Majorization in Quantum Control

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Outline

- Brief introduction to majorization
- Characterize majorization monotone dynamics
- Majorization in time optimal quantum control.

Definition of Majorization

Definition: $\forall x, y \in R^n$, x majorized by y($x \prec y$) means

$$x_1^{\downarrow} \leq y_1^{\downarrow}$$

$$x_1^{\downarrow} + x_2^{\downarrow} \leq y_1^{\downarrow} + y_2^{\downarrow}$$

$$\vdots$$

$$\sum_{i=1}^{n-1} x_i^{\downarrow} \leq \sum_{i=1}^{n-1} y_i^{\downarrow}$$

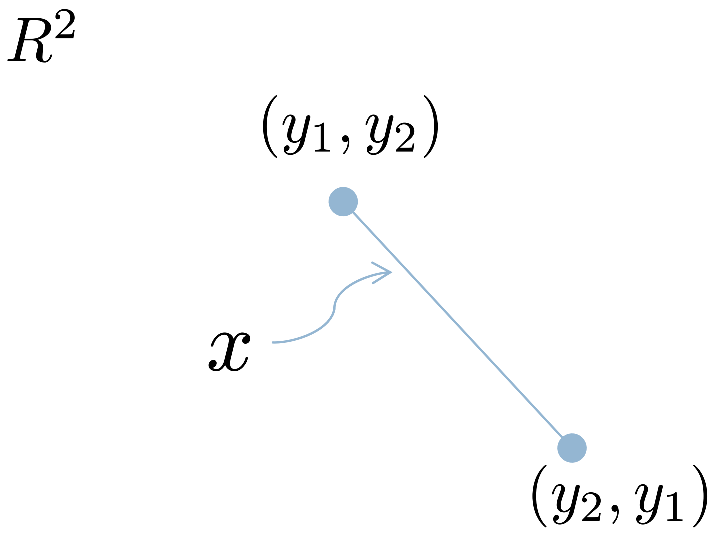
$$\sum_{i=1}^{n} x_i^{\downarrow} = \sum_{i=1}^{n} y_i^{\downarrow}$$

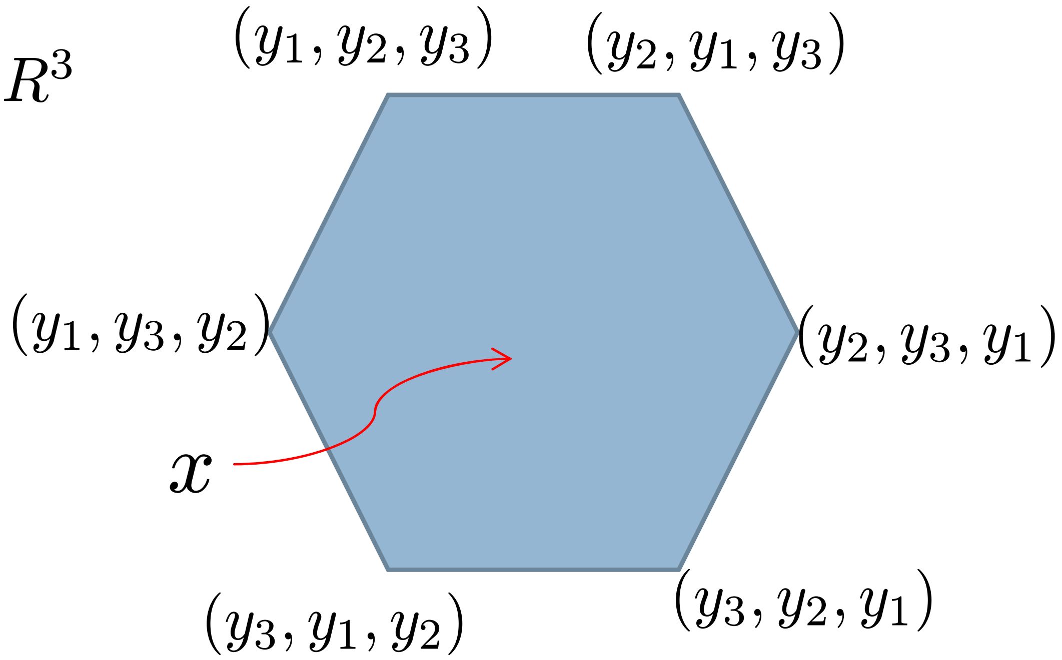
$\{x_1^{\downarrow}, x_2^{\downarrow}, \cdots, x_n^{\downarrow}\}$ is a permutation of $\{x_1, x_2, \cdots, x_n\}$ so that

$$x_1^{\downarrow} \geq x_2^{\downarrow} \geq \cdots \geq x_n^{\downarrow}$$

Geometrically

$x \prec y$ means x lies in the convex hull of all the permutations of y





Some properties of majorization

Proposition 1: $x \prec y$ if and only if

$$x = Dy$$

where D is doubly stochastic matrix:

$$d_{ij} \geq 0 \qquad \sum_i d_{ij} = 1 \qquad \sum_j d_{ij} = 1$$

Proposition 2: if $x \prec y$, and f is a convex (concave) function, then

$$\sum_i f(x_i) \leq \sum_i f(y_i) \qquad (\qquad \sum_i f(x_i) \geq \sum_i f(y_i) \qquad)$$

Ex: if $x \prec y$ are both probability vectors, and $f(\alpha) = -\alpha log(\alpha)$ which is concave, then $H(x) \geq H(y)$, where $H(x) = \sum_i -x_i log(x_i)$ is the Shannon entropy of probability distribution x.

Majorization of density matrix

ρ_1 is majorized by ρ_2 if $\lambda(\rho_1) \prec \lambda(\rho_2)$

Von Neumann entropy: The Von Neumann entropy of a density matrix is defined as

$$S(\rho) = -Tr(\rho log(\rho))$$

$$\lambda(\rho_1) \prec \lambda(\rho_2) \Longrightarrow \begin{array}{l} S(\rho_1) \geq S(\rho_2) \\ Tr(\rho_1^2) \leq Tr(\rho_2^2) \end{array}$$

$$\lambda(\rho_1) \prec \lambda(\rho_2) \Longleftrightarrow \rho_1 = \sum_i p_i U_i \rho_2 U_i^\dagger$$

Majorization monotone dynamics

$$\tfrac{d}{dt}\rho = -i[H,\rho] + L(\rho)$$

$$L(\rho) = \textstyle\sum_{i,j} a_{ij}(F_i \rho F_j^\dagger - \tfrac{1}{2}F_j^\dagger F_i \rho - \tfrac{1}{2}\rho F_j^\dagger F_i)$$

$$i, j \in \{1, 2, ..., N^2 - 1\}$$

$F_\alpha, \alpha \in \{1, 2, ..., N^2 - 1\}$ forms a basis of $N \times N$ trace 0 matrices

$A = (a_{ij})$ is positive semi-definite, $(N^2 - 1) \times (N^2 - 1)$ matrix

$$\lambda(\rho(t_2)) \prec \lambda(\rho(t_1)) \quad \text{when } t_2 > t_1$$

Necessary condition: $\frac{1}{N}I$ is a steady state, i.e., $L(\frac{1}{N}I) = 0$

Sufficient?

Is entropy monotone?

Suppose $L(\frac{1}{N}I) = 0$, is entropy monotone increasing?

Relative entropy:

$$S(\rho|\sigma) = Tr(\rho log \rho) - Tr(\rho log \sigma)$$

Take $\sigma = \frac{1}{N}I$

$$S(\rho|\sigma) = Tr(\rho log \rho) - log \frac{1}{N} Tr \rho$$

$$= -S(\rho) + log N$$

$S(\rho(t_2)|\frac{1}{N}I) \leq S(\rho(t_1)|\frac{1}{N}I)$ when $t_2 > t_1$?

It is!

$$S(\rho(t_2)|\frac{1}{N}I) = S(Tr_E[U_{t_2-t_1}\rho(t_1) \otimes \rho_E U^{\dagger}_{t_2-t_1}]|Tr_E[U_{t_2-t_1}\frac{1}{N}I \otimes \rho_E U^{\dagger}_{t_2-t_1}])$$

$$\leq S(U_{t_2-t_1}\rho(t_1) \otimes \rho_E U^{\dagger}_{t_2-t_1}|U_{t_2-t_1}\frac{1}{N}I \otimes \rho_E U^{\dagger}_{t_2-t_1})$$

$$= S(\rho(t_1) \otimes \rho_E|\frac{1}{N}I \otimes \rho_E)$$

$$= S(\rho(t_1)|\frac{1}{N}I)$$

⇒ $S(\rho(t_2)) \geq S(\rho(t_1))$

What are the conditions for L(I)=0?

$$L(\rho) = \sum_{i,j} a_{ij}\left(F_i \rho F_j^\dagger - \tfrac{1}{2} F_j^\dagger F_i \rho - \tfrac{1}{2} \rho F_j^\dagger F_i\right)$$

Choose $F_\alpha, \alpha \in \{1, 2, ..., N^2 - 1\}$ as a basis of $su(N)$

$$L(I) = 0 \Rightarrow \sum_{i,j} a_{ij}(F_j F_i - F_i F_j) = \sum_{i,j} a_{ij}[F_j, F_i] = \sum_{i,j,k} a_{ij} C_{jik} F_k = 0$$

In the single spin case:

$$F_1 = \tfrac{1}{\sqrt{2}}\sigma_x \qquad F_2 = \tfrac{1}{\sqrt{2}}\sigma_y \qquad F_3 = \tfrac{1}{\sqrt{2}}\sigma_z$$

$$L(I) = 0 \Rightarrow a_{ij} = a_{ji}$$

$\Rightarrow$ $A = (a_{ij})$ is real symmetric, positive semidefinite

Single spin case

$$\rho(t) = U(t)\begin{pmatrix} \frac{1}{2}+\lambda(t) & 0 \\ 0 & \frac{1}{2}-\lambda(t) \end{pmatrix} U^\dagger(t)$$

$$U \in SU(2)$$

$$\lambda \in [0, \tfrac{1}{2}]$$

$$\dot{\lambda} = -(a'_{11}(t) + a'_{22}(t))\lambda$$

$$A'(t) = O^T(t) A O(t) \qquad O = Ad(U) \in SO(3)$$

⇒ $\lambda(t_2) \leq \lambda(t_1)$ when $t_2 > t_1$

$\lambda(\rho(t_2)) \prec \lambda(\rho(t_1))$ when $t_2 > t_1$

Compute reachable set of controlled single spin

$$\tfrac{d}{dt}\rho = -i[H_0 + \textstyle\sum_i u_i H_i, \rho] + L(\rho)$$

$$\rho(t) = U(t) \begin{pmatrix} \frac{1}{2} + \lambda(t) & 0 \\ 0 & \frac{1}{2} - \lambda(t) \end{pmatrix} U^\dagger(t)$$

$$\dot{\lambda} = -(a'_{11}(t) + a'_{22}(t))\lambda$$

$$A'(t) = O^T(t) A O(t) \qquad \{O(t) = Ad(U(t))\} = SO(3)$$

A useful mathematical theorem

Theorem: If A is a symmetrical matrix with eigenvalues $\lambda_i, i \in \{1, 2, ..., n\}$,

then the diagonal of A is majorized by its eigenvalues, i.e.,

$$\underline{(a_{11}, a_{22}, ..., a_{nn}) \prec (\lambda_1, \lambda_2, ..., \lambda_n)}$$

Furthermore, $\forall (a'_{11}, a'_{22}, ..., a'_{nn}) \prec (\lambda_1, \lambda_2, ..., \lambda_n),$

$\exists O \in SO(n),$ such that the diagonal entries of $A' = O^T A O$ is $(a'_{11}, a'_{22}, ..., a'_{nn})$.

Reachable set of controlled single spin

$$\dot{\lambda} = -(a'_{11}(t) + a'_{22}(t))\lambda$$

$$A'(t) = O^T(t)AO(t) \qquad \{O(t) = Ad(U(t))\} = SO(3)$$

$\mu_1 \geq \mu_2 \geq \mu_3$ are eigenvalues of A

$$(a'_{11}, a'_{22}, a'_{33}) \prec (\mu_1, \mu_2, \mu_3)$$

$$\mu_3 + \mu_2 \leq a'_{11} + a'_{22} \leq \mu_2 + \mu_1$$

$$\lambda(T) \in [e^{-(\mu_1+\mu_2)T}\lambda(0), e^{-(\mu_2+\mu_3)T}\lambda(0)]$$

Reachable set of controlled single spin

The reachable set at time T for the density matrix of single spin is:

$$U \begin{pmatrix} \frac{1}{2} + \lambda(T) & 0 \\ 0 & \frac{1}{2} - \lambda(T) \end{pmatrix} U^\dagger$$

where $U \in SU(2)$

$$\lambda(T) \in [e^{-(\mu_1+\mu_2)T}\lambda(0), e^{-(\mu_2+\mu_3)T}\lambda(0)]$$

General case

$$\frac{d}{dt}\rho = -i[H,\rho] + L(\rho)$$

$$L(\rho) = \sum_{i,j} a_{ij}(F_i \rho F_j^\dagger - \tfrac{1}{2}F_j^\dagger F_i \rho - \tfrac{1}{2}\rho F_j^\dagger F_i)$$

$$\rho(t_2) = \sum_i V_i \rho(t_1) V_i^\dagger \qquad \sum_i {V_i}^\dagger V_i = I$$

$$L(I) = 0 \quad \Longrightarrow \quad \sum_i V_i {V_i}^\dagger = I$$

$$\rho(t_1) = U_1 Diag(\lambda(\rho(t_1))U_1^\dagger$$

$$\rho(t_2) = U_2 Diag(\lambda(\rho(t_2))U_2^\dagger$$

$$Diag(\lambda(\rho(t_2))) = \sum_i V_i' Diag(\lambda(\rho(t_1)))V_i'^\dagger$$

where $V_i' = U_2^\dagger V_i U_1$ $\qquad \sum_i V_i'^\dagger V_i' = I$ $\qquad \sum_i V_i' V_i'^\dagger = I$

General Case

$$Diag(\lambda(\rho(t_2))) = \sum_i V_i' Diag(\lambda(\rho(t_1))) V_i'^\dagger$$

⇒ $\lambda(\rho(t_2)) = D\lambda(\rho(t_1))$ **where** $D_{\alpha\beta} = \sum_i |(V_i')_{\alpha\beta}|^2$

$$\sum_i V_i'^\dagger V_i' = I \qquad \sum_i V_i' V_i'^\dagger = I$$

⇒ D is doubly stochastic matrix.

⇒ $\lambda(\rho(t_2)) \prec \lambda(\rho(t_1))$

$L(I) = 0$ ⟺ Majorization monotone

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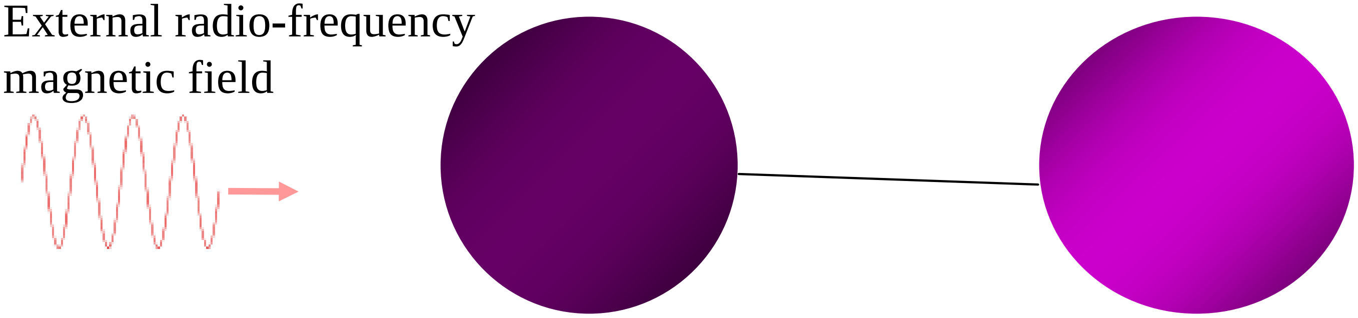
- Characterize majorization monotone dynamics
- Majorization in time optimal quantum control.

Two Spin System

External radio-frequency magnetic field



$$H_0 = \sum_{\alpha,\beta\in\{x,y,z\}} J_{\alpha\beta}(t)\sigma_\alpha \otimes \sigma_\beta$$

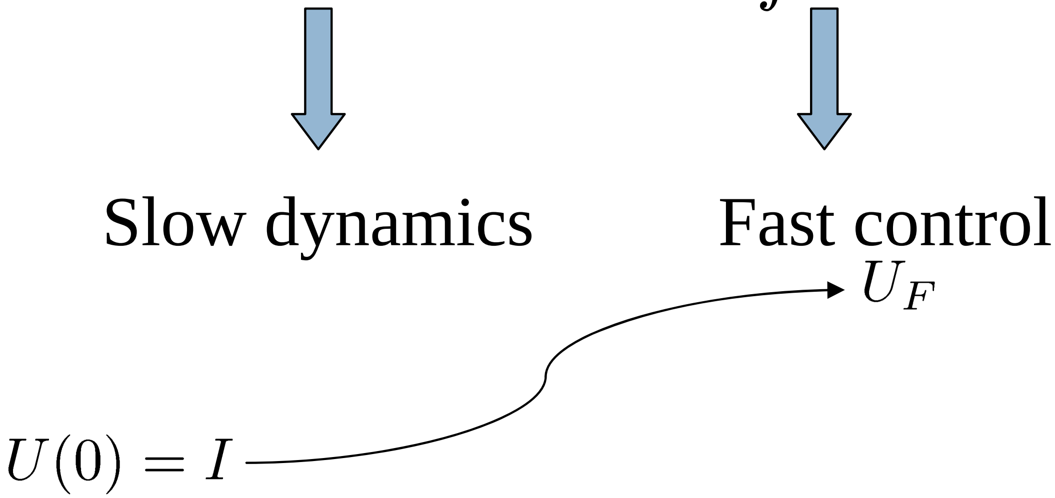
$$H_{rf}(t) = u_1(t)\sigma_x \otimes I + u_2(t)\sigma_y \otimes I + v_1(t) I \otimes \sigma_x + v_2(t) I \otimes \sigma_y$$

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad \mathbf{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Two Spin System

- Given any unitary matrix U in SU(4), find the minimum time that it can be generated
- Find all the unitary matrices in SU(4) that can be reached within any time T.

$$\frac{d}{dt}U(t) = -i[H_0(t) + H_{rf}(t)]U(t)$$



Slow dynamics

Fast control

U_F

$U(0) = I$

Choose a basis

$$\begin{matrix} |00\rangle & |01\rangle \\ |10\rangle & |11\rangle \end{matrix} \quad \Longrightarrow \quad \begin{matrix} \frac{|00\rangle+|11\rangle}{\sqrt{2}} & i\frac{|00\rangle-|11\rangle}{\sqrt{2}} \\ i\frac{|01\rangle+|10\rangle}{\sqrt{2}} & \frac{|01\rangle-|10\rangle}{\sqrt{2}} \end{matrix}$$

$$SU(2) \otimes SU(2) \quad \Longrightarrow \quad SO(4)$$

$$H_0 = \sum_{\alpha,\beta \in \{x,y,z\}} J_{\alpha\beta}(t)\sigma_\alpha \otimes \sigma_\beta \quad \Longrightarrow \quad \text{real symmetric}$$

Compute the reachable Set

$$\frac{d}{dt}U(t) = -i[H_0(t) + \sum_i u_i(t)H_i]U(t)$$

$$U = S_1 Diag(\psi_1, \psi_2, \psi_3, \psi_4)S_2 \qquad S_1, S_2 \in SO(4)$$

$$\frac{d}{dt}Diag(\psi_1, \psi_2, \psi_3, \psi_4) = -iDiag(SH_0S^T)Diag(\psi_1, \psi_2, \psi_3, \psi_4) \qquad S \in SO(4)$$

Result for two spin systems

$$\frac{dU}{dt} = -i[\sum_{\alpha,\beta} J_{\alpha\beta}(t)\sigma_\alpha \otimes \sigma_\beta + u_1\sigma_x \otimes I + u_2\sigma_y \otimes I + u_3 I \otimes \sigma_x + u_4 I \otimes \sigma_y]U$$

$$J(t) = \begin{pmatrix} J_{xx}(t) & J_{xy}(t) & J_{xz}(t) \\ J_{yx}(t) & J_{yy}(t) & J_{yz}(t) \\ J_{zx}(t) & J_{zy}(t) & J_{zz}(t) \end{pmatrix}$$

Singular values: $s_1(t) \geq s_2(t) \geq s_3(t)$

$$\alpha_1(t) = s_1(t),\ \alpha_2(t) = s_2(t),\ \alpha_3(t) = sgn(det(J(t)))s_3(t)$$

$$\boxed{\mu(T) = [\int_0^T \alpha_1(\tau)d\tau, \int_0^T \alpha_2(\tau)d\tau, \int_0^T \alpha_3(\tau)d\tau]}$$

Result for two spin systems

Theorem: The reachable set for the control system

$$\frac{dU}{dt} = -i[\sum_{\alpha,\beta} J_{\alpha\beta}(t)\sigma_\alpha \otimes \sigma_\beta + u_1\sigma_x \otimes I + u_2\sigma_y \otimes I + u_3 I \otimes \sigma_x + u_4 I \otimes \sigma_y]U$$

within time T are the set

$$K_1 \exp(iY)K_2 : \; K_1, K_2 \in SU(2) \otimes SU(2)$$

$$Y = c_1\sigma_x \otimes \sigma_x + c_2\sigma_y \otimes \sigma_y + c_3\sigma_z \otimes \sigma_z,$$

$$c_1 \geq c_2 \geq |c_3|$$

$$\left.\begin{array}{c} c_1 \leq \mu_1(T) \\ c_1 + c_2 - c_3 \leq \mu_1(T) + \mu_2(T) - \mu_3(T) \\ c_1 + c_2 + c_3 \leq \mu_1(T) + \mu_2(T) + \mu_3(T) \end{array}\right\} \quad (c_1, c_2, c_3) \prec_s \mu(T)$$

Result for two spin systems

Given a two-spin operator $U \in SU(4)$

$$U = K_1 e^{i(c_1 \sigma_x \otimes \sigma_x + c_2 \sigma_y \otimes \sigma_y + c_3 \sigma_z \otimes \sigma_z)} K_2$$

$$K_1, K_2 \in SU(2) \otimes SU(2)$$

$$\tfrac{\pi}{4} \geq c_1 \geq c_2 \geq |c_3|$$

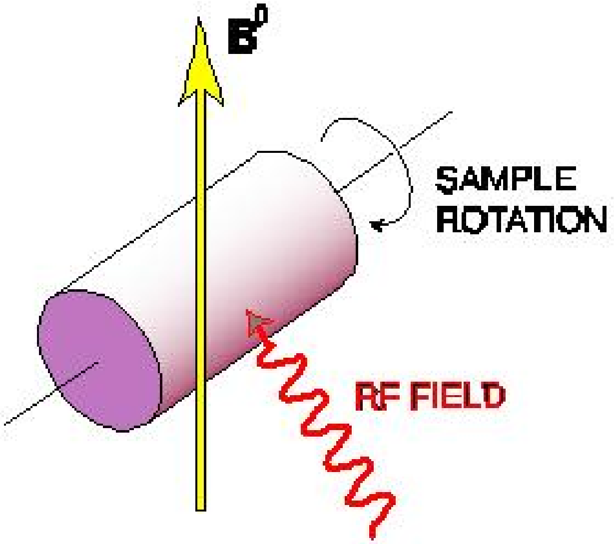
The minimum time required to simulate U is given by the minimum value of T such that either

$$(c_1, c_2, c_3) \prec_s \mu(T)$$

or $(c_1, c_2, c_3) + \frac{\pi}{2}(-1, 0, 0) \prec_s \mu(T)$ holds

Example: Solid State NMR

$$H_0(t) = D(t)(\sigma_x \otimes \sigma_x + \sigma_y \otimes \sigma_y - 2\sigma_z \otimes \sigma_z)$$

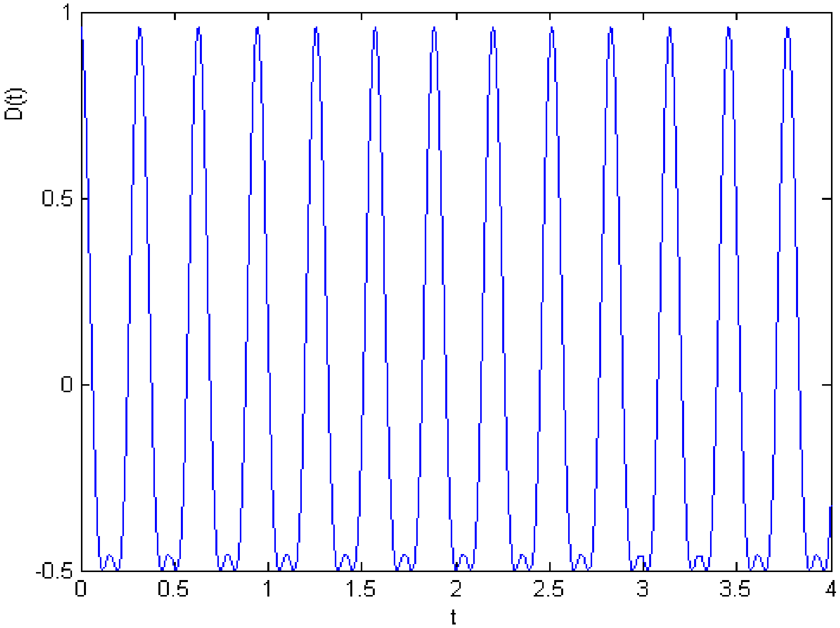


Swap gate

$$U = e^{-i\frac{\pi}{4}(\sigma_x\otimes\sigma_x+\sigma_y\otimes\sigma_y+\sigma_z\otimes\sigma_z)}$$

The minimum time to generate U is the minimum time T satisfies:

$$\frac{3\pi}{4} \leq \int_0^T 3|D(t)| - D(t)dt$$



Conclusion

Majorization is useful!