Literature Review

Batch Active Learning for Drug Discovery

rjb255

January 29, 2022

Abstract

Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Etiam lobortis facilisis sem. Nullam nec mi et neque pharetra sollicitudin. Praesent imperdiet mi nec ante. Donec ullamcorper, felis non sodales commodo, lectus velit ultrices augue, a dignissim nibh lectus placerat pede. Vivamus nunc nunc, molestie ut, ultricies vel, semper in, velit. Ut porttitor. Praesent in sapien. Lorem ipsum dolor sit amet, consectetuer adipiscing elit. Duis fringilla tristique neque. Sed interdum libero ut metus. Pellentesque placerat. Nam rutrum augue a leo. Morbi sed elit sit amet ante lobortis sollicitudin. Praesent blandit blandit mauris. Praesent lectus tellus, aliquet aliquam, luctus a, egestas a, turpis. Mauris lacinia lorem sit amet ipsum. Nunc quis urna dictum turpis accumsan semper.

I propose (1) where N represents the dimensionality of the model space, and r_i is the distance between x_j and x_i. The next test point is given by () where X_{known} is the set of labelled data points and X_{unknown} is the set of available data points for testing.

$$\rho_{x_j} = \sum_i \frac{1}{r^N_{x_i,x_j}} \tag{1}$$

$$x_{\text{next}} = \underset{X_{\text{Unknown}}}{\text{argmin}} \sum_{x=X_{\text{Known}}} \frac{1}{r^N_{X_{\text{Unknown}},x}} \tag{2}$$

$$x_{\text{next}} = \underset{x}{\text{argmax}} \left[s_x \times (\text{peakness}\, s_x)^{\alpha} \right]$$