Distributional Bellman Operators over Mean Embeddings

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Abstract

We propose a novel algorithmic framework for distributional reinforcement learning, based on learning finite-dimensional mean embeddings of return distributions. The framework reveals a wide variety of new algorithms for dynamic programming and temporal-difference algorithms that rely on the *sketch Bellman operator*, which updates mean embeddings with simple linear-algebraic computations. We provide asymptotic convergence theory using a novel error analysis approach, and examine the empirical performance of the algorithms on a suite of tabular tasks. Further, we show that this approach can be straightforwardly combined with deep reinforcement learning to give competitive performances.

1. Introduction

In distributional approaches to reinforcement learning (RL), the aim is to learn the full probability distribution of future returns (Morimura et al., 2010a; Bellemare et al., 2017; 2023), rather than just their expected values, as is typically the case in value-based reinforcement learning (Sutton & Barto, 2018). Distributional RL was proposed in the setting of deep reinforcement learning by Bellemare et al. (2017), with a variety of precursor work stretching back almost as far as Markov decision processes themselves (Jaquette, 1973; Sobel, 1982; Chung & Sobel, 1987; Morimura et al., 2010a;b). Beginning with the work in Bellemare et al. (2017), the distributional approach to reinforcement learning has been central across a variety of applications of deep RL in simulation and in the real world (Bodnar et al., 2020; Bellemare et al., 2020; Wurman et al., 2022; Fawzi et al., 2022), and has motivated new theories of how neurons in the brain represent uncertainties in rewards (Dabney et al., 2020; Tano et al., 2020; Muller et al., 2024)

Typically, predictions of return distributions are represented directly as approximate probability distributions, such as categorical distributions (Bellemare et al., 2017) and equally-weighted mixtures of Dirac deltas (Dabney et al., 2018b; Nguyen-Tang et al., 2021). Rowland et al. (2019) proposed an alternative framework where return distributions are represented via the values of *statistical functionals*, called a *sketch* by Bellemare et al. (2023). This provided a new space of distributional reinforcement learning algorithms, leading to improvements in deep RL agents, and hypotheses regarding distributional RL in the brain (Dabney et al., 2020; Lowet et al., 2020). On the other hand, a potential drawback of this approach is that, to perform each distributional Bellman update to this representation, these statistical functional values must be "decoded" back into an approximate distribution via an expensive *imputation strategy*. In practice, this can introduce significant computational overhead to Bellman updates, and is unlikely to be biologically plausible for distributional return learning in the brain (Tano et al., 2020).

Here, we focus on a notable instance of the sketch called the *mean embedding sketch*. In short, the mean embedding is the expectation of nonlinear functions under the distribution represented (Smola et al., 2007; Sriperumbudur et al., 2010; Berlinet & Thomas-Agnan, 2011), and is related to *frames* in signal processing (Mallat, 1999) and *distributed distributional code* in theoretical neuroscience (Sahani & Dayan, 2003; Vértes & Sahani, 2018).

The core contributions of this paper are to revisit the approach to distributional reinforcement learning based on sketches (Rowland et al., 2019), and to propose the *sketch Bellman operator* that updates the implicit distributional representation as a simple linear operation, obviating the need for the expensive imputation strategies converting between sketches and distributions. This leads to a rich new space of distributional RL algorithms that operate entirely in the space of sketches. We provide theoretical convergence analysis to accompany the framework, using a novel error analysis approach. We then investigate the practical behaviour of various instantiations of the proposed algorithms in tabular domains, and demonstrate the effectiveness in deep reinforcement learning, showing that our approach is robust enough to serve as the basis for a new variety of deep distributional reinforcement learning algorithms.

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2. Background

We consider a Markov decision process (MDP) with state space $\mathcal{X}$, action space $\mathcal{A}$, transition probabilities $P : \mathcal{X} \times \mathcal{A} \to \mathscr{P}(\mathcal{X})$, reward distribution function $P_R : \mathcal{X} \times \mathcal{A} \to \mathscr{P}(\mathbb{R})$, and discount factor $\gamma \in [0, 1)$. ($\mathscr{P}(\mathcal{X})$ denotes the space of probability distributions over $\mathcal{X}$.) Given a policy $\pi : \mathcal{X} \to \mathscr{P}(\mathcal{A})$ and initial state $x \in \mathcal{X}$, a random trajectory $(X_t, A_t, R_t)_{t \geq 0}$ is the sequence of random states, actions, and rewards encountered when using the policy π to select actions in this MDP. More precisely, we have $X_0 = x$, $A_t \sim \pi(\cdot|X_t)$, $R_t \sim P_R(X_t, A_t)$, $X_{t+1} \sim P(\cdot|X_t, A_t)$ for all $t \geq 0$. We write $\mathbb{P}_x^\pi$ and $\mathbb{E}_x^\pi$ for probabilities and expectations with respect to this distribution (conditioned on $X_0 = x$ and following π), respectively. The performance along the trajectory is measured by the discounted return, defined by

$$\sum_{t=0}^{\infty} \gamma^t R_t \,. \qquad (1)$$

In typical value-based RL, during policy evaluation, the agent learns the expectation of the return for each possible initial state $x \in \mathcal{X}$, which is encoded by the value function $V^\pi : \mathcal{X} \to \mathbb{R}$, given by $V^\pi(x) = \mathbb{E}_x^\pi[\sum_{t=0}^{\infty} \gamma^t R_t]$.

2.1. Distributional RL and Bellman Equation

In distributional RL (Bellemare et al., 2023), the problem of policy evaluation is to learn the probability distribution of return in Equation (1) generated by following a policy π from each possible initial state $x \in \mathcal{X}$. This is encoded by the return-distribution function $\eta^\pi : \mathcal{X} \to \mathscr{P}(\mathbb{R})$, which maps each initial state $x \in \mathcal{X}$ to the corresponding distribution of the random return. A central result in distributional reinforcement learning is the distributional Bellman equation, which relates the distribution of the random return under different combinations of initial states and actions.

To build the random variable formulation of the returns, we let $(G^\pi(x) : x \in \mathcal{X})$ be a collection of random variables with the property that $G^\pi(x)$ is equal to Equation (1) in distribution (random variables sharing the same distribution), conditioned on the initial state $X_0 = x$. This formulation implies that the random variable $G^\pi(x)$ is distributed as the *return distribution* $\eta^\pi(x)$ for all $x \in \mathcal{X}$. Consider a random transition (x, R, X') generated by π, independent of the G^π random variables. Then, the (random variable) distributional Bellman equation states that for each state x,

$$G^\pi(x) \overset{\mathcal{D}}{=} R + \gamma G^\pi(X') \quad | X = x \,,$$

where $\overset{\mathcal{D}}{=}$ denotes equality in distribution. Here, we use the slight abuse of the conditioning bar to set the distribution of X in the random transition. It is also useful to introduce the distributional Bellman operator $\mathcal{T}^\pi : \mathscr{P}(\mathbb{R})^{\mathcal{X}} \to \mathscr{P}(\mathbb{R})^{\mathcal{X}}$

to describe the transformation that occurs on the right-hand side for all $x \in \mathcal{X}$ (Morimura et al., 2010a; Bellemare et al., 2017). If $\eta \in \mathscr{P}(\mathbb{R})^{\mathcal{X}}$ is a collection of probability distributions, and $(G(x) : x \in \mathcal{X})$ is a collection of random variables such that $G(x) \sim \eta(x)$ for all x, and (X, R, X') is random transition generated by π, independent of $(G(x) : x \in \mathcal{X})$, then $(\mathcal{T}^\pi \eta)(x) = \text{Dist}(R + \gamma G(X')|X = x)$.

To implement algorithms of distributional RL, one needs to approximate the infinite-dimensional return-distribution function η^π with finite-dimensional representations. This is typically done via approximations in the space of return distributions; see e.g. Bellemare et al. (Chapter 5; 2023).

2.2. Statistical Functionals and Sketches

Rather than using representations in the space of return distributions, Rowland et al. (2019) proposed to represent return distributions indirectly via *functionals* of the return distribution, called *sketches* by Bellemare et al. (2023). In this work we consider a specific class of sketches below.

Definition 2.1 (Mean embedding sketches). A *mean embedding sketch* ψ is specified by a function $\phi : \mathbb{R} \to \mathbb{R}^m$, and defined by

$$\psi(\nu) := \mathbb{E}_{Z \sim \nu}[\phi(Z)] \,. \qquad (2)$$

For a given distribution ν, the embedding $\psi(\nu)$ can therefore be thought of as providing a *lossy* summary of the distribution. The name is motivated by the kernel literature, in which Equation (2) can be viewed as embedding the distribution ν into $\mathbb{R}^m$ based on the mean of ϕ under ν (Smola et al., 2007; Sriperumbudur et al., 2010; Berlinet & Thomas-Agnan, 2011). As we will show, the mean embedding sketch enables elegant distributional RL algorithms.

Statistical functional dynamic programming (SFDP; Rowland et al. (2019), see also Bellemare et al. (2023)) is an approach to distributional RL in which sketch values, rather than approximate distributions, are the primary object learned. Given a sketch ψ and estimated sketch values $U : \mathcal{X} \to \mathbb{R}^m$, SFDP proceed by first defining an *imputation strategy* $\iota : \mathbb{R}^m \to \mathscr{P}(\mathbb{R})$ mapping sketch values back to distributions, with the aim that $\psi(\iota(U)) \approx U$, so that ι acts as an approximate pseudo-inverse of ψ. The usual Bellman backup is then applied to this *imputed* distribution, and the sketch value extracted from this updated distribution. Thus, a typical update in SFDP takes the form $U \leftarrow \psi((\mathcal{T}^\pi \iota(U))(x))$; see Figure 1.

This approach led to expectile-regression DQN, a deep RL agent that aims to learn the sketch values associated with certain expectiles (Newey & Powell, 1987) of the return, and influenced a distributional model of dopamine signalling in the brain (Dabney et al., 2020; Muller et al., 2024), although the computation of the imputation strategy is often costly in
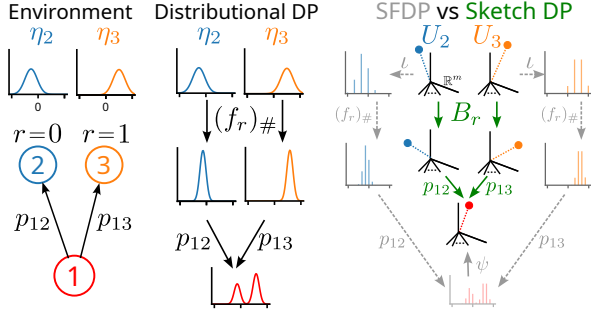
Figure 1. Example of DP update for a three-state environment. State 1 has two child states 2 and 3 associated with return distributions η_2 and η_3. In the exact distributional DP, the domain of η is scaled and shifted by $f_r(g) = r + \gamma g$ (pushed-forward by f_r, giving $(f_r)_\# \eta$), and then weighted by the transition probabilities. In SFDP (grey) (Rowland et al., 2019), the map ι imputes, from initial sketch values U, approximate (e.g. categorical) distributions on which the distribution DP is applied, followed by evaluating the sketch ψ. In our approach Sketch-DP (green), the updates are computed in the mean embedding space, facilitated by the Bellman coefficients B_r along the green paths, avoiding the expensive conversions using imputation in the grey paths.

applications and biologically implausible in neuroscience modelling (Tano et al., 2020).

3. The Bellman Sketch Framework

Our goal is to derive a framework for approximate computation of the mean embedding sketch ψ (with corresponding feature function ϕ) of the return distributions corresponding to a policy π, without needing to design, implement, or compute an imputation strategy as in the case of SFDP/TD. That is, we aim to compute $U^\pi : \mathcal{X} \to \mathbb{R}^m$, given by

$$U^\pi(x) := \psi(\eta^\pi(x)) = \mathbb{E}_x^\pi[\phi(\sum_{t=0}^\infty \gamma^t R_t)].$$

We refer to $U^\pi(x)$ as the mean embedding of η_x^π, a type of sketch value. We begin by considering environments with a finite set of possible rewards $\mathcal{R} \subseteq \mathbb{R}$; we discuss generalisations later. To motivate our method, we consider a special case; suppose that for each possible return $g \in \mathbb{R}$, and each possible immediate reward $r \in \mathcal{R}$, there exists a matrix B_r such that

$$\phi(r + \gamma g) = B_r \phi(g); \qquad (3)$$

note that B_r does not depend on g, and γ is a constant. In words, this says that the feature function ϕ evaluated at the bootstrap return $r + \gamma g$ is expressible as a linear transformation of the feature function evaluated at g itself. If such a relationship holds, then we have

$$U^\pi(x) \overset{(a)}{=} \mathbb{E}_x^\pi[\phi(R + \gamma G^\pi(X'))] \overset{(b)}{=} \mathbb{E}_x^\pi[B_R \phi(G^\pi(X'))]$$

$$\overset{(c)}{=} \mathbb{E}_x^\pi[B_R U^\pi(X')], \qquad (4)$$

where (a) follows from the distributional Bellman equation, (b) from Equation (3), and (c) from exchanging the linear map B_r and the conditional expectation given (R, X'), crucially relying on the linearity of the approximation in Equation (3). Note that for example with $\phi(g) = (1, g)^\top$ we have $B_r = \left(\begin{smallmatrix} 1 & 0 \\ r & \gamma \end{smallmatrix} \right)$, and Equation (4) reduces to the classical Bellman equation for V^π, with $U^\pi(x) = (1, V^\pi(x))^\top$. In Appendix B.2, we generalise the relation in Equation (4) to stochastic rewards under a condition that differs slightly from equation (4).

Thus, $U^\pi(x)$ satisfies its own linear Bellman equation, which motivates algorithms that work directly in the space of sketches, without recourse to imputation strategies. In particular, a natural dynamic programming algorithm to consider is based on the recursion

$$U(x) \leftarrow \mathbb{E}_x^\pi[B_R U(X')]. \qquad \text{(Sketch-DP)}$$

See Figure 1 for an example and comparison with SFDP. As this is an update applied directly to mean embeddings themselves, we introduce the *sketch Bellman operator* $\mathcal{T}_\phi^\pi$: $(\mathbb{R}^m)^\mathcal{X} \to (\mathbb{R}^m)^\mathcal{X}$, with $(\mathcal{T}_\phi^\pi U)(x)$ defined according to the right-hand side of Equation (Sketch-DP). Note that $\mathcal{T}_\phi^\pi$ is a *linear* operator, in contrast to the standard expected-value Bellman operator, which is affine. We recover the affine case by taking one component of ϕ to be constant, e.g. $\phi_1(g) \equiv 1$, and enforcing $U_1(x) \equiv 1$.

The right-hand side of Equation (Sketch-DP) can be unbiasedly approximated with a sample transition (x, r, x'). Stochastic approximation theory (Kushner & Yin, 1997; Bertsekas & Tsitsiklis, 1996) then naturally suggests the following temporal-difference learning update:

$$U(x) \leftarrow (1 - \alpha)U(x) + \alpha B_r U(x') \qquad \text{(Sketch-TD)}$$

given a learning rate α. Rowland et al. (2019) introduced the term *Bellman closed* for sketches for which an *exact* dynamic programming algorithm is available, and provided a characterisation of Bellman closed mean embedding sketches. The notion of Bellman closedness is similar to the relationship in Equation (3), and from Rowland et al. (Theorem 4.3; 2019), we can deduce that the only mean embedding sketches that satisfy Equation (3) are invertible linear combinations of the first-m moments.

Thus, our discussion above serves as a way of re-deriving known algorithms for computing moments of the return (Sobel, 1982; Lattimore & Hutter, 2014), but is insufficient to yield algorithms for computing other sketches. Additionally, since moments of the return distribution are naturally of widely differing magnitudes, it is difficult to learn a high-dimensional mean embedding based on moments; see Appendix D.1 for further details. To go further, we must weaken the assumption made in Equation (3).

3.1. General Sketches

To extend our framework to a much more general family of sketches, we relax our assumption of the exact predictability of $\phi(r+\gamma g)$ from $\phi(g)$ in Equation (3), by defining a matrix of *Bellman coefficients* B_r for each possible reward $r \in \mathcal{R}$ as the solution of the linear regression problem:

$$B_r := \arg\min_B \mathbb{E}_{G \sim \mu}\left[\|\phi(r + \gamma G) - B\phi(G)\|_2^2\right], \quad (5)$$

so that, informally, we have $\phi(r + \gamma g) \approx B_r \phi(g)$ for each g. Here, μ is a distribution to be specified that weights the returns G; we found that a uniform distribution on evenly supported atoms over an estimated return range produces good results (see Appendix B.4). Using the same motivation as in the previous section, we therefore obtain

$$U^\pi(x) \stackrel{(a)}{=} \mathbb{E}_x^\pi[\phi(R + \gamma G^\pi(X'))] \approx \mathbb{E}_x^\pi[B_R \phi(G^\pi(X'))]$$
$$\stackrel{(c)}{=} \mathbb{E}_x^\pi[B_R U^\pi(X')], \quad (6)$$

noting that informally we have *approximate* equality in the middle of this line. This still motivates the approaches expressed in Equations (Sketch-DP) and (Sketch-TD), though we have lost the property that the exact mean embeddings U^π are a fixed point of the dynamic programming procedure.

Algorithm 1 Sketch-DP/Sketch-TD

Precompute Bellman coefficients
Compute C as in Equation (7)
for $r \in \mathcal{R}$ **do**
  Compute C_r as in Equation (7)
  Set $B_r = C_r C^{-1}$
end for
Initialise $U : \mathcal{X} \to \mathbb{R}^m$
# Main loop
for $k = 1, 2, \ldots$ **do**
  if DP **then**
    $U(x) \leftarrow \sum_{r,x',a} P(r, x'|x, a)\pi(a|x)B_r U(x') \; \forall x$
  else if TD **then**
    Observe transition (x_k, a_k, r_k, x_k').
    $U(x_k) \leftarrow (1 - \alpha_k)U(x_k) + \alpha_k B_{r_k} U(x_k')$
  end if
end for

Computing Bellman coefficients. Under mild conditions (invertibility of C as follows) the matrix of Bellman coefficients B_r defined in Equation (5) can be solved as $B_r = C_r C^{-1}$, where $C, C_r \in \mathbb{R}^{m \times m}$ are defined by

$$\begin{aligned} C &:= \mathbb{E}_{G \sim \mu}[\phi(G)\phi(G)^\top], \\ C_r &:= \mathbb{E}_{G \sim \mu}[\phi(r + \gamma G)\phi(G)^\top]. \end{aligned} \quad (7)$$

A derivation is in Appendix B.3 where we also describe the choice of μ. The elements of these matrices are expressible as integrals over the real line, and hence several possibilities are available for (approximate) computation: if μ is finitely-supported, direct summation is possible; in certain cases the integrals may be analytically available, and otherwise numerical integration can be performed. Additionally, for certain feature maps ϕ, the Bellman coefficients B_r have particular structure that can be exploited computationally; see Appendix B.4 for further discussion. The generalisation to handle an infinite $\mathcal{R}$ is presented in Appendix B.5; and detailed properties of B_r are studied in Appendix B.6.

Algorithms. We summarise the two core algorithmic contributions, **sketch dynamic programming** (Sketch-DP) and **sketch temporal-difference learning** (Sketch-TD), that arise from our proposed framework in Algorithm 1. Pausing to take stock, we have proposed an algorithm framework for computing approximations of *lossy* mean embeddings for a wide variety of feature functions ϕ. Further, these algorithms operate directly within the space of mean embeddings.

Selecting feature maps. A natural question is what effect the choice of feature map ϕ has on the performance of the algorithm. There are several competing concerns. First, the richer the map ϕ, the more information about the return distribution can be captured by the corresponding mean embedding. However, in the worst case, the computational costs of our proposed Algorithm 1 scale cubically with m (the dimensionality of ϕ) prior to the iterative updates which then scale quadratically with m. In addition, the accuracy of the algorithm in approximating the mean embeddings of the true return distributions relies on having a low approximation error in Equation (6), which in turn relies on a low regression error in Equation (5) (see Proposition 4.1 below). Selecting an appropriate feature map is therefore somewhat nuanced, and involves trading off a variety of computational and approximation concerns.

A collection of feature maps that offer the potential for trade-offs along the dimensions above is the translation family

$$\phi_i(z) := \kappa(s(z - z_i)), \quad \forall i \in \{1, \cdots, m\}, \quad (8)$$

where $\kappa : \mathbb{R} \to \mathbb{R}$ is a *base feature function*, $s \in \mathbb{R}^+$ is the *slope*, and the set $\{z_1, \ldots, z_m\} \subseteq \mathbb{R}$ is the *anchors* of the feature map. We will often take κ to be commonly used bounded and smooth nonlinear functions, such as the Gaussian or the sigmoid functions, and spread the anchor points uniformly over the return range. We emphasise that the choice of feature maps for the Bellman sketch framework is flexible; see Appendix B.7 for other possible choices.

Remark 3.1 (Invariance). Given the m-dimensional function space obtained from the span of the coordinate functions $\phi_1, \ldots, \phi_m$, the algorithms above are essentially independent of the choice of basis for this space. For any invertible matrix $M \in \mathbb{R}^{m \times m}$, replacing ϕ by $M^{-1}\phi$, and *also* $\| \cdot \|_2$

by $|| \cdot ||_{M^\top M}$ in Equation (5) gives an equivalent algorithm. See Appendix B.8 for formal results.

Remark 3.2 (The need for *linear* regression). It is tempting to try and obtain a more general framework by allowing *non-linear* regression of $\phi(r + \gamma g)$ on $\phi(g)$ in Equation (5), to obtain a more accurate fit, for example fitting a function $H : \mathbb{R} \times \mathbb{R}^m \to \mathbb{R}^m$ so that $\phi(r + \gamma g) \approx H(r, \phi(g))$. The issue is that if H is not linear in the second argument, then generally $\mathbb{E}[H(r, \phi(G(X')))] \neq H(r, \mathbb{E}[\phi(G(X'))])$, and so step (c) in Equation (6) is not valid. However, there may be settings where it is desirable to *learn* such a function H, to avoid online computation of Bellman coefficients every time a new reward value is encountered in TD learning.

Remark 3.3 (Linear update). The sketch updates in Equations (Sketch-DP) and (Sketch-TD) are linearly, which is distinct from typical particle-based distributional RL algorithms (e.g. (Dabney et al., 2018b;a; Nguyen-Tang et al., 2021), where the updates involve non-linear operations. In particular, Nguyen-Tang et al. (2021) proposed a TD algorithm for updating particle locations by decreasing a sample MMD objective (Gretton et al., 2012). However, this does not yield a dynamic programming algorithm, and Nguyen-Tang et al. (2021) do not analyse the TD algorithm; further comparisons are more clearly described in Appendix B.9.

Remark 3.4 (Multidimensional rewards). Since the sketch algorithms operate fully in the mean embedding space, they generalise to multidimensional or source-dependent reward settings (Van Seijen et al., 2017; Lin et al., 2020; Zhang et al., 2021) by using a ϕ that takes vector-valued inputs.

3.2. Sketch-DP at Work

To give more intuition for the Bellman sketch framework, we provide a walk-through of using Algorithm 1 to estimate the return distributions for the environment in Figure 2A. We take a sinusoidal feature map ϕ that consists of $m = 13$ harmonics over the range $[-4.5, 4.5]$ (see Appendix D.2 for an example using feature map of the form Equation (8)). The Bellman regression problem in Equation (5) is set with $\mu =$ Uniform($[-4, 4]$), based on the typical returns observed in the environment. We then run the Sketch-DP algorithm with the initial estimates $U(x)$ set to $\phi(0)$ for all $x \in \mathcal{X}$.

To visualise how the estimated mean embeddings evolve over iterations, we project them onto their first two principal components in Figure 2C. To approximate the ground truth return distributions, we collected a large number of Monte Carlo samples from the MRP as (Figure 2D); see Appendix C.1 for details. We then estimate the ground-truth mean embeddings and project them on to the principal subspace in Figure 2C as crosses. The Sketch-DP estimates converge to close proximity of the ground-truth. The distinctive update pattern stems from the fact that all paths between rewarding states have length 3. The mean embedding of

state 2 is closer to state 4 due to more frequent transitions from state 2 to 4.

To aid interpretation of these results, we also include a comparison in which we "decode" the mean embeddings at selected iterations back into probability distributions (via an imputation strategy (Rowland et al., 2019)), and compare with the ground-truth return distributions projected (in Cramér distance) onto the anchor locations of the features (Rowland et al., 2018, Proposition 1), as shown in Figure 2D. Full details of the imputation strategy are in Appendix B.1. These decoded distributions are shown in Figure 2E. Initially, the imputed distributions of the Sketch-DP mean embedding estimates reflect the initialisation to the mean embedding of δ_0. As more iterations of Sketch-DP are applied, the imputed distributions of the evolving mean embedding estimates become close to the projected ground-truth. This indicates that, in this example, not only does Sketch-DP compute accurate mean embeddings of the return, but that this embedding is rich enough to recover a lot of information regarding the return distributions themselves.

Concluding the introduction of the Sketch-DP algorithmic framework, there are several natural questions that arise. Can we quantify how accurately Sketch-DP algorithms can approximate mean embeddings of return distributions? What effects do choices such as the feature map ϕ have on the algorithms in practice? The next sections are devoted to answering these questions in turn.

4. Convergence Analysis

We analyse the Sketch-DP procedure described in Algorithm 1, with a novel error analysis approach that can be mathematically described in the following succinct manner. We let $U_0 : \mathcal{X} \to \mathbb{R}^m$ denote the initial mean embedding estimates, and then note from Algorithm 1 that the collection of estimates after each DP update form a sequence $(U_k)_{k=0}^\infty$, with $U_{k+1} = \mathcal{T}_\phi^\pi U_k$. Our convergence analysis therefore focuses on the asymptotic behaviour of this sequence. We introduce the notation $\Phi : \mathscr{P}(\mathbb{R}) \to \mathbb{R}^m$ for the sketch associated with the feature function ϕ, so that $\Phi\mu = \mathbb{E}_{Z \sim \mu}[\phi(Z)]$, and define Φ for return-distribution functions (RDFs) by specifying for $\eta \in \mathscr{P}(\mathbb{R})^\mathcal{X}$ that $(\Phi\eta)(x) = \Phi(\eta(x))$. Ideally, we would like these iterates to approach $U^\pi : \mathcal{X} \to \mathbb{R}^m$, the mean embeddings of the true return distributions, given by $U^\pi(x) = \mathbb{E}_x^\pi[\phi(\sum_{t=0}^\infty \gamma^t R_t)]$. As already described, typically this is not possible when the sketch Φ is not Bellman closed, and so we can only expect to approximate U^π. Mathematically, this is because in general $\Phi\mathcal{T}^\pi \neq \mathcal{T}_\phi^\pi \Phi$ when ϕ is not Bellman closed.

The first step is to bound the error incurred in a single step of dynamic programming due to using $\mathcal{T}_\phi^\pi$ directly on the mean embeddings, rather taking mean embeddings after applying
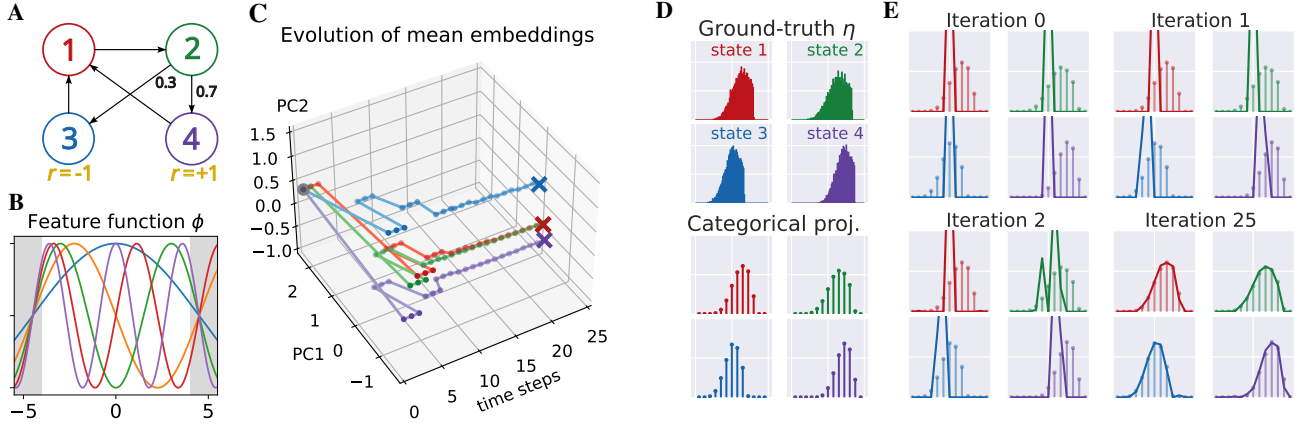
Figure 2. An example run of Sketch-DP. **A**, The MRP considered here. **B**, The first 5 of $m = 13$ sinusoidal feature functions ϕ. The regression Equation (5) is performed under a densely spaced grid over the white region $[-4, 4]$. **C**, Evolution of the estimated mean embeddings from initialisation (grey dot) onto the first two principal components. Crosses represent the ground-truth mean embeddings. **D**, Ground-truth return distributions (estimated by Monte-Carlo) and their categorical projections onto a regular grid. **E**, Imputed distributions from the mean embeddings onto the same grid for selected iterations (curves), compared against the categorical projections (stems).
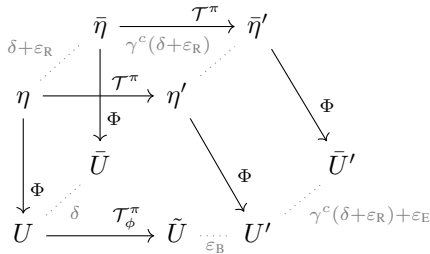

Figure 3. The objects and structure used to analyse the Sketch-DP.

the true distributional Bellman operator to the underlying distributions; this corresponds to the foreground of Figure 3.

Proposition 4.1. *(Regression error to Bellman approximation.) Let $\|\cdot\|$ be a norm on $\mathbb{R}^m$. Then for any RDF $\eta \in \mathscr{P}([G_{min}, G_{max}])^{\mathcal{X}}$, we have*

$$\max_{x \in \mathcal{X}} \|\Phi(\mathcal{T}^\pi \eta)(x) - (\mathcal{T}_\phi^\pi \Phi \eta)(x)\| \quad (9)$$

$$\leq \sup_{g \in [G_{min}, G_{max}]} \max_{r \in \mathcal{R}} \|\phi(r + \gamma g) - B_r \phi(g)\|.$$

The second step of the analysis is to chain together the errors that are incurred at each step of dynamic programming, so as to obtain a bound on the asymptotic distance of the sequence $(U_k)_{k=0}^\infty$ from U^π, motivated by error propagation analysis in the case of function approximation (Bertsekas & Tsitsiklis (1996); Munos (2003); see also Wu et al. (2023) in the distributional setting). The next proposition provides the technical tools required for this; the notation is chosen to match the illustration in Figure 3.

Proposition 4.2. *(Error propagation.) Consider a norm $\|\cdot\|$ on $\mathbb{R}^m$, and let $\|\cdot\|_\infty$ be the norm on $(\mathbb{R}^m)^{\mathcal{X}}$ defined by $\|U\|_\infty = \max_{x \in \mathcal{X}} \|U(x)\|$. Let d be a metric on RDFs such that $\mathcal{T}^\pi$ is a γ^c-contraction with respect to d (such as the supremum-Wasserstein and the supremum-Cramer distances). Suppose the following bounds hold.*

- *(Bellman approximation bound.) For any $\eta \in \mathscr{P}([G_{min}, G_{max}])^{\mathcal{X}}$,*

$$\max_{x \in \mathcal{X}} \|\Phi(\mathcal{T}^\pi \eta)(x) - (\mathcal{T}_\phi^\pi \Phi \eta)(x)\| \leq \varepsilon_B.$$

- *(Reconstruction error bound.) For any $\eta, \bar{\eta} \in \mathscr{P}([G_{min}, G_{max}])^{\mathcal{X}}$ with sketches $U, \bar{U}$, we have $d(\eta, \bar{\eta}) \leq \|U - \bar{U}\|_\infty + \varepsilon_R$.*

- *(Embedding error bound.) For any $\eta', \bar{\eta}' \in \mathscr{P}([G_{min}, G_{max}])^{\mathcal{X}}$ with sketches $U', \bar{U}'$, we have $\|U' - \bar{U}'\|_\infty \leq d(\eta', \bar{\eta}') + \varepsilon_E.$*

Then for any two return-distribution functions $\eta, \bar{\eta} \in \mathscr{P}([G_{min}, G_{max}])^{\mathcal{X}}$ with sketches $U, \bar{U}$ satisfying $\|U - \bar{U}\| \leq \delta$, we have

$$\|\Phi \mathcal{T}^\pi \eta - \mathcal{T}_\phi^\pi \bar{U}\|_\infty \leq \gamma^c(\delta + \varepsilon_R) + \varepsilon_R + \varepsilon_E.$$

A formal proof is given in Appendix A; Figure 3 (bottom) shows the intuition, propagating bounds through different intermediate stages of the analysis of the update. The main error bound result combines the two earlier results.

Proposition 4.3. *Suppose the assumptions of Proposition 4.2 hold, that $\mathcal{T}^\pi$ maps $\mathscr{P}([G_{min}, G_{max}])^{\mathcal{X}}$ to itself, and suppose $\mathcal{T}_\phi^\pi$ maps $\{\Phi\nu : \nu \in \mathscr{P}([G_{min}, G_{max}])^{\mathcal{X}}\}$ to itself. Then for a sequence of sketches $(U_k)_{k=0}^\infty$ defined iteratively via $U_{k+1} = \mathcal{T}_\phi^\pi U_k$, we have*

$$\limsup_{k \to \infty} \|U_k - U^\pi\| \leq \frac{1}{1 - \gamma^c}(\gamma^c \varepsilon_R + \varepsilon_B + \varepsilon_E).$$

Proof. For each U_k, let η_k be an RDF with the property $\Phi\eta_k = U_k$. Applying Proposition 4.2 to sketches U^π and U_k, we obtain $\|U_{k+1} - U^\pi\|_\infty \leq \gamma^c \|U_k - U^\pi\|_\infty + \gamma^c \varepsilon_R + \varepsilon_B + \varepsilon_E$. Taking a limsup on both sides over k and rearranging yields the result. $\square$

6

4.1. Concrete Example

The analysis presented above is abstract; it provides a generic template for conducting error propagation analysis to show that Sketch-DP converges to a neighbourhood of the true values, and moreover illustrates the dependence of this error on the "richness" of the sketch, and accuracy of the Bellman coefficients. To apply this abstract result to a concrete algorithm, we are required to establish the three error bounds that appear in the statement of Proposition 4.2. The result below shows how this can lead to a concrete result for a novel class of sketches; in particular, proving that computed mean embeddings under these features become arbitrarily accurate as the number of features increases.

Proposition 4.4. *Consider a sketch ϕ whose coordinates are feature functions of the form $\phi_i(z) = \mathbb{1}\{z_1 \leq z < z_{i+1}\}$ $(i = 1, \ldots, m - 1)$, and $\phi_m(z) = \mathbb{1}\{z_1 \leq z \leq z_{m+1}\}$, where $z_1, \ldots, z_{m+1}$ is an equally-spaced grid over $[G_{min}, G_{max}]$, with $G_{min} = \min \mathcal{R}/(1 - \gamma)$, $G_{max} = \max \mathcal{R}/(1 - \gamma)$. Let $\mathcal{T}_\phi^\pi$ be the corresponding Sketch-DP operator given by solving Equation (5) with $\mu = Unif([G_{min}, G_{max}])$, and define a sequence $(U_k)_{k=0}^\infty$ by taking $U_0(x)$ to be the sketch of some initial distribution in $\mathscr{P}([G_{min}, G_{max}])$, and $U_{k+1} = \mathcal{T}_\phi^\pi U_k$ for all $k \geq 0$. Let $U^\pi \in (\mathbb{R}^m)^{\mathcal{X}}$ be the mean embeddings of the true return distributions. Finally, let $\|\cdot\|$ be the norm on $\mathbb{R}^m$ defined by $\|u\| = \frac{G_{max}-G_{min}}{m} \sum_{i=1}^m |u_i|$. Then we have*

$$\limsup_{k \to \infty} \|U_k - U^\pi\|_\infty \leq \frac{(G_{max} - G_{min})(3 + 2\gamma)}{(1 - \gamma)m}.$$

5. Experiments

We first test quality of return distribution predictions by the sketch algorithms, investigating the effects of three key factors in Equation (8): the base feature κ, the number of features m, and the slope s, using three tabular MRPs (details in Appendix C.1, extended results in Appendix D.3). In **Random chain**, the transitions are random, and the rewards are deterministic; in **Directed chain** (DC), both transitions and rewards are deterministic; and in **DC+Gaussian R**, the transitions are deterministic and the rewards are Gaussian. We compare the mean embeddings estimated by Sketch-DP with ground-truth mean embeddings, reporting their squared L^2 distance (**mean embedding squared error**), and also compare the **Cramér distance** $\max_{x \in \mathcal{X}} \ell_2^2(\hat{\eta}(x), \eta^\pi(x))$ (see e.g. Rowland et al. (2018)) between the distribution $\hat{\eta}(x)$ imputed from the Sketch-DP estimate against the ground-truth $\eta^\pi(x)$ (grey dotted line). To aid interpretation of the Cramér distance results, we also report the Cramér distance between the ground truth $\eta^\pi(x)$ and two baselines. First, the Dirac delta $\delta_{V^\pi(X)}$ at the mean return; we expect Sketch-DP to outperform this naïve baseline by better capturing properties of the return distribution beyond the mean.

Second, the return distribution estimate computed by categorical DP (Rowland et al., 2018; Bellemare et al., 2023), a well-understood approach to distrbutional RL based on categorical distributions.

The results for sweeps over feature count m and slope s are shown in Figure 4. By sweeping over m, we see that the estimated mean embedding goes towards the ground-truth as we use more features. This is consistent with our intuition that more features should improve the estimates. Further, the Cramér distance also decreases as m increases, suggesting that the distribution represented also approaches the ground-truth. To highlight differences between various Sketch-DP algorithms, we also compute the **excess Cramér distance**: the Cramér distance as above, minus the corresponding distance between the categorical (Carmér) projection of η^π and η^π itself; the latter gives the theoretical lower bound achievable by any distribution on a given finite support. All distributional methods perform well on these tasks, and significantly outperform the Dirac estimator in stochastic environments; we note that all methods have tunable hyperparameters (bin locations for CDRL, feature parameters for Sketch-DP), which should inform direct comparison between methods. We see that the sketch algorithm, in combination with the imputation strategy described in Appendix B.1, can give lower Cramér distances than the CDRL algorithm, especially when using the sigmoidal or Gaussian base features. The results of the sweep on the slope parameter s show different trends depending on the metric. For smoother ϕ, generally we can obtain smaller error on the mean embeddings, but the Cramér distances are only small for intermediate range of slope values. This result is expected: when the features are too smooth or too sharp, there exists regions within the return range where the feature values do not vary meaningfully. This results in a more lossy encoding of the return distribution, indicating the importance of tuning the slope parameter of the translation family (Equation (8)).

We include additional experiments in Appendix D.4 showing that Sketch-DP outperforms and is substantially faster in wallclock run-time than SFDP based on imputation strategies (Rowland et al., 2019; Bellemare et al., 2023). The faster speed of Sketch-DP is because its updates involve simple linear-algebraic operations, as opposed to the more involved DP update, using imputation strategies, in SFDP.

5.1. Deep Reinforcement Learning

The primary motivation of our work has been to develop principled novel approaches to distributional RL based on mean embeddings. Here, we also verify that the Bellman sketch framework is robust enough to apply in combination with deep reinforcement learning. We train neural-network predictions $U_\theta(x, a)$ of mean embeddings for each
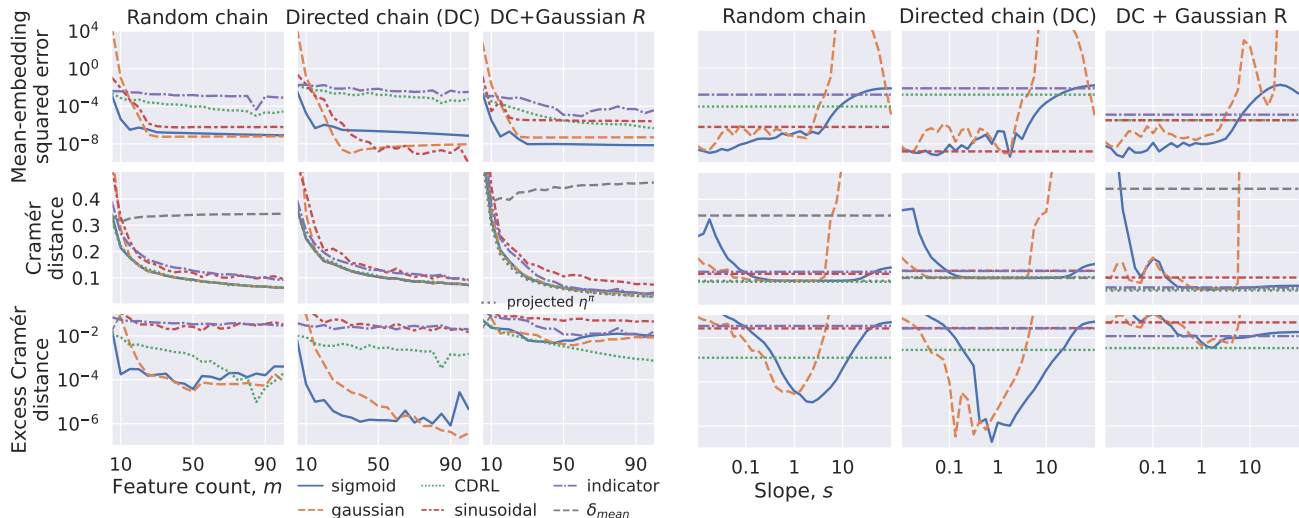
Figure 4. Results of running Sketch-DP (Algorithm 1) on tabular environments. First row shows the squared L^2 distance between ground-truth mean embeddings to the Sketch-DP estimates. The grey dotted line in the second row is the Cramér distance between the ground-truth η^π and its categorical projection. The third row shows the difference between the Cramér distance and the projected η^π.
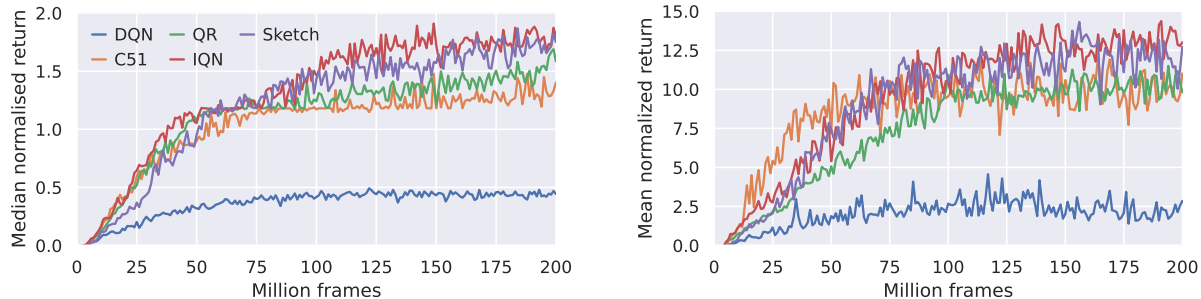

Figure 5. Median (left) and mean (right) human-normalised scores on the Atari 57 suite.

state-action pair (x, a). To be able to define greedy policy improvements based on estimated mean embeddings, we precompute *value-readout coefficients* $\beta \in \mathbb{R}^m$ by solving

$$\min_\beta \mathbb{E}_{G \sim \mu}[(G - \langle \beta, \phi(G) \rangle)^2],$$

so that we can approximate the expected returns from the mean embedding estimates as $\langle \beta, U_\theta(x, a) \rangle$ by linearity of expectation. This allows us to define a Q-learning-style update rule: given a transition (x, a, r, x'), first compute $a' = \arg\max_{\tilde{a}} \langle \beta, U_{\bar{\theta}}(x', \tilde{a}) \rangle$, and then the gradient: $\nabla_\theta \|U_\theta(x, a) - B_r U_{\bar{\theta}}(x', a')\|_2^2$, where $\bar{\theta}$ are the target network parameters. In our experiments, we parametrise U_θ according to the architecture of QR-DQN (Dabney et al., 2018b), so that the m outputs of the network predict the values of the m coordinates of the corresponding mean embedding. We use the sigmoid function as the base feature κ. Full experimental details for replication are in Appendix C.2; further results are in Appendix D.5.

Figure 5 shows the mean and median human-normalised performance on the Atari suite of environments (Bellemare et al., 2013) across 200M training frames, and includes comparisons against DQN (Mnih et al., 2015), as well

as the distributional agents C51 (Bellemare et al., 2017), QR-DQN (Dabney et al., 2018b), and IQN (Dabney et al., 2018a). Sketch-DQN attains higher performance on both metrics relative to the comparator agents C51 and QR-DQN, and approaches the performance of IQN, which uses a more complex prediction network to make non-parametric predictions of the quantile function of the return. In addition, Sketch-DQN runs faster than QR-DQN and IQN; see Appendix D.6. These results indicate that the sketch framework can be reliably applied to deep RL, and we believe further investigation of the combination of this framework and deep RL agents is a promising direction for future work. Code is available at https://github.com/google-deepmind/sketch_dqn.

6. Related Work

Typical approaches to distributional RL focus on learning approximate distributions of the true return distributions (see, e.g., Bellemare et al. (2017); Dabney et al. (2018b); Yang et al. (2019); Nguyen-Tang et al. (2021); Wu et al. (2023)). Much prior work has considered statistical functionals of the

random return, at varying levels of generality with regard to the underlying Markov decision process model. See for example Mandl (1971); Farahmand (2019) for work on characteristic functions, Chung & Sobel (1987) for the Laplace transform, Tamar et al. (2013; 2016) for variance, and Sobel (1982) for higher moments.

Our use of finite-dimensional mean embeddings is inspired by distributed distributional codes (DDCs) from theoretical neuroscience (Sahani & Dayan, 2003; Vértes & Sahani, 2018; Wenliang & Sahani, 2019), which can be regarded as neural activities encoding return distributions. DDCs were previously used to model transition dynamics and successor features in partially observable MDPs (Vértes & Sahani, 2019). Tano et al. (2020) consider applying non-linearities to rewards themselves, rather than the return, and learning with a variety of discount factors, to encode the distribution of rewards at each timestep. In addition, Tano et al. (2020) showed that learning with a variety of discount factors encode the distribution of rewards at each timestep, complementary to modelling return distributions. Tano et al. (2020) were also motivated by a biologically plausible mechanism for distributional reinforcement learning in the brain (i.e. not requiring the non-local optimisation in the imputation strategies described by Rowland et al. (2019)). The approach proposed here is also biologically plausible, as all computations for value estimation are linear and can be easily implemented with neuronal circuits, and there may be value in further investigation of the consequences of our framework for dopamine modelling in the brain.

The sketches in this paper are in fact mean embeddings into finite-dimensional reproducing kernel Hilbert spaces (RKHSs; the kernel corresponding to the feature function ϕ is $K(z, z') = \langle \phi(z), \phi(z') \rangle$). Kernel mean embeddings have been used in RL for representing state-transition distributions (Grünewälder et al., 2012; Boots et al., 2013; Lever et al., 2016; Chowdhury & Oliveira, 2023), and maximum mean discrepancies (MMDs) (Gretton et al., 2012) have been used to define losses in distributional RL by Nguyen-Tang et al. (2021). Nguyen-Tang et al. (2021) combine an MMD loss and distributional bootstrapping to define an incremental learning algorithm, but it does not naturally lead to a DP formulation, and its convergence is not analysed. In contrast, our sketch framework not only generalises their approach to define both DP and TD algorithms but also allows rigorous analysis of DP convergence as presented in Section 4. We elaborate the comparisons to MMDRL and a few other distributional RL methods in Appendix B.9. Similar to their work, our method generalises to multidimensional or source-dependent reward settings (Van Seijen et al., 2017; Lin et al., 2020; Zhang et al., 2021), as discussed in Remark 3.4.

7. Conclusion

We have proposed a framework for distributional RL based on Bellman updates that take place entirely within the sketch domain. This has yielded new dynamic programming and temporal-difference learning algorithms and a novel error propagation analysis. We have provided empirical validation on a suite of tabular MRPs and demonstrated that the approach can be successfully applied as a variant of the DQN. While convergence analysis for general sketches and mean embedding feature functions is an immediate future work, we expect that there will be benefits from further exploration of algorithmic possibilities opened up by this framework, and potential consequences for modelling value representations in the brain.

Acknowledgments

Impact Statement

This paper presents work whose goal is to advance the field of Machine Learning. There are many potential societal consequences of our work, none which we feel must be specifically highlighted here.

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Distributional Bellman Operators over Mean Embeddings:
Supplementary Material

A. Proofs

Proposition 4.1. *(**Regression error to Bellman approximation.**) Let $\| \cdot \|$ be a norm on $\mathbb{R}^m$. Then for any RDF $\eta \in \mathscr{P}([G_{min}, G_{max}])^{\mathcal{X}}$, we have*

$$\max_{x \in \mathcal{X}} \| \Phi(\mathcal{T}^\pi \eta)(x) - (\mathcal{T}^\pi_\phi \Phi \eta)(x) \| \tag{9}$$
$$\leq \sup_{g \in [G_{min}, G_{max}]} \max_{r \in \mathcal{R}} \| \phi(r + \gamma g) - B_r \phi(g) \| .$$

Proof. Let $(G(x) : x \in \mathcal{X})$ be an instantiation of η (Bellemare et al., 2023); that is, a collection of random variables such that for each $x \in \mathcal{X}$, we have $G(x) \sim \eta(x)$. First, note that the distribution $(\mathcal{T}^\pi \eta)(x)$ is exactly the distribution of $R + \gamma G(X')$ (when the transition begins at x and is generated by π). So we have

$$\Phi(\mathcal{T}^\pi \eta)(x) = \mathbb{E}_{Z \sim (\mathcal{T}^\pi \eta)(x)}[\phi(Z)] = \mathbb{E}^\pi_x[\phi(R + \gamma G(X'))] .$$

It then follows that:

$$\max_{x \in \mathcal{X}} \| \Phi(\mathcal{T}^\pi \eta)(x) - (\mathcal{T}^\pi_\phi \Phi \eta)(x) \| = \max_{x \in \mathcal{X}} \left\| \mathbb{E}^\pi_x \left[\phi(R + \gamma G(X')) \right] - \mathbb{E}^\pi_x \left[B_R \mathbb{E}[\phi(G(X'))|X'] \right] \right\|$$
$$= \max_{x \in \mathcal{X}} \left\| \mathbb{E}^\pi_x \left[\phi(R + \gamma G(X')) - B_R \phi(G(X')) \right] \right\|$$
$$\leq \max_{x \in \mathcal{X}} \mathbb{E}^\pi_x \left[\left\| \phi(R + \gamma G(X')) - B_R \phi(G(X')) \right\| \right]$$
$$\leq \max_{g \in [G_{min}, G_{max}]} \max_{r \in \mathcal{R}} \| \phi(r + \gamma g) - B_r \phi(g) \| ,$$

as required. $\qquad \square$

Proposition 4.2. *(**Error propagation.**) Consider a norm $\| \cdot \|$ on $\mathbb{R}^m$, and let $\| \cdot \|_\infty$ be the norm on $(\mathbb{R}^m)^{\mathcal{X}}$ defined by $\|U\|_\infty = \max_{x \in \mathcal{X}} \|U(x)\|$. Let d be a metric on RDFs such that $\mathcal{T}^\pi$ is a γ^c-contraction with respect to d (such as the supremum-Wasserstein and the supremum-Cramér distances). Suppose the following bounds hold.*

- *(Bellman approximation bound.) For any $\eta \in \mathscr{P}([G_{min}, G_{max}])^{\mathcal{X}}$,*

$$\max_{x \in \mathcal{X}} \| \Phi(\mathcal{T}^\pi \eta)(x) - (\mathcal{T}^\pi_\phi \Phi \eta)(x) \| \leq \varepsilon_B .$$

- *(Reconstruction error bound.) For any $\eta, \bar{\eta} \in \mathscr{P}([G_{min}, G_{max}])^{\mathcal{X}}$ with sketches $U, \bar{U}$, we have $d(\eta, \bar{\eta}) \leq \|U - \bar{U}\|_\infty + \varepsilon_R$.*

- *(Embedding error bound.) For any $\eta', \bar{\eta}' \in \mathscr{P}([G_{min}, G_{max}])^{\mathcal{X}}$ with sketches $U', \bar{U}'$, we have $\|U' - \bar{U}'\|_\infty \leq d(\eta', \bar{\eta}') + \varepsilon_E$.*

Then for any two return-distribution functions $\eta, \bar{\eta} \in \mathscr{P}([G_{min}, G_{max}])^{\mathcal{X}}$ with sketches $U, \bar{U}$ satisfying $\|U - \bar{U}\| \leq \delta$, we have

$$\| \Phi \mathcal{T}^\pi \eta - \mathcal{T}^\pi_\phi \bar{U} \|_\infty \leq \gamma^c (\delta + \varepsilon_R) + \varepsilon_R + \varepsilon_E .$$

Proof. We follow the illustration laid out in Figure 3:

$$\|\mathcal{T}_\phi^\pi U - \Phi\mathcal{T}^\pi\bar\eta\|_\infty \overset{(a)}{\leq} \|\mathcal{T}_\phi^\pi U - \Phi\mathcal{T}^\pi\eta\|_\infty + \|\Phi\mathcal{T}^\pi\eta - \Phi\mathcal{T}^\pi\bar\eta\|_\infty$$

$$\overset{(b)}{\leq} \varepsilon_\mathrm{B} + \|\Phi\mathcal{T}^\pi\eta - \Phi\mathcal{T}^\pi\bar\eta\|_\infty$$

$$\overset{(c)}{\leq} \varepsilon_\mathrm{B} + d(\mathcal{T}^\pi\eta, \mathcal{T}^\pi\bar\eta) + \varepsilon_\mathrm{E}$$

$$\overset{(d)}{\leq} \varepsilon_\mathrm{B} + \gamma^c d(\eta, \bar\eta) + \varepsilon_\mathrm{E}$$

$$\overset{(e)}{\leq} \varepsilon_\mathrm{B} + \gamma^c(\delta + \varepsilon_\mathrm{R}) + \varepsilon_\mathrm{E},$$

as required, where (a) follows from the triangle inequality, (b) follows from the Bellman approximation bound, (c) follows from the embedding error bound, (d) follows from γ^c-contractivity of $\mathcal{T}^\pi$ with respect to d, and (e) follows from the reconstruction error bound. □

Proposition 4.4. *Consider a sketch ϕ whose coordinates are feature functions of the form $\phi_i(z) = \mathbb{1}\{z_1 \leq z < z_{i+1}\}$ ($i = 1, \ldots, m-1$), and $\phi_m(z) = \mathbb{1}\{z_1 \leq z \leq z_{m+1}\}$, where $z_1, \ldots, z_{m+1}$ is an equally-spaced grid over $[G_{min}, G_{max}]$, with $G_{min} = \min \mathcal{R}/(1-\gamma)$, $G_{max} = \max \mathcal{R}/(1-\gamma)$. Let $\mathcal{T}_\phi^\pi$ be the corresponding Sketch-DP operator given by solving Equation (5) with $\mu = \mathrm{Unif}([G_{min}, G_{max}])$, and define a sequence $(U_k)_{k=0}^\infty$ by taking $U_0(x)$ to be the sketch of some initial distribution in $\mathscr{P}([G_{min}, G_{max}])$, and $U_{k+1} = \mathcal{T}_\phi^\pi U_k$ for all $k \geq 0$. Let $U^\pi \in (\mathbb{R}^m)^\mathcal{X}$ be the mean embeddings of the true return distributions. Finally, let $\|\cdot\|$ be the norm on $\mathbb{R}^m$ defined by $\|u\| = \frac{G_{max}-G_{min}}{m}\sum_{i=1}^m |u_i|$. Then we have*

$$\limsup_{k\to\infty} \|U_k - U^\pi\|_\infty \leq \frac{(G_{max} - G_{min})(3 + 2\gamma)}{(1-\gamma)m}.$$

Proof. We begin by obtaining reconstruction and embedding error bounds for this sketch. We introduce the shorthand $\Delta = (G_{\max} - G_{\min})/m$. To obtain a reconstruction error bound, for any distribution $\nu \in \mathscr{P}([z_1, z_{m+1}])$, define $\Pi\nu$ to be the distribution obtained by mapping each point of support z of ν to the greatest z_i less than or equal to z. Mathematically, if we define $f(z) = \max\{z_i : z_i \leq z\}$, then $\Pi\nu = f_\#\nu$, i.e. $\Pi\nu$ is the pushforward of ν through f. We then have $w_1(\nu, \Pi\nu) \leq \Delta$ for all ν supported on $[z_1, z_m]$, where w_1 is the 1-Wasserstein distance, since f transports mass by at most Δ. Introducing another distribution ν' and the projection $\Pi\nu'$, we note that $w_1(\Pi\nu, \Pi\nu') = \|\Phi\nu - \Phi\nu'\|$. Combining these observations with the triangle inequality yields

$$w_1(\nu, \nu') \leq w_1(\nu, \Pi\nu) + \|\Phi\nu - \Phi\nu'\| + w_1(\nu', \Pi\nu') \leq \|\Phi\nu - \Phi\nu'\| + 2\Delta,$$

which gives the required form of reconstruction bound, with $\varepsilon_\mathrm{R} = 2\Delta$, for the supremum-Wasserstein distance $\overline{w}_1(\eta, \eta') = \max_{x\in\mathcal{X}} w_1(\eta(x), \eta'(x))$ defined over RDFs $\eta, \eta' \in \mathscr{P}(\mathbb{R})^\mathcal{X}$. We can also essentially reverse the argument to get

$$\|\Phi\nu - \Phi\nu'\| = w_1(\Pi\nu, \Pi\nu') \leq w_1(\Pi\nu, \nu) + w_1(\nu, \nu') + w_1(\nu', \Pi\nu') \leq w_1(\nu, \nu') + 2\Delta$$

which gives the required form of the embedding error bound, with $\varepsilon_\mathrm{E} = 2\Delta$.

Additionally, we can analyse the worst-case regression error $\|\phi(r + \gamma g) - B_r\phi(g)\|$ to get a bound on the Bellman approximation ε_B, by Proposition 4.1. Observe that $\phi(g)$ is constant for $g \in [z_i, z_{i+1})$, and equal to

$$(\underbrace{1, \ldots, 1}_{i \text{ times}}, 0, \ldots, 0)^\top.$$

The minimum regression error in

$$\mathbb{E}_{G\sim\mathrm{Unif}([z_1, z_m])}[\|\phi(r + \gamma G) - B_r\phi(G)\|] \tag{10}$$

is therefore obtained by setting the ith column of B_r so that

$$B_r\phi(z_i) = \mathbb{E}_{G\sim\mathrm{Unif}([z_i, z_{i+1}))}[\phi(r + \gamma G)];$$

14

note the support of the distribution in the line above. Since $r + \gamma G$ in this expectation varies over an interval of width $\gamma\Delta$, the integrand $\phi(r + \gamma G)$ takes on at most two distinct values. It then follows that we can bound the minimum regression error in Equation (10) by Δ, and hence we can take $\varepsilon_B = \Delta$.

Finally, we observe that $\mathcal{T}^\pi$ maps $\mathscr{P}([G_{\min}, G_{\max}])$ to itself, since for any $g \in [G_{\min}, G_{\max}]$ and any $r \in \mathcal{R}$, we have by construction of $G_{\min}$, $G_{\max}$ that $r + \gamma g \in [G_{\min}, G_{\max}]$. In addition, we have $\{\Phi\nu : \nu \in \mathscr{P}([G_{\min}, G_{\max}]\} = \{u \in \mathbb{R}^m : 0 \leq u_1 \leq \cdots \leq u_{m-1} \leq u_m = 1\}$, and by the inspection of the columns of B_r above, it follows that $\mathcal{T}^\pi_\phi$ maps $\{\Phi\nu : \nu \in \mathscr{P}([G_{\min}, G_{\max}]\}^{\mathcal{X}}$ to itself. Therefore the conclusion of Proposition 4.3 holds, and we obtain

$$\limsup_{k\to\infty} \|U_k - U^\pi\|_\infty \leq \frac{1}{1-\gamma}(\gamma\varepsilon_R + \varepsilon_B + \varepsilon_E)$$
$$\leq \frac{1}{1-\gamma}(\gamma 2\Delta + \Delta + 2\Delta)$$
$$= \frac{\Delta(3 + 2\gamma)}{1-\gamma}$$
$$= \frac{(G_{\max} - G_{\min})(3 + 2\gamma)}{(1-\gamma)m}$$

as required. $\square$

B. Further details and extensions

In this section, we collect further details on a number of topics raised in the main paper.

B.1. Categorical imputation

In the tabular experiments in Sections 3.2 and 5, we include comparisons of distributions imputed from the learned mean embeddings, to provide an interpretable comparison between the different Sketch-DP methods studied. Here, we provide a detailed description of the imputation method.

For a given feature map ϕ, and a learned mean embedding u, the goal is to define an imputation strategy $\iota : \mathbb{R}^m \to \mathscr{P}(\mathbb{R})$ (Rowland et al., 2019; Bellemare et al., 2023); that is, a function with the property $\mathbb{E}_{Z\sim\iota(u)}[\phi(Z)] \approx u$, so that ι serves as an approximate pseudo-inverse to the mean embedding. Here, we follow the approach of Song et al. (2008), and impute probability distributions supported on a finite support set $\{z_1, \ldots, z_n\}$. We define $\iota(s)$ implicitly through the following (convex) quadratic program

$$\arg\min_{p\in\Delta_n} \left\| \sum_{i=1}^n p_i\phi(z_i) - s \right\|_2^2.$$

Note that the left-hand term inside is the expectation of $\phi(Z)$ with $Z \sim \sum_{i=1}^n p_i\delta_{z_i}$, and so the objective is simply aiming to minimise the squared error between the learned mean embedding and the mean embedding from this discrete distribution. Since this quadratic program is convex, it is solvable efficiently; in our implementations, we use SciPy's MINIMIZE algorithm (Virtanen et al., 2020).

B.2. Alternative condition for Bellman-closedness

In the main paper, we relied on the condition equation (3) to derive the Bellman coefficients. Here we derive a condition slightly different from equation (3) when the rewards are stochastic. We begin by writing the mean embedding of the return in terms of the random variables involved explicitly:

$$U^\pi(x) = \mathbb{E}_{G\sim\eta^\pi_x}[\phi(G)] = \mathbb{E}^\pi_{R,X',G'|x}[\phi(R + \gamma G'(X'))]$$

We can decompose the target by

$$\mathbb{E}^\pi_{X',R,G'|x}[\phi(R + \gamma G'(X'))] = \mathbb{E}^\pi_{X'|x}\mathbb{E}^\pi_{G'|X'}\mathbb{E}^\pi_{R|X',x}[\phi(R + \gamma G'(X'))] \tag{11}$$

where we assumed that G' is independent of the previous state x given the current state X', and the immediate reward R does not depend on G'. Usually, the reward R depends only on x. Suppose now that the last (conditional) mean embedding

is linear in the mean embedding of the return distributions of state x'; that is, there exists a matrix $W_{x',x}$ for each pair of states such that, for all $g \in \mathbb{R}$,

$$\mathbb{E}^\pi_{R|X',x}[\phi(R + \gamma g)] = W_{X',x}\phi(g), \tag{12}$$

then substituting this in equation (11) gives

$$U^\pi(x) = \mathbb{E}^\pi_{X',R,G'|x}[\phi(R + \gamma G'(X'))] = \mathbb{E}^\pi_{X'|X}[W_{X',x}\mathbb{E}^\pi_{G'|X'}[\phi(G'(X'))]] = \mathbb{E}^\pi_x[W_{X',x}U^\pi(X')]$$

Here, the matrix $W_{x',x}$ plays a similar role to B_R in Equation (4), although the former has the random reward marginalised out explicitly. If R is deterministic, then the condition in Equation (12) reduces to Equation (4). If R is stochastic, then Equation (12) may be weaker than Equation (4) as it only needs to hold in expectation over R.

B.3. Computational properties of Bellman coefficients

Under many choices of feature maps ϕ, the matrix B_r has structure that may be exploited computationally. We provide sketches of several cases of interest. For "binning features", even for overlapping bins, B_r is a very narrow band matrix, and hence is sparse, leading to linear-time matrix-vector product computation. This remains approximately true for other forms of localised features, such as low-bandwidth Gaussians and related bump-like functions, and in particular applying truncation to near-zero coefficient in the Bellman coefficients in such cases will also lead to sparse matrices.

Bellman coefficients as least-squares coefficients. The closed-form solution for the Bellman coefficients B_r in Equation (7) can be derived by viewing the optimisation problem in Equation (5) as a vector-valued linear regression problem, and using the usual expression for the optimal prediction coefficients. The derivation is the same in content to the usual derivation of least-squares coefficients, which we provide below for completeness, to illustrate how it is obtained in our case. We begin by differentiating the (quadratic) objective in Equation (7) with respect to B, and setting the resulting expression equal to the zero vector, to obtain

$$-2\mathbb{E}_{G\sim\mu}[\phi(r + \gamma G)\phi(G)^\top] + 2\mathbb{E}_{G\sim\mu}[B_r\phi(G)\phi(G)^\top] = 0.$$

Rearranging, we obtain

$$B_r\mathbb{E}_{G\sim\mu}[\phi(G)\phi(G)^\top] = \mathbb{E}_{G\sim\mu}[\phi(r + \gamma G)\phi(G)^\top].$$

Finally, under the assumption of invertibility of $\mathbb{E}_{G\sim\mu}[\phi(G)\phi(G)^\top]$, we obtain the expression for the Bellman coefficients in Equation (7):

$$B_r = \mathbb{E}_{G\sim\mu}[\phi(r + \gamma G)\phi(G)^\top]\mathbb{E}_{G\sim\mu}[\phi(G)\phi(G)^\top]^{-1}.$$

Online computation of Bellman coefficients in the case of unknown rewards. In settings where the set of possible rewards $\mathcal{R}$ is not known in advance, is infinite, or is too large to cache Bellman coefficients for all possible rewards $r \in \mathcal{R}$, we may exploit the structure of the Bellman coefficients described above to speed up the computation of the coefficients online. Rather than solving the regression problem from scratch, an alternative is to cache the matrix $\mathbb{E}_{G\sim\mu}[\phi(G)\phi(G)^\top]^{-1}$ above, and construct the matrix $\mathbb{E}_{G\sim\mu}[\phi(r + \gamma G)\phi(G)^\top]$ as required, upon observing a new reward r. This reduces the marginal cost of computing the Bellman coefficients B_r to a matrix-matrix product.

B.4. Choices of regression distribution μ

In the main paper, we note that the one-dimensional integrals defining the matrices C and C_r which in turn define the Bellman coefficients B_r can be computed in a variety of ways, depending on the choice of μ and feature map ϕ. In our experiments, we take ν to be a finitely-supported grid in the range $[\hat{G}_{\min} - b\hat{L}, \hat{G}_{\max} + b\hat{L}]$, where b is casually chosen to be around 0.2. The support of ν is thus slightly wider than the estimated return range and slightly narrower than the anchor range described in Section B.7. The intuition for using a wider anchor range is that we need the features to cover the return distribution (and ν) with the non-trivial support of the features. We validate this intuition in an additional experiment in Appendix D.3. With this ν, Equation (5) is a standard regression problem, and C and C_r can be computed with standard linear-algebraic operations.

Another possibility, particularly if one wishes to use μ which is not finitely supported, is to use numerical integration to compute these integrals. Additionally, in certain settings the integrals may be computed analytically. For example, with
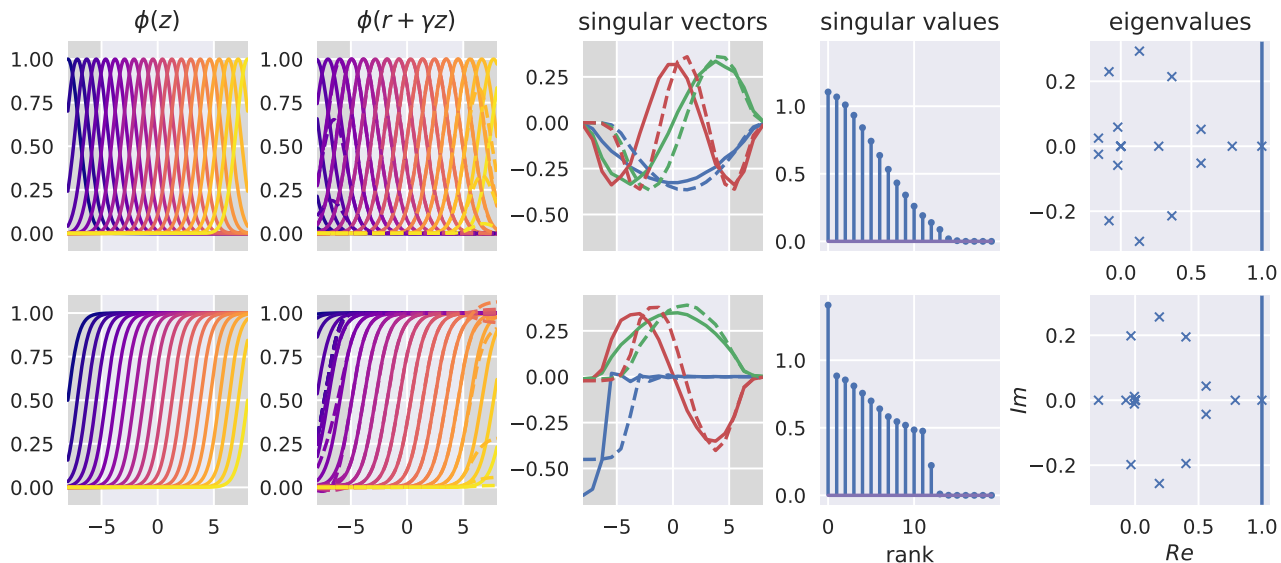
Figure 6. In-depth analysis of Bellman coefficients in the setting described in Section B.6. In the third column, solid curves are the most significant input/right singular vectors, and dashed lines with matching colours are the corresponding output/left singular vectors.

Gaussian $\phi_i(x) = \exp(-s^2(x - z_i)^2/2)$ and Gaussian μ, or μ as Lebesgue measure (in which case, technically, we modify the expectation in Equation (5) into an integral against an unnormalised measure), C and C_r can be computed analytically. In the case of μ as Lebesgue measure, we have

$$C_{ij} = \sqrt{\frac{\pi}{2s}} \exp\left(-\frac{s}{2}(z_i - z_j)^2\right) \text{ and } (C_r)_{ij} = \sqrt{\frac{\pi}{s(1 + \gamma^2)}} \exp\left(-\frac{s(r + \gamma z_i - \gamma z_j)^2)}{1 + \gamma^2}\right).$$

B.5. Knowledge of rewards

In distributional approaches to dynamic programming, it is necessary to know all aspects of the environment's transition structure and reward structure in advance, including the set $\mathcal{R}$ required for precomputing the Bellman coefficients. However, in temporal-difference learning, this is a non-trivial assumption. In many environments, this information is available in advance (in the Atari suite with standard reward clipping post-processing (Mnih et al., 2015), rewards are known to lie in $\{-1, 0, 1\}$, for example). When this information is not available, one may modify Algorithm 1 to instead compute Bellman coefficients for observed rewards *just-in-time*; that is, when these rewards are encountered in a transition. This makes the algorithm more broadly applicable, but clearly incurs a significant cost of computing Bellman coefficients for rewards for which these coefficients are not already cached. As Remark 3.2, one possibility in this setting is to learn an approximator $H : \mathbb{R} \to \mathbb{R}^{m \times m}$ that maps from rewards to Bellman coefficients, and use the predictions of the approximator as proxies for the true Bellman coefficients to reduce the need to solve for the Bellman coefficients every time a new reward is encountered.

B.6. Mathematical properties of Bellman coefficients

The Bellman coefficients B_r play a crucial role in our Bellman sketch framework. Here, we present various properties of B_r in a worked example, derived from both a sigmoid and a Gaussian base feature in Figure 6. For each base feature, we choose 20 evenly spaced anchors in $[-8, 8]$, and find B_r for $r = 1$ and $\gamma = 0.8$, and μ uniformly supported on a dense grid of 10,000 evenly spaced points in $[-5, 5]$. We apply a small L^2 regulariser with weight 10^{-6} in the regression problem.

First, we assess how accurate approximation in Equation (6) is when B_r is found via the regression problem in Equation (5). In the left two columns of Figure 6, we show the feature functions $\phi(z)$ and $\phi(r + \gamma z)$ in the first two columns. In the second column, we also show $B_r\phi(z)$ in dashed lines evaluated on $[-8, 8]$, wider than the grid over which we minimised the error. The error is tiny and virtually invisible within the interval $[-5, 5]$, but is larger outside. Quantitatively, the maximum absolute difference between $\phi(r + \gamma z)$ and $B_r\phi(z)$ over the dense grid in $[-5, 5]$ is less than 0.002 for both base features. By Proposition 4.1, we expect a small error in a single step of dynamical programming.

Had B_r been a contraction, we would have been able to prove contraction for Algorithm 1. However, we show empirically that B_r is not in general a contraction in L^2 norm, but the dynamics from repeated multiplication of B_r may converge to a stable fixed point. First, we performed a singular value decomposition of the B_r for the two base features. We see that the singular vectors in Figure 6 (third column) are similar to harmonic functions. Importantly, in the largest singular values (operator norms) in Figure 6 (fourth column) are greater than 1, suggesting that a single application of B_r may expand the input. Further, we show the eigenvalues of B_r in the fifth column of Figure 6. Interestingly, all eigenvalues have real parts less or very close to 1.0 suggesting that there exists fixed points in the dynamics induced by B_r. As such, the Bellman coefficients B_r exhibit transient dynamics (typical for non-normal matrices) but is stable after repeated applications to an initial vector. Further studies into these dynamical properties are important for future work. Given the important role of non-normal dynamics hypothesised to be present in the nervous system (Hennequin et al., 2012; Bondanelli & Ostojic, 2020), these observations allude to the possibility that the Bellman sketch framework could contribute to a biological implementation of distributional RL.

B.7. Choices of feature function

In the main paper, we note that any set of features spanning the degree-m polynomials is Bellman closed, as described by Rowland et al. (2019), and hence exact dynamic programming is possible with this feature set, as shown by Sobel (1982). However, in preliminary experiments we found these features difficult to learn with temporal-difference methods beyond small values of m, due to the widely varying magnitude of moments as m grows, making learning rate selection problematic in stochastic environments; further details are provided in Appendix D.1.

In this paper, we tested the following functions as the base feature κ in the translation family Equation (8):

- Sigmoid: $\kappa(x) = \frac{1}{1+\exp(-x)}$;

- Gaussian: $\kappa(x) = \exp(-x^2/2)$;

- Parabolic: $\kappa(x) = 1 - x^2$ for $|x| \leq 1$, zero otherwise.

- Hyperbolic tangent: $\kappa(x) = \tanh(x)$

In Appendix D.3, we provide further experimental results for a wide variety of feature maps from this family. In addition, we also consider the indicator feature used in Proposition 4.4 as well as sinusoidal features shown in Figure 2B.

We found that the anchor points must be chosen carefully so that the features produce variations within the return range. This can be done by choosing the range of the anchors to be slightly wider than and estimated return range, and setting the slope so that there does not exist a region of the return range that produce no change in the feature functions. In the tabular experiments, we set the extremum anchor points to be $\hat{G}_{\min} - a\hat{L}$ and $\hat{G}_{\max} + a\hat{L}$, where $\hat{L} = \hat{G}_{\min} - \hat{G}_{\min}$ is the estimated return range, and a is a small positive value around 0.4 casually chosen and not tuned. The return limits $\hat{G}_{\min}$ and $\hat{G}_{\max}$ are estimated by the sample minimum and maximum from samples collected by first-visit Monte Carlo; see Appendix C.1.

The slope parameter should depend on the feature and the return range, and we applied the following intuition. Most of the base feature κ have an "non-trivial support" that produces the most variations in the function value. For example, the "non-trivial" support for the sigmoidal and Gaussian κ can be chosen as $[-2, 2]$; and for base features that are nonzero only in $[-1, 1]$, this support is $[-1, 1]$. We define the width w of a base function as the length of the non-trivial support. Crudely, the feature with slope s has width w/s, as sharper features tend to have shorter non-trivial support. In addition, for the set of features to cover return range uniformly, we set each adjacent feature functions to overlap by 50%. Finally, we want the union of the non-trivial supports of 10 (arbitrary chosen) such overlapping features to equal the return range. We must then have $0.5 \times 10w/s = \hat{G}_{\min} - \hat{G}_{\max}$. This is the *default slope* for each feature and each environment with known return range. As such, the sigmoidal and Gaussian base features have default slope equal to $s = 20/(\hat{G}_{\min} - \hat{G}_{\max})$.

B.8. Invariance of sketch algorithm to linear transformation of sketch features.

Suppose we instead choose to work with a collection of feature functions $\varphi, \ldots, \varphi$ which serve as an alternative basis for the finite-dimensional vector space $\langle \phi_1, \ldots, \phi_m \rangle$. Specifically, consider an invertible matrix $M \in \mathbb{R}^{m \times m}$, and suppose we have

$$\varphi(g) = M\phi(g)$$

for all $g \in \mathbb{R}$. By definition, the mean embeddings of the return distribution $\eta^\pi(x)$ under the two features are related by

$$S^\pi(x) = \mathbb{E}_{G \sim \eta^\pi(x)}[\varphi(G)] = \mathbb{E}_{G \sim \eta^\pi(x)}[M\phi(G)] = MU^\pi(x)$$

Let us write B^φ for the Bellman coefficients associated with φ. It can be shown that B^φ is related to B_r in the following sense: for all $g \in \mathbb{R}$, we have

$$B^\varphi \varphi(g) = \varphi(r + \gamma g) \qquad \Longleftrightarrow \qquad B^\varphi M\phi(g) = M\phi(r + \gamma g) \qquad \Longleftrightarrow \qquad M^{-1}B^\varphi M\phi(g) = \phi(r + \gamma g).$$

But now by linear independence of the ϕ, we must have $M^{-1}B^\varphi M = B_r$, or equivalently

$$B^\varphi = MB_r M^{-1}.$$

The corresponding Sketch-DP update to an approximate mean embeddings $S \in \mathbb{R}^{\mathcal{X} \times m}$ is (c.f. Equation (Sketch-DP))

$$S(x) \leftarrow \mathbb{E}_x^\pi[B^\varphi S(X')].$$

The right-hand side of this update is

$$\mathbb{E}_x^\pi[B^\varphi S(X') = \mathbb{E}_x^\pi[MB_R M^{-1}S(X')] = \mathbb{E}_x^\pi[MB_R M^{-1}M\phi(X')] = M\mathbb{E}_x^\pi[B_R\phi(X')].$$

Thus, a Sketch-DP update (using B_r^φ) on the mean embeddings associated with φ is equal to the same update applied to the mean embeddings of the original feature ϕ (using B_r).

Likewise, we can show a similar result for Sketch-TD. Following the transition (x, r, x'), the corresponding sketch-TD update to an approximate $S \in \mathbb{R}^{\mathcal{X} \times m}$ to mean embeddings under φ is given by

$$S(x) \leftarrow (1 - \alpha)S(x) + \alpha B^\varphi S(x').$$

The right-hand side of this update is

$$\begin{aligned}
&(1 - \alpha)S(x) + \alpha B_r^\varphi S(x') \\
=&(1 - \alpha)MU(x) + \alpha MB_r M^{-1}MU(x') \\
=&M((1 - \alpha)U(x) + \alpha B_r U(x')).
\end{aligned}$$

Thus, we have shown that both Sketch-DP and Sketch-TD algorithms with respect to φ and ϕ are equivalent: one can perform updates for one choice of features, and then with the transformation M or M^{-1}, obtain the updated predictions that would have been obtained had we worked with the other set of features in the first place.

This shows that in the tabular setting, with a scalar learning rate, it does not matter which choice of basis for polynomial features we use. However, there are factors that could make the choice of basis important, including function approximation, adaptive optimisers (such as Adam), and floating point numerical issues (e.g. if the condition number of B^φ becomes large).

B.9. Comparison with other approaches to distributional RL

In this section, we provide additional comparisons against existing approaches to distributional RL. As distributional RL is a quickly evolving field, we focus our comparison on a few main classes of algorithms related to our work, which illustrate some key axes of variation within the field: (i) categorical approaches (Bellemare et al., 2017); (ii) quantile approaches (Dabney et al., 2018a;b; Yang et al., 2019); (iii) approaches related to maximum mean discrepancy (MMD; Gretton et al., 2012), such as Nguyen-Tang et al. (2021); Zhang et al. (2021); Sun et al. (2022); and (iv) sketch-based approaches (Sobel, 1982; Rowland et al., 2019).

Distribution representation. Categorical, quantile, and MMD approaches are typically presented as learning approximate return distributions directly. In categorical approaches, the approximate distribution is parametrised as

$$\sum_{i=1}^m p_i \delta_{z_i},$$

with fixed particle locations $(z_i)_{i=1}^m$, and learnable probabilities $(p_i)_{i=1}^m$ for each state-action pair at which the return distribution is to be approximated. In contrast, quantile and MMD approaches learn fixed-weight particle approximations, of the form

$$\sum_{i=1}^m \frac{1}{m} \delta_{z_i} \,, \tag{13}$$

in which the particle locations $(z_i)_{i=1}^m$ are learnable. Work on sketches has instead focused on learning the values of particular statistical functionals of the return, rather than explicitly approximating return distributions.

Rowland et al. (2019) also shows that standard categorical- and quantile-based algorithms can also be viewed through the lens of sketch-based distributional RL. Other work in this vein includes Sobel (1982), who analysed the case of moments specifically, and Marthe et al. (2023), who extend the work of Rowland et al. (2019) to the undiscounted, finite-horizon case. The approach proposed in this paper sits firmly in the camp of sketch-based approaches, without ever representing approximated distributions directly. We highlight generative models of distributions as another prominent class of (non-parametric) representation (see, e.g., Doan et al. 2018; Freirich et al. 2019; Dabney et al. 2018a; Yang et al. 2019; Wu et al. 2023).

Algorithm types. Most prior algorithmic contributions to distributional reinforcement learning have focused on sample-based temporal-difference approaches, in which prediction parameters are iteratively and incrementally updated based on the gradient of a sampled approximation to a loss function. These approaches include the original C51 (Bellemare et al., 2017), QR-DQN (Dabney et al., 2018b), MMDRL (Nguyen-Tang et al., 2021), and EDRL (Rowland et al., 2019) algorithms. Dynamic programming algorithms, in which parameters are not updated incrementally via loss gradients, but instead according to the application of an implementable operator, have also been considered (see Rowland et al. (2018; 2023); Wu et al. (2023) for categorical dynamic programming, quantile dynamic programming, and fitted likelihood estimation, respectively). In this paper, our algorithmic contributions include both DP and TD methods.

Losses, projections, and convergence theory. One of the core axes of variation across distributional RL approaches is the loss used to define updates in incremental algorithms, and to define projections in dynamic programming. Categorical approaches use a projection in Cramér metric (Rowland et al., 2018) to define a target distribution for both dynamic programming and incremental versions of the algorithm; the incremental algorithm updates predictions via the gradient of a KL loss between the current and target distributions. Quantile-based approaches use either the quantile regression loss in incremental settings, or a Wasserstein-1 projection in dynamic programming (Dabney et al., 2018b).

The approach proposed in this paper works entirely with mean embeddings of probability distributions. Earlier approaches to sketched-based distributional RL, both in dynamic programming and incremental forms, have defined losses via imputation strategies, which compute updates by converting sketches into approximate distributions (Rowland et al., 2019; Bellemare et al., 2023).

Here, we contribute a novel perspective on the work of Nguyen-Tang et al. (2021), who propose a sample-based TD algorithm for updating particle locations (as in Equation (13)) by using an MMD loss, specifically taking the form

$$\text{MMD}_K^2 \left(\sum_{i=1}^m \frac{1}{m} \delta_{z_i(x,a)}, \sum_{i=1}^m \frac{1}{m} \delta_{r+\gamma z_i(x',a')} \right) \,, \tag{14}$$

for some choice of kernel K. Although not described in this manner by Nguyen-Tang et al. (2021), this can be seen as an incremental update on approximate mean embeddings for the RKHS $\mathcal{H}_K$ corresponding to the kernel K, amongst the class of mean embeddings of the form

$$\sum_{i=1}^m \frac{1}{m} K(z_i, \cdot) \in \mathcal{H}_K \,, \tag{15}$$

where the particle locations $(z_i)_{i=1}^m$ are optimised. We note that Nguyen-Tang et al. (2021) do not provide theoretical analysis for their algorithm. They provide contraction analysis of $\mathcal{T}^\pi$ (Theorem 2), and MMD approximation bounds for fixed target distributions (Theorem 3 and Proposition 2), but these do not constitute a proof of convergence of the incremental algorithm described therein. A key reason why the proposed algorithm may not yield clean convergence theory is that the space of mean embeddings described in Equation (15), where only the particles $(z_i)_{i=1}^m$ can vary, is a non-convex subset of

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an infinite-dimensional RKHS. As such, tractable global optimisation of the objective may not be possible, along with the definition of a straightforward dynamic programming version of this approach. In other words, it is not straightforward to define a dynamic programming method to optimise the particle locations $(z_i)_{i=1}^m$.

In contrast, the Sketch-DP and Sketch-TD algorithms introduced in this paper work with finite-dimensional RKHS, and define updates via matrix-vector products with the Bellman coefficients derived in Equation (5). This naturally yields tractable dynamic programming and temporal-difference learning algorithms, and also allows us to develop convergence theory, as described in Section 4.

Contrasting against the Sketch-DP/Sketch-TD approaches described above, earlier approaches to sketched-based distributional RL, both in dynamic programming and incremental forms, have defined losses via imputation strategies, which compute updates by converting sketches into approximate distributions (Rowland et al., 2019; Bellemare et al., 2023). Foreshadowing the remarks on theoretical analysis below, we remark that neither MMDRL nor the earlier sketch-based approach described above have been analysed for convergence, while Section 4 in this paper deals with convergence analysis of the approach proposed in this paper.

In general, convergence analysis of dynamic programming algorithms has been obtained for several classes of distributional algorithms beyond the theory described in this paper; see Rowland et al. (2018) for the case of categorical dynamic programming, Dabney et al. (2018b) for the case of a quantile dynamic programming algorithm, Bellemare et al. (2023); Rowland et al. (2023) for later generalisations of this work, and Wu et al. (2023) in the case of fitted likelihood evaluation. This analysis typically centres around (i) proving contractivity of the distributional Bellman operator $\mathcal{T}^\pi$ with respect to some metric d, and proving non-contractivity of the specific distributional projection used by the dynamic programming algorithm under this same metric. Notably, the metric d used in the *analysis* need not be the same as any metrics used in *defining* the algorithm; this is the case for quantile dynamic programming, for which Wasserstein-1 distance is used to define the algorithm, while Wasserstein-∞ distance is used to analyse the algorithm (Dabney et al., 2018b; Bellemare et al., 2023; Rowland et al., 2023). Our proof technique in this paper, in particular, makes use of contraction of the distributional Bellman operator in Wasserstein distances, though such distances do not feature in the definition of the Sketch-DP/TD algorithms.

In general, there has been less work on the convergence analysis of sample-based incremental algorithms. Rowland et al. (2023) recently showed convergence of quantile temporal-difference learning, though the question of convergence for many other sample-based incremental distributional reinforcement learning algorithms is currently open. The analysis of incremental algorithms is generally more mathematically involved than in the dynamic programming case, principally owing to the fact that rather than analysing the iterated application of a fixed operator, one needs to analyse the continuous dynamical system associated with incremental updates.

C. Experimental details

In this section, we provide additional details on the experimental results reported in the main paper.

C.1. Tabular environments

We describe the setup in the main paper. In Appendix D.3, we show extended results of more features and more environments.

Environments. In the main paper, we reported results on the on the following environments,

- **Random chain:** Ten states $\{x_1, x_2, \ldots, x_{10}\}$ are arranged in a chain. There is equal probability of transitioning to either neighbour at each state, and state x_{10} has a deterministic reward of +1;

$$\text{terminal} \leftarrow x_1 \longleftrightarrow x_2 \longleftrightarrow x_3 \longleftrightarrow \cdots \longleftrightarrow x_{10} \rightarrow \text{terminal} .$$

- **Directed chain (DC):** Five states are arranged in a directed chain, but the agent can only move along the arrow deterministically until termination. A deterministic reward of +1 is given at state x_5;

$$x_1 \longrightarrow x_2 \longrightarrow x_3 \longrightarrow \cdots \longrightarrow x_5 \rightarrow \text{terminal} .$$

- **DC with Gaussian reward:** A variant of the directed chain above, with the only difference that x_5 has a Gaussian reward with mean 1 and unit variance.

The discount factor is $\gamma = 0.9$. These environments cover stochastic and deterministic rewards and state transitions, giving a range of different types of return distributions.

Feature functions. We use features of translation family Equation (8), with κ chosen from a subset of base features described in equation (B.7). We also include the indicator features used in Proposition 4.4. For the sweep over slope, we set the slope s to be the default slope (described in Appendix B.7) multiplied by a scaling factor, and sweep over this factor. from 0.001 to 10.0. This is done primary because the return range varies a lot across different environments, and the default slope is adjusted to the return range. The results serve as justification for the heuristics on choosing the default slope.

Ground-truth distribution. We approximate the ground-truth mean embeddings and the ground-truth return distributions by collecting a large number of return samples from the MRPs. To do so, we use first-visit Monte Carlo with a sufficiently long horizon (after the first visit to each state) to ensure that the samples are unbiased and has bounded error caused by truncating the rollout to a finite horizon. For environments with deterministic rewards, truncating the horizon at L steps induces maximum truncation error $|r|_{\max}\gamma^L/(1-\gamma)$, where $|r|_{\max}$ is the maximum reward magnitude. We bound this error at 10^{-4}, giving $L > 110$, so we set the horizon after the first visit to 110. For environments with Gaussian rewards, we set the horizon to 200. We initialise the rollout at each state in the environment, and for initial each state this is repeated 10^5 times. This gives us at least 10^5 samples each state.

Sketch DP under conditional independence. Many RL environments, including the tabular environments tested in this paper, have the property that $R \perp\!\!\!\perp X'|X$ for the trajectory X, A, R, X', so the Sketch-DP update Equation (Sketch-DP) simplifies to

$$U(x) \leftarrow \mathbb{E}_x^\pi[B_R]\mathbb{E}_x^\pi[U(X')] = \mathbb{E}_x^\pi[B_R]\sum_{x' \in \mathcal{X}} P(x'|x)U(x').$$

This means we need to evaluate the expected Bellman coefficient $\mathbb{E}_x^\pi[B_R]$. This is trivial for deterministic rewards. For stochastic rewards with known distributions, we approximate the expectation via numerical integration. We run all DP methods for 200 iterations.

Jittered imputation support. The support on which we impute the distribution are the anchors of the features. Some tabular environments have states with deterministic returns that directly align with the feature anchors, which interferes in unintuitive ways with the finite support on which we impute distributions, producing non-monotonic trends in the results. To avoid this unnecessary complication, we jitter the support before imputing the distribution: for points in the support, we add noise uniformly distributed over $[-\Delta/2, \Delta/2]$, where Δ is the distance between consecutive support points. Likewise, we project ground truth distribution using the same jittered support to. In Figure 4, we report the average of the metrics computed from 100 independent jitters. Note that since the imputation (from mean embedding) and projection (from ground-truth) share the same support for each of the 100 jitters, the average Cramér distance between the projected and the ground-truth still lower-bounds the average Cramér distance between the imputed distribution and the ground-truth.

C.2. Deep reinforcement learning implementation details

In this section, we provide further details on the deep reinforcement learning experiments described in the main paper, in particular describing hyperparameters and relevant sweeps.

Environment. We used the exact same Atari suite environment for benchmarking QR-DQN (Bellemare et al., 2013; Dabney et al., 2018b). In all experiments, we run three random seeds per environment.

Feature map ϕ. The results in Figure 5 uses the sigmoid base feature $\kappa(x) = 1/(e^{-x} + 1)$ with slope $s = 5$, and the anchors to be 401 (tuned from 101, 201 and 401) evenly spaced points between -12 and 12. These values are loosely motivated by the range used in C51 (Bellemare et al., 2017). We did not use the heuristic in Appendix B.7 to choose the slope parameter, instead we set this to 10 by tuning from $\{1, 2, \ldots, 12\}$. Larger slope values typically resulted in Bellman coefficients with a worst-case regression error $\max_{r \in \mathcal{R}} \max_{g \in \text{supp}(\mu)} \|\phi(r + \gamma g) - B_r\phi(g)\|$ greater than 0.01. In these cases, we regard the regression error as too large, and did not perform agent training with these hyperparameter settings. In addition, ϕ is appended with a constant feature of ones, which we found to be very crucial for a good performance; as noted in the main paper, this ensures that the sketch operator is truly affine, not linear. We also tried a several other feature functions, including the Gaussian, the hyperbolic tangent and the (Gaussian) error function, and found that the sigmoid reliably performed the best.

Solving the regression problems. To compute the Bellman coefficients as well as the value readout weights β described

in Section 5.1, we solve the corresponding regression problem with μ set to be 100,000 points evenly spaced between -10 and 10. We also add a L^2 regulariser with strength set to 10^{-9} to avoid numerical issues, which is tuned from $\{10^{-15}, 10^{-12}, 10^{-9}, 10^{-6}, 10^{-3}\}$.

Neural network. We implement Sketch-DQN based on the QR-DQN architecture, using almost the same convolutional torso and fully-connected layers to estimate the mean embeddings, with the differences being:

- We add a sigmoid or tanh nonlinearity, depending on the base feature output range to the final layer. This helps bound the predicted mean embedding and improved the results.

- The network only predicts the non-constant dimensions of the mean embedding, and the constant feature is appended as a hard-coded value.

- We use the pre-computed mean readout coefficients β to predict state-action values for state-action pairs in the Q-learning objective, and at current states to determine the greedy policy.

Training. We use the exact same training procedure as QR-DQN (Dabney et al., 2018b). Notably, the learning rate, exploration schedule, buffer design are all the same. We tried a small hyperparameter sweep on the learning rate, and found the default learning rate 0.00005 to be optimal for performance taken at 200 million frames.

Evaluation. The returns are normalised against random and human performance, as reported by Mnih et al. (2015). We use the mean and median over all games and three random seeds for each game.

Baseline methods. We also tuned the number of atoms of the approximating distributions in the baseline methods. In particular, we found that C51 performed the best compared to using more atoms; IQN did best when using 51 quantiles; and QR-DQN did best using 201 quantiles. Increasing the number of atoms in these methods lead to worse performance. We report the results of these best variants of the corresponding baseline methods in Figure 5.

D. Further experiments

In this section, we collect further experimental results to complement those reported in the main paper.

D.1. Temporal-difference learning with polynomial features

As noted in the main text, the sketch corresponding to the polynomial feature function $\phi(g) = (1, g, g^2, \ldots g^m)$ is Bellman closed, and the Bellman coefficients B_r obtain zero regression error in Equation (5). In addition, there has been much prior work on dynamic programming (Sobel, 1982) for moments of the return, and temporal-difference learning specifically in the case of the first two moments (Tamar et al., 2013; 2016). However, such polynomial feature functions are difficult to use as the basis of learning high-dimensional feature embeddings. This stems from several factors, including that the typical scales of the coordinates of the feature function often vary over many orders of magnitude, making tuning of learning rates difficult, as well as the fact that polynomial features are *non-local*, making it more difficult to decode distributional information via an imputation strategy.

To quantify these informal ideas, we ran an experiment comparing Sketch-TD updates for a 50-dimensional mean embedding based on the translation family (Equation (8)) with a sigmoid base feature κ, as well as polynomial features with $m = 5$, and $m = 50$. The sigmoid features are chosen according to the intuitions in Appendix B.7. We ran 100,000 synchronous TD updates on mean embedding estimates initialised at $\phi(0)$ for all state. Each run uses a fixed learning rate chosen from 10^{-6} to 1.

In Figure 7, we plot the Cramér distance of imputed distributions from ground-truth after running TD for each of these three methods, on a variety of the environments described in Section D.3. In all environments, there is a similar pattern. For the Sketch-TD algorithm based on sigmoid non-linearities, there is a reasonably wide basin of good learning rates, with performance degrading as the learning rate becomes too small or too large. On several environments this pattern is reflected also in the performance of the degree-5 polynomial embedding, though the minimal Cramér error is generally significantly worse than that of the sigmoid embedding. This supports our earlier observations; this mean embedding captures relatively coarse information about the return distribution, and in addition different feature components have different magnitudes, meaning that a constant learning rate cannot perform well. The mean embedding with degree-50 polynomials generally

performs very badly on all environments, as the components of the embedding are at such different magnitudes that no appropriate learning rate exists.

D.2. Sketch DP example with sigmoidal features

To given an example of how to use the translation family described in Equation (8), we include another example of Sketch-DP execution in Figure 8. The results are largely similar to using sinusoidal features, except that the evolution is smoother and compared to using sinusoids. We also found that the first two principal components explained >97% variance, higher than using sinusoids. Please see Appendices B.4 and B.7 for how to the heuristics on selecting the anchors and μ.

D.3. Extended tabular results

We tested Sketch-DP using the following additional MRPs. If unspecified, the default reward distribution for each state is a Dirac delta at 0, and the transition probabilities from a state to its child states are equal.

- Tree: State 1 transitions to states 2 and 3; state 3 transitions to states 4 and 5. State 2 has mean reward 5; state 4 has mean reward -10, and state 5 has mean reward 10. All leaf states are terminal.

- Loopy tree: Same as Tree, but with a connection from state 2 back to state 1.

- Cycle: Five states arranged into a cycle, with only a single state having mean reward 1.

- Rowland '23: The environment in Example 6.5 of Rowland et al. (2023).

- S&B '18: The environment in Example 6.4 of Sutton & Barto (2018).

- Loopy fork: The environment shown in Figure 2(A).

All environments have discount factor $\gamma = 0.9$. For each environment, except Rowland '23 and S&B'18, the reward distributions for the non-zero-reward states are either Dirac deltas at the specified mean, or Gaussian with specified mean and unit standard deviation.

The results, extending those in Figure 4, are illustrated in Figure 9. The results are in general consistent with the main Figure 4. In particular, the Cramér distances decay as the number of features increases, and can be closer to the corresponding projected ground-truths than the CDRL baseline.

In Appendix B.7, we suggested that the range of the anchors should be wider than the range of the uniform grid μ on which we measure the regression loss. We validate this intuition by performing another experiment, sweeping the ratio of the width of the anchor range relative to the width of the grid μ, fixing the mid points between these two ranges the same. Here, we use $m = 50$ features for each base feature function and apply the default slope described in Appendix B.7. The results in Figure 10 shows that a slightly wider anchor range produces reliably small Cramér distances for almost all base features. When the anchor range decreases from 1 to 0, there is a much sharper increase in the Cramér distance, because the support on which we impute the distribution is too narrow and can miss substantial probability mass outside the support. On the other hand, when the anchor range increases from 1, the Cramér distance also increases because the support points get further away from each other, lowering the resolution of the imputed distribution. Since the grid is chosen to be slightly wider than the true return range, we see that the smallest Cramér distances can be attained at anchor range ratio slightly less than 1, but this does not hold universally (see, e.g., random chain and cycle results). Choosing this ratio to be slightly greater than 1, as suggested in Appendices B.4 and B.7, is more reliable at the cost of a small increase in distributional mismatch.
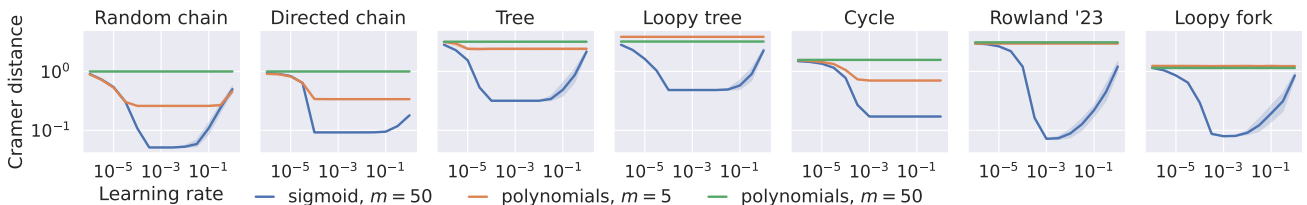

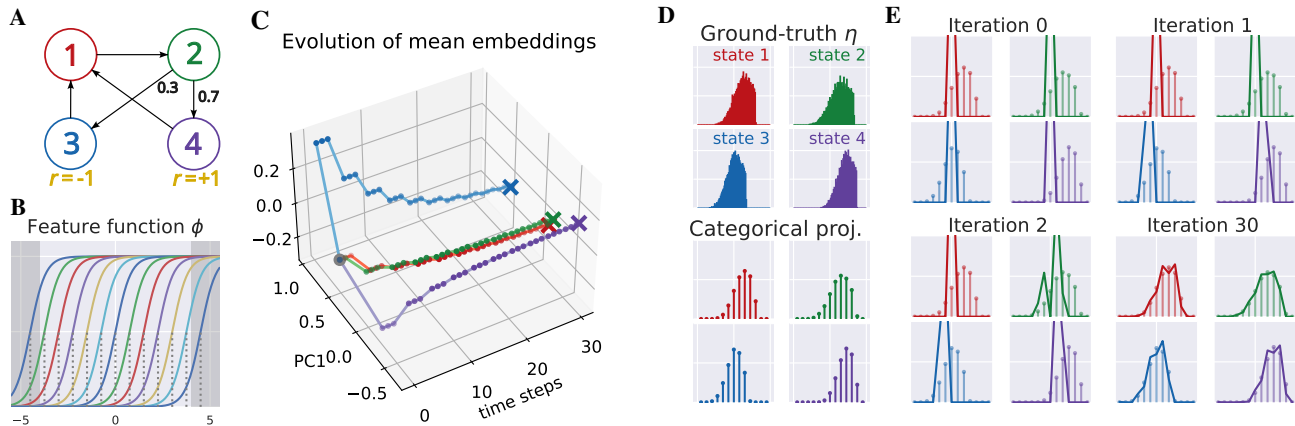*Figure 7.* Results comparing Sketch-TD with sigmoidal and polynomial features.

Figure 8. An example run of Sketch-DP as in Figure 2 but using sigmoidal features as shown in **B**. We use $m = 13$ sigmoidal features with anchors evenly spaced in $[-4.5, 4.5]$ at locations indicated by the dotted lines. The regression Equation (5) is performed under a densely spaced grid over the white region $[-4, 4]$.

D.4. Comparison with statistical functional dynamic programming

The Sketch-DP methods developed in this paper were motivated in Section 2 with the aim of having distributional dynamic programming algorithms that operate directly on mean embeddings, without the need for the computationally intensive imputation strategies associated with SFDP algorithms. In this section, we empirically compare Sketch-DP and SFDP methods, to quantitatively measure the extent to which this has been achieved. We give details below of the Sketch-DP and SFDP algorithms we compare, and provide comparisons of per-update wallclock time to assess computational efficiency, and distribution reconstruction error to assess accuracy.

Sketch-DP. We consider the Sketch-DP algorithm based on sigmoid features as described in Section 3.1, and implemented as described in Section 5 and Appendix C.1.

SFDP. We consider the SFDP algorithm for learning expectile values as described by Bellemare et al. (2023, Section 8.6). We use SciPy's default `minimize` implementation (Virtanen et al., 2020) to solve the imputation strategy optimisation problem given in Equation (8.15) in Bellemare et al. (2023). For a given sketch dimension m, we use expectiles at linearly spaced levels $\tau_i = (2i - 1)/(2m)$ for $i = 1, \ldots, m$.

Results. These two algorithms, for varying numbers of feature/expectiles m, were run on a selection of deterministic-reward environments as described in Appendix D.3. In Figure 11, we plot the Cramér distance and the excess Cramér distance of reconstructed distributions to ground truth, as described in Section 5 and plotted in Figure 4. In addition, we also plot two wallclock times in each case: the average time it takes to run one iteration of the dynamic programming procedure, and the time it takes to setup the Bellman operator, which includes solving for B_r for Sketch-DP. As predicted, the run time is significantly higher for the SFDP algorithm, due to its use of imputation strategies. The approximation errors measured by Cramér distances are also smaller for Sketch-DP, particularly as the number of features/expectiles is increased. Considering the per-update wallclock times in the third row of the figure, there is consistently a speed up of at least 100x associated with the Sketch-DP algorithm relative to SFDP. This is due to the fact that the Sketch-DP update consists of simple linear-algebraic operations, while the SFDP update includes calls to an imputation strategy, which must solve an optimisation problem. The one-off computation of the Bellman coefficients takes around 0.1–4 seconds, depending on the number of features m, which is only at most a couple of SFDP iterations, and hence a small fraction of the total run time of the SFDP algorithm.

### D.5. Extended results on Atari suite

We show in Figure 12 the advantage of the Sketch-DQN method to other baselines. On one hand, we see that Sketch-DQN surpasses DQN on almost all games. Compared to IQN and QR-DQN, Sketch-DQN is consistently better on CRAZY CLIMBER, SPACE INVADERS, RIVER RAID, ROAD RUNNERS and VIDEO PINBALL, while worse on ASSAULT, ASTERIX, DOUBLE DUNK, KRULL, PHOENIX, and STAR GUNNER.

To show how sensitive are the results depending on the feature parameters, we ran the full Atari suite using a few sigmoidal
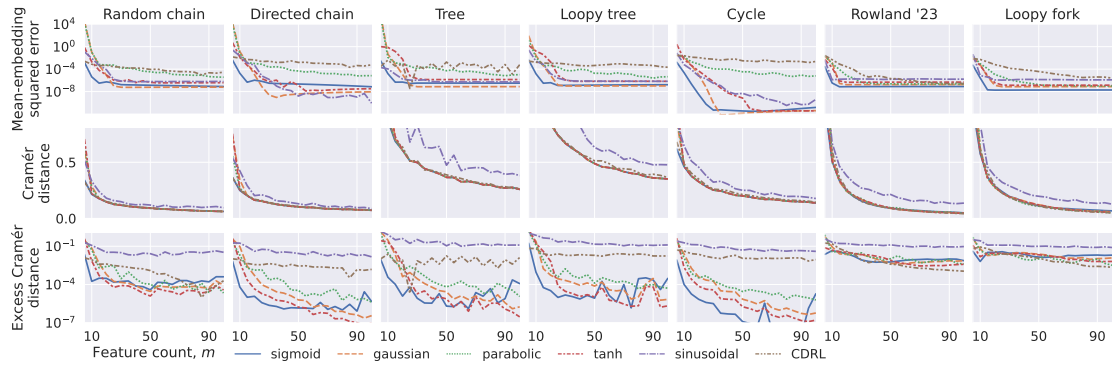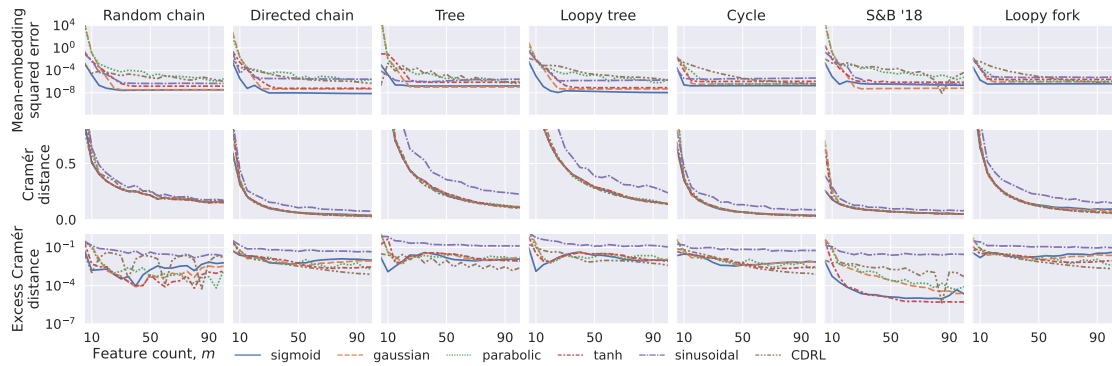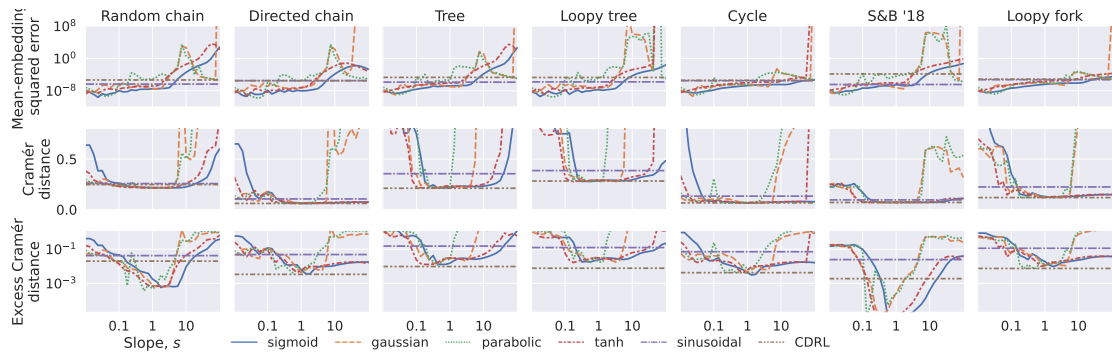
(a) Environments with deterministic rewards, sweeping over feature count m.
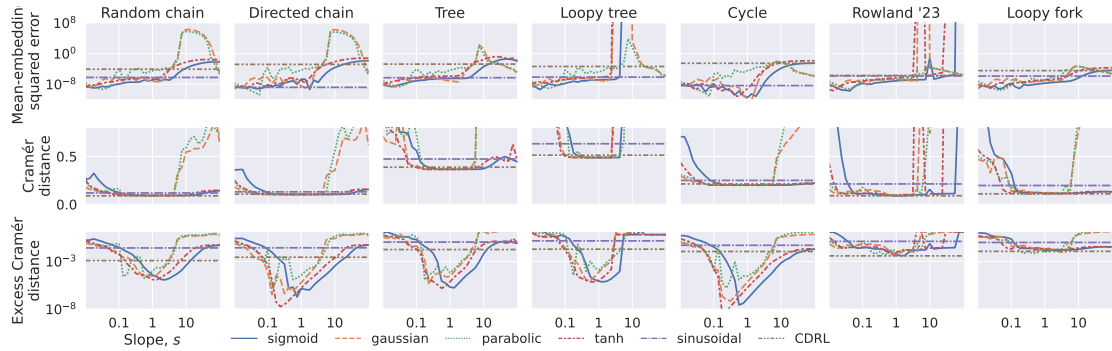
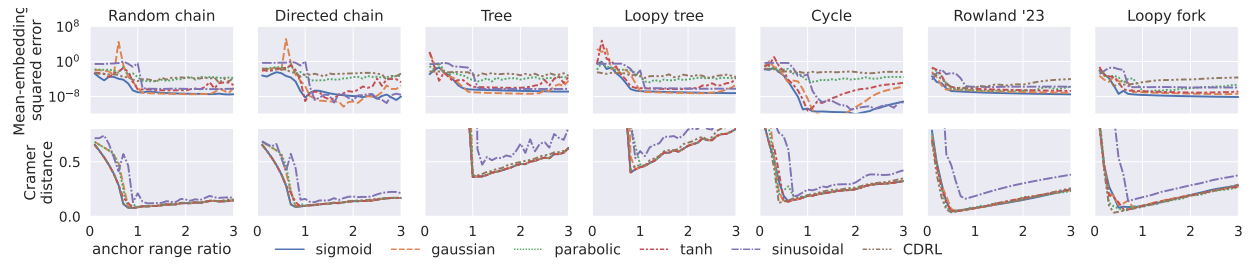(b) Environments with deterministic rewards, sweeping over slope s.

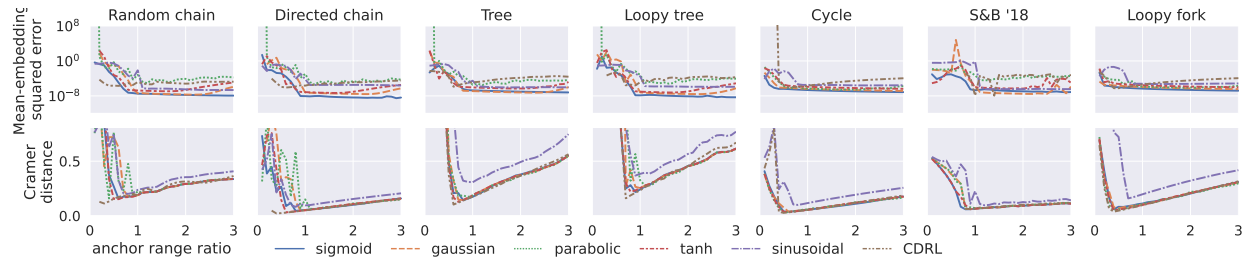(c) Environments with Gaussian rewards, sweeping over feature count m.

(d) Environments with Gaussian rewards, sweeping over slope s.

Figure 9. Additional tabular results extending Figure 4.

(a) Environments with deterministic rewards.

(b) Environments with Gaussian rewards.

Figure 10. Additional tabular results from sweeping over the range of the anchors relative to the width of the uniform grid given by the support of μ.
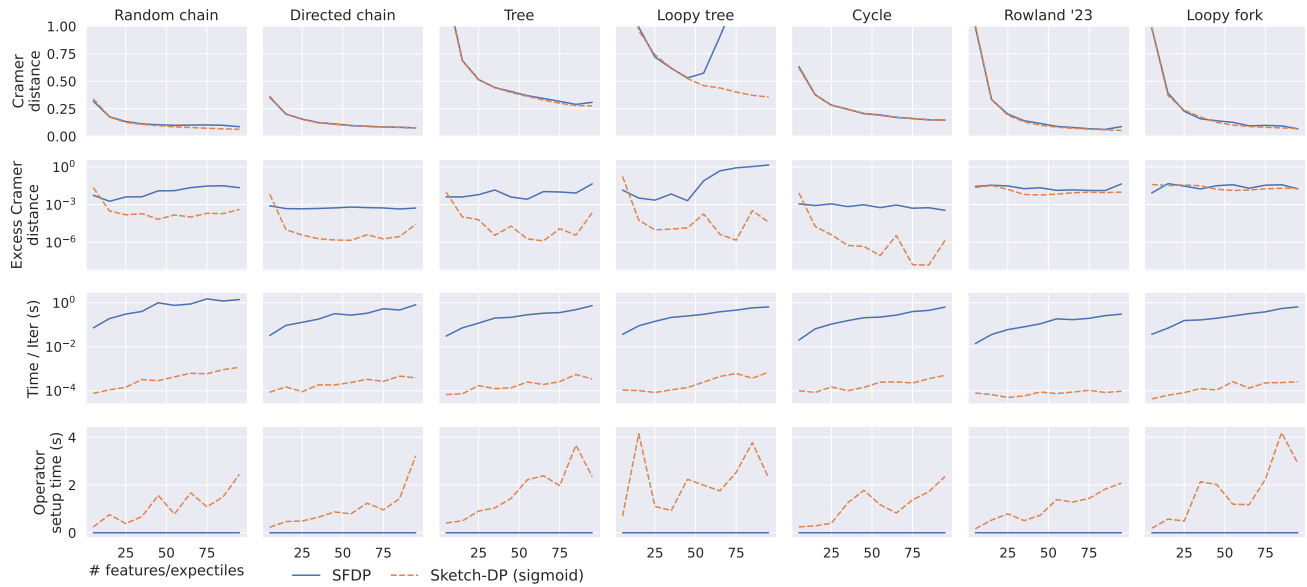
Figure 11. Results comparing Cramér distances as in Figure 4 (first two rows), and wallclock runtimes for each DP iteration (third row) and for setting the corresponding Bellman operator (bottom row), for Sketch-DP and SFDP algorithms, varying the numbers of features/expectiles m.
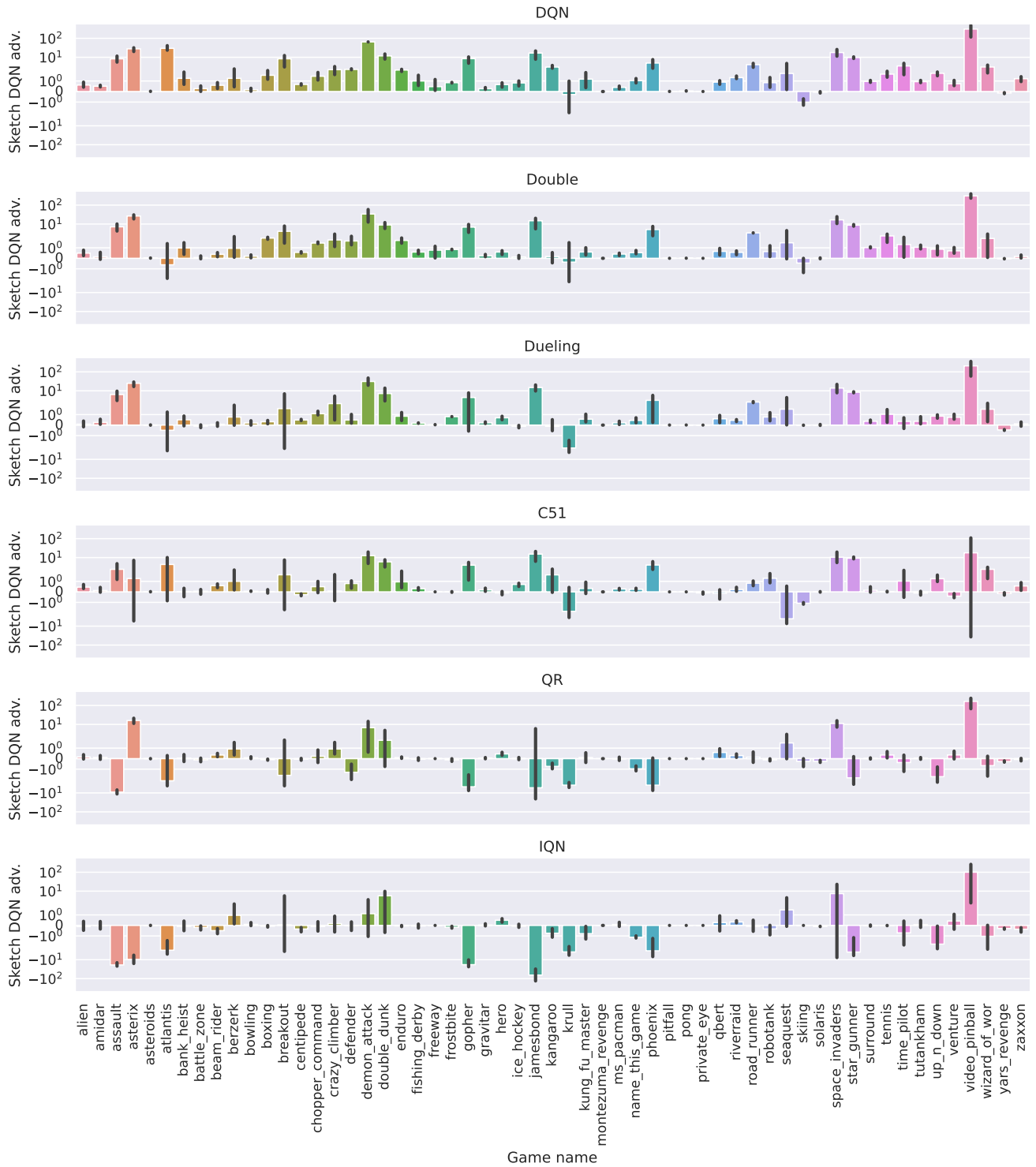
Figure 12. Advantage of Sketch-DQN, measured as Sketch-DQN's normalised return minus the returns of other baseline methods. Positive values means Sketch-DQN is better. We show the mean and standard error over 3 seeds for each game.

| Method | Number of features / atoms | | | |
	51	64	201	401
Sketch-DQN	-	-	1326 ± 107	1320 ± 110
Categorical-DQN	(C51) 1309 ± 146	1306 ± 139	1293 ± 152	1291 ± 154
QR-DQN	-	-	1258 ± 107	1256 ± 106
IQN	-	1120 ± 90	698 ± 41	400 ± 16

Table 1. Frame rate for selected methods. Higher is faster.

and Gaussian features, and show the results in Figure 13. Overall, we see that the choice on feature parameters is important; in particular, the sigmoidal feature outperforms Gaussian features. For the sigmoidal feature, the performance improved from using 101 to 201 features. On the contrary, for Gaussian features, increasing the feature count does not produce much change.

D.6. Runtime comparison

Here, we report the mean (±s.d.) rate (per second) at which frames are processed during training in our Atari experiments, with each agent running on a single V100 GPU. These frame-processing times reflect the wallclock time associated with all aspects of the DQN training, including network forward passes for action selection, environment simulation, and periodic gradient updates. These statistics are averaged across all games and seeds.

The results are shown in Table 1. Note that, by default, C51 uses 51 atoms, QR-DQN uses 201 quantiles, and IQN uses 64 quantiles. The Sketch-DQN method has the highest frame rate, and C51 and QR-DQN has slightly lower average frame rates. IQN with default 64 quantiles has a slightly lower average frame rate still, and is much lower when the number of quantiles is increased to match the number of predictions made by QR-DQN and Sketch-DQN. This is because the IQN architecture requires one forward pass through the MLP component of the network for each predicted quantile level. By contrast, the Sketch & QR architectures simply modify the original DQN architecture to produce multiple predictions of mean embeddings/quantiles from the final hidden layer of the network.
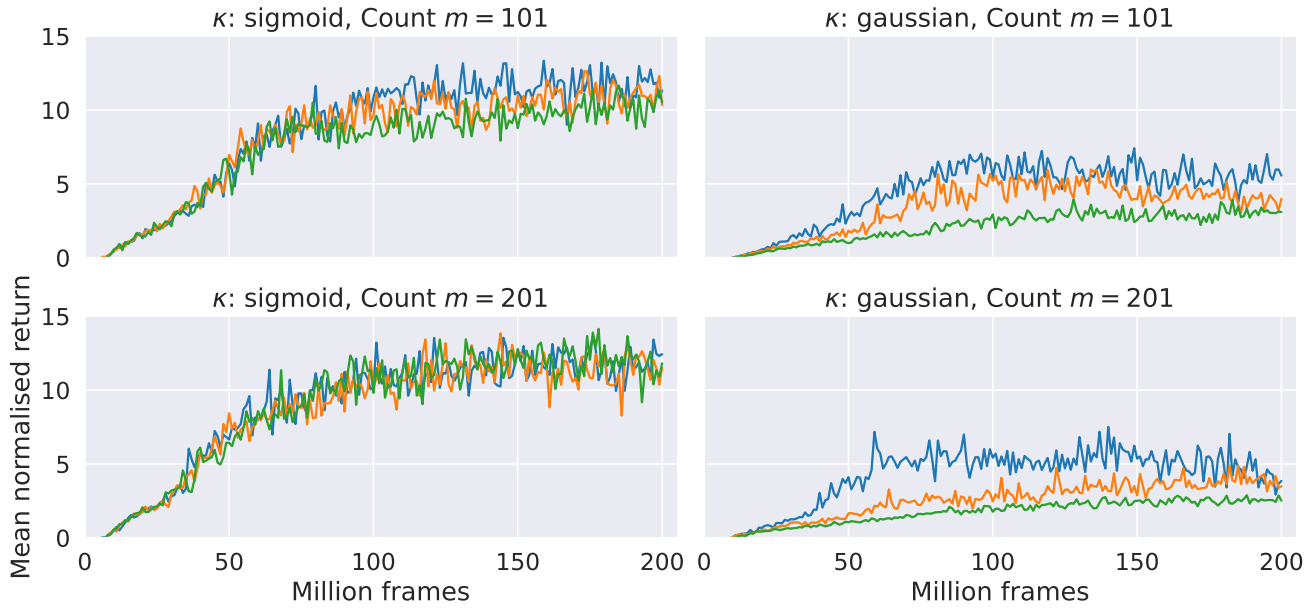
(a) Mean normalised return.
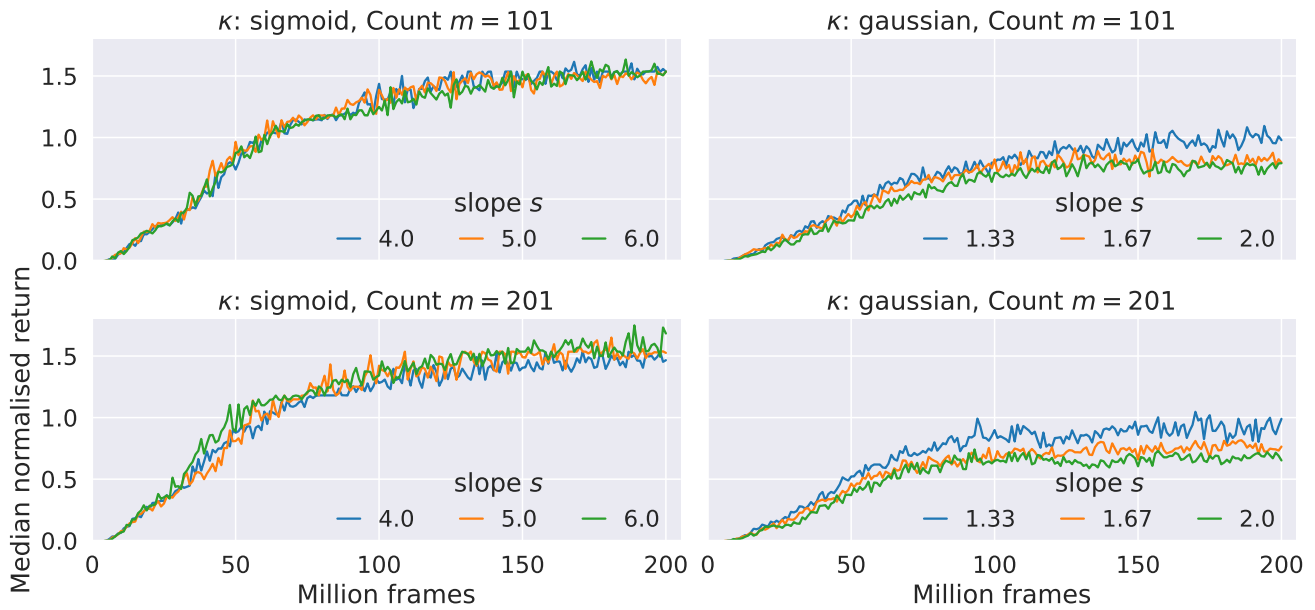
(b) Median normalised return.

Figure 13. Results on Atari suite for different feature parameters.