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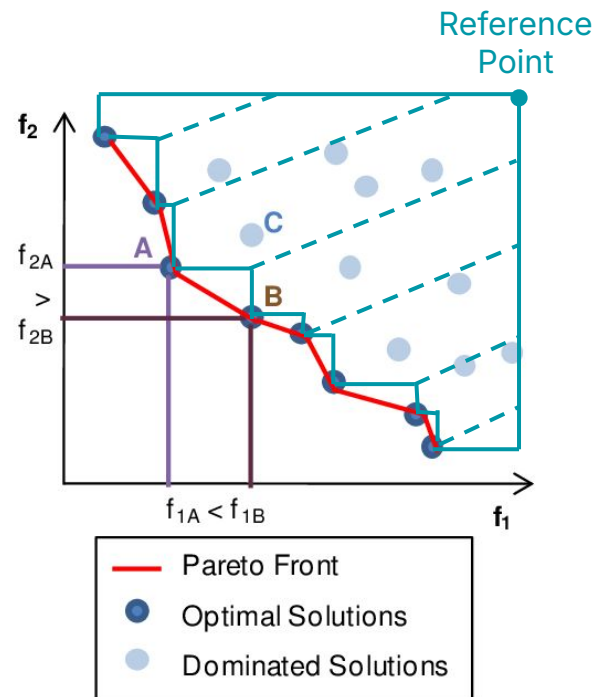
Pareto-Conditioned Diffusion Models for Offline Multi-Objective Optimization

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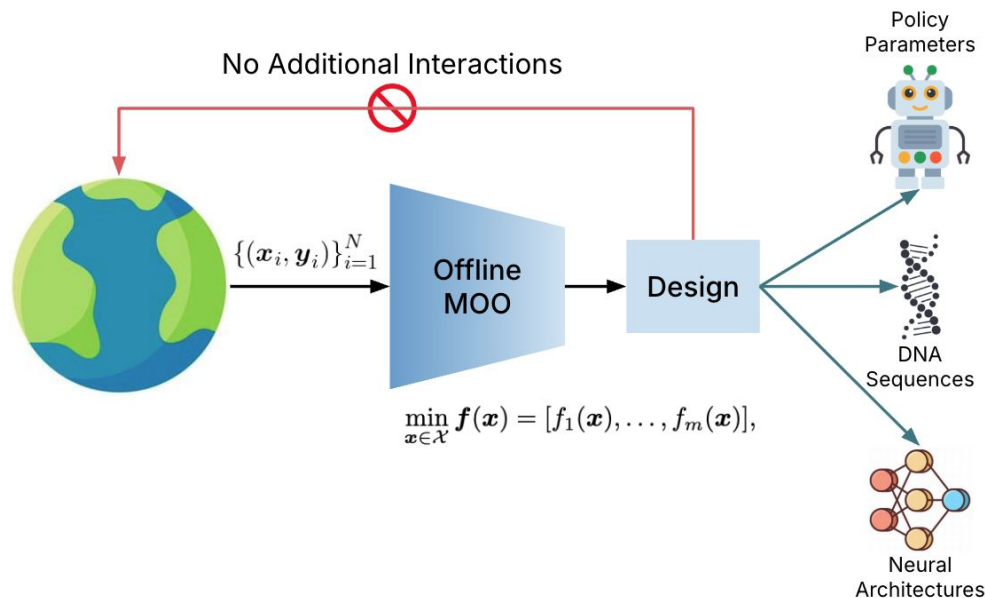
Motivation

- Many real-world optimization problems are **multi-objective**
 - *Biological Sequence Design*
 - *Neural Architecture Search*
- We aim to find the set of all **non-dominated solutions** that forms the **Pareto Front**
- **Hypervolume** measures the quality of a solution set with respect to the **reference point**



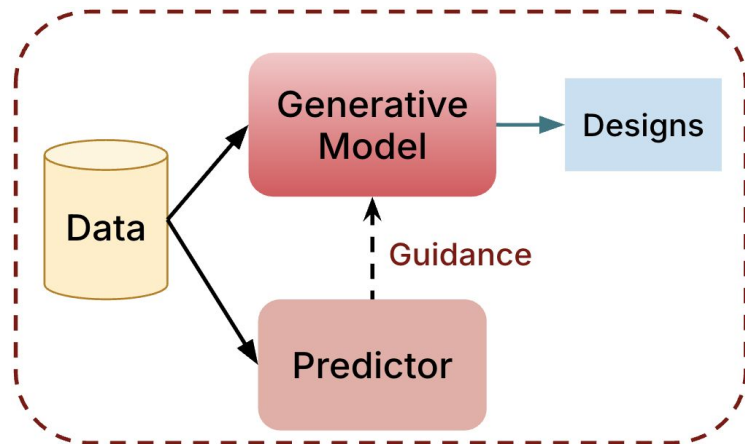
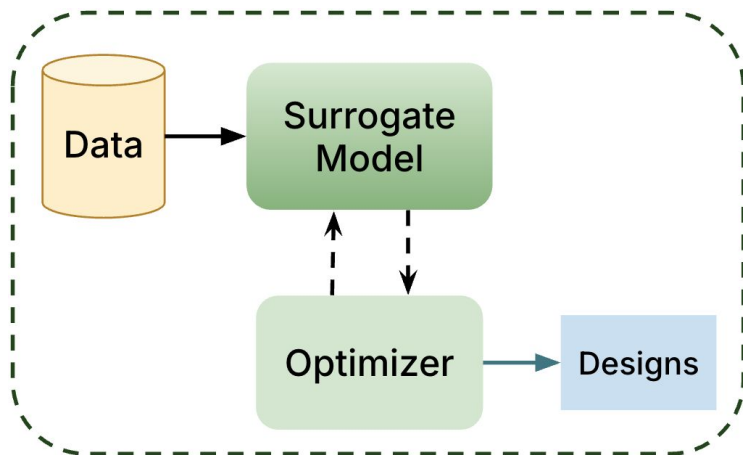
Offline Multi-Objective Optimization

- **Challenge:** Evaluating real-world designs is prohibitively expensive or risky
- **The "Offline" Setting:** Optimize using only a static, pre-collected dataset



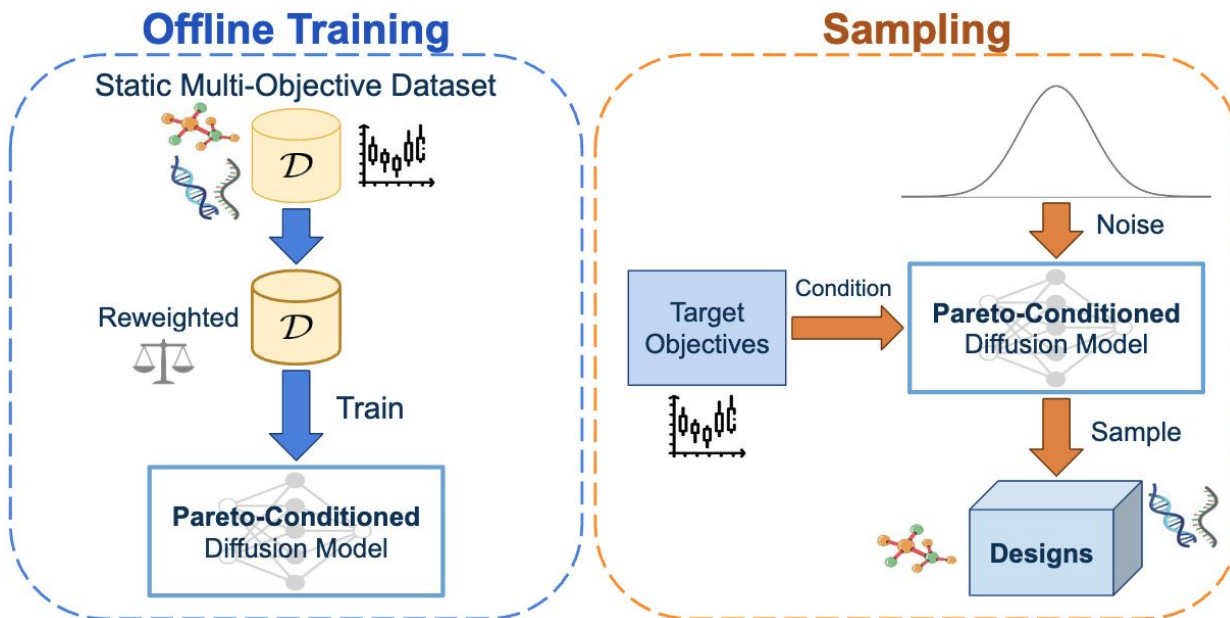
Prior Work

- **The Dominant Paradigm:** Multi-stage pipelines relying on explicit **surrogate models** or **predictors**
- **The Bottleneck:** Performance is limited by the accuracy of the **surrogate model** or **predictor**



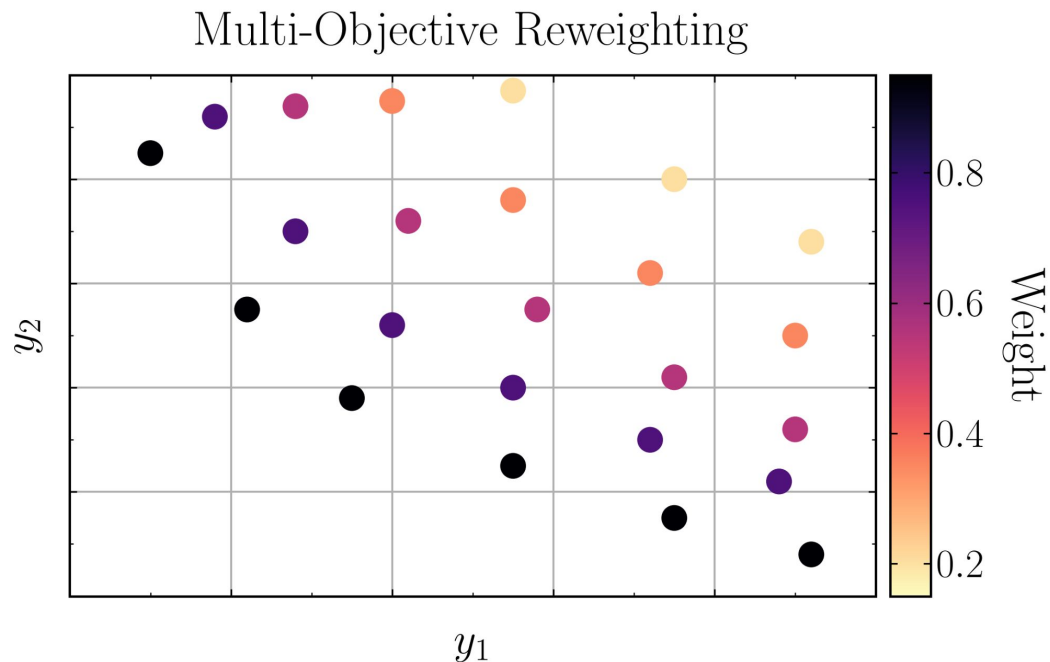
Pareto-Conditioned Diffusion Models

- **Our Solution:** We propose **Pareto-Conditioned Diffusion (PCD)**, which reframes offline MOO as a **conditional sampling problem**



Training Via Multi-Objective Reweighting

- **Goal:** Focus on **optimal** designs, not average ones
- **Issue:** How to compare points in multi-objective solution space?
- **Solution:** Reweight the dataset using the **dominance number** of each point

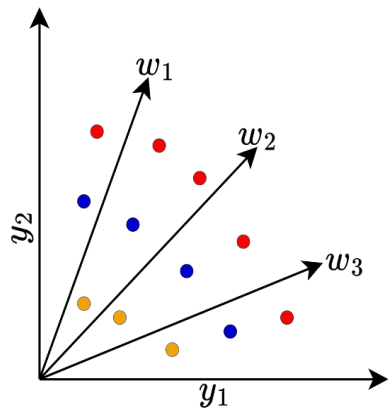


Generating Conditioning Points

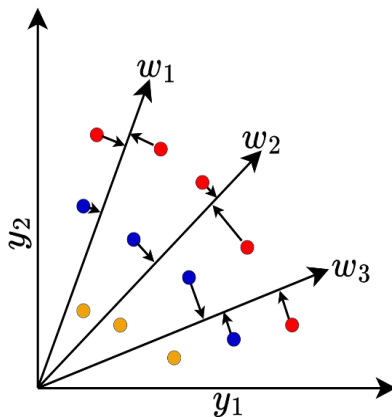
How do we generate target trade-offs that offer better **coverage** and **performance** than the offline dataset?

Generating Conditioning Points

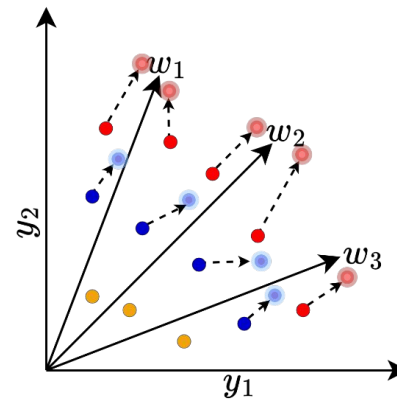
1) Partition solution space via direction vectors



2) Assign points to direction vectors

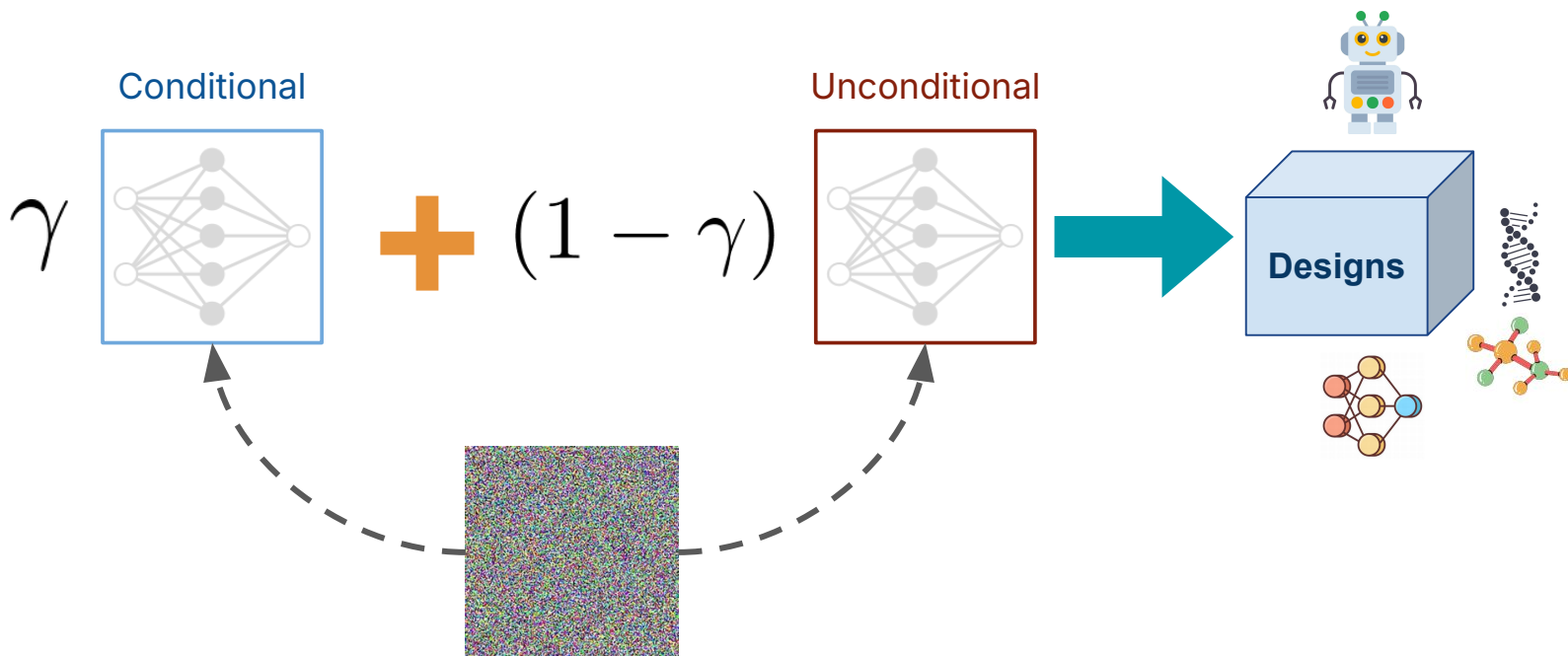


3) Extrapolate and add noise



Sampling via Predictor-free Guidance

- Generate **designs** that are highly faithful to the **target trade-offs**



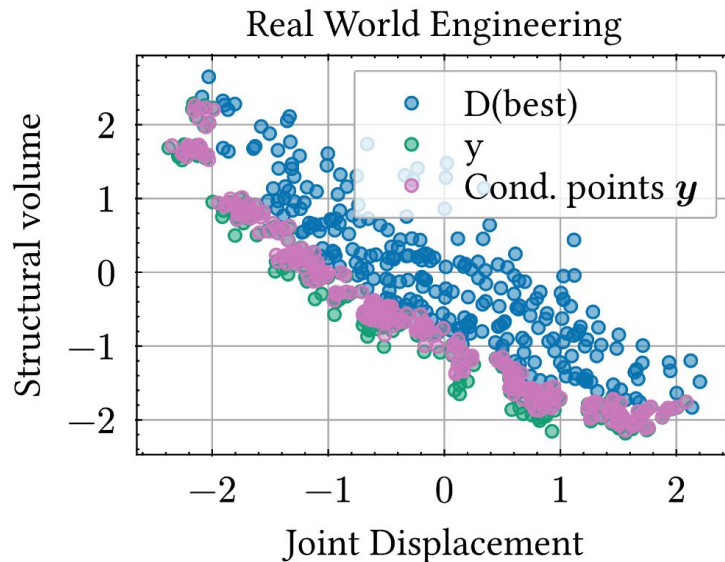
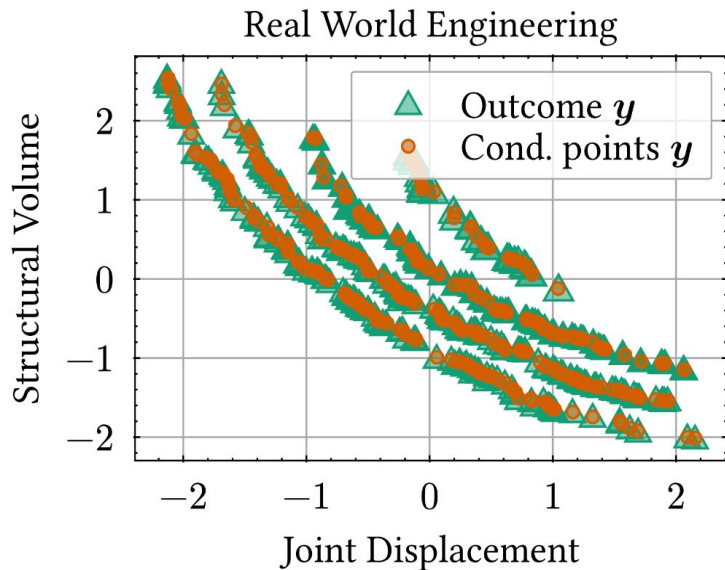
Main Results

- PCD is highly **competitive** and **consistent** across diverse offline MOO tasks with a single set of hyperparameters

Method	Synthetic	MORL	RE	Scientific	MONAS	Avg. rank
$D(\text{best})$	5.45 ± 0.19	1.70 ± 0.27	2.60 ± 0.07	9.35 ± 0.14	11.53 ± 0.06	7.43 ± 0.05
MOBO	8.69 ± 0.30	14.60 ± 0.42	10.00 ± 0.33	6.75 ± 0.47	8.11 ± 0.80	8.81 ± 0.34
E2E + GN	7.33 ± 0.55	5.70 ± 2.14	7.06 ± 0.32	5.35 ± 1.38	9.33 ± 0.53	7.82 ± 0.40
E2E + PC	5.93 ± 0.25	<u>3.50 ± 1.22</u>	6.22 ± 0.33	4.30 ± 1.32	6.60 ± 0.40	6.01 ± 0.29
E2E	6.16 ± 0.30	9.70 ± 2.08	6.06 ± 0.30	4.20 ± 1.40	<u>5.13 ± 0.22</u>	<u>5.71 ± 0.16</u>
MH + GN	8.82 ± 0.53	8.90 ± 2.16	8.14 ± 0.94	5.05 ± 2.14	12.57 ± 0.40	9.84 ± 0.33
MH + PC	8.87 ± 0.45	10.90 ± 1.08	6.74 ± 0.68	6.15 ± 0.91	7.46 ± 0.30	7.68 ± 0.33
MH	6.18 ± 0.53	8.00 ± 1.41	6.14 ± 0.29	5.80 ± 0.89	5.88 ± 0.49	6.10 ± 0.22
MM + COMs	8.02 ± 0.47	3.60 ± 1.29	6.54 ± 0.17	3.85 ± 0.68	7.22 ± 0.43	6.80 ± 0.13
MM + ICT	6.73 ± 0.46	9.10 ± 1.95	5.44 ± 0.32	5.05 ± 0.74	8.42 ± 0.40	7.08 ± 0.13
MM + IOM	5.16 ± 0.51	12.70 ± 0.91	5.76 ± 0.52	4.40 ± 1.15	5.77 ± 0.50	5.80 ± 0.20
MM + TM	6.55 ± 0.82	7.90 ± 2.16	5.78 ± 0.25	5.90 ± 1.29	7.87 ± 0.39	6.91 ± 0.20
MM	6.07 ± 0.50	9.50 ± 0.79	5.94 ± 0.41	6.55 ± 0.93	4.97 ± 0.46	5.80 ± 0.21
ParetoFlow	2.44 ± 0.28	8.50 ± 1.32	<u>1.74 ± 0.17</u>	9.05 ± 0.27	11.19 ± 0.52	6.74 ± 0.23
PCD (ours)	<u>3.38 ± 0.20</u>	5.50 ± 3.30	1.51 ± 0.13	<u>4.05 ± 0.33</u>	7.54 ± 0.50	4.80 ± 0.30

How Effective is the Conditioning in PCD?

- PCD faithfully **reconstructs** the original conditioning points
- Matches or exceeds **extrapolated** conditioning targets



Conclusion

- We introduced **PCD**, reframing offline MOO as a **conditional sampling problem**
- Leverages **dominance-based reweighting** and **extrapolated targets** to generate diverse, novel **Pareto-optimal** solutions
- **PCD** achieves highly **competitive** and **consistent** performance across diverse benchmarks
- **Future work:** Extending PCD with discrete diffusion models for combinatorial optimization!

Thank you



Project website

