Python for early-stage design of sustainable aviation fuels

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Design a cake!

- Make a recipe

- Goals:
  - Taste
  - Cost
  - Appearance

Why is it difficult?

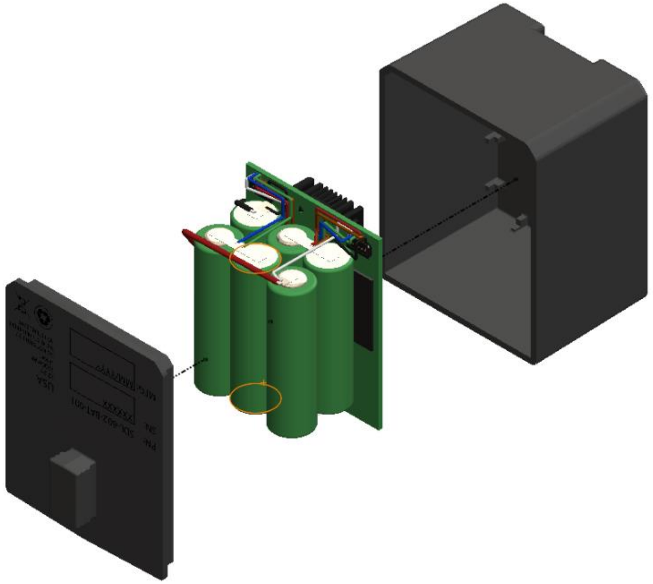
- Multi-objective
  - Taste
  - Cost
  - Appearance

- Multi-parameter
  - Flour
  - Sugar
  - Egg

No-recipe Cakes in the Real World

- Manufacture of disintegrating tablets[1]

- Battery design[2]



- Transportation decarbonization

Transportation Decarbonization

- Different modes have different pathways
- Gasoline vehicles → electric vehicles

- Aviation 2-3% of global CO_2 emissions
- Difficult to decarbonize

Conventional Aviation Fuel

- Liquid, petroleum fuel
- Stringent requirements
  - Freezing point
  - Flash point
  - Viscosity
  - Density

Sustainable Aviation Fuel

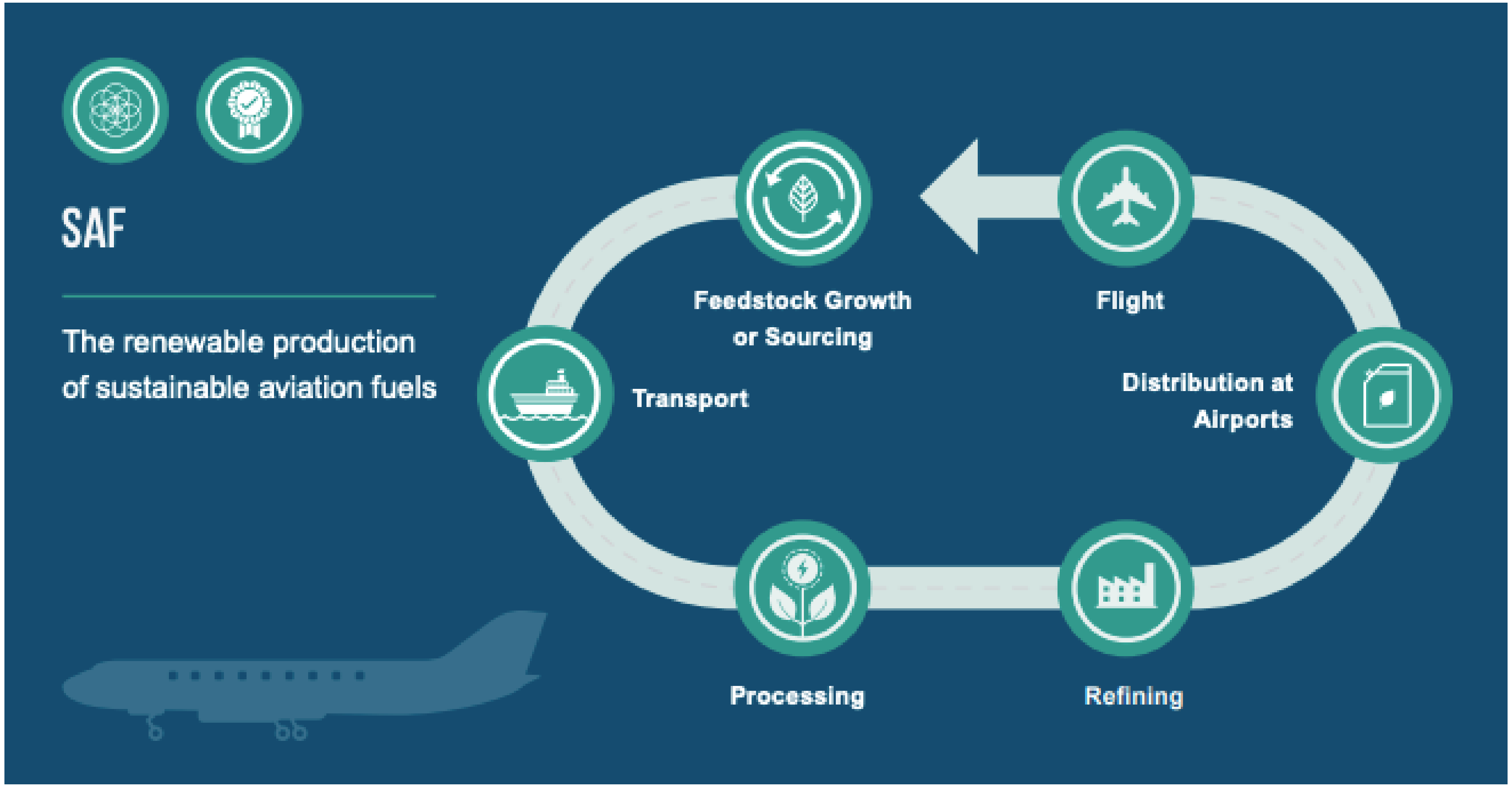
- Primary decarbonization opportunity

- Derived from biomass feedstocks
  - Cooking/plant oil
  - Agricultural residue

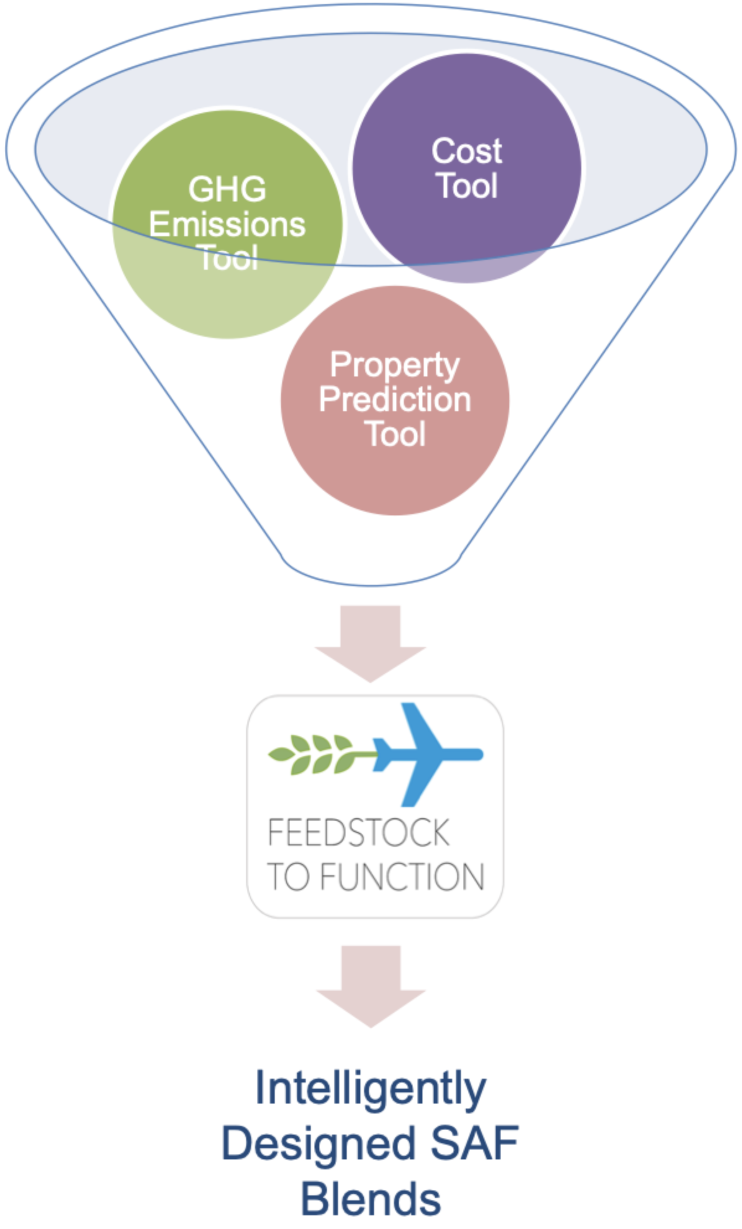
- Comparable performance to conventional fuel

Sustainable Fuel Implementation Challenges

- Cost
- Scale-up
- Slow development



Create an optimization tool for early-stage design of novel sustainable aviation fuels



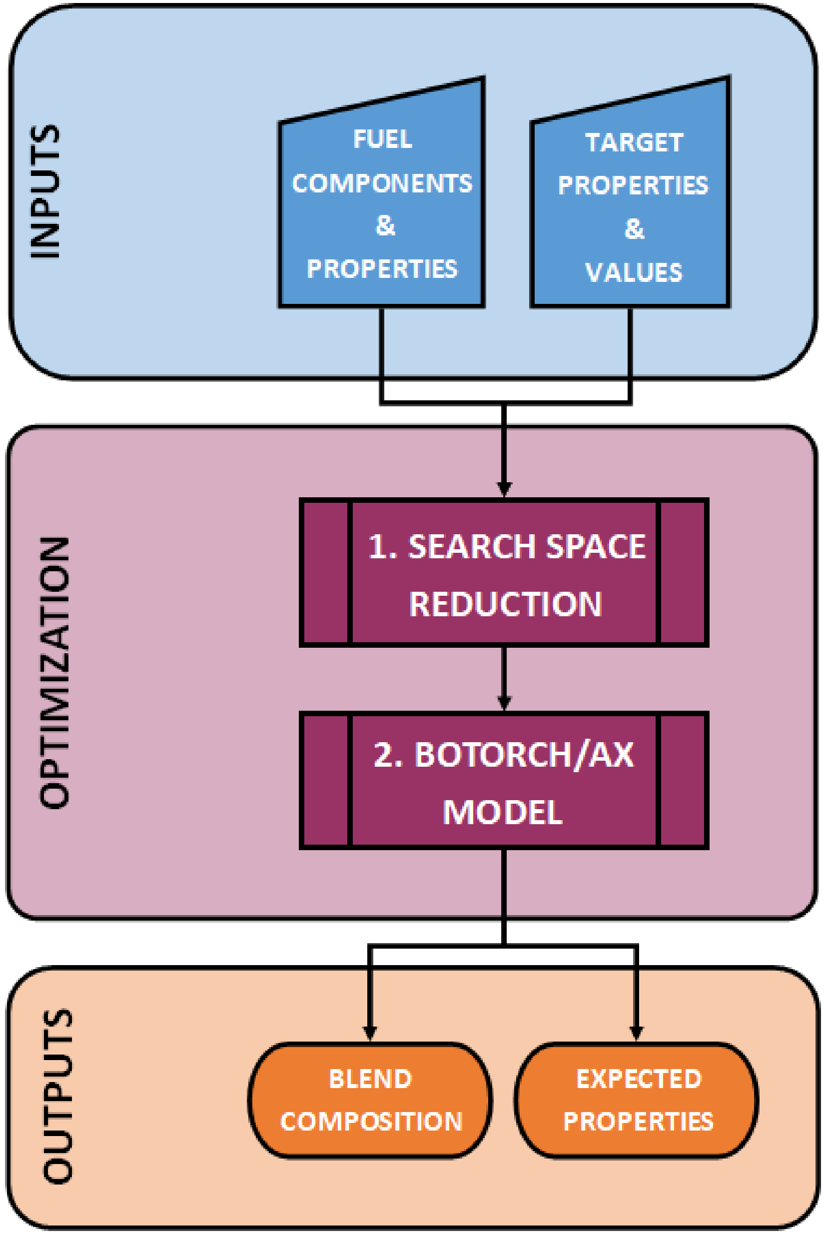
Methods

Sequential optimization:

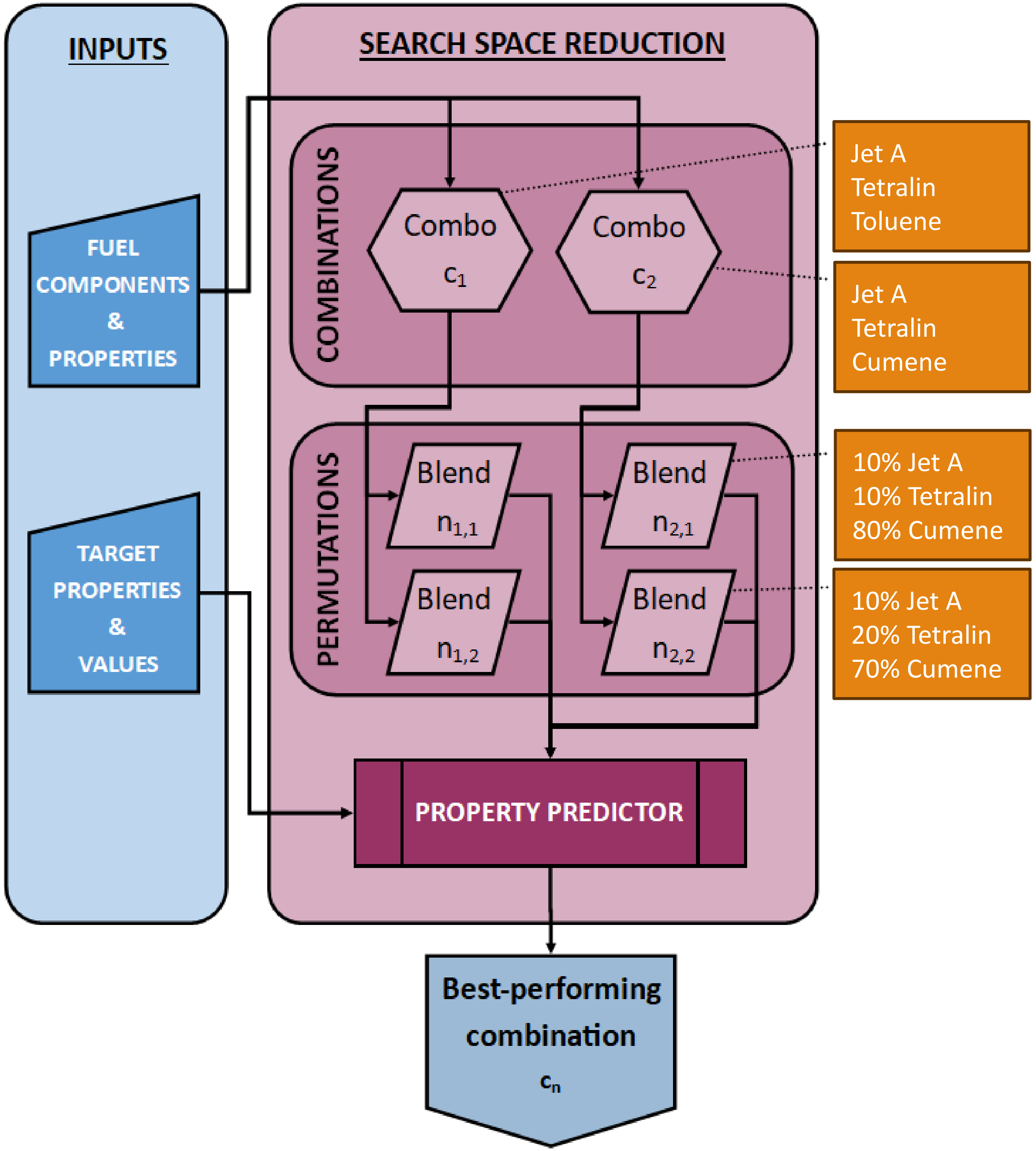
1. Search space reduction
2. Multi-objective Bayesian optimization

BoTorch

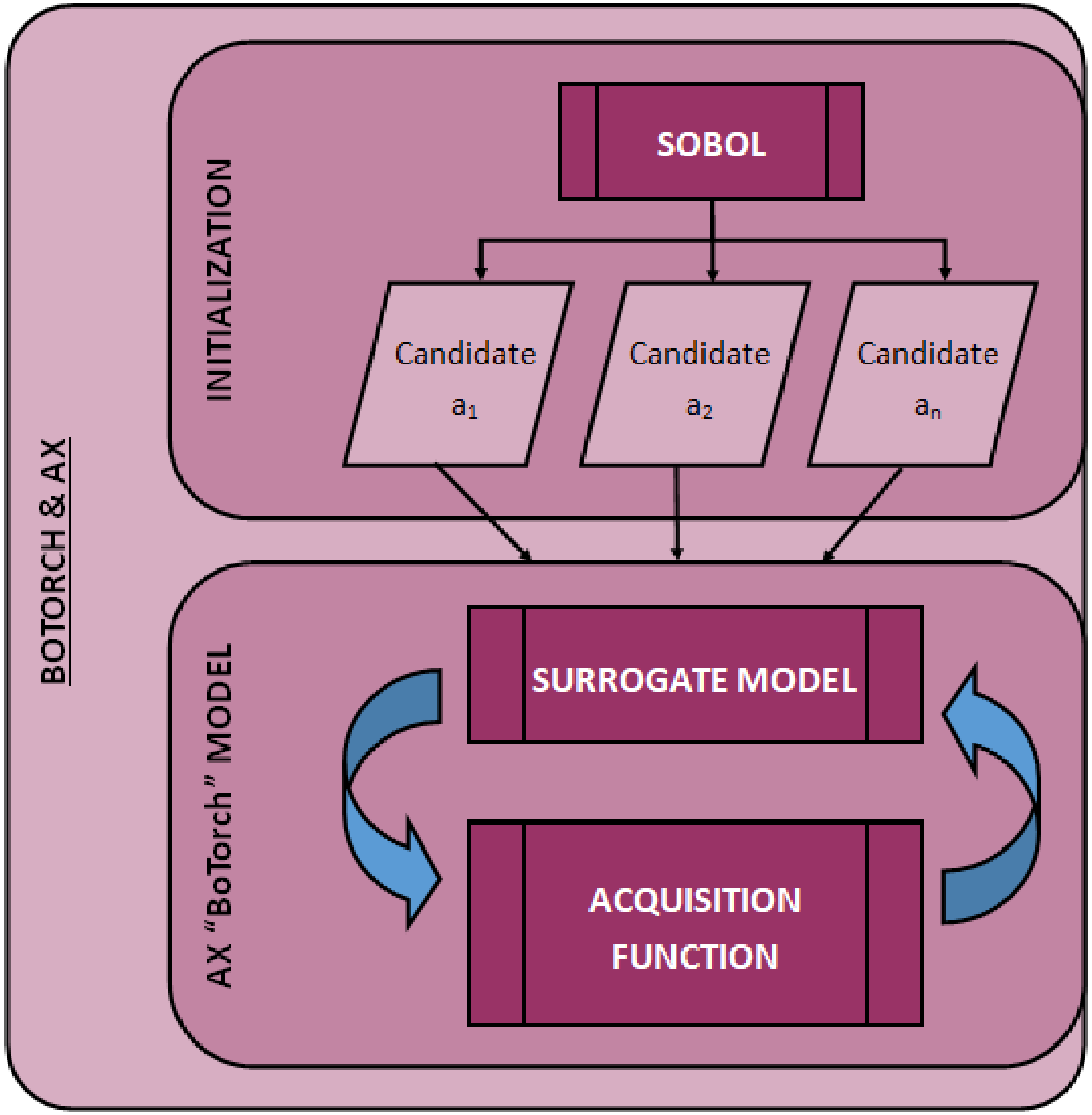
Ax

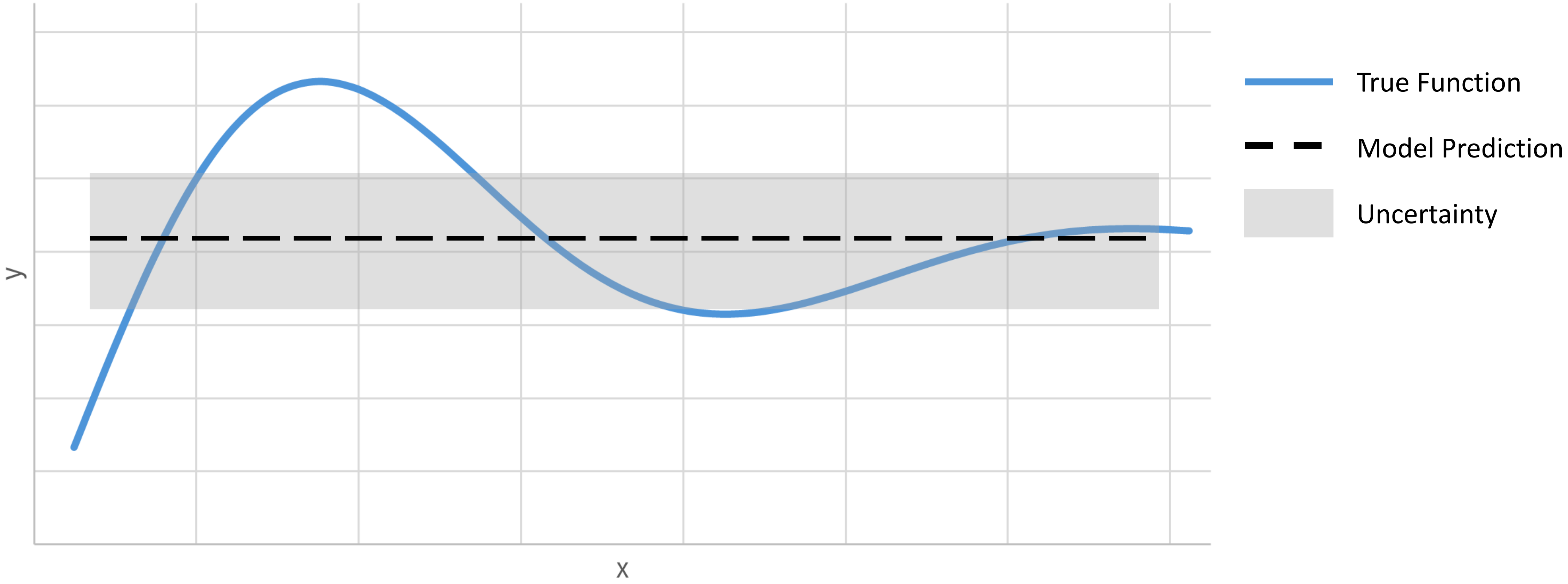


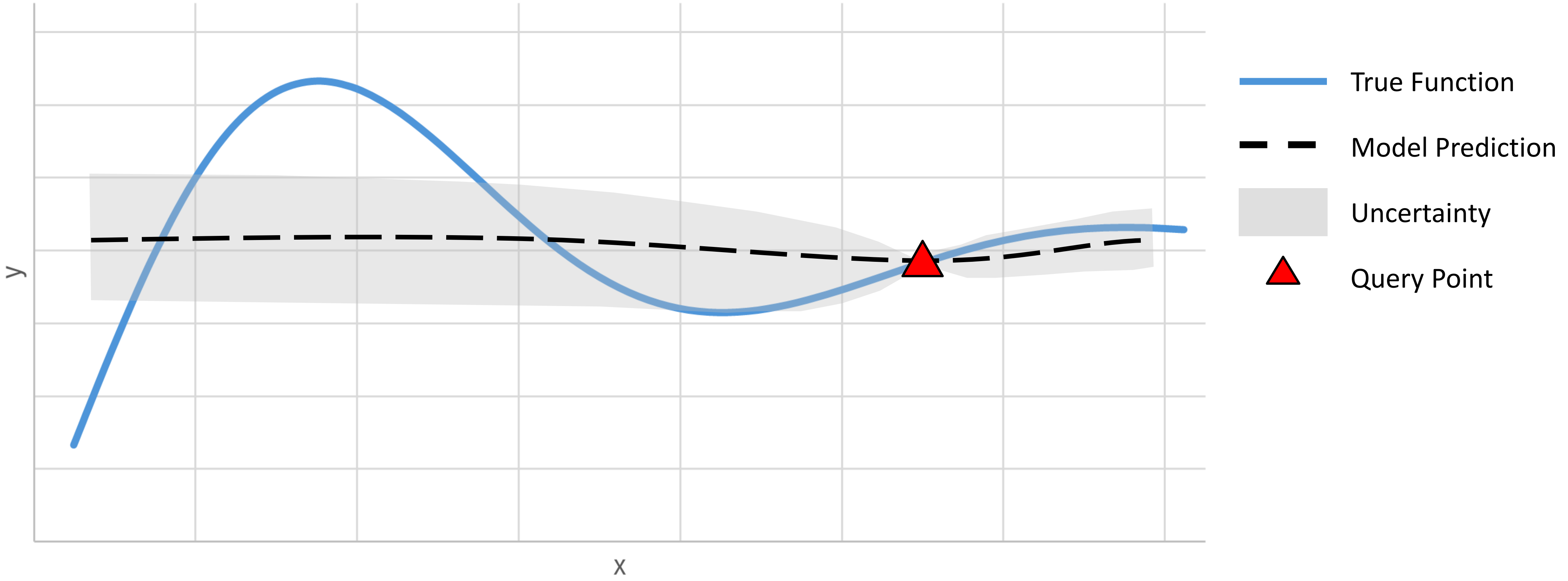
Search Space Reduction



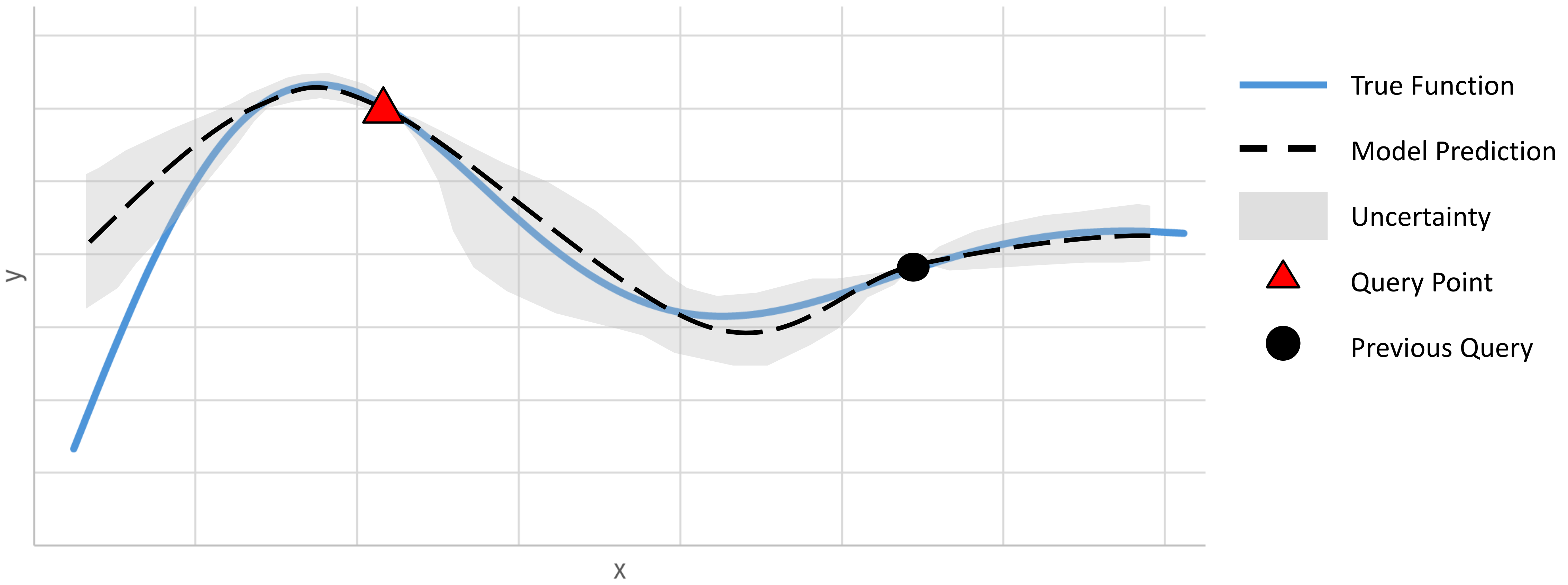
BoTorch/Ax Bayesian Optimization



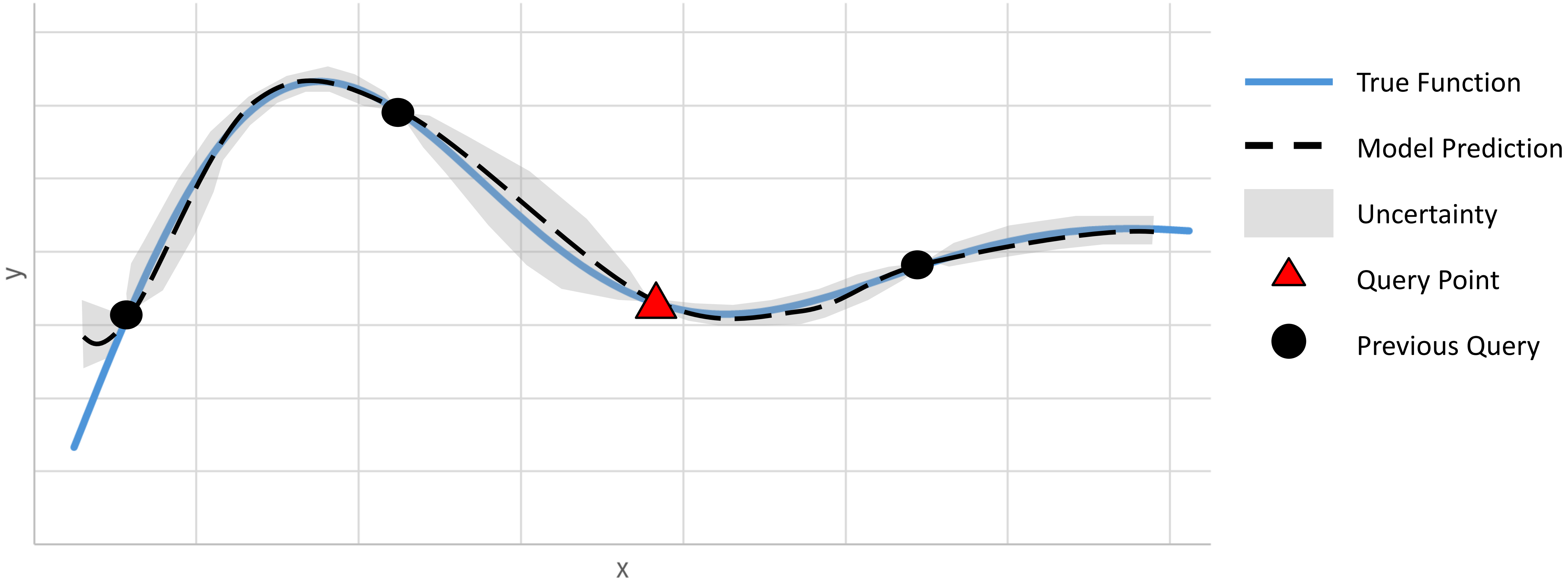

True Function
Model Prediction
Uncertainty
y
x



True Function
Model Prediction
Uncertainty
Query Point
y
x



y
x
True Function
Model Prediction
Uncertainty
Query Point
Previous Query


y
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True Function
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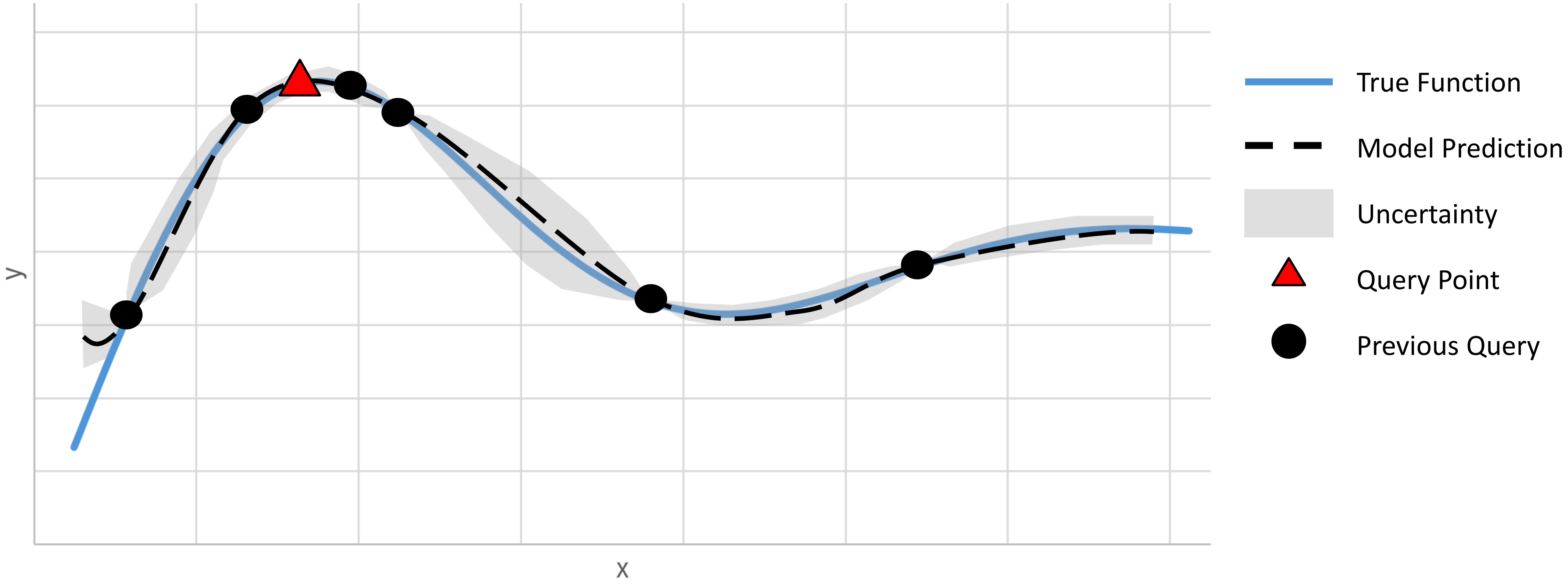
True Function
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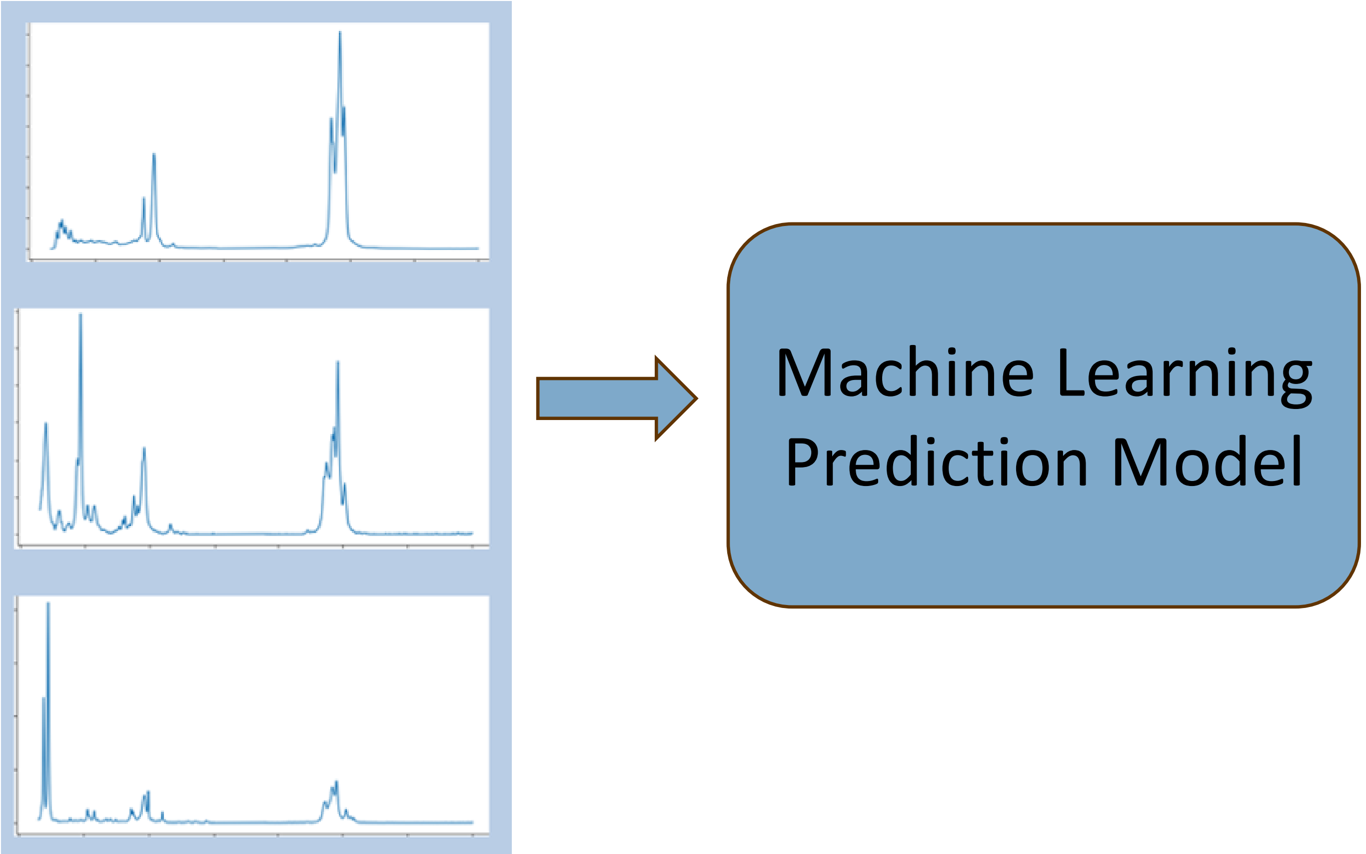
x

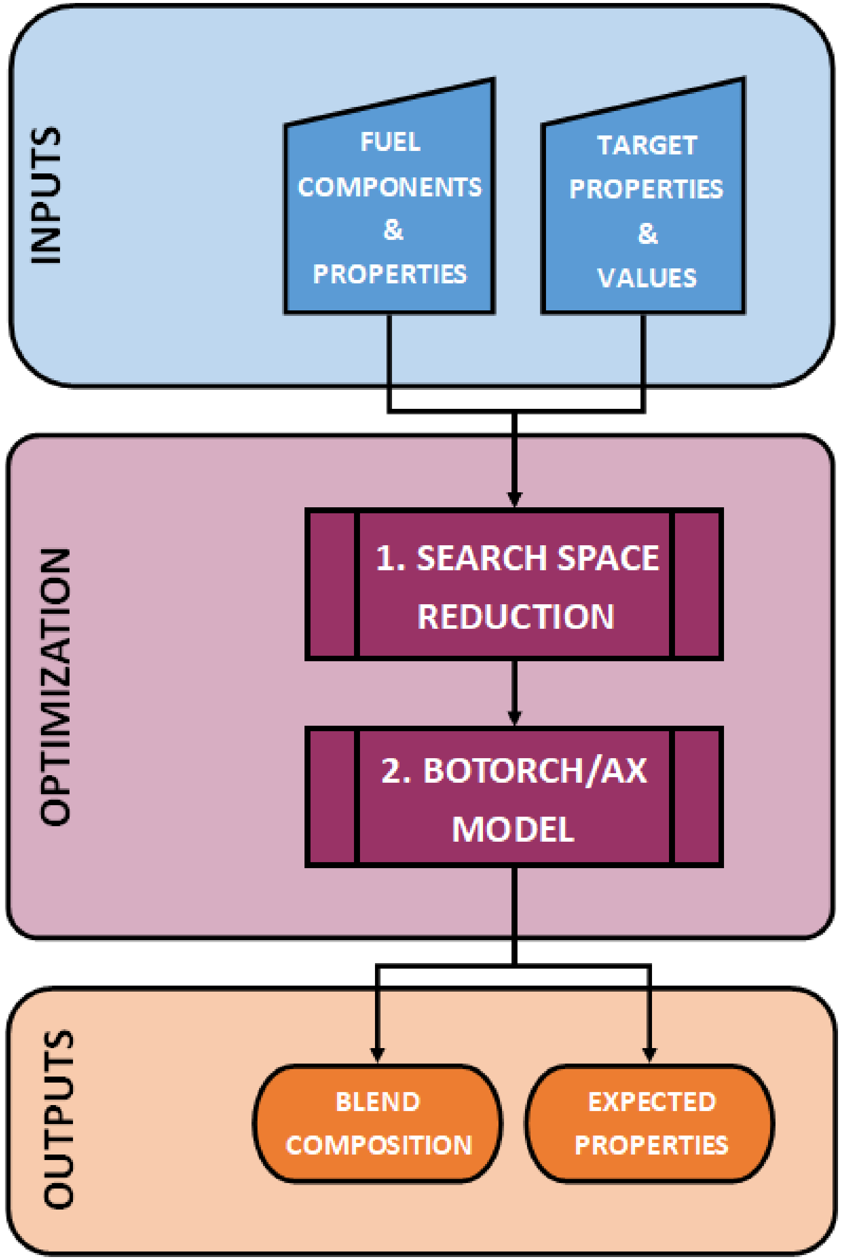
Property Predictors

- “Black box” prediction
- Modular substitution

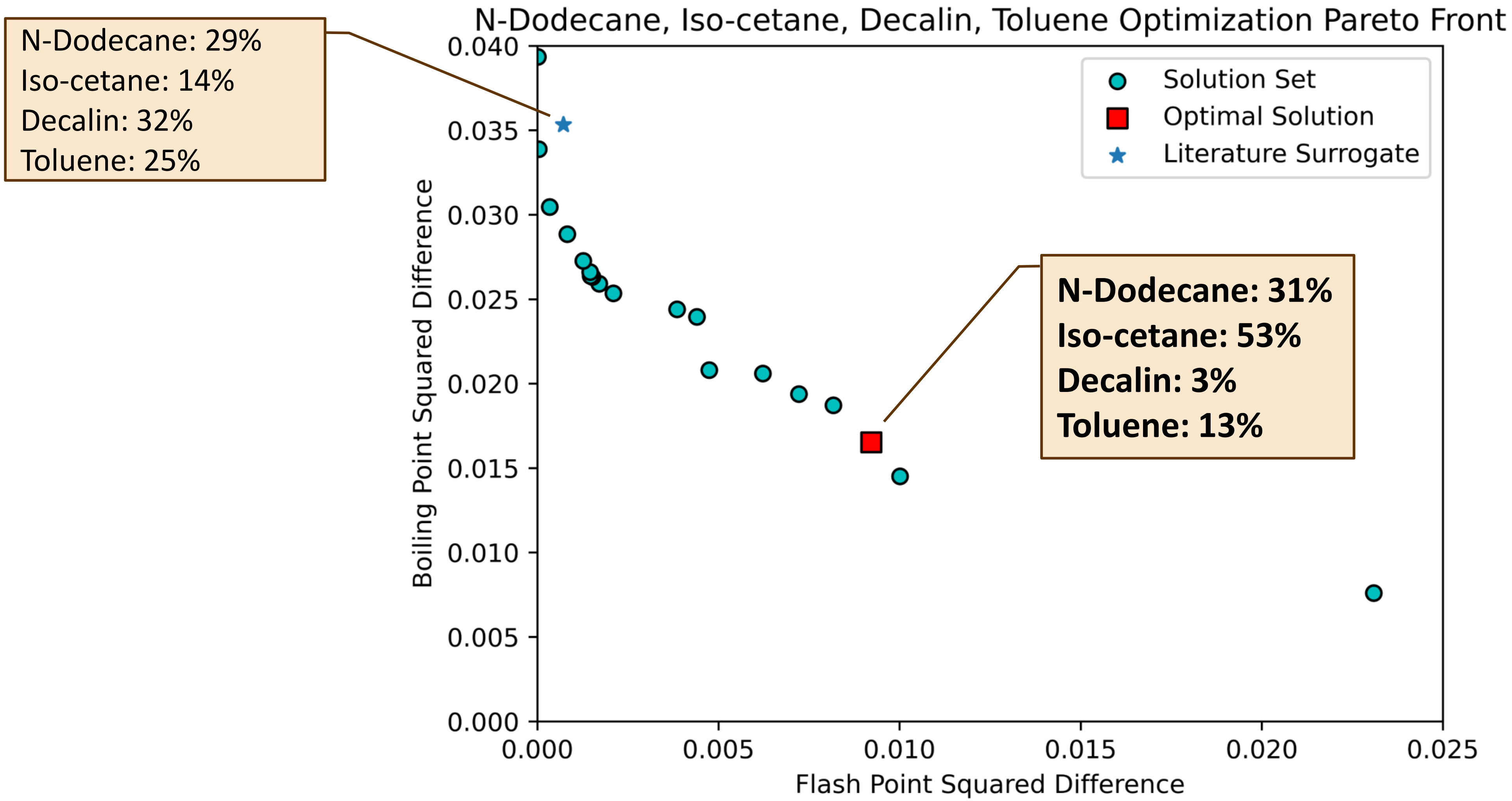
- Linear by Volume
- Data-driven predictor



Review


INPUTS
FUEL COMPONENTS & PROPERTIES
TARGET PROPERTIES & VALUES
OPTIMIZATION
1. SEARCH SPACE REDUCTION
2. BOTORCH/AX MODEL
OUTPUTS
BLEND COMPOSITION
EXPECTED PROPERTIES

Surrogate Comparison [3]



Design Challenge #1

Possible components:

cumene, methylcyclohexane, toluene, cyclopentane, hexene, isooctane

	Cumene	**Methylcyclohexane**	**Hexene**
Blend Ratio	0.18	0.21	0.61

	Boiling Point (K)	Flash Point (K)	Melting Point (K)	Density (kg/m^3)	Viscosity (mm^2/s)
Target Values	400	280	150	750	1.3
Blended Estimate	376	292	164	742	1.319
+/-	*-24*	*+12*	*+14*	*-8*	*+0.019*

Design Challenge #2

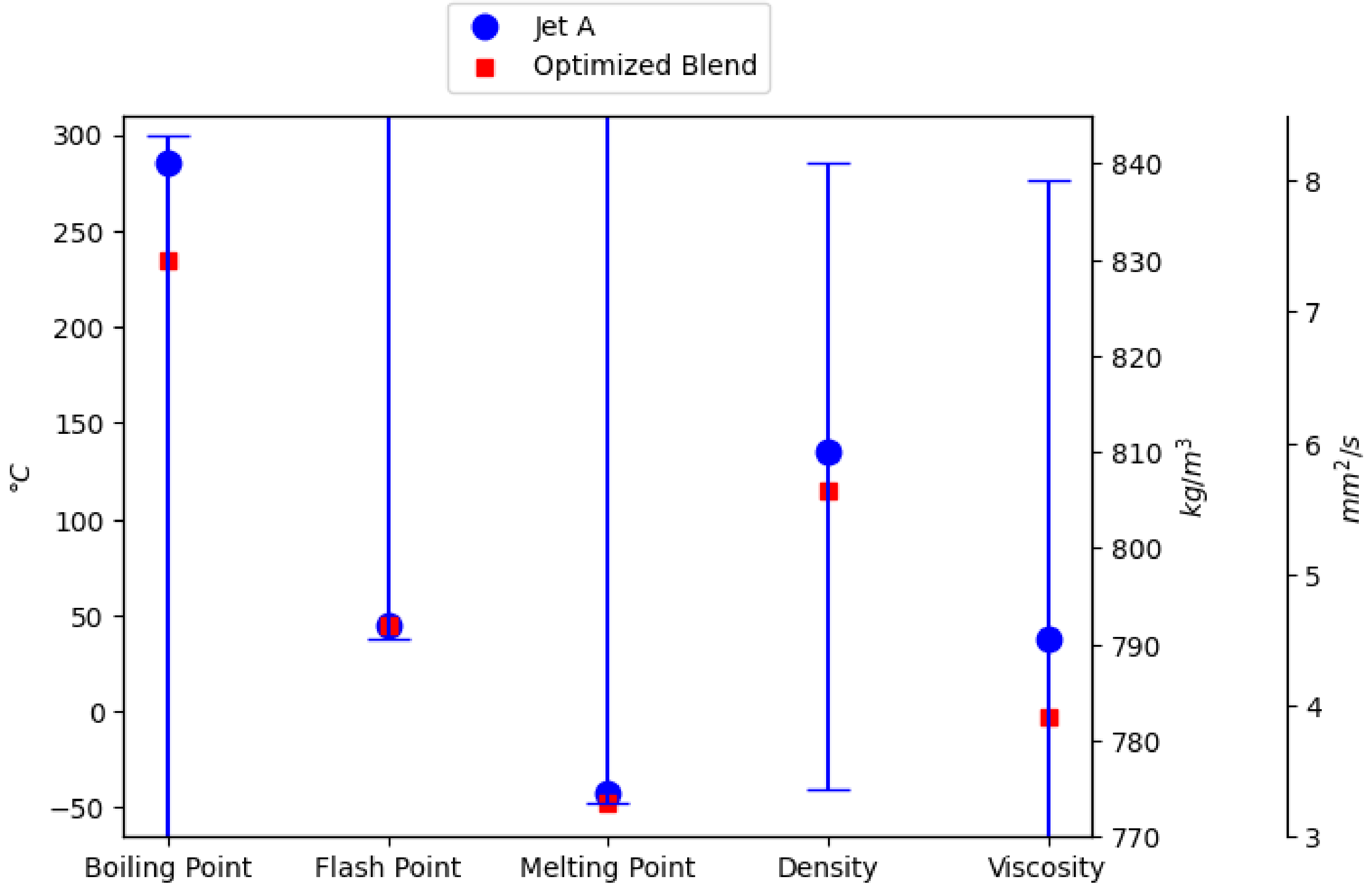
Requirement: 0-75% Jet A

Possible components:

- 60% heptane/40% isooctane, tetralin, cumene, toluene, methylpentane, isooctane

Blend Ratio:

- 74% Jet A
- 08% 60/40 heptane/isooctane
- 08% Tetralin
- 10% Cumene



Summary

- Developed multi-objective, multi-parameter optimization approach

- Tool designed for variability
  - Number of components
  - Required components
  - Predictors

- Expanded Feedstock to Function capabilities

https://feedstock-to-function.lbl.gov/

Credits

[1] Sano, Syusuke, et al. “Application of Bayesian Optimization for Pharmaceutical Product Development.” *Journal of Pharmaceutical Innovation*, vol. 15, no. 3, Sept. 2020, pp. 333–43. *Springer Link*, https://doi.org/10.1007/s12247-019-09382-8.

[2] Thelen, Adam, et al. “Sequential Bayesian Optimization for Accelerating the Design of Sodium Metal Battery Nucleation Layers.” *Journal of Power Sources*, vol. 581, Oct. 2023, p. 233508. *ScienceDirect*, https://doi.org/10.1016/j.jpowsour.2023.233508.

[3] Kim, Doohyun, Jason Martz, and Angela Violi. “A Surrogate for Emulating the Physical and Chemical Properties of Conventional Jet Fuel.” *Combustion and Flame*, vol. 161, no. 6, June 2014, pp. 1489–98. *ScienceDirect*, https://doi.org/10.1016/j.combustflame.2013.12.015