UQ of the 4th kind, Uncertainty Quantification of the 4th kind; optimal posterior accuracy-uncertainty tradeoff with the minimum enclosing ball,

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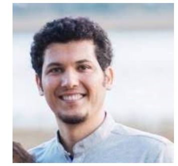
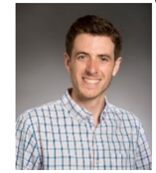




Supported by AFOSR, JPL and BL with the following target applications

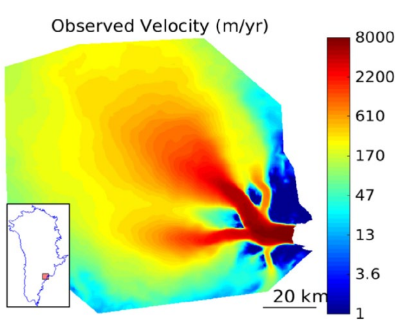
Greenland contribution to sea level by 2050 : The role of meltwater in shaping the future ice sheet

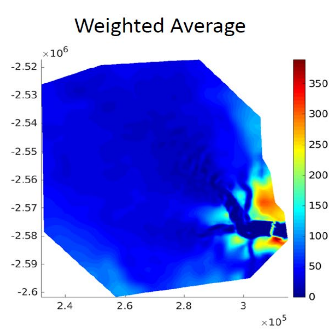
Helene Seroussi (JPL)

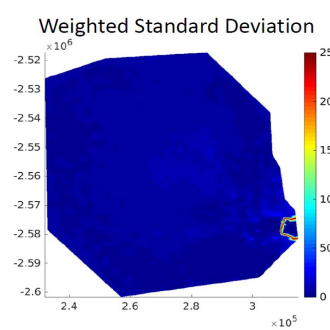
Peyman Tavallali (JPL)

Reservoir modeling

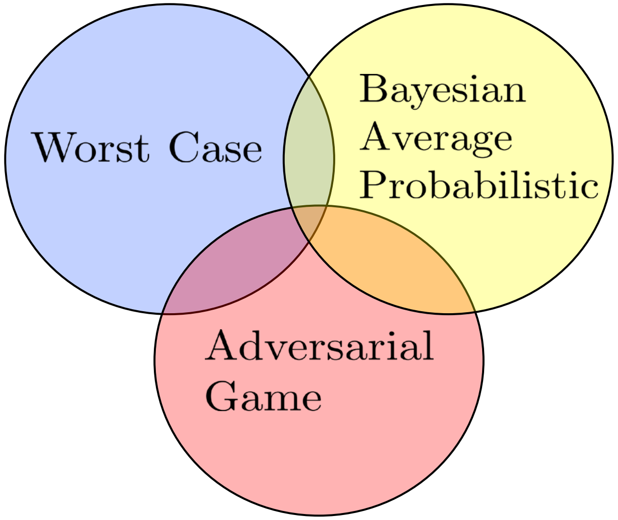
M. Shirdel (BL)







3 main approaches to uncertainty quantification

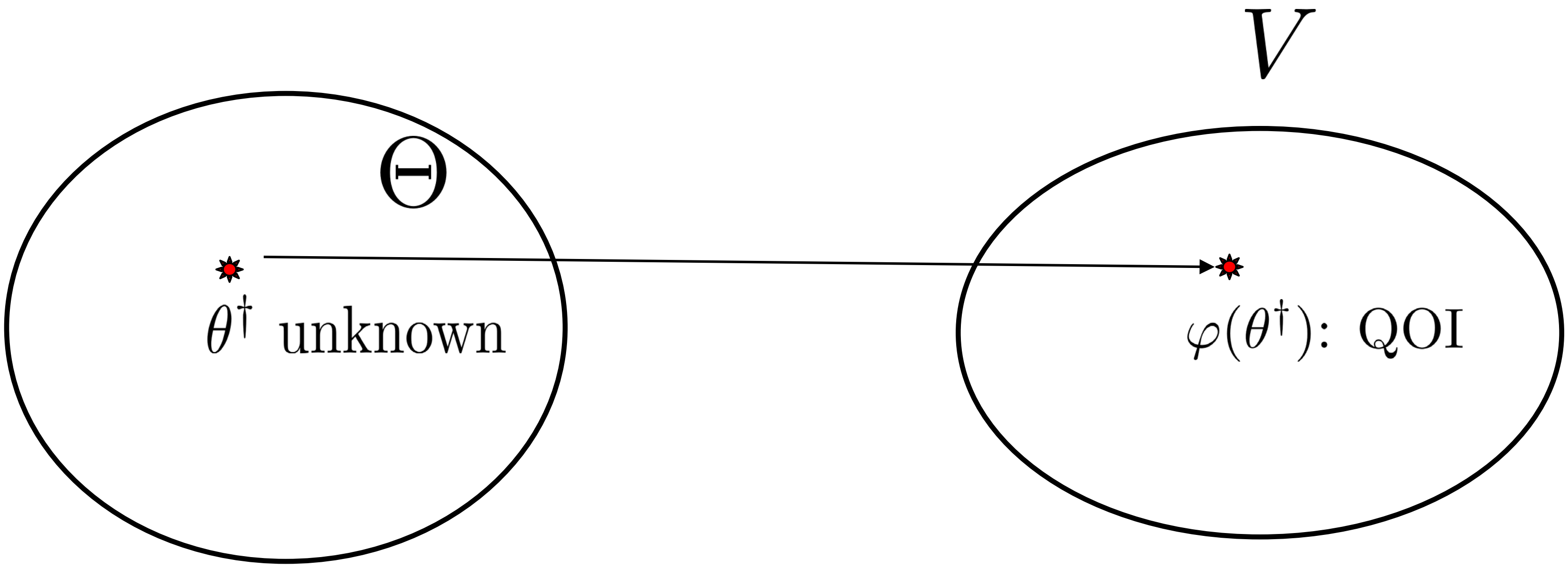


- **Worst case**: min and max (conservative)
  Not good at assimilating data.
- **Bayesian:** Brittle with respect to the choice of prior. MCMC to compute posteriors (slow)
- **Decision/Game Theory** (Minimax, identifies a prior). Suffers from the curse of dimensionality in approximating an optimal prior. The notion of risk is an averaged one (average with respect to data)

We have discovered a 4^{th} one

- Hybrid between all 3 above and hypothesis testing
- Does not suffer from the curse of dimensionality
- Fast
- Notion of risk posterior to measurements
- Contains a Bayesian interpretation (direct computation of an optimal posterior)
- Optimal in the robustness vs accuracy tradeoff

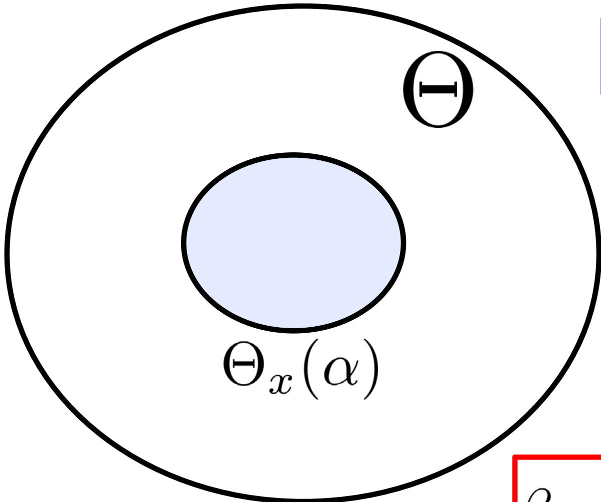
Problem



Given $x \sim P(\cdot|\theta^\dagger)$ estimate $\varphi(\theta^\dagger)$
and quantify the uncertainty of the estimate

Solution

$\theta \in \Theta_x(\alpha)$: Non-rarity assumption on the data



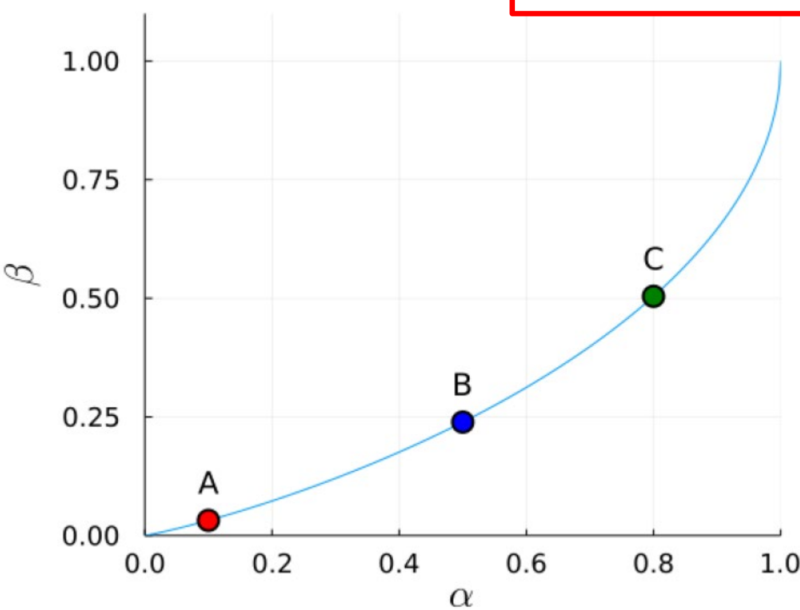
$\Theta_x(\alpha) := \{\theta \in \Theta : \bar{p}(x|\theta) \geq \alpha\}$: Likelihood region

$\bar{p}(x|\theta) := \frac{p(x|\theta)}{\sup_{\theta \in \Theta} p(x|\theta)}$: Relative likelihood

$p(\cdot|\theta)$: density of $P(\cdot|\theta)$

$0 \leq \alpha \leq 1$

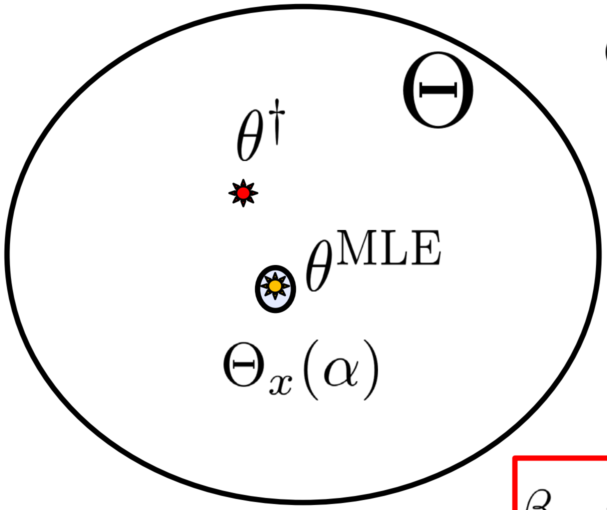
$\beta_\alpha := \sup_{\theta \in \Theta} P\Big(\{x' \in X : \theta \notin \Theta_{x'}(\alpha)\}\Big|\theta\Big)$: p-value



Significance level: (max in θ) probability that the assumption is wrong

$1 - \beta_\alpha$: Confidence level that the assumption is true

$\theta \in \Theta_x(\alpha)$: Non-rarity assumption on the data



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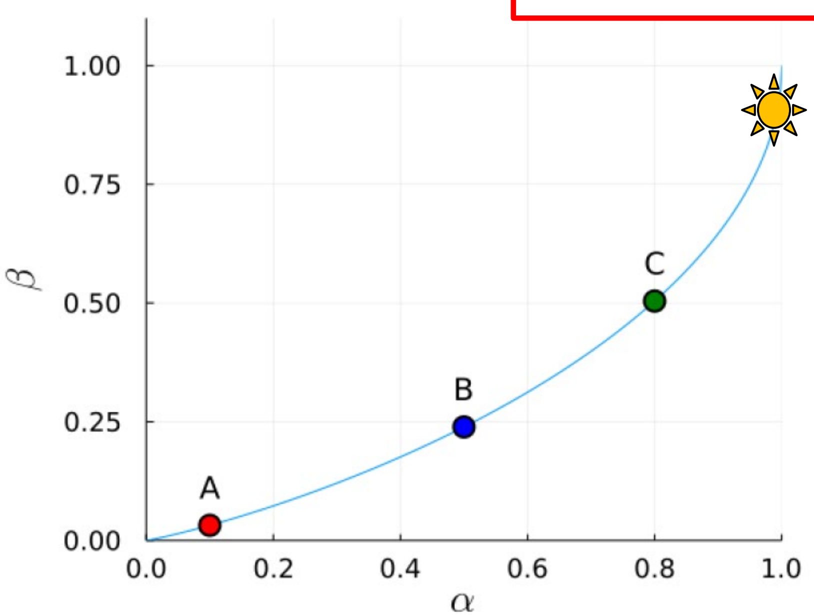
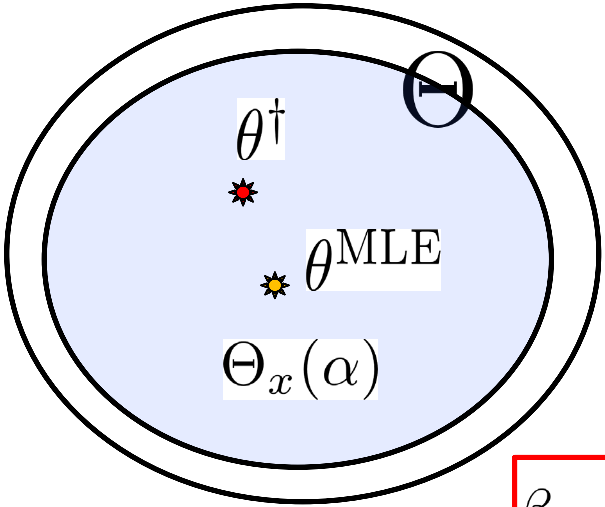


$\alpha \approx 1$

When $\alpha \approx 1$, $\Theta_x(\alpha)$ concentrates around the MLE but the max probability β_α that $\theta^\dagger \notin \Theta_x(\alpha)$ is high.

$\theta \in \Theta_x(\alpha)$: Non-rarity assumption on the data



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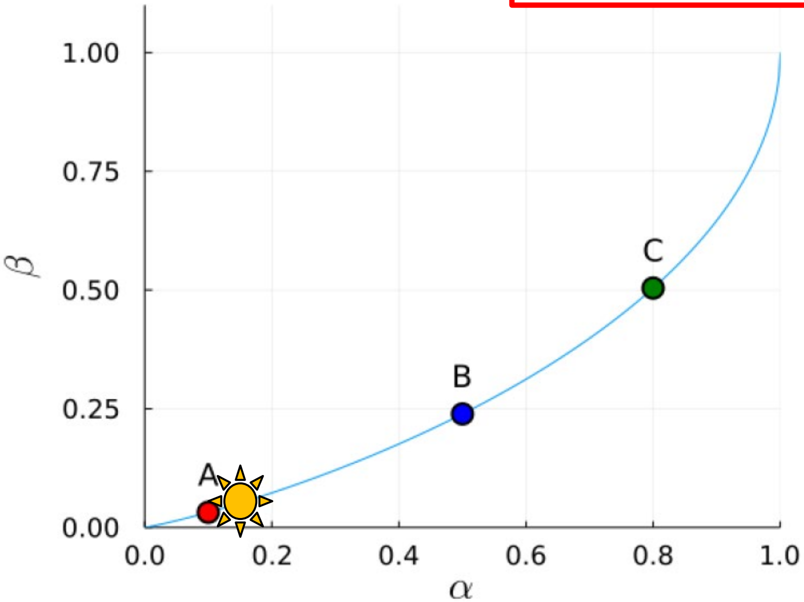
$\beta_\alpha := \sup_{\theta \in \Theta} P\Big(\{x' \in X : \theta \notin \Theta_{x'}(\alpha)\}\Big|\theta\Big)$: p-value

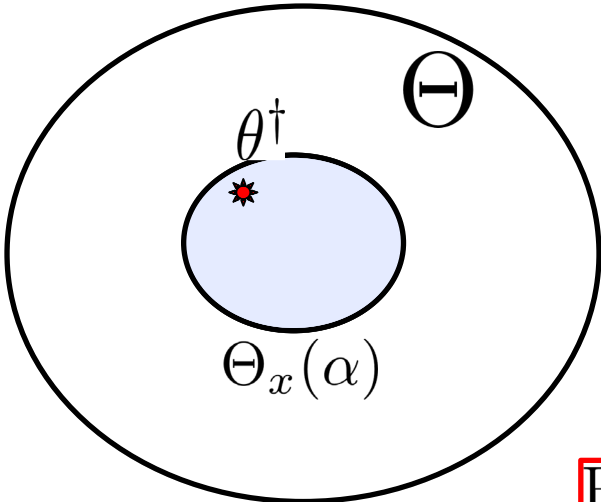


$\alpha \approx 0$

When $\alpha \approx 0$, $\Theta_x(\alpha)$ covers most of the domain and the max probability β_α that $\theta^\dagger \notin \Theta_x(\alpha)$ is low.

Choose

$$\alpha := \max\{\alpha' \mid 1 - \beta_{\alpha'} \geq 0.95\}$$



With probability at least 0.95, $\theta_x(\alpha)$ contains the true (data generating) parameter $\theta^\dagger$.

Play adversarial game in $\Theta_x(\alpha)$

Player I

Selects $\pi \in \mathcal{P}(\Theta_x(\alpha))$

Player II

Selects $d \in V$

max

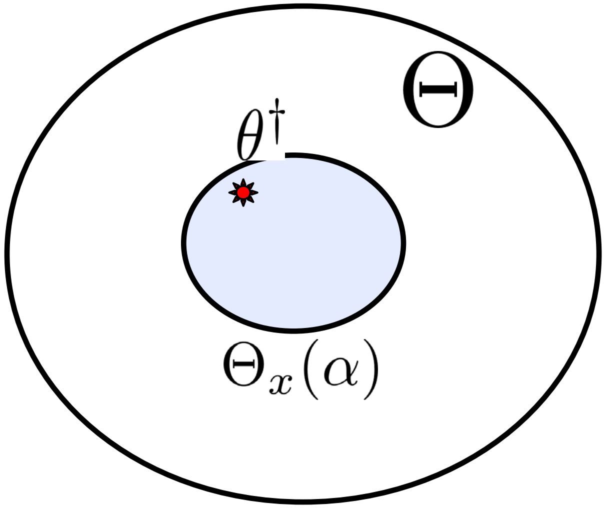
min

$$\mathbb{E}_{\theta \sim \pi_x}\left[\|\varphi(\theta) - d\|^2\right]$$

$$\pi_x := \frac{\bar{p}(x|\cdot)\pi}{\int_\Theta \bar{p}(x|\theta)d\pi(\theta)}$$

Choose

$$\alpha := \max\{\alpha' \mid \beta_{\alpha'} \leq 0.05\}$$



With probability at least 0.95, $\theta_x(\alpha)$ contains the true (data generating) parameter $\theta^\dagger$.

Identification of optimal posterior

Player I

Selects $\pi \in \mathcal{P}(\Theta_x(\alpha))$

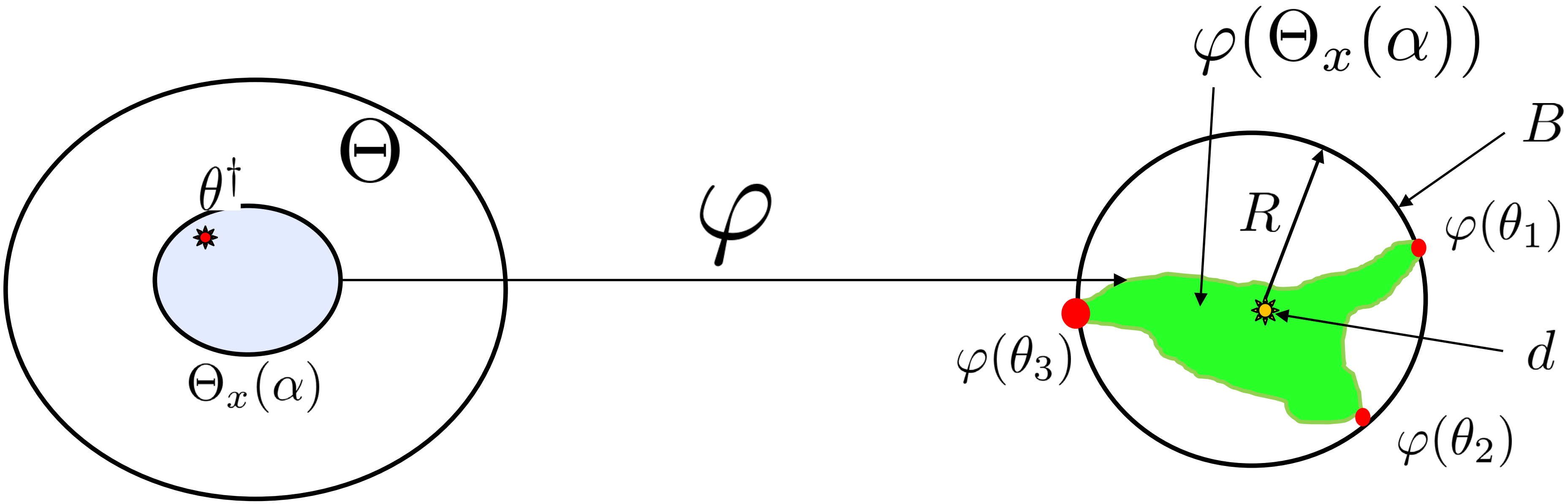
Player II

Selects $d \in V$

max

min

$$\mathbb{E}_{\theta\sim\pi}\left[\|\varphi(\theta) - d\|^2\right]$$



Theorem

B: Min enclosing ball of $\varphi(\Theta_x(\alpha))$

Optimal decision d: Center of B

Optimal posterior: $\pi = \sum_{i=1}^{\dim(V)+1} \pi_i \delta_{\theta_i}$

$$\varphi(\theta_i) \in \partial B$$

Risk $\mathbb{E}_{\theta\sim\pi}\left[\|\varphi(\theta) - d\|^2\right]$: Squared radius R^2 of B

Example

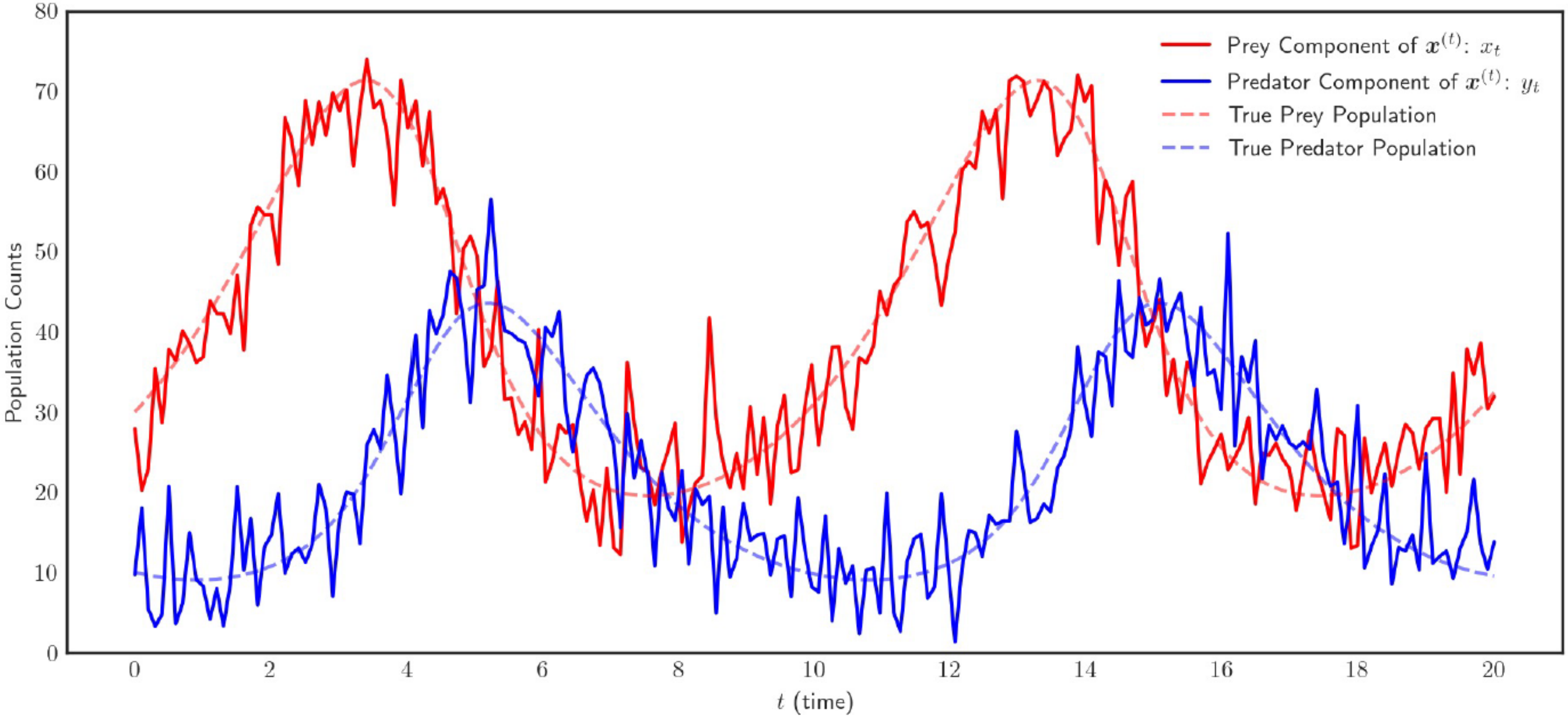
Consider the Lotka-Volterra predator-prey model.

$$\frac{dx}{dt} = \theta_1 x - \eta x y$$
$$\frac{dy}{dt} = \xi x y - \theta_2 y$$

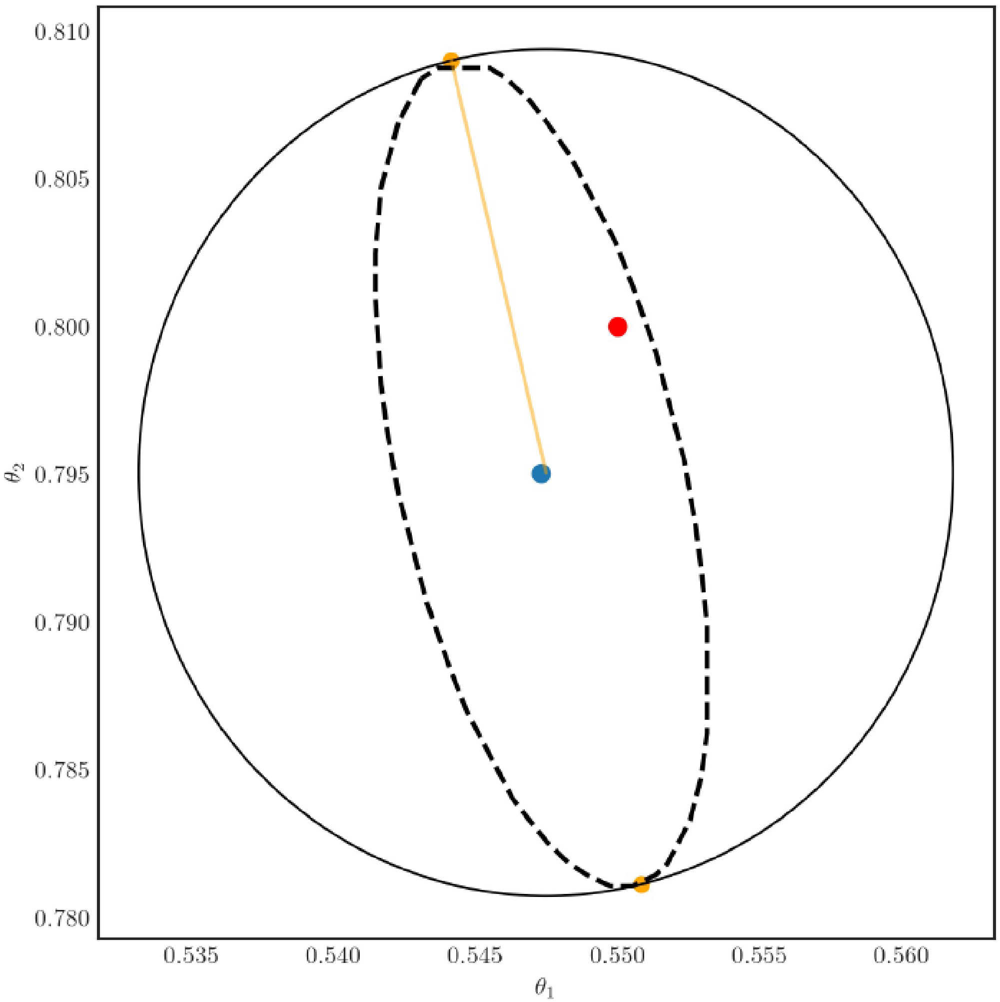
Given

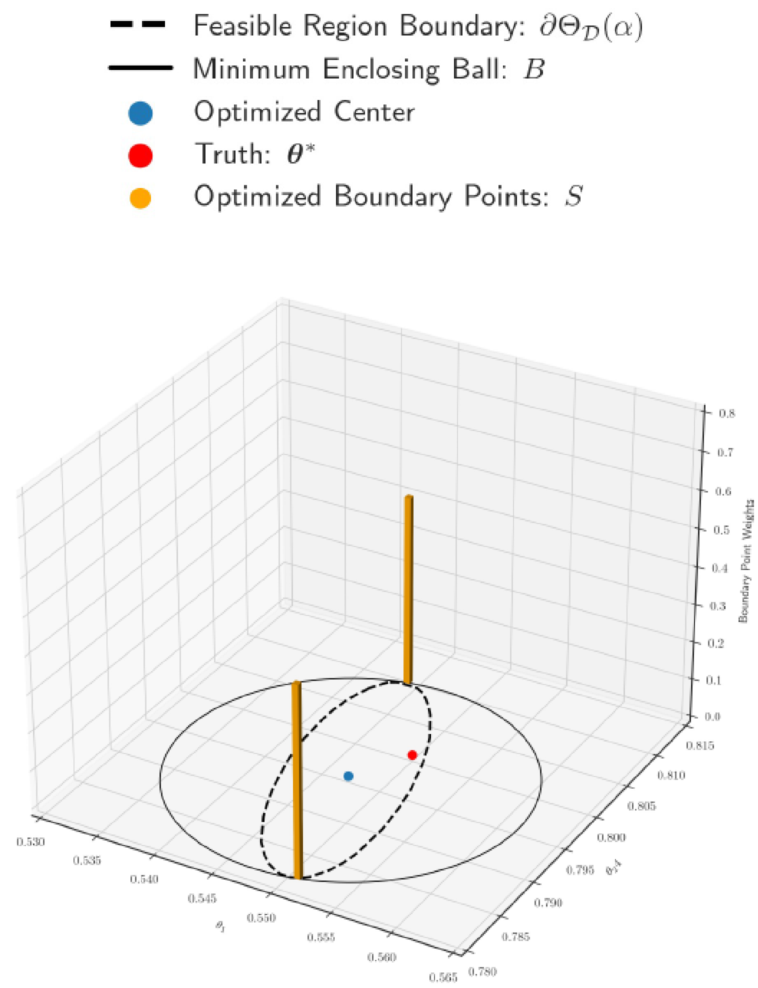
$$\boldsymbol{x}^{(t)} = \begin{bmatrix} x_t \\ y_t \end{bmatrix} = \boldsymbol{m}(t; \boldsymbol{\theta}) + \epsilon_t, \quad \epsilon_t \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I}), \quad t \in \{0, \tfrac{1}{10}, \ldots, 20\}$$

Estimate (θ_1, θ_2)



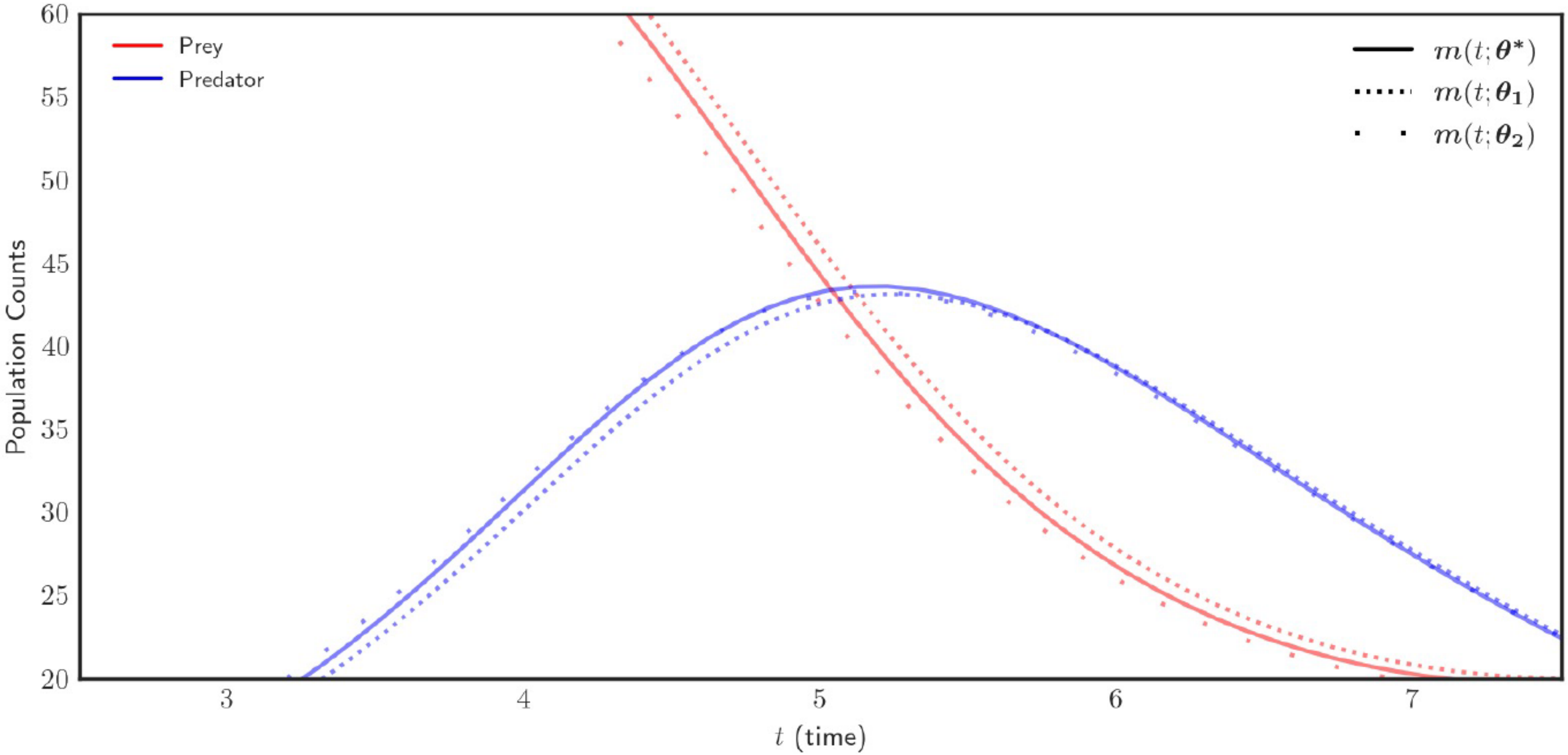
Min enclosing ball and optimal decision





Solution map and support points of optimal posterior

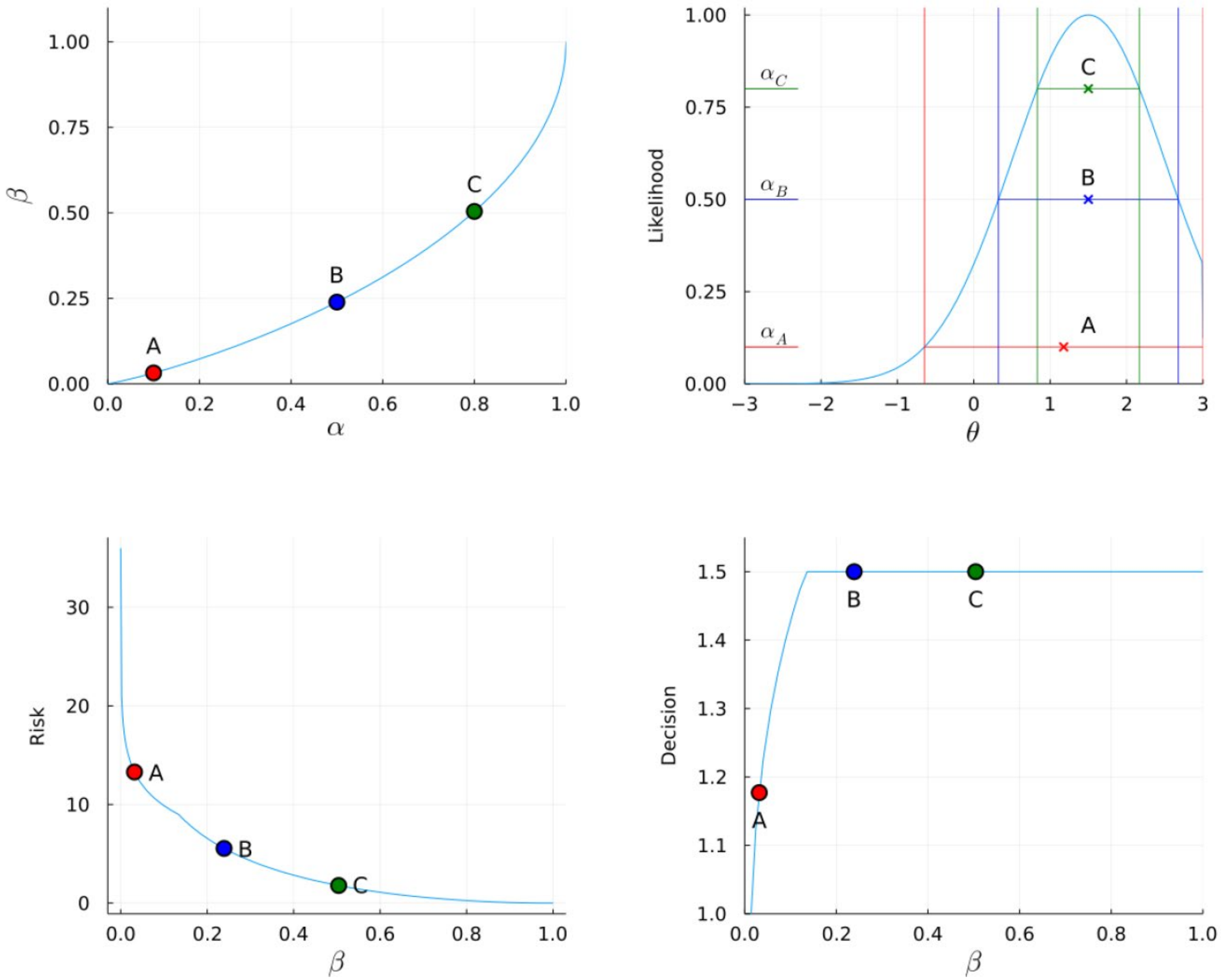
$$\boldsymbol{\theta} \mapsto \boldsymbol{m}(t;\boldsymbol{\theta}), t \in T,$$



Example $\theta^\dagger \in [-\tau, \tau]$ unknown

Given $x \sim \mathcal{N}(\theta^\dagger, \sigma^2)$ estimate $\theta^\dagger$

Solution $x = 1.5,\ \sigma = 1,\ \tau = 3$



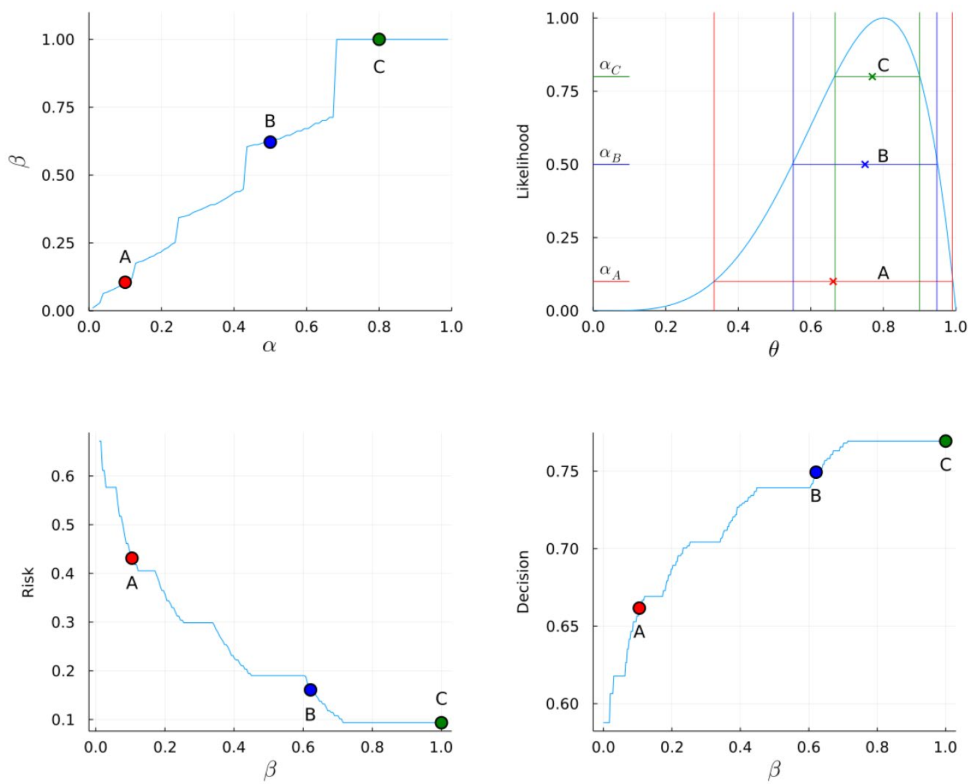
Example

Estimate the probability that a biased coin lands on heads from the observation of n independent tosses of that coin.

$\theta^\dagger \in [0,1]$

Given $Y_1,\dots,Y_n$ i.i.d. $(P(Y_i=1)=\theta^\dagger,\ P(Y_i=0)=1-\theta^\dagger)$ estimate $\theta^\dagger$.

Solution $n=5,\ 4$ heads



Example

Consider two independent biased coins with unknown probabilities $\theta_1^\dagger$ and $\theta_2^\dagger$ of landing on head. Given n_1 tosses of coin 1 and n_2 tosses of coin 2 estimate $\theta_1^\dagger$ and $\theta_2^\dagger$.

Likelihood regions
And min enclosing balls

$$n_1 = 4, \text{ 3 heads and 1 tail for coin 1}$$
$$n_2 = 6, \text{ 5 heads and 1 tail for coin 2}$$