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Curiosity: a tool for exploring maps

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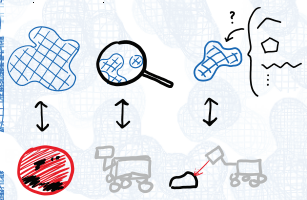
Motivation

There are many tools available for assessing the correctness of a molecular model. We set out instead to find not-yet-modeled features in a map.



Curiosity and its moving parts are named in analogy to the Mars rover. Instead of exploring a planet, we are exploring a map. Our program explores a new combination of map(s) and models on each new "expedition." Each test it conducts on a region of the map is one of the "probes" it is equipped with, and it keeps the results of these tests for later examination by human eyes.

Design

Curiosity is designed to traverse an existing model and search nearby each residue or other component to find recognizable features in the map. These characteristic map features are then used to model the new atoms or make the necessary changes to existing atoms to better fit the density.

Different features can be identified by different "probes," each independently comparing density sampled from one or more maps to their expected patterns. This modular design allows probes to be used only where applicable — on the appropriate residues, for example, or only when the necessary combination of maps is supplied.

Implementation

Curiosity starts with the same basic framework as qPTxM, a similar tool designed specifically to identify posttranscriptional modifications, and is also built with *cctbx/Phenix* tools in python. Instead of choosing specific positions in the map *a priori* that ought to be the most informative points to sample, however, Curiosity reads the map in a 3D grid and feeds all these values into a neural network trained to recognize a given feature. With successful training, the network reduces the dimensionality of the input density values while retaining the most salient features. Networks may be designed to incorporate other sources of information as well, if desired.

Code: https://github.com/fraser-lab/curiosity

Feedback/bugs: irisdyoung-at-gmail.com

Ion Detection Probe

We are first exploring using Curiosity to identify ions mismodeled as waters, recognising them by their coordination environments. In this case we examine each position modeled as a water, normalize an orientation relative to the locations of the nearest two coordination partners, and read a grid of densities 5 Å in each direction at 0.2 Å intervals.

This probe has a precision of 73%, a recall of 70%, and overall 99% accuracy. In the context of the cross-validation dataset...

On a Venn diagram the size of this poster representing all the positions in a map reasonably modeled as waters, about this much should be ions:

And these would be the error rates: