Introduction to Lcpp

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The R package `Lcpp` provides convenient R wrapper functions for the **forward algorithm** that can be used to fit a wide range of **latent Markov models** like **hidden Markov models** (HMMs), **hidden semi-Markov models** (HSMMs) and **state space models** (SSMs) via **direct numerical maximum likelihood estimation**. To make writing bespoke likelihood functions faster and more convenient, it also includes many auxiliary functions that to be used in the likelihood computation.

The three main families of functions therefore are `forward`, `tpm` and `stationary` and we showcasse the simplest versions in the following introductory example.

Introductory example: Homogeneous HMM

In this vignette, we start from the most simple HMM we can think of. Such a basic N**-state HMM** is a doubly stochastic process in discrete time, i.e. in such a model observations are generated by one of N possible distributions $f_j(x_t)$, $j = 1, \dots N$ with an unobserved N**-state Markov chain** selecting which distribution is active at any given time point. Therefore, HMMs can be interpreted as correlated mixture models and are very popular accross a wide range of disciplines like ecology, sports, finance where time-series data with underlying sequential dependencies are to be analyzed. They statements above already hint at the two main assumptions in such a model, namely

1. $f(s_t \mid s_{t-1}, s_{t-2}, \dots, s_1) = f(s_t \mid s_{t-1})$ (Markov assumption)
2. $f(x_t \mid x_1, \dots, x_{t-1}, x_{t-1}, x_T, s_1, \dots, s_T) = f(x_t \mid s_t)$ (conditional independence assumption).

The hidden state process is described by a Markov chain, as such a stochastic process can easily be characterized by its **initial distribution**

$$\delta^{(1)} = (\Pr(S_1 = 1), \dots, \Pr(S_1 = N))$$

and the one-step **transition probabilities**

$$\gamma_{ij} = \Pr(S_t = j \mid S_{t-1} = i), \quad i, j = 1, \dots, N$$

which are typically summarized in the so-called **transition probability matrix** (t.p.m.)

$$\Gamma = (\gamma_{ij})_{i,j=1,\dots,N}$$

where row i is the conditional one-step ahead distribution of the state process given that the current state is i. For HMMs with homogeneous transition probabilities, we often assume **stationarity** of the underlying Markov chain, as well-behaved Markov chains converge to a unique stationary distribution. When we e.g. observe an animial and model its behavioral states by a Markov chain, it is reasonable to assume that the chain has been running for a long time prior to our observation and thus already converged to its stationary distribution. This distribution (which we call δ) can be computed by solving the system of equations

$$\delta\Gamma = \delta, \quad \text{s.t.} \sum_{j=1}^{N} \delta_j = 1,$$

which is implemented in the function `stationary()`. For stationary HMMs, we then replace the initial distribution $\delta^{(1)}$ by this stationary distribution.

For the conditional distributions of the observations $f_j(x_t)$, a typical choice would be some kind of parametric family like normal or gamma distributions with state-specific means and standard deviations. For a more exhaustive description of such models see Zucchini, MacDonald, and Langrock (2016).

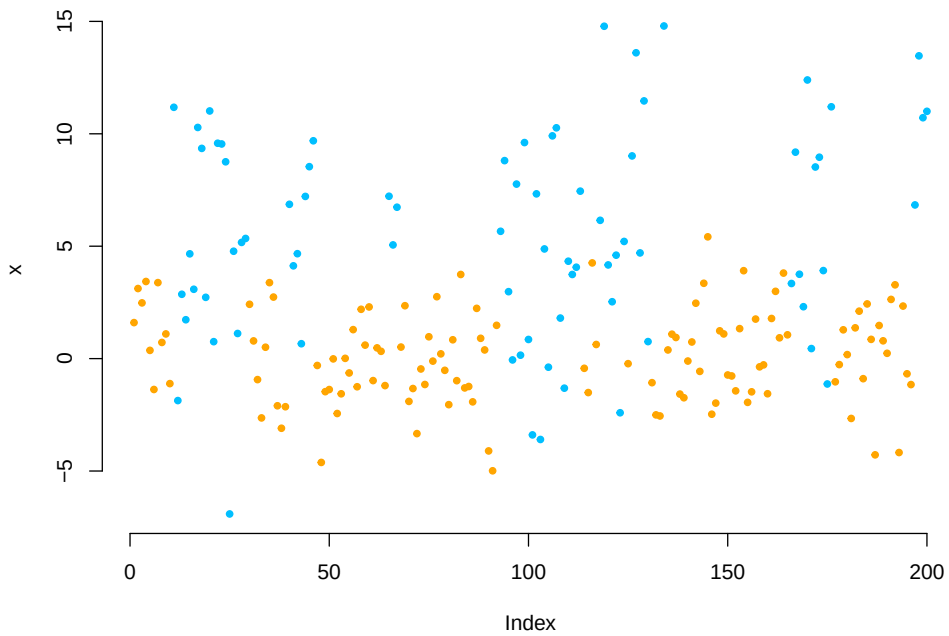
Generating data from a 2-state HMM

Here we can already use `stationary()` to compute the stationary distribution.

```
# parameters
mu = c(0, 6)
sigma = c(2, 4)
Gamma = matrix(c(0.95, 0.05, 0.15, 0.85), nrow = 2, byrow = TRUE)
delta = stationary(Gamma) # stationary HMM

# simulation
n = 1000
set.seed(123)
s = x = rep(NA, n)
s[1] = sample(1:2, 1, prob = delta)
x[1] = stats::rnorm(1, mu[s[1]], sigma[s[1]])
for(t in 2:n){
  # we draw the next state conditional on the last one
  s[t] = sample(1:2, 1, prob = Gamma[s[t-1],])
  # we draw the observation conditional on the current state
  x[t] = rnorm(1, mu[s[t]], sigma[s[t]])
}

color = c("orange", "deepskyblue")
plot(x[1:200], bty = "n", pch = 20, ylab = "x",
     col = color[s[1:200]])
```



Writing the negative log-likelihood function

Inference for HMMs is more difficult compared to e.g. regression modeling, as the observations are not independent. We would like to estimate model parameters via maximum likelihood estimation, due to the nice properties possessed by the maximum likelihood estimator. However, computing the HMM likelihood for observed data points $x_1, \ldots, x_T$ is not a trivial task, as we do not observe the underlying states. We thus need to *sum out* all possible state sequences which would be infeasible for general state processes. We can, however, exploit the Markov property and thus calculate the likelihood recursively as a matrix product using the so-called **forward algorithm**. In closed form, the HMM likelihood then becomes

$$L(\theta) = \delta^{(1)} P(x_1) \Gamma P(x_2) \Gamma \ldots \Gamma P(x_T) 1^t,$$

where $\delta^{(1)}$ and Γ are as defined above, $P(x_t)$ is a diagonal matrix with state-dependent densities or probability mass functions $f_j(x_t) = f(x_t \mid S_t = j)$ on its diagonal and 1 is a row vector of ones with length N. All model parameters are here summarized in the vector θ. Being able to evaluate the likelihood function, it can be numerically maximized by popular optimizers like `nlm()` or `optim()`.

The algorithm explained above suffers from numerical underflow and for T only moderately large the likelihood is rounded to zero. Thus, one can use a scaling strategy, detailed by Zucchini, MacDonald, and Langrock (2016), to avoid this and calculate the log-likelihood recursively. This version of the forward algorithm is implemented in `Lcpp` and written in C++. For HMMs we often need to constrain the domains of several of the model parameters in θ (i.e. positive standard deviations or a transition probability matrix with elements between 0 and 1 and rows that sum to one). One could now resort to contraint numerical optimziation but in practice one usually maximizes the likelihood w.r.t. a transformed version (to the real number line) of the model parameters by using suitable invertible and differenentiable link functions, which we denote here as θ^* (also in the code). For example we use the log-link for parameters that need to be strictly positive and the multinomial logistic link for the transition probability matrix. While the former can easily be coded by hand, the latter is implemented by the functions `tpm()` and `tpm_g()` for convenience and computational speed. For efficiency, it is also advisable to evaluate the state-dependent densities (or probability mass functions) vectorized outside the recursive forward algorithm. This results in a matrix containing the state-dependent likelihoods for each data point conditioned on each state (i.e. of dimension `c(n,N)`) which, throughout the package, we call the `allprobs` matrix.

In this example, within the negative log-likelihood function we build the homogeneous transition probability matrix using the `tpm()` function and compute the stationary distribution of the Markov chain using `stationary()`. We then build the `allprobs` matrix and calculate the log-likelihood using `forward()` in the last line. It is returned negative such that the function can be numerically minimized by e.g. `nlm()`.

```
mllk = function(theta.star, x){
  # parameter transformations for unconstraint optimization
  Gamma = Lcpp::tpm(theta.star[1:2])
  delta = Lcpp::stationary(Gamma) # stationary HMM
  mu = theta.star[3:4]
  sigma = exp(theta.star[5:6])
  # calculate all state-dependent probabilities outside the forward algorithm
  allprobs = matrix(1, length(x), 2)
  for(j in 1:2){ allprobs[,j] = stats::dnorm(x, mu[j], sigma[j]) }
  # return negative for minimization
  -Lcpp::forward(delta, Gamma, allprobs)
}
```

Fitting an HMM to the data

```
theta.star = c(-1,-1,1,4,log(1),log(3))
# initial transformed parameters: not chosen too well
s = Sys.time()
mod = stats::nlm(mllk, theta.star, x = x)
Sys.time()-s
#> Time difference of 0.01744413 secs
```

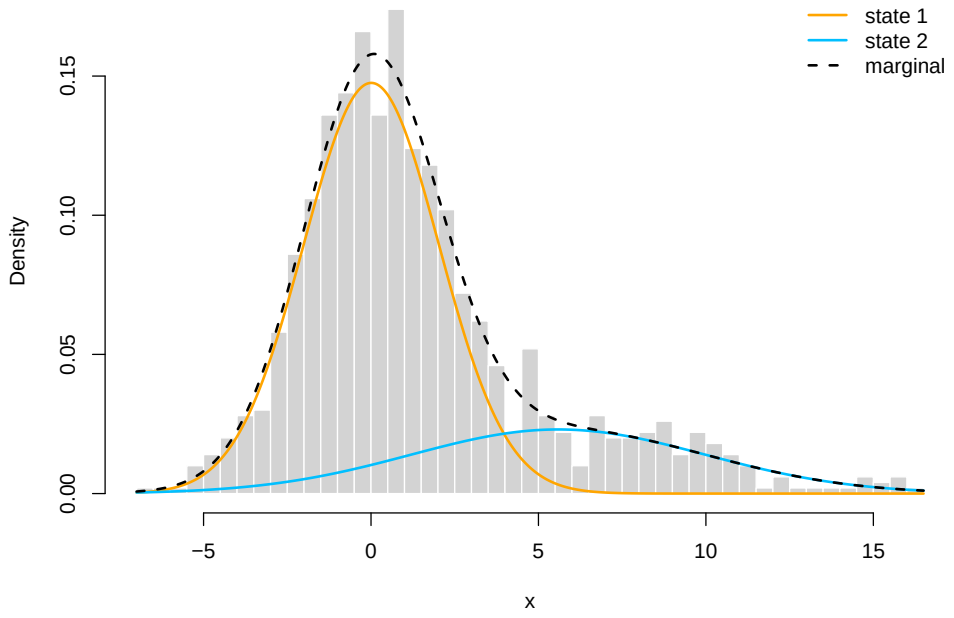
We see that implementation of the forward algorithm in C++ leads to really fast estimation speeds.

Visualizing results

Again, we use `tpm()` and `stationary()` to tranform the unconstraint parameters to working parameters.

```
# transform parameters to working
Gamma = tpm(mod$estimate[1:2])
delta = stationary(Gamma) # stationary HMM
mu = mod$estimate[3:4]
sigma = exp(mod$estimate[5:6])

hist(x, prob = TRUE, bor = "white", breaks = 40, main = "")
curve(delta[1]*dnorm(x, mu[1], sigma[1]), add = TRUE, lwd = 2, col = "orange", n=500)
curve(delta[2]*dnorm(x, mu[2], sigma[2]), add = TRUE, lwd = 2, col = "deepskyblue", n=500)
curve(delta[1]*dnorm(x, mu[1], sigma[1])+delta[2]*dnorm(x, mu[2], sigma[2]),
      add = TRUE, lwd = 2, lty = "dashed", n=500)
legend("topright", col = c(color, "black"), lwd = 2, bty = "n",
       lty = c(1,1,2), legend = c("state 1", "state 2", "marginal"))
```

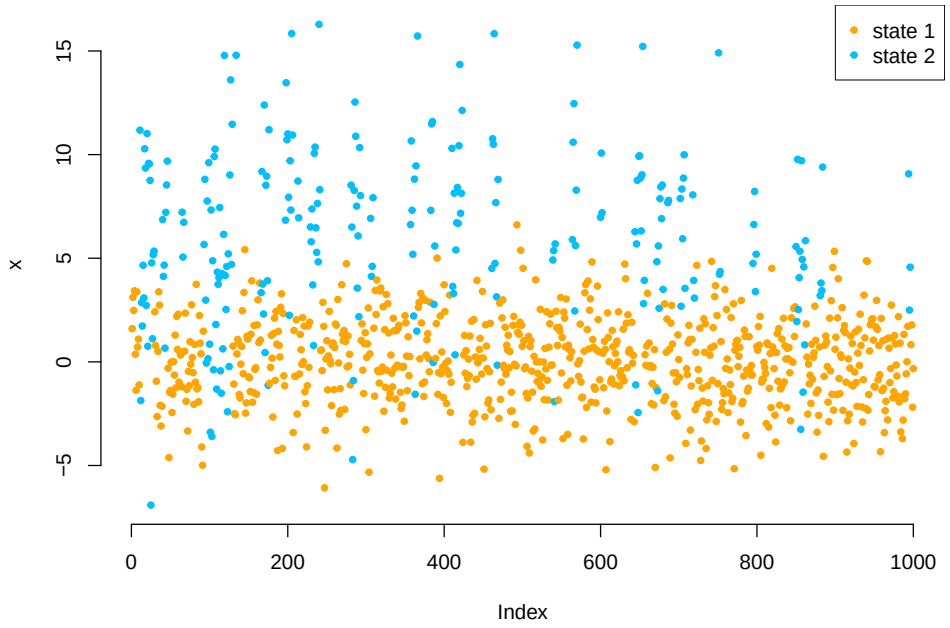


We can also decode the most probable state sequence with the `viterbi()` function, when first computing the `allprobs` matrix:

```r
allprobs = matrix(1, length(x), 2)
for(j in 1:2){ allprobs[,j] = dnorm(x, mu[j], sigma[j]) }

states = viterbi(delta, Gamma, allprobs)

plot(x, pch = 20, bty = "n", col = color[states])
legend("topright", pch = 20, legend = c("state 1", "state 2"),
       col = color, box.lwd = 0)
```



References

Zucchini, Walter, Iain L. MacDonald, and Roland Langrock. 2016. *Hidden Markov Models for Time Series: An Introduction Using R*. Boca Raton: Chapman & Hall/CRC.