Design of Experiments for Model Discrimination using Gaussian Process Surrogate Models

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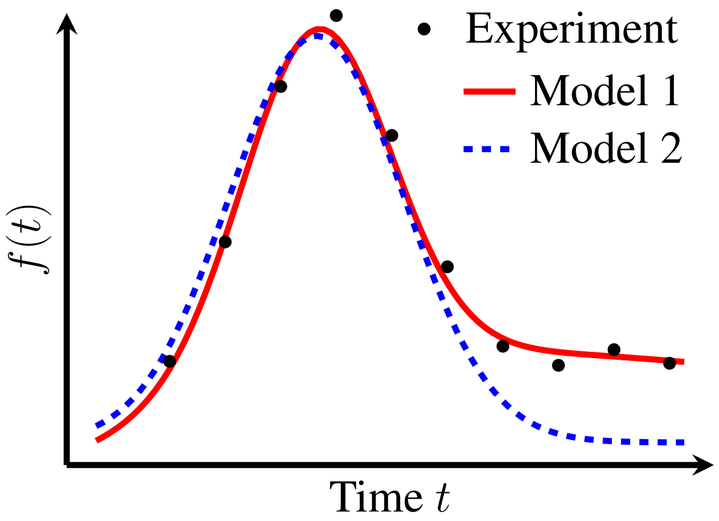
1. Model Discrimination

Assume we are studying a complex **physical system** (e.g. a human organ interacting with a new pharmaceutical).

We may have rival **models** (i.e. hypotheses) for some underlying system mechanism. We perform **model discrimination** by discarding models whose predictions do not agree with experimental results.



Example of rival models.

Common in industry to lack sufficient experimental results to perform model discrimination. This issue e.g. slows down development of new pharmaceuticals.
⇒ **Need additional experiments!**

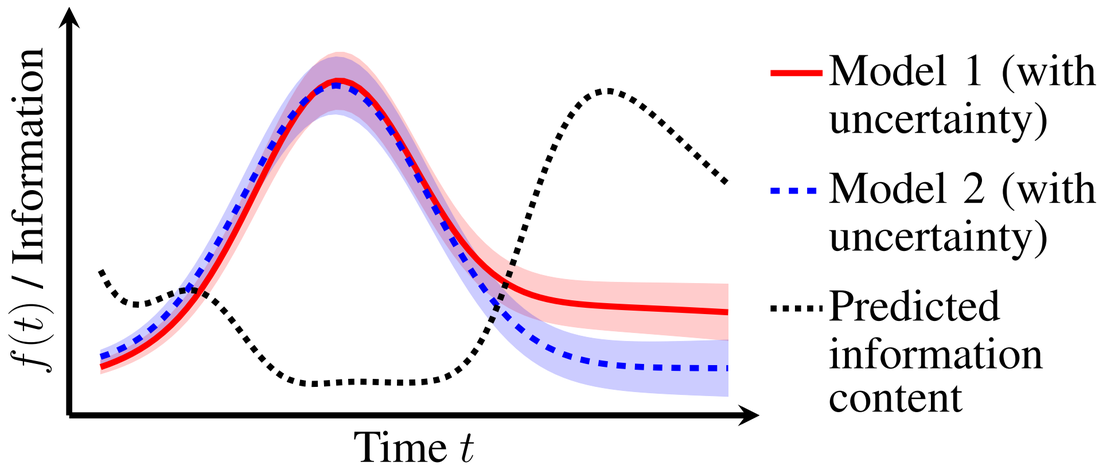
Challenge: Design the most informative experiments to help with model discrimination.

Classical approach vs. Data-driven approach

How can we find the most informative next experiment, taking model uncertainty into account?

2.1 Classical Approach

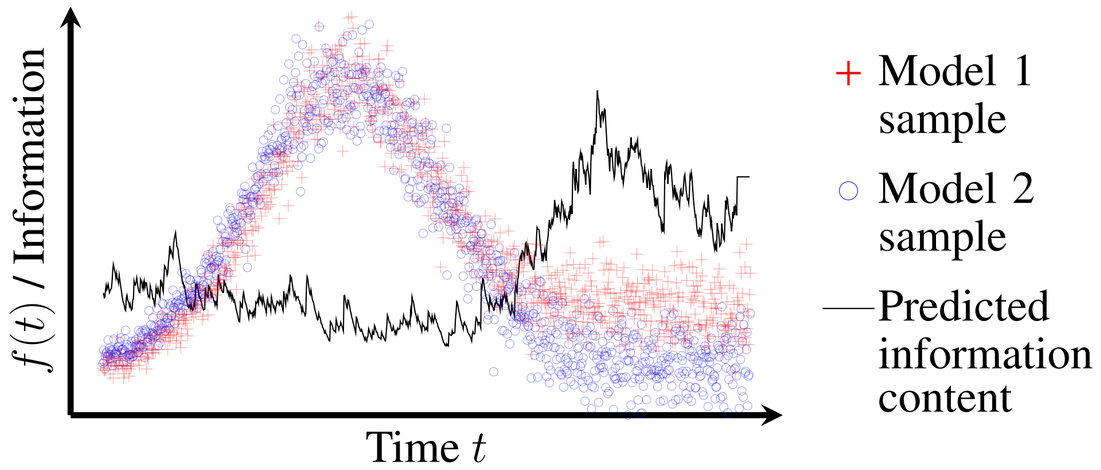
Find optimal next experiment by exploiting the models' mathematical structure.



\+ Computationally cheap.
– Limits our choice of model structure.

2.2 Data-Driven Approach

Exploit power of computers to find the optimal next experiment through brute force.

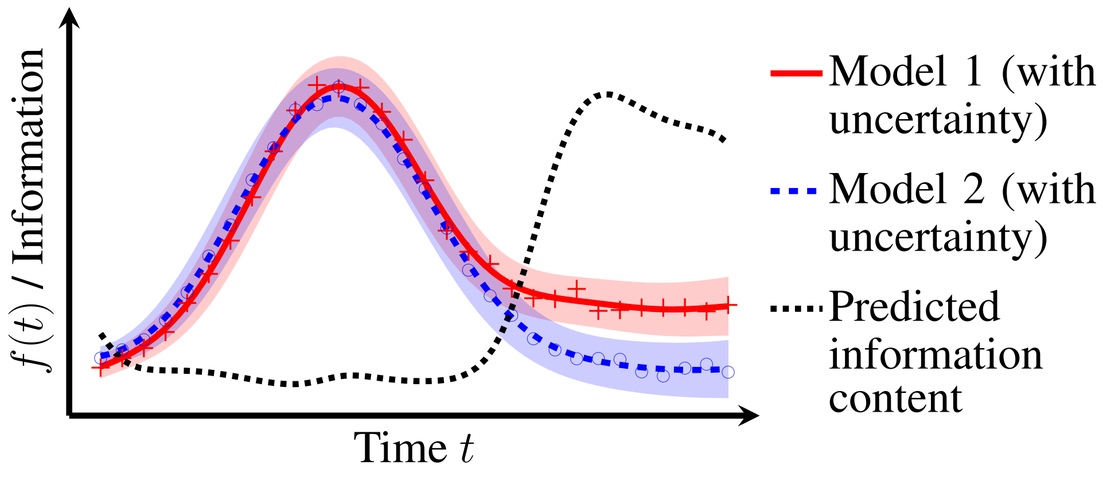


\+ Flexible with regards to model structure.
– Computationally expensive.

Using machine learning, we hybridise the two approaches

3. Novel Approach

We introduce data-driven surrogate models, whose mathematical structure can be exploited.



\+ Flexible with regards to models structure.
\+ Computationally cheap.

4. Conclusion

Difficulties with model discrimination often slows down e.g. **development of new pharmaceuticals**.

We hybridise two existing approaches, leveraging advantages of both, by use of **machine learning**.

The novel approach is implemented and available as free **open-source software**.

References

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Acknowledgement. This work has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement no. 675251, and an EPSRC Research Fellowship to R.M. (EP/P016871/1).