Process optimisation using machine learning techniques

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About this workshop....

Introduction to Perceptive Engineering

Challenges in Process Development/Optimisation and How Machine Learning Can Help

About the Nelder-Mead Self Learning Optimisation Algorithm

Introduction to the Experimental Rig

Optimisation runs

About Adaptive Model Predictive Control

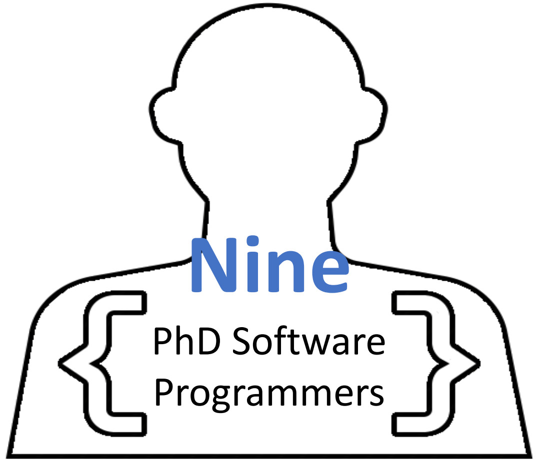
About Gaussian Optimisation

Results and Discussion

Perceptive Engineering

2-Minute Capability Pitch

Solely focussed on software and solutions applying Advanced Process Control **techniques**



Dedicated
Support Team

ISO 9001:2015 CERTIFIED COMPANY

Technology partners:

SIEMENS

GEA

Support
Eight
Research
Centres

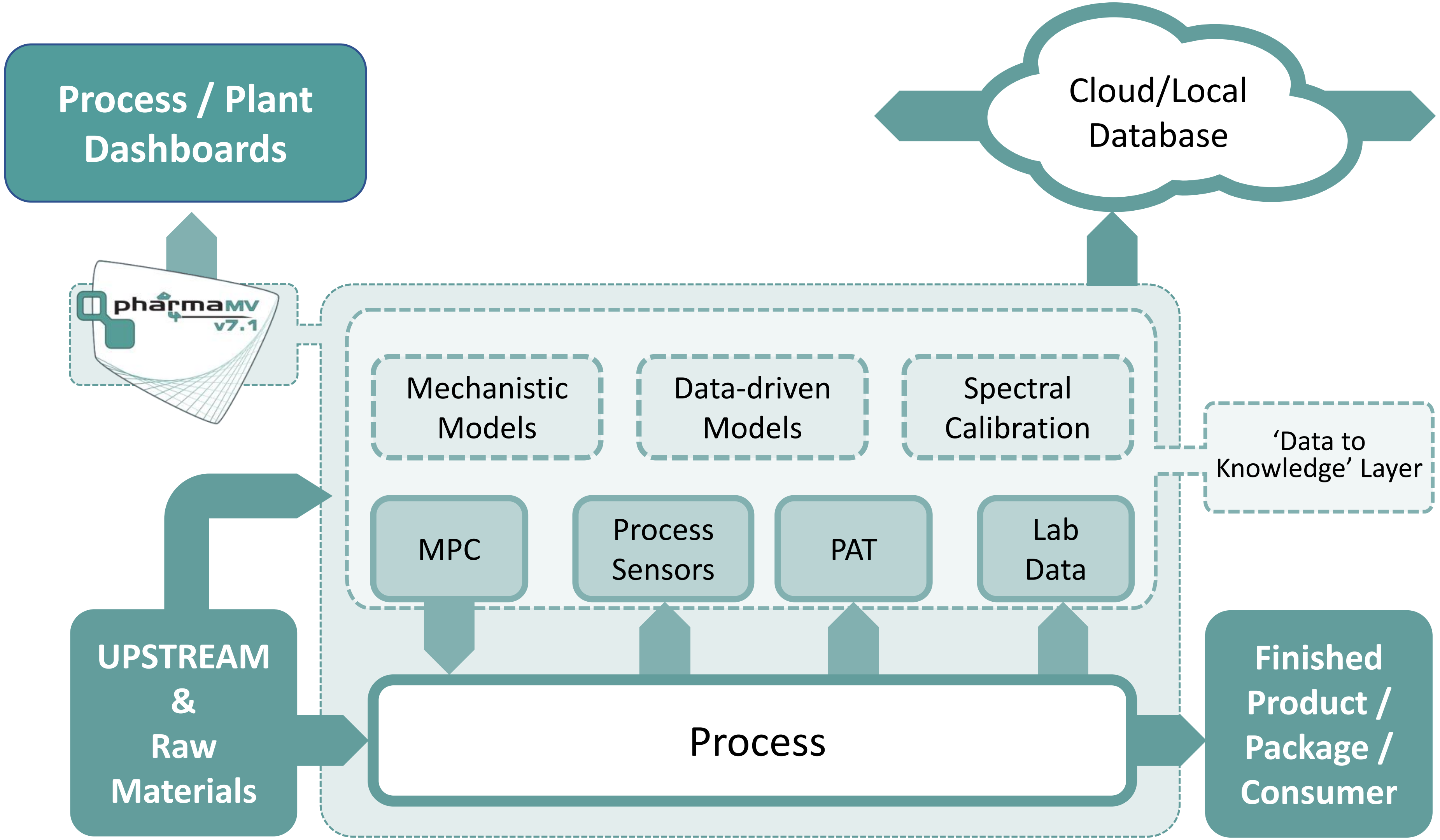
Rutgers NFC CMAC MMIC RCPE PMTC ASTAR SSPC

DANONE Arla Unilever VISY FOR A BETTER WORLD Pfizer MERCK gsk

PharmaMV
Process Control & Monitoring

In the lab, PharmaMV can act as a SCADA/HMI to pull control and monitoring of discrete pieces of equipment into a single interface

allowing **ALL** data to be accessed from a single interface and used in modelling and process understanding



Philosophy of "Data"

DATA
- Process
- Lab/Offline
- PAT/Spectral
- Contextual information

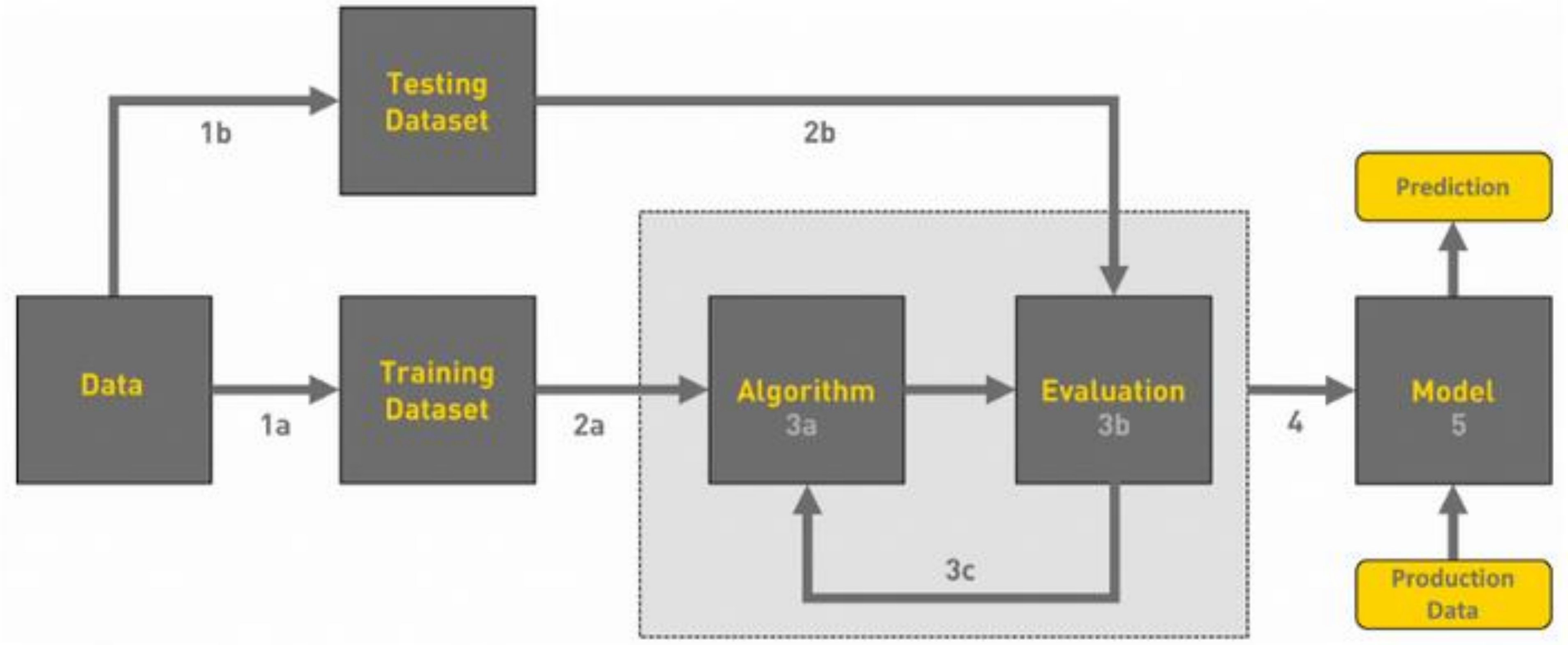
INFORMATION
- Data Alignment
- Pre-processing
- Pre-treatment
- Key-Performance Indicators

KNOWLEDGE
- DoE Execution
- Rapid Development
- Data-Driven and hybrid modelling

WISDOM
Robust, real-time prediction, soft-sensors, monitoring, control and optimisation

Teaching the machine

Today….



Overview of the Workflow of ML

https://towardsdatascience.com/workflow-of-a-machine-learning-project-ec1dba419b94

Motivations and Benefits

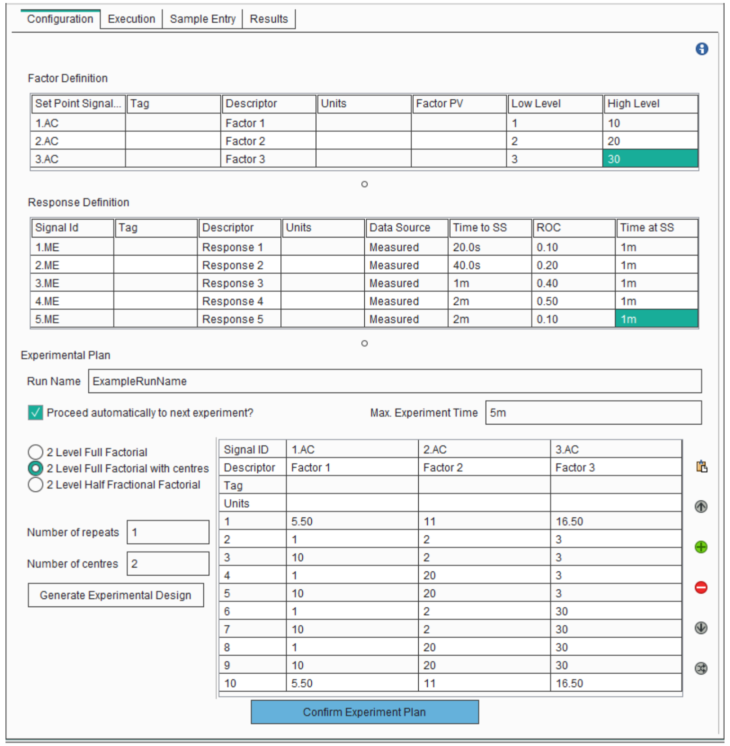
Process Development Approaches

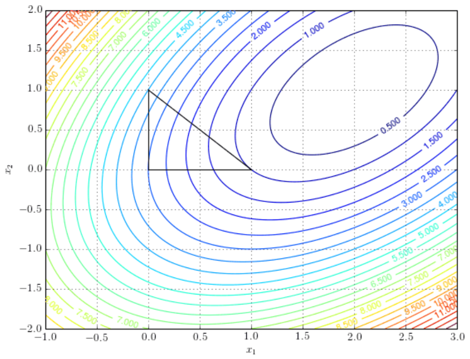
Traditional "One at a Time" approach

- Trial and error optimisation of the reaction
- Significant human input – depends of the know-how of the chemist

Quality by Design Approach

- Application of Design of Experiments
- Automation can be used to execute pre-defined experimental conditions
- Extensive experimental effort required





ML – Recursive Learning Approach

- Automation and online analysis combined with a "curiosity" algorithm
  - Outperforms a human to get to the optimum
- No human interaction required after initialisation

**An Autonomous Self-Optimizing Flow Reactor for the Synthesis of Natural Product*
The Journal of Organic Chemistry 2018 83 (23), 14286-14299

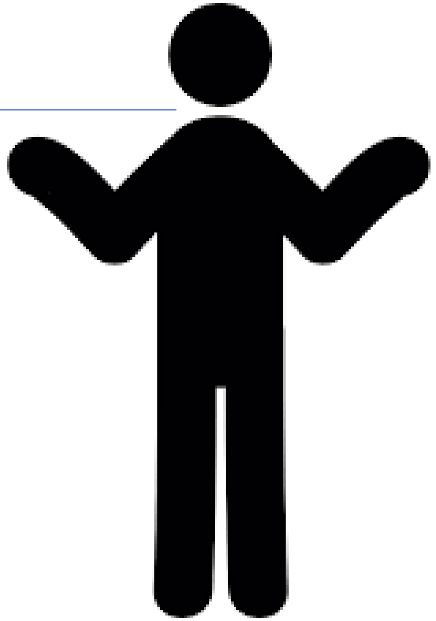
Nelder-Mead Self-Optimisation

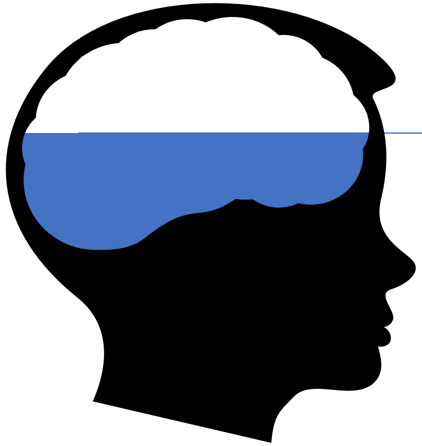
Smart Data Generation. . . Nelder Mead Method

What and Why?

What is it?

Iterative “DoE” which calculates next experiment based on previous results





Why do you want it?

Benefit

Run less trials to find optimal process parameters

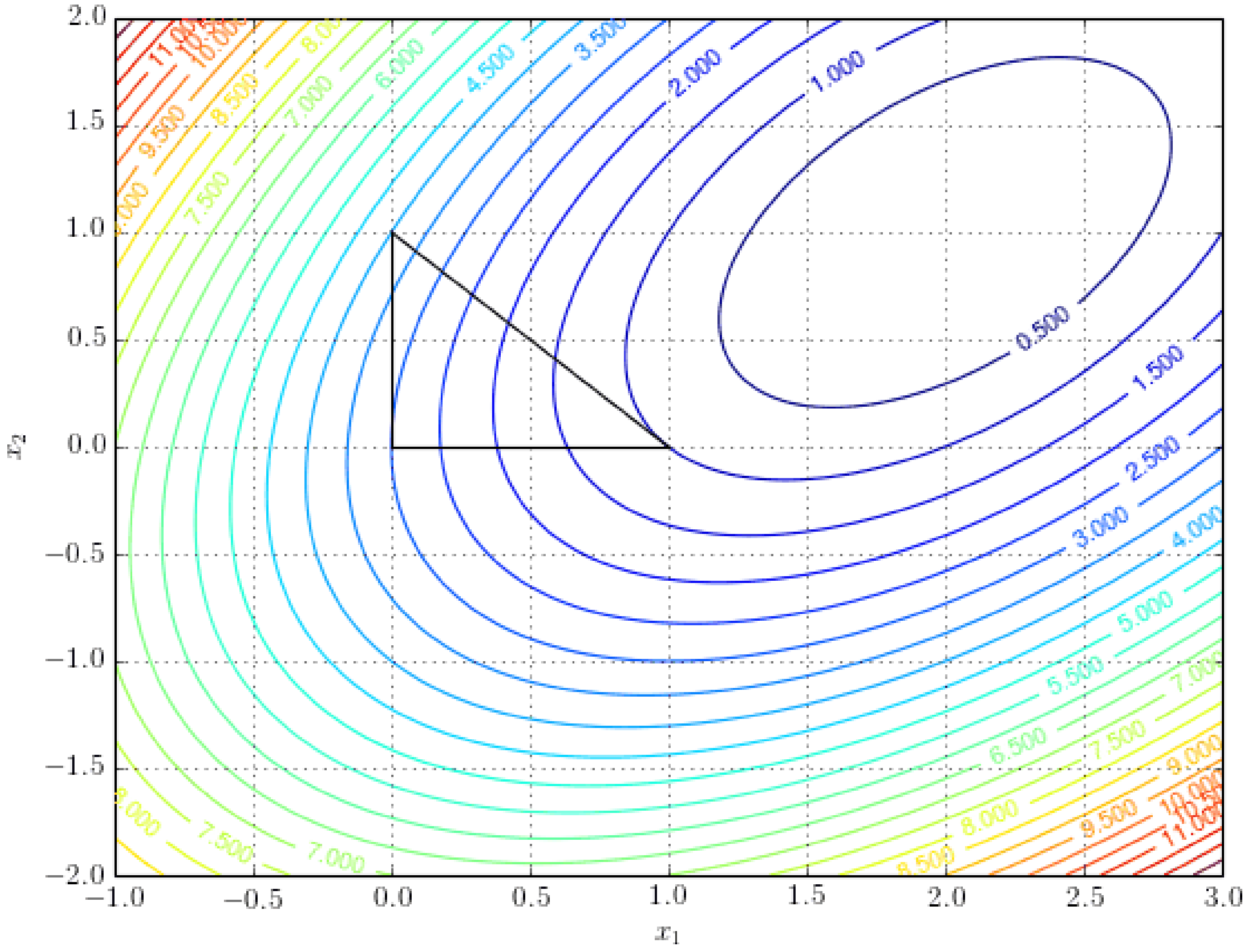
1

Value

Cost & time savings, less wasted batches

Smart Data Generation. . . Nelder Mead Method

Simple Overview

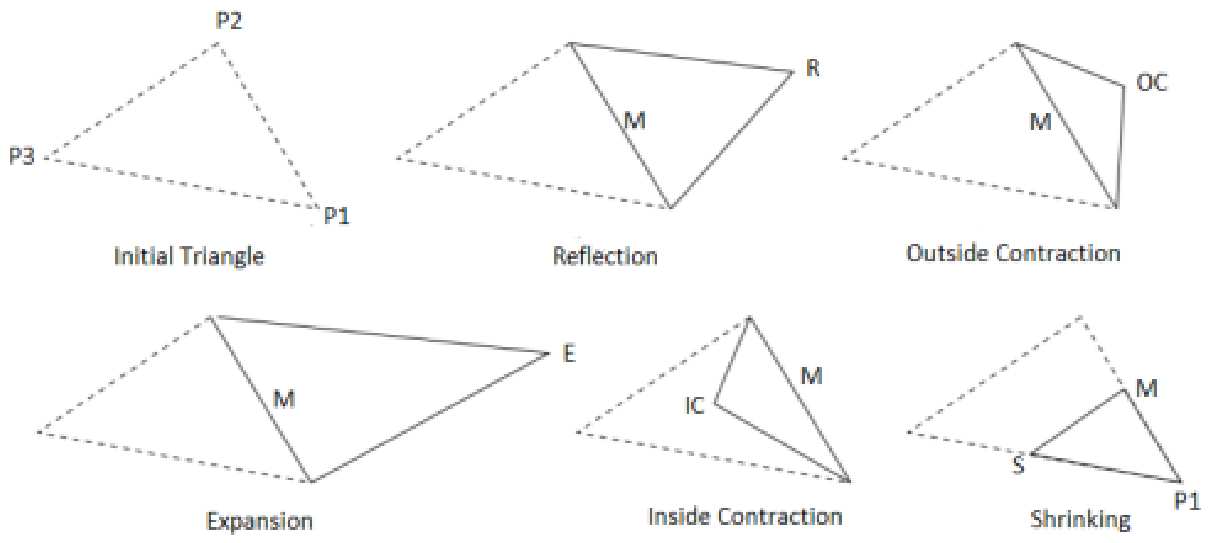


*An Autonomous Self-Optimizing Flow Reactor for the Synthesis of Natural Product
The Journal of Organic Chemistry 2018 83 (23), 14286-14299*

How?

- Optimisation *via* customised Nelder-Mead type algorithm

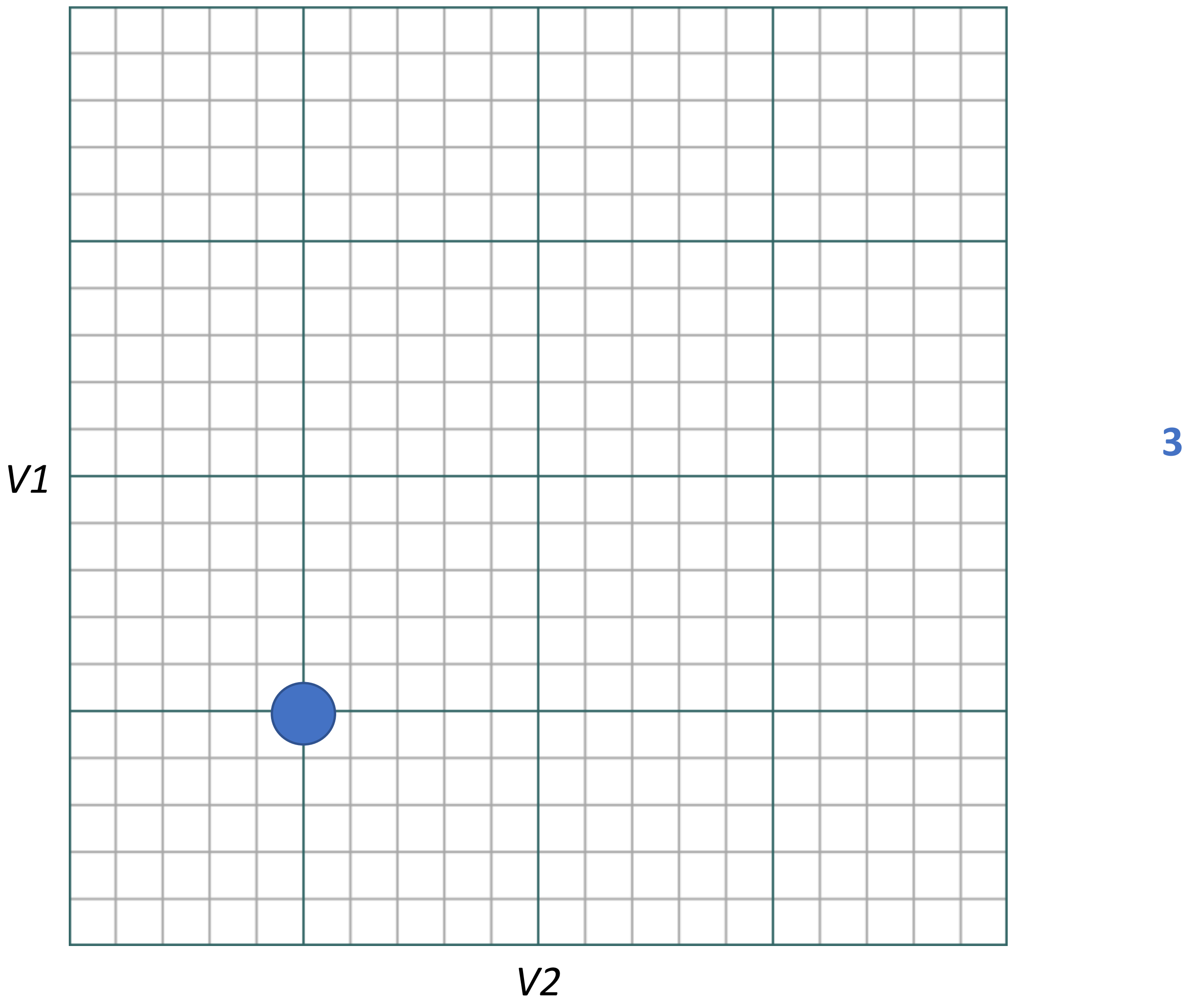
- Customised?
  - Objective function style redefined for target-aiming type of problem
    - $f(x) = \sqrt{\left((Target\ - Experimental\,Value)^2\right)}$
  - Stopping parameters re-defined
    - *i.e.* stop when *Target* is within threshold



How?

Example for a 2 variable problem

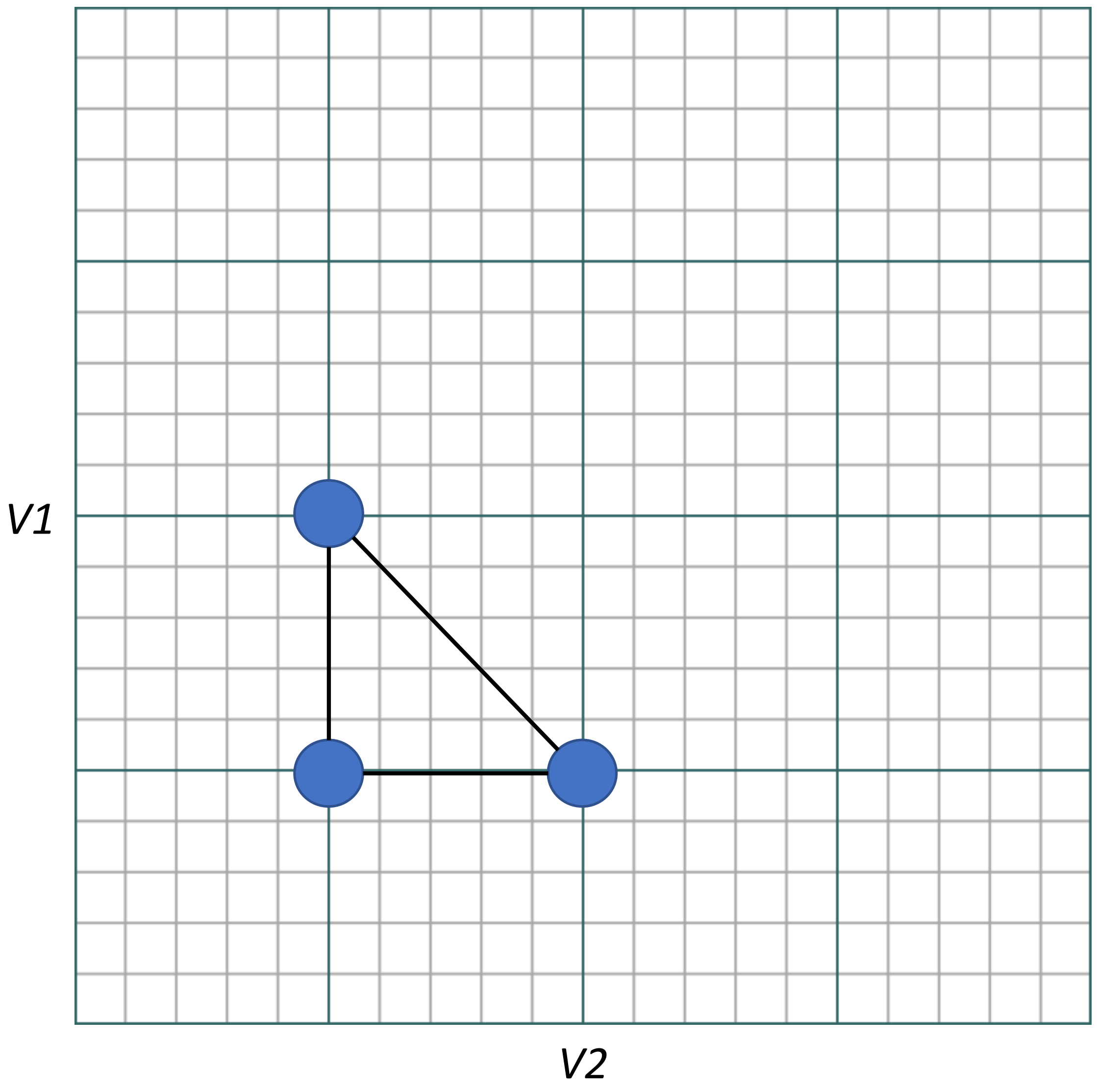
1. Initial Parameters



How?

Example for a 2 variable problem

1. Initial Parameters
2. Construct initial simplex (n + 1) vertices



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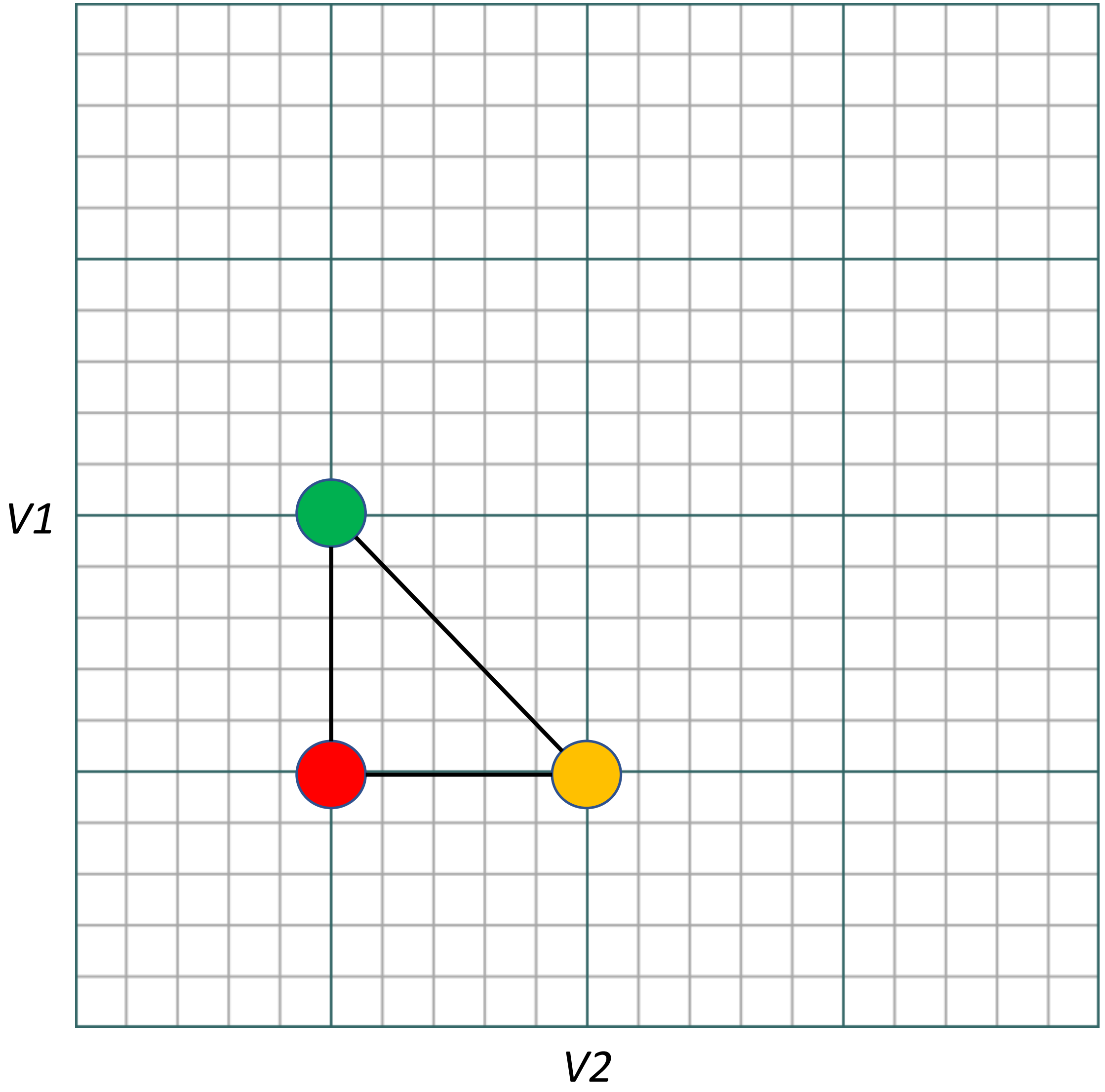
How?

Example for a 2 variable problem

1. Initial Parameters
2. Construct initial simplex (n + 1) vertices
3. Evaluate and Rank



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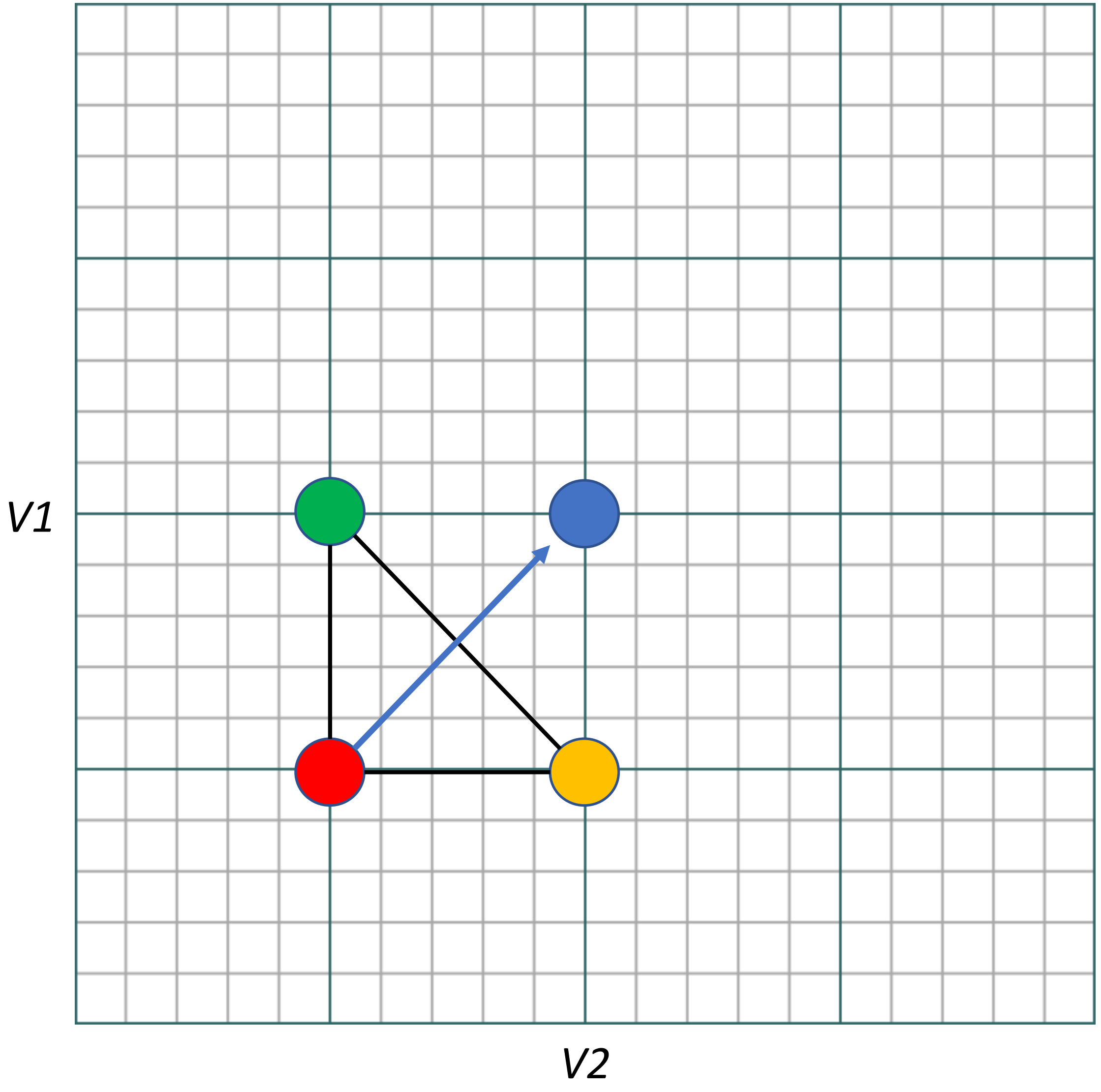
How?

Example for a 2 variable problem

1. Initial Parameters
2. Construct initial simplex (n + 1) vertices
3. Evaluate and Rank
4. Reflect away from worst result to generate new set of parameters



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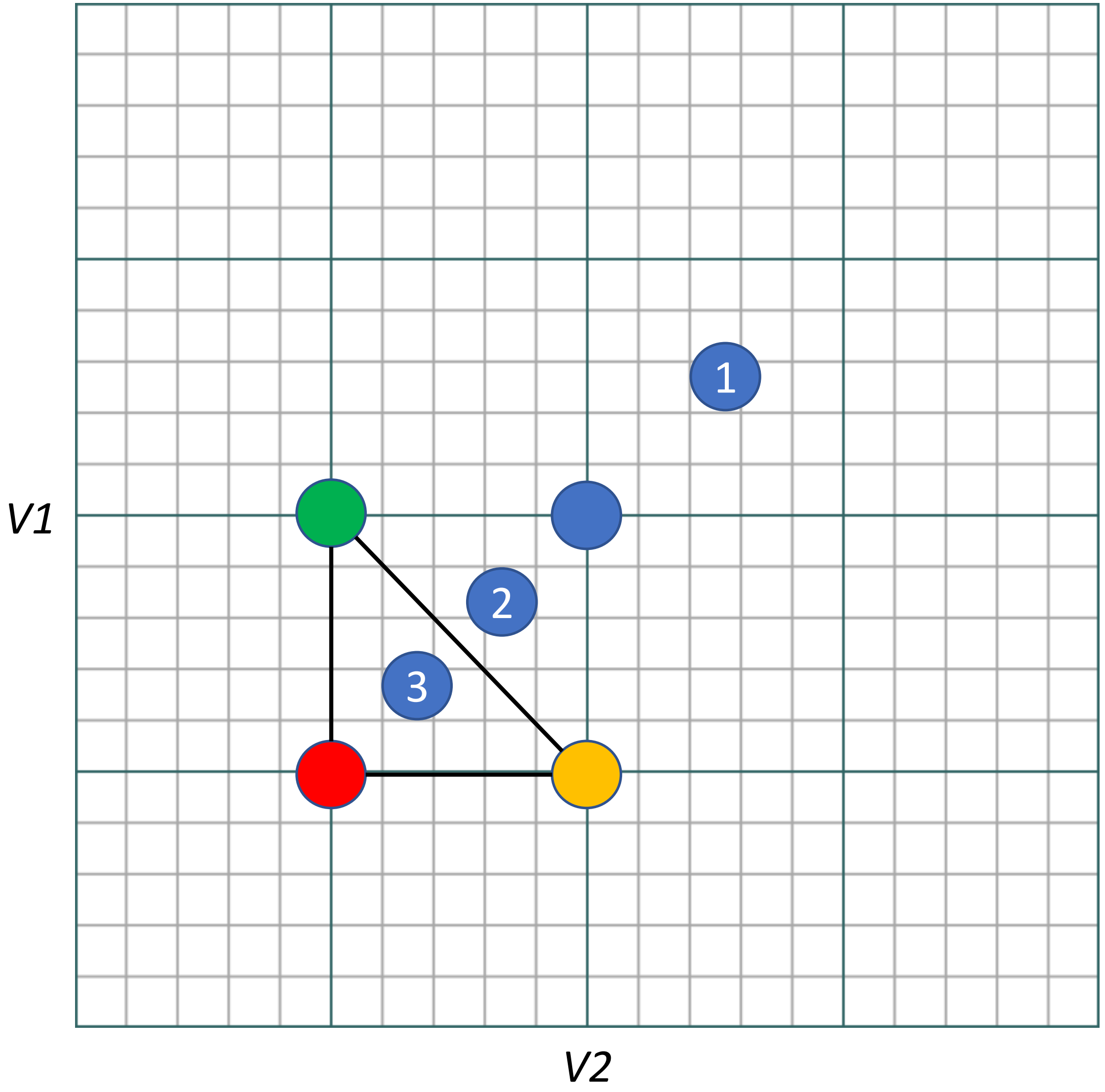
How?

Example for a 2 variable problem

1. Initial Parameters
2. Construct initial simplex (n + 1) vertices
3. Evaluate and Rank
4. Reflect away from worst result to generate new set of parameters
5. Evaluate new point, if favourable expand (1), if not contract (2,3)



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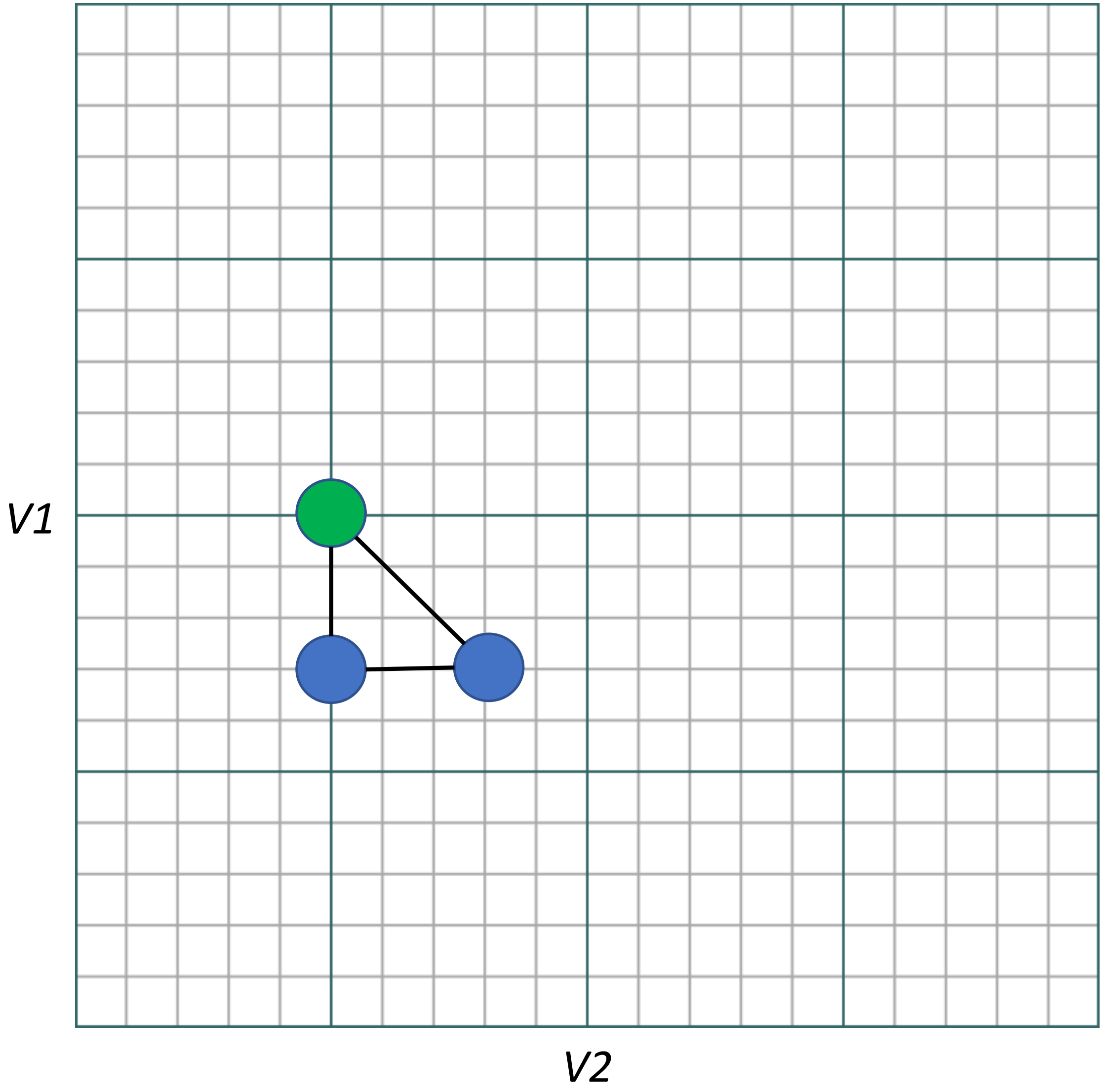
How?

Example for a 2 variable problem

1. Initial Parameters
2. Construct initial simplex (n + 1) vertices
3. Evaluate and Rank
4. Reflect away from worst result to generate new set of parameters
5. Evaluate new point, if favourable expand (1), if not contract (2,3)
6. If none of these points are better than the current best then the simplex is shrunk toward the best. But . . .



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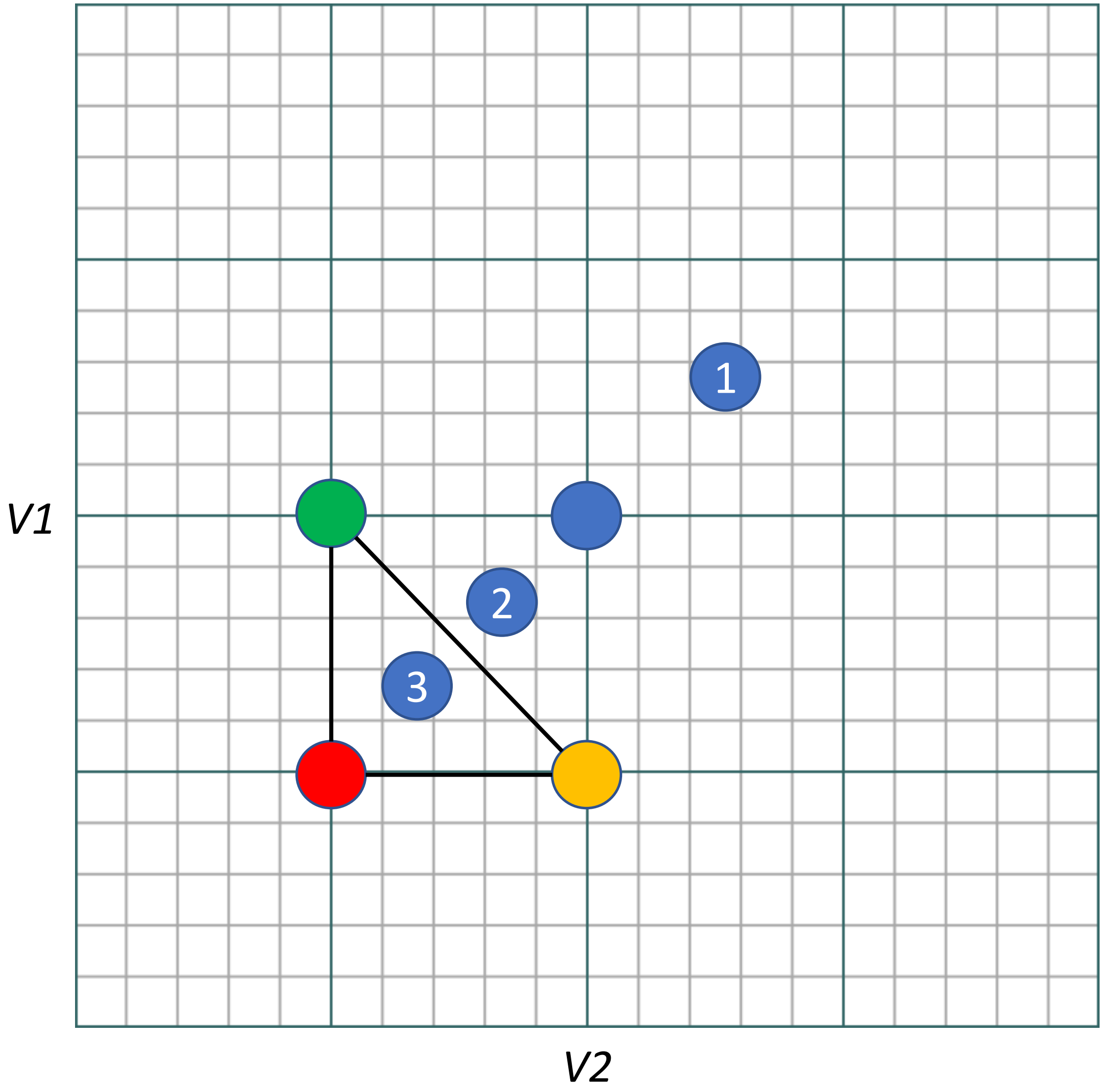
6. But. .



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How?

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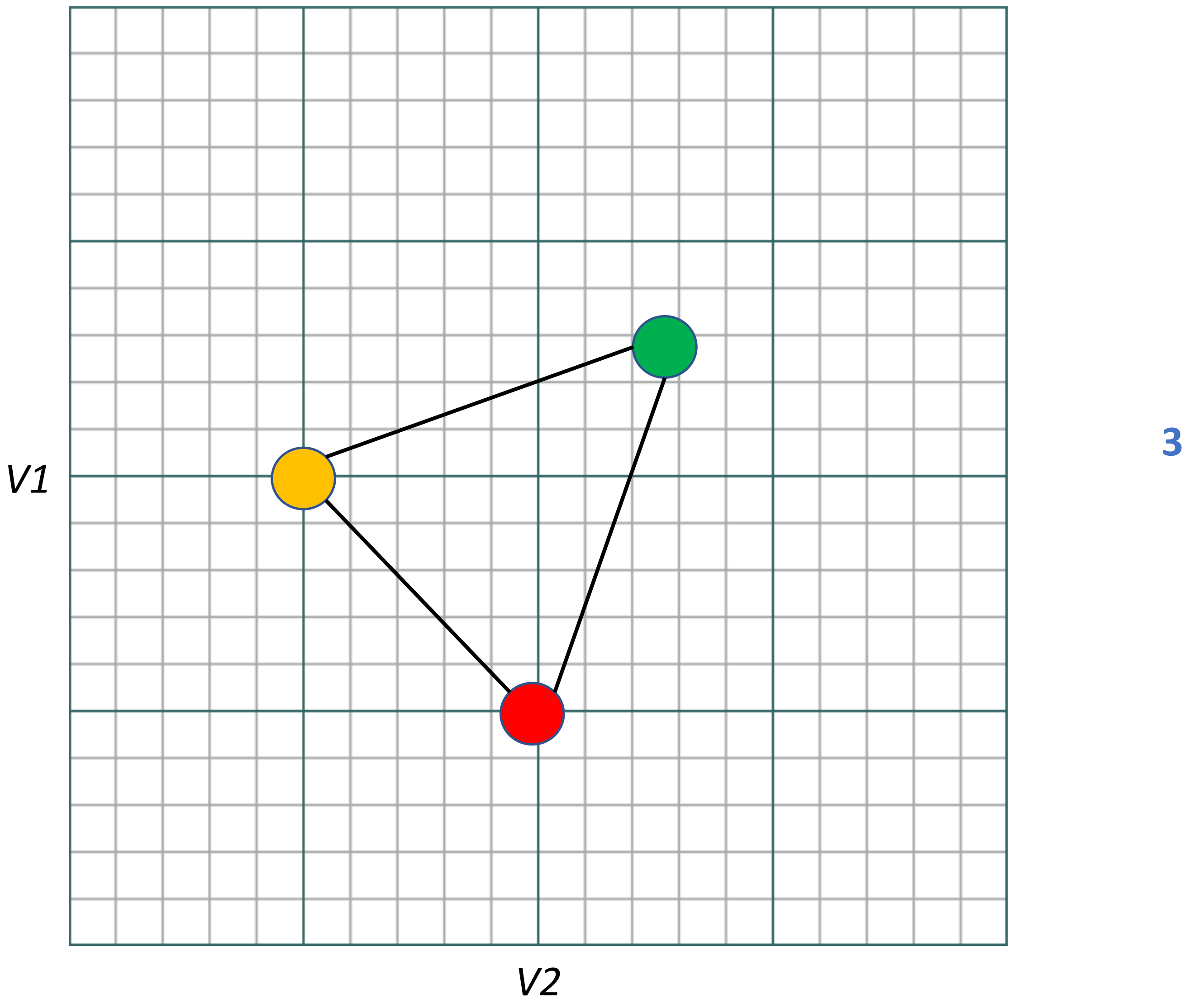
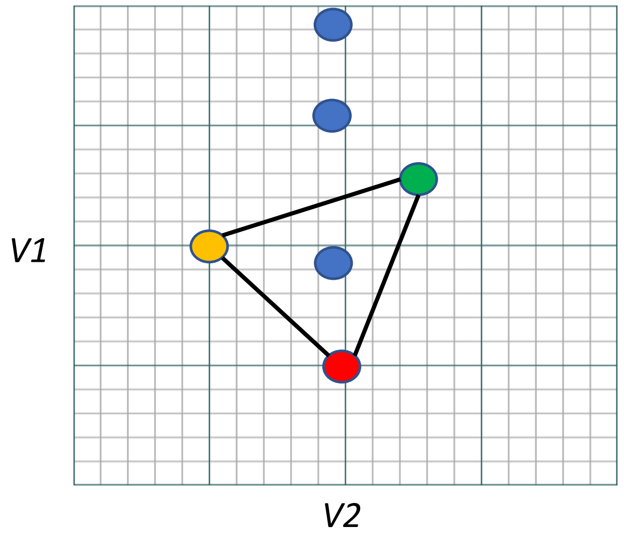
1. Initial Parameters
2. Construct initial simplex (n + 1) vertices
3. Evaluate and Rank
4. Reflect away from worst result to generate new set of parameters
5. Evaluate new point, if favourable expand (1), if not contract (2,3)
6. But. . If we accept then the new point becomes part of the simplex

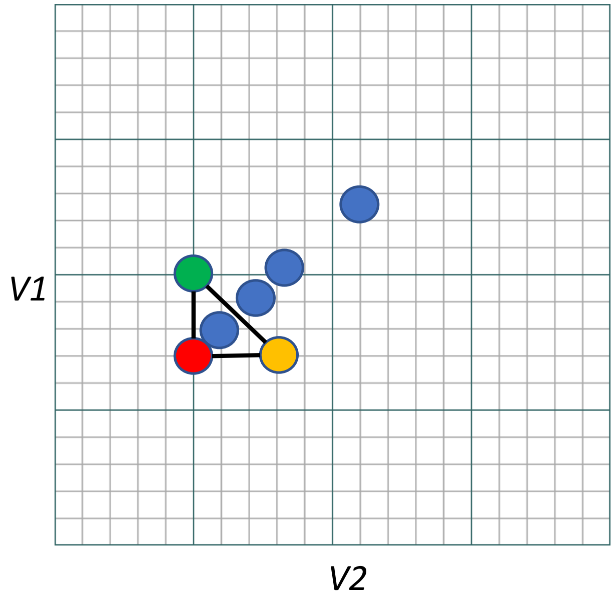


How?

Example for a 2 variable problem

1. Initial Parameters
2. Construct initial simplex (n + 1) vertices
3. Evaluate and Rank
4. Reflect away from worst result to generate new set of parameters
5. Evaluate new point, if favourable expand (1), if not contract (2,3)
6. Either way the steps repeat with the new simplex
7. Until the stopping parameter is met





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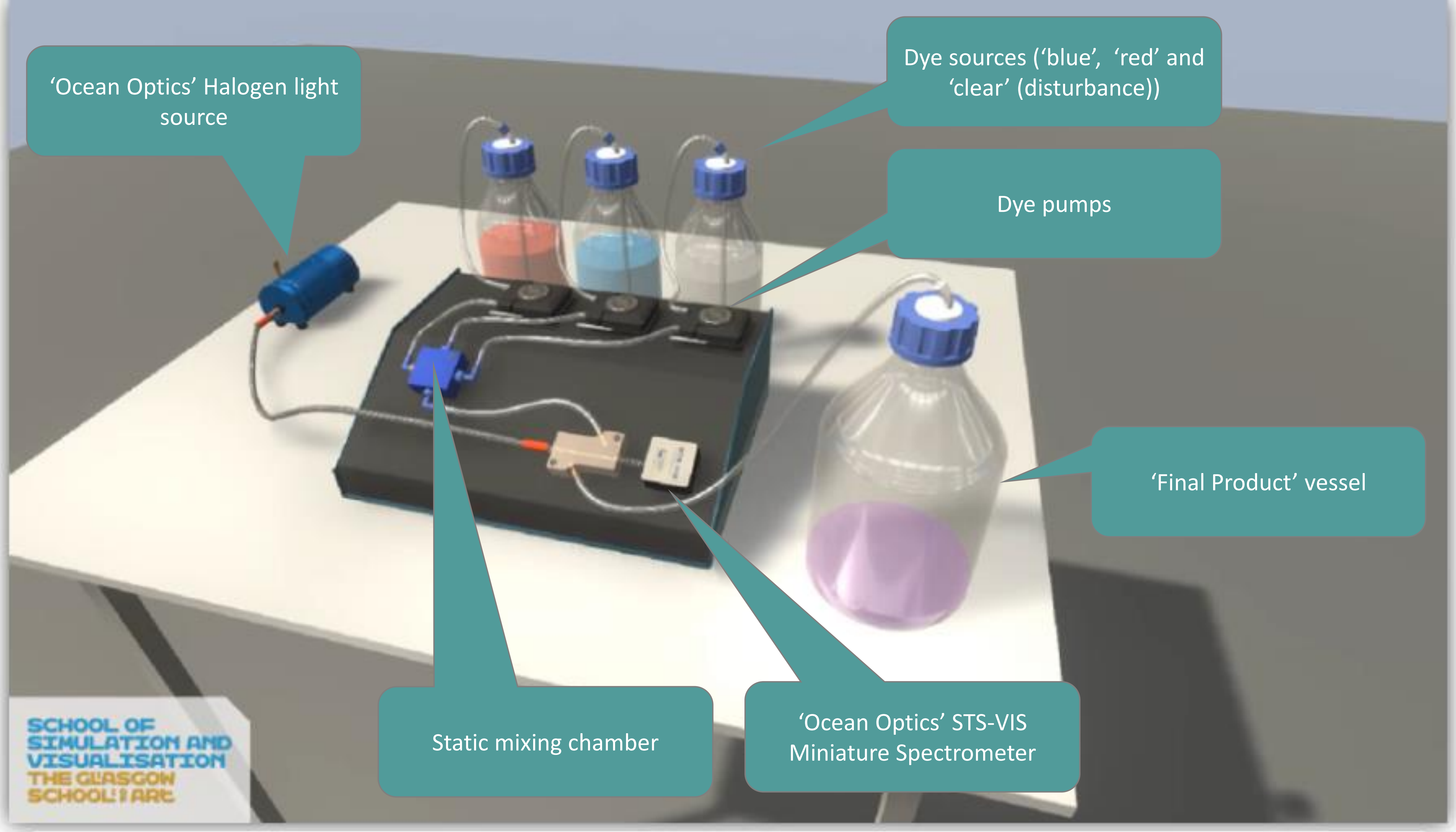
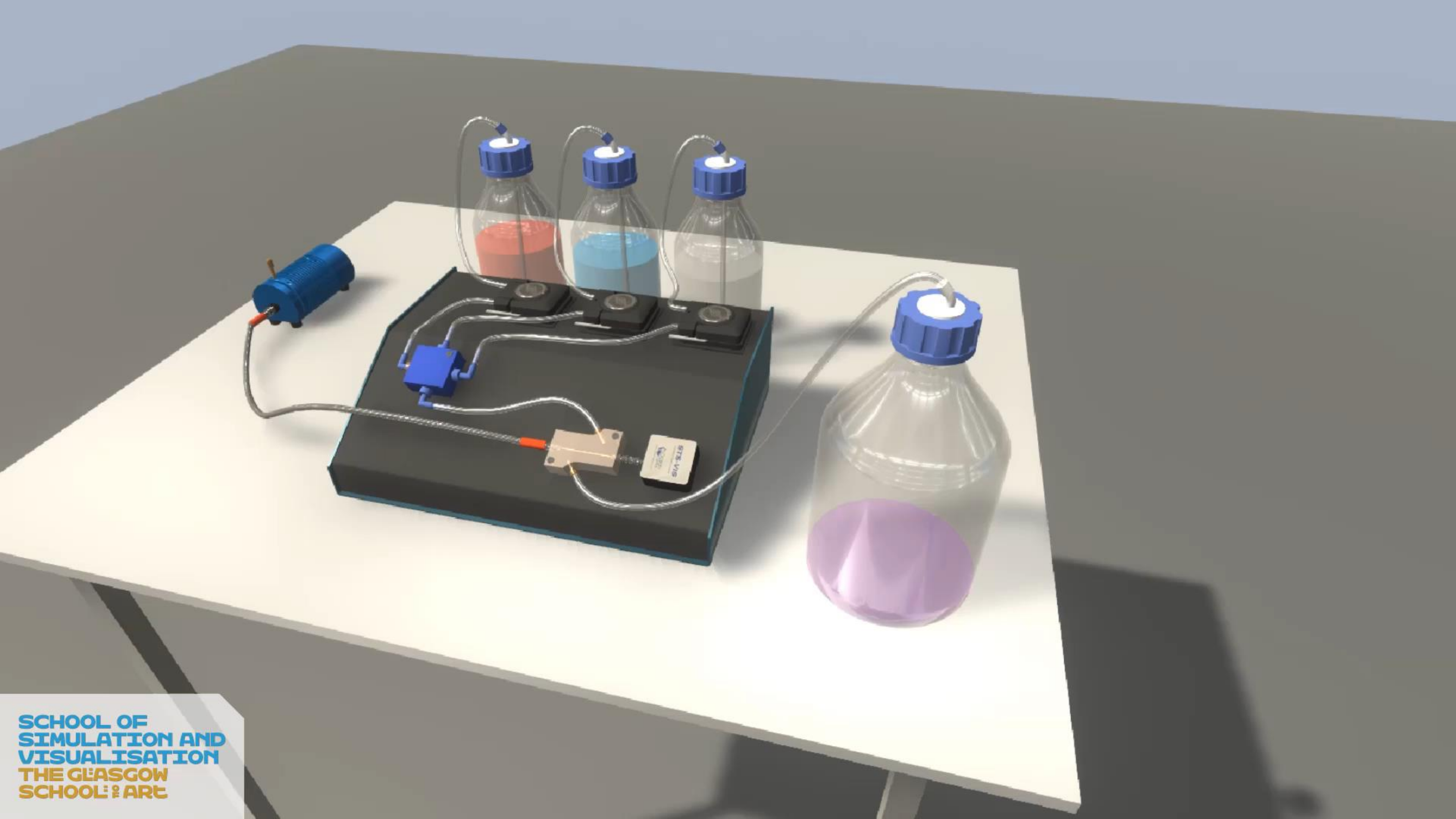
Our Experimental Rig


'Ocean Optics' Halogen light source
Dye sources ('blue', 'red' and 'clear' (disturbance))
Dye pumps
'Final Product' vessel
Static mixing chamber
'Ocean Optics' STS-VIS Miniature Spectrometer
SCHOOL OF SIMULATION AND VISUALISATION
THE GLASGOW SCHOOL of ART


SCHOOL OF
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Rig Demonstration Run

Adaptive Model Predictive Control

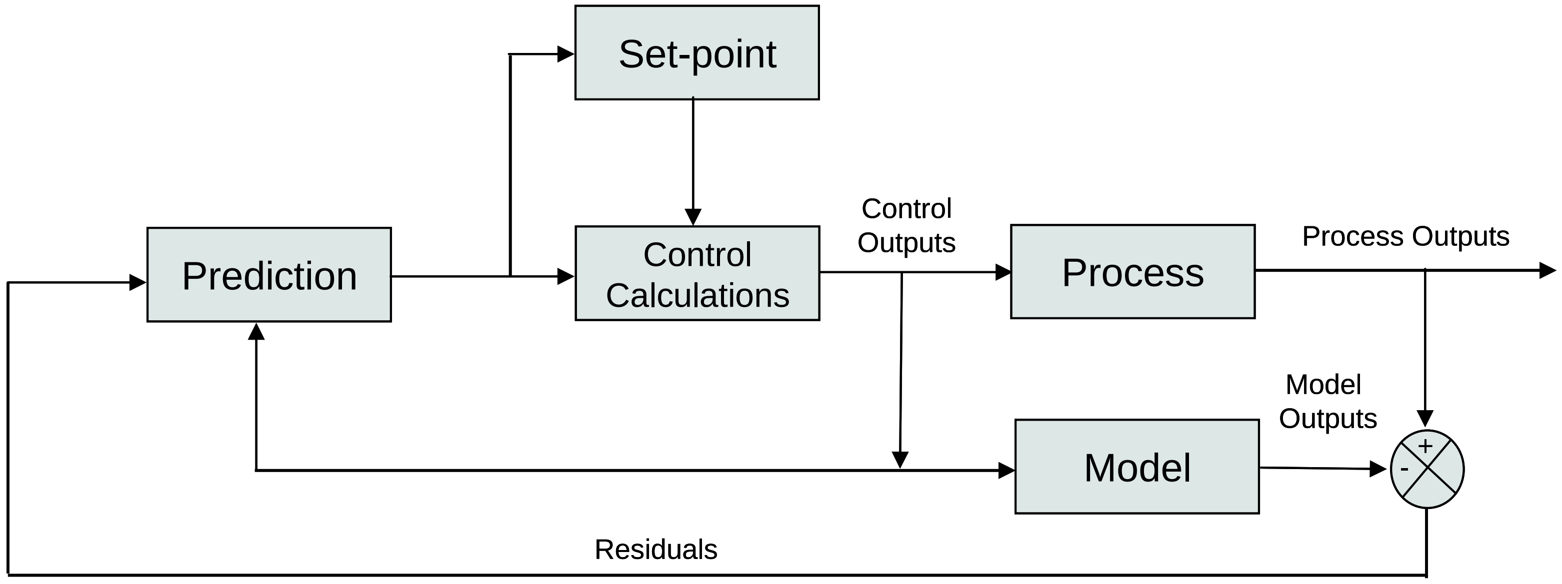
Model Predictive Control –
Principle of Operation

To obtain control moves, need:

- The current and recent past state of the process
- the model, and
- an optimisation algorithm

To calculate the moves

- first, predict the future behaviour of the process (using a model)
- then work out the “best” way to manipulate the MVs in order to achieve the control objectives.
- “Best” is defined through a cost function that is minimised by the optimisation procedure to yield the control moves.
- Minimisation of the cost function can directly consider the process constraints.



Model Predictive Control

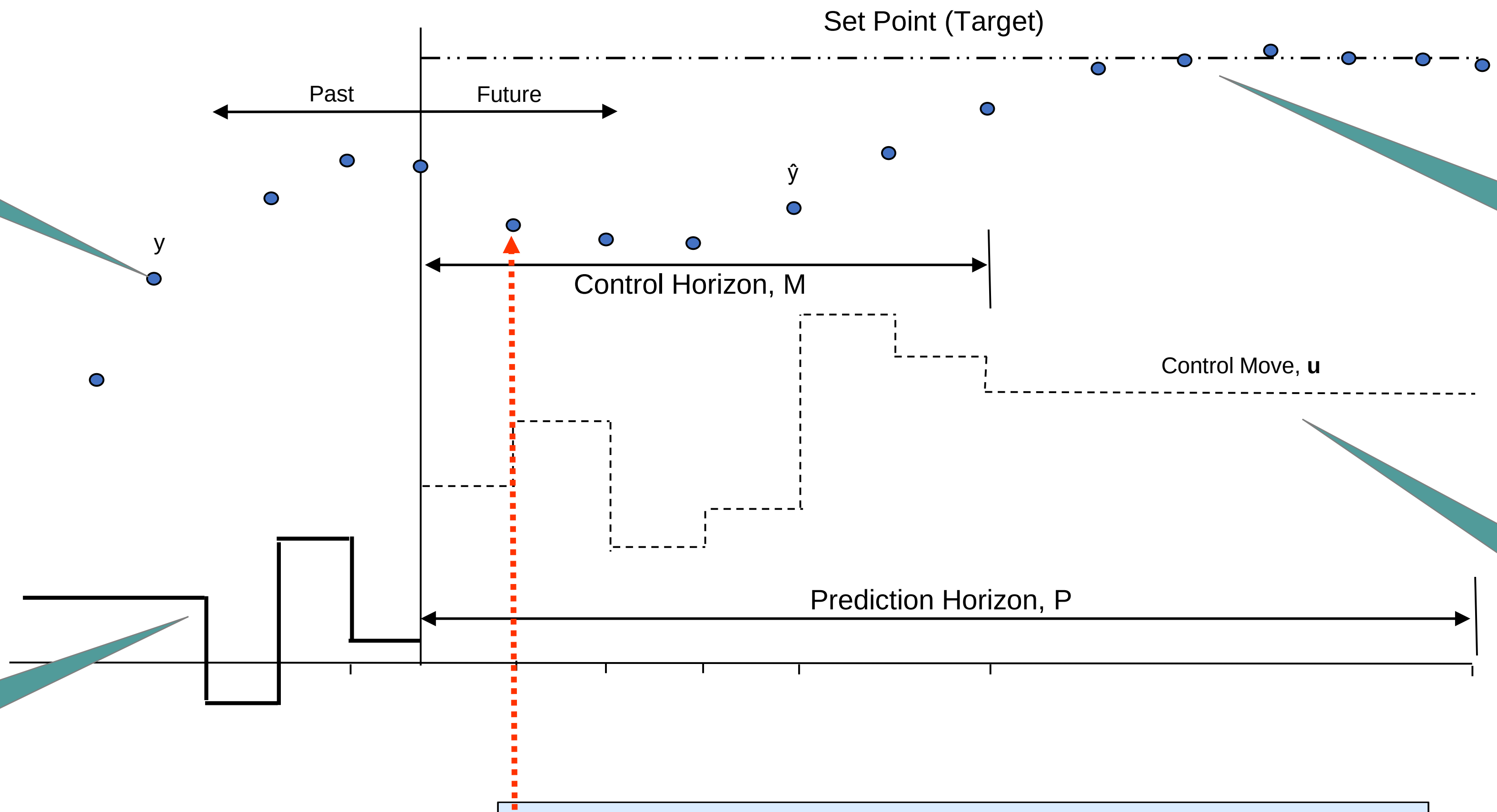
Simple Overview

Previous Sensor Values

Predict Future Behaviour

Calculate Control Moves

Previous Control Moves

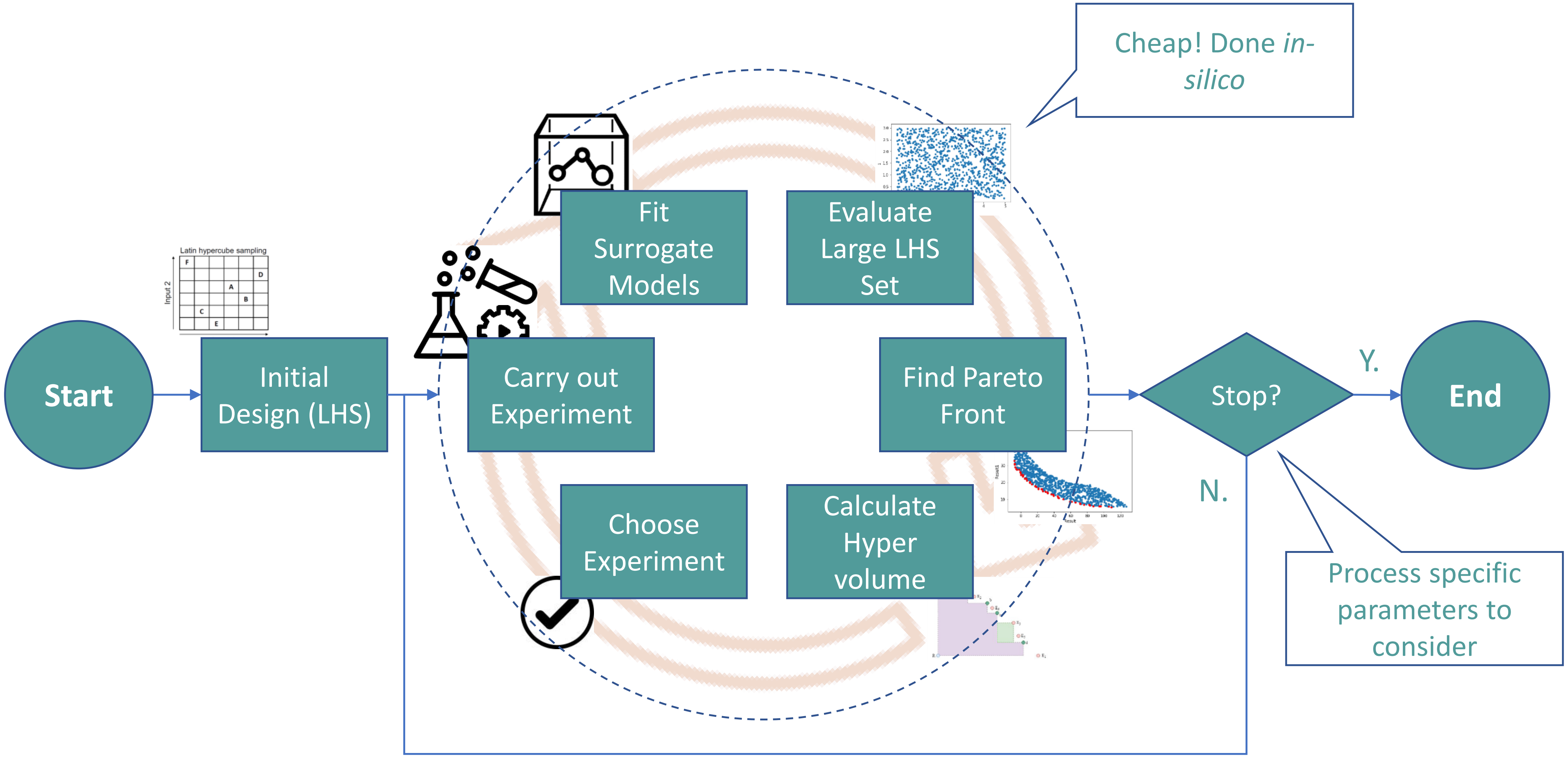


$$\underline{y}_{k+1} = \underline{\alpha}\begin{bmatrix} \underline{y}_k \\ \underline{y}_{k-1} \\ \cdot \\ \cdot \\ \underline{y}_{k-R} \end{bmatrix} + \underline{\beta 1}\begin{bmatrix} u1_k - u1_{k-1} \\ u1_{k-1} - u1_{k-2} \\ u1_{k-2} - u1_{k-3} \\ \cdot \\ \cdot \end{bmatrix} + \underline{\beta 2}\begin{bmatrix} u2_k - u2_{k-1} \\ u2_{k-1} - u2_{k-2} \\ u2_{k-2} - u2_{k-3} \\ \cdot \\ \cdot \end{bmatrix} + \ldots + \underline{\beta q}\begin{bmatrix} v1_k - v1_{k-1} \\ v1_{k-1} - v1_{k-2} \\ v1_{k-2} - v1_{k-3} \\ \cdot \\ \cdot \end{bmatrix} + \ldots$$

‘Gaussian’ Multi-Objective Optimisation

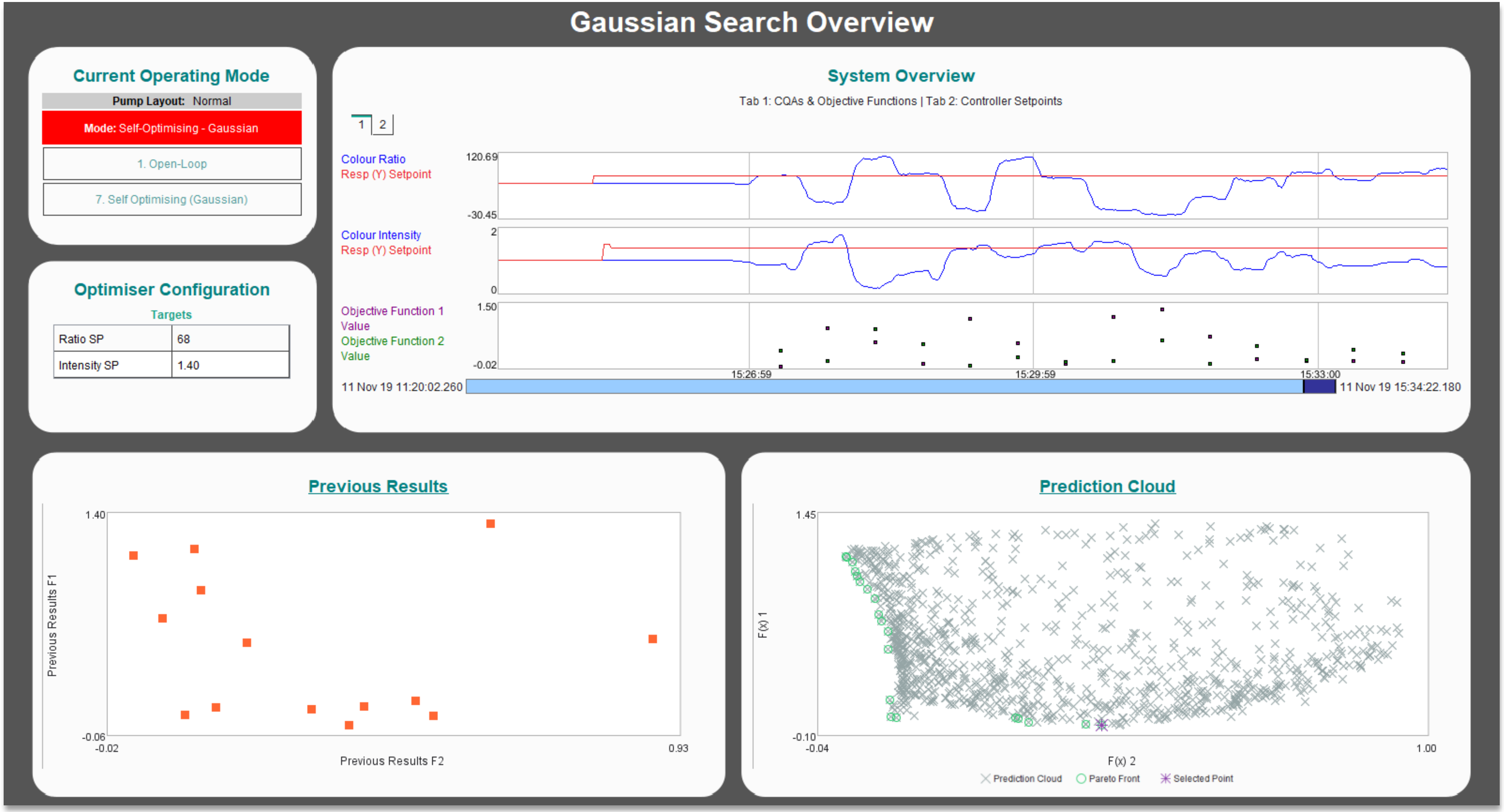
True Multi-objective Optimisation

Gaussian Search



True Multi-objective Optimisation

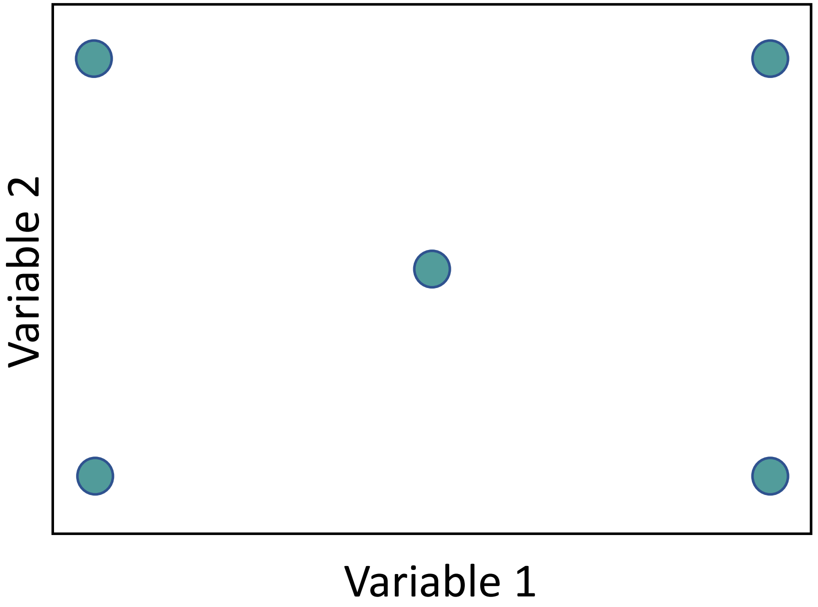
Gaussian Search



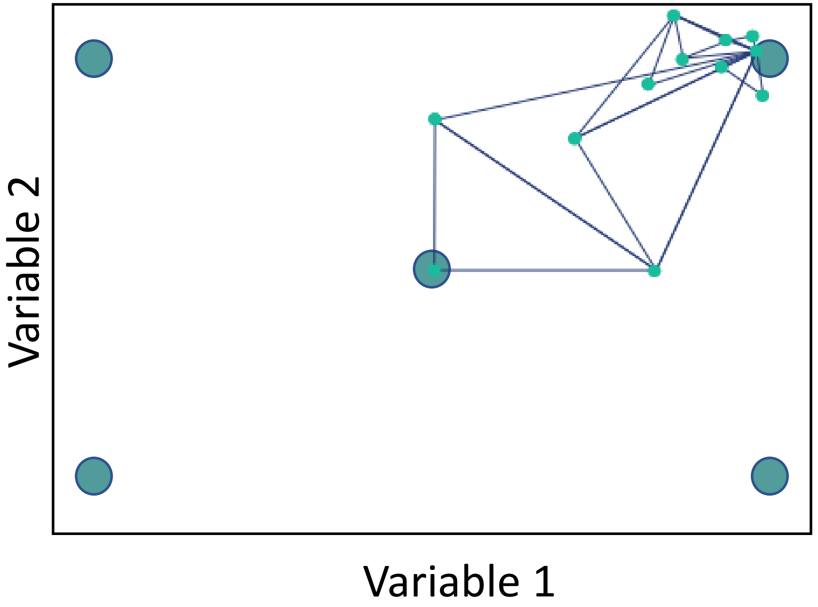
Data Generation

Exploration vs Exploitation

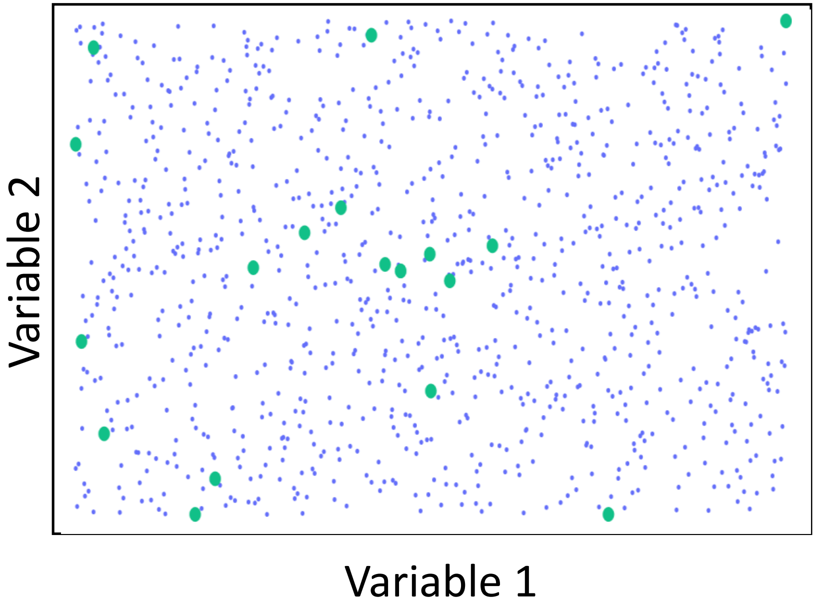
DoE:
Pure Exploration



Nelder-Mead:
Pure Exploitation



Gaussian Search:
Both via Surrogate Models



Surrogate Points
Experiment Points

Nelder Mead and MPC

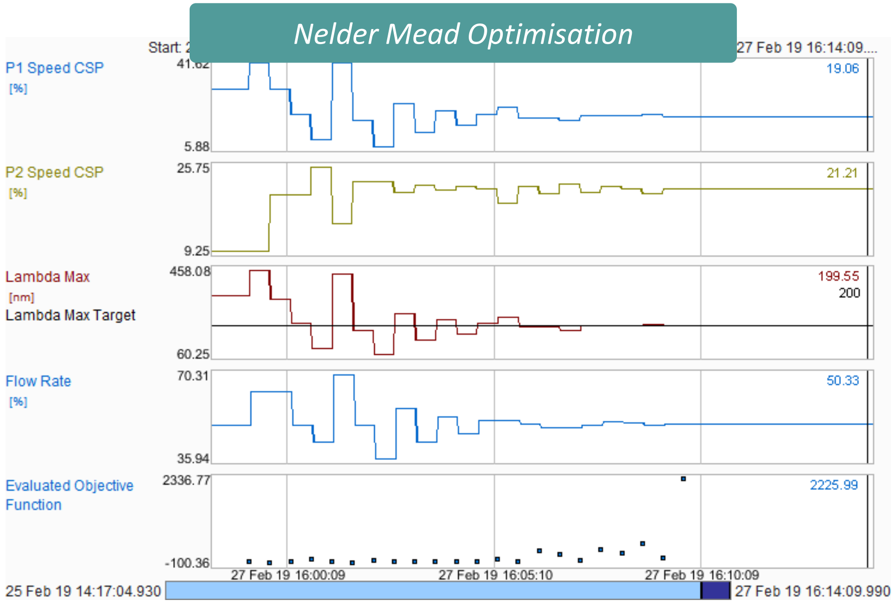
Does each algorithm *Learn?*

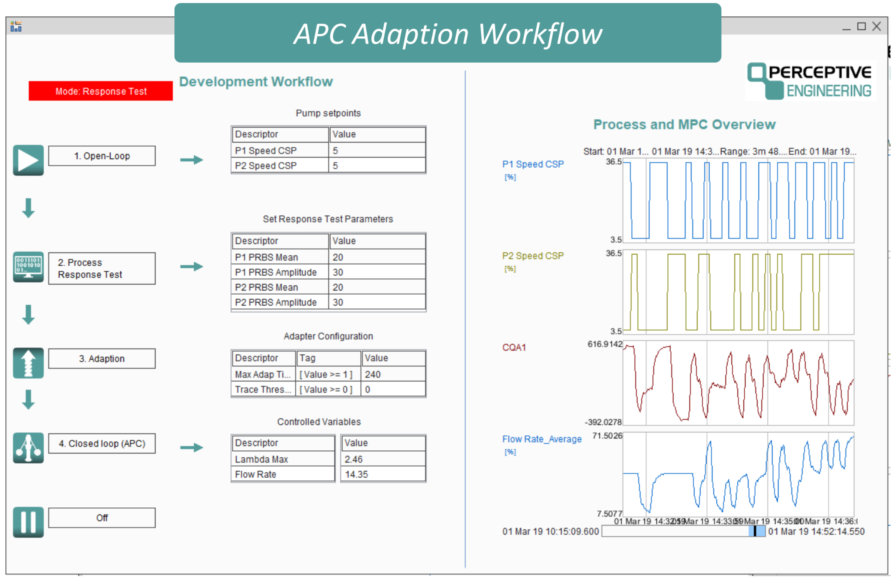
The Nelder Mead curiosity algorithm doesn't *learn* in the same way as other AI (Neural Networks for example):

- Constrained "trial and error" learning
- Minimising or maximising the objective function.
- Systematic approach leads to a (local) optimum
- No "predictive" capacity

MPC *predicts* future behaviour using it's dynamic model.

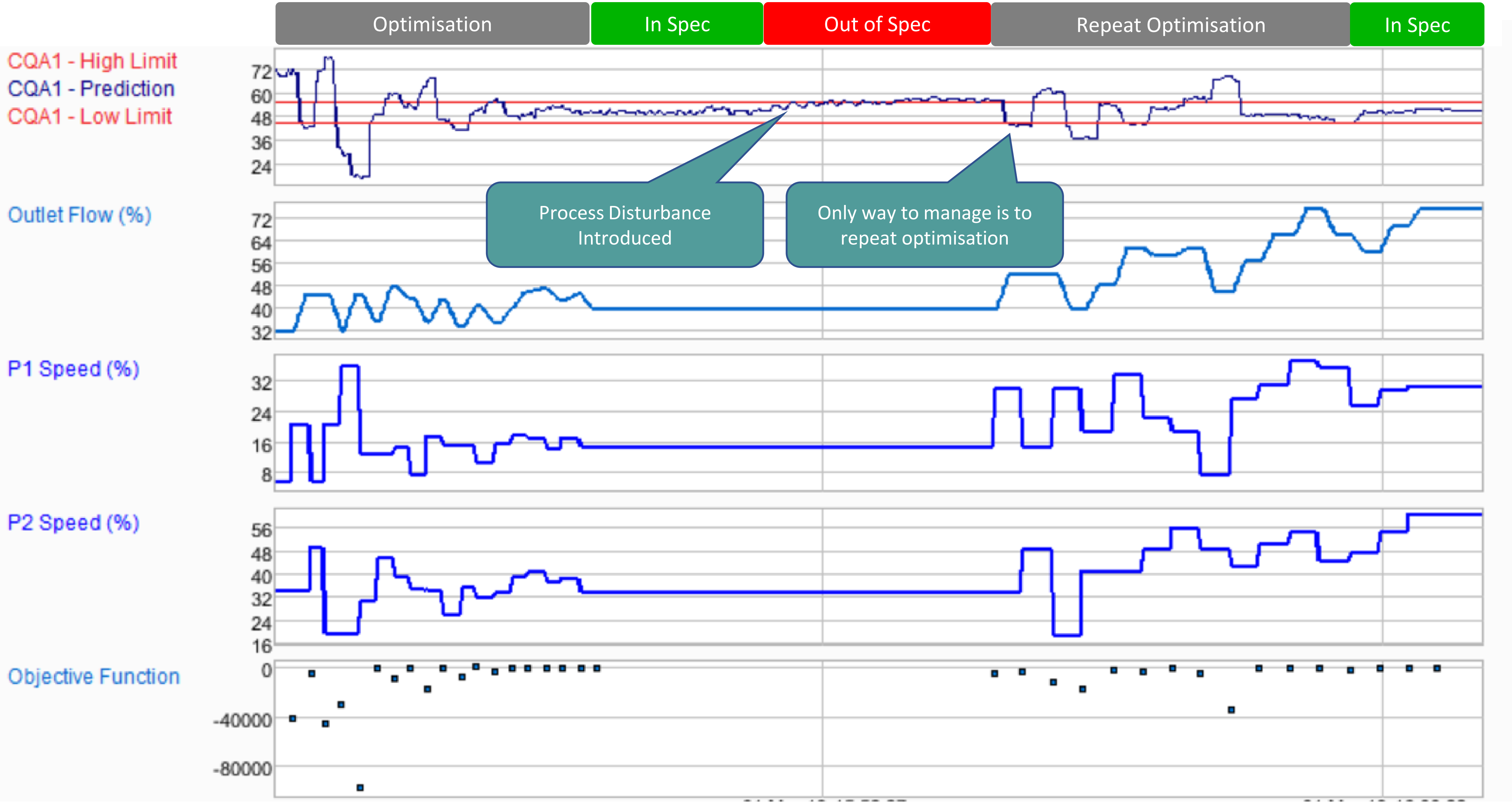
- Traditionally the model is built offline from process data
- A linear representation around a defined operating point
- Online Adaption can be used to update the model (regression based on new information).
- Narrow learning under human supervision.





Optimisation as a controller?

Effect of Process Disturbances



Self-Optimising Reactor Case-Study

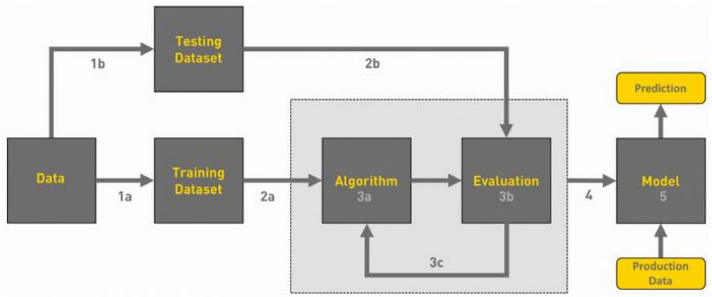
Combining algorithmic approaches

These two approaches are complimentary:

Self Optimisation
Hit the optimum efficiently and generate useful data in doing so.

Advanced Control
build model on process data, keep the process at that optimum, whilst compensating for raw material and process disturbances.

SMART DATA GENERATION

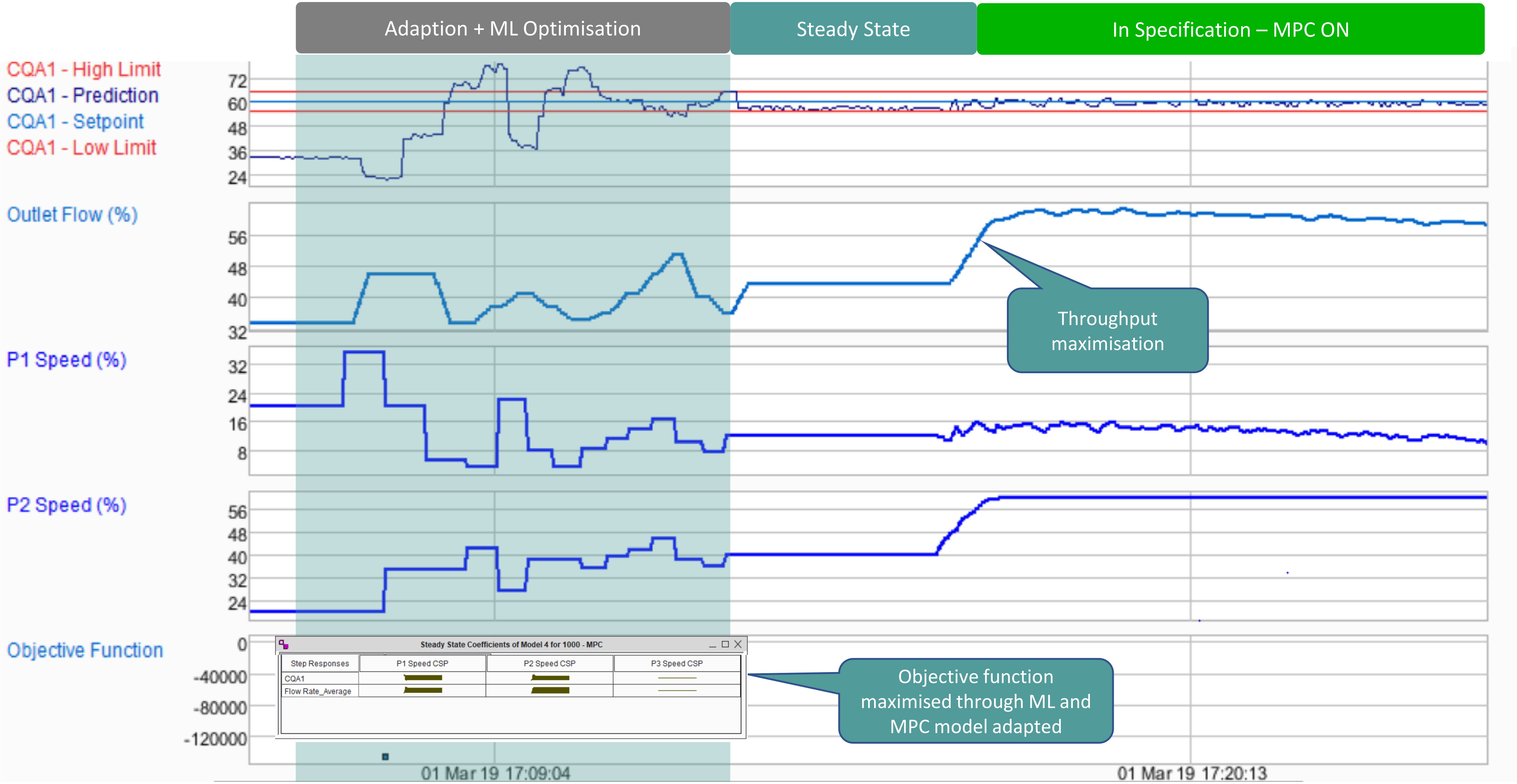


Overview of the Workflow of ML

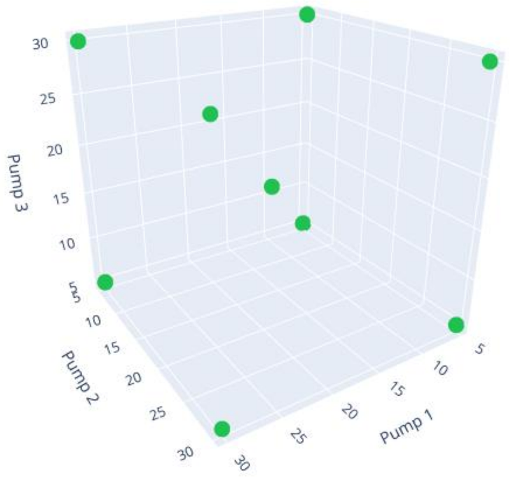
CONTROL

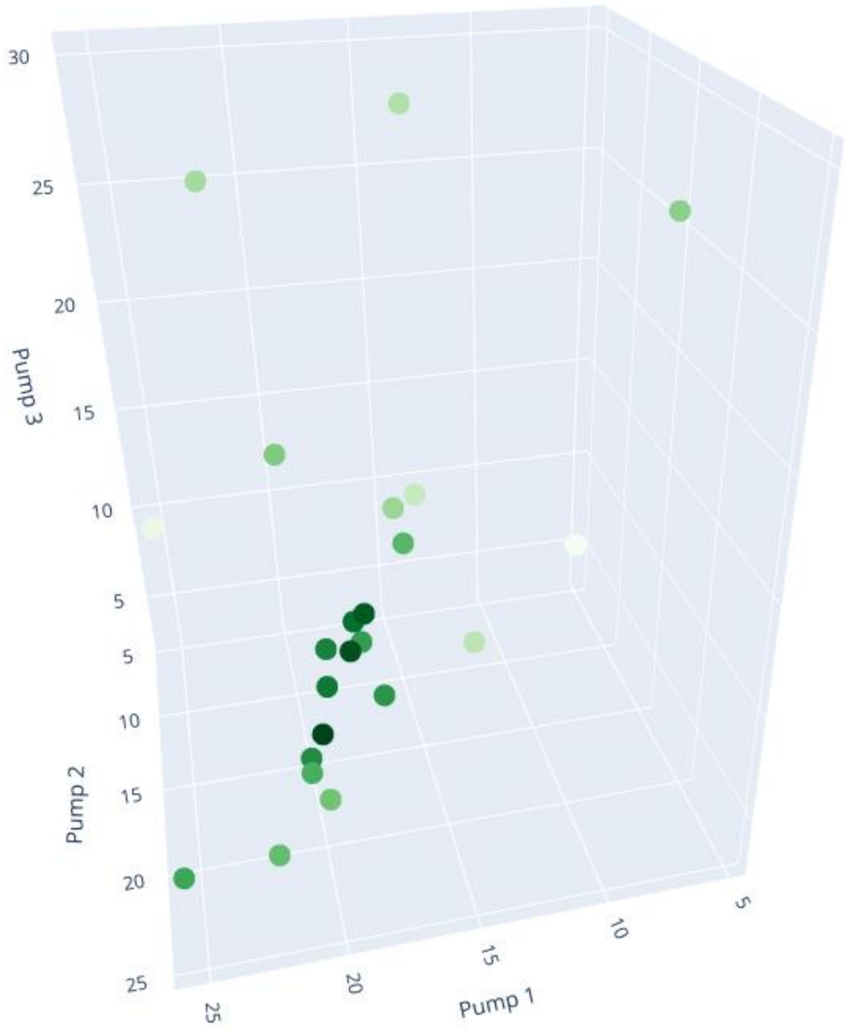
Self Optimisation + Model Predictive Control

Combined Advanced Process Control And Machine Learning
Example

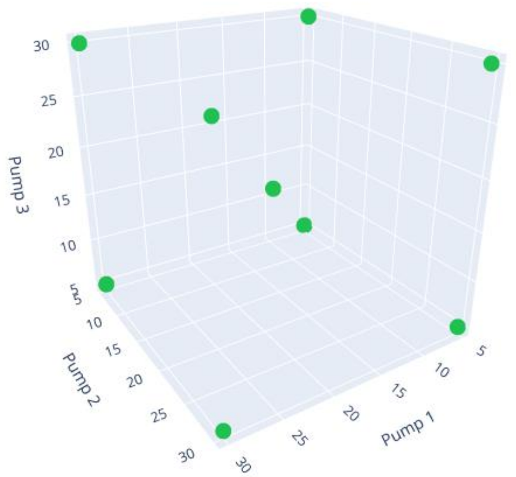


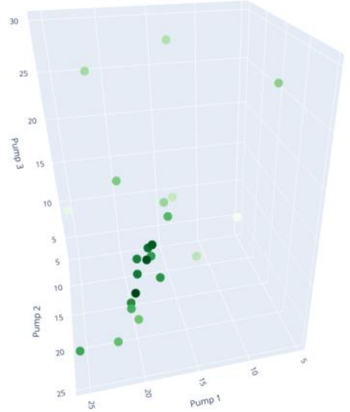
Nelder-Mead Space Filling

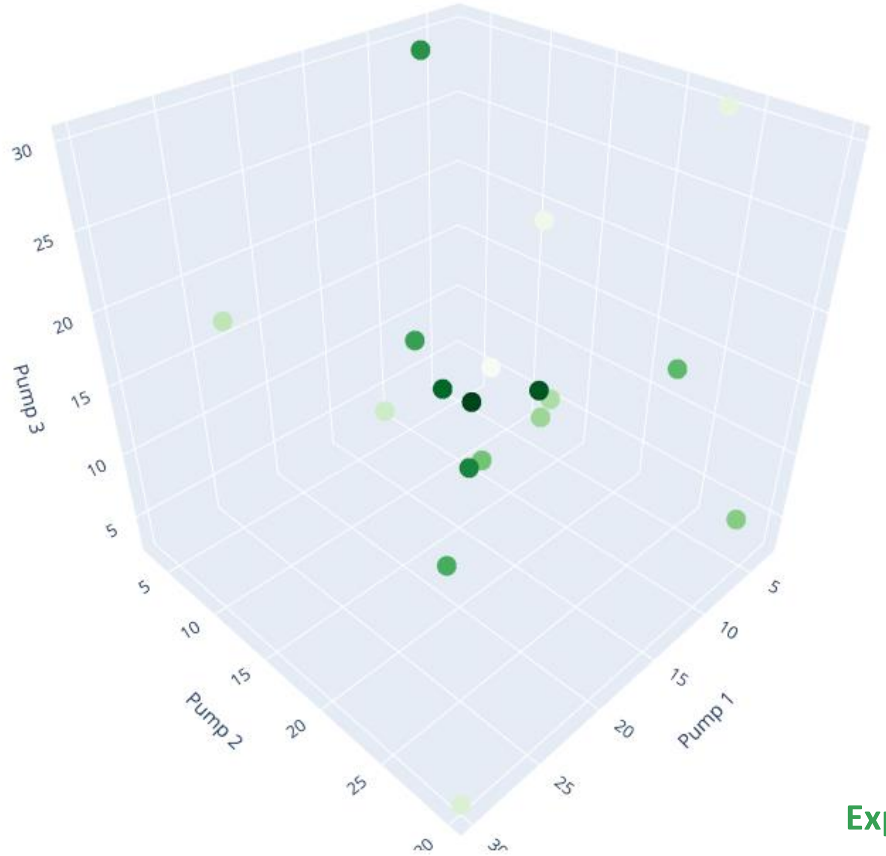




Gaussian Search Space Filling

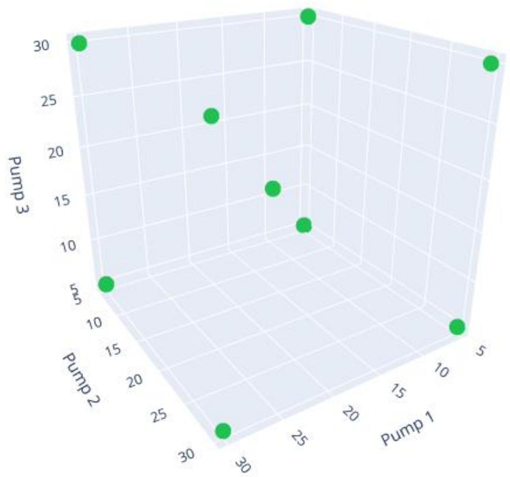


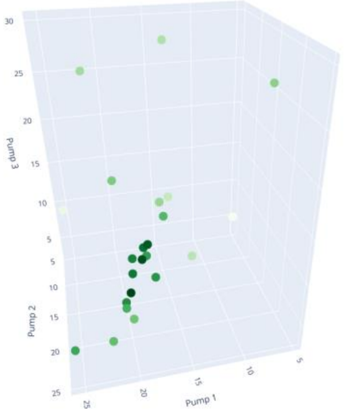


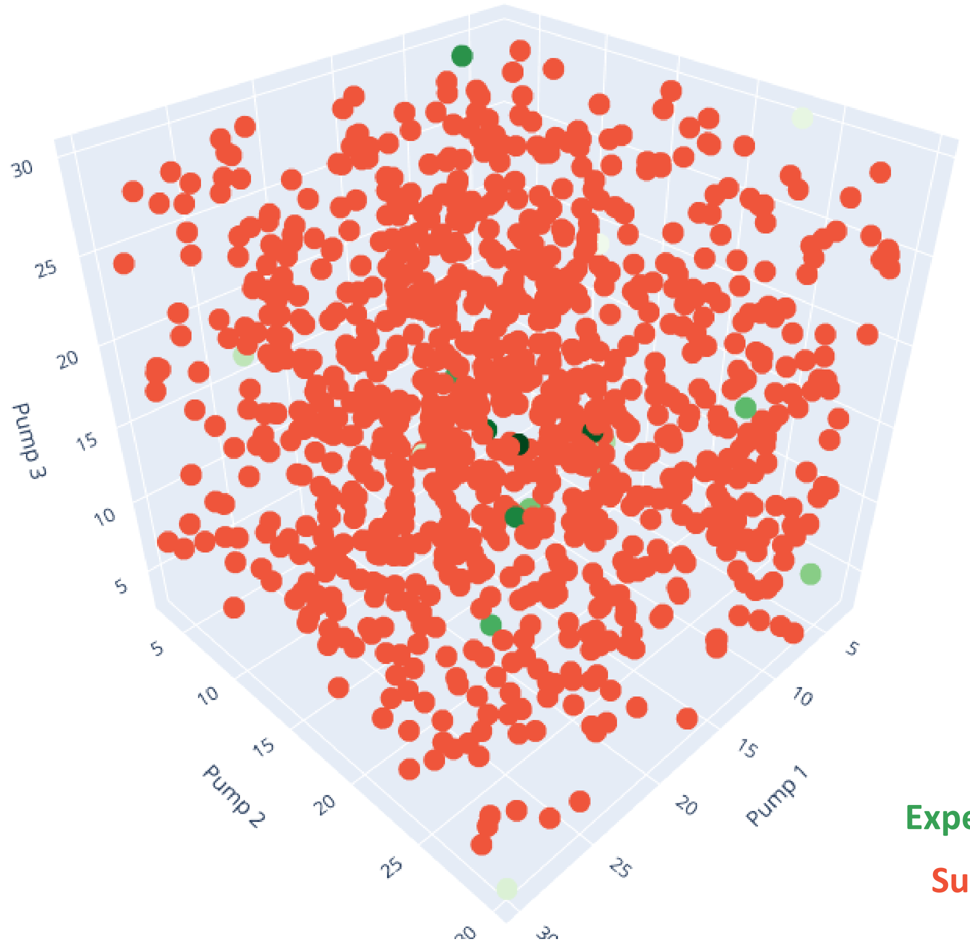


Experimental Points

Gaussian Search Space Filling



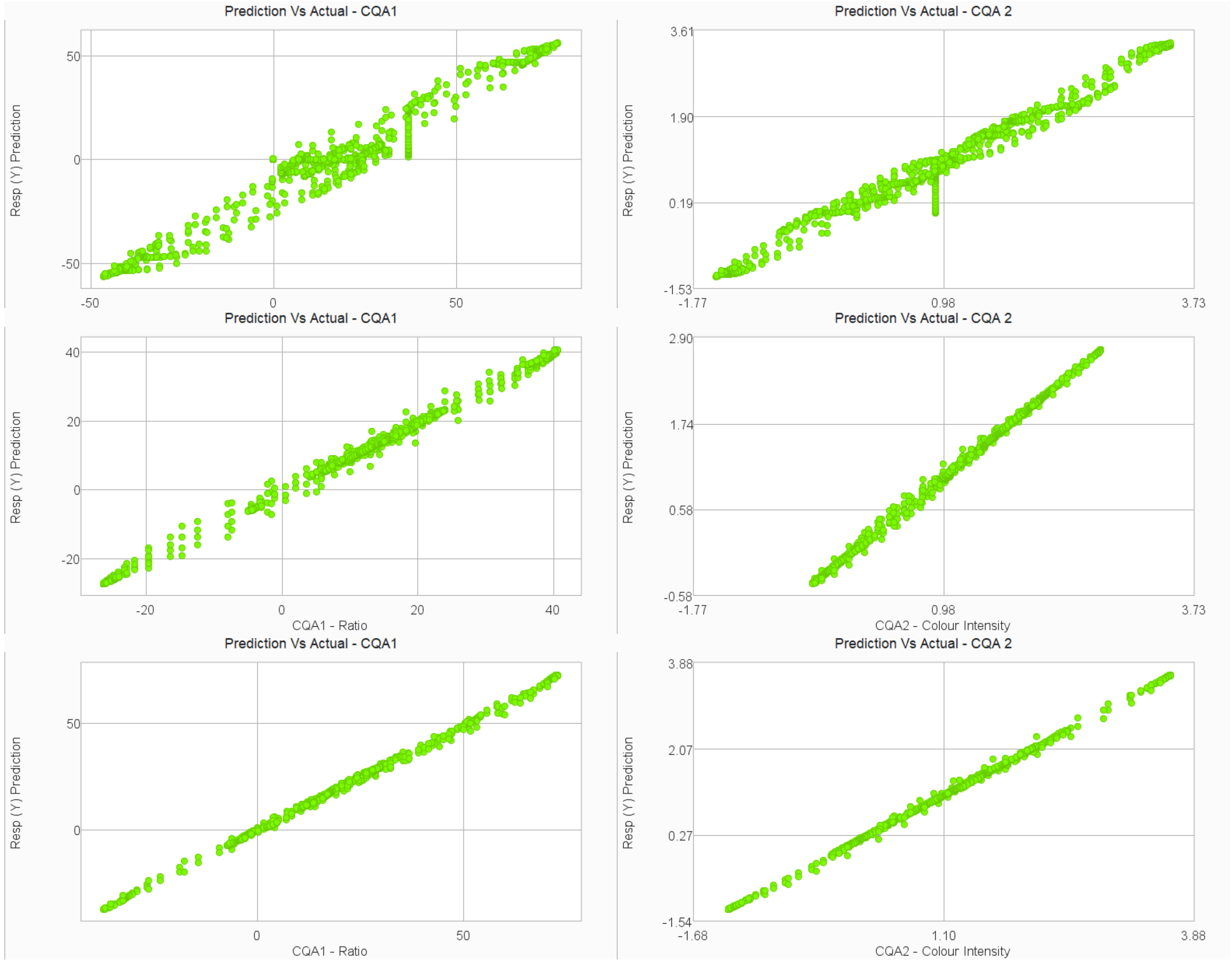




Smart Data Creation

How 'Rich' is the Data for Generating an MPC Model?

	RMSEP CQA1	RMSEP CQA2
DoE	6.8	0.12
NM	1.05	0.030
GS	0.51	0.013



Comparison

Does the Machine Learning algorithm do what we want?

	Automated DoE	Adaptive MPC	Nelder-Mead	Gaussian Search
Optimised Process			"Single Objective" Pseudo-Multi-Objective Possible	"Multi-Objective"
Static Process Model	Anova and Linear Model at Best (Further Modelling Step)		(Further Modelling Step)	Linear and/or Non-Linear for Each Objective
PAT Calibration	Unlikely	Unlikely		
Rich enough Data for MPC			Sometimes	

Real-Time Machine Learning for Process Optimisation

Webinar Summary

ML has brought along with it a whole new set of terminology for existing techniques

The potential of these techniques is significant provided they are selected with care

Beyond the Hype:

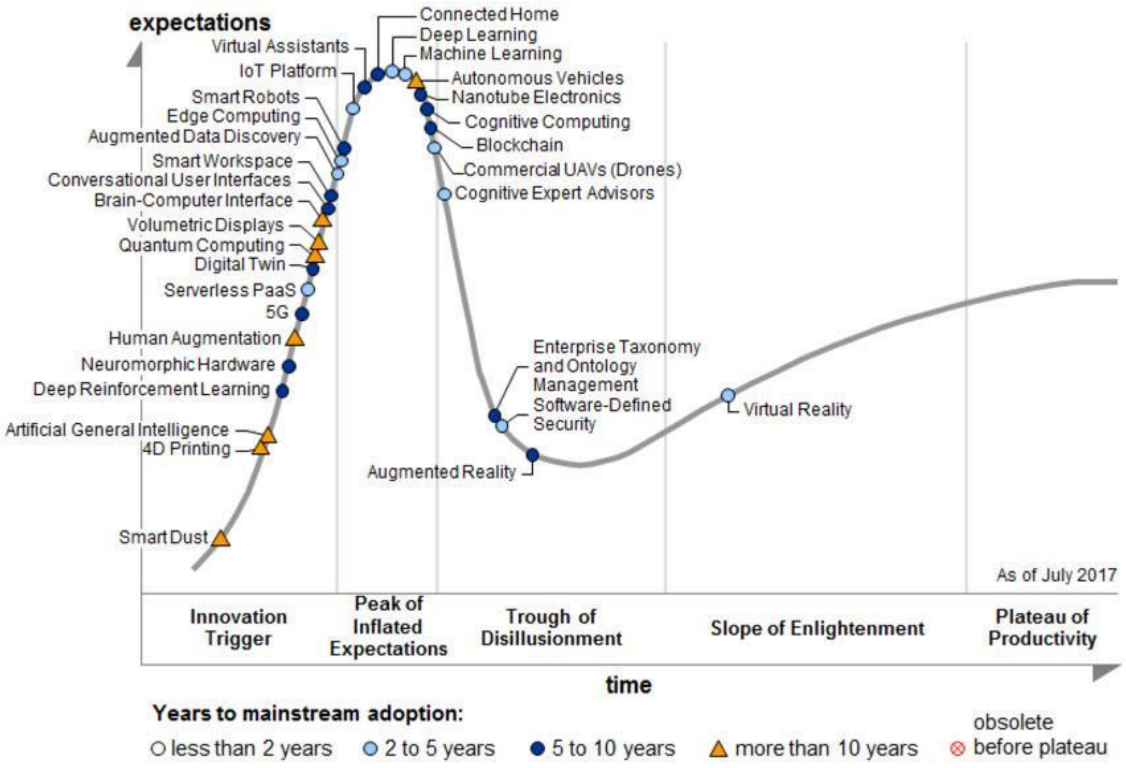
Within ML are a lot of methodologies that bring genuine value

Most appropriate when dealing with large data sets

Like all technology, these have strengths and weaknesses

These methodologies require insightful application

Hype Cycle for Emerging Technologies, 2017



Note: PaaS = platform as a service; UAVs = unmanned aerial vehicles

Source: Gartner (July 2017)

Gartner Hype Cycle for Emerging Tech (2017)

Thank you for listening!

To learn more:

www.perceptiveapc.com

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