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Knowledgeable Language Models as Black-Box Optimizers for Personalized Medicine

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Personalized Medicine as an Optimization Problem



Design a **treatment strategy** to optimally treat a **patient**



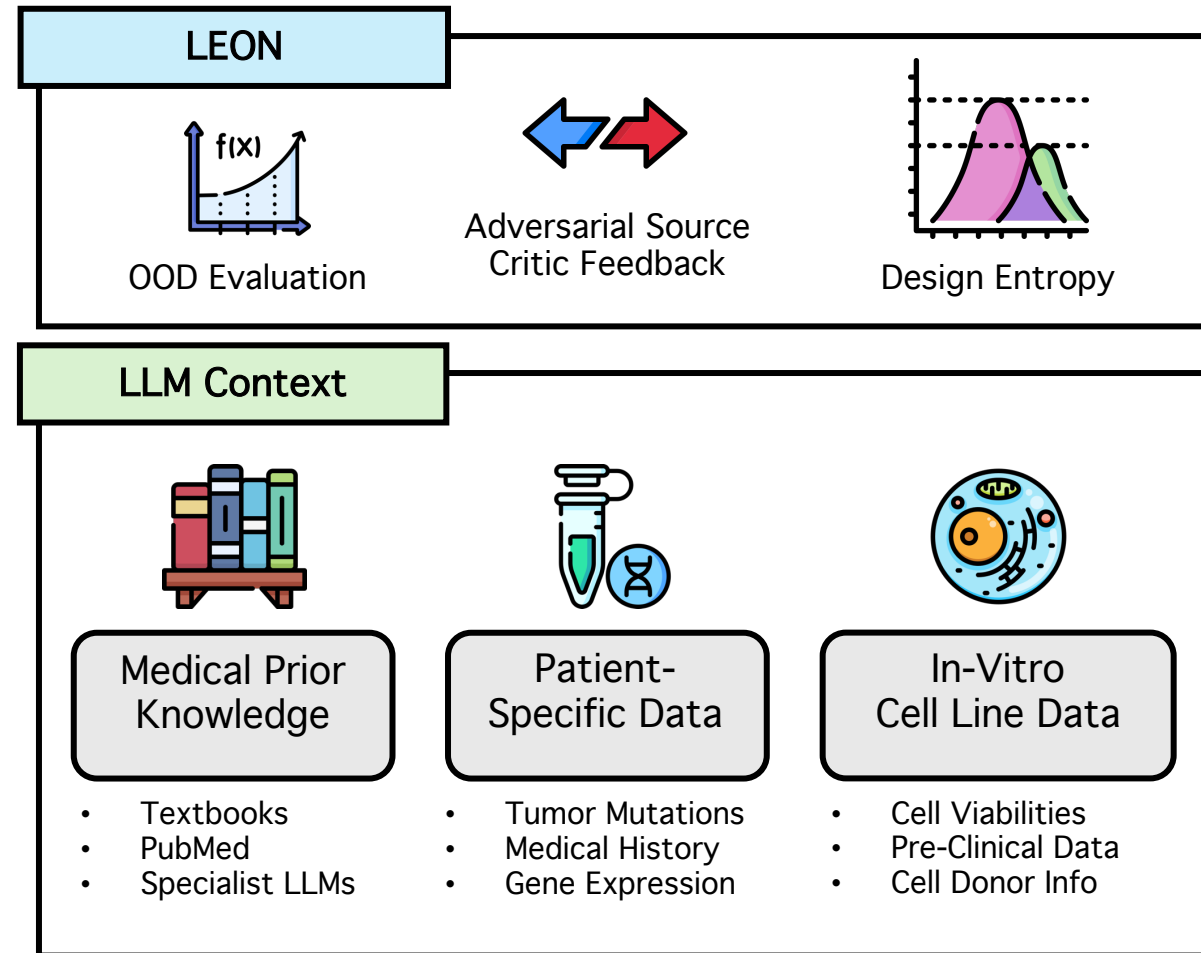
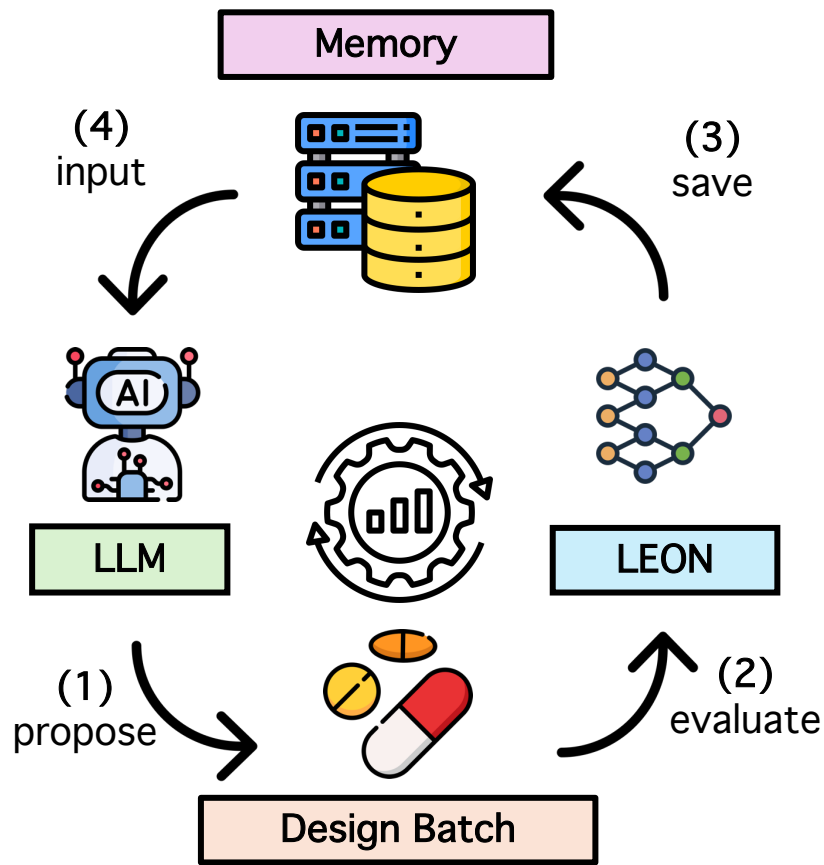
Design a **medication dose** to optimally treat a **disease**

We can't test all possible treatments and doses!

Our work: Let's use LLMs to evaluate alternative treatments *in silico*

Hypothesis: LLMs can use text-encoded knowledge to determine good treatment options for patients.

LLM Entropy-guided Optimization with Knowledgeable priors (LEON)



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Method	Warfarin ↓ RMSE Loss (<i>mg/week</i>)	HIV ↓ Viral Load (<i>copies/mL</i>)	Breast ↑ TTNTD (<i>months</i>)	Lung ↑ TTNTD (<i>months</i>)	ADR ↓ NLL Loss (<i>no units</i>)	Rank
Majority	3.46 ± 0.70	4.55 ± 0.07	25.95 ± 0.75	20.13 ± 0.13	1.41 ± 0.05	8.0
Human	2.68 ± 0.86	4.55 ± 0.07	29.65 ± 1.14	21.10 ± 0.27	—	8.5
Grad.	<u>1.37 ± 0.13</u>	<u>4.52 ± 0.04</u>	65.23 ± 2.03	24.09 ± 0.44	23.7 ± 1.7	5.2
BO-qEI	1.36 ± 0.13	4.53 ± 0.04	67.05 ± 1.87	27.97 ± 0.65	23.2 ± 1.7	<u>3.4</u>
Sim. Anneal	1.38 ± 0.12	4.55 ± 0.03	66.62 ± 2.62	<u>29.29 ± 0.74</u>	23.8 ± 1.7	5.0
CMA-ES	1.90 ± 0.14	4.53 ± 0.04	59.48 ± 2.76	27.43 ± 0.68	23.4 ± 1.7	6.2
GA	1.49 ± 0.26	4.62 ± 0.05	<u>69.90 ± 2.28</u>	27.53 ± 0.81	20.0 ± 2.3	5.2
LLAMBO	3.28 ± 0.10	<u>4.52 ± 0.05</u>	48.83 ± 2.48	20.60 ± 0.31	20.6 ± 1.9	7.0
OPRO	1.40 ± 0.13	4.55 ± 0.04	55.68 ± 2.86	24.35 ± 0.43	23.8 ± 1.7	7.0
Eureka	1.54 ± 0.25	4.58 ± 0.04	63.48 ± 3.52	25.10 ± 0.69	21.3 ± 2.0	6.8
LEON	1.36 ± 0.13	4.50 ± 0.04	72.43 ± 2.86	32.71 ± 0.32	<u>12.4 ± 1.6</u>	1.2



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