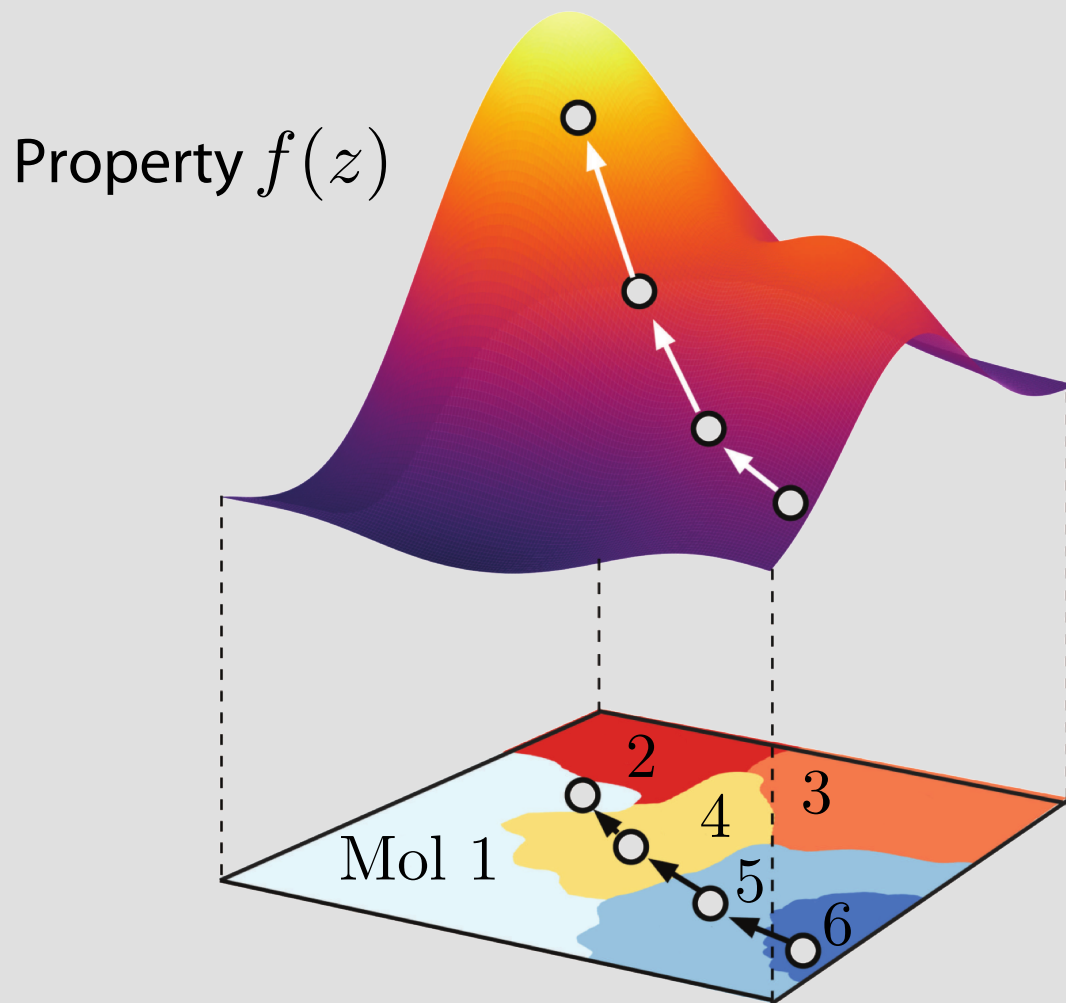


Bayesian optimization



Optimize property like effectiveness against cancer.

While **True**:

1. Find maximum of acquisition function
2. Perform trials on new molecule

