

Cover letter

Hello.

I have several related implemented projects done for myself:

1. Global optimization better than Multistart (and GlobalOptimization from Matlab). 3 times faster, 90% in global optimum vs 45% in multistart. (Without basins of attractions)

[Global optimization better, than Matlab has](#)

2. Meta model for machine learning. There are many ways to combine different machine learning models to get better results. I get 5% better results than ensemble (mean of many models).

[Ensemble learning with the grid, best model selection, geometrical primitives for any dimension number](#)

How I planned to do research.

Well, that is the quite simple model. We have a convex hull of the RNA, gRNA and a protein where one or two gRNA is located.

And we can specify forms of interactions (Most commonly interaction between those three atoms: N,O,H).

1. So in first we must perform geometrical analysis (how close our target RNA can be located inside our complex). It's a simplest analysis, and I plan to use global optimization with the sum of the distances between nearest N O H as a score function (more links is better).

Or simply build a hashing based on intervals (make a sphere that contains all nearest atoms) and determine how strong that complex binds to each other. (temperature when they unbind or mean radius of "vibrations" from quantum chemistry simulator)

2. Then we must determine distances between most attractive points (more distance we have – more energy we can get from that segment to "break" our binding).

Here I will use another model – sphere, but with respect to the nearest spheres (some linkage vector). And use the same metrics – radius of vibration or unbind temperature.

At that point I will get model of binding anything to anything with some improvised score.

I can use that model to check constructed proteins\gRNA\protein gRNA complexes in a fast way.

That allows me to build better gRNA tools faster and more efficient.

And I already have best Global Optimization method :)