Putting quantum machine learning algorithms to the test

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Introduction

Quantum Computing & Qubits

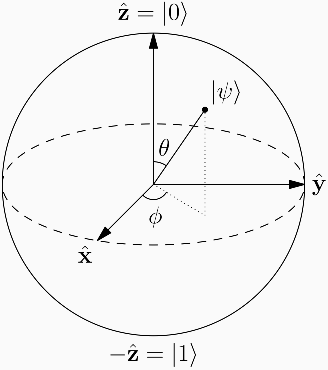

Figure 1: Arbitrary two-dimensional qubit $|\psi\rangle$ visualized on the Bloch sphere[1]

Most general form of a 2-D qubit:

$$|q\rangle = \alpha\,|0\rangle + \beta\,|1\rangle \qquad (1)$$

where $\alpha, \beta \in \mathbb{C}$.

Can also be visualized in spherical polar coords on the unit or Bloch sphere as follows:

$$|q\rangle = \cos\frac{\theta}{2}\,|0\rangle + e^{i\phi}\sin\frac{\theta}{2}\,|1\rangle \qquad (2)$$

where $0 \leq \theta \leq \pi$ and $0 \leq \phi \leq 2\pi$

[1] Reprinted from Wikipedia, n.d., Retrieved September 7, 2016, from `https://en.wikipedia.org/wiki/Bloch_Sphere`. Copyright 2012 by Glosser.ca. Reprinted with permission.

Machine Learning

- Approximately 2.5 quintillion (10^{18}) bytes of digital data are created every day[1]
- Need for advanced algorithms that can make sense of data content, retrieve patterns and reveal correlations $\rightarrow$ Machine learning (ML)
- ML algorithms often involve
  - solving large systems of linear equations
  - inverting large matrices
  - distance computations
- Performing these computations on large data sets gets increasingly difficult[2]

[1] IBM. (2016). What is big data? https://www-01.ibm.com/software/data/bigdata/what-is-big -data.html. (Accessed: 2016-09-08)
[2] Bekkerman, R., Bilenko, M., & Langford, J. (2011). Scaling up machine learning: Parallel and distributed approaches. Cambridge University Press.

Machine Learning

Machine learning can be subdivided into three major fields.

Supervised ML

- Based on *input* and *output* data

"I know how to classify this data but I need the algorithm to do the computations for me."

Unsupervised ML

- Based on *input* data only

"I have no clue how to classify this data, can the algorithm create a classifier for me?"

Reinforcement learning

- Based on *input* data only

"I have no clue how to classify this data, can the algorithm classify this data and I'll give it a reward if it's correct or I'll punish it if it's not."

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Quantum Machine Learning

- ML involves manipulation of large vectors and matrices
- Quantum mechanics is about vectors $\in$ complex Hilbert spaces
- Quantum computers are performing linear operations on qubits
- Hence, we can manipulate large vectors in parallel on quantum computers
- So can we use QC to improve classical ML algorithms??

- Classical ML is a very practical topic
- BUT, QML has been of almost entirely theoretical nature

Classical k-nearest neighbour

- kNN is a non-parametric classifier
- k is a positive integer, usually chosen small

Given training data set:

$D_T = v_0, v_1, .., v_{10}$

$v_i \in \{A, B\}$

Given a new vector $\tilde{x}$ (red star):

- consider k nearest neighbours
- classify $\tilde{x}$, based on majority vote, as A or B

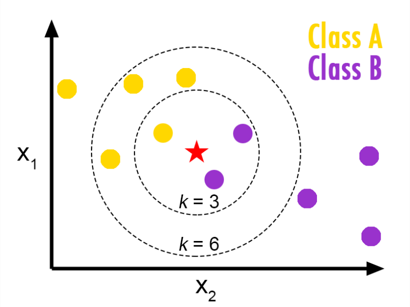

Figure 2: Visualization of a kNN classifier[1]

[1] Reprinted from GitHub, Burton de Wilde, Retrieved September 13, 2016, from http://bdewilde.github.io/blog/blogger/2012/10/26/classification-of-hand-written-digits-3/. Copyright 2012 by Burton de Wilde. Reprinted with permission.

Quantum k-nearest neighbour

Two different algorithms with respect to initial state preparation:

Data encoded into qubits

k-dimensional probability vector requires $4k$ classical bits which are encoded one-to-one into $4k$ qubits, e.g.

$$\begin{pmatrix} 0.6 \\ 0.4 \end{pmatrix} * 10 \rightarrow \begin{pmatrix} 6 \\ 4 \end{pmatrix} \rightarrow \begin{pmatrix} 0110 \\ 0100 \end{pmatrix} \rightarrow n = 01100100 \rightarrow |n\rangle = |01100100\rangle$$

Data encoded into amplitudes

k-dimensional probability vector is encoded into $log_2(k)$ qubits, e.g.

$$\begin{pmatrix} 0.6 \\ 0.4 \end{pmatrix} \quad \rightarrow \quad |n\rangle = \sqrt{0.6}\,|0\rangle + \sqrt{0.4}\,|1\rangle$$

Quantum k-nearest neighbour

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Amplitude-based kNN algorithm

The algorithm

$$\frac{1}{\sqrt{2M}} \sum_{m=1}^{M} \left(|0\rangle |\Psi_{\tilde{x}}\rangle + |1\rangle |\Psi_{x^m}\rangle \right) |y^m\rangle |m\rangle \tag{3}$$

where

$$|\Psi_{\tilde{x}}\rangle = \sum_{i=1}^{N} \tilde{x}_i |i\rangle \qquad |\Psi_{x^m}\rangle = \sum_{i=1}^{N} x_i^m |i\rangle \tag{4}$$

$$\frac{1}{2\sqrt{M}} \sum_{m=1}^{M} \left(|0\rangle \left[|\Psi_{\tilde{x}}\rangle + |\Psi_{x^m}\rangle \right] + |1\rangle \left[|\Psi_{\tilde{x}}\rangle - |\Psi_{x^m}\rangle \right] \right) |y^m\rangle |m\rangle \tag{5}$$

The algorithm

After successful conditional measurement, the state is proportional to

$$\frac{1}{2\sqrt{M}} \sum_{m=1}^{M} \sum_{i=1}^{N} (\tilde{x}_i + x_i^m) |0\rangle |i\rangle |y^m\rangle |m\rangle \tag{6}$$

$$p(|y^m\rangle = |0\rangle) = \sum_{m|y^m=0} 1 - \frac{1}{4M} \mid \tilde{x} - x^m \mid^2 \tag{7}$$

Overall algorithmic complexity

$\mathcal{O}(\frac{1}{p_{acc}})$ where p_{acc} is the probability of measuring ancilla in the $|0\rangle$ state

Simple binary classification case

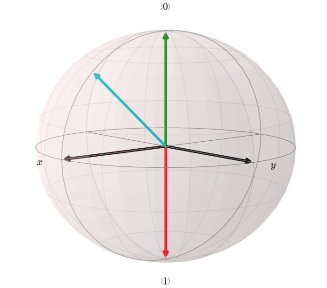


Figure 3: Simple binary classification problem of a quantum state

$$\frac{1}{\sqrt{2M}}\sum_{m=1}^{M}(|0\rangle|\Psi_{\tilde{x}}\rangle + |1\rangle|\Psi_{x^m}\rangle)|y^m\rangle|m\rangle \tag{8}$$

where

$$|\Psi_{\tilde{x}}\rangle = \sum_{i=1}^{N}\tilde{x}_i|i\rangle \qquad |\Psi_{x^m}\rangle = \sum_{i=1}^{N}x_i^m|i\rangle \tag{9}$$

Procedure to load the input vector $\tilde{x}$:

$$|\Psi_0\rangle = \frac{1}{2}\sum_{m=1}^{2}(|0\rangle|0\rangle + |1\rangle|0\rangle)|y^m\rangle|m\rangle \tag{10}$$

Apply controlled rotation ${}^1_0CR_y(\frac{\pi}{4})$ s.t.

$${}^1_0CR_y(\frac{\pi}{4})|\Psi_0\rangle = |\Psi_1\rangle = \frac{1}{2}\sum_{m=1}^{2}(|0\rangle|0\rangle + |1\rangle|\Psi_{\tilde{x}}\rangle)|y^m\rangle|m\rangle \tag{11}$$

Flip the ancilla qubit in the first register

$$(X\otimes\mathbb{1}\otimes\mathbb{1}\otimes\mathbb{1})|\Psi_1\rangle = |\Psi_2\rangle = \frac{1}{2}\sum_{m=1}^{2}(|0\rangle|\Psi_{\tilde{x}}\rangle + |1\rangle|0\rangle)|y^m\rangle|m\rangle \tag{12}$$

Implementation with IBM's quantum computer

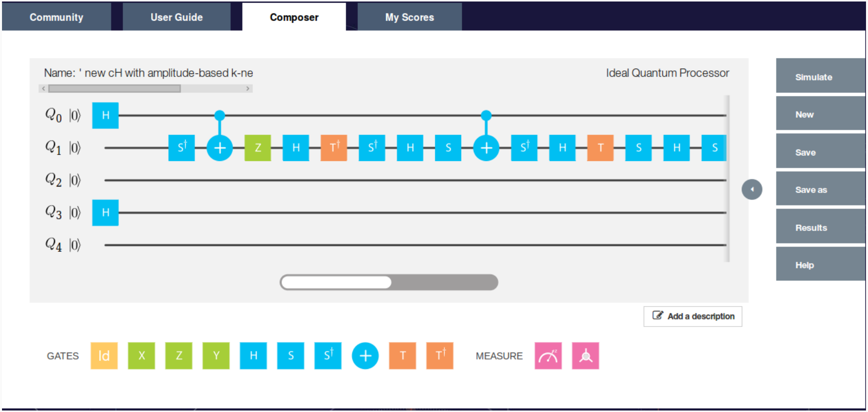


Figure 4: IBM's quantum composer

- Accessible to the public
- Allows for ideal + real simulations
- 5 superconducting qubits
- 40 gates (39 gates + 1 measurement)

Controlled U gate

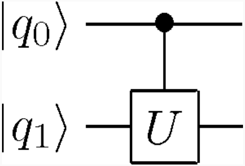


Figure 5: Controlled U-gate

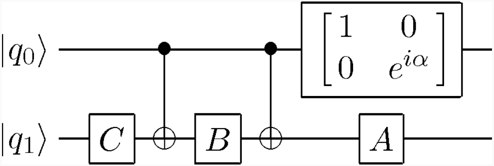


Figure 6: Decomposition of a controlled U-gate[1]

Choose A,B,C and α s.t.

$$e^{i\alpha} * A * X * B * X * C = U \quad and \quad A * B * C = \mathbb{1} \tag{13}$$

Need to solve the following equation[1]

$$U = \begin{pmatrix} e^{i(\alpha - \frac{\beta}{2} - \frac{\delta}{2})} \cos \frac{\gamma}{2} & -e^{i(\alpha - \frac{\beta}{2} + \frac{\delta}{2})} \sin \frac{\gamma}{2} \\ e^{i(\alpha + \frac{\beta}{2} - \frac{\delta}{2})} \sin \frac{\gamma}{2} & e^{i(\alpha + \frac{\beta}{2} + \frac{\delta}{2})} \cos \frac{\gamma}{2} \end{pmatrix} \tag{14}$$

Overall algorithmic complexity

$\mathcal{O}(\frac{1}{p_{acc}}) + \mathcal{O}(k)$ where k is number of root finding iterations[2]

[1] Nielsen, M. A., & Chuang, I. L. (2010). Quantum computation and quantum information. Cambridge University Press.
[2] Jat, R. N., & Ruhela, D. S. (2011). Comparative study of complexity of algorithms for iterative solution of non-linear equations. Journal of International Academy Of Physical Sciences, 15(4).

Problems with universal gate sets

In our case we need to find A, B, C and α for ${}^1_0 CR_y(\frac{\pi}{4})$:

Using a root finding algorithm for non-linear equations we find:

$$\alpha = \pi; \quad \beta = 2\pi; \quad \delta = \frac{7}{8}\pi; \quad \gamma = 0 \tag{15}$$

Then,

$$A = R_z(\beta)R_y(\frac{\gamma}{2}) = R_z(2\pi) = \mathbb{1} \tag{16}$$

$$B = R_y(-\frac{\gamma}{2})R_z(-\frac{\delta+\beta}{2}) = R_z(-\frac{23}{16}\pi) = ??? \tag{17}$$

$$C = R_z(\frac{\delta-\beta}{2}) = R_z(-\frac{9}{16}\pi) = ??? \tag{18}$$

$$\begin{pmatrix} 1 & 0 \\ 0 & e^{i\alpha} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & e^{i\pi} \end{pmatrix} = Z \tag{19}$$

[1] Dawson, C. M., & Nielsen, M. A. (2005). The Solovay-Kitaev algorithm. arXiv preprint quant-ph/0505030.

The Solovay-Kitaev theorem

$$B = R_z(-\frac{23}{16}\pi) = ??? \tag{20}$$
$$C = R_z(-\frac{9}{16}\pi) = ??? \tag{21}$$

The Solovay-Kitaev theorem guarantees that given a set of single-qubit quantum gates which generates a dense subset of $SU(2)$, then that set is guaranteed to fill $SU(2)$ quickly.[1]

$\rightarrow$ **Hence, given any universal gate set it is possible to obtain good approximations to any desired gate.**

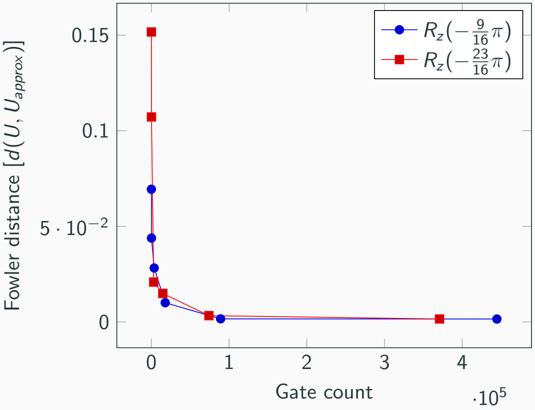
$\rightarrow$ **But needs to be computed classically!**

[1] Dawson, C. M., & Nielsen, M. A. (2005). The Solovay-Kitaev algorithm. arXiv preprint quant-ph/0505030.

The Solovay-Kitaev algorithm

Fowler distance[1]:

$$dist(U, U_{approx}) = \sqrt{\frac{2 - \mid tr(U \cdot U_{approx}^{\dagger}) \mid}{2}} \tag{22}$$



[1] Booth Jr, J. (2012). Quantum compiler optimizations. arXiv preprint arXiv:1206.3348.

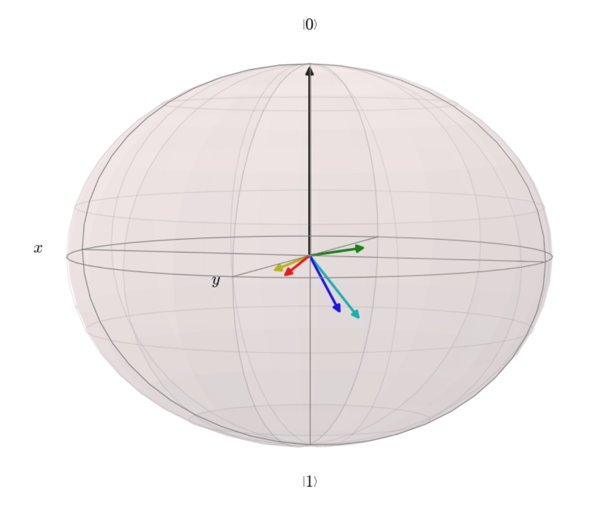


Figure 7: Various Fowler distances visualized on Bloch sphere

$$d = 0.22739 \quad (23)$$

$$d = 0.15165 \quad (24)$$

$$d = 0.10722 \quad (25)$$

$$d = 0.02086 \quad (26)$$

$$d = 0.00156 \quad (27)$$

The Solovay-Kitaev algorithm

IBM's quantum computer needs **130ns for single-qubit gates** and **500ns for CNOT gates.**

IBM qubit decoherence times:

$49.5\,\mu s \leq T_1 \leq 85.3\,\mu s$ "amplitude damping"
$56.0\,\mu s \leq T_2 \leq 139.7\,\mu s$ "phase damping"

Approx. Gate	Distance	Gate count	Execution time
$R_z(-\frac{23}{16}\pi)$	0.15165	25	$\sim 3\,\mu s$
	0.10722	109	$\sim 14\,\mu s$
	0.02086	2997	$\sim 390\,\mu s$
	0.01494	14721	$\sim 1914\,\mu s$
	0.003327	74009	$\sim 9621\,\mu s$
	0.001578	370813	$\sim 48\,206\,\mu s$

Table 1: SK algorithm results

Adding complexities

Executing the SK algorithm adds to our overall algorithmic complexity:

Overall algorithmic complexity

$\mathcal{O}(\frac{1}{p_{acc}}) + \mathcal{O}(k) + \mathcal{O}(m * log^{2.71}(\frac{m}{\epsilon}))$ for ϵ-approximations of m gates[1]

Due to state preparation we went from

$$\mathcal{O}(\frac{1}{p_{acc}}) \tag{28}$$

suddenly to

$$\mathcal{O}(m * log^{2.71}(\frac{m}{\epsilon})) \tag{29}$$

where m is the number of gates that need approximation to ϵ-accuracy

[1] Dawson, C. M., & Nielsen, M. A. (2005). The Solovay-Kitaev algorithm. arXiv preprint quant-ph/0505030.

Liqui$|\rangle$ simulations

Currently impossible to implement the quantum algorithm on IBM's quantum computer! $\rightarrow$ can only simulate it with i.e. Liqui$|\rangle$

In Liqui$|\rangle$ we can directly implement the controlled R_y rotation!

Conclusion

Summary

- Initial state preparation is non-trivial! (even for very simple examples)
- In this case, state preparation dominates the overall algorithmic complexity
- Universal gate sets are only useful when combined with long qubit lifetimes
- Solovay-Kitaev yields very long gate sequences for good approximations
- **Need for better quantum compiling and more general state preparation algorithms!**

Taking it further

- Complexity analysis of the qubit-based kNN algorithm
- Classification of gaussian probability distributions
- Implementing more general state preparation algorithms

References

Bekkerman, R., Bilenko, M., & Langford, J. (2011). Scaling up machine learning: Parallel and distributed approaches. Cambridge University Press.

Booth Jr, J. (2012). Quantum compiler optimizations. arXiv preprint arXiv:1206.3348.

Dawson, C. M., & Nielsen, M. A. (2005). The Solovay-Kitaev algorithm. arXiv preprint quant-ph/0505030.

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Jat, R. N., & Ruhela, D. S. (2011). Comparative study of complexity of algorithms for iterative solution of non-linear equations. Journal of International Academy Of Physical Sciences, 15(4).

Nielsen, M. A., & Chuang, I. L. (2010). Quantum computation and quantum information. Cambridge University Press.

Questions?

Backup slide: Qubit decoherence times

We expect exponential decay:

$$e^{t/T_i} \tag{30}$$

T_1: **Longitudinal coherence time (amplitude damping)**

- Prepare $|0\rangle$ state
- Apply the X (NOT) gate s.t. qubit is in $|1\rangle$ state
- Wait for time t
- Measure the probability of being in $|1\rangle$ state

T_2: **Transversal coherence time (phase damping)**

- Prepare $|0\rangle$ state
- Apply Hadamard $\rightarrow$ $\frac{|0\rangle+|1\rangle}{\sqrt{2}}$
- Wait for time t
- Apply Hadamard again
- Measure the probability of being in $|0\rangle$ state

We expect this probability to go to 0.5 $\rightarrow$ qubit lost quantum behaviour

Backup Slide II: Experimental realizations

Only few experimental verifications of QML algorithms:

- Li, Liu, Xu, and Du (2015) successfully distinguished a handwritten six from a nine using a quantum support vector machine on a four-qubit nuclear magnetic resonance test bench[1]

- Cai et al. (2015) were first to experimentally demonstrate quantum machine learning on a photonic QC and showed that the distance between two vectors and their inner product can indeed be computed quantum mechanically[2]

- Rist et al. (2015) solved a learning parity problem with five superconducting qubits and found that a quantum advantage can already be observed in non error-corrected systems[3]

[1] Li, Z., Liu, X., Xu, N., & Du, J. (2015). Experimental realization of a quantum support vector machine. Physical Review Letters, 114 (14), 15. doi: 10.1103/PhysRevLett.114.140504

[2] Cai, X. D., Wu, D., Su, Z. E., Chen, M. C., Wang, X. L., Li, L., . . . Pan, J. W. (2015). Entanglement- based machine learning on a quantum computer.

Liqui|⟩ simulations: Taking it further

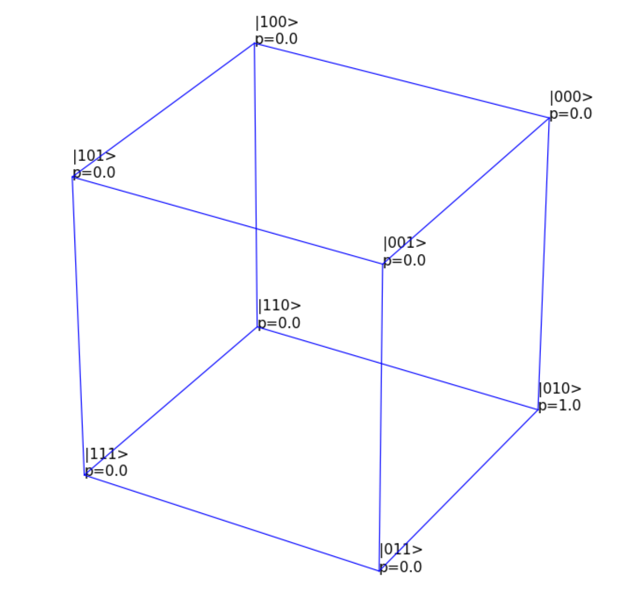


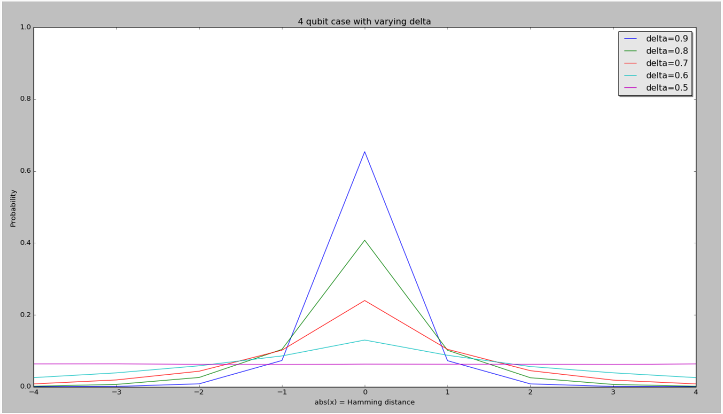
Figure 8: Representation of hamming distance on 3D cube

Liqui|⟩ simulations: Taking it further

Applying the following matrix

$$\begin{pmatrix} \sqrt{\delta} & 1-\sqrt{\delta} \\ 1-\sqrt{\delta} & -\sqrt{\delta} \end{pmatrix} \tag{31}$$

to all qubits in the data register leads to a gaussian distribution over the "Hamming distance" cube:



Liqui|⟩ simulations: Taking it further

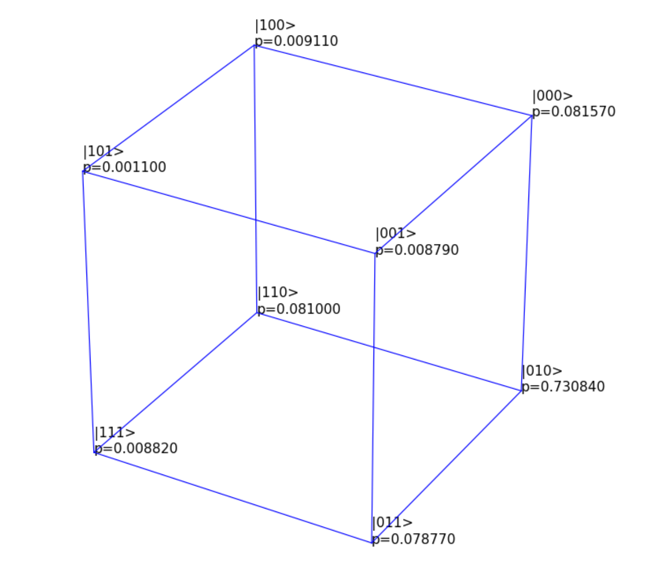


Figure 10: Representation of gaussian diffusion on 3D cube

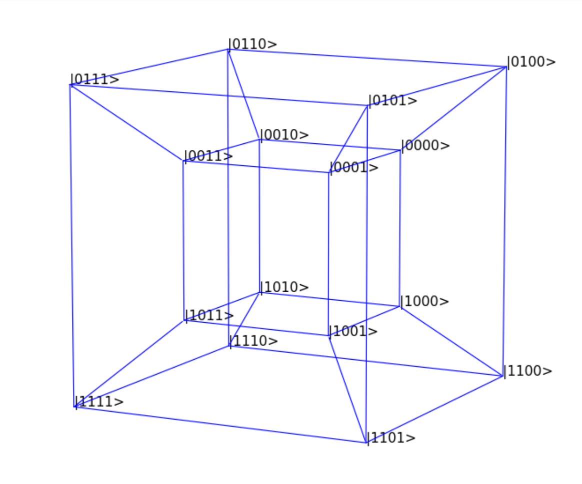


Figure 11: Representation of gaussian diffusion on 3D cube

Backup slide II I

IBM.

What is big data?

https://www-01.ibm.com/software/data/bigdata/what-is-big-data.html, 2016.

Accessed: 2016-09-08.

Qubit-based kNN quantum algorithm

Typography

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\emph{emphasize} text, \alert{accent} parts
or show \textbf{bold} results.
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References go here

Font feature test

- Regular
- *Italic*
- SmallCaps
- **Bold**
- **Bold Italic**
- **Bold SmallCaps**
- `Monospace`
- *`Monospace Italic`*
- `Monospace Bold`
- *`Monospace Bold Italic`*

References go here

Lists

Items

- Milk
- Eggs
- Potatos

Enumerations

1. First,
2. Second and
3. Last.

Descriptions

PowerPoint Meeh.

Beamer Yeeeha.

Animation

- This is important

Animation

- This is important
- Now this

Animation

- This is important
- Now this
- And now this

Animation

- This is really important
- Now this
- And now this

Figures

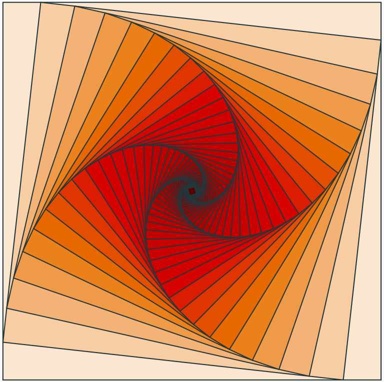

Figure 12: Rotated square from texample.net.

Tables

Table 2: Largest cities in the world (source: Wikipedia)

City	Population
Mexico City	20,116,842
Shanghai	19,210,000
Peking	15,796,450
Istanbul	14,160,467

Blocks

Three different block environments are pre-defined and may be styled with an optional background color.

Default

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Alert

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Example

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Default

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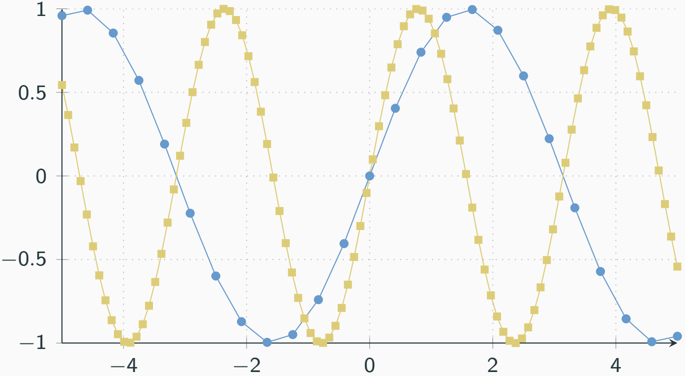
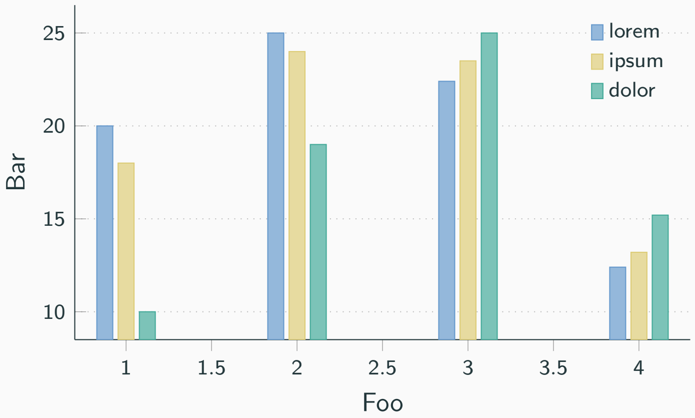
Math

$$e = \lim_{n \to \infty} \left(1 + \frac{1}{n}\right)^n$$

Line plots



Bar charts



Quotes

Veni, Vidi, Vici