Neural Uncertainty

Max Cohen

September 24, 2020

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,

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

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

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:

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

$$Q(\hat{\Theta}_p, \Theta) = \mathbb{E}_{\hat{\Theta}_p} \left[\log \ p_\Theta(X_{1:T}, y_{1:T}, u_{1:T}) | y_{1:T} \right] \tag{1.2}$$

Let's develop the interior of the expectation:

$$p_\Theta(X_{1:T}, y_{1:T}, u_{1:T}) = \frac{1}{T} \log \left(\prod_{k=1}^{T} p_\Theta(x_k|x_{k-1}, u_k) p_\Theta(y_k|x_k) \right)$$

$$= \frac{1}{T} \sum_{k=1}^{T} \log \, p_\Theta(x_k|x_{k-1}, u_k) + \log \, p_\Theta(y_k|x_k)$$

$$= \frac{1}{T} \sum_{k=1}^{T} \log \left(\det(2\pi\Sigma_x)^{-1/2} \exp(-\frac{1}{2}(x_k - g_\Theta(x_{k-1}, u_k))^T \Sigma_x^{-1}(x_k - g_\Theta(x_{k-1}, u_k))) \right)$$

$$+ \log \left(det(2\pi\Sigma_y)^{-1/2} \exp(-\frac{1}{2}(y_k - f_\Theta(x_k))^T \Sigma_y^{-1}(y_k - f_\Theta(x_k))) \right)$$

$$= -\frac{1}{2} \log|\Sigma_x| - \frac{1}{2} \log|\Sigma_y|$$

$$- \frac{1}{2T} \sum_{k=1}^{T} (x_k - g_\Theta(x_{k-1}, u_k))^T \Sigma_x^{-1}(x_k - g_\Theta(x_{k-1}, u_k))$$

$$- \frac{1}{2T} \sum_{k=1}^{T} (y_k - f_\Theta(x_k))^T \Sigma_y^{-1}(y_k - f_\Theta(x_k))$$

In order to find the minimal value of Σ_x, we can search for the zeros of the derivate of the concave function $\Sigma_x \mapsto p_\Theta(X_{1:T}, y_{1:T}, u_{1:T})$.

$$\frac{\partial p_\Theta(X_{1:T}, y_{1:T}, u_{1:T})}{\partial \Sigma_x^{-1}} = \frac{1}{2}\Sigma_x - \frac{1}{2T} \sum_{k=1}^{T} 2\Sigma_x^{-1}(x_k - f_\Theta(x_{k-1}, u_k))$$

$$= \frac{1}{2}\Sigma_x - \frac{\Sigma_x^{-1}}{T} \sum_{k=1}^{T} x_k - f_\Theta(x_{k-1}, u_k)$$

$$\frac{\partial p_\Theta(X_{1:T}, y_{1:T}, u_{1:T})}{\partial \Sigma_x^{-1}} = 0 \implies diag(\Sigma_x) = \sum_{k=1}^{T} x_k - f_\Theta(x_{k-1}, u_k)$$