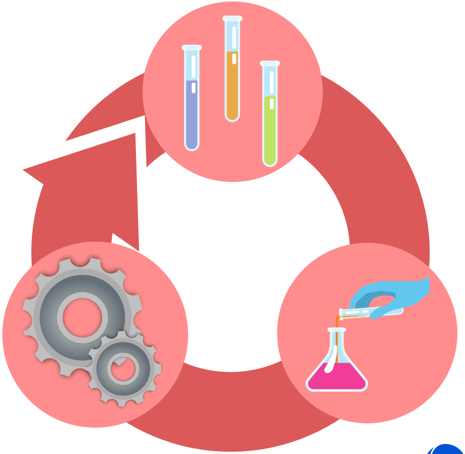
DeepMind

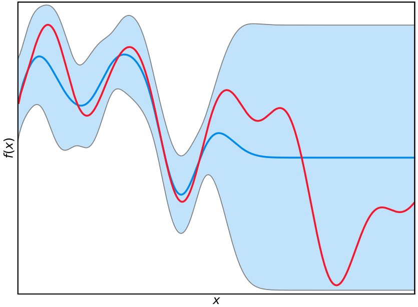
Scaling GP Optimization by Evaluating a Few Unique Candidates Multiple Times

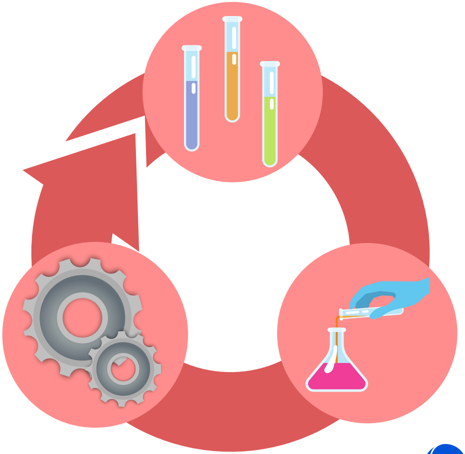
D. Calandriello, L. Carratino, A. Lazaric, M. Valko, L. Rosasco

Running example: optimizing a chemical mixture



Running example: optimizing a chemical mixture with GP-Opt





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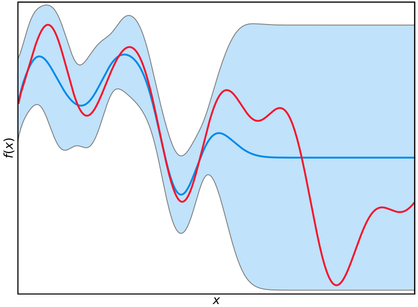
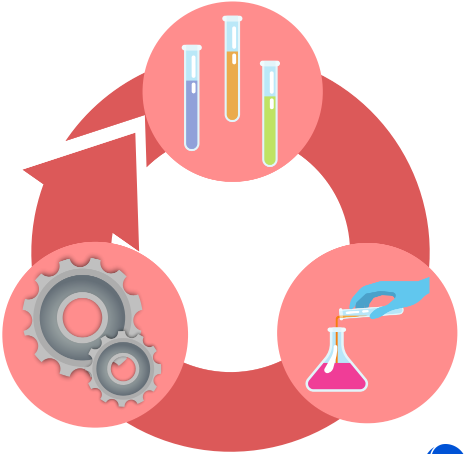


GP-Opt can balance exploration/exploitation



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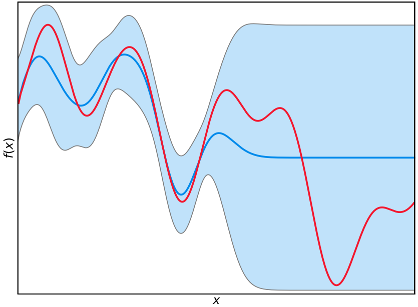
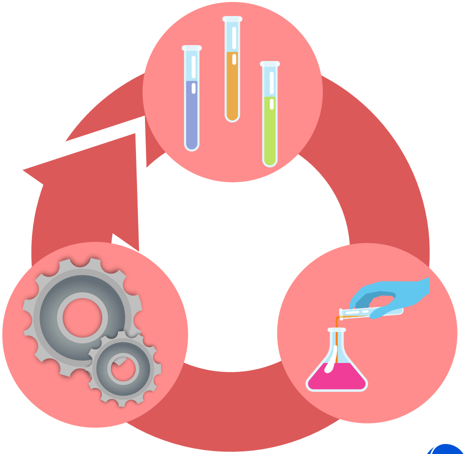


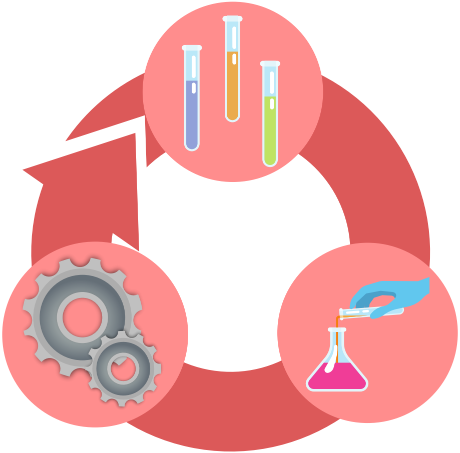
GP-Opt can balance exploration/exploitation but:

- poor experimental scalability (sequential feedback)
- high computational complexity (slow model update)



One easy trick to scale

Keep choosing and evaluating the same candidate



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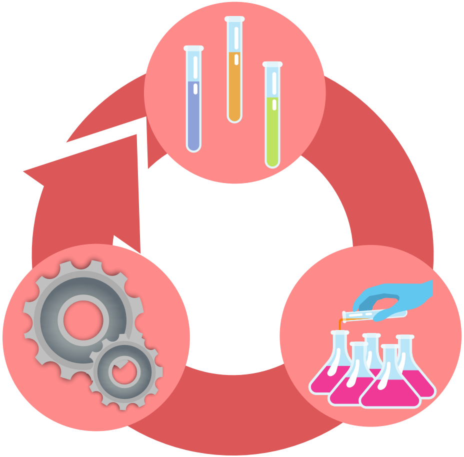
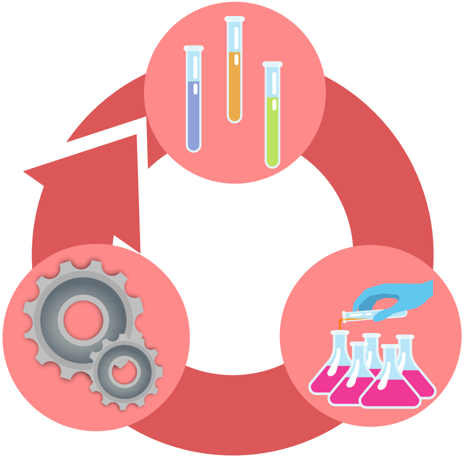


One easy trick to scale

Keep choosing and evaluating the same candidate but **not for too long!**



Too late

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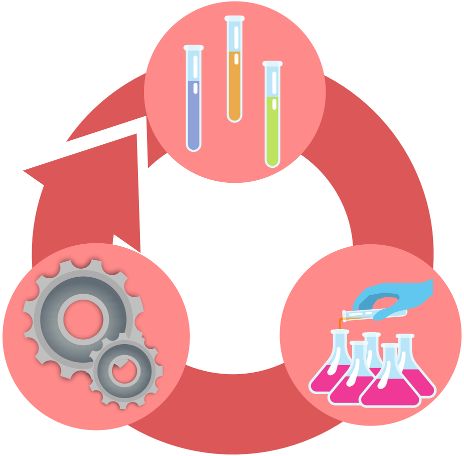

Too early

Too late

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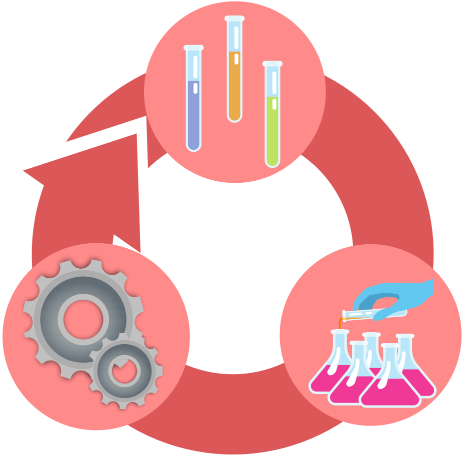

Too early

"Just right"

Too late

Mini-META: making GP-Opt scalable

Contribution: an automatic “just right” detector to choose when to switch candidates

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  - Unlocks experimental parallelism
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Mini-META: making GP-Opt scalable

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Weaknesses:

- Cannot be applied when repeated choices are not possible (e.g., personalized news)
- Not very useful for noiseless scenarios

Bonus properties: few unique candidates

Low number of switches + selecting same candidate = few unique candidates in the GP

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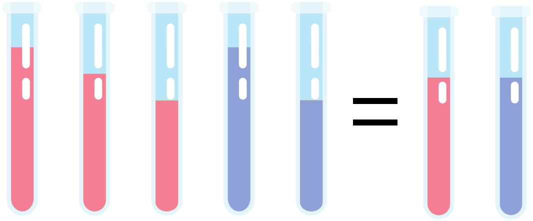

GP reformulation, not GP approximation!

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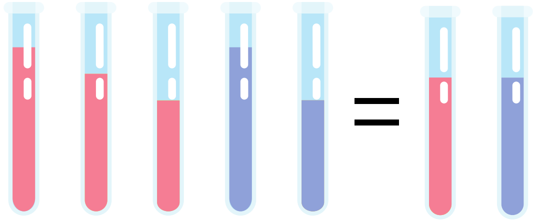

GP reformulation, not GP approximation!

vs.

Existing scalable GP-Opt methods [5, 3, 1, 4]

Randomized GP approximation

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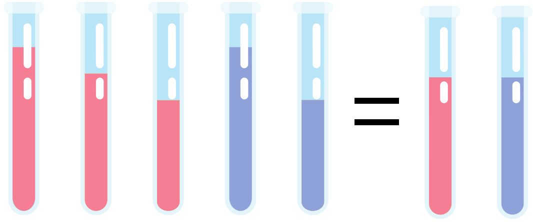

vs.

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GP reformulation, not GP approximation!

Randomized GP approximation

Special case of stratified sampling [2], inapplicable to GPs with i.i.d. samples

Bonus property: low setup costs

vs.

Wrapping up

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See us at the poster/virtual session to check if your GP-Opt algorithm can be Mini-fied!

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Thanks!

[1] Maximilian Balandat et al. "Botorch: Programmable bayesian optimization in pytorch". In: *arXiv preprint arXiv:1910.06403* (2019).

[2] Mickaël Binois et al. "Replication or exploration? Sequential design for stochastic simulation experiments". In: *Technometrics* 61.1 (2019), pp. 7–23.

[3] Daniele Calandriello et al. "Near-linear Time Gaussian Process Optimization with Adaptive Batching and Resparsification". In: *ICML*. 2020.

[4] Jacob R Gardner et al. "Gpytorch: Blackbox matrix-matrix Gaussian process inference with GPU acceleration". In: *NeurIPS* (2018).

[5] Mojmir Mutny et al. "Efficient High Dimensional Bayesian Optimization with Additivity and Quadrature Fourier Features". In: *NeurIPS*. 2018.

[6] Niranjan Srinivas et al. "Gaussian Process Optimization in the Bandit Setting: No Regret and Experimental Design". In: *ICML*. 2010.

[7] Ziyu Wang et al. "Bayesian multi-scale optimistic optimization". In: *Artificial Intelligence and Statistics*. 2014, pp. 1005–1014.