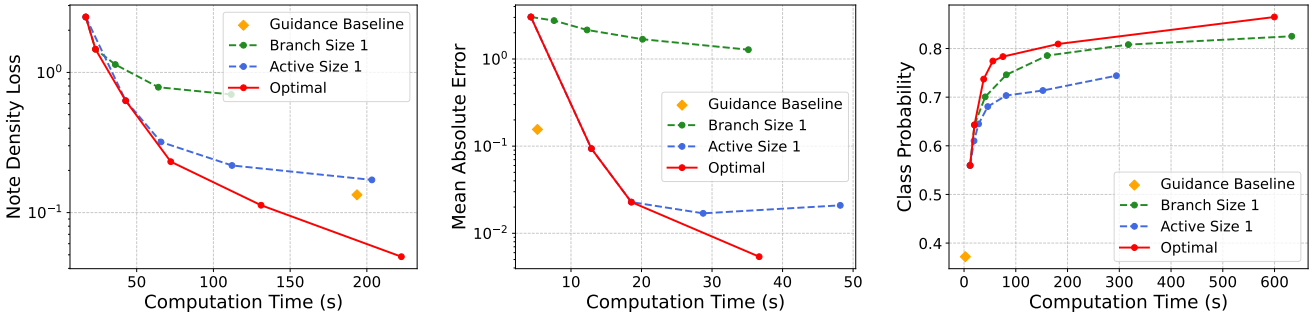
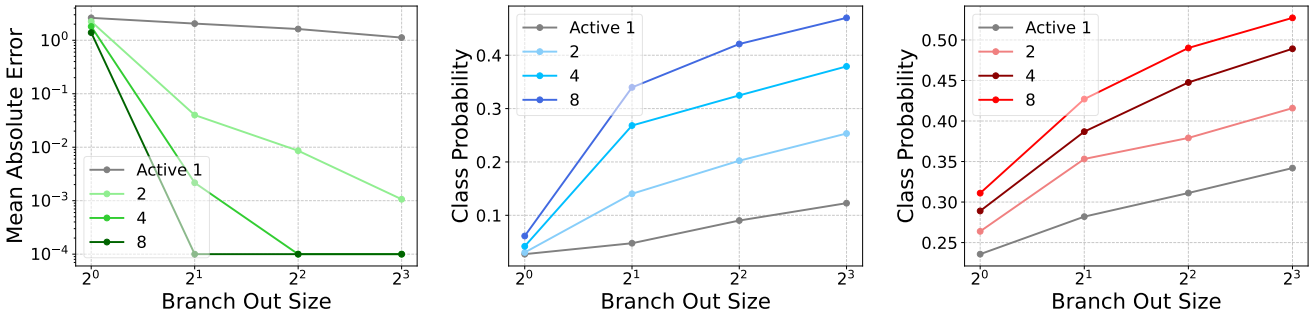
# 1 New Figure 2




(a) Symbolic Music Generation (Loss ↓) (b) Small Molecule Generation (MAE ↓) (c) Enhancer DNA Design (Prob ↑)

Figure 1: **SPS outperforms the guidance baseline, with the optimization effect of the objective function following a scaling behavior with inference time.** We evaluate SPS with varying active set and branch-out sizes. **"Optimal"** refers to the combination of active set and branch-out sizes that achieve the best performance within the same inference time. The optimal line shows that SPS outperforms the guidance baseline and the scaling behavior of inference time.




(a) SPS-SD for Small Molecule Generation (b) SPS-SC for Enhancer DNA Design (c) SPS-G for Enhancer DNA Design

Figure 2: **Scaling Behavior with Fixed Active or Branch-Out Size:** Increasing either the active size or the branch-out size enhances performance. (a): The MAEs are capped at $10^{-4}$; (b) & (c): The results are for Class 3 in DNA enhancer design with strength 20 for SPS-G.

## 2 New Figure 3

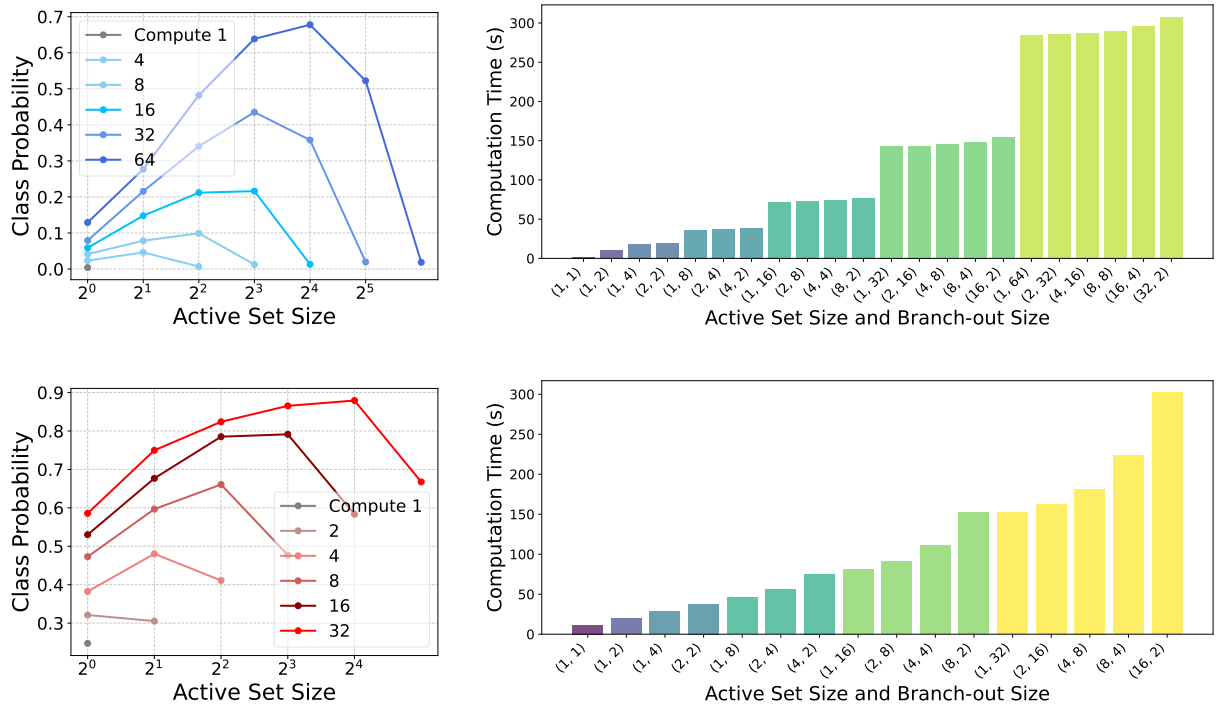



Figure 3: **Trade-Off between Active Set Size $A$ and Branch-Out Size $K$ with Fixed Computation:** SPS-SC (Top) and SPS-G (Bottom) vary $(A, K)$ with fixed total compute $A * K$ for DNA enhancer design. Performance peaks when $A$ and $K$ are in the moderate range. Fixed $A * K$ can be viewed as a fixed computation budget where the actual inference time is shown on the right. The results are for Class 1 and $\gamma = 20$ for SPS-G.