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Variational Inference for Inverse Reinforcement Learning with Gaussian Processes

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ABSTRACT

We prove the validity of performing variational inference on the Gaussian process-based inverse reinforcement learning model that preserves and approximates the full joint probability distribution of rewards across states of the Markov decision process.

1. INTRODUCTION

Inverse reinforcement learning (IRL)—a problem proposed by Russell in 1998 [25]—asks us to find a reward function for a Markov decision process (MDP) that best explains a set of given demonstrations. IRL is important because reward functions can be hard to define manually [1, 2], and rewards are not entirely specific to a given environment, allowing one to reuse the same reward structure in previously unseen environments [2, 10, 15]. Moreover, IRL has seen a wide array of applications in autonomous vehicle control [11, 12] and learning to predict another agent's behaviour [5, 27, 28, 29, 30]. Most approaches in the literature (see Section 2) make a convenient yet unjustified assumption that the reward function can be expressed as a linear combination of features. One proven way to abandon this assumption is by representing the reward function as a Gaussian process (GP) [10, 15, 21]. The original approach used maximum likelihood estimation [15], whereas we use variational inference (VI) instead, which learns approximate posterior probability distributions instead of point estimates. This approach can prove useful in three major ways:

1. Modelling full posterior distributions for various parameters can result in more precise reward predictions, as the model simply holds more information.
2. Having variance estimates for rewards can direct our choice in what data should be collected next.
3. An approximate Bayesian treatment of many parameters in the model guards against overfitting [10].

1.1 Statement of the Problem

Definition 1.1 (MDP). *A* Markov decision process *is a set $\mathcal{M} = \{\mathcal{S}, \mathcal{A}, \mathcal{T}, \gamma, \mathbf{r}\}$, where $\mathcal{S}$ and $\mathcal{A}$ are sets of states and actions, respectively; $\mathcal{T} : \mathcal{S} \times \mathcal{A} \times \mathcal{S} \to [0, 1]$ is a function defined so that $\mathcal{T}(s, a, s')$ is the probability of moving to state s' after taking action a in state s; $\gamma \in [0, 1)$ is the discount factor; and $\mathbf{r} \in \mathbb{R}^{|\mathcal{S}|}$ is the reward vector*[1].

[1]Depending on the situation, we will sometimes represent rewards as a function $r : \mathcal{S} \to \mathbb{R}$.

Definition 1.2 (IRL). *Given an MDP without rewards $\mathcal{M} \setminus \{\mathbf{r}\}$, an $|\mathcal{S}| \times d$ feature matrix $\mathbf{X}$ (where d is the number of features), and a set of expert demonstrations $\mathcal{D} = \{\zeta_i\}_{i=1}^{N}$, where each demonstration $\zeta_i = \{(s_{i,t}, a_{i,t})\}_{t=1}^{T}$ is a multiset of state-action pairs representing optimal actions executed by an expert, find the reward function that maximises the probability of observing the demonstrations, i.e.,*

$$\arg\max_{\mathbf{r}} p(\mathcal{D} \mid \mathbf{r}).$$

The optimal *policy* $\pi : \mathcal{S} \to \mathcal{A}$ (i.e., a choice of actions for each state that maximises reward over time) is usually constructed by defining a *value (utility) function* $V_{\mathbf{r}} : \mathcal{S} \to \mathbb{R}$ that measures how good a state is based on the reward $\mathbf{r}$ as well as the structure of the MDP. One can then find $V_{\mathbf{r}}$ by applying the Bellman backup operator until convergence to every $s \in \mathcal{S}$ (the technique is known as *value iteration*) [26]:

$$V_{\mathbf{r}}(s) \coloneqq r(s) + \gamma \max_{a \in \mathcal{A}} \sum_{s' \in \mathcal{S}} \mathcal{T}(s, a, s') V_{\mathbf{r}}(s').$$

However, we follow previous work on GP IRL [15, 10], and use a *linearly solvable* (or *maximum causal entropy*) MDP with stochastic policy that define probability distributions over actions (instead of suggesting a single action for each state) [28]. This type of MDP can be solved by applying the 'soft' version of the operator [15, 16]:

$$V_{\mathbf{r}}(s) \coloneqq \log \sum_{a \in \mathcal{A}} \exp\left(r(s) + \gamma \sum_{s' \in \mathcal{S}} \mathcal{T}(s, a, s') V_{\mathbf{r}}(s') \right). \quad (1)$$

With this model, we can express the likelihood as [10, 15]

$$\begin{aligned} p(\mathcal{D} \mid \mathbf{r}) &= \prod_{i=1}^{N} \prod_{t=1}^{T} p(a_{i,t} \mid s_{i,t}) \\ &= \exp\left(\sum_{i=1}^{N} \sum_{t=1}^{T} Q_{\mathbf{r}}(s_{i,t}, a_{i,t}) - V_{\mathbf{r}}(s_{i,t}) \right), \end{aligned} \quad (2)$$

where

$$Q_{\mathbf{r}}(s, a) = r(s) + \gamma \sum_{s' \in \mathcal{S}} \mathcal{T}(s, a, s') V_{\mathbf{r}}(s').$$

However, a reward function learned by maximising this likelihood is not transferable to new situations [10, 15]. One needs to model the reward structure in a way that would allow reward predictions for previously unseen states.

One way to model rewards without assumptions of linearity is with a *Gaussian process* (GP). A GP is a collection of random variables, any finite combination of which has a joint Gaussian distribution [23]. We write $r \sim \mathcal{GP}(0, k)$ to

say that r is a GP with mean 0 and covariance function k. *Covariance functions* (also known as *kernels*) take two state feature vectors as input and quantify how similar the two states are, in a sense that we would expect them to have similar rewards.

As training a GP with n data points has a time complexity of $\mathcal{O}(n^3)$ [23], numerous approximation methods have been suggested, many of which select a subset of data called *inducing points* and focus most of the training effort on them [17]. Let $\mathbf{X_u}$ be the matrix of features at inducing states, $\mathbf{u}$ the rewards at those states. Then the full joint probability distribution can be factorised as

$$p(\mathcal{D}, \mathbf{u}, \mathbf{r}) = p(\mathbf{u}) \times p(\mathbf{r} \mid \mathbf{u}) \times p(\mathcal{D} \mid \mathbf{r}), \tag{3}$$

where

$$\begin{aligned} p(\mathbf{u}) &= \mathcal{N}(\mathbf{u}; \mathbf{0}, \mathbf{K_{u,u}}) \\ &= \frac{1}{(2\pi)^{m/2}|\mathbf{K_{u,u}}|^{1/2}} \exp\left(-\frac{1}{2}\mathbf{u}^\intercal \mathbf{K_{u,u}^{-1}}\mathbf{u}\right) \\ &= \exp\left(-\frac{1}{2}\mathbf{u}^\intercal \mathbf{K_{u,u}^{-1}}\mathbf{u} - \frac{1}{2}\log|\mathbf{K_{u,u}}| - \frac{m}{2}\log 2\pi\right) \end{aligned}$$

is the GP prior [23], and $m \in \mathbb{N}$ is the number of inducing points. The GP posterior is then a multivariate Gaussian [15]

$$p(\mathbf{r} \mid \mathbf{u}) = \mathcal{N}(\mathbf{r}; \mathbf{K_{r,u}^\intercal}\mathbf{K_{u,u}^{-1}}\mathbf{u}, \mathbf{K_{r,r}} - \mathbf{K_{r,u}^\intercal}\mathbf{K_{u,u}^{-1}}\mathbf{K_{r,u}}), \tag{4}$$

and $p(\mathcal{D} \mid \mathbf{r})$ is as in (2). The matrices such as $\mathbf{K_{r,u}}$ are called *covariance matrices* and are defined as $[\mathbf{K_{r,u}}]_{i,j} = k(\mathbf{x}_{\mathbf{r},i}, \mathbf{x}_{\mathbf{u},j})$, where $\mathbf{x}_{\mathbf{r},i}$ and $\mathbf{x}_{\mathbf{u},j}$ denote feature vectors for the ith state in $\mathcal{S}$ and the jth state in $\mathbf{X_u}$, respectively [10].

Given this model, data $\mathcal{D}$, and inducing feature matrix $\mathbf{X_u}$, our goal is then to find optimal values of parameters $\boldsymbol{\lambda}$, inducing rewards $\mathbf{u}$, and the rewards for all relevant states $\mathbf{r}$. While the previous paper to consider this IRL model computed maximum likelihood (ML) estimates for $\boldsymbol{\lambda}$ and $\mathbf{u}$, and made an assumption that $\mathbf{r}$ in (4) has zero variance [15], we aim to avoid this assumption and use VI to approximate the full posterior distribution $p(\mathbf{u}, \mathbf{r} \mid \mathcal{D})$. *Variational inference* is an approximation technique for probability densities [4]. Let $q(\mathbf{u}, \mathbf{r})$ be our approximating family of probability distributions for $p(\mathbf{u}, \mathbf{r} \mid \mathcal{D})$. Then the job of VI is to optimise the parameters of the approximating distribution in order to minimise the *Kullback-Leibler* (KL) divergence between the original probability distribution and our approximation. KL divergence (asymmetrically) measures how different the two distributions are, and can be defined as [4]

$$\begin{aligned} D_{\mathrm{KL}}(q(\mathbf{u}, \mathbf{r}) \parallel p(\mathbf{u}, \mathbf{r} \mid \mathcal{D})) &= \mathbb{E}[\log q(\mathbf{u}, \mathbf{r}) - \log p(\mathbf{u}, \mathbf{r} \mid \mathcal{D})] \\ &= \mathbb{E}[\log q(\mathbf{u}, \mathbf{r}) - \log p(\mathcal{D}, \mathbf{u}, \mathbf{r})] \\ &\quad + \mathbb{E}[\log p(\mathcal{D})]. \end{aligned}$$

The last term is both hard to compute and constant w.r.t. $q(\mathbf{u}, \mathbf{r})$ [4], so we can remove it from our optimisation objective. The negation of what remains is often called the *evidence lower bound* (ELBO) and is defined as[2] [3, 4]

$$\begin{aligned} \mathcal{L} &= \mathbb{E}\left[\log \frac{p(\mathcal{D}, \mathbf{u}, \mathbf{r})}{q(\mathbf{u}, \mathbf{r})}\right] \\ &= \iiint \log \frac{p(\mathcal{D}, \mathbf{u}, \mathbf{r})}{q(\mathbf{u}, \mathbf{r})} q(\mathbf{u}, \mathbf{r})\, d\mathbf{r}\, d\mathbf{u}. \end{aligned} \tag{5}$$

[2]Throughout the proposal, all integrals should be interpreted as definite integrals over the entire sample space.

By considering full probability distributions instead of point estimates—as long as the approximations are able to capture important features of the posterior—our predictions are likely to be more accurate and rely on fewer assumptions. Moreover, we hope to make use of various recent advancements in VI for both time complexity and approximation distribution fit (see Section 2), making the resulting algorithm competitive both in terms of running time and model fit.

2. BACKGROUND

2.1 Linear Algebra, Numerical Analysis, and Measure Theory

Here we introduce a few definitions and results that will be used later in the paper. Namely, we will use several different vector and matrix norms, consider how an inverse of a matrix changes with a small perturbation, and use Lebesgue's dominated convergence theorem in order to justify the validity of our approach.

DEFINITION 2.1 (NORMS). *For any finite-dimensional vector* $\mathbf{x} = (x_1, \ldots, x_n)^\intercal$, *its* maximum norm *is*

$$\|\mathbf{x}\|_\infty = \max_i |x_i|$$

whereas its taxicab *(or* Manhattan*)* norm *is*

$$\|\mathbf{x}\|_1 = \sum_{i=1}^{n} |x_i|.$$

Let $\mathbf{A}$ *be a matrix. For any vector norm* $\|\cdot\|_p$, *we can also define its* induced norm *for matrices as*

$$\|\mathbf{A}\|_p = \sup_{\mathbf{x} \neq \mathbf{0}} \frac{\|\mathbf{A}\mathbf{x}\|_p}{\|\mathbf{x}\|_p}.$$

In particular, for $p = \infty$, *we have*

$$\|\mathbf{A}\|_\infty = \max_i \sum_j |A_{i,j}|.$$

LEMMA 2.2 (PERTURBATION LEMMA [14]). *Let* $\|\cdot\|$ *be any matrix norm, and let* $\mathbf{A}$ *and* $\mathbf{E}$ *be matrices such that* $\mathbf{A}$ *is invertible and* $\|\mathbf{A}^{-1}\|\|\mathbf{E}\| < 1$, *then* $\mathbf{A} + \mathbf{E}$ *is invertible, and*

$$\|(\mathbf{A} + \mathbf{E})^{-1}\| \leq \frac{\|\mathbf{A}^{-1}\|}{1 - \|\mathbf{A}^{-1}\|\|\mathbf{E}\|}.$$

THEOREM 2.3 (DOMINATED CONVERGENCE THEOREM [24]). *Let* $(X, \mathcal{M}, \mu)$ *be a measure space and* $\{f_n\}$ *a sequence of measurable functions on* X *for which* $\{f_n\} \to f$ *pointwise a.e. on* X *and the function* f *is measurable. Assume there is a non-negative function* g *that is integrable over* X *and dominates the sequence* $\{f_n\}$ *on* X *in the sense that*

$$|f_n| \leq g \text{ a.e. on } X \text{ for all } n.$$

Then f *is integrable over* X *and*

$$\lim_{n\to\infty} \int_X f_n\, d\mu = \int_X f\, d\mu.$$

3. SOLUTION

For any matrix $\mathbf{A}$, we will use either $A_{i,j}$ or $[\mathbf{A}]_{i,j}$ to denote the element of $\mathbf{A}$ in row i and column j. Moreover, we use $\mathrm{tr}(\mathbf{A})$ to denote its *trace* and $\mathrm{adj}(\mathbf{A})$ for its *adjugate*

(or *classical adjoint*). For any vector $\mathbf{x}$, we write $\mathbb{R}_d[\mathbf{x}]$ to denote a vector space of polynomials with degree at most d, where variables are elements of $\mathbf{x}$, and coefficients are in $\mathbb{R}$.

In this paper, all references to measurability are with respect to the Lebesgue measure. Similarly, whenever we consider the existence of an integral, we use the Lebesgue definition of integration.

3.1 Details of the Model

We keep the covariance function the same as in the work by Levine et al. [15], which is a version of the automatic relevance detection kernel [15, 18]:

$$k(\mathbf{x}_i, \mathbf{x}_j) = \lambda_0 \exp\Bigg(-\frac{1}{2}(\mathbf{x}_i - \mathbf{x}_j)^\intercal \mathbf{\Lambda}(\mathbf{x}_i - \mathbf{x}_j) - \mathbb{1}[i \neq j]\sigma^2 \operatorname{tr}(\mathbf{\Lambda}) \Bigg).$$

Here, λ_0 is the overall 'scale' factor for how similar or distant the states are, $\mathbf{\Lambda} = \operatorname{diag}(\lambda_1, \ldots, \lambda_d)$ is a diagonal matrix that determines the relevance of each feature (where d denotes the number of features), $\mathbb{1}$ is defined as

$$\mathbb{1}[b] = \begin{cases} 1 & \text{if } b \text{ is true} \\ 0 & \text{otherwise,} \end{cases}$$

and σ^2 is set to $10^{-2}/2$ (as the original paper noted that the value makes little difference to the performance of the algorithm [15]). We will write $\boldsymbol{\lambda} = (\lambda_0, \ldots, \lambda_d)^\intercal$ to refer to both λ_0 and $\mathbf{\Lambda}$ at the same time.

Ideally, we would like to model $\boldsymbol{\lambda}$ with an approximating distribution. However, due to how $p(\mathbf{u})$ has $\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}$ in its expression, and the ELBO is defined as an expectation, we are unable to show that the ELBO is well-defined. More generally, we pose the following problem, which is open to the best of our knowledge:

Open Problem 3.1. *Let $\mathbf{A}$ be a $n \times n$ matrix of coefficients, X be a random variable, and $\mathbf{M}$ be an $n \times n$ matrix such that $M_{i,j} = f(X, A_{i,j})$, where f is an arbitrary function. Under what circumstances does $\mathbb{E}[\mathbf{M}^{-1}]$ exist?*

While there are some obvious examples of when the required expected value exists (e.g., $f(X, A_{i,j}) = A_{i,j}X$ for an invertible $\mathbf{A}$ and many distributions of X), it would be particularly interesting to know whether the answer is 'always'. A proof of such a result would allow us to model $\boldsymbol{\lambda}$ instead of treating it as a variational parameter, and would thus guard against overfitting. For now, $\boldsymbol{\lambda}$ will have to be treated as a variational parameter.

It remains to decide on the model for $\mathbf{u}$ and $\mathbf{r}$. As is commonly done when applying VI to GPs, we set

$$q(\mathbf{u}, \mathbf{r}) = q(\mathbf{u})q(\mathbf{r} \mid \mathbf{u}), \tag{6}$$

where $q(\mathbf{r} \mid \mathbf{u}) = p(\mathbf{r} \mid \mathbf{u})$ and $q(\mathbf{u}) = \mathcal{N}(\mathbf{u}; \boldsymbol{\mu}, \mathbf{\Sigma})$ [7].

Ong et al. [19] have recently suggested that, in order to make variational approximation of a multivariate Gaussian more scalable, the covariance matrix should be decomposed as $\mathbf{\Sigma} = \mathbf{B}\mathbf{B}^\intercal + \mathbf{D}^2$, where $\mathbf{B}$ is a lower triangular $m \times p$ matrix with positive diagonal entries, and $\mathbf{D}$ is a diagonal matrix. Typically, we would set p so that $p \ll m$ to get an efficient approximation. However, as our goal is precision rather than scalability, we will set $p = m$ and $\mathbf{D} = \mathbf{O}_m$ in order to retain full covariance structure.

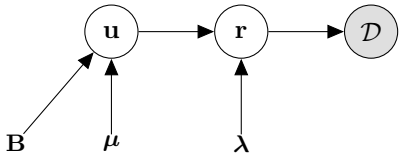

Figure 1: Our VI problem expressed as a (simplified) Bayesian network. The only observed variable (representing the demonstrations) is in a gray circle, modelled latent variables are in white circles, and the variational parameters are at the bottom.

The resulting model is summarised in Figure 1. We rely on $p(\mathcal{D} \mid \mathbf{r})$ as the only link between data and the model. Since the expression for $q(\mathbf{r} \mid \mathbf{u})$ has both $\mathbf{u}$ and covariance matrices in it, $\mathbf{r}$ depends on both $\mathbf{u}$ and the parameters of the kernel, $\boldsymbol{\lambda}$. The two remaining dependencies stem from the fact that the approximating distribution for $\mathbf{u}$ is $\mathcal{N}(\boldsymbol{\lambda}, \mathbf{B}\mathbf{B}^\intercal)$.

As we want to restrict some parameters (namely, $\boldsymbol{\lambda}$ and the diagonal of $\mathbf{B}$) to positive values, we express them as exponentials and later adjust their derivatives accordingly. Specifically, we can set $\lambda_i = e^{\lambda_i'}$ and optimise λ_i' using the chain rule:

$$\frac{\partial \mathcal{L}}{\partial \lambda_i'} = e^{\lambda_i'} \frac{\partial \mathcal{L}}{\partial \lambda_i}.$$

This way, we restrict λ_i to positive values while allowing λ_i' to range over $\mathbb{R}$.

Finally, the parameters are initialised as follows:

$$\begin{aligned} \mu_i &\sim \mathcal{U}(0,1) && \text{for } i = 1, \ldots, m, \\ \lambda_0 &\sim \chi^2_5, \\ \lambda_i &\sim \chi^2_1 && \text{for } i = 1, \ldots, d, \\ \operatorname{diag}(\mathbf{B}) &\sim \chi^2_4, \\ \text{the rest of } \mathbf{B} &\sim \mathcal{N}(0,1). \end{aligned}$$

The initialisation of $\boldsymbol{\mu}$ mirrors the initialisation of $\mathbf{r}$ in previous work by Levine et al. [15]. While they have constant initial values for $\boldsymbol{\lambda}$, we sample from χ^2 distributions centred around those values (5 for λ_0 and 1 for any other λ_i). The distributions for initial values of $\mathbf{B}$ are simply set to provide a reasonable spread of positive values for the diagonal, and both positive and negative values for all other entries in the matrix.

3.2 Evidence Lower Bound

In this section, we derive and simplify the ELBO for this (now fully specified) model. Note that in order to keep the derivation simple, we drop all constant terms in the expression of $\mathcal{L}$, i.e., equality is taken to mean 'equality up to an additive constant'. Also note that all expected values are with respect to $(\mathbf{u}, \mathbf{r}) \sim q(\mathbf{u}, \mathbf{r})$.

In order to derive the ELBO, let us go back to (5) and write

$$\mathcal{L} = \mathbb{E}[\log p(\mathcal{D}, \mathbf{u}, \mathbf{r})] - \mathbb{E}[\log q(\mathbf{u}, \mathbf{r})].$$

By substituting in (3) and (6), we get

$$\begin{aligned} \mathcal{L} = \mathbb{E}[&\log p(\mathbf{u}) + \log p(\mathbf{r} \mid \mathbf{u}) + \log p(\mathcal{D} \mid \mathbf{r})] \\ &- \mathbb{E}[\log q(\mathbf{u}) + \log q(\mathbf{r} \mid \mathbf{u})]. \end{aligned}$$

Since $q(\mathbf{r} \mid \mathbf{u}) = p(\mathbf{r} \mid \mathbf{u})$, they cancel each other out. Also

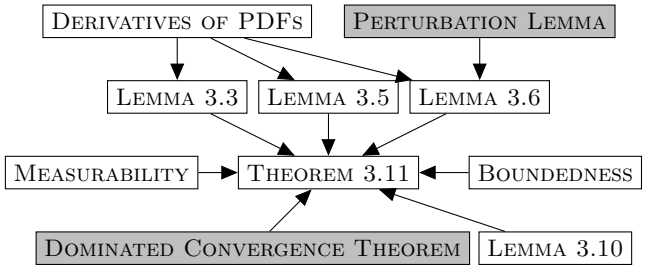

Figure 2: A graphical representation of dependencies between our theoretical results. An arrow from A to B means that A was used to prove B. Results from the literature are in gray.

notice that

$$\begin{aligned}\mathbb{E}[\log p(\mathbf{u}) - \log q(\mathbf{u})] &= -D_{\mathrm{KL}}(q(\mathbf{u}) \parallel p(\mathbf{u})) \\ &= -\frac{1}{2}(\operatorname{tr}(\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\boldsymbol{\Sigma}) + \boldsymbol{\mu}^\intercal \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\boldsymbol{\mu} - m \\ &\quad + \log|\mathbf{K}_{\mathbf{u},\mathbf{u}}| - \log|\boldsymbol{\Sigma}|),\end{aligned}$$

by the definition of KL divergence between two multivariate Gaussians [8]. Hence,

$$\begin{aligned}\mathcal{L} &= \mathbb{E}\left[\sum_{i=1}^{N}\sum_{t=1}^{T} Q_{\mathbf{r}}(s_{i,t}, a_{i,t}) - V_{\mathbf{r}}(s_{i,t})\right] \\ &\quad - \frac{1}{2}\left(\operatorname{tr}\left(\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\boldsymbol{\Sigma}\right) + \boldsymbol{\mu}^\intercal \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\boldsymbol{\mu} + \log|\mathbf{K}_{\mathbf{u},\mathbf{u}}| - \log|\boldsymbol{\Sigma}|\right).\end{aligned}$$

Using the expressions for $Q_{\mathbf{r}}$ we get

$$\begin{aligned}\mathcal{L} &= \mathbb{E}\left[\sum_{i=1}^{N}\sum_{t=1}^{T} r(s_{i,t}) - V_{\mathbf{r}}(s_{i,t}) + \gamma\sum_{s'\in\mathcal{S}}\mathcal{T}(s_{i,t}, a_{i,t}, s')V_{\mathbf{r}}(s')\right] \\ &\quad - \frac{1}{2}\left(\operatorname{tr}\left(\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\boldsymbol{\Sigma}\right) + \boldsymbol{\mu}^\intercal \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\boldsymbol{\mu} + \log|\mathbf{K}_{\mathbf{u},\mathbf{u}}| - \log|\boldsymbol{\Sigma}|\right).\end{aligned}$$

We can simplify $\sum_{i=1}^{N}\sum_{t=1}^{T} r(s_{i,t})$ by defining a new vector $\mathbf{t} = (t_1, \ldots, t_{|\mathcal{S}|})^\intercal$, where t_i is the number of times the state associated with the reward r_i has been visited across all demonstrations. Then

$$\begin{aligned}\mathbb{E}\left[\sum_{i=1}^{N}\sum_{t=1}^{T} r(s_{i,t})\right] &= \mathbb{E}[\mathbf{t}^\intercal\mathbf{r}] = \mathbf{t}^\intercal\mathbb{E}[\mathbf{r}] \\ &= \mathbf{t}^\intercal\mathbb{E}\left[\mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{u}\right] = \mathbf{t}^\intercal\mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\boldsymbol{\mu}.\end{aligned}$$

This allows us to simplify $\mathcal{L}$ to

$$\begin{aligned}\mathcal{L} &= \mathbf{t}^\intercal\mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\boldsymbol{\mu} - \mathbb{E}[v] \\ &\quad - \frac{1}{2}\left(\operatorname{tr}\left(\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\boldsymbol{\Sigma}\right) + \boldsymbol{\mu}^\intercal\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\boldsymbol{\mu} + \log|\mathbf{K}_{\mathbf{u},\mathbf{u}}| - \log|\boldsymbol{\Sigma}|\right),\end{aligned}$$

where

$$v = \sum_{i=1}^{N}\sum_{t=1}^{T} V_{\mathbf{r}}(s_{i,t}) - \gamma\sum_{s'\in\mathcal{S}}\mathcal{T}(s_{i,t}, a_{i,t}, s')V_{\mathbf{r}}(s').$$

3.3 Theoretical Justification

The typical way to optimise a quantity (the ELBO, in this case) involves computing its gradient. Unfortunately, some of the terms in $\mathcal{L}$ are still left as expected values. The goal of this section is to show how Theorem 2.3 can be applied to our model in order to derive the gradient anyway[3]. After showing that the theorem applies to our situation, given any term expressed as an expected value $\mathbb{E}[f(\mathbf{u}, \mathbf{r})]$, we can estimate its gradient as

$$\nabla\mathbb{E}[f(\mathbf{u}, \mathbf{r})] = \mathbb{E}[\nabla f(\mathbf{u}, \mathbf{r})] \approx \frac{1}{S}\sum_{s=1}^{S}\nabla f(\mathbf{u}_s, \mathbf{r}_s),$$

which can be computed by drawing S Monte Carlo samples $(\mathbf{u}_s, \mathbf{r}_s) \sim q(\mathbf{u}, \mathbf{r})$.

Our main goal is Theorem 3.11, which allows us to move differentiation inside the integral. In order to prove it, we use a number of intermediate results. We start by stating a few derivatives of probability density functions (PDFs) and covariance matrices, and bound their values with some easy-to-deal-with polynomials. We then provide a sketch proof of the measurability of MDP value functions, which is non-obvious due to their non-trivial definition. Afterwards, we establish bounds for the value functions, and, after another quick lemma, tackle the main proof of this paper. See Figure 2 for an overview of how these results fit together.

Before that, however, we define a few extra variables in order to simplify expressions of derivatives:

$$\begin{aligned}\mathbf{U} &= (\mathbf{u} - \boldsymbol{\mu})(\mathbf{u} - \boldsymbol{\mu})^\intercal, \\ \mathbf{S} &= \mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}, \\ \boldsymbol{\Gamma} &= \mathbf{K}_{\mathbf{r},\mathbf{r}} - \mathbf{S}\mathbf{K}_{\mathbf{r},\mathbf{u}}, \\ \mathbf{R} &= \mathbf{S}\frac{\partial\mathbf{K}_{\mathbf{r},\mathbf{u}}}{\partial\lambda_i} - \frac{\partial\mathbf{K}_{\mathbf{r},\mathbf{r}}}{\partial\lambda_i} + \left(\frac{\partial\mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal}{\partial\lambda_i} - \mathbf{S}\frac{\partial\mathbf{K}_{\mathbf{u},\mathbf{u}}}{\partial\lambda_i}\right)\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{K}_{\mathbf{r},\mathbf{u}}, \\ Q &= (\mathbf{u} - \boldsymbol{\mu})^\intercal\boldsymbol{\Sigma}^{-1}(\mathbf{u} - \boldsymbol{\mu}).\end{aligned}$$

Lemma 3.2 (Derivatives of PDFs).

1. $\frac{\partial q(\mathbf{u})}{\partial\boldsymbol{\mu}} = \frac{1}{2}q(\mathbf{u})(\boldsymbol{\Sigma}^{-1} + \boldsymbol{\Sigma}^{-\intercal})(\mathbf{u} - \boldsymbol{\mu})$.
2. (a) $\frac{\partial q(\mathbf{u})}{\partial\boldsymbol{\Sigma}} = \frac{1}{2}q(\mathbf{u})(\boldsymbol{\Sigma}^{-\intercal}\mathbf{U}\boldsymbol{\Sigma}^{-\intercal} - \boldsymbol{\Sigma}^{-\intercal})$.
   (b) $\frac{\partial q(\mathbf{u})}{\partial\mathbf{B}} = q(\mathbf{u})(\boldsymbol{\Sigma}^{-1}\mathbf{U}\boldsymbol{\Sigma}^{-1} - |\boldsymbol{\Sigma}|^{-1}\operatorname{adj}(\boldsymbol{\Sigma}))\mathbf{B}$.
3. *For* $i = 0, \ldots, d$,
   (a)
   $$\begin{aligned}\frac{\partial q(\mathbf{r} \mid \mathbf{u})}{\partial\lambda_i} &= \frac{1}{2}q(\mathbf{r} \mid \mathbf{u})(|\boldsymbol{\Gamma}|^{-1}\operatorname{tr}(\mathbf{R}\operatorname{adj}(\boldsymbol{\Gamma})) \\ &\quad - (\mathbf{r} - \mathbf{S}\mathbf{u})^\intercal\boldsymbol{\Gamma}^{-1}\mathbf{R}\boldsymbol{\Gamma}^{-1}(\mathbf{r} - \mathbf{S}\mathbf{u})).\end{aligned}$$
   (b) *For any covariance matrix* $\mathbf{K}$,
   $$\frac{\partial\mathbf{K}}{\partial\lambda_i} = \begin{cases}\frac{1}{\lambda_i}\mathbf{K} & \text{if } i = 0, \\ \mathbf{L} & \text{otherwise,}\end{cases}$$
   where
   $$L_{j,k} = k(\mathbf{x}_j, \mathbf{x}_k)\left(-\frac{1}{2}(x_{j,i} - x_{k,i})^2 - \mathbb{1}[j \neq k]\sigma^2\right).$$

Lemma 3.3. *Let* $i \in \{0, \ldots, d\}$ *and* $\epsilon > 0$ *be arbitrary. Furthermore, let* $c : \mathbb{R}^{|\mathcal{S}|} \times \mathbb{R}^m \to (\lambda_i - \epsilon, \lambda_i + \epsilon) \subset \mathbb{R}$ *be a function with a codomain arbitrarily close to* λ_i*. Then*

$$\left.\frac{\partial q(\mathbf{r} \mid \mathbf{u})}{\partial\lambda_i}\right|_{\lambda_i = c(\mathbf{r},\mathbf{u})}$$

[3]This technique is inspired by black box VI [22], but takes a more detailed look at the problem and requires significantly more work to prove correctness.

has upper and lower bounds of the form $q(\mathbf{r} \mid \mathbf{u})d(\mathbf{u})$, where $d(\mathbf{u}) \in \mathbb{R}_2[\mathbf{u}]$.

PROOF. Remember that

$$\frac{\partial q(\mathbf{r} \mid \mathbf{u})}{\partial \lambda_i} = \frac{1}{2} q(\mathbf{r} \mid \mathbf{u})(|\mathbf{\Gamma}|^{-1} \operatorname{tr}(\mathbf{R} \operatorname{adj}(\mathbf{\Gamma})) - (\mathbf{r} - \mathbf{S}\mathbf{u})^\intercal \mathbf{\Gamma}^{-1} \mathbf{R} \mathbf{\Gamma}^{-1} (\mathbf{r} - \mathbf{S}\mathbf{u})).$$

by Lemma 3.2.

Given any covariance matrix $\mathbf{K}$, we can easily establish constant upper and lower bounds on $\mathbf{K}|_{\lambda_i = c(\mathbf{r},\mathbf{u})}$ by the boundedness of c and continuity of the covariance function. Similar reasoning combined with the expressions for derivatives of covariance matrices in Lemma 3.2 gives constant upper and lower bounds on the elements of

$$\left.\frac{\partial \mathbf{K}}{\partial \lambda_i}\right|_{\lambda_i = c(\mathbf{r},\mathbf{u})}$$

as well.

First, we will show that $\mathbf{K}^{-1}|_{\lambda_i = c(\mathbf{r},\mathbf{u})}$ has constant bounds. If $i = 0$, then $\mathbf{K}|_{\lambda_i = c(\mathbf{r},\mathbf{u})} = c(\mathbf{r}, \mathbf{u})\mathbf{A}$, where $\mathbf{A}$ is a constant matrix defined by

$$\mathbf{A} = \frac{1}{\lambda_0}\mathbf{K},$$

and, thus, is invertible. Therefore,

$$\mathbf{K}^{-1}|_{\lambda_i = c(\mathbf{r},\mathbf{u})} = \frac{1}{c(\mathbf{r}, \mathbf{u})}\mathbf{A}^{-1}.$$

Since λ_0 cannot be zero, we can make ϵ small enough so that either $\lambda_0 - \epsilon > 0$ or $\lambda_0 + \epsilon < 0$, i.e., the values of $c(\mathbf{r}, \mathbf{u})$ are either all positive or all negative. Then, by continuity of $x \mapsto \frac{1}{x}$, $\mathbf{K}^{-1}|_{\lambda_i = c(\mathbf{r},\mathbf{u})}$ has constant bounds.

Let

$$S = \sum_{n \in \{1,\dots,d\} \setminus \{i\}} \frac{\lambda_n}{2}(x_{j,n} - x_{k,n})^2 + \mathbb{1}[j \neq k]\sigma^2 \lambda_n$$

and $\delta = c(\mathbf{r}, \mathbf{u}) - \lambda_i$ so that $c(\mathbf{r}, \mathbf{u}) = \lambda_i + \delta$. If $i > 0$, then

$$\begin{aligned}
k(\mathbf{x}_j, \mathbf{x}_k)|_{\lambda_i = c(\mathbf{r},\mathbf{u})} &= \lambda_0 \exp\Big(-\frac{1}{2} c(\mathbf{r}, \mathbf{u})(x_{j,i} - x_{k,i})^2 \\
&\qquad - \mathbb{1}[j \neq k]\sigma^2 c(\mathbf{r}, \mathbf{u}) - S \Big) \\
&= \lambda_0 \exp\Big(-\frac{1}{2}(\lambda_i + \delta)(x_{j,i} - x_{k,i})^2 \\
&\qquad - \mathbb{1}[j \neq k]\sigma^2(\lambda_i + \delta) - S \Big) \\
&= \lambda_0 \exp\Big(-\frac{1}{2}(\mathbf{x}_j - \mathbf{x}_k)^\intercal \mathbf{\Lambda}(\mathbf{x}_j - \mathbf{x}_k) - \mathbb{1}[j \neq k]\sigma^2 \operatorname{tr}(\mathbf{\Lambda}) \\
&\qquad - \frac{\delta}{2}(x_{j,i} - x_{k,i})^2 - \mathbb{1}[j \neq k]\sigma^2\delta \Big) \\
&= k(\mathbf{x}_j, \mathbf{x}_k) \exp\Big(-\frac{\delta}{2}(x_{j,i} - x_{k,i})^2 - \mathbb{1}[j \neq k]\sigma^2\delta \Big) \\
&= k(\mathbf{x}_j, \mathbf{x}_k) + k(\mathbf{x}_j, \mathbf{x}_k) \Big(\exp\Big(-\frac{\delta}{2}(x_{j,i} - x_{k,i})^2 \\
&\qquad - \mathbb{1}[j \neq k]\sigma^2\delta \Big) - 1 \Big)
\end{aligned}$$

Hence, we can express $\mathbf{K}|_{\lambda_i = c(\mathbf{r},\mathbf{u})}$ as $\mathbf{K}|_{\lambda_i = c(\mathbf{r},\mathbf{u})} = \mathbf{K} + \mathbf{E}$, where

$$E_{j,k} = k(\mathbf{x}_j, \mathbf{x}_k) \left(\exp\left(-\frac{\delta}{2}(x_{j,i} - x_{k,i})^2 - \mathbb{1}[j \neq k]\sigma^2\delta \right) - 1 \right).$$

Note that $E_{j,k} \to 0$ as $\delta \to 0$ and δ can be made arbitrarily small via ϵ. Then, since $\mathbf{K}$ is invertible, we can make δ small enough so that $\|\mathbf{K}^{-1}\|_\infty \|\mathbf{E}\|_\infty < 1$, and Lemma 2.2 shows the existence of $\mathbf{K}^{-1}_{\lambda_i = c(\mathbf{r},\mathbf{u})}$ and gives upper and lower bounds on all of its elements.

This is enough to prove constant upper and lower bounds on $\mathbf{S}$, $\mathbf{\Gamma}$, and $\mathbf{R}$ (all with λ_i replaced with $c(\mathbf{r}, \mathbf{u})$), which means that $(\mathbf{r} - \mathbf{S}\mathbf{u})^\intercal \mathbf{\Gamma}^{-1} \mathbf{R} \mathbf{\Gamma}^{-1} (\mathbf{r} - \mathbf{S}\mathbf{u})|_{\lambda_i = c(\mathbf{r},\mathbf{u})}$ has upper and lower bounds in $\mathbb{R}_2[\mathbf{u}]$.

Since $\mathbf{\Gamma}|_{\lambda_i = c(\mathbf{r},\mathbf{u})}$ is bounded, so is $\det(\mathbf{\Gamma})|_{\lambda_i = c(\mathbf{r},\mathbf{u})}$. Assuming that $\mathbf{\Gamma}$ is invertible so that $q(\mathbf{r} \mid \mathbf{u})$ exists, we can make $\mathbf{\Gamma}|_{\lambda_i = c(\mathbf{r},\mathbf{u})}$ close enough to $\mathbf{\Gamma}$ to ensure that

$$\det(\mathbf{\Gamma})|_{\lambda_i = c(\mathbf{r},\mathbf{u})} \neq 0.$$

Moreover, boundedness of $\mathbf{\Gamma}|_{\lambda_i = c(\mathbf{r},\mathbf{u})}$ gives boundedness of $\det(\mathbf{\Gamma})|_{\lambda_i = c(\mathbf{r},\mathbf{u})}$.

Combined with the fact that $ab > 0$ (i.e., both endpoints together are either positive or negative), this gives boundedness of $\det(\mathbf{\Gamma})^{-1}_{\lambda_i = c(\mathbf{r},\mathbf{u})}$.

Recall that

$$\mathbf{\Gamma} = \mathbf{K}_{\mathbf{r},\mathbf{r}} - \mathbf{S}\mathbf{K}_{\mathbf{r},\mathbf{u}} = \mathbf{K}_{\mathbf{r},\mathbf{r}} - \mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1} \mathbf{K}_{\mathbf{r},\mathbf{u}}.$$

We have already demonstrated that for $\mathbf{K} \in \{\mathbf{K}_{\mathbf{r},\mathbf{r}}, \mathbf{K}_{\mathbf{r},\mathbf{u}}, \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\}$, $\lim_{\epsilon \to 0} \mathbf{K}|_{\lambda_i = c(\mathbf{r},\mathbf{u})} = \mathbf{K}$. We can use a general fact that if $\lim_{x \to 0} f(x) = f$, then $f(x) = f + g(x)$ for some function g such that $\lim_{x \to 0} g(x) = 0$ to define matrices $\mathbf{E}_{\mathbf{r},\mathbf{r}}$, $\mathbf{E}_{\mathbf{r},\mathbf{u}}$, and $\mathbf{E}_{\mathbf{u},\mathbf{u}}$ such that

$$\begin{aligned}
&\mathbf{K}_{\mathbf{r},\mathbf{r}}|_{\lambda_i = c(\mathbf{r},\mathbf{u})} = \mathbf{K}_{\mathbf{r},\mathbf{r}} + \mathbf{E}_{\mathbf{r},\mathbf{r}}, && \mathbf{E}_{\mathbf{r},\mathbf{r}} \to \mathbf{O}_{|\mathcal{S}|}, \\
&\mathbf{K}_{\mathbf{r},\mathbf{u}}|_{\lambda_i = c(\mathbf{r},\mathbf{u})} = \mathbf{K}_{\mathbf{r},\mathbf{u}} + \mathbf{E}_{\mathbf{r},\mathbf{u}}, \quad \text{and} && \mathbf{E}_{\mathbf{r},\mathbf{u}} \to \mathbf{O}_{|\mathcal{S}|,m}, \\
&\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}|_{\lambda_i = c(\mathbf{r},\mathbf{u})} = \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1} + \mathbf{E}_{\mathbf{u},\mathbf{u}}, && \mathbf{E}_{\mathbf{u},\mathbf{u}} \to \mathbf{O}_m.
\end{aligned}$$

as $\epsilon \to 0$. Then, $\mathbf{\Gamma}|_{\lambda_i = c(\mathbf{r},\mathbf{u})} = \mathbf{\Gamma} + \mathbf{E}$, where

$$\begin{aligned}
\mathbf{E} &= \mathbf{E}_{\mathbf{r},\mathbf{r}} - \mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1} \mathbf{E}_{\mathbf{r},\mathbf{u}} - \mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal \mathbf{E}_{\mathbf{u},\mathbf{u}} (\mathbf{K}_{\mathbf{r},\mathbf{u}} + \mathbf{E}_{\mathbf{r},\mathbf{u}}) \\
&\quad - \mathbf{E}_{\mathbf{r},\mathbf{u}}^\intercal (\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1} + \mathbf{E}_{\mathbf{u},\mathbf{u}})(\mathbf{K}_{\mathbf{r},\mathbf{u}} + \mathbf{E}_{\mathbf{r},\mathbf{u}}) \\
&\quad \to \mathbf{O}_{|\mathcal{S}|}
\end{aligned}$$

as $\epsilon \to 0$. Thus, Lemma 2.2 shows that $\mathbf{\Gamma}^{-1}|_{\lambda_i = c(\mathbf{r},\mathbf{u})}$ exists and provides constant bounds on its elements.

Since we already know that $\mathbf{\Gamma}^{-1}|_{\lambda_i = c(\mathbf{r},\mathbf{u})}$ and $\det(\mathbf{\Gamma})|_{\lambda_i = c(\mathbf{r},\mathbf{u})}$ are bounded, so is $\operatorname{adj}(\mathbf{\Gamma}) = \det(\mathbf{\Gamma})\mathbf{\Gamma}^{-1}|_{\lambda_i = c(\mathbf{r},\mathbf{u})}$. Thus, we have constant bounds on $|\mathbf{\Gamma}|^{-1} \operatorname{tr}(\mathbf{R} \operatorname{adj}(\mathbf{\Gamma}))|_{\lambda_i = c(\mathbf{r},\mathbf{u})}$, which means that

$$\left.\frac{\partial q(\mathbf{r} \mid \mathbf{u})}{\partial \lambda_i}\right|_{\lambda_i = c(\mathbf{r},\mathbf{u})}$$

has the required bounds. □

REMARK 3.4. *In order to find a derivative such as $\frac{\partial q(\mathbf{u})}{\partial \mu_i}$, we can find $\frac{\partial q(\mathbf{u})}{\partial \boldsymbol{\mu}}$ and simply take the ith element. A similar line of reasoning applies to matrices as well. Thus, we only need to consider derivatives with respect to $\boldsymbol{\mu}$ and $\mathbf{\Sigma}$.*

LEMMA 3.5. *Let $c : \mathbb{R}^{|\mathcal{S}|} \times \mathbb{R}^m \to (a, b) \subset \mathbb{R}$ be an arbitrary bounded function. Then, for $i = 1, \dots, m$, every element of*

$$\left.\frac{\partial q(\mathbf{u})}{\partial \boldsymbol{\mu}}\right|_{\mu_i = c(\mathbf{r},\mathbf{u})}$$

has upper and lower bounds of the form $q(\mathbf{u})d(\mathbf{u})$, where $d(\mathbf{u}) \in \mathbb{R}_1[\mathbf{u}]$.

PROOF. Using Lemma 3.2,

$$\left.\frac{\partial q(\mathbf{u})}{\partial \boldsymbol{\mu}}\right|_{\mu_i=c(\mathbf{r},\mathbf{u})} = \frac{1}{2}q(\mathbf{u})(\boldsymbol{\Sigma}^{-1}+\boldsymbol{\Sigma}^{-\intercal})(\mathbf{u}-\mathbf{c}(\mathbf{r},\mathbf{u})),$$

where $\mathbf{c}(\mathbf{r},\mathbf{u}) = (\mu_1,\ldots,\mu_{i-1},c(\mathbf{r},\mathbf{u}),\mu_{i+1}\ldots,\mu_m)^\intercal$. Since $c(\mathbf{r},\mathbf{u})$ is bounded and $\boldsymbol{\Sigma}^{-1}+\boldsymbol{\Sigma}^{-\intercal}$ is a constant matrix, we can use the bounds on $c(\mathbf{r},\mathbf{u})$ to manufacture both upper and lower bounds on

$$\left.\frac{\partial q(\mathbf{u})}{\partial \boldsymbol{\mu}}\right|_{\mu_i=c(\mathbf{r},\mathbf{u})}$$

of the required form. □

LEMMA 3.6. *Let $i,j=1,\ldots,m$, and let $\epsilon>0$ be arbitrary. Furthermore, let*

$$c:\mathbb{R}^{|\mathcal{S}|}\times\mathbb{R}^m\to(\Sigma_{i,j}-\epsilon,\Sigma_{i,j}+\epsilon)\subset\mathbb{R}$$

be a function with a codomain arbitrarily close to $\Sigma_{i,j}$. Then every element of

$$\left.\frac{\partial q(\mathbf{u})}{\partial \boldsymbol{\Sigma}}\right|_{\Sigma_{i,j}=c(\mathbf{r},\mathbf{u})}$$

has upper and lower bounds of the form $q(\mathbf{u})d(\mathbf{u})$, where $d(\mathbf{u})\in\mathbb{R}_2[\mathbf{u}]$.

PROOF. Using Lemma 3.2,

$$\left.\frac{\partial q(\mathbf{u})}{\partial \boldsymbol{\Sigma}}\right|_{\Sigma_{i,j}=c(\mathbf{r},\mathbf{u})} = \frac{1}{2}q(\mathbf{u})(\mathbf{C}(\mathbf{r},\mathbf{u})^{-\intercal}\mathbf{U}\mathbf{C}(\mathbf{r},\mathbf{u})^{-\intercal}-\mathbf{C}(\mathbf{r},\mathbf{u})^{-\intercal}),$$

where

$$[\mathbf{C}(\mathbf{r},\mathbf{u})]_{k,l}=\begin{cases}c(\mathbf{r},\mathbf{u}) & \text{if } (k,l)=(i,j),\\ \Sigma_{k,l} & \text{otherwise.}\end{cases}$$

We can also express $\mathbf{C}(\mathbf{r},\mathbf{u})$ as $\mathbf{C}(\mathbf{r},\mathbf{u})=\boldsymbol{\Sigma}+\mathbf{E}(\mathbf{r},\mathbf{u})$, where

$$[\mathbf{E}(\mathbf{r},\mathbf{u})]_{k,l}=\begin{cases}c(\mathbf{r},\mathbf{u})-\Sigma_{i,j} & \text{if } (k,l)=(i,j),\\ 0 & \text{otherwise.}\end{cases}$$

We begin by establishing upper and lower bounds on $\mathbf{C}(\mathbf{r},\mathbf{u})^{-1}$. For this, we use the maximum norm $\|\cdot\|_\infty$ on both vectors and matrices. We can apply Lemma 2.2 to $\boldsymbol{\Sigma}$ and $\mathbf{E}(\mathbf{r},\mathbf{u})$ since

$$\|\mathbf{E}(\mathbf{r},\mathbf{u})\|_\infty=\max_k\sum_l|[\mathbf{E}(\mathbf{r},\mathbf{u})]_{k,l}|=|c(\mathbf{r},\mathbf{u})-\Sigma_{i,j}|<\epsilon$$

can be made arbitrarily small so that $\|\boldsymbol{\Sigma}^{-1}\|_\infty\|\mathbf{E}(\mathbf{r},\mathbf{u})\|_\infty<1$. Then $\mathbf{C}(\mathbf{r},\mathbf{u})$ is invertible, and

$$\|\mathbf{C}(\mathbf{r},\mathbf{u})^{-1}\|_\infty\le\frac{\|\boldsymbol{\Sigma}^{-1}\|_\infty}{1-\|\boldsymbol{\Sigma}^{-1}\|_\infty\|\mathbf{E}(\mathbf{r},\mathbf{u})\|_\infty}<\frac{\|\boldsymbol{\Sigma}^{-1}\|_\infty}{1-\|\boldsymbol{\Sigma}^{-1}\|_\infty\epsilon},$$

which means that

$$\max_k\sum_l\left|[\mathbf{C}(\mathbf{r},\mathbf{u})^{-1}]_{k,l}\right|<\frac{\|\boldsymbol{\Sigma}^{-1}\|_\infty}{1-\|\boldsymbol{\Sigma}^{-1}\|_\infty\epsilon},$$

i.e., for any row k and column l,

$$\left|[\mathbf{C}(\mathbf{r},\mathbf{u})^{-1}]_{k,l}\right|<\frac{\|\boldsymbol{\Sigma}^{-1}\|_\infty}{1-\|\boldsymbol{\Sigma}^{-1}\|_\infty\epsilon},$$

which bounds all elements of $\mathbf{C}(\mathbf{r},\mathbf{u})^{-1}$ as required. Since every element of $\mathbf{U}=(\mathbf{u}-\boldsymbol{\mu})(\mathbf{u}-\boldsymbol{\mu})^\intercal$ is in $\mathbb{R}_2[\mathbf{u}]$, and the elements of $\mathbf{C}(\mathbf{r},\mathbf{u})^{-1}$ are bounded, the desired result follows. □

REMARK 3.7. *MDP values are characterised by both a state and a reward function/vector. In this section, we think of the value function as $V:\mathcal{S}\to\mathbb{R}^{|\mathcal{S}|}\to\mathbb{R}$, i.e., V takes a state $s\in\mathcal{S}$ and returns a function $V(s):\mathbb{R}^{|\mathcal{S}|}\to\mathbb{R}$ that takes a reward vector $\mathbf{r}\in\mathbb{R}^{|\mathcal{S}|}$ and returns a value of the state s, $V_\mathbf{r}(s)\in\mathbb{R}$. Given a reward vector, the function $V(s)$ computes the values of all states and returns the value of state s.*

PROPOSITION 3.8 (MEASURABILITY). *MDP value functions $V(s):\mathbb{R}^{|\mathcal{S}|}\to\mathbb{R}$ (for $s\in\mathcal{S}$) are Lebesgue measurable.*

PROOF. For any reward vector $\mathbf{r}\in\mathbb{R}^{|\mathcal{S}|}$, the collection of converged value functions $\{V_\mathbf{r}(s)\mid s\in\mathcal{S}\}$ satisfy

$$V_\mathbf{r}(s)=\log\sum_{a\in\mathcal{A}}\exp\left(r(s)+\gamma\sum_{s'\in\mathcal{S}}\mathcal{T}(s,a,s')V_\mathbf{r}(s')\right)\quad(7)$$

for all $s\in\mathcal{S}$. Let $s_0\in\mathcal{S}$ be an arbitrary state. In order to prove that $V(s_0)$ is measurable, it is enough to show that for any $\alpha\in\mathbb{R}$, the set

$$\left\{\mathbf{r}\in\mathbb{R}^{|\mathcal{S}|}\;\middle|\;\begin{array}{l}V_\mathbf{r}(s_0)\in(-\infty,\alpha);\\ V_\mathbf{r}(s)\in\mathbb{R}\text{ for all }s\in\mathcal{S}\setminus\{s_0\};\\ (7)\text{ is satisfied by all }s\in\mathcal{S}\end{array}\right\}$$

is measurable. Since this set can be constructed in Zermelo-Fraenkel set theory *without* the axiom of choice, it is measurable [9], which proves that $V(s)$ is a measurable function for any $s\in\mathcal{S}$. □

PROPOSITION 3.9 (BOUNDEDNESS). *If the initial values of the MDP value function satisfy the following bound, then the bound remains satisfied throughout value iteration:*

$$|V_\mathbf{r}(s)|\le\frac{\|\mathbf{r}\|_\infty+\log|\mathcal{A}|}{1-\gamma}.\quad(8)$$

PROOF. We begin by considering (8) without taking the absolute value of $V_\mathbf{r}(s)$, i.e.,

$$V_\mathbf{r}(s)\le\frac{\|\mathbf{r}\|_\infty+\log|\mathcal{A}|}{1-\gamma},\quad(9)$$

and assuming that the initial values of $\{V_\mathbf{r}(s)\mid s\in\mathcal{S}\}$ already satisfy (9). Recall that for each $s\in\mathcal{S}$, the value of $V_\mathbf{r}(s)$ is updated by applying (1). Note that both log and exp are increasing functions, $\gamma>0$, and the $\mathcal{T}$ function gives a probability (a non-negative number). Thus

$$\begin{aligned}V_\mathbf{r}(s)&\le\log\sum_{a\in\mathcal{A}}\exp\left(r(s)+\gamma\sum_{s'\in\mathcal{S}}\mathcal{T}(s,a,s')\frac{\|\mathbf{r}\|_\infty+\log|\mathcal{A}|}{1-\gamma}\right)\\ &=\log\sum_{a\in\mathcal{A}}\exp\left(r(s)+\frac{\gamma(\|\mathbf{r}\|_\infty+\log|\mathcal{A}|)}{1-\gamma}\sum_{s'\in\mathcal{S}}\mathcal{T}(s,a,s')\right)\\ &=\log\sum_{a\in\mathcal{A}}\exp\left(r(s)+\frac{\gamma(\|\mathbf{r}\|_\infty+\log|\mathcal{A}|)}{1-\gamma}\right)\end{aligned}$$

by the definition of $\mathcal{T}$. Then

$$\begin{aligned}
V_{\mathbf{r}}(s) &\le \log\left(|\mathcal{A}|\exp\left(r(s)+\frac{\gamma(\|\mathbf{r}\|_\infty+\log|\mathcal{A}|)}{1-\gamma}\right)\right)\\
&= \log\left(\exp\left(\log|\mathcal{A}|+r(s)+\frac{\gamma(\|\mathbf{r}\|_\infty+\log|\mathcal{A}|)}{1-\gamma}\right)\right)\\
&= \log|\mathcal{A}|+r(s)+\frac{\gamma(\|\mathbf{r}\|_\infty+\log|\mathcal{A}|)}{1-\gamma}\\
&= \frac{\gamma(\|\mathbf{r}\|_\infty+\log|\mathcal{A}|)+(1-\gamma)(\log|\mathcal{A}|+r(s))}{1-\gamma}\\
&\le \frac{\gamma(\|\mathbf{r}\|_\infty+\log|\mathcal{A}|)+(1-\gamma)(\log|\mathcal{A}|+\|\mathbf{r}\|_\infty)}{1-\gamma}\\
&= \frac{\|\mathbf{r}\|_\infty+\log|\mathcal{A}|}{1-\gamma}
\end{aligned}$$

by the definition of $\|\mathbf{r}\|_\infty$.

The proof for

$$V_{\mathbf{r}}(s) \ge \frac{\|\mathbf{r}\|_\infty+\log|\mathcal{A}|}{\gamma-1} \tag{10}$$

follows the same argument until we get to

$$\begin{aligned}
V_{\mathbf{r}}(s) &\ge \frac{\gamma(\|\mathbf{r}\|_\infty+\log|\mathcal{A}|)+(\gamma-1)(\log|\mathcal{A}|+r(s))}{\gamma-1}\\
&\ge \frac{\gamma(\|\mathbf{r}\|_\infty+\log|\mathcal{A}|)+(\gamma-1)(-\log|\mathcal{A}|-\|\mathbf{r}\|_\infty)}{\gamma-1}\\
&= \frac{\|\mathbf{r}\|_\infty+\log|\mathcal{A}|}{\gamma-1},
\end{aligned}$$

where we use the fact that $r(s) \ge -\|\mathbf{r}\|_\infty - 2\log|\mathcal{A}|$. Combining (9) and (10) gives (8). □

LEMMA 3.10.

$$\int \|\mathbf{r}\|_\infty q(\mathbf{r}\mid\mathbf{u})\,d\mathbf{r} \le a + \|\mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{u}\|_1,$$

where a is a constant independent of $\mathbf{u}$.

PROOF. Since $\|\mathbf{r}\|_\infty \le \|\mathbf{r}\|_1$,

$$\int \|\mathbf{r}\|_\infty q(\mathbf{r}\mid\mathbf{u})\,d\mathbf{r} \le \int \|\mathbf{r}\|_1 q(\mathbf{r}\mid\mathbf{u})\,d\mathbf{r} = \sum_{i=1}^{|\mathcal{S}|}\mathbb{E}[|r_i|].$$

As each $\mathbb{E}[|r_i|]$ is a mean of a folded Gaussian distribution,

$$\mathbb{E}[|r_i|] = \sigma_i\sqrt{\frac{2}{\pi}}\exp\left(-\frac{\xi_i^2}{2\sigma_i^2}\right)+\xi_i\left(1-2\Phi\left(-\frac{\xi_1}{\sigma_1}\right)\right),$$

where $\xi_i = \left[\mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{u}\right]_i$, $\sigma_i = \sqrt{[\mathbf{K}_{\mathbf{r},\mathbf{r}}-\mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{K}_{\mathbf{r},\mathbf{u}}]_{i,i}}$[4], and Φ is the cumulative distribution function of the standard Gaussian. Furthermore,

$$\mathbb{E}[|r_i|] \le \sigma_i\sqrt{\frac{2}{\pi}}+|\xi_i|,$$

as σ_i is non-negative, and $\Phi(x)\in[0,1]$ for all x. Since

$$\sum_{i=1}^{|\mathcal{S}|}|\xi_i| = \|\mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{u}\|_1,$$

we can set

$$a = \sum_{i=1}^{|\mathcal{S}|}\sigma_i\sqrt{\frac{2}{\pi}}$$

to get the desired result. □

Our main theorem is a specialised version of an integral differentiation result by Chen [6].

THEOREM 3.11. *Whenever the derivative exists,*

$$\frac{\partial}{\partial t}\iint V_{\mathbf{r}}(s)q(\mathbf{r}\mid\mathbf{u})q(\mathbf{u})\,d\mathbf{r}\,d\mathbf{u} = \iint\frac{\partial}{\partial t}[V_{\mathbf{r}}(s)q(\mathbf{r}\mid\mathbf{u})q(\mathbf{u})]\,d\mathbf{r}\,d\mathbf{u},$$

where t is any scalar part of $\boldsymbol{\mu}$, $\boldsymbol{\Sigma}$, or $\boldsymbol{\lambda}$.

PROOF. Let

$$f(\mathbf{r},\mathbf{u},t) = V_{\mathbf{r}}(s)q(\mathbf{r}\mid\mathbf{u})q(\mathbf{u}),$$
$$F(t) = \iint f(\mathbf{r},\mathbf{u},t)\,d\mathbf{r}\,d\mathbf{u},$$

and fix the value of t. Let $(t_n)_{n=1}^\infty$ be any sequence such that $\lim_{n\to\infty}t_n = t$, but $t_n \ne t$ for all n. We want to show that

$$F'(t) = \lim_{n\to\infty}\frac{F(t_n)-F(t)}{t_n-t} = \iint\left.\frac{\partial f}{\partial t}\right|_{(\mathbf{r},\mathbf{u},t)}d\mathbf{r}\,d\mathbf{u}. \tag{11}$$

We have

$$\begin{aligned}
\frac{F(t_n)-F(t)}{t_n-t} &= \iint\frac{f(\mathbf{r},\mathbf{u},t_n)-f(\mathbf{r},\mathbf{u},t)}{t_n-t}\,d\mathbf{r}\,d\mathbf{u}\\
&= \iint f_n(\mathbf{r},\mathbf{u})\,d\mathbf{r}\,d\mathbf{u},
\end{aligned}$$

where

$$f_n(\mathbf{r},\mathbf{u}) = \frac{f(\mathbf{r},\mathbf{u},t_n)-f(\mathbf{r},\mathbf{u},t)}{t_n-t}.$$

Since

$$\lim_{n\to\infty}f_n(\mathbf{r},\mathbf{u}) = \left.\frac{\partial f}{\partial t}\right|_{(\mathbf{r},\mathbf{u},t)},$$

(11) follows from Theorem 2.3 as soon as we show that both f and f_n are measurable and find a non-negative integrable function g such that for all n, $\mathbf{r}$, $\mathbf{u}$,

$$|f_n(\mathbf{r},\mathbf{u})| \le g(\mathbf{r},\mathbf{u}).$$

The MDP value function is measurable by Proposition 3.8. The result of multiplying or adding measurable functions (e.g., probability density functions) to a measurable function is still measurable. Thus, both f and f_n are measurable.

It remains to find g. For notational simplicity and without loss of generality, we will temporarily assume that t is a parameter of $q(\mathbf{r}\mid\mathbf{u})$. Then

$$|f_n(\mathbf{r},\mathbf{u})| = |V_{\mathbf{r}}(s)|\left|\frac{q(\mathbf{r}\mid\mathbf{u})|_{t=t_n}-q(\mathbf{r}\mid\mathbf{u})}{t_n-t}\right|q(\mathbf{u})$$

since PDFs are non-negative. An upper bound for $|V_{\mathbf{r}}(s)|$ is given by Proposition 3.9, while

$$\frac{q(\mathbf{r}\mid\mathbf{u})|_{t=t_n}-q(\mathbf{r}\mid\mathbf{u})}{t_n-t} = \left.\frac{\partial q(\mathbf{r}\mid\mathbf{u})}{\partial t}\right|_{t=c(\mathbf{r},\mathbf{u})}$$

for some function $c:\mathbb{R}^{|\mathcal{S}|}\times\mathbb{R}^m\to(\min\{t,t_n\},\max\{t,t_n\})$ due to the mean value theorem (since q is a continuous and differentiable function of t, regardless of the specific choices of q and t).

[4]The expression under the square root sign is non-negative because $\mathbf{K}_{\mathbf{r},\mathbf{r}}-\mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{K}_{\mathbf{r},\mathbf{u}}$ is a covariance matrix of a Gaussian distribution, hence also positive semi-definite, which means that its diagonal entries are non-negative.

We then have that

$$|f_n(\mathbf{r},\mathbf{u})| \leq \frac{\|\mathbf{r}\|_\infty + \log|\mathcal{A}|}{1-\gamma} \left| \frac{\partial q(\mathbf{r} \mid \mathbf{u})}{\partial t} \Big|_{t=c(\mathbf{r},\mathbf{u})} \right| q(\mathbf{u}).$$

The bound is clearly non-negative and measurable. It remains to show that it is also integrable. Depending on what t represents, we can use one of the Lemmas 3.3, 3.5, and 3.6, which gives us two polynomials $p_1(\mathbf{u}), p_2(\mathbf{u}) \in \mathbb{R}_2[\mathbf{u}]$ such that

$$p_1(\mathbf{u})q(\mathbf{r} \mid \mathbf{u}) < \frac{\partial q(\mathbf{r} \mid \mathbf{u})}{\partial t}\Big|_{t=c(\mathbf{r},\mathbf{u})} < p_2(\mathbf{u})q(\mathbf{r} \mid \mathbf{u}).$$

Then

$$\left| \frac{\partial q(\mathbf{r} \mid \mathbf{u})}{\partial t}\Big|_{t=c(\mathbf{r},\mathbf{u})} \right| < q(\mathbf{r} \mid \mathbf{u}) \max\{|p_1(\mathbf{u})|, |p_2(\mathbf{u})|\}.$$

We can now apply Lemma 3.10, which allows us to integrate out $\mathbf{r}$, and we are left with showing the existence of

$$\int \left(a + \|\mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{u}\|_1\right) \max\{|p_1(\mathbf{u})|, |p_2(\mathbf{u})|\} q(\mathbf{u})\, d\mathbf{u}, \tag{12}$$

where a is a constant. The integral

$$\int \max\left\{ \begin{matrix} |p_1(\mathbf{u})|, \\ |p_2(\mathbf{u})| \end{matrix} \right\} q(\mathbf{u})\, d\mathbf{u} = \int \max\left\{ \begin{matrix} |p_1(\mathbf{u})q(\mathbf{u})|, \\ |p_2(\mathbf{u})q(\mathbf{u})| \end{matrix} \right\} d\mathbf{u}$$

exists because $p_1(\mathbf{u})q(\mathbf{u})$ and $p_2(\mathbf{u})q(\mathbf{u})$ are both integrable, hence their absolute values are integrable, and the maximum of two integrable functions is also integrable. Since $\|\mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{u}\|_1 \in \mathbb{R}_1[\mathbf{u}]$, a similar argument can be applied to the rest of (12) as well. □

4. EVALUATION

In order to fully understand the model's behaviour, we focus on a three-state MDP where the agent can deterministically move from any state to any other state. More formally, we set $\mathcal{S} = \{s_1, s_2, s_3\}$, $\mathcal{A} = \{a_1, a_2\}$,

$$\begin{aligned} \mathcal{T}(s_1, a_1, s_2) &= 1, \quad \mathcal{T}(s_1, a_2, s_3) = 1, \\ \mathcal{T}(s_2, a_1, s_1) &= 1, \quad \mathcal{T}(s_1, a_2, s_3) = 1, \\ \mathcal{T}(s_3, a_1, s_1) &= 1, \quad \mathcal{T}(s_1, a_2, s_2) = 1, \end{aligned}$$

all other values of $\mathcal{T}$ to zero, and vary the value of γ. We also set the inducing points to be equal to the three states in $\mathcal{S}$, add a single feature $f : \mathcal{S} \to \mathbb{R}$ such that

$$f(s_1) = 1, \quad f(s_2) = 2, \quad f(s_3) = 3,$$

and create two demonstrations: $\zeta_1 = \{(s_1, a_1)\}$ and $\zeta_2 = \{(s_3, a_2)\}$. In other words, the demonstrations move from s_1 and s_3 to s_2. Therefore, we would expect the reward (and value) of s_2 to be the highest.

Observation from a plot not worth including here. The policy behaves as expected: if we fix $r(s_1)$, $\pi(s_1, a_1)$ increases with higher $r(s_2)$ as well as lower $r(s_3)$ values.

5. CONCLUSIONS

More variables/information. Fewer assumptions.

We show how to avoid the deterministic training conditional assumption.

5.1 Future Work

An interesting extension to our work would be to consider IRL in the context of a reinforcement learning (RL) agent. Suppose we have an agent whose purpose is to learn optimal behaviour from observing other agents using IRL. It could then take reward variance estimates into account when choosing what states to visit next. It would have to handle the balance between exploration and exploitation similarly to many RL agents, but the information about rewards would come from observing (presumably near-optimal) behaviour exhibited by other agents rather than directly from the environment.

It is also worth noting the approach presented in this paper requires solving S MDPs for every iteration of optimising the parameters (where S is the number of samples drawn from $q(\mathbf{u}, \mathbf{r})$). There are at least two ways to reduce or eliminate this performance bottleneck:

- The MDP value function could be approximated, allowing for some minor mistakes in the resulting policy.
- Perhaps there is a good way to use information about previously computed value functions for similar rewards to hasten the current computation. One simple way to do this would be by initialising the current values to the optimal values of the previous MDP value function computation.

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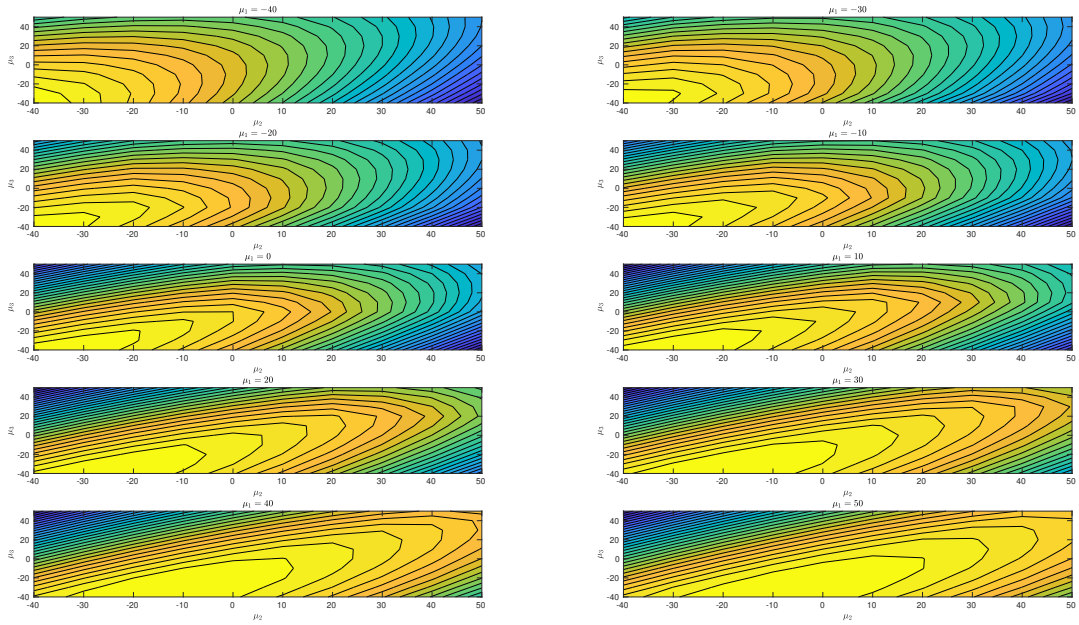

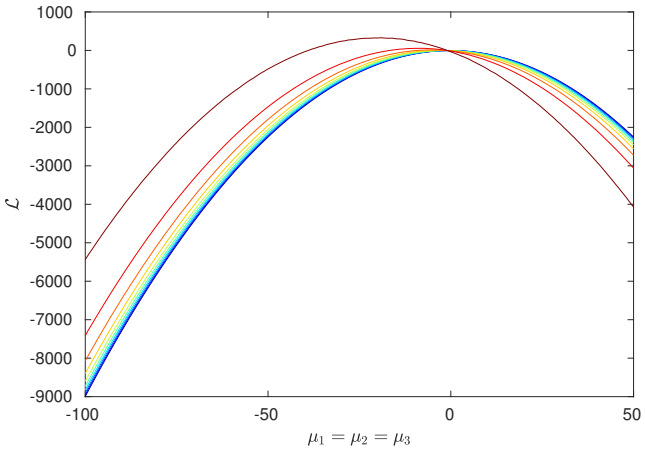

Figure 3: Changes in $\mathcal{L}$ as a function of μ, where $\mu_1 = \mu_2 = \mu_3$, and $\gamma = 0, 0.1, \ldots, 0.9$. Each of the ten curves plots a different value of γ, ranging from 0 in dark blue to 0.9 in dark red.

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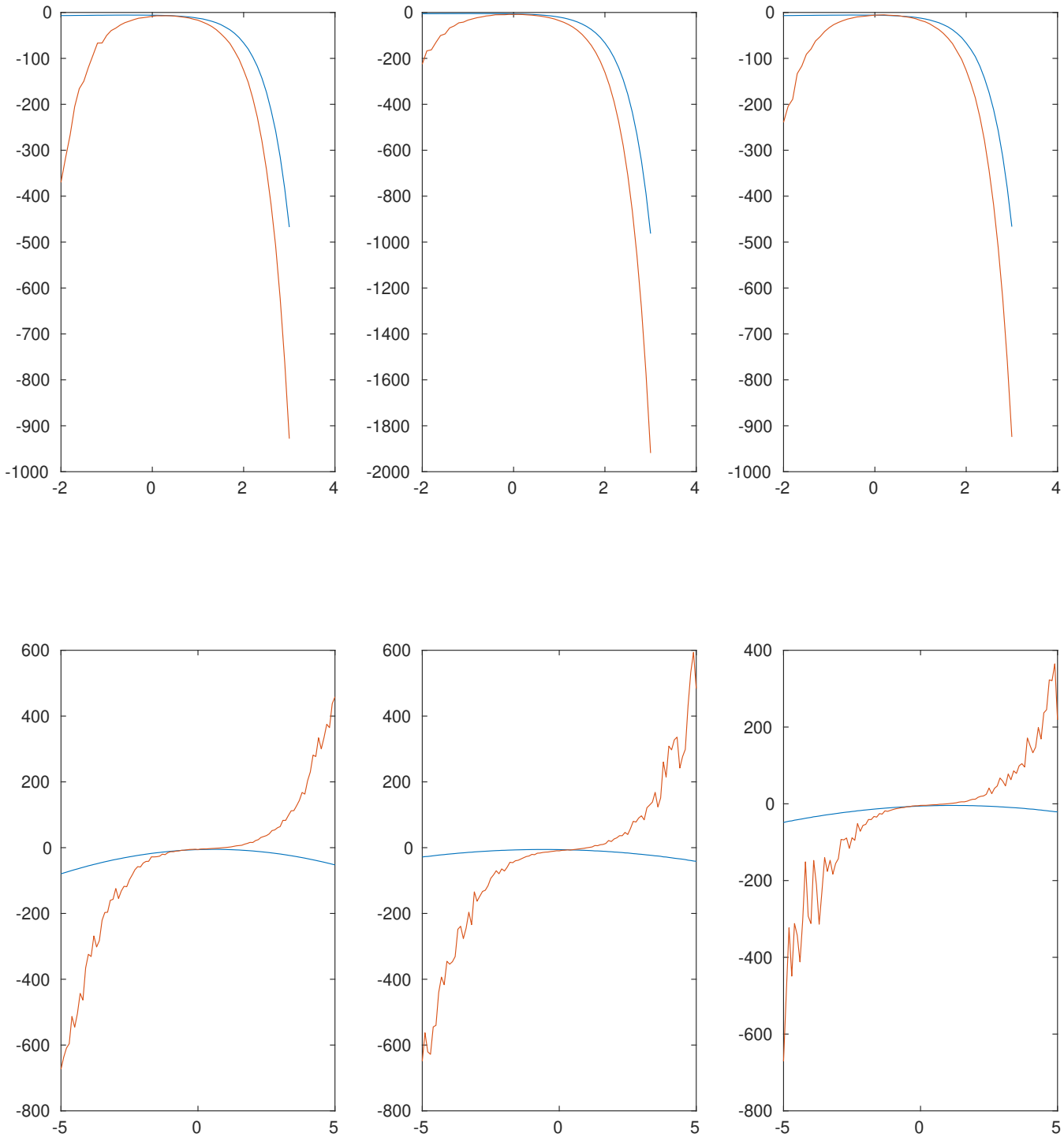

Figure 4: ELBO in blue, derivative in red. The first row is for diagonal values of B, the second row is for non-diagonal values.

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APPENDIX

A. PROOFS

LEMMA 3.2 (DERIVATIVES OF PDFS).

1. $\frac{\partial q(\mathbf{u})}{\partial \boldsymbol{\mu}} = \frac{1}{2} q(\mathbf{u})(\boldsymbol{\Sigma}^{-1} + \boldsymbol{\Sigma}^{-\intercal})(\mathbf{u} - \boldsymbol{\mu})$.
2. (a) $\frac{\partial q(\mathbf{u})}{\partial \boldsymbol{\Sigma}} = \frac{1}{2} q(\mathbf{u})(\boldsymbol{\Sigma}^{-\intercal}\mathbf{U}\boldsymbol{\Sigma}^{-\intercal} - \boldsymbol{\Sigma}^{-\intercal})$.
   (b) $\frac{\partial q(\mathbf{u})}{\partial \mathbf{B}} = q(\mathbf{u})(\boldsymbol{\Sigma}^{-1}\mathbf{U}\boldsymbol{\Sigma}^{-1} - |\boldsymbol{\Sigma}|^{-1}\operatorname{adj}(\boldsymbol{\Sigma}))\mathbf{B}$.
3. *For* $i = 0, \ldots, d$,
   (a)

$$\frac{\partial q(\mathbf{r} \mid \mathbf{u})}{\partial \lambda_i} = \frac{1}{2} q(\mathbf{r} \mid \mathbf{u})(|\boldsymbol{\Gamma}|^{-1} \operatorname{tr}(\mathbf{R} \operatorname{adj}(\boldsymbol{\Gamma})) - (\mathbf{r} - \mathbf{S}\mathbf{u})^{\intercal}\boldsymbol{\Gamma}^{-1}\mathbf{R}\boldsymbol{\Gamma}^{-1}(\mathbf{r} - \mathbf{S}\mathbf{u})).$$

   (b) *For any covariance matrix* $\mathbf{K}$,

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

where

$$L_{j,k} = k(\mathbf{x}_j, \mathbf{x}_k)\left(-\frac{1}{2}(x_{j,i} - x_{k,i})^2 - \mathbb{1}[j \neq k]\sigma^2\right).$$

PROOF.

1.

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

2. An online tool by Laue et al.[5] [13] can be used to find both derivatives.

3. (a) Since

$$\begin{aligned}q(\mathbf{r} \mid \mathbf{u}) &= \mathcal{N}(\mathbf{r}; \mathbf{K}_{\mathbf{r},\mathbf{u}}^{\intercal}\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{u}, \mathbf{K}_{\mathbf{r},\mathbf{r}} - \mathbf{K}_{\mathbf{r},\mathbf{u}}^{\intercal}\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{K}_{\mathbf{r},\mathbf{u}}) \\ &= \mathcal{N}(\mathbf{r}; \mathbf{S}\mathbf{u}, \boldsymbol{\Gamma}),\end{aligned}$$

we have

$$\frac{\partial q(\mathbf{r} \mid \mathbf{u})}{\partial \lambda_i} = -\frac{1}{2}q(\mathbf{r} \mid \mathbf{u})\frac{\partial}{\partial \lambda_i}[(\mathbf{r}-\mathbf{S}\mathbf{u})^{\intercal}\boldsymbol{\Gamma}^{-1}(\mathbf{r}-\mathbf{S}\mathbf{u})+\log|\boldsymbol{\Gamma}|].$$

The same online tool can be used to show that

$$\frac{\partial}{\partial \lambda_i}\log|\boldsymbol{\Gamma}| = -|\boldsymbol{\Gamma}|^{-1}\operatorname{tr}(\mathbf{R}\operatorname{adj}(\boldsymbol{\Gamma})),$$

and

$$\frac{\partial}{\partial \lambda_i}\boldsymbol{\Gamma}^{-1} = \boldsymbol{\Gamma}^{-1}\mathbf{R}\boldsymbol{\Gamma}^{-1}.$$

[5] http://www.matrixcalculus.org/

(b) If $i = 0$, then

$$\frac{\partial \mathbf{K}}{\partial \lambda_i} = \frac{1}{\lambda_i}\mathbf{K}$$

by the structure of each element of $\mathbf{K}$. If $i \neq 0$, then each element of $\frac{\partial \mathbf{K}}{\partial \lambda_i}$ is

$$\begin{aligned}
L_{j,k} &= \frac{\partial k(\mathbf{x}_j, \mathbf{x}_k)}{\partial \lambda_i} \\
&= k(\mathbf{x}_j, \mathbf{x}_k)\frac{\partial}{\partial \lambda_i}\Bigg[-\frac{1}{2}(\mathbf{x}_j - \mathbf{x}_k)^\intercal \mathbf{\Lambda}(\mathbf{x}_j - \mathbf{x}_k) \\
&\qquad - \mathbb{1}[j \neq k]\sigma^2 \operatorname{tr}(\mathbf{\Lambda})\Bigg] \\
&= k(\mathbf{x}_j, \mathbf{x}_k)\frac{\partial}{\partial \lambda_i}\Bigg[-\frac{1}{2}\sum_{l=1}^{d} \lambda_l (x_{j,l} - x_{k,l})^2 \\
&\qquad - \mathbb{1}[j \neq k]\sigma^2 \sum_{l=1}^{d} \lambda_l \Bigg] \\
&= k(\mathbf{x}_j, \mathbf{x}_k)\left(-\frac{1}{2}(x_{j,i} - x_{k,i})^2 - \mathbb{1}[j \neq k]\sigma^2\right).
\end{aligned}$$

□

B. DERIVATIVES OF THE ELBO

B.1 $\partial/\partial\boldsymbol{\mu}$

We begin by removing terms independent of $\boldsymbol{\mu}$:

$$\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}} = \frac{\partial}{\partial \boldsymbol{\mu}}[\mathbf{t}^\intercal \mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\boldsymbol{\mu}] - \frac{1}{2}\frac{\partial}{\partial \boldsymbol{\mu}}\left[\boldsymbol{\mu}^\intercal \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\boldsymbol{\mu}\right] - \frac{\partial}{\partial \boldsymbol{\mu}}\mathbb{E}[v].$$

Here

$$\frac{\partial}{\partial \boldsymbol{\mu}}\left[\boldsymbol{\mu}^\intercal \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\boldsymbol{\mu}\right] = (\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1} + \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-\intercal})\boldsymbol{\mu}$$

by Petersen and Pedersen [20], and

$$\begin{aligned}
\frac{\partial}{\partial \boldsymbol{\mu}}\mathbb{E}[V_{\mathbf{r}}(s)] &= \frac{\partial}{\partial \boldsymbol{\mu}}\iint V_{\mathbf{r}}(s) q(\mathbf{r} \mid \mathbf{u}) q(\mathbf{u})\, d\mathbf{r}\, d\mathbf{u} \\
&= \iint V_{\mathbf{r}}(s) q(\mathbf{r} \mid \mathbf{u}) \frac{\partial q(\mathbf{u})}{\partial \boldsymbol{\mu}}\, d\mathbf{r}\, d\mathbf{u} \\
&= \frac{1}{2}\mathbb{E}[V_{\mathbf{r}}(s)(\mathbf{\Sigma}^{-1} + \mathbf{\Sigma}^{-\intercal})(\mathbf{u} - \boldsymbol{\mu})]
\end{aligned}$$

by Theorem 3.11 and Lemma 3.2. Hence,

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \boldsymbol{\mu}} &= \mathbf{t}^\intercal \mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1} - \frac{1}{2}(\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1} + \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-\intercal})\boldsymbol{\mu} \\
&\quad - \frac{1}{2}\mathbb{E}\left[(\mathbf{\Sigma}^{-1} + \mathbf{\Sigma}^{-\intercal})(\mathbf{u} - \boldsymbol{\mu})v\right].
\end{aligned}$$

B.2 $\partial/\partial\mathbf{B}$

$$\frac{\partial \mathcal{L}}{\partial \mathbf{B}} = \frac{1}{2}\left(\frac{\partial}{\partial \mathbf{B}}\log|\mathbf{\Sigma}| - \frac{\partial}{\partial \mathbf{B}}\operatorname{tr}\left(\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{\Sigma}\right)\right) - \frac{\partial}{\partial \mathbf{B}}\mathbb{E}[v].$$

By Theorem 3.11,

$$\frac{\partial}{\partial \mathbf{B}}\mathbb{E}[V_{\mathbf{r}}(s)] = \iint V_{\mathbf{r}}(s) q(\mathbf{r} \mid \mathbf{u}) \frac{\partial q(\mathbf{u})}{\partial \mathbf{B}}\, d\mathbf{r}\, d\mathbf{u}.$$

Then, using the aforementioned tool by Laue et al. [13], we get

$$\frac{\partial}{\partial \mathbf{B}}\log|\mathbf{\Sigma}| = 2\mathbf{\Sigma}^{-1}\mathbf{B}, \quad \frac{\partial}{\partial \mathbf{B}}\operatorname{tr}\left(\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{\Sigma}\right) = 2\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{B},$$

and Lemma 3.2 gives

$$\frac{\partial q(\mathbf{u})}{\partial \mathbf{B}} = q(\mathbf{u})(\mathbf{\Sigma}^{-1}\mathbf{U}\mathbf{\Sigma}^{-1} - |\mathbf{\Sigma}|^{-1}\operatorname{adj}(\mathbf{\Sigma}))\mathbf{B}.$$

Therefore,

$$\frac{\partial \mathcal{L}}{\partial \mathbf{B}} = \left(\mathbf{\Sigma}^{-1} - \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\right)\mathbf{B} - \mathbb{E}[(\mathbf{\Sigma}^{-1}\mathbf{U}\mathbf{\Sigma}^{-1} - |\mathbf{\Sigma}|^{-1}\operatorname{adj}(\mathbf{\Sigma}))\mathbf{B}v].$$

B.3 $\partial/\partial\lambda_j$

For $j = 0, \ldots, d$,

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \lambda_j} &= \mathbf{t}^\intercal \frac{\partial}{\partial \lambda_j}\left[\mathbf{K}_{\mathbf{r},\mathbf{u}}\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\right]\boldsymbol{\mu} - \frac{\partial}{\partial \lambda_j}\mathbb{E}[v] \\
&\quad - \frac{1}{2}\left(\frac{\partial}{\partial \lambda_j}\operatorname{tr}\left(\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{\Sigma}\right) + \boldsymbol{\mu}^\intercal \frac{\partial \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}}{\partial \lambda_j}\boldsymbol{\mu} + \frac{\partial}{\partial \lambda_j}\log|\mathbf{K}_{\mathbf{u},\mathbf{u}}|\right),
\end{aligned}$$

where

$$\begin{aligned}
\frac{\partial \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}}{\partial \lambda_j} &= -\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\frac{\partial \mathbf{K}_{\mathbf{u},\mathbf{u}}}{\partial \lambda_j}\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}, \\
\frac{\partial}{\partial \lambda_j}\left[\mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\right] &= \frac{\partial \mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal}{\partial \lambda_j}\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1} + \mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal \frac{\partial \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}}{\partial \lambda_j} \\
&= \left(\frac{\partial \mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal}{\partial \lambda_j} - \mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\frac{\partial \mathbf{K}_{\mathbf{u},\mathbf{u}}}{\partial \lambda_j}\right)\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}, \\
\frac{\partial}{\partial \lambda_j}\operatorname{tr}(\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{\Sigma}) &= \operatorname{tr}\left(\frac{\partial}{\partial \lambda_j}\left[\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{\Sigma}\right]\right) = \operatorname{tr}\left(\frac{\partial \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}}{\partial \lambda_j}\mathbf{\Sigma}\right) \\
&= -\operatorname{tr}\left(\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\frac{\partial \mathbf{K}_{\mathbf{u},\mathbf{u}}}{\partial \lambda_j}\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{\Sigma}\right), \\
\frac{\partial}{\partial \lambda_j}\log|\mathbf{K}_{\mathbf{u},\mathbf{u}}| &= \operatorname{tr}\left(\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\frac{\partial \mathbf{K}_{\mathbf{u},\mathbf{u}}}{\partial \lambda_j}\right)
\end{aligned}$$

by Petersen and Pedersen [20], and

$$\begin{aligned}
\frac{\partial}{\partial \lambda_j}\mathbb{E}[V_{\mathbf{r}}(s)] &= \iint V_{\mathbf{r}}(s)\frac{\partial q(\mathbf{r} \mid \mathbf{u})}{\partial \lambda_j} q(\mathbf{u})\, d\mathbf{r}\, d\mathbf{u} \\
&= \frac{1}{2}\mathbb{E}[V_{\mathbf{r}}(s)(|\mathbf{\Gamma}|^{-1}\operatorname{tr}(\mathbf{R}\operatorname{adj}(\mathbf{\Gamma})) \\
&\qquad - (\mathbf{r} - \mathbf{S}\mathbf{u})^\intercal \mathbf{\Gamma}^{-1}\mathbf{R}\mathbf{\Gamma}^{-1}(\mathbf{r} - \mathbf{S}\mathbf{u}))]
\end{aligned}$$

by Theorem 3.11 and Lemma 3.2. Thus,

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \lambda_j} &= \mathbf{t}^\intercal \left(\frac{\partial \mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal}{\partial \lambda_j} - \mathbf{K}_{\mathbf{r},\mathbf{u}}^\intercal \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\frac{\partial \mathbf{K}_{\mathbf{u},\mathbf{u}}}{\partial \lambda_j}\right)\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\boldsymbol{\mu} \\
&\quad + \frac{1}{2}\Bigg[\operatorname{tr}\left(\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\frac{\partial \mathbf{K}_{\mathbf{u},\mathbf{u}}}{\partial \lambda_j}\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\mathbf{\Sigma}\right) + \boldsymbol{\mu}^\intercal \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\frac{\partial \mathbf{K}_{\mathbf{u},\mathbf{u}}}{\partial \lambda_j}\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\boldsymbol{\mu} \\
&\qquad - \operatorname{tr}\left(\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}\frac{\partial \mathbf{K}_{\mathbf{u},\mathbf{u}}}{\partial \lambda_j}\right)\Bigg] \\
&\quad - \frac{1}{2}\mathbb{E}[(|\mathbf{\Gamma}|^{-1}\operatorname{tr}(\mathbf{R}\operatorname{adj}(\mathbf{\Gamma})) \\
&\qquad - (\mathbf{r} - \mathbf{S}\mathbf{u})^\intercal \mathbf{\Gamma}^{-1}\mathbf{R}\mathbf{\Gamma}^{-1}(\mathbf{r} - \mathbf{S}\mathbf{u}))v],
\end{aligned}$$

where the remaining derivatives can be found in Lemma 3.2.