When is Bayesian Optimization Beneficial? A Critical Assessment of Optimization Strategies in High-Throughput Organic Photovoltaic Manufacturing

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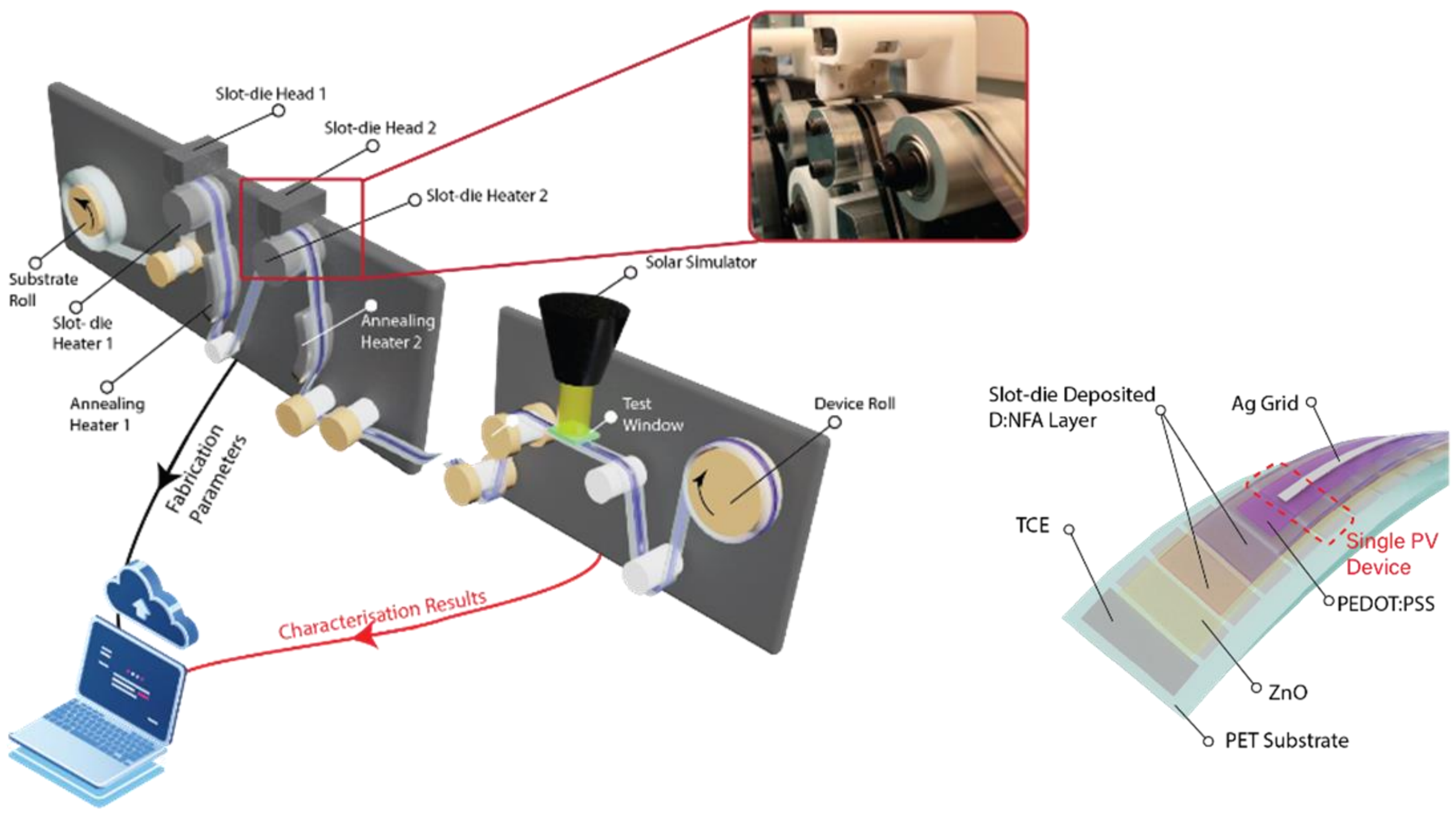
Introduction

- High-throughput OPV manufacturing requires optimizing 12+ controllable parameters while involving environmental noises
- We must assess whether Bayesian Optimization (BO) provides real-world advantages over simpler, computationally cheaper methods like Random Search (RS) in this setting.
- In noisy high-throughput environments, does BO outperform RS in finding optimal parameters, or are its advantages lost

Method

1. Manufacturing



- Derived from high-throughput roll-to-roll OPV microfactory (Ng et al., 2024).
- Stack: PET/TCE/PEDOT:PSS/ PBF-QxF:Y6 /ETL/Ag.
- Initial 36 process parameters reduced to 12 via:
  - Removal of highly correlated features (|r| > 0.8)
  - Elimination of non-controllable variables
  - Filtering of low-variance parameters
- Dataset: 11,587 OPV devices, fabricated and characterized within 24-hours

2. Simulation

$$\hat{f}(x) = \begin{cases} f(x) & \text{if } x \text{ exists in initial dataset} \\ \sum_{i=1}^{11} f(x_i)\, \bar{w}_{i,x} & \text{otherwise} \end{cases}$$

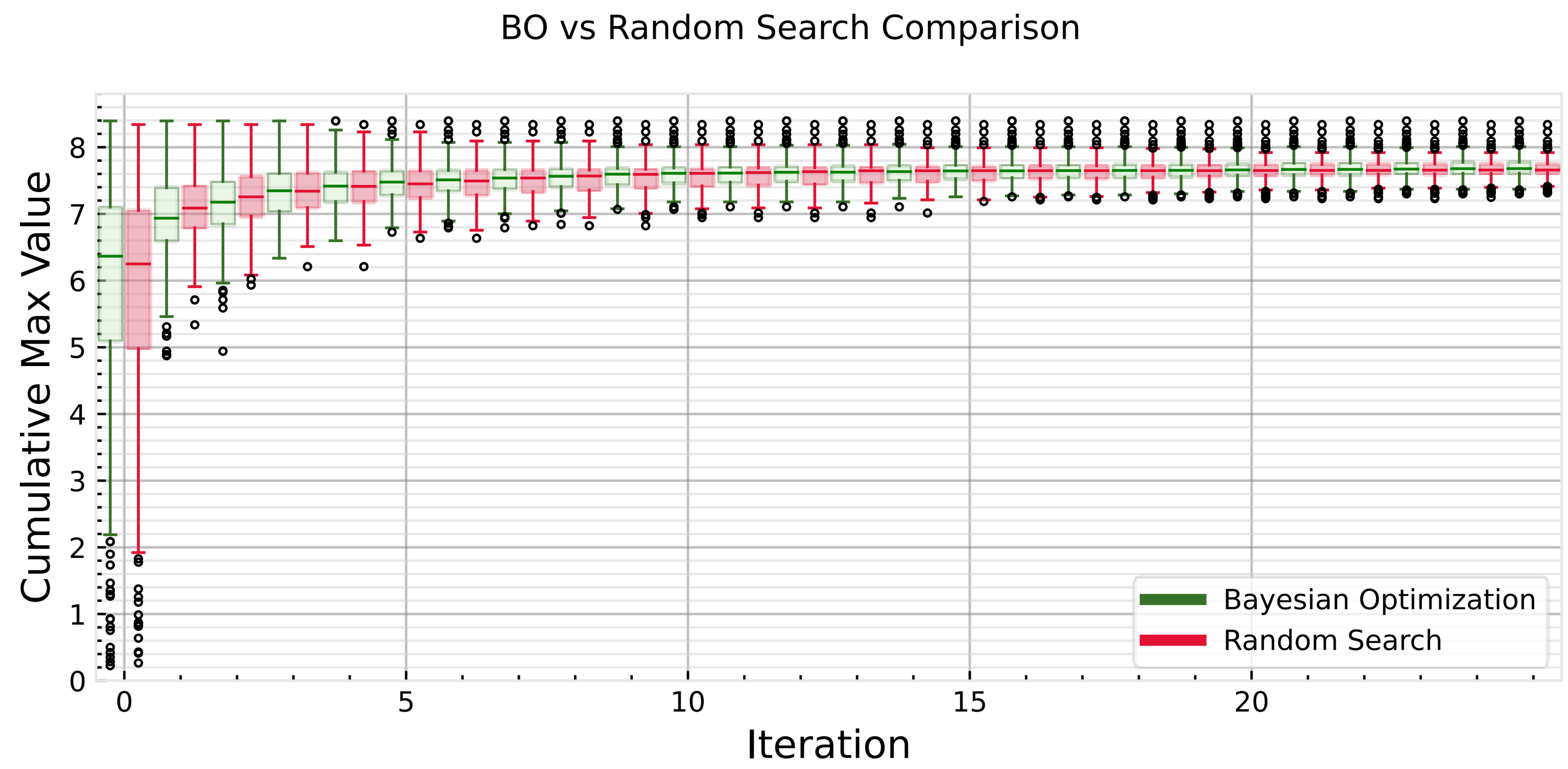
where x_i is the i-th nearest point to x in the dataset, and $\bar{w}_{i,x} = \dfrac{\frac{1}{\|x-x_i\|}}{\sum_{k=1}^{11} \frac{1}{\|x-x_k\|}}$

Implementation	BO	Random Search
Surrogate Model	Gaussian RBF	None
Acquisition Function	Expected Improvement	NA
Candidate Pool	100	25
GPU Utilization	EI Optimization	None
CPU Utilization	Function Evaluation; Candidate Generation	
Initialization	2 Points	
Iteration batch size	25	
Total Iterations	25	

All comparisons were averaged across 300 independent optimization cycles to ensure statistical significance

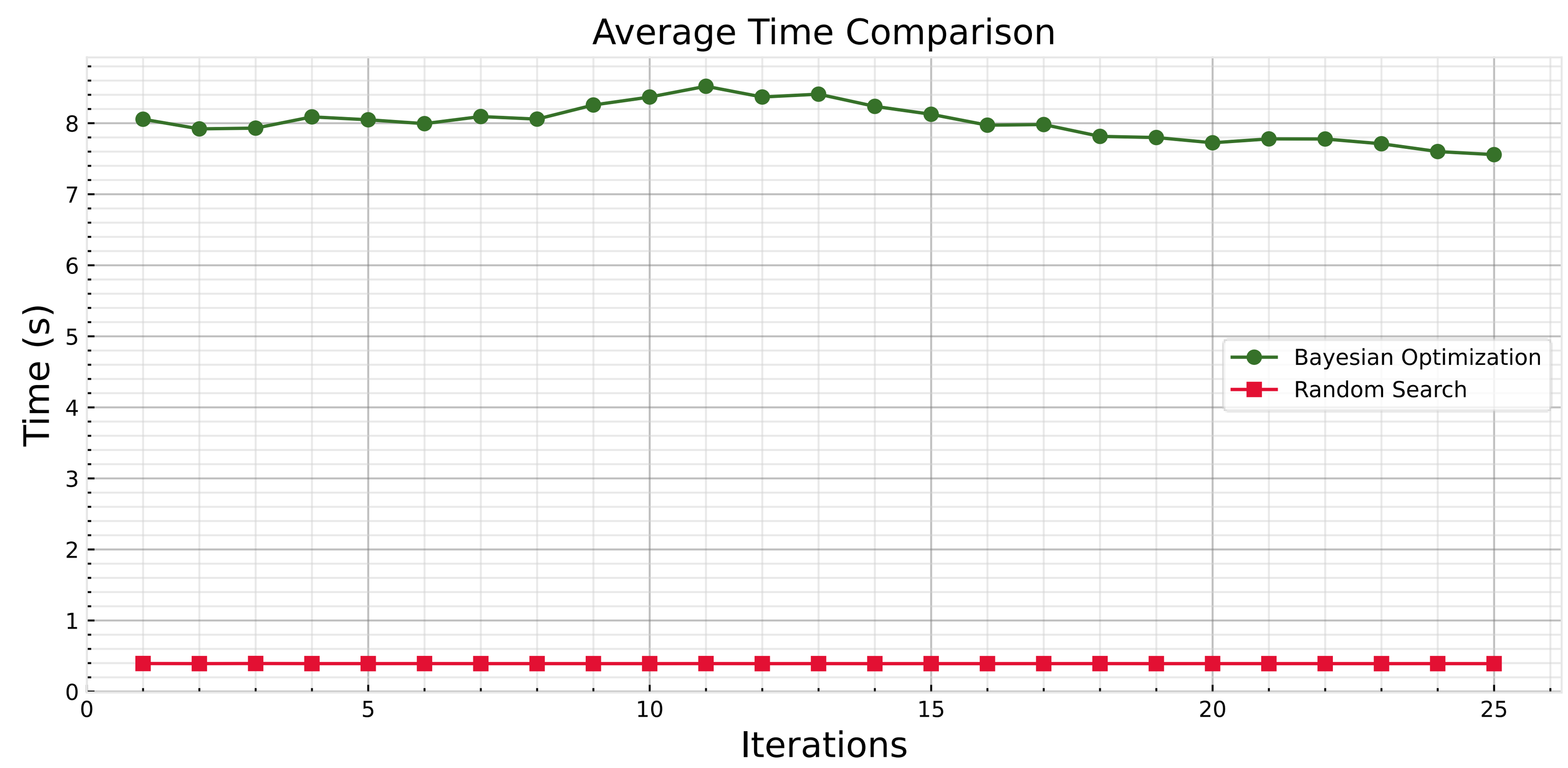
Result

1. Optimization Performance



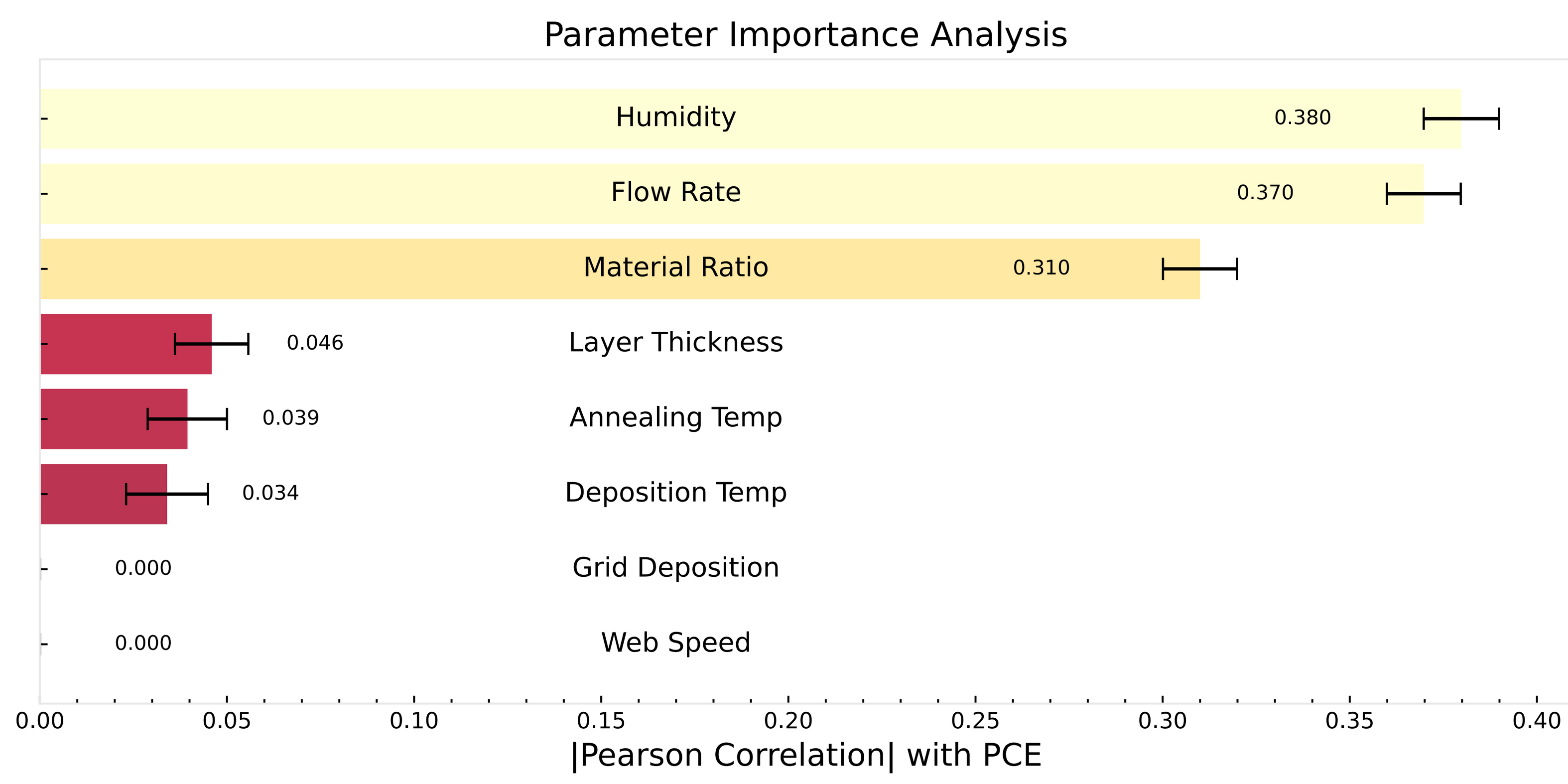
- BO achieved 7.69% vs RS's 7.66%, a negligible 0.03% gain that was not statistically significant (p > 0.05).
- RS performed better in early iterations, while BO showed marginal improvement later—but both plateaued way below the known maximum (8.35%).

2. Computational Time



- BO required ~8 seconds per iteration making it ~20× slower than RS, which averaged ~0.4 seconds per iteration.

3. Parameter Importance



- High humidity correlation (r = 0.38) and system tolerances created a noisy, locally complex space. This made RS more effective than BO under real-world conditions.

Conclusion

- Environmental and process parameters, especially humidity, had greater impact on PCE than optimization strategy, highlighting that robust process control is more critical than algorithmic choice.
- BO's limited gains in a noisy, multimodal space suggest that hybrid or adaptive methods combining RS efficiency with targeted exploration may better balance performance and practicality.