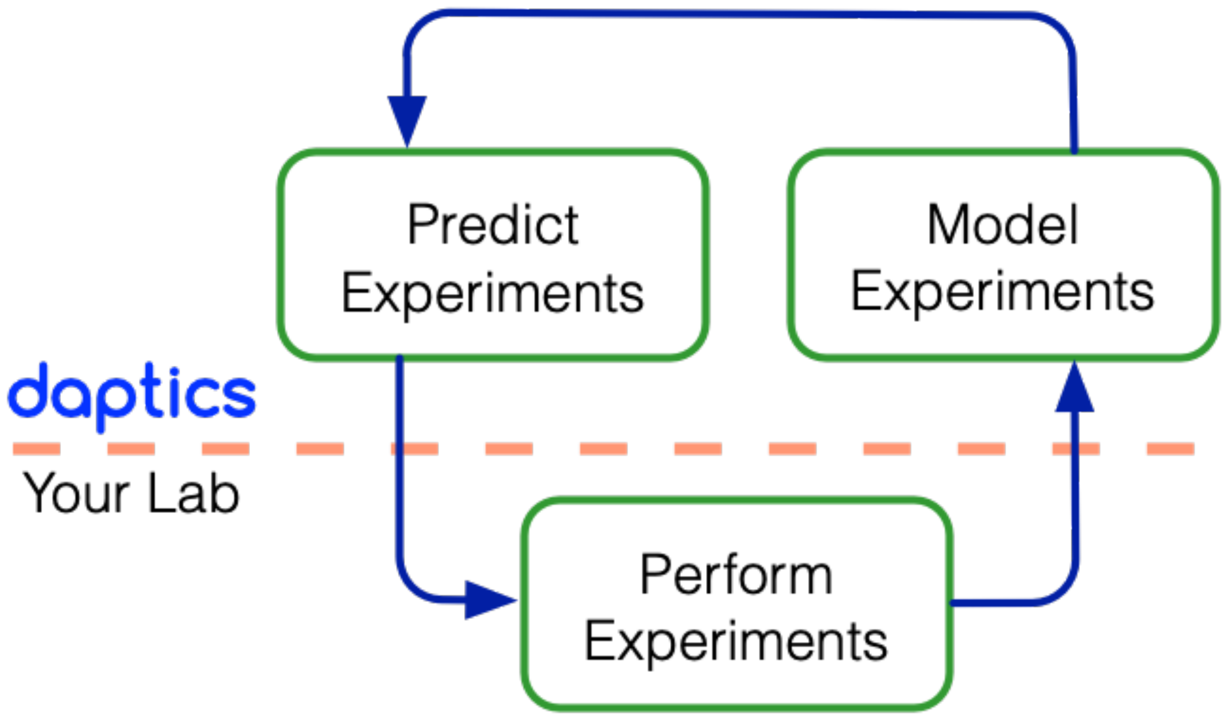
daptics

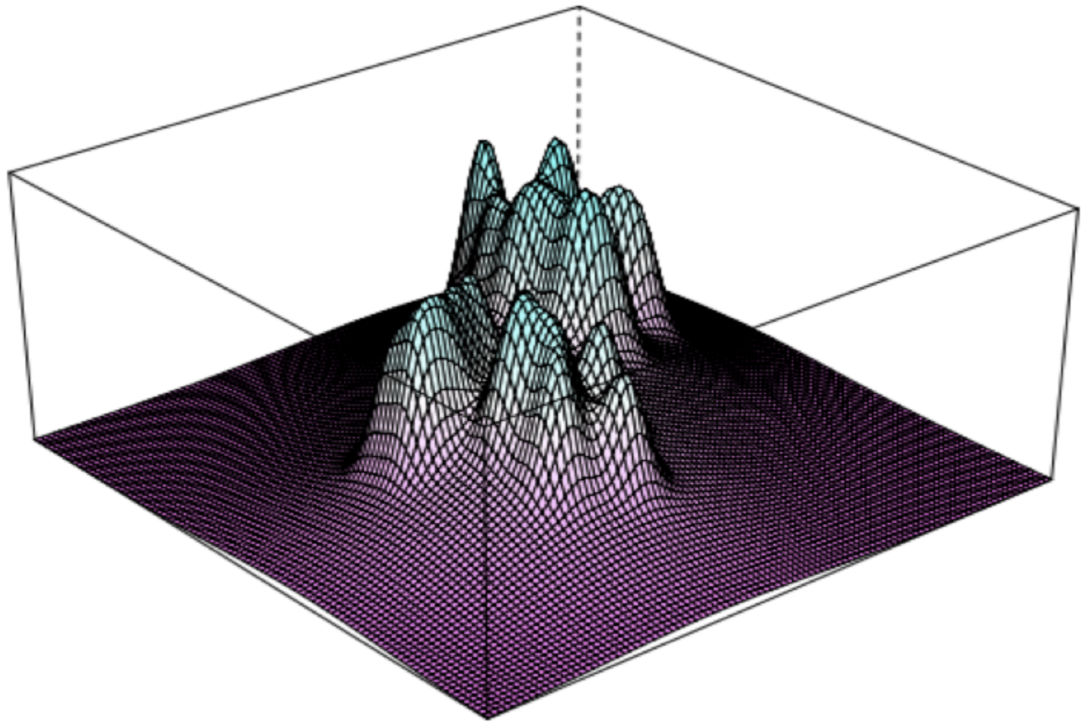
Daptics, Inc.

The Experimental Loop



- Experiments are *expensive* $\Rightarrow$ data is limited and needs to be efficiently leveraged
- Predictive models are built and refined after each set (*generation*) of experiments is performed
- Models are used to discover increasingly better experiments

Experimental Response Surface



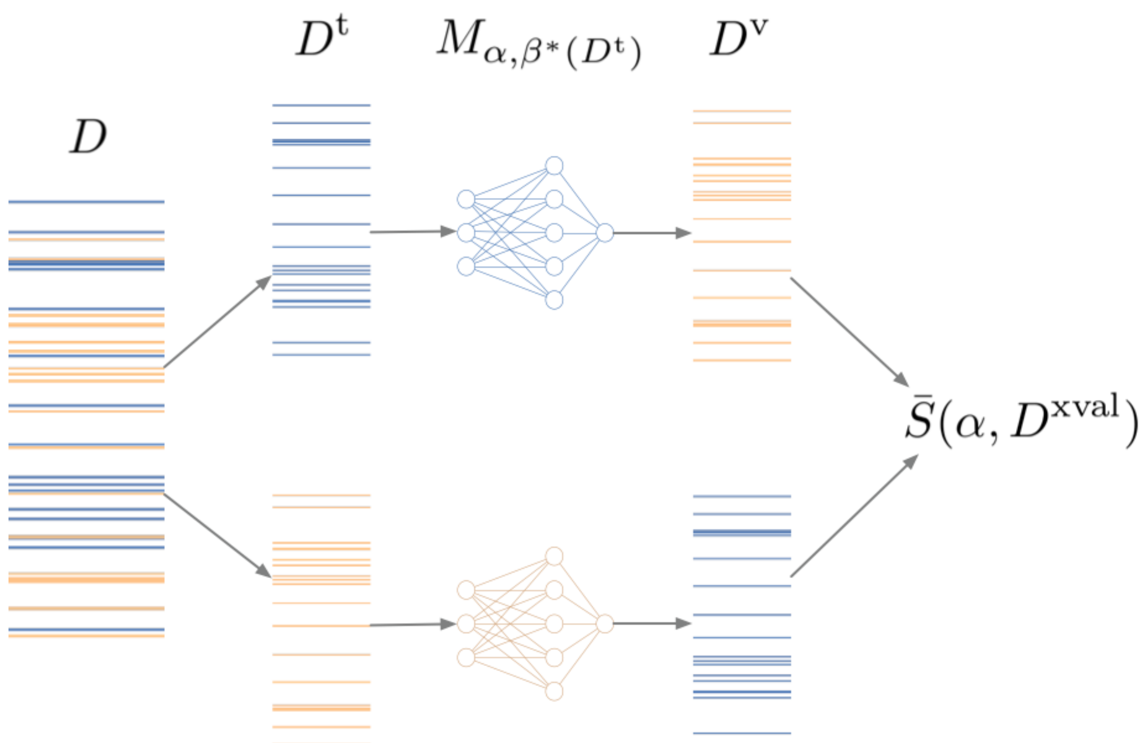
- A complex response surface contains several local maxima, due to strong non-linear synergy between experimental parameters.
- *X*, *Y* axes: two (of potentially many) experimental parameters
- *Z* axis: experimental response

Experimental Space Definition

Name	Type	Value.1	Value.2	Value.3	Value.4	Value.5
Quench	categorical	Yes	No			
StepNum	numerical	1.000	2.000	3.000		
Duration	numerical	60.000	120.000	180.000		
Buffer	numerical	7000.000	7900.000	8850.000	10550.000	
DNAType	categorical	A	B	C	D	
AmphiLogRatio	numerical	-1.100	-0.220	1.230	1.890	3.200
Catalyst	numerical	100.000	180.000	260.000	311.000	400.000

- The experimental space is defined by a set of experimental parameters and their corresponding possible values
- The number of experimental parameters (i.e., the dimension of the experimental space) in this space is 7
- This experimental space contains a total of 2 * 3 * 3 * 4 * 4 * 5 * 5 = 7200 experiments

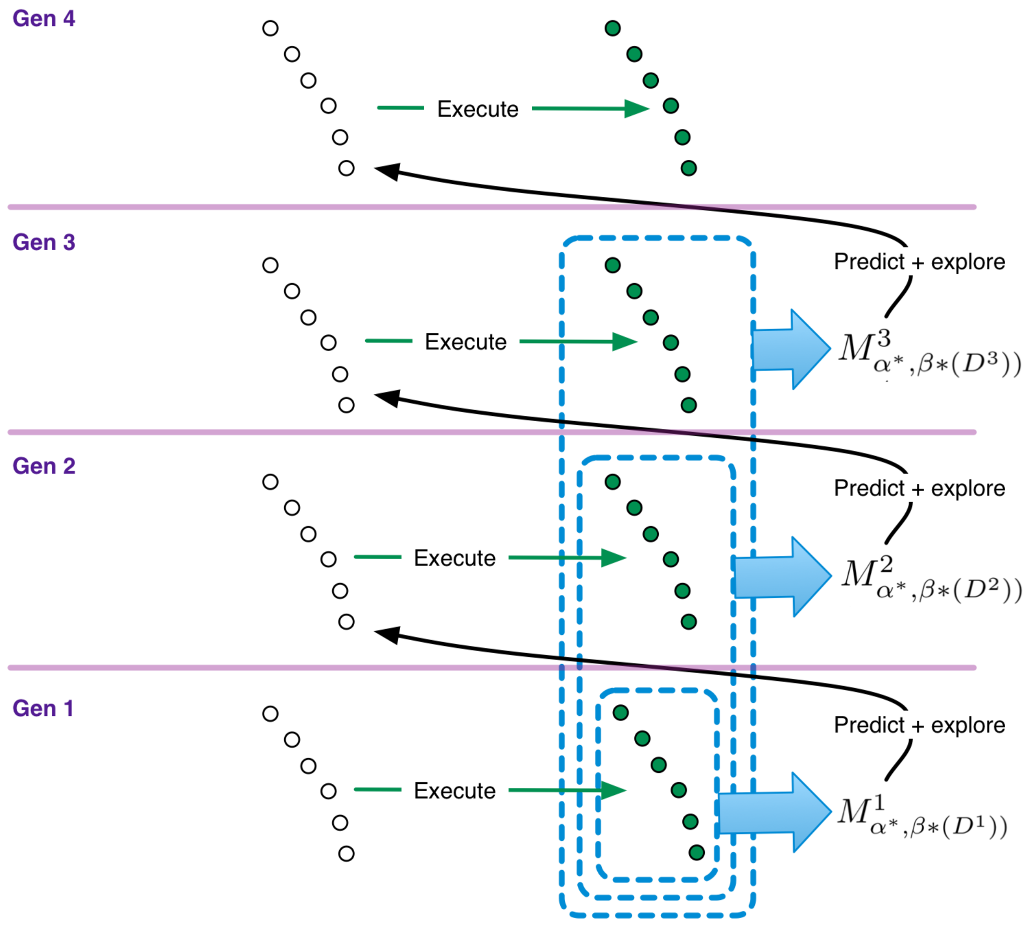
Cross-Validation for Hyper-Parameter Optimization



- *D*: Available dataset
- D^t : training subset
- D^v : validation subset
- $M_{\alpha,\beta}{}^*(D^t)$: model with hyper-parameters trained on D^t
- *$S(\alpha, D^{xval})$: average cross-validation performance of the model with hyper-parameters α.*

- The available data is partitioned into disjoint subsets
- A model with hyper-parameters α is trained on one subset and its performance measured (validated) on another.
- This process is repeated on tens of different partitions and tens–hundreds of different hyper-parameters α.
- The hyper-parameters α with the best average validation performance are finally selected for the current generation's model.

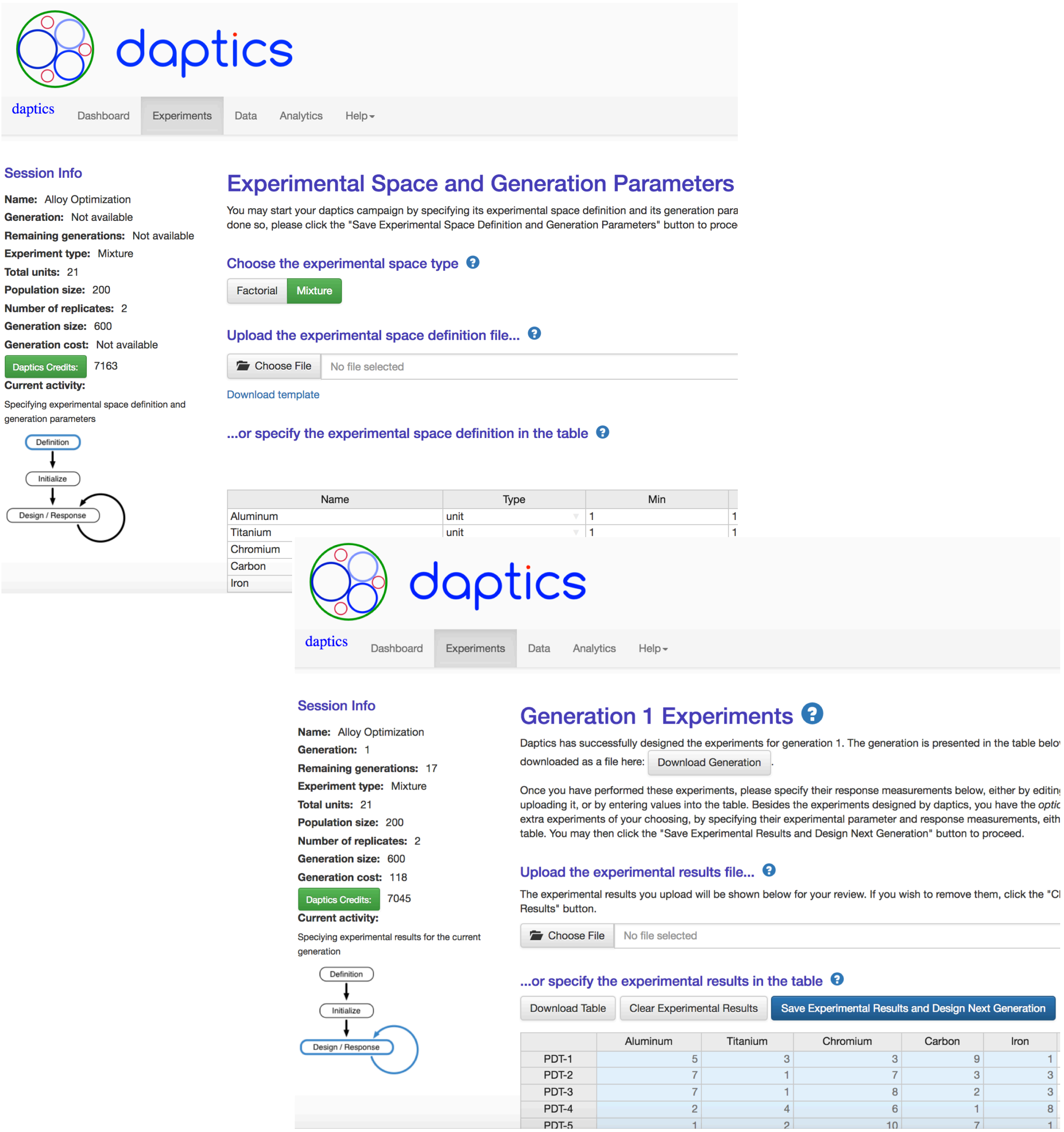
Model Evolution



- White circles: experiments
- Green circles: experimental results
- Green arrows: experiment execution
- Blue arrows: model training via cross-validated hyper-parameter optimization.
- Black arrows: selection of experiments for the next generation by means of:
    - Predictions from the model trained on the data collected up to the current generation
    - Exploration to improve experimental space coverage

- Predictive models evolve over successive generations of experiments, and become increasingly effective in discovering new good experiments

Web interface



- An intuitive and easy-to-use web interface to Daptics is available at https://daptics.ai

- Powerful artificial intelligence will automatically deploy models and algorithms on your data for you

- Skills in data science, machine learning, programming, or design of experiments are not required on your part

- Sign up for a **free** Daptics account at https://daptics.ai/register

- Check out the **free** Daptics demo at https://daptics.ai/demo