Sequential Stein Variational Gradient Descent for Time Series Model Estimation

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Introduction

State-Space models have become popular tools in the analysis of time-series. They allow for arbitrary transition and observation dynamics. The researcher can assign a latent data generating process, while simultaneously allowing for observational error on that process. The classic algorithm for fitting non-Gaussian SSMs is given by the particle filter. Although many variations exist, we generally refer to the sampling importance re-sampling (SIR) filter when discussing particle filtering. Although a powerful inference tool, particle filtering suffers from several well known drawbacks. The first is the problem of filter degeneracy. This occurs when the observations are far from the state predicted by the latent dynamics. The second is the excessive run-times on longer time series with complex dynamics. We propose an alternative approach that we hope will do better than particle filtering in practice. In this approach, Stein Variational Gradient Descent (SVGD) is used to sequentially estimate the distribution of state variables in each time step, conditional on observed data up through that time.

Overview of SVGD

Stein Variational Gradient Descent can be used to estimate a continuous distribution by a set of particles. By iteratively transporting samples from an initial distribution in the direction of the likelihood, we are able to generate compute Monte Carlo estimates of the posterior. The usefulness of this approximation is apparent in Bayesian statistics, where the usually intractable normalizing constant disappears in the particle update step. The particles are subject to the following gradient ascent procedure.

$$x_i^{l+i} \leftarrow x_i^l + \epsilon_l \hat{\phi^*}(x_i^l)$$

$$\hat{\phi^*}(x) = \frac{1}{n}\sum_{j=1}^{n}[k(x_j^l, x)\nabla_{x_j^l} log\ p(x_j^l) + \nabla_{x_j^l} k(x_j^l, x)]$$

for an arbitrary positive definite kernel function $k(.,.)$ usually chosen to be a Gaussian kernel.

State Space Models

Suppose we are given a time series $Y_1, Y_2, ..., Y_t$ for $Y \in \mathbb{R}$. We model the sequence as a state-space model parameterized by an observation density $p(y_t|x_t)$ and a transition density $p(x_t|x_{t-1})$ Figure 1.

We are interested in the filtering distribution $p(x_1, ..., x_n|y_1, ..., y_n)$ which by Bayes formula is

$$p(x_1, ..., x_n|y_1, ..., y_n) = \frac{p(y_1, ..., y_n|x_1, ..., x_n)p(x_1, ..., x_n)}{Z}$$

.

Because computing the normalizing constant Z is intractable for many choices of $p(y_t|x_t)$ and $p(x_t|x_{t-1})$, we must resort to Monte Carlo algorithms. The classic approach that incorporates the sequential nature of the

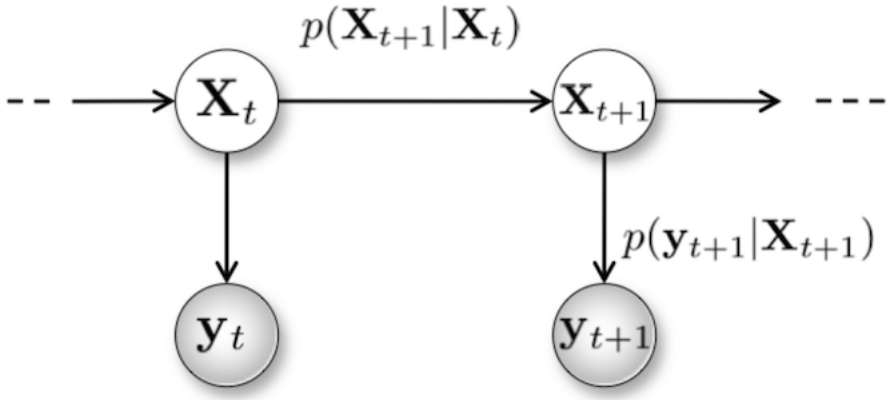

Figure 1: State-Space Model Setup

data is given by the particle filtering algorithm. Particle filtering approximates the filtering density using sequential importance sampling. We instead focus on the following recursion.

$$p(x_t|y_{1:t}) = \int p(x_{0:t}|y_{1:t}) d_{x_0:t-1}$$

$$= \frac{p(y_t|x_t)}{\int p(y_t|x_t)p(x_t|y_{1:t-1})dx_t} p(x_t|y_{1:t-1})$$

$$\propto p(y_t|x_t)p(x_t|y_{1:t-1})$$

$$\propto p(y_t|x_t)p(x_t|y_{1:t-1})$$

$$\propto p(y_t|x_t) \int_{x_{t-1}} p(x_t, x_{t-1}|y_{1:t-1}) d_{x_{t-1}}$$

$$\propto p(y_t|x_t) \int_{x_{t-1}} p(x_t|x_{t-1})p(x_{t-1}|y_{1:t-1}) d_{x_{t-1}}$$

which we can approximate using svgd as

$$\approx p(y_t|x_t) \frac{1}{n} \sum_{i=1}^{n} p(x_t|x_{t-1}^{(i)})$$

We can now estimate $p(x_{t+1}|y_{1:t+1})$ using the same algebra as above. (proof in apendix A)

Model Structure

States:

- $X_1 \sim g_1(x_1; \xi)$
- $X_t|X_{t-1} \sim g(x_t|x_{t-1}; \xi)$ for all $t = 2, \ldots, T$

Observations:

- $Y_t|X_t \sim h(y_t|x_t; \zeta)$

Here, $g_1(\cdot)$ and $g(\cdot)$ are appropriately defined probability density functions depending on parameters ξ and $h(\cdot)$ is an appropriately defined probability density function or probability mass function depending on parameters ζ.

Define $\theta = (\xi, \zeta)$ to be the full set of model parameters.

Filtering

There are two types of filtering:

1. sample of particles $x_{1:T}^{(k)} \sim f(x_{1:T}|y_{1:T})$
2. sample of particles $x_t^{(k)} \sim f(x_t|y_{1:t})$ for each $t = 1, \ldots, T$

Let's look at the second one. Assume we have a sample $x_{t-1}^{(k)} \sim f(x_{t-1}|y_{1:t-1})$

$$\begin{aligned}
p(x_t|y_{1:t}) &= \frac{f(x_t, y_t|y_{1:t-1})}{f(y_t|y_{1:t-1})} \\
&\propto f(x_t, y_t|y_{1:t-1}) \\
&= f(y_t|x_t) f(x_t|y_{1:t-1}) \\
&= f(y_t|x_t) \int f(x_t, x_{t-1}|y_{1:t-1}) dx_{t-1} \\
&= f(y_t|x_t) \int f(x_t|x_{t-1}) f(x_{t-1}|y_{1:t-1}) dx_{t-1} \\
&\approx f(y_t|x_t) \sum_{x_{t-1}^{(k)}} f(x_t|x_{t-1}^{(k)})
\end{aligned}$$

So $\log\{p(x_t|y_{1:t})\}$ is approximately proportional to $\log\{f(y_t|x_t)\} + \log\{\sum_{x_{t-1}^{(k)}} f(x_t|x_{t-1}^{(k)})\}$

Locally Level Gaussian Noise Model

In order to demonstrate that the approximation is reasonable we evaluate the predictive accuracy under an analytically tractable model, the locally level Gaussian model. This model takes the form

$$X_t \sim N(X_{t-1}, \sigma_1^2)$$

$$Y_t \sim N(X_t, \sigma_2^2)$$

```
##
## Attaching package: 'dlm'
```

```
## The following object is masked from 'package:ggplot2':
##
##     %+%
```

```
## [1] "python /home/gcgibson/ssvgd/python/locally_level_gaussian.py  -0.257101984753462, 2.93940091932
```

```
##
## Attaching package: 'cowplot'
```

```
## The following object is masked from 'package:ggplot2':
##
##     ggsave
```

```
## Warning: Removed 1 rows containing missing values (geom_path).

## Warning: Removed 1 rows containing missing values (geom_path).

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```
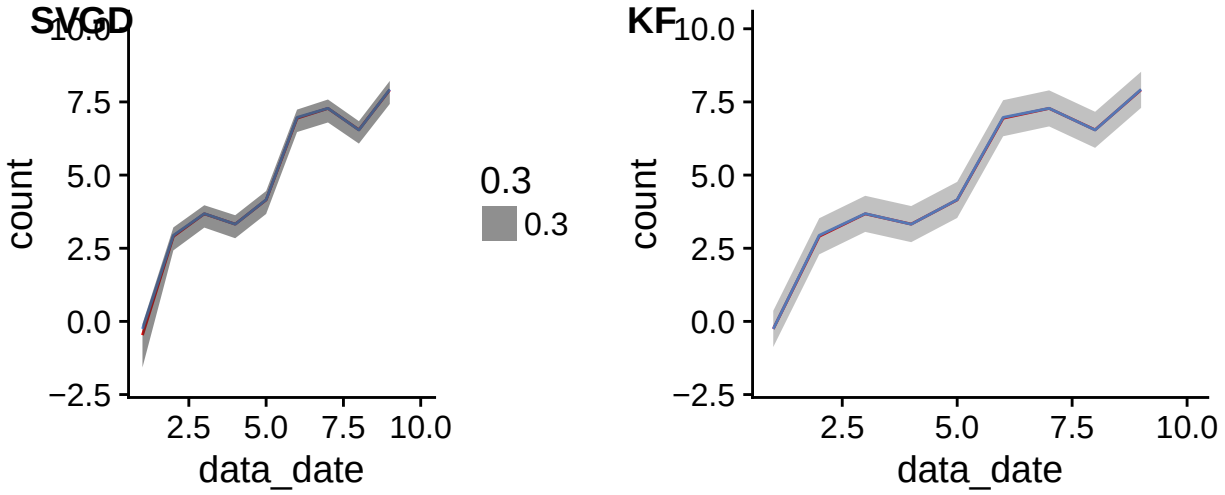



Poisson Observation Model With Seasonal State-Space Dynamics

In order to evaluate the performance on more involved dynamics we consider the following state-space model.

$$\begin{pmatrix} X_{t,1} \\ X_{t,2} \end{pmatrix} = \begin{pmatrix} cos(2\pi/s) & sin(2\pi/s) \\ -sin(2\pi/s) & cos(2\pi/s) \end{pmatrix} \begin{pmatrix} X_{t-1,1} \\ X_{t-1,2} \end{pmatrix}$$

$$Y_t \sim Pois(e^{X_{t,1}})$$

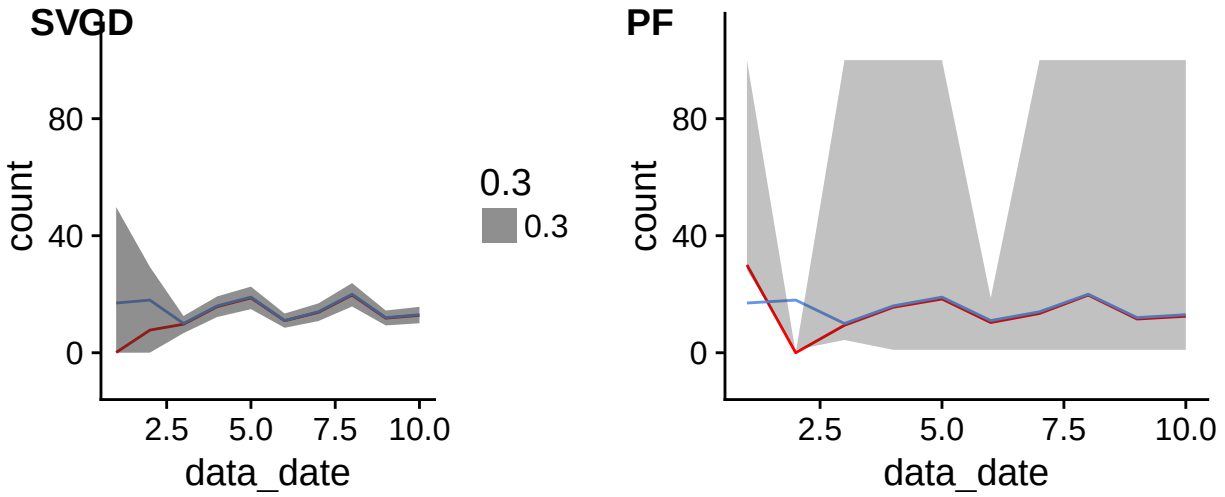
```
## Loading required package: rbiips

## Loading required package: coda

## Loading required package: MASS

##
## Attaching package: 'MASS'

## The following object is masked from 'package:dplyr':
##
##     select

## ##
## ## Markov Chain Monte Carlo Package (MCMCpack)

## ## Copyright (C) 2003-2018 Andrew D. Martin, Kevin M. Quinn, and Jong Hee Park

## ##
## ## Support provided by the U.S. National Science Foundation

## ## (Grants SES-0350646 and SES-0350613)
## ##

## * Parsing model in: /home/gcgibson/ssvgd/bug_files/seasonal_pois.bug
```

```
## Warning in biips_model(seasonal_model_file, data = seasonal_data,
## sample_data = FALSE): Unused variables in data: G, mean_sigma_init,
## cov_sigma_init, mean_x_init
```

```
## * Compiling model graph
##   Declaring variables
##   Resolving undeclared variables
##   Allocating nodes
##   Graph size: 121
```

```
## * Assigning node samplers
## * Running SMC forward sampler with 100000 particles
##   |-------------------------------------------------| 100%
##   |*************************************************| 11 iterations in 9.29 s
```

```
## [1] "python /home/gcgibson/ssvgd/python/seasonal.py  17, 18, 10, 16, 19, 11, 14, 20, 12, 13"
```



Divergent Particle Filter

We next investigate the ability of SSVGD to perform in the presence of poor initialization. This is a well known issue with current particle filter implementations: starting far from a plausible value of x_0 forces all particles to receive weight 0 under the likelihood, leading to a degenerate filtering distribution. However, under SSVGD, we can simply increase the number of iterations, allowing for arbitrarily poor starting points. Standard particle filtering algorithms use effective sample size as a measure of degeneracy. This is commonly defined as

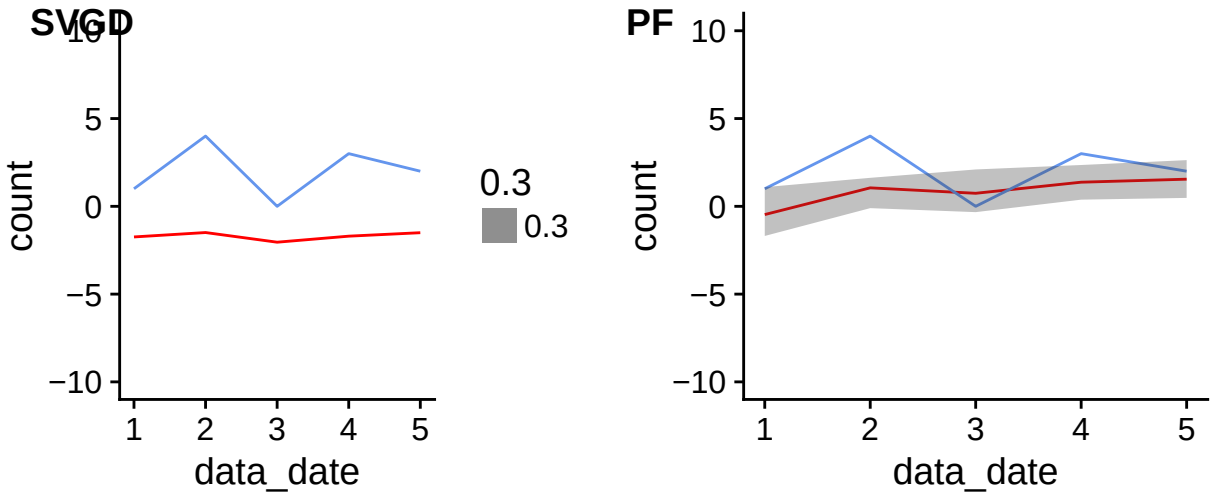
$$S_{eff}^{pf} = \frac{1}{\sum_i (w_t^i)^2}$$

. The common rule of thumb is to not allow this quantity to drop below 50. The natural translation of this metric into particle filtering is compute the same metric based on the samples obtained by SSVGD.

```
## * Parsing model in: /home/gcgibson/ssvgd/bug_files/locally_level_1.bug
## * Compiling model graph
##   Declaring variables
##   Resolving undeclared variables
##   Allocating nodes
##   Graph size: 14
```

```
## * Assigning node samplers
## * Running SMC forward sampler with 100 particles
```

```
##   |-------------------------------------------------| 100%
##   |*************************************************| 5 iterations in 0.00 s

## * Diagnosis of variable: x[1:5]
##   Filtering: POOR
##     The minimum effective sample size is too low: 8.152
##     Estimates may be poor for some variables.
##     You should increase the number of particles
## .  Smoothing: POOR
##     The minimum effective sample size is too low: 4.629
##     Estimates may be poor for some variables.
##     You should increase the number of particles
## .

## [1] -0.4692  1.0525  0.7421  1.3743  1.5461

## [1] "python /home/gcgibson/ssvgd/python/llg.py  1, 4, 0, 3, 2"
```




```
## NULL
```

Diagnostics

Standard particle filtering algorithms use effective sample size as a measure of degeneracy. This is commonly defined as

$$S_{eff} = \frac{1}{\sum_i (w_i)^2}$$

. The common rule of thumb is to not allow this quantity to fall below 50. Indeed, software implementations such as Biips throws an error if the number of effective particles falls below 50. We compute the effective sample size in an analogous way to the particle filter, where w_i is defined as in the SIR particle filter.

```
library(knitr)

ess_df <- data.frame(seq(1:5),effect_size,out_smc$x$f$ess)
colnames(ess_df) <- c("t","SSVGD ESS", "PF ESS")
kable(ess_df,caption="Effective Sample size")
```

Table 1: Effective Sample size

t	SSVGD ESS	PF ESS
1	3.4573	100.000

t	SSVGD ESS	PF ESS
2	0.2284	8.152
3	23.1824	86.440
4	1.2917	76.115
5	2.2782	62.245

Results

In order to assess the accuracy of SSVGD we consider multiple different evaluation metrics. We evaluate the forecasts on both mean-square-error and log-score. Log-scores were computed as follows,

$$p(y_{1:n}) = \int_{x_{1:n}} p(y_{1:n}|x_{1:n})p(x_{1:n})d_{x_{1:n}}$$

This can be approximated as

$$\frac{1}{k}\sum_{i=1}^{k} p(y_{1:n}|x_{1:n}^{(i)})$$

That is, we take a full trajectory $x_{1:n}$ and compute the log-probability of $y_{1:n}$. Note that this is equivalent to taking the average weight at each step.

```
log_p <- c()
for (i in 1:nrow(weights)){
  log_p <- c(log_p,mean(weights[i,]))
}



ll_df <- data.frame(sum(log_p),out_smc$log_marg_like)
colnames(ll_df) <- c("SSVGD","PF")
kable(ll_df,caption="Log Score")
```

Table 2: Log Score

SSVGD	PF
-4.928	-16.42

Discussion

Sequential Stein Variational Gradient Descent offers a useful alternative to traditional particle filtering. We are able to increase the effective sample size using the same number of particles. We are also able to approximate the true likelihood of the Kalman Filter with a small number of particles. Further work is required to understand the impact of the bandwith heuristic on the resulting predictive intervals.

Bibliography