Learning-to-defer for sequential medical decision-making under uncertainty

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Paper under double-blind review

Abstract

Learning-to-defer is a framework to automatically defer decision-making to a human expert when ML-based decisions are deemed unreliable. Existing learning-to-defer frameworks are not designed for sequential settings. That is, they defer at every instance independently, based on immediate predictions, while ignoring the potential long-term impact of these interventions. As a result, existing frameworks are myopic. Further, they do not defer adaptively, which is crucial when human interventions are costly. In this work, we propose Sequential Learning-to-Defer (SLTD), a framework for learning-to-defer to a domain expert in sequential decision-making settings. Contrary to existing literature, we pose the problem of learning-to-defer as model-based reinforcement learning (RL) to i) account for long-term consequences of ML-based actions using RL and ii) adaptively defer based on the dynamics (model-based). Our proposed framework determines whether to defer (at each time step) by quantifying whether a deferral now will improve the value compared to delaying deferral to the next time step. To quantify the improvement, we account for potential future deferrals. As a result, we learn a pre-emptive deferral policy (i.e. a policy that defers early if using the ML-based policy could worsen long-term outcomes). Our deferral policy is adaptive to the non-stationarity in the dynamics. We demonstrate that adaptive deferral via SLTD provides an improved trade-off between long-term outcomes and deferral frequency on synthetic, semi-synthetic, and real-world data with non-stationary dynamics. Finally, we interpret the deferral decision by decomposing the propagated (long-term) uncertainty around the outcome, to justify the deferral decision.

1 Introduction

Machine learning (ML) has the potential to be deployed for decision-making in complex domains such as healthcare, lending, and legal systems. In many cases, ML-based policy may not generalize to situations not encountered during training. In practice, it may be safer to defer to a human expert when using the ML policy may not improve outcomes or cause active harm. Automatically deferring to a human expert is called 'Learning-to-defer.' Earlier works have considered the problem of learning-to-defer in non-sequential settings (Mozannar and Sontag, 2020; Madras et al., 2017)..

In situations such as managing health, however, two key challenges remain. First, deferral decisions can significantly alter long-term outcomes. Thus modeling the long-term outcome is critical to decide *when* to defer to an expert. Deferring too late may lead to unintended and irreversible harm. Deferring too early may increase the burden on the human expert. Second, when human interventions (after deferral) are costly, learning-to-defer *adaptively* and only when critical is crucial. To defer adaptively, we need a well-characterized model of the environment, a challenging estimation issue, especially under non-stationarity, i.e., when the dynamics of the environment change over time.

Existing learning-to-defer methods defer based on immediate outcomes e.g. Mozannar and Sontag (2020); Madras et al. (2017); Gennatas et al. (2020), and are therefore myopic. Further, the objective to defer is to improve the performance of some prediction tasks (such as the ability to predict a patient outcome). These frameworks either defer based on the probability of correct short-term prediction or characterizing the trade-off of paying a cost (to defer). Instead, interventions based on an ML system can have long-term consequences that are crucial to the model. Further, in many cases, merely deferring to optimize for decision/

prediction accuracy in a supervised learning setting does not suffice to improve long-term outcomes. Existing approaches also do not leverage the potential of modeling the environment to defer *adaptively*, especially beneficial if the environment is non-stationary.

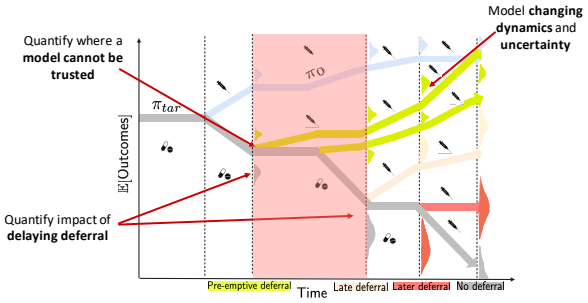

Figure 1: Overview of deferral strategies in a medical setting. The target policy π_{tar} recommends continuing a pill-based therapy, while the domain expert (π_0) suggests switching to a shot. SLTD (green) defers in the shaded region where π_{tar} is unlikely to improve expected future outcomes. To do so, SLTD models changing dynamics, and accounts for the impact of delayed deferral to identify and defer in the shaded region.

Algorithmic Motivation. To address these challenges, we deviate significantly from existing learning-to-defer methods, which use a supervised learning framework. Instead, we model the learning-to-defer problem for sequential settings as offline model-based reinforcement learning (RL). SLTD is the first RL-based learning-to-defer framework. We focus on settings where online experimentation is prohibitive for safety reasons, such as healthcare.

We assume access to batch data collected by human experts (such as clinicians) using a behavior policy. Our goal is to learn a deferral policy with respect to a fixed ML-based policy (called the target policy). SLTD decides whether or not to defer (to the expert behavior policy) at each instance by modeling the impact of *delaying deferral* (by one time step) on the long-term outcomes. SLTD defers if delaying deferral does not improve outcomes compared to deferring in the current instance. To quantify long-term outcomes, we also account for all future deferrals. In doing so, SLTD precisely identifies the regions of the state space where the target ML-based policy will not improve outcomes. As a result, our method is pre-emptive, i.e., *it defers in all regions where the ML policy is unlikely to improve long-term outcomes*. See Figure 1 for a conceptual overview of SLTD.

Human expert interventions are often costly. Hence deferring too often is not desirable. To defer *adaptively*, we propose to leverage an estimate of the environment dynamics and the associated uncertainty. Modeling the dynamics allows us to reliably quantify the impact of delaying deferral on long-term outcomes, which is particularly beneficial in non-stationary settings. We show that modeling the non-stationarity provides a better trade-off of improving outcomes versus the frequency of deferrals. In a myopic environment (i.e., when the effect of interventions are observed in the near future), it may seem unnecessary to model the dynamics. However, we demonstrate that deferral methods that defer myopically, based on immediate outcomes still benefit from modeling the dynamics, and consequently the impact of potential future myopic deferrals. When SLTD defers, human experts can benefit from an additional justification of the deferral decision to determine potential interventions. Hence, we also interpret SLTD's decision to defer at any given time by quantifying the long-term uncertainty in the outcome and decomposing the sources of uncertainty. We justify how the decomposition can guide experts to potential interventions.

Clinical Motivation. We are motivated by clinical settings where a target policy is learned from batch data to work well across multiple institutions. Such a policy may perform well on average, but when deployed to a new environment, encounter a different or an evolving patient population. Clinicians might also follow a slightly different treatment protocol than this learned policy. Regulatory constraints may prevent significantly adapting our target policy completely to the new site. In this case, it is safer to leverage batch data from the new site to quantify when it is reliable to deploy the learned target policy. In situations where the policy does not improve outcomes compared to the human expert, exacerbated by challenges like non-stationarity,

it is safer to defer to human experts. Beyond healthcare, our work is applicable in many safety-focused, data-scarce, non-stationary settings where online policy improvement is not allowed due to ethical or practical constraints.

2 Related Work & Background

Mixture-of-Experts (MoE). Many methods focus on deciding to deploy two or more policies. For example, Jacobs et al. (1991); Jordan and Jacobs (1994) switch between different policies in decision-making by partitioning the input space into regions assigned to different specialized sub-models. Variants of this framework enforce an explicit preference for a specific expert, e.g., a human expert, and train other experts to complement the human expert (Pradier et al., 2021). In sequential settings, Parbhoo et al. (2017); Gottesman et al. (2019); Parbhoo et al. (2018) combine parametric and non-parametric experts to learn more accurate estimates of the value function. On the other hand, we focus on *deferral to human experts when future outcomes using the current ML-based policy are potentially undesirable*. Further, we defer based on explicitly quantifying the impact of delayed deferral to decide *when* to defer.

Policy Improvement with Expert Supervision. Sonabend et al. (2020) use hypothesis testing to assess whether, at each state, a policy from a human expert would improve value estimates over a target policy *during training* to improve the target policy. In contrast, our work identifies the value of *delaying deferral to a human expert at test time*. Improvements using expert supervision are unlikely to be always feasible due to safety and regulatory constraints. Learning-to-defer with respect to a fixed target policy is crucial as a safeguard. Some works focus on safe policy improvement in a non-stationary MDP setting (Chandak et al., 2020b;a). Chandak et al. (2020a) assume that the non-stationarity is governed by an exogenous process, and so past actions do not impact the underlying non-stationarity. Our work differs in two ways: first, we argue that model misspecification, specifically ignoring non-stationarity induced by (deferral) actions, affects the likelihood of future deferrals. Accounting for this non-stationarity is crucial to avoid costly deferrals. Second, we incorporate human expertise by explicitly measuring the impact of delaying deferral.

Learning-to-defer to Human Expertise. Madras et al. (2017); Mozannar and Sontag (2020) propose supervised models to defer to the expert. Here, the classifiers are trained on the samples of an expert's decisions. Madras et al. (2017) train a separate rejection and prediction function, while Mozannar and Sontag (2020) learn a joint predictor for all targets and deferral. Madras et al. (2017) is conceptually closer to our work but in a non-sequential setting. Other approaches such as Raghu et al. (2019); Wilder et al. (2020) first train a standard classifier on the data and then compute uncertainty estimates for this classifier and the human expert. The models defer to the expert if the model is highly uncertain or can significantly benefit from deferral. Liu et al. (2021) incorporate uncertainty in Learning-to-Defer algorithms for classification tasks. Instead, we focus on learning-to-defer in non-stationary, sequential settings.

Decomposing Uncertainty for Interpreting Policies. Uncertainty, if well calibrated can help decision-makers understand the failure modes of a model (Bhatt et al., 2020; Tomsett et al., 2020; Zhang et al., 2020). Several methods estimate predictive uncertainty in ML (Gal and Ghahramani, 2016; Guo et al., 2017). Here, we focus on capturing the *propagated uncertainty* in sequential settings to interpret deferral decisions. We interpret the (different) sources of propagated uncertainty when SLTD defers to the expert. Decomposing the sources of uncertainty into modeling and irreducible uncertainty over predictions has been explored in classification and prediction settings (Yao et al., 2019; Depeweg et al., 2018) but remains significantly under-explored for sequential settings.

Background and Notation. We consider our environment to be a finite horizon MDP defined by $\mathcal{M} \equiv (\mathcal{S}, \mathcal{A}, \mathcal{P}, r, p_0)$ where $\mathcal{S}$ indicates the state-space, $\mathcal{A}$ indicates the action-space, $\mathcal{P}$ the transition dynamics, $r : s \times a \rightarrow \mathbb{R}_+$ the reward function, p_0 the initial state distribution. The action-space is assumed to be discrete, while the state space can be discrete or continuous. Any intervention policy (usually stochastic in our case) is given by $\pi =: \mathcal{S} \times \mathcal{A} \rightarrow [0, 1]$. We consider a non-stationary environment such that the dynamics at any time t are governed by a specific MDP $\mathcal{M}_t$. Thus the environment is a sequence of MDPs. We assume the existence of a true set of non-stationary dynamics governing all episodes and denote it by $\boldsymbol{\mathcal{M}}^* := \{\mathcal{M}_t^*\}_t$. In the rest of the draft, $\boldsymbol{\mathcal{M}} := \{\mathcal{M}_t\}_t$ denotes an estimate of the true dynamics $\boldsymbol{\mathcal{M}}^*$. Let T

be the episode-length. The value of a policy π at t is given by $V^{\boldsymbol{\mathcal{M}}}_{\pi,t}(s) = \mathbb{E}_{\boldsymbol{\mathcal{M}}}[\sum_{j=t}^{T} r^j(s,a)|s_t = s, \pi]$. The action value is given by $Q^{\boldsymbol{\mathcal{M}}}_{\pi,t}(s,a) = r(s,a) + \sum_{s' \in \mathcal{S}} \mathcal{P}(s'|s,a) V^{\boldsymbol{\mathcal{M}}}_{\pi,t}(s')$.

3 Sequential Learning-to-Defer

Problem Setup. Assume we are given a policy π_{tar} that may be learned from batch data from one or more environments. π_{tar} is intended to be deployed in a new environment. We have access to batch data, denoted by $\mathcal{D}^* = \{s_{i,0}, a_{i,0}, r_{i,0}, \cdots, s_{i,T}, a_{i,T}, r_{i,T}\}_{i=1}^{N}$ collected in the new non-stationary environment $\boldsymbol{\mathcal{M}}^* = \{\boldsymbol{\mathcal{M}}^*_t\}_t$, from some (potentially non-stationary) behavior policy π_0. Here N denotes the number of episodes. Our goal is to learn a deferral policy $g_{\pi_{\text{tar}}}(s,t) : \mathcal{S} \times T \to \{0,1\}$ (where 1 corresponds to defer or $\perp$) with respect to π_{tar} to defer to the expert policy π_0.

Deferral to the expert is denoted by the action $\perp$. That is, we will augment the action space of existing MDP $\boldsymbol{\mathcal{M}}^*$ to include a new deferral action $\mathcal{A}_\perp := \mathcal{A} \cup \perp$. At every step, the agent decides whether or not to defer. If the agent defers, π_0 will be deployed for that time step. We describe the formulation assuming strict adherence to π_0 at deferral to emphasize other aspects of our contribution such as the impact of non-stationarity and how to account for relevant sources of uncertainty to compare outcomes. SLTD can easily account for the uncertainty of expert actions in the framework.

In practice, the target policy π_0 may not uniformly improve over π_{tar} for all states. That is guaranteeing that $V^{\boldsymbol{\mathcal{M}}^*}_{\pi_{\text{tar}},0}(s) \geq V^{\boldsymbol{\mathcal{M}}^*}_{\pi_0,0}(s)$ for all $s \in \mathcal{S}$, is challenging. Even when fine-tuning is allowed, it is challenging to ensure that the target policy is indeed better than π_0 in all regions of the state space. Hence, we would like to get the best of both worlds. We can deploy π_{tar}, to reduce the costs of relying on human expertise, and learn to automatically defer to the costlier policy π_0 (i.e. human expert) when relying on π_{tar} does not improve outcomes. In regions of the state-space where the value of π_{tar} is lower than π_0, it is better to defer to the human as a "safety protocol".

SLTD. To determine whether to defer at each time step, we quantify whether deferring (relying on the behavior policy) or not deferring (using the target policy) at the current time step improves the long-term outcome. Long-term outcomes are affected by potential future deferrals. Thus comparing the consequences of deferring versus relying on the ML policy at the current instance is equivalent to comparing the impact of deferring now versus delaying deferral by one time step.

Future deferrals imply that some unknown mixture of π_{tar} and π_0 is used in the future. We denote such a mixture policy as π_{mix}. To minimize cumbersome notation, we denote a policy where π_{tar} is deployed at instance t and π_{mix} in the future as: $\pi_{\text{tar}(t),\text{mix}(t_+)}$. Similarly, if we defer *now*, then the policy that is deployed at time t is π_0 , and π_{mix} in the future. We denote this mixture as $\pi_{0(t),\text{mix}(t_+)}$. Thus, at any instance t, we want to defer if $V^{\boldsymbol{\mathcal{M}}}_{\pi_{\text{tar}(t),\text{mix}(t_+)}}(s) < V^{\boldsymbol{\mathcal{M}}}_{\pi_{0(t),\text{mix}(t_+)}}(s)$. Note that we consider deferral to π_0 as a costly one. This is accounted through a constant cost $c > 0$ in terms of the value. That is, deferral incurs cost c and the resulting value is: $V^{\boldsymbol{\mathcal{M}}}_{\pi_{0(t),\text{mix}(t_+)}}(s) - c$. We can now formalize our stochastic deferral policy:

Definition 1. *Let $\pi_{tar,t}$ be such that such that there exists $s^t \subseteq \mathcal{S} \forall t \in \{0, 1, \cdots, T\}$ where $P(V^{\boldsymbol{\mathcal{M}}}_{\pi_{tar(t),mix(t_+)}}(s) < V^{\boldsymbol{\mathcal{M}}}_{\pi_{0(t),mix(t_+)}}(s) - c) > \tau$ for constant cost of deferral $c > 0$ and threshold $\tau > 0$, $\forall s \in s^t$. Then the deferral policy $g_{\pi_{tar}}(s,t) \triangleq \mathbf{1}[P(V^{\boldsymbol{\mathcal{M}}}_{\pi_{tar(t),mix(t_+)}}(s) < V^{\boldsymbol{\mathcal{M}}}_{\pi_{0(t),mix(t_+)}}(s) - c) > \tau] \triangleq \mathbf{1}[\tilde{g}_{\pi_{tar}}(s,t) > \tau]$.*

Corollary 1. *By Definition 1, $g_{\pi_{tar}}(s,t)$, includes the earliest time in the episode where $\tilde{g}_{\pi_{tar}}(s,t) \triangleq P(V^{\boldsymbol{\mathcal{M}}}_{\pi_{tar(t),mix(t_+)}} < V^{\boldsymbol{\mathcal{M}}}_{\pi_{0(t),mix(t_+)}} - c) > \tau$. Thus, $g_{\pi_{tar}}(s,t)$ is a pre-emptive deferral policy.*

The cost c determines how conservative SLTD is and trades-off frequency of deferral to the value attained.This parameter should be tuned by domain experts aware of the trade-off and risks involved. For instance, in a critical care setting, we may be more conservative and use a smaller c than in a chronic care situation. τ is a safety threshold on the probability of worse outcome beyond which we deem that deferral is necessary.

Definition 1 indicates that to reliably learn the deferral policy, we need to estimate $\tilde{g}_{\pi_{\text{tar}}}(s,t) \triangleq P(V^{\boldsymbol{\mathcal{M}}}_{\pi_{\text{tar}(t),mix(t_+)}}(s) < V^{\boldsymbol{\mathcal{M}}}_{\pi_{0(t),mix(t_+)}}(s) - c)$. To estimate this probability, we should model all sources of uncertainty in the system, including the non-stationary dynamics, and the uncertainty associated with our

modeling assumptions. We use a Bayesian RL approach to account for all sources of uncertainty. We motivate this by first describing our dynamic programming approach to learn-to-defer.

Our dynamic programming procedure maintains an estimate of the deferral probability $\tilde{g}_{\pi_{\text{tar}}}(s,t)$ and refines it as we train on the batch data. Given an estimate of $\tilde{g}_{\pi_{\text{tar}}}(s,t)$, we outline the procedure to i) estimate the value under mixture policies corresponding to deferral (and delayed deferral), ii) modeling the probability of improvement under various sources of uncertainty, and finally iii) obtaining a new estimate of the deferral probability $\tilde{g}_{\pi_{\text{tar}}}(s,t) \forall s \in \mathcal{S}$ at the given time t using i) and ii). We then bootstrap this procedure over our batch data to refine our deferral probabilities. We describe the procedure for the discrete setting.

Algorithm 1 Sequential Learning to Defer

Input: $\mathcal{D}^*$, behavior policy π_0, target policy π_{tar}.
Estimate Posterior Distributions $\{\mathcal{M}_t \triangleq p_t(\cdot|\mathcal{D}^*)\}_{t=0}^T$ (posteriors over rewards not shown here)
Initialization: Deferral function $g_{\pi_{\text{tar}}}(s,t) = 0$ for all $s \in \mathcal{S}$ and $t \in \{1, 2, \cdots, T\}$.
for $n \in$ BOOTSTRAPS($\mathcal{D}^*$) **do**
  Sample $\boldsymbol{\mathcal{M}}_k \triangleq \{\mathcal{M}_{k,t} \sim p_t(|\mathcal{D}*)\} \forall t \in \{1, 2, \cdots, T\}, \forall k \in \{1, 2, \cdots, K\}$
  for $t \in \{T, T-1, \cdots, 1\}$ **do**
    for $s \in \mathcal{S}$ **do**
      Compute $V^{\boldsymbol{\mathcal{M}}}_{\pi_{\text{tar}(t),\text{mix}(t_+)}}, V^{\boldsymbol{\mathcal{M}}}_{\pi_{0(t),\text{mix}(t_+)}} - c \forall \boldsymbol{\mathcal{M}}$
      $\tilde{g}_{\pi_{\text{tar}}}(s,t) \leftarrow\approx \frac{1}{K} \sum_{\boldsymbol{\mathcal{M}}_k \sim \{p_{t'}(\cdot|\mathcal{D})\}_{t'=t}^T} [\mathbf{1}(V^{\boldsymbol{\mathcal{M}}_k}_{\pi_{\text{tar}(t),\text{mix}(t_+)}} < V^{\boldsymbol{\mathcal{M}}_k}_{\pi_{0(t),\text{mix}(t_+)}} - c)]$
    end for
  end for
end for
return $g_{\pi_{\text{tar}}}(s,t) = \mathbf{1}(\tilde{g}_{\pi_{\text{tar}}}(s,t) > \tau) \forall s, t \in \mathcal{S} \times \{1, 2, \cdots, T\}$

Estimating Value function. At any instance we defer based on current estimates of $g_{\pi_{\text{tar}}}(s,t)$ (or equivalently $\tilde{g}_{\pi_{\text{tar}}}(s,t)$). We sample actions from π_{tar} if $g_{\pi_{\text{tar}}}(s,t) = 0$ and π_0 otherwise (equivalent to $\perp$). Note that the current estimate of $g_{\pi_{\text{tar}}}(s,t)$ determines the future mixture policy as well. We now estimate the value of the mixture policies using the Bellman Equation of the state and action value functions. For the mixture policy $\pi_m \triangleq \pi_{tar(t),mix(t_+)}$ (corresponding to no deferral at t), the Q-function is:

$$Q^{\boldsymbol{\mathcal{M}}}_{\pi_m,t}(s,a) = r(s,a) + \sum_{s' \in \mathcal{S}} \mathcal{P}^{\boldsymbol{\mathcal{M}}}(s'|s,a) V^{\boldsymbol{\mathcal{M}}}_{\pi_{\text{mix}(t_+)},t+1}(s') \tag{1}$$

and the Value function is:

$$V^{\boldsymbol{\mathcal{M}}}_{\pi_m,t}(s) = \sum_{a \in \mathcal{A}} \pi_{\text{tar}(t)}(a|s) Q^{\boldsymbol{\mathcal{M}}}_{\pi_m,t}(s,a) \tag{2}$$

Similarly for the mixture policy if we defer at t.

Estimating the probability of improving outcomes by delaying deferral. At each instance t, for all states s, we can estimate the indicator function $\mathbf{1}[V^{\boldsymbol{\mathcal{M}}^*}_{\pi_{\text{tar}(t),\text{mix}(t_+)}}(s) < V^{\boldsymbol{\mathcal{M}}^*}_{\pi_{0(t),\text{mix}(t_+)}}(s) - c]$ given an estimate of $\tilde{g}_{\pi_{\text{tar}}}$ as described above. However, we do not have access to the true dynamics $\boldsymbol{\mathcal{M}}^*$. In batch settings, such as ours, we often estimate the dynamics using maximum-likelihood estimation. Such methods make specific assumptions about the distribution governing the dynamics. Our assumptions about the dynamics may be incorrect resulting in potential misspecification of our dynamics model. This increases the uncertainty in the outcome and potentially over-estimates the probability that relying on the model may improve outcomes. To account for this additional source of uncertainty, we use a Bayesian RL approach. We describe the procedure for the dynamics. The procedure for rewards follows an analogous process.

Suppose the parameters of the distributions governing the dynamics are denoted by $\theta_t \, \forall t \in \{0, \cdots, T\}$. We denote the full set of parameters by $\boldsymbol{\theta} = \{\theta_t\}_t$. We assume a prior distribution over the parameters of the distribution governing the dynamics $\mathcal{P}^{\boldsymbol{\mathcal{M}}}_{\theta}(s'|s,a)$ and the rewards $r(s,a)$. Given batch samples $\mathcal{D}^*$, we can estimate the posterior distribution over the non-stationary MDPs and rewards using Bayesian inference:

$$p(\boldsymbol{\theta}|\mathcal{D}^*) \propto p(\mathcal{D}^*|\boldsymbol{\theta}) p(\boldsymbol{\theta})$$

More specifically, we assume conjugate priors for our parameters $\boldsymbol{\theta}$. By relying on conjugate priors in our inference, the parameters of posterior distributions over the dynamics and rewards are obtained in closed form. For discrete state dynamics (and rewards), we assume a Dirichlet prior distribution and model the observations $p(\mathcal{D}^*|\boldsymbol{\theta})$ using a Multinomial distribution. For continuous states, $p(\mathcal{D}^*|\boldsymbol{\theta})$ is assumed to be normally distributed with $\boldsymbol{\theta}$ being the mean and variance parameters. The prior distributions over the mean and precision (inverse of the variance) is the Normal-gamma prior. This is a domain-dependent choice and SLTD is agnostic so long as we can sample from the posterior distributions of the learned model dynamics. A detailed derivation of how the data is leveraged to estimate the posterior distributions over the dynamics are provided in Appendix A.1. By allowing flexibility of modeling the dynamics via Bayesian RL, we can account for uncertainty over our modeling assumptions.

Finally, based on our assumption that the non-stationary environment is governed by a sequence of MDPs, we estimate the MDP for each time step independently from batch data. This allows us to make fewer assumptions about the *type* of non-stationarity. Any additional domain knowledge about the nature of non-stationarity can be leveraged for data efficiency. We can now estimate the impact of delayed deferral by sampling non-stationary MDPs from our posterior distributions and averaging to obtain our final probability:

$$\begin{aligned}
&\tilde{g}_{\pi_{\text{tar}}}(s,t) \triangleq P(V^{\boldsymbol{\mathcal{M}}^*}_{\pi_{\text{tar}(t),\text{mix}(t_+)}}(s) < V^{\boldsymbol{\mathcal{M}}^*}_{\pi_{0(t),\text{mix}(t_+)}}(s) - c) \\
&= \mathbb{E}_{\boldsymbol{\mathcal{M}}\sim p(\cdot|\mathcal{D}^*)}[\mathbf{1}[V^{\boldsymbol{\mathcal{M}}}_{\pi_{\text{tar}(t),\text{mix}(t_+)}}(s) < V^{\boldsymbol{\mathcal{M}}}_{\pi_{0(t),\text{mix}(t_+)}}(s) - c]] \\
&\approx \frac{1}{K} \sum_{\boldsymbol{\mathcal{M}}_k\sim\{p_{t'}(\cdot|\mathcal{D}^*)\}_{t'=t}^{T}} \mathbf{1}[V^{\boldsymbol{\mathcal{M}}_k}_{\pi_{\text{tar}(t),\text{mix}(t_+)}}(s) < V^{\boldsymbol{\mathcal{M}}_k}_{\pi_{0(t),\text{mix}(t_+)}}(s) - c]
\end{aligned} \tag{3}$$

where the second line comes from the definition due to the randomness over the dynamics, and the last term comes from approximating the expectation using K samples from the posterior distribution of the dynamics $p(\cdot|\mathcal{D}^*)$. Thus, for every instant t, in a given state s, our deferral policy $g_{\pi_{\text{tar}}}(s,t)$ is given by, $g_{\pi_{\text{tar}}}(s,t) := \mathbf{1}[\tilde{g}_{\pi_{\text{tar}}}(s,t) > \tau]$.

Dynamic Programming to estimate $g_{\pi_{\text{tar}}}(s,t)$. Our dynamic programming procedure is summarized in Algorithm 1. We initialize $g_{\pi_{\text{tar}}}(s,t) = 0$ for all $s \in \mathcal{S}$. We estimate $V^{\boldsymbol{\mathcal{M}}}_{\pi_{\text{tar}(t),\text{mix}(t_+)}}(s), V^{\boldsymbol{\mathcal{M}}}_{\pi_{0(t),\text{mix}(t_+)}}(s)$ for a given t using Bellman Equations 1 and 2. Following that, we can update our estimate of $g_{\pi_{\text{tar}}}(s,t)$ using our posterior MDPs, i.e. Equation 3. We repeat (over t) using the *updated* estimates of $g_{\pi_{\text{tar}}}(s,t)$.

4 Decomposing the uncertainty at deferral

SLTD defers at time t because the probability that relying on π_{tar} improves the outcome is below our safety threshold, i.e. SLTD is uncertain of an improved outcome. Conveying this uncertainty can help the domain expert take over decision-making. We interpret this deferral decision in terms of the total and decomposed uncertainty on long-term outcomes. We convey two different sources of uncertainty at deferral. First, we consider *epistemic/modeling uncertainty*, which captures whether our model specification has resulted in high uncertainty and the *aleatoric uncertainty* which mainly results from the stochasticity of the environment itself. A high relative value of the former suggests that adding more data to train SLTD can improve the confidence of the model. High aleatoric uncertainty suggests that the environment itself is highly variable leading to the lack of confidence in relying on π_{tar}.

Concretely, let t_d be a time when SLTD defers. The agent is in state s_{t_d}. We are interested in the reward (and uncertainty over the reward) at time T due to deferral at t_d, i.e., $\mathbb{E}[r_T|s_{t_d}, \mu_{t_d}, \pi_{0(t_d),mix(t_d+)}]$. We denote the posterior MDP samples for any state-action pair by μ_t. The variability in these samples captures modeling uncertainty. The dynamics parameters are denoted by $\theta_t(s,a)$ for each state-action pair. First, we sample the parameters of the dynamics from posterior distribution $p(\theta_{t'}|\mathcal{D}^*)$, followed by sampling the MDPs $\mu_{t'} \sim p(\mu_{t'}|\theta'_t(s_{t'}, a_{t'}))$. Once we defer, we sample actions from π_0 at time $t' = t_d$ and π_{mix} for $t' > t_d$ where the mixture probability is determined by the learned $g_{\pi_{\text{tar}}}$ for future deferrals. The expected long-term outcome is given by:

$$\mathbb{E}[r_T|s_{t_d}, \mu_{t_d}] = \int_{s_{t_d+1}}^{s_T} \int_{a_{t_d}}^{a_T} \int_{\mu_{t_d+1}}^{\mu_T} \int_{\theta_{t_d}}^{T} r(s_T, a_T) \times \prod_{t'=t_d+1}^{T} p_{t'}(s_{t'}|\mu_{t'}) p_{t'}(\mu_{t'}|\theta'_t(s_{t'}, a_{t'})) \pi_{t'}(a_{t'}|s_{t'}) p_{t'}(\theta_{t'}|\mathcal{D}) d\mathbf{s} d\mathbf{a} d\boldsymbol{\mu} d\boldsymbol{\theta}$$

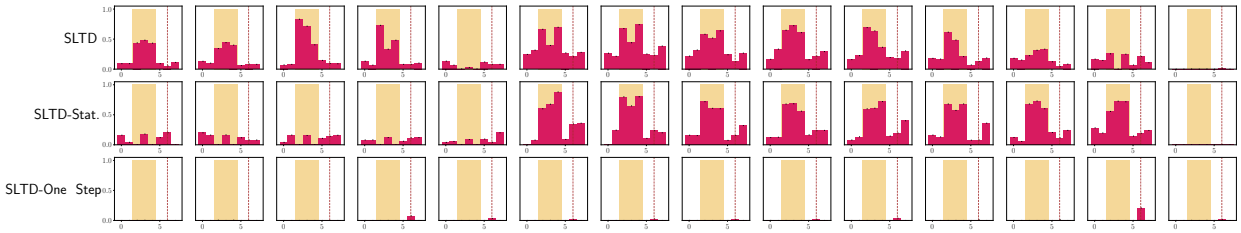

Figure 2: Learned deferral probabilities for SLTD (top row), SLTD stationary (second row), SLTD one-step (third row), and Augmented-MDP (red dotted line) for $c = 0$. Each row shows the deferral histogram $\tilde{g}_{\pi_{\text{tar}}}(s, t)$ over the length of the episode T (major x-axis) for Synthetic data. Each box is the histogram with respect to the states at a fixed time. According to Synthetic data design, target policy always takes suboptimal actions in the yellow region. Further the dynamics changes over time so that the optimal action flips, as well as the noise increases, when $5 \leq t \leq 12$ requiring deferral more often. Thus, shaded yellow regions is the region of pre-emptive deferral. SLTD, which models non-stationarity defers adaptively and early in the shaded yellow region (top row), and increases the deferral probability when dynamics change. SLTD-stationary does not learn calibrated probabilities in the yellow region over time and only defers when the *average* dynamics of the environment require deferral. SLTD-one-step and Augmented-MDP (dotted red line) only defer in state 6 when the reward is negative, and are not pre-emptive.

Integrands are written in short-hand: $\mathbf{s} = \{s_{t_d+1}, s_{t_d+2}, \cdots, s_T\}$ (analogously for other quantities). We maintain one estimate of parameter $\theta_{t'}$ and sample K MDPs $\mu_{t'}$ from this distribution. Thus, the epistemic uncertainty we capture is due to the uncertainty over dynamics under fixed parameters. The total uncertainty can now be decomposed using the law of total variance:

$$\underbrace{\text{Var}(r_T|s_{t_d}, \mathcal{D})}_{\text{Total Uncertainty}} = \underbrace{\mathbb{E}_{\mu_{t_d}\sim p(\mu_{t_d}|\mathcal{D})}[\text{Var}(r_T|\mu_{t_d}, s_{t_d}, \mathcal{D})]}_{\text{Irreducible/ Aleatoric Uncertainty}} + \underbrace{\text{Var}_{\mu_{t_d}\sim p(\mu_{t_d}|\mathcal{D})}(\mathbb{E}[r_T|\mu_{t_d}, s_{t_d}, \mathcal{D}])}_{\text{Epistemic/Modeling Uncertainty}}$$

The second term is the variance *conditioned* on knowledge of the model μ_{t_d}. This is the *propagated uncertainty due to modeling uncertainty at* t_d and can be reduced by data collection. The first term averages over the variance due to μ_{t_d} and captures *propagated uncertainty due to aleatoric uncertainty at* t_d, which conveys stochasticity of the environment itself. This uncertainty can only be reduced by careful interventions at t_d. We estimate these using Monte-Carlo sampling. Additional details on the derivation are provided in Appendix A.2. As suggested before, a high *propagated epistemic uncertainty* conveys that the current uncertainty of model prediction (of the dynamics) is high but could be improved if additional data could be collected. High *propagated aleatoric uncertainty* indicates high variability in the dynamics that can only be reduced with careful interventions and is otherwise not manageable.

5 Experiments

We evaluate SLTD's ability to defer adaptively in sequential settings with respect to a known and fixed π_{tar} to the expert policy π_0. We test the utility of: i) deferring based on long-term outcomes, ii) adaptively deferring by quantifying the impact of delaying deferral, i.e., in regions where delayed deferral can worsen outcomes, iii) modeling the non-stationarity on deferral frequency, iv) quantifying multiple sources of uncertainty to estimate the probability of different outcomes under delayed deferral. We test our method on synthetic data, a non-stationary diabetes simulator[1] modified from Chandak et al. (2020b), and real-world HIV data.

Synthetic Data. In this synthetic simulation, the region of deferral is known apriori by careful design of π_{tar}. This environment has 8 discrete states and binary actions $\{a_0, a_1\}$. All samples start at state 0 and progress toward a sink state 7. The episode length is 15. State 6 has low reward (-5) while all other states have a reward of $+1$. The initial dynamics are set up such that action a_0 reduces the probability of landing in stage 6, and action a_1 increases the probability of reaching state 6. π_{tar} increases the chances to reach state 6 unfavourably by taking action a_1 in states $2, 3, 4$ when $t < 5$ or $t > 12$. We expect to defer in states $2, 3, 4$ even though rewards are favorable, if a method is pre-emptive. When $5 \leq t \leq 12$, the dynamics flip such that a_0 becomes an unfavourable action that increases the probability of landing in 6, while a_1 reduces this

[1] Jinyu Xie. Simglucose v0.2.1 (2018) [Online]. Available: `https://github.com/jxx123/simglucose`. Accessed on: 07-24-2021.

Method	Synthetic		Diabetes		HIV - Case Study I		HIV - Case Study II	
	Value (mean ± 2 s.e.)	Defer Frequency	Value (mean ± 2 s.e.)	Defer Frequency	Value (mean ± 2 s.e.)	Defer Frequency	Value (mean ± 2 s.e.)	Defer Frequency
SLTD	**8.029 ± 0.039**	0.509	**36.931 ± 0.166**	0.396	**14.792 ± 0.267**	0.342	**8.754 ± 0.125**	0.461
SLTD-Stat.	5.588 ± 0.048	1.000	34.326 ± 0.172	1.000	11.020 ± 0.230	0.629	4.291 ± 0.218	0.317
SLTD-One Step	5.578 ± 0.050	1.000	36.819 ± 0.23	0.412	9.671 ± 0.129	0.531	4.588 ± 0.178	0.337
SLTD (K=1)	8.011 ± 0.025	0.511	36.678 ± 0.289	0.297	9.311 ± 0.162	0.517	6.492 ± 0.388	0.372
SLTD-Stat. (K=1)	5.575 ± 0.036	1.000	34.320 ± 0.175	1.000	8.659 ± 0.027	0.571	3.662 ± 0.059	0.263
SLTD-One Step (K=1)	5.595 ± 0.038	1.000	36.482 ± 0.284	0.328	8.640 ± 0.104	0.318	3.959 ± 0.130	0.387
Augmented-MDP	3.044 ± 0.023	0.512	13.273 ± 0.126	0.000	N/A	N/A	N/A	N/A
Mozannar et. al.	6.369 ± 2.226	0.468	-15.155 ± 0.675	0.010	3.820 ± 0.231	0.291	4.726 ± 0.295	0.416
Madras et. al.	5.731 ± 0.223	1.000	35.388 ± 0.475	0.332	3.330 ± 0.481	0.400	4.972 ±0.125	0.360
π_{tar}	-1.80 ± 0.071	N/A	13.202 ± 0.162	N/A	5.837 ± 0.171	N/A	3.292 ± 0.274	N/A
π_0	5.485 ± 0.035	N/A	34.241 ± 0.151	N/A	14.124 ± 0.592	N/A	5.629 ± 0.159	N/A

Table 1: Expected Value for SLTD compared with baselines. The table shows the value of using π_{tar} with our deferral method SLTD, its variants, and other baselines. Higher values indicate better performance. Note that none of the values shown are cost-penalized, i.e. all values are true values within the system, irrespective of the deferral cost. Results show the best performing policy after tuning the respective hyperparameters (see Appendix A.4). We further show how often each method defers to the expert policy (lower is better). $K = 1$ variants of SLTD indicate ablations of SLTD that ignore modeling uncertainty. SLTD outperforms baselines in for all datasets with fewer (though not the lowest) deferral frequency.

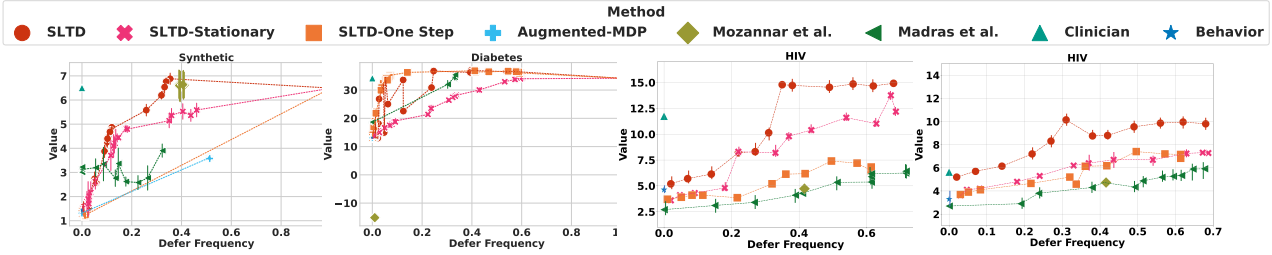

Figure 3: Trade-off of deferral frequency and value attained. Plot shows expected value (higher is better) for a sweep over deferral cost (and any other method specific hyperparamters) in relation to the deferral frequency (lower is better). SLTD achieves the best trade-off and better value by deferring pre-emptively. The stationary variant defers significantly more to achieve better outcomes. The One-Step variant cannot improve over π_{tar} in MDPs where effect of interventions are not myopic (Synthetic and HIV) and achieve good performance by virtue of modeling dynamics in Diabetes, compared to existing learning-to-defer baselines Mozannar et. al. and Madras et. al. (which are myopic). Augmented-MDP is unable to achieve good performance even at upto 50% deferral and unable to improve value in Diabetes indicating the benefits of deferring by explicitly quantifying the impact of delaying deferral as in SLTD over Augmented-MDP's Value Iteration method.

probability. Here, π_{tar} again increases the chances of landing in 6, by taking a_0 more often in states $2, 3, 4$. By flipping the better action to a_0 in this region, it becomes crucial to *estimate the dynamics* over predicting the best action. The dynamics are non-stationary and the probability of landing in state 6 progressively increases when $5 \leq t \leq 12$.

Real-world simulator: Diabetes Data. We use an open-source implementation of the FDA approved Type-1 Diabetes Mellitus simulator (T1DMS) for modelling treatment of Type-1 diabetes. We sample 10 adolescent patient trajectories (episodes) over 24 hours (aggregated at 15 minute intervals). Glucose levels are discretized into 13 states. Combination interventions of insulin and bolus are discretized to generate a total of 25 actions. We introduce non-stationarity in each episode by increasingly changing the adolescent patient properties to an alternative patient. This significantly affects the utility of the initial target policy which is learned on the dynamics of the original patient, thus necessitating deferral as the patient properties change over time. The non-stationary behavior policy π_{tar} for this task is estimated using Q-learning. We

defer to a clinician policy, here simulated by learning an epsilon-greedy version of a policy learned using Q-learning under (estimated) non-stationary dynamics on the target data.

Real-world: HIV Data. We identified individuals between 18-72 years of age from the EuResist database (Zazzi et al., 2012) comprising of genotype, phenotype and clinical information of over 65,000 individuals in response to antiretroviral therapy administered between 1983-2018. We focus on a subset of $32,960$ patients' genotype, treatment response, CD4+ and viral load measurements, gender, age, risk group, number of past treatments collected over on average 14 years (aggregated at 4-6 month intervals). Our action space consists of the 25 most frequently occurring drug combinations, while our state space consists of 100 continuous states of cell counts and viral loads. Since the virus evolves in response to drug pressure, the problem is inherently non-stationary. For our first case study, we investigate whether deferring to a second line therapy as proposed by standard medical guidelines (Saag et al., 2020) in response to potential drug resistance improves long-term outcomes. The non-stationary behaviour policy is the first line therapy estimated using Q-learning. For our second case study, the non-stationary behaviour policy corresponds to a first line therapy typically used for treating patients of subtype C. We then examine whether deferring to a first line therapy, given by clinical collaborators, for patients of subtype M (due to potential drug resistance) improves long-term outcomes.

Baselines. We compare to the following baselines.

Mozannar et. al. (Mozannar and Sontag, 2020): This is a supervised method using a consistent loss function to learn-to-defer. It learns an augmented regressor to defer or recommend treatment myopically (independently at every time-step). When the model defers, clinician policy is used.

Madras et. al. (Madras et al., 2017): This is an alternative supervised learning-to-defer method. This baseline learns separate regressors to defer and recommend treatments. We modify it to use π_{tar} to recommend and learn the rejection function to defer to π_0.

Augmented-MDP: A conceptual contribution of SLTD is to defer by comparing outcomes by delaying deferral with some knowledge of the expert policy. The deferral action itself is considered to augment the MDP action-space. We explore a baseline that uses Value Iteration in this augmented MDP. Comparing with this baseline helps evaluate the utility of deferring based on outcomes on delayed versus immediate deferral. This baseline will defer permanently to the expert, and knowledge of an expert policy is not assumed. This augmented MDP has action-space is $\mathcal{A} \cup \perp$, an augmented state-space $\mathcal{S} \cup s_{defer}$ (s_{defer} is the deferred state), and defers based on the cost c. This baseline models non-stationary dynamics, and is designed for sequential settings. However since this method defers permanently to the expert, it incurs a larger deferral cost. In our experiments all values are plotted *without* the cost to reflect actual environment outcomes.

SLTD-Stationary: To assess the impact of mis-specifying the non-stationarity, we compare to a variant of SLTD that assumes the dynamics (and rewards) are stationary while allowing the method the flexibility of learning a non-stationary deferral policy.

SLTD-One Step: We compare to a myopic version of SLTD that defers based on the immediate reward. The key difference with the myopic Madras et. al., Mozannar et. al. baselines is that SLTD-One Step models the dynamics and the uncertainty on the immediate reward. Thus, this baseline accounts for future deferrals while deferring myopically.

Ablations for Uncertainty Modeling: For all SLTD variants, we evaluate the utility of accounting for different sources of uncertainty, more specifically the *modeling uncertainty* to estimate the probability of improving outcomes via delayed deferral. In SLTD, *modeling uncertainty* is accounted for by sampling multiple (K) MDPs (Equation 3) from the posterior dynamics distribution, over which our outcomes are averaged. Higher variability across K indicates higher modeling uncertainty. Hence, in Equation 3, using $K = 1$ assumes a perfect estimate of the dynamics model and only accounts for the irreducible stochasticity of the environment. A larger K accounts for potential variability in estimation (original SLTD formulation). If our modeling uncertainty in the environment is indeed large, we anticipate choice of K to have a larger effect on SLTD's performance. Modeling uncertainty can be large when there is insufficient data to fit the target function class of the dynamics.

6 Results

Optimizing for long-term outcomes learns qualitatively different deferral policies. Our deferral policy is a non-stationary stochastic function $\tilde{g}_{\pi_{\text{tar}}}(s,t)$ which we threshold. Visualizing $\tilde{g}_{\pi_{\text{tar}}}(s,t)$ enables us to understand the utility of various modeling choices of SLTD. Figure 2 shows the histograms of $\tilde{g}_{\pi_{\text{tar}}}$ for SLTD and its Stationary and One-Step variant when the cost $c = 0$ for Synthetic data. Visualizing without deferral cost allows us to see the how adaptive SLTD is without a penalty. Each row corresponds to a method; x-axis corresponds to time over the horizon T. Each box in a row corresponds to one time point. For a fixed t, $\tilde{g}_{\pi_{\text{tar}}}$ is a stochastic function of the states, shown as a histogram.

Yellow shaded region indicates the state space where π_{tar} takes unfavorable actions. Over time, the dynamics change so that the favorable action flips $5 \leq t \leq 12$ and the stochasticity in the dynamics increases requiring more frequent deferrals. Deferring in the yellow region is desirable to pre-emptively avoid landing in state 6. SLTD is highly adaptive, and pre-emptively defers in the yellow region. As the stochasticity increases, probability of deferrals appropriately increases. The stationary variant significantly under-estimates the need to defer in states $2, 3, 4$ when $t < 5$. It is only able to pre-emptively defer in regions where the average stochasticity of the estimated dynamics aligns with the environment. The One-Step variant defers only in state 6 and is therefore not-preemptive. Augmented-MDP (red vertical line) deterministically defers in state 6. Thus deferring based on probability of improved outcomes of immediate and delayed deferrals is desirable over alternatives (see also Figures 4, 5, and 6 in Appendix).

SLTD improves long-term outcomes. Table 1 shows the value (higher is better) for all baselines corresponding to best performing parameters. For all datasets, we see a significant benefit from SLTD. Augmented-MDP baseline is not preemptive in spite of modeling the non-stationary dynamics. Hence, deferring by comparing outcomes of delayed deferral is better alternatives, specifically Value Iteration on the Augmented MDP. Additional benefits of modeling the dynamics is clear from improved performance of all SLTD variants compared to the myopic baselines. However, mis-specification of dynamics (SLTD-Stat.) results in worse performance. SLTD-Stat. defers more often to achieve comparable performance. Figure 3 demonstrates this trade-off is general, for all choices of deferral costs and other parameters. The x-axis corresponds to deferral frequency (lower is better) and y-axis the value attained (higher is better). SLTD achieves the best trade-off. Further pre-emptive deferral allows SLTD to reach higher value than the expert policy itself. SLTD-One Step only relies on immediate rewards failing to improve long-term outcomes for synthetic data and HIV. However as long as we model the dynamics appropriately, even myopic deferral using SLTD One Step is beneficial for Diabetes compared to Mozannar et. al., Madras et. al.. This is possible when effect of interventions are observed myopically, as is the case in Diabetes data since modeling the dynamics and impact of future deferral is beneficial to characterize. Madras et. al., Mozannar et. al. baselines are unable to maximize long-term rewards. Madras et. al. performs well on Diabetes data suggesting optimal actions don't significantly deviate in target data and that its design of training a rejection function worked better than the loss function design of Mozannar et. al.

	Defer Time t_d	Total Uncertainty	Modeling Uncertainty	Mean Outcome
Synthetic data	3	26.190	0.233	3.42
Diabetes	3	3418.17	34.160	73.669

Table 2: Interpreting first time of deferral for a sample trajectory. Modeling uncertainty remains low in all cases whereas in comparison, total variance is high. This indicates irreducible stochasticity of the dynamics is the primary source of uncertainty. Additional results are in Appendix.

Ablations for uncertainty modeling. We study the utility of accounting for modeling uncertainty in our framework. As described in Section 4, multiple sources of propagated uncertainty contribute to variability in estimated outcomes. Modeling uncertainty is crucial to account for in a model-based framework. Here we evaluate the impact of not accounting for this uncertainty on SLTD's performance.

If modeling uncertainty is high, variability of the sampled MDPs used to estimate Equation 3 will be higher. Evaluating for $K = 1$, will evaluate the impact of ignoring this uncertainty. In Table 1 (see also Figure 8 in Appendix), we demonstrate the results with $K = 1$ for all SLTD variants. We do not observe significant

differences for Synthetic data and Diabetes indicating that our modeling uncertainty is low in these data. The difference is higher in HIV suggesting the importance of accounting for this uncertainty for real-world HIV data. Such analysis is crucial to understanding whether our modeling assumptions are reasonable.

Decomposing uncertainty in SLTD can help interpret deferral. Conveying the type of uncertainty to a domain expert can help identify the dominant source of uncertainty that resulted in a deferral to their own standard practice (expert policy). Table 2 shows this decomposition for one time point for discrete data. In each case, the modeling uncertainty is a small fraction of the total uncertainty. This suggests that the systematic non-stationarity is the dominant source of uncertainty which generally cannot be reduced by collecting data and may require careful interventions beyond standard policy. Knowledge of the amount of model uncertainty can enable users to further improve decision-making through data collection or improving model assumptions.

7 Discussion

We proposed SLTD, a learning-to-defer framework for sequential settings using offline model-based RL. We learn a deferral policy by quantifying the impact of delaying deferral to the future. SLTD is able to defer based on long-term outcomes, and learns a pre-emptive deferral policy. Further, we emphasize a model-based RL method that captures the dynamics of the environment, particularly non-stationarity. Modeling non-stationarity of the environment allows to defer adaptively. Misspecifying non-stationarity leads to significantly more deferrals to improve long-term outcomes. We demonstrate that existing learning-to-defer frameworks are myopic. That is, these methods do not learn a pre-emptive policy even in sequential settings as they focus on immediate consequences of actions. We further demonstrate the utility of accounting for all potential sources of stochasticity to quantify the impact of delayed deferral. Explicit characterization of probability of improving outcomes is beneficial to prevent over-estimation of benefits of delaying deferral. We further interpret deferral decisions of SLTD by decomposing the *long-term* propagated uncertainty. While quantifying the uncertainty is useful, modeling uncertainty through non-stationarity is costly. Developing a model-free framework is left for future work. SLTD can account for some deviations to the expert policy, though significant deviations could be modeled as a human-in-the-loop and is left to future work.

Ethical considerations. SLTD is a technical proof-of-concept to defer to an expert by accounting for long-term effects, assuming that the expert is better at increasing value over the current policy in certain regions. In practice, an expert policy may not be bias free. Thus, deferral may result in biased decisions if the expert is biased. While we are not focused on addressing bias, exposing uncertainties may encourage expert introspection. Nonetheless, deferring is better when an automated decision may be harmful.

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