Adding Conditional Control to Diffusion Models with Reinforcement Learning

Genentech
A Member of the Roche Group

Yulai Zhao[1]*, Masatoshi Uehara[2]*, Gabriele Scalia[2], Tommaso Biancalani[2], Sergey Levine[3], Ehsan Hajiramezanali[2]
[1]Princeton University, [2]Genentech, [3]University of California, Berkeley

Biology Research | AI Development

Background

- A pre-trained conditional diffusion model excels at modeling p(x|c).
  - For example, in Stable Diffusion, c∈C is a prompt, and x∈X is the image generated according to this prompt.
  - Many tailored DMs are able to generate biological sequences (e.g., DDSM).
- In practice, **we are often interested in adding new controls into pre-trained diffusion models**, e.g.
  - Stable Diffusion.
    - existing condition: prompts
    - new condition: certain layouts or backgrounds.
  - DDSM that generates DNA enhancers.
    - existing condition: activity level in HepG2
    - new condition: activity level in other cell lines such as K562.

Settings

- Given the pre-trained model, which enables us to sample from $p^{pre}(x|c)$: $C \mapsto \Delta(X)$.
- Our goal is to add new conditional controls y∈Y such that we can sample from p(x|c,y).
- Assume we can access to offline data:

  $$D = \{(c^{(i)}, x^{(i)}, y^{(i)})\}_{i=1}^{n}.$$

  We denote the conditional distribution by $p^{\diamond}(y|x,c)$.

Target Distribution

our goal is to obtain a diffusion model such that we can sample from

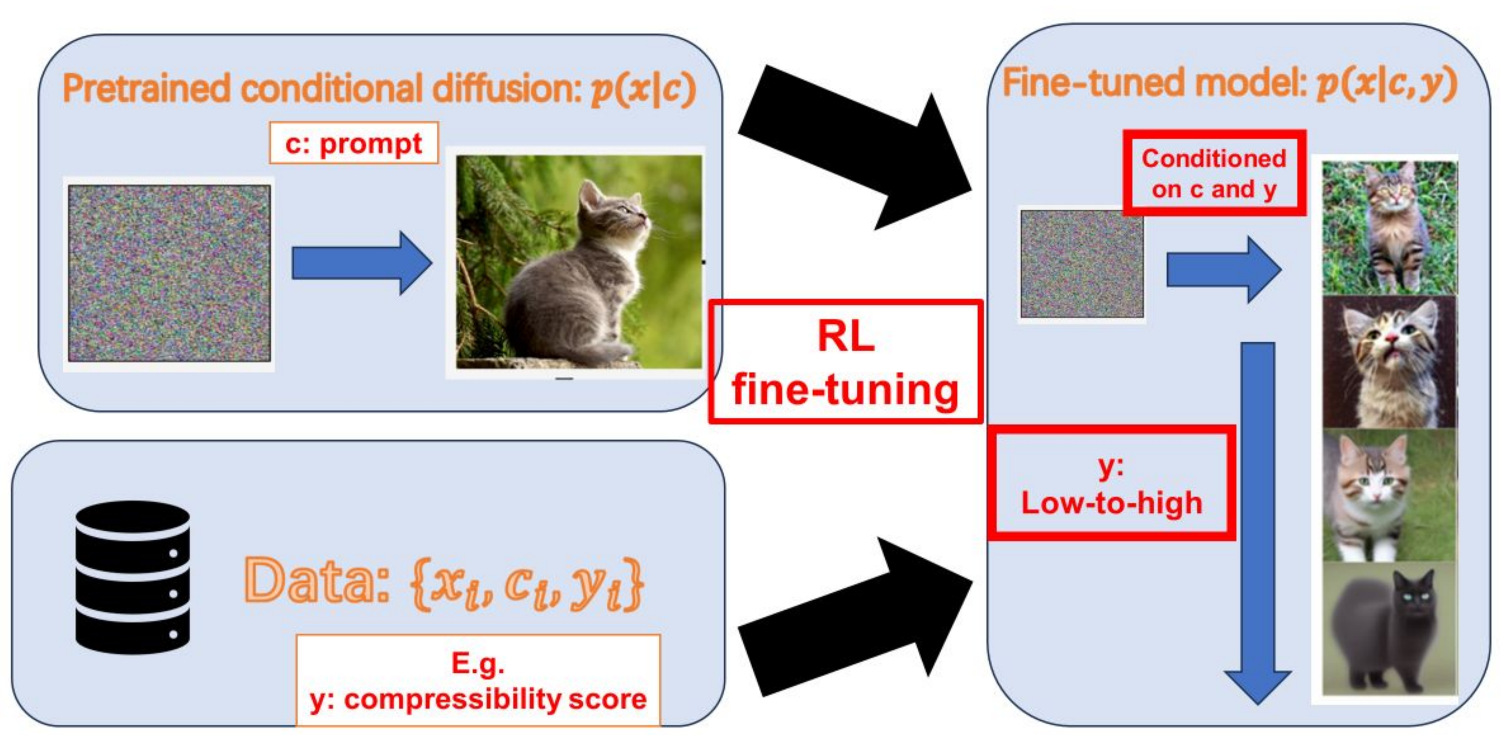
$$p_{\gamma}(\cdot|c,y) \propto (p^{\diamond}(y|\cdot,c))^{\gamma}\, p^{pre}(\cdot|c)$$

where γ represents the strength of the additional guidance.

Methodology & Results

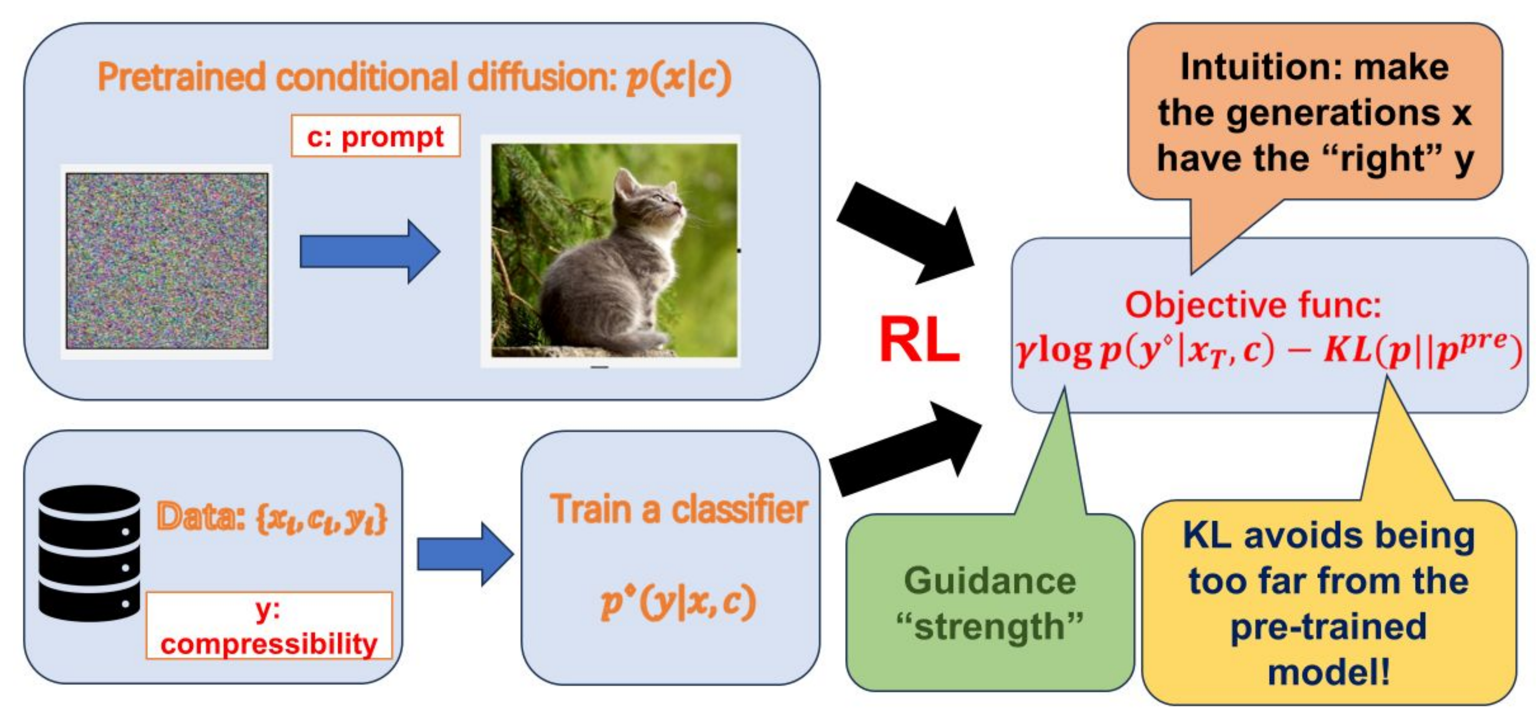
Roadmap

Our goal: adding control via fine-tuning



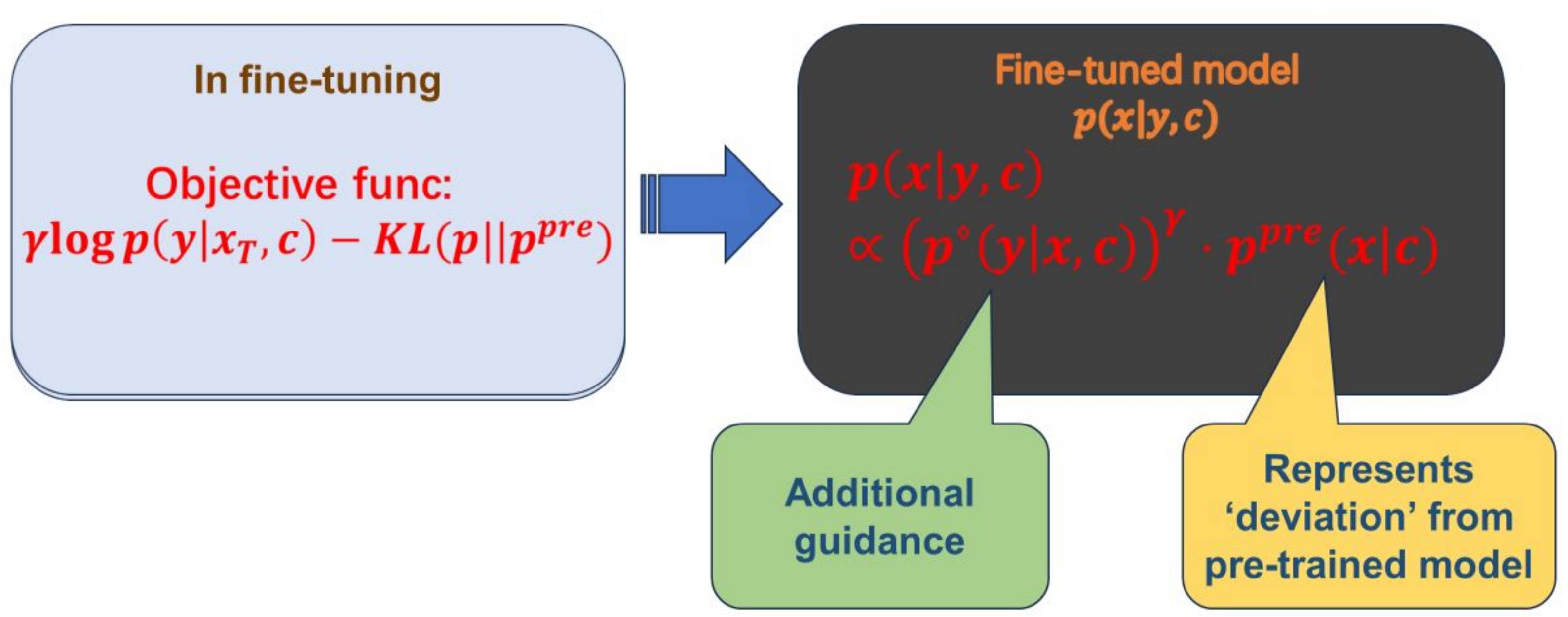
RL-based Fine-tuning

Methodology

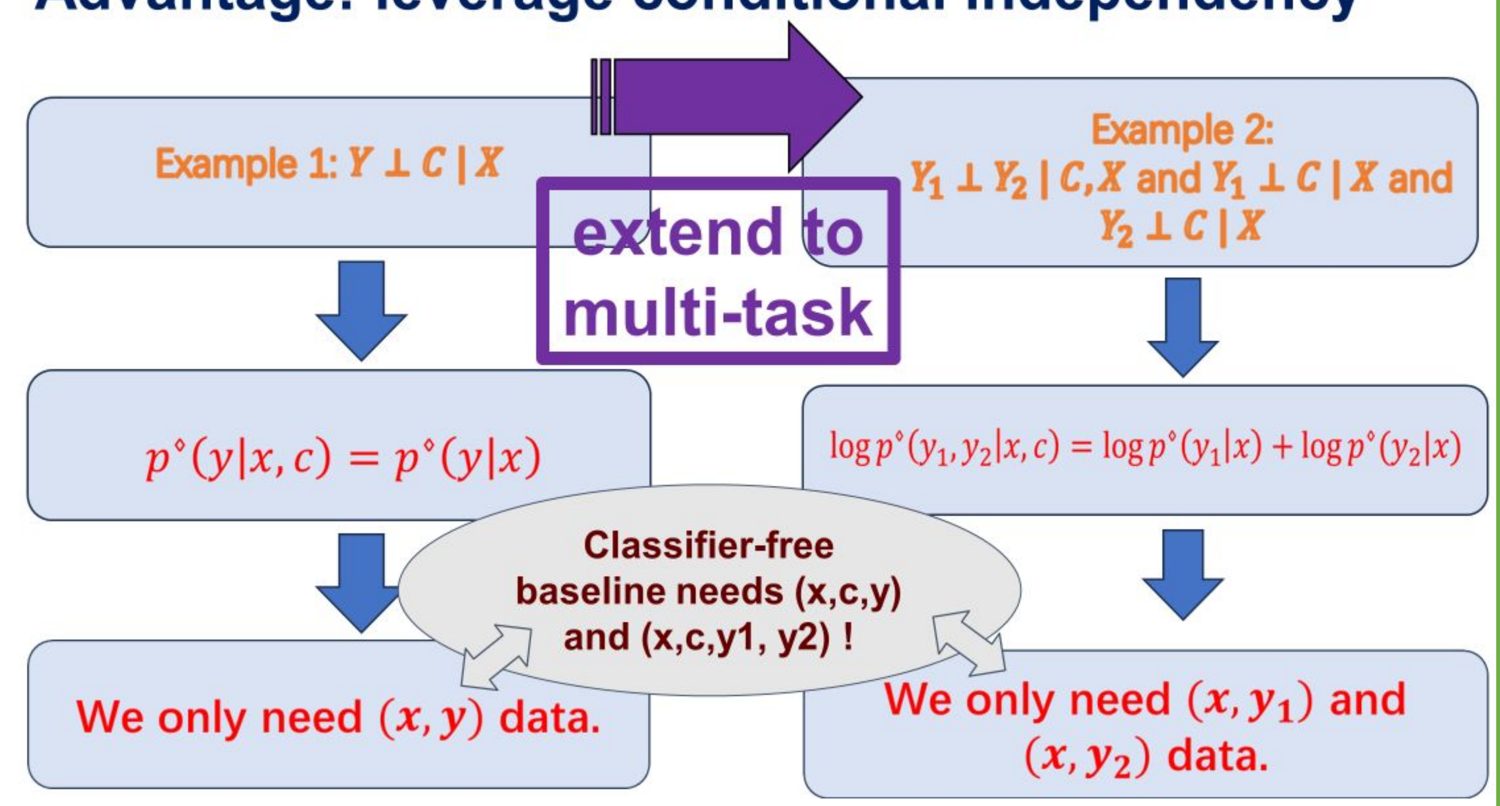


Benefits of Our Approach

Theoretical justification (incomplete)



Advantage: leverage conditional independency



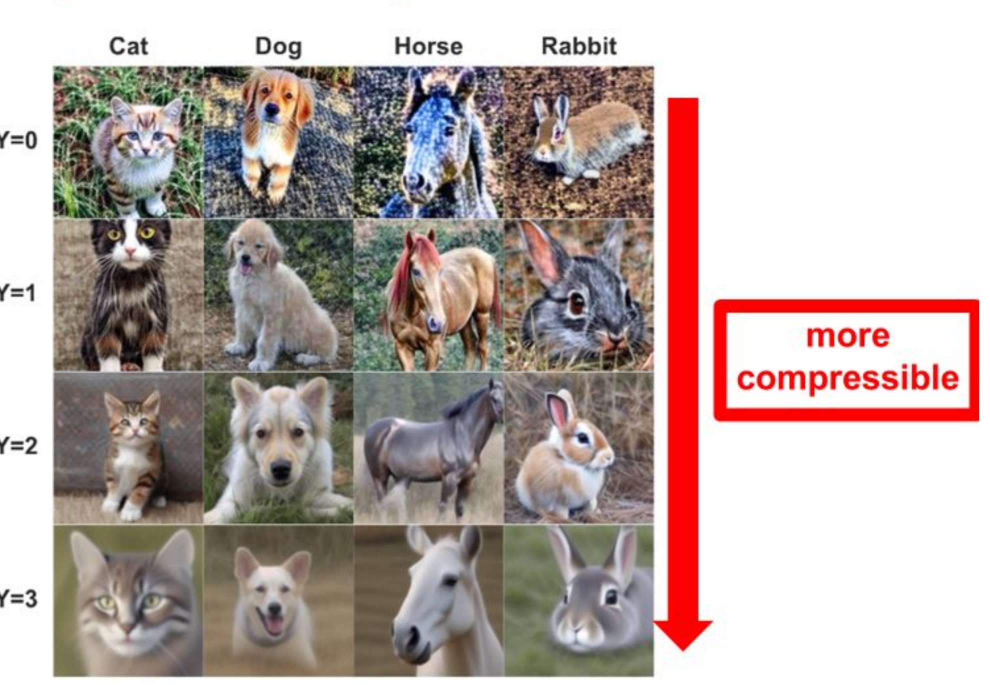
Experimental Results

Example 1: Compressibility

(a) Training curve

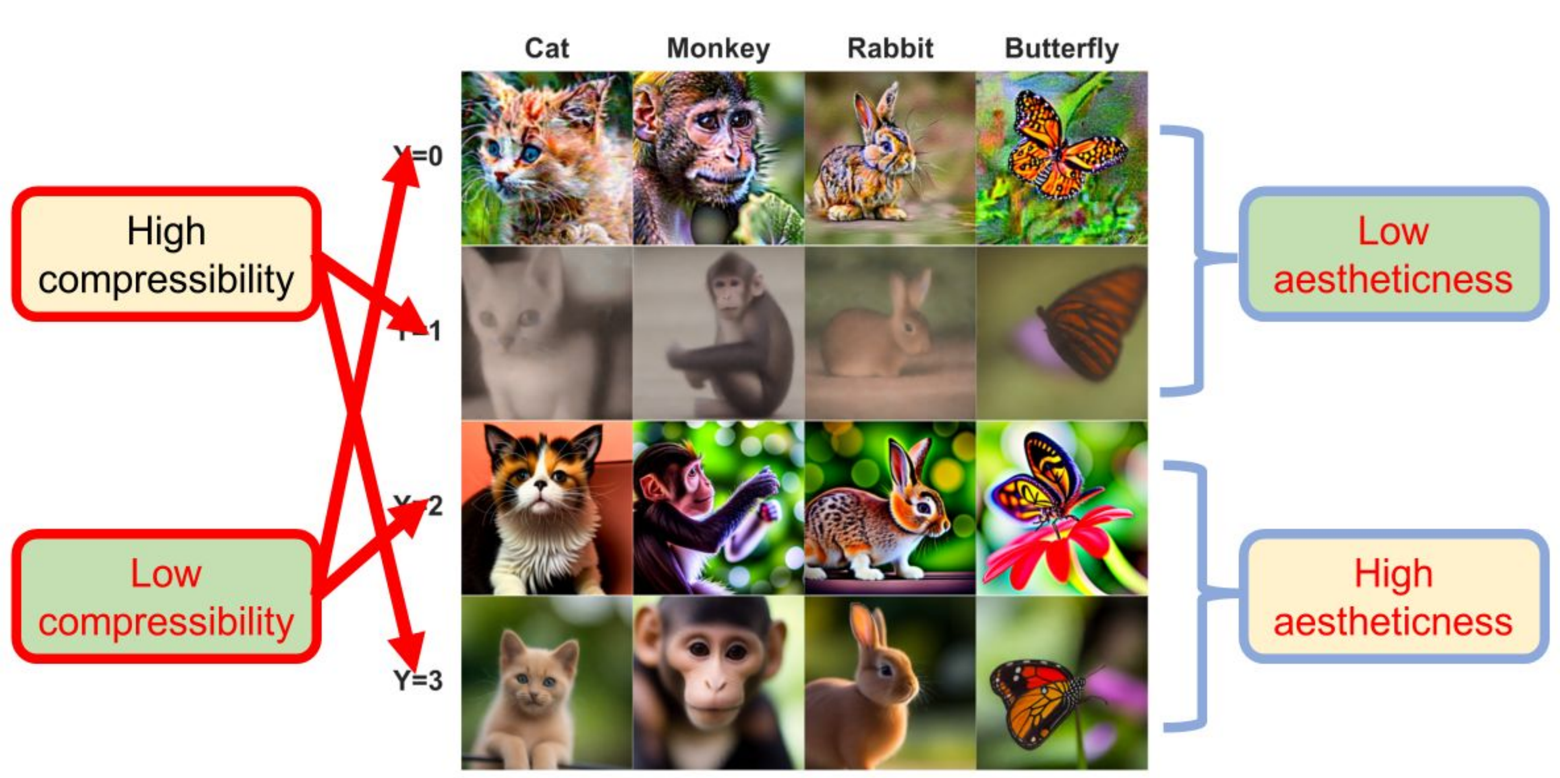
	Accuracy ↑	Macro F1 score ↑
DPS	0.45	0.44
CTRL (Ours)	1.0	1.0

(b) Evaluation of conditional generations



(c) Generated images

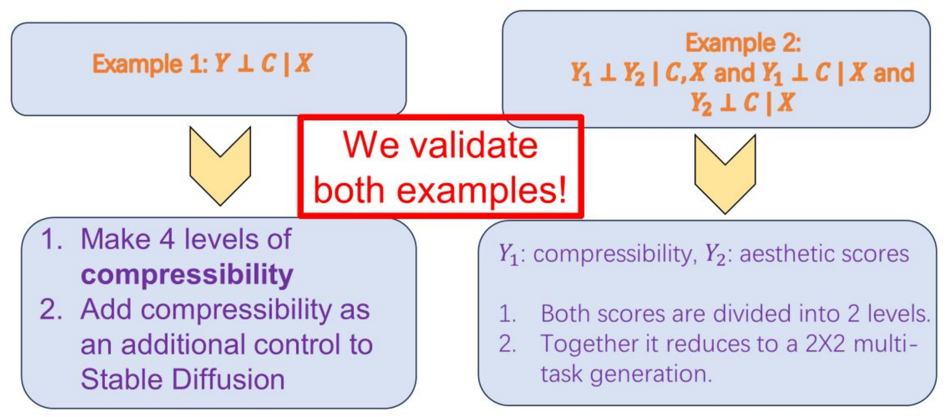
Example 2: Compressibility & Aestheticness



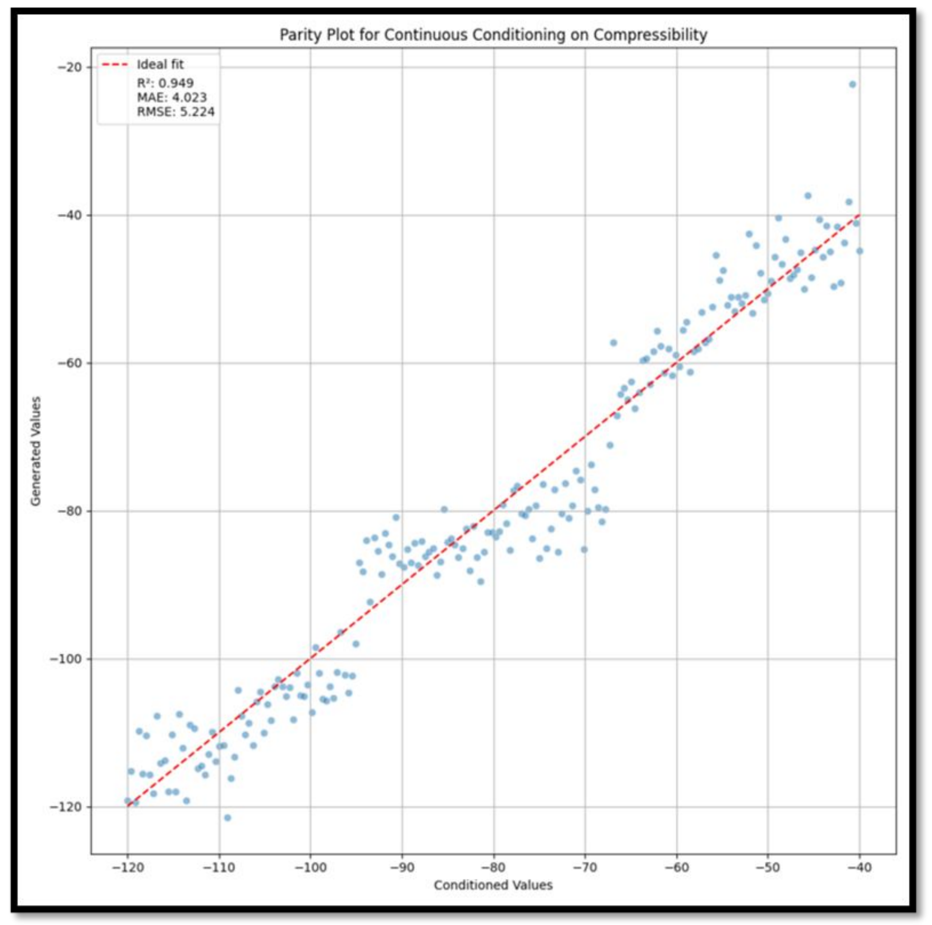
Experimental Details

Settings

Experiments



Extension: continuous condition



Conclusions & Future Work

- We introduce an **RL-based fine-tuning** approach for conditioning pre-trained diffusion models on new additional labels.
- Compared to **classifier-free guidance**, our proposed method allows for **leveraging the conditional independence**, thereby greatly simplifying the construction of the offline dataset.
- We also theoretically justify our approach and **build the connection with classifier-based guidance**.
- We are working on extending this work to **DNA enhancers** and **RNA 5'UTR** design.
- The goal is achieve **cell-specific promoters design**!

ArXiv