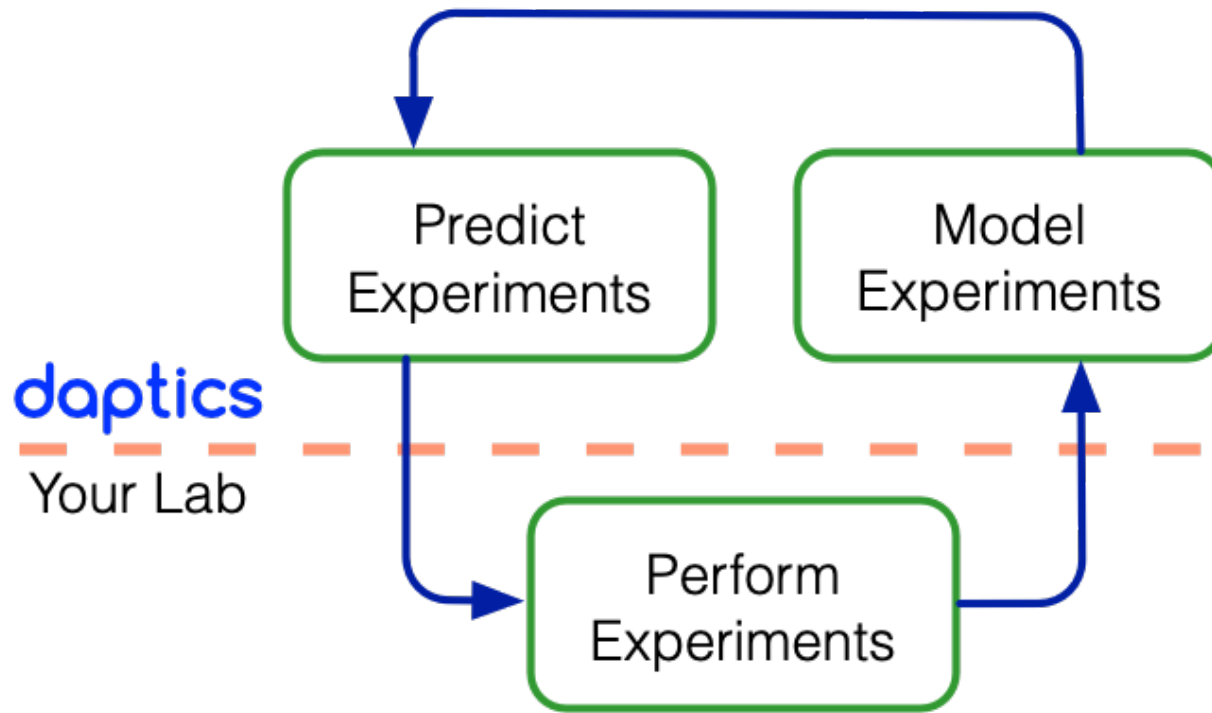


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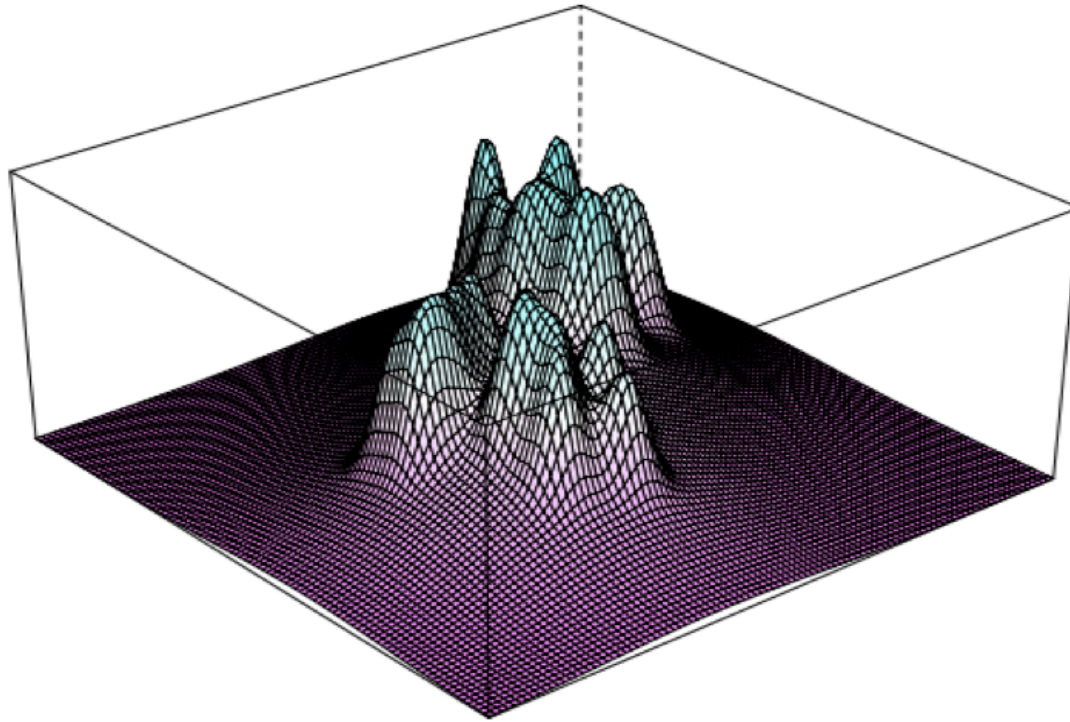
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The Experimental Loop



- 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



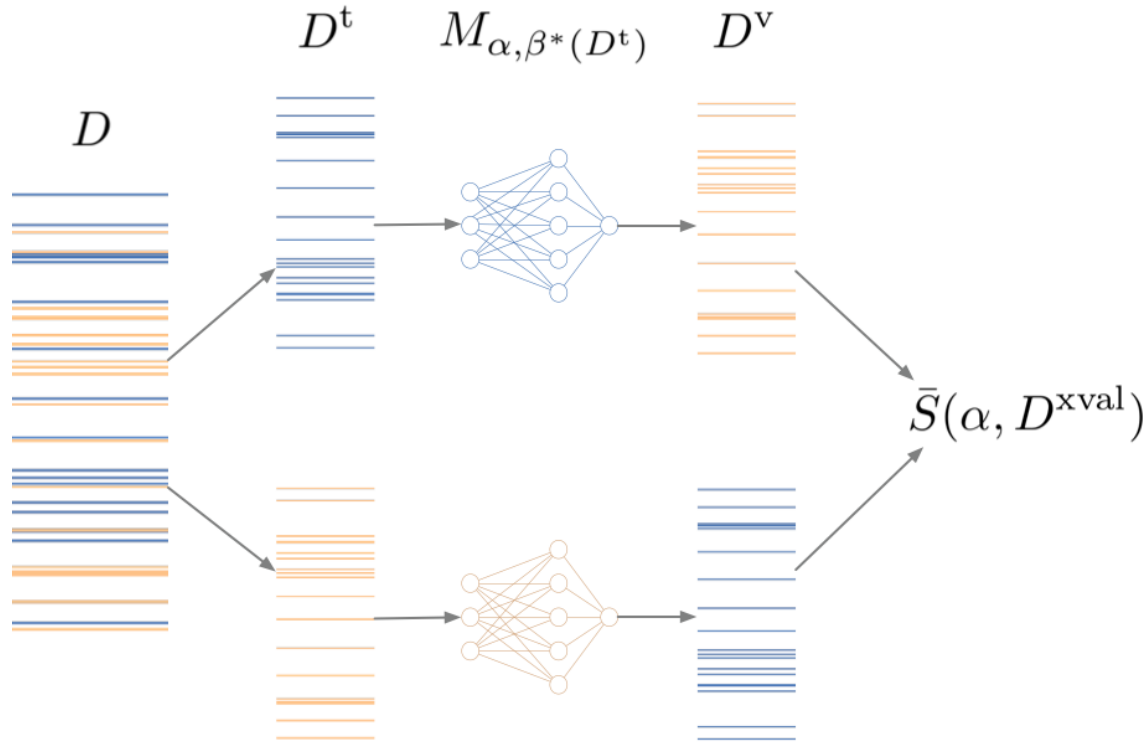
- A complex response surface contains several local maxima, due to strong non-linear synergy between experimental parameters.
- X, Y axes: two (of potentially many) experimental parameters
- Z axis: experimental response

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

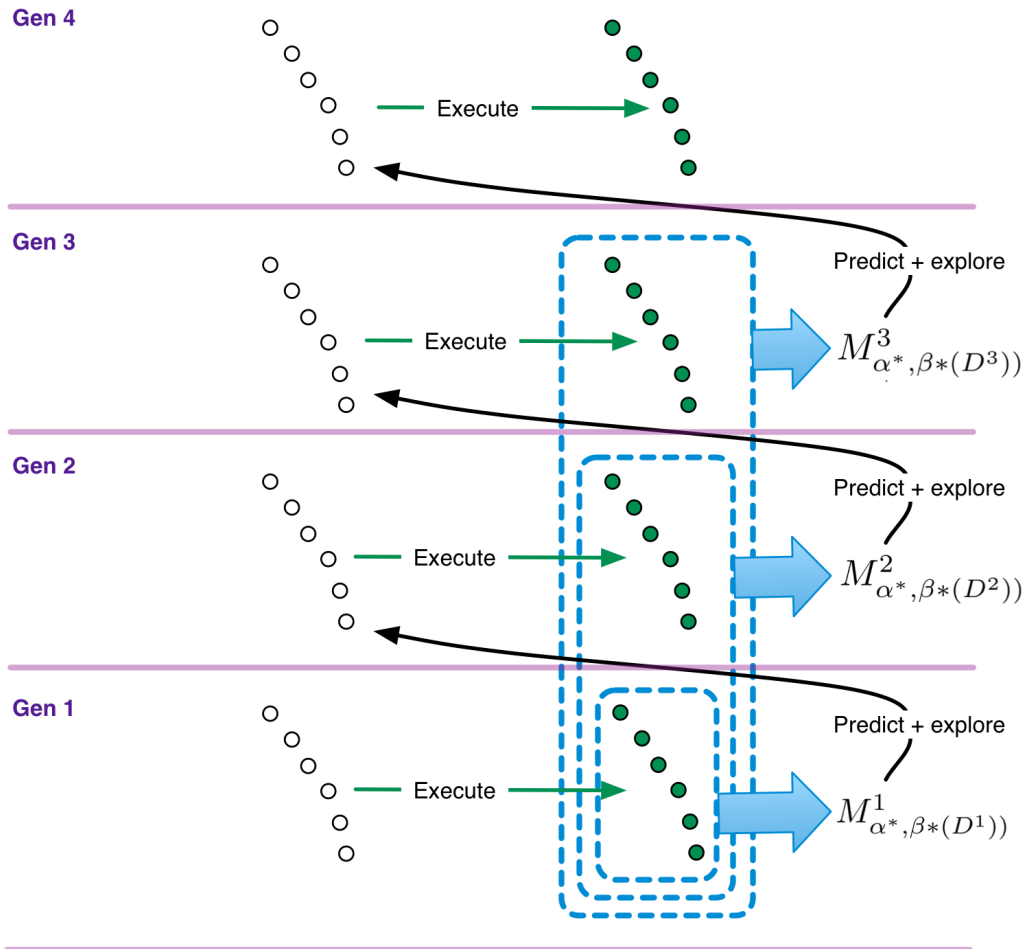
Cross-Validation for Hyper-Parameter Optimization



- D : Available dataset
- D^t : training subset
- D^v : validation subset
- $M_{\alpha, \beta^*}(D^t)$: model with hyper-parameters trained on D^t
- $\bar{S}(\alpha, D^{xval})$: 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

The screenshot displays the Daptics web interface. At the top, there's a navigation bar with the Daptics logo and links for Dashboard, Experiments, Data, Analytics, and Help. The main content area is titled 'Experimental Space and Generation Parameters'. It includes a 'Session Info' sidebar on the left with details like Name (Alloy Optimization), Generation (Not available), Remaining generations (Not available), Experiment type (Mixture), Total units (21), Population size (200), Number of replicates (2), Generation size (600), Generation cost (Not available), Daptics Credits (7163), and Current activity (Specifying experimental space definition and generation parameters). The main area has a 'Choose the experimental space type' section with buttons for Factorial and Mixture. Below that is an 'Upload the experimental space definition file...' section with a 'Choose File' button and a 'No file selected' message. A 'Download template' link is also present. A section titled '...or specify the experimental space definition in the table' includes a table with columns Name, Type, and Min. The table lists Aluminum, Titanium, Chromium, Carbon, and Iron, all with a Type of 'unit' and a Min value of 1. A flowchart on the left shows the process: Definition -> Initialize -> Design / Response -> back to Definition. The Daptics logo and navigation bar are repeated at the bottom of the main content area.

Session Info

Name: Alloy Optimization
Generation: Not available
Remaining generations: Not available
Experiment type: Mixture
Total units: 21
Population size: 200
Number of replicates: 2
Generation size: 600
Generation cost: Not available
Daptics Credits: 7163
Current activity: Specifying experimental space definition and generation parameters

Experimental Space and Generation Parameters

You may start your daptics campaign by specifying its experimental space definition and its generation parameters done so, please click the "Save Experimental Space Definition and Generation Parameters" button to proceed.

Choose the experimental space type

Factorial Mixture

Upload the experimental space definition file...

Choose File No file selected

[Download template](#)

...or specify the experimental space definition in the table

Name	Type	Min
Aluminum	unit	1
Titanium	unit	1
Chromium		
Carbon		
Iron		

Session Info

Name: Alloy Optimization
Generation: 1
Remaining generations: 17
Experiment type: Mixture
Total units: 21
Population size: 200
Number of replicates: 2
Generation size: 600
Generation cost: 118
Daptics Credits: 7045
Current activity: Specifying experimental results for the current generation

Generation 1 Experiments

Daptics has successfully designed the experiments for generation 1. The generation is presented in the table below downloaded as a file here: [Download Generation](#).

Once you have performed these experiments, please specify their response measurements below, either by editing, uploading it, or by entering values into the table. Besides the experiments designed by daptics, you have the *opti* extra experiments of your choosing, by specifying their experimental parameter and response measurements, either table. You may then click the "Save Experimental Results and Design Next Generation" button to proceed.

Upload the experimental results file...

Choose File No file selected

...or specify the experimental results in the table

[Download Table](#) [Clear Experimental Results](#) [Save Experimental Results and Design Next Generation](#)

	Aluminum	Titanium	Chromium	Carbon	Iron
PDT-1	5	3	3	9	1
PDT-2	7	1	7	3	3
PDT-3	7	1	8	2	3
PDT-4	2	4	6	1	8
PDT-5	1	2	10	7	1

- 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>