

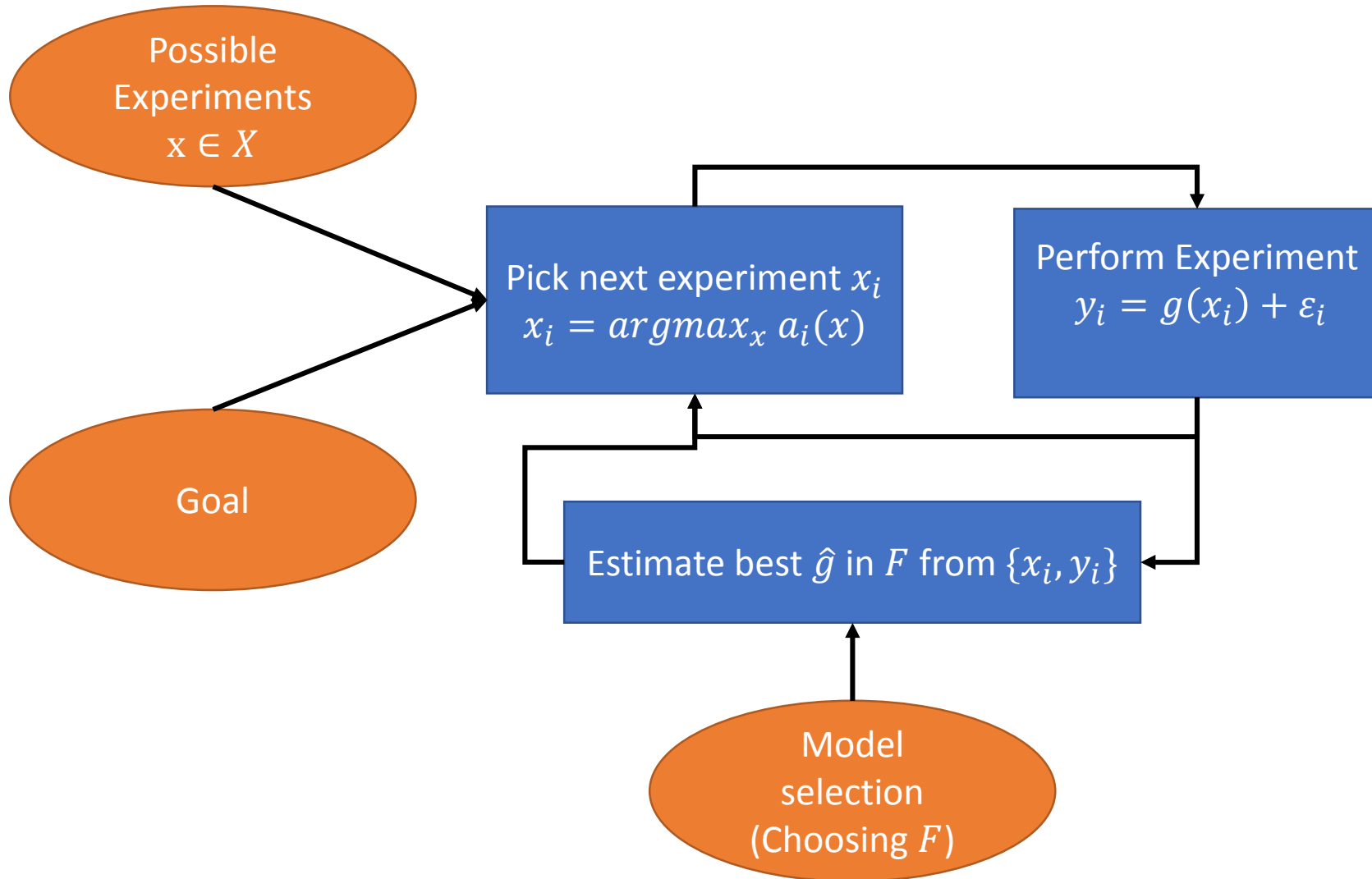
# Optimization for Knowledge Discovery

Modern design of statistical experiments

Mojmír Mutný, ETH Zürich

Joint work with Andreas, Johannes and others

# Experiment Design



- How many iterations do we need to finish with the goal?
- What is the right goal?
- How to select  $F$ ?
- How to be robust to noise?
- Can we efficiently pick the experiment?
- How to select the right  $F$ ?

In one sentence:

*“How to make sequential decision making scale to more realistic and modern model assumptions and requirements?”*

Unknown  
Model

Sequential hypothesis testing

Complex  
models beyond  
GPs

MKL, neural networks

New Tasks

Subspace estimation, level sets

New noise  
models

Poisson sensing, heavy tail bandits,  
likelihood

Scalable  
Assumptions

Additive models, subspaces,  
Projection pursuit

Efficient  
Algorithms

LineBO, Batching,  
Sketching

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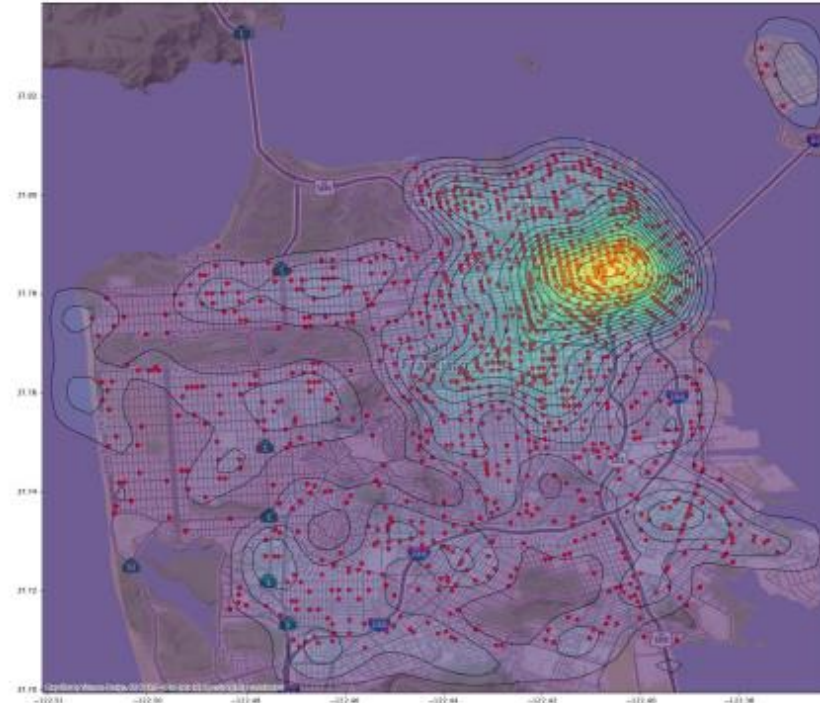
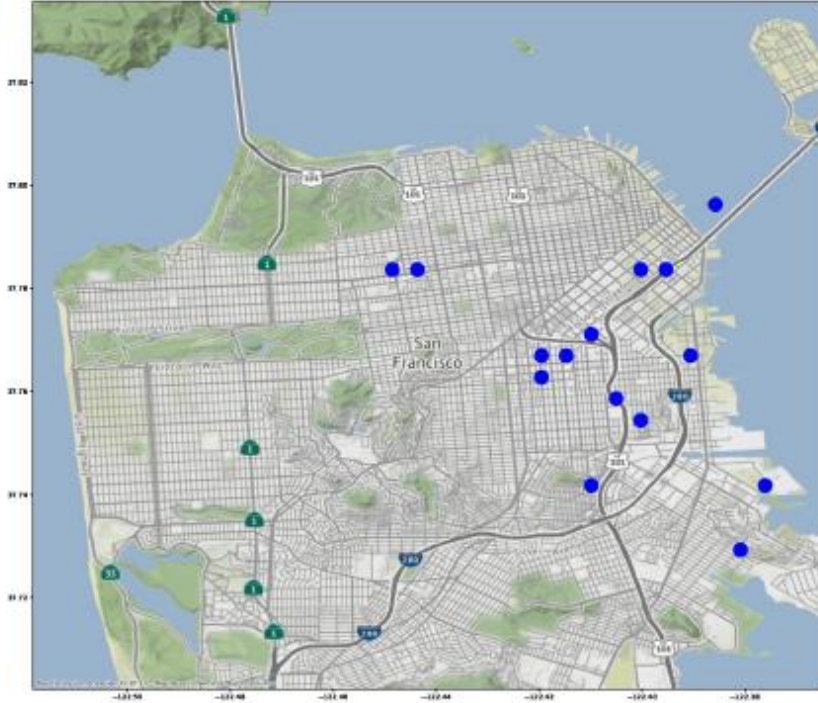
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# Tolerance to Noise: Poisson Sensing

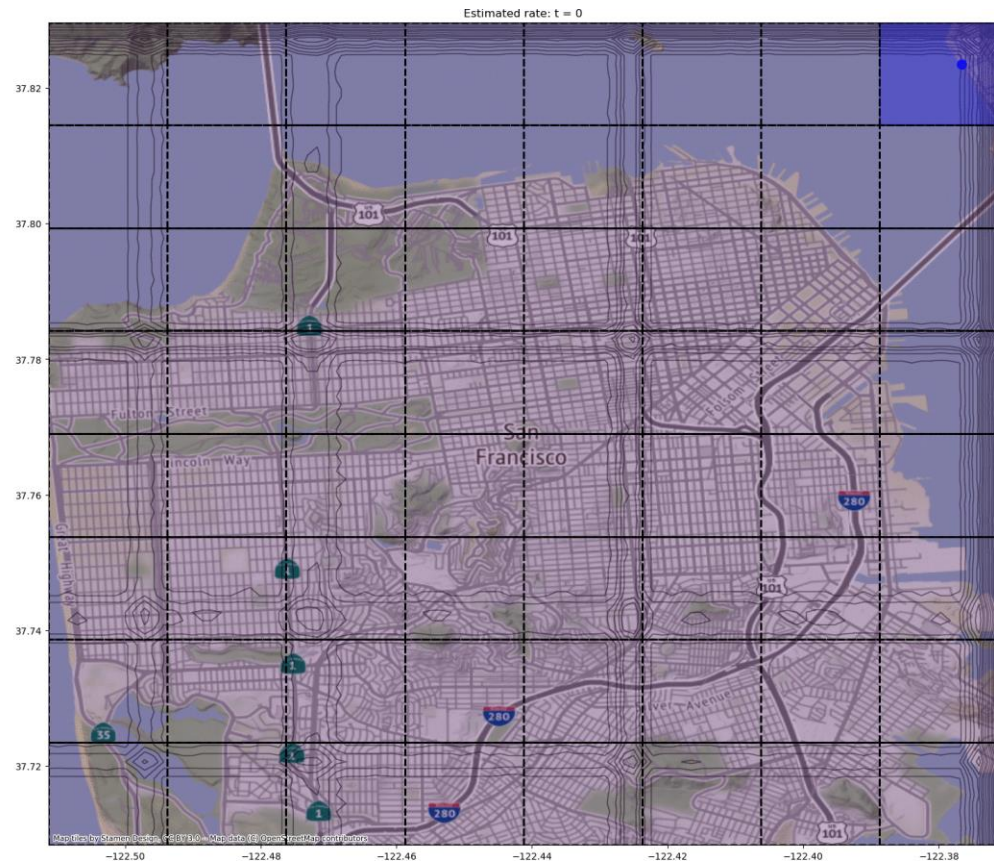
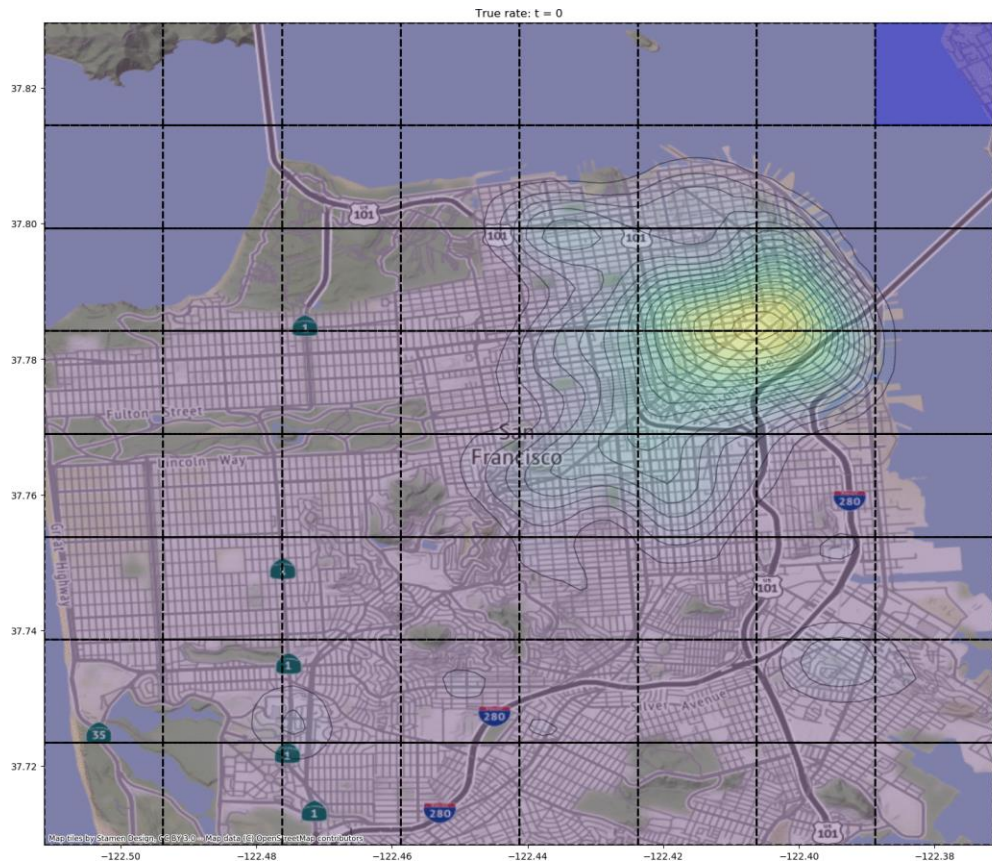
New noise models



$$N(A) \sim \text{Poisson} \left( \Delta \int_A \lambda(x) dx \right).$$

# Tolerance to Noise: Poisson Sensing

New noise models



# Scalable models: additive models

Scalable  
Assumptions

- **Statistical** → needs assumptions

## Additive functions

$$g(\underbrace{x_1}_{\text{blue}} \underbrace{x_2}_{\text{orange}} \underbrace{x_3}_{\text{grey}} \underbrace{x_4}_{\text{green}}) = g_1(\underbrace{x_1}_{\text{blue}} \underbrace{x_2}_{\text{orange}}) + g_2(\underbrace{x_2}_{\text{orange}} \underbrace{x_3}_{\text{grey}}) + g_3(\underbrace{x_4}_{\text{green}})$$

$\bar{d} := \text{size of largest group}$

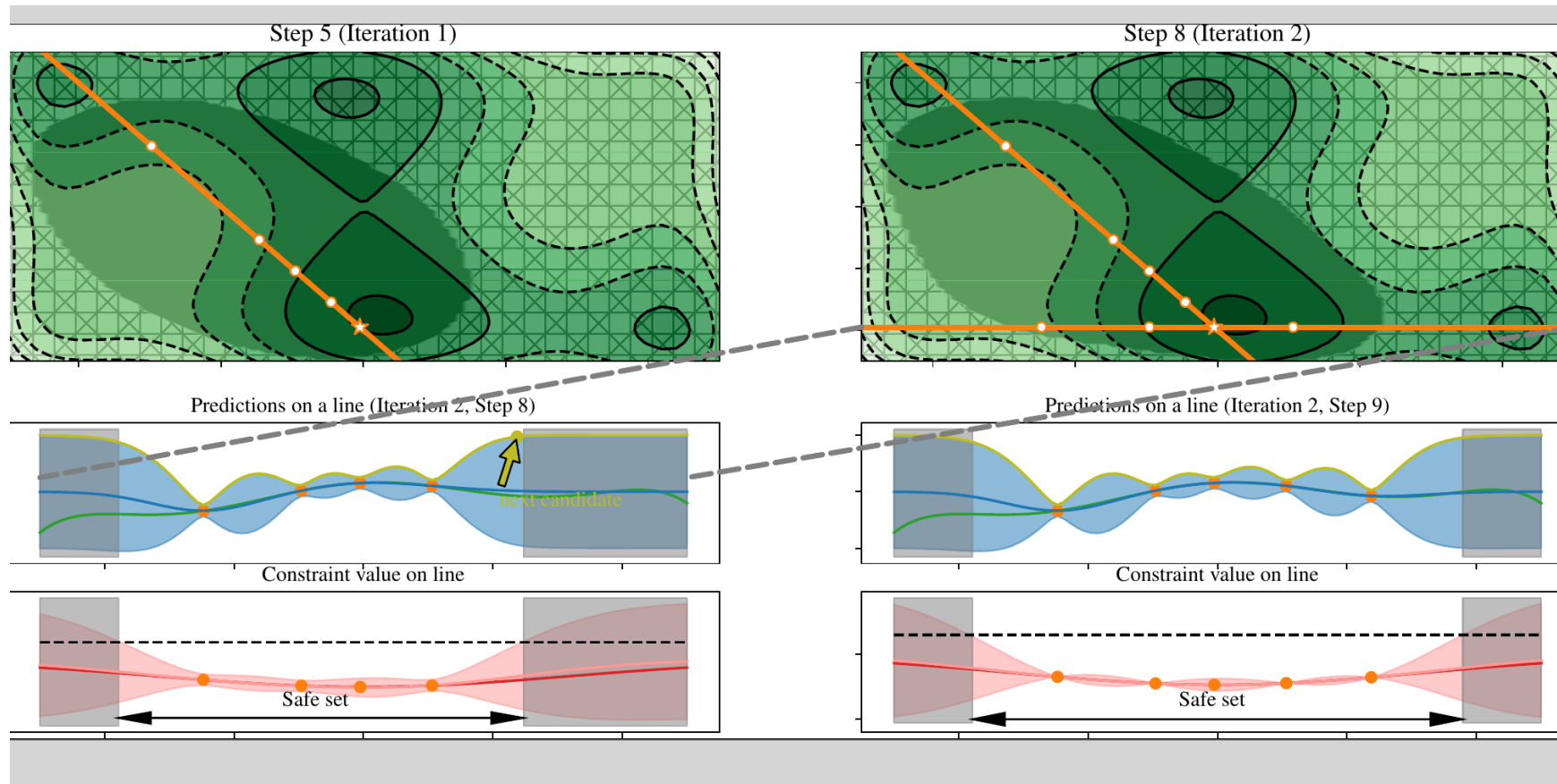
- **Computational**

- Kernel inversion  $\mathcal{O}(T^3) \rightarrow \mathcal{O}(T \log T)$
- Optimization of the acquisition function → **coordinate optimization**

# Scalable Algorithms - LineBO

Efficient Algorithms

- Prior joint work with PSI, **Johannes**, Nicole, Jochem, Rasmus and Andreas



Pick next experiment  $x_i$   
 $x_i = \operatorname{argmax}_x a_i(x)$