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Subject: evolutionary algorithm

Posted by [pc419714@ohio.edu](mailto: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

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Subject: Re: evolutionary algorithm

Posted by [thomas](#) on Thu, 07 Mar 2019 16:52:21 GMT

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Hi Patrick,

during the creation of the new generation structures DataWarrior does not look at any fitness criteria. It just creates compounds with small changes from the previous generation, which have not been generated in any of the previous generations. Thus, it may be that the best compound of the generation has a worse fitness than the best compound of the previous generation.

Thomas

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