

Lecture 5 – Controllability and reachability

Consider the evolution of a closed quantum system governed by Schrödinger's equation:

$$\frac{\partial}{\partial t} |\psi(t)\rangle = -i\mathbf{H}(t) |\psi(t)\rangle \quad (1)$$

where the Hamiltonian $\mathbf{H}(t)$ is a linear combination of the drift operator $\mathbf{H}_0$ and a number of control operators $\mathbf{H}_k$ whose coefficients $c_k(t)$ the instrument can vary:

$$\mathbf{H}(t) = \mathbf{H}_0 + \sum_{k=1}^K c_k(t) \mathbf{H}_k \quad (2)$$

In this lecture we will only consider unitary dynamics of closed quantum systems for which questions of controllability and reachability are mostly settled and convenient conditions exist.

1. Controllability types

In the context of Eqs (1) and (2), *state controllability* is the ability to drive the system from any initial state $|\psi_A\rangle$ to any final state $|\psi_B\rangle$ in the system's Hilbert space using control inputs. State controllability is achieved if, for any pair of states $|\psi_A\rangle$ and $|\psi_B\rangle$, there exists a set of functions $\{c_k(t)\}$ such that:

$$|\psi_B\rangle = \overleftarrow{\exp} \left[-i \int_0^T \mathbf{H}(t) dt \right] |\psi_A\rangle \quad (3)$$

where T is a finite experiment time and the time-ordered exponential notation is used for the propagator that performs the evolution. This definition may be extended to density matrices, in which case the time propagation rule is double-sided (see LvN equation lecture):

$$\rho_B = \mathbf{P} \rho_A \mathbf{P}^\dagger, \quad \mathbf{P} = \overleftarrow{\exp} \left[-i \int_0^T \mathbf{H}(t) dt \right] \quad (4)$$

A stronger condition is *full controllability*. The system is fully controllable if, for any unitary transformation $\mathbf{U}$ of its Hilbert space, there exists a set of functions $\{c_k(t)\}$ such that, for some experiment time T :

$$\overleftarrow{\exp} \left[-i \int_0^T \mathbf{H}(t) dt \right] = \mathbf{U} \quad (5)$$

It is clear from Eqs (3) and (5) that full controllability guarantees state controllability. However, state controllability may still exist in the absence of full controllability.

When a system is not state controllable, an important question is about which states (wavefunctions or density matrices) may be reached from a given starting point. The *reachable set* $\mathcal{R}(|\psi_A\rangle)$ of an initial wavefunction $|\psi_A\rangle$ is defined as the set of all wavefunctions of the form:

$$|\psi\rangle = \overleftarrow{\exp} \left[-i \int_0^T \mathbf{H}(t) dt \right] |\psi_A\rangle \quad (6)$$

for a given set of control operators and functions. Common situations where reachable sets are smaller than the full Hilbert space involve symmetries and conservation laws: a system that started its evolution in a particular symmetry, or with particular values of conserved quantities, will not be able to change those under a Hamiltonian that respects those symmetries and conservation laws.

2. Full controllability criterion

Consider the *dynamical Lie algebra* $\mathfrak{g}$ of the system (using the physicists' $\exp[-i\mathbf{A}]$ exponential map) spanned by the set of all nested commutators of the drift and the control operators:

$$\mathfrak{g} = \text{Lie}\{\mathbf{H}_0, \mathbf{H}_1, \dots, \mathbf{H}_K\} \quad (7)$$

The structure of $\mathfrak{g}$ determines the controllability of the system. In particular, if $\mathfrak{g}$ is equal to the dynamical algebra of the system – $\mathfrak{su}(n)$ for a quantum system with n energy levels and traceless Hamiltonians – then the system is fully controllable.

2.1 Example 1: spin-½ under Zeeman controls

The Lie algebra of a spin-½ particle is $\mathfrak{su}(2)$; it is spanned by the three spin operators $\{\mathbf{S}_x, \mathbf{S}_y, \mathbf{S}_z\}$. The following situations are encountered in magnetic resonance systems:

1. Static external field with X and Y control:

$$\mathbf{H}_0 = \omega_0 \mathbf{S}_z, \quad \mathbf{H}_1 = \mathbf{S}_x, \quad \mathbf{H}_2 = \mathbf{S}_y \quad (8)$$

The system is fully controllable because $\{\mathbf{H}_0, \mathbf{H}_1, \mathbf{H}_2\}$ are already the basis set of $\mathfrak{su}(2)$.

2. Static external field with X control only:

$$\mathbf{H}_0 = \omega_0 \mathbf{S}_z, \quad \mathbf{H}_1 = \mathbf{S}_x \quad (9)$$

The system is still fully controllable because $[\mathbf{S}_z, \mathbf{S}_x] = i\mathbf{S}_y$, and the set of nested commutators of does therefore still span $\mathfrak{su}(2)$.

3. Static external field with Z control only:

$$\mathbf{H}_0 = \omega_0 \mathbf{S}_z, \quad \mathbf{H}_1 = \mathbf{S}_z \quad (10)$$

The system is not fully controllable because commutators of $\mathbf{H}_0$ and $\mathbf{H}_1$ do not produce $\mathbf{S}_x$ or $\mathbf{S}_y$ and therefore do not span $\mathfrak{su}(2)$.

2.1 Example 2: J -coupled ^1H - ^{13}C system

The dynamical Lie algebra of a J -coupled ^1H - ^{13}C system is $\mathfrak{su}(4)$, its generators are:

	$\mathbf{S}_x$	$\mathbf{S}_y$	$\mathbf{S}_z$
$\mathbf{L}_x$	$\mathbf{L}_x \mathbf{S}_x$	$\mathbf{L}_x \mathbf{S}_y$	$\mathbf{L}_x \mathbf{S}_z$
$\mathbf{L}_y$	$\mathbf{L}_y \mathbf{S}_x$	$\mathbf{L}_y \mathbf{S}_y$	$\mathbf{L}_y \mathbf{S}_z$
$\mathbf{L}_z$	$\mathbf{L}_z \mathbf{S}_x$	$\mathbf{L}_z \mathbf{S}_y$	$\mathbf{L}_z \mathbf{S}_z$

It is clear from this table that, in the absence of J -coupling, the system is not fully controllable because commutators within the set $\{\mathbf{L}_x, \mathbf{L}_y, \mathbf{L}_z, \mathbf{S}_x, \mathbf{S}_y, \mathbf{S}_z\}$ are all single-spin operators:

$$[\mathbf{L}_i, \mathbf{L}_j] = \varepsilon_{ijk} \mathbf{L}_k, \quad [\mathbf{S}_i, \mathbf{S}_j] = \varepsilon_{ijk} \mathbf{S}_k, \quad [\mathbf{L}_i, \mathbf{S}_j] = 0 \quad (11)$$

Consider then the following drift Hamiltonian (Zeeman offsets and a weak J -coupling):

$$\mathbf{H}_0 = \omega_L \mathbf{L}_z + \omega_S \mathbf{S}_z + 2\pi J \mathbf{L}_z \mathbf{S}_z \quad (12)$$

and the following control sets:

1. Two-channel (X and Y) controls on both ^1H and ^{13}C :

$$\mathbf{H}_1 = \mathbf{L}_X, \quad \mathbf{H}_2 = \mathbf{L}_Y, \quad \mathbf{H}_3 = \mathbf{S}_X, \quad \mathbf{H}_4 = \mathbf{S}_Y \quad (13)$$

The system is fully controllable because $[\mathbf{L}_Z \mathbf{S}_Z, \mathbf{L}_X] = i\mathbf{L}_Y \mathbf{S}_Z$ etc., and the two-spin part of the generator table is contained within the set of nested commutators of drift and controls.

2. One channel (X or Y) controls on both ^1H and ^{13}C , for example:

$$\mathbf{H}_1 = \mathbf{L}_X, \quad \mathbf{H}_2 = \mathbf{S}_X \quad (14)$$

Still fully controllable because $[\mathbf{L}_Z, \mathbf{L}_X] = i\mathbf{L}_Y$ and likewise for the other spin. As a result, the Y operators reappear and the problem becomes identical to Case 1 above.

3. One or two controls on just one spin, for example:

$$\mathbf{H}_1 = \mathbf{L}_X, \quad \mathbf{H}_2 = \mathbf{L}_Y \quad (15)$$

Restricted controllability: fully controllable with respect to the state of spin L, but not fully controllable as a system because nested commutators of $\{\mathbf{H}_0, \mathbf{H}_1, \mathbf{H}_2\}$ do not contain two-spin operators where spin S is transverse.

3. Sørensen bound

A convenient best-case bound for the maximum unitary transfer efficiency between two density matrices under any conceivable control sequence was given in the context of NMR spectroscopy by Ole W. Sørensen in 1989 (see Eq 186 in [https://doi.org/10.1016/0079-6565\(89\)80006-8](https://doi.org/10.1016/0079-6565(89)80006-8)). To derive the bound, we first need to consider a simple lemma.

Sørensen's lemma: Consider two n -dimensional real vectors $\mathbf{a}$ and $\mathbf{b}$, written in a basis chosen so that $a_1 \geq a_2 \geq a_3 \geq \dots \geq a_n$. Then, among the set of element permutations of the $\mathbf{b}$ vector, the permutation with the largest inner product with $\mathbf{a}$ is the one where also $b_1 \geq b_2 \geq b_3 \geq \dots \geq b_n$. **Proof:** no time.

Now we proceed to derive the bound itself. Let $\mathbf{A}$ be the initial density matrix and let $\mathbf{D}$ be the desired part (whose contribution we seek to maximise) of the final density matrix $\mathbf{F}$:

$$\mathbf{F} = \alpha \mathbf{D} + \beta \mathbf{G}, \quad \text{Tr}(\mathbf{D}^\dagger \mathbf{G}) = 0 \quad (16)$$

We assume that $\mathbf{F}$ is produced at the end of an experiment in which we are not restricted in the choice or amplitudes of control operators – and can therefore produce any unitary transformation. In Eq (16), $\mathbf{G}$ is “garbage” that is orthogonal to the desired state (with respect to the Frobenius inner product, as indicated) and α is the coefficient that we seek to maximise; it can only be real because all matrices in this discussion are Hermitian – therefore diagonalisable with real eigenvalues.

We start by picking a basis in which $\mathbf{A}$ is diagonal and its eigenvalues are sorted in the order prescribed by Sørensen's lemma; in practice we need to diagonalise it and reorder the eigenvector array $\mathbf{V}$:

$$\text{diag}(\mathbf{a}) = \mathbf{V} \mathbf{A} \mathbf{V}^{-1} \quad (17)$$

where $\mathbf{a}$ is now a vector of eigenvalues of $\mathbf{A}$ sorted so that $a_1 \geq a_2 \geq a_3 \geq \dots \geq a_n$. We then ask what is the unitary evolution operator $\mathbf{U}$ acting on $\mathbf{A}$ that would maximise the overlap $\text{Tr}(\mathbf{D}^\dagger \mathbf{U} \mathbf{A} \mathbf{U}^{-1})$ of the evolved density matrix $\mathbf{U} \mathbf{A} \mathbf{U}^{-1}$ with the desired density matrix $\mathbf{D}$.

After noting that $\mathbf{D}^\dagger = \mathbf{D}$ and rotating the matrix product under the trace, we obtain $\text{Tr}(\mathbf{U}^{-1}\mathbf{D}\mathbf{U}\mathbf{A})$ where (as per our initial assumption), $\mathbf{U}$ is an arbitrary unitary transformation. We may choose it to be such as to use Sørensen's lemma again, and thus the overlap becomes $\langle \mathbf{a} | \mathbf{d} \rangle$ where $\mathbf{d}$ is a vector of the eigenvalues of the desired density matrix:

$$\text{diag}(\mathbf{d}) = \mathbf{W}\mathbf{D}\mathbf{W}^{-1} \quad (18)$$

sorted so that $d_1 \geq d_2 \geq d_3 \geq \dots \geq d_n$. Finally we note that $\mathbf{D}$ need not be normalised (valid density matrices have a unit trace but not necessarily a unit norm), and therefore the expression for $\alpha_{\max}$ acquires a denominator where the Frobenius norm $\sqrt{\langle \mathbf{d} | \mathbf{d} \rangle}$ occurs twice: once to normalise $\mathbf{D}$ in the inner product, and another time to normalise it in the expansion in Eq (16). Therefore, finally:

$$a_{\max} = \langle \mathbf{a} | \mathbf{d} \rangle / \langle \mathbf{d} | \mathbf{d} \rangle \quad (19)$$

This is called *Sørensen bound*; it is very optimistic (we have assumed operator controllability) and rarely in practice achievable, except in the smallest systems. It also assumes unitary evolution and may therefore break in dissipative systems.

4. Literature

1. Ramakrishna, Viswanath, Murti V. Salapaka, Mohammed Dahleh, Herschel Rabitz, and Anthony Peirce, "Controllability of molecular systems", Physical Review A 51, no. 2 (1995): 960.
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