INTRODUCTION TO POMP: INFERENCE FOR PARTIALLY-OBSERVED MARKOV PROCESSES

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1. Partially-observed Markov processes

Partially-observed Markov process models are also known as state-space models or stochastic dynamical systems. The R package pomp provides facilities for fitting such models to uni- or multi-variate time series, for simulating them, for assessing model adequacy, and for comparing among models. The methods implemented in pomp are all "plug-and-play" in the sense that they require only that one be able to simulate the process portion of the model. This property is desirable because it will typically be the case that a mechanistic model will not be otherwise amenable to standard statistical analyses, but will be relatively easy to simulate. Even when one is interested in a model for which one can write down an explicit likelihood, for example, there are probably models that are "nearby" and equally interesting for which the likelihood cannot explicitly be written. The price one pays for this flexibility is primarily in terms of computational expense.

A partially-observed Markov process has two parts. First, there is the true underlying process which is generating the data. This is typically the thing we are most interested in: our goal is usually to better understand this process. Specifically, we may have various alternate hypotheses about how this system functions and we want to see whether time series data can tell us which hypotheses explain the data better. The challenge, of course, is that the data shed light on the system only indirectly.

pomp assumes that we can translate our hypotheses about the underlying, unobserved process into a Markov process model: That is, we are willing to assume that the system has a true state process, X_t that is Markovian. In particular, given any sequence of times t_0, t_1, \ldots, t_n , the Markov property allows us to write

$$X_{t_{k+1}} \sim f(X_{t_k}, \theta), \tag{1}$$

for each k = 1, ..., n, where f is some density. [In this document, we will be fairly cavalier about abusing notation, using the letter f to denote a probability distribution function generically, assuming that the reader will be able to unambiguously tell which probability distribution we're talking about from the arguments to f and the context.] That is, we assume that the state at time t_{k+1} depends only on the state at time t_k and on some parameters θ .

In addition to the state process X_t , there is some measurement or observation process Y_t which models the process by which the data themselves are generated and links the data therefore to the state process. In particular, we assume that

$$Y_t \sim f(X_t, \theta) \tag{2}$$

for all times t. That is, that the observations Y_t are random variables that depend only on the state at that time as well as on some parameters.

So, to specify a partially-observed Markov process model, one has to specify a process (unobserved or state) model and a measurement (observation) model. This seems straightforward enough, but from the computational point of view, there are actually two aspects to each model that may be important. On the one hand, one may need to evaluate the probability density of the state-transition $X_{t_k} \to X_{t_{k+1}}$, i.e., to compute $f(X_{t_{k+1}} | X_{t_k}, \theta)$. On the other hand, one may need to simulate this distribution, i.e., to draw random samples from the distribution of $X_{t_{k+1}} | X_{t_k}$. Depending on the model and on what one wants specifically to do, it may be technically easier or harder to do one of these or the other. Likewise, one may want to simulate, or evaluate the likelihood of, observations Y_t . At it's most basic level pomp is an infrastructure that allows you to encode your model by specifying some or all of these four basic components:

- (1) rprocess: a simulator of the process model
- (2) dprocess: an evaluator of the process model probability density function
- (3) rmeasure: a simulator of the measurement model
- (4) dmeasure: an evaluator of the measurement model probability density function

Once you've encoded your model, pomp provides a number of algorithms you can use to work with it: you can simulate the model, evaluate the likelihood of various parameter sets, and fit the model to the data using a variety of algorithms. Finally pomp provides an applications programming interface (API) upon which new algorithms for partially-observed Markov process models can be built. In this document, we'll see how this all works using relatively simple examples.

2. A FIRST EXAMPLE: A DISCRETE-TIME BIVARIATE AUTOREGRESSIVE PROCESS.

For simplicity, we'll begin with a very simple discrete-time model. The plug-and-play methods in pomp were designed to work on much more complicated models, and for our first example, they'll be extreme overkill, but starting with a simple model will help make the implementation of more general models clear. Our first example will be moreover a model for which plug-and-play methods are not even necessary. This will allow us to compare the results we obtain with the generalizable plug-and-play methods with exact results obtainable by the specialized methods appropriate to this particular model. Later we'll look at a continuous-time model for which no such special tricks are available.

Consider a two-dimensional AR(1) process with noisy observations. The state process $X_t \in \mathbb{R}^2$ satisfies

$$X_t = \alpha X_{t-1} + \sigma \, \xi_t. \tag{3}$$

The measurement process is

$$Y_t = \beta X_t + \tau \varepsilon_t. \tag{4}$$

In these equations, α and and β are 2×2 constant matrices. ξ_t and ε_t are mutually-independent families of i.i.d. bivariate standard normal random variables. σ is a lower-triangular matrix such that $\sigma\sigma^T$ is the variance-covariance matrix of $X_{t+1}|X_t$. We'll assume that each component of X is measured independently and with the same error, τ , so that the variance-covariance matrix of $Y_t|X_t$ has τ^2 on the diagonal and zeros elsewhere.

Given a data set, one can for this model obtain exact maximum likelihood estimates of the parameters using the Kalman filter. We will demonstrate this below. Here, we'll approach this model as we would a more complex model for which no such exact estimator is available.

3. Defining a partially observed Markov process in pomp.

In order to fully specify this partially-observed Markov process, we must implement both the process model (i.e., the unobserved process) and the measurement model (the observation process). As we saw before, we would like to be able to:

- (1) simulate from the process model, i.e., make a random draw from $X_{t+1} | X_t = x$ for arbitrary x and t (rprocess),
- (2) compute the probability density function (pdf) of state transitions, i.e., compute $f(X_{t+1} = x' | X_t = x)$ for arbitrary x, x', and t (dprocess),
- (3) simulate from the measurement model, i.e., make a random draw from $Y_t \mid X_t = x$ for arbitrary x and t (rmeasure),
- (4) compute the measurement model pdf, i.e., $f(Y_t = y \mid X_t = x)$ for arbitrary x, y, and t (dmeasure), and
- (5) compute the deterministic skeleton. In discrete-time, this is the map $x \mapsto \mathbb{E}[X_{t+1} \mid X_t = x]$ for arbitrary x.

For this simple model, all this is easy enough. More generally, it will be difficult to do some of these things. Depending on what we wish to accomplish, however, we may not need all of these capabilities and in particular, to use any particular one of the algorithms in pomp, we never need to specify all these. For example, to simulate data, all we need is 1 and 3. To run a particle filter (and hence to use iterated filtering, mif), one needs 1 and 4. To do MCMC, one needs 2 and 4. Nonlinear forecasting (nlf) requires 1 and 3. Trajectory matching (traj.match) requires 4 and 5.

Using pomp, the first step is always to construct an object (of class pomp, naturally enough), the key step of which is to specify functions to do some or all of 1–5, along with data and (optionally) other information. The package provides several algorithms for fitting the models to the data, for simulating the models, studying deterministic skeletons, and so on. The documentation (?pomp) spells out the usage of the pomp constructor, including detailed specifications for all its arguments and a worked example.

Let's see how to implement the AR(1) model in pomp. Here, we'll take the shortest path to this goal. In the "advanced topics in pomp" vignette, we show how one can make the codes much more efficient using compiled native (C or FORTRAN) code.

First, we write a function that implements the process model simulator. This is a function that will simulate a single step $(t \to t + 1)$ of the unobserved process (3).

The translation from the mathematical description (3) to the simulator is straightforward. When this function is called, the argument \mathbf{x} contains the state at time \mathbf{t} . The parameters (including the matrix α and the process noise s.d. matrix σ) are passed in the argument params. Notice that these arguments are named numeric vectors and that the output must be named numeric vector. In fact, the names of the output vector (here xnew) must be the same as those of the input vector \mathbf{x} . The algorithms in pomp all make heavy use of the names attributes of vectors and matrices. The argument delta.t tells how big the time-step is. In this case, our time-step will be 1 unit: we'll see below how that gets specified.

Next, we'll implement a simulator for the observation process (4).

```
ou2.meas.sim <- function (x, t, params, ...) {
  y <- rnorm(n=2,mean=x[c("x1","x2")],sd=params["tau"])
  names(y) <- c("y1","y2")
  y
}</pre>
```

Again the translation is straightforward. When this function is called, the unobserved states at time t will be in the named numeric vector x and the parameters in params as before. The function returns a named numeric vector that represents a single draw from the observation process (4).

4. Simulating the model

With the two functions above, we already have all we need to simulate the entire model. The first step is to construct an R object of class pomp which will serve as a container to hold the model and data. This is done with a call to pomp:

The first argument (data) specifies a data-frame that holds the data and the times at which the data were observed. Since this is a toy problem, we have no data. In a moment, however, we'll simulate some data so we can explore pomp's various methods for fitting models to data. The second argument (times) specifies which of the columns of data is the time variable. The third argument (rprocess) specifies that

the process model simulator will be in discrete-time, one step at a time. The function euler.sim belongs to the package pomp. It takes several arguments, one of which, step.fun, is the particular function that actually takes the step. Its second argument, delta.t, sets the size of the time-step. The argument rmeasure specifies the measurement model simulator function. to fixes t_0 for this model; here we have chosen this to be one time unit before the first observation.

Before we can simulate the model, we need to settle on some parameter values. We do this by specifying a named numeric vector that contains at least all the parameters needed by the functions ou.proc.sim and ou.meas.sim. The parameter vector needs to specify the initial conditions $X(t_0) = x_0$ as well.

In terms of the mathematical formulation of the model (Eqs. 3–4), we have

$$\alpha = \begin{pmatrix} \alpha_1 & \alpha_3 \\ \alpha_2 & \alpha_4 \end{pmatrix} \qquad \sigma = \begin{pmatrix} \sigma_1 & 0 \\ \sigma_2 & \sigma_3 \end{pmatrix} \qquad \beta = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad X(0) = \begin{pmatrix} -3 \\ 4 \end{pmatrix}.$$

The initial conditions are specified by the x1.0 and x2.0 elements. Here, the fact that the names end in ".0" is significant. This is the default operation of pomp: it is possible to parameterize the initial conditions in an arbitrary way using the optional initializer argument to pomp: see the documentation (?pomp) for details.

Now we can simulate the model:

```
ou2 <- simulate(ou2, params=theta)
```

Now ou2 is identical to what it was before, but the data that were there before have been replaced by simulated data. The parameters (theta) at which the simulations were performed have also been saved internally to ou2. We can plot the simulated data via

```
plot(ou2, variables=c("v1", "v2"))
```

Fig. 1 shows the results of this operation.

Since some parameter estimation algorithms in the pomp package only require simulations of the full process, we are already in a position to use them. At present, the only such algorithm is nonlinear forecasting (nlf). In the near future, probe-matching algorithms that require only rprocess and rmeasure will be included in the package. If we want to work with likelihood-based methods, however, we will need to be able to compute the likelihood of the data Y_t given the states X_t . To implement this in pomp, we write another function:

ou2

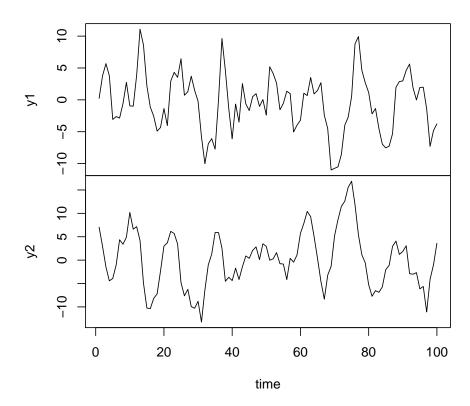


FIGURE 1. Simulated data and unobserved states from the Ornstein-Uhlenbeck process (Eqs. 3–4). This displays the results of the command plot(ou2).

```
if (log) f else exp(f)
}
```

This function computes the likelihood of the observation y at time t given the states x and the parameters params. Here, the named vector y contains data at a single timepoint (t) and x contains a single realization of the unobserved process at the same time. The extra argument log specifies whether likelihood or log-likelihood is desired.

To incorporate this into the pomp object, we'll make another call to pomp, giving our new function to the dmeasure argument:

```
t0=0
)
coef(ou2) <- theta
```

Note that we've first extracted the data from our old ou2 and set up the new one with the same data and parameters. The calls to coef and coef<- in the lines above make sure the parameters have the same values they had before.

5. Computing likelihood using particle filtering

To compute the likelihood of the data, we can use the function pfilter. This runs a plain vanilla particle filter (AKA sequential Monte Carlo) algorithm and results in an unbiased estimate of the likelihood. To do this, we must decide how many concurrent realizations (particles) to use: the larger the number of particles, the smaller the Monte Carlo error but the greater the computational effort. Let's run pfilter with 1000 particles and evaluate the likelihood at the true parameters:

```
pf <- pfilter(ou2,params=theta,Np=1000)
loglik.truth <- pf$loglik
loglik.truth
[1] -479.4467</pre>
```

Since the true parameters (i.e., the parameters that generated the data) are stored within the pomp object ou2 and can be extracted by the coef function, we could have done

```
pf <- pfilter(ou2,params=coef(ou2),Np=1000)
or even just
pf <- pfilter(ou2,Np=1000)</pre>
```

since the parameters are stored in the pomp object ou2. Now let's compute the log likelihood at a different point in parameter space:

```
theta.true <- coef(ou2)
theta.guess <- theta.true
theta.guess[c("alpha.2","alpha.3","tau")] <- 1.5*theta.true[c("alpha.2","alpha.3","tau")]
pf <- pfilter(ou2,params=theta.guess,Np=1000)
loglik.guess <- pf$loglik</pre>
```

As we mentioned before, for this particular example, we can compute the likelihood exactly using the Kalman filter, using this as a check on the validity of the particle filtering algorithm. An implementation of the Kalman filter is given in Box 1. Let's run the Kalman filter on the example data we generated above:

Box 1 Implementation of the Kalman filter for the AR(1) process.

```
require(mvtnorm)
kalman.filter <- function (y, x0, a, b, sigma, tau) {</pre>
  n \leftarrow nrow(y)
  ntimes <- ncol(y)</pre>
  sigma.sq <- sigma%*%t(sigma)
  tau.sq <- tau%*%t(tau)</pre>
  inv.tau.sq <- solve(tau.sq)</pre>
  cond.loglik <- numeric(ntimes)</pre>
  filter.mean <- matrix(0,n,ntimes)</pre>
  pred.mean <- matrix(0,n,ntimes)</pre>
  pred.var <- array(0,dim=c(n,n,ntimes))</pre>
  m <- x0
  v \leftarrow diag(0,n)
  for (k in seq_len(ntimes)) {
    pred.mean[,k] <- M <- a%*%m
    q \leftarrow b%*%V%*%t(b)+tau.sq
    r <- y[,k]-b%*%M
    cond.loglik[k] <- dmvnorm(x=y[,k],mean=as.numeric(b%*%M),sigma=q,log=TRUE)</pre>
    q \leftarrow t(b) *%inv.tau.sq%*%b+solve(V)
    v \leftarrow solve(q)
    filter.mean[,k] \leftarrow m \leftarrow v \% \% (t(b) \% \% inv.tau.sq \% \% [,k] + solve(V,M))
  }
  list(
        pred.mean=pred.mean,
        pred.var=pred.var,
        filter.mean=filter.mean,
        cond.loglik=cond.loglik,
        loglik=sum(cond.loglik)
}
tau <- diag(theta.guess['tau'],2,2)
```

tau <- diag(theta.guess['tau'],2,2)
x0 <- init.state(ou2)
kf <- kalman.filter(y,x0,a,b,sigma,tau)

In this case, the Kalman filter gives us a log likelihood of -497.07, while the particle filter with 1000 particles gives -498.16. Since the particle filter gives an unbiased estimate of the likelihood, the difference is due to Monte Carlo error in the particle filter. One can reduce this error by using a larger number of particles and/or by re-running pfilter multiple times and averaging the resulting estimated likelihoods. The latter approach has the advantage of allowing one to estimate the Monte Carlo error itself.

6. Utility functions for extracting and changing pieces of a pomp object

The pomp package provides a number of functions to extract or change pieces of a pomp-class object. One can read the documentation on all of these by doing class?pomp and methods?pomp. For example, as we've already seen, one can coerce a pomp object to a data frame:

```
as(ou2, 'data.frame')
```

and if we print a pomp object, the resulting data frame is what is shown, together with the call that created the pomp object. One can access the data and the observation times using

```
data.array(ou2)
time(ou2)
time(ou2,t0=TRUE)

The times can be changed using
time(ou2) <- 1:10
time(ou2,include.t0=T) <- seq(from=0,to=10,by=1)

One can read and change parameters associated with the pomp object using, e.g.,
coef(ou2)
coef(ou2,c("sigma.1","sigma.2")) <- c(1,0)</pre>
```

7. ESTIMATING PARAMETERS USING ITERATED FILTERING: MIF

Iterated filtering is a technique for maximizing the likelihood obtained by filtering. In pomp, the particle filter is used as a basis for iterated filtering. Iterated filtering is implemented in the mif function.

The key idea of iterated filtering is to replace the model we are interested in fitting—which has time-invariant parameters—with a model that is just the same except that its parameters take a random walk in time. As the intensity of this random walk approaches zero, the modified model approaches the original model. Adding additional variability in this way has three positive effects: (i) it smooths the likelihood surface, which makes optimization easier, (ii) it combats particle depletion, the fundamental difficulty associated with the particle filter, and (iii) the additional variability can be exploited to estimate of the gradient of the (smoothed) likelihood surface with no more computation than is required to estimate of the value of the likelihood. Iterated filtering exploits these effects to optimize the likelihood in a computationally efficient manner. As the filtering is iterated, the additional variability is decreased according to a cooling schedule. The cooling schedule can be adjusted in mif, as can the intensity of the parameter-space random walk and the other algorithm parameters. See the documentation (?mif) for details.

Let's use iterated filtering to obtain an approximate MLE for the data in ou2. We'll initiate the algorithm at theta.guess and just estmate the parameters α_1 , α_4 , and τ along with the initial conditions:

```
mf <- replicate(</pre>
                 n=3,
                 mif(
                      ou2,
                      Nmif=120,
                      start=theta.guess,
                      pars=c('alpha.2', 'alpha.3', 'tau'),
                      ivps=c('x1.0','x2.0'),
                      rw.sd=c(
                        x1.0=5, x2.0=5,
                        alpha. 2=0.02, alpha. 3=0.02, tau=0.05
                        ),
                      Np=1000,
                      var.factor=4,
                      ic.lag=10,
                      cooling.factor=0.97,
```

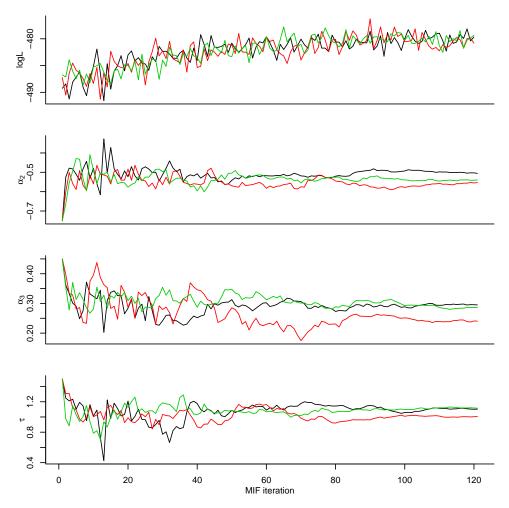


FIGURE 2. Convergence plots can be used to help diagnose convergence of the iterated filtering algorithm. This shows part of the output of compare.mif(mf).

```
max.fail=10
 fitted.pars <- c("alpha.2", "alpha.3", "tau", "x1.0", "x2.0")</pre>
 pf <- lapply(mf,pfilter)</pre>
 loglik.mle <- log(mean(exp(480+sapply(pf,function(x)x$loglik))))-480</pre>
 loglik.mle.sd <- sd(sapply(pf,function(x)x$loglik))</pre>
 theta.mle <- apply(sapply(mf,coef),1,mean)</pre>
           guess
                       mle
                            truth
alpha.2
           -0.75
                    -0.533
                              -0.5
alpha.3
            0.45
                     0.274
                               0.3
            1.50
                     1.080
tau
                               1.0
x1.0
           -3.00
                    -2.790
                              -3.0
            4.00
                     5.910
                               4.0
x2.0
loglik -498.20 -478.900 -479.4
```

8. Nonlinear forecasting: NLF

To be added.

9. Trajectory matching: traj.match

To be added.

10. A more complex example: A seasonal epidemic model

The SIR model is a mainstay of theoretical epidemiology. It has the deterministic skeleton

$$\frac{dS}{dt} = \mu (N - S) + \beta(t) \frac{I}{N} S$$
$$\frac{dI}{dt} = \beta(t) \frac{I}{N} S - \gamma I - \mu I$$
$$\frac{dR}{dt} = \gamma I - \mu R$$

Here N = S + I + R is the (constant) population size and β is a time-dependent contact rate. We'll assume that the contact rate is periodic and implement it as a covariate. As an additional wrinkle, we'll assume that the rate of the infection process $\beta I/N$ is perturbed by white noise.

As in the earlier example, we need to write a function that will simulate the process. We can use gillespie.sim to implement this using the exact stochastic simulation algorithm of Gillespie (1977). This will be quite slow and inefficient, however, so we'll use the so-called "tau-leap" algorithm, one version of which is implemented in pomp using Euler-multinomial processes. Before we do this, we'll first define the basis functions that will be used for the seasonality. It is convenient to use periodic B-splines for this purpose. The following codes set up this basis.

```
tbasis <- seq(0,25,by=1/52)
basis <- periodic.bspline.basis(tbasis,nbasis=3)
colnames(basis) <- paste("seas",1:3,sep='')</pre>
```

Now we'll define the process model simulator. Since we have covariates now, our function will have one additional argument, covars, which will contain the value of each covariate at time t, established using linear interpolation if necessary.

```
reulermultinom(n=1,size=R,rate=c(mu),dt=delta.t)
)
c(
    S=S+trans[1]-trans[2]-trans[3],
    I=I+trans[2]-trans[4]-trans[5],
    R=R+trans[4]-trans[6],
    cases=cases+trans[4],
    W=if (beta.sd>0) W+(dW-delta.t)/beta.sd else W
)
}
}
```

Let's look at this definition in a bit of detail. We will be log-transforming the parameters: the first line untransforms them. Here, we use with to make the codes a bit easier to read. The variable beta will be the transmission rate: the time-dependence of this rate is parameterized using the basis functions, the current values have been passed via the covars argument. The next lines make a draw, dW, from a Gamma random variable which will model environmental stochasticity as white noise in the transmission process (Bretó et al., 2009; He et al., 2010). The next line computes the force of infection, foi. trans is next filled with random draws of all the transitions between the S, I, and R compartments. Births are modeled using a Poisson distribution, the number of births is stored in trans[1]. Individuals leave the S class through either death or infection: trans[2] will contain the number infected, trans[3] the number dead. The number leaving the I and R classes are handled similarly. See the documentation on reulermultinom for a more thorough explanation of how this function works. Finally, a named vector is returned that contains the new values of the state variables, each of which is the old value, adjusted by the transitions. Note that the state variable cases accumulates the number of I→R transitions and W accumulates the (standardized) white noise.

Now we're ready to construct the pomp object.

```
pomp(
     data=data.frame(
        time=seq(1/52,4,by=1/52),
        reports=NA
        ),
      times="time",
      t0=0,
      tcovar=tbasis,
      covar=basis,
     rprocess=euler.sim(
        step.fun=sir.proc.sim,
        delta.t=1/52/20
        ),
     measurement.model=reports~binom(size=cases,prob=exp(rho)),
     zeronames=c("cases"),
      initializer=function(params, t0, comp.names, ...){
        p <- exp(params)</pre>
        snames <- c("S", "I", "R", "cases", "W")</pre>
        fracs <- p[paste(comp.names, "0", sep=".")]</pre>
        x0 <- numeric(length(snames))</pre>
        names(x0) \leftarrow snames
        x0[comp.names] <- round(p['pop']*fracs/sum(fracs))</pre>
        x0
```

```
},
comp.names=c("S","I","R")
) -> sir
```

The specification of data, times, and to should be familiar. The covariates are specified using the arguments tcovar and covar. Again, we use euler.sim to specify the process simulator (rprocess): we use a time-step of 1/20 of a week. Both rmeasure and dmeasure can be specified at once using the measurement.model argument. Here, we model the observation process using a binomial process, where the reporting rate, rho, is the probability that a case is reported.

As we noted before, the state variable cases accumulates the number of cases (i.e., the number of $I \rightarrow R$ transitions). However, the data are not the cumulative number of cases, but the number of cases that have occurred since the last report. Specifying cases in the zeronames argument has the effect of re-setting the state variable cases to zero after each observation.

Finally, in this example, we do not use the default parameterization of the initial states. Instead, we specify a custom initializer argument. We want instead to parameterize the initial states in terms of the fractions of the total population contained in each compartment. In particular, as we see in the initializer argument to pomp, we normalize so that the sum of S.O, I.O, and R.O is 1, then multiply by the initial population size, and then round to the nearest whole number. Note that the initializer we have specified needs an argument comp.names (the names of the S, I, and R state variables). This is set in the last line. More generally, one can give any number or kind of additional arguments to pomp: they will be passed to the initializer, rprocess, dprocess, rmeasure, dmeasure, and skeleton functions, if these exist. This feature aids in the writing of customized pomp objects.

Now we'll simulate data using the parameters

Figure 3 shows the simulated data and state variable trajectories.

References

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```
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URL: http://pomp.r-forge.r-project.org
```

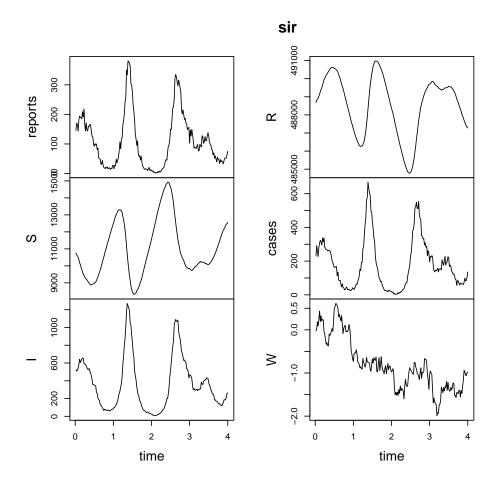


FIGURE 3. Results of plot(sir).