcal{F}''(u^k)\right)\delta u = -u^k + H_\gamma(\mathcal{F}'(u^k)),$$

which can be realized using a matrix-free Krylov method such as GMRES (where $\mathcal{F}''(u)$ can be computed using the solution of two linearized (adjoint) Bloch equations).

5. NUMERICAL EXAMPLES

Figure 2 illustrates the above approach for the simultaneous control of $J = 4$ isochromats with from $\mathbf{M}_0 = (0,0,1)^T$ to $\mathbf{M}_d^{(\omega_j)} = (0,0,1)$ for $j = 3$, $\mathbf{M}_0$ else, and $M = 6$ admissible values with equidistant phases (marked with dashed lines in Fig. 2a), where the implementation of the discrete (linearized) Bloch and adjoint equations is taken from Aigner et al. (2015). For more details and examples, see Clason et al. (2016).
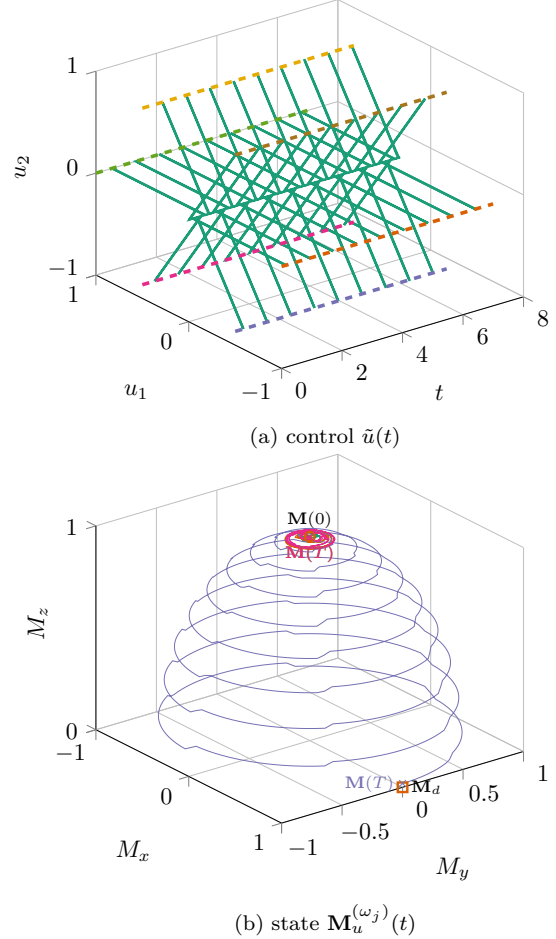

(a) control $\tilde{u}(t)$

(b) state $\mathbf{M}_u^{(\omega_j)}(t)$

Fig. 2. Optimal control and state for $M = 6$, $J = 4$

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