



University of Glasgow | School of
Computing Science

Variational Inference for Inverse Reinforcement Learning with Gaussian Processes

Paulius Dilkas

School of Computing Science
Sir Alwyn Williams Building
University of Glasgow
G12 8QQ

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1 Introduction

Inverse reinforcement learning (IRL)—a problem proposed by Russell in 1998 [57]—asks us to find a reward function for a Markov decision process that best explains a set of given demonstrations. IRL is important because reward functions can be hard to define manually [1, 3], and rewards are not entirely specific to a given environment, allowing one to reuse the same reward structure in previously unseen environments [3, 30, 35]. Moreover, IRL has seen a wide array of applications in autonomous vehicle control [31, 33] and learning to predict another agent’s behaviour [9, 70, 77, 78, 79]. Most approaches in the literature (see Section 3) 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 [30, 35, 48].

2 Statement of the Problem

Definition 1. A *Markov decision process* (MDP) is a set $\mathcal{M} = \{\mathcal{S}, \mathcal{A}, \mathcal{T}, \gamma, r\}$, where \mathcal{S} and \mathcal{A} are sets of states and actions, respectively; $\mathcal{T} : \mathcal{S} \times \mathcal{A} \times \mathcal{S} \rightarrow [0, 1]$ 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 (with higher γ values, it makes little difference whether a reward is received now or later, while with lower γ values the future becomes gradually less and less important); and $r : \mathcal{S} \rightarrow \mathbb{R}$ is the reward function.

In *inverse reinforcement learning*, one is presented with an MDP without a reward function $\mathcal{M} \setminus \{r\}$ and a set of expert demonstrations $\mathcal{D} = \{\zeta_i\}_{i=1}^N$, where each demonstration $\zeta_i = \{(s_{i,0}, a_{i,0}), \dots, (s_{i,T}, a_{i,T})\}$ is a multiset of state-action pairs representing the actions taken by the expert during a particular recorded session. Each state is also characterised by a number of features. The goal of IRL is then to find r such that the optimal policy under r

$$\pi^* = \arg \max_{\pi} \mathbb{E} \left[\sum_{t=0}^{\infty} \gamma^t r(s_t) | \pi \right]$$

matches the actions in \mathcal{D} .

The likelihood of the data can be written down as [30, 35]

$$p(\mathcal{D}|r) = \prod_{i=1}^N \prod_{t=1}^T p(a_{i,t}|s_{i,t}) = \exp \left(\sum_{i=1}^N \sum_{t=1}^T Q_r(s_{i,t}, a_{i,t}) - V_r(s_{i,t}) \right), \quad (1)$$

where

$$Q_r(s_{i,t}, a_{i,t}) = r(s_{i,t}) + \gamma \sum_{s' \in \mathcal{S}} \mathcal{T}(s_{i,t}, a_{i,t}, s') V_r(s'), \quad (2)$$

and $V_r(s)$ can be obtained by repeatedly applying the equation [36]

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

However, a reward function learned by maximising this likelihood is not transferable to new situations [30, 35]. 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 [54]. We write $r \sim \mathcal{GP}(0, k_\Theta)$ to say that r is a GP with mean 0 and covariance function k_Θ , which uses a set of hyperparameters Θ . Covariance functions 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 $\mathcal{O}(n^3)$ [54], 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 [39]. Let \mathbf{X}_u be the matrix of features at inducing states, \mathbf{u} the rewards at those states, and \mathbf{r} a vector with $r(\mathcal{S})$ as elements. Then the full joint probability distribution can be factorised as

$$p(\mathcal{D}, \Theta, \mathbf{X}_u, \mathbf{u}, \mathbf{r}) = p(\mathbf{X}_u) \times p(\Theta | \mathbf{X}_u) \times p(\mathbf{u} | \Theta, \mathbf{X}_u) \times p(\mathbf{r} | \Theta, \mathbf{X}_u, \mathbf{u}) \times p(\mathcal{D} | \mathbf{r}). \quad (3)$$

Here $p(\mathbf{X}_u)$ and $p(\Theta | \mathbf{X}_u)$ are customisable priors,

$$\begin{aligned} p(\mathbf{u} | \Theta, \mathbf{X}_u) &= \mathcal{N}(\mathbf{u}; \mathbf{0}, \mathbf{K}_{u,u}) \\ &= \frac{1}{(2\pi)^{m/2} |\mathbf{K}_{u,u}|^{1/2}} \exp \left(-\frac{1}{2} \mathbf{u}^\top \mathbf{K}_{u,u}^{-1} \mathbf{u} \right) \\ &= \exp \left(-\frac{1}{2} \mathbf{u}^\top \mathbf{K}_{u,u}^{-1} \mathbf{u} - \frac{1}{2} \log |\mathbf{K}_{u,u}| - \frac{m}{2} \log 2\pi \right) \end{aligned} \quad (4)$$

is the GP prior [54], where $m \in \mathbb{N}$ is the number of inducing points. The GP posterior is a multivariate Gaussian [35]

$$p(\mathbf{r} | \Theta, \mathbf{X}_u, \mathbf{u}) = \mathcal{N}(\mathbf{r}; \mathbf{K}_{r,u}^\top \mathbf{K}_{u,u}^{-1} \mathbf{u}, \mathbf{K}_{r,r} - \mathbf{K}_{r,u}^\top \mathbf{K}_{u,u}^{-1} \mathbf{K}_{r,u}), \quad (5)$$

and $p(\mathcal{D} | \mathbf{r})$ is as in (1). The matrices such as $\mathbf{K}_{r,u}$ are called *covariance matrices* and are defined as $[\mathbf{K}_{r,u}]_{i,j} = k_\Theta(\mathbf{x}_{r,i}, \mathbf{x}_{u,j})$, where $\mathbf{x}_{r,i}$ and $\mathbf{x}_{u,j}$ denote feature vectors for the i th state in \mathcal{S} and the j th state in \mathbf{X}_u , respectively [30].

Given this model, data \mathcal{D} , and inducing feature matrix \mathbf{X}_u , our goal is then to find optimal values of hyperparameters Θ , inducing rewards \mathbf{u} , and the reward function r . While the previous paper that considered this IRL model computed maximum likelihood estimates for Θ and \mathbf{u} , and made an assumption that \mathbf{r} in (5) has zero variance [35], we aim to avoid this assumption and use variational inference to approximate the full posterior distribution $p(\Theta, \mathbf{u}, \mathbf{r} | \mathcal{D}, \mathbf{X}_u)$. *Variational inference* (VI) is an approximation technique for probability densities [8]. Let $q_\nu(\Theta, \mathbf{u}, \mathbf{r})$ be our approximating family of probability distributions for $p(\Theta, \mathbf{u}, \mathbf{r} | \mathcal{D}, \mathbf{X}_u)$ with its own hyperparameter vector ν . Then it is up to VI algorithms to optimise ν 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 in this case can be defined as follows [8]:

$$D_{\text{KL}}(q_\nu(\Theta, \mathbf{u}, \mathbf{r}) || p(\Theta, \mathbf{u}, \mathbf{r} | \mathcal{D}, \mathbf{X}_u)) = \mathbb{E}_{(\Theta, \mathbf{u}, \mathbf{r}) \sim q_\nu(\Theta, \mathbf{u}, \mathbf{r})} \left[\log \frac{q_\nu(\Theta, \mathbf{u}, \mathbf{r})}{p(\Theta, \mathbf{u}, \mathbf{r} | \mathcal{D}, \mathbf{X}_u)} \right].$$

Since KL divergence is typically hard to compute, instead of minimising it, VI typically tries to maximise the *evidence lower bound* (ELBO) defined as [7, 8]

$$\begin{aligned}\mathcal{L}(\boldsymbol{\nu}) &= \mathbb{E}_{(\Theta, \mathbf{u}, \mathbf{r}) \sim q_{\boldsymbol{\nu}}(\Theta, \mathbf{u}, \mathbf{r})} \left[\log \frac{p(\mathcal{D}, \Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u}, \mathbf{r})}{q_{\boldsymbol{\nu}}(\Theta, \mathbf{u}, \mathbf{r})} \right] \\ &= \iiint q_{\boldsymbol{\nu}}(\Theta, \mathbf{u}, \mathbf{r}) \log \frac{p(\mathcal{D}, \Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u}, \mathbf{r})}{q_{\boldsymbol{\nu}}(\Theta, \mathbf{u}, \mathbf{r})} d\Theta d\mathbf{u} d\mathbf{r}.\end{aligned}\tag{6}$$

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 3), making the resulting algorithm competitive both in terms of speed and model fit.

3 Literature Survey

Variational inference has seen a recent increase in interest among academics, with different approaches focusing on different goals: better time complexity, handling a wider variety of models, making approximations more accurate, and using more complex function approximation techniques (such as neural networks) to infer local latent variable values without having to calculate them individually for each data point [75]. As our IRL model is based on a GP, we will begin by reviewing some of the VI approaches applied specifically to GP regression. Based on a recent review of scalable GPs [75], we will concentrate on *stochastic variational sparse approximations*, as they have achieved modelling accuracy close to that of the full GP with no approximations, while providing a time complexity of $\mathcal{O}(m^3)$. Below we provide a short overview of various assumptions that have been used in approximating *sparse* GPs (i.e., GPs that use inducing points), following on a paper by Quinonero-Candela and Rasmussen [49].

Subset of data ($\mathcal{O}(m^3)$) is a baseline method of simply using a subset of data points.

Subset of regressors ($\mathcal{O}(nm^2)$) [62, 63, 71] is a degenerate approximation that uses a weight for each inducing point. A GP is called *degenerate* if the covariance function has a finite number of non-zero eigenvalues, restricting the prior distribution to only a finite number of linearly independent functions [49].

Deterministic training conditional ($\mathcal{O}(nm^2)$) [60] approximation imposes a zero-variance normal distribution for $\mathbf{r}|\mathbf{u}$, resulting in the same mean but different variance predictions compared to the subset of regressors.

Fully independent training conditional ($\mathcal{O}(nm^2)$) [64] has the assumption that the GP values are independent of each other when conditioned on the inducing values:

$$q(\mathbf{r}|\mathbf{u}) = \prod_{i=1}^n p(r_i|\mathbf{u}).$$

Authors, year	Inducing points	Hyperparameters	Complexity
Titsias, 2009 [67]	variational	variational	$\mathcal{O}(nm^2)$
Hensman et al., 2013 [22]	fixed	variational	$\mathcal{O}(m^3)$
Gal et al., 2014 [19]	variational	variational	$\mathcal{O}(nm^2)$
Hoang et al., 2015 [24]	fixed	fixed	$\mathcal{O}(m^3)$
Cheng and Boots, 2017 [12]	variational	variational	$\mathcal{O}(nm_\alpha + nm_\beta^2)$
Hensman et al., 2017 [21]	fixed	variational	$\mathcal{O}(nm)$
Peng et al., 2017 [45]	variational	variational	$\mathcal{O}(m^3)$

Table 1: Summary of relevant VI approximations to GPs. For both inducing points and hyperparameters, ‘fixed’ means ‘chosen before the algorithm starts’ and ‘variational’ means ‘included amongst the variational parameters’. Hyperparameters m_α and m_β refer to the number of bases used to represent the GP’s mean and covariance, respectively.

Partially independent training conditional ($\mathcal{O}(nm^2)$) [68, 59] approximates the same distribution as the fully independent training conditional, but considers a block diagonal rather than a diagonal covariance matrix.

Transduction tailors the predictive distribution to specific test inputs [49]. As we are not too concerned about a specific set of test inputs in the IRL setting, transduction is of limited interest to us.

Augmentation [53] aims to improve predictive accuracy by adding each test input to the inducing points.

Nyström approximation ($\mathcal{O}(nm^2)$) [72] approximates the prior covariance of \mathbf{r} , but can lead to negative predictive variances.

Relevance vector machine ($\mathcal{O}(m^3)$) [66] is a degenerative approximation supporting a limited range of covariance functions.

Table 1 further summarises some of the recent and/or influential GP approximation approaches that might be suitable for our GP IRL model. In order to derive a reliable ELBO, the inducing points should be either fixed or modelled by a probability distribution (none of the approaches do that), while hyperparameters cannot be variational (the reason will be explained in Section 4).

- We would also like to avoid having the hyperparameters fixed, as learning them efficiently would introduce a separate problem. As the approach by Hoang et al. does not seem to be easily extendable to modelled hyperparameters, it is unsuitable to our needs.
- (TODO: this will have comments about other papers as well and will be restructured into a paragraph) The variational Fourier features (VFF) algorithm by Hensman et al. [21] is only defined for Matérn kernels, which is likely to be too restrictive for our

situation (the original paper on using GPs for IRL [35] used the automatic relevance detection kernel that has weights controlling how important each feature is). While extending VFF to support a flexible class of kernels defined by Wilson and Adams [73] is an interesting and promising avenue of work, it is likely to be beyond the scope of this project.

- The derivation of the ELBO in the work of Peng et al. [45] relies primarily on the fact that the evidence for a GP is a Gaussian, while in our case the evidence can be defined in several ways depending on the model, but must always involve \mathcal{D} , making the main idea of the paper inapplicable to IRL.

Since we expect $p(\Theta, \mathbf{u}, \mathbf{r} | \mathcal{D}, \mathbf{X}_{\mathbf{u}})$ to be highly irregular, we would like our approximation to be capable of representing a wide range of possible probability distributions. The primary way to represent complex posteriors in VI is by using *normalising flows*, i.e., a collection of invertible functions—parametrised by additional variational parameters—that are applied to latent variables [55]. Unfortunately, this parametrisation also means that the gradient of the joint probability distribution w.r.t. variational parameters $\nabla_{\nu} p(\mathcal{D}, \Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u}, \mathbf{r})$ is no longer zero, making an analytic expression for ELBO impossible using the usual methods. While it may be possible to have an approximating distribution for the flow parameters, it is uncertain how such an algorithm would behave, as it would have to perform optimisation in a space with significantly more dimensions.

4 Proposed Approach

In order to properly investigate the difference between variational inference and maximum likelihood estimation for the model, we keep other parts of the model the same. Namely, we set the covariance function to a version of the automatic relevance detection kernel [35, 42]

$$k_{\Theta}(\mathbf{x}_i, \mathbf{x}_j) = \lambda_0 \exp \left(-\frac{1}{2} (\mathbf{x}_i - \mathbf{x}_j)^{\top} \mathbf{\Lambda} (\mathbf{x}_i - \mathbf{x}_j) - \mathbb{1}[i \neq j] \sigma^2 \text{Tr}[\mathbf{\Lambda}] \right),$$

where λ_0 is the overall “scale” factor for how similar or distant the states are,

$$\mathbf{\Lambda} = \text{diag}(\lambda_1, \dots, \lambda_d)$$

is a diagonal matrix that determines how relevant each feature is (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 [35]). Thus we can set $\boldsymbol{\lambda} = (\lambda_0, \dots, \lambda_d)^{\top}$, and $\Theta = \{\boldsymbol{\lambda}\}$. Similarly, we keep the expression for the prior of Θ :

$$p(\Theta | \mathbf{X}_{\mathbf{u}}) = \exp \left(-\frac{1}{2} \text{Tr}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-2}] - \sum_{i=1}^d \log(\lambda_i + 1) \right). \quad (7)$$

Next, we can rewrite the posterior by using the chain rule and Bayes' theorem in order to get a better sense of what we are trying to approximate:

$$\begin{aligned}
p(\Theta, \mathbf{u}, \mathbf{r} | \mathcal{D}, \mathbf{X}_{\mathbf{u}}) &= p(\Theta | \mathbf{X}_{\mathbf{u}}, \mathcal{D}) \times p(\mathbf{u} | \Theta, \mathbf{X}_{\mathbf{u}}, \mathcal{D}) \times p(\mathbf{r} | \Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u}, \mathcal{D}) \\
&\propto p(\Theta | \mathbf{X}_{\mathbf{u}}, \mathcal{D}) \times p(\mathbf{u} | \Theta, \mathbf{X}_{\mathbf{u}}, \mathcal{D}) \times p(\mathcal{D} | \mathbf{r}) \times p(\mathbf{r} | \Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u}) \\
&\propto p(\Theta | \mathbf{X}_{\mathbf{u}}, \mathcal{D}) \times p(\mathcal{D} | \Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u}) \times p(\mathbf{u} | \Theta, \mathbf{X}_{\mathbf{u}}) \times p(\mathcal{D} | \mathbf{r}) \times p(\mathbf{r} | \Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u}) \\
&\propto p(\mathcal{D} | \Theta, \mathbf{X}_{\mathbf{u}}) \times p(\Theta | \mathbf{X}_{\mathbf{u}}) \times p(\mathcal{D} | \Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u}) \times p(\mathbf{u} | \Theta, \mathbf{X}_{\mathbf{u}}) \times p(\mathcal{D} | \mathbf{r}) \times p(\mathbf{r} | \Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u})
\end{aligned}$$

Note that now there are only two unknown probability distributions: $p(\mathcal{D} | \Theta, \mathbf{X}_{\mathbf{u}})$ and $p(\mathcal{D} | \Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u})$, which can be computed as follows:

$$\begin{aligned}
p(\mathcal{D} | \Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u}) &= \int p(\mathcal{D} | r) \times p(\mathbf{r} | \Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u}) \, d\mathbf{r}, \\
p(\mathcal{D} | \Theta, \mathbf{X}_{\mathbf{u}}) &= \iint p(\mathcal{D} | r) \times p(\mathbf{r} | \Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u}) \times p(\mathbf{u} | \Theta, \mathbf{X}_{\mathbf{u}}) \, d\mathbf{u} \, d\mathbf{r}.
\end{aligned}$$

This suggests the following form for the approximation:

$$q_{\nu}(\Theta, \mathbf{u}, \mathbf{r}) = q(\Theta) \times q(\mathbf{u} | \Theta) \times q(\mathbf{r} | \Theta, \mathbf{u}). \quad (8)$$

4.1 The Structure of the Approximating Distribution

At this point we are forced to make assumptions about the approximate posterior in order to arrive at an implementable solution. Time permitting, ways to relax the assumptions may be investigated towards the end of the project.

First, as is common in the literature for applying VI to GPs [12, 22, 24, 67], we simply set

$$q(\mathbf{r} | \Theta, \mathbf{u}) = p(\mathbf{r} | \Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u}). \quad (9)$$

We can make a similarly justified choice for $q(\mathbf{u} | \Theta)$:

$$q(\mathbf{u} | \Theta) = q(\mathbf{u}) = \mathcal{N}(\mathbf{u}; \mathbf{m}, \mathbf{S}) \quad (10)$$

for some variational parameters $\mathbf{m} \in \mathbb{R}^m$ and a positive semi-definite matrix $\mathbf{S} \in \mathbb{R}^{m \times m}$. [12, 21, 23].

In order to have a reasonable way of calculating/approximating the ELBO (see Section 4.4), we need to have an approximating distribution for Θ , but unfortunately all the papers in Table 1 either fix it or treat it as a variational parameter. Hence we make our first assumption without justification from previous literature:

$$q(\Theta) = \prod_{i=0}^d q(\lambda_i). \quad (11)$$

We want to restrict λ_0 to be positive so that k_{Θ} would produce non-negative values and not become trivial. Similarly, we want that $\lambda_i \geq 0$ for $i = 1, \dots, d$ so that $\mathbf{\Lambda}$ is a positive-definite matrix. Considering the possible distributions for all $d + 1$ variables, we would

like the mean to be flexible (i.e., not tied to zero, like with the exponential distribution), and the tails to converge to zero as the value of the random variable moves away from the mean. We might want to support some right skew, but the distribution should be close to symmetric with at least some parameter values. This limits our choice of distributions quite significantly, and we decide to go with the gamma distribution as it is fairly flexible and commonly used [27]. We then define the probability density functions as

$$q(\lambda_i) = \Gamma(\lambda_i; \alpha_i, \beta_i) = \frac{\beta_i^{\alpha_i}}{\Gamma(\alpha_i)} \lambda_i^{\alpha_i-1} e^{-\beta_i \lambda_i}, \quad i = 0, \dots, d, \quad (12)$$

where $\alpha_i > 0$ and $\beta_i > 0$ are parameters of the distribution, and $\Gamma(\cdot)$ is the gamma function. This gives us our vector of variational parameters $\boldsymbol{\nu} = (\mathbf{m}, \mathbf{S}, \alpha_0, \beta_0, \dots, \alpha_d, \beta_d)^\top$.

4.2 Evidence Lower Bound

In this section we derive and simplify the ELBO for this (now fully specified) model. In order to derive the ELBO, let us go back to (6) and write¹

$$\mathcal{L}(\boldsymbol{\nu}) = \mathbb{E}[\log p(\mathcal{D}, \Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u}, \mathbf{r})] - \mathbb{E}[\log q_{\boldsymbol{\nu}}(\Theta, \mathbf{u}, \mathbf{r})].$$

By plugging in (3) and (8), we get

$$\begin{aligned} \mathcal{L}(\boldsymbol{\nu}) &= \mathbb{E}[\log p(\mathbf{X}_{\mathbf{u}}) + \log p(\Theta | \mathbf{X}_{\mathbf{u}}) + \log p(\mathbf{u} | \Theta, \mathbf{X}_{\mathbf{u}}) + \log p(\mathbf{r} | \Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u}) + \log p(\mathcal{D} | r)] \\ &\quad - \mathbb{E}[\log q(\Theta) + \log q(\mathbf{u}) + \log q(\mathbf{r} | \Theta, \mathbf{u})]. \end{aligned}$$

Note that $\mathbb{E}[\log p(\mathbf{X}_{\mathbf{u}})]$ is just a constant, so we can simply drop it from the expression. Furthermore, since $q(\mathbf{r} | \Theta, \mathbf{u}) = p(\mathbf{r} | \Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u})$, they cancel each other out. Then we can substitute various terms with their definitions to get

$$\begin{aligned} \mathcal{L}(\boldsymbol{\nu}) &= \mathbb{E} \left[-\frac{1}{2} \text{Tr}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-2}] - \sum_{i=1}^d \log(\lambda_i + 1) \right] + \mathbb{E}[\log \mathcal{N}(\mathbf{u}; \mathbf{0}, \mathbf{K}_{\mathbf{u}, \mathbf{u}})] \\ &\quad + \mathbb{E} \left[\sum_{i=1}^N \sum_{t=1}^T Q_r(s_{i,t}, a_{i,t}) - V_r(s_{i,t}) \right] - \sum_{i=0}^d \mathbb{E} \left[\log \left(\frac{\beta_i^{\alpha_i}}{\Gamma(\alpha_i)} \lambda_i^{\alpha_i-1} e^{-\beta_i \lambda_i} \right) \right] \\ &\quad - \mathbb{E}[\log \mathcal{N}(\mathbf{u}; \mathbf{m}, \mathbf{S})]. \end{aligned}$$

We can simplify the last term by noting that $-\mathbb{E}[\log \mathcal{N}(\mathbf{u}; \mathbf{m}, \mathbf{S})] = \frac{1}{2} \log |\mathbf{S}|$ up to an additive constant that depends on the number of dimensions of the distribution [2]. Also note that we cannot use this fact for $\mathbb{E}[\log \mathcal{N}(\mathbf{u}; \mathbf{0}, \mathbf{K}_{\mathbf{u}, \mathbf{u}})]$ because $\mathbf{K}_{\mathbf{u}, \mathbf{u}}$ depends on Θ . We

¹At this point, we will drop the subscript denoting which variables the expectation is taken over. Also note that throughout the derivation equality is taken to mean “equality up to an additive constant”.

also plug in the definitions of $\mathcal{N}(\mathbf{u}; \mathbf{0}, \mathbf{K}_{\mathbf{u},\mathbf{u}})$ and Q_r , and get:

$$\begin{aligned}\mathcal{L}(\boldsymbol{\nu}) &= \frac{1}{2} \log |\mathbf{S}| + \mathbb{E} \left[-\frac{1}{2} \text{Tr}[\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-2}] - \sum_{i=1}^d \log(\lambda_i + 1) \right] \\ &+ \mathbb{E} \left[-\frac{1}{2} \mathbf{u}^\top \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1} \mathbf{u} - \frac{1}{2} \log |\mathbf{K}_{\mathbf{u},\mathbf{u}}| - \frac{m}{2} \log 2\pi \right] \\ &+ \mathbb{E} \left[\sum_{i=1}^N \sum_{t=1}^T r(s_{i,t}) - V_r(s_{i,t}) + \gamma \sum_{s' \in \mathcal{S}} \mathcal{T}(s_{i,t}, a_{i,t}, s') V_r(s') \right] \\ &- \sum_{i=0}^d \mathbb{E}[\alpha_i \log \beta_i - \log \Gamma(\alpha_i) + (\alpha_i - 1) \log \lambda_i - \beta_i \lambda_i]\end{aligned}$$

Now we can remove $\mathbb{E} \left[-\frac{m}{2} \log 2\pi \right]$ since it is constant w.r.t. both the variational parameters and the variables the expectation is over, and move constants (or variational parameters) independent of the approximated variables outside of the expectations. Also note that $\mathbb{E}[\lambda_i] = \alpha_i/\beta_i$ and $\mathbb{E}[\log \lambda_i] = \psi(\alpha_i) - \log \beta_i$, where ψ is the digamma function defined as $\psi(x) = \frac{d}{dx} \log \Gamma(x)$ [7]. Moreover, we can simplify $\sum_{i=1}^N \sum_{t=1}^T r(s_{i,t})$ by choosing to represent all visited states in $\mathbf{r} = (r_1, \dots, r_k)^\top$, and defining a new vector $\mathbf{t} = (t_1, \dots, t_k)^\top$, where t_i is the number of times the state associated with the reward r_i has been visited across all demonstrations. Then

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

Finally, as $\mathbf{u}^\top \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1} \mathbf{u}$ is a function of \mathbf{u} and Θ , we can take the expectation of \mathbf{u} , leaving the expectation of Θ :

$$\mathbb{E}[\mathbf{u}^\top \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1} \mathbf{u}] = \mathbb{E}[\text{Tr}[\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1} \mathbf{S}] + \mathbf{m}^\top \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1} \mathbf{m}] = \text{Tr}[\mathbb{E}[\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}] \mathbf{S}] + \mathbf{m}^\top \mathbb{E}[\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}] \mathbf{m}.$$

This allows us to simplify $\mathcal{L}(\boldsymbol{\nu})$ to the following:

$$\begin{aligned}\mathcal{L}(\boldsymbol{\nu}) &= \frac{1}{2} \log |\mathbf{S}| - \frac{1}{2} \text{Tr}[\mathbb{E}[\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-2}]] - \sum_{i=1}^d \mathbb{E}[\log(\lambda_i + 1)] - \frac{1}{2} \text{Tr}[\mathbb{E}[\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}] \mathbf{S}] \\ &- \frac{1}{2} \mathbf{m}^\top \mathbb{E}[\mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}] \mathbf{m} - \frac{1}{2} \mathbb{E}[\log |\mathbf{K}_{\mathbf{u},\mathbf{u}}|] + \sum_{i=0}^d \alpha_i - \log \beta_i + \log \Gamma(\alpha_i) + (1 - \alpha_i) \psi(\alpha_i) \\ &+ \mathbf{t}^\top \mathbb{E}[\mathbf{K}_{\mathbf{r},\mathbf{u}}^\top \mathbf{K}_{\mathbf{u},\mathbf{u}}^{-1}] \mathbf{m} - \sum_{i=1}^N \sum_{t=1}^T \mathbb{E}[V_r(s_{i,t})] - \gamma \sum_{s' \in \mathcal{S}} \mathcal{T}(s_{i,t}, a_{i,t}, s') \mathbb{E}[V_r(s')].\end{aligned}$$

4.3 Derivatives

4.3.1 $\partial/\partial \mathbf{m}$

We begin by removing terms independent of \mathbf{m} :

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \mathbf{m}} = & -\frac{1}{2} \frac{\partial}{\partial \mathbf{m}} [\mathbf{m}^\top \mathbb{E}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1}] \mathbf{m}] + \frac{\partial}{\partial \mathbf{m}} [\mathbf{t}^\top \mathbb{E}[\mathbf{K}_{\mathbf{r}, \mathbf{u}}^\top \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1}] \mathbf{m}] \\ & - \sum_{i=1}^N \sum_{t=1}^T \frac{\partial}{\partial \mathbf{m}} \mathbb{E}[V_r(s_{i,t})] - \gamma \sum_{s' \in \mathcal{S}} \mathcal{T}(s_{i,t}, a_{i,t}, s') \frac{\partial}{\partial \mathbf{m}} \mathbb{E}[V_r(s')]. \end{aligned}$$

Here

$$\begin{aligned} \frac{\partial}{\partial \mathbf{m}} [\mathbf{m}^\top \mathbb{E}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1}] \mathbf{m}] &= (\mathbb{E}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1}] + \mathbb{E}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1}]^\top) \mathbf{m}, \\ \frac{\partial}{\partial \mathbf{m}} [\mathbf{t}^\top \mathbb{E}[\mathbf{K}_{\mathbf{r}, \mathbf{u}}^\top \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1}] \mathbf{m}] &= \mathbf{t}^\top \mathbb{E}[\mathbf{K}_{\mathbf{r}, \mathbf{u}}^\top \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1}], \end{aligned}$$

and

$$\begin{aligned} \frac{\partial}{\partial \mathbf{m}} \mathbb{E}[V_r(s)] &= \frac{\partial}{\partial \mathbf{m}} \iiint V_r(s) p(\mathbf{r}|\Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u}) \mathcal{N}(\mathbf{u}; \mathbf{m}, \mathbf{S}) q(\boldsymbol{\lambda}) d\mathbf{r} d\mathbf{u} d\boldsymbol{\lambda} \\ &= \iiint V_r(s) p(\mathbf{r}|\Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u}) \frac{\partial}{\partial \mathbf{m}} \mathcal{N}(\mathbf{u}; \mathbf{m}, \mathbf{S}) q(\boldsymbol{\lambda}) d\mathbf{r} d\mathbf{u} d\boldsymbol{\lambda}, \end{aligned} \tag{13}$$

where

$$\begin{aligned} \frac{\partial}{\partial \mathbf{m}} \mathcal{N}(\mathbf{u}; \mathbf{m}, \mathbf{S}) &= \mathcal{N}(\mathbf{u}; \mathbf{m}, \mathbf{S}) \frac{\partial}{\partial \mathbf{m}} \left[-\frac{1}{2} (\mathbf{u} - \mathbf{m})^\top \mathbf{S}^{-1} (\mathbf{u} - \mathbf{m}) \right] \\ &= \mathcal{N}(\mathbf{u}; \mathbf{m}, \mathbf{S}) \left(-\frac{1}{2} \right) (\mathbf{S}^{-1} + \mathbf{S}^{-\top}) (\mathbf{u} - \mathbf{m}) \frac{\partial}{\partial \mathbf{m}} [\mathbf{u} - \mathbf{m}] \\ &= \mathcal{N}(\mathbf{u}; \mathbf{m}, \mathbf{S}) \frac{1}{2} (\mathbf{S}^{-1} + \mathbf{S}^{-\top}) (\mathbf{u} - \mathbf{m}). \end{aligned}$$

Substituting it back into (13) gives

$$\begin{aligned} \frac{\partial}{\partial \mathbf{m}} \mathbb{E}[V_r(s)] &= \frac{1}{2} \iiint V_r(s) (\mathbf{S}^{-1} + \mathbf{S}^{-\top}) (\mathbf{u} - \mathbf{m}) p(\mathbf{r}|\Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u}) \mathcal{N}(\mathbf{u}; \mathbf{m}, \mathbf{S}) q(\boldsymbol{\lambda}) d\mathbf{r} d\mathbf{u} d\boldsymbol{\lambda} \\ &= \frac{1}{2} \mathbb{E}[V_r(s) (\mathbf{S}^{-1} + \mathbf{S}^{-\top}) (\mathbf{u} - \mathbf{m})]. \end{aligned}$$

Hence

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \mathbf{m}} = & -\frac{1}{2} (\mathbb{E}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1}] + \mathbb{E}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1}]^\top) \mathbf{m} + \mathbf{t}^\top \mathbb{E}[\mathbf{K}_{\mathbf{r}, \mathbf{u}}^\top \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1}] \mathbf{m} \\ & - \frac{1}{2} \sum_{i=1}^N \sum_{t=1}^T \mathbb{E}[V_r(s_{i,t}) (\mathbf{S}^{-1} + \mathbf{S}^{-\top}) (\mathbf{u} - \mathbf{m})] \\ & - \gamma \sum_{s' \in \mathcal{S}} \mathcal{T}(s_{i,t}, a_{i,t}, s') \mathbb{E}[V_r(s') (\mathbf{S}^{-1} + \mathbf{S}^{-\top}) (\mathbf{u} - \mathbf{m})]. \end{aligned}$$

4.3.2 $\partial/\partial \mathbf{S}$

Similarly to the previous section,

$$\begin{aligned} \frac{\partial \mathcal{L}}{\partial \mathbf{S}} &= \frac{1}{2} \frac{\partial}{\partial \mathbf{S}} \log |\mathbf{S}| - \frac{1}{2} \frac{\partial}{\partial \mathbf{S}} \text{Tr}[\mathbb{E}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1}] \mathbf{S}] \\ &\quad - \sum_{i=1}^N \sum_{t=1}^T \frac{\partial}{\partial \mathbf{S}} \mathbb{E}[V_r(s_{i,t})] - \gamma \sum_{s' \in \mathcal{S}} \mathcal{T}(s_{i,t}, a_{i,t}, s') \frac{\partial}{\partial \mathbf{S}} \mathbb{E}[V_r(s')], \end{aligned}$$

where

$$\frac{\partial}{\partial \mathbf{S}} \log |\mathbf{S}| = \mathbf{S}^{-\top},$$

and

$$\frac{\partial}{\partial \mathbf{S}} \text{Tr}[\mathbb{E}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1}] \mathbf{S}] = \mathbb{E}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1}]^{\top}$$

by *The Matrix Cookbook* [46]. Then

$$\frac{\partial}{\partial \mathbf{S}} \mathbb{E}[V_r(s)] = \iiint V_r(s) q(\mathbf{r}) \frac{\partial}{\partial \mathbf{S}} \mathcal{N}(\mathbf{u}; \mathbf{m}, \mathbf{S}) q(\boldsymbol{\lambda}) d\mathbf{r} d\mathbf{u} d\boldsymbol{\lambda},$$

where

$$\begin{aligned} \frac{\partial}{\partial \mathbf{S}} \mathcal{N}(\mathbf{u}; \mathbf{m}, \mathbf{S}) &= \frac{\partial}{\partial \mathbf{S}} \left[\frac{1}{(2\pi)^{m/2} |\mathbf{S}|^{1/2}} \exp \left(-\frac{1}{2} (\mathbf{u} - \mathbf{m})^{\top} \mathbf{S}^{-1} (\mathbf{u} - \mathbf{m}) \right) \right] \\ &= \frac{\partial}{\partial \mathbf{S}} \left[\frac{1}{(2\pi)^{m/2} |\mathbf{S}|^{1/2}} \right] \exp \left(-\frac{1}{2} (\mathbf{u} - \mathbf{m})^{\top} \mathbf{S}^{-1} (\mathbf{u} - \mathbf{m}) \right) \\ &\quad + \frac{1}{(2\pi)^{m/2} |\mathbf{S}|^{1/2}} \frac{\partial}{\partial \mathbf{S}} \left[\exp \left(-\frac{1}{2} (\mathbf{u} - \mathbf{m})^{\top} \mathbf{S}^{-1} (\mathbf{u} - \mathbf{m}) \right) \right] \\ &= \frac{1}{(2\pi)^{m/2}} \frac{\partial}{\partial \mathbf{S}} \left[\frac{1}{|\mathbf{S}|^{1/2}} \right] \exp \left(-\frac{1}{2} (\mathbf{u} - \mathbf{m})^{\top} \mathbf{S}^{-1} (\mathbf{u} - \mathbf{m}) \right) \\ &\quad - \frac{1}{2} \mathcal{N}(\mathbf{u}; \mathbf{m}, \mathbf{S}) \frac{\partial}{\partial \mathbf{S}} [(\mathbf{u} - \mathbf{m})^{\top} \mathbf{S}^{-1} (\mathbf{u} - \mathbf{m})]. \end{aligned}$$

The two remaining derivatives can be taken with the help of *The Matrix Cookbook* [46]:

$$\begin{aligned} \frac{\partial}{\partial \mathbf{S}} \left[\frac{1}{|\mathbf{S}|^{1/2}} \right] &= -\frac{1}{2} |\mathbf{S}|^{-3/2} \frac{\partial |\mathbf{S}|}{\partial \mathbf{S}} = -\frac{1}{2} |\mathbf{S}|^{-3/2} |\mathbf{S}| \mathbf{S}^{-\top} = -\frac{1}{2 |\mathbf{S}|^{1/2}} \mathbf{S}^{-\top}, \\ \frac{\partial}{\partial \mathbf{S}} [(\mathbf{u} - \mathbf{m})^{\top} \mathbf{S}^{-1} (\mathbf{u} - \mathbf{m})] &= -\mathbf{S}^{-\top} (\mathbf{u} - \mathbf{m}) (\mathbf{u} - \mathbf{m})^{\top} \mathbf{S}^{-\top}. \end{aligned}$$

Plugging them back in gives

$$\frac{\partial}{\partial \mathbf{S}} \mathcal{N}(\mathbf{u}; \mathbf{m}, \mathbf{S}) = -\frac{1}{2} \mathbf{S}^{-\top} \mathcal{N}(\mathbf{u}; \mathbf{m}, \mathbf{S}) + \frac{1}{2} \mathcal{N}(\mathbf{u}; \mathbf{m}, \mathbf{S}) \mathbf{S}^{-\top} (\mathbf{u} - \mathbf{m}) (\mathbf{u} - \mathbf{m})^{\top} \mathbf{S}^{-\top},$$

and

$$\begin{aligned} \frac{\partial}{\partial \mathbf{S}} \mathbb{E}[V_r(s)] &= \frac{1}{2} \iiint V_r(s) (\mathbf{S}^{-\top} (\mathbf{u} - \mathbf{m}) (\mathbf{u} - \mathbf{m})^{\top} \mathbf{S}^{-\top} - \mathbf{S}^{-\top}) q(\mathbf{r}) \mathcal{N}(\mathbf{u}; \mathbf{m}, \mathbf{S}) q(\boldsymbol{\lambda}) d\mathbf{r} d\mathbf{u} d\boldsymbol{\lambda} \\ &= \frac{1}{2} \mathbb{E}[V_r(s) (\mathbf{S}^{-\top} (\mathbf{u} - \mathbf{m}) (\mathbf{u} - \mathbf{m})^{\top} \mathbf{S}^{-\top} - \mathbf{S}^{-\top})]. \end{aligned}$$

Therefore

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial \mathbf{S}} &= \frac{1}{2} \mathbf{S}^{-\top} - \frac{1}{2} \mathbb{E}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1}]^{\top} - \frac{1}{2} \sum_{i=1}^N \sum_{t=1}^T \mathbb{E}[V_r(s_{i,t}) (\mathbf{S}^{-\top} (\mathbf{u} - \mathbf{m}) (\mathbf{u} - \mathbf{m})^{\top} \mathbf{S}^{-\top} - \mathbf{S}^{-\top})] \\ &\quad - \gamma \sum_{s' \in \mathcal{S}} \mathcal{T}(s_{i,t}, a_{i,t}, s') \mathbb{E}[V_r(s') (\mathbf{S}^{-\top} (\mathbf{u} - \mathbf{m}) (\mathbf{u} - \mathbf{m})^{\top} \mathbf{S}^{-\top} - \mathbf{S}^{-\top})].\end{aligned}$$

4.3.3 $\partial/\partial\alpha_j$

We begin in the usual way:

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial \alpha_j} &= -\frac{1}{2} \frac{\partial}{\partial \alpha_j} \mathbb{E}[\text{Tr}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-2}]] - \frac{1}{2} \frac{\partial}{\partial \alpha_j} \mathbb{E}[\text{Tr}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{S}]] - \frac{1}{2} \frac{\partial}{\partial \alpha_j} \mathbb{E}[\mathbf{m}^{\top} \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{m}] - \frac{1}{2} \frac{\partial}{\partial \alpha_j} \mathbb{E}[\log |\mathbf{K}_{\mathbf{u}, \mathbf{u}}|] \\ &\quad + \frac{\partial}{\partial \alpha_j} \mathbb{E}[\mathbf{t}^{\top} \mathbf{K}_{\mathbf{r}, \mathbf{u}}^{\top} \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{m}] + \frac{\partial}{\partial \alpha_j} [\alpha_j + \log \Gamma(\alpha_j) + (1 - \alpha_j) \psi(\alpha_j)] \\ &\quad - \sum_{i=1}^N \sum_{t=1}^T \frac{\partial}{\partial \alpha_j} \mathbb{E}[V_r(s_{i,t})] - \gamma \sum_{s' \in \mathcal{S}} \mathcal{T}(s_{i,t}, a_{i,t}, s') \frac{\partial}{\partial \alpha_j} \mathbb{E}[V_r(s')].\end{aligned}$$

First,

$$\frac{\partial}{\partial \alpha_j} [\alpha_j + \log \Gamma(\alpha_j) + (1 - \alpha_j) \psi(\alpha_j)] = 1 + \psi(\alpha_j) - \psi(\alpha_j) + (1 - \alpha_j) \psi'(\alpha_j) = 1 + (1 - \alpha_j) \psi'(\alpha_j)$$

by the definition of ψ . The remaining terms can all be treated in the same way, as they all contain expectations of scalar functions that are independent of α_j , and α_j only occurs in $\Gamma(\lambda_j; \alpha_j, \beta_j)$. Thus we can work with an abstract function as follows:

$$\begin{aligned}\frac{\partial}{\partial \alpha_j} \mathbb{E}[f(k_{\Theta}, \mathbf{r})] &= \frac{\partial}{\partial \alpha_j} \iiint f(k_{\Theta}, \mathbf{r}) q(\boldsymbol{\lambda}) q(\mathbf{r}) q(\mathbf{u}) d\boldsymbol{\lambda} d\mathbf{r} d\mathbf{u} \\ &= \iiint f(k_{\Theta}, \mathbf{r}) q(\lambda_0) \cdots q(\lambda_{j-1}) \frac{\partial}{\partial \alpha_j} \left[\frac{\beta_j^{\alpha_j}}{\Gamma(\alpha_j)} \lambda_j^{\alpha_j-1} \right] e^{-\beta_j \lambda_j} \\ &\quad q(\lambda_{j+1}) \cdots q(\lambda_d) q(\mathbf{r}) q(\mathbf{u}) d\boldsymbol{\lambda} d\mathbf{r} d\mathbf{u}.\end{aligned}$$

Then

$$\begin{aligned}\frac{\partial}{\partial \alpha_j} \left[\frac{\beta_j^{\alpha_j}}{\Gamma(\alpha_j)} \lambda_j^{\alpha_j-1} \right] &= \frac{\frac{\partial}{\partial \alpha_j} [\beta_j^{\alpha_j} \lambda_j^{\alpha_j-1}] \Gamma(\alpha_j) - \beta_j^{\alpha_j} \lambda_j^{\alpha_j-1} \Gamma'(\alpha_j)}{(\Gamma(\alpha_j))^2} \\ &= \frac{\beta_j^{\alpha_j} \lambda_j^{\alpha_j-1} \frac{\partial}{\partial \alpha_j} [\alpha_j \log \beta_j + (\alpha_j - 1) \log \lambda_j] \Gamma(\alpha_j) - \beta_j^{\alpha_j} \lambda_j^{\alpha_j-1} \Gamma'(\alpha_j)}{(\Gamma(\alpha_j))^2} \\ &= \frac{\beta_j^{\alpha_j} \lambda_j^{\alpha_j-1} (\log \beta_j + \log \lambda_j) \Gamma(\alpha_j) - \beta_j^{\alpha_j} \lambda_j^{\alpha_j-1} \Gamma'(\alpha_j)}{(\Gamma(\alpha_j))^2} \\ &= \frac{\beta_j^{\alpha_j} \lambda_j^{\alpha_j-1}}{\Gamma(\alpha_j)} \left(\log \beta_j + \log \lambda_j - \frac{\Gamma'(\alpha_j)}{\Gamma(\alpha_j)} \right),\end{aligned}$$

which means that

$$\begin{aligned}
\frac{\partial}{\partial \alpha_j} \mathbb{E}[f(k_\Theta, \mathbf{r})] &= \iiint f(k_\Theta, \mathbf{r}) q(\lambda_0) \cdots q(\lambda_{j-1}) \frac{\beta_j^{\alpha_j}}{\Gamma(\alpha_j)} \lambda_j^{\alpha_j-1} e^{-\beta_j \lambda_j} \left(\log \beta_j + \log \lambda_j - \frac{\Gamma'(\alpha_j)}{\Gamma(\alpha_j)} \right) \\
&\quad q(\lambda_{j+1}) \cdots q(\lambda_d) q(\mathbf{r}) q(\mathbf{u}) d\boldsymbol{\lambda} d\mathbf{r} d\mathbf{u} \\
&= \iiint f(k_\Theta, \mathbf{r}) \left(\log \beta_j + \log \lambda_j - \frac{\Gamma'(\alpha_j)}{\Gamma(\alpha_j)} \right) q(\boldsymbol{\lambda}) q(\mathbf{r}) q(\mathbf{u}) d\boldsymbol{\lambda} d\mathbf{r} d\mathbf{u} \\
&= \mathbb{E} \left[f(k_\Theta, \mathbf{r}) \left(\log \beta_j + \log \lambda_j - \frac{\Gamma'(\alpha_j)}{\Gamma(\alpha_j)} \right) \right] \\
&= \left(\log \beta_j - \frac{\Gamma'(\alpha_j)}{\Gamma(\alpha_j)} \right) \mathbb{E}[f(k_\Theta, \mathbf{r})] + \mathbb{E}[f(k_\Theta, \mathbf{r}) \log \lambda_j].
\end{aligned}$$

With these results in mind, we can simplify the initial expression to

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \alpha_j} &= 1 + (1 - \alpha_j) \psi'(\alpha_j) + \left(\log \beta_j - \frac{\Gamma'(\alpha_j)}{\Gamma(\alpha_j)} \right) \left(-\frac{1}{2} \mathbb{E}[\text{Tr}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-2}]] - \frac{1}{2} \mathbb{E}[\text{Tr}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{S}]] \right. \\
&\quad - \frac{1}{2} \mathbb{E}[\mathbf{m}^\top \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{m}] - \frac{1}{2} \mathbb{E}[\log |\mathbf{K}_{\mathbf{u}, \mathbf{u}}|] + \mathbb{E}[\mathbf{t}^\top \mathbf{K}_{\mathbf{r}, \mathbf{u}}^\top \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{m}] \\
&\quad \left. - \sum_{i=1}^N \sum_{t=1}^T \mathbb{E}[V_r(s_{i,t})] - \gamma \sum_{s' \in \mathcal{S}} \mathcal{T}(s_{i,t}, a_{i,t}, s') \mathbb{E}[V_r(s')] \right) \\
&\quad - \frac{1}{2} \mathbb{E}[\text{Tr}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-2}] \log \lambda_j] - \frac{1}{2} \mathbb{E}[\text{Tr}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{S}] \log \lambda_j] - \frac{1}{2} \mathbb{E}[\mathbf{m}^\top \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{m} \log \lambda_j] \\
&\quad - \frac{1}{2} \mathbb{E}[\log |\mathbf{K}_{\mathbf{u}, \mathbf{u}}| \log \lambda_j] + \mathbb{E}[\mathbf{t}^\top \mathbf{K}_{\mathbf{r}, \mathbf{u}}^\top \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{m} \log \lambda_j] \\
&\quad - \sum_{i=1}^N \sum_{t=1}^T \mathbb{E}[V_r(s_{i,t}) \log \lambda_j] - \gamma \sum_{s' \in \mathcal{S}} \mathcal{T}(s_{i,t}, a_{i,t}, s') \mathbb{E}[V_r(s') \log \lambda_j].
\end{aligned}$$

4.3.4 $\partial/\partial \beta_j$

Finally,

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial \beta_j} &= -\frac{1}{2} \frac{\partial}{\partial \beta_j} \mathbb{E}[\text{Tr}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-2}]] - \frac{1}{2} \frac{\partial}{\partial \beta_j} \mathbb{E}[\text{Tr}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{S}]] - \frac{1}{2} \frac{\partial}{\partial \beta_j} \mathbb{E}[\mathbf{m}^\top \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{m}] \\
&\quad - \frac{1}{2} \frac{\partial}{\partial \beta_j} \mathbb{E}[\log |\mathbf{K}_{\mathbf{u}, \mathbf{u}}|] + \frac{\partial}{\partial \beta_j} \mathbb{E}[\mathbf{t}^\top \mathbf{K}_{\mathbf{r}, \mathbf{u}}^\top \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{m}] - \frac{\partial}{\partial \beta_j} [\log \beta_j] \\
&\quad - \sum_{i=1}^N \sum_{t=1}^T \frac{\partial}{\partial \beta_j} \mathbb{E}[V_r(s_{i,t})] - \gamma \sum_{s' \in \mathcal{S}} \mathcal{T}(s_{i,t}, a_{i,t}, s') \frac{\partial}{\partial \beta_j} \mathbb{E}[V_r(s')].
\end{aligned}$$

Similarly to the previous section, we can handle all derivatives of expectations in the same way:

$$\begin{aligned}\frac{\partial}{\partial \beta_j} \mathbb{E}[f(k_\Theta, \mathbf{r})] &= \frac{\partial}{\partial \beta_j} \iiint f(k_\Theta, \mathbf{r}) q(\boldsymbol{\lambda}) q(\mathbf{r}) q(\mathbf{u}) d\boldsymbol{\lambda} d\mathbf{r} d\mathbf{u} \\ &= \iiint f(k_\Theta, \mathbf{r}) q(\lambda_0) \cdots q(\lambda_{j-1}) \frac{\lambda_j^{\alpha_j-1}}{\Gamma(\alpha_j)} \frac{\partial}{\partial \beta_j} [\beta_j^{\alpha_j} e^{-\beta_j \lambda_j}] \\ &\quad q(\lambda_{j+1}) \cdots q(\lambda_d) q(\mathbf{r}) q(\mathbf{u}) d\boldsymbol{\lambda} d\mathbf{r} d\mathbf{u}.\end{aligned}$$

Since

$$\frac{\partial}{\partial \beta_j} [\beta_j^{\alpha_j} e^{-\beta_j \lambda_j}] = \alpha_j \beta_j^{\alpha_j-1} e^{-\beta_j \lambda_j} - \beta_j^{\alpha_j} e^{-\beta_j \lambda_j} \lambda_j = \beta_j^{\alpha_j} e^{-\beta_j \lambda_j} \left(\frac{\alpha_j}{\beta_j} - \lambda_j \right),$$

we have that

$$\begin{aligned}\frac{\partial}{\partial \beta_j} \mathbb{E}[f(k_\Theta, \mathbf{r})] &= \iiint f(k_\Theta, \mathbf{r}) q(\lambda_0) \cdots q(\lambda_{j-1}) \frac{\beta_j^{\alpha_j}}{\Gamma(\alpha_j)} \lambda_j^{\alpha_j-1} e^{-\beta_j \lambda_j} \left(\frac{\alpha_j}{\beta_j} - \lambda_j \right) \\ &\quad q(\lambda_{j+1}) \cdots q(\lambda_d) q(\mathbf{r}) q(\mathbf{u}) d\boldsymbol{\lambda} d\mathbf{r} d\mathbf{u} \\ &= \iiint f(k_\Theta, \mathbf{r}) \left(\frac{\alpha_j}{\beta_j} - \lambda_j \right) q(\boldsymbol{\lambda}) q(\mathbf{r}) q(\mathbf{u}) d\boldsymbol{\lambda} d\mathbf{r} d\mathbf{u} \\ &= \mathbb{E} \left[f(k_\Theta, \mathbf{r}) \left(\frac{\alpha_j}{\beta_j} - \lambda_j \right) \right] = \frac{\alpha_j}{\beta_j} \mathbb{E}[f(k_\Theta, \mathbf{r})] - \mathbb{E}[f(k_\Theta, \mathbf{r}) \lambda_j].\end{aligned}$$

This gives us the final expression of $\frac{\partial \mathcal{L}}{\partial \beta_j}$:

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial \beta_j} &= -\frac{1}{\beta_j} - \frac{1}{2} \mathbb{E} \left[\text{Tr}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-2}] \left(\frac{\alpha_j}{\beta_j} - \lambda_j \right) \right] - \frac{1}{2} \mathbb{E} \left[\text{Tr}[\mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{S}] \left(\frac{\alpha_j}{\beta_j} - \lambda_j \right) \right] \\ &\quad - \frac{1}{2} \mathbb{E} \left[\mathbf{m}^\top \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{m} \left(\frac{\alpha_j}{\beta_j} - \lambda_j \right) \right] - \frac{1}{2} \mathbb{E} \left[\log |\mathbf{K}_{\mathbf{u}, \mathbf{u}}| \left(\frac{\alpha_j}{\beta_j} - \lambda_j \right) \right] \\ &\quad + \mathbb{E} \left[\mathbf{t}^\top \mathbf{K}_{\mathbf{r}, \mathbf{u}}^\top \mathbf{K}_{\mathbf{u}, \mathbf{u}}^{-1} \mathbf{m} \left(\frac{\alpha_j}{\beta_j} - \lambda_j \right) \right] \\ &\quad - \sum_{i=1}^N \sum_{t=1}^T \mathbb{E} \left[V_r(s_{i,t}) \left(\frac{\alpha_j}{\beta_j} - \lambda_j \right) \right] - \gamma \sum_{s' \in \mathcal{S}} \mathcal{T}(s_{i,t}, a_{i,t}, s') \mathbb{E} \left[V_r(s') \left(\frac{\alpha_j}{\beta_j} - \lambda_j \right) \right].\end{aligned}$$

4.4 Variational Inference Algorithms

The typical way to optimise a quantity (the ELBO, in this case) involves computing its gradient [8]. Due to terms involving \mathcal{D} that are computed by solving an MDP and do not resemble a typical probability distribution, we turn our attention to the *black box variational inference* [52] paper that suggests a convenient trick:

$$\nabla_{\boldsymbol{\nu}} \mathcal{L} = \mathbb{E}_{(\Theta, \mathbf{u}, \mathbf{r}) \sim q_{\boldsymbol{\nu}}(\Theta, \mathbf{u}, \mathbf{r})} [\nabla_{\boldsymbol{\nu}} \log q_{\boldsymbol{\nu}}(\Theta, \mathbf{u}, \mathbf{r}) (\log p(\mathcal{D}, \Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u}, \mathbf{r}) - \log q_{\boldsymbol{\nu}}(\Theta, \mathbf{u}, \mathbf{r}))].$$

With this trick in mind, we only need to evaluate $\log p(\mathcal{D}, \Theta, \mathbf{X}_{\mathbf{u}}, \mathbf{u}, \mathbf{r})$ and take the gradient of $\log q_{\nu}(\Theta, \mathbf{u}, \mathbf{r})$. Following the same paper, $\nabla_{\nu} \mathcal{L}$ then has an unbiased estimate

$$\nabla_{\nu} \mathcal{L} \approx \frac{1}{S} \sum_{s=1}^S \nabla_{\nu} \log q_{\nu}(\Theta_s, \mathbf{u}_s, \mathbf{r}_s) (\log p(\mathcal{D}, \Theta_s, \mathbf{X}_{\mathbf{u}}, \mathbf{u}_s, \mathbf{r}_s) - \log q_{\nu}(\Theta_s, \mathbf{u}_s, \mathbf{r}_s))$$

computed by drawing S Monte Carlo samples $(\Theta_s, \mathbf{u}_s, \mathbf{r}_s) \sim q_{\nu}(\Theta, \mathbf{u}, \mathbf{r})$.

5 Work Plan

show how you plan to organize your work, identifying intermediate deliverables and dates.

6 Notes on papers (to be removed)

6.1 Miscellaneous

(Directed) similarity between MDPs using restricted Boltzmann machines [10]

Chapter 6 on distance measures [41]

The PhD thesis behind maximum causal entropy [76]

6.2 Gaussian Processes

Simple introduction to GPs for time-series modelling [56]

GPs over graphs instead of vectors (haven't actually read) [69]

Another introduction from physics (skimmed through) [29]

Learning a GP from very little data [47]

One GP for multiple correlated output variables [6]

Kernels for categorical and count data [58]

Scalability/Approximations thesis [28]

6.3 Interpretability

Learning latent factors [38]

The behaviour of Reddit users [16]

6.4 Inverse Reinforcement Learning

One of the first papers on the topic [44]

Bayesian setting [51]

Learning optimal composite features [14]

A different take on IRL with GPs [48]

IRL for large state spaces (haven't read) [11]

Multiple reward functions [13]

A recent survey [3]

Some not-very-successful method [43]

6.4.1 Multiple Strategies

EM clustering [4]

Structured priors [17]

There are more, but I haven't gotten to them yet.

6.5 Variational Inference

Part IV on probabilities and inference [40]

Stochastic VI [26]

Structured stochastic VI [25]

Another review of recent advances [75]

Tighter ELBOs are not necessarily better [50]

For details on Lebesgue's dominated convergence theorem [15]

Still looking for the relevant version of the theorem [32]

Approximation as a multivariate Gaussian (haven't read) [65]

How black box VI can be even more black box [37]

Evaluating VI [74]

6.5.1 for GPs

Linear VI for GPs [12]

Sparse VI for GP [21]

Stochastic VI for sparse spectral GPs (no inducing points, so not that relevant) [23]

Sparse GPs 2 [19]

The 3 papers I need to focus on:

SVI for sparse GPs [22]

distributed 1 [24]

distributed 2 (haven't read) [45]

The paper at the core of the 3 approaches (approximates posterior) [67]

Generalized version? [61]

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