

Variational Inference for Inverse Reinforcement Learning with Gaussian Processes: Supplementary Material

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Proof.

1.

$$\begin{aligned}\frac{\partial q(\mathbf{u})}{\partial \mathbf{m}} &= q(\mathbf{u}) \frac{\partial}{\partial \boldsymbol{\mu}} \left[-\frac{1}{2}(\mathbf{u} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{u} - \boldsymbol{\mu}) \right] \\ &= -\frac{1}{2} q(\mathbf{u}) (\boldsymbol{\Sigma}^{-1} + \boldsymbol{\Sigma}^{-\top})(\mathbf{u} - \boldsymbol{\mu}) \frac{\partial}{\partial \boldsymbol{\mu}} [\mathbf{u} - \boldsymbol{\mu}] \\ &= \frac{1}{2} q(\mathbf{u}) (\boldsymbol{\Sigma}^{-1} + \boldsymbol{\Sigma}^{-\top})(\mathbf{u} - \boldsymbol{\mu}).\end{aligned}$$

2. For $\mathbf{S} \in \{\boldsymbol{\Sigma}, \mathbf{B}, \mathbf{D}\}$,

$$\begin{aligned}\frac{\partial q(\mathbf{u})}{\partial \mathbf{S}} &= \frac{\partial}{\partial \mathbf{S}} \left[\frac{1}{(2\pi)^{m/2} |\boldsymbol{\Sigma}|^{1/2}} \exp \left(-\frac{1}{2}(\mathbf{u} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{u} - \boldsymbol{\mu}) \right) \right] \\ &= \frac{\partial}{\partial \mathbf{S}} \left[\frac{1}{(2\pi)^{m/2} |\boldsymbol{\Sigma}|^{1/2}} \right] \exp \left(-\frac{1}{2}(\mathbf{u} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{u} - \boldsymbol{\mu}) \right) \\ &\quad + \frac{1}{(2\pi)^{m/2} |\boldsymbol{\Sigma}|^{1/2}} \frac{\partial}{\partial \mathbf{S}} \left[\exp \left(-\frac{1}{2}(\mathbf{u} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{u} - \boldsymbol{\mu}) \right) \right] \\ &= -\frac{1}{2} q(\mathbf{u}) \left(|\boldsymbol{\Sigma}|^{-3/2} \frac{\partial |\boldsymbol{\Sigma}|}{\partial \mathbf{S}} + \frac{\partial}{\partial \mathbf{S}} [(\mathbf{u} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{u} - \boldsymbol{\mu})] \right).\end{aligned}\tag{1}$$

For derivatives with respect to $\boldsymbol{\Sigma}$, we can refer to Petersen and Pedersen [2]:

$$\begin{aligned}\frac{\partial |\boldsymbol{\Sigma}|}{\partial \boldsymbol{\Sigma}} &= |\boldsymbol{\Sigma}| \boldsymbol{\Sigma}^{-\top}, \\ \frac{\partial}{\partial \mathbf{S}} [(\mathbf{u} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{u} - \boldsymbol{\mu})] &= -\boldsymbol{\Sigma}^{-\top} \mathbf{U} \boldsymbol{\Sigma}^{-\top},\end{aligned}\tag{2}$$

while we can use an online tool by Laue et al.¹ [1] for the remaining ones:

$$\begin{aligned}\frac{\partial |\boldsymbol{\Sigma}|}{\partial \mathbf{B}} &= (\text{adj}(\mathbf{T}) + \text{adj}(\boldsymbol{\Sigma})) \mathbf{B}, \\ \frac{\partial |\boldsymbol{\Sigma}|}{\partial \mathbf{D}} &= \text{adj}(\mathbf{T}) \mathbf{D}^\top + \mathbf{D}^\top \text{adj}(\mathbf{T}), \\ \frac{\partial}{\partial \mathbf{B}} [(\mathbf{u} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{u} - \boldsymbol{\mu})] &= -(\mathbf{T} \mathbf{U} \mathbf{T} + \boldsymbol{\Sigma}^{-1} \mathbf{U} \boldsymbol{\Sigma}^{-1}) \mathbf{B}, \\ \frac{\partial}{\partial \mathbf{D}} [(\mathbf{u} - \boldsymbol{\mu})^\top \boldsymbol{\Sigma}^{-1}(\mathbf{u} - \boldsymbol{\mu})] &= -\mathbf{T} \mathbf{U} \mathbf{T} \mathbf{D}^\top - \mathbf{D}^\top \mathbf{T} \mathbf{U} \mathbf{T}.\end{aligned}\tag{3}$$

¹<http://www.matrixcalculus.org/>

Substituting results from (2) and (3) back into (1) gives:

$$\begin{aligned}\frac{\partial q(\mathbf{u})}{\partial \boldsymbol{\Sigma}} &= \frac{1}{2}q(\mathbf{u})(\boldsymbol{\Sigma}^{-\top} \mathbf{U} \boldsymbol{\Sigma}^{-\top} - \boldsymbol{\Sigma}^{-\top}), \\ \frac{\partial q(\mathbf{u})}{\partial \mathbf{B}} &= \frac{1}{2}q(\mathbf{u})\{|\boldsymbol{\Sigma}|^{-3/2}(\text{adj}(\mathbf{T}) + \text{adj}(\boldsymbol{\Sigma})) + \mathbf{T} \mathbf{U} \mathbf{T} + \boldsymbol{\Sigma}^{-1} \mathbf{U} \boldsymbol{\Sigma}^{-1}\} \mathbf{B}, \\ \frac{\partial q(\mathbf{u})}{\partial \mathbf{D}} &= \frac{1}{2}q(\mathbf{u})\{\mathbf{T} \mathbf{U} \mathbf{T} \mathbf{D}^\top + \mathbf{D}^\top \mathbf{T} \mathbf{U} \mathbf{T} - |\boldsymbol{\Sigma}|^{-3/2}(\text{adj}(\mathbf{T}) \mathbf{D}^\top + \mathbf{D}^\top \text{adj}(\mathbf{T}))\}.\end{aligned}$$

3. Using a result by Rasmussen and Williams [3],

$$\frac{\partial q(\mathbf{r} | \mathbf{u})}{\partial \lambda_i} = q(\mathbf{r} | \mathbf{u}) \frac{\partial}{\partial \lambda_i} \left[-\frac{1}{2} \mathbf{u}^\top \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{u} - \frac{1}{2} \log |\mathbf{K}_{\mathbf{u}, \mathbf{u}}| \right] = \frac{1}{2} q(\mathbf{r} | \mathbf{u}) \text{tr} \left((\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{u} \mathbf{u}^\top \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} - \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1}) \frac{\partial \mathbf{K}_{\mathbf{u}, \mathbf{u}}}{\partial \lambda_i} \right).$$

The remaining derivative is

$$\frac{\partial \mathbf{K}_{\mathbf{u}, \mathbf{u}}}{\partial \lambda_i} = \begin{cases} \frac{1}{\lambda_i} \mathbf{K}_{\mathbf{u}, \mathbf{u}} & \text{if } i = 0, \\ \mathbf{L}_{\mathbf{u}, \mathbf{u}} & \text{otherwise,} \end{cases}$$

where

$$\begin{aligned}[\mathbf{L}_{\mathbf{u}, \mathbf{u}}]_{j,k} &= \frac{\partial}{\partial \lambda_i} k_\lambda(\mathbf{x}_{\mathbf{u},j}, \mathbf{x}_{\mathbf{u},k}) \\ &= k_\lambda(\mathbf{x}_{\mathbf{u},j}, \mathbf{x}_{\mathbf{u},k}) \frac{\partial}{\partial \lambda_i} \left[-\frac{1}{2} (\mathbf{x}_{\mathbf{u},j} - \mathbf{x}_{\mathbf{u},k})^\top \boldsymbol{\Lambda} (\mathbf{x}_{\mathbf{u},j} - \mathbf{x}_{\mathbf{u},k}) - \mathbb{1}[j \neq k] \sigma^2 \text{tr}(\boldsymbol{\Lambda}) \right] \\ &= k_\lambda(\mathbf{x}_{\mathbf{u},j}, \mathbf{x}_{\mathbf{u},k}) \frac{\partial}{\partial \lambda_i} \left[-\frac{1}{2} \sum_{l=1}^d \lambda_l (x_{\mathbf{u},j,l} - x_{\mathbf{u},k,l})^2 - \mathbb{1}[j \neq k] \sigma^2 \sum_{l=1}^d \lambda_l \right] \\ &= k_\lambda(\mathbf{x}_{\mathbf{u},j}, \mathbf{x}_{\mathbf{u},k}) \left(-\frac{1}{2} (x_{\mathbf{u},j,i} - x_{\mathbf{u},k,i})^2 - \mathbb{1}[j \neq k] \sigma^2 \right).\end{aligned}$$

□

References

- [1] S. Laue, M. Mitterreiter, and J. Giesen. Computing higher order derivatives of matrix and tensor expressions. In S. Bengio, H. M. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, *Advances in Neural Information Processing Systems 31: Annual Conference on Neural Information Processing Systems 2018, NeurIPS 2018, 3-8 December 2018, Montréal, Canada.*, pages 2755–2764, 2018.
- [2] K. B. Petersen, M. S. Pedersen, et al. The matrix cookbook. *Technical University of Denmark*, 7(15):510, 2008.
- [3] C. E. Rasmussen and C. K. I. Williams. *Gaussian processes for machine learning*. Adaptive computation and machine learning. MIT Press, 2006.

