A Comparative Study of Techniques for Estimation and Inference of Nonlinear Stochastic Time Series

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Masters Thesis Defence
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2. Stochastic SIR Model
3. Hamiltonian HMCMC
4. Iterated Filtering 2
5. Forecasting Frameworks
6. S-maps & Seasonal Outbreaks
7. Spatiotemporal Epidemics
8. Parallelism & Future Directions

Framing

1


SIResampling
ParticleMCMC
ParticleFilter
Dewdrop
SIS
SeasonalARIMA
EnsembleKF
GARMA
DewdropRegression
ASIR
IF
RPF
MIF2
HMM
RHF
GLM
ParticleFilter
Simplex
ABC
S-map
SGEnKF
KalmanFilter
SimplexProjection
MCMC
HamiltonianMCMC
ARIMA

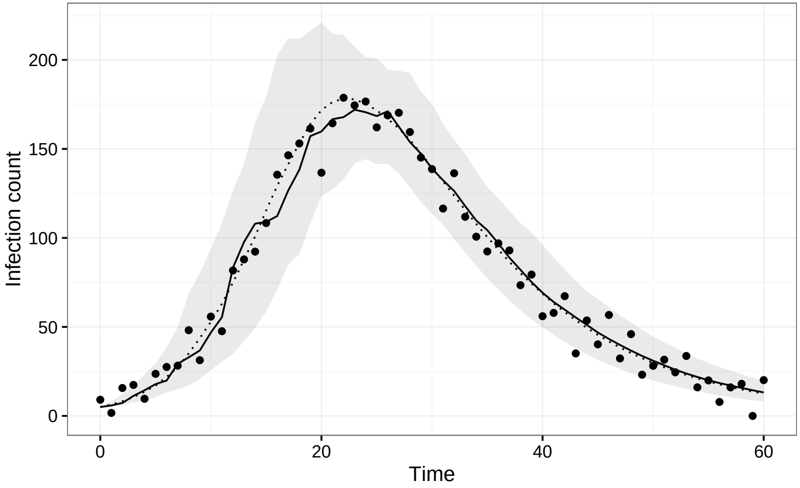
2 Stochastic SIR Model

Stochastic SIR model

$$\frac{dS}{dt} = -\beta SI$$
$$\frac{dI}{dt} = \beta SI - \gamma I$$
$$\frac{dR}{dt} = \gamma I$$

$$+$$

$$\beta_{t+1} = \exp\left[\beta_t + \eta\left(\bar{\beta} - \beta_t\right) + \mathcal{N}(0, \sigma_{proc})\right]$$



Infection count
200
150
100
50
0
0
20
40
60
Time

3 Hamiltonian MCMC

MCMC

Iteratively construct Markov chain to approximate posterior

1. Choose starting parameter set
2. Generate N samples by
   2.1 Propose new sample
   2.2 Compute acceptance ratio
   2.3 Accept/reject sample

/* Select a starting point */
Input : Initialize $\theta^{(1)}$
for $i = 2 : N$ **do**
  /* Sample */
  $\theta^* \sim q(\cdot|\theta^{(i-1)})$
  $u \sim \mathcal{U}(0, 1)$
  /* Evaluate acceptance ratio */
  $r \leftarrow \frac{\mathcal{L}(\theta^*)p(\theta^*)}{\mathcal{L}(\theta)p(\theta)}$
  /* Step acceptance criterion */
  if $u < \min\{1, r\}$ **then**
    $\theta^{(i)} = \theta^*$
  else
    $\theta^{(i)} = \theta^{(i-1)}$

/* Samples from approximated posterior distribution */
Output: Chain of samples $(\theta^{(1)}, \theta^{(2)}, \ldots, \theta^{(N)})$

Hamiltonian Dynamics

Energy

Kinetic $$K(r) = \frac{1}{2} r^T M^{-1} r$$

Potential $$U(\theta) = -\log(\mathcal{L}(\theta)p(\theta))$$

Hamiltonian $$H(\theta, r) = U(\theta) + K(r)$$

Dynamics simulation
$$\frac{d\theta}{dt} = M^{-1} r$$
$$\frac{dr}{dt} = -\nabla U(\theta)$$

HMCMC algorithm

1. Choose starting parameter set
2. Generate N samples by
   2.1 Resampling moments
   2.2 Simulate Hamiltonian dynamics using Leapfrog integration
   2.3 Compute acceptance ratio
   2.4 Accept/reject sample

/* Select a starting point */

Input : Initialize $\theta^{(1)}$

for $i = 2 : N$ **do**

  /* Resample moments */

  for $i = 1 : n$ **do**

    $r(i) \leftarrow \mathcal{N}(0, 1)$

  /* Leapfrog initialization */

  $\theta_0 \leftarrow \theta^{(i-1)}$

  $r_0 \leftarrow r - \nabla U(\theta_0) \cdot \varepsilon/2$

  /* Leapfrog intermediate steps */

  for $j = 1 : L - 1$ **do**

    $\theta_j \leftarrow \theta_{j-1} + M^{-1} r_{j-1} \cdot \varepsilon$

    $r_j \leftarrow r_{j-1} - \nabla U(\theta_j) \cdot \varepsilon$

  /* Leapfrog last steps */

  $\theta^* \leftarrow \theta_{L-1} + M^{-1} r_{L-1} \cdot \varepsilon$

  $r^* \leftarrow \nabla U(\theta_L) \cdot \varepsilon/2 - r_{L-1}$

  /* Evaluate acceptance ratio */

  $r = \exp\left[H(\theta^{(i-1)}, r) - H(\theta^*, r^*)\right]$

  /* Sample */

  $u \sim \mathcal{U}(0, 1)$

  /* Step acceptance criterion */

  if $u < \min\{1, r\}$ **then**

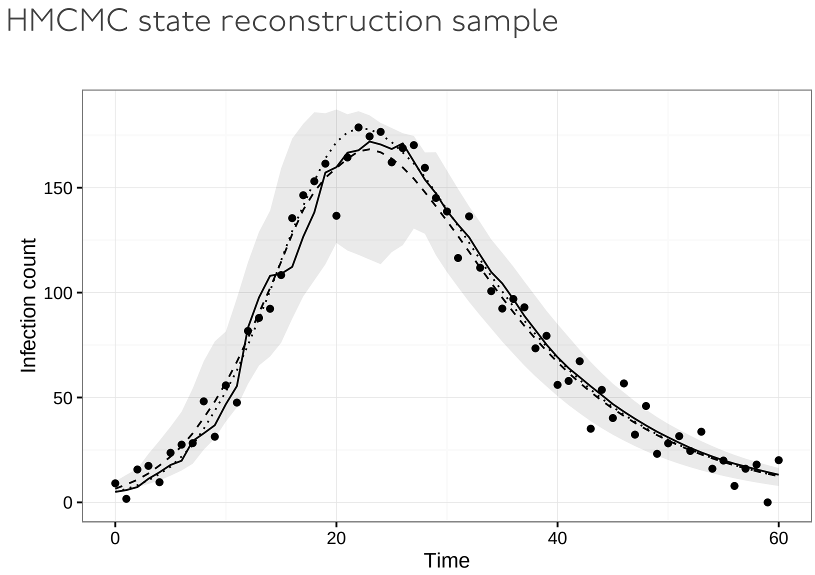
    $\theta^{(i)} = \theta^*$

  else

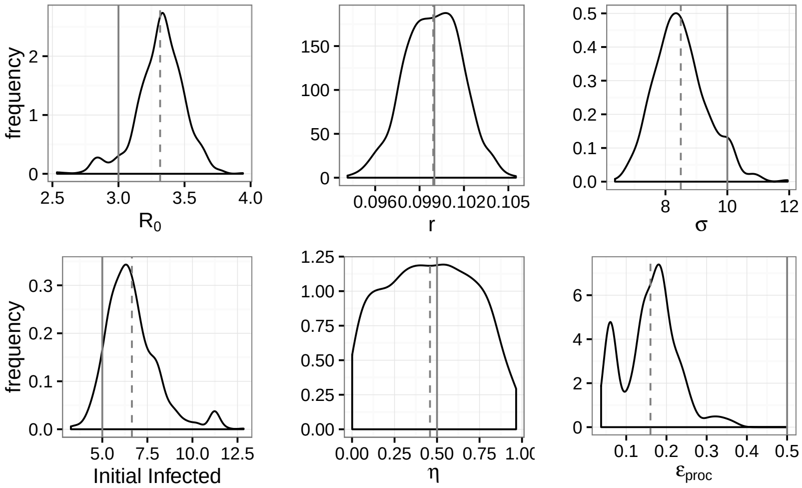
    $\theta^{(i)} = \theta^{(i-1)}$

/* Samples from approximated posterior distribution */

Output: Chain of samples $(\theta^{(1)}, \theta^{(2)}, \ldots, \theta^{(N)})$


HMCMC state reconstruction sample
Infection count
Time
0
50
100
150
0
20
40
60

HMCMC parameter estimation kernels sample



Iterated Filtering 2

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Basic Particle Filter

Iterative prediction-update cycle prunes particle cohort of poor parameter estimates

1. Initialize particles with parameter sets
2. For each data point
   - 2.1 Evolve particle states
   - 2.2 Weight via likelihood
   - 2.3 Resample proportional to weights

/* Select a starting point */
Input : Observations $D = y_1, y_2, \ldots, y_T$, initial particle distribution P_0 of size J

/* Setup */
Initialize particle cohort by sampling $(p^{(1)}, p^{(2)}, \ldots, p^{(J)})$ from P_0

for $t = 1 : T$ **do**

  /* Evolve */
  for j = 1:J **do**
    $X_t^{(j)} \leftarrow f_1(X_{t-1}^{(j)}, \theta^{(j)})$

  /* Weight */
  for j = 1:J **do**
    $w^{(j)} \leftarrow P(y_t | X_t^{(j)}, \theta^{(j)}) = f_2(X_t^{(j)}, \theta^{(j)})$

  /* Normalize */
  for j = 1:J **do**
    $w^{(j)} \leftarrow w^{(j)} / \sum_1^J w^{(j)}$

  /* Resample */
  $p^{(1:J)} \leftarrow \text{sample}(p^{(1:J)}, \text{prob} = w, \text{replace} = \text{true})$

/* Samples from approximated posterior distribution */
Output: Cohort of posterior samples $(\theta^{(1)}, \theta^{(2)}, \ldots, \theta^{(J)})$

Iterated Filtering 2

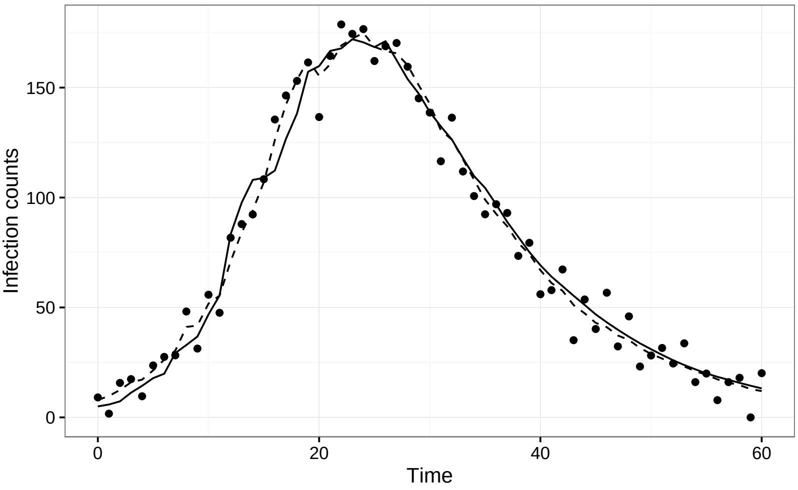
Treat parameter estimates as stochastic processes

Multiple passes through data (a la Data cloning)

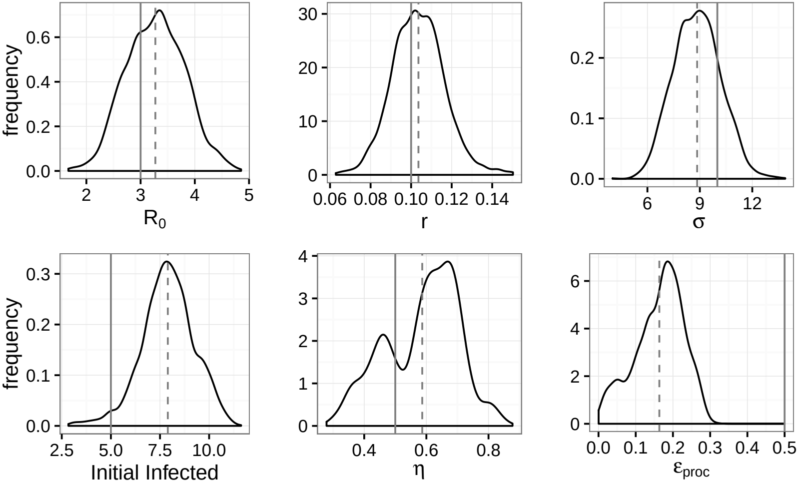
/* Setup */
Initialize particle cohort by sampling $(p^{(1)}, p^{(2)}, \ldots, p^{(J)})$ from P_0
/* Particle seeding distribution */
$\Theta \leftarrow P_0$
for $m = 1 : M$ **do**
    /* Pass perturbation */
    for j = 1:J **do**
        $p^{(j)} \sim h(\Theta^{(j)}, \sigma_m)$
    for $t = 1 : T$ **do**
        for j = 1:J **do**
            /* Iteration perturbation */
            $p^{(j)} \sim h(p^{(j)}, \sigma_m)$
            /* Evolve */
            $X_t^{(j)} \leftarrow f_1(X_{t-1}^{(j)}, \theta^{(j)})$
            /* Weight */
            $w^{(j)} \leftarrow P(y_t | X_t^{(j)}, \theta^{(j)}) = f_2(X_t^{(j)}, \theta^{(j)})$
        /* Normalize */
        for j = 1:J **do**
            $w^{(j)} \leftarrow w^{(j)} / \sum_1^J w^{(j)}$
        /* Resample */
        $p^{(1:J)} \leftarrow \text{sample}(p^{(1:J)}, \text{prob} = w, \text{replace} = \text{true})$
    /* Collect particles for next pass */
    for $j = 1 : J$ **do**
        $\Theta^{(j)} \leftarrow p^{(j)}$

/* Samples from approximated posterior distribution */
Output: Cohort of posterior samples $(\theta^{(1)}, \theta^{(2)}, \ldots, \theta^{(J)})$

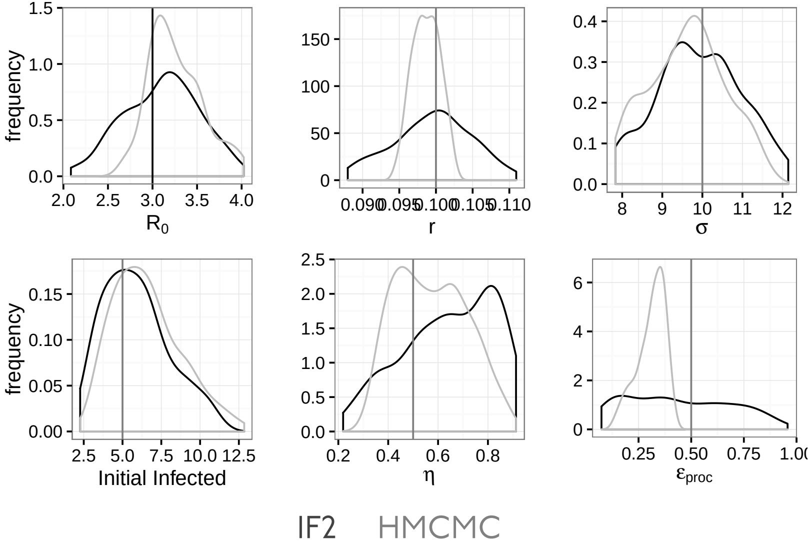
IF2 state reconstruction sample



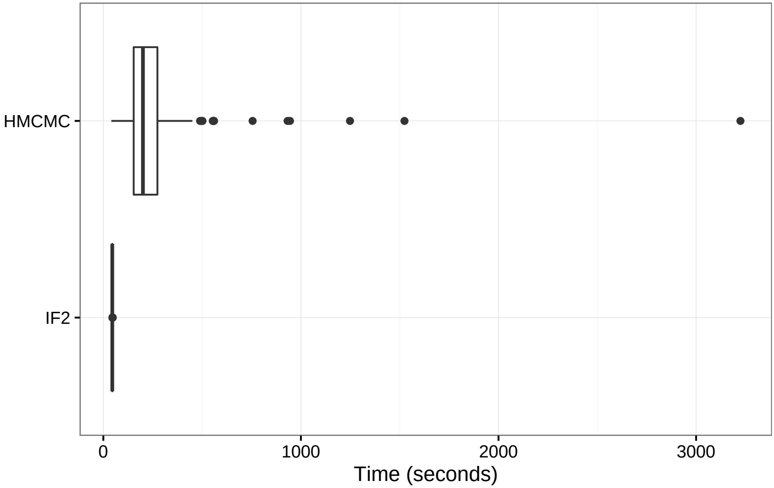
IF2 parameter estimation kernels sample



Mean parameter estimation distributions



Running times



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Forecasting Frameworks

IF2 + Parametric bootstrapping + Forward simulation

- Provides additional samples from posterior distribution
- Forward simulation using states point estimate, posterior samples

Input : Forward simulator $S(\theta)$, data set D

/* Initial fit */
$\theta^* \leftarrow \mathrm{IF2}(D)$

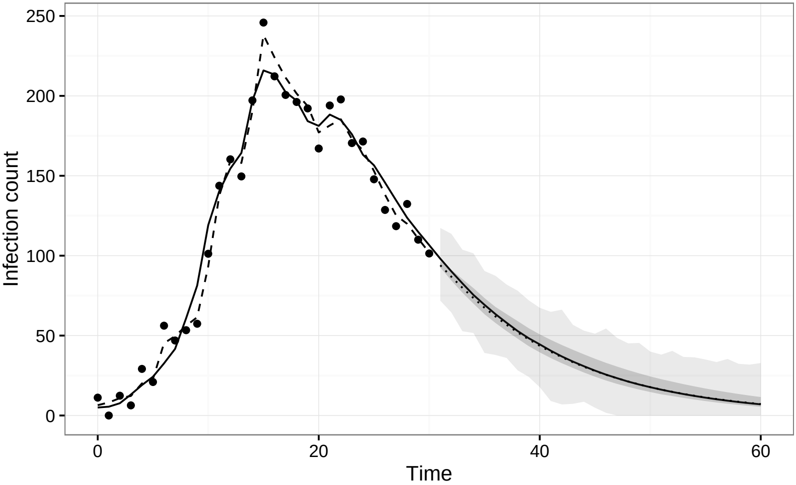
/* Generate artificial data sets */
for $i = 1 : M$ **do**
  $D_i \leftarrow S(\theta^*)$

/* Fit to new data sets */
for $i = 1 : M$ **do**
  $\theta_i \leftarrow \mathrm{IF2}(D_i)$

/* Simulate forward to produce forecasts */
for $i = 1 : M$ **do**
  $F_i \leftarrow S(D, \theta_i)$

Output: Forecast trajectories $F_1, F_2, \ldots, F_M$

IF2 parametric bootstrapping forecast



HMCMC + State reconstructions + Forward simulation

- Reconstruct states using latent process noise samples
- Simulate forward

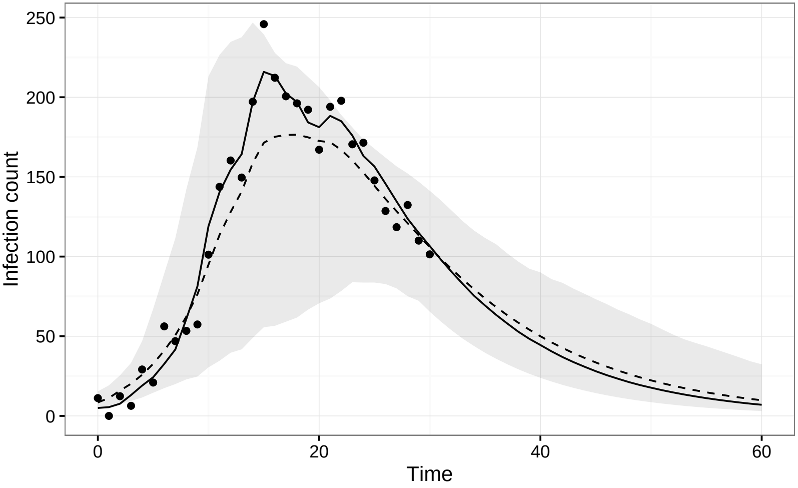
/* Sample from the posterior */
Input : Posterior samples $\theta_1, \theta_2, \ldots, \theta_M$

/* Reconstruct state estimates */
for $i = 1 : M$ **do**
    $D_i \leftarrow S(\theta_i)$

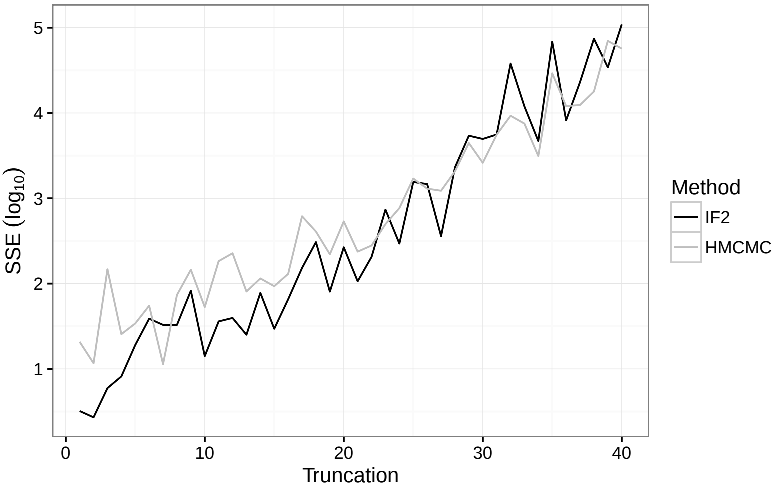
/* Simulate forward to produce forecasts */
for $i = 1 : M$ **do**
    $F_i \leftarrow S(D_i, \theta_i)$

Output: Forecast trajectories $F_1, F_2, \ldots, F_M$

HMCMC parametric bootstrapping forecast



Forecast accuracy comparison



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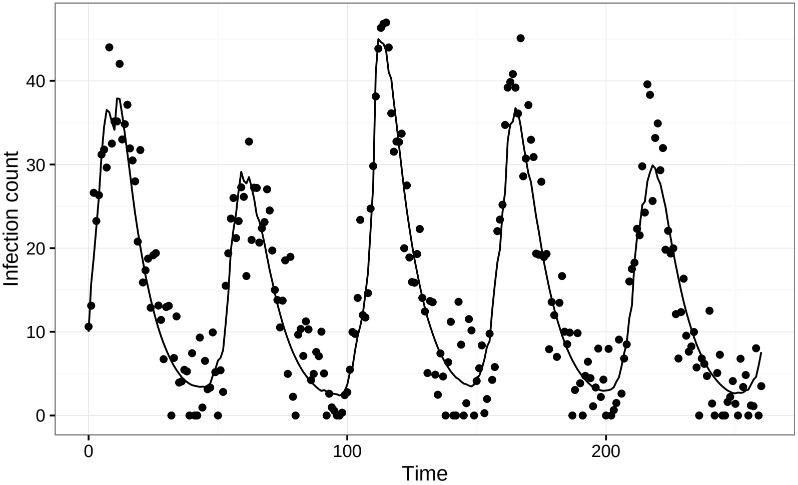
S-maps & Seasonal Outbreaks

Stochastic SIRS model

$$\frac{dS}{dt} = -\beta SI + \alpha R$$
$$\frac{dI}{dt} = \beta SI - \gamma I$$
$$\frac{dR}{dt} = \gamma I - \alpha R$$

$$+$$

$$\beta_{t+1} = \exp\left[\beta_t + \eta\left(\bar{\beta} - \beta_t\right) + \mathcal{N}(0, \sigma_{\text{proc}})\right]$$


Infection count
0
10
20
30
40
0
100
200
Time

S-map

- Construct global mapping of time-lagged vectors (the library) to future states
- Weightings are used to penalize poorly matching library vectors

/* Select a starting point */

Input : Time series $x_1, x_2, \ldots, x_T$, embedding dimension E, distance penalization θ, forecast length L, predictor vector $\mathbf{x_t}$

/* Construct library $\{x_i\}$ */

for $i = E : T$ **do**

  $x_i = (x_i, x_{i-1}, \ldots, x_{i-E-1})$

/* Construct mapping from library vectors to predictions */

for $i = 1 : (T_E + 1)$ **do**

  for $j = 1 : E$ **do**

    $A(i, j) = w(||x_i - \mathbf{x_t}||)x_i(j)$

for $i = 1 : (T_E + 1)$ **do**

  $b(i) = w(||x_i - \mathbf{x_t}||)y_i$

/* Use SVD to solve the mapping system, Ac = b */

$\mathrm{SVD}(Ac = b)$

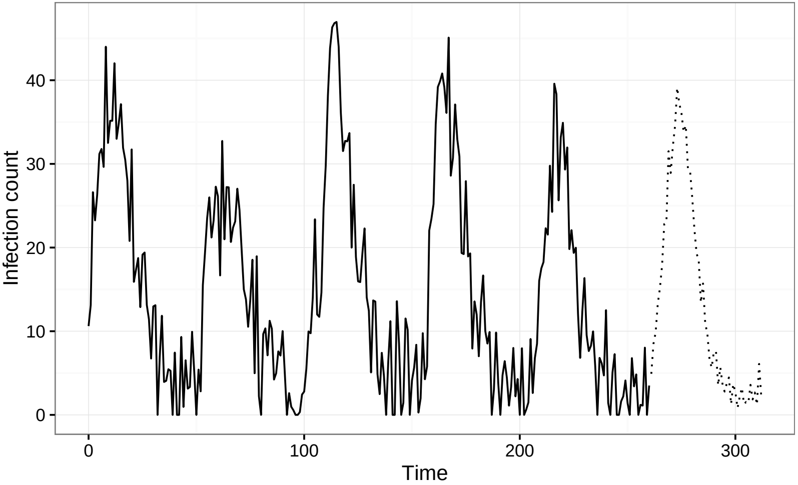
/* Compute forecast */

$\hat{y_t} = \sum_{j=0}^{E} c_t(j)\mathbf{x_t}(j)$

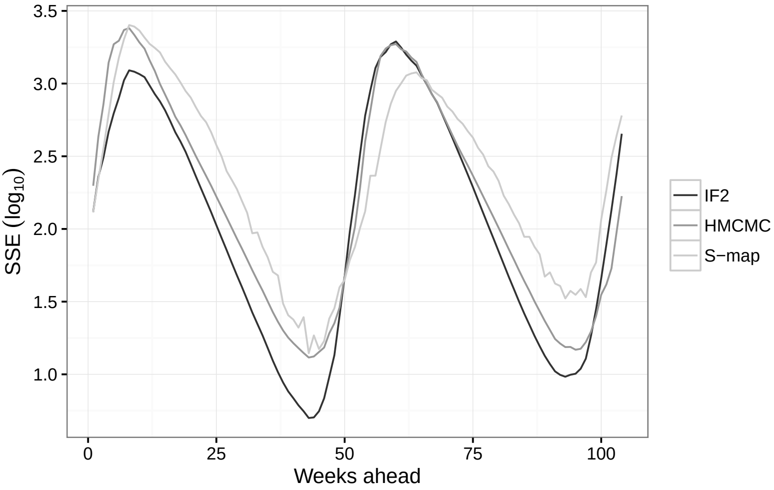
/* Forecasted value in time series */

Output: Forecast $\hat{y_t}$

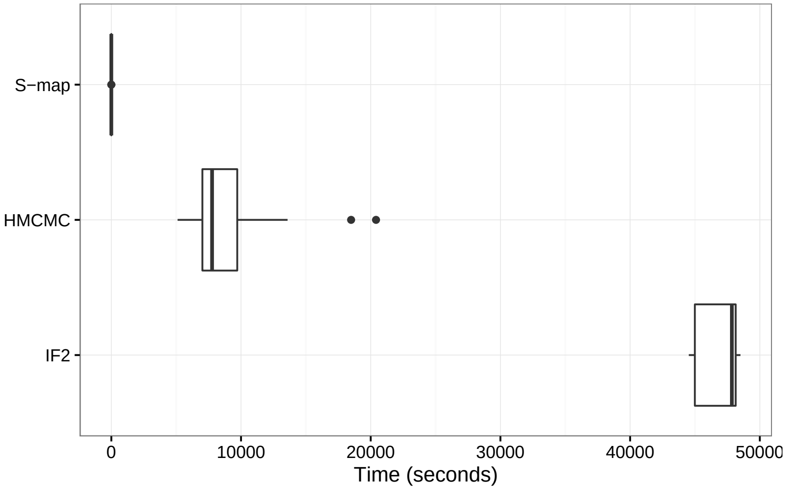
S-map forecast



SIRS model forecasting error



SIRS model forecasting runtimes



S-map: 316,000x faster than IF2, 61,800x faster than HMCMC

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Spatiotemporal Epidemics

Stochastic Spatial SIR model

$$\frac{dS_i}{dt} = -\left(1 - \phi\frac{M}{M+1}\right)\beta_i S_i I_i - \frac{\phi}{M+1} S_i \sum_{j=1}^{M} \beta_{ij} I_j$$

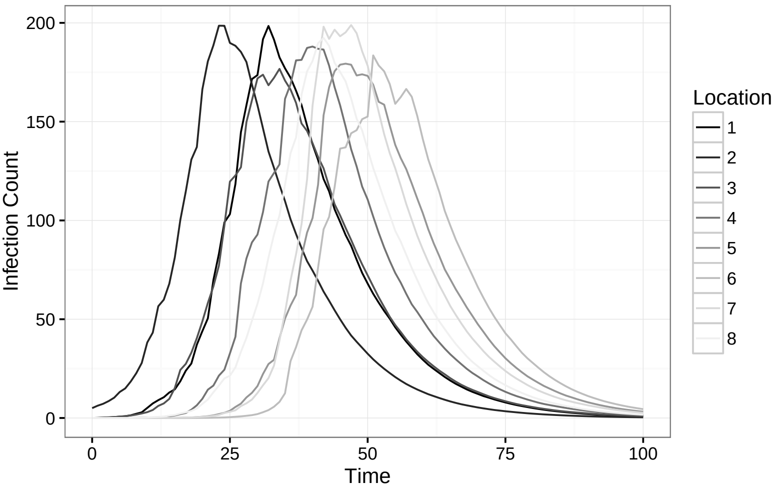
$$\frac{dI_i}{dt} = \left(1 - \phi\frac{M}{M+1}\right)\beta_i S_i I_i + \frac{\phi}{M+1} S_i \sum_{j=1}^{M} \beta_{ij} I_j - \gamma I_i$$

$$\frac{dR_i}{dt} = \gamma I_i$$

$$+$$

$$\beta_{i,t+1} = \exp\left[\beta_{i,t} + \eta\left(\bar{\beta} - \beta_{i,t}\right) + \mathcal{N}(0, \sigma_{proc})\right]$$

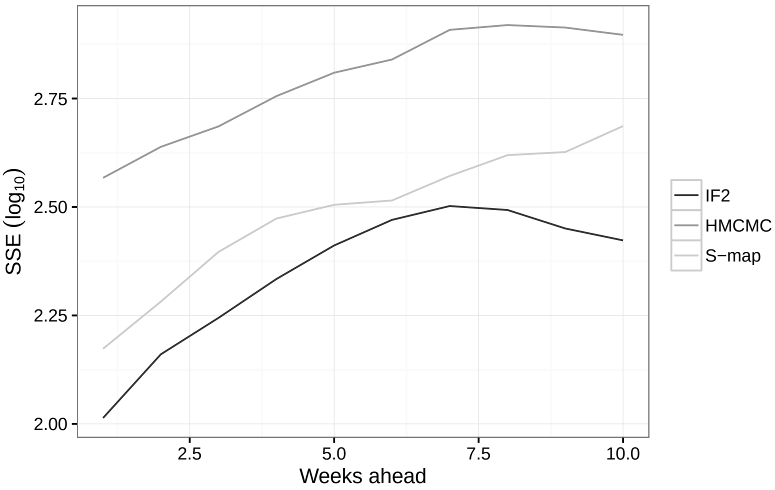
Stochastic spatial SIR model simulation (ring topology)

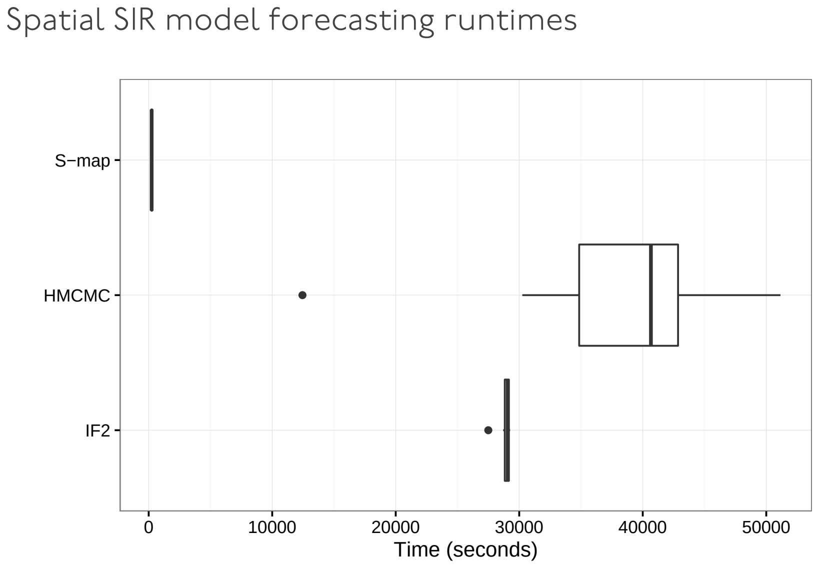


Dewdrop Regression

- “Stitching” together multiple short time series into single library
- Requires scaling

Stochastic SIR model forecasting error




Spatial SIR model forecasting runtimes
S−map
HMCMC
IF2
0
10000
20000
30000
40000
50000
Time (seconds)

8

Parallelism & Future Directions

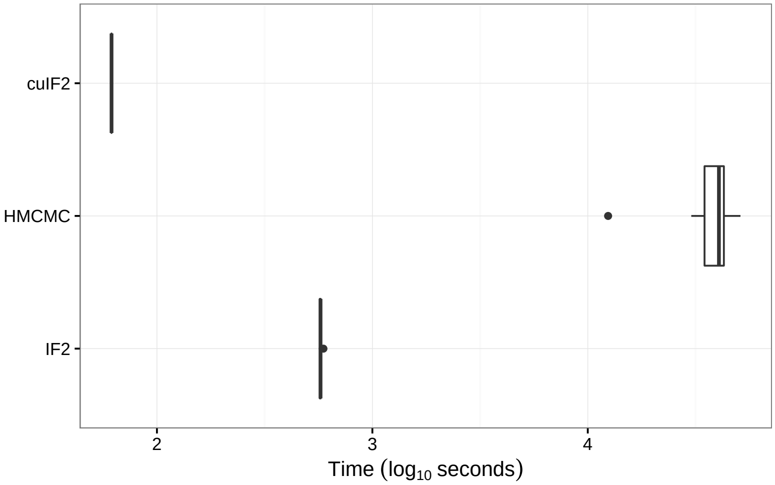
Conclusions

- IF2 produces superior forecasts in all scenarios
- S-mapping runs orders of magnitude faster than other methods

More than Moore

- Moore's Law is ceasing to hold
- Focus now on distributed computing
- MCMC-based methods are resistant to parallelization
    - Chain construction requires iterative dependence
- IF2 exhibits high parallel potential
    - Preliminary CUDA (GPU-accelerated) implementation - `cuIF2`

Spatial SIR model fitting times



`cuIF2`: 9.33x faster than IF2, 617x faster than HMCMC

THE BEST THESIS DEFENSE IS A GOOD THESIS OFFENSE.