GA for CELL

in here I try to explain what I do in - the GA implementation to find Unit Cell - from experimentall XRD pattern

To do the Genetic Algorithm I defined a class that define a unit cell called

" Cell "

Where giving the
- unit cell params
- wavelenght used
- kind of unit cell
- Unit cell limits

- it defines a cell, allowing me to see if the unit cell params are correct giving the kind of unit cell presented.

Done by the Function "_enforce_structure_constrains"

- it allow me to calculate the expected peaks

Done by the Function "give_theta2"

In this class I define a discrete space for each of the

$a, b, c, \alpha, \beta, \gamma$

(This was done to better explore the Space)

And it allow us to do

- MUTATION: We can have the cell to mutate in three ways

1. Each parameter can alter its value if we choose a random number smaller them change_prob.

It can walk between min_step until max_step defined differently to the lenghts and angles.

2. Change the kind of Structure if we obtain a random number smaller them struct_change_prob

(This may cause problem, so I only use in the "kids")

3. Shuffle the (a,b,c) and (α,β,γ) parameter if we obtain a Random number smaller them change_shuffle

(Done to go to very distant points in space)

after we pass it all I "_enforce_Structure_Constrains"

- CROSSOVER: make a children, by giving other cell I take the average of each parameter giving the weight inherit_prob.

if the cells have different kind of cells it inherit the other

cell only if we randomly get a number smaller than "inherit_cell".

After we do this I generated functions

- diversity: which calculate the distance between two points in a space of

$$(a, b, c, \alpha, \beta, \gamma)$$

to allow me to get a measurement of how far the cells are from the best obtained

- Cosine_fitness: is the minimization function where I generate an array of all possible angle and based on it I generate vectors that have

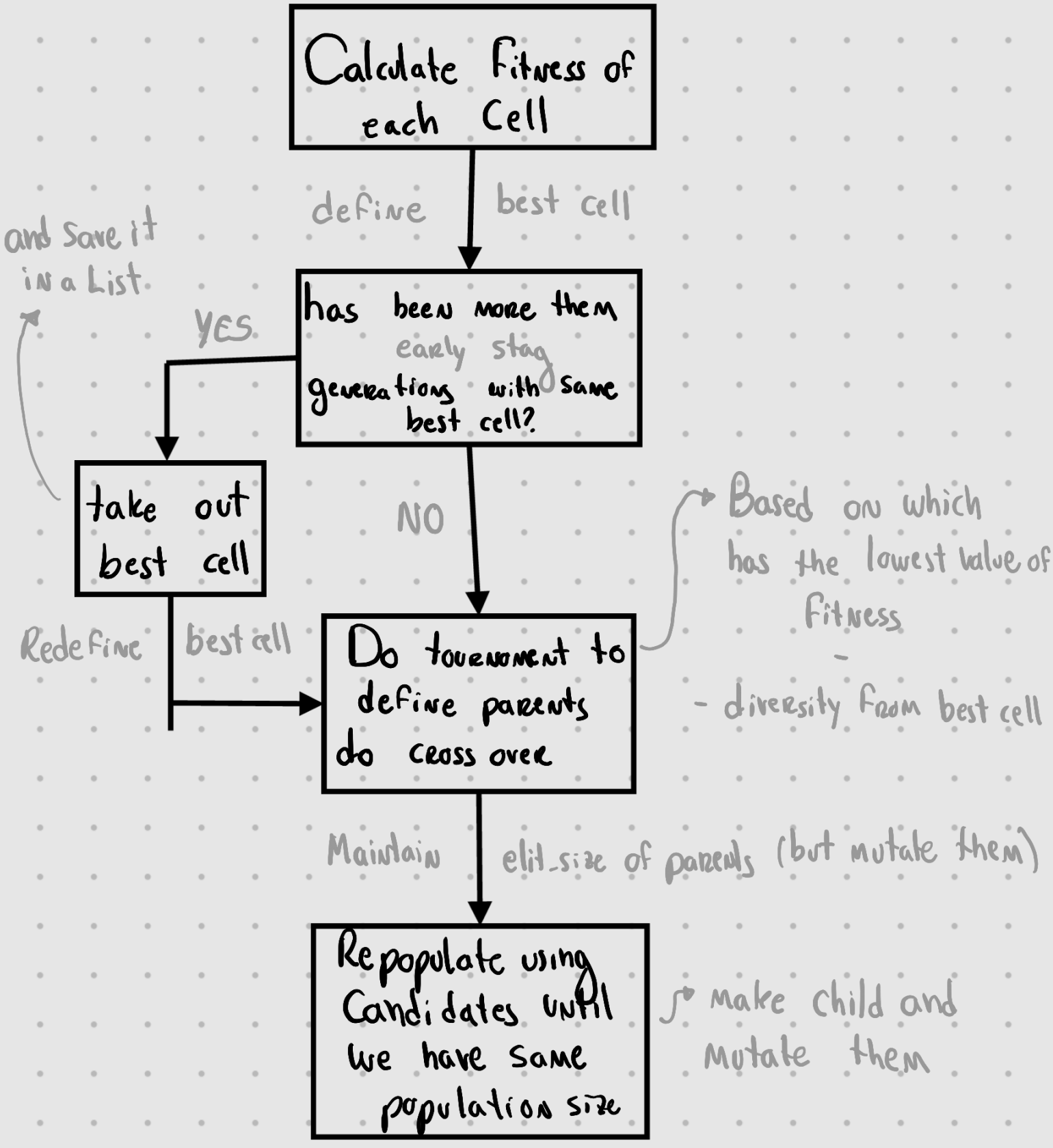
defined by me "can change"
- 0 → No peak in angle
- 30 → if no experimental peak in angle
- intensity of peak → if experimental peak in angle

and I calculate the -Normalized dot product between this vector for exp. peaks and for unit cell peaks.

Giving this I do the Genetic Algorithm through

"RUN_GA_LIST"

Where we generate population giving possible kinds of Unit cell, them follow



do that for a speific number of generation

This way we end up with a List of best cell candidates

(but there may be duplicated cells)

need to fix...