## DS-GA 3001.001 Special Topics in Data Science: Modeling Time Series Handout: Kalman filtering and smoothing derivations

## 1 LSD model specification

The latents have first order Markov structure with linear dynamics and i.i.d. gaussian noise:

$$\mathbf{z}_i = \mathbf{A}\mathbf{z}_{i-1} + \mathbf{w}_i \tag{1}$$

where  $\mathbf{z}_0 \sim \mathcal{N}(\mu_0, \Sigma_0)$  and  $\mathbf{w}_i \sim \mathcal{N}(0, \mathbf{Q})$  (to avoid degeneracy, we usually take  $\mathbf{Q} = \mathbf{I}$ ). Observations are obtained by another linear projection with i.i.d. gaussian noise:

$$\mathbf{x}_i = \mathbf{C}\mathbf{z}_i + \mathbf{v}_i \tag{2}$$

with  $\mathbf{v}_i \sim \mathcal{N}(0, \mathbf{R})$ .

## 2 Kalman filter

The goal is to compute the posterior distribution of the latent state  $\mathbf{z}_i$  given past observations  $\{\mathbf{x}_1, \dots, \mathbf{x}_i\}$ . The proof proceeds by induction: we start by inferring the posterior distribution of latent variable  $\mathbf{z}_1$  condition on observation  $\mathbf{x}_1$  (marginalizing out the unobserved initial state  $\mathbf{z}_0$ ). The resulting posterior is also gaussian so it can be treated as prior for inferring the next latent state and so on.

To compute the posterior  $P(\mathbf{z}_1|\mathbf{x}_1)$  we start from the joint distribution  $P(\mathbf{z}_1,\mathbf{x}_1)$  and then use the general formula for conditioning in multivariate Gaussians:

$$\mu_{z|x} = \mu_z + \Sigma_{zx} \Sigma_{xx}^{-1} \left( \mathbf{x} - \mu_x \right) \tag{3}$$

$$\Sigma_{z|x} = \Sigma_{zz} - \Sigma_{zx} \Sigma_{xx}^{-1} \Sigma_{xz} \tag{4}$$

To compute the means, we start with  $\mathbf{z}_1 = \mathbf{A}\mathbf{z}_{i-1} + \mathbf{w}_i$  which is a sum of 2 independent multivariate gaussian distributions with means  $\mathbf{A}\mu_0$  and 0, and covariances  $\mathbf{A}\Sigma_0\mathbf{A}^t$  and  $\mathbf{Q}$ , respectively. Putting the two together, yields the prior  $\mathbf{z}_1 \sim \mathcal{N}\left(\mu_{1|0}, \Sigma_{1|0}\right)$ , with parameters: <sup>1</sup>

$$\mu_z = \mu_{1|0} = \mathbf{A}\mu_0 \tag{5}$$

$$\Sigma_{zz} = \Sigma_{1|0} = \mathbf{A}\Sigma_0 \mathbf{A}^{t} + \mathbf{Q} \tag{6}$$

Since  $\mathbf{x}_1$  is generated using the same kind of process, we can get the corresponding moments exactly in the same way:

$$\mu_x = \mathbf{C}\mu_{1|0} \tag{7}$$

$$\Sigma_{xx} = \mathbf{C}\Sigma_{1|0}\mathbf{C}^{t} + \mathbf{R} \tag{8}$$

Lastly, we need to compute the covariance:<sup>2</sup>

$$\Sigma_{zx} = \text{cov}[\mathbf{z}_1, \mathbf{x}_1] = \text{cov}[\mathbf{z}_1, \mathbf{C}\mathbf{z}_1 + \mathbf{v}_t] = \Sigma_{1|0}\mathbf{C}^t$$
(9)

where we have used the fact that the observation noise is independent (so the second term cancels out). Plugging the different elements in Eq. 3 we obtain the posterior mean for  $\mathbf{z}_1$ :

$$\mu_{1|1} = \mu_{1|0} + \mathbf{K} \left( x_1 - \mathbf{C} \mu_{1|0} \right) \tag{10}$$

where we use matrix  $\mathbf{K} = \Sigma_{zx}\Sigma_{xx}^{-1}$  as shorthand for the Kalman gain.

<sup>&</sup>lt;sup>1</sup>Notational convention for the double indexing of  $\mu_{i|j}$  and  $\Sigma_{i|j}$  means that we are computing the moments of latent  $\mathbf{z}_i$ , conditioned on observations up to j,  $\{\mathbf{x}_1, \dots, \mathbf{x}_j\}$ .

<sup>&</sup>lt;sup>2</sup>Remember that linear combinations distribute when computing covariances.

The corresponding posterior covariance matrix is (using Eq. 4):

$$\Sigma_{1|1} = \Sigma 1|0 - \mathbf{KC}\Sigma_{1|0}. \tag{11}$$

In general, for i > 1 we first compute the prior for  $\mathbf{z}_{i+1}$  as:

$$\mu_{i|i-1} = \mathbf{A}\mu_{i-1|i-1} \tag{12}$$

$$\Sigma_{i|i-1} = \mathbf{A}\Sigma_{i-1|i-1}\mathbf{A}^{t} + \mathbf{Q}$$
 (13)

Then we incorporate the evidence, to obtain the posterior with parameters:

$$\mu_{i|i} = \mu_{i|i-1} + \mathbf{K}_i \left( x_i - \mathbf{C} \mu_{i|i-1} \right) \tag{14}$$

$$\Sigma_{i|i} = \Sigma_{i|i-1} - \mathbf{K}_i \mathbf{C} \Sigma_{i|i-1} \tag{15}$$

where the Kalman gain is  $\mathbf{K}_i = \Sigma_{i|i-1} \mathbf{C}^t \left( \mathbf{C} \Sigma_{i|i-1} \mathbf{C}^t + R \right)^{-1}$ .

## 3 Kalman smoothing

The goal of smoothing is to compute the posterior distribution of the latent state  $\mathbf{z}_i$  but given the full sequence of observations observations  $\{\mathbf{x}_1, \dots, \mathbf{x}_t\}$ . There are very different ways of deriving the smoother; here we use the approach of Ainsley and Kohn (1982), as presented in Chapter 6 of Shumway and Stoffer.

The starting point of this version of the derivation is focusing on the dependency between  $\mathbf{z}_i$  and  $\mathbf{z}_{i+1}$ , and explicitly separating out different components of the generative model such that the parts are (conditionally) independent. Specifically, we start by defining some shorthand variables  $\mathbf{x}_{1:i} = \{\mathbf{x}_1, \dots, \mathbf{x}_i\}$  and  $\eta_{i+1} = \{\mathbf{w}_{i+2}, \dots, \mathbf{w}_t, \mathbf{v}_{i+1}, \dots, \mathbf{v}_t\}$ .

We also introduce an additional auxiliary random variable  $m_i$ , defined as follows:

$$m_i = \mathbb{E}[\mathbf{z}_i|\mathbf{x}_{1:i}, \mathbf{z}_{i+1} - \mu_{i+1|i}, \eta_{i+1}] \tag{16}$$

This estimates the uncertainty about  $\mathbf{z}_i$  after taking into account observations up to  $\mathbf{x}_i$ , the prediction error at step i+1 (which depends implicitly on  $\mathbf{w}_i$ ) and all the subsequent noise terms, which are independent of  $\mathbf{z}_i$ . Note also that the variables  $\mathbf{x}_{1:i}$ ,  $z_{i+1} - \mu_{i+1|i}$ ,  $\eta_i$  are mutually independent.

To compute  $m_i$  we use again the trick of computing joint statistics for  $\mathbf{z}_i$  and  $(\mathbf{z}_{i+1} - \mu_{i+1|i})$ , conditioned on the rest and then recovering  $m_i$  via the multivariate normal conditioning formula, as done for the Kalman filter above.

First, the moments of  $\mathbf{z}_i$  conditioned on  $\mathbf{x}_{1:i}$  are  $\mu_{i|i}$  and  $\Sigma_{i|i}$ , according to our original definition. Second, the corresponding moments for random variable  $(\mathbf{z}_{i+1} - \mu_{i+1|i})$  are: <sup>3</sup>

$$\mathbb{E}[\mathbf{z}_{i+1} - \mu_{i+1|i}|\mathbf{x}_{1:i}] = \mathbb{E}[\mathbf{z}_{i+1}|\mathbf{x}_{1:i}] - \mu_{i+1|i} = 0$$
(17)

$$\operatorname{Var}[\mathbf{z}_{i+1} - \mu_{i+1|i}|\mathbf{x}_{1:i}] = \Sigma_{i+1|i}$$
(18)

Lastly the covariance term is:

$$cov[\mathbf{z}_{i}, \mathbf{z}_{i+1} - \mu_{i+1|i}|\mathbf{x}_{1:i}] = cov[\mathbf{z}_{i}, \mathbf{A}\mathbf{z}_{i+1} + w_{t} - \mu_{i+1|i}|\mathbf{x}_{1:i}] = \Sigma_{i|i}\mathbf{A}^{t}$$
(19)

since the rest of the terms cancel out.

Putting everything together (Eq. 3) we get the final expression for  $m_i$ :

$$m_i = \mu_{i|i} + \mathbf{F}_i \left( \mathbf{z}_{i+1} - \mu_{i+1|i} \right) \tag{20}$$

where  $\mathbf{F}_i = \Sigma_{i|i} \mathbf{A}^t \Sigma_{i+1|i}^{-1}$ .

<sup>&</sup>lt;sup>3</sup>After conditioning,  $\mathbf{z}_{i+1|i}$  is just a constant.

Lastly, we use  $m_i$  to compute the mean of  $\mathbf{z}_i$  conditioned on the full sequence of observations  $\mathbf{x}_{1:t}$ :

$$\mu_{i|t} = \mathbb{E}[m_i|\mathbf{x}_{1:t}] \tag{21}$$

$$= \mathbb{E}[\mu_{i|i} + \mathbf{F}_i \left( \mathbf{z}_{i+1} - \mu_{i+1|i} \right) | \mathbf{x}_{1:t}]$$
 (22)

$$= \mu_{i|i} + \mathbf{F}_i \left( \mathbb{E}[\mathbf{z}_{i+1}|\mathbf{x}_{1:t}] - \mu_{i+1|i} \right)$$
 (23)

$$= \mu_{i|i} + \mathbf{F}_i \left( \mu_{i+1|t} - \mu_{i+1|i} \right). \tag{24}$$

For the covariance update rules, we start from the expression derived from the mean,  $\mu_{i|t} = \mu_{i|i} + \mathbf{F}_i \left(\mu_{i+1|t} - \mu_{i+1|i}\right)$ , subtracting  $\mathbf{z}_i$  on both sides and rewriting slightly we get:

$$\mathbf{z}_i - \mu_{i|t} + \mathbf{F}_i \mu_{i+1|t} = \mathbf{z}_i - \mu_{i|i} + \mathbf{F}_i \mathbf{A} \mu_{i|i}$$
(25)

where we have used  $\mu_{i+1|i} = \mathbf{A}\mu_{i|i}$ . We then multiply each side with its transpose and take expectations (for  $\mathbf{z}_i$ ). With some appropriate ordering of terms this yields:

$$\mathbb{E}[(\mathbf{z}_{i} - \mu_{i|t})(\mathbf{z}_{i} - \mu_{i|t})^{t}] + \mathbf{F}_{i}\mathbb{E}[\mu_{i+1|t}\mu_{i+1|t}^{t}]\mathbf{F}_{i}^{t} = \mathbb{E}[(\mathbf{z}_{i} - \mu_{i|i})(\mathbf{z}_{i} - \mu_{i|i})^{t}] + \mathbf{F}_{i}\mathbf{A}\mathbb{E}[(\mu_{i|i})(\mu_{i|i})^{t}]\mathbf{A}^{t}\mathbf{F}_{i}^{t}$$

$$\Sigma_{i|t} + \mathbf{F}_{i}\mathbb{E}[\mu_{i+1|t}\mu_{i+1|t}^{t}]\mathbf{F}_{i}^{t} = \Sigma_{i|i} + \mathbf{F}_{i}\mathbf{A}\mathbb{E}[\mu_{i|i}\mu_{i|i}^{t}]\mathbf{A}^{t}\mathbf{F}_{i}^{t}$$

$$(27)$$

where we used the fact that the cross-products cancel out. Finally, the remaining expectations can be rewritten as:<sup>4</sup>:

$$\mathbb{E}[\mu_{i+1|t}\mu_{i+1|t}^{t}] = \mathbb{E}[\mathbf{z}_{i+1}, \mathbf{z}_{i+1}^{t}] - \Sigma_{i+1|t}$$

$$(28)$$

$$= \mathbf{A}\mathbb{E}[\mathbf{z}_i, \mathbf{z}_i^t]\mathbf{A}^t + \mathbf{Q} - \Sigma_{i+1|t}$$
 (29)

$$\mathbb{E}[\mu_{i|i}\mu_{i|i}^{t}] = \mathbb{E}[\mathbf{z}_{i}, \mathbf{z}_{i}^{t}] - \Sigma_{i|i}. \tag{30}$$

where we have used the one step linear dependence between  $\mathbf{z}_i$  and  $\mathbf{z}_{i+1}$ .

Including these expressions, and rewriting  $\mathbf{A}\Sigma_{i|i}\mathbf{A}^{t} + \mathbf{Q}$  back as  $\Sigma_{i+1|i}$ , the posterior covariance for smoothing simplifies to the final expression:

$$\Sigma_{i|t} = \Sigma_{i|i} + \mathbf{F}_i \left( \Sigma_{i+1|t} - \Sigma_{i+1|i} \right) \mathbf{F}_i^{t}. \tag{31}$$

Overall, filtering (forward pass) includes information flowing rightwards from index 1 to t with the current state  $\mathbf{z}_i$  being updates as a function of past state  $\mathbf{z}_{i-1}$  and current observation  $\mathbf{x}_i$ . In contrast, during smoothing (backward pass) the current state  $\mathbf{z}_i$  is updated based on posterior for the next state  $\mathbf{z}_{i+1}$  which already incorporates information from the full sequence.

<sup>&</sup>lt;sup>4</sup>Here we use the fact that the covariance is 2nd moment - squared mean.