Algorithmic Least Squares Estimation: From Numerical Linear Algebra to Quantum Control

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Linear Systems Snapshots

Recent joint work with Paul: We Go Tensor!!

- **Greetings and Apologies**

  why Paul cannot come and why this talk is not about linear systems

- **Invariant Factors/Jordan Structure of $A \otimes B$**

  polynomial models versus Clebsch-Gordan formula (SL_2-reps)

- **Polynomial Sylvester Equations**

  How to solve $AX + BX = C$ or $\sum_{i=1}^{m} A_i X B_i = C$

- **Tensor Products of Behaviors**

  tensor product of vector spaces $B_1 \otimes_F B_2$ ($2D$**-behavior!**)

  tensor product of modules $B_1 \otimes_{F[z]} B_2$ (**smaller** $1D$**-bahavior**)

- **Realization Theory for Tensored Behaviors**

  Parametrizations of Yang–Mills instantons; separable $2D$-systems

Back to the Talk: Motivation

Algorithmic Engineering: Design of Algorithms

Most computational tasks can be reformulated as optimization tasks on Riemannian manifolds. This includes most computational tasks form e.g.

- **Numerical Linear Algebra**
  eigenvalues, singular values, ...
- **Control Theory**
  Riccati equations, balanced realizations,...
- **Robotics; Quantum Control and Computer Vision**
  grasping problems, quantum computation, camera estimation problems

Motivation: The Core Problem

- **Riemannian Optimization:** For $a \notin M$, find the optimum x_* of the least squares distance function

$$||x - a||^2$$

  on a Riemannian manifold M.

- **Optimal Control:** Find a control $u(t)$ for the control system

$$\dot{x} = f(x, u)$$

  on M, that steers an initial point $x_0 \in M$ optimally to $x_* \in M$.

Motivation: The Core Problem

- Standard numerical recipes often not applicable or too ad hoc.
  $\rightarrow$ Iterative Methods! Follow your nose to find solutions!

- Standard optimization methods (Lagrange multipliers, augmented Lagrangians,...) are often not applicable nor well-adapted to structure
  Good algorithm design employs the geometry of constraint set. $\rightarrow$ Riemannian Optimization Methods!

- Result of optimization process often has to be realized experimentally.
  $\rightarrow$ Algorithms as Control Systems/Control of Algorithms!

- Need good examples/prototypes for the theory.
  Develop a theory for Riemannian symmetric spaces!

Motivation: Linear Algebra

Least Squares Eigenvalue Computation:

- **Matrix Diagonalization:**
  Minimize $\|A - X\|^2$ on $M = \{SX_0S^{-1} | S \quad \text{invertible}\}$.

- **C-Numerical Range:**
  Minimize $\|A - X\|^2$ on $M = \{UCU^{-1} | U \quad \text{unitary}\}$.

- **Singular Value Computation:**
  Minimize $\|A - X\|^2$ on $M = \{UX_0V^{-1} | U, V \quad \text{unitary}\}$.

- **Lower Rank Approximation:**
  Minimize $\|A - X\|^2$ on $M = \{X \in \mathbb{R}^{n \times m} | \mathrm{rkX} \leq \mathrm{r}\}$.

Motivation: Control Theory

Least Squares Model Reduction:

- **Hankel/Toeplitz Approximation:**
  Minimize $\|A - X\|^2$ on $M = \{X \quad \text{Hankel} \quad \text{operator} | \quad \text{rkX} \leq \text{r}\}$.

- **Proper Orthogonal Decomposition (POD):**
  Minimize $\|A - XX^\top\|^2$ on $M = \{X \in \mathbb{R}^{n \times r} | X^\top X = I_r\}$.

- **Norm Balanced Realizations:**
  Minimize $\|F - SAS^{-1}\|^2 + \|G - SB\|^2 + \|H - CS^{-1}\|^2$ on $S \in GL(n)$.

Motivation: Control Theory Cont'd

$$\dot{x} = Ax + Bu, \quad y = Cx.$$

Controllability/Observability Gramians

$$W_c = \int_0^\infty e^{tA} B B^\top e^{tA^\top} dt, \quad W_o = \int_0^\infty e^{tA^\top} C^\top C e^{tA} dt.$$

Goal: Find balancing state space transformation such that

$$S W_c S^\top = S^{-\top} W_o S^{-1} = \text{diagonal}.$$

Solution: For $N := diag(1, ..., n)$ find minimizer of $f_N : GL(n, \mathbb{R}) \to \mathbb{R}$

$$f_N(S) := \operatorname{tr}(N(S W_c S^\top + S^{-\top} W_o S^{-1})).$$

Where are the optimal control problems?

Motivation: Control of Spin Systems

The time evolution of N coupled spin $\frac{1}{2}$ particles is governed by

$$\dot{X}(t) = -\mathrm{i}\Big(H_d + \sum_{j=1}^{m} u_j(t) H_j\Big) X(t), \quad X(0) = I.$$

Schrödinger Equation on $SU(2^N)$

Optimal Control Problems:

- Find controls $u_1(\cdot), \ldots, u_m(\cdot)$ that steer the Schrödinger Equation to a maximum of the transfer function

$$f : SU(2^N) \to \mathbb{R}, \quad f(X) := \mathrm{Re}\,\mathrm{tr}(C^* X A X^*).$$

- If the above problem has at least one solution, then try to find a time-optimal one.

Motivation: Control of Density Operators

In presence of spin relaxation, the time evolution on density operators is

$$\dot\rho = -\mathrm{i}\Big[H_d + \sum_{j=1}^{m} u_j H_j, \rho\Big] - \sum_{i=1}^{r}\Big[\lambda_i, \big[\lambda_i, \rho\big]\Big]$$

Lindblad Master Equation

Optimal Control Problems:

- Find controls $u_1(\cdot), \ldots, u_m(\cdot)$ that steer the Lindblad Equation to a maximum of the transfer function

$$f(\rho) := \mathrm{Re}\,\mathrm{tr}(C^*\rho).$$

- If the above problem has at least one solution, then try to find a time-optimal one.

Lie Groups & Lie Algebras

Tutorial: Lie Groups and Lie Algebras

Examples:

(a) The *real orthogonal group*

$$O(n, \mathbb{R}) := \{X \in \mathbb{R}^{n\times n} |\ XX^\top = I_n\}$$

(b) The *special unitary group*

$$SU(n) := \{X \in \mathbb{C}^{n\times n} |\ XX^* = I_n,\ \det X = 1\}$$

(c) The *local unitary group*

$$SU_{\rm loc}(2^N) := \{X_1 \otimes \ldots \otimes X_N \mid X \in SU(2)\},$$

where $\otimes$ denotes the Kronecker product of matrices.

Tutorial: Lie Groups and Lie Algebras

Definition. A vector space V with a bilinear operation $[\ ,\ ] : V \times V \to V$

(i) $[x, y] = -[y, x]$

(ii) $[x, [y, z]] + [z, [x, y]] + [y, [z, x]] = 0$ (Jacobi Identity)

is called a **Lie Algebra**.

Theorem. Let $G \subset GL(n, \mathbb{R})$ be a matrix Lie group. Then the tangent space $\mathfrak{g} := T_I G$ at the identity is a Lie algebra with Lie bracket:

$$[X, Y] = XY - YX.$$

Tutorial: Lie Groups and Lie Algebras

Examples

(a) The Lie algebra of $O(n, \mathbb{R})$ is

$$\mathfrak{o}(n, \mathbb{R}) := \{\Omega \in \mathbb{R}^{n \times n} | \ \Omega^\top = -\Omega\}.$$

(b) The Lie algebra of $SU(n)$ is

$$\mathfrak{su}(n) := \{\Omega \in \mathbb{C}^{n \times n} | \ \Omega^* = -\Omega, \ \operatorname{tr}\Omega = 0\}$$

(c) The Lie algebra of $SU_{\rm loc}(4)$ is

$$\{\Omega_1 \otimes I_2 + I_2 \otimes \Omega_2 \mid \Omega_1, \Omega_2 \in \mathfrak{su}(2)\} \subset \mathfrak{su}(4).$$

Controllability on Lie Groups

Controllability on Lie Groups

History

- **Geometric Function Theory**: Bieberbach Conjecture; Semigroups of univalent functions, Löwner-, Beltrami equation (C. Löwner)
- **Nonlinear Control Theory**: Controllability, Observability (R. Hermann, R.W. Brockett, A. Krener, I. Kupka, H. Sussmann,...)
- **Lie Theory of Semigroups**: Lie wedges; Cones in Lie Algebras (J. Hilgert, K.-H. Hoffmann, J. Lawson, G.I. Ol'shanskii)
- **Control Sets & Dynamical Systems**: Chain-Recurrency, Transitivity (F. Colonius, W. Kliemann, L. San Martin)

Controllability on Lie Groups

- G connected matrix Lie group with Lie algebra $\mathfrak{g}$.
- **Bilinear control system** on G

$$(\Sigma) \quad \dot{X} = \left(A_d + \sum_{j=1}^{m} u_j A_j \right) X, \quad X(0) = I,$$

where $A_d, A_1, ..., A_m \in \mathfrak{g}$.

- **Reachable set**

$$\mathcal{R}(I) = \{X_F \in G \mid \exists u_1, ..., u_m \text{ and } T \geq 0 : X(T) = X_F\}$$

Controllability on Lie Groups

Structure of reachable sets:

Theorem (R.W. Brockett, H. Sussmann, V. Jurdjevic)

(i) The closure $\overline{\mathcal{R}(I)}$ of the reachable set is an (infinitesimally generated) **Lie subsemigroup** of G.

(ii) If there is **no drift**, i.e. $A_d = 0$, then $\overline{\mathcal{R}(I)}$ is a **Lie subgroup** of G.

(iii) If G is **compact**, then the closure $\overline{\mathcal{R}(I)}$ is a **Lie subgroup** of G.

Controllability on Lie Groups

Controllability Concepts:

- **Accessibility:** The reachable set $\mathcal{R}(I)$ has an interior point.
- **Controllability:**

$$\mathcal{R}(I) = G.$$

- **System Lie Algebra**:

  $\mathcal{L} :=$ smallest Lie subalgebra of $\mathfrak{g}$ containing $A_1, ..., A_m, A_d$, i.e. the smallest subspace containing all the iterated Lie brackets

$$A_d, A_1, ..., A_m, [A_d, A_i], [A_i, A_j], [A_d, [A_i, A_j]], ...$$

Controllability on Lie Groups

Controllability Results

Theorem (Jurdjevic/Sussmann)

- Σ is **accessible** if and only if the system Lie algebra is $\mathcal{L} = \mathfrak{g}$.
- A bilinear system Σ is **controllable** if and only if (i) Σ is accessible. (ii) $\mathcal{R}(I)$ is a subgroup of G.
- Let G be a **compact** connected Lie group. Then Σ is controllable if and only if it is accessible.

Controllability on Lie Groups: Spin Systems

Example: Nuclear Magnetic Resonance (NMR)

$$\dot{X} = -\mathrm{i}\Big(A_d + \sum_{j=1}^{2N} u_j A_j\Big) X, \quad X(0) = I$$

Schrödinger equation on $SU(2^N)$

- Drift Term: $A_d = \sum_{k<l} \lambda_{k,l}\, \sigma_{kz} \cdot \sigma_{lz}$
- Control Hamiltonians:

$$\begin{aligned} A_j &= \sigma_{jx} \quad \text{for } j = 1, \ldots, N \\ A_j &= \sigma_{jy} \quad \text{for } j = N+1, \ldots, 2N \end{aligned}$$

Controllability on Lie Groups: Spin Systems

Pauli Matrices

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

$$\sigma_{kx} = \overbrace{I_2 \otimes \cdots \otimes I_2 \otimes \underbrace{\sigma_x}_{k\text{-th position}} \otimes I_2 \otimes \cdots \otimes I_2}^{N \text{ factors}}$$

and σ_{ky}, σ_{kz} analogously.

Controllability on Lie Groups: Spin Systems

- $N = 2$:

$$A_1 = \frac{1}{2}\begin{bmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}, \quad A_2 = \frac{1}{2}\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix},$$

$$A_3 = \frac{1}{2}\begin{bmatrix} 0 & 0 & -\mathrm{i} & 0 \\ 0 & 0 & 0 & -\mathrm{i} \\ \mathrm{i} & 0 & 0 & 0 \\ 0 & \mathrm{i} & 0 & 0 \end{bmatrix}, \quad A_4 = \frac{1}{2}\begin{bmatrix} 0 & -\mathrm{i} & 0 & 0 \\ \mathrm{i} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\mathrm{i} \\ 0 & 0 & \mathrm{i} & 0 \end{bmatrix},$$

$$A_d = \frac{1}{4}\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

Controllability on Lie Groups: Spin Systems

Structure of reachable sets of the Schrödinger equation

Theorem (Schulte-Herbrüggen '98): For coupling terms $\lambda_{k,l}$ describing a connecting spin-spin interaction graph, the NMR-Schrödinger equation is controllable on $\mathrm{SU}(2^N)$.

Theorem (Albertini/Alessandro '01): The closures of the reachable sets of the NMR-Schrödinger equation are exactly the Lie subgroups

$$K = SU(m_1) \otimes ... \otimes SU(m_r), m_1 + ... + m_r = 2^N.$$

Controllability on Lie Groups: Spin Systems

Structure of reachable sets of the Lindblad equation

- The Liouville Master equation

$$\dot{\rho} = -\mathrm{i}\Big[H_d + \sum_{j=1}^{m} u_j H_j, \rho\Big]$$

is controllable on each isospectral set $\{U\rho U^* | U \in SU(2^N)\}$, iff the spin-spin coupling graph is connected.

- The Lindblad equation

$$\dot{\rho} = -\mathrm{i}\Big[H_d + \sum_{j=1}^{m} u_j H_j, \rho\Big] - \sum_{i=1}^{r} \Big[\lambda_i, \Big[\lambda_i, \rho\Big]\Big]$$

is generically accessible, but is never controllable!

Description of reachable sets for Lindblad equation: unknown!

Controllability on Lie Groups: Spin Systems

Accessibility of the Lindblad equation

The Lindblad equation

$$\dot{\rho} = -\mathrm{i}\Big[H_d + \sum_{j=1}^{m} u_j H_j, \rho\Big] - \sum_{i=1}^{r} \Big[\lambda_i, \big[\lambda_i, \rho\big]\Big]$$

is accessible, if and only if the system Lie algebra is one of the 14 following types.

Controllability on Lie Groups: Spin Systems

Accessibility of the Lindblad equation

Theorem: Let $H_d, H_1, \ldots, H_m \in \mathfrak{gl}(N, \mathbb{R})$ with $N \geq 2$. The Lindblad equation is accessible on $\mathbb{R}^N \setminus \{0\}$ if and only if the system Lie algebra $\mathcal{A} \subset \mathfrak{gl}(N, \mathbb{R})$ is conjugate to one of the following types:

- $\mathfrak{sl}(2, \mathbb{R})$, $\mathfrak{gl}(2, \mathbb{R})$ and $\mathfrak{gl}(N/2, \mathbb{C})$, if $N = 2$.
- $\mathfrak{so}(N) \oplus \mathbb{R}$, if $N \geq 3$.
- $\mathfrak{su}(N/2) \oplus \mathrm{e}^{\mathrm{i}\alpha}\mathbb{R}$ and $\mathfrak{su}(N/2) \oplus \mathbb{C}$, if N is even and $N \geq 3$.
- $\mathfrak{sp}(N/4) \oplus \mathrm{e}^{\mathrm{i}\alpha}\mathbb{R}$, $\mathfrak{sp}(N/4) \oplus \mathbb{C}$ and $\mathfrak{sp}(N/4) \oplus \mathbb{H}$, if $N = 4k$.
- $\mathfrak{g}_2 \oplus \mathbb{R}$, if $N = 7$.
- $\mathfrak{spin}(7) \oplus \mathbb{R}$, if $N = 8$.
- $\mathfrak{spin}(9) \oplus \mathbb{R}$, if $N = 16$.
- $\mathfrak{sl}(N, \mathbb{R})$ and $\mathfrak{gl}(N, \mathbb{R})$, if $N \geq 3$.

Controllability on Lie Groups: Spin Systems

Accessibility of the Lindblad equation

- $\mathfrak{sl}(N/2, \mathbb{C})$, $\mathfrak{sl}(N/2, \mathbb{C}) \oplus \mathrm{e}^{\mathrm{i}\beta}\mathbb{R}$ and $\mathfrak{gl}(N/2, \mathbb{C})$, if N is even and $N \geq 3$.
- $\mathfrak{sl}(N/4, \mathbb{H})$, $\mathfrak{sl}(N/4, \mathbb{H}) \oplus \mathrm{e}^{\mathrm{i}\beta}\mathbb{R}$ and $\mathfrak{sl}(N/4, \mathbb{H}) \oplus \mathbb{C}$, if $N = 4k$.
- $\mathfrak{sl}(N/4, \mathbb{H}) \oplus \mathfrak{sp}(1)$ and $\mathfrak{sl}(N/4, \mathbb{H}) \oplus \mathbb{H}$, if $N = 4k$.
- $\mathfrak{sp}(N, \mathbb{R})$ and $\mathfrak{sp}(N, \mathbb{R}) \oplus \mathbb{R}$, if N is even and $N \geq 3$. $\mathfrak{sp}(N/2, \mathbb{C})$, $\mathfrak{sp}(N/2, \mathbb{C}) \oplus \mathrm{e}^{\mathrm{i}\beta}\mathbb{R}$ and $\mathfrak{sp}(N/2, \mathbb{C}) \oplus \mathbb{C}$, if $N = 4k$.
- $\mathfrak{spin}(9, 1, \mathbb{R})$ and $\mathfrak{spin}(9, 1, \mathbb{R}) \oplus \mathbb{R}$, if $N = 16$.

Here, α and β have to satisfy $\alpha \in (\frac{\pi}{2}, -\frac{\pi}{2})$ and $\beta \in [\frac{\pi}{2}, -\frac{\pi}{2}]$.

Optimization on Reachable Sets

Optimization on Reachable Sets

History

- **Optimization on Riemannian Manifolds**: Conjugate Gradient, Newton-, Jacobi Methods on Manifolds
(U.H., K. Hüper, R. Mahony, M. Shub, S. Smith, J. Manton)
- **Isospectral Flows**: Gradient and Hamiltonian flows
(A. Bloch, R.W. Brockett, P. Deift, U. H., J. Moser, A.P. Veselov)
- **Geometric Integration of ODEs & PDEs**: Runge-Kutta Methods on Manifolds; Butcher Trees; Magnus Expansions
(P. Crouch, E. Hairer, A. Iserles, G. Wanner, H. Munte-Kaas,..)

Optimization on Reachable Sets

Final Point Characterization: NMR Spin Systems

Find a unitary matrix $X_{\max} \in K$ that maximizes the *transfer function*

$$f : K \to \mathbb{R}, \quad f(X) := \mathrm{Re}\,\mathrm{tr}(C^* X A X^*)$$

over the closure of the reachable set

$$K = SU(m_1) \otimes \ldots \otimes SU(m_r).$$

Relative Numerical Range

Range of $f = \mathrm{Re}\, W_K(C, A)$, where

$$W_K(C, A) := \{\mathrm{tr}(C^* X A X^*) \mid X \in K\}$$

denotes the **relative C-numerical range** of A.

Optimization on Reachable Sets

Example 1: The C-numerical range

- For $C, A \in \mathbb{C}^{2^N \times 2^N}$ the C-**numerical range** of A is

$$W(C,A) := \{\mathrm{tr}\,(C^\dagger U A U^\dagger) \mid U \in SU(2^N)\} \subset \mathbb{C}.$$

- **Basic Properties:**
  - It generalizes the **classical numerical range** of A

$$W(A) := \{x^\dagger A x \mid \|x\| = 1\}.$$

  - $W(C,A)$ is *compact and connected*.
  - $W(C,A)$ is *star-shaped*. [Cheung & Tsing '96]
  - $W(A)$ is *convex*. [Hausdorff 1919], [Töplitz 1918]

Optimization on Reachable Sets

The C-numerical range

- **Basic Properties:**

• $W(C, A)$ is *convex* if C or A are Hermitian. [Westwick '75]

Proof via symplectic geometry; convexity of images of moment maps (Atiyah..).

• $W(C, A)$ is a *circular disk centered at the origin* if C or A are unitary block-shift matrices. [Li & Tsing '91]

No symplectic geometry proof known!

Optimization on Reachable Sets

Example 2: The local C-numerical range

- For $C, A \in \mathbb{C}^{2^N \times 2^N}$ the **local C-numerical range** of A is given by

$$W_{\mathrm{loc}}(C, A) := \{\mathrm{tr}\,(C^\dagger U A U^\dagger) \mid U \in SU_{\mathrm{loc}}(2^N)\} \subset \mathbb{C}.$$

- **Basic Properties:**

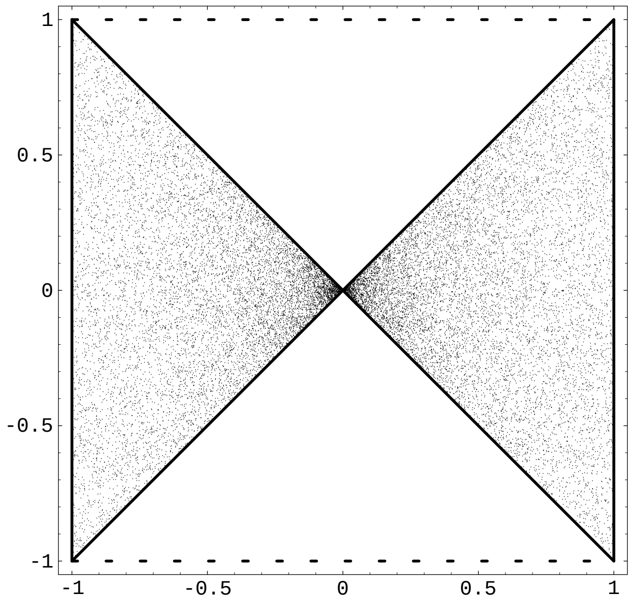
  • $W_{\mathrm{loc}}(C, A)$ is compact and connected.

  • However, $W_{\mathrm{loc}}(C, A)$ is in general neither convex nor star-shaped.

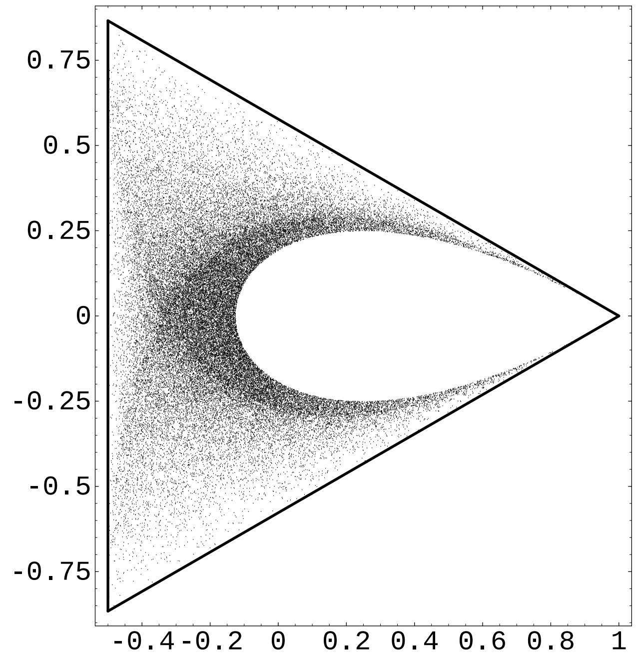
  • An Lie-theoretic analog of Li and Tsing's circular disk result is in preparation.

Optimization on Reachable Sets

Shapes of the Local C-Numerical Range



$N = 2$ Spins



$N = 3$ Spins

Optimization on Reachable Sets

Open Problems

- When is the local numerical range a disc? What is the radius of this disc?
- When is the relative C-numerical range $W_K(C, A)$ convex?

Develop numerical methods for computing the local C-numerical radius!

Optimization on Reachable Sets

Geometric Optimization Methods:

- **Gradient Method**
- **Jacobi-type Method**
- **Newton Method**
- **Conjugate Gradient Method**

All of them exploit the intrinsic manifold structure of the reachable sets of the Schrödinger Equation (Riemannian geometry and Lie Theory) and do not use the ambient vector space.

Optimization on Reachable Sets

Gradient Method:

$$x_{k+1} := \exp_{x_k}\left(-\alpha_k \nabla f(x_k)\right),$$

where $\nabla f(x)$ is the gradient of f, α_n a step size and $\exp_x(\cdot)$ the Riemannian exponential map at x.

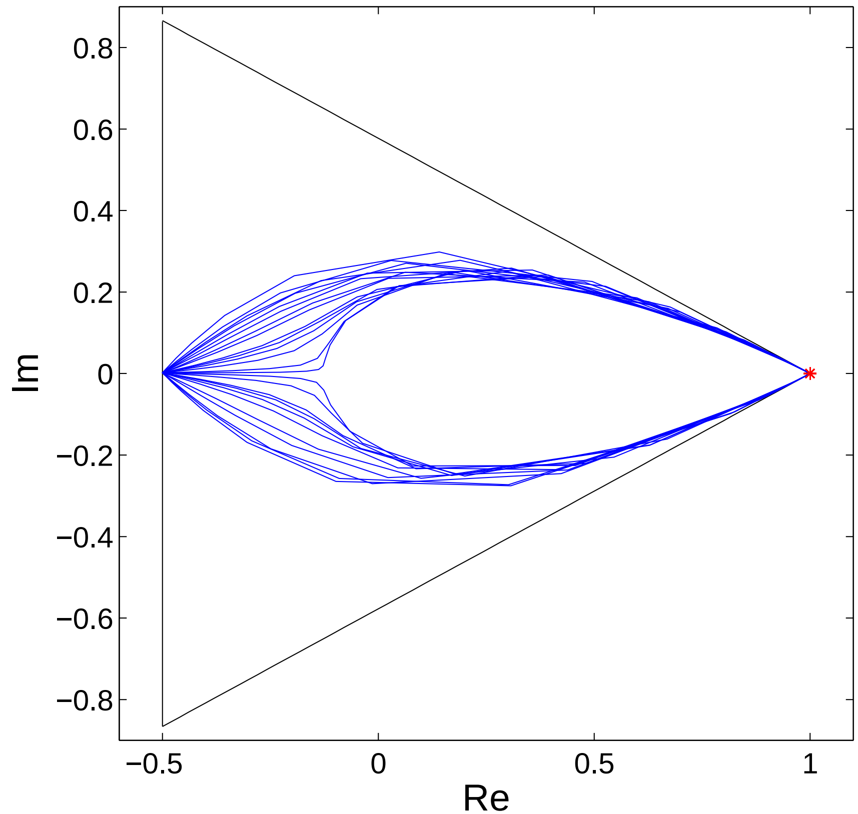
Newton Method:

$$x_{k+1} := \exp_{x_k}\Big(\big(-\mathrm{H}_f(x_k)\big)^{-1}\nabla f(x_k)\Big),$$

where $\mathrm{H}_f(x)$ is the Hessian operator of f and $\exp_x(\Omega)$ the Riemannian exponential map at x.

Geometric Optimization Methods

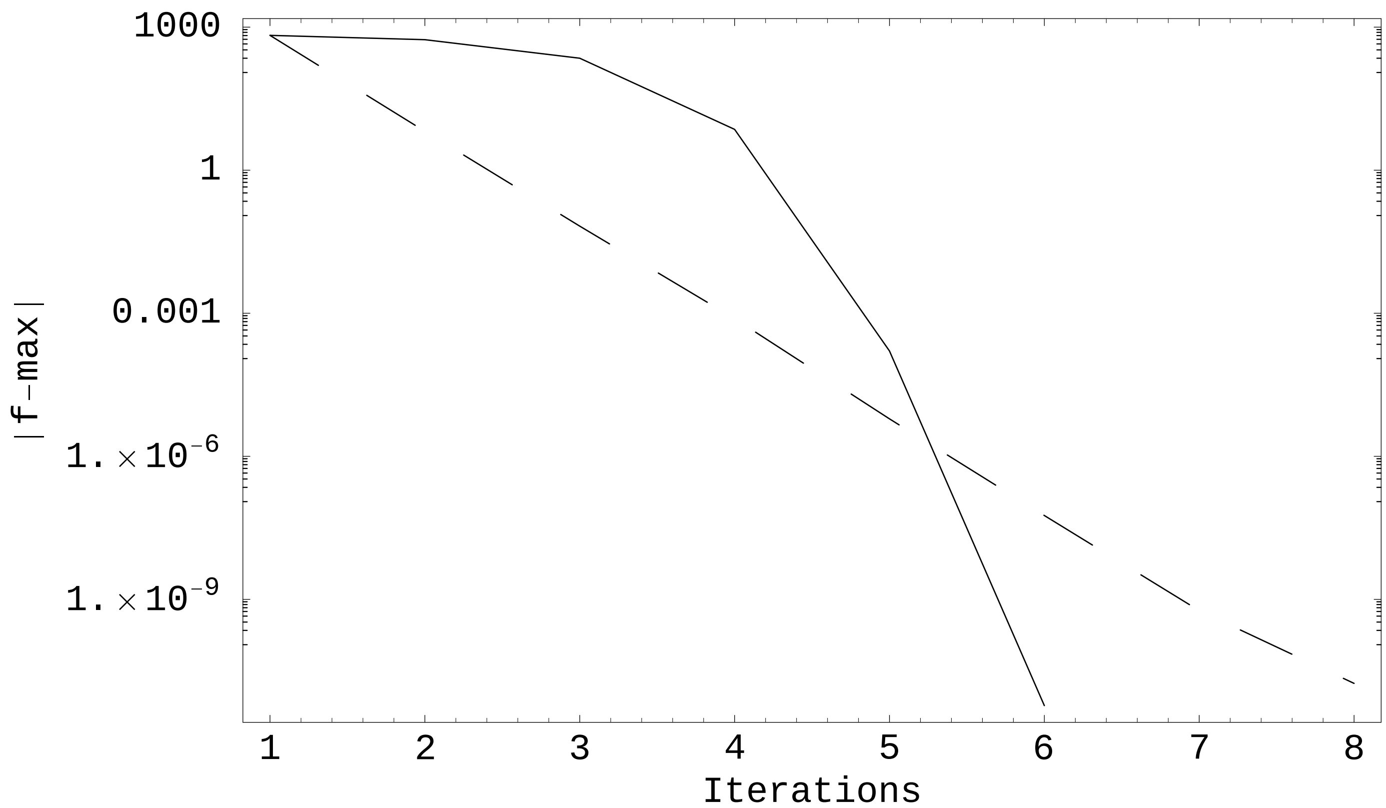
Numerical Experiments for $SU_{\mathrm{loc}}(2^N)$: Gradient Flow



$N = 3$, $n = 8$: Gradient flow for Example II

Geometric Optimization Methods

Numerical Experiments for $SU_{\mathrm{loc}}(2^N)$:



$N = 5$, $n = 32$: C randomly chosen; $A = U_0 C U_0^\dagger$.

Solid line: Newton method; dashed line: conjugate gradient

Time-Optimal Control on Lie Groups

Time-Optimal Control on Lie Groups

- **Pontryagin Maximum Principle** (Jurdjevic, Sussmann)
  - *Advantage:* Always possible. Necessary condition.
  - *Disadvantage:* Little information on optimal control!
- **Lie Theory on Symmetric Spaces** (Brockett, Khaneja)
  - *Advantage:* Full information on optimal control.
  - *Disadvantage:* Restricted to Riemannian symmetric spaces!

Time-Optimal Control on Lie Groups

General Notation:

- G **compact**, connected Lie Group with Lie algebra $\mathfrak{g}$.
- Bilinear control system on G

$$(\Sigma) \qquad \dot{X} = \Big(A_d + \sum_{j=1}^{m} u_j A_j\Big) X, \quad X(0) = I$$

with $A_d, A_1, \ldots, A_m \in \mathfrak{g}$. Let $\mathfrak{k}$ denote the Lie algebra generated by $A_1, \ldots, A_m$.

- Assumptions:
  - (Σ) is controllable, i.e. $\mathfrak{g} = \mathcal{L}$.
  - The **"fast" subgroup** $K := \exp(\mathfrak{k})$ is compact.

Time-Optimal Control on Lie Groups

- Given: Initial state $X_0 = I$ and final state $X_F \in G$
- Problem: Find controls $u_1(\cdot), \ldots, u_m(\cdot)$ and minimal time $T = T_{\text{opt}}(X_F)$ s.t. the corresponding solution $X(t)$ of (Σ) satisfies

$$X(0) = X_0, \; X(T) = X_F.$$

Remark:

- This is difficult! Solutions known only for **small dimensional problems ($n \leq 4$)**!
- Note, there are *no* bounds on the controls.

Time-Optimal Control on Lie Groups

Time-Optimal Torus Theorem

Theorem (Khaneja, Brockett, Glaser '01). Let G/K be a compact *Riemannian symmetric space*, defined by a Cartan decomposition $\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}, \quad \mathfrak{p} := \mathfrak{k}^\perp$. Let $A_d^\perp$ be the orthogonal projection of A_d onto $\mathfrak{p}$ and $\mathfrak{a}$ be a maximal abelian subalgebra of $\mathfrak{p}$ containing $A_d^\perp$. Then:

- Each $X \in G$ has a decomposition

$$X = U\Sigma V \qquad \text{with } U, V \in K \text{ and } \Sigma \in \exp \mathfrak{a}.$$

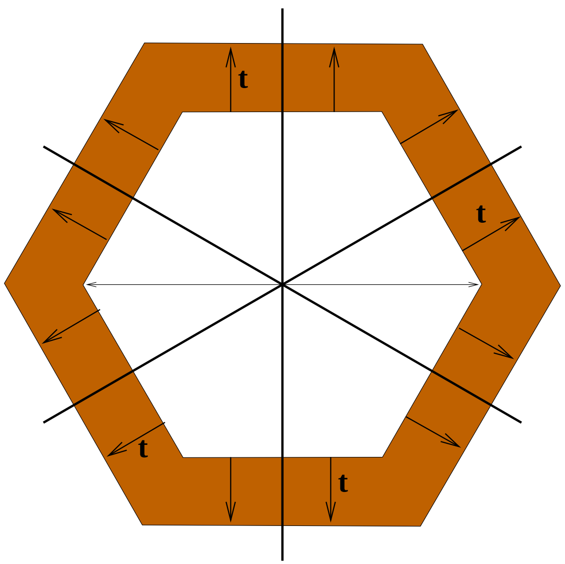
- The minimal time is

$$T_{\mathrm{opt}}(X) = \min \left\{ t \geq 0 \,\middle|\, \left(t \cdot \operatorname{conv} \mathcal{W}(A_d^\perp) \right) \cap \exp^{-1}(\Sigma) \neq \emptyset \right\},$$

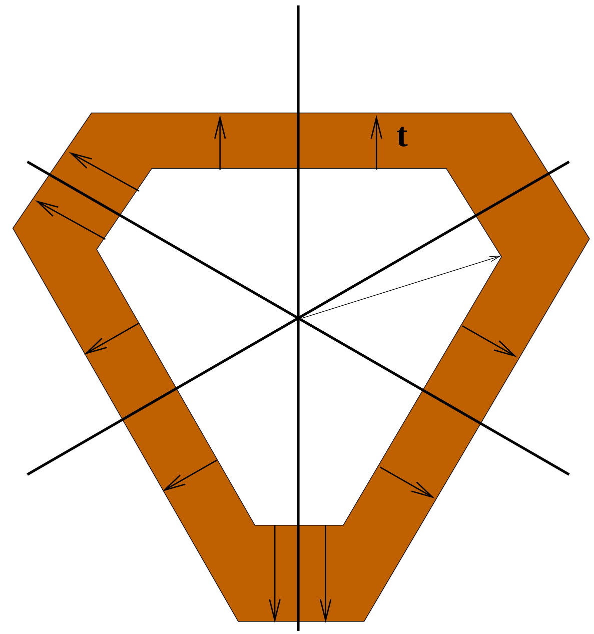
where $X = U\Sigma V$ and $\mathcal{W}(A_d^\perp)$ denotes the Weyl orbit of $A_d^\perp$.

Time-Optimal Control on Lie Groups

Time-Optimal Torus Theorem



Convex hull of the Weyl Orbit of a "symmetric" drift term A_d



Convex hull of the Weyl Orbit of an arbitrary A_d.

Time-Optimal Control on Lie Groups

Examples of Riemannian Symmetric Spaces

- $SU(n)/SO(n)$ is a compact Riemannian symmetric space
- $SU(4)/\big(SU(2) \otimes SU(2)\big)$ is a Riemannian symmetric space (good news!)
- $SU(8)/\big(SU(2) \otimes SU(2) \otimes SU(2)\big)$ is *NOT* a Riemannian symmetric space (bad news!)

Theory works well for 2-Spins, but not for $N \geq 3$ Spins!

Computation of Time-Optimal Trajectories

Global Optimal Control Approach.

- **Combines simulated annealing & gradient descent. Works on any Riemannian symmetric space**.
- **Example: NMR-Schrödinger equation on** $\mathrm{SU}(4)$

$$\dot{X} = -2\pi \mathrm{i}\Big(H_d + \sum_{i=1}^{4} u_i H_i\Big), \quad X(0) = \mathrm{I},$$

$H_d := \sigma_z \otimes \sigma_z,\ H_1 := \mathrm{I}_2 \otimes \sigma_x,\ H_2 := \mathrm{I}_2 \otimes \sigma_y,\ H_3 := \sigma_x \otimes \mathrm{I}_2,$
$H_4 := \sigma_y \otimes \mathrm{I}_2.$

- $K = \mathrm{SU}(2) \otimes \mathrm{SU}(2).$

Computation of Time-Optimal Trajectories

Optimization Algorithm for the NMR-Case:

Let $X(t,u) = U(u_1, ..., u_6)\Sigma(t_1, t_2, t_3)V(u_7, ..., u_{12})$,

$$U(u_1, \ldots, u_6) = \mathrm{e}^{-\mathrm{i}2\pi u_1 H_1}\mathrm{e}^{-\mathrm{i}2\pi u_2 H_2}\mathrm{e}^{-\mathrm{i}2\pi u_3 H_1}\mathrm{e}^{-\mathrm{i}2\pi u_4 H_3}\mathrm{e}^{-\mathrm{i}2\pi u_5 H_4}\mathrm{e}^{-\mathrm{i}2\pi u_6 H_3}$$

$$V(u_7, \ldots, u_{12}) = \mathrm{e}^{-\mathrm{i}2\pi u_7 H_1}\mathrm{e}^{-\mathrm{i}2\pi u_8 H_2}\mathrm{e}^{-\mathrm{i}2\pi u_9 H_1}\mathrm{e}^{-\mathrm{i}2\pi u_{10} H_3}\mathrm{e}^{-\mathrm{i}2\pi u_{11} H_4}\mathrm{e}^{-\mathrm{i}2\pi u_{12} H}$$

$$\Sigma = \mathrm{e}^{t_1 2\pi\mathrm{i}(\sigma_x \otimes \sigma_x)}\mathrm{e}^{t_2 2\pi\mathrm{i}(\sigma_y \otimes \sigma_y)}\mathrm{e}^{t_3 2\pi\mathrm{i}(\sigma_z \otimes \sigma_z)}$$

To compute the minimal time $T(X)$, we combine simulated annealing with gradient methods to solve the nonlinear optimization problem:

$$\begin{aligned} \min \quad & f(t,u) := |t_1| + |t_2| + |t_3|, \\ \text{subject to} \quad & g(t,u) := 4 - \mathrm{Re}\,\mathrm{tr}(X_F^* X(t,u)) = 0 \end{aligned}$$

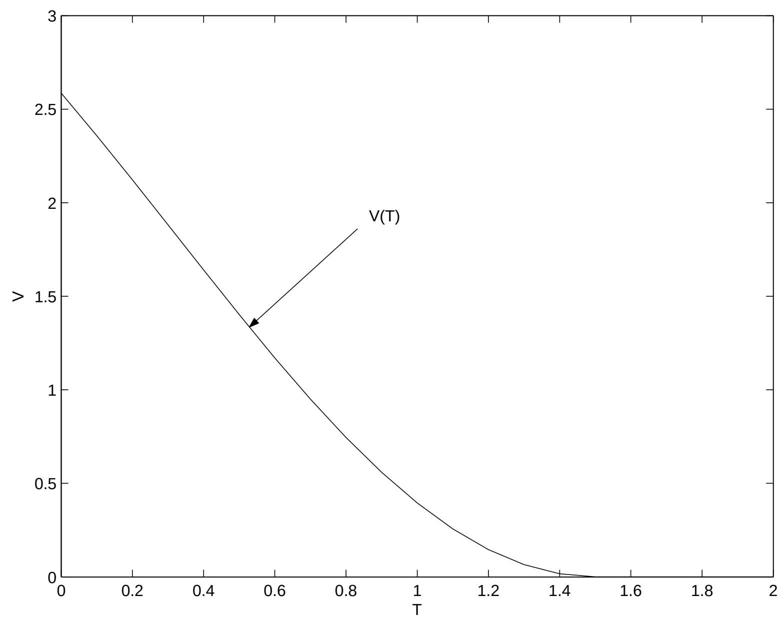
where $t = [t_1, t_2, t_3], u = [u_1, u_2, ..., u_{12}] \in [-1, 1] \times \cdots \times [-1, 1]$

Computation of Time-optimal Trajectories

Numerical Results:

$$X_F = \mathrm{e}^{-\frac{\mathrm{i}\pi}{4}} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$ **Swap Gate**

$$T_{\mathrm{opt}}(X_F) = 1.499996 \qquad t = [0.499993 \mid 0.500017 \mid 0.499986]$$



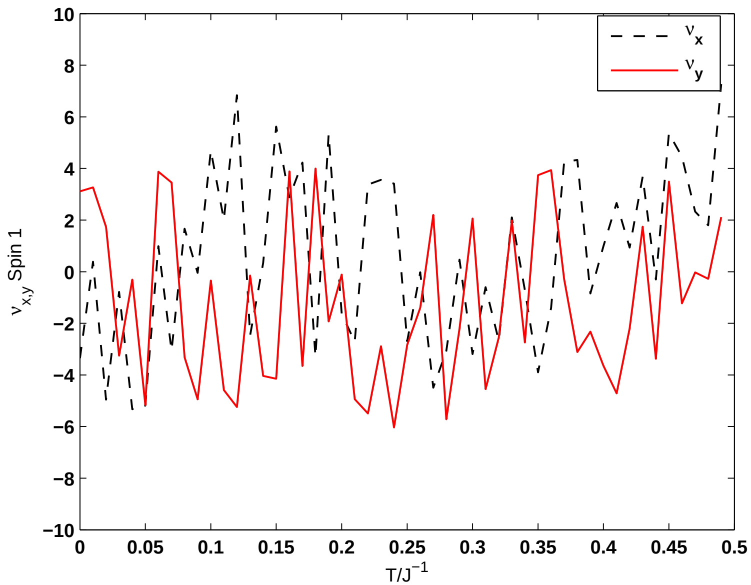
Plot of $V(T)$ over $[0, 3]$.

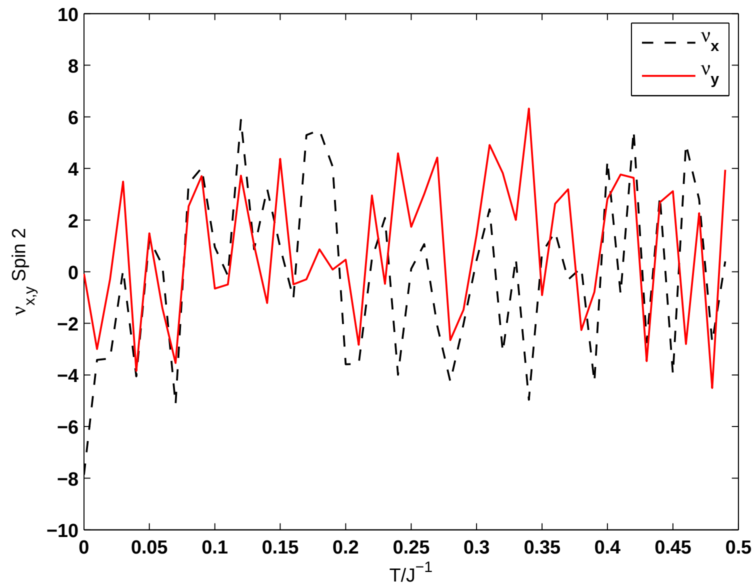
Optimization in Quantum Control

Alternative Approach: GRAPE Algorithm:

- Use piecewise constant controls (M switches, time length T).
- Optimize cost function via gradient descent on finite-dimensional space of input values $\mathbb{R}^M$ (using Armijo step size)
- Plot achieved optimal inputs and transfer function as function of T.

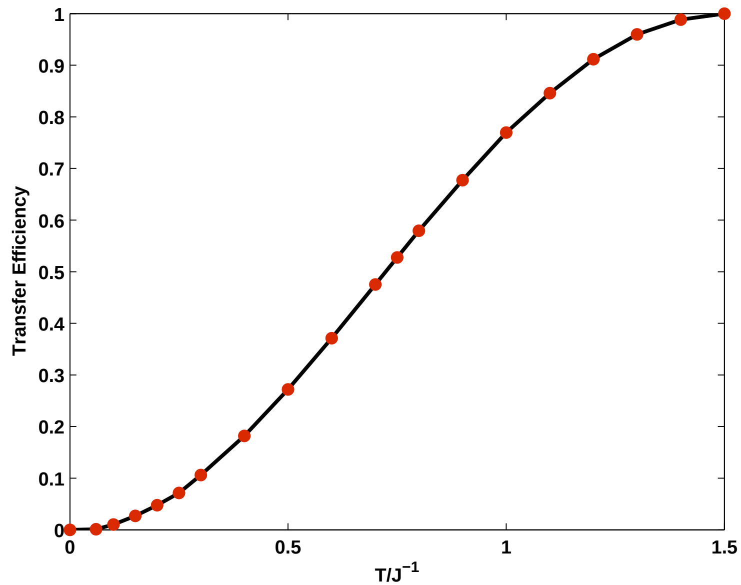
Optimal Control of Spin Systems





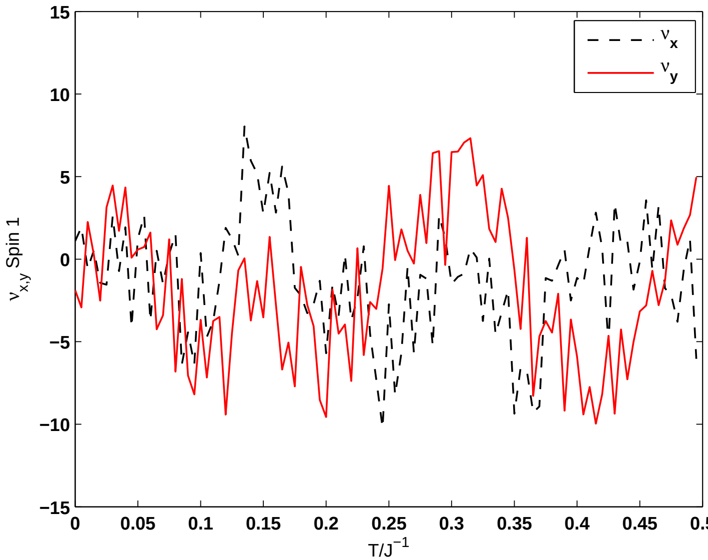
2-Spin Case: Optimal inputs at spin 1, resp. spin 2 for $T = 0.5$ seconds

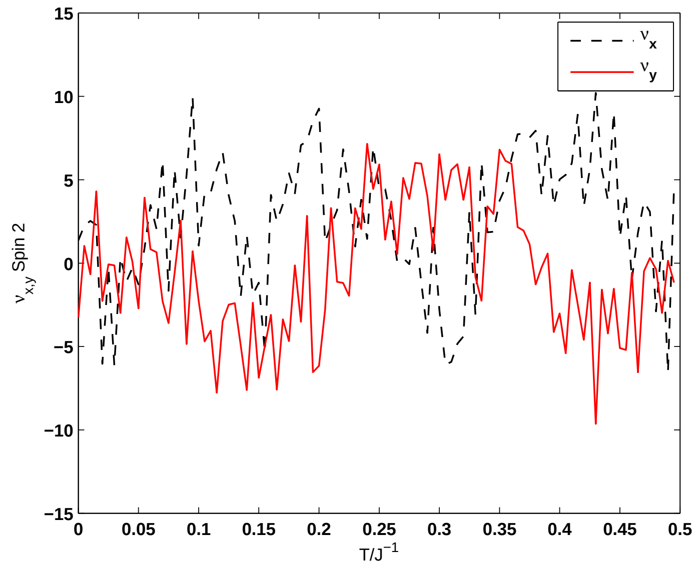
Optimal Control of Spin Systems

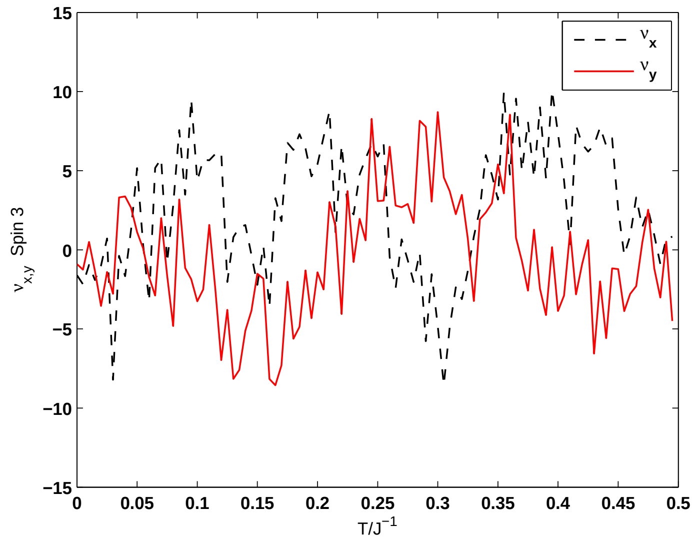


2-Spin Case: Optimal Transfer Efficiencies. The accuracy is 10^{-6}.

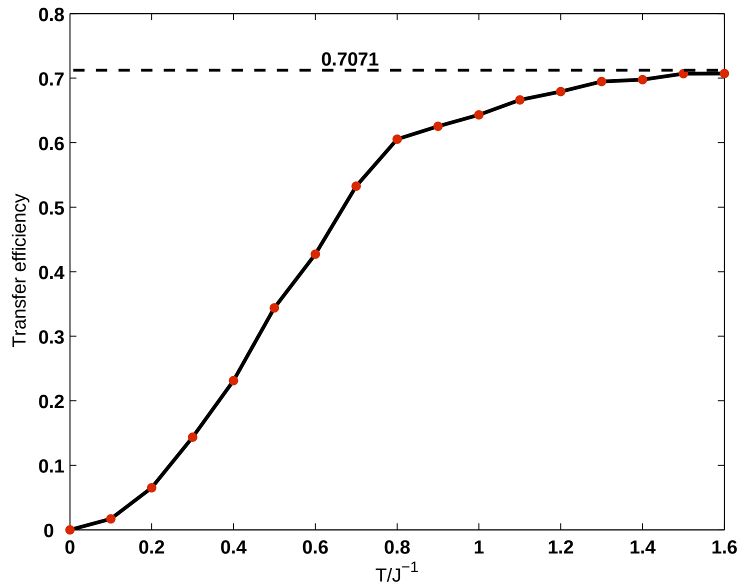
Optimal Control of Spin Systems



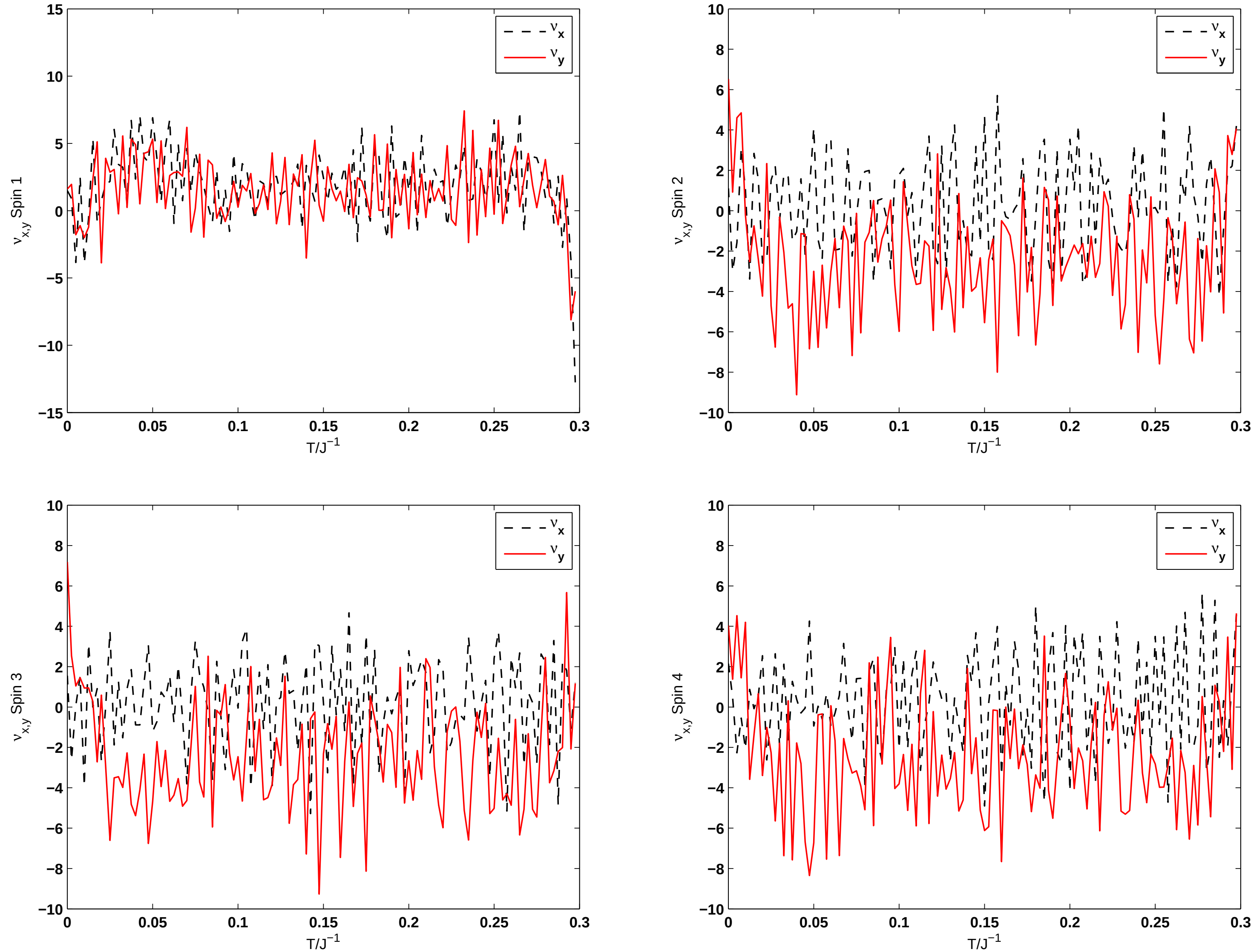




Optimal Control of Spin Systems

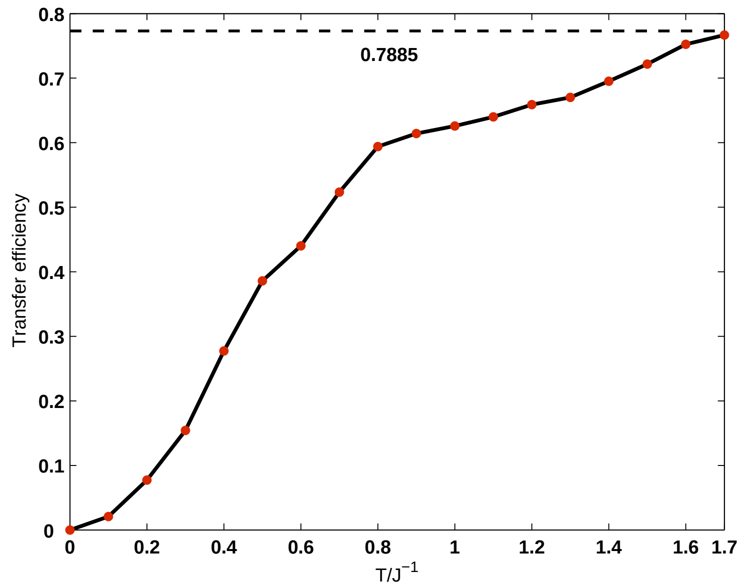


3-Spin Case: Optimal Transfer Efficiencies. The accuracy is 10^{-5}.



4-Spin Case: Optimal inputs at spin 1, spin 2, spin 3, resp. spin 4 for $T = 0.3$ s

Optimal Control of Spin Systems



4-Spin Case: Optimal Transfer Efficiencies. The accuracy is 10^{-3}.

Optimization for Quantum Control

Conclusions and Open Problems:

- Resonably well developed optimal control theory is emerging for Riemannian symmetric spaces.

Many challenging open problem in different mathematical areas:

- **Control Theory:** A complete description of the reachable sets of the Schrödinger equation in terms of couplings, i.e. in terms of the spin-spin interaction graph. Fast optimal control algorithms.
- **Linear Algebra:** Reliable algorithms for computing relative numerical ranges.
- **Geometric Optimization/Computing:** Riemannian optimization algorithms proved to be efficient tools for small $N \sim 5$; however for large $N \sim 20$ there is still work to do.