Lecture 1: AI and Quantum Physics and Quantum Computation

Andreas Wichert

Department of Computer Science and Engineering

Técnico Lisboa

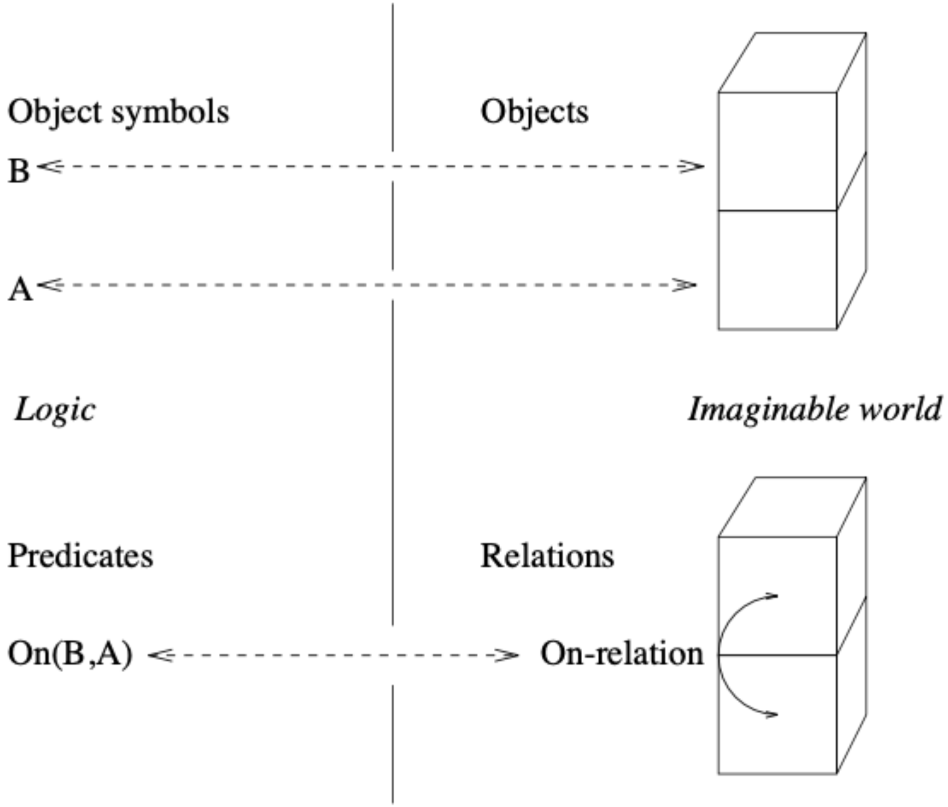
Overview

- Artificial Intelligence
    - Symbolical AI
    - Machine Learning
- Quantum Physics
- Principles of Quantum Computation
    - Qubits, Linear Operators
- Compound System
    - Computation with one and several Qubits
- Entanglement
- Cloning
- Phase Kick-Back
- Quantum Boolean Gates

- Artificial intelligence (AI) is a subfield of computer science that models the mechanisms of intelligent human behavior (intelligence).
- This approach is accomplished via simulation with the help of artificial artifacts, typically with computer programs on a machine that performs calculations.
- However, the term “intelligence” and “intelligent human behavior” are not very well defined and understood.
- That is why over the years the definition of artificial intelligence changed

What is Symbolical AI

Predicates



Object represented by symbols and relation represented by predicate

Symbolical AI

- Rules and Operators

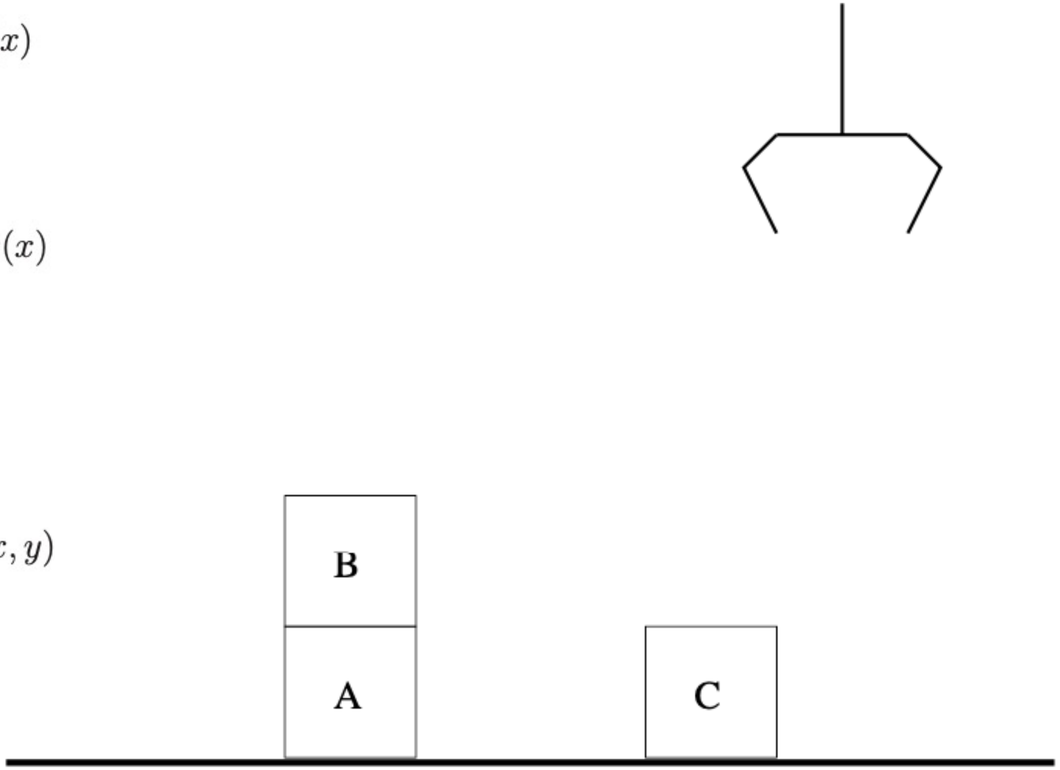
$$pickup(x)\begin{cases} P: & gripping() \wedge clear(x) \wedge ontable(x) \\ A: & gripping(x) \\ D: & ontable(x) \wedge gripping() \end{cases}$$

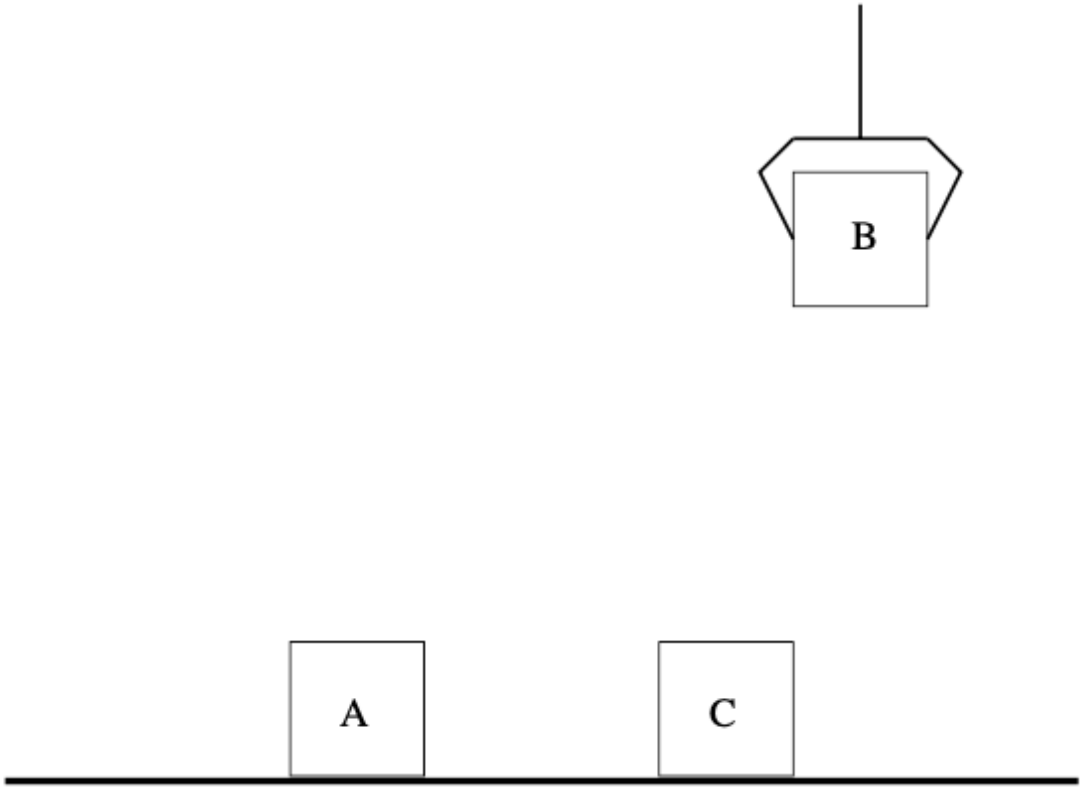
$$putdown(x)\begin{cases} P: & gripping(x) \\ A: & ontable(x) \wedge gripping() \wedge clear(x) \\ D: & gripping(x) \end{cases}$$

$$stack(x,y)\begin{cases} P: & gripping(x) \wedge clear(x) \\ A: & on(x,y) \wedge gripping() \wedge clear(x) \\ D: & clear(y) \wedge gripping(x) \end{cases}$$

$$unstack(x,y)\begin{cases} P: & gripping() \wedge clear(x) \wedge on(x,y) \\ A: & gripping(x) \wedge clear(y) \\ D: & on(x,y) \wedge gripping() \end{cases}$$

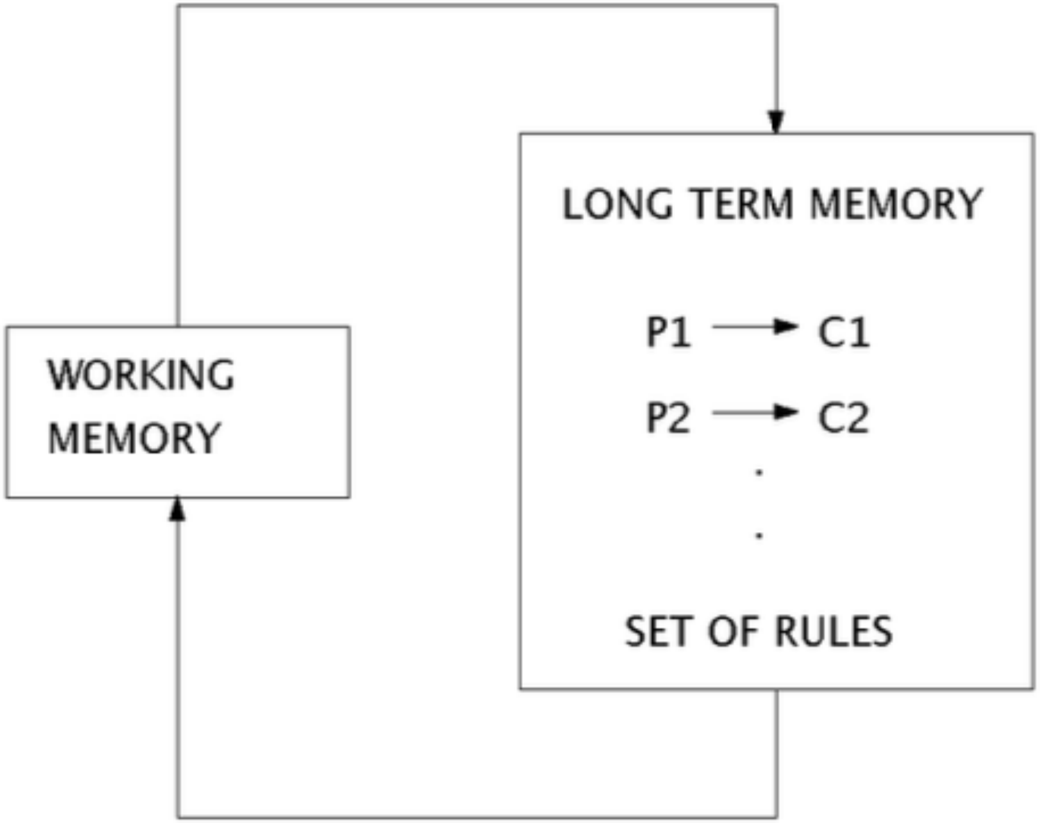
$ontable(A).$
$ontable(C).$
$on(B,A).$
$clear(B).$
$clear(C).$
$gripping().$





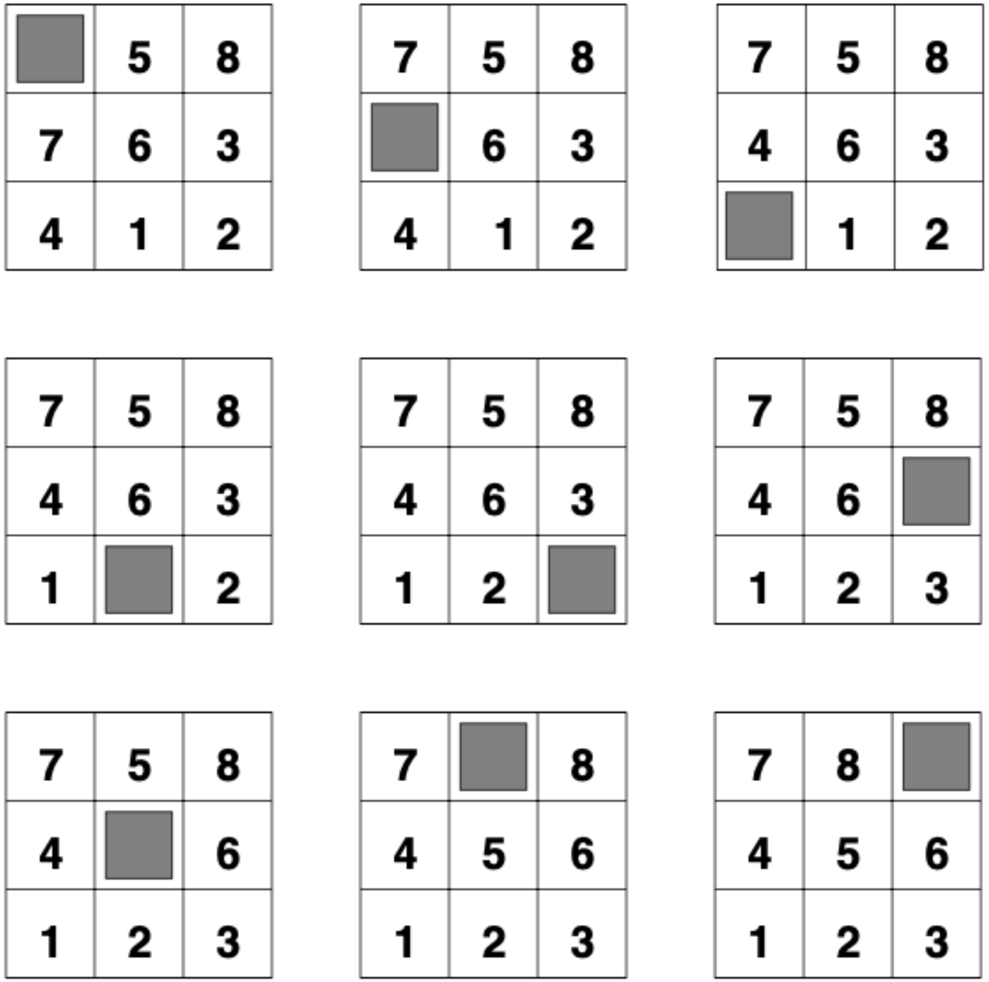
The state after the operator pickup(B) was applied

Production Systems



8-Puzzle

- If the empty cell is not on the top edge, then move the empty cell up;
- If the empty cell is not on the left edge, then move the empty cell left;
- If the empty cell is not on the right edge, then move the empty cell right;
- If the empty cell is not on the bottom edge, then move the empty cell
- down.



■	5	8
7	6	3
4	1	2

7	5	8
■	6	3
4	1	2

7	5	8
4	6	3
■	1	2

7	5	8
4	6	3
1	■	2

7	5	8
4	6	3
1	2	■

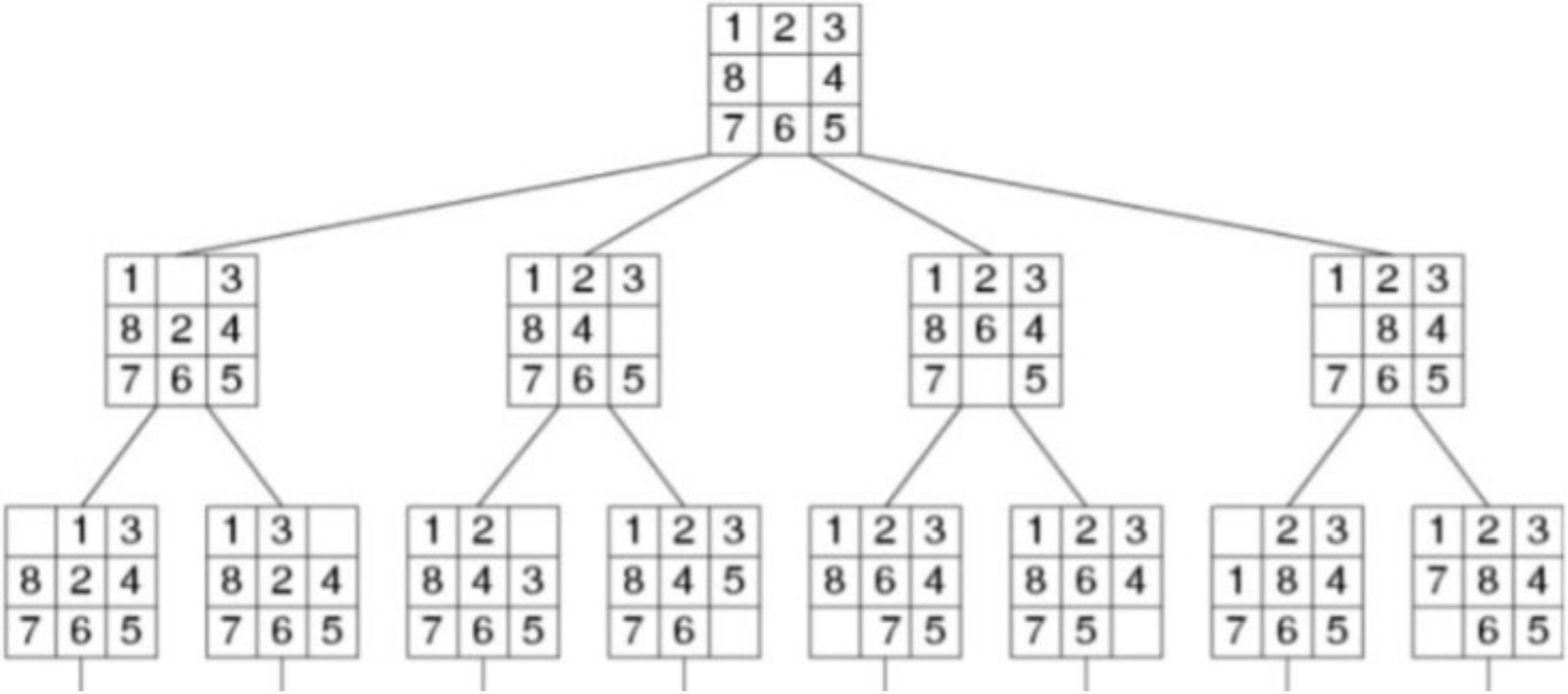
7	5	8
4	6	■
1	2	3

7	5	8
4	■	6
1	2	3

7	■	8
4	5	6
1	2	3

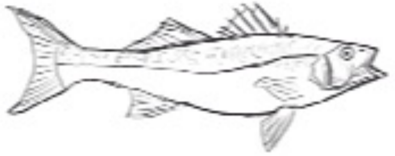
7	8	■
4	5	6
1	2	3

Tree Search

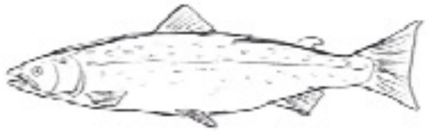


What is Machine Learning ?

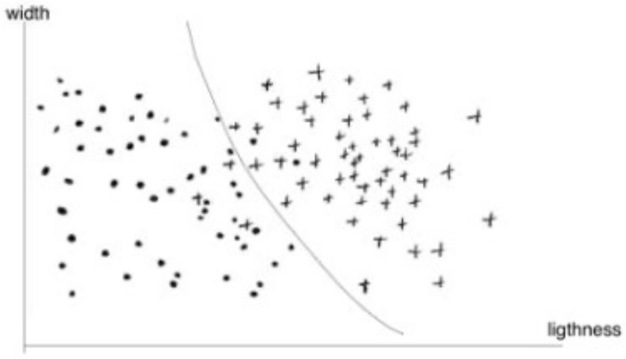
- A) Symbolical Machine Learning
    - Decision Trees: Greedy Search
- B) Subsymbolic - Statistical Machine Learning



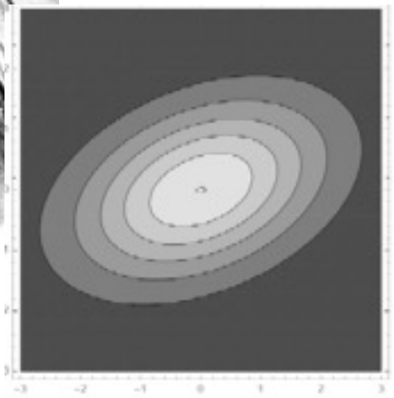
(a)

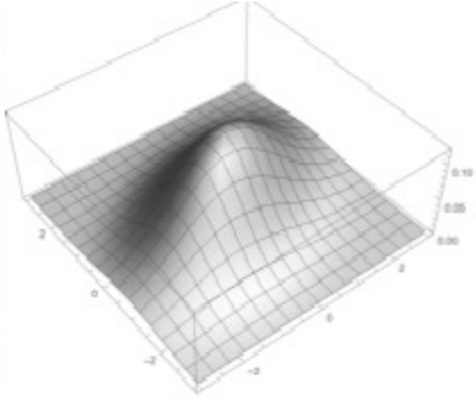


(b)

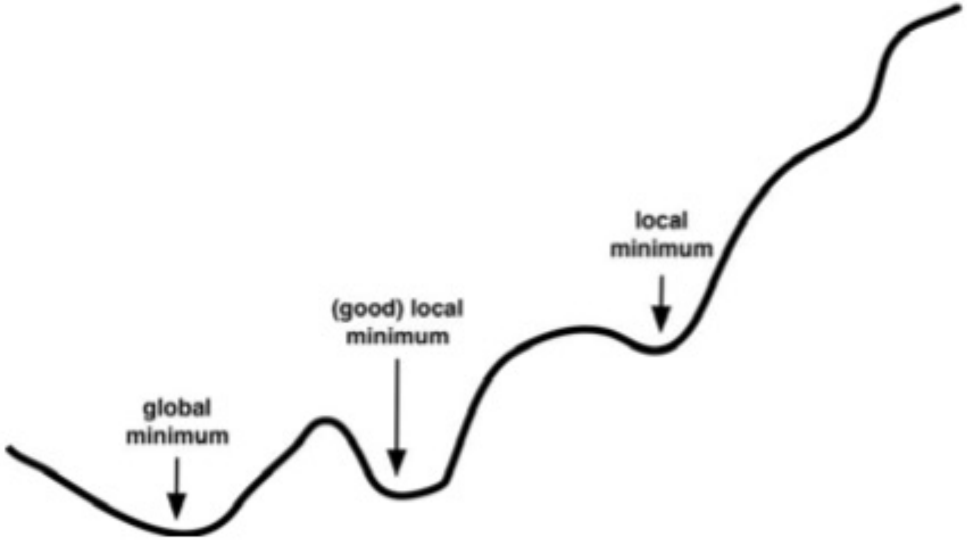


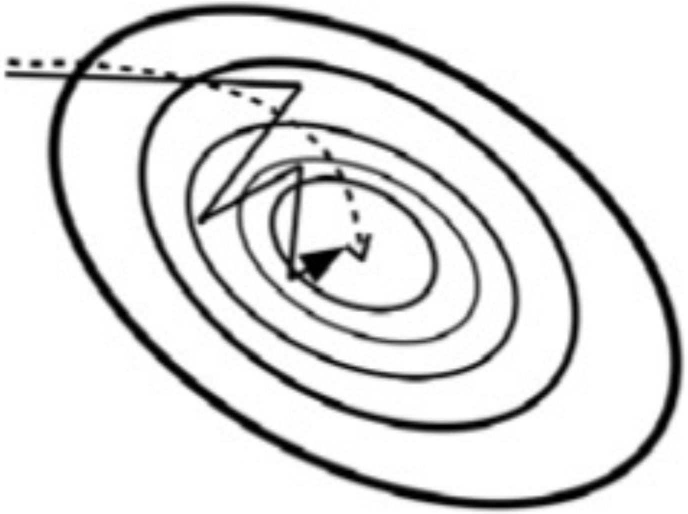
Probability and Information





Linear Algebra and Optimization

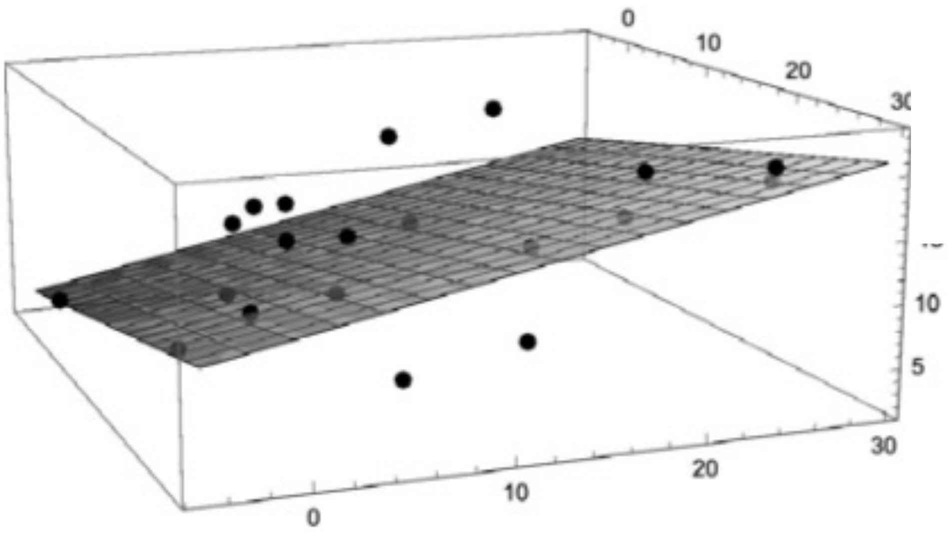




Second Order Optimization:
Hessian matrix positive definite,
does not work well with saddle points,
expensive

Linear and Nonlinear Regression

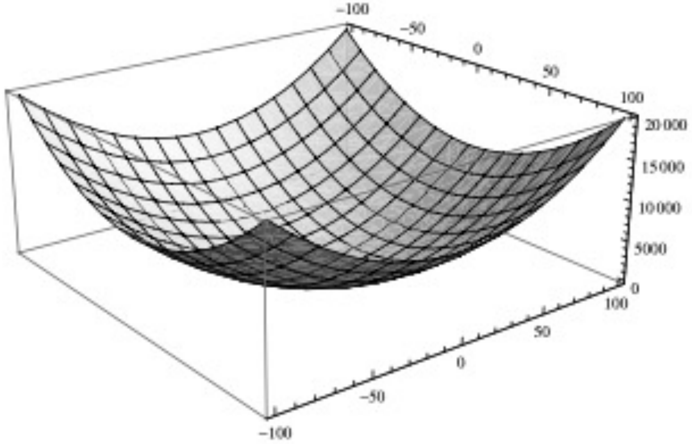
- Multilinear Regression

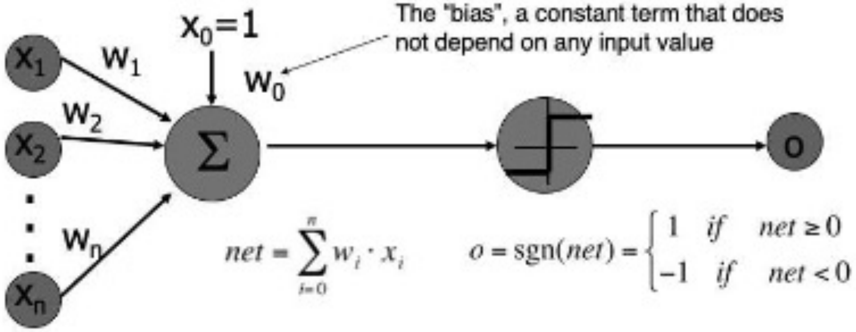



(a)


(b)

Perceptron and Logistic Regression



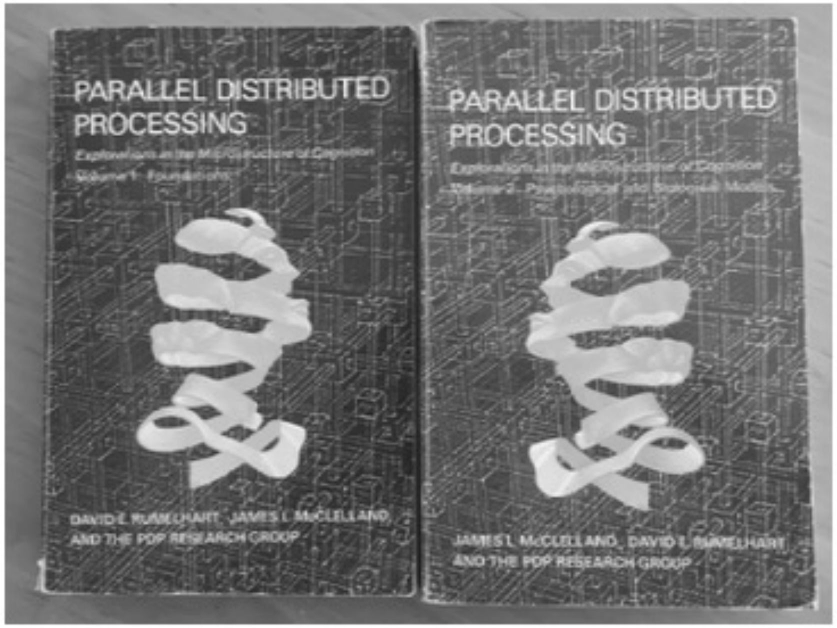


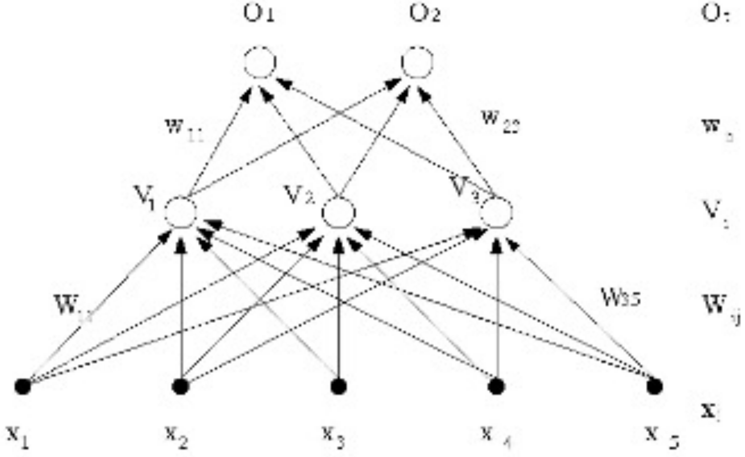
The "bias", a constant term that does not depend on any input value

$$net = \sum_{i=0}^{n} w_i \cdot x_i$$

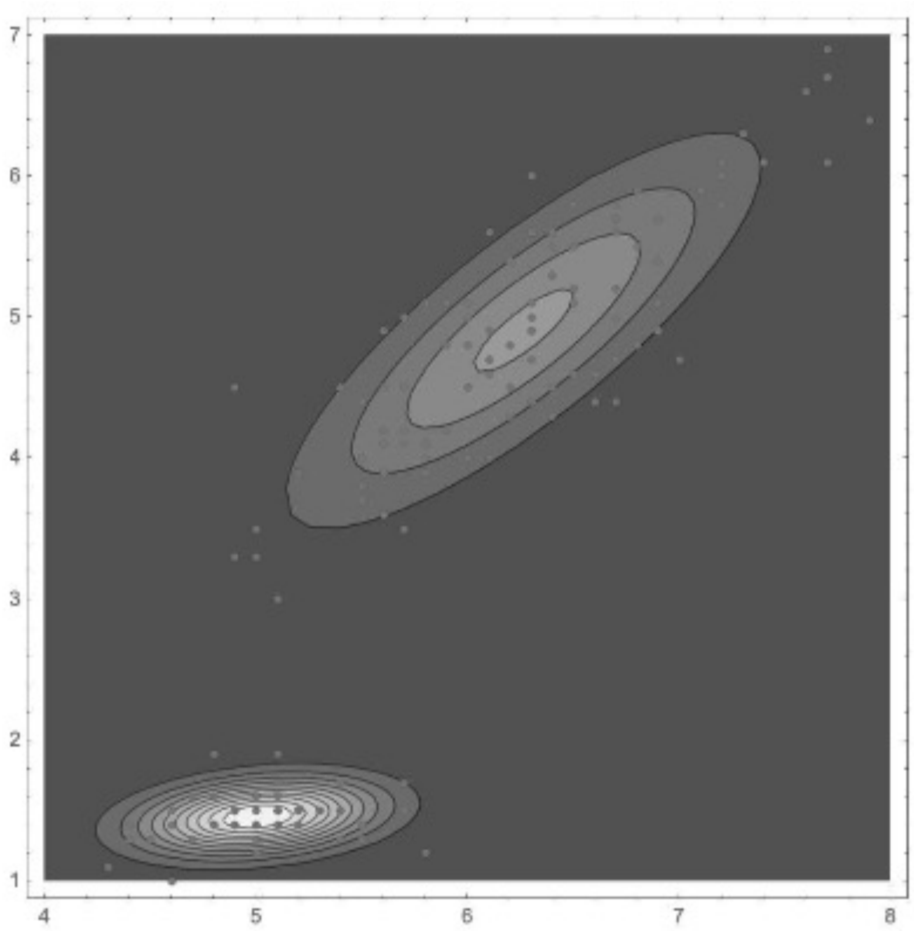
$$o = \operatorname{sgn}(net) = \begin{cases} 1 & if \quad net \ge 0 \\ -1 & if \quad net < 0 \end{cases}$$

Multilayer Perceptron

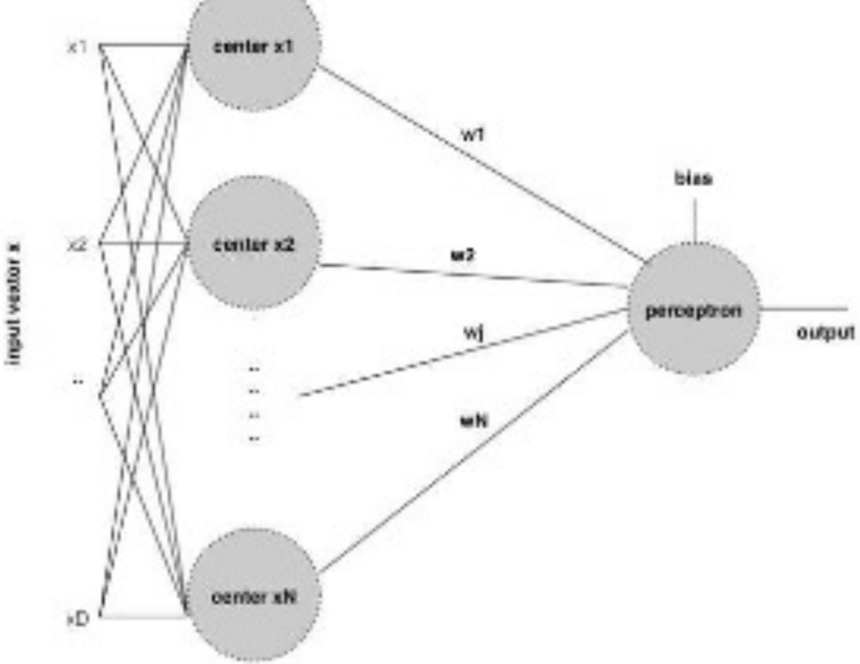




K-Means, EM-Clustering

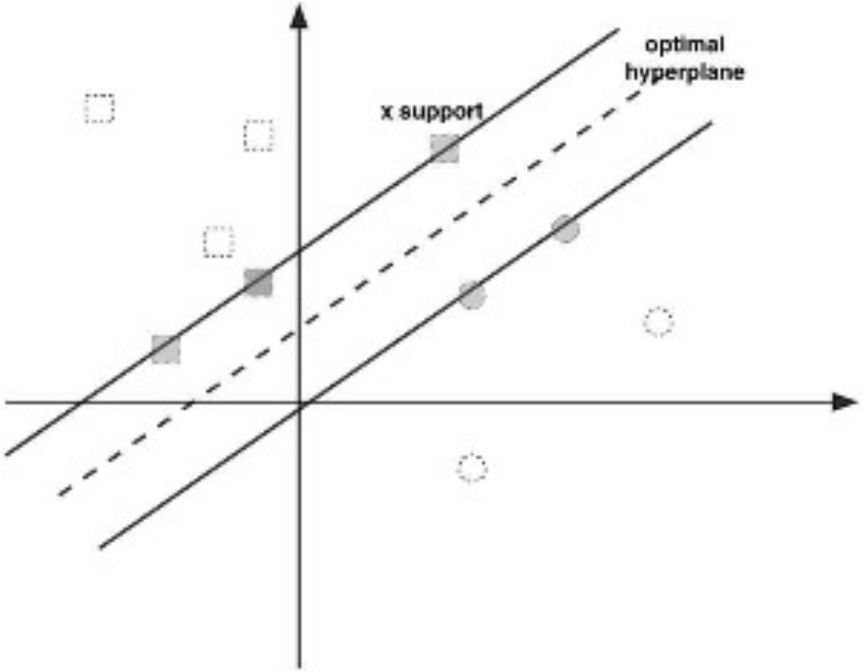


Kernel Methods and RBF



Micchelli's Theorem interpolation matrix Φ is nonsingular (Gram matrix)
Charles A. Micchelli recieved a doctor honoris causa from the university of Zaragoza (Spain) 1994.

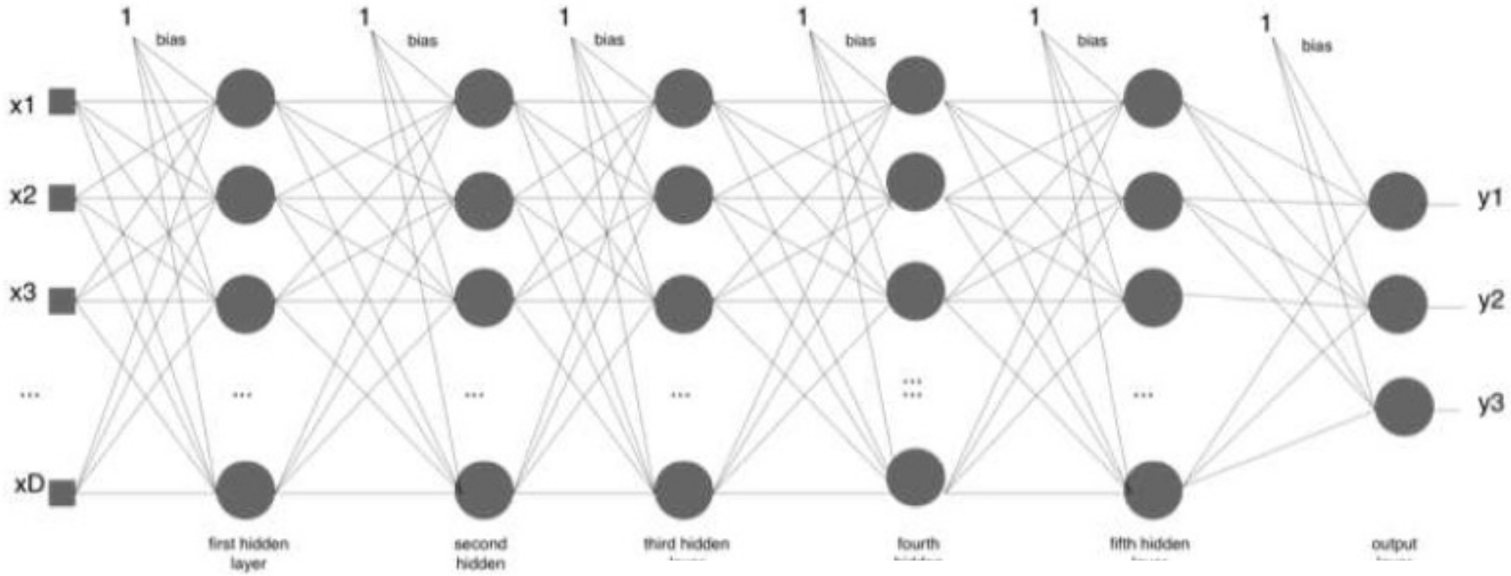
Support Vector Machines

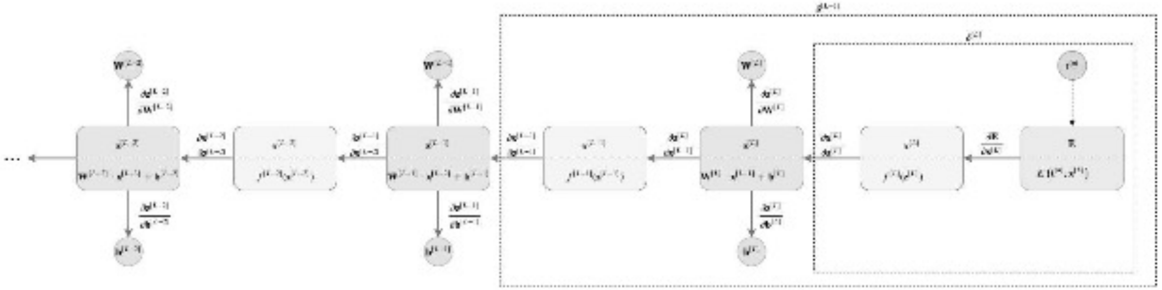


James Mercer (1883 - 1932) was a British mathematician. **Mercer’s theorem**, which states that positive-definite kernels can be expressed as a dot product in a high-dimensional space

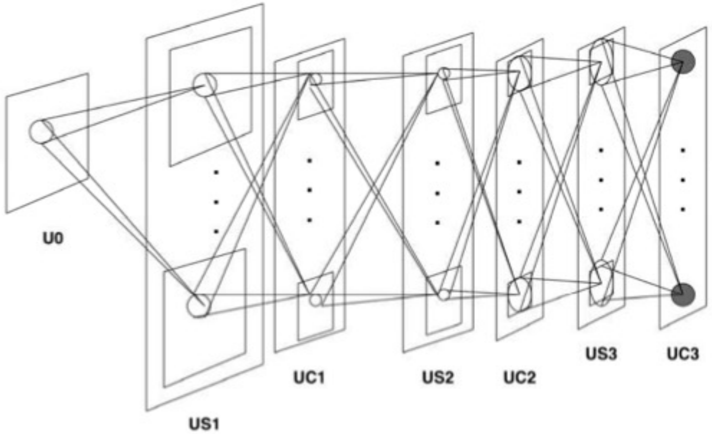
Corinna Cortes is a Danish computer scientist that developed together with Vladimir Vapnik the SVM learning algorithm

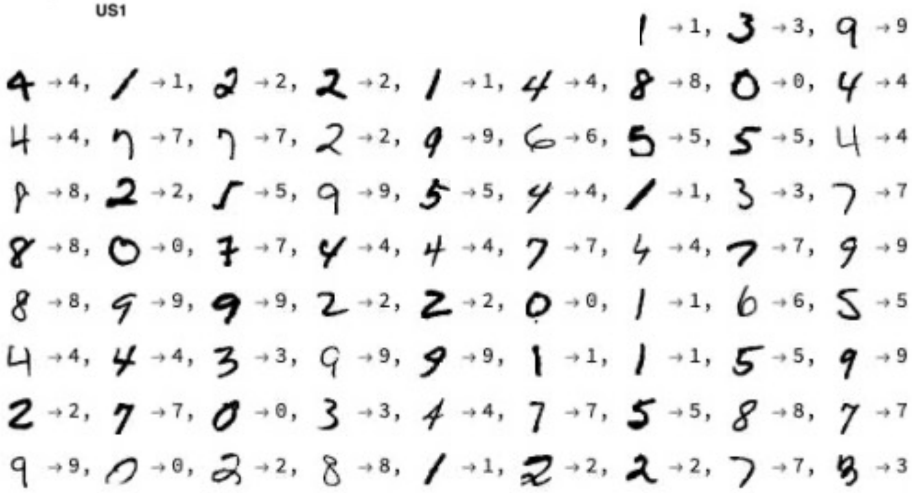
Deep Learning





Convolutional Neural Networks





What Is Quantum Physics?

- Statistical laws govern the totality of observations in physics.
- An object can be described in classical mechanics by a vector which describes the position and its momentum.
- Classical mechanics is usually valid at the macro scale.
- The changes in the position and the momentum of the object over time are described by the Hamiltonian equation of motion
- At micro scale the observations are described by quantum physics

- Light appears only in chunks that can be quantized
- An individual chunk is called quantum, a quantum of light is called a photon
- Quantum theory gets its name from this property, which it attributes to all measurable physical quantities
- A photon can be described by a wave function if it is isolated from its environment
- The wave function in quantum mechanics, if unobserved, evolves in a smooth and continuous way according to Schrödinger equation

Schrödinger Equation

- This equation describes a linear superposition of different states at time *t*, which is represented by the vector ***x(t)***

$$i \cdot h \cdot \frac{d}{dt}\mathbf{x}(t) = H \cdot \mathbf{x}(t)$$

  - with *i* =$\sqrt{-1}$ and *h* being the Planck's constant.
    - For simplification we set *h = 1*.
  - *H* is the Hamiltonian operator, which is related to the total energy of the system.

H is the Hamiltonian operator

- H self-adjoint operator is represented by a Hermitian matrix $H^* = H$ with $h_{ij} = h_{ji}^*$.
- For real values the Hermitian matrix is a symmetrical matrix with $H^T = H$.
- Example:

$$\begin{bmatrix} 0 & a-ib & c-id \\ a+ib & 1 & m-in \\ c+id & m+in & 2 \end{bmatrix}$$

  - The diagonal elements must be real, as they must be their own complex conjugate

Unitary Evolution

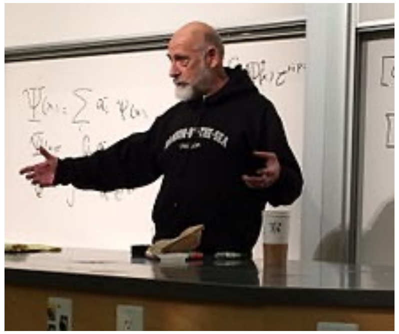
- A general solution of the Schrödinger equation (for the time-independent Hamiltonian) represents the unitary evolution with

$$\mathbf{x}(t) = e^{-i \cdot t \cdot H} \cdot \mathbf{x}(0) = U_t \cdot \mathbf{x}(0)$$

- where $U_t = e^{-i \cdot t \cdot H}$ is the evolutionary operator, which can be represented by a unitary matrix
- In Unitary matrices, its conjugate transpose is equal to its inverse

  $U^* = U^{-1}$

- Unitary evolution is **deterministic and reversible**



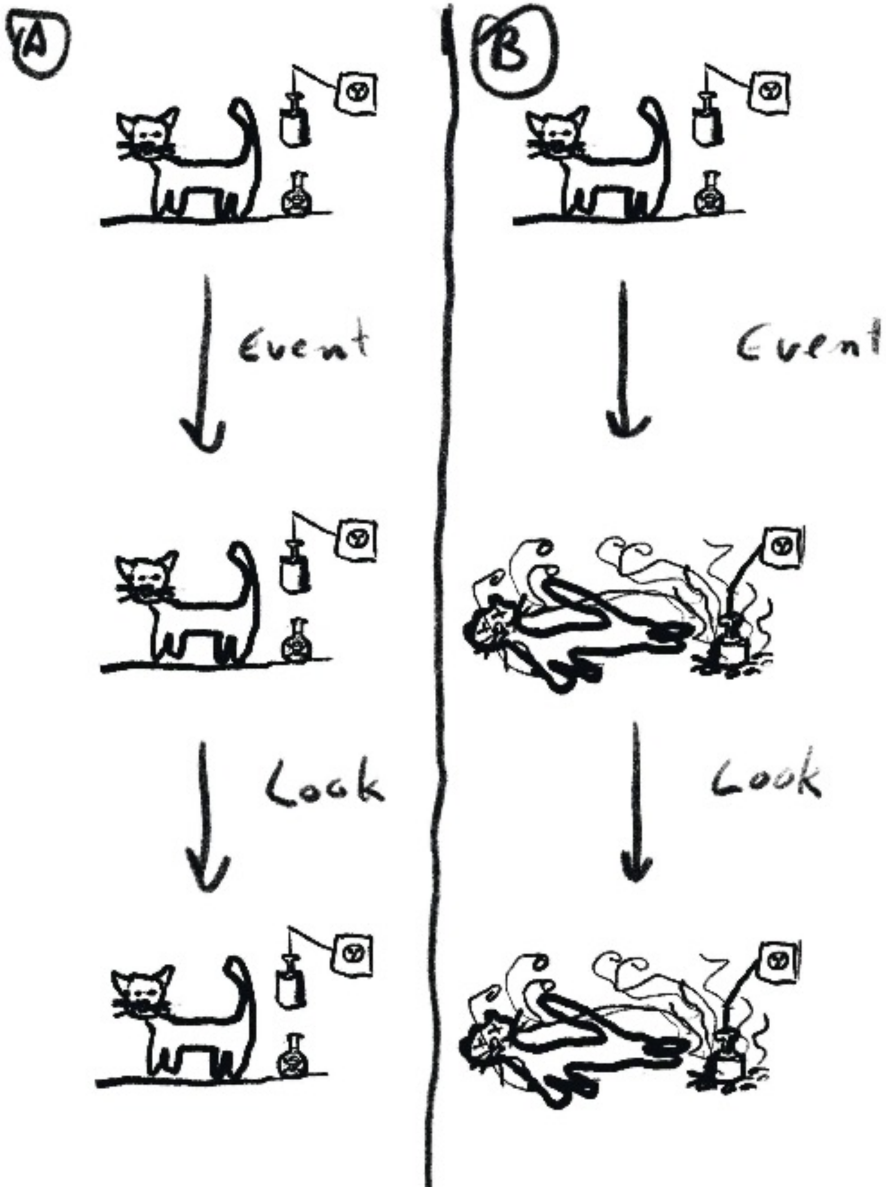
- Reversible means that no information is lost
  - According to Susskind this is the “Zero law” of physics
- For example, a NOT gate is reversible in the sense that one can infer the output from the input
- However, neither the AND or OR gates are reversible in the sense that one cannot infer the output from the input.
- For example:

(1 AND *0)=(0* AND *1)=(0* AND *0)=0*

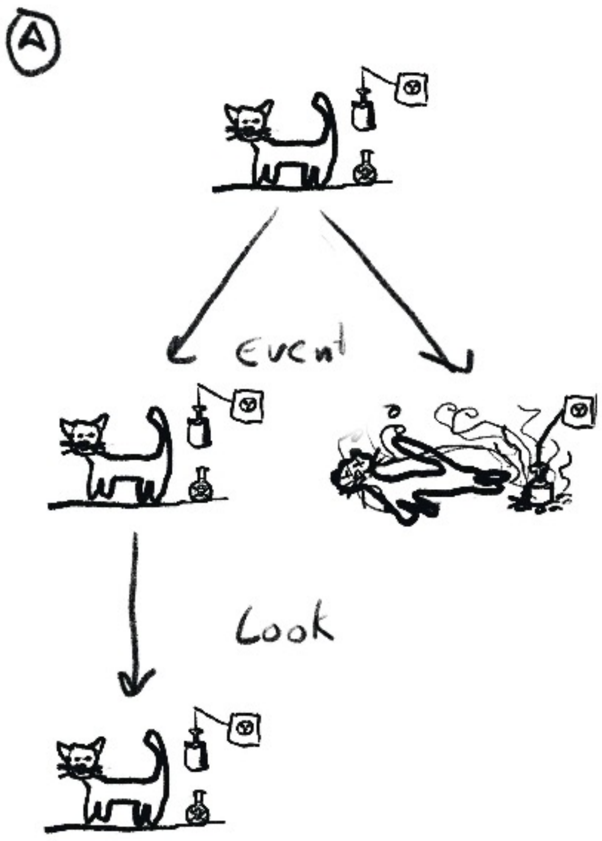
Bennett (1973) showed that irreversible overwriting of one bit causes at least k · T · log2 joules of energy dissipation, where k is Boltzmann’s constant and T is the absolute temperature

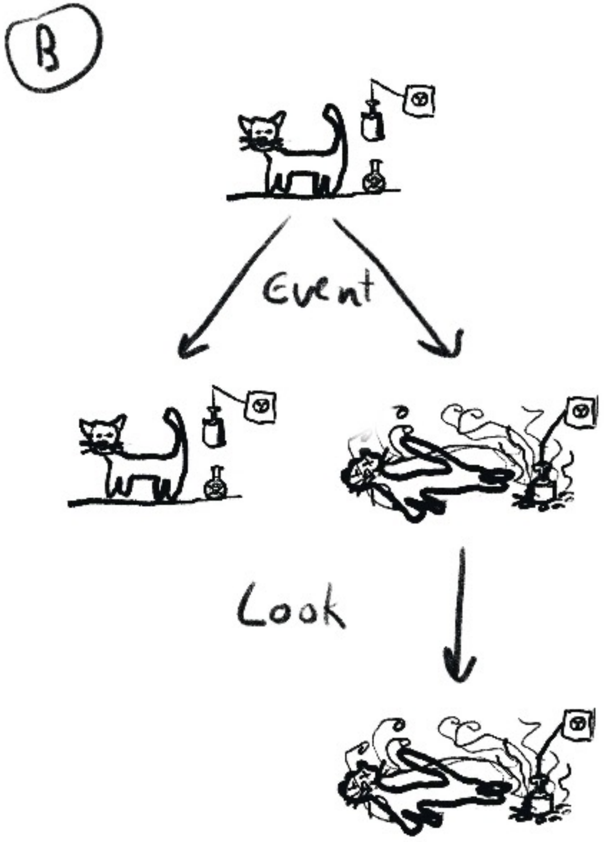
- Unitary evolution is deterministic and reversible
- The vector ***x**(t)* (wave function) describes the probability of the presence of certain states when measured
- Measurements always find the physical system to be in a definite state, which does something to the wavefunction represented by the vector ***x**(t)*
- This state corresponds to one dimension of the vector ***x**(t)*
- It does something to the wave function represented by the vector ***x**(t)*
  - *This something is not explained by quantum theory*

Classical Physics



Quantum Physics



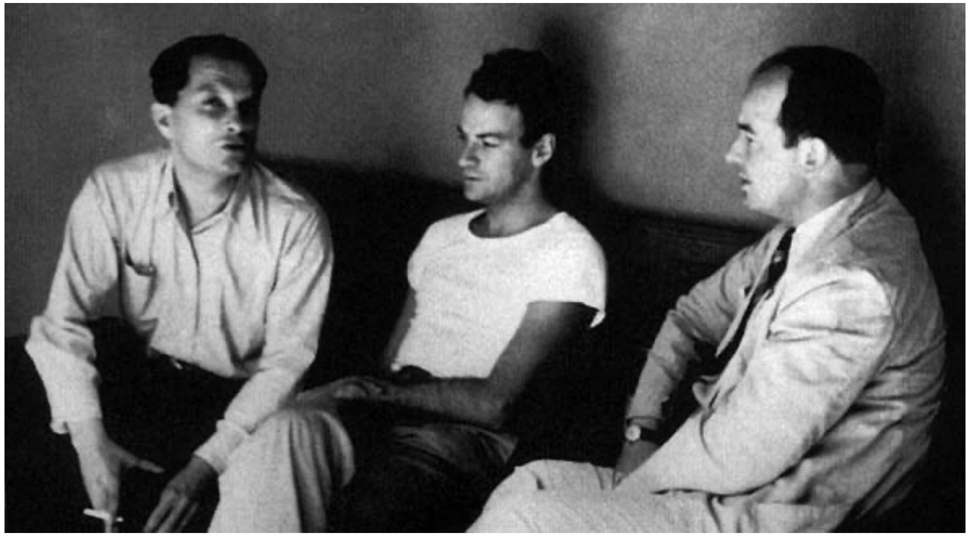


- A quantum system that is perfectly isolated maintains its wave representation, its coherence.
- If it is not perfectly isolated, during interaction with the environment the wave representation of an event is lost, this is called the quantum decoherence.
- Quantum decoherence happens during the measurement.
- Decoherence is usually viewed as the loss of information from a system into the environment.
- Since quantum systems are not isolated a large scale (macro scale), the effects are mostly present at the scale of atoms, and subatomic particles (micro scale)

Two Common Interpretations

- The most popular interpretation, the Copenhagen interpretation
    - Quantum mechanics is a mathematical tool that is used in the calculation of probabilities and has no physical existence; all other questions are metaphysical and should be avoided.

- The many-worlds theory views reality as a many-branched tree in which every possible quantum outcome is realized.
    - Every possible outcome to every event exists in its own world.
    - In one world, randomness exists, but not in the universe (multiverse) that describes all possible worlds



Stanislaw Ulam, Richard Feynman, John Von Neumann

- The hypothesis that the universe is equivalent to a Turing machine, which is related to the Church-Turing thesis, is similar to that stated in digital physics.
- Richard Feynman observed in the early eighties that it did not appear possible for a Turing machine to simulate certain quantum physical processes without incurring an exponential slowdown.
- This fact would contradict the strong Church-Turing thesis, which led Feynman to ask whether a quantum system can be simulated on an imaginary quantum computer.

- Strong Church-Turing thesis:
  - Any physically reasonable algorithmic process can be simulated on a Turing machine, with at most a polynomial slowdown in the number of steps required to do the simulation
- Deutsch: Maybe computers based on quantum mechanics might violate the strong Church-Turing thesis?

Strong Church-Turing thesis

- New formulation:

- The strong Church-Turing thesis implies that the problems in P are precisely those for which a polynomial-time solution is the best possible, in any **physically reasonable** model of computation

- In quantum computation there are two principles (algorithms) that speed up the computation by changing the probability distribution so that we can measure the desired solution.
- In addition to their being “faster” and their ability to generate true randomness, quantum computers have identical computational power to a Turing machine
- The access of the corresponding information has some additional costs

Representation

- Described by a vector in Hilbert space.
  - Extends the two- or three-dimensional Euclidean space into spaces that have any finite or infinite number of dimensions.
  - In such a space, the Euclidean norm is induced by the inner product

$$\|\mathbf{x}\| = \sqrt{\langle \mathbf{x} | \mathbf{x} \rangle}.$$

- Without a scalar product there is no orthogonality.
- In a Hilbert space, two vectors are orthogonal if and only if the scalar product is zero

A 2-state system

- For the basis "*computational basis*" $\mathbf{e}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \mathbf{e}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$
  - the system is described by a vector **x**= $\begin{pmatrix} \omega_1 \\ \omega_2 \end{pmatrix}$

  with complex numbers ω_1, ω_2 that represent the amplitude of each dimension

  - The probabilities are real numbers between 0 and 1
  - The probability that the system is in $\mathbf{e}_1$ and $\mathbf{e}_2$ is $|\omega_1|_2$ and $|\omega_2|_2$

$$\omega^* \cdot \omega = (x - y \cdot i) \cdot (x + y \cdot i) = x^2 + y^2 = |\omega|^2.$$

This is because the product of complex number with is conjugate is always a real number

- The vector representing a state is normalized
- Its length in l_2 norm is **one**. The amplitudes correspond to the probability with

$$\omega^* \cdot \omega = (x - y \cdot i) \cdot (x + y \cdot i) = x^2 + y^2 = |\omega|^2.$$

- Paul Dirac introduced the following notation for a vector **x** describing a state

$$|x\rangle = \omega_1 \cdot |e_1\rangle + \omega_2 \cdot |e_2\rangle = \omega_1 \cdot |x_1\rangle + \omega_2 \cdot |x_2\rangle = \begin{pmatrix} \omega_1 \\ \omega_2 \end{pmatrix}$$

$$|e_1\rangle = |x_1\rangle, |e_2\rangle = |x_2\rangle.$$

Bra(c)ket Notation (Dirac notation)

- It is a shorthand notation for a column vector.
- Related to the scalar product $\langle \mathbf{x}|\mathbf{x}\rangle$
- row vector are $\langle \mathbf{x}|$ "bra"
- column vectors are $|\mathbf{x}\rangle$ "kets" from bra(c)kets
- A state vector is just a particular instance of a ket vector. It is specified by a particular **choice of basis** and refers to **observable** that can have some system properties
  - However, we will use the *computational basis* $\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$, …

Linear Operators

- The operators are represented by unitary matrices

  inverse matrix is the conjugate transpose of the matrix

$$U^* = U^{-1}$$

- A **quantum coin** is a system with two basis states 0 and 1 with

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

- And the mapping:

$$|0\rangle \rightarrow \frac{1}{\sqrt{2}} \cdot |0\rangle + \frac{1}{\sqrt{2}} \cdot |1\rangle$$

$$|1\rangle \rightarrow \frac{1}{\sqrt{2}} \cdot |0\rangle - \frac{1}{\sqrt{2}} \cdot |1\rangle.$$

Destructive Interference

- The corresponding operator is indicated by

$$H = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} = \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

  - called a Hadamard (*H*) or Hadamard Walsh (*W*), matrix

- If the system starts in state $|0\rangle$ and undergoes the time evolution,

$$|0\rangle \rightarrow \frac{1}{\sqrt{2}} \cdot |0\rangle + \frac{1}{\sqrt{2}} \cdot |1\rangle$$

the probability of observing 0 or 1 is $\left|\frac{1}{\sqrt{2}}\right|^2 = \frac{1}{2}$.

Compound Systems

$$|x_1\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |x_2\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$|x\rangle = \omega_1 \cdot |x_1\rangle + \omega_2 \cdot |x_2\rangle = \begin{pmatrix} \omega_1 \\ \omega_2 \end{pmatrix}$$

- corresponds to a qubit with the basis $|0\rangle = |x_1\rangle, \quad |1\rangle = |x_2\rangle.$
- The unitary matrix *H* (Hadamard matrix) performs the following mapping in the ket notation

$$H \cdot |0\rangle = \frac{1}{\sqrt{2}} \cdot |0\rangle + \frac{1}{\sqrt{2}} \cdot |1\rangle$$

- And the vector notation

$$\frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

Quantum Coin Evolution

$$H \cdot \left(\frac{1}{\sqrt{2}} \cdot |0\rangle + \frac{1}{\sqrt{2}} \cdot |1\rangle \right) = H \cdot \frac{1}{\sqrt{2}} \cdot |0\rangle + H \cdot \frac{1}{\sqrt{2}} \cdot |1\rangle = |0\rangle$$

$$\frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \cdot \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

- Comparing to stochastic Markov evolution
  - Information is lost
- Modeling a coin:
  - the fixed distribution is reached after one step

$$\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \end{pmatrix} = \begin{pmatrix} \frac{p_1+p_2}{2} \\ \frac{p_1+p_2}{2} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{pmatrix} \cdot \begin{pmatrix} p_1 \\ p_2 \end{pmatrix}$$

Two Qubits

- The register of two qubits is represented as a direct product of |**x**⟩ and |**y**⟩

$$|x\rangle \otimes |y\rangle = |x\rangle|y\rangle = |xy\rangle = \begin{pmatrix} \omega_0 \\ \omega_1 \end{pmatrix} \otimes \begin{pmatrix} \omega_0 \\ \omega_1 \end{pmatrix} = \begin{pmatrix} \omega_0 \cdot \omega_0 \\ \omega_0 \cdot \omega_1 \\ \omega_1 \cdot \omega_0 \\ \omega_1 \cdot \omega_1 \end{pmatrix} = \begin{pmatrix} \omega_0 \\ \omega_1 \\ \omega_2 \\ \omega_3 \end{pmatrix}$$

$$|xy\rangle = (\omega_0 \cdot |0\rangle + \omega_1 \cdot |1\rangle) \otimes (\omega_0 \cdot |0\rangle + \omega_1 \cdot |1\rangle)$$

$$|xy\rangle = \omega_0 \cdot |00\rangle + \omega_1 \cdot |01\rangle + \omega_2 \cdot |10\rangle + \omega_3 \cdot |11\rangle$$

Computational Basis

- New basis for two qubits $|xy\rangle = \omega_0 \cdot |00\rangle + \omega_1 \cdot |01\rangle + \omega_2 \cdot |10\rangle + \omega_3 \cdot |11\rangle$

$$|00\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, |01\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, |10\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, |11\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

  - A register of three qubits represents 2^3 different states represented in a Hilbert space

$$|xyz\rangle = |x\rangle \otimes |y\rangle \otimes |z\rangle =$$

$$\omega_0 \cdot |00\rangle + \omega_1 \cdot |001\rangle + \omega_2 \cdot |010\rangle + \omega_3 \cdot |011\rangle +$$

$$+\omega_4 \cdot |100\rangle + \omega_5 \cdot |001\rangle + \omega_6 \cdot |110\rangle + \omega_7 \cdot |111\rangle.$$

n-dimensional Hilbert space

- A quantum register of length *m* represents *m* qubits in a Hilbert space of dimension $n = 2^m$.
- A state in a n-dimensional Hilbert space $\boldsymbol{H}_n$ is defined by an orthonormal basis

$$|x_1\rangle, |x_1\rangle, \cdots |x_n\rangle$$

- and is represented as a unit-length vector

$$\omega_1 \cdot |x_1\rangle + \omega_2 \cdot |x_2\rangle + \cdots + \omega_n \cdot |x_n\rangle$$

- The state is in a basis state $|\mathbf{x}_i\rangle$ with a probability $|\omega_i|^2$

Compound System

- The compound system of the Hilbert space $\boldsymbol{H}_n$ and a w-dimensional Hilbert space $\boldsymbol{H}_w$ defined by an orthonormal basis $|\mathbf{y}_1\rangle$, $|\mathbf{y}_1\rangle. \cdots |\mathbf{y}_w\rangle$ is defined by the tensor product $\mathcal{H}_{n\cdot w} = \mathcal{H}_n \otimes \mathcal{H}_w$

$$H \cdot (\omega_0 \cdot |0\rangle + \omega_1 \cdot |1\rangle) \otimes H \cdot (\omega_0 \cdot |0\rangle + \omega_1 \cdot |1\rangle) =$$

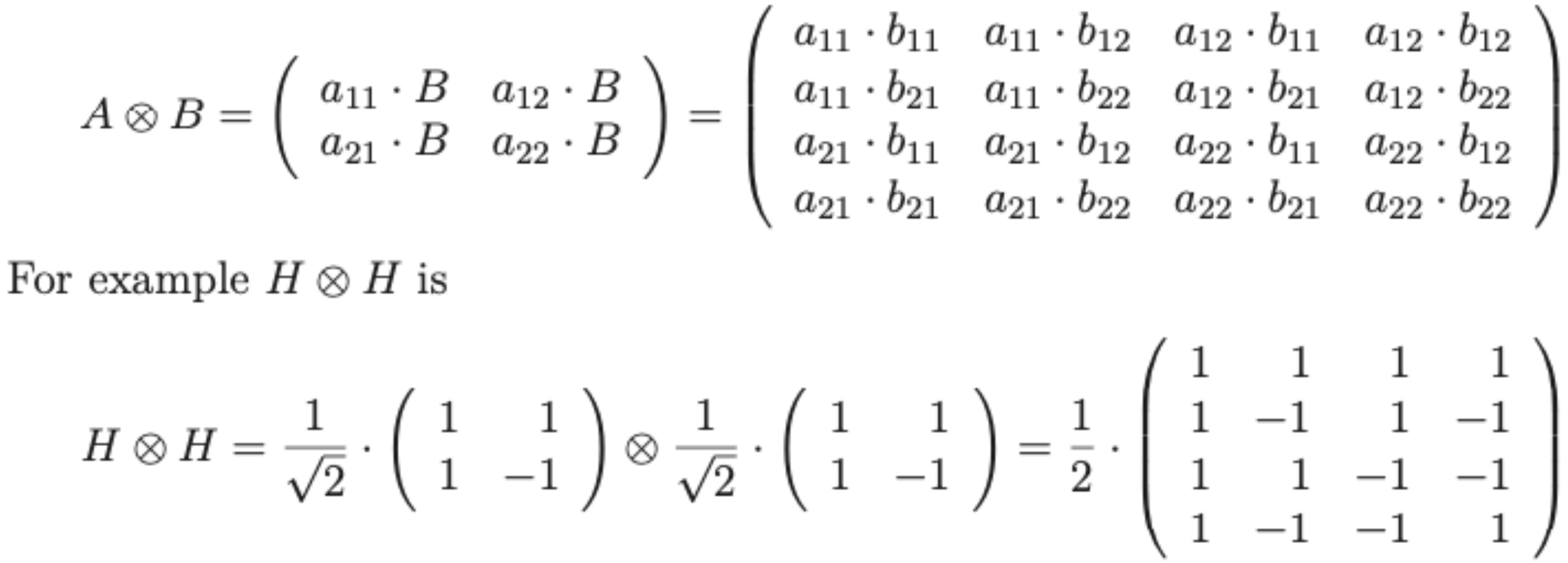
$$\left(H \cdot \begin{pmatrix} \omega_0 \\ \omega_1 \end{pmatrix}\right) \otimes \left(H \cdot \begin{pmatrix} \omega_0 \\ \omega_1 \end{pmatrix}\right)$$

$$(H \otimes H) \cdot (\omega_0 \cdot |0\rangle + \omega_1 \cdot |1\rangle) \otimes (\omega_0 \cdot |0\rangle + \omega_1 \cdot |1\rangle) = (H \otimes H) \cdot \begin{pmatrix} \omega_0 \\ \omega_1 \\ \omega_2 \\ \omega_3 \end{pmatrix}$$

it follows

$$\left(H \cdot \begin{pmatrix} \omega_0 \\ \omega_1 \end{pmatrix}\right) \otimes \left(H \cdot \begin{pmatrix} \omega_0 \\ \omega_1 \end{pmatrix}\right) = (H \otimes H) \cdot \begin{pmatrix} \omega_0 \\ \omega_1 \\ \omega_2 \\ \omega_3 \end{pmatrix}.$$

Tensor Product between Matrices



$$A \otimes B = \begin{pmatrix} a_{11} \cdot B & a_{12} \cdot B \\ a_{21} \cdot B & a_{22} \cdot B \end{pmatrix} = \begin{pmatrix} a_{11} \cdot b_{11} & a_{11} \cdot b_{12} & a_{12} \cdot b_{11} & a_{12} \cdot b_{12} \\ a_{11} \cdot b_{21} & a_{11} \cdot b_{22} & a_{12} \cdot b_{21} & a_{12} \cdot b_{22} \\ a_{21} \cdot b_{11} & a_{21} \cdot b_{12} & a_{22} \cdot b_{11} & a_{22} \cdot b_{12} \\ a_{21} \cdot b_{21} & a_{21} \cdot b_{22} & a_{22} \cdot b_{21} & a_{22} \cdot b_{22} \end{pmatrix}$$

For example $H \otimes H$ is

$$H \otimes H = \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{1}{2} \cdot \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}$$

Measurement

- The measurement corresponds to the collapse of the state vector, a projection into **one** basis state
- The projection is not reversible and it is not consistent with the unitary time evolution

$$\begin{tikzcd}
\omega_1 \cdot |x_1\rangle + \omega_2 \cdot |x_2\rangle + \cdots + \omega_n \cdot |x_n\rangle \arrow[d, "\text{Measurement}"] \\
1 \cdot |x_k\rangle.
\end{tikzcd}$$

Measurement of Compound System

- The state of a compound system is projected to the subspace that corresponds to the observed state
- The vector representing the state is renormalized to the unit length
- An observable describes a subspace for some dimensions with a special case of one dimension
- A part of the system can be observed by a projection in a subspace with a dimension higher one

- The compound system of n-dimensional Hilbert space |**x**⟩ ∈ $\boldsymbol{H}_n$ and a w-dimensional Hilbert space **|y⟩ ∈ $\boldsymbol{H}_w$** defined by an orthonormal basis |**xy**⟩ ∈ $\boldsymbol{H}_{n\cdot w}$

$$|xy\rangle = \sum_{i=1}^{n}\sum_{j=1}^{w} \omega_{ij}|x_i\rangle|y_j\rangle.$$

Example:

$$|xy\rangle = \sum_{i=1}^{2}\sum_{j=1}^{2} \omega_{ij}|x_i\rangle|y_j\rangle =$$

$$= \omega_{11}\cdot|x_1\rangle|y_1\rangle + \omega_{12}\cdot|x_1\rangle|y_2\rangle + \omega_{21}\cdot|x_2\rangle|y_1\rangle + \omega_{22}\cdot|x_2\rangle|y_2\rangle$$

$$|xy\rangle = \omega_0\cdot|00\rangle + \omega_1\cdot|01\rangle + \omega_2\cdot|10\rangle + \omega_3\cdot|11\rangle$$

$$|xy\rangle = \sum_{i=1}^{n} \sum_{j=1}^{w} \omega_{ij} |x_i\rangle |y_j\rangle$$

- The probability of observing $\boldsymbol{x}_k$ is $\sum_{j=1}^{w} |\omega_{kj}|^2$

- If we observe $\boldsymbol{x}_k$, the system after the observation is projected into

$$|xy\rangle = \frac{1}{\sqrt{\sum_{j=1}^{w} |\omega_{kj}|^2}} \sum_{j=1}^{w} \omega_{kj} |x_k\rangle |y_j\rangle.$$

- Suppose the two qubits are in the following state

$$\sqrt{0.25} \cdot |00\rangle + \sqrt{0.25} \cdot |01\rangle + \sqrt{0.25} \cdot |10\rangle + \sqrt{0.25} \cdot |11\rangle = \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}$$

- The observed first qubit is |0⟩. The probability of the observation is

$$|\omega_{00}|^2 + |\omega_{01}|^2 = |\omega_0|^2 + |\omega_1|^2 = |\sqrt{0.25}|^2 + |\sqrt{0.25}|^2 = 0.25 + 0.25 = 0.5$$

- The system after the observation is projected into

$$\frac{\sqrt{0.25} \cdot |00\rangle + \sqrt{0.25} \cdot |01\rangle}{\sqrt{0.5}} = \sqrt{0.5} \cdot |00\rangle + \sqrt{0.5} \cdot |01\rangle = \begin{pmatrix} \sqrt{\frac{1}{2}} \\ \sqrt{\frac{1}{2}} \\ 0 \\ 0 \end{pmatrix}$$

Computation with one Qubit

- NOT gate X does the not operation on a qubit

$$X|0\rangle = |1\rangle, X|1\rangle = |0\rangle$$

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

- It is represented by the unitary matrix

$$X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Square Root of the NOT gate

$$X = \sqrt{X} \cdot \sqrt{X} \qquad \sqrt{X} = \begin{pmatrix} \frac{1+i}{2} & \frac{1-i}{2} \\ \frac{1-i}{2} & \frac{1+i}{2} \end{pmatrix}$$

$$X = \begin{pmatrix} \frac{1+i}{2} & \frac{1-i}{2} \\ \frac{1-i}{2} & \frac{1+i}{2} \end{pmatrix} \cdot \begin{pmatrix} \frac{1+i}{2} & \frac{1-i}{2} \\ \frac{1-i}{2} & \frac{1+i}{2} \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

Unitary because:

$$\begin{pmatrix} \frac{1+i}{2} & \frac{1-i}{2} \\ \frac{1-i}{2} & \frac{1+i}{2} \end{pmatrix} \cdot \begin{pmatrix} \frac{1-i}{2} & \frac{1+i}{2} \\ \frac{1+i}{2} & \frac{1-i}{2} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

$$\sqrt{X}\,|0\rangle = \frac{1+i}{2}\cdot|0\rangle + \frac{1-i}{2}\cdot|1\rangle$$

$$\sqrt{X}\,|1\rangle = \frac{1-i}{2}\cdot|0\rangle + \frac{1+i}{2}\cdot|1\rangle$$

- The probability of measuring |0⟩ and |1⟩ is 0.5

$$\left|\frac{1-i}{2}\right|^2 = \left|\frac{1+i}{2}\right|^2 = \frac{1}{2}$$

Computation with m Qubits

$$|0000\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, |0001\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, |0010\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \cdots, |1111\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

- A Hadamard operator for m qubits H_m is represented by a $2^m \times 2^m$ dimensional matrix built by a direct product of m H_1 matrices.

$$H_m = \bigotimes^m H_1 = H_1 \otimes H_1 \cdots \otimes H_1$$

$$H_m = \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} H_{m-1} & H_{m-1} \\ H_{m-1} & -H_{m-1} \end{pmatrix}$$

$$H_3 = H_1 \otimes H_1 \otimes H_1$$

$$H_3 = \frac{1}{\sqrt{2}} \cdot \begin{pmatrix} H_2 & H_2 \\ H_2 & -H_2 \end{pmatrix} = \frac{1}{\sqrt{2^3}} \cdot \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 & 1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 \end{pmatrix}$$

$$\begin{aligned} H_3|000\rangle &= H_1|0\rangle \otimes H_1|0\rangle \otimes H_1|0\rangle = \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right) \cdot \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right) \cdot \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right) \\ &= \frac{1}{\sqrt{2^3}} \left(|000\rangle + |001\rangle + |000\rangle + |010\rangle + |011\rangle + |100\rangle + |101\rangle + |111\rangle\right) \end{aligned}$$

- The Hadamard operator H_m maps *m* qubits |***z***⟩ representing a basis state in a Hilbert space $\boldsymbol{H}_2^m$ with **z** ∈ B^m (B^m stands for binary string of length m representing a binary number

$$H_m|z\rangle = \frac{1}{\sqrt{2^m}} \sum_{x \in B^m} (-1)^{\langle z|x\rangle} \cdot |x\rangle$$

  - with a scalar product (⟨***z***|***x***⟩) over the binary field with two elements corresponding to the bits 0 and 1

$$0 \cdot 0 = 0 \wedge 0 = 0, \quad 0 \cdot 1 = 0 \wedge 1 = 0, \quad 1 \cdot 0 = 1 \wedge 0 = 0, \quad 1 \cdot 1 = 1 \wedge 1 = 1$$

$$H_2|11\rangle = H_1|1\rangle \otimes H_1|1\rangle = \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right) \cdot \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right)$$

$$H_2|11\rangle = \frac{1}{2} \cdot (|00\rangle - |01\rangle - |10\rangle + |11\rangle)\,.$$

Serial and Parallel Operations

- Serial operations: multiplication of matrices is usually not commutative

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} \cdot \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \neq \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix}$$

$$\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \neq \begin{pmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}$$

- Parallel operations:

$$X \otimes I_1 \otimes H_1 \cdot |000\rangle = (X \cdot |0\rangle) \otimes (I_1 \cdot |0\rangle) \otimes (H_1 \cdot |0\rangle) =$$

$$|10\rangle \cdot \frac{|0\rangle + |1\rangle}{\sqrt{2}} = \frac{|100\rangle + |101\rangle}{\sqrt{2}}$$

$$X \otimes I_1 \otimes H_1 \cdot |000\rangle = (X \cdot |0\rangle) \otimes (I_1 \cdot |0\rangle) \otimes (H_1 \cdot |0\rangle) =$$

$$|10\rangle \cdot \frac{|0\rangle + |1\rangle}{\sqrt{2}} = \frac{|100\rangle + |101\rangle}{\sqrt{2}}$$

$$\left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}\right) \otimes \left(\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}\right) \otimes \left(\begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix}\right) =$$

$$\begin{pmatrix} 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ 0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} & 0 & 0 & 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \\ \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \\ 0 \\ 0 \end{pmatrix}$$

Entanglement

- If two qubits are entangled in a state, then observing one of them will result in the same value of the other one
- Both qubits behave as one unit and are called an ebit
- The two qubits in an ebit behave as one unit, even if the qubits are separated
- Once either qubit of an ebit is measured, the states of both qubits become definite
- Experiments have shown that this correlation can remain even if the qubits are separated over a distance of several kilometers.

Controlled NOT

- The following operator cX is unitary and defends an injective mapping on two qubits that is reversible

$$cX|00\rangle = |00\rangle, \quad cX|01\rangle = |01\rangle,$$

$$cX|10\rangle = |11\rangle, \quad cX|11\rangle = |10\rangle.$$

- The operator cX is called a controlled not gate
  - The first qubit counting from the left is not changed
  - The second qubit is only flipped in the case that the first qubit is 1

CX cannot be expressed as a tensor product of 2×2 matrices

$$CX = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

- We start with the state |00⟩

$$H_1 \otimes I \cdot |00\rangle = (H_1 \cdot |0\rangle) \otimes |0\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes |0\rangle = \frac{|00\rangle + |10\rangle}{\sqrt{2}}$$

- To this state represented by the two qubit we apply CX (=cX) gate

$$CX \cdot \left(\frac{|00\rangle + |10\rangle}{\sqrt{2}} \right) = \frac{CX \cdot |00\rangle + CX \cdot |10\rangle}{\sqrt{2}} = \frac{|00\rangle + |11\rangle}{\sqrt{2}}$$

- $\frac{|00\rangle + |11\rangle}{\sqrt{2}}$ is not decomposable

Proof by Contradiction

$$\frac{|00\rangle + |11\rangle}{\sqrt{2}} = (a_o \cdot |0\rangle + a_1|1\rangle) \otimes (b_o \cdot |0\rangle + b_1|1\rangle) =$$

$$= a_0 \cdot b_0 \cdot |00\rangle + a_0 \cdot b_1 \cdot |01\rangle + a_1 \cdot b_0 \cdot |10\rangle + a_1 \cdot b_1 \cdot |11\rangle$$

$$\rightarrow \quad a_0 \cdot b_0 = \frac{1}{\sqrt{2}}, \quad a_0 \cdot b_1 = 0, \quad a_1 \cdot b_0 = 0, \quad a_1 \cdot b_1 = \frac{1}{\sqrt{2}}$$

- There are four known ebits:

$$\frac{|00\rangle + |11\rangle}{\sqrt{2}}, \quad \frac{|00\rangle - |11\rangle}{\sqrt{2}}, \quad \frac{|01\rangle + |10\rangle}{\sqrt{2}}, \quad \frac{|01\rangle - |10\rangle}{\sqrt{2}}.$$

Cloning

- A linear operation that would produce a copy of an arbitrary quantum state is not possible.
- We cannot copy an unknown amplitude distribution of a state.
- This has profound implications in the field of quantum computing, since we cannot reuse an arbitrary quantum state.

Cloning

$$U_{copy}(|x\rangle, |x_1\rangle) = |x\rangle|x\rangle.$$

- Does U_{copy} exist?
- For basis states U_{copy} is defined.
- It can be realized for example by CX with $|x_1\rangle = |0\rangle$ and $|x_2\rangle = |1\rangle$

$$U_{copy}(|x_1\rangle, |x_1\rangle) = |x_1\rangle|x_1\rangle, \quad U_{copy}(|x_2\rangle, |x_1\rangle) = |x_2\rangle|x_2\rangle.$$

- If the state is in a superposition, it is not defined

$$|x\rangle = \frac{|x_1\rangle + |x_2\rangle}{\sqrt{2}}$$

Proof by Contradiction

$$U_{copy}(|x\rangle, |x_1\rangle) = |x\rangle|x\rangle = \left(\frac{|x_1\rangle + |x_2\rangle}{\sqrt{2}}\right) \otimes \left(\frac{|x_1\rangle + |x_2\rangle}{\sqrt{2}}\right) =$$

$$\frac{1}{2} \cdot (|x_1\rangle|x_1\rangle + |x_1\rangle|x_2\rangle + |x_2\rangle|x_1\rangle + |x_2\rangle|x_2\rangle)\,.$$

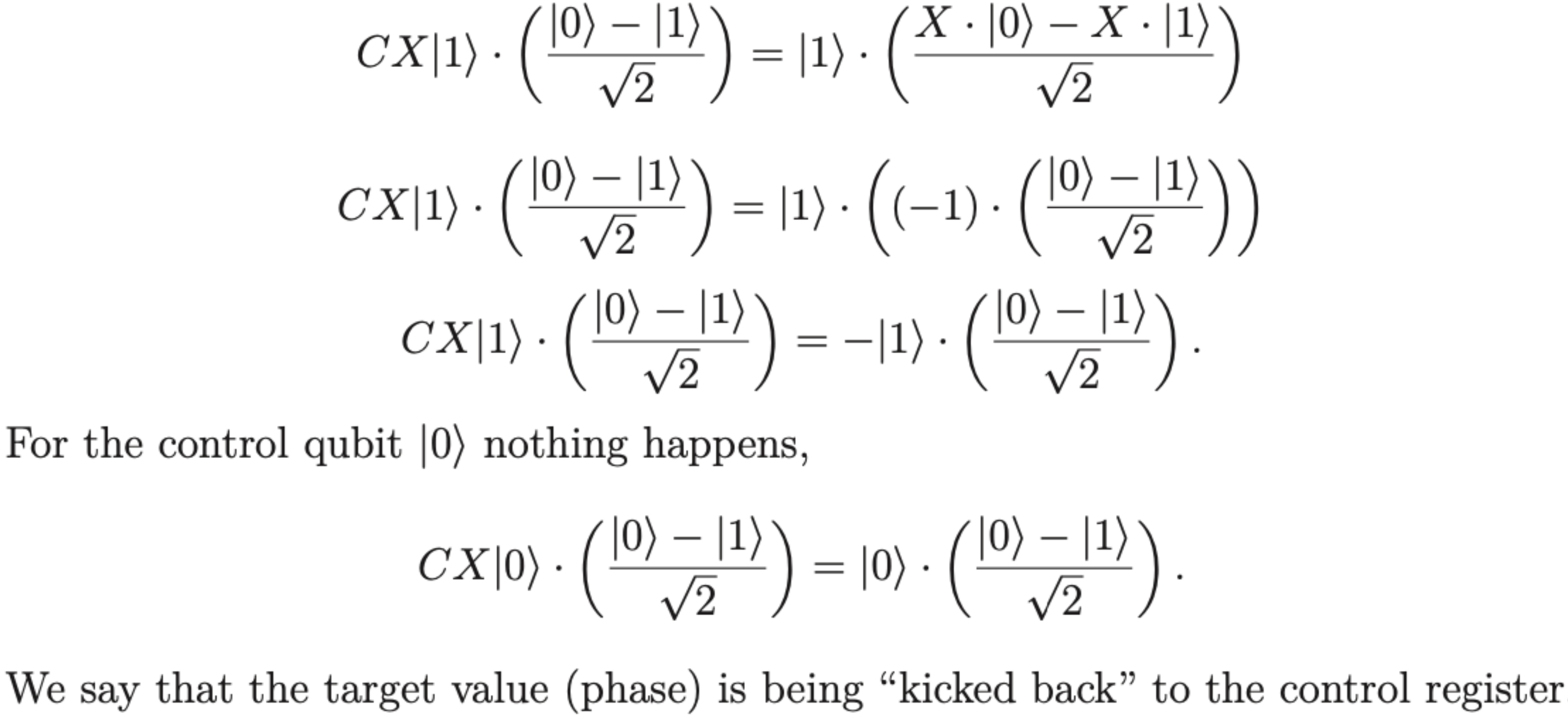
Because of the linearity of U_{copy} it follows,

$$U_{copy}(|x\rangle, |x_1\rangle) = U_{copy}\left(\frac{|x_1\rangle + |x_2\rangle}{\sqrt{2}}, |x_1\rangle\right) =$$

$$U_{copy}(|x\rangle, |x_1\rangle) = U_{copy}\left(\frac{|x_1\rangle|x_1\rangle + |x_2\rangle|x_1\rangle}{\sqrt{2}}\right) =$$

$$\frac{U_{copy}(|x_1\rangle|x_1\rangle) + U_{copy}(|x_2\rangle|x_1\rangle)}{\sqrt{2}} = \frac{1}{\sqrt{2}} \cdot (|x_1\rangle|x_1\rangle + |x_2\rangle|x_2\rangle)$$

Phase Kick-Back



$$CX|1\rangle \cdot \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right) = |1\rangle \cdot \left(\frac{X \cdot |0\rangle - X \cdot |1\rangle}{\sqrt{2}}\right)$$

$$CX|1\rangle \cdot \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right) = |1\rangle \cdot \left((-1) \cdot \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right)\right)$$

$$CX|1\rangle \cdot \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right) = -|1\rangle \cdot \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right).$$

For the control qubit $|0\rangle$ nothing happens,

$$CX|0\rangle \cdot \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right) = |0\rangle \cdot \left(\frac{|0\rangle - |1\rangle}{\sqrt{2}}\right).$$

We say that the target value (phase) is being “kicked back” to the control register

Quantum Boolean Gates

- A reversible Boolean circuit that is composed of *m* bits corresponds to a unitary mapping that represents a permutation on *m* bits, defining an injective mapping $B^m \rightarrow B^m$
- A unitary permutation matrix can represent this unitary mapping
- The following quantum gates are Boolean quantum gates:
  - The identity gate I
  - The not gate X
  - The control not gate cX
    - The control not gate performs the essential fan- out operation

AND and OR

- A reversible Toffoli gate ccX is a unitary mapping
- It defines a quantum gate on **three** qubits and can be represented by a unitary matrix CCX in Hilbert space $\boldsymbol{H}_8$

$$CCX \cdot |xyz\rangle = CCX \cdot |x\rangle|y\rangle|z\rangle = |x\rangle|y\rangle|(x \wedge y) \oplus z\rangle$$

XOR

$$CCX = \begin{pmatrix} I_1 & 0 & 0 & 0 \\ 0 & I_1 & 0 & 0 \\ 0 & 0 & I_1 & 0 \\ 0 & 0 & 0 & X \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

Hilbert space $\boldsymbol{H}_8$

$$|000\rangle = \begin{pmatrix}1\\0\\0\\0\\0\\0\\0\\0\end{pmatrix}, |001\rangle = \begin{pmatrix}0\\1\\0\\0\\0\\0\\0\\0\end{pmatrix}, |010\rangle = \begin{pmatrix}0\\0\\1\\0\\0\\0\\0\\0\end{pmatrix}, |011\rangle = \begin{pmatrix}0\\0\\0\\1\\0\\0\\0\\0\end{pmatrix},$$

$$|100\rangle = \begin{pmatrix}0\\0\\0\\0\\1\\0\\0\\0\end{pmatrix}, |101\rangle = \begin{pmatrix}0\\0\\0\\0\\0\\1\\0\\0\end{pmatrix}, |110\rangle = \begin{pmatrix}0\\0\\0\\0\\0\\0\\1\\0\end{pmatrix}, |111\rangle = \begin{pmatrix}0\\0\\0\\0\\0\\0\\0\\1\end{pmatrix}$$

- The unitary matrix CCX can be decomposed into several ways using non Boolean quantum gates
- However, each decomposition involves the CX matrix, indicating that an entanglement may arise when applying a quantum Toffoli gate

AND and OR

$$CCX \cdot |xyz\rangle = CCX \cdot |x\rangle|y\rangle|z\rangle = |x\rangle|y\rangle|(x \wedge y) \oplus z\rangle$$

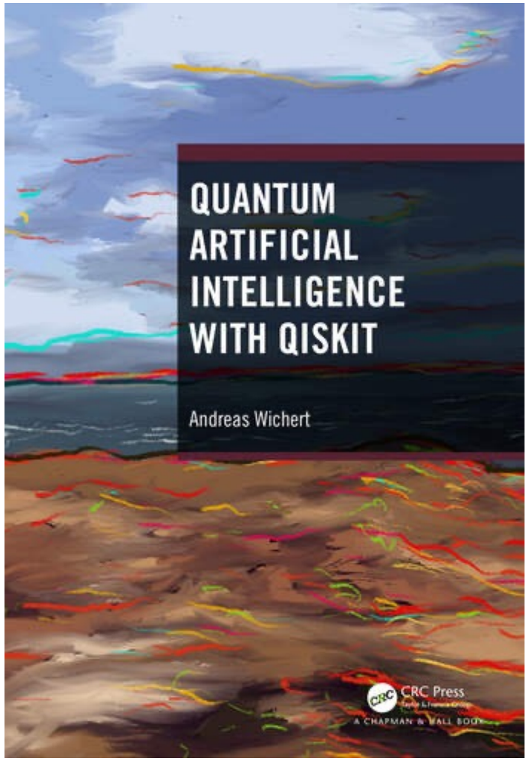
For the *AND* operation, the ancilla bit z is set to 0

$$CCX \cdot |x\rangle|y\rangle|0\rangle = |x\rangle|y\rangle|(x \wedge y)\rangle.$$

The *OR* operation is represented by the unitary mapping according to the De Morgan's laws

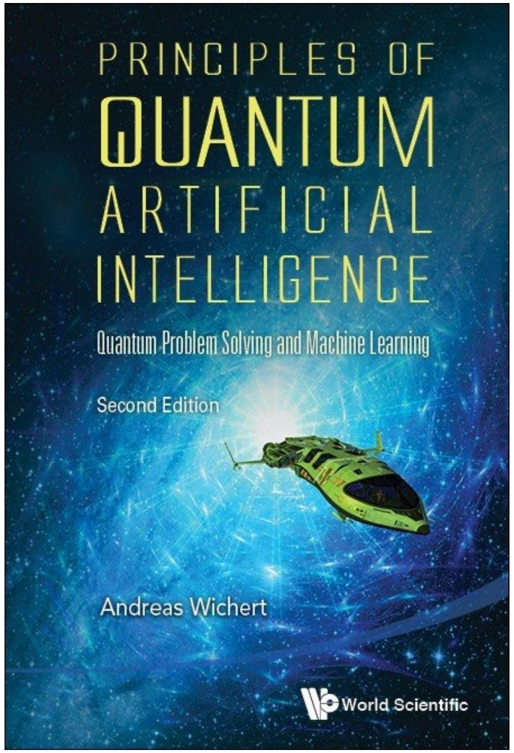
$$x_1 \vee x_2 = \neg(\neg x_1 \wedge, \neg x_2)$$

$$((I_2 \otimes X) \cdot CCX \cdot (X \otimes X \otimes I_1)) \cdot |xy0\rangle = xy(x \vee y)\rangle.$$



- Chapter 1
- Chapter 2

Quantum Artificial Intelligence with Qiskit, A. Wichert, Chapman and Hall/CRC, 2024



- Chapter 1
- Chapter 3
- Chapter 7
- Chapter 8

Principles of Quantum Artificial Intelligence: Quantum Problem Solving and Machine Learning, 2nd Edition, A. Wichert, World Scientific, 2020