Design of optimal RF pulses for NMR as a discrete-valued control problem

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joint work with Carla Tameling (Göttingen) and Benedikt Wirth (Münster)

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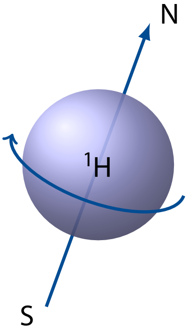
Motivation: MRT

Magnetic resonance tomography (MRT):

- based on measurement of resonance frequency of hydrogen nuclei
- hydrogen nucleus (proton) acts like rotating magnet
- “angular momentum”: nuclear spin, “axis” randomly aligned



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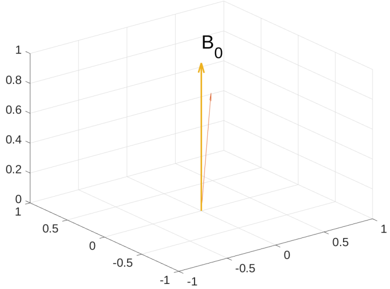
nuclear spin in magnetic field:

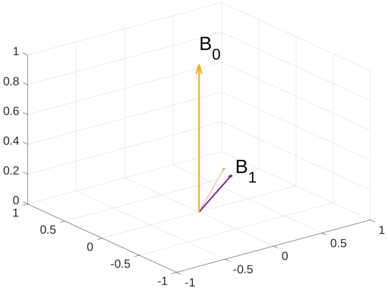
- axis aligns with external field
- precesses around field direction



Motivation: MRT

nuclear spin in rotating magnetic field:

- axis aligns with external field
- precesses around field direction
- field rotating at resonance frequency: energy is absorbed
- resonance frequency proportional to field strength



Motivation: MRT

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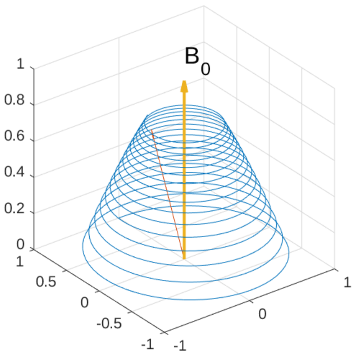

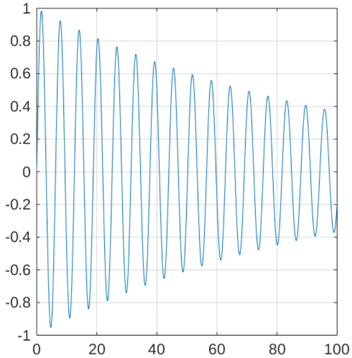

magnetic field off: spin relaxes… …induces current in coil

⇝ measurement

Mathematical model

Bloch equation

$$\frac{d}{dt}M(t) = M(t) \times B(t), \qquad M(0) = M_0$$

- $M(t) \in \mathbb{R}^3$ describes temporal evolution of spin ensemble
- $B(t) = (u_1(t), u_2(t), \omega)^T$ controlled time-dependent magnetic field
- ω resonance frequency
- control-to-state mapping $S^{(\omega)} : u \rightarrow M(T)$

Optimal control problem

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Goal:

- compute control $u(t) = (u_1(t), u_2(t))$ such that $M(T) \approx M_d$
- M_d desired magnetization state
- $M_d = M_d^{(\omega)}$ selective to resonance frequency
  ($\rightsquigarrow$ spectroscopy, slice selection)
- in addition: control with minimal specific absorption rate (SAR)

$$\min_{u \in L^2} \frac{1}{2} \sum_{\omega} \|S^{(\omega)}(u) - M_d^{(\omega)}\|_2^2 + \frac{\alpha}{2} \int_0^T |u(t)|_2^2 \, dt$$

Discrete control

Technical limitation: device can only realize control from discrete set

$$U = \left\{ u \in L^2(0,T;\mathbb{R}^2) : u(t) \in \{u_1, \dots, u_d\} \text{ a.e.} \right\}$$

- $u_1, \dots, u_d \in \mathbb{R}^2$ given (fixed amplitude, phases)
- non-convex discrete-valued control problem

$$\min_{u \in U} \frac{1}{2} \sum_{\omega} \|S^{(\omega)}(u) - M_d^{(\omega)}\|_2^2 + \frac{\alpha}{2} \int_0^T |u(t)|_2^2 \, dt$$

Multi-bang penalty

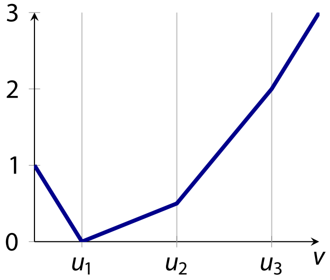
- convex relaxation: replace U by convex hull
- works only for $d = 2$, cf. bang-bang control ($\alpha = 0$)
- $\rightsquigarrow$ promote $u(x) \in \{u_1, \dots, u_d\}$ by convex pointwise penalty

$$\mathcal{G}(u) = \int_\Omega g(u(x))\,dx$$

- generalize L^1 norm: polyhedral epigraph with vertices $u_1, \dots, u_d$
- not exact relaxation/penalization (in general)!

Multi-bang penalty

- generalize L^1 norm: polyhedral epigraph with vertices $u_1, \ldots, u_d$



- motivation: convex envelope of $\frac{1}{2}\|u\|^2 + \delta_U$
- multi-bang (generalized bang-bang) control
- $\rightsquigarrow$ non-smooth optimization in function spaces

Fenchel duality

$f : V \to \overline{\mathbb{R}} := \mathbb{R} \cup \{+\infty\}$ convex, V Banach space, V^* dual space

- subdifferential

$$\partial f(\bar{v}) = \left\{ v^* \in V^* : \langle v^*, v - \bar{v} \rangle_{V^*,V} \leqslant f(v) - f(\bar{v}) \quad \text{for all } v \in V \right\}$$

- Fenchel conjugate (always convex)

$$f^* : V^* \to \overline{\mathbb{R}}, \qquad f^*(v^*) = \sup_{v \in V} \langle v^*, v \rangle_{V^*,V} - f(v)$$

- "convex inverse function theorem":

$$v^* \in \partial f(v) \quad \Leftrightarrow \quad v \in \partial f^*(v^*)$$

Fenchel duality: application

$$\mathcal{F}(\bar{u}) + \mathcal{G}(\bar{u}) = \min_u \mathcal{F}(u) + \mathcal{G}(u)$$

1. Fermat principle: $0 \in \partial\left(\mathcal{F}(\bar{u}) + \mathcal{G}(\bar{u})\right)$
2. sum rule: $0 \in \partial\mathcal{F}(\bar{u}) + \partial\mathcal{G}(\bar{u})$, i.e., there is $\bar{p} \in V^*$ with

$$\begin{cases} -\bar{p} \in \partial\mathcal{F}(\bar{u}) \\ \bar{p} \in \partial\mathcal{G}(\bar{u}) \end{cases}$$

3. Fenchel duality:

$$\begin{cases} -\bar{p} \in \partial\mathcal{F}(\bar{u}) \\ \bar{u} \in \partial\mathcal{G}^*(\bar{p}) \end{cases}$$

Regularization

$\mathcal{G}$ non-smooth $\rightsquigarrow$ subdifferential $\partial\mathcal{G}^*$ set-valued $\rightsquigarrow$ regularize

$u, p \in L^2(\Omega)$ Hilbert space $\rightsquigarrow$ consider for $\gamma > 0$

Proximal mapping

$$\operatorname{prox}_{\gamma\mathcal{G}^*}(p) = \arg\min_w \mathcal{G}^*(w) + \frac{1}{2\gamma}\|w - p\|^2$$

- single-valued, Lipschitz continuous
- coincides with resolvent $(\mathrm{Id} + \gamma\partial\mathcal{G}^*)^{-1}(p)$
- (also required for primal-dual first-order methods)

Regularization

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Proximal mapping

$$\mathrm{prox}_{\gamma\mathcal{G}^*}(p) = \arg\min_w \mathcal{G}^*(w) + \frac{1}{2\gamma}\|w - p\|^2$$

Complementarity formulation of $u \in \partial\mathcal{G}^*(p)$

$$u = \frac{1}{\gamma}\left((p + \gamma u) - \mathrm{prox}_{\gamma\mathcal{G}^*}(p + \gamma u)\right)$$

- equivalent for every $\gamma > 0$
- single-valued, Lipschitz continuous, implicit

Regularization

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Proximal mapping

$$\text{prox}_{\gamma\mathcal{G}^*}(p) = \arg\min_w \mathcal{G}^*(w) + \frac{1}{2\gamma}\|w - p\|^2$$

Moreau–Yosida regularization of $u \in \partial\mathcal{G}^*(p)$

$$u = \frac{1}{\gamma}\left(p - \text{prox}_{\gamma\mathcal{G}^*}(p)\right) =: \partial\mathcal{G}^*_\gamma(p)$$

- $\partial\mathcal{G}^*_\gamma = \partial\left(\mathcal{G} + \frac{\gamma}{2}\|\cdot\|^2\right)^* \to \partial\mathcal{G}^*$ as $\gamma \to 0$
- single-valued, Lipschitz continuous, explicit
  $\rightsquigarrow$ nonsmooth operator equation, Newton method

Semismooth Newton method

f locally Lipschitz, piecewise C^1:

$$f(v) = 0, \qquad f : \mathbb{R}^n \to \mathbb{R}$$

Newton derivative

$$D_N f(v)\delta v \in \partial_C f(v)\delta v$$

Clarke generalized gradient: convex hull of piecewise derivatives

semismooth Newton method

$$D_N f(v^k)\delta v = -f(v^k), \qquad v^{k+1} = v^k + \delta v$$

converges locally superlinearly

Semismooth Newton method

f locally Lipschitz, piecewise C^1:

$$F(u) = 0, \qquad F : L^p(\Omega) \to L^q(\Omega), \quad [F(u)](x) = f(u(x))$$

Newton derivative

$$[D_N F(u)\delta u](x) \in \partial_C f(\delta u(x))\delta u(x)$$

any measurable selection of Clarke generalized gradient

semismooth Newton method

$$D_N F(u^k)\delta u = -F(u^k), \qquad u^{k+1} = u^k + \delta u$$

converges locally superlinearly if $p > q$

Vector-valued multi-bang: penalty

Here: admissible control set U of d radially distributed states, origin

$$U = \left\{ \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} \omega_0 \cos\theta_1 \\ \omega_0 \sin\theta_1 \end{pmatrix}, \dots, \begin{pmatrix} \omega_0 \cos\theta_d \\ \omega_0 \sin\theta_d \end{pmatrix} \right\}$$

- fixed amplitude $\omega_0 > 0$
- phases $0 \leqslant \theta_1 < \dots < \theta_d < 2\pi$

multi-bang penalty $g = \left(\frac{1}{2}|\cdot|_2^2 + \delta_U\right)^{**}$ convex envelope

$$g^*(q) = \left(\left(\tfrac{1}{2}|\cdot|_2^2 + \delta_U\right)^{**}\right)^*(q) = \left(\tfrac{1}{2}|\cdot|_2^2 + \delta_U\right)^*(q)$$

$$= \begin{cases} 0 & \langle q, u_i\rangle \leqslant \frac{1}{2}\omega_0^2 \text{ for all } 1 \leqslant i \leqslant d \\ \langle q, u_i\rangle - \frac{1}{2}\omega_0^2 & \frac{\theta_{i-1}+\theta_i}{2} \leqslant \angle q \leqslant \frac{\theta_i+\theta_{i+1}}{2}, \langle q, u_i\rangle \geqslant \frac{1}{2}\omega_0^2 \end{cases}$$

Vector-valued multi-bang: subdifferential

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Fenchel conjugate

$$g^*(q) = \begin{cases} 0 =: u_0 & q \in \overline{Q}_0 \\ \langle q, u_i \rangle - \frac{1}{2}\omega_0^2 & q \in \overline{Q}_i \end{cases}$$

Subdifferential

$$\partial g^*(q) = \begin{cases} \{u_i\} & q \in Q_i & 0 \leqslant i \leqslant d \\ \operatorname{co}\{u_{i_1}, \ldots, u_{i_k}\} & q \in Q_{i_1 \ldots i_k} & 0 \leqslant i_1, \ldots, i_k \leqslant d \end{cases}$$

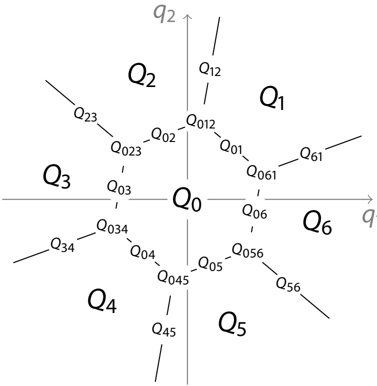
Vector-valued multi-bang: subdifferential

Subdifferential

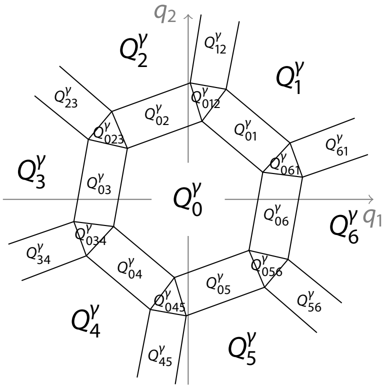
$$\partial g^*(q) = \begin{cases} \{u_i\} & q \in Q_i \qquad 0 \leqslant i \leqslant d \\ \operatorname{co}\{u_{i_1}, \ldots, u_{i_k}\} & q \in Q_{i_1 \ldots i_k} \qquad 0 \leqslant i_1, \ldots, i_k \leqslant d \end{cases}$$

Moreau–Yosida regularization

$$(\partial g^*)_\gamma(q) = \begin{cases} u_i & q \in Q_i^\gamma \\ \left(\frac{\langle q, u_i \rangle}{\gamma \omega_0^2} - \frac{\alpha}{2\gamma}\right) u_i & q \in Q_{0,i}^\gamma \\ \frac{u_i + u_{i+1}}{2} + \frac{\langle q, u_i - u_{i+1} \rangle (u_i - u_{i+1})}{\gamma |u_i - u_{i+1}|_2^2} & q \in Q_{i,i+1}^\gamma \\ \frac{q}{\gamma} - \frac{\alpha}{\gamma}\left(\frac{\omega_0}{|u_i + u_{i+1}|_2}\right)^2 (u_i + u_{i+1}) & q \in Q_{0,i,i+1}^\gamma \end{cases}$$



(a) subdomains for ∂g^*



(b) subdomains for $(\partial g^*)_\gamma$

Vector-valued multi-bang: Newton method

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Newton derivative

$$D_N(\partial g_\gamma^*)(q) = \begin{cases} 0 & q \in Q_i^\gamma \\ \frac{u_i u_i^T 1}{\gamma \omega_0^2} & q \in Q_{0,i}^\gamma \\ \frac{(u_i - u_{i+1})(u_i - u_{i+1})^T}{\gamma |u_i - u_{i+1}|_2^2} & q \in Q_{i,i+1}^\gamma \\ \frac{1}{\gamma}\,\mathrm{Id} & q \in Q_{0,i,i+1}^\gamma \end{cases}$$

Superposition operator:

$$\left[D_N H_\gamma(p)\right](t) := D_N\left(\partial g_\gamma^*\right)(p(t)) \quad \text{a.e.} \quad t \in [0,T]$$

Vector-valued multi-bang: Newton method

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Newton system

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

- matrix-free Krylov method for semismooth Newton step
- $\mathcal{F}'$, $\mathcal{F}''$ via linearized, adjoint Bloch equation
- discretization, adjoint from [Aigner/Clason/Rund/Stollberger '16]

Numerical examples

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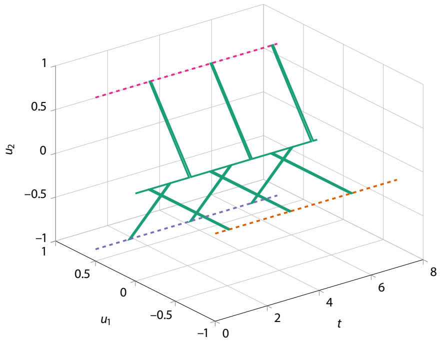
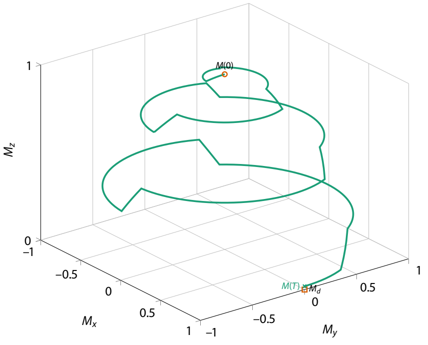
- goal: shift magnetization from $M_0 = (0, 0, 1)^T$ at $t = 0$
  to $M_d = (1, 0, 0)^T$ at $t = T$
- $d = 3, 6$ radially distributed admissible control states
- $n = 1, 4$ isochromats with different resonance frequencies
  1. shift all isochromats
  2. shift only one isochromat
- $\alpha = 10^{-1}, \omega_0 = 1$
- example motivated by [Dridi/Lapert/Salomon/Glaser/Sugny '15]



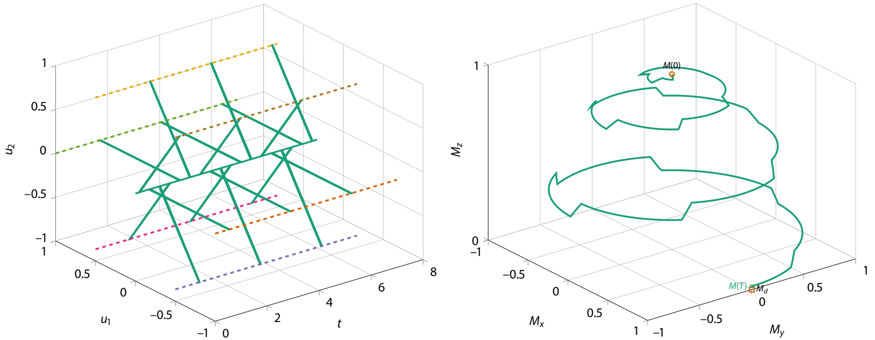
(a) control $u(t)$



(b) state $M(t)$

Figure: $n = 1$ isochromat, $d = 3$ control states

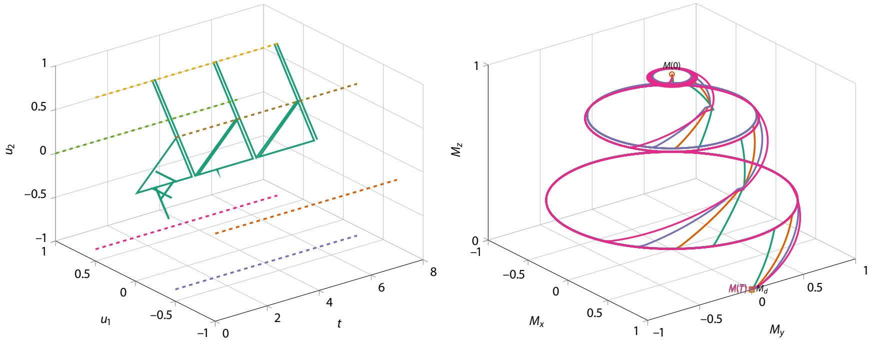
Numerical examples



(a) control $u(t)$ (b) state $M(t)$

Figure: $n = 1$ isochromat, $d = 6$ control states

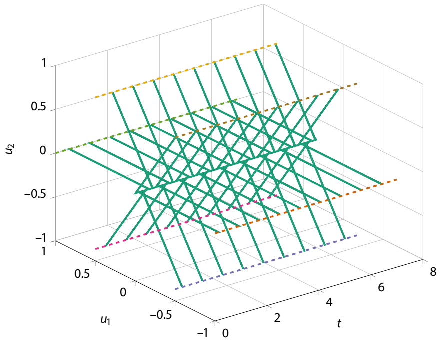
Numerical examples



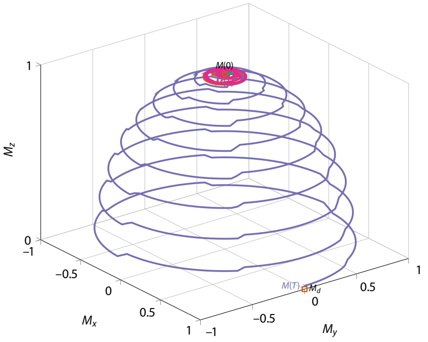
(a) control $u(t)$ (b) state $M(t)$

Figure: $n = 4$ isochromats, same target

Numerical examples



(a) control $u(t)$



(b) state $M(t)$

Figure: $J = 4$ isochromats, different targets

Conclusion

Discrete controls in NMR:

- can be promoted by convex penalties
- linear complexity in number of parameter values
- $\rightsquigarrow$ efficient numerical solution (superlinear convergence)
- applicable to nonlinear, vector-valued problems

Outlook:

- robust optimization, e.g., with respect to static field
- include signal acquisition
- other discrete–continuous problems: switching, networks

Preprint, MATLAB/Python codes:

`http://www.uni-due.de/mathematik/agclason/clason_pub.php`