

# Sample-Efficient Optimization in the Latent Space of Deep Generative Models via Weighted Retraining

Erik Daxberger\*, Austin Tripp\* & José Miguel Hernández-Lobato

ReaIML @ ICML2020

2020-07-18



UNIVERSITY OF  
CAMBRIDGE

# Problem

Optimization of **expensive**, **black box** functions on **structured input spaces**.

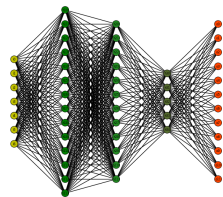
Examples:



Drug Design



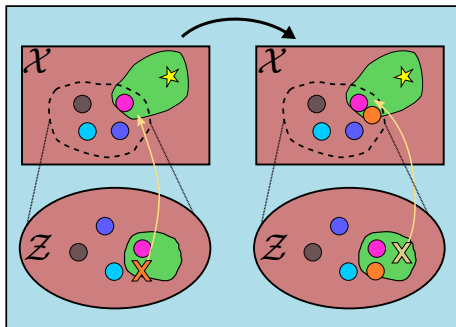
Materials Discovery



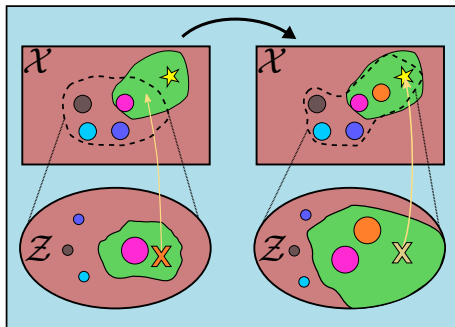
Neural Architecture Search

# Latent Space Optimization

Optimize in the **latent space  $\mathcal{Z}$**  of a deep generative model  
(instead of **data space  $\mathcal{X}$** )



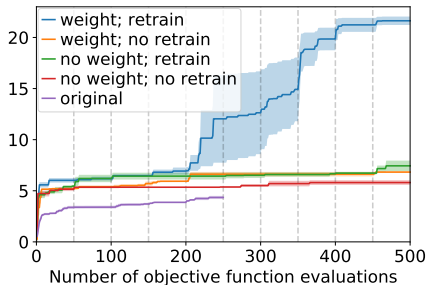
Normal



With weighted retraining

# Results

## Chemical Design Task



- works with a variety of models
- easy to implement
- huge increase in performance and sample efficiency

*More results in the paper!*