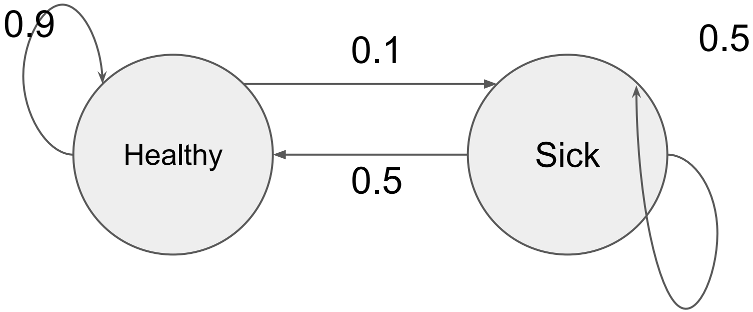
Markov Chain and Matrices Methods

Diego Useche - dh.useche@uniandes.edu.co

Metodos Computacionales I

Physics Department, Universidad de los Andes, Bogotá

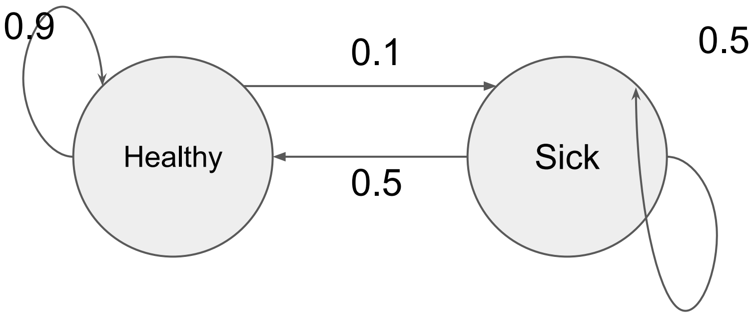
Markov Chain



It can start in any state

T	Healthy	Sick
0	1	0
1	0.9	0.1
2	(0.9*0.9) + (0.1*0.5) = 0.86	(0.9*0.1) + (0.1*0.5) = 0.14
3	(0.86*0.9) + (0.14*0.5) = 0.844	(0.86*0.1) + (0.14*0.5) = 0.156
	...	...
$t \rightarrow \infty$	0.833	0.167

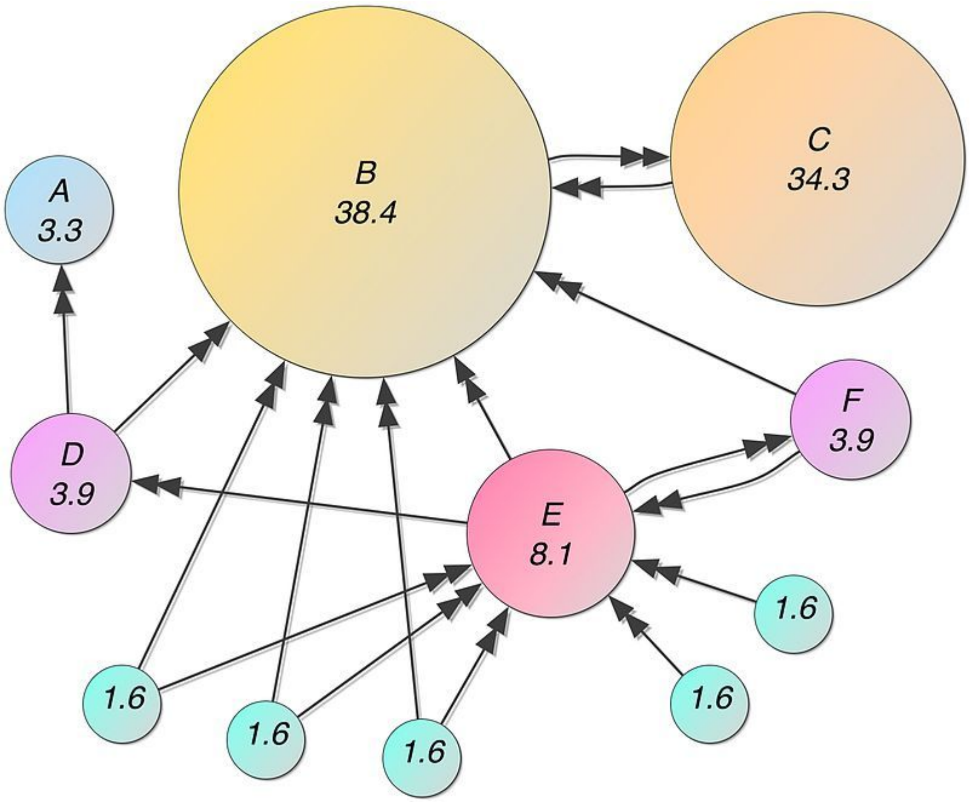
Stationary Distribution



T	Healthy	Sick
$t \rightarrow \infty$	0.833	0.167

Page Rank

- Similar to a Markov Chain to determine the connected web pages.
- Built as product of a PhD research by Sergei Brin and Larry Page.
- Used to improve web searching.
- The origin of google.



Gaussian Elimination Algorithm

$$\begin{bmatrix} 1 & 2 & -1 & 1 \\ 2 & 7 & 4 & 2 \\ -1 & 4 & 13 & -1 \end{bmatrix} \rightsquigarrow \begin{bmatrix} 1 & 2 & -1 & 1 \\ 0 & 3 & 6 & 0 \\ -1 & 4 & 13 & -1 \end{bmatrix}$$

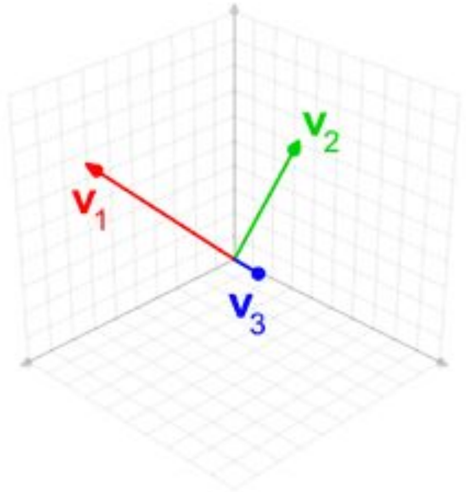
$$\rightsquigarrow \begin{bmatrix} 1 & 2 & -1 & 1 \\ 0 & 3 & 6 & 0 \\ 0 & 6 & 12 & 0 \end{bmatrix} \rightsquigarrow \begin{bmatrix} 1 & 2 & -1 & 1 \\ 0 & 3 & 6 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

QR Decomposition

- Let A and mxn matrix
- Then $A = QR$
  - Where Q is an ortogonal matrix (the rows are all orthonormal) , R is an upper triangular matrix.
- Algorithm
  - Gram–Schmidt Algorithm
- Applications:
  - Least Squares

Gram-Schmidt Algorithm

- Let A be a matrix
- Normalize the first row vector , that is our first orthonormal vector(v1)
- Project the second row vector of A over v1, find the span of the projection and normalize (v2), Etc
- Save the coordinates of the original vectors, on the orthonormal basis, in the R matrix.



QR Decomposition

$$A = \begin{bmatrix} 1 & 3 & 1 \\ 1 & 1 & 1 \\ 1 & -1 & 3 \\ 1 & 1 & 3 \end{bmatrix}$$

$$Q = \begin{bmatrix} 1/2 & 1/\sqrt{2} & 0 \\ 1/2 & 0 & -1/\sqrt{2} \\ 1/2 & -1/\sqrt{2} & 0 \\ 1/2 & 0 & 1/\sqrt{2} \end{bmatrix}$$

$$R = \begin{bmatrix} 2 & 2 & 4 \\ 0 & 2\sqrt{2} & -\sqrt{2} \\ 0 & 0 & \sqrt{2} \end{bmatrix}$$

Spectral Decomposition

- Let A be a symmetric matrix ($A^T = A$)
- Then $A = V\Delta V^T$
  - Where Δ is a diagonal matrix, and V is an orthonormal matrix.
  - Δ is formed by the eigenvalues of A, V by the eigenvectors
- Algorithm
  - QR Algorithm, divide-and-conquer, Jacobi Algorithm , $O(n^3)$
- Applications:
  - Find the eigenstate of a system.

Spectral Decomposition $\quad A = UDU.T$

$$A = \begin{bmatrix} 9 & 3 & 9 \\ 3 & 17 & -3 \\ 9 & -3 & 9 \end{bmatrix};$$

$$\begin{bmatrix} u_1 & u_2 & u_3 \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{38}} & \frac{3}{\sqrt{19}} \\ 0 & -\frac{6}{\sqrt{38}} & -\frac{1}{\sqrt{19}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{38}} & -\frac{3}{\sqrt{19}} \end{bmatrix};$$

$$D = \begin{bmatrix} 18 & 0 & 0 \\ 0 & 18 & 0 \\ 0 & 0 & -1 \end{bmatrix}$$

https://www.chegg.com/homework-help/

QR Algorithm

Find a series of unitary operations

$$(U_k^* \cdots U_1^*)A(U_1 \cdots U_k) \to T \text{ (triangular) as } k \to \infty.$$

$$A = \begin{matrix} 1 & 1 & 1 & 1 & 1 \\ 16 & 8 & 4 & 2 & 1 \\ 81 & 27 & 9 & 3 & 1 \\ 256 & 64 & 16 & 4 & 1 \\ 625 & 125 & 25 & 5 & 1 \end{matrix}$$

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>> for k=1:20, [Q,R]=qr(A); A=Q'*A*Q;  end
>> A
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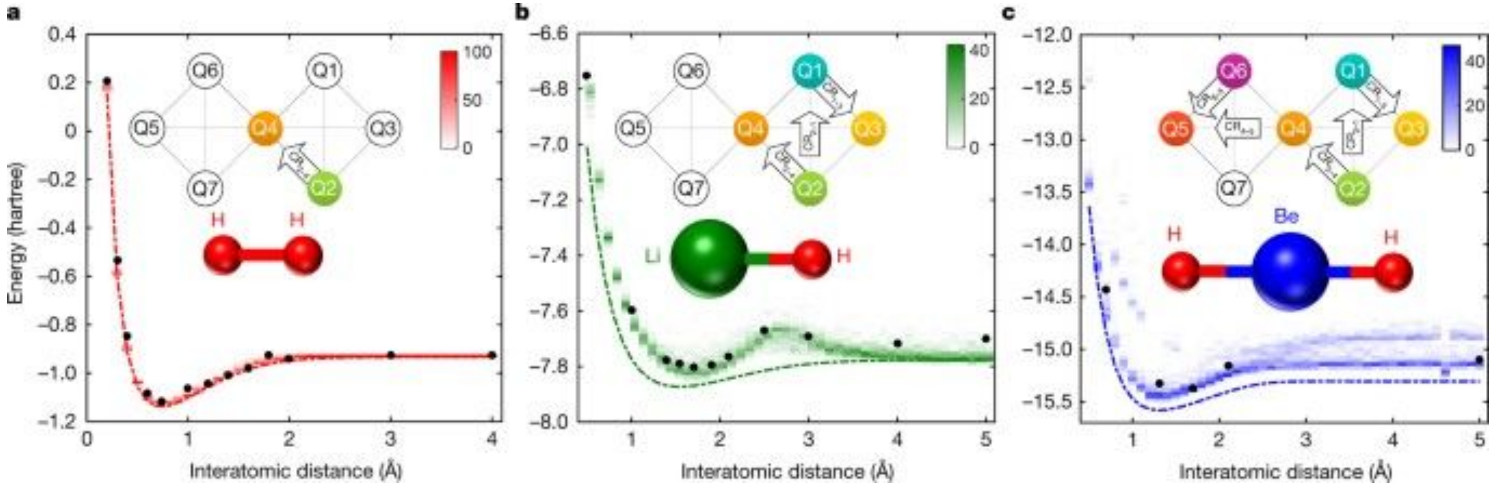
$$\begin{matrix} 45.9604 & \lambda_1 \\ -28.9437 & \\ 6.7954 & \\ -0.8496 & \\ 0.0375 & \lambda_5 \end{matrix}$$

$$A = \begin{matrix} 45.9697 & 333.0696 & -514.7544 & 307.7187 & -66.7932 \\ -0.0021 & -28.9530 & 62.9322 & -47.4590 & 12.6896 \\ -0.0000 & -0.0000 & 6.7954 & -9.3745 & 3.5876 \\ -0.0000 & -0.0000 & 0.0000 & -0.8496 & 0.6473 \\ -0.0000 & -0.0000 & 0.0000 & -0.0000 & 0.0375 \end{matrix}$$

Solving Ground States of Molecules with VQE

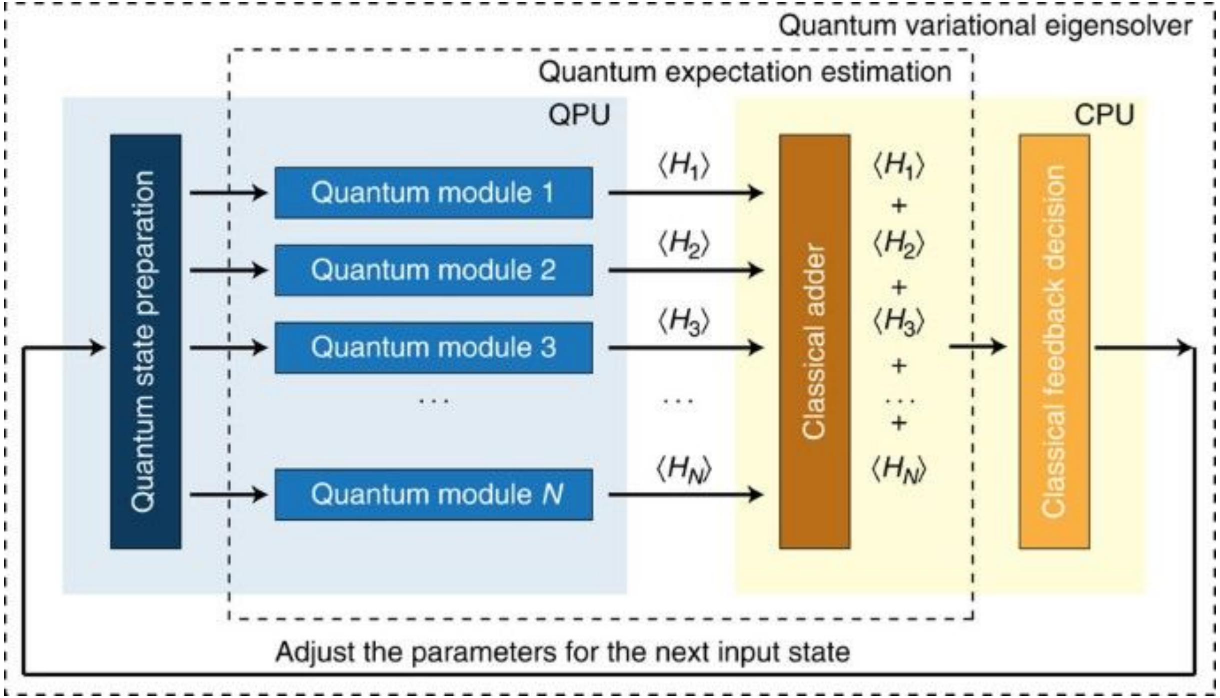
Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets

Abhinav Kandala, Antonio Mezzacapo, Kristan Temme, Maika Takita, Markus Brink, Jerry M. Chow & Jay M. Gambetta



A variational eigenvalue solver on a photonic quantum processor

Alberto Peruzzo, Jarrod McClean, Peter Shadbolt, Man-Hong Yung, Xiao-Qi Zhou, Peter J. Love, Alán Aspuru-Guzik & Jeremy L. O'Brien



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Kandala, A., Mezzacapo, A., Temme, K. *et al.* Hardware-efficient variational quantum eigensolver for small molecules and quantum magnets. *Nature* 549, 242–246 (2017). https://doi.org/10.1038/nature23879

Peruzzo, A., McClean, J., Shadbolt, P. *et al.* A variational eigenvalue solver on a photonic quantum processor. *Nat Commun* 5, 4213 (2014). https://doi.org/10.1038/ncomms5213