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Detailed Derivations of Eqs (13) & (14) in NeuroMHE paper.

Notation: $\frac{d(\cdot)}{d(\cdot)}$: total derivative, $\frac{\partial(\cdot)}{\partial(\cdot)}$: partial derivative

e.g., $f(x, y, p): \mathbb{R}^{\dim(x)} \times \mathbb{R}^{\dim(y)} \times \mathbb{R}^{\dim(p)} \rightarrow \mathbb{R}^{\dim(f)}$ where x and y are functions of p.

$$\frac{df}{dp} = \frac{\partial f}{\partial x}\cdot\frac{\partial x}{\partial p} + \frac{\partial f}{\partial y}\cdot\frac{\partial y}{\partial p} + \frac{\partial f}{\partial p},$$ accounting for dependence of x and y on p.

* in the paper, we denote $\frac{\partial}{\partial \cdot}$ by ∇.

The KKT conditions (10) can be rewritten in the following form:

$$\nabla_{\hat{x}_{t-N|t}}\mathcal{L}\left(\hat{x}_{t-N|t}, \hat{x}_{t-N}, y_{t-N}, \hat{w}_{t-N|t}, \lambda^*_{t-N}, \theta\right) = 0 \quad (10a)$$

* The analytical expression of $\nabla_{\hat{x}_{t-N|t}}\mathcal{L}$ is shown in Eq. (10a) of the paper.

$$\nabla_{\hat{x}_{k|t}}\mathcal{L}\left(\hat{x}_{k|t}, y_k, \hat{w}_{k|t}, \lambda^*_k, \lambda^*_{k-1}, \theta\right) = 0 \quad (10b)$$

$$\nabla_{\hat{w}_{k|t}}\mathcal{L}\left(\hat{x}_{k|t}, \hat{w}_{k|t}, \lambda^*_k, \theta\right) = 0 \quad (10c)$$

$$\nabla_{\lambda^*_k}\mathcal{L}\left(\hat{x}_{k+1|t}, \hat{x}_{k|t}, \overset{u_k}{\downarrow}\ \hat{w}_{k|t}\right) = 0 \quad (10d)$$

* Note that y_k (measurement) and u_k (control signal) do not explicitly depend on θ.
* Please refer to Appendix-A for the dependence of $\hat{x}_{t-N}$ on θ.
* The optimization variables $\hat{x}_{k|t}$, $\hat{w}_{k|t}$, and λ^*_k (dual variable) depend on θ.

Differentiate the KKT conditions (10) on both sides w.r.t θ using chain rule and the notation.

$$\frac{d\nabla_{\hat{x}_{t-N|t}}\mathcal{L}}{d\theta} = \underbrace{\frac{\partial \nabla_{\hat{x}_{t-N|t}}\mathcal{L}}{\partial \hat{x}_{t-N|t}}}_{\text{denoted}\Downarrow\ L^{xx}_{t-N}\ (14)}\cdot\frac{\partial \hat{x}_{t-N|t}}{\partial\theta} + \underbrace{\frac{\partial \nabla_{\hat{x}_{t-N|t}}\mathcal{L}}{\partial \hat{x}_{t-N}}}_{\Downarrow\ -P}\cdot\frac{\partial \hat{x}_{t-N}}{\partial\theta} + \underbrace{\frac{\partial \nabla_{\hat{x}_{t-N|t}}\mathcal{L}}{\partial \hat{w}_{t-N|t}}}_{\text{denoted}\Downarrow\ L^{xw}_{t-N}\ (14)}\cdot\frac{\partial \hat{w}_{t-N|t}}{\partial\theta} + \underbrace{\frac{\partial \nabla_{\hat{x}_{t-N|t}}\mathcal{L}}{\partial \lambda^*_{t-N}}}_{\Downarrow\ -F^T_{t-N}\ (11)}\cdot\frac{\partial \lambda^*_{t-N}}{\partial\theta} + \underbrace{\frac{\partial \nabla_{\hat{x}_{t-N|t}}\mathcal{L}}{\partial\theta}}_{\text{denoted}\Downarrow\ L^{x\theta}_{t-N}\ (14)} = 0$$

$$\left(\text{i.e., } \frac{d\nabla_{\hat{x}_{t-N|t}}\mathcal{L}}{d\theta} = L^{xx}_{t-N}\frac{\partial \hat{x}_{t-N|t}}{\partial\theta} - P\cdot\frac{\partial \hat{x}_{t-N}}{\partial\theta} + L^{xw}_{t-N}\cdot\frac{\partial \hat{w}_{t-N|t}}{\partial\theta} - F^T_{t-N}\cdot\frac{\partial \lambda^*_{t-N}}{\partial\theta} + L^{x\theta}_{t-N} = 0 \quad (13a)\right)$$

$$\frac{d\nabla_{\hat{x}_{k|t}}\mathcal{L}}{d\theta} = \underbrace{\frac{\partial \nabla_{\hat{x}_{k|t}}\mathcal{L}}{\partial \hat{x}_{k|t}}}_{\text{denoted}\Downarrow\ L^{xx}_{k}\ (14)}\cdot\frac{\partial \hat{x}_{k|t}}{\partial\theta} + \underbrace{\frac{\partial \nabla_{\hat{x}_{k|t}}\mathcal{L}}{\partial \hat{w}_{k|t}}}_{\text{denoted}\Downarrow\ L^{xw}_{k}\ (14)}\cdot\frac{\partial \hat{w}_{k|t}}{\partial\theta} + \underbrace{\frac{\partial \nabla_{\hat{x}_{k|t}}\mathcal{L}}{\partial \lambda^*_{k}}}_{\Downarrow\ -F^T_{k}\ (11)}\cdot\frac{\partial \lambda^*_{k}}{\partial\theta} + \underbrace{\frac{\partial \nabla_{\hat{x}_{k|t}}\mathcal{L}}{\partial \lambda^*_{k-1}}}_{\Downarrow\ I\ (\text{identity matrix})}\cdot\frac{\partial \lambda^*_{k-1}}{\partial\theta} + \underbrace{\frac{\partial \nabla_{\hat{x}_{k|t}}\mathcal{L}}{\partial\theta}}_{\text{denoted}\Downarrow\ L^{x\theta}_{k}\ (14)} = 0$$

$$\frac{d\nabla_{\hat{w}_{k|t}}\mathcal{L}}{d\theta} = \underbrace{\frac{\partial \nabla_{\hat{w}_{k|t}}\mathcal{L}}{\partial \hat{x}_{k|t}}}_{\text{denoted}\Downarrow\ L^{wx}_{k}\ (14)}\cdot\frac{\partial \hat{x}_{k|t}}{\partial\theta} + \underbrace{\frac{\partial \nabla_{\hat{w}_{k|t}}\mathcal{L}}{\partial \hat{w}_{k|t}}}_{\text{denoted}\Downarrow\ L^{ww}_{k}\ (14)}\cdot\frac{\partial \hat{w}_{k|t}}{\partial\theta} + \underbrace{\frac{\partial \nabla_{\hat{w}_{k|t}}\mathcal{L}}{\partial \lambda^*_{k}}}_{\Downarrow\ -G^T_{k}\ (11)}\cdot\frac{\partial \lambda^*_{k}}{\partial\theta} + \underbrace{\frac{\partial \nabla_{\hat{w}_{k|t}}\mathcal{L}}{\partial\theta}}_{\text{denoted}\Downarrow\ L^{w\theta}_{k}} = 0$$

$$\frac{d\nabla_{\lambda^*_k}\mathcal{L}}{d\theta} = \underbrace{\frac{\partial \nabla_{\lambda^*_k}\mathcal{L}}{\partial \hat{x}_{k+1|t}}}_{\Downarrow\ I\ (\text{identity matrix})}\cdot\frac{\partial \hat{x}_{k+1|t}}{\partial\theta} + \underbrace{\frac{\partial \nabla_{\lambda^*_k}\mathcal{L}}{\partial \hat{x}_{k|t}}}_{\Downarrow\ -F_k\ (11)}\cdot\frac{\partial \hat{x}_{k|t}}{\partial\theta} + \underbrace{\frac{\partial \nabla_{\lambda^*_k}\mathcal{L}}{\partial \hat{w}_{k|t}}}_{\Downarrow\ -G_k\ (11)}\cdot\frac{\partial \hat{w}_{k|t}}{\partial\theta} = 0$$

θ: weightings in the MHE cost
Dynamics f does not depend on θ.

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