Chapter 1

Model definition

1.1 Notations

We consider the prediction task of a set of observations $(y^1, \cdots y^T)$ given a set of input $(u^1, \cdots u^T)$.

1.2 Model

We define a L layer RNN followed by a fully connected layer. At time step t,

$$\begin{cases} y_{t+1} = \tanh(W_y x_{t+1}^L + b_y) \\ x_{t+1}^l = \tanh(W_{xx}^l x_t^l + W_{xu}^l x_{t+1}^{l-1} + b_x^l) \quad \forall 1 \leq l \leq L \end{cases}$$

with $x_t^0 \equiv u_t \; \forall t$ and $x_0^l \equiv 0 \; \forall 1 \leq l \leq L$.

Let's consider the weights of the last RNN and fully connected layers as $\theta \equiv (W_{xx}^L, W_{xu}^L, b_x^L, W_y, b_y)$. We can define a new matrix y_t at each time step corresponding to the concatenation of all RNN layers: $x_t \equiv (x_t^1 \cdots x_t^L)$. We also introduce two sequences of random noises as i.i.d real valued random variables ϵ and η. We can now write our model in terms of two functions f and g as:

$$\begin{cases} y_{t+1} = f_\theta(x_{t+1}) + \epsilon_{t+1} & \text{observation model} \\ x_{t+1} = g_\theta(x_t, u_{t+1}) + \eta_{t+1} & \text{state model} \end{cases} \tag{1.1}$$

In the following section, we will focus on minimizing the log likelihood

$$\log \; p_\mu(X_{1:T}, y_{1:T}, u_{1:T}) \tag{1.2}$$

1.3 Minimization

In order to minimize 1.2, we apply an EM strategy. Let $\mu_p = (\theta_p, \Sigma_{x,p}, \Sigma_{y,p})$, we will compute at each EM step:

$$Q(\hat{\mu}_p, \mu) = \mathbb{E}_{\hat{\mu}_p} \left[\log\ p_\mu(X_{1:T}, y_{1:T}, u_{1:T}) | y_{1:T} \right] \tag{1.3}$$

We can start by developing the log likelihood:

$$\begin{aligned}
\log p_\mu(X_{1:T}, y_{1:T}, u_{1:T}) &= \frac{1}{T} \log \left(\prod_{k=1}^{T} p_\mu(x_k|x_{k-1}, u_k) p_\mu(y_k|x_k) \right) \\
&= \frac{1}{T} \sum_{k=1}^{T} \log\ p_\mu(x_k|x_{k-1}, u_k) + \log\ p_\mu(y_k|x_k) \\
&= \frac{1}{T} \sum_{k=1}^{T} \log \left(\det(2\pi\Sigma_x)^{-1/2} \exp(-\frac{1}{2}(x_k - g_\theta(x_{k-1}, u_k))^T \Sigma_x^{-1} (x_k - g_\theta(x_{k-1}, u_k)) \right) \\
&+ \log \left(det(2\pi\Sigma_y)^{-1/2} \exp(-\frac{1}{2}(y_k - f_\theta(x_k))^T \Sigma_y^{-1} (y_k - f_\theta(x_k)) \right) \\
&= -\frac{1}{2} \log |\Sigma_x| - \frac{1}{2} \log |\Sigma_y| \\
&- \frac{1}{2T} \sum_{k=1}^{T} (x_k - g_\theta(x_{k-1}, u_k))^T \Sigma_x^{-1} (x_k - g_\theta(x_{k-1}, u_k)) \\
&- \frac{1}{2T} \sum_{k=1}^{T} (y_k - f_\theta(x_k))^T \Sigma_y^{-1} (y_k - f_\theta(x_k))
\end{aligned}$$

We will jointly update Σ_x, Σ_y and θ iteratively. We can start by computing the explicit form of the minimum of both covariance matrices.

For Σ_y, we search the zeros of the derivate of the convex function $\Sigma_y \mapsto p_\mu(X_{1:T}, y_{1:T}, u_{1:T})$.

$$\frac{\partial p_\mu(X_{1:T}, y_{1:T}, u_{1:T})}{\partial \Sigma_y^{-1}} = \frac{1}{2}\Sigma_y - \frac{1}{2T} \sum_{k=1}^{T} (x_k - f_\theta(x_k)) \cdot (x_k - f_\theta(x_k))'$$

$$\frac{\partial p_\mu(X_{1:T}, y_{1:T}, u_{1:T})}{\partial \Sigma_y^{-1}} = 0 \implies \Sigma_y = \frac{1}{T} \sum_{k=1}^{T} (y_k - f_\theta(x_k))(y_k - f_\theta(x_k))'$$

$$\frac{\partial p_\mu(X_{1:T}, y_{1:T}, u_{1:T})}{\partial \Sigma_x^{-1}} = 0 \implies \Sigma_x = \frac{1}{T} \sum_{k=1}^{T} (x_k - g_\theta(x_{k-1}, u_k))(x_k - g_\theta(x_{k-1}, u_k))'$$

We now have an expression for minimizing both Σ matrices given a value of θ, but we can't compute an explicit form for minimizing θ. We can identify two approaches to jointly minimizing μ:

1. At each step of the EM algorithm, we can compute the maximum expectation for both covariant matrices given the previous value of θ, then approximate the new θ by minimizing an argmin, through gradient descent for example.

$$\Sigma_{y,p+1} = \frac{1}{T}\sum_{k=1}^{T} \mathbb{E}_{\hat{\mu}_p}\left[(y_k - f_{\theta_p}(x_k))(y_k - f_{\theta_p}(x_k))'|y_{1:T}\right]$$
$$\Sigma_{x,p+1} = \frac{1}{T}\sum_{k=1}^{T} \mathbb{E}_{\hat{\mu}_p}\left[(x_k - g_{\theta_p}(x_{k-1},u_k))(x_k - g_{\theta_p}(x_{k-1},u_k))'|y_{1:T}\right]$$
$$\begin{aligned}\theta_{p+1} = \underset{\theta}{\operatorname{argmin}} \frac{1}{T}\sum_{k=1}^{T} \mathbb{E}_{\hat{\mu}_p}[&(y_k - f_{\theta_p}(x_k))'\Sigma_{y,p+1}^{-1}(y_k - f_{\theta_p}(x_k)) \\ &+ (x_k - g_{\theta_p}(x_{k-1},u_k)'\Sigma_{x,p+1}^{-1}(x_k - g_{\theta_p}(x_{k-1},u_k))|y_{1:T}]\end{aligned}$$

2. We can also ignore the explicit expression for the covariant matrices, and approximate both θ and Σ by gradient descent at each time step. Although we're putting aside a valuable result about Σ, this method could prove more efficient from an implementation perspective.

1.4 Sequential Monte Carlo Approach

In order to compute the conditional expectations in the previous expressions, we will sample trajectories $\xi^m_{1:T}$ associated with the weights ω^m_T with respect to the density $p_\theta(x|y)$, using a sequential Monte Carlo particle filter.

We sample particles iteratively. At time step $k = 0$, $(\xi^l_0)^N_{l=1}$ are sampled independently from the instrumental density ρ_0 and each particle is associated with the standard importance sampling weight:

$$\omega^l_0 = \chi(\xi^l_0)g_0(\xi^l_0)/\rho_0(\xi^l_0)$$

At time k, we choose to propagate the previous particle (ξ^l_{k-1}) with density:

$$\pi_k(l,x) \propto \omega^l_{k-1}\nu(\xi^l_{k-1})p_k(\xi^l_{k-1},x)$$

Particles are associated with weights:

$$\omega^l_k = \frac{q(\xi^{I^l_k}_{k-1},\xi^l_k)}{p_k(\xi^{I^l_k}_{k-1},\xi^l_k)}\frac{g_k(\xi^l_k)}{\nu_k(\xi^{I^l_k}_{k-1})}$$

Using the poor man filter, we get N trajectories:

$$\xi^l_{0:k+1} = (\xi^{I^l_{k+1}}_{0:k},\xi^l_{k+1})$$

We can now approximate this conditional expectation for any measurable bounded function h:

$$\begin{aligned}\Phi_k^M[h] &= \mathbb{E}_{\hat{\mu}_p}\left[h(x_k)|y_{1:T}\right] \\ &= \sum_{l=1}^{N} \omega_T^l h(\xi_{0:T}^l)\end{aligned}$$

1.5 Gradient descent

At each iteration of the EM algorithm, we start by generating a set of particles under the law $p(x|y)$, that allows us to compute a explicit value for the expectation. We can then minimize this expectation, in order to approximate the new θ candidate, using a gradient descent.

$$\begin{aligned}\theta_{p+1} = \underset{\theta}{\operatorname{argmin}} \frac{1}{T} \sum_{k=1}^{T} \sum_{m=1}^{M} & \omega_T^m (y_k - f_{\theta_p}(\xi_k^m))' \Sigma_{y,p+1}^{-1} (y_k - f_{\theta_p}(\omega_k^m)) \\ &+ \omega_T^m (\xi_k^m - g_{\theta_p}(\xi_{k-1}^m, u_k)' \Sigma_{x,p+1}^{-1} (\xi_k^m - g_{\theta_p}(\xi_{k-1}^m, u_k))\end{aligned}$$