Filling in the blanks

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A key aspect of drug discovery is identifying interactions between disease-causing proteins and potential disease-treating drug compounds. Since conducting experiments on every possible compound-protein pair is far too expensive and time-consuming to be possible, companies, like our collaborators e-Therapeutics, use mathematical techniques to make predictions from a relatively small amount of experimental data.

In many ways, the challenge is similar to that faced in e-commerce by companies such as Netflix, Amazon and Tesco, who are interested in predicting interactions between products and customers. Applications span from identifying speech and language patterns to recommending films and Christmas gifts.

The question we are tackling is whether, by expressing our database as a product of two binary matrices which contain information about patterns of interaction, we can predict interactions. Within the realm of drug discovery, this means finding groups of proteins and compounds that interact with each other. This is particularly useful for complex diseases such as cancer and Alzheimer's disease, where you might be interested in understanding interactions across multiple proteins, or identifying compounds from different areas of chemical space. To answer this question, we've been developing an algorithm that splits the database by patterns of interaction.

The goal of our research is to find accurate, interpretable predictions. In particular, our collaboration with e-Therapeutics offers a cheaper and faster way to develop the drugs needed to tackle the complex diseases that impact so many within society.