# Control Theoretic Aspects of Matrix Factorizations

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# Motivation

- Quantum Computing
- Quantum Control, Control of Spin Systems
- Control of Numerical Algorithms
- Constructive Controllability, Motion Planning in Robotics

# Time-optimal Factorization Problem

- $G$ compact connected Lie group with Lie Algebra $\mathfrak{g}$
- $\omega := \{\Omega_1^+, ..., \Omega_r^+, \Omega_1^-, ..., \Omega_s^-\}$ finite set of LA generators of $\mathfrak{g}$
- $\Omega_i^+$: "slow, cost expensive" directions
  $\Omega_i^-$: "fast, cheap" directions
- Given $X \in G$, define

$$T_{\min}(X) = \inf \left\{ \sum_i |t_i^+| \mid X = \prod_{\text{finite}} e^{t_i^\pm \Omega_i^\pm} \right\}$$

## Problem:

- Is $T_{\min} < \infty$ always? Compute $T_{\min}$!
- When does there exist a *finite, time-optimal* factorization?

# Example

## Optimal Condition Numbers

- $G = GL(n)$ general linear group of invertible matrices
- $\omega := \{\Omega_1^+, ..., \Omega_r^+, \Omega_1^-, ..., \Omega_s^-\}$ finite set of LA generators of $\mathfrak{gl}(\mathfrak{n})$
- $\Omega_i^+$: "hyperbolic Jacobi rotations"
  $\Omega_i^-$: "standard Jacobi directions"
- Given $X \in G$, define ($\kappa$ denotes the condition number)

$$T_{\min}(X) = \inf \left\{ \sum_i \kappa(e^{t_i^+ \Omega_i^+})| \mid X = \prod_{\text{finite}} e^{t_i^{\pm} \Omega_i^{\pm}} \right\}$$

## Problem:

- This factorization task with minimal total condition number!
- Does there exists factorization with better condition numbers than for $X$?

# Lie Groups & Lie Algebras

# Intermezzo: Lie Groups and Lie Algebras

Example. General linear group of invertible $n \times n$ matrices

$$GL(n, \mathbb{R}) := \{X \in \mathbb{R}^{n \times n} \mid \det X \neq 0\}.$$

Definition. A matrix *Lie group* is any subgroup $G \subset GL(n, \mathbb{R})$ that is also a (locally closed) submanifold of $\mathbb{R}^{n \times n}$.

Dynamics & Control

# Intermezzo: Lie Groups and Lie Algebras

## Examples, cont'd:

(a) The *real orthogonal group*

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

(b) The *special unitary group*

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

(c) The *Euclidean group*

$$E(n) := \left\{ \begin{bmatrix} R & p \\ 0 & 1 \end{bmatrix} \middle| \; R \in O(n), p \in \mathbb{R}^n \right\}.$$

The first two examples are compact groups, while the third is not.

# Intermezzo: Lie Groups and Lie Algebras

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

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

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

is called a *Lie Algebra*.

# Intermezzo: Lie Groups and Lie Algebras

- Lie algebras are the tangent spaces of Lie groups.

- **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 matrix is a Lie algebra with commutator as the Lie bracket:

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

# Intermezzo: Lie Groups and Lie Algebras

## Examples

(a) The Lie algebra of $O(n)$ is

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

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

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

(c) The Lie algebra of $E(n)$ is

$$\mathfrak{e}(n) := \left\{ \begin{bmatrix} \Omega & v \\ 0 & 0 \end{bmatrix} \middle| \ \Omega^\top = -\Omega, v \in \mathbb{R}^n \right\}.$$

# Control on Lie Groups

# Control on Lie Groups

- $G$ Lie Group with Lie Algebra $\mathfrak{g}$.
- Bilinear control system on $G$

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

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

- Reachable Set at time $T > 0$

$$\mathcal{R}(T) = \{ X_F \in G | \; \exists u_1, ..., u_m \text{ and } s \leq T : X(s) = X_F \}$$

- Reachable Set

$$\mathcal{R} = \cup_T \mathcal{R}(T)$$

# Control on Lie Groups

## Definition

- **Accessibility:** The reachable set $\mathcal{R}(T)$ has an interior point
- **Local Controllability:** The identity $I \in \mathcal{R}(T)$ is an interior point
- **Controllability:** For any $X_F \in G$ there exist controls $u_1(\cdot), ..., u_m(\cdot)$ and $T > 0$ s.t. the solution of $(\Sigma)$ satisfies $X(0) = I, X(T) = X_F$.

# Control on Lie Groups

Problem 1 (Accessibility)

- Definition (*System Lie Algebra*)

  $\mathcal{L} :=$ smallest Lie subalgebra of $\mathfrak{g}$, containing $A_1, ..., A_m, A_d$

  *Generators*: $([A, B] = AB - BA)$

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

- **Theorem.** $(\Sigma)$ is accessible if and only if the system Lie algebra is $\mathcal{L} = \mathfrak{g}$.

# Control on Lie Groups

- **Theorem** (Lian et al. 1994) Suppose

  (i) For some constant controls $u_1, ..., u_m$

  $$(\Sigma_{const}) \quad \dot{X} = (A_d + \sum_j u_j A_j)X$$

  is weakly positively Poisson stable.

  (ii) The system Lie algebra $\mathcal{L}$ satisfies $\mathcal{L} = \mathfrak{g}$.

  Then the bilinear control system is controllable.

**Accessability** $+$ **Poisson Stability** $\Rightarrow$ **Controllability**

# Control on Lie Groups

**Definition** (Poisson Stability)

Flow of $(\Sigma_{const})$: $\Phi : G \times \mathbb{R} \to G; \ (z, t) \mapsto \Phi(z, t)$

- $(\Sigma_{const})$ is **Weakly Positively Poisson Stable** if for all $z \in G$, any neighborhood $B(z)$ of $z$ and all $T > 0$, there exists $t > T$ such that $\Phi(U_z, t) \cap B(z) \neq \emptyset$.

Examples: a swing (no damping), satellite attitude, ball rolling in a bowl.

# Control on Lie Groups

- Theorem (Jurdjevic-Sussmann) Assume:

  (i) There exist constant controls such that $A_d + \sum_j u_j A_j$ lies in a **compact** subalgebra $\mathfrak{k}$ of $\mathfrak{g}$.

  (ii) The system Lie algebra $\mathcal{L}$ satisfies $\mathcal{L} = \mathfrak{g}$.

  Then the system $(\Sigma)$ is controllable.

# Control on Lie Groups

- Corollary

  Let $G$ be a **compact** connected Lie group. Then $(\Sigma)$ is controllable if and only if

$$\mathcal{L} = \mathfrak{g}.$$

# Time-Optimal Control on Lie Groups

# Time-Optimal Control on Lie Groups

## General Notation:

- Let $G$ be a compact Lie Group with Lie algebra $\mathfrak{g}$; $K \subset G$ a compact connected Lie subgroup with LA $\mathfrak{k}$ . Consider the bilinear control system on $G$

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

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

- Assumption:
  - $\Sigma$ is controllable, i.e. $\mathfrak{g}$ =LA generated by $A_d, A_1, ..., A_m$
  - $\mathfrak{k} =$ LA generated by $A_1, ..., A_m$

# Time-Optimal Control on Lie Groups

- Given: Initial state $X_0 = I$, Final state $X_F \in G$
- Problem 1.Find controls $u_1(\cdot), ..., u_m(\cdot)$ s.t. the corresponding solution $X(t)$ of $(\Sigma)$ satisfies

$$X(0) = X_0, \; X(T) = X_F \quad \text{for some} \quad T > 0$$

- Problem 2.If problem 1 has at least one solution, then find a time-optimal one, i.e. one with *minimal* $T = T_{\text{opt}}(X_F)$.
- Problem 1 is always solvable, provided $(\Sigma)$ is controllable!

# Time-Optimal Control on Lie Groups

## Fast versus slow directions

- $A_d$ is called the *drift term*, $A_1, ..., A_m$ the *fast directions*
- Fact 1. If $A_d = 0$ and $(\Sigma)$ controllable, then can control to $X_F$ in *arbitrarily small time*: $T_{\text{opt}}(X_F) = 0$, always!
- Fact 2. The presence of drift term $A_d \neq 0$ is responsible for $T_{\text{opt}} > 0$.
- Idea: Factor out fast directions!

# Time-Optimal Control on Lie Groups

## Quotient System and Equivalence Principle

- Consider the quotient space

$$G/K := \{Kg \mid g \in G\}$$

  of left co-sets $Kg$, $K = \exp(\mathfrak{k})$ Lie Group generated by fast controls.

- $G/K$ is a smooth manifold

# Time-Optimal Control on Lie Groups

Example: (NMR)

- For the NMR Schrödinger Equation on $G = SU(2^N)$

$$\dot{X} = -\mathrm{i}\left(H_d + \sum_{j=1}^{2N} u_j H_j\right) X, \quad X(0) = I$$

$\mathfrak{k} :=$ LA generated by $\mathrm{i}H_1, ..., \mathrm{i}H_{2N}$
$K := \exp(\mathfrak{k})$ compact, connected Lie subgroup of $SU(2^N)$, generated by $\exp(\mathrm{i}tH_j), t \in \mathbb{R}, j = 1, ..., 2N$.

One verifies $K = SU(2) \otimes ... \otimes SU(2)$

- For $N = 1 : K = SU(2) = G$
- For $N = 2 : K = SU(2) \otimes SU(2) \simeq SO(4) \subset SU(4)$

# Time-Optimal Control on Lie Groups

## Quotient System and Equivalence Principle

- The *quotient system* of

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

is the control system on $G/K$

$$(\Sigma/K) \qquad \dot{P} = \mathrm{Ad}_{U(t)}(A_d) P, \quad P(0) = K, \quad P(T) = K X_F$$

$\mathrm{Ad}_g(A_d) = g A_d g^{-1}, \ g \in K$. The control functions for $(\Sigma/K)$ are arbitrary $L^1_{\mathrm{loc}}$ functions $t \mapsto U(t) \in K$.

# Time-Optimal Control on Lie Groups

## Quotient System and Equivalence Principle

- Theorem (Equivalence Principle).

  $(\Sigma)$ is controllable on $G$ iff $(\Sigma/K)$ is controllable on $G/K$. Moreover, the optimal times on $G$ and $G/K$ coincide.

  $$T_{\mathrm{opt}}^{G}(X_F) = T_{\mathrm{opt}}^{G/K}(KX_F)$$

  Proof: PhD thesis by Khaneja

- The optimal time $T_{\mathrm{opt}}^{G/K}$ has an interpretation within Sub-Riemannian Geometry.

# Time-Optimal Control on Lie Groups

## Sub-Riemannian Geometry

- Let $M$ be a Riemannian manifold, $E \subset TM$ a constant dimensional subbundle that satisfies the *Hörmander Condition*

  For any $p \in M$, the LA of the sections of $E$ evaluated in $p$ is equal to $T_pM$ (controllability cond.)

- For any two points $x, y \in M$, the *Sub-Riemannian distance* is

$$d(x,y) := \inf\left\{ \int_0^1 ||\dot{\alpha}(t)||dt \mid \alpha(0) = x, \alpha(1) = y, \dot{\alpha}(t) \in E_{\alpha(t)} \right\}.$$

- Example: $M = G/K, E_p := \mathrm{span}\{kA_dk^{-1} \mid k \in K\}P$, $P \in M$ satisfies the Hörmander Cond. (Equivalence principle)
- NMR: $M = SU(2^N)/SU(2) \otimes \ldots \otimes SU(2)$ Sub-Riemannian space

# Time-Optimal Control on Lie Groups

## Sub-Riemannian Geometry

- **Theorem.**

$$T_{\mathrm{opt}}^{G/K}(KX_F) = d(K, KX_F)$$

  Sub-Riemannian distance

- **Remark.** The Sub-Riemannian distance $d(x,y)$ is greater than or equal the Riemannian distance on $G/K$:

$$d(x,y) \geq \text{ geodesic distance between } x, y$$

- There is one case where these distances are equal: *Riemannian symmetric spaces.*

# Time-Optimal Control on Lie Groups

## Sub-Riemannian Geometry

- **Theorem.** If $G/K$ is a Riemannian Symmetric Space, then

  $T_{\mathrm{opt}}(X_F) =$ length of a geodesic in $G/K$ that connects $K$ with $KX_F$

- **Main Advantage:** Riemannian distances (i.e. lengths of geodesics) are much easier to compute than Sub-Riemannian distances.

# Time-Optimal Control on Lie Groups

- **Theorem.** The homogenous space $G/K$ is a Riemannian symmetric space, provided $(\mathfrak{g}, \mathfrak{k})$ is a Cartan-pair, i.e. $\mathfrak{g}$ is semisimple and

$$\mathfrak{g} = \mathfrak{k} \oplus \mathfrak{p}, \quad \mathfrak{p} := \mathfrak{k}^{\perp}$$

  satisfies

$$[\mathfrak{k}, \mathfrak{k}] \subset \mathfrak{k}, \quad [\mathfrak{k}, \mathfrak{p}] \subset \mathfrak{p}, \quad [\mathfrak{p}, \mathfrak{p}] \subset \mathfrak{k}$$

# Time-Optimal Control on Lie Groups

## Riemannian Symmetric Spaces

- $SU(n)/SO(n)$ is a Riemannian Symmetric Space
- $SU(4)/SU(2) \otimes SU(2)$ is a Riemannian Symmetric Space (good! 2-Spin Case)
- $SU(8)/SU(2) \otimes SU(2) \otimes SU(2)$ is *NOT* a Riemannian Symmetric Space (bad!)

# Time-Optimal Factorization

# Time-optimal Factorization

- Let $G$ be a connected, compact Lie group with Lie algebra $\mathfrak{g}$.
- Let $K \subset G$ be a connected compact subgroup with Lie algebra $\mathfrak{k}$.
- Let $\Delta \in \mathfrak{g}$ be a drift term s.t. $\langle \Delta, \mathfrak{k} \rangle_L = \mathfrak{g}$.
- Consider the discrete control System:

$$(\Sigma_d) \qquad X_{n+1} = K_n \mathrm{e}^{t_n \Delta} L_n X_n, \quad X_0 = I \quad K_n, L_n \in K, t_n \geq 0.$$

For $X \in G$ let $T^d_{\mathrm{opt}}(X) :=$

$$\inf \left\{ \sum_{n=1}^{\infty} t_n \;\middle|\; \exists \, (K_n, L_n, t_n) : \prod_{n=1}^{\infty} K_n \mathrm{e}^{t_n \Delta} L_n = X \right\}.$$

# Time-optimal Factorization

## Problem:

- Is $(\Sigma_d)$ controllable, i.e. does $T^d_{\mathrm{opt}}(X) < \infty$ hold for all $X \in G$?
- Determine the "minimal" time $T^d_{\mathrm{opt}}(X)$ for $X \in G$.

# Time-optimal Factorization

## Generalized Version (multiple drifts)

- $G$ compact connected Lie group with LA $\mathfrak{g}$
- $\omega := \{\Omega_1^+, ..., \Omega_r^+, \Omega_1^-, ..., \Omega_s^-\}$ finite set of LA generators of $\mathfrak{k}$
- $\Omega_i^+$: "slow, cost expensive" directions
  $\Omega_i^-$: "fast, cheap" directions
- Given $X \in G$, define

$$T_{\min}(X) = \inf \left\{ \sum_i |t_i^+| \mid X = \prod_{\text{finite}} e^{t_i^\pm \Omega_i^\pm} \right\}$$

# Time-optimal Factorization

## Problem

- Is $T_{\min} < \infty$ always? Compute $T_{\min}$!
- When does there exist a *finite, time-optimal* factorization?

# Time-optimal Factorization

Example 1 (Euler Angles)

- $SO(3)$, $\omega = \{\Omega_1^+, \Omega_1^-\}$,

$$\Omega_1^+ := \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \Omega_1^- := \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

- *Euler Angles*:

$$X = \mathrm{e}^{\theta_1 \Omega_1^-} \mathrm{e}^{\theta_2 \Omega_1^+} \mathrm{e}^{\theta_3 \Omega_1^-}, \quad \theta_i \in [-\pi, \pi]$$

- We will show: Euler Angles are time-optimal and

$$T_{\min} = |\theta_2| \in [0, \pi]$$

# Time-optimal Factorization

Example 2 (Euler Angles)

- $SO(3)$, $\omega = \{\Omega_1^+, \Omega_2^+\}$, $\Omega_2^+ := \Omega_1^-$
- Then Euler angles are i.g. *NOT* time-optimal:

$$T_{\min} < \theta_1 + \theta_2 + \theta_3 \; ! \quad \text{(Mittenhuber)}$$

Dynamics & Control

# Time-optimal Factorization

## Equivalence Principle

- Let $G$ be a connected, compact Lie group with Lie algebra $\mathfrak{g}$.
- Let $\mathfrak{k} := \langle A_1, ..., A_m \rangle_L$, $K := \exp \mathfrak{k}$.
- Let $\Delta \in \mathfrak{g}$ be a drift term such that $\langle \Delta, \mathfrak{k} \rangle_L = \mathfrak{g}$.
- Theorem.
  - (a) The discrete control system $(\Sigma_d)$ on $G$ is controllable and thus $T^d_{\text{opt}}(X) < \infty$
  - (b) For any $X \in G$ the minimal times $T^d_{\text{opt}}(X) = T_{\text{opt}}(X)$ coincide, where $T_{\text{opt}}(X)$ is the minimal time for the control problem

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

# Time-optimal Factorization

- **Problem:** I.g. time optimal factorizations are infinite

  Under what conditions on the drift term $\Delta$ are they *finite*?

- **Definition** [Haselgrove, Nielsen, Osborne]: A drift term $\Delta$ is called *lazy*, if there exists $\varepsilon > 0$ such that

$$T_{\mathrm{opt}}(\mathrm{e}^{t\Delta}) < t \qquad \text{for all } t \in (0, \varepsilon). \qquad (**)$$

  If $\Delta$ is not lazy, we call it *fast*.

Dynamics & Control

# Time-optimal Factorization

- **Theorem.** If $\Delta$ is lazy, there are no finite, time optimal factorizations for any element $X \in G - K$.

# Time-optimal Factorization

- **Conjecture 1:** There exists a finite, time optimal factorization for all $X \in G$ iff $\Delta$ is fast.
- **Conjecture 2:** $\Delta$ fast $\iff$ $[\Delta, \Delta^{\perp}] = 0$.
- **Remark:** Conjecture 2 implies Conjecture 1.

# Computation of Optimal Time

Theorem (Khaneja). Let $(\mathfrak{g}, \mathfrak{k})$ be a Cartan pair. Let $\Delta^\perp$ be the orthogonal projection of $\Delta$ onto $\mathfrak{p}$ and let $\mathfrak{a}$ be a maximal abelian subalgebra of $\mathfrak{p}$ that contains $\Delta^\perp$. Then:

- Each $X \in G$ has a decomposition of the form

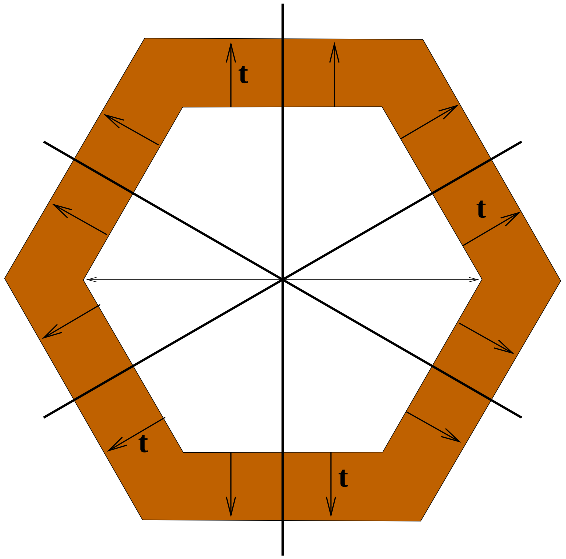
$$X = U\Sigma V \qquad \text{with } U, V \in K \text{ and } \Sigma \in \exp \mathfrak{a}.$$

- The minimal time is given by

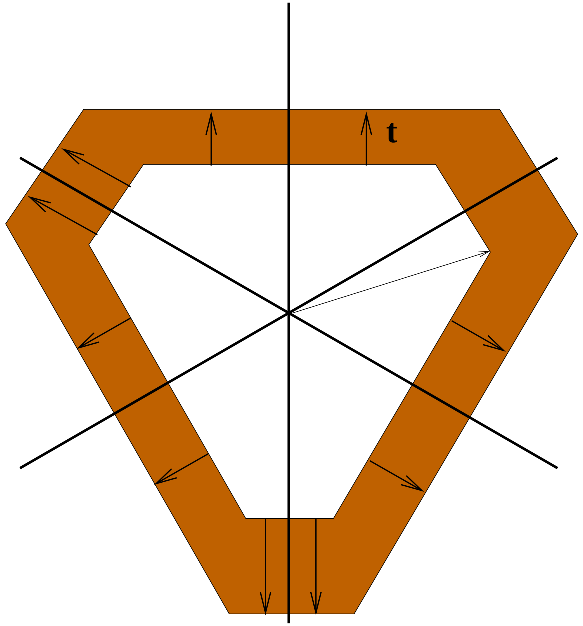
$$T_{\mathrm{opt}}(X) = \min \left\{ t \geq 0 \,\middle|\, \left( t \cdot \operatorname{conv} \mathcal{W}(\Delta^\perp) \right) \cap \exp^{-1}(\Sigma) \neq \emptyset \right\},$$

where $X = U\Sigma V$ is an arbitrary factorization of the above type and $\mathcal{W}(\Delta^\perp)$ denotes the Weyl orbit of $\Delta^\perp$.

# Computation of Optimal Time




Convex hull of the Weyl Orbit of a "symmetric" drift term $\Delta$




Convex hull of the Weyl Orbit of an arbitrary $\Delta$.

# Computation of Optimal Time

## Example 1, cont'd:

- $G := \mathrm{SO}(3)$ and $\mathfrak{g} := \mathfrak{so}(3)$,

$$\Omega_1 := \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}, \Omega_2 := \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

- $\Delta := \alpha\Omega_1 + \beta\Omega_2$, $\mathfrak{k} := \langle\Omega_2\rangle$

Euler Angles: $X = \mathrm{e}^{\theta_1\Omega_2}\mathrm{e}^{\theta_2\Omega_1}\mathrm{e}^{\theta_3\Omega_2}$, $\theta_i \in [-\pi, \pi]$

- $T_{\mathrm{opt}}(X) = \alpha^{-1}|\theta_2|$,
- $\Delta$ fast $\iff$ $\beta = 0$.

# Computation of minimal time

Example: (NMR cont'd)

- NMR-Schrödinger equation on $\mathrm{SU}(4)$

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

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

- $K = \mathrm{SU}(2) \otimes \mathrm{SU}(2)$.
- $\Delta = -2\pi \mathrm{i} H_d$ and $\mathfrak{a} := \mathrm{i}\langle \sigma_x \otimes \sigma_x, \sigma_y \otimes \sigma_y, \sigma_z \otimes \sigma_z \rangle$.

# Computation of minimal time

Example: (NMR cont'd)

**Theorem.** For all $X = U\Sigma V \in SU(4)$ and $U, V \in K$, and $\Sigma \in \exp \mathfrak{a}$ fixed it holds

- $T(X) = \min \left\{ \sum_{n=1}^{3} |t_n| \,\Big|\, \mathrm{e}^{t_1 2\pi \mathrm{i}(\sigma_x \otimes \sigma_x)} \mathrm{e}^{t_2 2\pi \mathrm{i}(\sigma_y \otimes \sigma_y)} \mathrm{e}^{t_3 2\pi \mathrm{i}(\sigma_z \otimes \sigma_z)} = \Sigma \right\}$
- $T(X) \leq \frac{3}{2}$

# Computation of minimal time

## Optimization Algorithm (NMR cont'd)

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

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

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

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

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

# Computation of Time-optimal Pulse Sequences

Consists of two sub-problems:

- Given $T \geq 0$, solve

$$\begin{aligned} \min_{t,u} \quad & g(t,u), \\ \text{subject to} \quad & f(t,u) \leq T, \\ & t \geq 0. \end{aligned}$$

- Let $V(T)$ be the global optimal value of $g(t,u)$, associated with a given $T \geq 0$.

$$\begin{aligned} \text{Minimize} \quad & T \\ \text{subject to} \quad & V(T) = 0, \\ & T \geq 0. \end{aligned}$$

# Computation of Time-optimal Pulse Sequences

## Example

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

$$\begin{aligned} T(X_F) &= 1.499996 \\ t &= [0.499993 \mid 0.500017 \mid 0.499986] \end{aligned}$$