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BAYESIAN CALIBRATION OF STOCHASTIC AGENT BASED MODEL VIA PCA BASED SURROGATE MODELING

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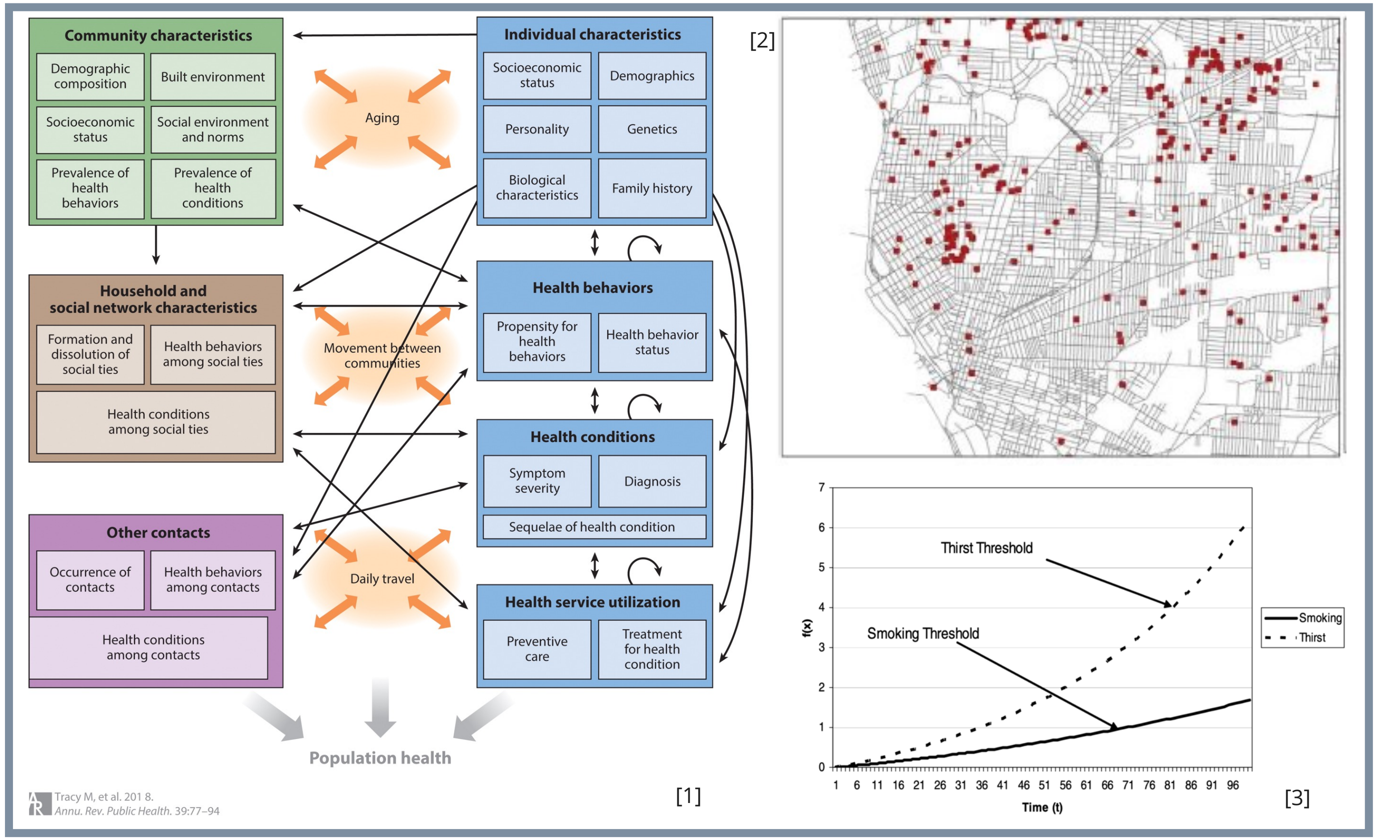
OVERVIEW

1. Agent based models
2. CityCOVID
3. PCA + Random Forest surrogate model
4. Parameter estimation outline
5. Calibration results and comparison
6. Challenges / future work

AGENT BASED MODELS - OVERVIEW

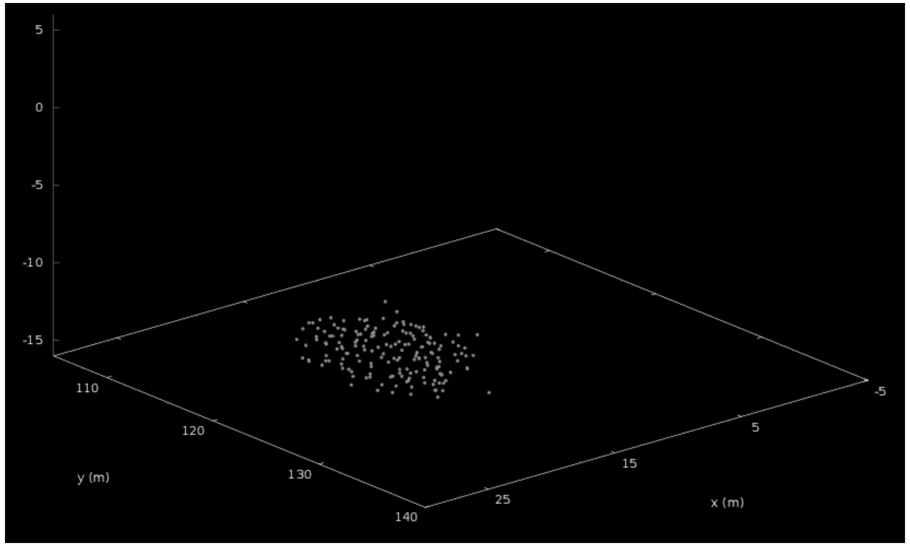
- **Agent based models (ABMs)** simulate interactions of discrete agents in an environment
  - Agents can have a variety of attributes and behaviors
  - Environment can influence and be influenced by agents (often graphs or continuum)
- **Features:**
  - Can capture emergent behavior in diverse populations
  - Usually, nonlinear, discrete, and stochastic
- **Examples:**
  - Epidemiology
  - Biology (cellular, ecological, etc.)
  - Economics



AGENT BASED MODELS - CHARACTERISTICS

Emergent behaviors:

Flocking



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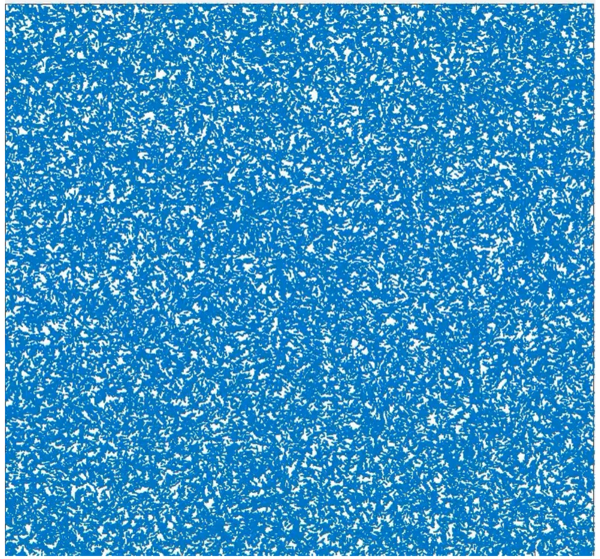
Swarming



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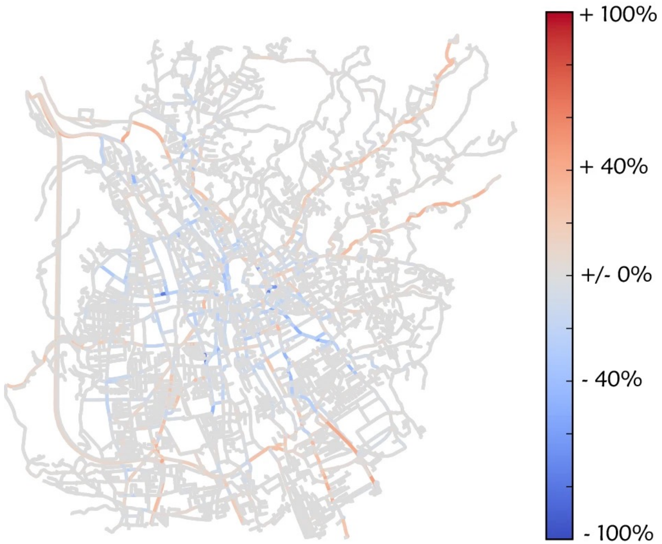
Traffic jams



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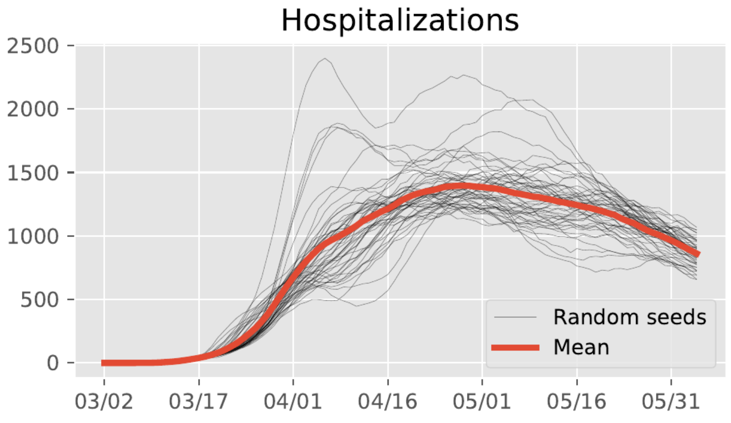
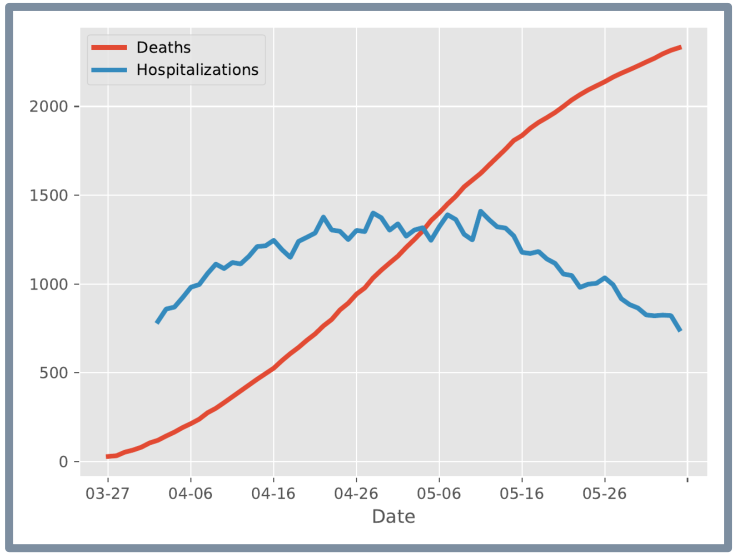
Stochasticity:

* Population-level measurements are heavily influenced by initial conditions



CITYCOVID – OVERVIEW

- Models COVID19 spread in Chicago metropolitan area
(2.7 million agents, 1.2 million locations)
- **Characteristics:**
  - Models protective behaviors and alternative schedules
  - Graph geometry
  - 100 CPU hrs per 70 day simulation



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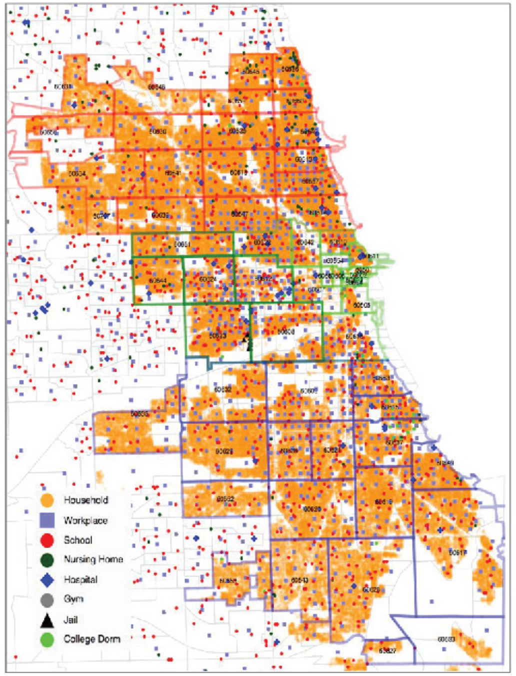
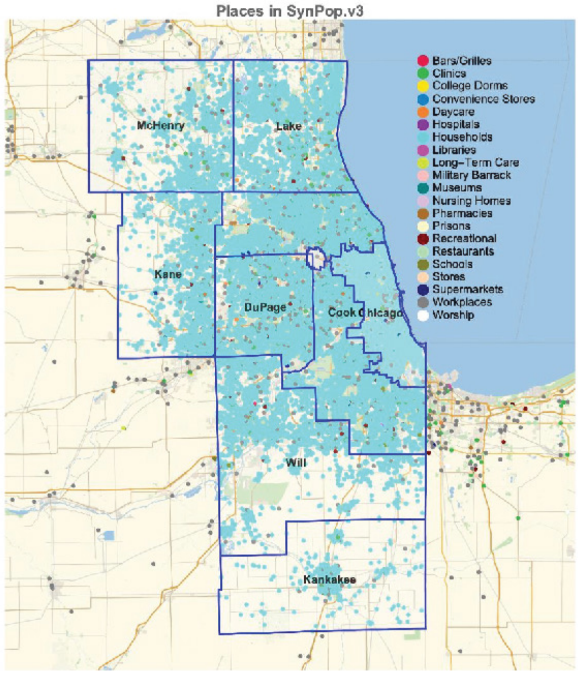
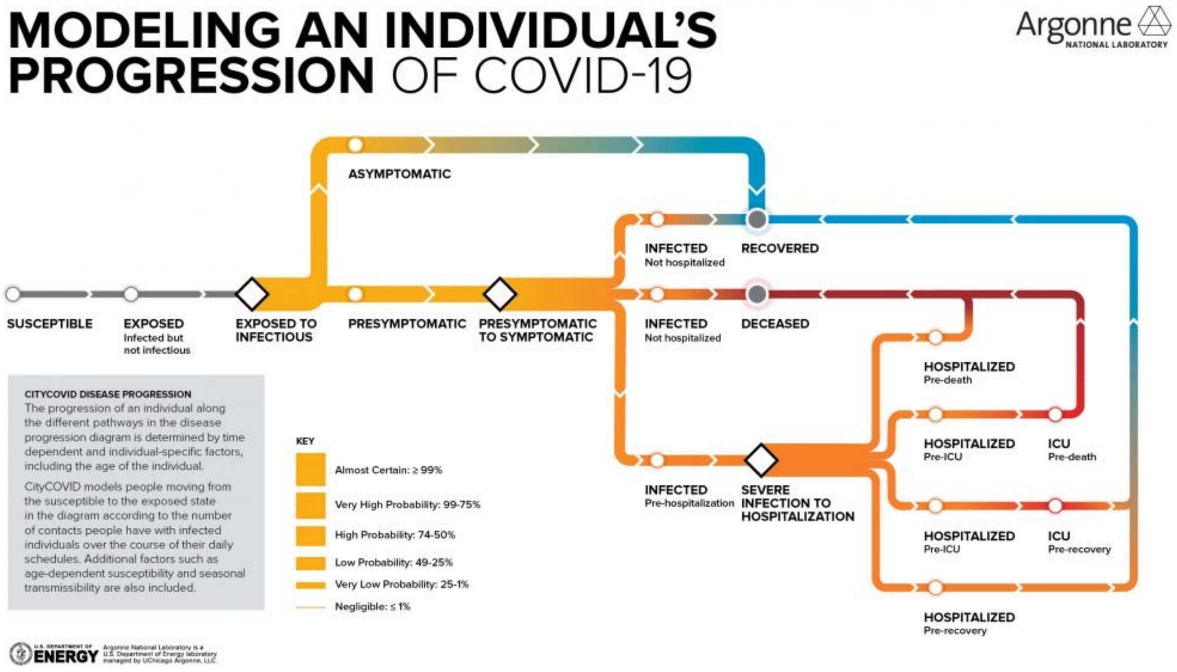






SURROGATE – MODEL

- Hospitalization, death data concatenated and decomposed with PCA
  - Captures temporal modes across all parameter samples
- Random forest mapping from CityCOVID parameters to PCA weights (100 trees)

$$\begin{bmatrix} h_{1,1} & \dots & h_{1,n} & d_{1,1} & \dots & d_{1,n} \\ h_{2,1} & \dots & h_{2,n} & d_{2,1} & \dots & d_{2,n} \\ \vdots & \dots & \vdots & \vdots & \dots & \vdots \\ h_{m,1} & \dots & h_{m,n} & d_{m,1} & \dots & d_{m,n} \end{bmatrix} \rightarrow \begin{bmatrix} \alpha_{1,1} \\ \alpha_{2,1} \\ \vdots \\ \alpha_{m,1} \end{bmatrix} \odot \vec{c}_1 + \dots + \begin{bmatrix} \alpha_{1,2n} \\ \alpha_{2,2n} \\ \vdots \\ \alpha_{m,2n} \end{bmatrix} \odot \vec{c}_{2n}$$

$h_{i,j}$ – Hospitalizations for parameter set i at time step j

$d_{i,j}$ – Deaths for parameter set i at time step j

$\vec{c}_j$ – PCA component j

$\alpha_{i,j}$ – PCA weight multiplying component j for parameter set i

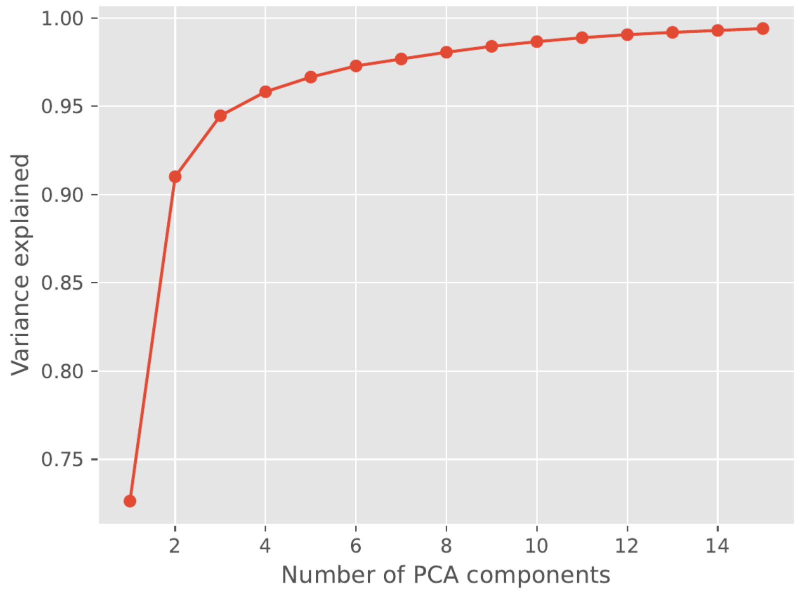
$r_f : \vec{\theta}_i \rightarrow \vec{\alpha}_i$ – Random forest mapping from parameter set i to PCA weights $\vec{\alpha}_i$

Model	q5	q50	q95
LinReg	<1%	6%	23%
Ridge	<1%	6%	23%
SVR	2%	21%	61%
KNN	2%	22%	66%
GP	<1%	5%	21%
MLP	2%	10%	66%
Tree	<1%	7%	35%
RF	**<1%**	**4%**	**24%**
GBRF	<1%	5%	20%

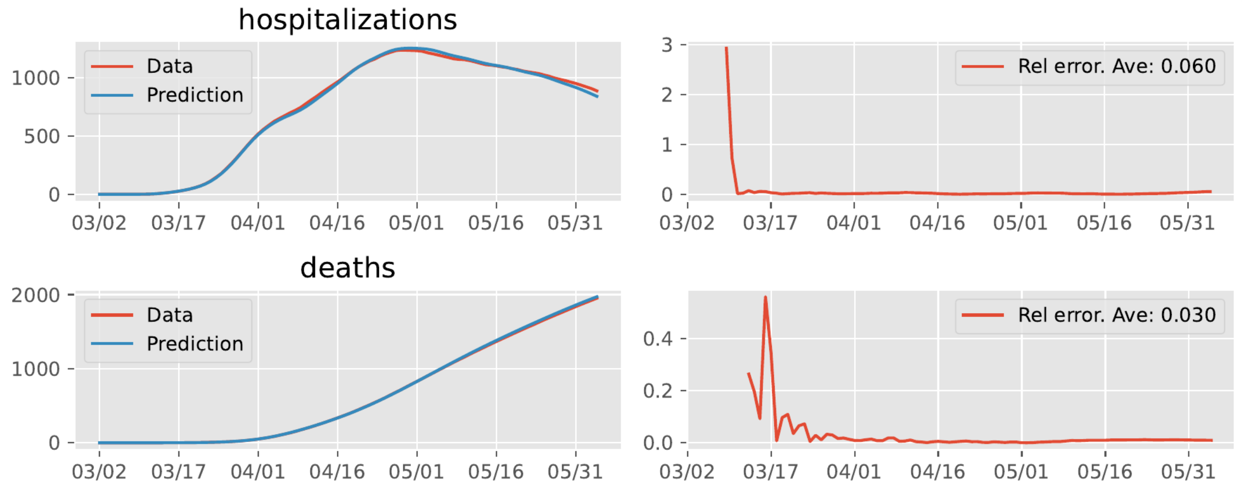
SURROGATE – PERFORMANCE

- PCA decomposition is able to recover accurately temporal trends
  - Only 4 modes required to recover 95% of data variance
- PCA + RF – 5% median abs relative error

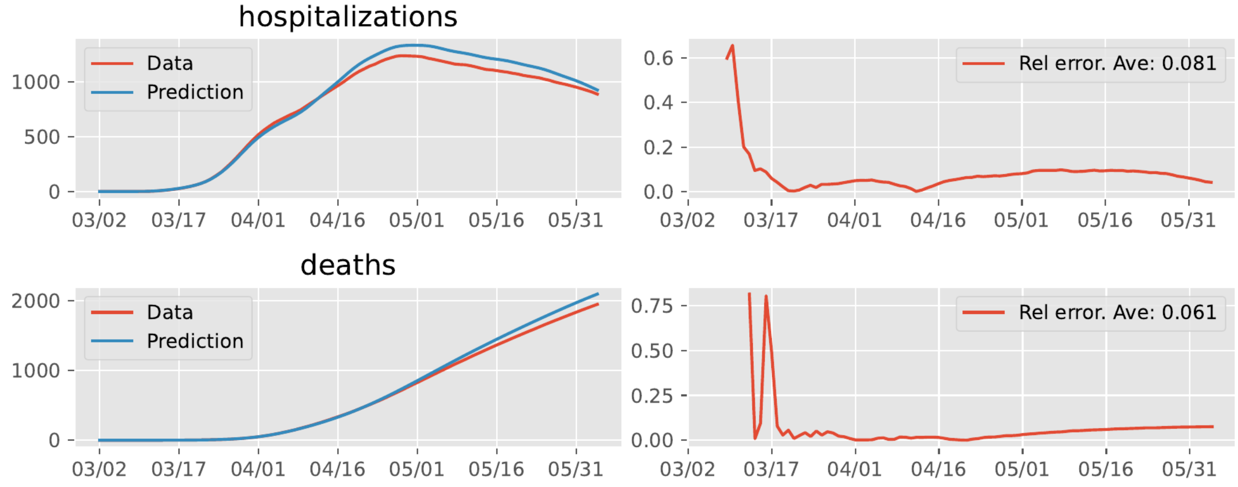
# of PCA components



PCA Reconstruction



PCA+RF Reconstruction



PARAMETER ESTIMATION FORMULATION

- Surrogate sensitivity identified 4 key parameters
- 4D Latin hypercube sampling minimally reduced around real observations from Chicago
- Daily counts used for estimation (more stationary)

Parameter	Gini	Perm
Infection susceptibility	0.39	0.56
First exposure date	0.32	0.54
Stay-at-home probability	0.21	0.27
Protective behavior factor	0.08	0.03

Parameter estimation formulation

$$\hat{h}^\circ \sim \mathrm{MvNormal}(h^\circ, \sigma_h | \vec{\theta})$$

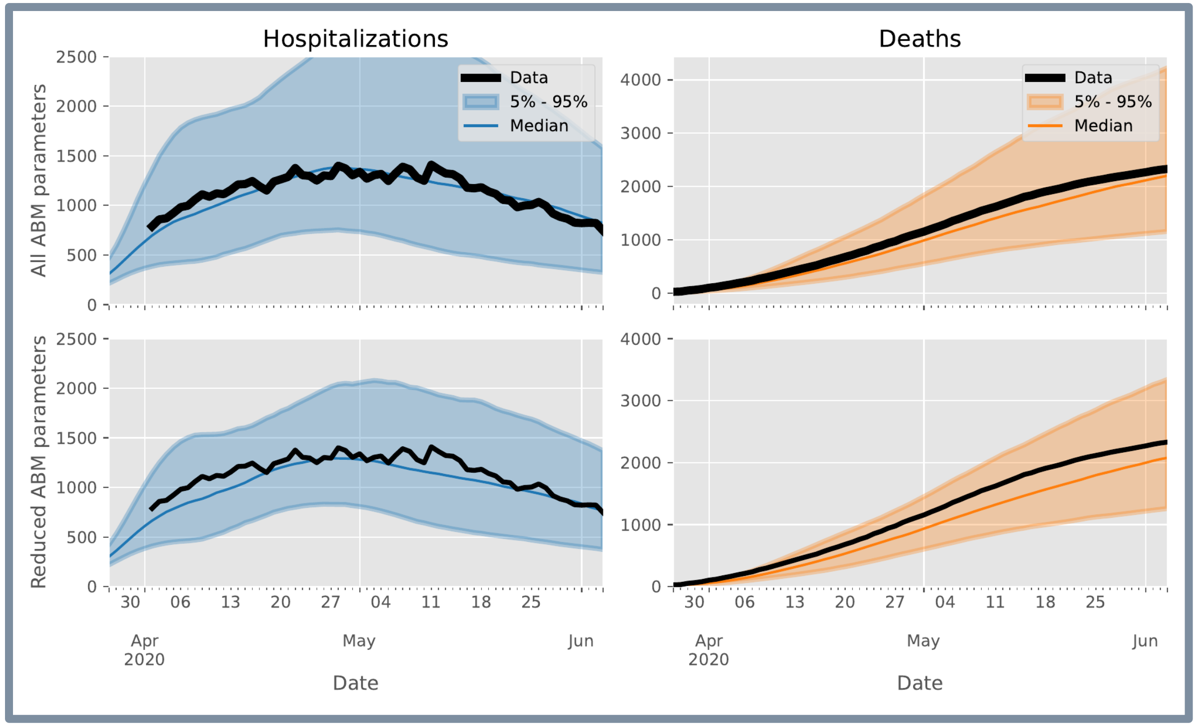
$$\hat{d}^\circ \sim \mathrm{MvNormal}(d^\circ, \sigma_d | \vec{\theta})$$

$$\sigma_h^{-2} \sim \mathrm{Gamma}\left(\frac{n_s + n}{2}, \frac{n_s \sigma_{h_0}^2 + S_h(\vec{\theta})}{2}\right)$$

$$\sigma_d^{-2} \sim \mathrm{Gamma}\left(\frac{n_s + n}{2}, \frac{n_s \sigma_{d_0}^2 + S_d(\vec{\theta})}{2}\right)$$

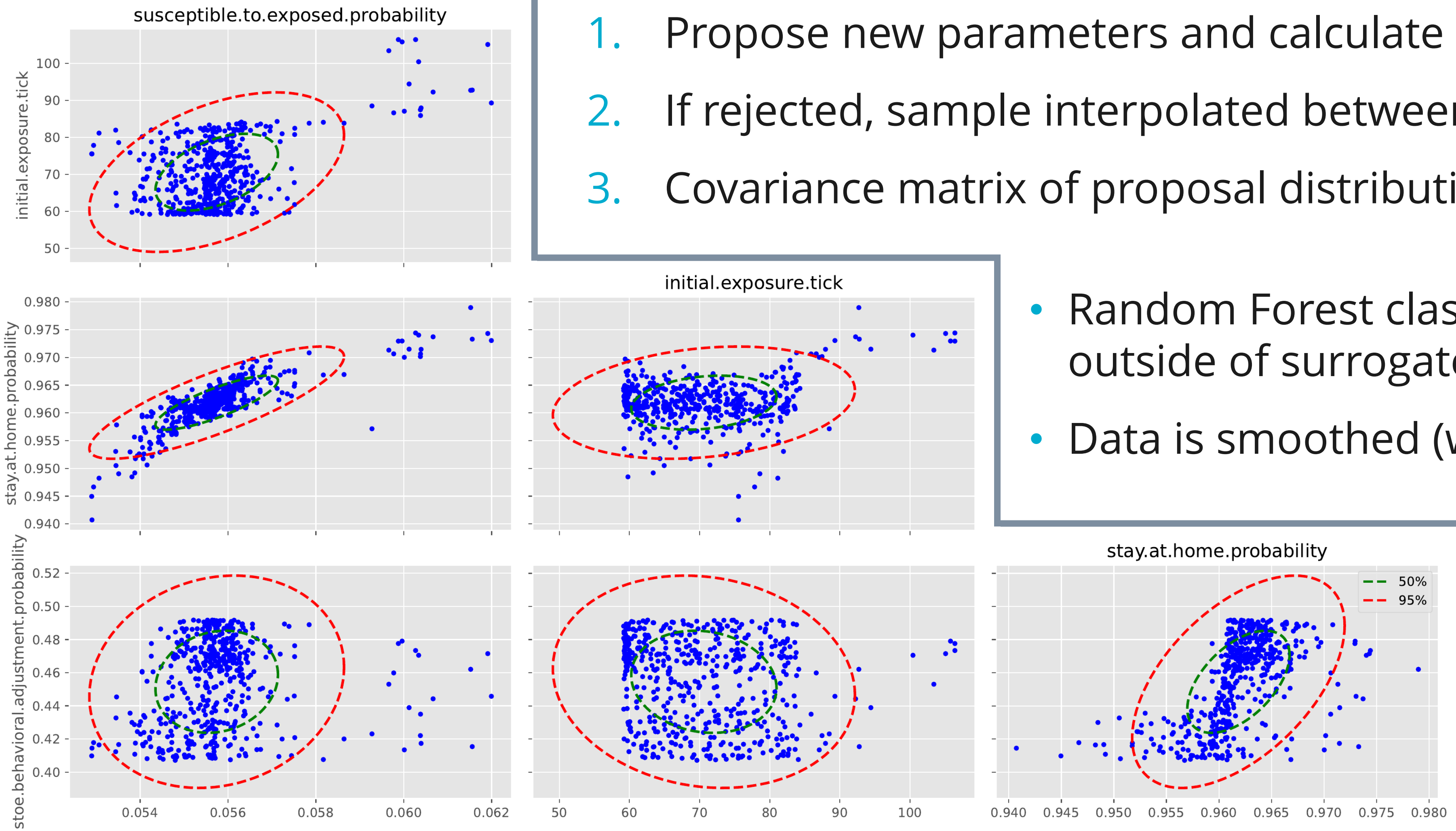
$$S_h(\vec{\theta}) = \sum_j^n (\hat{h}_j^\circ - h_j^\circ(\vec{\theta}))^2, \quad S_d(\vec{\theta}) = \sum_j^n (\hat{d}_j^\circ - d_j^\circ(\vec{\theta}))^2$$

$$\sigma_{h_0} = S_h(\vec{\theta}_0), \quad \sigma_{d_0} = S_d(\vec{\theta}_0), \quad \theta_i \sim C(\vec{\theta})$$



BAYESIAN INFERENCE – SAMPLING

- Samples from posterior taken via Delayed Rejection Adaptive Metropolis-Hastings (DRAM):

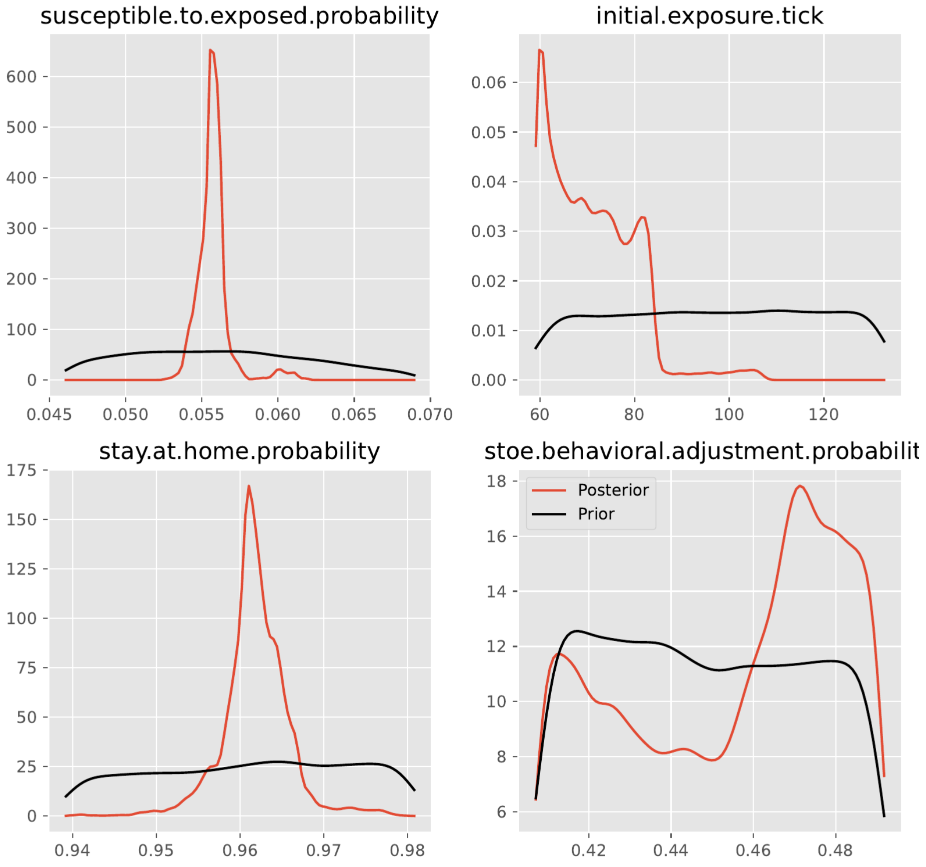


1. Propose new parameters and calculate acceptance ratio
2. If rejected, sample interpolated between proposal and previous
3. Covariance matrix of proposal distribution adjusts with samples

- Random Forest classifier to remove proposals outside of surrogate training set
- Data is smoothed (weekly windows)

BAYESIAN INFERENCE – RESULTS

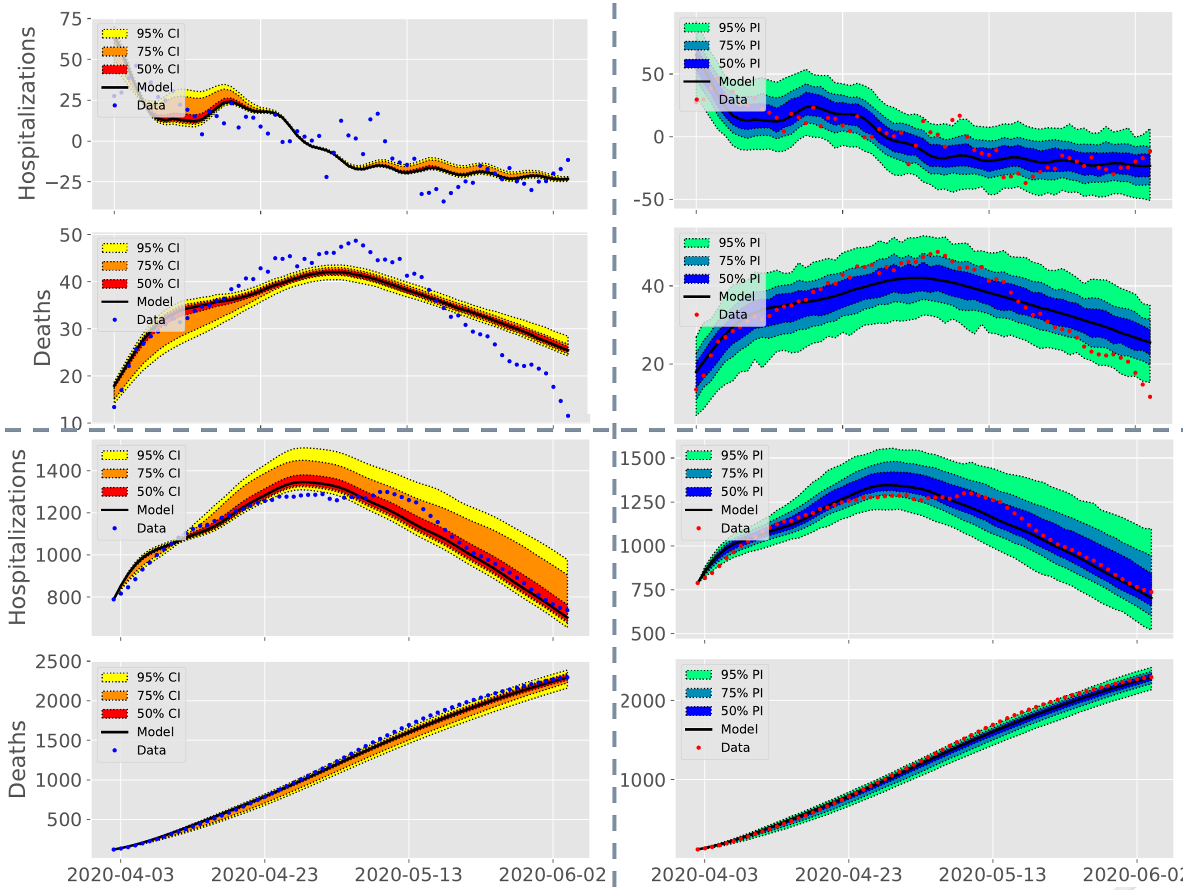
- Posteriors show clear MAP in all but least important parameter (behavior adjustment)
- Posterior predictions capture daily data fairly well but also population rates after cumulative sum



Pushforward **Predictive**

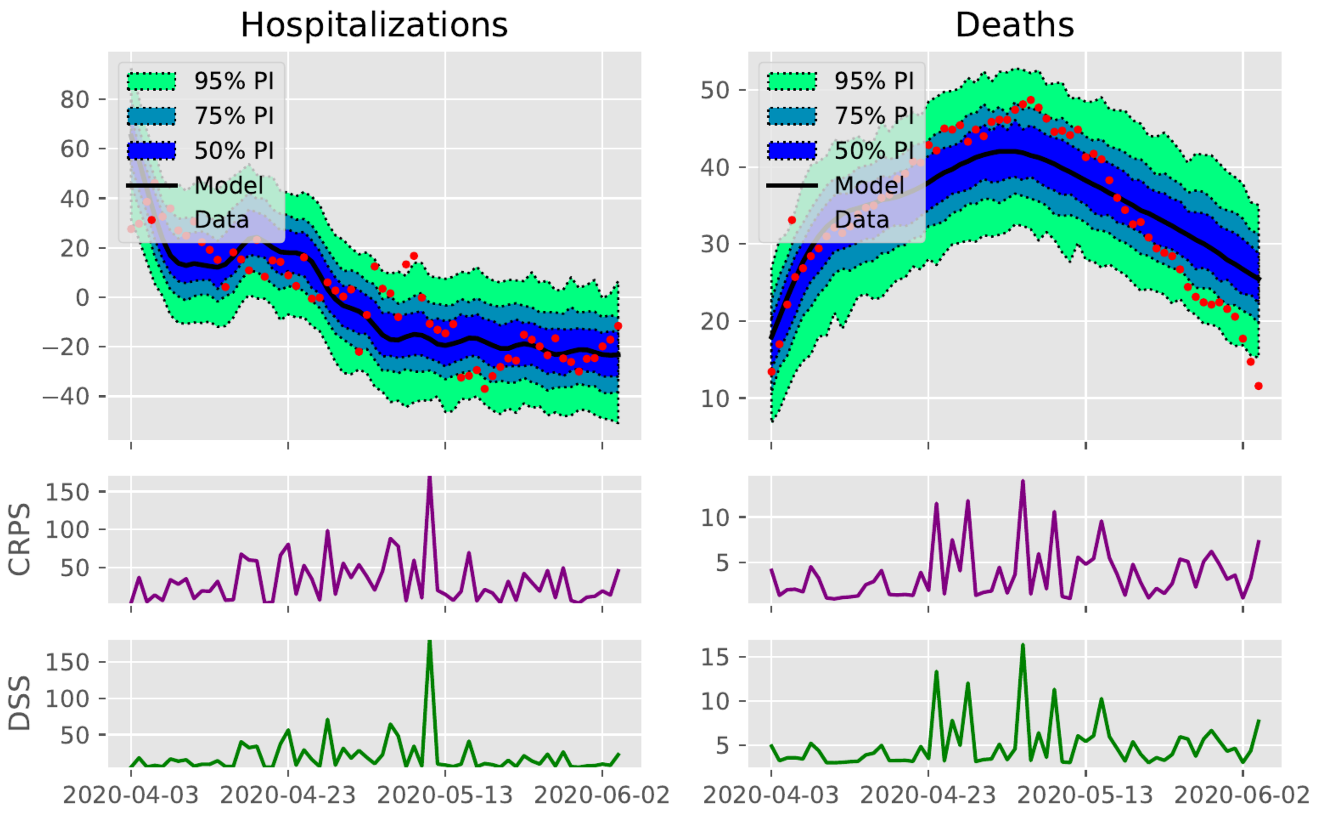
Daily

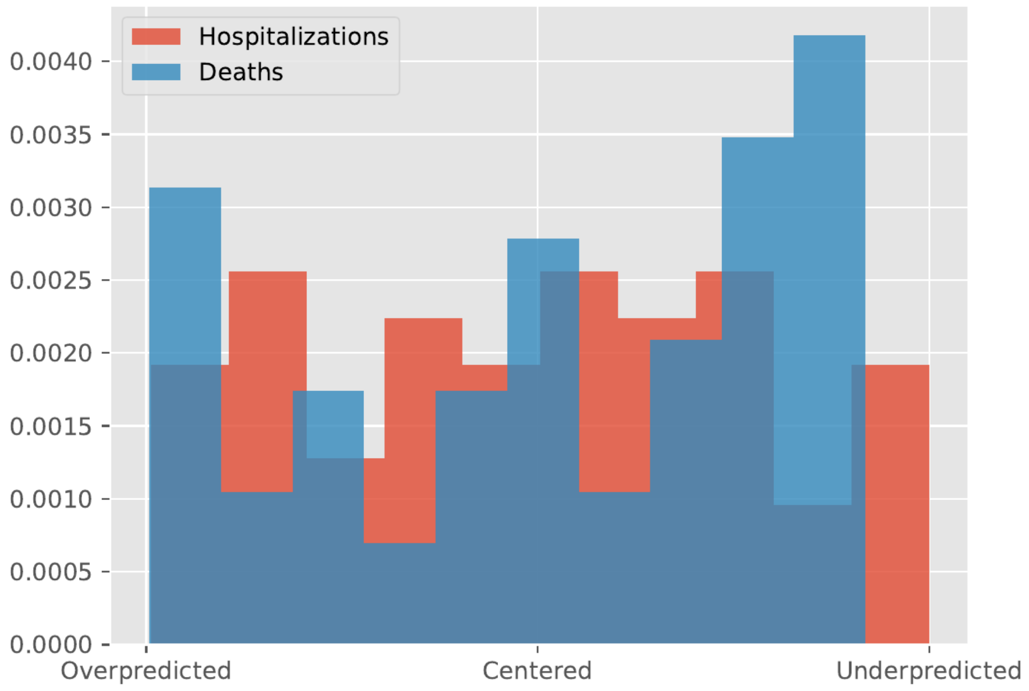
Cumulative



BAYESIAN INFERENCE – SCORING

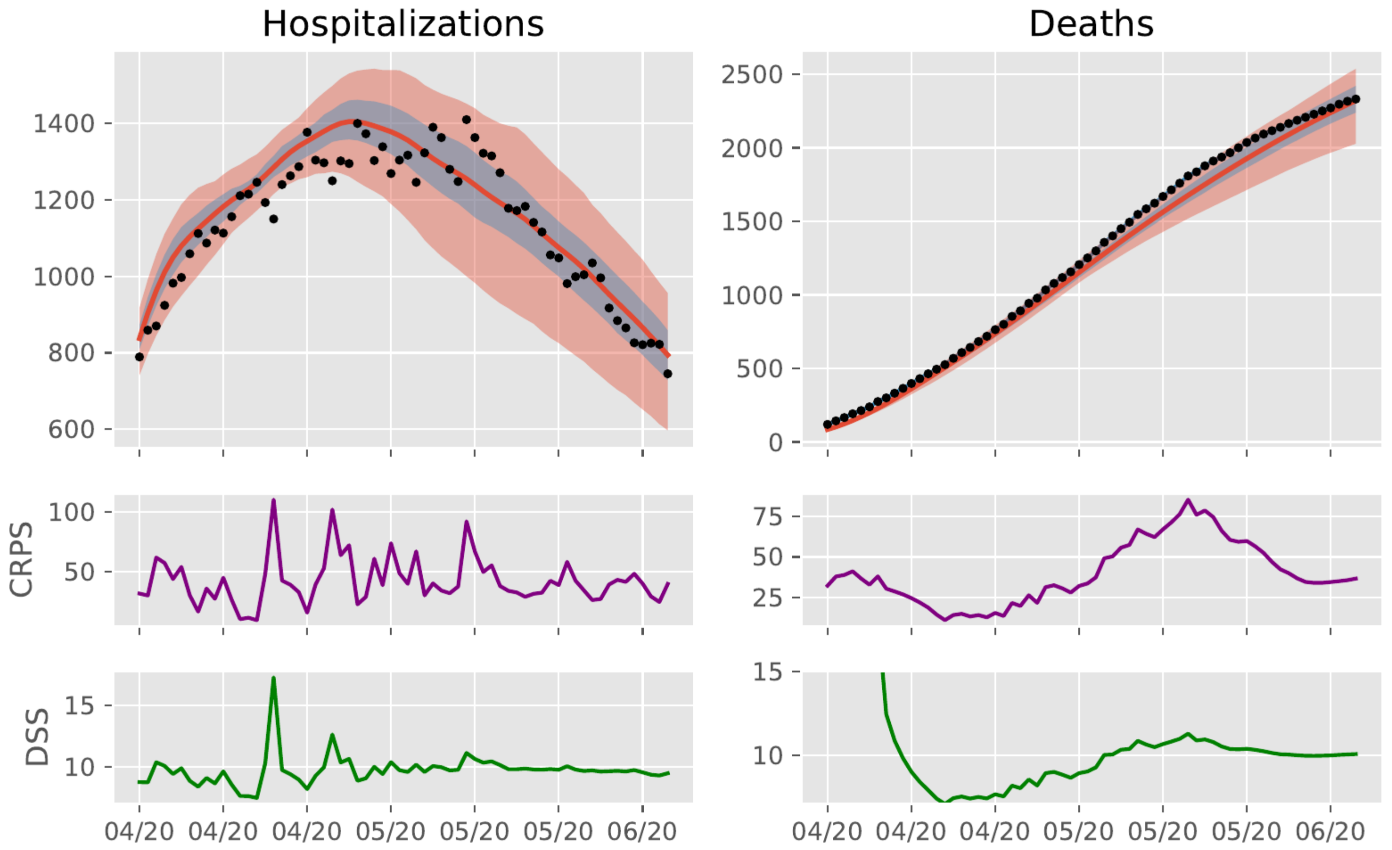
- **CRPS** – measure of absolute error and inter-sample variance (from posterior)
- **DSS** – similar to CRPS but with additional penalization on overconfidence
- **Rank verification histogram** – death predictions are often either under or over predicted

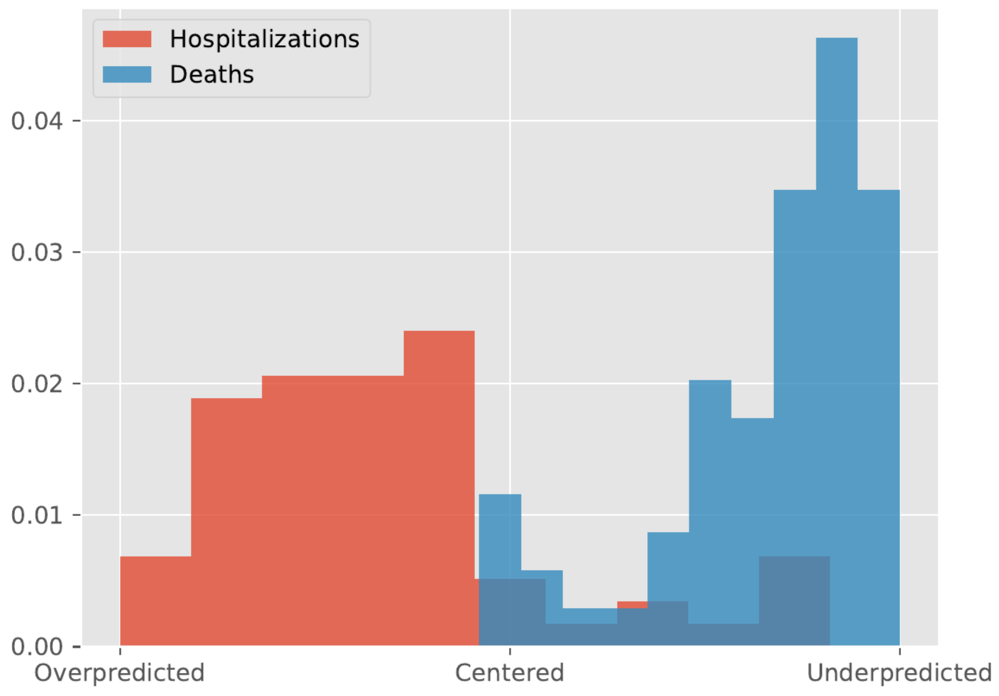




PUSHFORWARD RESULTS – OUTLINE

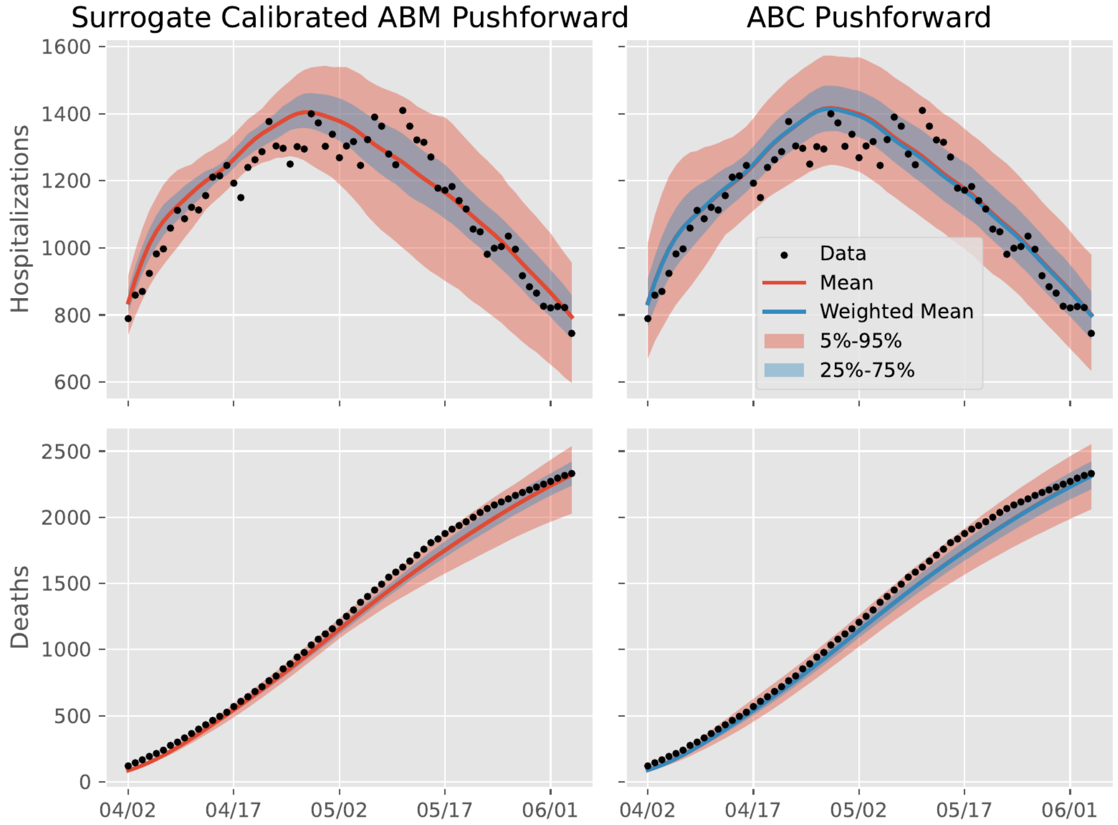
- Posterior samples fed into ABM with 50 initial conditions – resulting trajectories averaged
- Average **over**-prediction of hospitalizations and **under**-prediction of deaths for early times
- Improved accuracy at late times though increased uncertainty

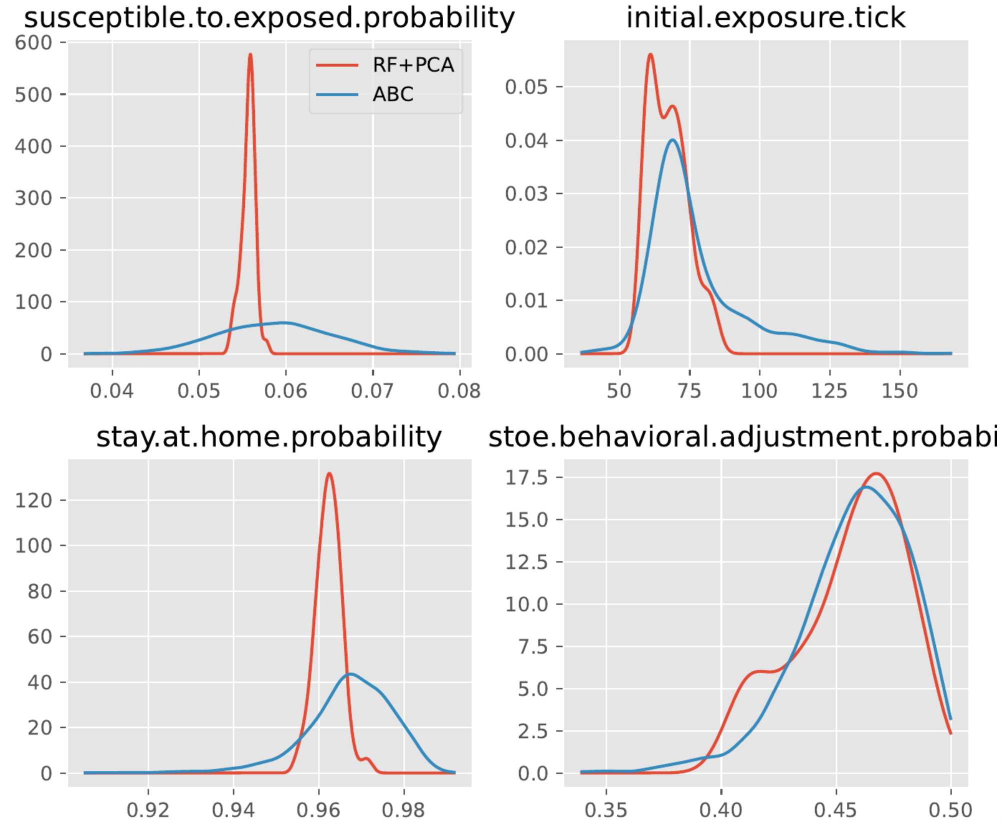




PUSHFORWARD RESULTS – COMPARISON

- rABC calibration of CityCOVID required 3000 ABM samples ($3{\times}10^6$ CPU hrs)
- PCA + RF assisted calibration used 500 samples ($5{\times}10^5$ CPU hrs) with <5 CPU hrs for MCMC
- Almost equally resolved pushforward prediction, but much tighter parameter calibration





CONCLUSION

- PCA based temporal mode decomposition with RF mapping was:
  - Able to adequately approximate mean behavior of population stats in CityCOVID ABM
  - Sampled with control using additional RF classifier
- Bayesian inference yielded more concise posterior distributions than original ABC sampling
- Pushforward population values were comparable with ABC sampling

Challenges / Future work

- Surrogate inadequate for calibration using fixed-seed ABM runs (not averaged)
- Further efforts needed to include measure of ABM stochasticity