# IDC451: Seminar Delivery

## Using Genetic Algorithms to calculate $\Psi_{gs}$

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Saturday 16$^{th}$ October, 2021

1. What are Genetic Algorithms?
2. Applying to quantum systems

## Introduction

It is a computational optimization scheme which imitates natural selection in nature. Optimization generally refers to such a problem:

| | |
|---|---|
| Maximize/Minimize: | $y = f(x)$ |
| Subject to constraints: | $g_i(x) = 0; \quad x \in [x_i, x_f]$ |

The key idea is "survival of the fittest" $\rightarrow$ fitter members pass on their genes more often than the weaker members. Stated without proof, the net effect is evolution of the population towards an optimum.

# The Algorithm

1. Generate initial population of N individuals $\rightarrow$ encode.
2. Calculate cost functions $\rightarrow$ assign fitness. (**Selection**)
3. Sort the population based on fitness $\rightarrow$ reproduce to create new generation. (**Crossover**)
4. Replace weakest member of the new gen with best member of previous gen.
5. Replace old gen with the new gen, and repeat (2-5).
6. **When do we break the loop?**

# A simple example

Consider the problem of maximizing

$$f(x) = (x - 15)(x - 20)(x - 70)$$

such that $x \in [0, 63]$ is an integer

- **Encoding:** Integer $\rightarrow$ 6-bit binary string
- **Cost/Fitness**: $f(x)$
- **Crossover:** ??

# Crossover

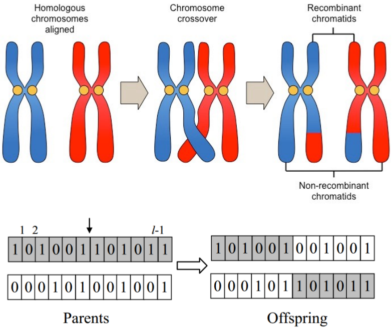


Figure 1: Crossing over in (a) real chromosomes[4] (b) bit string[5]

# Results

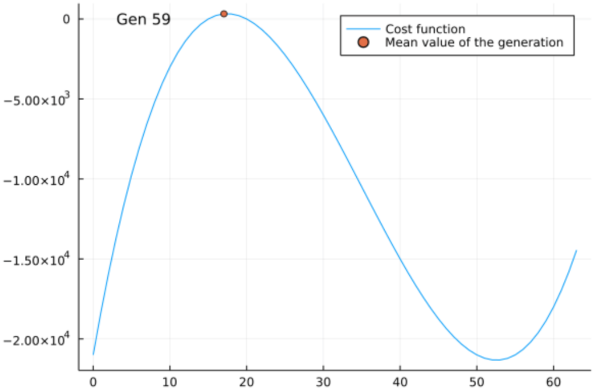


Figure 2: Results of the algorithm for $f(x) = (x - 15)(x - 20)(x - 70)$.

# The problem statement

We will restrict ourselves to a 1-D discussion here. Given a potential V(x), we must determine the ground state energy, $E_{gs}$ and wavefunction $\Psi_{gs}(x)$ such that:

$$\left[-\frac{1}{2}\frac{d^2}{dx^2} + V(x)\right]\Psi_{gs}(x) = E_{gs}\Psi_{gs}$$

The cost/fitness function is the energy:

$$E = \frac{\langle\psi|\, H \,|\psi\rangle}{\langle\psi|\psi\rangle} \geq E_{gs}$$

# The chromosomes

Choose discretized domain:

$$\{x_0, x_1, ..., x_N\} \quad \leftarrow \quad x_k = x_i + (k-1) \cdot \Delta x$$

Discretized wave-function will be:

$$\Psi(x) \equiv [\Psi(x_0), \Psi(x_1), ..., \Psi(x_N)] \quad \leftarrow \quad \text{chromosomes}$$

Crossover mechanism:

$$\Psi_1^{new}(x) = S(x) \cdot \Psi_1^{old}(x) + (1 - S(x)) \cdot \Psi_2^{old}(x)$$

$$\Psi_2^{new}(x) = (1 - S(x)) \cdot \Psi_1^{old}(x) + S(x) \cdot \Psi_2^{old}(x)$$

# The chromosomes (Contd.)

Smooth crossover function:

$$S(x) = \frac{1}{2}\left(1 + \tanh\left((x - x_0)/k_c^2\right)\right)$$

- $x_0 \in [x_i, x_f]$ chosen randomly.
- $k_c$ - parameter to tune the sharpness of crossover.

# Calculating the energy

Discrete evaluation of the energy integral:

$$\langle\Psi| H |\Psi\rangle = [\Psi \cdot (H\Psi^T)] \cdot \Delta x$$

Second derivative can be evaluated by a central difference scheme:

$$\frac{d^2 f(x_n)}{dx^2} = \frac{f(x_{n+1}) - 2f(x_n) + f(x_{n-1})}{(\Delta x)^2}$$

# Calculating the energy (Contd.)

More explicitly, this can be done by the following matrix multiplications:

$$\frac{d^2\Psi}{dx^2} = \frac{1}{(\Delta x)^2}\begin{pmatrix} -2 & 1 & 0 & \dots & \dots & \dots & 0 \\ 1 & -2 & 1 & 0 & . & . & . \\ 0 & 1 & -2 & 1 & 0 & . & . \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ . & . & 0 & 1 & -2 & 1 & 0 \\ . & . & . & 0 & 1 & -2 & 1 \\ 0 & \dots & \dots & \dots & 0 & 1 & -2 \end{pmatrix}\begin{pmatrix} \Psi(x_0) \\ \Psi(x_1) \\ \vdots \\ \vdots \\ \Psi(x_{n-1}) \\ \Psi(x_n) \end{pmatrix}$$

# Results

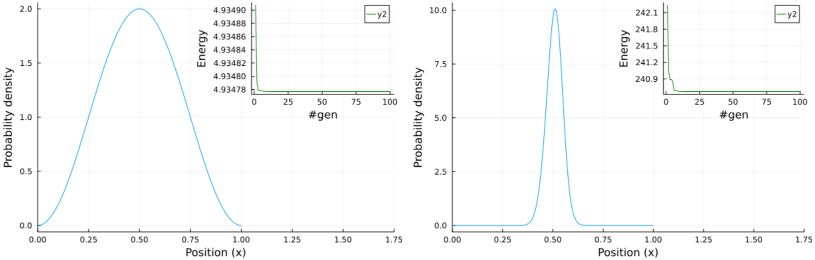


Figure 3: Results for (a) Inf. sq. well (b) Harmonic potential

# Results (Contd.)

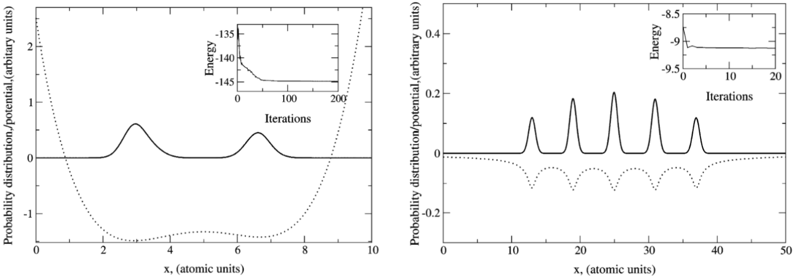


Figure 4: Results for V(x)[3]

$$(a) k_0 - k_2x^2 + k_3x^3 + k_4x^4 \qquad (b) \sum_{i=1}^{5} \frac{Q}{(x-x_i)^2 + a^2}$$

# Results (Contd.)

Working in atomic units; $m_e = \hbar = e = 1$. The ground state energy of Inf. sq. well is given by:

$$E_{gs} = \frac{\pi^2}{2a^2} \approx 4.93480 \text{ a.u.}$$

Obtained valued was: $E_{gs} = 4.93478$ which is within a margin of $10^{-3}$ %. For a more detailed analysis, refer the paper[3] by Grigorenko, M.E Garcia.

`https://github.com/20akshay00/GeneticAlgorithm`

# References I

[1] Jitendra R Raol and Abhijit Jalisatgi, *From Genetics to Genetic Algorithms*, Resonance Aug 1996 [LINK]

[2] *Efficiency of genetic algorithm and determination of ground state energy of impurity in a spherical quantum dot*, arXiv:cond-mat/0403249 [LINK]

[3] I Grigorenko, M.E Garcia, *An evolutionary algorithm to calculate the ground state of a quantum system*, Physica A: Statistical Mechanics and its Applications, Volume 284, Issues 1-4, 2000, Pages 131-139.

[4] *Crossing Over,* [LINK]

[5] Yu and M. Gen, *Introduction to Evolutionary Algorithms*, ser. Decision Engineering. Springer, 2010.