Multi-objective optimization in perovskite processing scaleup

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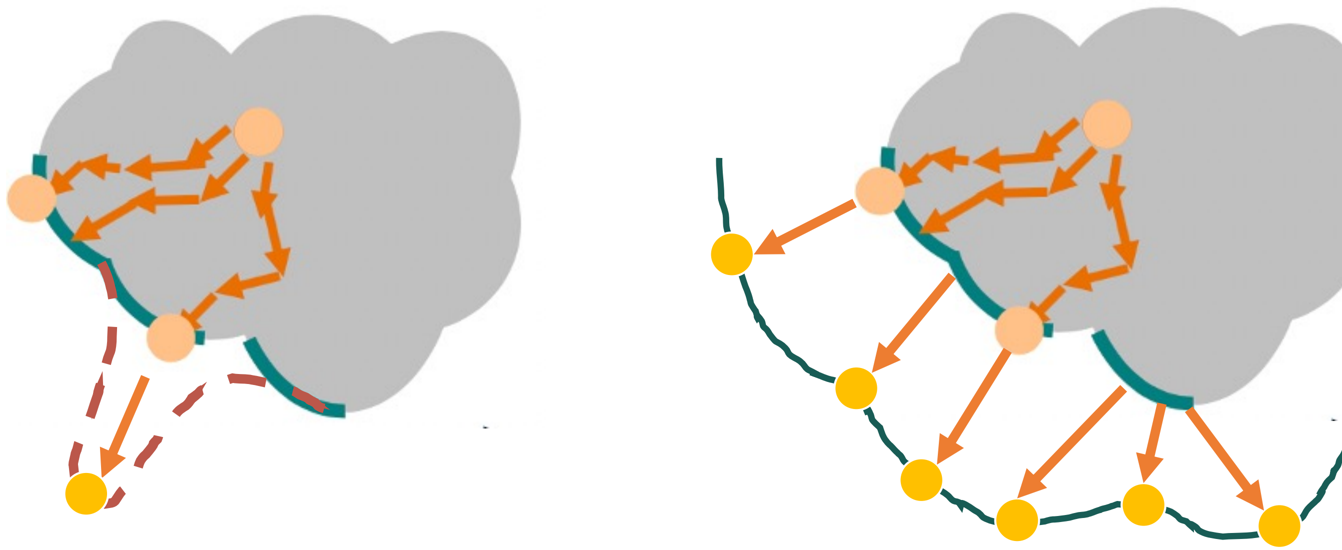
07/20

Photovoltaic
Research
Laboratory

Multi-objective optimization + active learning

Bayesian Optimization Objective function Surrogate model Acquisition function

New experiments that best expand the pareto front should be prioritized.



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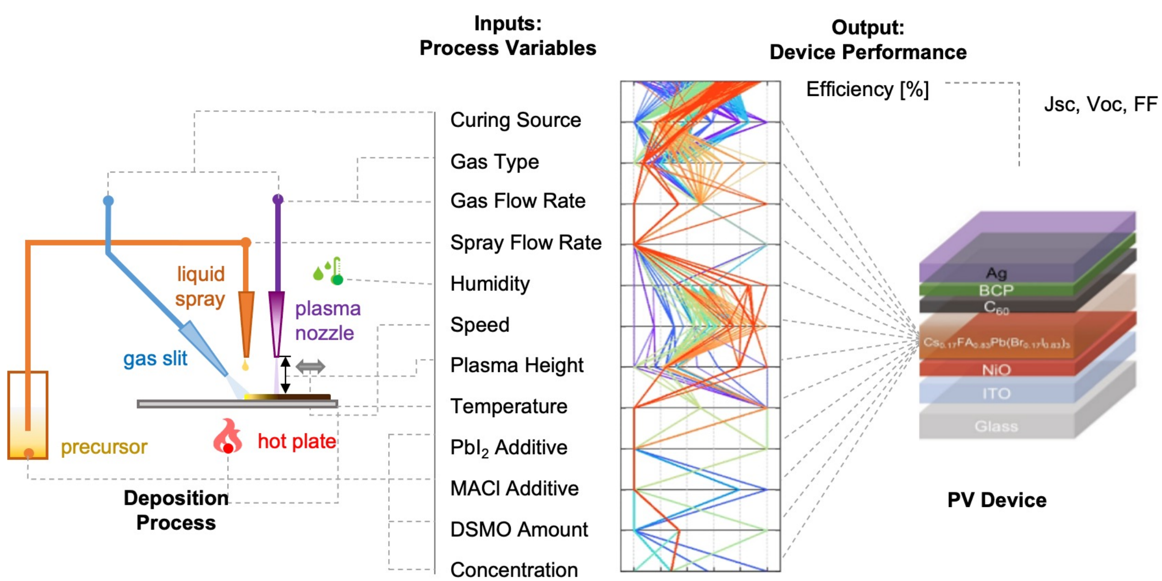
Case study and POC

Currently available $$Jsc \cdot Voc \cdot FF = \frac{P_{MAX}}{c} \propto PCE$$

Future PCE & Degradation



SIPS dataset for MOBO demo

X (6 dimensional)

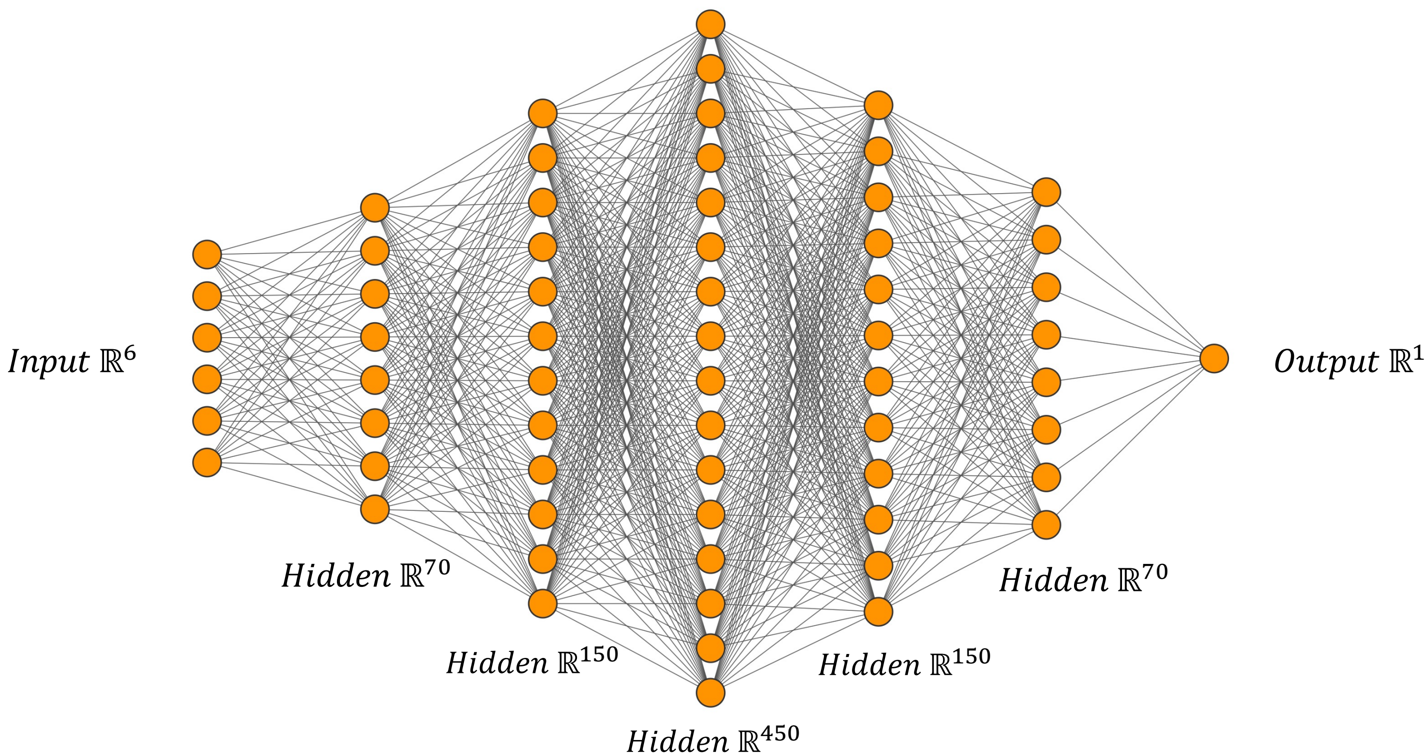
max y_1 max y_2 max y_3

400

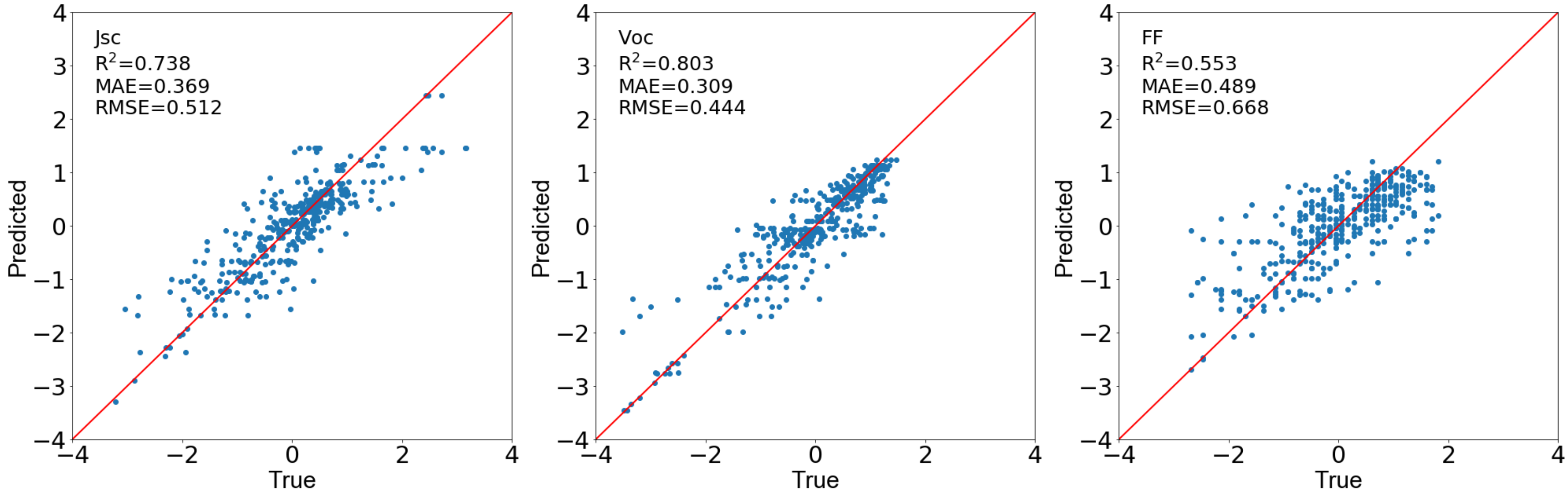
	Temp [degC]	speed [mm/s]	sprayFL [uL/min]	plamsaH [cm]	gasFL [L/min]	plasmaDC [%]	Jsc	Voc	FF
0	150	275	2000	1.0	25	100	12.766660	0.675600	0.37
1	155	150	3000	1.2	20	50	13.819050	0.839975	0.37
2	155	150	4500	1.2	25	25	20.452380	0.859849	0.37
3	145	125	3500	1.0	25	50	25.580952	0.866390	0.37
4	140	200	5000	1.2	20	50	26.180950	0.763086	0.38
...	...	...	...	...	...	...	...	...	...
395	135	175	4000	1.2	20	50	22.185710	0.997484	0.77
396	135	150	4000	0.8	20	50	22.405000	1.007000	0.77
397	145	125	3500	1.0	25	50	22.295200	1.031000	0.77
398	135	150	3500	1.2	20	25	23.666670	0.919288	0.78
399	145	175	3000	1.0	16	25	22.042860	0.972841	0.78

400 rows × 9 columns

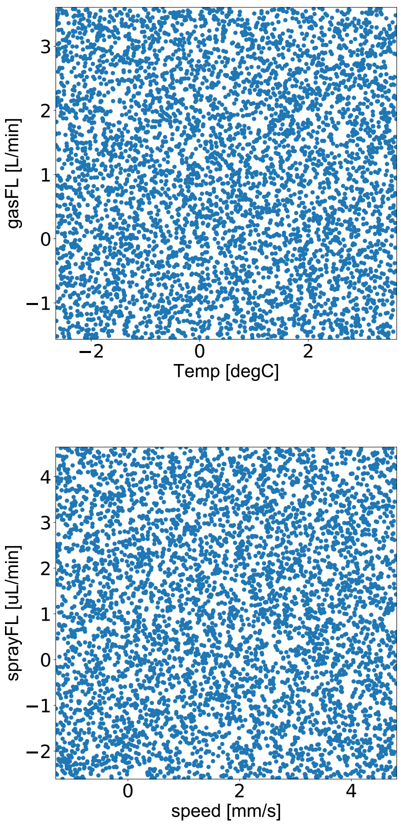
NN “ground truth” models

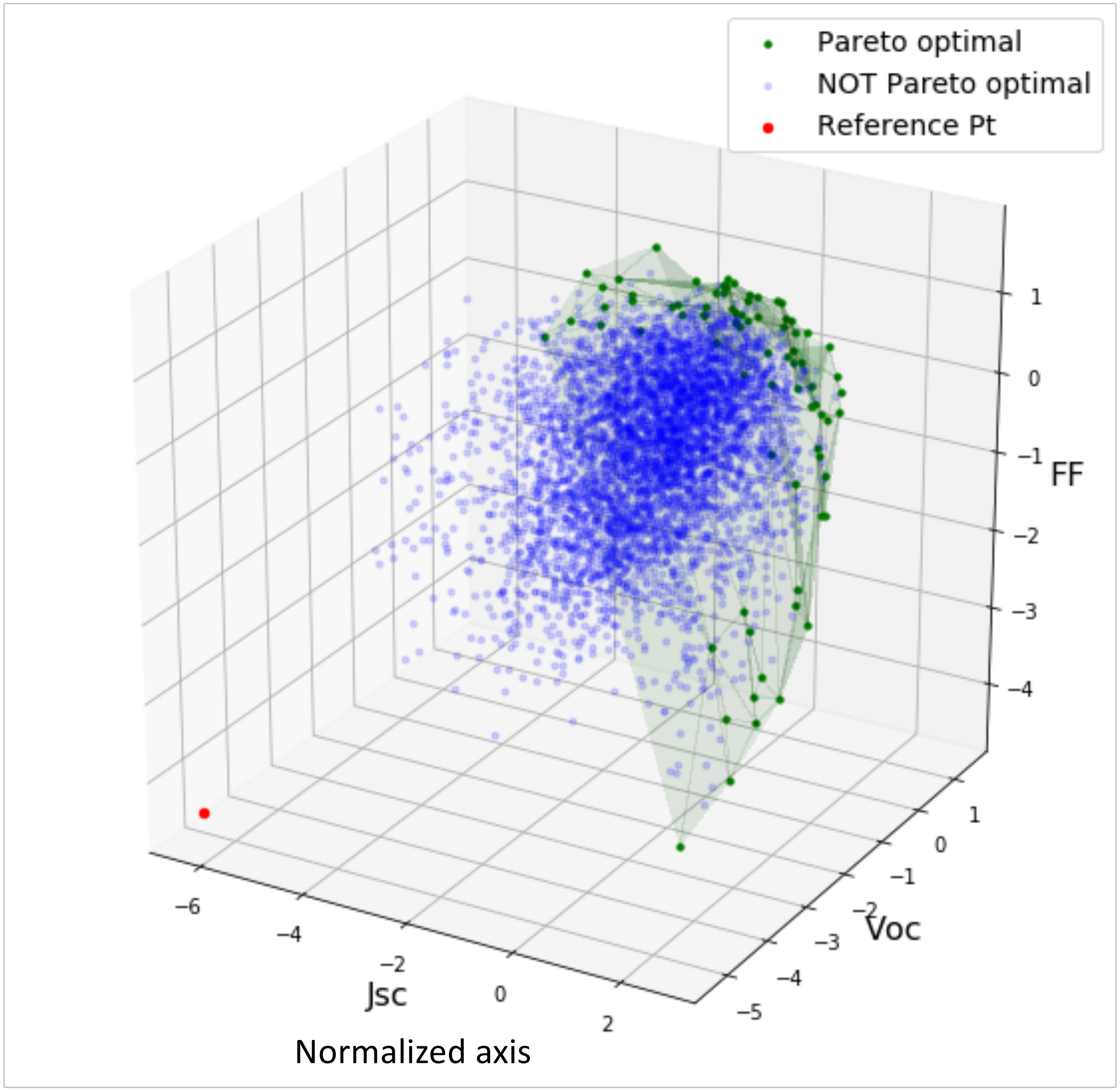


Parity plots for NN "ground truth" models



‘Ground truth’





SIPS dataset for Retrospective MOBO demo

X (6 dimensional)

max y_1 max y_2 max y_3

5000

	Temp [degC]	speed [mm/s]	sprayFL [uL/min]	plamsaH [cm]	gasFL [L/min]	plasmaDC [%]	Jsc	Voc	FF
0	0.038594	4.787340	-2.520705	-0.007977	-0.620975	1.283714	-1.414222	-3.740918	0.162440
1	0.563656	1.445652	-1.206571	-0.935139	3.393827	-0.860181	-3.334766	0.069202	-0.512193
2	3.454014	1.500614	3.023343	-0.201919	3.174462	0.282355	-0.866588	-0.161780	-1.855402
3	-2.461107	1.157407	-1.632031	0.814202	0.801796	0.597884	-0.170123	-1.430053	0.648208
4	2.035842	2.216341	-0.612670	0.866140	1.805497	-0.219867	-2.467092	-0.413279	0.437571
...	...	...	...	...	...	...	...	...	...
4995	-2.394532	0.656643	0.379102	-0.660527	1.244666	0.761434	-0.502961	-0.646321	0.573376
4996	1.713016	3.904284	-1.427288	-0.334528	1.696849	-0.060174	-2.128265	-1.476419	1.168108
4997	1.172880	0.932674	3.887332	0.665016	-0.894147	-1.169537	1.102211	-1.256820	-2.229904
4998	-2.528938	1.790081	-1.237065	0.901503	0.646585	1.924799	0.068143	-3.538066	0.275859
4999	-1.421031	4.229170	-2.095245	-1.082667	1.267431	1.629329	-1.288464	-3.374500	0.159917

Multi-objective BO (MOBO) demo

Total design space size = 5000

Initial experiments (LHS Sampling) = 20/50

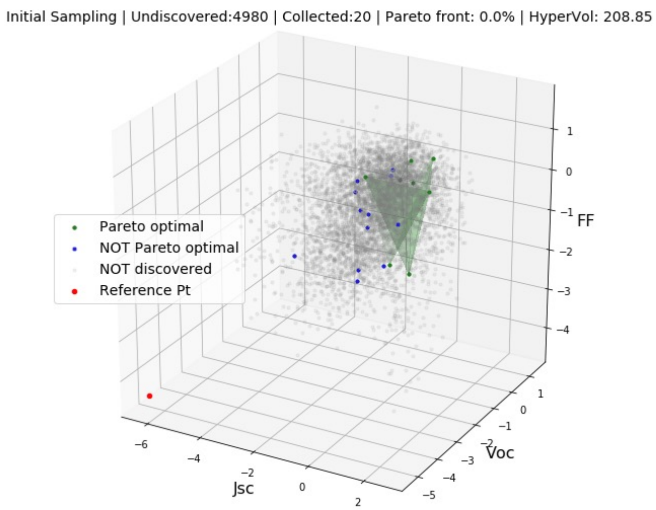
Batch size = 5/20/50

Surrogate model: Default Multivariate GP ARD Matern kernel from BOTorch

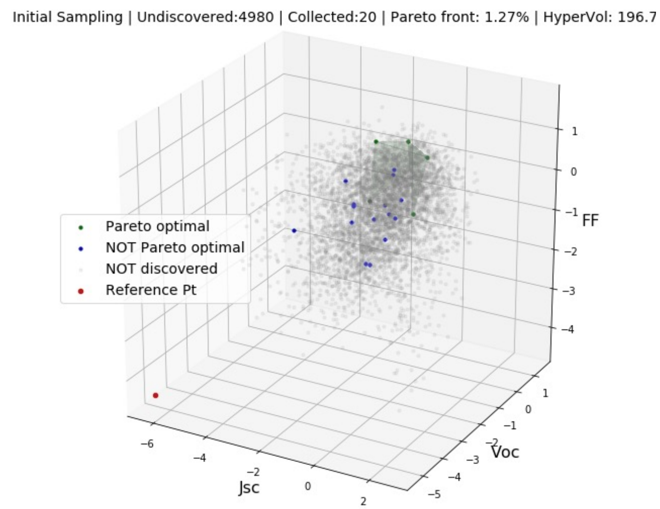
Acquisition function: $EHVI$ (Expected Hypervolume Improvement)

In real time

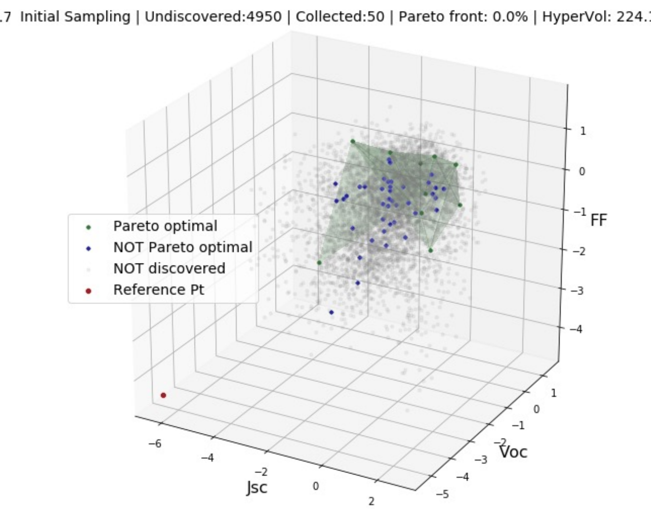
Batch = 5



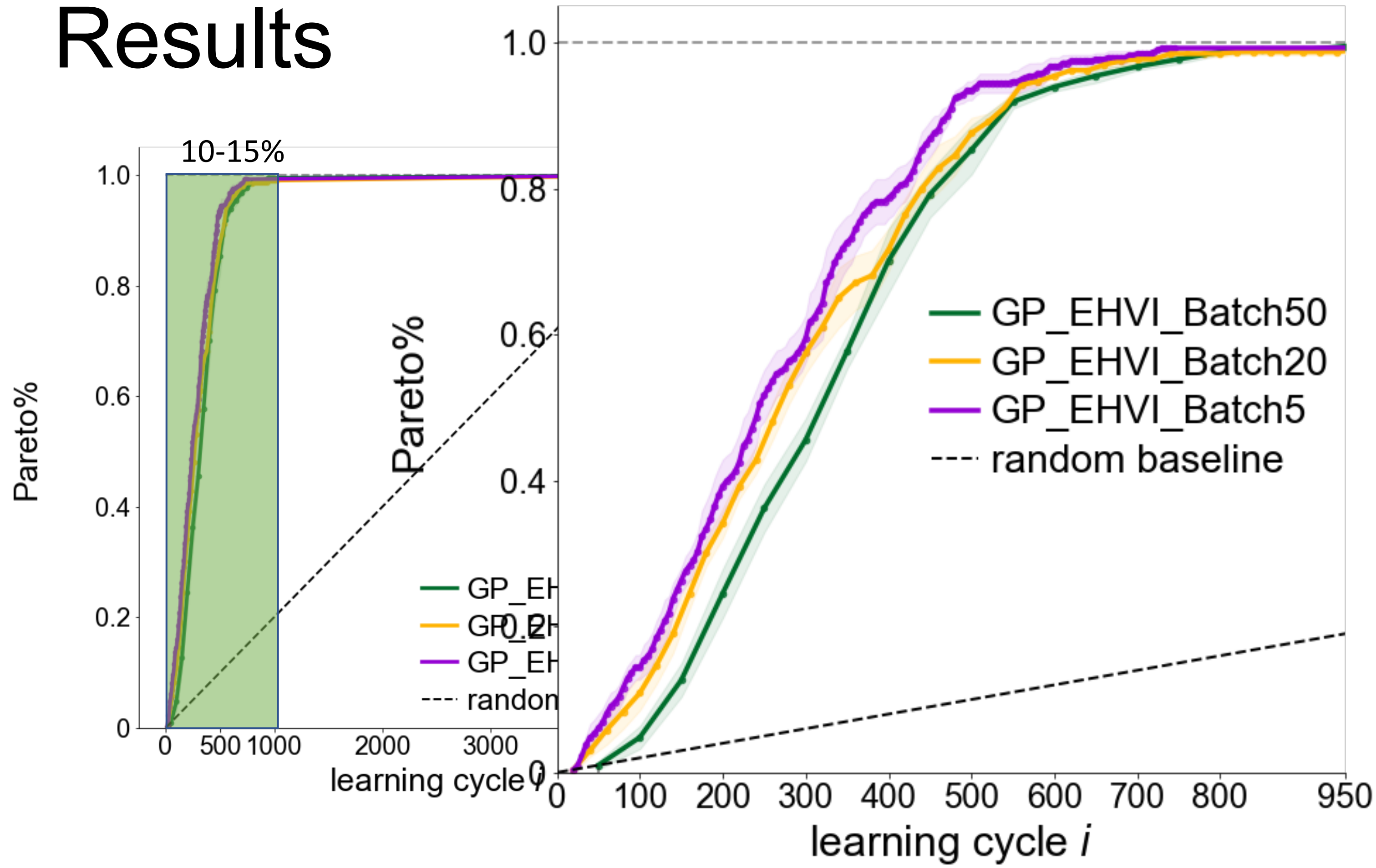
Batch = 20



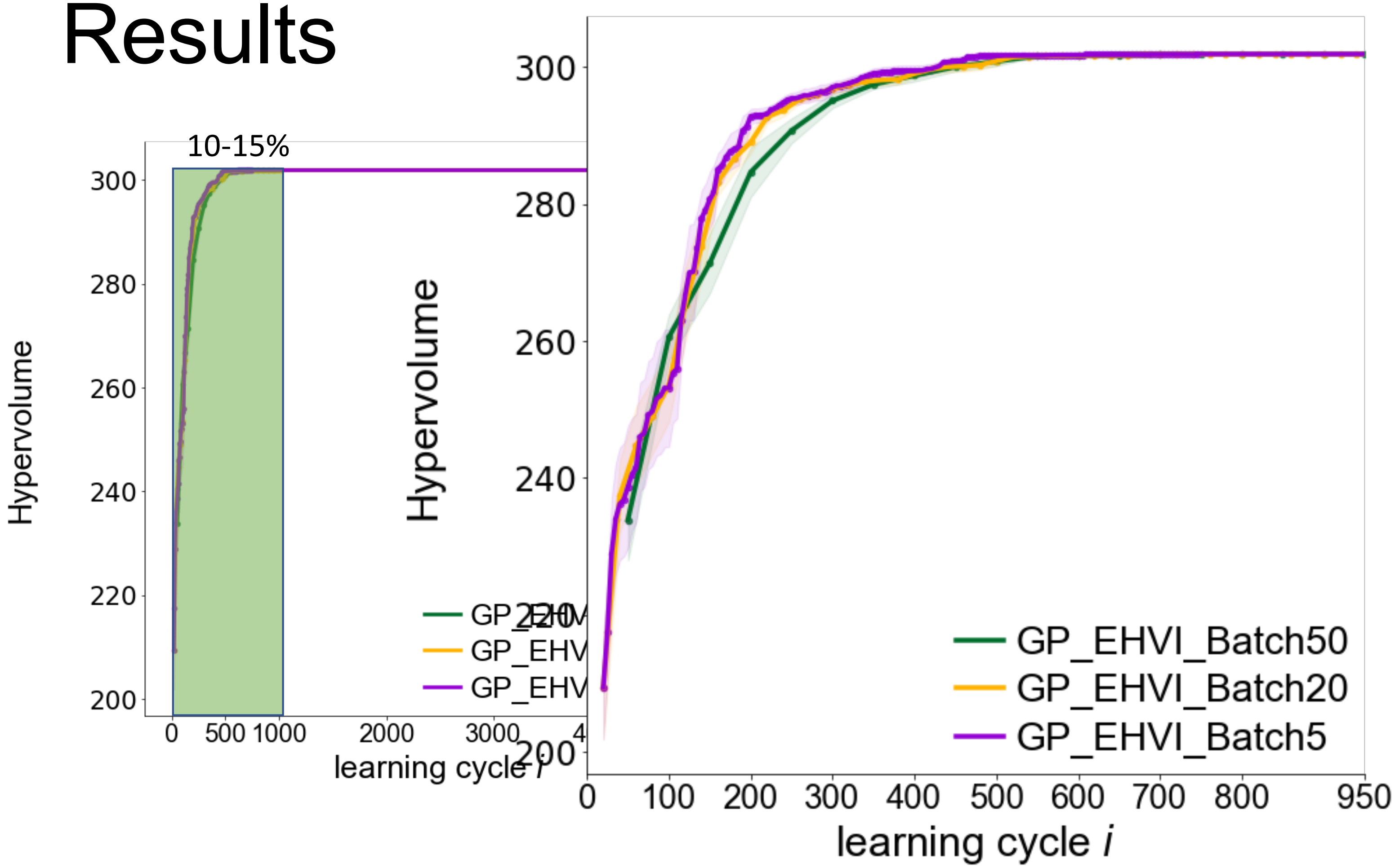
Batch = 50

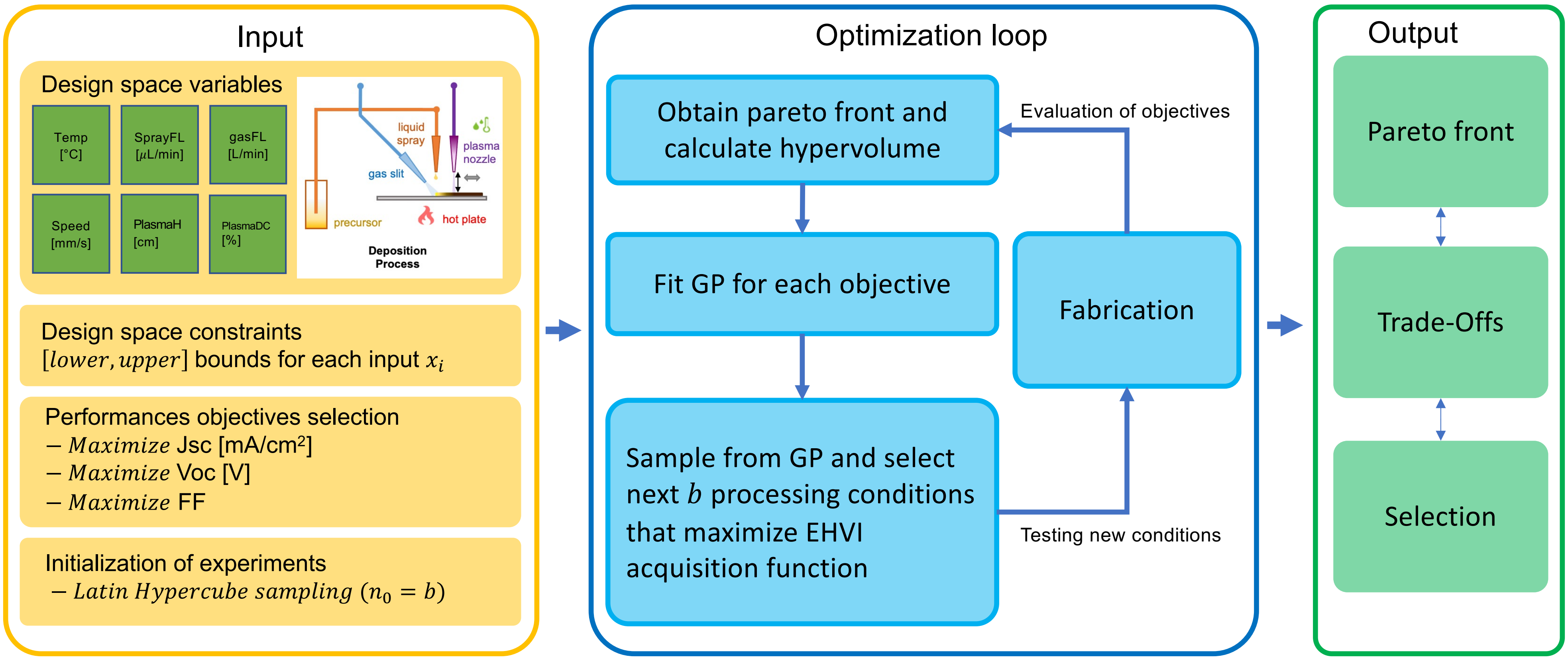


Results


10-15%
1.0
0.8
0.6
0.4
0.2
0
Pareto%
0
500
1000
2000
3000
learning cycle
GP_EH
GP_EH
GP_EH
random
1.0
0.8
0.6
0.4
0.2
0
Pareto%
0
100
200
300
400
500
600
700
800
950
learning cycle i
GP_EHVI_Batch50
GP_EHVI_Batch20
GP_EHVI_Batch5
random baseline

Results


10-15%
Hypervolume
learning cycle i
Hypervolume
learning cycle i
GP_EHVI_Batch50
GP_EHVI_Batch20
GP_EHVI_Batch5



- Demo
- Seeking suggestions of scientific intuition, Important ranges in objective space
- Thoughts are appreciated.

Expected hypervolume improvement

Definition 8 (*Expected hypervolume improvement*) Given parameters of the multivariate predictive distribution $\boldsymbol{\mu}, \boldsymbol{\sigma}$ and the Pareto-front approximation set $\mathcal{P}$, the *expected hypervolume improvement* is defined as:

$$EHVI(\boldsymbol{\mu}, \boldsymbol{\sigma}, \mathcal{P}, \mathbf{r}) := \int_{\mathbb{R}^d} \text{HVI}(\mathcal{P}, \mathbf{y}, \mathbf{r}) \cdot \boldsymbol{\xi}_{\boldsymbol{\sigma},\boldsymbol{\mu}}(\mathbf{y}) d\mathbf{y} \tag{17}$$