Subject: evolutionary algorithm
Posted by pc419714@ohio.edu on Thu, 21 Feb 2019 21:59:52 GMT
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Thomas,

Could you describe how the evolutionary algorithm was written? I have some scaffolds that it evolved, however I am wondering why the fitness sometimes appears to decrease before increasing in a stepwise fashion. If I had it set up to generate 4096 compounds per generation, unlimited generations, with 32 compounds surviving each generation, and generate compounds similar to my scaffold without anything in the structure selected, how does it determine which compounds to start the next generation with? It just appears to increase and then decrease sometimes.... I thought it would just keep increasing in fitness every time.... Does it just improve upon the lower fitness molecules from the previous generation? How is fitness defined? I read the documentation. I just wondered if you used a formula or anything to make the algorithm.

Thank you

Patrick Chirdon