IDC451: Seminar Delivery

Using Genetic Algorithms to calculate Ψ_{gs}

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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 → encode.
2. Calculate cost functions → assign fitness. (**Selection**)
3. Sort the population based on fitness → 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

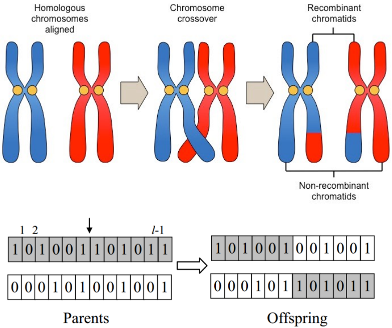

Figure 1: Crossing over in (a) real chromosomes[4] (b) bit string[5]

Results

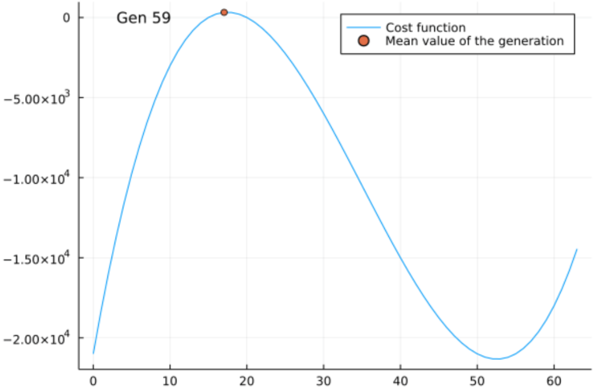

Figure 2: Results of the algorithm for $f(x) = (x - 15)(x - 20)(x - 70)$.

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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:

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

Discretized wave-function will be:

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

Crossover mechanism:

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

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

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

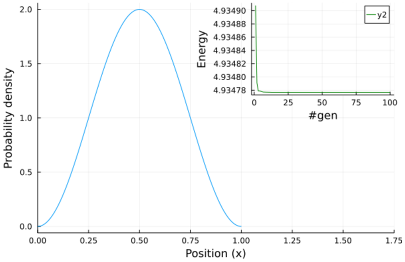
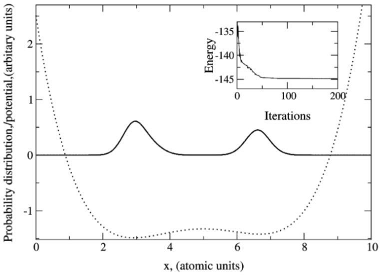


Figure 3: Results for (a) Inf. sq. well (b) Harmonic potential

Results (Contd.)



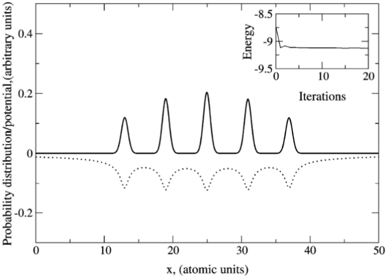


Figure 4: Results for V(x)[3]

(a)$k_0 - k_2x^2 + k_3x^3 + k_4x^4$ (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.