INTRODUCTION TO POMP BY EXAMPLE

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1. A FIRST EXAMPLE: A TWO-DIMENSIONAL RANDOM-WALK.

In order to specify a partially-observed Markov process, we must define the process model and the measurement model. In particular, we will need to be able to simulate from and compute the p.d.f. of both models. The following function will simulate the process model. The documentation (?pomp) spells out the specifications for this function.

Some methods will require the probability density of a given state transition. The function dprocess will evaluate this for a sequences of state transitions.

```
> rw.dprocess <- function(x, times, params, log = FALSE,
      nsims <- ncol(params)</pre>
      ntimes <- length(times)</pre>
       dt <- diff(times)</pre>
       d \leftarrow array(0, dim = c(2, nsims, ntimes - 1))
      noise.sds <- params[c("s1", "s2"), ]
       for (j \text{ in } 2:\text{ntimes}) d[, , j - 1] \leftarrow \text{dnorm}(x[,
            , j] - x[, , j - 1], mean = 0, sd = noise.sds *
           dt[j - 1], log = TRUE)
       if (log) {
           apply(d, c(2, 3), sum)
       }
       else {
            exp(apply(d, c(2, 3), sum))
+
+ }
```

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Now we specify the function that will simulate the measurement process. Again, the documentation spells out how.

```
> bvnorm.rmeasure <- function(x, times, params,
      ...) {
      nsims \leftarrow dim(x)[2]
      ntimes <- dim(x)[3]
      y \leftarrow array(0, dim = c(2, nsims, ntimes))
      rownames(y) <- c("y1", "y2")
      for (k in 1:nsims) {
           for (j in 1:ntimes) {
               y[, k, j] \leftarrow rnorm(2, mean = x[, k,
                    j], sd = params["tau", k])
           }
      }
      у
+ }
Finally, we have to specify how to evaluate the likelihood of an observation given the underlying state.
> bvnorm.dmeasure <- function(y, x, times, params,</pre>
      log = FALSE, ...) {
      d1 \leftarrow dnorm(x = y["y1", ], mean = x["x1",
           , ], sd = params["tau", ], log = TRUE)
      d2 \leftarrow dnorm(x = y["y2", ], mean = x["x2",
           , ], sd = params["tau", ], log = TRUE)
      if (log) {
           sum(d1, d2, na.rm = T)
      }
      else {
           exp(sum(d1, d2, na.rm = T))
+
      }
+ }
The following builds a pomp object called rw2.
> rw2 <- pomp(rprocess = rw.rprocess, dprocess = rw.dprocess,
      rmeasure = bvnorm.rmeasure, dmeasure = bvnorm.dmeasure,
      times = 1:100, data = rbind(y1 = rep(0, 100),
           y2 = rep(0, 100), t0 = 0, useless = 23)
  Now we'll specify some parameters and initial states.
> p \leftarrow rbind(s1 = c(2, 2, 3), s2 = c(0.1, 1, 2),
      tau = c(1, 5, 0))
    [,1] [,2] [,3]
             2
s1
     2.0
s2
     0.1
             1
                  2
tau 1.0
             5
                  0
> x0 \leftarrow rbind(x1 = c(0, 0, 5), x2 = c(0, 0, 0))
   [,1] [,2] [,3]
x1
      0
            0
                 5
Each column is a different initial state or parameter vector. Note that we must use rownames!
  When we defined rw2, the data were all missing. We can generate simulated data by:
> examples <- simulate(rw2, xstart = x0, params = p)</pre>
> rw2 <- examples[[1]]
```

By default simulate will generate a list of new pomp objects. It can also be used to obtain the simulated state and/or measurement trajectories:

A plot method exists for pomp objects (Fig. 1).

Access to the individual components of the pomp object is available by means of a few *methods*. To extract the data and the observation times, use data.array and time, respectively:

```
> x <- data.array(rw2)
> t <- time(rw2)</pre>
```

To run the process model, users should use simulate with the states=T option. Lower-level access is available via the rprocess method:

```
> x <- rprocess(rw2, xstart = x0, times = 0:100,
+ params = p)
```

Similarly, low-level access to the measurement-model simulator can be had through rmeasure:

```
> y <- rmeasure(rw2, x = x[, , -1, drop = F], times = 1:100,
+ params = p)</pre>
```

Access to the process-model p.d.f. is available via dprocess:

```
> dprocess(rw2, x[, , 6:11], times = 5:10, params = p)
            [,1]
                        [,2]
                                     [,3]
[1,] 0.022463149 0.05927096 0.3798196689 0.16176447
[2,] 0.076592028 0.03247796 0.0623806264 0.05983027
[3,] 0.005067855 0.02172208 0.0007791167 0.01897462
           [,5]
[1,] 0.33734907
[2,] 0.04705575
[3,] 0.01421167
> dprocess(rw2, x[, , 6:11], times = 5:10, params = p,
      log = T)
          [,1]
                    [,2]
                                [,3]
                                          [,4]
                                                     [,5]
[1,] -3.795879 -2.825636 -0.9680587 -1.821614 -1.086637
[2,] -2.569262 -3.427194 -2.7745005 -2.816244 -3.056422
```

[3,] -5.284838 -3.829426 -7.1573497 -3.964653 -4.253692

Note that dprocess returns a matrix: the rows correspond to independent simulations, the columns to distinct state transitions. The measurement-model p.d.f. is accessed via the dmeasure method, which like dprocess, returns a matrix. The rows correspond to independent simulations, the columns to distinct times.

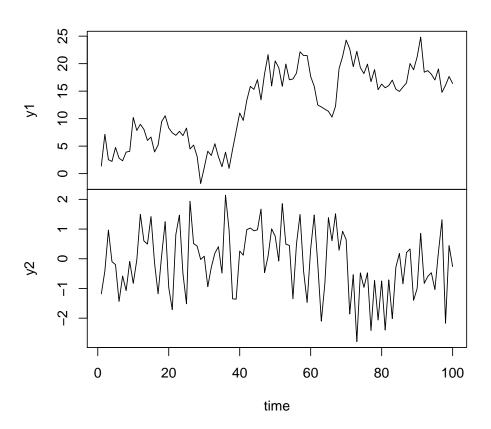


FIGURE 1. A plot method exists for pomp objects.

2. A TWO-DIMENSIONAL ORNSTEIN-UHLENBECK PROCESS.

To keep things simple, we will study a discrete-time process. The tricks below will continue to be useful even in the case of a continuous-time process, but the computational effort will be greater. The unobserved Ornstein-Uhlenbeck (OU) process $X_t \in \mathbb{R}^2$ satisfies

$$X_t = A X_{t-1} + \xi_t.$$

The observation process is

$$Y_t = B X_t + \varepsilon_t$$
.

In these equations, A and and B are 2×2 constant matrices; ξ_t and ε_t are mutually-independent families of i.i.d. bivariate normal random variables. We let $\sigma\sigma^T$ be the variance-covariance matrix of ξ_t , where σ is lower-triangular; likewise, we let $\tau\tau^T$ be that of ε_t .

We build the pomp object by specifying the three basic elements. The process model simulator and density functions:

```
> ou2.rprocess <- function(xstart, times, params,
      ...) {
      nsims <- ncol(xstart)</pre>
      ntimes <- length(times)</pre>
      alpha <- array(params[c("alpha.1", "alpha.2",</pre>
          "alpha.3", "alpha.4"), ], dim = c(2, 2, 4)
          nsims))
      sigma <- array(params[c("sigma.1", "sigma.2",</pre>
+
          nsims))
      sigma[1, 2, ] <- 0
      x \leftarrow array(0, dim = c(2, nsims, ntimes))
      rownames(x) <- rownames(xstart)</pre>
      x[, , 1] \leftarrow xstart
      for (k in 1:nsims) {
          for (j in 2:ntimes) {
              x[, k, j] \leftarrow alpha[, k] %*% x[,
                  k, j - 1] + sigma[, , k] %*% rnorm(2)
+
          }
      }
+
      X
+ }
> ou2.dprocess <- function(x, times, params, log = FALSE,
      ...) {
+
      nsims \leftarrow ncol(x)
      ntimes <- length(times)</pre>
      alpha <- array(params[c("alpha.1", "alpha.2",</pre>
          "alpha.3", "alpha.4"), ], \dim = c(2, 2, 2, 1)
      sigma <- array(params[c("sigma.1", "sigma.2",</pre>
          nsims))
+
      sigma[1, 2, ] <- 0
      d \leftarrow array(0, dim = c(nsims, ntimes - 1))
      for (k in 1:nsims) {
          for (j in 2:ntimes) {
              z <- forwardsolve(sigma[, , k], x[,</pre>
                  k, j] - alpha[, , k] %*% x[, k,
                  j - 1])
```

```
if (log) {
                   d[k, j-1] \leftarrow sum(dnorm(z, mean = 0,
+
                     sd = 1, log = TRUE)
               }
               else {
                   d[k, j-1] \leftarrow \exp(sum(dnorm(z,
                     mean = 0, sd = 1, log = TRUE)))
          }
      }
      d
+ }
The measurement model is the same as that for the random walk example above. We build the pomp object:
> ou2 <- pomp(times = seq(1, 100), data = rbind(y1 = rep(0,
      100), y2 = rep(0, 100)), t0 = 0, rprocess = ou2.rprocess,
      dprocess = ou2.dprocess, rmeasure = bvnorm.rmeasure,
      dmeasure = bvnorm.dmeasure)
  Now we'll specify the "true" parameters and initial states.
> x0 \leftarrow c(x1 = 50, x2 = -50)
x1 x2
50 -50
> p < -c(alpha.1 = 0.9, alpha.2 = 0, alpha.3 = 0,
      alpha.4 = 0.99, sigma.1 = 1, sigma.2 = 0,
      sigma.3 = 2, tau = 1)
alpha.1 alpha.2 alpha.3 alpha.4 sigma.1 sigma.2 sigma.3
   0.90
           0.00
                    0.00
                            0.99
                                     1.00
                                              0.00
    t.an
   1.00
As before, we'll fill in the missing values with simulated data.
> tic <- Sys.time()</pre>
> ou2 <- simulate(ou2, xstart = x0, params = p,
      nsim = 1000)[[1]]
> toc <- Sys.time()</pre>
> print(toc - tic)
Time difference of 8.59457 secs
  Let's make sure everything works.
> x \leftarrow rprocess(ou2, xstart = as.matrix(x0), times = c(0,
      time(ou2)), params = as.matrix(p))
> y <- rmeasure(ou2, x = x[, , -1, drop = F], times = time(ou2),
      params = as.matrix(p))
> dprocess(ou2, x[, , 36:41, drop = F], times = time(ou2)[35:40],
      params = as.matrix(p))
          Γ.17
                      [,2]
                                  [.3]
                                              [,4]
                                                          [.5]
[1,] 0.0202328 0.01875074 0.04594179 0.04462344 0.04895929
> \exp(dprocess(ou2, x[, , 36:41, drop = F], times = time(ou2)[35:40],
      params = as.matrix(p), log = T))
                      [,2]
          [,1]
                                  [,3]
                                              [,4]
[1,] 0.0202328 0.01875074 0.04594179 0.04462344 0.04895929
> dmeasure(ou2, y = y[, 1, 1:4], x = x[, , 2:5,
      drop = F], times = time(ou2)[1:4], params = as.matrix(p))
```

3. Linking in compiled code for computational efficiency.

The functions we've just written are (relatively) easy to read, but they will be slow to evaluate because, being written in R, they must be interpreted. Since many of the methods we will use require us to simulate the process and/or measurement models many times, it is a good idea to translate these codes into a compiled language. The package includes some C codes that were written to implement the OU example. Read the source (file 'ou2.c') for details. The following wrapper functions make use of these compiled codes.

```
> ou2.rprocess <- function(xstart, times, params,
      ...) .Call("ou2_simulator", xstart, times,
      params)
> ou2.dprocess <- function(x, times, params, log = FALSE,
      ...) .Call("ou2_density", x, as.numeric(times),
      params, log)
> bvnorm.dmeasure <- function(y, x, times, params,
      log = FALSE, ...) .Call("bivariate_normal_dmeasure",
      y, x, as.numeric(times), params, log)
> bvnorm.rmeasure <- function(x, times, params,</pre>
      ...) .Call("bivariate_normal_rmeasure", x,
      as.numeric(times), params)
To take advantage of the compiled functions, we need to reconstruct the pomp object.
> ou2 <- pomp(times = seq(1, 100), data = rbind(y1 = rep(0,
      100), y2 = rep(0, 100)), t0 = 0, rprocess = ou2.rprocess,
      dprocess = ou2.dprocess, rmeasure = bvnorm.rmeasure,
      dmeasure = bvnorm.dmeasure, ivpnames = c("x1.0",
          "x2.0"), parnames = c("alpha.1", "alpha.2",
          "alpha.3", "alpha.4", "sigma.1", "sigma.2",
          "sigma.3", "tau"))
> tic <- Sys.time()</pre>
> ou2 <- simulate(ou2, xstart = x0, params = p,
      nsim = 1000)[[1]]
> toc <- Sys.time()
> print(toc - tic)
```

Time difference of 0.878233 secs

Notice that we have added two objects, ivpnames and parnames to the pomp object. These will be passed to each of the functions and will come in handy later when we do particle filtering. Fig. 2 plots the data. Let's make sure everything works.

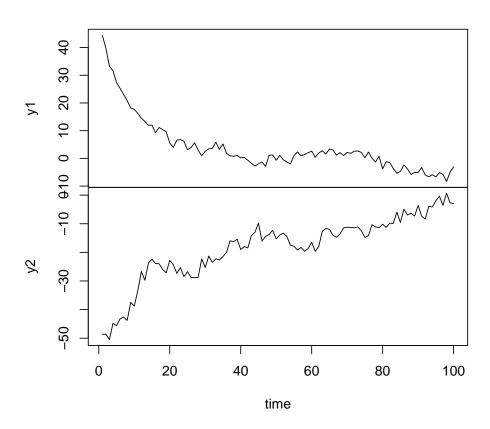


FIGURE 2. The OU process.

```
> dprocess(ou2, x[, , 36:41, drop = F], times = time(ou2)[35:40],
      params = as.matrix(p), log = T)
                              [,3]
                                         [,4]
[1,] -4.296176 -2.092207 -2.254465 -2.592138 -3.769548
> log(dmeasure(ou2, y = y[, 1, 1:4], x = x[, , 2:5,
      drop = F], times = time(ou2)[1:4], params = as.matrix(p)))
                    [,2]
                              [,3]
[1,] -2.085597 -2.176366 -2.092416 -3.867857
> dmeasure(ou2, y = y[, 1, 1:4], x = x[, , 2:5,
      drop = F], times = time(ou2)[1:4], params = as.matrix(p),
      log = T)
          [,1]
                    [,2]
                              [,3]
                                         [,4]
[1,] -2.085597 -2.176366 -2.092416 -3.867857
```

The pomp object we just created is included in the package: use data(ou2) to retrieve it.

4. Particle filter.

We can run a particle filter as follows:

```
> X0 <- matrix(x0, 2, 2000)
> rownames(X0) <- c("x1", "x2")
> fit1 <- pfilter(ou2, X0, p, filter.mean = T, pred.mean = T,
+ pred.var = T)</pre>
```

We can compare the results against those of the Kalman filter, which is exact in this case. First, we need to implement the Kalman filter.

```
> kalman.filter <- function(y, x0, a, b, sigma,
      tau) {
      n \leftarrow nrow(y)
      ntimes <- ncol(y)</pre>
      sigma.sq <- sigma %*% t(sigma)
      tau.sq <- tau %*% t(tau)
      inv.tau.sq <- solve(tau.sq)</pre>
      cond.dev <- numeric(ntimes)</pre>
      filter.mean <- matrix(0, n, ntimes)
      pred.mean <- matrix(0, n, ntimes)</pre>
      pred.var \leftarrow array(0, dim = c(n, n, ntimes))
      dev <- 0
      m <- x0
      v <- diag(0, n)
      for (k in seq(length = ntimes)) {
           pred.mean[, k] <- M <- a %*% m</pre>
           pred.var[, , k] <- V <- a %*% v %*% t(a) +
               sigma.sq
           q <- b %*% V %*% t(b) + tau.sq
           r \leftarrow y[, k] - b \% * \% M
           cond.dev[k] \leftarrow n * log(2 * pi) + log(det(q)) +
               t(r) \% \% solve(q, r)
           dev <- dev + cond.dev[k]</pre>
           q \leftarrow t(b) \% \% inv.tau.sq \% \% b + solve(V)
           v \leftarrow solve(q)
           filter.mean[, k] <- m <- v %*% (t(b) %*%
               inv.tau.sq %*% y[, k] + solve(V, M))
      }
+
      list(pred.mean = pred.mean, pred.var = pred.var,
           filter.mean = filter.mean, cond.loglik = -0.5 *
               cond.dev, loglik = -0.5 * dev)
Now we can run it on the example data we generated above.
> y <- data.array(ou2)</pre>
> a <- matrix(p[c("alpha.1", "alpha.2", "alpha.3",</pre>
       "alpha.4")], 2, 2)
> b < - diag(1, 2)
> sigma <- matrix(c(p["sigma.1"], p["sigma.2"],</pre>
      0, p["sigma.3"]), 2, 2)
> tau <- diag(p["tau"], 2, 2)</pre>
> fit2 <- kalman.filter(y, x0, a, b, sigma, tau)
```

In this case, the Kalman filter gives us a log likelihood of fit2\$loglik=-418.341737503386, while the particle filter gives us fit1\$loglik=-418.80655108131.

5. The MIF algorithm

In order to use MIF, we need to specify the distribution of particles in the state-parameter space. This distribution must be such that, when sd=0, all the particles are identical. For this example, we'll just draw our particles from a multivariate normal distribution.

```
> normal.particles <- function(Np, center, sd, ivpnames,
+ ...) {
+ params <- matrix(rnorm(Np * length(center),
+ mean = center, sd = sd), length(center),
+ Np, dimnames = list(names(center), NULL))
+ states <- params[ivpnames, , drop = FALSE]
+ rownames(states) <- gsub(".0", "", ivpnames)
+ list(states = states, params = params)
+ }</pre>
```

Now we'll run MIF to maximize the likelihood over two of the parameters and the initial conditions. We'll use 1000 particles, an exponential cooling factor of 0.95, and a fixed-lag smoother with lag 10 for the initial conditions.

```
> ou2 <- mif(ou2, Nmif = 0, start = c(x1.0 = 50,
      x2.0 = -50, p), pars = c("alpha.1", "alpha.4"),
      ivps = c("x1.0", "x2.0"), particles = normal.particles,
      rw.sd = c(x1.0 = 5, x2.0 = 5, alpha.1 = 0.1,
          alpha.2 = 0, alpha.3 = 0, alpha.4 = 0.1,
          sigma.1 = 0, sigma.2 = 0, sigma.3 = 0,
          tau = 0), alg.pars = list(Np = 1000, var.factor = 1,
          ic.lag = 10, cooling.factor = 0.95), max.fail = 100)
Just to make it interesting, we'll start far from the true parameter values:
> coef(ou2, c("x1.0", "x2.0", "alpha.1", "alpha.4")) <- <math>c(45, -1)
      -60, 0.8, 0.9)
> tic <- Sys.time()</pre>
> fit <- mif(ou2, Nmif = 2, max.fail = 100)
> fit <- continue(fit, Nmif = 78, max.fail = 100)</pre>
> toc <- Sys.time()</pre>
> print(toc - tic)
Time difference of 1.003212 mins
> coef(fit)
       x1.0
                    x2.0
                              alpha.1
                                           alpha.2
                                                        alpha.3
 48.7900861 -52.1461654
                            0.9047399
                                         0.0000000
                                                     0.000000
    alpha.4
                 sigma.1
                              sigma.2
                                           sigma.3
                                                            tau
  0.9683325
               1.0000000
                            0.0000000
                                        2.0000000
                                                     1.0000000
```

The log likelihood of the random-parameter model at the end of the mif iterations, which should be a rough approximation of that of the fixed-parameter model, is logLik(fit)=-416.520477148688. To get the log likelihood of the fixed-parameter model (up to Monte Carlo error) we can use pfilter:

```
> pfilter(fit)$loglik
```

```
[1] -414.7529
```

We can diagnose convergence of the MIF algorithm using "convergence plots" (Fig. 3).

Like pomp objects, mif objects can be simulated (Fig. 4).

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```
E-mail address: kingaa at umich dot edu URL: http://www.umich.edu/~kingaa
```

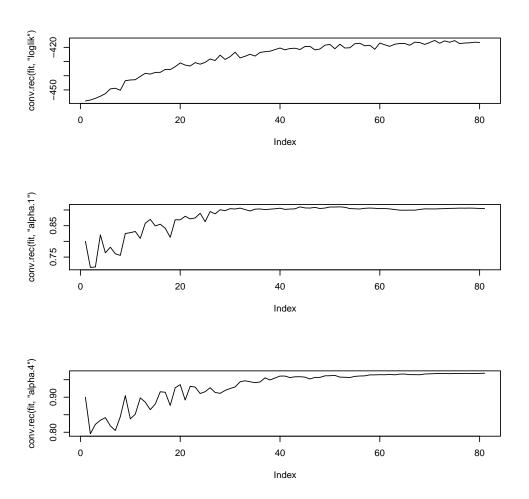


FIGURE 3. Convergence plots can be used to help diagnose convergence of the MIF algorithm.

simulate(fit)[[1]]

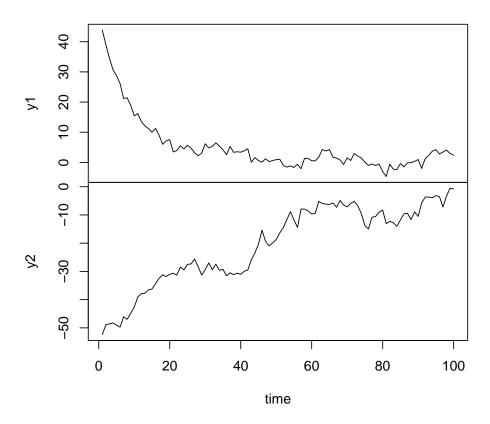


FIGURE 4. mif objects can be simulated.