Phoenics: A Bayesian optimizer for Chemistry

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HARVARD UNIVERSITY

aisc

Materials challenges of the 21st century

Chemistry is the study of matter and the changes in undergoes

Functional molecules / materials promise solutions to key global challenges:

- Clean energy
  (e.g. solar cells, flow batteries)
- Global health
  (e.g. drugs, water purifier)
- Sustainability
  (e.g. biodegradable plastics)
- and many more

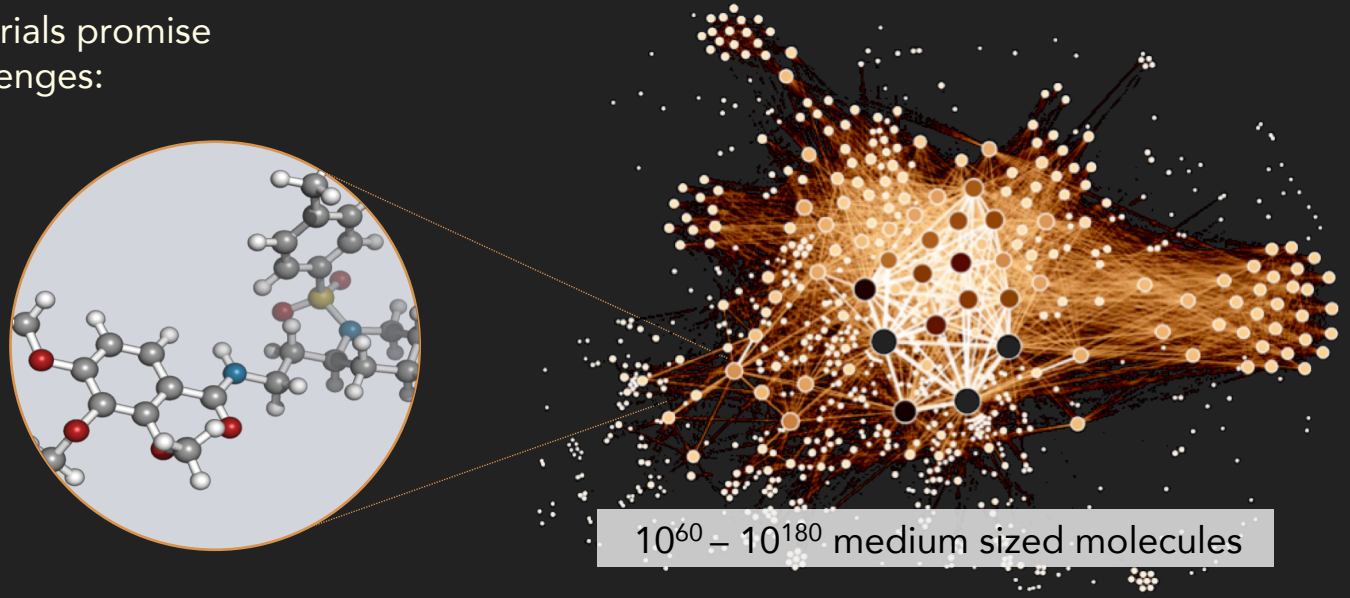


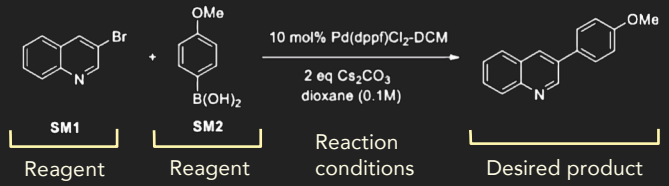
Illustration of the molecular space

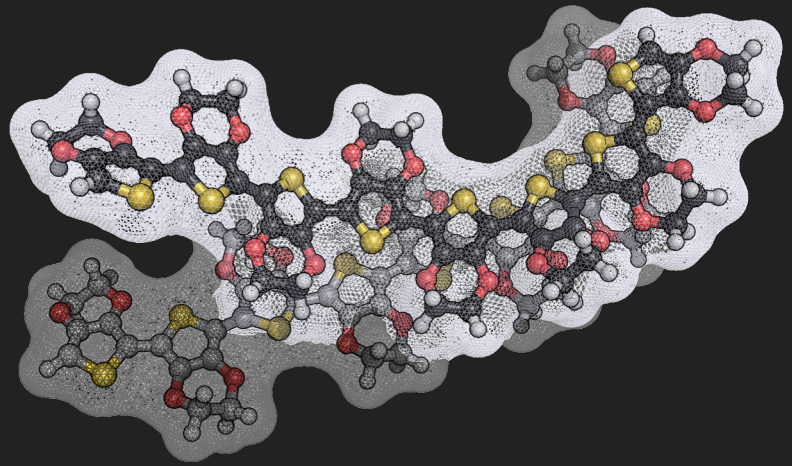
How do we find these materials?

Materials challenges of the 21st century

How do we make these materials?

(i). Find a synthesis route
(ii). Find suitable reaction conditions,
(i.e. *make the reaction work*)





Materials challenges of the 21st century

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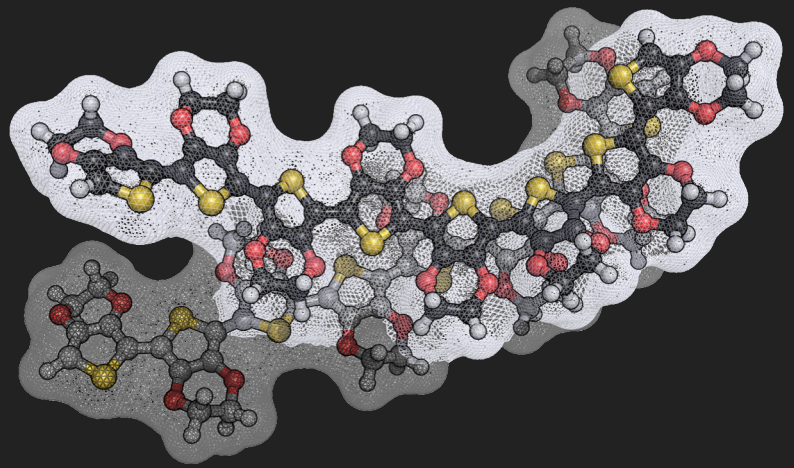
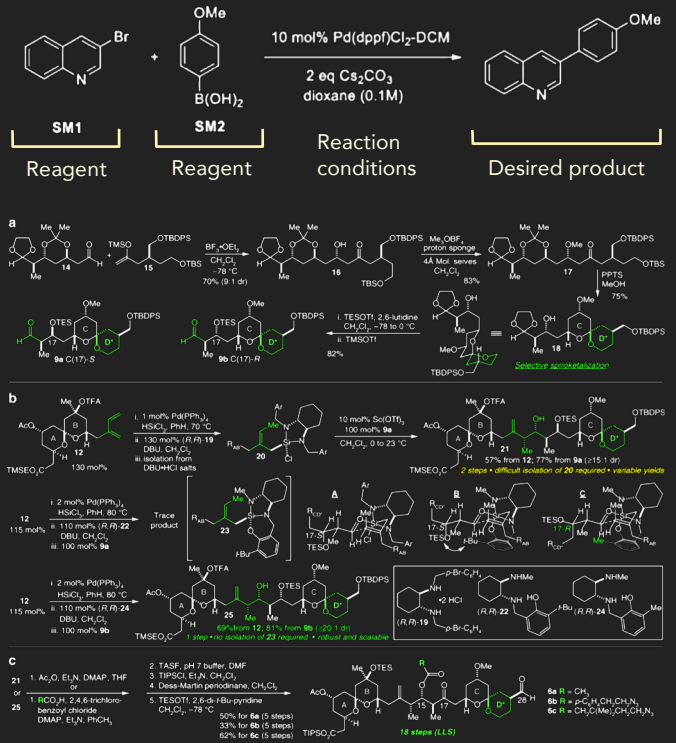




Suen et al. *Nature communications* 9.1 (2018): 4710.

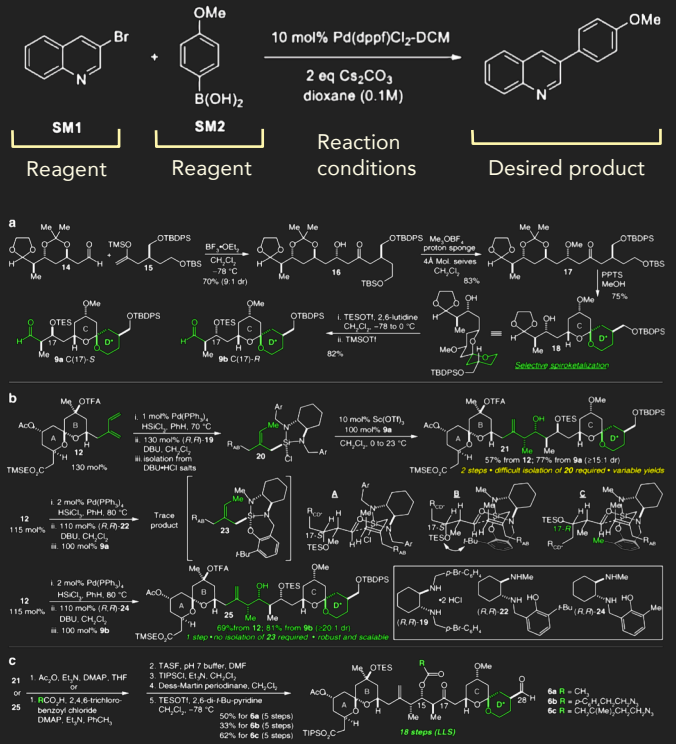
Materials challenges of the 21st century

How do we make these materials?

(i). Find a synthesis route
(ii). Find suitable reaction conditions, (i.e. *make the reaction work*)

Challenges

- Many parameters to tune
- Time constraints delay feedback
- Resource constraints often prevent exhaustive screening
- Large, well curated databases do not exist

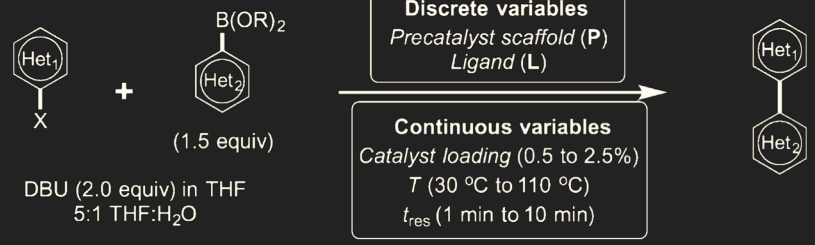


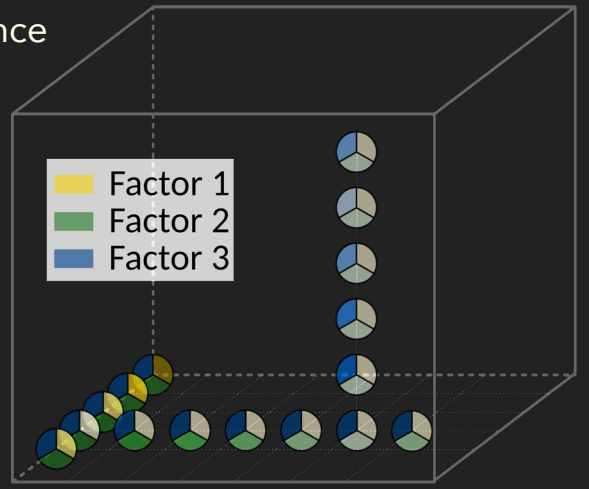
Suen et al. *Nature communications* 9.1 (2018): 4710.

Traditional routes to designing experiments

- Intuition of researchers based on prior knowledge and experience
- Systematic approaches:

  one-factor-at-a-time (OFAT)





1.5 %

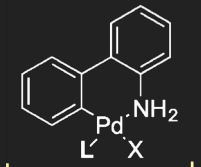
Catalyst loading

60 °C

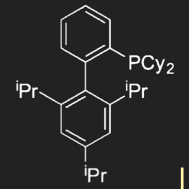
Temperature

2 min

Residence time



Catalyst

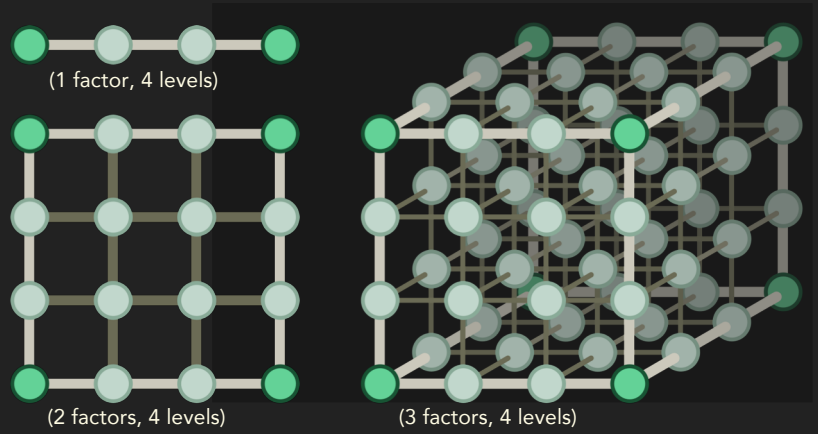


Ligand

Traditional routes to designing experiments

Design of experiments (DoE)

- Similar to grid searches
- Probes hypothesized relations between parameters (factors) and measurements



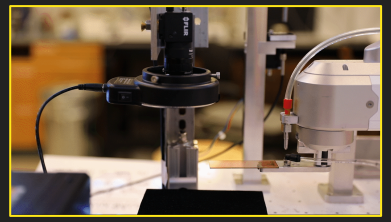
- Subsequent campaigns might be executed with finer grids

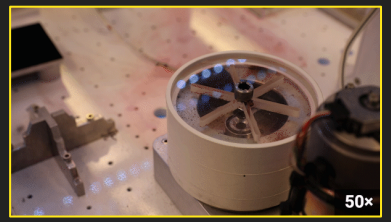
Advantage:

experiments are massively parallelizable (resource permitting)

Drawback:

design choices cannot be refined *on-the-fly*





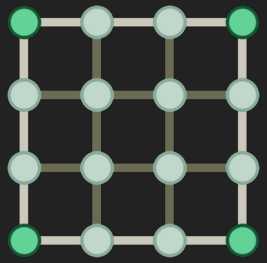
Traditional routes to designing experiments

Design of experiments (DoE)

- implicitly constructs *Taylor expansion* to the experimental response surface

$$f(\boldsymbol{x}) = \sum_{|\boldsymbol{\alpha}|<k} \frac{1}{\boldsymbol{\alpha}} \frac{\partial^{|\alpha|} f(\boldsymbol{x})}{\partial_{x_1}^{\alpha_1} \dots \partial_{x_n}^{\alpha_n}}\Bigg|_{\boldsymbol{x}=\boldsymbol{\alpha}} (\boldsymbol{x}-\boldsymbol{\alpha})^{\boldsymbol{\alpha}}$$

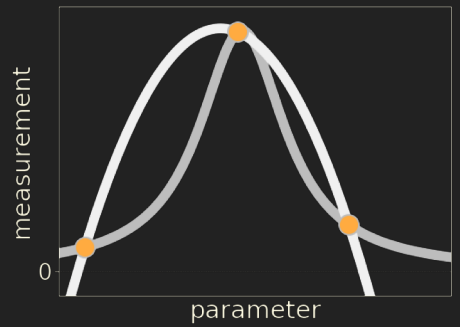
- shows adverse exponential scaling with the number of parameters



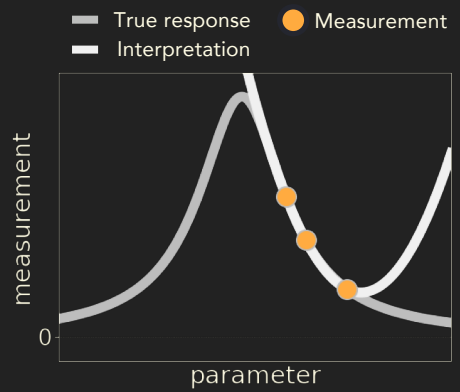
(2 factors, 4 levels)

$$\#\,\text{exp} = (\#\,\text{levels})^{\#\,\text{parameters}}$$

Only applicable to small spaces



Physical constraints can be violated



Misleading trends might be detected

Experimental campaign is executed without constant refinement

Rethinking the experimentation process

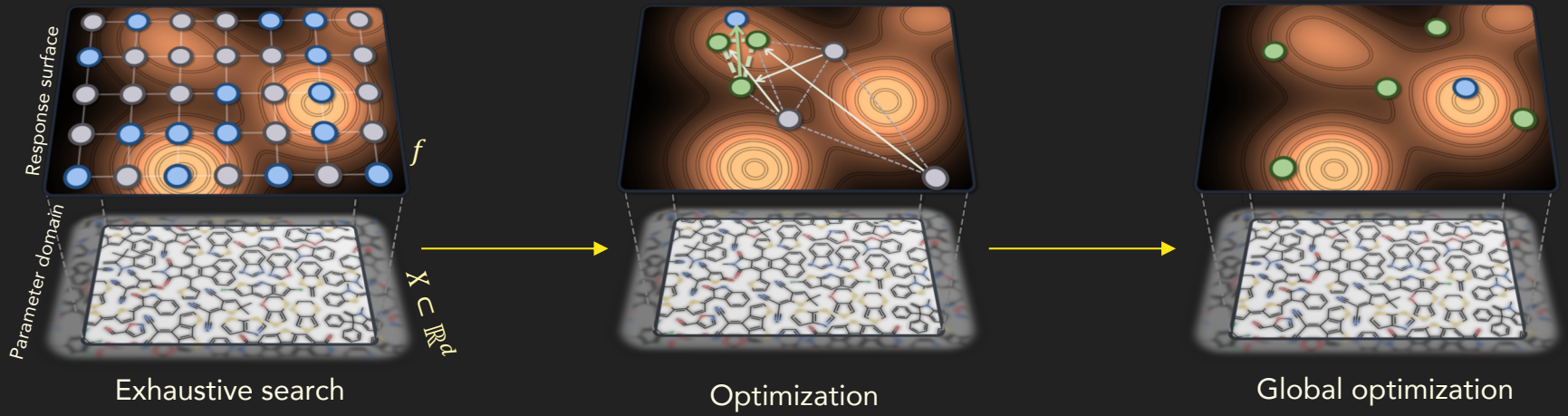
Alternative approaches

- formulate experiment planning as an optimization problem

$$x^* = \underset{x \in X \subset \mathbb{R}^d}{\operatorname{argmin}} f(x)$$

Assumptions about f:

- evaluations expensive (take minutes, hours, days)
- evaluations are noisy
- f is mostly well-behaved
- f is defined on a moderately large space ($d \leq 20$)

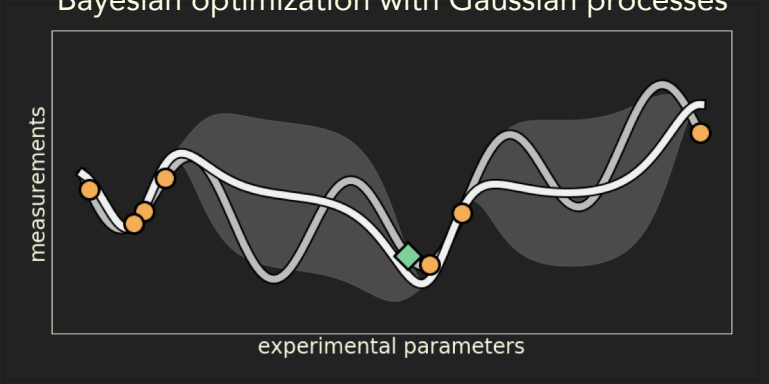


Bayesian optimization

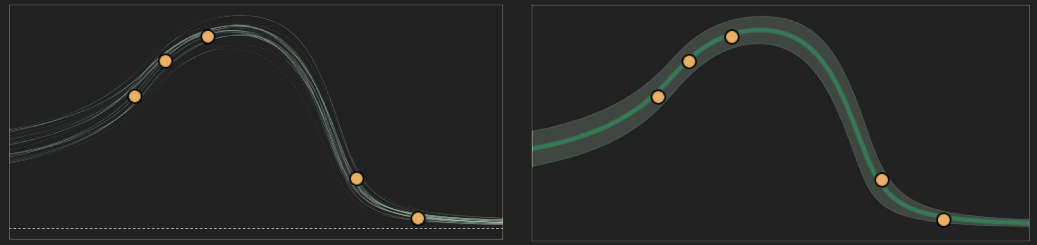
Bayesian optimization relies on
probabilistic universal function approximators.

The *true response surface* is modelled as the *maximum likelihood estimate* of the *distribution of functions.*

Bayesian optimization with Gaussian processes



Regression with a Bayesian neural network



individual samples

average prediction

Assumptions about f:

- evaluations expensive (minutes, hours, days)
- evaluations are noisy
- f is mostly well-behaved
- f is defined on a moderately large space ($d \leq 20$)

Bayesian optimization

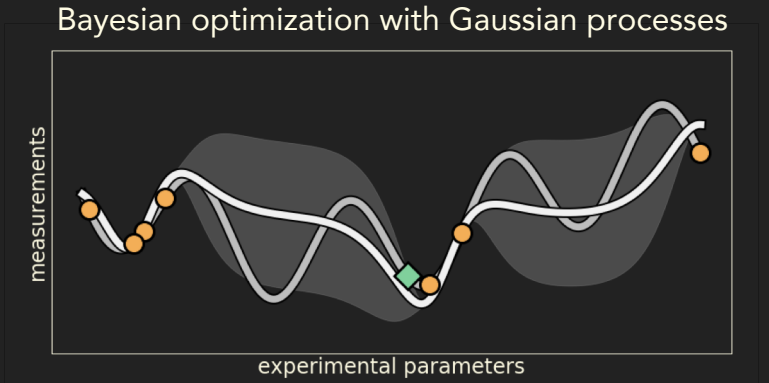
(i). Construct a surrogate using a model which provides uncertainty information

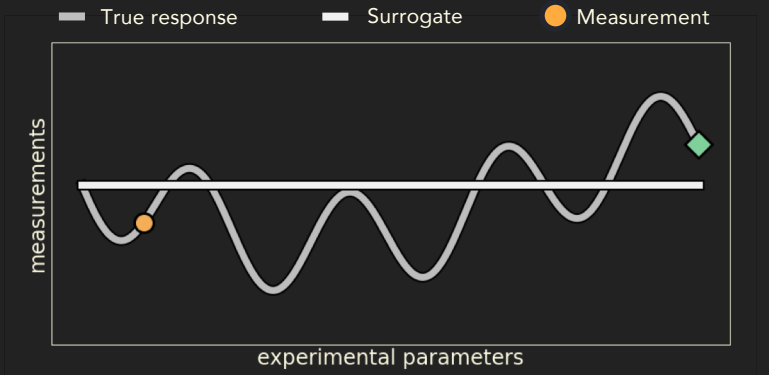
Gaussian processes, random forests, Bayesian neural networks, etc.

(ii). Formulate an acquisition function which balances space exploration and knowledge exploitation

expected improvement, upper confidence bound, entropy search

(iii). Speculate about the information gain when evaluating parameters and suggest the most promising

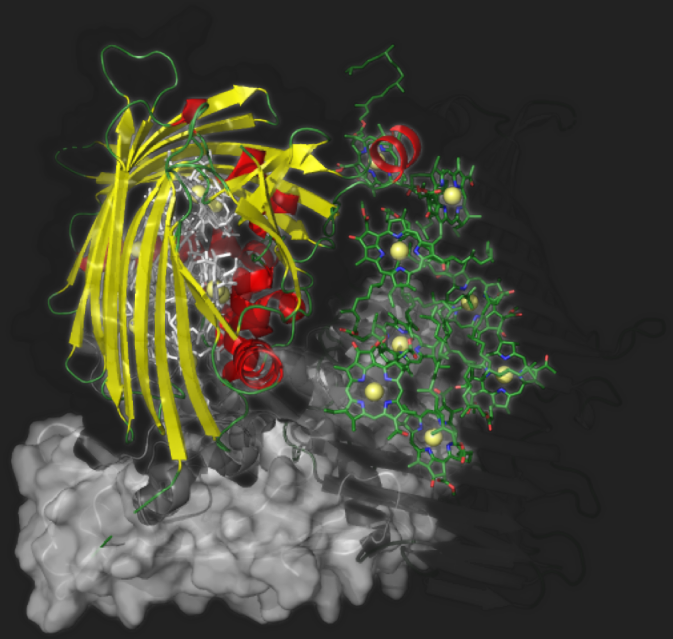




[1] Snoek, J., Larochelle, H., & Adams, R. P. (2012). Practical bayesian optimization of machine learning algorithms. In *Advances in neural information processing systems* (pp. 2951-2959).
[2] Frazier, Peter I. "A tutorial on Bayesian optimization." *arXiv preprint arXiv:1807.02811* (2018).
[3] Hutter, Frank, Holger H. Hoos, and Kevin Leyton-Brown. "Sequential model-based optimization for general algorithm configuration." *International Conference on Learning and Intelligent Optimization*. Springer, Berlin, Heidelberg, 2011.

A brief introduction to metadynamics

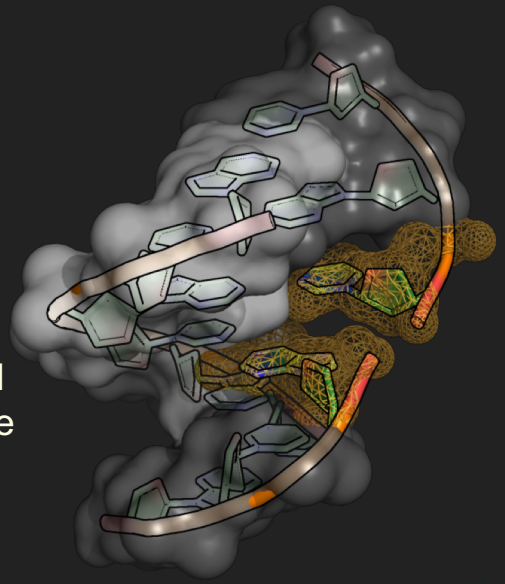
Molecular dynamics is a computational approach to simulate the dynamics of *many-particle systems*, e.g. biologically relevant protein complexes at atomic resolution.



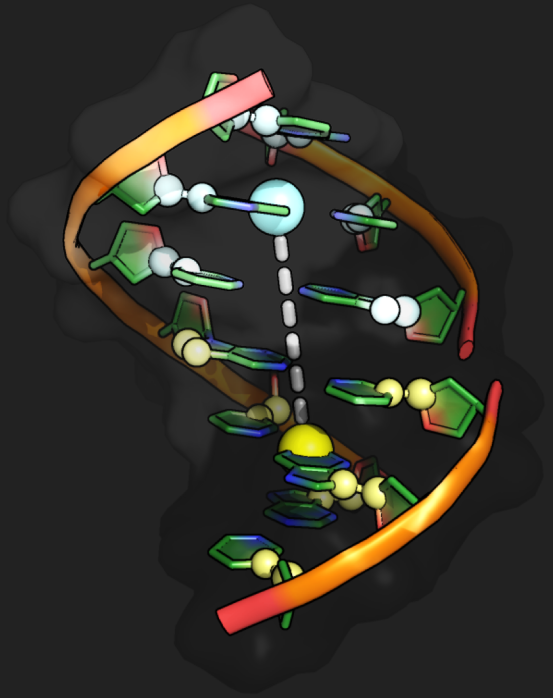
Typically 100,000s atoms and more than 10^9 integration steps

$$\boldsymbol{F}(\boldsymbol{r}) = -\nabla U(\boldsymbol{r}) = m\dot{\boldsymbol{v}}(\boldsymbol{t})$$
$$\boldsymbol{v}(t) = \dot{\boldsymbol{r}}(t)$$

Metadynamics describes an enhanced sampling method to reduce the runtime of molecular dynamics simulations.

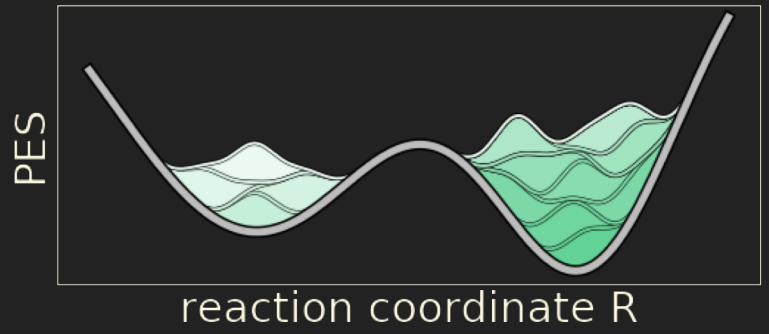


A brief introduction to metadynamics



Exploration of the potential energy surface (PES) is encouraged by adding penalty terms to previously visited regions.

$$\mathrm{PES}_{\mathrm{eff}}(\boldsymbol{r}, t) = \mathrm{PES}(\boldsymbol{r}) + \int_0^t dt' \, \omega \exp\left(-\frac{\boldsymbol{R}(\boldsymbol{r}) - \boldsymbol{R}(\boldsymbol{r}(t'))^2}{2\,\sigma^2}\right)$$



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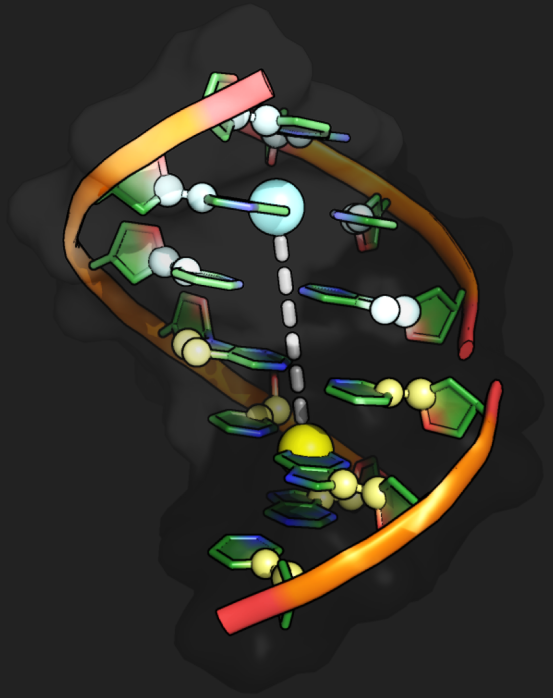
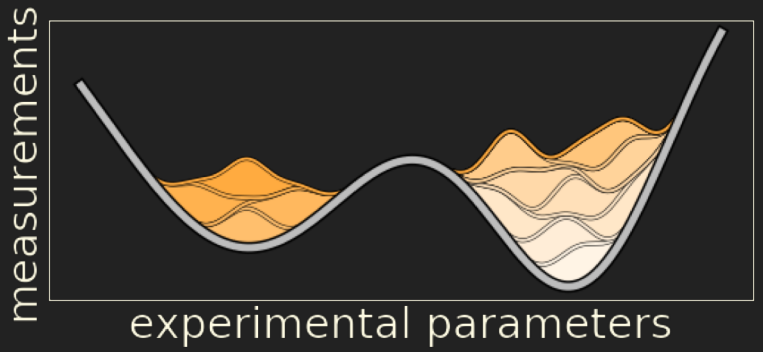


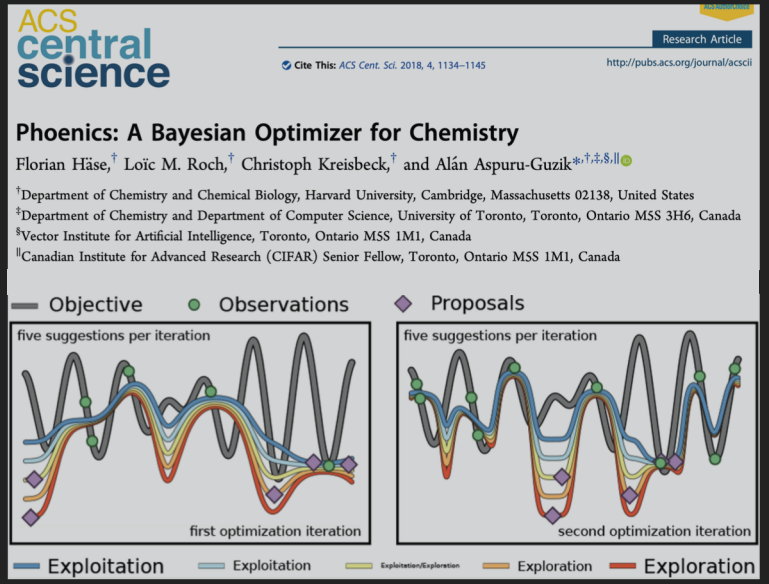
Can we use similar ideas to determine the optimal parameters for an experiment?

$$\mathrm{PES}_{\mathrm{eff}}(\boldsymbol{r},t) = \mathrm{PES}(\boldsymbol{r}) + \int_0^t dt' \, \omega \exp\left(-\frac{\boldsymbol{R}(\boldsymbol{r}) - \boldsymbol{R}(\boldsymbol{r}(t'))^2}{2\,\sigma^2}\right)$$

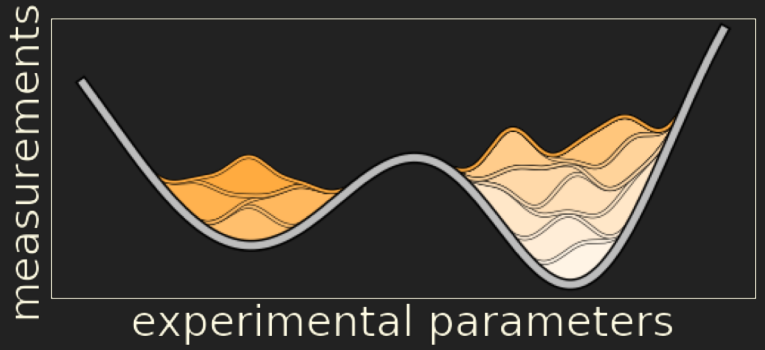


Phoenics: A Bayesian optimizer for chemistry

Phoenics implements global optimization by combining ideas from Bayesian optimization with concepts from Bayesian kernel density estimation.



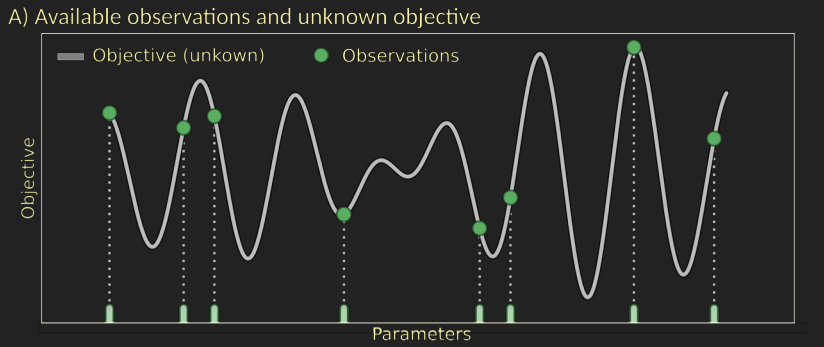
- natively supports batch optimization
- favorable linear scaling with the number of measurements

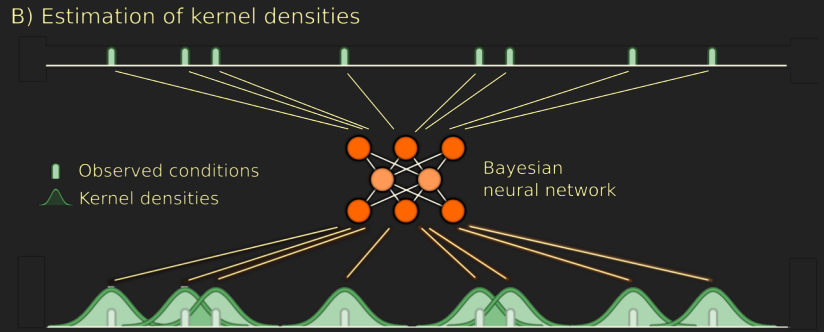


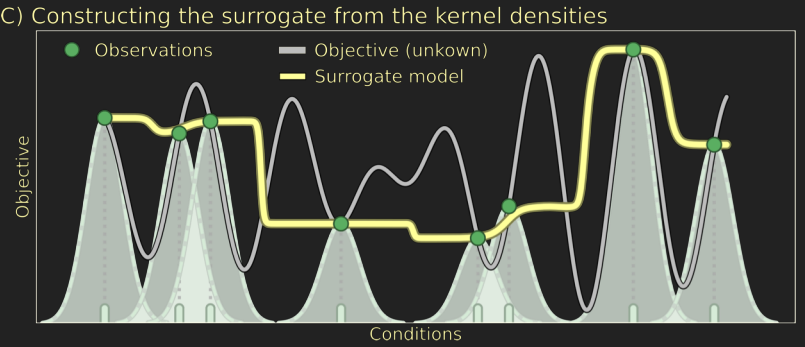
Häse et al. *ACS Central Science* 4.9 (2018): 1134-1145.

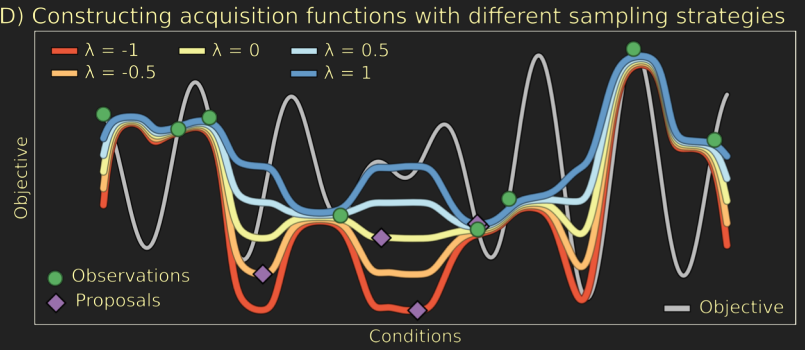
Phoenics: A Bayesian optimizer for chemistry

Phoenics implements a four-step process to propose experimental parameters for future evaluation.









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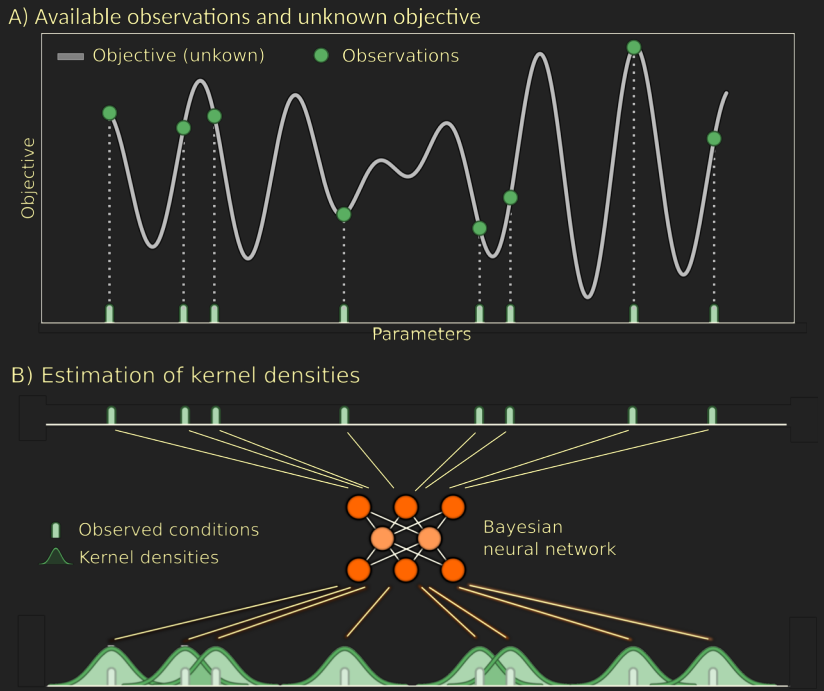
Phoenics: A Bayesian optimizer for chemistry

Phoenics estimates parameter kernel densities using a Bayesian neural network:



Posterior kernel densities are modeled with variational probability distributions, where

$$p(\boldsymbol{x}_i \,|\theta, \{\boldsymbol{x}_0, \ldots, \boldsymbol{x}_n\}) = \mathrm{Normal}(\boldsymbol{x}_i \mid \mathrm{BNN}(\boldsymbol{x}_i; \boldsymbol{\theta}), \sigma^2)$$

with

$$\phi_1(\boldsymbol{x}_i) = \tanh(\boldsymbol{x}_i \cdot \boldsymbol{w}_0 + \boldsymbol{b}_0)$$

$$\phi_2(\phi_1) = \tanh(\phi_1 \cdot \boldsymbol{w}_1 + \boldsymbol{b}_1)$$

$$\mathrm{BNN}(\phi_2) = \mathrm{sigmoid}(\phi_2 \cdot \boldsymbol{w}_2 + \boldsymbol{b}_2)$$

and priors are chosen as

$$\boldsymbol{w}_k \sim \mathrm{Normal}(0, \mathrm{I}) \qquad b_k \sim \mathrm{Normal}(0, \mathrm{I})$$

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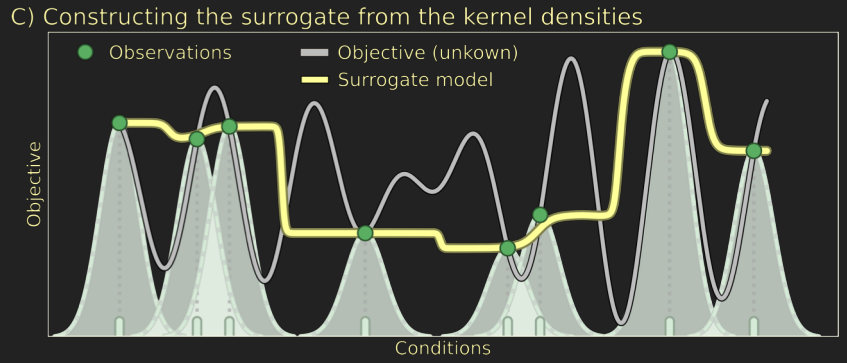
Phoenics: A Bayesian optimizer for chemistry

The kernel densities provide the basis for the surrogate.

Given a set of *n* observations

$$D_n = \{(\boldsymbol{x}_k, f_k)\}_{k=1}^{n}$$



Note, that

$$\sigma^2 = {}^{1}/_{\tau}, \qquad \tau \sim \mathrm{Gamma}(\mathrm{n}^2, 1)$$

the surrogate is constructed similar to a *partition function*

$$\alpha(\boldsymbol{x}) = \frac{\sum_{k=1}^{n} f_k p_k(\boldsymbol{x})}{\sum_{k=1}^{n} p_k(\boldsymbol{x})}$$

where

$$p_k(\boldsymbol{x}) = p_k(\boldsymbol{x}|\theta, \{\boldsymbol{x}_0, \ldots, \boldsymbol{x}_n\}) = \mathrm{Normal}(\boldsymbol{x}_i \mid \mathrm{BNN}(\boldsymbol{x}_i; \boldsymbol{\theta}), \sigma^2)$$

and

$$\alpha(\boldsymbol{x}) \cong p_k(\boldsymbol{x}) \quad \text{for} \quad \boldsymbol{x} \cong \boldsymbol{x}_k$$

where the approximation becomes exact in the limit of infinitely many distinct observations.

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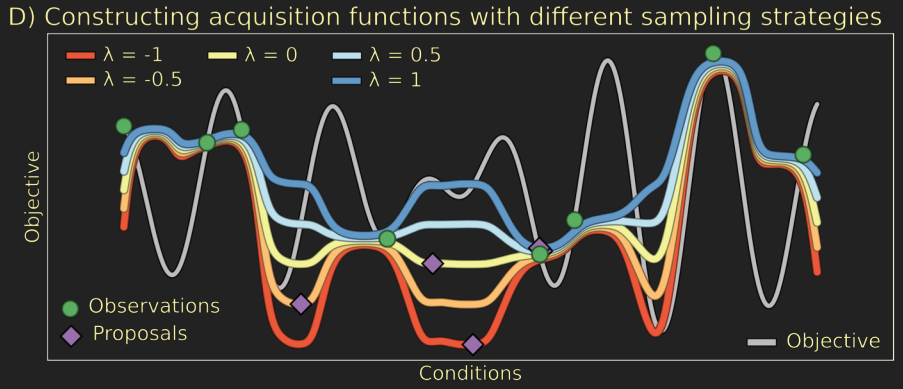
Phoenics: A Bayesian optimizer for chemistry

The kernel densities provide the basis for the surrogate.



Without any prior knowledge, the ***optimum*** $\boldsymbol{x}^*$ could be located ***anywhere*** in the domain $\boldsymbol{X} \subset \mathbb{R}^{\boldsymbol{d}}$ with ***equal probability***.

$$p_{\text{prior}}\,(\boldsymbol{x} = \boldsymbol{x}^*) = {}^{1}/_{\text{Volume}(X)} = p_{\text{uniform}}(\boldsymbol{x})$$

The surrogate is inaccurate in low-density regions

$$\alpha(\boldsymbol{x}) = \frac{\sum_{k=1}^{n} f_k p_k(\boldsymbol{x})}{\sum_{k=1}^{n} p_k(\boldsymbol{x})}$$

Confidence can be built into the surrogate by adding $p_{\text{uniform}}(\boldsymbol{x})$ to indicate this lack of information

$$\alpha(\boldsymbol{x}) = \frac{\sum_{k=1}^{n} f_k p_k(\boldsymbol{x}) + \lambda\, p_{\text{uniform}}(\boldsymbol{x})}{\sum_{k=1}^{n} p_k(\boldsymbol{x}) + p_{\text{uniform}}\,(\boldsymbol{x})}$$

The number of evaluations of the Bayesian network is independent of the number of evaluations of this acquisition function.

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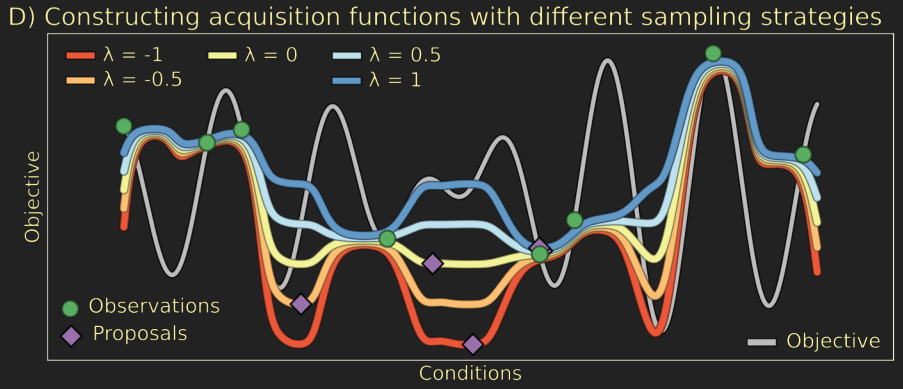

Suggesting parameters with different sampling strategies, e.g. $\lambda \in \{-1, 0, 1\}$, only requires one kernel density estimation.

The surrogate now contains a sampling parameter $\lambda \in \mathbb{R}$ indicating the trust we put in the prior

$$\alpha(\boldsymbol{x}) = \frac{\sum_{k=1}^{n} f_k p_k(\boldsymbol{x}) + \lambda\, p_{\text{uniform}}(\boldsymbol{x})}{\sum_{k=1}^{n} p_k(\boldsymbol{x}) + p_{\text{uniform}}\,(\boldsymbol{x})}$$

When suggesting parameters based on the global optimum of the surrogate $\alpha(\boldsymbol{x})$:

- $\lambda < 0$ biases towards explorative behavior
- $\lambda > 0$ biases towards exploitative behavior

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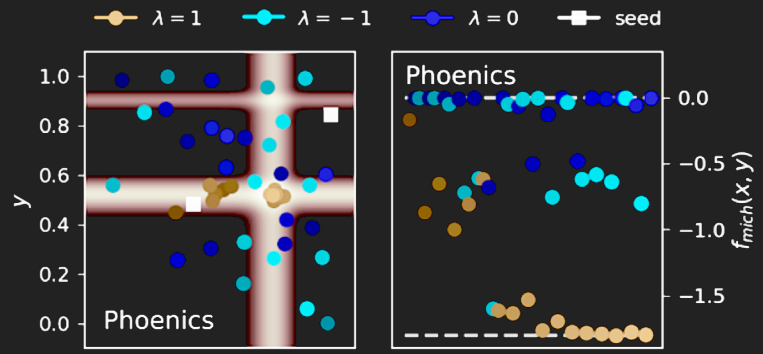
Break

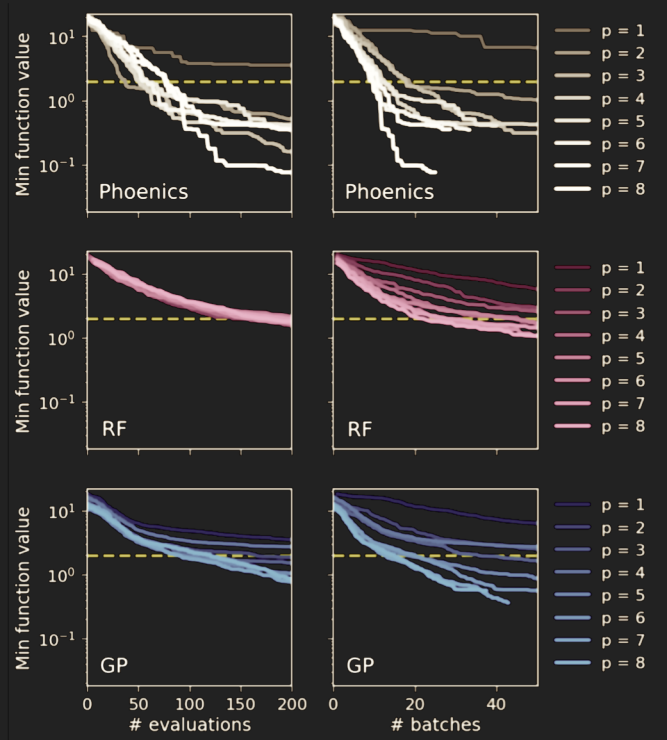
Performance on analytic benchmarks

Benchmarks on 15 different analytic functions in two and higher dimensions

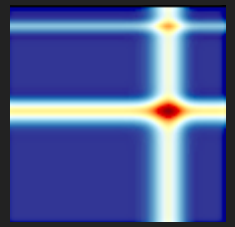
- Compared to *spearmint* (GP), *SMAC* (RF), *particle swarm search* and *CMA-ES* (not shown)
- only slightly outperformed by *spearmint* on purely convex functions



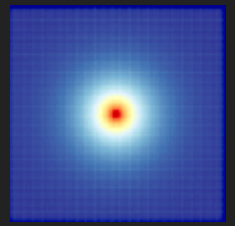
Optimization on the two-dimensional *Michalewicz* function



Optimization on the two-dimensional *Ackley path* function



Michalewicz function



Ackley path function

Häse et al. *ACS Central Science* 4.9 (2018): 1134-1145.

(i) Chemical oscillators

Scheme 1. Subreactions of the Belousov–Zhabotinsky Reaction[78]

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$$2\,Ce^{IV} + 2\,CH_2(COOH)_2 + BrCH(COOH)_2 + HBrO + 2\,H_2O \longrightarrow 2\,Ce^{III} + 2\,Br^- + 3\,HOCH(COOH)_2 + 4\,H^+$$

Goal: finding parameters which yield a desired dynamic behavior

The reaction dynamics can be described with a set of coupled non-linear different equations (*Oregonator*)* with 11 parameters

$$\frac{dX}{dt} = k_1 AY - k_2 XY + k_3 BX - 2k_4 X^2$$

$$\frac{dY}{dt} = -k_1 AY - k_2 XY + f k_5 Z$$

$$\frac{dZ}{dt} = k_3 BX - k_5 Z$$

Non-dimensionalizing these equations yields three effective concentrations (α, η, ρ) and 4 independent effective reaction rates (s, q, w, f)

$$\frac{d\alpha}{d\tau} = s\,(\eta - \eta\alpha + \alpha - q\alpha^2)$$

$$\frac{d\eta}{d\tau} = s^{-1}(-\eta - \eta\alpha + f\rho)$$

$$\frac{d\rho}{d\tau} = w\,(\alpha - \rho)$$

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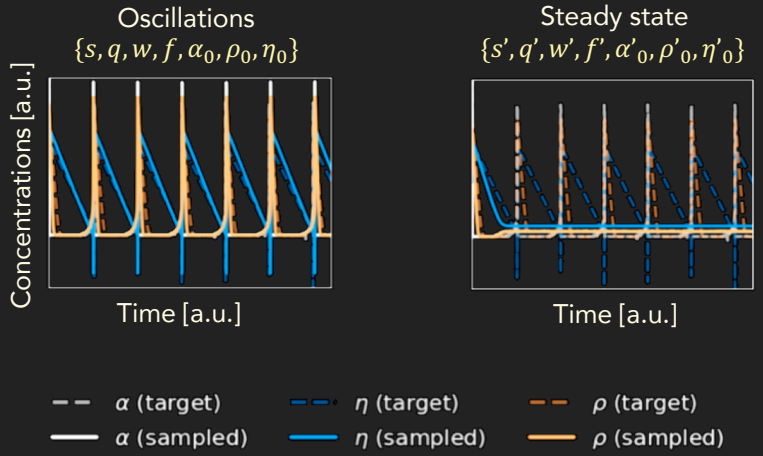

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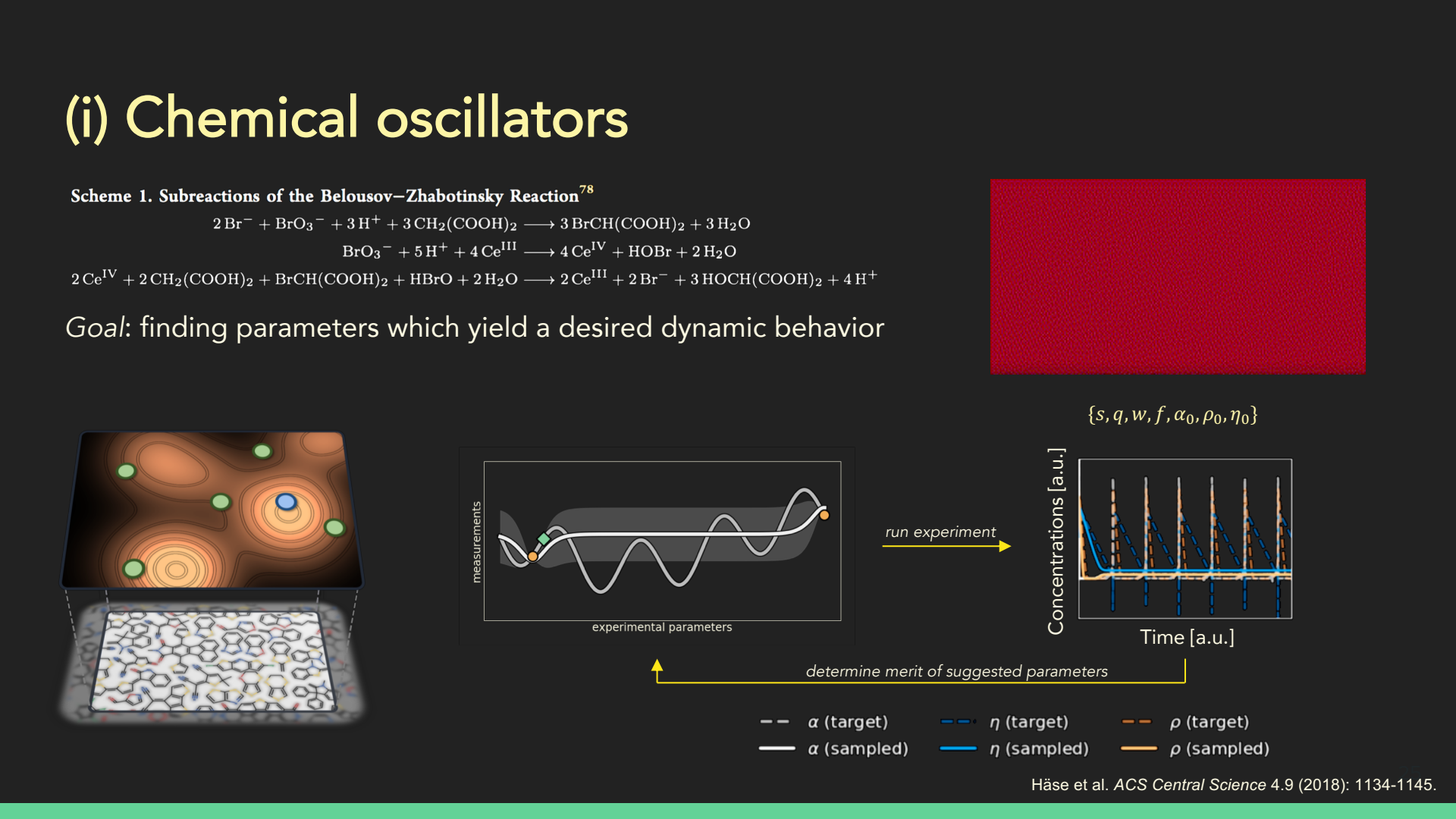

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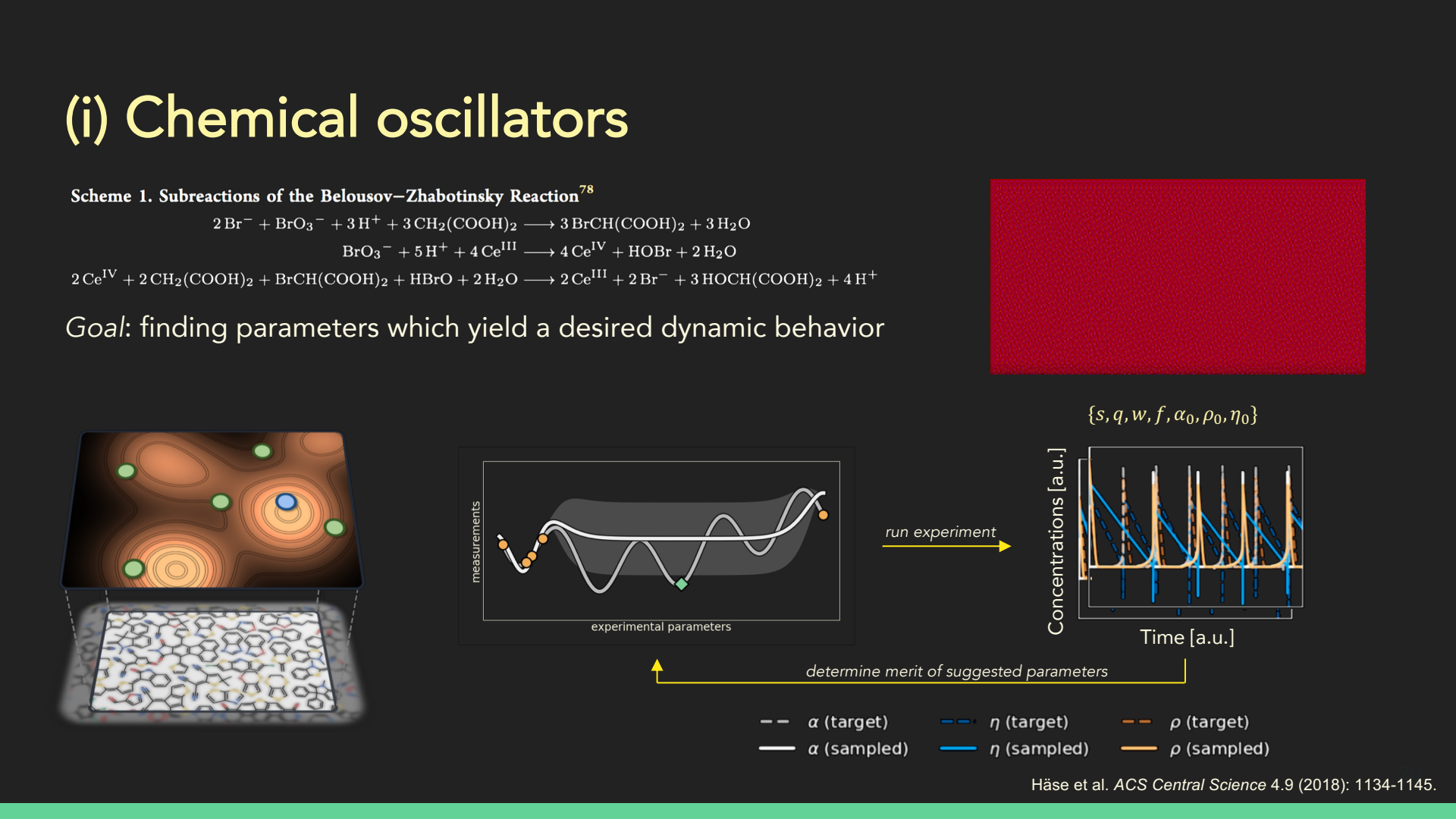

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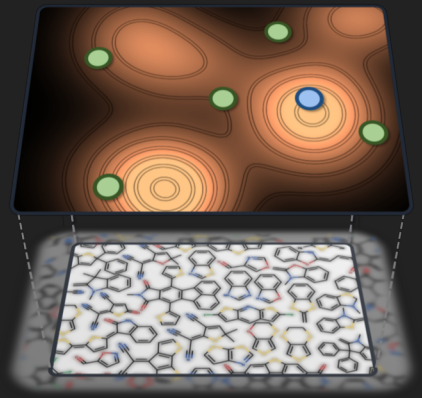
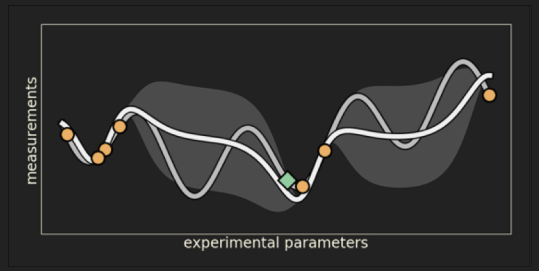
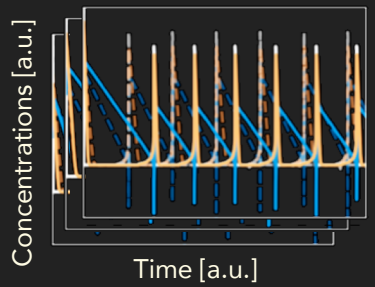




run experiment

$\{s, q, w, f, \alpha_0, \rho_0, \eta_0\}$



determine merit of suggested parameters

α (target) α (sampled) η (target) η (sampled) ρ (target) ρ (sampled)

Häse et al. *ACS Central Science* 4.9 (2018): 1134-1145.

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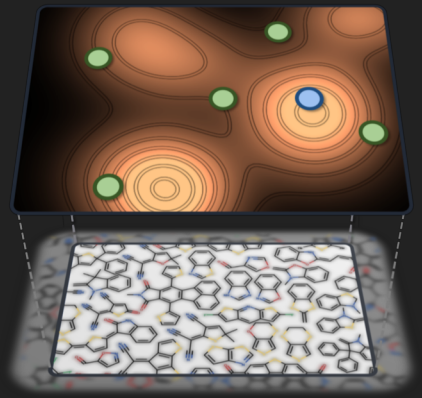

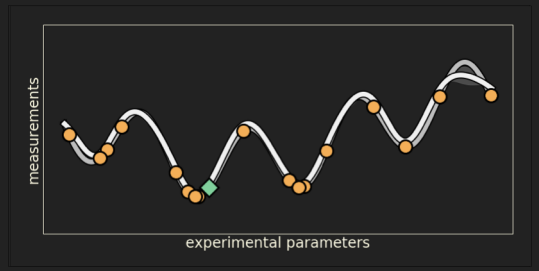

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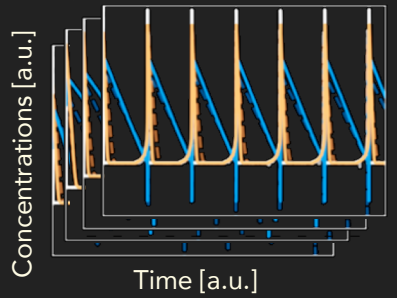

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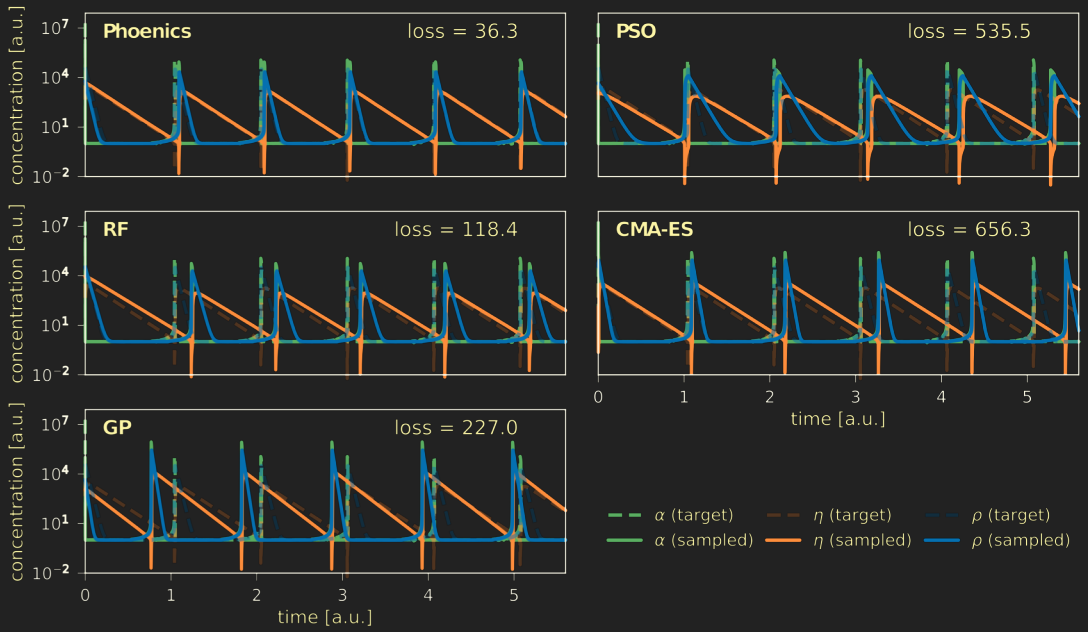

Executed 50 independent runs with a budget of 150 evaluations per run:

- Each set of parameters was integrated for 10^7 steps with adaptive Runge-Kutta scheme
- Compared to *spearmint* (GP), *SMAC* (RF), *particle swarm search* (PSO) and *CMA-ES*
- Inspected traces with best agreement across all runs for each method

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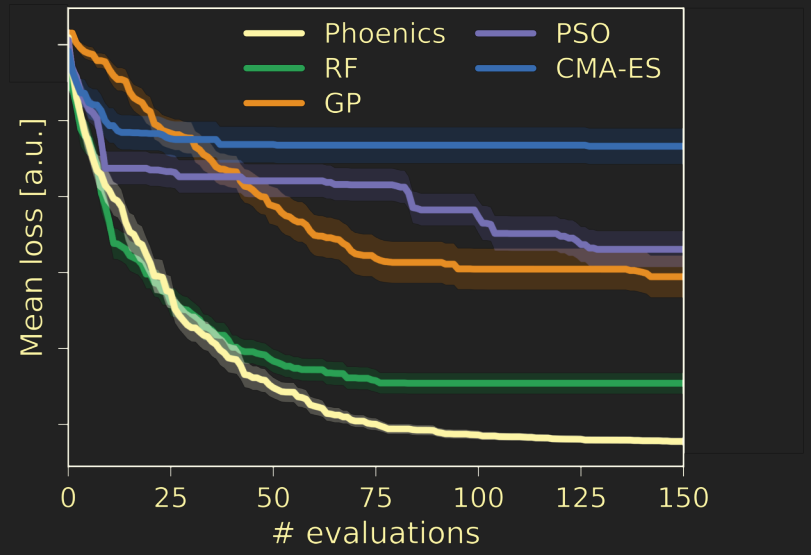

Executed 50 independent runs with a budget of 150 evaluations per run:

- Each set of parameters was integrated for 10^7 steps with adaptive Runge-Kutta scheme
- Compared to *spearmint* (GP), *SMAC* (RF), *particle swarm search* (PSO) and *CMA-ES*
- Average performance of tested optimization algorithms

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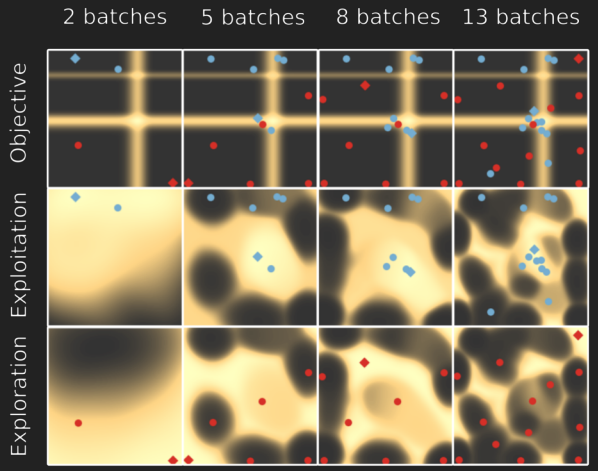
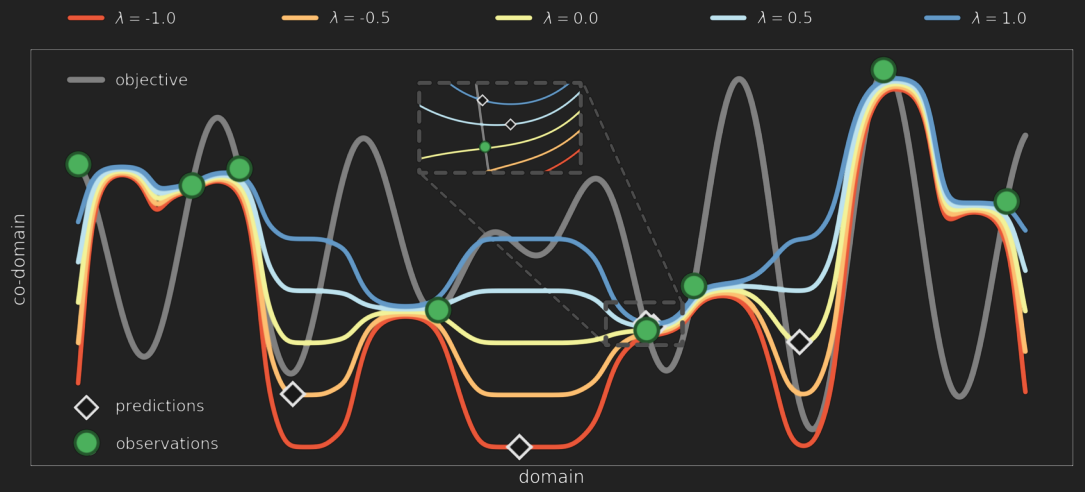
Summary

Phoenics is a global optimization algorithm inspired by *metadynamics*, which combines ideas from *Bayesian optimization* with concepts from *Bayesian kernel density estimation*.





Häse et al. *ACS Central Science* 4.9 (2018): 1134-1145.

Acknowledgments

Aspuru-Guzik group

Loïc Roch
Christoph Kreisbeck
Teresa Tamayo-Mendoza
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Brabec group

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Thomas Heumüller
Christoph Brabec

Hein group

Lars Yunker
Elena Liles
Sebastian Steiner
Jason Hein

Berlinguette group

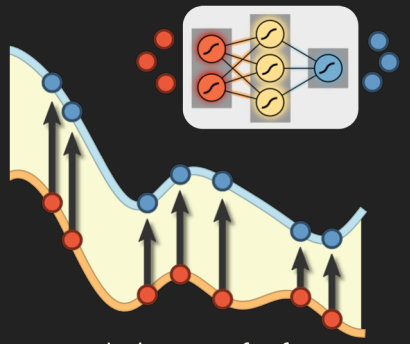
Fraser Parlane
Ben MacLeod
Maddie Eghtesad
Curtis Berlinguette

Aspuru-Guzik group (incomplete)

Discussion Points

Providing domain knowledge

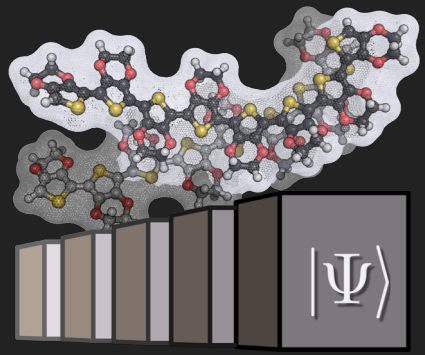
- How can we exploit knowledge acquired from related experiments?
- How can we provide scientific expectations?



Knowledge transfer from related experiments

Interpreting algorithmic choices

- Can we improve on existing methods for analyzing collected experimental data to simplify its interpretation and enable the formulation of (new) scientific concepts?

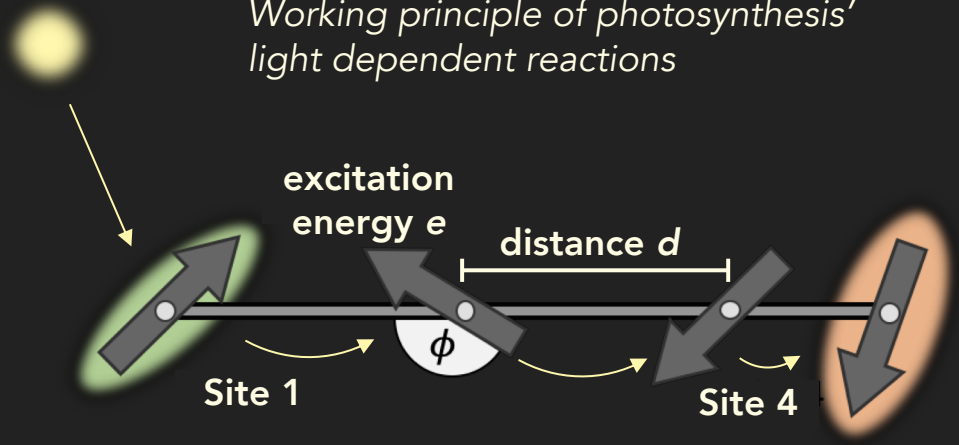


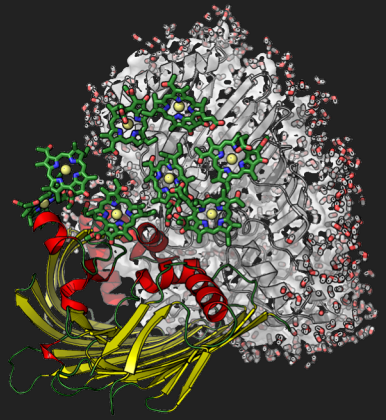
Ab initio calculations of materials properties

(ii) Designing systems for excitation energy transport

- incoming photons locally excite molecular pigments
- excitation is transferred to nearby pigments

Working principle of photosynthesis' light dependent reactions



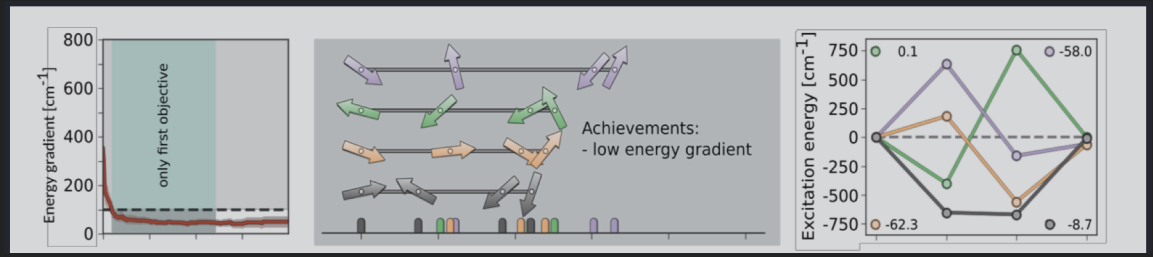


Each system is characterized by:
- **4** transition dipole angles
- **3** excitation energies
- **3** distances between pigments

Total number of parameters: **10**

Häse et al. *Chemical Science 9* (2018): 7642.

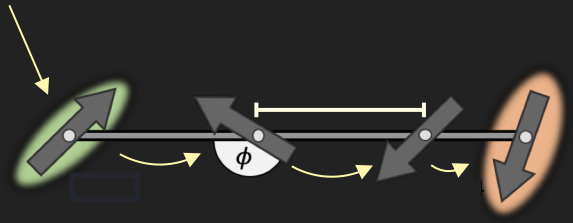
(ii) Designing systems for excitation energy transport



Goal of the optimization:

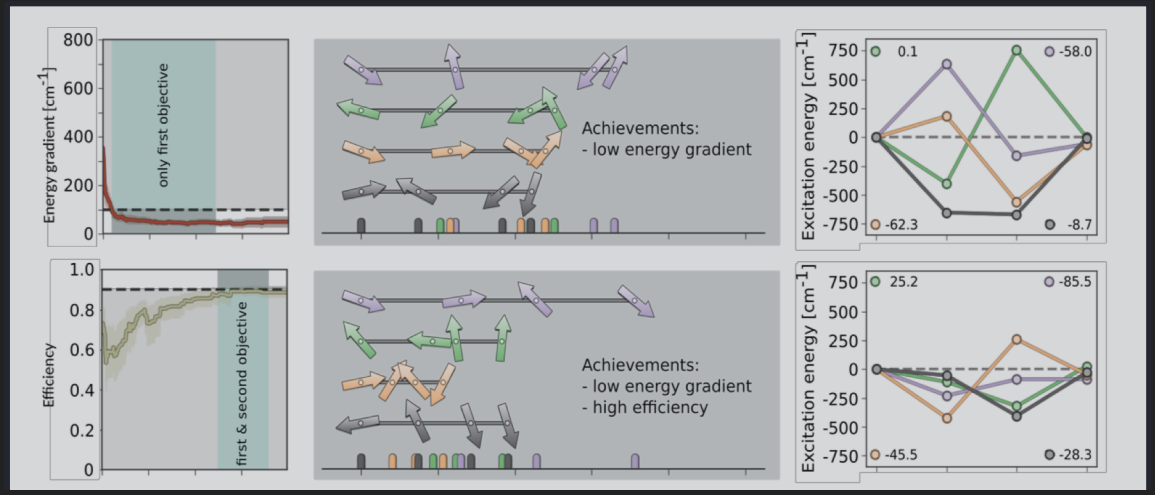
Small energy gradient

25 independent runs with
400 evaluations per run



Häse et al. *Chemical Science* 9 (2018): 7642.

(ii) Designing systems for excitation energy transport

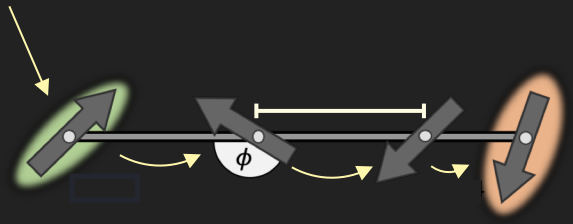


Goal of the optimization:

Small energy gradient

Large transfer efficiency

Chimera enables a priori multi-target optimization



Häse et al. *Chemical Science 9* (2018): 7642.

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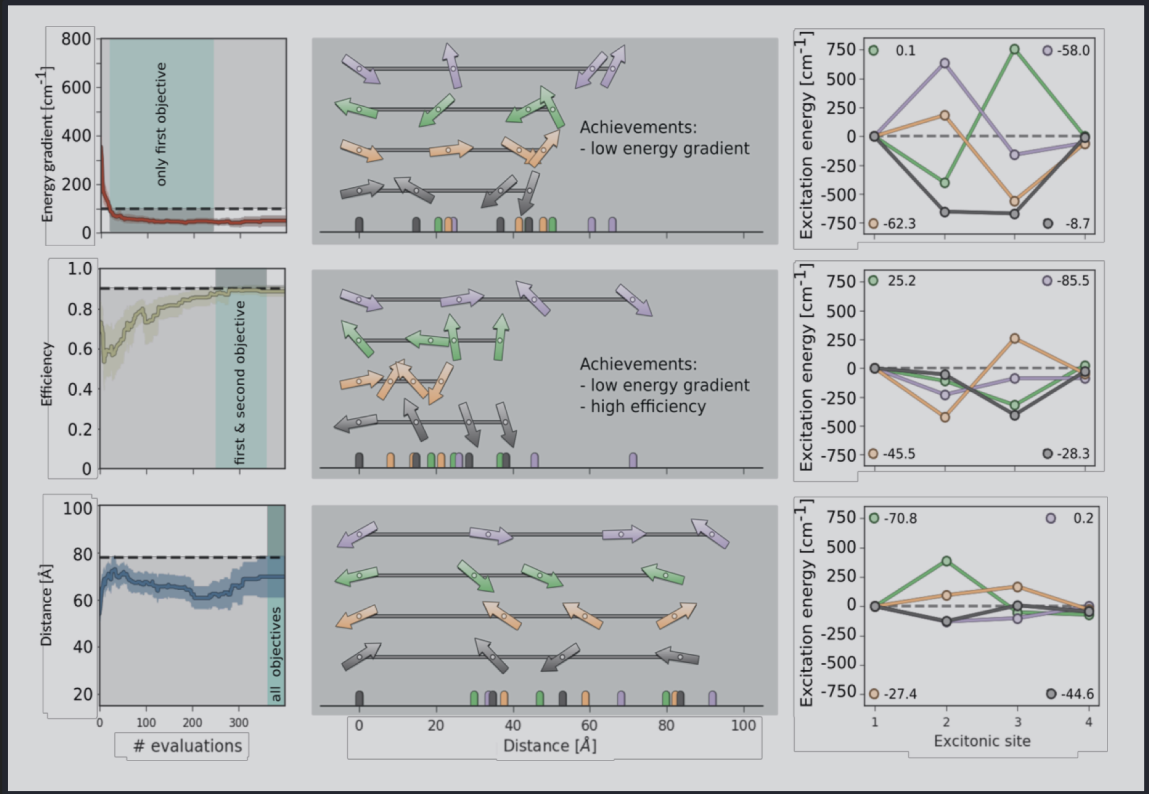


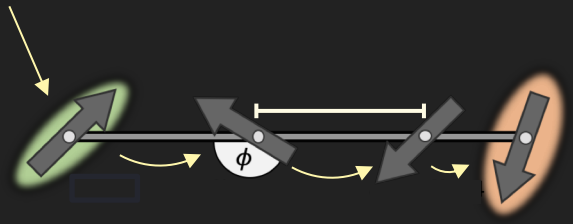
Goal of the optimization:

Small energy gradient

Large transfer efficiency

Large total distance

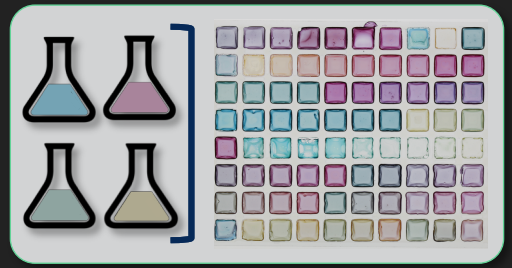
Chimera enables a priori multi-target optimization



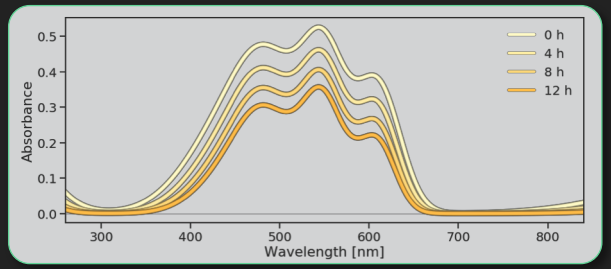
Häse et al. *Chemical Science 9* (2018): 7642.

(iii) Designing photostable OPV candidates

Goal: Identify blends for *organic photovoltaics* (OPVs) which do not degrade when exposed to sunlight.



Suggest polymer blend



Measure photo-stability

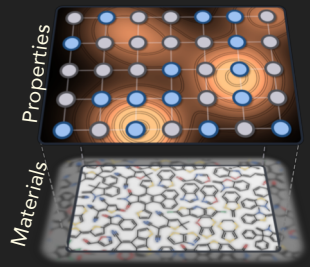
Direct integration of *Phoenics* with automated platform for OPV fabrication.

Experiments are conducted in Germany, but remotely controlled from Toronto.

ChemOS
SELF-DRIVING LABORATORIES

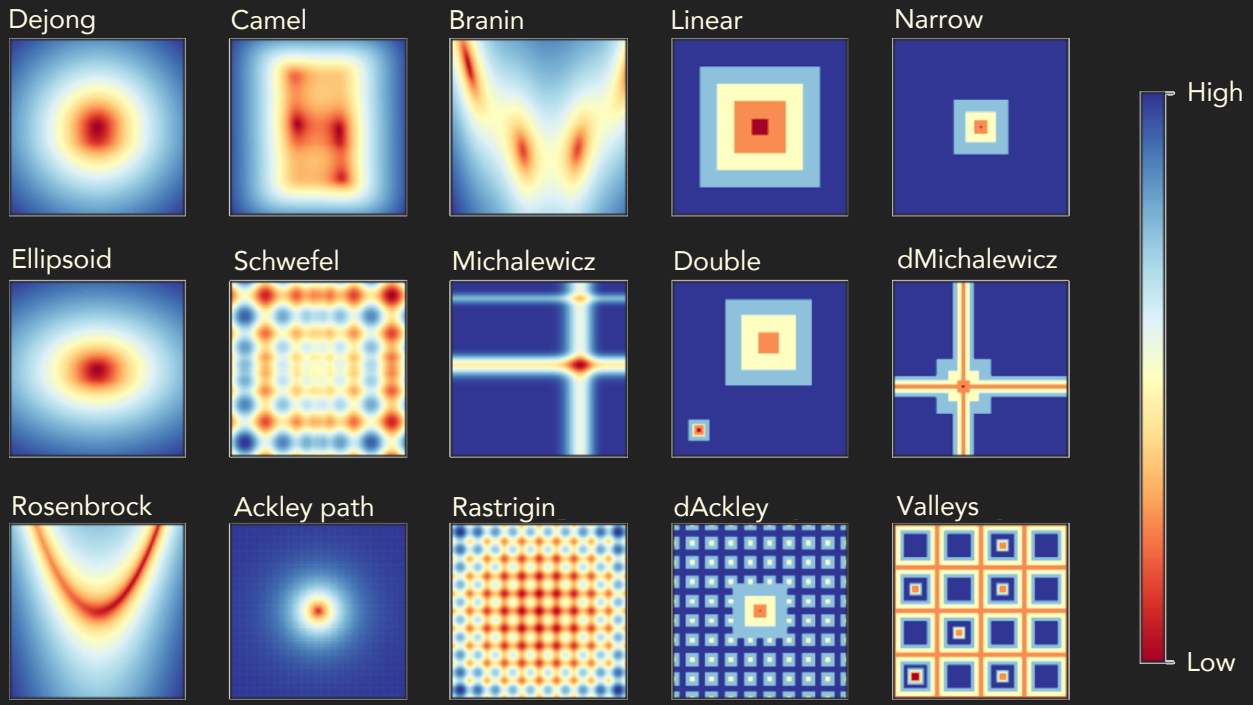
(iii) Designing photostable OPV candidates

High-throughput screening (HTS)



HTS		Phoenics
1022	*experiments*	30
2 blends/ week	*throughput*	9 blends/ week
15 mg/material 100 mL solvent	*consumption*	0.9 mg/material 6 mL solvent

Analytic benchmark functions



Performance on analytic benchmark functions