Understanding Performance of Protein Surface Classifiers

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The Problem

Surface classifiers make predictions as to which regions of the molecules have target properties. These classifiers can help determine the functionality of previously uncharacterized proteins and help elucidate the structural features that lead to a particular function. Current strategies for assessing the performance of these structural classifiers depend on aggregate summary statistics, which are insufficient and limit analysis.

MCC = 0.3

Summary statistic PyMol representation Our representation

Visualizing a Solution

To understand how the classifier behaves, we must be able to see performance over the corpus and on the molecule. This suggests an overview+detail visualization. Special considerations need to be made to display spatial data in a way that decreases unnecessary visual complexity and allows inspection of all data.

To investigate performance across the test corpus, the corpus overview uses a re-orderable small multiples framework with glyphs designed for aggregate judgment.

To see data on individual proteins, the molecular detail view uses the protein surface as a scaffold to display spatial classifications and input features in three dimensions. This representation affords bivariate layering using textures and automatic camera touring of classifications.

Corpus Overview

Each protein is represented by a small multiple. The visualization in the glyphs can be changed to afford different views of the data and the corpus can be reordered to discover patterns in performance.

Reordering the corpus

Ordering by MCC score, best for finding outliers; using quilted blocks, best for extracting mean distributions
Ordering by percentage of positive labels, best for discovering the role of initial bias
Ordering by PDB ID, best to regain bearings over the corpus

Changing the glyph

Using the heatmap glyph, best for high-fidelity numerosity judgments
Using the histogram glyph, best for explicit classification distributions
Using the proportion plot glyph, best for determining classification correctness

Detail View

Clustering classifications on the protein surface helps simplify the localization of classifications and transforms a large amount of tiny spatial decisions to a much smaller number of decisions grouped together. This simplifies spatial analysis and allows for automated camera touring.

Using textures to layer classifications over an input variable affords a separable bivariate encoding of features and classification. The user has control over the transfer function for the color.

Changing the decision boundary of the classifications allows the user to reclassify classifier predictions and see the resulting distribution of classifications in the histogram.

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References are available in the abstract submission.