

# Expectation maximization of a linear dynamical system with a separate offset for each data set and an emissions matrix with columns that sum to 1

The goal of this derivation is to find the EM update for the  $C$  and  $\mathbf{d}^{(i)}$  parameters of an LDS. Specifically, we want to fit a separate  $\mathbf{d}^{(i)}$  for each data set. Finally, we also want to restrict  $C$  such that all the columns sum to 1.

LDS equations where data sets indexed with  $i$

$$\begin{aligned}\mathbf{x}_t^{(i)} &= A\mathbf{x}_{t-1}^{(i)} + B\mathbf{u}_t^{(i)} + \mathbf{w}_t^{(i)} \\ \mathbf{y}_t^{(i)} &= C\mathbf{x}_t^{(i)} + D\mathbf{u}_t^{(i)} + \mathbf{d}^{(i)} + \mathbf{v}_t^{(i)} \\ \mathbf{w}_t^{(i)} &\sim \mathcal{N}(0, Q), \mathbf{v}_t^{(i)} \sim \mathcal{N}(0, R)\end{aligned}$$

Consider the term of the complete data log likelihood  $L_y$  which deals with emissions  $\mathbf{y}$ . This is taken from equation 73 in Jonathan's Kalman Filter tutorial.  $T$  is the number of time points and  $W$  is the number of worms (data sets). All vectors are assumed to be column vectors

$$\begin{aligned}L_y &= \mathbb{E} \left[ \sum_{t=1}^{T^{(i)}} \log \mathcal{N}(\mathbf{y}_t^{(i)}; C\mathbf{x}_t^{(i)} + D\mathbf{u}_t^{(i)} + \mathbf{d}^{(i)}, R) \right] = \\ &= -\frac{1}{2} \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ (\mathbf{y}_t^{(i)} - C\mathbf{x}_t^{(i)} - D\mathbf{u}_t^{(i)} - \mathbf{d}^{(i)})^\top R^{-1} (\mathbf{y}_t^{(i)} - C\mathbf{x}_t^{(i)} - D\mathbf{u}_t^{(i)} - \mathbf{d}^{(i)}) \right] \\ &\quad - \frac{1}{2} \sum_{i=1}^W T^{(i)} \log |2\pi R|\end{aligned} \quad (1)$$

Expand the quadratic into all of its terms

$$L_y = -\frac{1}{2} \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \begin{aligned} &\mathbf{y}_t^{(i)\top} R^{-1} \mathbf{y}_t^{(i)} \\ &- \mathbf{y}_t^{(i)\top} R^{-1} C\mathbf{x}_t^{(i)} - \mathbf{x}_t^{(i)\top} C^\top R^{-1} \mathbf{y}_t^{(i)} \\ &- \mathbf{y}_t^{(i)\top} R^{-1} D\mathbf{u}_t^{(i)} - \mathbf{u}_t^{(i)\top} D^\top R^{-1} \mathbf{y}_t^{(i)} \\ &- \mathbf{y}_t^{(i)\top} R^{-1} \mathbf{d}^{(i)} - \mathbf{d}^{(i)\top} R^{-1} \mathbf{y}_t^{(i)} \\ &+ \mathbf{x}_t^{(i)\top} C^\top R^{-1} C\mathbf{x}_t^{(i)} \\ &+ \mathbf{x}_t^{(i)\top} C^\top R^{-1} D\mathbf{u}_t^{(i)} + \mathbf{u}_t^{(i)\top} D^\top R^{-1} C\mathbf{x}_t^{(i)} \\ &+ \mathbf{x}_t^{(i)\top} C^\top R^{-1} \mathbf{d}^{(i)} + \mathbf{d}^{(i)\top} R^{-1} C\mathbf{x}_t^{(i)} \\ &+ \mathbf{u}_t^{(i)\top} D^\top R^{-1} D\mathbf{u}_t^{(i)} \\ &+ \mathbf{u}_t^{(i)\top} D^\top R^{-1} \mathbf{d}^{(i)} + \mathbf{d}^{(i)\top} R^{-1} D\mathbf{u}_t^{(i)} \\ &+ \mathbf{d}^{(i)\top} R^{-1} \mathbf{d}^{(i)} \end{aligned} \right] - \frac{1}{2} \sum_{i=1}^W T^{(i)} \log |2\pi R| \quad (2)$$

Because this entire term is a scalar, the entire thing can be written as a trace. Trace distributes across addition and matrix multiplication within a trace can be circularly permuted. Permute all the terms so that  $R^{-1}$  is on the left

$$L_y = -\frac{1}{2} \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \begin{array}{c} \text{Tr} \left[ R^{-1} \mathbf{y}_t^{(i)} \mathbf{y}_t^{(i)\top} \right] \\ -\text{Tr} \left[ R^{-1} C \mathbf{x}_t^{(i)} \mathbf{y}_t^{(i)\top} \right] - \text{Tr} \left[ R^{-1} \mathbf{y}_t^{(i)} \mathbf{x}_t^{(i)\top} C^\top \right] \\ -\text{Tr} \left[ R^{-1} D \mathbf{u}_t^{(i)} \mathbf{y}_t^{(i)\top} \right] - \text{Tr} \left[ R^{-1} \mathbf{y}_t^{(i)} \mathbf{u}_t^{(i)\top} D^\top \right] \\ -\text{Tr} \left[ R^{-1} \mathbf{d}^{(i)} \mathbf{y}_t^{(i)\top} \right] - \text{Tr} \left[ R^{-1} \mathbf{y}_t^{(i)} \mathbf{d}^{(i)\top} \right] \\ +\text{Tr} \left[ R^{-1} C \mathbf{x}_t^{(i)} \mathbf{x}_t^{(i)\top} C^\top \right] \\ +\text{Tr} \left[ R^{-1} D \mathbf{u}_t^{(i)} \mathbf{x}_t^{(i)\top} C^\top \right] + \text{Tr} \left[ R^{-1} C \mathbf{x}_t^{(i)} \mathbf{u}_t^{(i)\top} D^\top \right] \\ +\text{Tr} \left[ R^{-1} \mathbf{d}^{(i)} \mathbf{x}_t^{(i)\top} C^\top \right] + \text{Tr} \left[ R^{-1} C \mathbf{x}_t^{(i)} \mathbf{d}^{(i)\top} \right] \\ +\text{Tr} \left[ R^{-1} D \mathbf{u}_t^{(i)} \mathbf{u}_t^{(i)\top} D^\top \right] \\ +\text{Tr} \left[ R^{-1} \mathbf{d}^{(i)} \mathbf{u}_t^{(i)\top} D^\top \right] + \text{Tr} \left[ R^{-1} D \mathbf{u}_t^{(i)} \mathbf{d}^{(i)\top} \right] \\ +\text{Tr} \left[ R^{-1} \mathbf{d}^{(i)} \mathbf{d}^{(i)\top} \right] \end{array} \right] - \frac{1}{2} \sum_{i=1}^W T^{(i)} \log |2\pi R| \quad (3)$$

Distribute the expectation and the sums

$$L_y = -\frac{1}{2} \left[ \begin{array}{c} \text{Tr} \left[ R^{-1} \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \mathbf{y}_t^{(i)} \mathbf{y}_t^{(i)\top} \right] \right] \\ -\text{Tr} \left[ R^{-1} C \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \mathbf{x}_t^{(i)} \mathbf{y}_t^{(i)\top} \right] \right] - \text{Tr} \left[ R^{-1} \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \mathbf{y}_t^{(i)} \mathbf{x}_t^{(i)\top} \right] C^\top \right] \\ -\text{Tr} \left[ R^{-1} D \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \mathbf{u}_t^{(i)} \mathbf{y}_t^{(i)\top} \right] \right] - \text{Tr} \left[ R^{-1} \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \mathbf{y}_t^{(i)} \mathbf{u}_t^{(i)\top} \right] D^\top \right] \\ -\text{Tr} \left[ R^{-1} \sum_{i=1}^W \mathbf{d}^{(i)} \sum_{t=1}^T \mathbb{E} \left[ \mathbf{y}_t^{(i)\top} \right] \right] - \text{Tr} \left[ R^{-1} \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \mathbf{y}_t^{(i)} \right] \mathbf{d}^{(i)\top} \right] \\ +\text{Tr} \left[ R^{-1} C \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \mathbf{x}_t^{(i)} \mathbf{x}_t^{(i)\top} \right] C^\top \right] \\ +\text{Tr} \left[ R^{-1} D \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \mathbf{u}_t^{(i)} \mathbf{x}_t^{(i)\top} \right] C^\top \right] + \text{Tr} \left[ R^{-1} C \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \mathbf{x}_t^{(i)} \mathbf{u}_t^{(i)\top} \right] D^\top \right] \\ +\text{Tr} \left[ R^{-1} \sum_{i=1}^W \mathbf{d}^{(i)} \sum_{t=1}^T \mathbb{E} \left[ \mathbf{x}_t^{(i)\top} \right] C^\top \right] + \text{Tr} \left[ R^{-1} C \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \mathbf{x}_t^{(i)} \right] \mathbf{d}^{(i)\top} \right] \\ +\text{Tr} \left[ R^{-1} D \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \mathbf{u}_t^{(i)} \mathbf{u}_t^{(i)\top} \right] D^\top \right] \\ +\text{Tr} \left[ R^{-1} \sum_{i=1}^W \mathbf{d}^{(i)} \sum_{t=1}^T \mathbb{E} \left[ \mathbf{u}_t^{(i)\top} \right] D^\top \right] + \text{Tr} \left[ R^{-1} D \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \mathbf{u}_t^{(i)} \right] \mathbf{d}^{(i)\top} \right] \\ +\text{Tr} \left[ R^{-1} \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \mathbf{d}^{(i)} \mathbf{d}^{(i)\top} \right] \right] \end{array} \right] - \frac{1}{2} \sum_{i=1}^W T^{(i)} \log |2\pi R| \quad (4)$$

apply the expectation and calculate the following suff stats. Note that  $Y$  and  $\tilde{Y}$  get modified by imputing missing  $y$  values, though no other stats are affected. I skip that here, but adjust in the code.

$$\begin{array}{lll} Y = \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \mathbf{y}_t^{(i)} \mathbf{y}_t^{(i)\top} \right] & \tilde{Y} = \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \mathbf{x}_t^{(i)} \mathbf{y}_t^{(i)\top} \right] & \bar{Y}^{(i)} = \sum_{t=1}^T \mathbb{E} \left[ \mathbf{y}_t^{(i)\top} \right] \\ M_{(1,T)} = \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \mathbf{x}_t^{(i)} \mathbf{x}_t^{(i)\top} \right] & U_y = \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \mathbf{u}_t^{(i)} \mathbf{y}_t^{(i)\top} \right] & \bar{M}^{(i)\top} = \sum_{t=1}^T \mathbb{E} \left[ \mathbf{x}_t^{(i)\top} \right] \\ U_{(1,T)} = \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \mathbf{u}_t^{(i)} \mathbf{u}_t^{(i)\top} \right] & \tilde{U}_{(1,T)} = \sum_{i=1}^W \sum_{t=1}^T \mathbb{E} \left[ \mathbf{u}_t^{(i)} \mathbf{x}_t^{(i)\top} \right] & \bar{U}^{(i)} = \sum_{t=1}^T \mathbb{E} \left[ \mathbf{u}_t^{(i)\top} \right] \end{array} \quad (5)$$

$$L_y = -\frac{1}{2} \left[ \begin{array}{c} \text{Tr} [R^{-1}Y] \\ -\text{Tr} [R^{-1}C\tilde{Y}] - \text{Tr} [R^{-1}\tilde{Y}^\top C^\top] \\ -\text{Tr} [R^{-1}DU_y] - \text{Tr} [R^{-1}U_y^\top D^\top] \\ -\text{Tr} [R^{-1} \sum_{i=1}^W \mathbf{d}^{(i)} \bar{Y}^{(i)\top}] - \text{Tr} [R^{-1} \sum_{i=1}^W \bar{Y}^{(i)} \mathbf{d}^{(i)\top}] \\ +\text{Tr} [R^{-1}CM_{(1,T)}C^\top] \\ +\text{Tr} [R^{-1}D\tilde{U}_{(1,T)}C^\top] + \text{Tr} [R^{-1}C\tilde{U}_{(1,T)}^\top D^\top] \\ +\text{Tr} [R^{-1} \sum_{i=1}^W \mathbf{d}^{(i)} \bar{M}^{(i)\top}C^\top] + \text{Tr} [R^{-1}C \sum_{i=1}^W \bar{M}^{(i)} \mathbf{d}^{(i)\top}] \\ +\text{Tr} [R^{-1}DU_{(1,T)}D^\top] \\ +\text{Tr} [R^{-1} \sum_{i=1}^W \mathbf{d}^{(i)} \bar{U}^{(i)\top}D^\top] + \text{Tr} [R^{-1}D \sum_{i=1}^W \bar{U}^{(i)} \mathbf{d}^{(i)\top}] \\ +\text{Tr} [R^{-1} \sum_{i=1}^W T^{(i)} \mathbf{d}^{(i)} \mathbf{d}^{(i)\top}] \end{array} \right] - \frac{1}{2} \sum_{i=1}^W T^{(i)} \log |2\pi R| \quad (6)$$

Finally, add a lagrange multiplier such that the columns of  $C$  sum to the 1 vector.  $-\boldsymbol{\lambda}^\top(1 - C1) = -\boldsymbol{\lambda}^\top 1 + \boldsymbol{\lambda}^\top C1$

$$L_y = -\frac{1}{2} \left[ \begin{array}{c} \text{Tr} [R^{-1}Y] \\ -\text{Tr} [R^{-1}C\tilde{Y}] - \text{Tr} [R^{-1}\tilde{Y}^\top C^\top] \\ -\text{Tr} [R^{-1}DU_y] - \text{Tr} [R^{-1}U_y^\top D^\top] \\ -\text{Tr} [R^{-1} \sum_{i=1}^W \mathbf{d}^{(i)} \bar{Y}^{(i)\top}] - \text{Tr} [R^{-1} \sum_{i=1}^W \bar{Y}^{(i)} \mathbf{d}^{(i)\top}] \\ +\text{Tr} [R^{-1}CM_{(1,T)}C^\top] \\ +\text{Tr} [R^{-1}D\tilde{U}_{(1,T)}C^\top] + \text{Tr} [R^{-1}C\tilde{U}_{(1,T)}^\top D^\top] \\ +\text{Tr} [R^{-1} \sum_{i=1}^W \mathbf{d}^{(i)} \bar{M}^{(i)\top}C^\top] + \text{Tr} [R^{-1}C \sum_{i=1}^W \bar{M}^{(i)} \mathbf{d}^{(i)\top}] \\ +\text{Tr} [R^{-1}DU_{(1,T)}D^\top] \\ +\text{Tr} [R^{-1} \sum_{i=1}^W \mathbf{d}^{(i)} \bar{U}^{(i)\top}D^\top] + \text{Tr} [R^{-1}D \sum_{i=1}^W \bar{U}^{(i)} \mathbf{d}^{(i)\top}] \\ +\text{Tr} [R^{-1} \sum_{i=1}^W T^{(i)} \mathbf{d}^{(i)} \mathbf{d}^{(i)\top}] \end{array} \right] - \frac{1}{2} \sum_{i=1}^W T^{(i)} \log |2\pi R| - \boldsymbol{\lambda}^\top 1 + \boldsymbol{\lambda}^\top C1 \quad (7)$$

Take the derivative of  $L_y$  with respect to  $C$ ,  $\boldsymbol{\lambda}$ , and  $\mathbf{d}^{(i)}$  using the trace derivative equations in the appendix. Treat  $D$  as a constant. Note that all the transposed terms end up with the same derivative. Don't forget the  $-\frac{1}{2}$  in front

$$\begin{aligned} \frac{\partial L_y}{\partial C} &= R^{-1}\tilde{Y}^\top - R^{-1}CM_{(1,T)} - R^{-1}D\tilde{U}_{(1,T)} - R^{-1} \sum_{i=1}^W \mathbf{d}^{(i)} \bar{M}^{(i)\top} + \boldsymbol{\lambda}1^\top \\ \frac{\partial L_y}{\partial \boldsymbol{\lambda}} &= C1 - 1 \\ \frac{\partial L_y}{\partial \mathbf{d}^{(i)}} &= R^{-1}\bar{Y}^{(i)} - R^{-1}C\bar{M}^{(i)} - R^{-1}D\bar{U}^{(i)} - T^{(i)}R^{-1}\mathbf{d}^{(i)} \end{aligned} \quad (8)$$

Set all terms to 0, multiply by  $R$  and gather terms that don't include  $C$ ,  $\boldsymbol{\lambda}$ , or  $\mathbf{d}^{(i)}$

$$\begin{aligned} \tilde{Y}^\top - D\tilde{U}_{(1,T)} &= CM_{(1,T)} + \sum_{i=1}^W \mathbf{d}^{(i)} \bar{M}^{(i)\top} - R\boldsymbol{\lambda}1^\top \\ 1 &= C1 \\ \bar{Y}^{(i)} - D\bar{U}^{(i)} &= C\bar{M}^{(i)} + T^{(i)}\mathbf{d}^{(i)} \end{aligned} \quad (9)$$

Transpose and rewrite as a linear equation. Because  $R$  is diagonal, we could solve this equation column by column and treat  $R$  like a scalar. However, all it does it change the amplitude of  $\boldsymbol{\lambda}$ , without affecting any other parameter. We don't use  $\boldsymbol{\lambda}$  anywhere so we can safely remove the  $-R$  term.

$$\begin{aligned} \tilde{Y} - \tilde{U}_{(1,T)}^\top D^\top &= M_{(1,T)}C^\top + \bar{M}^{(i)} \sum_{i=1}^W \mathbf{d}^{(i)\top} + 1\boldsymbol{\lambda}^\top(-R) \\ 1^\top &= 1^\top C^\top \\ \bar{Y}^{(i)\top} - \bar{U}^{(i)\top} D^\top &= \bar{M}^{(i)\top}C^\top + T^{(i)}\mathbf{d}^{(i)\top} \end{aligned} \quad (10)$$

$$\begin{bmatrix} \tilde{Y} - \tilde{U}_{(1,T)}^\top D^\top \\ 1^\top \\ \bar{Y}^{(i)\top} - \bar{U}^{(i)\top} D^\top \end{bmatrix} = \begin{bmatrix} M_{(1,T)} & 1 & \bar{M}^{(1)} & \dots & \bar{M}^{(W)} \\ 1^\top & 0 & 0 & 0 & 0 \\ \bar{M}^{(1)\top} & 0 & T^{(1)} & 0 & 0 \\ \vdots & 0 & 0 & \ddots & 0 \\ \bar{M}^{(W)\top} & 0 & 0 & 0 & T^{(W)} \end{bmatrix} \begin{bmatrix} C^\top \\ \boldsymbol{\lambda}^\top \\ \mathbf{d}^{(1)\top} \\ \vdots \\ \mathbf{d}^{(W)\top} \end{bmatrix} \quad (11)$$

Here is an example with two data sets

$$\begin{bmatrix} \tilde{Y} - \tilde{U}_{(1,T)}^\top D^\top \\ 1^\top \\ \bar{Y}^{(1)\top} - \bar{U}^{(1)\top} D^\top \\ \bar{Y}^{(2)\top} - \bar{U}^{(2)\top} D^\top \end{bmatrix} = \begin{bmatrix} M_{(1,T)} & 1 & \bar{M}^{(1)} & \bar{M}^{(2)} \\ 1^\top & 0 & 0 & 0 \\ \bar{M}^{(1)\top} & 0 & T^{(1)} & 0 \\ \bar{M}^{(2)\top} & 0 & 0 & T^{(2)} \end{bmatrix} \begin{bmatrix} C^\top \\ \boldsymbol{\lambda}^\top \\ \mathbf{d}^{(1)\top} \\ \mathbf{d}^{(2)\top} \end{bmatrix} \quad (12)$$

## Solving for $R$

Derivative rules are in the appendix

$$\frac{\partial L_y}{\partial R^{-1}} = -\frac{1}{2} \begin{bmatrix} Y \\ -C\tilde{Y} - \tilde{Y}^\top C^\top \\ -DU_y - U_y^\top D^\top \\ -\sum_{i=1}^W \mathbf{d}^{(i)} \bar{Y}^{(i)\top} - \sum_{i=1}^W \bar{Y}^{(i)} \mathbf{d}^{(i)\top} \\ +CM_{(1,T)}C^\top \\ +D\tilde{U}_{(1,T)}C^\top + C\tilde{U}_{(1,T)}^\top D^\top \\ +\sum_{i=1}^W \mathbf{d}^{(i)} \bar{M}^{(i)\top} C^\top + C\sum_{i=1}^W \bar{M}^{(i)} \mathbf{d}^{(i)\top} \\ +DU_{(1,T)}D^\top \\ +\sum_{i=1}^W \mathbf{d}^{(i)} \bar{U}^{(i)\top} D^\top + D\sum_{i=1}^W \bar{U}^{(i)} \mathbf{d}^{(i)\top} \\ +\sum_{i=1}^W T^{(i)} \mathbf{d}^{(i)} \mathbf{d}^{(i)\top} \end{bmatrix} + \frac{1}{2} \sum_{i=1}^W T^{(i)} R \quad (13)$$

Set the derivative to 0 and solve for  $R$

$$R = \frac{1}{\sum_{i=1}^W T^{(i)}} \begin{bmatrix} Y \\ -C\tilde{Y} - \tilde{Y}^\top C^\top \\ -DU_y - U_y^\top D^\top \\ -\sum_{i=1}^W \mathbf{d}^{(i)} \bar{Y}^{(i)\top} - \sum_{i=1}^W \bar{Y}^{(i)} \mathbf{d}^{(i)\top} \\ +CM_{(1,T)}C^\top \\ +D\tilde{U}_{(1,T)}C^\top + C\tilde{U}_{(1,T)}^\top D^\top \\ +\sum_{i=1}^W \mathbf{d}^{(i)} \bar{M}^{(i)\top} C^\top + C\sum_{i=1}^W \bar{M}^{(i)} \mathbf{d}^{(i)\top} \\ +DU_{(1,T)}D^\top \\ +\sum_{i=1}^W \mathbf{d}^{(i)} \bar{U}^{(i)\top} D^\top + D\sum_{i=1}^W \bar{U}^{(i)} \mathbf{d}^{(i)\top} \\ +\sum_{i=1}^W T^{(i)} \mathbf{d}^{(i)} \mathbf{d}^{(i)\top} \end{bmatrix} \quad (14)$$

## Appendix

### Trace and determinant derivatives

$$\frac{\partial}{\partial X} \text{Tr}[AXB] = A^\top B^\top \quad (15)$$

$$\frac{\partial}{\partial X} \text{Tr}[AX^\top B] = BA \quad (16)$$

If  $C$  is the identity and  $A$  and  $B$  are symmetric

$$\frac{\partial}{\partial X} \text{Tr}[A_{\text{sym}} X B_{\text{sym}} X^\top] = 2AXB \quad (17)$$

$$\frac{\partial}{\partial X^{-1}} \log |X| = -X \tag{18}$$