AI for Materials Science: Tuning Laser-Induced Graphene Production and Beyond

Lars Kotthoff and others who did the actual work
Artificially Intelligent Manufacturing Center
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University of Wyoming

Leiden, 29 August 2019

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THE WORLD NEEDS
MORE COWBOYS.

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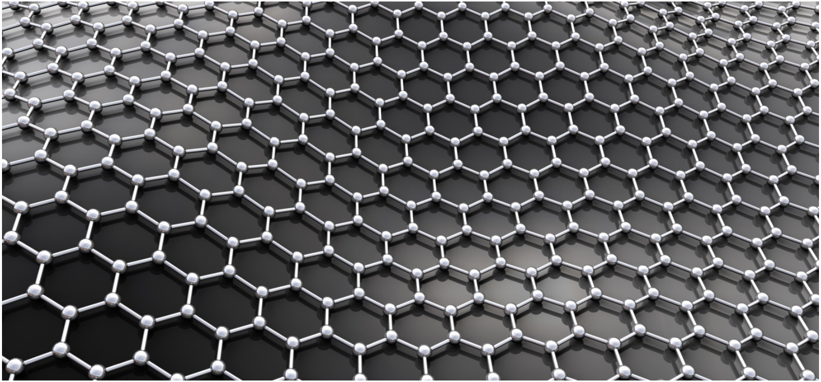
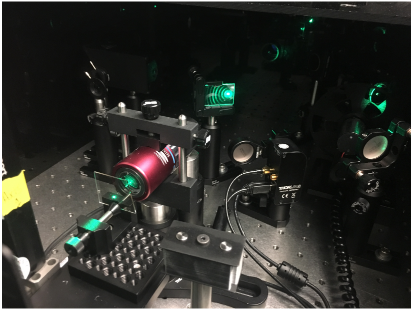


Automated Parameter Tuning

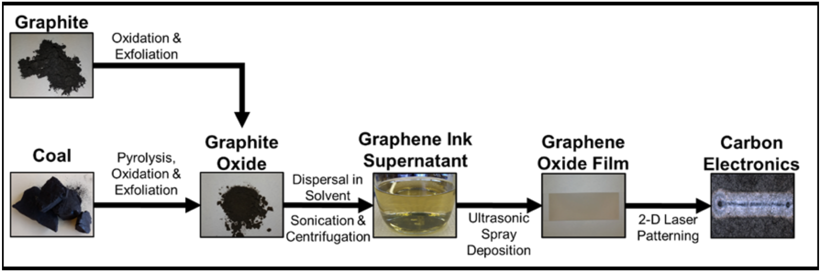
- ▷ treat tunable process as black box – no knowledge of inner workings required
- ▷ intelligently and iteratively select parameter settings likely to improve performance
- ▷ mature techniques used in many areas of AI

Optimizing Graphene Oxide Reduction

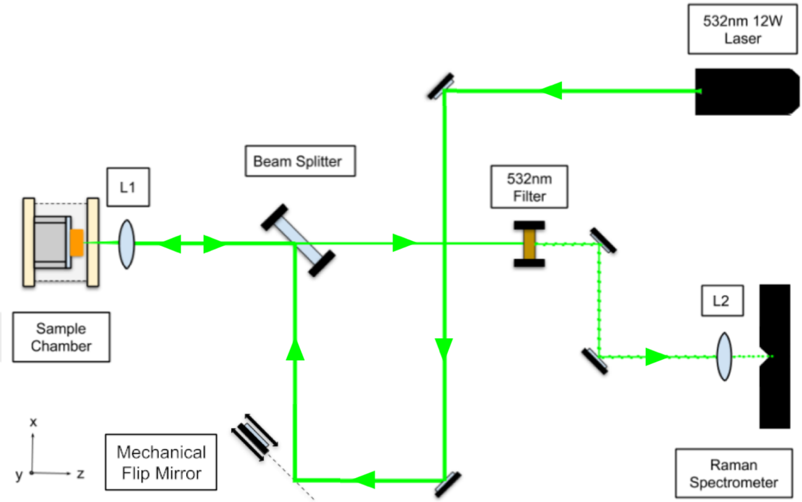
- reduce graphene oxide to graphene through laser irradiation
- allows to create electrically conductive lines in insulating material
- laser parameters need to be tuned carefully to achieve good results



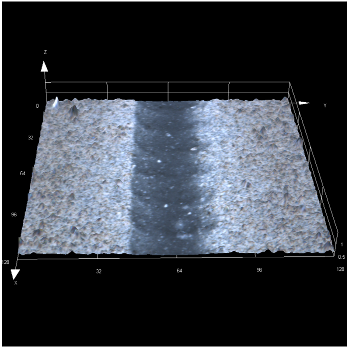
From Graphite/Coal to Carbon Electronics

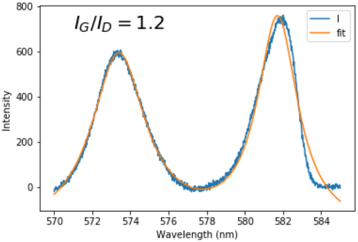


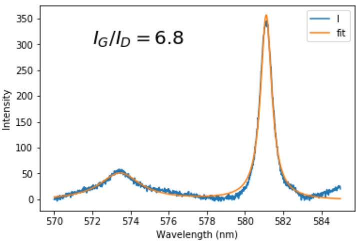
Experimental Setup



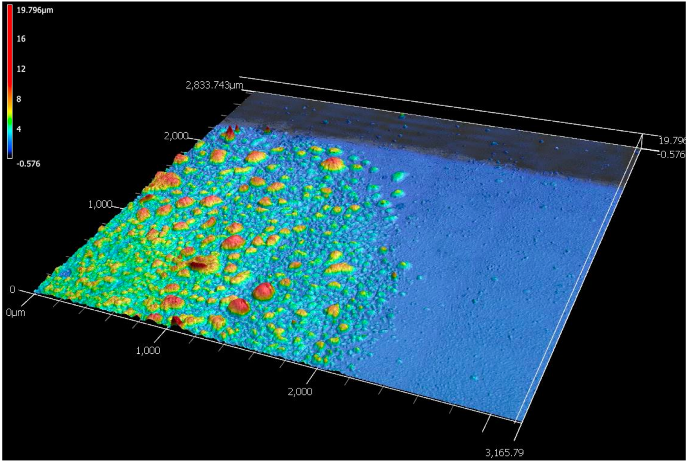
Evaluation of Irradiated Material







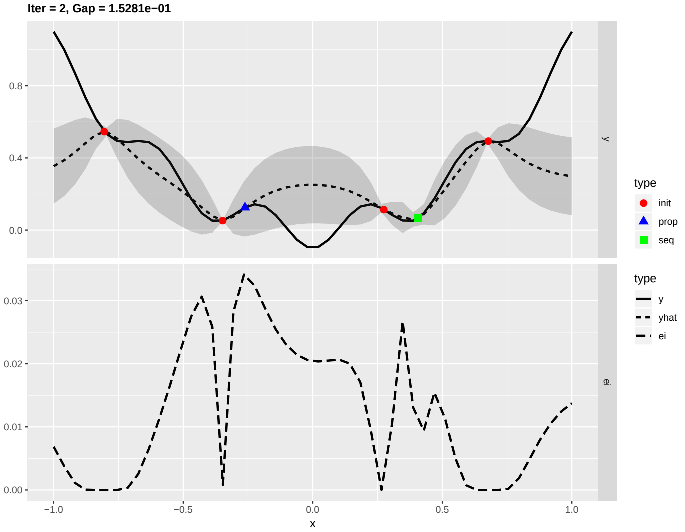
Morphology of Irradiated Material



Bayesian Optimization with Surrogate Models

- evaluate small number of initial (random) configurations
- build surrogate model of parameter-performance surface based on this
- use model to predict where to evaluate next
- repeat
- allows targeted exploration of new configurations

Bayesian Optimization with Surrogate Models



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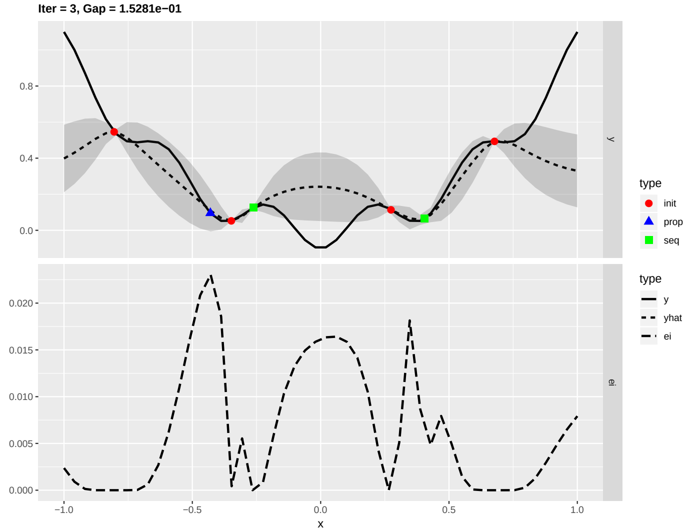

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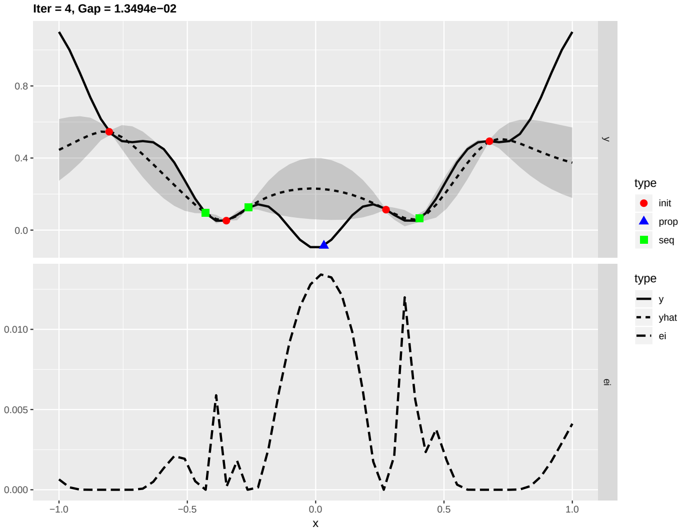

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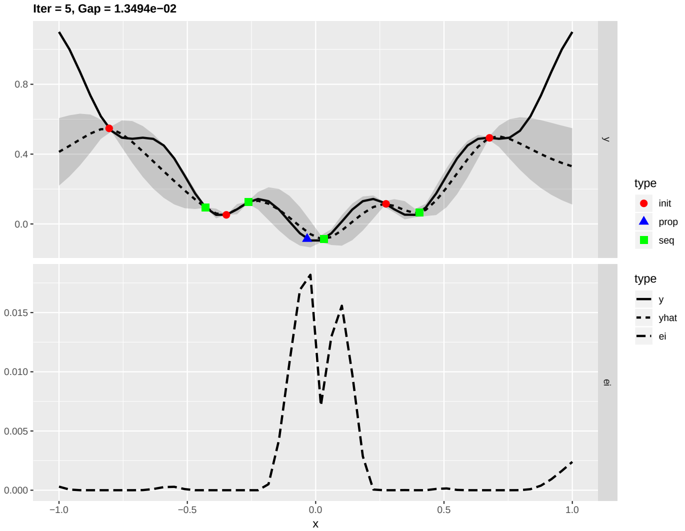

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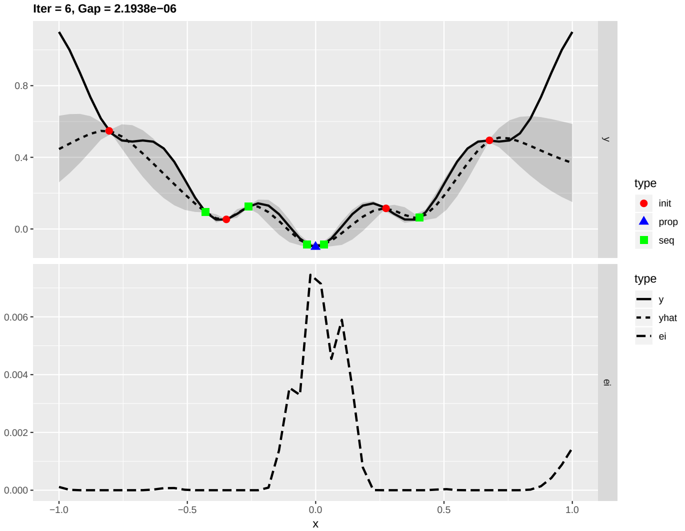

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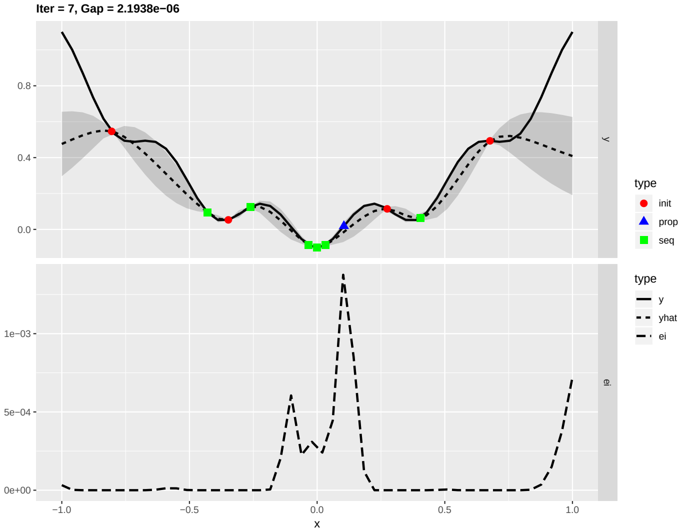

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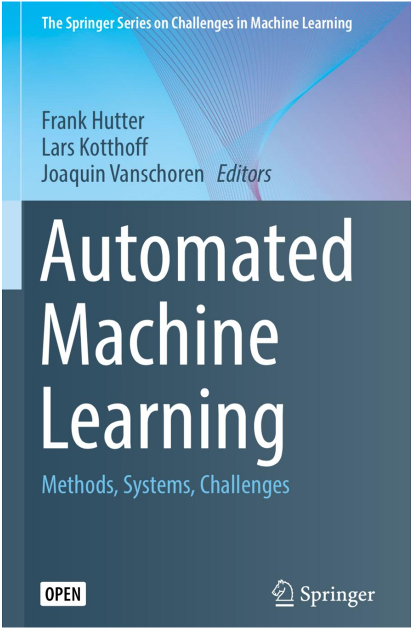
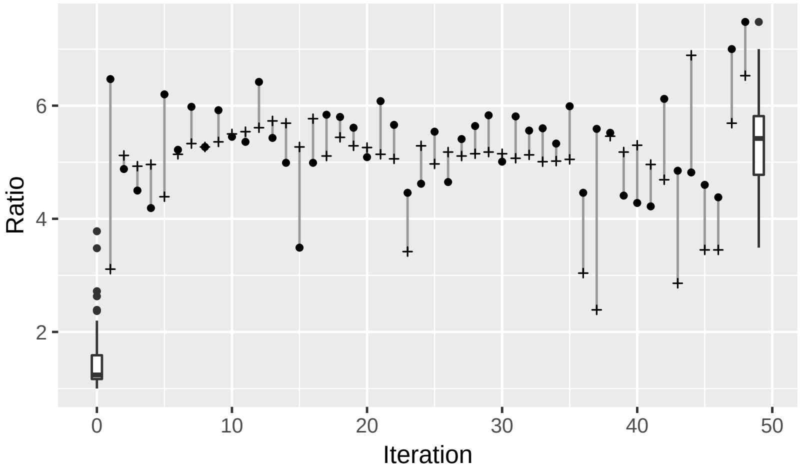


https://www.automl.org/book/

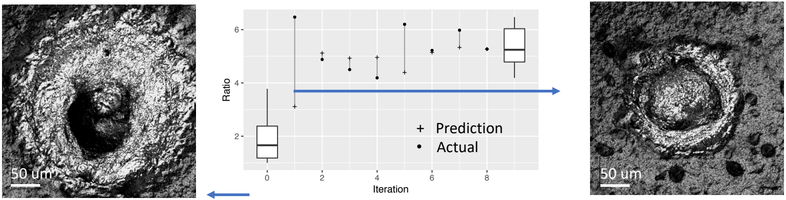
Tuned Parameters

- laser power (1 mW to 4400 mW), duration for irradiating spot (710 ms to 20 210 ms), pressure in reaction chamber (10 psi to 100 psi)
- ≈7.8 billion configurations
- individual graphene oxide sample allows for max 361 evaluations, about 2 weeks of human operator time

Tuned Parameters

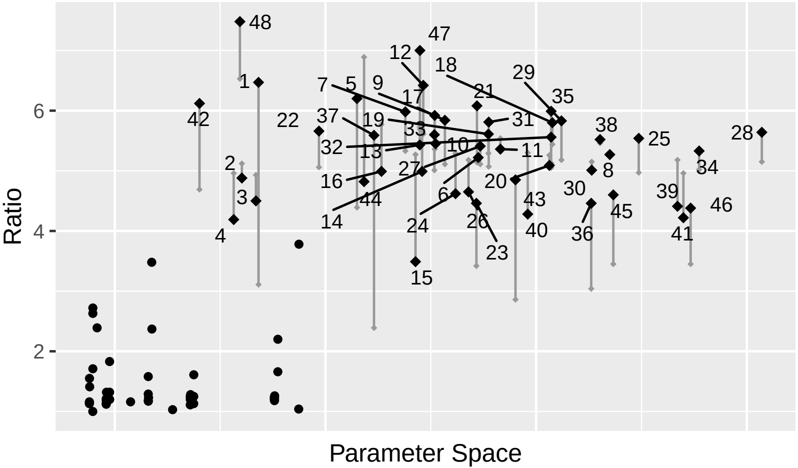


Tuned Parameters



- improvement of factor of two over best result in literature
- good results even with small amount of initial data (19 evaluations)
- code can be used by domain experts with no background in machine learning

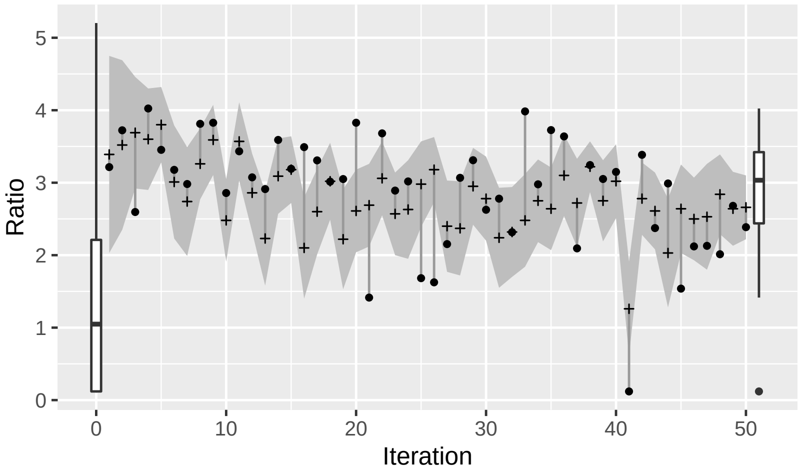
Explored Parameter Space



Tuned Parameters – Kapton

- extend parameter space with gas in reaction chamber – air, argon, nitrogen
- extend ranges of other parameters
- more and longer experimental campaigns

Tuned Parameters – Kapton



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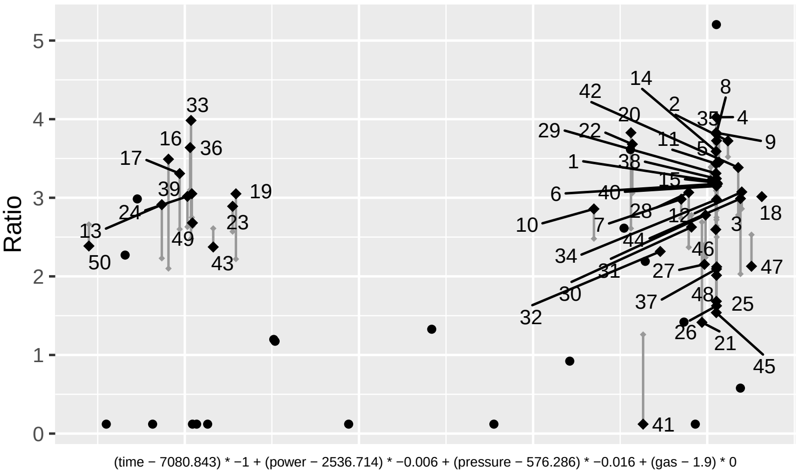
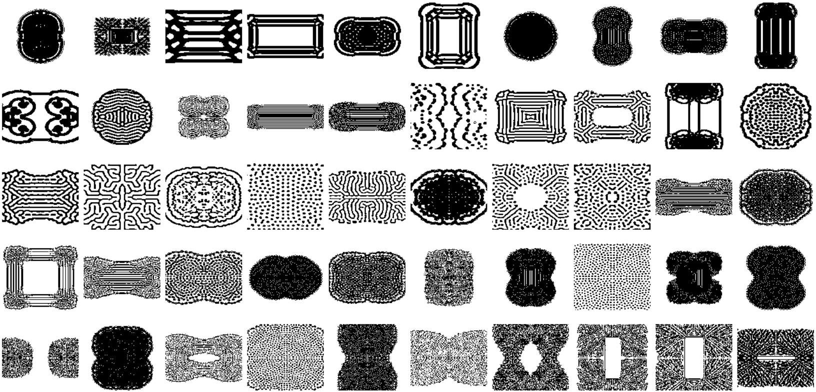
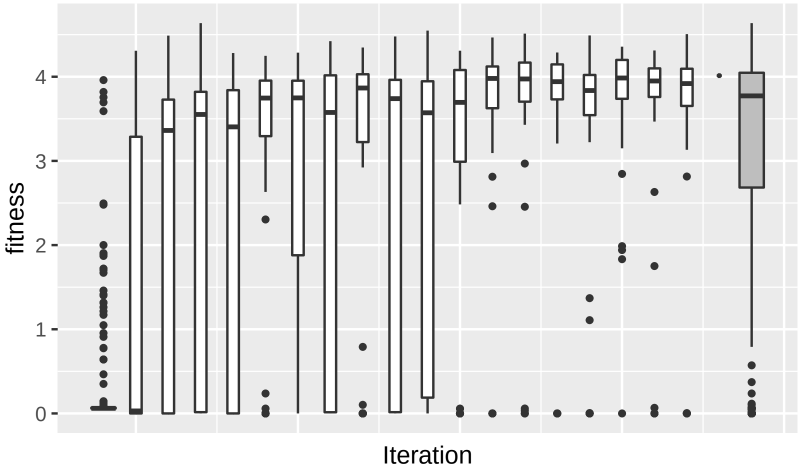


Design of New Materials



- optimize parameters of pattern generator for energy absorption of material
- six numeric parameters
- computational evaluation of candidates

ML-Optimized Generator Parameters



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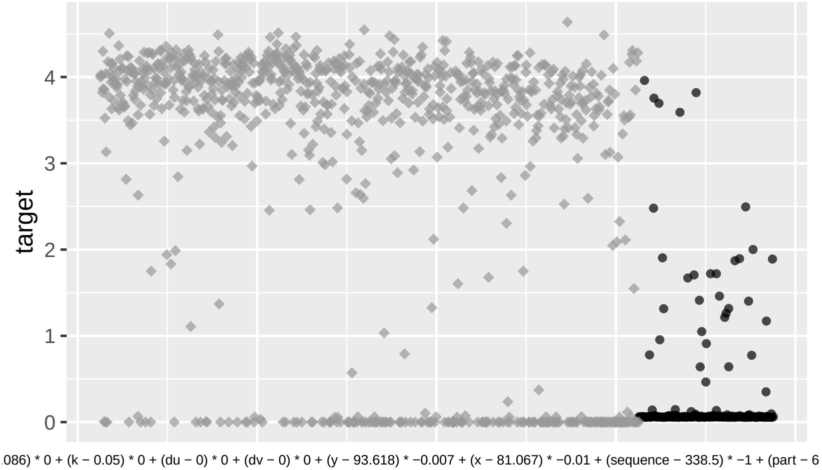

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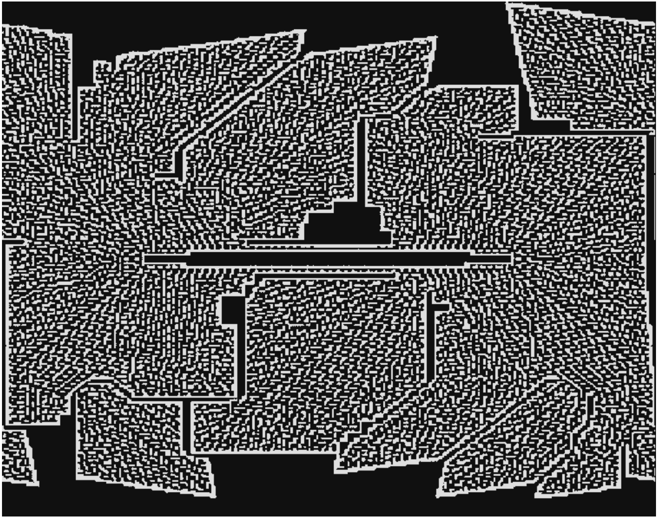


Outlook

- ▷ automate experimental setup
- ▷ application to other materials
- ▷ more in-depth investigation of Bayesian Optimization performance (and other approaches)
- ▷ inform understanding of process by what surrogate model has learned

Other Projects

- optimization of wear of buttons
- density functional theory (DFT) calculations of properties of graphene
- optimization of DFT calculations

Challenges and Opportunities

- sparsity of data
- multi-scale measurements
- combination of optimization with experiments and simulations

Do Try This at Home

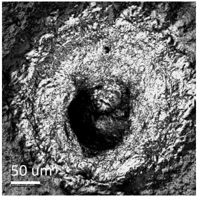
Tutorial on AI for Materials Science @ IJCAI 2019

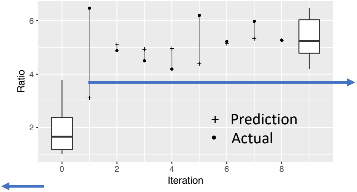
`https://www.cs.uwyo.edu/~larsko/aimat-tut/`

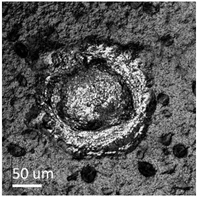
Simulator optimizers available

- build surrogate model based on (relatively) large amount of data
- Bayesian Optimization based on this surrogate model
- playground to try your own approaches

Summary







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