Robust Autonomous Adaptive Experimentation
(FA9550-16-1-0053)

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AFOSR Program Review:
Computational Cognition and Machine Intelligence Program
(October 6-8, 2020, Arlington, VA)

Robust Autonomous Adaptive Experimentation
(Mark Pitt & Jay Myung, Ohio State University)

Objective:

- Improve the efficiency and informativeness of inference in experimentation
- Develop and apply robust algorithms for autonomous experimentation systems (ARES)

Approach:

- Nonparametric Bayesian framework
- Active learning

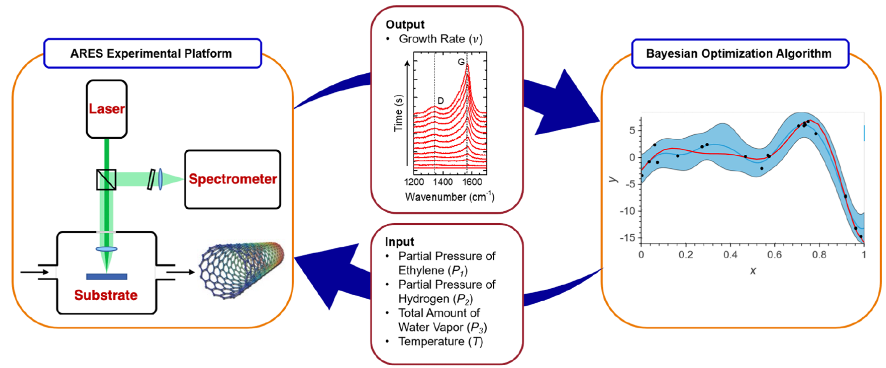
DoD Benefits:

- Optimize autonomous experimentation in materials development (e.g., carbon nanotube synthesis, additive manufacturing)
- Improve human-machine teaming in scientific discovery

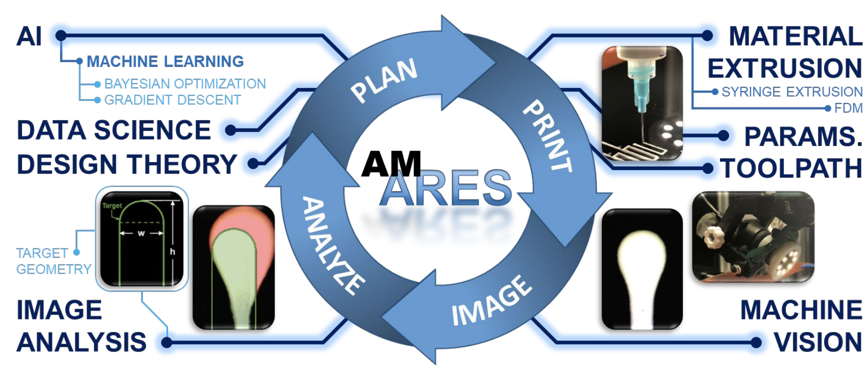
Progress:

- Validated the algorithms in two domains of materials science: carbon nanotube synthesis (CNT) and additive manufacturing (AM)
- Applied the algorithms in two domains of cognitive science: delay discounting and numerical cognition

CNT-ARES system



AM-ARES system



<u>List of Project Goals</u>

1. Develop computational methods to make autonomous adaptive experimentation *informative*, *efficient*, and *<u>robust</u>* to model misspecification

   a) Bayesian optimization (BO)
   b) Gaussian Processes (GP)

2. Validate the methods in two substantive fields

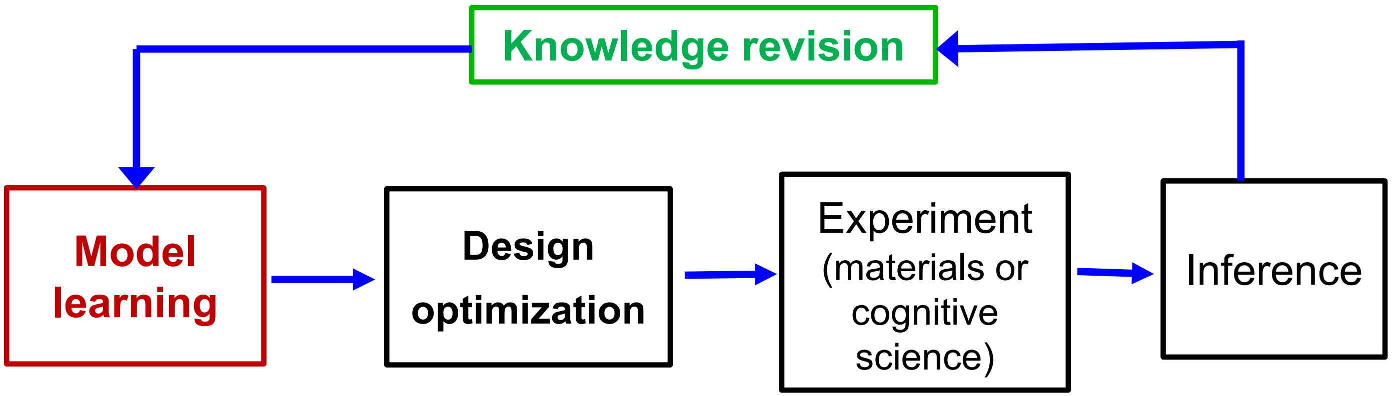
   a) Materials science (AFRL collaboration)
   b) Cognitive science

Progress Towards Goals

1. Develop computational methods….
   1) *Adapted Bayesian Optimization (BO) algorithms to autonomous materials development*
   2) *Developed a Gaussian Process Active Learning (GPAL) method for rapid function learning in cognitive science*

2. Validate the methods in two substantive fields
   1. *Validated BO in autonomous carbon nanotube (CNT) synthesis experiments*
   2. *Validated BO in autonomous additive manufacturing (3D printing) experiments*
   3. *Demonstrated the usefulness of GPAL in two content areas of cognitive science: delay discounting and numerical cognition*

Autonomous Experimentation Loop
Robust **A**utonomous **A**daptive **S**ystem (**RAAS**)



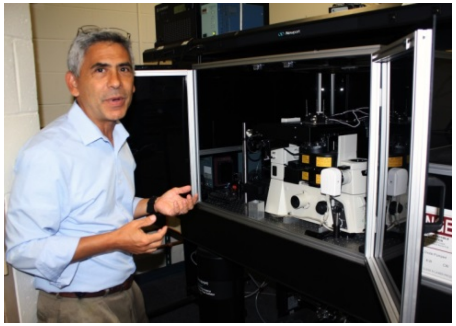
- **Robust:** The data-generating model is not pre-assumed but is learned as the data are collected.
- **Autonomous:** Closed feedback loop
- **Adaptive:** Decide optimally what next experiment to conduct based on the history of observations already collected.

1. Optimizing Autonomous Carbon Nanotubes Synthesis

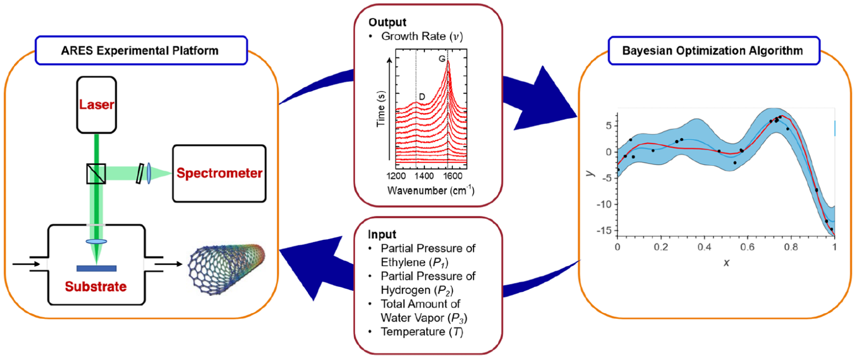
(in collaboration with Dr. Maruyama’s lab at AFRL)

Carbon **N**ano**t**ubes Synthesis **A**utonomous **Re**search **S**ystem (**CNT-ARES**; AFRL Lab)

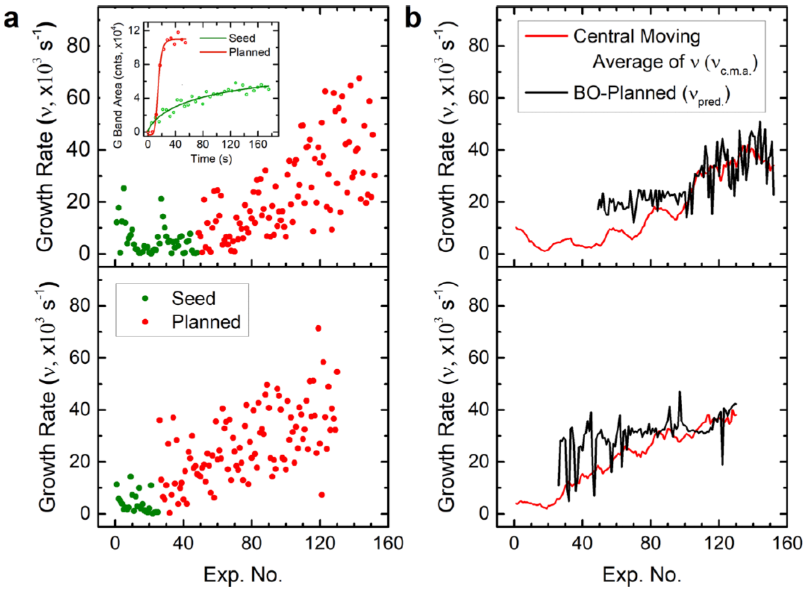
Schematic illustration of Bayesian optimization (BO) based **CNT-ARES**



Dr. Maruyama with the actual CNT-ARES system.



Improved CNT growth rate in BO-planner experiments (red dots) over baseline experiments (green dots)

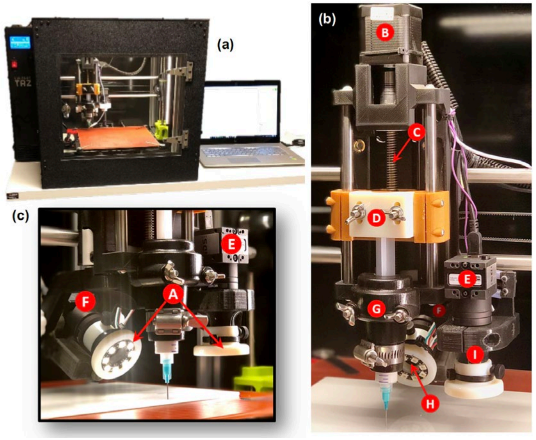


Chang et al (2020). *Scientific Reports*

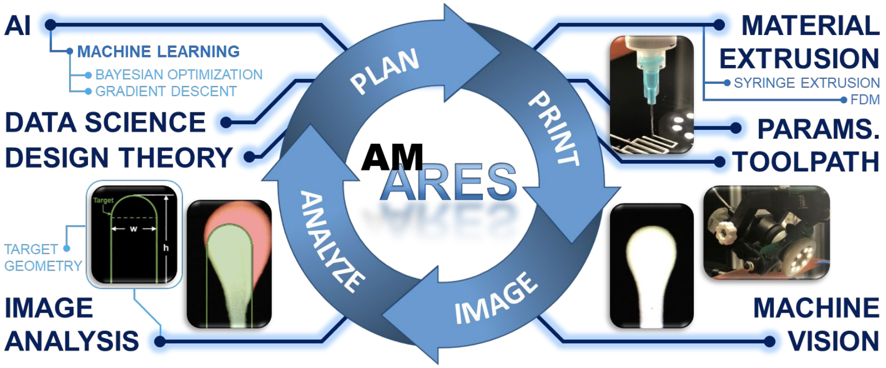
2. Optimizing Autonomous Additive Manufacturing (3D Printing)

(in collaboration with Dr. Maruyama's lab at AFRL)

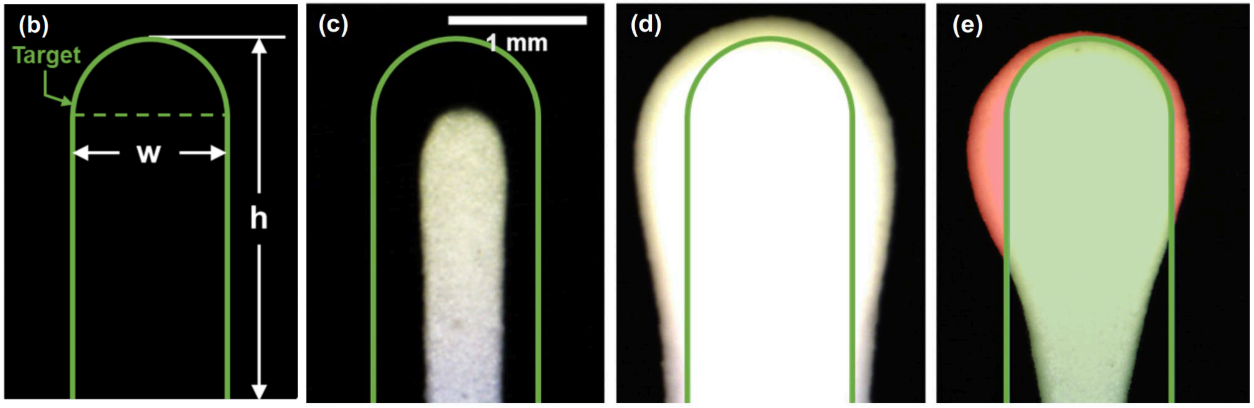
Additive Manufacturing Autonomous Research System (AM-ARES; AFRL Lab)



Prototype **AM-ARES** test platform for closed-loop autonomous printing



Work flowchart of **AM-ARES**



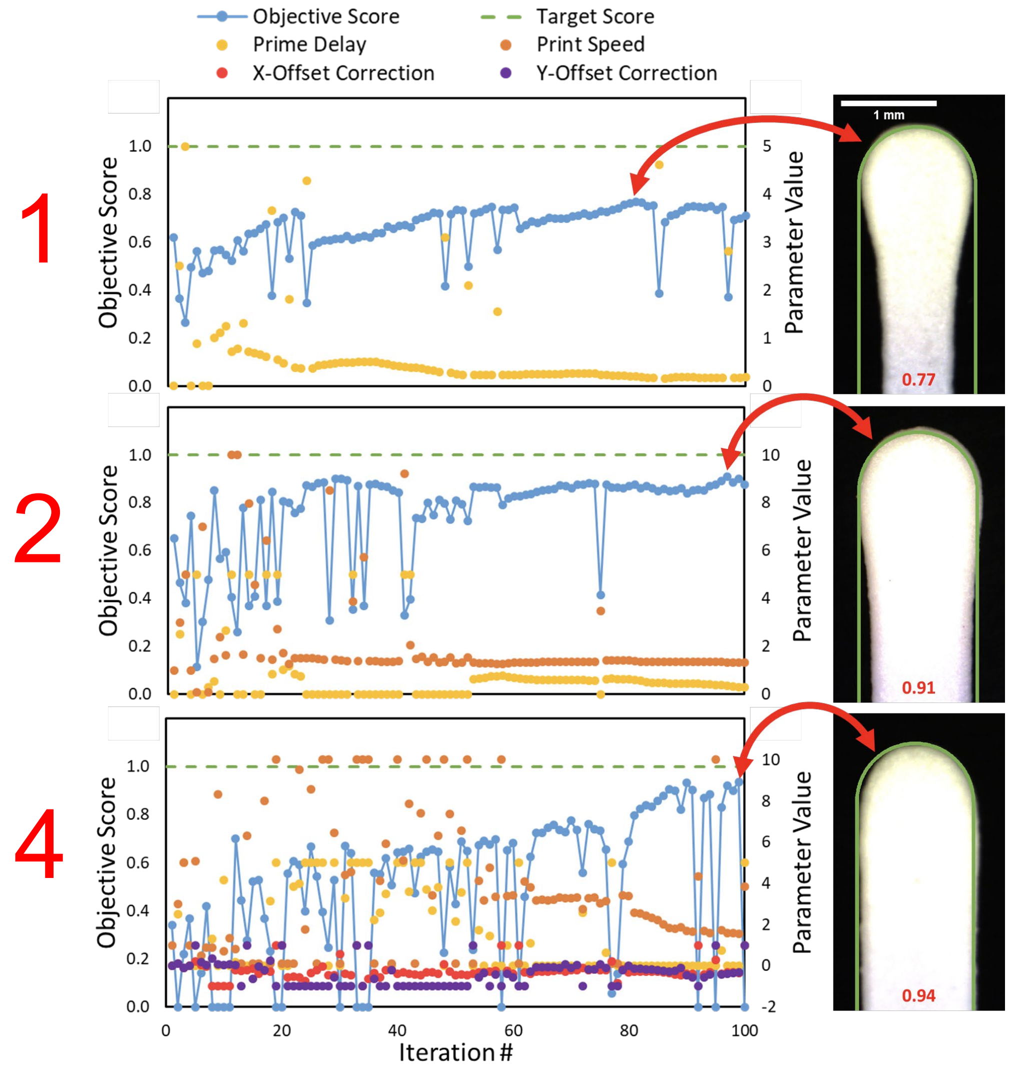
Optimizing the geometry of the segment of printed lines in the **AM-ARES** system. (b) target region; (c) & (d) under- and over-extruded segments; (e) combination of both.

$$\text{objective score} = \frac{A_{\text{inside}} - A_{\text{outside}}}{A_{\text{desired}}} = \frac{A_{\text{effective}}}{A_{\text{desired}}}$$

$$A_{\text{desired}} = w \times \left(h - \frac{w}{2}\right) + \frac{1}{2}\pi\left(\frac{w}{2}\right)^2$$

AM-ARES print optimization using 1, 2, and 4 syringe extrusion parameters via a remote cloud-based BO-planner

Successfully optimized an elementary print feature of up to 4 parameters in under 100 experimental iterations

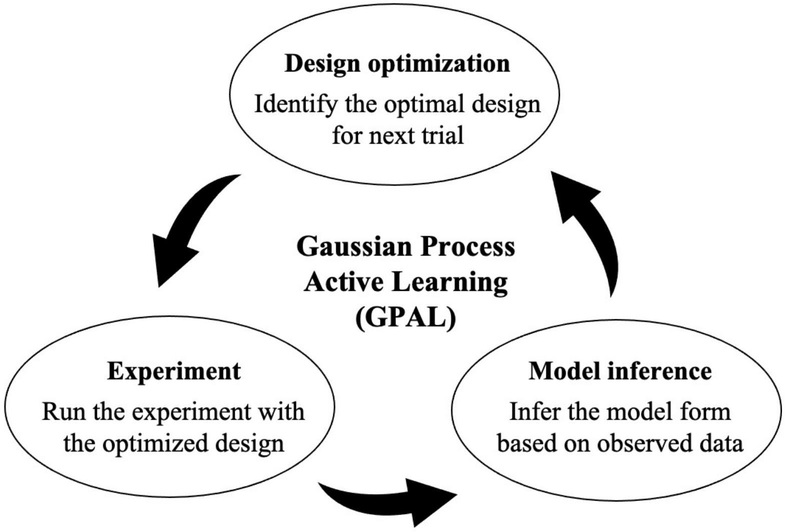


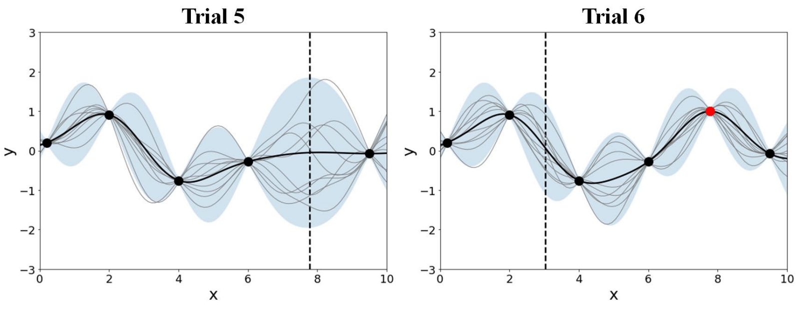
Deneault et al (2020, in revision). *MRS Bulletin*

3. Autonomous Function Learning in Cognitive Science

Gaussian Process Active Learning (GPAL)

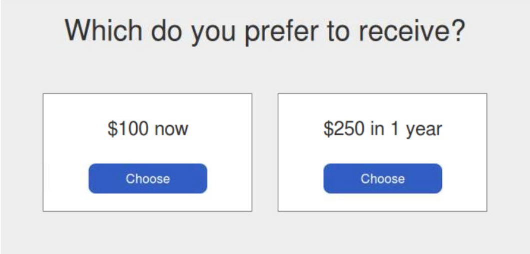
- Objective: Develop a data-driven (model-free) cognitive modeling framework
- Approach combines Gaussian Process (GP) with active learning (AL)
- GPAL efficiently learns the function underlying task performance, without making a priori assumptions about underlying functional form, in contrast to the model-based approach

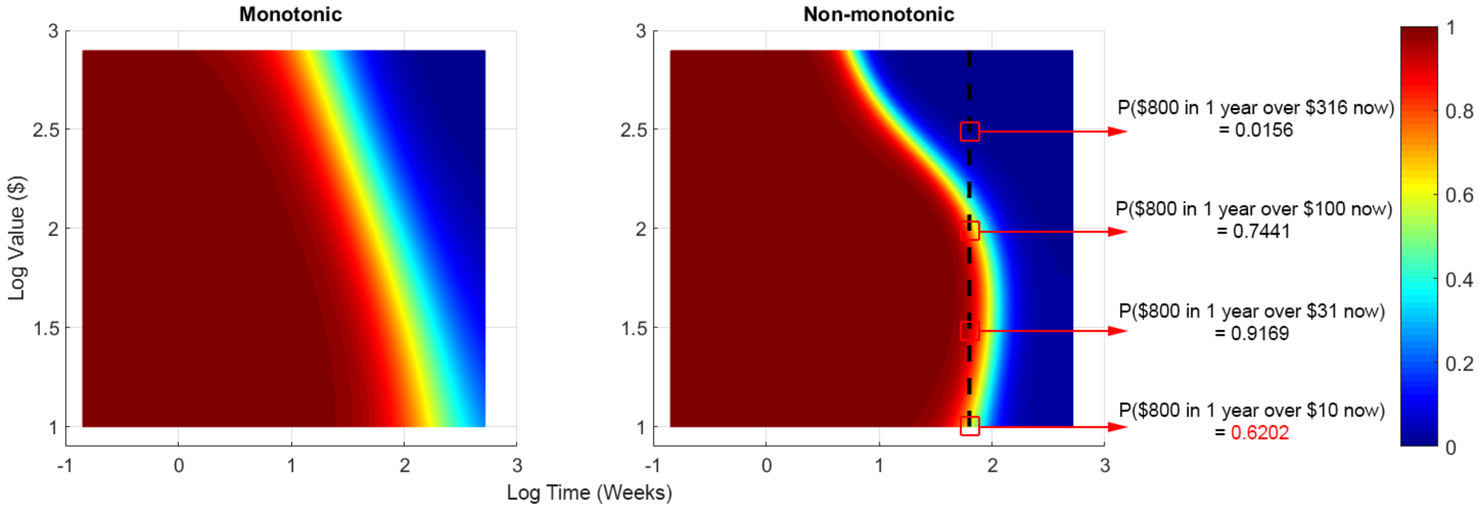




Chang et al (2019). *Proc. Cognitive Science Conference*

Delay Discounting Task





Observed examples of normal (left) and abnormal (right) discounting behavior. Shown are 2-dim plots of the probability of choosing the later-larger reward over the smaller-sooner reward. Chang et al (in press, *Cognitive Psychology).*

- GPAL quickly maps an observer's response function
- The GP's flexibility enables it to identify anomalies in performance, making it well suited for measuring individual differences in decision making
- GPAL is a promising tool for developing unbiased models of cognition

Conclusion

- In this 4-year project (2016 -2020), we have developed a suite of general-purpose algorithms for robust autonomous adaptive experimentation
- In collaboration with AFRL materials science lab, we have validated the efficiency and success of the algorithms in two domains of materials design, namely, carbon nanotubes synthesis and additive manufacturing.
- We have also demonstrated the promise of the algorithms to modeling in two domains of cognitive science, delay discounting and numerical cognition.

List of Publications, Awards, Honors, etc. Attributed to the Grant

- Chang, J., Nikolaev, P., Carpena-Nunez, J., Rao, R. Decker, K., Islam, A. E., Kim, J., Pitt, M. A., Myung, J. I., & Maruyama, B. (2020). Efficient closed-loop maximization of carbon nanotube growth rate using Bayesian optimization. *Scientific Reports* 10:9040.
- Deneault, J. R., Chang, J., Myung, J., Hooper, D., Armstrong, A., Pitt, M., & Maruyama, B. (revision). Autonomous additive manufacturing: Artificial intelligence learns to 3D print. *MRS Bulletin Impact.*
- Chang, J., Kim, J., Zhang, B.-T., Pitt, M. A., & Myung, J. I. (in press). Data-driven experimental design and model development using Gaussian Process with active learning. *Cognitive Psychology*.
- Lee, S. H., Kim, D., Opfer, J. , Pitt, M. A. & Myung, J. I. (submitted). Machine learning provides insights into the development of numerocity estimation.
- Chang, J., Kim, J., Zhang, B.-T., Pitt, M. A., & Myung, J. I. (2019). Modeling delay discounting using Gaussian Process with active learning. *Proceedings of the 41-th Annual Conference of the Cognitive Science Society* (pp. 1479-1485). Austin, TX: Cognitive Science Society.