When Gauss Met Bernoulli
– how differential geometry solves time-optimal quantum control

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(arXiv:1408.2465)


Louisiana State University, March 6, 2015

Our main results

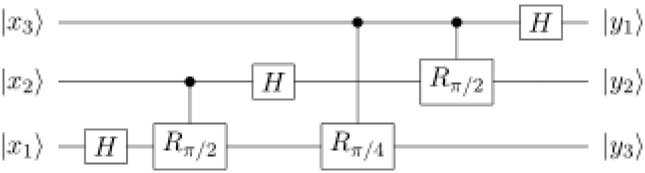
For a quantum system under two common constraints:

- the system has a finite energy bandwidth;
- only certain forms of the Hamiltonian can be physically generated,

we

- established the connection between the time-minimal (brachistochrone) and the distance-minimal(geodesics) curves;
- developed an efficient numerical method that can solve the time-optimal boundary value problem which otherwise cannot be solved by conventional methods for high dimensions;
- utilize Pontryagin maximum principle to answer the question when the time-optimal control can be solved in this way, and when it cannot. (Drift case and drift-free case)

Gate generation and optimal control



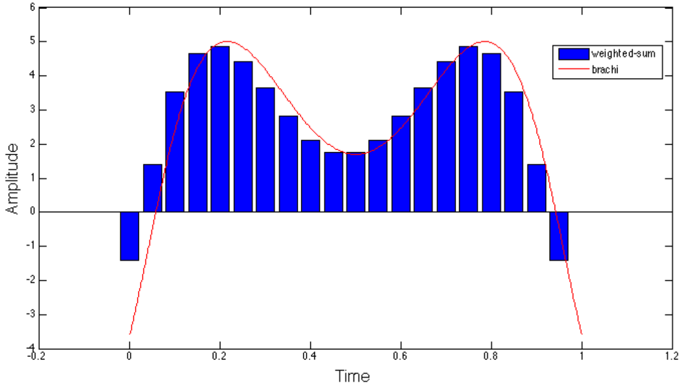
Under the dynamics:

$$\dot{U}(t) = -\frac{i}{\hbar}(H_0 + H_c(t))U(t)$$
$$H_c(t) = \sum_k u_k(t)H_k$$

we hope to find the control protocol $\mathbf{u}(t)$, s.t.:

$$\max \mathcal{J} = Fi(U(t_f), U_d),$$
$$\text{where } U(t_f) = U(t_f)[\mathbf{u}^{(1)}, \mathbf{u}^{(2)}, \cdots, \mathbf{u}^{(m)}]$$

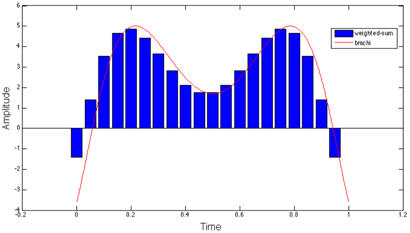
Gate generation and optimal control:CNOT



$$\max \mathcal{J} = Fi(U(t_f), U_d),$$

$$\text{where } U(t_f) = U(t_f)[\mathbf{u}^{(1)}, \mathbf{u}^{(2)}, \cdots, \mathbf{u}^{(m)}]$$

Time-optimal control: max *Fi* and min *T*



$$\min \mathcal{J} = -Fi(U(t_f), U_d) + \alpha \int_0^{t_f} dt,$$

where $U(t_f) = U(t_f)[\mathbf{u}^{(1)}, \mathbf{u}^{(2)}, \cdots, \mathbf{u}^{(m)}]$

Drawback: this is only an approximated time-optimal solution.
Question: can we characterize the accurate time-optimal solution?

- Quantum brachistochrone equation(A. Carlini, 2006);
- Quantum computation as geometry (M. Nielsen, 2006)

Motivation for studying time-optimal problems

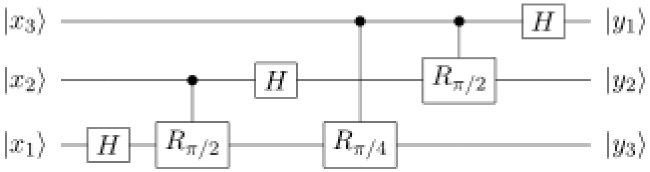
Why do we care about time-optimal problem?

"Better three hours too soon, than one minute too late."

— William Shakespeare

- to reduce noise and increase fidelity;
- to study the complexity problem;
- to challenge ourself and challenge other colleagues.

e.g. Quantum Fourier Transform: $\mathcal{O}(n^2)$, can be improved to: $\mathcal{O}(n \log n)$.



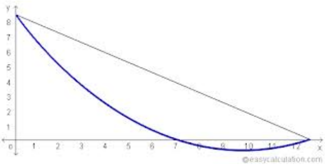
Main characters of the story

Figure: Johann Bernoulli, 1667-1748

Figure: Carl Friedrich Gauss, 1777-1855

Shortest time v.s. shortest distance

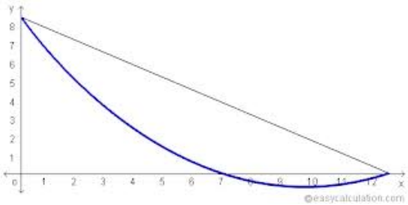
- Bernoulli: given points A and B in a vertical plane, what is the curve that an object travels from A to B in the shortest time? – Brachistochrone curve: cycloid.



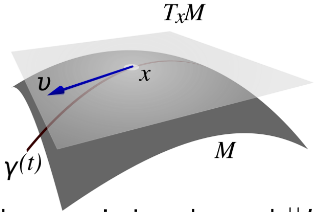
- Gauss: what is the shortest curve that connects A and B on a given manifold? – Geodesic equation.
- Imagine through time travel, Bernoulli and Gauss sit together discussing math problems:
  When does the shortest-time curve coincide with the shortest-distance curve?

Brachistochrone curve

- By definition, brachistochrone curve is the time-minimal path.
- $V = -mgy = -T = -\frac{1}{2}mv^2$, $v = \sqrt{2gy}$.
- $$\int dt = \int \frac{ds}{v} = \int \frac{\sqrt{1 + \left(\frac{dy}{dx}\right)^2}}{\sqrt{2gy}} dx = \int f(\frac{dy}{dx}, y) dx$$
- Apply Euler-Lagrange equation: The curve is a cycloid.



Time-optimal quantum gate generation on $\mathrm{SU}(n)$



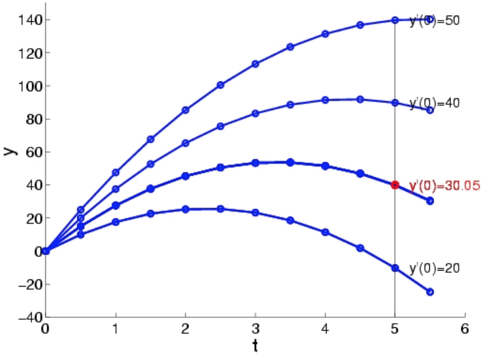
- Case 1: no further restrictions beyond $||H(t)|| \leq E$, the time-optimal solution: $H(t) \equiv \bar{H}$.
- Case 2: $H(t) \in \mathcal{A}$, i.e., $f_k(H) = \mathrm{Tr}(HB_k) = 0$, $B_k \in \mathcal{B}$, forbidden space.
  Brachistochrone equation(A. Carlini, PRL 96, 060503 (2006)):

$$\dot{H} + \sum_k \dot{\lambda}_k B_k = -i \sum_k \lambda_k [H, B_k],$$
$$\dot{U} = -\frac{i}{\hbar} H(t) U$$

- How to solve this boundary value ODE problem?

Numerical methods to solve BVP: shooting method

- Popular method for boundary-value ODE: shooting method.
- Solve a nonlinear equation: $U(t_f, H(0)) = U_d$.
- Efficient only when the initial guess solution is close to the actual solution. Example: 1-D case.
- Other methods: finite-difference, finite element(allocation), all fail for high dimensions.



Differential geometry on $\mathrm{SU}(n)$

- Define a metric that includes the constraints $H(t) \in \mathcal{A}$;
- $H(t) = \sum_{\mathcal{A}} \alpha_j A_j + \sum_{\mathcal{B}} \beta_k B_k$, where $\{A_j, B_k\}$ form a basis.
- Define a penalty q-metric:

$$||H_q||_q^2 = \langle H_q, H_q \rangle_q \equiv \sum_j \alpha_j^{(q)} \alpha_j^{(q)} + q \sum_k \beta_k^{(q)} \beta_k^{(q)}$$

- Geodesic equation under q-metric:

$$\mathcal{G}_q(\dot{H}_q) = i[H_q, \mathcal{G}_q(H)]$$
$$\mathcal{G}_q(H_q) \equiv \mathcal{P}_{\mathcal{A}}(H_q) + q\mathcal{P}_{\mathcal{B}}(H_q)$$

(Dowling & Nielsen, Quant. Inf. Comput. 10, 0861 (2008))

Brachistochrone-geodesic connection

Brachistochrone equation in the component form:

$$\dot{\mu}_j = i \sum_{k'} \lambda_{k'} \, \mathrm{Tr}(H[A_j, B_{k'}]),$$

$$\dot{\lambda}_k = i \sum_{k'} \lambda_{k'} \, \mathrm{Tr}(H[B_k, B_{k'}]).$$

Geodesic equation in the component form:

$$\dot{\alpha}_j^q = i \sum_{j'} \alpha_{j'}^q \, \mathrm{Tr}(H_q[A_j, A_{j'}]) + i \sum_{k'} q\beta_{k'}^q \, \mathrm{Tr}(H_q[A_j, B_{k'}])$$

$$q\dot{\beta}_k^q = i \sum_{j'} \alpha_{j'}^q \, \mathrm{Tr}(H_q[B_k, A_{j'}]) + i \sum_{k'} q\beta_{k'}^q \, \mathrm{Tr}(H_q[B_k, B_{k'}])$$

In the large q limit:

$$\dot{\alpha}_j^q = i \sum_{k'} q\beta_{k'}^q \, \mathrm{Tr}(H_q[A_j, B_{k'}]),$$

$$q\dot{\beta}_k^q = i \sum_{k'} q\beta_{k'}^q \, \mathrm{Tr}(H_q[B_k, B_{k'}])$$

Numerical simulation: "q-jumping" method

Example: a 2-qubit system:

$$H = \hbar \sum_{l,m} \omega_m^{(l)} \sigma_m^{(l)} + \hbar\kappa \sum_m \sigma_m^{(1)} \otimes \sigma_m^{(2)}, \quad ||H|| \leq E$$

- Let's choose a random U_d in $SU(4)$:

$$U_d = \begin{pmatrix} -0.147 + 0.356i & 0.047 - 0.130i & 0.050 - 0.734i & -0.136 - 0.521i \\ -0.08 + 0.335i & -0.426 + 0.063i & 0.541 + 0.127i & -0.578 + 0.223i \\ -0.770 + 0.073i & -0.165 + 0.470i & -0.360 - 0.034i & 0.039 + 0.139i \\ 0.344 - 0.116i & -0.247 + 0.695i & 0.037 + 0.130i & -0.008 - 0.551i \end{pmatrix}$$

- At $q = 1$, fixing $T = 1$, we can analytically solve $H_{q=1}(0) = i \log U_d$.
- For $q > 1$, we can sequentially solve $H_{q_k}(0)$ from $H_{q_{k-1}}(0)$, $1 = q_1 < q_2 < \cdots q_{k-1} < q_k < \cdots$.

Illustration of "q-jumping" method

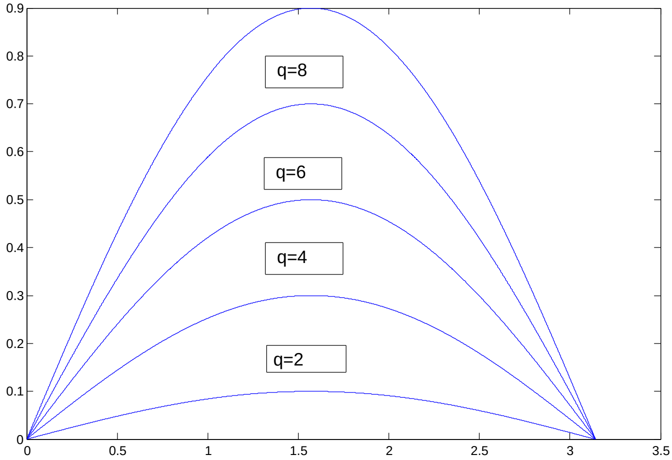


Figure: geodesic deviation with 2 fixed ends

Example: 2-qubit random U_d, q-jumping

q	Geodesic solution: $H_q(0) = (\alpha_j^q(0), \beta_k^q(0))$, $j = 1, \cdots, 7$, $k = 1, \cdots, 8$	Fidelity
1	(1.2200 -0.1238 -0.6603 -1.3985 -2.4579 1.6768 -0.7312 0.4938 0.4424 $\cdots$ -0.6108)	0.7612
2	(0.9034 0.0337 -0.6488 -1.3562 -2.6288 1.7150 -0.8652 0.3377 0.4857 $\cdots$ -0.5384)	0.7818
3	(0.5851 0.1617 -0.6198 -1.3278 -2.7493 1.7308 -0.9837 0.2508 0.4839 $\cdots$ -0.5086)	0.7992
4	(0.2747 0.2575 -0.5888 -1.3071 -2.8308 1.7388 -1.0848 0.1920 0.4702 $\cdots$ -0.4932)	0.8146
5	(-0.0214 0.3244 -0.5592 -1.2916 -2.8822 1.7421 -1.1688 0.1478 0.4525 $\cdots$ -0.4839)	0.8282
$\vdots$	$\vdots$	$\vdots$
39	(-2.9985 -0.0496 0.8486 -0.3773 -2.3631 0.4896 -2.4435 -0.0778 0.2137 $\cdots$ -0.4464)	0.9266
40	(-2.9972 -0.0388 0.8888 -0.3574 -2.3680 0.4507 -2.4622 -0.0787 0.2103 $\cdots$ -0.4463)	0.9273
$\vdots$	$\vdots$	$\vdots$
59	(-2.8716 1.2846 -0.6363 -0.8567 -3.2048 2.0340 -1.4730 -0.1193 0.0566 $\cdots$ -0.3967)	0.9559
60	(-2.8693 1.2953 -0.6781 -0.8527 -3.2025 2.0753 -1.4622 -0.1201 0.0526 $\cdots$ -0.3932)	0.9567
99	(-3.5774 0.5188 -2.4764 -0.0207 -1.7913 3.8783 -1.1532 -0.0784 0.0019 $\cdots$ -0.1488)	0.9920
100	(-3.5776 0.4989 -2.4919 -0.0148 -1.7645 3.8928 -1.1452 -0.0774 0.0019 $\cdots$ -0.1465)	0.9922
	Brachistochrone solution: $(H(0), \lambda_k^q(0)) = (\mu_j^q(0), \lambda_k^q(0))$, $j = 1, \cdots, 7$, $k = 1, \cdots, 8$	Fidelity
approx.	(-3.5776 0.4989 -2.4919 -0.0148 -1.7645 3.8928 -1.1452 -7.7391 0.1918 $\cdots$ -14.6530)	0.9916
exact	(-4.0194 0.1372 -2.8829 0.2481 -1.0109 4.2998 -0.8674 -6.7600 0.0926 $\cdots$ -9.7607)	1

Table: For a randomly chosen U_d, geodesic solutions $H_q(0)$, $q = 1, \cdots, 100$, are calculated from $H^0_{q=1} = \bar{H}^{(1)}$. The brachistochrone solution $H(t)$ is found using shooting method with the good approximated solution derived from $H_{q=100}(t)$.

Method 2: "direct geodesic" method

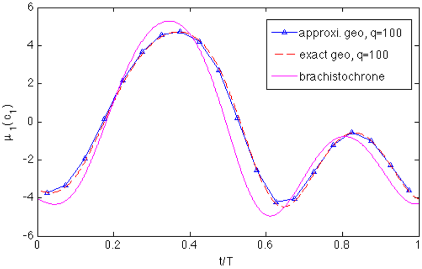


Figure: We have plotted the first component $\mu_1(t)(\alpha_1(t))$ of the optimal Hamiltonian for: (1) the approximated geodesic solution at $q = 100$(solid line with markers) derived from weighted-sum optimization; (2) the accurate geodesic solution at $q = 100$(dashed line); (3) the corresponding brachistochrone solution(solid line).

$$J = 1 - \frac{1}{N}||\text{Tr}[U_d^\dagger U(T)]|| + \alpha \int_0^T ||H_q(t)||_q dt,$$

“direct geodesic” method CNOT gate

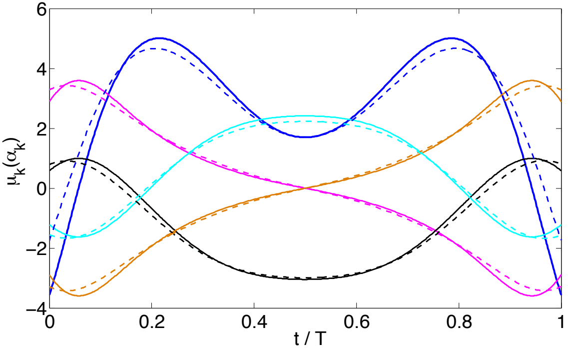


Figure: Here we show the 7 control functions that implement the minimal-time CNOT gate (solid curves), along with those for the geodesic solution at $q = 100$ (dashed curves).

Complexity analysis of geodesic numerical methods

Assuming the dimension of the quantum system is N:

- weighted-sum optimization: quasi-Newton method, $poly(N)$;
- solving initial-value ODE, $poly(N)$.
- shooting method, $poly(N)$ as long as it converges.

However, for a quantum system, the complexity increases as 2^N.
Any classical time-optimal method will become intractable for large quantum system.

Drift-case time-optimal control

Assuming there is a drift component in $H_{\text{tot}}(t)$ which cannot be controlled:

- $H_{\text{tot}}(t) = H_0 + H(t)$;
- $||H(t)|| \leq E$;
- $H(t) \in \mathcal{A}$, i.e., $\text{Tr}(H(t)\mathcal{B}) = 0$.

The time-optimal solution can be classified as being: (1) nonsingular: $||H_{opt}(t)|| = E$, (2) singular $||H_{opt}(t)|| < E$. (Pontryagin maximum principle)
For nonsingular solution, we can write down the corresponding brachistochrone equation and the geodesic equation.

$$\dot{\lambda} H + \lambda \dot{H} + \sum_k \dot{\lambda}_k B_k = -i[H_0 + H, \lambda H + \sum_k \lambda_k B_k] \quad (1)$$

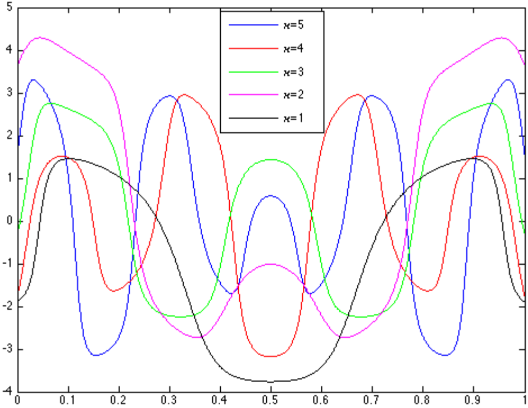
$$\dot{\bar{\lambda}} \mathcal{G}_q(H_q) + \bar{\lambda} \mathcal{G}_q(\dot{H}_q) = -i\bar{\lambda}[H_0 + H_q, \mathcal{G}_q(H_q)] \quad (2)$$

Drift-case time-optimal control

- We can prove that when $H_0 \in \mathcal{A}$, then all optimal protocols satisfy $||H(t)|| = E$, i.e., nonsingular.
- For single qubit system, with $\mathcal{A} = \text{span}\{\sigma_x, \sigma_y\}$, and $\sigma_0 = \sigma_z$, all time-optimal solutions are nonsingular.
- When $H_0 \notin \mathcal{A}$, if span $\mathcal{A} = \mathfrak{su}(N)$, then the optimal solutions are nonsingular; if span $\mathcal{A} \neq \mathfrak{su}(N)$, and when $\kappa \equiv \frac{||H_0||}{E} \ll 1$, then the optimal solutions will become singular, and for other value of κ, time-optimal solutions are still nonsingular.

Numerical examples: drift-case CNOT

$$H = H_0 + H_c(t) = \hbar\kappa \sum_m \sigma_m^{(1)} \otimes \sigma_m^{(2)} + \hbar \sum_{l,m} \omega_m^{(l)}(t)\sigma_m^{(l)}, \quad ||H|| \leq E$$



Numerical examples: drift-case CNOT

κ	brachi solution: $H_q(0) = (\alpha_j^{(q)}(0), \beta_k^{(q)}(0))$	phase	T_{opt}
0.4		-i	7.6266
0.5		-i	6.3628
0.6		1	6.4756
0.7		-i	5.2935
0.8		-i	5.4701
0.9	(1.2200 -0.1238 -0.6603 -1.3985 -2.4579 1.6768 -0.7312 0.4938 0.4424 $\cdots$)	-i	5.5766
1	(1.2200 -0.1238 -0.6603 -1.3985 -2.4579 1.6768 -0.7312 0.4938 0.4424 $\cdots$)	-i	5.5661
2	(0.9034 0.0337 -0.6488 -1.3562 -2.6288 1.7150 -0.8652 0.3377 0.4857 $\cdots$)	-1	5.6741
3	(0.5851 0.1617 -0.6198 -1.3278 -2.7493 1.7308 -0.9837 0.2508 0.4839 $\cdots$)	-1	4.4965
4	(0.2747 0.2575 -0.5888 -1.3071 -2.8308 1.7388 -1.0848 0.1920 0.4702 $\cdots$)	i	4.4965
5	(-0.0214 0.3244 -0.5592 -1.2916 -2.8822 1.7421 -1.1688 0.1478 0.4525 $\cdots$)	1	4.7855

Table: For different values of κ, we calculate the time-optimal solution if it is nonsingular.

Connections to other topics

We have discussed how to formulate and solve the time-optimal control problem under two constraints: (1) $||H(t)|| \leq E$; and (2) $\mathrm{Tr}(H(t)\mathcal{B}) = 0$. Dependent on being nonsingular or singular, with a drift or drift-free, the brachistochrone-geodesics connection can be derived, and an efficient numerical method can be obtained.

- Ultimate physical limit to computation(Nature Review, S. LLloyd, 2000);
- Zermelo Navigation problem and Randers metric (B. Russel, PRA, 2014);
- Solovay-Kitaev theorem. Given error ϵ, numerical time cost: $\mathcal{O}(\log^{2.71}(\frac{1}{\epsilon}))$ and sequence length: $\mathcal{O}(\log^{3.97}(\frac{1}{\epsilon}))$.
- Machine learning algorithm and big data.

The End

“We are time’s subjects, and time bids be gone.”

— William Shakespeare