The Constructive Lie Algebra Rank Condition and its Applications to Quantum Control

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Introduction

Systems in (finite dimensional) Coherent Quantum Control

$$\dot{X} = -iH(u)X, \quad X(0) = \mathbf{1}$$

- X varies in the unitary (matrix) Lie group $U(n)$.
- H is a matrix function of the controls u, which is Hermitian for every value of u. The controls u attain values in a set $\mathcal{U} \subseteq R^m$.
- $\mathbf{1}$ is the identity in the group.

Important feature of these systems: Right Invariance: If $X(t, S, u_{[0,t)})$ is the solution corresponding to initial condition S and control function $u_{[0,t)}$, then

$$X(t, S, u_{[0,t)}) = X(t, \mathbf{1}, u_{[0,t)})S.$$

Consequence for control: If u_1 (u_2) drives X from the identity $\mathbf{1}$ to S_1 (S_2), then $u_2 \circ u_1$ (concatenation of the two controls) drives the identity $\mathbf{1}$ to S_2S_1.

Controllability

What is the set reachable $\mathcal{R}$ from the identity $\mathbf{1}$ by appropriately varying the controls?
Theorem [Jurdjevic-Sussmann, 1973] Lie Algebra Rank Condition (LARC)

- Let
$$\tilde{\mathcal{F}} := \{-iH(u) | u \in \mathcal{U}\}.$$
- Let $\mathcal{L}$ by the Lie algebra generated by $\tilde{\mathcal{F}}$ and $e^{\mathcal{L}}$ the associated connected Lie group.
- If $e^{\mathcal{L}}$ is compact, then
$$e^{\mathcal{L}} = \mathcal{R}$$
- This result has been elaborated upon in many papers on quantum systems.
- In particular the structure of the *dynamical Lie algebra* $\mathcal{L}$ has been studied in [Polack, Suchowski, Tannor, PRA 2009] and [D'Alessandro, IEEE TAC 2009 (submitted)].
- For quantum systems $\mathcal{L}$ is always the direct sum of an Abelian subalgebra of $u(n)$ and a semisimple one. $e^{\mathcal{L}}$ is always the direct product of an Abelian Lie group and a semisimple (compact) one. That is, modulo an Abelian Lie group which commutes with everything, $e^{\mathcal{L}}$ is compact.

Constructive Control Set-up

Can we make LARC theorem constructive? That is: Given $X_f \in e^{\mathcal{L}}$ can we find a control u to drive $\mathbf{1} \to X_f$?

Reformulate problem:

- Select a maximal linearly independent set $\mathcal{F} \subseteq \tilde{\mathcal{F}}$

$$\mathcal{F} = \{-iH_1, \ldots, -iH_m\}.$$

To each $-iH_j$ there corresponds a control $u_j \in \mathcal{U}$ and trajectory $\{e^{-iH_j t} | t \geq 0\}$.

- $\mathcal{F}$ generates $\mathcal{L}$ (just like $\tilde{\mathcal{F}}$)
- With a piecewise constant control with values $u_1, \ldots, u_r$ a typical trajectory is

$$e^{-i\tilde{H}_r t_r} \cdots e^{-i\tilde{H}_2 t_2} e^{-i\tilde{H}_1 t_1},$$

with $-i\tilde{H}_1, \ldots, -i\tilde{H}_r \in \mathcal{F}$ and $t_1, \ldots, t_r > 0$.

Constructive Control Set-up (ctd.)

- Control problem: Given $X_f \in e^{\mathcal{L}}$ find a sequence of elements $-i\tilde{H}_k \in \mathcal{F}$ and $t_k > 0$ such that

$$X_f = \prod_{k=1}^{r} e^{-i\tilde{H}_k t_k}.$$

- Initially we are going to relax the requirement $t_k > 0$ and allow general $t_k \in R$.

Achieving More Exponentials

- $$\mathcal{F} := \{-iH_1, \ldots, -iH_m\}$$

  typically is not a basis of the dynamical Lie algebra $\mathcal{L}$. We want to be able to implement more exponentials of linearly independent matrices in $\mathcal{L}$.

- Assume span $\mathcal{F} \neq \mathcal{L}$. Since $\mathcal{F}$ generates $\mathcal{L}$, there exist indexes j and k such that

  $$[-iH_j, -iH_k] \qquad \text{linearly independent of } \mathcal{F}.$$

- Look at $H(t) := e^{-iH_j t} H_k e^{iH_j t}$, $t \in R$.
  There exists a $\bar{t} \in R$ such that $H(\bar{t})$ is linearly independent of $\mathcal{F}$.
  If this was not the case we would have $H(t) = -i \sum_{j=1}^{m} a_j(t) H_j$, for every t.
  This implies

  $$\frac{d}{dt} H(t)|_{t=0} := \frac{d}{dt} e^{-iH_j t} H_k e^{iH_j t}, |_{t=0} = [-iH_j, -iH_k] = -i \sum_{j=1}^{m} \dot{a}_j(0) H_j,$$

  which contradicts the assumption that $[-iH_j, -iH_k]$ is linearly independent of $\mathcal{F}$.

Achieving More Exponentials (ctd.)

- Define
$$-iH_{m+1} := H(\bar{t}) = e^{-iH_j\bar{t}}(-iH_k)e^{iH_j\bar{t}}.$$
$$\mathcal{F}_+ := \mathcal{F}\bigcup\{-iH_{m+1}\} = \{-iH_1, -iH_2, \ldots, -iH_m, -iH_{m+1}\}$$
is a linearly independent set in $\mathcal{L}$
- $\mathcal{F}_+$ generates $\mathcal{L}$.
- The exponential of $-iH_{m+1}$ can be expressed in terms of the available exponentials since
$$e^{-iH_{m+1}x} = e^{-iH_j\bar{t}}e^{-iH_kx}e^{iH_j\bar{t}}, \quad \forall x \in R.$$
- Therefore $\mathcal{F}_+$ can replace $\mathcal{F}$ and the procedure can be iterated.
- This way, we obtain a basis of $\mathcal{L}$,
$$\mathcal{S} := \{-iH_1, -iH_2, \ldots, -iH_m, -iH_{m+1}, \ldots, -iH_s\}, \quad s = \dim\mathcal{L},$$
and the exponential of every element of $\mathcal{S}$ can be expressed as the product of available exponentials.

Constructive Controllability Method 1

- The set

$$\mathcal{N} := \{e^{-iH_1t_1}e^{-iH_2t_2}\ldots e^{-iH_mt_m}e^{-iH_{m+1}t_{m+1}}\ldots e^{-iH_st_s}|t_1,\ldots t_s \in R\},$$

  is an open neighborhood of $\mathbf{1}$ in $e^{\mathcal{L}}$.
- Since $e^{\mathcal{L}}$ is compact the exponential map is *surjective*. Therefore, given $X_f \in e^{\mathcal{L}}$, we can choose $A \in \mathcal{L}$ so that $X_f = e^A$.
- for m sufficiently large $e^{\frac{A}{m}} \in \mathcal{N}$ and the equation

$$e^{\frac{A}{m}} = e^{-iH_1t_1}e^{-iH_2t_2}\ldots e^{-iH_mt_m}e^{-iH_{m+1}t_{m+1}}\ldots e^{-iH_st_s}, \qquad (1)$$

  has a solution.
- Method: Solve equation (1) for m sufficiently large. Then

$$X_f = e^A = \left[e^{-iH_1t_1}e^{-iH_2t_2}\ldots e^{-iH_mt_m}e^{-iH_{m+1}t_{m+1}}\ldots e^{-iH_st_s}\right]^m$$

Constructive Controllability Method 2

- Recall Calculus' limit (1^∞ indeterminate form)

$$\lim_{x\to\infty}\left(e^{\frac{k}{x}}+O\left(\frac{1}{x^{1+\delta}}\right)\right)^x=e^k,\quad \delta>0.$$

- Matrix version of this result (see e.g. [Horn-Johnson, TMA]) for a matrix A

$$\lim_{n\to\infty}\left(e^{\frac{A}{n}}+O\left(\frac{1}{n^{1+\delta}}\right)\right)^n=e^A,\quad \delta>0.$$

- If $X_f=e^A$, write

$$A=\sum_{j=1}^{s}a_j(-iH_j).$$

- Then

$$e^{\frac{A}{n}}=e^{\left(\sum_{j=1}^{s}a_j(-iH_j)\right)\frac{1}{n}}=\prod_{j=1}^{s}e^{-i\frac{a_jH_j}{n}}+O\left(\frac{1}{n^2}\right).$$

Constructive Controllability Method 2 (ctd)

- From

$$e^{\frac{A}{n}} = \prod_{j=1}^{s} e^{-i\frac{a_j H_j}{n}} + O\left(\frac{1}{n^2}\right),$$

  applying formula

$$\lim_{n \to \infty} \left(e^{\frac{A}{n}} + O\left(\frac{1}{n^{1+\delta}}\right)\right)^n = e^A, \quad \delta > 0,$$

  we have

$$\lim_{n \to \infty} \left[\prod_{j=1}^{s} e^{-i\frac{a_j H_j}{n}}\right]^n = e^A = X_f$$

- Method: Repeat $\prod_{j=1}^{s} e^{-i\frac{a_j H_j}{n}}$, n times, for n sufficiently large.

Method 2 Error analysis

- Formula

$$\lim_{n\to\infty}\left[\prod_{j=1}^{s} e^{\frac{A_j}{n}}\right]^n = e^{\sum_{j=1}^{s} A_j},$$

is *generalized Trotter formula*.

- Error can be obtained applying an induction to error formula known in the $s = 2$ case.
- Error formula is given, with $A = \sum_{j=1}^{s} A_j$, by

$$\left\| e^{A} - \left(\prod_{j=1}^{s} e^{\frac{A_j}{n}}\right)^n \right\| \leq \frac{1}{2n}\sum_{j=1}^{s-1}\left\| \left[\sum_{l=1}^{j} A_l \, , A_{j+1}\right] \right\|.$$

- Upper bound on error increases with the number of matrices used and the size of their commutators.
- Remark: The procedure allows for a lot of *flexibility* in the choices of the A_j's (which are the $-iH_j$) (e.g., the choice of the initial set $\mathcal{F}$, the choice of the similarity transformations at every step) which could be used to make this error small.

Constructive Controllability Method 3

- Method 3, like Method 2, uses formula

$$\lim_{n \to \infty} \left(e^{\frac{A}{n}} + O\left(\frac{1}{n^{1+\delta}} \right) \right)^n = e^A, \quad \delta > 0,$$

  but differs from Method 2 in the way e^{Ax} for x small is approximated.

- Starting from

$$\mathcal{F} := \{-iH_1, \ldots, -iH_m\},$$

  generate a basis of $\mathcal{L}$ by repeated Lie brackets of elements in $\mathcal{F}$,

$$\{-iH_1, \ldots, -iH_m, -iH_{m+1}, \ldots, -iH_s\}.$$

- Given $X_f = e^A$ expand A as

$$A = \sum_{j=1}^{s} a_j(-iH_j).$$

Constructive Controllability Method 3 (ctd)

- For x small (positive)

$$e^{Ax} = \prod_{j=1}^{s} e^{-ia_j H_j x} + O(x^{1+\delta}), \qquad \delta > 0. \qquad (3)$$

- If $-iH_j$ is one of the available one (i.e., it is in $\mathcal{F}$), then it can be implemented with the available exponentials.

- If $-iH_j \notin \mathcal{F}$, then $-iH_j = [B, C]$, for some B and C. Use the *exponential formula*

$$e^{-iH_j x} = e^{[B,C]x} = e^{-B\sqrt{x}} e^{-C\sqrt{x}} e^{B\sqrt{x}} e^{C\sqrt{x}} + O(x^{\frac{3}{2}}).$$

Constructive Controllability Method 3 (ctd)

- Iterate the process. Eventually, we obtain an approximation for e^{Ax} in terms of the original exponentials, i.e.,

$$e^{Ax} = \prod_{j=1}^{k} e^{-i\tilde{H}_j f_j(x)} + O(x^{1+\delta}),$$

for some functions f_j, $\delta > 0$ and $-i\tilde{H}_j \in \mathcal{F}$.

- From this we obtain

$$\lim_{n\to\infty} \left[\prod_{j=1}^{k} e^{-i\tilde{H}_j f_j(\frac{1}{n})} \right]^n = e^A = X_f.$$

- This method is more complicated than Method 2 and normally converges more slowly (number of iterations larger). However it may be more convenient in some cases and may lead to faster convergence in terms of time.

Summary

- I have proposed three methods for control of right invariant systems on compact Lie groups.
- All methods employ piecewise constant controls.
- The first method requires a finite (small) number of iterations of the same sequence of controls but also requires the solution of an algebraic equation. The other two methods require a (large) number of iterations of the same control sequence but present no mathematical difficulty.
- In all cases we have assumed that we can go both forward and backward in time (alternatively we have both H and $-H$ Hamiltonians available).

Exponentials e^{At} with $t < 0$

- If the elements of $\mathcal{F} := \{-iH_1, \ldots, -iH_m\}$ give periodic orbits $\{e^{-iH_j t} | t \in R\}$, then we can implement exactly $e^{-iH_j t_1}$, $t_1 < 0$ with $e^{-iH_j t_2}$ with $t_2 > 0$. To this purpose notice that
  - We have flexibility in choosing the matrices in $\mathcal{F}$ we begin with.
  - It is not necessary to choose a maximal linearly independent set, we only need an independent set which generates $\mathcal{L}$.
  - In fact, if the problem is to reach e^{At}, we only need to generate enough elements $-iH_j$, $j = 1, \ldots, f$, so as to write

$$A = \sum_{j=1}^{f} -ia_j H_j.$$

- We can use several methods in the physics literature to *cancel* the effect of an Hamiltonian $e^{-iHt} \rightarrow e^{-iH(-t)}$.
- *In any case* using the compactness of the Lie group $e^{\mathcal{L}}$, $e^{-A|t|}$ can be approximated with arbitrary accuracy with e^{At_1} with $t_1 > 0$.

Exponentials e^{At} with $t < 0$ (ctd)

- Original Argument [Jurdjevic-Sussmann, 1973]
  - Consider e^{At} and the sequence $\left\{e^{nA|t|}\right\}$.
  - By compactness of $e^{\mathcal{L}}$, $\left\{e^{nA|t|}\right\}$ has a converging subsequence $\{e^{n(k)A|t|}\}$.
  - Then, Consider the sequence $\left\{e^{n(k+1)A|t|-n(k)A|t|-A|t|}\right\}$

$$\lim_{k\to\infty} e^{n(k+1)A|t|-n(k)A|t|-A|t|} = e^{-A|t|}$$

- Given $x > 0$, we would like to have a constructive method to find $t > 0$ so that

$$e^{At} \approx e^{-Ax}, \qquad e^{A(t+x)} \approx \mathbf{1}$$

Exponentials e^{At} with $t < 0$ (ctd)

- Assume $\mathcal{L} \subseteq u(n)$ (Quantum Control Scenario).
- Using Frobenius norm $e^{A(t+x)} \approx \mathbf{1}$ if and only if

$$Tr\left(e^{A(t+x)} + e^{A^{\dagger}(t+x)}\right) \approx 2n \qquad (4)$$

- Fix $\epsilon > 0$ and let $i\omega_k$, $k = 1, \ldots, n$, denote the eigenvalues of A.
- Then condition (4) is verified if and only if

$$n - \sum_{k=1}^{n} \cos(\omega_k(t+x)) < \epsilon.$$

Exponentials e^{At} with $t < 0$ (ctd)

- This is certainly verified if we choose t so that

$$\cos(\omega_k(t+x)) > 1 - \frac{\epsilon}{n}, \quad k = 1, \ldots, n \Leftrightarrow |\omega_k(t+x) - 2\pi n_k| < \arccos(1 - \frac{\epsilon}{n}),$$

  for some integers n_k $k = 1, \ldots, n$.
- Equivalently define
  - $\alpha_k := \frac{\omega_k x}{2\pi}$,
  - $y := \frac{t+x}{x}$
  - $\epsilon' := \frac{\arccos(1-\frac{\epsilon}{n})}{2\pi}$
- Then given n numbers α_k, and (small) $\epsilon' > 0$ we want to choose $y \geq 1$ and k integers n_k such that

$$|\alpha_k y - n_k| < \epsilon'$$

Exponentials e^{At} with $t < 0$ (ctd)

- Dirichlet's approximation theorem of number theory:
  - Given n numbers α_k and an integer N there exist a positive integer y and n integers $n_1, \ldots, n_n$ such that
$$|\alpha_k y - n_k| < \frac{1}{N}.$$
  - Moreover $1 \leq y \leq N^n$.
- Therefore we can choose N so that $\frac{1}{N} < \epsilon'$ and we will have
$$|\alpha_k y - n_k| < \epsilon'.$$
- This looks like only an existence result. However we only need $y := \frac{t+x}{x}$ and we can obtain it (at least) with an exhaustive search since $1 \leq y \leq N^n$. Moreover $y \geq 1$ ensures that $t \geq 0$, as desired.
- There exist algorithms to calculate Dirichlet's approximation (i.e., the numbers y and n_k), cf. [B. Just, *SIAM J. Comput.* 1992]

Conclusions

- Presented three methods to obtain control of general systems on compact Lie groups to an arbitrary target. Notice the compactness of the Lie group $e^{\mathcal{L}}$ is used only in two places:
  - The exponential map is surjective ($X_f = e^A$).
  - We are able to approximate exponentials e^{At} with $t < 0$ with exponentials e^{At} with $t > 0$.
- Method 1 allows (possibly) to control exactly and in finite time but requires solving a (nonlinear) algebraic equation.
- Method 2 allows to control with arbitrary accuracy to any desired target and does not involve any mathematical difficulties.
- Method 3 differs from Method 2 in the way exponentials are generated.
- These methods allow the coherent control of closed quantum systems in every case.
- They provide an alternative constructive proof of the LARC
- On a case by case basis one may refine these methods to obtain, e.g., faster convergence in terms of time and-or number of switches.

Main Reference and Acknowledgments

The main reference of this talk is:

D. D'Alessandro, General Methods to control right-invariant systems on compact Lie groups and multilevel quantum systems, arXiv:0904.2793v1 [quant-ph].

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