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Sensitivity properties describe how changes to the input of a program affect the output, typically by upper bounding the distance between the outputs of two runs by a monotone function of the distance between the corresponding inputs. When programs are probabilistic, the distance between outputs is a distance between distributions. The Kantorovich lifting provides a general way of defining a distance between distributions by lifting the distance of the underlying sample space; by choosing an appropriate distance on the base space, one can recover other usual probabilistic distances, such as the Total Variation distance. We develop a relational pre-expectation calculus to upper bound the Kantorovich distance between two executions of a probabilistic program. We illustrate our methods by proving algorithmic stability of a machine learning algorithm, convergence of a reinforcement learning algorithm, and fast mixing for card shuffling algorithms. We also consider some extensions: proving lower bounds on the Total Variation distance and convergence to the uniform distribution. Finally, we describe an asynchronous extension of our calculus to reason about pairs of program executions with different control flow.

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1 INTRODUCTION

Sensitivity properties describe how changes in program inputs affect program outputs, with respect to particular distances on program inputs and program outputs. By varying these distances, sensitivity properties are relevant in many application areas, including: (i) numerical computations, where distances are taken between real numbers, (ii) numerical queries, where program inputs are databases, and the distance between them is the number of differing entries, and (iii) learning algorithms, where the distance between two training sets is the number of differing examples, and the distance between outputs measures the difference in errors labeling unseen examples. This paper is concerned with sensitivity properties of probabilistic programs. As such programs return distributions over their output space, the corresponding notions of sensitivity use distances over distributions. The *Total Variation* (TV) distance (a.k.a. statistical distance), for example, is a widely

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used notion of distance that measures the maximal difference of probabilities for two distributions. One key benefit of the TV distance is that it is defined for distributions over arbitrary spaces. However, it is sometimes desirable to consider distances inherited from the underlying space. It is common to consider classes of distances on distributions that are obtained by lifting a distance on an underlying space. This lifting is defined by the so-called *Kantorovich metric*, which yields a family of probabilistic metrics obtained by lifting a distance \mathcal{E} on a ground set X to a distance $\mathcal{E}^{\#}$ on distributions over X. The class of Kantorovich metrics cover many notions of distance, including the TV distance which can be obtained by applying the Kantorovich lifting to the discrete distance.

Approach. We develop a relational pre-expectation calculus for reasoning about sensitivity of probabilistic computations under the Kantorovich metric. Relational pre-expectations are mappings expressing a quantitative relation (e.g., a distance or metric) between states, and are modelled as maps of the form State × State $\rightarrow [0, \infty]$. Our calculus takes as input a probabilistic program c written in a core imperative language and a pre-expectation \mathcal{E} between output states and determines a pre-expectation $rpe(c, \mathcal{E})$ between input states. The calculus is a sound approximation of sensitivity, in the sense that running the program c on inputs at distance smaller than $rpe(c, \mathcal{E})$ yields output distributions at distance smaller than $\mathcal{E}^{\#}$.

Technically, our calculus is inspired by early work on probabilistic dynamic logic due to Kozen [22] in which maps $\mathcal{E}:$ **State** $\rightarrow [0, \infty]$ serve as quantitative counterparts of Boolean predicates P: **State** $\rightarrow \{0, 1\}$. McIver and Morgan [23] later coined the term *expectation*—not to be confused with expected values—for such maps \mathcal{E} . Moreover, they developed a weakest pre-expectation calculus for the probabilistic imperative language PGCL. Their calculus was designed as a generalization of Dijkstra's weakest pre-conditions supporting both probabilistic and non-deterministic choice. The basic idea is to define an operator $wpe(c, \mathcal{E})$ that transforms an expectation \mathcal{E} averaged over the *output* distribution of a program *c* into an expectation evaluated over the *input* state. In this way, the expectation is transformed by the effects of the probabilistic program in a backwards fashion, much like how predicates are transformed through Dijkstra's weakest pre-conditions.

Our pre-expectation calculus operates similarly, but—as it aims to measure distances between distributions of outputs in terms of inputs—manipulates *relational* expectations instead. We next motivate the need for relational expectations, and explain why they are challenging.

Why do we need relational pre-expectations? The classical weakest pre-expectation calculus enjoys strong theoretical properties: in particular, it is both sound and complete (in an extensional sense) w.r.t. common program semantics (cf. Gretz et al. [17]). Therefore, weakest pre-expectations can—in principle—be applied to reason about bounds on the Total Variation distance: Given a program c, (i) take a copy c' over a fresh set of program variables—e.g. if variable x appears in c, substitute it by x' in c'—and (ii) determine the weakest pre-expectation $wpe(c; c', \mathcal{E})$, where the expectation \mathcal{E} measures the distance between variables in c and their counterparts in c'.

However, this naïve approach is not practical for analyzing sensitivity: the TV distance, for example, is defined as a maximum of a difference of probabilities over all events of the output space. While the output space—and thus potentially the TV distance—is often *unbounded*, the calculus of McIver and Morgan [23] is restricted to bounded expectations. Moreover, the above approach pushes the difficulty of reasoning about sensitivity properties into the task of finding suitable invariants for probabilistic programs—a highly challenging task on its own. In particular, finding invariants may involve reasoning about probabilistic independence, which is not readily available when using weakest pre-expectations. In fact, mathematicians have long observed that reasoning about the TV distance or the Kantorovich metric directly from their definition is inappropriate. Rather, they rely on *probabilistic couplings* [32], a mathematical tool for relating two different distributions. Relational

pre-expectations naturally connect with probabilistic couplings, and capture well-established proof principles used by mathematicians for reasoning about the TV distance.

Challenges of relational pre-expectations. Relational pre-expectations pose a number of specific challenges compared to their unary counterpart. First, the Kantorovich distance cannot be defined inductively on the structure of programs. More specifically, the Kantorovich distance between two runs of c; c' is not a simple combination of the Kantorovich distances between two runs of c and two runs of c' (we provide a counterexample in Section 3). Instead, we define a pre-expectation calculus $\widetilde{rpe}(c, \mathcal{E})$ that can compute a compositional *upper-bound* of the Kantorovich distance—this is sufficient for proving sensitivity properties.

Second, proofs of soundness and continuity for our relational pre-expectation calculus are significantly more involved than for the usual weakest pre-expectation calculus, and use non-elementary results from optimal transport theory. In particular, we are only able to prove continuity for finitely supported distributions, and soundness for discrete distributions.

Third, relational calculi are naturally better suited to reason about two executions that follow the same control-flow. We offer useful support for reasoning about executions with different control-flow, through a careful generalization of the rules for conditionals and loops. While our rules do not suffice for arbitrary examples (it remains an open problem to develop relatively complete verification approaches for relational properties of probabilistic programs), they suffice for non-trivial examples that exhibit asynchronous behavior.

Applications. We demonstrate our technique on several applications. In our first application, we formalize an *algorithmic stability* property of machine-learning algorithms. Informally, algorithmic stability describes how much the output parameters from a learning algorithm are affected when one input training example is changed; this notion of probabilistic sensitivity is known to imply generalization and prevent overfitting [11]. We use our calculus for proving algorithmic stability of a commonly-used learning algorithm: stochastic gradient descent (SGD). We use these examples to constrast our approach with prior work.

Then, we consider a pair of applications showing convergence properties. We first formalize convergence of a reinforcement learning algorithm [31], following a recent analysis by Amortila et al. [2]. Then, we show convergence and rapid mixing of several card shuffling algorithms [1]. We show that the TV distance between the outputs of two probabilistic loops decreases to 0 as the number of loop iterations increases—that is, the output distributions from any two inputs *converge* to the same distribution. Moreover, our technique is precise enough to describe the rate of this convergence. Upper bounds on convergence speed are key properties in algorithms that generate samples form complex distributions, such as Markov Chain Monte Carlo.

Extensions: uniformity and lower bounds. Next, we show how to formalize other properties complementing our bounds on convergence rate. First, we prove with our system that some card shuffling examples converge to the uniform distribution. Second, we study lower bounds–a task already challenging in the non-relational *wpe* calculus [19]. While upper bounds on convergence speed are often the main focus of formal analyses of probabilistic processes, lower bounds are also useful to understand how far apart the output distributions must be. The Monge-Kantorovich theorem provides a general method for proving lower bounds on the Kantorovich metric by using the unary *wpe* transformer from McIver and Morgan [23]. However, proving lower bounds poses some challenges [19]: we have to find a separating event and establish both upper and lower bounds on its probability. We show how to solve these challenges for card shuffling examples.

Extensions: asynchronous reasoning. Finally, we describe extensions to our calculus for asynchronous reasoning. We show how to prove relational properties when pairs of program executions have

different control flow. We demonstrate our asynchronous extensions to reason about a program generating a binomial distribution.

Contributions and outline. After introducing preliminaries on probability theory and the Kantorovich distance (§ 2), we present our main contributions:

- We define a sound, compositional, relational pre-expectation calculus for computing upperbounds on the Kantorovich distance. We introduce convenient proof rules for sampling commands and loops, and we show that the core fragment of probabilistic relational Hoare logics, namely PRHL [8] and EPRHL [7], can be embedded into our calculus (§ 3).
- We apply our calculus to three case studies. As a warmup example, we use our calculus to provide a clean proof of algorithmic stability of stochastic gradient descent [18] (§ 4). Second, we formalize convergence of TD(0), an algorithm from the Reinforcement Learning literature [31] (§ 5). Third, we apply our calculus to show rapid convergence of random walks and card shuffling algorithms [1] (§ 6).
- We show two complementary extensions to the previous examples: we use the weakest pre-expectation transformer from McIver and Morgan to compute lower bounds for the distance between distributions, and we use our calculus to show that the limiting distribution is uniform (§ 7).
- We present proof rules for reasoning about programs with asynchronous control flow (§ 8).

Finally, we survey related work (§ 9) and conclude (§ 10).

2 MATHEMATICAL PRELIMINARIES

We briefly recap the foundations required for relational reasoning about sensitivity properties: (1) probability theory, (2) probabilistic programming languages, and (3) distances on probability distributions. A comprehensive treatment of these topics is found, e.g., in the textbooks [3, 23, 32].

2.1 Basic probability concepts

We will use sub-distributions to model probabilistic behavior. A *sub-distribution* over a countable set *A* is a function $\mu: A \to [0, 1]$ assigning a probability to each element of *A*. Probabilistic *events* are subsets $B \subseteq A$; the probability of *B* is denoted $\mu(B)$ and defined by $\mu(B) = \sum_{b \in B} \mu(b)$. The *support* of μ is the set of all events $a \in A$ with $\mu(a) > 0$. Moreover, we let $|\mu| = \mu(A)$. As usual, the probabilities in any sub-distribution must sum up to at most 1: $|\mu| \leq 1$. We call μ a distribution if $|\mu| = 1$. We let **Dist**(*A*) denote the set of *sub-distributions* over *A*.

Given a sub-distribution $\mu \in \text{Dist}(A_1 \times A_2)$ over a product, its left and right marginals, $\pi_1(\mu)$ and $\pi_2(\mu)$, are sub-distributions over A_1 and A_2 , respectively, which are given by $\pi_1(\mu)(x_1) = \sum_{x_2 \in X} \mu(x_1, x_2)$, and $\pi_2(\mu)(x_2) = \sum_{x_1 \in X} \mu(x_1, x_2)$.

The *Dirac distribution* $\delta(a) \in \text{Dist}(A)$ is the point distribution at $a \in A$, $\delta(a)(a') = [a = a']$, where the right-hand-side is an *Iverson-bracket* which evaluates to 1 if the formula inside (in this case, a = a') evaluates to true, and to 0 otherwise. If $f : A \to \mathbb{R}_{\geq 0}^{\infty}$ is a function mapping into the extended reals, we can take its *expected value* $\mathbb{E}_{\mu}[f]$ with respect to some sub-distribution $\mu \in \text{Dist}(A)$: $\mathbb{E}_{\mu}[f] = \sum_{a \in A} f(a) \cdot \mu(a)$. If the sum diverges, the expected value is ∞ . We assume that addition and multiplication are extended in the natural way, with the convention $0 \cdot \infty = \infty \cdot 0 = 0$.

2.2 Programming language and semantics

We work with a standard probabilistic imperative language PWHILE. This language has commands defined by the following grammar:

 $c\coloneqq \mathsf{skip}\mid x\leftarrow e\mid x\xleftarrow{\hspace{0.1cm}{\scriptscriptstyle\bullet}} d\mid c;c\mid \mathsf{if}\ e\ \mathsf{then}\ c\ \mathsf{else}\ c\mid \mathsf{while}\ e\ \mathsf{do}\ c\ .$

Variables x are drawn from an arbitrary but finite set **Var** of variable names. Expressions e are largely standard, formed from variables and basic operations (e.g., integer addition, boolean conjunction). To handle programs with (static) arrays, we assume expressions include basic array operations for accessing and updating. For instance, when a is an array variable we have syntactic sugar:

$$a[e] \triangleq \text{Lookup}(a, e)$$
 (expression) and $a[e] \leftarrow e' \triangleq a \leftarrow \text{Update}(a, e, e')$ (command)

The random sampling command $x \triangleq d$ takes a sample from some primitive distribution d and stores it in x. For simplicity, we assume that primitive distributions do not have free program variables, and we interpret them as full distributions $\llbracket d \rrbracket$: **Dist**(D) over some countable set D, possibly different for different distributions. We will often use the uniform distribution U(S) when S is a finite, non-empty set; for instance, for a positive integer N we will write [N] for the set of integers $\{0, \ldots, N-1\}$, so that $x \triangleq U([N])$ samples each number in [N] with probability 1/N and stores it in x. The distributions can also be parameterized by some more complex expression, for instance in $x \triangleq [y]$ for a program variable y.

PWHILE programs transform *states*, which are finite maps $s: \text{Var} \to D$; we write **State** for the set of all states. The semantics of a program *c* is a map $[c]: \text{State} \to \text{Dist}(\text{State})$ assigning a subdistribution over possible outputs to each input. For example, for the random sampling command, we define

$$(\llbracket x \xleftarrow{s} d \rrbracket s)(s') \triangleq \begin{cases} s(d)(s'(x)) & : s(y) = s'(y) \text{ for all } y \neq x \\ 0 & : \text{ otherwise} \end{cases}$$

The semantics of the remaining language constructs is standard and deferred to the appendix. As we only work with discrete primitive distributions and states have finitely many variables, output distributions programs always have countable support.

To express properties about pairs of states we use *relational expectations*, which are maps of type **State**×**State** $\rightarrow \mathbb{R}_{\geq 0}^{\infty}$; we write **Exp** for the set of all relational expectations. This set is equipped with the pointwise order inherited from the order on $\mathbb{R}_{\geq 0}^{\infty}$, i.e., $\mathcal{E} \leq \mathcal{E}'$ if and only if $\mathcal{E}(s_1, s_2) \leq \mathcal{E}'(s_1, s_2)$ for all pairs (s_1, s_2) of states. Since $\mathbb{R}_{\geq 0}^{\infty}$ is a complete lattice and **Exp** has the pointwise order, **Exp** is also a complete lattice; the top and bottom elements are the constant relational expectations ∞ and 0, which send all pairs of states to ∞ and 0 respectively.

For denoting specific relational expectations, we borrow notation from relational Hoare logic [10]: We tag variables with $\langle 1 \rangle$ or $\langle 2 \rangle$ to refer to their value in the first or the second state, respectively. For instance, $[x\langle 1 \rangle = x\langle 2 \rangle]$ is a relational expectation encoding the predicate $\lambda \langle s_1, s_2 \rangle$. $[s_1(x) = s_2(x)]$.

2.3 Distances between probability distributions

Various notions of distances between distributions allow us to specify sensitivity properties of probabilistic programs. A popular example is the following:

DEFINITION 1 (TOTAL VARIATION DISTANCE). The Total Variation (TV) distance between $\mu_1, \mu_2 \in$ Dist(X) is defined as: $TV(\mu_1, \mu_2) \triangleq \frac{1}{2} \sum_{x \in X} |\mu_1(x) - \mu_2(x)|$.

The term distance (or *metric*) is justified as $TV(\mu_1, \mu_2)$ is symmetric, satisfies the triangle inequality, and maps to zero if and only if $\mu_1 = \mu_2$. The normalization factor of $\frac{1}{2}$ ensures that the TV distance is within [0, 1]. Roughly speaking, the TV distance measures the largest difference in probabilities of any event between two given distributions.

Note that the TV distance does not require a metric space, i.e., the underlying set X is not necessarily equipped with any metric. If X is a metric space, we can define:

DEFINITION 2 (KANTOROVICH DISTANCE). Let X be a (extended) metric space with a distance $\mathcal{E}: X \times X \to \mathbb{R}^{\infty}_{>0}$. The Kantorovich distance is a canonical lifting of \mathcal{E} to a function $\mathcal{E}^{\#}: \text{Dist}(X) \times \mathbb{R}^{\infty}$

 $\mathbf{Dist}(X) \to \mathbb{R}^{\infty}_{>0}$ that defines a metric on $\mathbf{Dist}(X)$. This distance is defined as

$$\mathcal{E}^{\#}(\mu_1,\mu_2) = \inf_{\mu \in \Gamma(\mu_1,\mu_2)} \mathbb{E}_{\mu}[\mathcal{E}],$$

where $\Gamma(\mu_1, \mu_2)$ is the set of probabilistic couplings of μ_1, μ_2 , given by

$$\Gamma(\mu_1, \mu_2) = \{ \mu \in \text{Dist}(X \times X) \mid \pi_i(\mu) = \mu_i, \text{ for } i = 1, 2 \}.$$

The set $\Gamma(\mu_1, \mu_2)$ is non-empty provided $|\mu_1| = |\mu_2|$. Otherwise, $\Gamma(\mu_1, \mu_2) = \emptyset$ and $\mathcal{E}^{\#}(\mu_1, \mu_2) = \infty$.

The coupling-based definition of the Kantorovich distance is more abstract than other distances between distributions, but its generality turns out to be a strength. First, we can recover the TV distance as a lifting of the discrete metric:

THEOREM 1 (TOTAL VARIATION AND KANTOROVICH DISTANCE). Let $\mu_1, \mu_2 \in \text{Dist}(X)$ such that $|\mu_1| = |\mu_2| = 1$. If the discrete metric $\mathcal{E}: X \times X \to \{0, 1\}$ is given by $\mathcal{E}(x_1, x_2) = [x_1 \neq x_2]$, then $TV(\mu_1, \mu_2) = \mathcal{E}^{\#}(\mu_1, \mu_2)$.

Another advantage of the Kantorovich distance is that it is defined as an infimum. For our goal of proving continuity, it suffices to compute an upper bound of the distance, which corresponds to determining $\mathbb{E}_{\mu}[\mathcal{E}]$ for some particular coupling μ .

Traditionally, the definition of $\mathcal{E}^{\#}$ is restricted to functions \mathcal{E} defining a metric on X. However, the definition of $\mathcal{E}^{\#}$ extends *mutatis mutandis* to arbitrary functions \mathcal{E} . We abuse terminology and use the term Kantorovich distance also in the more general case. For instance, we can use this more general notion to bound the difference between the expected values of two functions on the outputs of two program runs:

THEOREM 2 (ABSOLUTE EXPECTED DIFFERENCE). Let $\mu_1, \mu_2 \in \text{Dist}(X)$ such that $|\mu_1| = |\mu_2| = 1$, and let $f_1, f_2: X \to \mathbb{R}_{\geq 0}^{\infty}$. Let $\mathcal{E}: X \times X \to \mathbb{R}_{\geq 0}^{\infty}$ be defined by $\mathcal{E}(x_1, x_2) = |f_1(x_1) - f_2(x_2)|$. Then $|\mathbb{E}_{\mu_1}[f_1] - \mathbb{E}_{\mu_2}[f_2]| \leq \mathcal{E}^{\#}(\mu_1, \mu_2)$.

We can also obtain bounds on the TV distance when lifting other base distances that assign a minimum, non-zero distance to all pairs of distinct elements.

THEOREM 3 (SCALED TV DISTANCE). Let $\mu_1, \mu_2 \in \text{Dist}(X)$ with $|\mu_1| = |\mu_2| = 1$, let $\mathcal{E}_{\rho} \colon X \times X \to [0, 1]$, and let $\rho \in \mathbb{R}_{>0}$ be a strictly positive constant with $\mathcal{E}_{\rho}(x_1, x_2) \ge \rho \cdot [x_1 \neq x_2]$. Then, $TV(\mu_1, \mu_2) \le \frac{1}{\rho} \cdot \mathcal{E}_{\rho}^{\#}(\mu_1, \mu_2)$.

3 BOUNDING EXPECTED SENSITIVITY WITH RELATIONAL PRE-EXPECTATIONS

As we have seen, the Kantorovich distance encompasses many specific distances on distributions. To reason about probabilistic and expected sensitivity, we would like to bound the Kantorovich distance between two output distributions in terms of the distance between two program inputs. In this section, we develop a relational pre-expectation operation to prove these bounds.

3.1 A first unsuccessful attempt: a relational pre-expectation for exact bounds

Since we want to reason about the Kantorovich distance lifting of a relational expectation \mathcal{E} : State × State $\rightarrow \mathbb{R}^{\infty}_{\geq 0}$ between output distributions of a program *c*, an initial idea is to define a relational pre-expectation operator *rpe*(*c*, \mathcal{E}) coinciding exactly with the Kantorovich distance:

$$rpe(c, \mathcal{E})(s_1, s_2) = \mathcal{E}^{\#}([\![c]\!]s_1, [\![c]\!]s_2),$$

and then prove bounds of the form $rpe(c, \mathcal{E}_{out}) \leq \mathcal{E}_{in}$ in order to bound the Kantorovich distance between outputs by some distance between inputs. While this definition is appealing, it turns out to be inconvenient for formal reasoning because it does not behave well under sequential composition:

the expected sequence rule $rpe(c; c', \mathcal{E}) = rpe(c, rpe(c', \mathcal{E}))$ does *not* hold. Roughly, this is because choosing local infima on each step does not necessarily amount to a global infimum. In fact, in some cases *no local choice* amounts to a *global infimum*.

EXAMPLE 1. The Bernoulli distribution B(p) with bias p returns 1 with probability p and 0 with probability 1-p. Consider the following programs:

Moreover, consider the relational expectation $\mathcal{E} = [x\langle 1 \rangle \neq x\langle 2 \rangle \lor y\langle 1 \rangle \neq y\langle 2 \rangle]$. *If we fix* $b\langle 1 \rangle =$ true *and* $b\langle 2 \rangle =$ false *throughout, then*

$$rpe(c', \mathcal{E})(s'_1, s'_2) = \inf_{\Gamma(\llbracket y \stackrel{\&}{\leftarrow} B^{(1/2)} \rrbracket s'_1, \llbracket x \stackrel{\&}{\leftarrow} B^{(1/2)} \rrbracket s'_2)} \mathbb{E}[\mathcal{E}] .$$

To compute the above relational pre-expectation, we first need to understand the possible couplings. Hence, we compute the marginals of the involved distributions:

$$\mu_1 \triangleq \llbracket y \nleftrightarrow B(1/2) \rrbracket s'_1 = \begin{cases} \frac{1}{2} : x \mapsto s'_1(x), y \mapsto 0\\ \frac{1}{2} : x \mapsto s'_1(x), y \mapsto 1 \end{cases}$$
$$\mu_2 \triangleq \llbracket x \twoheadleftarrow B(1/2) \rrbracket s'_2 = \begin{cases} \frac{1}{2} : x \mapsto 0, y \mapsto s'_2(y)\\ \frac{1}{2} : x \mapsto 1, y \mapsto s'_2(y) \end{cases}$$

The marginal conditions for couplings (Def. 2) then yield that any coupling in $\Gamma(\mu_1, \mu_2)$ is of the form

$$\begin{aligned} \mu_{\rho}(s_1, s_2) &= \rho \cdot [s_1(x) = s_1'(x) \land s_1(y) = 1] \cdot [s_2(x) = 1 \land s_2(y) = s_2'(y)] \\ &+ \left(\frac{1}{2} - \rho\right) \cdot [s_1(x) = s_1'(x) \land s_1(y) = 1] \cdot [s_2(x) = 0 \land s_2(y) = s_2'(y)] \\ &+ \left(\frac{1}{2} - \rho\right) \cdot [s_1(x) = s_1'(x) \land s_1(y) = 0] \cdot [s_2(x) = 1 \land s_2(y) = s_2'(y)] \\ &+ \rho \cdot [s_1(x) = s_1'(x) \land s_1(y) = 0] \cdot [s_2(x) = 0 \land s_2(y) = s_2'(y)] .\end{aligned}$$

for some $0 \le \rho \le \frac{1}{2}$ and the previously fixed states s'_1 and s'_2 . Hence,

$$\mathbb{E}_{\mu_{\rho}}[\mathcal{E}] = \rho \cdot [s_{1}'(x) \neq 1 \lor s_{2}'(y) \neq 1] + \left(\frac{1}{2} - \rho\right) [s_{1}'(x) \neq 0 \lor s_{2}'(y) \neq 1] \\ + \left(\frac{1}{2} - \rho\right) [s_{1}'(x) \neq 1 \lor s_{2}'(y) \neq 0] + \rho \cdot [s_{1}'(x) \neq 0 \lor s_{2}'(y) \neq 0] .$$

Since $rpe(c', \mathcal{E})$ takes the minimum over all couplings, i.e., the minimum over all $\rho \in [0, \frac{1}{2}]$, by simple computation we get that $rpe(c', \mathcal{E})(s'_1, s'_2) = 1/2$, setting $\rho = 1/2$ if $s'_1(x) = s'_2(y)$ and $\rho = 0$ otherwise. Since $s'_1(x), s'_2(y)$ are sampled from $[c]s_1$ and $[c]s_2$, for any way to couple them $rpe(c, rpe(c', \mathcal{E}))(s_1, s_2) = \frac{1}{2} > 0$. However, $[c; c']s_1$ and $[c; c']s_2$ have the same marginal distributions for (x, y) and thus distance 0. Therefore,

$$0 = rpe(c; c', \mathcal{E})(s_1, s_2) < rpe(c, rpe(c', \mathcal{E}))(s_1, s_2) = \frac{1}{2}.$$

Fortunately, we generally do not need to compute the exact Kantorovich distance to prove sensitivity properties: an upper bound suffices. Since the Kantorovich distance is an infimum over *all* couplings, we can establish upper bounds by exhibiting a *specific* coupling—of course, the tightness of these upper bounds will depend on the particular coupling we chose. Crucially, couplings *can* be constructed compositionally: a coupling for a sequential composition c; c' can be obtained by combining a coupling for c with a coupling for c'. We leverage this observation into our compositional relational pre-expectation calculus, which provides upper bounds on the Kantorovich distance.

$$\begin{split} \widetilde{ppe}(\operatorname{skip}, \mathcal{E}) &\triangleq \mathcal{E} \\ \widetilde{ppe}(\operatorname{skip}, \mathcal{E}) &\triangleq \mathcal{E}\{e\langle 1 \rangle, e\langle 2 \rangle / x \langle 1 \rangle, x \langle 2 \rangle\} \\ &\triangleq \lambda s_1 s_2. \mathcal{E}(s_1[x \mapsto e\langle 1 \rangle], s_2[x \mapsto e\langle 2 \rangle]) \\ \widetilde{ppe}(x \Leftrightarrow d, \mathcal{E}) &\triangleq \lambda s_1 s_2. \mathcal{E}^{\#}([x \And d]] s_1, [x \And d]] s_2) \text{, where } \mathcal{E}^{\#}(\mu_1, \mu_2) &\triangleq \inf_{\mu \in \Gamma(\mu_1, \mu_2)} \mathbb{E}_{\mu}[\mathcal{E}] \\ \widetilde{ppe}(c; c', \mathcal{E}) &\triangleq \widetilde{ppe}(c, \widetilde{ppe}(c', \mathcal{E})) \\ \widetilde{ppe}(\operatorname{if} e \operatorname{then} c \operatorname{else} c', \mathcal{E}) &\triangleq [e\langle 1 \rangle \wedge e\langle 2 \rangle] \cdot \widetilde{ppe}(c, \mathcal{E}) + [\neg e\langle 1 \rangle \wedge \neg e\langle 2 \rangle] \cdot \widetilde{ppe}(c', \mathcal{E}) + [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot \infty \\ \widetilde{ppe}(\operatorname{while} e \operatorname{do} c, \mathcal{E}) &\triangleq \operatorname{lpt} X. \Phi_{\mathcal{E}, c}(X), \\ \operatorname{where} \Phi_{\mathcal{E}, c}(X) &\triangleq [e\langle 1 \rangle \wedge e\langle 2 \rangle] \cdot \widetilde{ppe}(c, X) + [\neg e\langle 1 \rangle \wedge \neg e\langle 2 \rangle] \cdot \mathcal{E} + [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot \infty \end{split}$$

Fig. 1. Definition of the relational pre-expectation operator $\widetilde{rpe}(c, \mathcal{E})$.

3.2 Compositional upper bounds by relational pre-expectation

To facilitate compositional reasoning, we define an upper bound $\widetilde{rpe}(c, \mathcal{E})$ of the Kantorovich distance \mathcal{E} with respect to program c. Technically, $\widetilde{rpe}(c, \mathcal{E})$ is a relational pre-expectation calculus defined by induction on the structure of *c*, similarly to the calculus by McIver and Morgan [25]. The rules of our calculus are shown in Figure 1. We take the indicator expectation $[\mathcal{P}]$ to be 1 if \mathcal{P} is true, otherwise 0, and we define addition and multiplication on expectations pointwise. The cases of skipping, assignments and sequential composition are straightforward and apply the backwards semantics of commands. The relational pre-expectation of sampling is expressed directly in terms of the Kantorovich distance, i.e., an infimum is taken over the set of all couplings, which is not always possible in practice. We give more details on this problem in Section 3.3. The relational pre-expectation for conditionals assumes the two runs are synchronized. If not, $[e(1) \neq e(2)] = 1$ and the distance is (trivially) upper bounded by ∞ , since the branches may not terminate with the same probability, so the set of couplings may be empty. Finally, in the case of while loops, we take the least fixed point of the characteristic functional $\Phi_{\mathcal{E},c}$ of the loop. It is not hard to show that $\Phi_{\mathcal{E}, \mathcal{C}}(-)$: Exp \rightarrow Exp is monotonic (see Lemma 3 in the Appendix), so by the Knaster-Tarski theorem the least fixed point is well-defined. As in the previous case, the relational pre-expectation returns ∞ when runs are not synchronized, i.e., only one loop guard is true. Computing the least fixed point is usually not possible. We present an invariant-based rule in Section 3.3.

Remark (Synchronous vs. asynchronous control flow). In contrast to the Kantorovich distance operator $rpe(c, \mathcal{E})$, cour compositional relational pre-expectation operator $\tilde{rpe}(c, \mathcal{E})$ only gives useful (i.e., finite) bounds when the control flows in the two executions of *c* can be *synchronized.* For deterministic guards, this means that pairs of related executions always take the same branches; for randomized guards, this means that we can relate the random samplings so that pairs of related executions always take the same branches. In Section 8, we describe extensions of our calculus that can give more useful bounds when reasoning asynchronously.

Remark (Tightness of bounds). It is also complicated to estimate the exact loss between $\widetilde{rpe}(c, \mathcal{E})$ and $rpe(c, \mathcal{E})$, since lower bounds on $rpe(c, \mathcal{E})$ are not given by a witness coupling. Nonetheless, in our setting this limitation is not exclusive to our technique—in the statistical literature, lower bounds for stochastic processes such as the ones we analyze in Section 6 are in general hard to compute and so the exact distance is often not known. We will return to this topic in Section 7.

We now study the metatheory of our calculus. Our first result is that our calculus is sound: it correctly upper bounds the Kantorovich distance.

$$\begin{split} \frac{\mathcal{E} \leq \mathcal{E}'}{\widetilde{rpe}(c,\mathcal{E}) \leq \widetilde{rpe}(c,\mathcal{E}')} & \text{Mono} & \frac{FV(\mathcal{E}') \cap MV(c) = \emptyset}{\widetilde{rpe}(c,\mathcal{E}) + \mathcal{E}'} & \text{Const} \\ \hline \\ \overline{\widetilde{rpe}(c,\mathcal{E}) \leq \widetilde{rpe}(c,\mathcal{E}')} & \text{SupAdd} & \frac{f: \mathbb{R}_{\geq 0} \to \mathbb{R}_{\geq 0} \text{ linear, with } f(\infty) \triangleq \infty}{\widetilde{rpe}(c,\mathcal{E}) + \widetilde{rpe}(c,\mathcal{E})} & \text{Scale} \\ \hline \\ \frac{M: \text{ State} \times \text{State} \times \text{State} \to \Gamma(\llbracket d \rrbracket, \llbracket d \rrbracket)}{\widetilde{rpe}(x \ll d, \mathcal{E}) \leq \mathbb{E}_{(v_1, v_2) \sim M(-, -)} [\mathcal{E}\{v_1, v_2/x\langle 1 \rangle, x\langle 2 \rangle\}]} & \text{Samp} \\ \hline \\ \frac{f: \text{ State} \times \text{State} \to (D \to D) \text{ bijection}}{\widetilde{rpe}(x \And U(D), \mathcal{E}) \leq \frac{1}{|D|} \sum_{v \in D} \mathcal{E}\{v, f(-, -)(v)/x\langle 1 \rangle, x\langle 2 \rangle\}} & \text{UNIF} \\ \hline \\ \frac{[e\langle 1 \rangle \wedge e\langle 2 \rangle] \cdot \widetilde{rpe}(c, I) + [\neg e\langle 1 \rangle \wedge \neg e\langle 2 \rangle] \cdot \mathcal{E} + [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot \infty \leq I}{\widetilde{rpe}(\text{while } e \text{ do } c, \mathcal{E}) \leq I} & \text{Inv} \end{split}$$

Fig. 2. Properties of relational pre-expectation operator $\widetilde{rpe}(c, \mathcal{E})$.

THEOREM 4 (SOUNDNESS OF \widetilde{rpe}). Let c be a PWHILE program and $\mathcal{E} \in \mathbf{Exp}$ be a relational expectation. Then $rpe(c, \mathcal{E}) \leq \widetilde{rpe}(c, \mathcal{E})$, i.e., if $\widetilde{rpe}(c, \mathcal{E})(s_1, s_2) < \infty$ for $s_1, s_2 \in \mathbf{State}$ then

 $\mathbb{E}_{\mu_{s_1,s_2}}[\mathcal{E}] \leq \widetilde{rpe}(c,\mathcal{E})(s_1,s_2) \quad \text{for some coupling} \quad \mu_{s_1,s_2} \in \Gamma(\llbracket c \rrbracket s_1, \llbracket c \rrbracket s_2) \;.$

PROOF SKETCH. By induction on *c*. The most challenging cases are for sampling and loops. The case for sampling requires first showing that there exists a coupling realizing the infimum defining the Kantorovich distance; such existence results belong to the theory of optimal transport [32].

The case for loops is challenging for another reason: it is not clear how to show that the preexpectation operator is continuous in its second argument (but see Thm. 5). Instead, our proof relies on extracting a convergent sequence of couplings. We defer the details to Appendix D. \Box

While it is not clear whether our relational pre-expectation operator is continuous for *all* programs, continuity does hold for programs that sample from *finite* distributions. Note that such programs can still produce distributions with infinite support by sampling in a loop.

THEOREM 5 (CONTINUITY OF \widetilde{rpe}). Let c be a PWHILE program where all primitive distributions have finite support, and let $\mathcal{E}_n \in \operatorname{Exp}$ for $n \in \mathbb{N}$ be a monotonically increasing chain of relational expectations converging pointwise to $\mathcal{E} \in \operatorname{Exp}$. Then,

$$\widetilde{rpe}(c, \mathcal{E}) = \sup_{n \in \mathbb{N}} \widetilde{rpe}(c, \mathcal{E}_n).$$

PROOF SKETCH. By induction on the structure of c. The most challenging case is for sampling instructions, where the proof depends on a continuity property for the Kantorovich distance. We establish this property for distributions with finite support, and complete the proof of continuity for relational pre-expectations. We defer details to Appendix D.

3.3 Reasoning with relational pre-expectations

The definition of \widetilde{rpe} in Fig. 1 is sufficient to prove relational properties of probabilistic programs in theory, but there are some practical obstacles:

• Comparing different relational pre-expectations for the same program is difficult—using the definition to compute each relational pre-expectation separately is tedious.

- Computing the relational pre-expectation for random sampling is difficult: it requires computing a minimum over all couplings.
- Computing the relational pre-expectation for loops is also difficult: in general, it is not possible to compute the least fixed point in closed form.

To make our operator easier to use, we introduce a collection of auxiliary properties in Fig. 2. We briefly describe the rules below.

Basic properties. The first four rules are basic properties of relational pre-expectations. Rule MONO states that the \tilde{rpe} transformer is monotone, and CONST intuitively states that the relational pre-expectation of \mathcal{E} is \mathcal{E} if c doesn't modify \mathcal{E} ; the rule is carefully stated to behave correctly when $\tilde{rpe}(c, \mathcal{E})$ is infinite.

The next two rules encode linearity-like properties of relational pre-expectations. SUPADD states that the property is super-additive: the relational pre-expectation of a sum can be greater than the sum of the relational pre-expectations. Intuitively, this is because $\widetilde{rpe}(c, \mathcal{E})$ involves an infimum for random sampling, and the infimum of a sum is always less than the sum of the infima. SCALE states that the relational pre-expectation is preserved by scaling. The requirement that the scaling function satisfies $f(\infty) = \infty$ is needed for correctly handle scaling by 0: $\widetilde{rpe}(c, \mathcal{E})$ may be infinite, even if \mathcal{E} is identically zero.

Bounding the pre-expectation for sampling. Using the Kantorovich distance for defining the relational pre-expectation of a sampling command $x \stackrel{\$}{\leftarrow} d$ is theoretically clean, but inconvenient in practice for two reasons. First, the set of couplings $\Gamma(\llbracket x \stackrel{\$}{\leftarrow} d \rrbracket s_1, \llbracket x \stackrel{\$}{\leftarrow} d \rrbracket s_2)$ over which the infimum is computed is a set of distributions over pairs of states. Given denotations of primitive distributions $\llbracket d \rrbracket \in \text{Dist}(D)$, it would be more convenient to reason about the set $\Gamma(\llbracket d \rrbracket, \llbracket d \rrbracket)$ —this is a set of distributions over pairs of sampled values $D \times D$, rather than pairs of memories. Second, computing the infimum is often difficult, and moreover unnecessary for establishing upper bounds.

Corresponding to the SAMP rule, the following result states that we can actually upper bound this Kantorovich distance by picking *any* coupling of the primitive distribution with itself; we call such a function M: **State** \times **State** $\rightarrow \Gamma(\llbracket d \rrbracket, \llbracket d \rrbracket)$ a *coupling function* (on *d*).

PROPOSITION 6. Let d be a primitive distribution, and let M be a coupling function on d. For any relational expectation $\mathcal{E} \in \text{Exp}$, we have:

$$\widetilde{rpe}(x \notin d, \mathcal{E}) \leq \mathbb{E}_{(v_1, v_2) \sim M(-, -)}[\mathcal{E}\{v_1, v_2/x\langle 1 \rangle, x\langle 2 \rangle\}]$$

We can reuse common couplings of primitive distributions across different proofs. For example, let D be a finite, non-empty set and let f: **State** × **State** → $(D \rightarrow D)$ map pairs of program states to bijections on D. Then the *bijection coupling* M_f , the coupling function on U(D) is defined by

$$f(s_1, s_2)(x_1, x_2) = \begin{cases} 1/|D| & : f(s_1, s_2)(x_1) = x_2 \\ 0 & : \text{ otherwise} \end{cases}$$

where x_1 and x_2 are elements in *D*. Specialized to this case, Proposition 6 gives UNIF:

$$\begin{split} \widetilde{rpe}(x \leftarrow U(D), \mathcal{E}) &\leq \widetilde{rpe}(x \leftarrow d, \mathcal{E}) \leq \mathbb{E}_{(v_1, v_2) \sim M_f(-, -)}[\mathcal{E}\{v_1, v_2/x\langle 1 \rangle, x\langle 2 \rangle\}] \\ &\leq \mathbb{E}_{v \sim \llbracket U(D) \rrbracket} [\mathcal{E}\{v, f(-, -)(v)/x\langle 1 \rangle, x\langle 2 \rangle\}] \\ &= \frac{1}{|D|} \sum_{v \in D} \mathcal{E}\{v, f(-, -)(v)/x\langle 1 \rangle, x\langle 2 \rangle\} \,. \end{split}$$

Different coupling functions can give upper bounds of different strengths—selecting appropriate couplings to show the target property is the key part of reasoning by couplings. This technique is well-known to probability theory, where it is called the *coupling method* [1].

Bounding the pre-expectation for loops. As in the case of sampling, it may not always be desirable or possible to compute the fixed point for loops. Instead, we can upper bound the relational pre-expectation by a relational expectation I, called an *invariant*—intuitively, if the relational pre-expectation of I with respect to the loop body is at most I, then the relational pre-expectation of the loop is also at most I. Formally, this reasoning is captured by INV and the following theorem:

THEOREM 7. Let $I \in Exp$ be a relational expectation. If

$$[e\langle 1\rangle \wedge e\langle 2\rangle] \cdot \widetilde{rpe}(c, \mathcal{I}) + [\neg e\langle 1\rangle \wedge \neg e\langle 2\rangle] \cdot \mathcal{E} + [e\langle 1\rangle \neq e\langle 2\rangle] \cdot \infty \leq \mathcal{I},$$

then $\widetilde{rpe}($ while $e \operatorname{do} c, \mathcal{E}) \leq I$.

PROOF. Let Φ be the characteristic functional of the loop, as defined for the relational preexpectation. The hypothesis implies $\Phi(\mathcal{I}) \leq \mathcal{I}$, so \mathcal{I} is a prefixed point of Φ . By Park induction [28], the least fixed point $\widetilde{rpe}(\text{while } e \text{ do } c, \mathcal{E})$ is less than \mathcal{I} .

3.4 Embedding **EpRHL**

Expectation Probabilistic Relational Hoare Logic (\mathbb{E} PRHL) is a quantitative extension of PRHL [7]. Judgments of \mathbb{E} PRHL are of the form: {*P*; *E*} $c_1 \sim_f c_2$ {*Q*; *E*'} where *P*, *Q* are boolean-valued assertions, \mathcal{E} , \mathcal{E}' are relational expectations, *f* is an affine function of the form ax + b, where $a, b \in \mathbb{R}_{\geq 0}$, and c_1 and c_2 are PWHILE programs. This judgment states that for every pair of input states s_1, s_2 satisfying the pre-condition *P*, there is a coupling μ of $[[c_1]](s_1), [[c_2]](s_2)$ whose support lies within the post-condition *Q*, and moreover $\mathbb{E}_{\mu}[\mathcal{E}'] \leq f(\mathcal{E}(s_1, s_2))$. We can embed the core inference rules of \mathbb{E} PRHL in our proof system (see Appendix E for details).

THEOREM 8 (EMBEDDING EPRHL). Let \vdash {P; E} c ~_f c {Q; E'} be a valid EPRHL judgment derived using the rules of Figure 6 in Appendix E, with finite E and E'. Then:

$$\widetilde{rpe}(c, \mathcal{E}' + [\neg Q] \cdot \infty) \le f(\mathcal{E}) + [\neg P] \cdot \infty.$$

Furthermore, this inequality can be derived using just the definition of $\widetilde{rpe}(c, \mathcal{E})$ for skip, assignment, sequence, and conditionals in Figure 1, and the auxiliary proof rules in Figure 2.

Intuitively, the bound on the relational pre-expectation captures the validity of the original $\mathbb{E}PRHL$ judgment. For any pair of states (s_1, s_2) , if (s_1, s_2) does not satisfy P, then the right-hand side is infinite and the bound trivially holds. If (s_1, s_2) satisfies P, then the right-hand side is finite (since \mathcal{E} is finite) and the relational pre-expectation is finite. This implies that Q must be satisfied almost surely in the coupling and $\widetilde{rpe}(c, \mathcal{E}') \leq f(\mathcal{E})$. This last inequality recovers the $\mathbb{E}PRHL$ judgment's bound on the output distance in terms of the input distance. Furthermore, the embedding shows that the bound is derivable in our calculus without computing infimums over couplings for sampling, or computing least fixed points for loops.

4 WARMUP EXAMPLE: STABILITY OF SGD

To demonstrate our relational pre-expectation operator, we analyze the stability of Stochastic Gradient Descent (SGD) as our warmup example. SGD is a core tool in modern machine learning; SGD is the most common learning algorithm used in practice for training neural networks. Its stability was first established in Hardt et al. [18], and it was later formalized in a relational program logic EPRHL [7]. The corresponding proof in EPRHL involves complex proof rules—our calculus can establish the same property with significantly cleaner reasoning.

	TDO(V)
sgd(S)	$n \leftarrow 0;$
$w \leftarrow w_0;$	while $n < N$ do
$t \leftarrow 0;$	$i \leftarrow 0;$
while $t < T$ do	while $i < S $ do
s ∉ [S];	$a \stackrel{\hspace{0.1em}\scriptscriptstyle\$}{\leftarrow} \pi(i); r \stackrel{\hspace{0.1em}\scriptscriptstyle\$}{\leftarrow} \mathcal{R}(i,a); j \stackrel{\hspace{0.1em}\scriptscriptstyle\$}{\leftarrow} \mathcal{P}(i,a);$
$q \leftarrow \nabla \ell(s, -)(w);$	$W[i] \leftarrow (1 - \alpha) \cdot V[i] + \alpha \cdot (r + \gamma \cdot V[j]);$ $i \leftarrow i + 1$
$w \leftarrow w - \alpha_t \cdot q$:	
$t \leftarrow t + 1$:	$V \leftarrow W; n \leftarrow n+1;$
,	

(a) Stochastic Gradient Descent (SGD)

(b) TD(0) learning algorithm

Fig. 3. Example programs: Stability and convergence

4.1 Background

Let *Z* be a space of labeled *examples*, e.g., images annotated with the main subject. A *learning algorithm* $A: S \to \mathbb{R}^d$ takes a set $S \in Z^n$ of examples as input and produces ("learns") *parameters* $w \in \mathbb{R}^d$. The algorithm is tailored to a given *loss function* $\ell: Z \to \mathbb{R}^d \to [0, 1]$, which describes how well an example is labeled by some parameters. The goal is to find parameters that have low loss on examples.

In machine learning, *uniform stability* is a useful property for learning algorithms. In a nutshell, a randomized learning algorithm *A* is ϵ -*uniformly stable* if for all pairs *S*, *S'* of training sets differing in exactly one example, and for all examples $z \in Z$, the expected losses of z are close:

$$|\mathbb{E}_{A(S)}[\ell(z)] - \mathbb{E}_{A(S')}[\ell(z)]| \le \epsilon .$$

Stable learning algorithms *generalize*: their performance on new, unseen examples is similar to their performance on the training set [11]. In particular, stability controls how much a learning algorithm can *overfit* the training set.

4.2 Verifying stability for stochastic gradient descent

We consider the program **sgd** in Figure 3a. The gradient ∇ is a higher-order function¹ with type $\nabla : (\mathbb{R}^d \to [0, 1]) \to (\mathbb{R}^d \to \mathbb{R}^d)$; we assume that it is well-defined and given. In SGD, the true gradient of a function is approximated by a gradient g at a single sample s. The step sizes α_t (with $t \in \mathbb{N}$) are a sequence of real numbers that control (together with the local gradient g) how to adjust the parameters in each iteration of SGD. Following Hardt et al. [18], we make the following assumptions:

- (1) The loss function ℓ is convex and *L*-Lipschitz in its second argument, i.e., $|\ell(z, w) \ell(z, w')| \le L \cdot ||w w'||$ for all parameters $w, w' \in \mathbb{R}^d$.
- (2) The gradient $\nabla \ell(z, -) : \mathbb{R}^d \to \mathbb{R}^d$ is β -Lipschitz for every $z \in Z$.
- (3) The step sizes satisfy $0 \le \alpha_t \le 2/\beta$.

To show uniform stability, for any two training sets S(1), S(2) differing in one element and every example $z \in Z$, our proof obligation is

$$|\mathbb{E}_{\mathrm{sgd}(S\langle 1\rangle)}[\ell(z)] - \mathbb{E}_{\mathrm{sgd}(S\langle 2\rangle)}[\ell(z)]| \le \gamma L \qquad \text{where } \gamma \triangleq \frac{2L}{n} \sum_{t=0}^{T-1} \alpha_t \,.$$

¹This makes our states non-discrete, but the distributions over them will still have discrete support, since they are generated by a composition of discrete samplings.

Rather than working with the loss function directly, we will first bound the pre-expectation of the distance $||w\langle 1\rangle - w\langle 2\rangle||$ and then use the *L*-Lipschitz property of ℓ to conclude uniform stability. As usual, the main part of the proof is bounding the pre-expectation of the loop. We use the following loop invariant:

$$I \triangleq [t\langle 1 \rangle \neq t\langle 2 \rangle] \cdot \infty + [t\langle 1 \rangle = t\langle 2 \rangle] \cdot \left(\|w\langle 1 \rangle - w\langle 2 \rangle\| + \frac{2L}{n} \sum_{j=t\langle 1 \rangle}^{T-1} \alpha_j \right).$$

By the loop rule (Theorem 7), it suffices to show the following invariant condition:

$$[e\langle 1\rangle \wedge e\langle 2\rangle] \cdot \widetilde{rpe}(bd, I) + [\neg e\langle 1\rangle \wedge \neg e\langle 2\rangle] \cdot ||w\langle 1\rangle - w\langle 2\rangle|| + [e\langle 1\rangle \neq e\langle 2\rangle] \cdot \infty \leq I .$$
(1)

The main case corresponds to the first term, where both loop guards $e\langle 1 \rangle$ and $e\langle 2 \rangle$ are true. To bound the pre-expectation $\widetilde{rpe}(bd, I)$, we consider $\widetilde{rpe}(bd, I) = \widetilde{rpe}(s \triangleq U(S), I')$ where

$$I' \triangleq [t\langle 1 \rangle + 1 \neq t\langle 2 \rangle + 1] \cdot \infty + [t\langle 1 \rangle + 1 = t\langle 2 \rangle + 1] \cdot P, \text{ with}$$
$$P \triangleq \frac{2L}{n} \sum_{j=t\langle 1 \rangle + 1}^{T-1} \alpha_j + \left\| \begin{array}{c} (w\langle 1 \rangle - \alpha_{t\langle 1 \rangle} \nabla \ell(s\langle 1 \rangle, -)(w\langle 1 \rangle)) \\ -(w\langle 2 \rangle - \alpha_{t\langle 2 \rangle} \nabla \ell(s\langle 2 \rangle, -)(w\langle 2 \rangle)) \end{array} \right\|.$$

To handle the random sampling command, we apply the sampling rule (Proposition 6) with the coupling function *M* for the two uniform distributions $[S\langle 1 \rangle]$ and $[S\langle 2 \rangle]$ induced by the bijection $f : S\langle 1 \rangle \rightarrow S\langle 2 \rangle$ mapping the differing example in $S\langle 1 \rangle$ to its counterpart in $S\langle 2 \rangle$, and fixing all other examples. We then have $\widetilde{rpe}(s \stackrel{\text{s}}{\leftarrow} U(S), I') \leq I''$, where

$$\begin{split} I'' &\triangleq \left[t\langle 1 \rangle + 1 \neq t\langle 2 \rangle + 1 \right] \cdot \infty + \left[t\langle 1 \rangle + 1 = t\langle 2 \rangle + 1 \right] \cdot P', \text{ with} \\ P' &= \frac{2L}{n} \sum_{j=t\langle 1 \rangle + 1}^{T-1} \alpha_j + \frac{1}{n} \sum_{s \in S\langle 1 \rangle}^{n-1} \left\| \begin{array}{c} (w\langle 1 \rangle - \alpha_{t\langle 1 \rangle} \nabla \ell(s, -)(w\langle 1 \rangle)) \\ -(w\langle 2 \rangle - \alpha_{t\langle 2 \rangle} \nabla \ell(f(s), -)(w\langle 2 \rangle)) \end{array} \right\| \end{split}$$

We focus on the terms of the last sum. Using the *L*-Lipschitz property of ℓ , when *s* is the differing example, we can bound the absolute difference by $||w\langle 1\rangle - w\langle 2\rangle|| + 2\alpha_{t\langle 1\rangle}L$. When *s* is not the differing example, we have $s\langle 1\rangle = s\langle 2\rangle$. By the β -Lipschitz property of $\nabla \ell$, convexity, and $0 \le \alpha_t \le 2/\beta$, we can bound each of the terms by $||w\langle 1\rangle - w\langle 2\rangle||$. Combining the two cases gives

$$\widetilde{rpe}(bd, I) \leq \left(\|w\langle 1\rangle - w\langle 2\rangle\| + \frac{2L}{n} \sum_{j=t\langle 1\rangle}^{T-1} \alpha_j \right)$$

for all input states with $t\langle 1 \rangle = t\langle 2 \rangle$ and $e\langle 1 \rangle \wedge e\langle 2 \rangle$. This establishes (1). Theorem 7 gives

$$\widetilde{rpe}($$
while e do bd , $||w\langle 1\rangle - w\langle 2\rangle||) \leq I$.

Finally, taking the pre-expectations of both sides with respect to the initial assignments yields

$$\widetilde{rpe}(\operatorname{sgd}(S), \|w\langle 1\rangle - w\langle 2\rangle\|) \leq \frac{2L}{n} \sum_{j=0}^{T-1} \alpha_j = \gamma,$$

when S(1) and S(2) differ in exactly one training example. Since ℓ is *L*-Lipschitz, we conclude

$$\widetilde{rpe}(\operatorname{sgd}(S), |\ell(z, w)\langle 1 \rangle - \ell(z, w)\langle 2 \rangle|) \leq \gamma L$$

for any example $z \in Z$. By Theorem 2, the expected losses are at most γL apart:

$$|\mathbb{E}_{\mathrm{sgd}(S\langle 1\rangle)}[\ell(z)] - \mathbb{E}_{\mathrm{sgd}(S\langle 2\rangle)}[\ell(z)]| \leq \gamma L \, ,$$

and so SGD satisfies γL -uniform stability.

REMARK. This stability bound for SGD was previously verified in the program logic $\mathbb{E}PRHL$ [7], using a complex rule for sequential composition (SEQCASE) that required bounding the probability of selecting two differing examples. Our proof using \overline{rpe} is much simpler, involving just compositional reasoning for sequencing and a loop invariant.

REMARK. While our calculus was designed for probabilistic programs, it is also a useful tool for proving relational properties of deterministic programs. In the Appendix G, we show how to prove a sensitivity bound for projected gradient descent, a deterministic version of SGD.

5 EXAMPLE: CONVERGENCE OF REINFORCEMENT LEARNING ALGORITHMS

In the previous section, the stability guarantee weakens as the program progresses: starting from two initially-equal parameter settings, the learned parameters may drift apart as SGD runs for more iterations. In the following two sections, we will apply our technique to prove a different style of guarantee: probabilistic convergence of two outputs, starting from two different inputs. Our first example shows convergence for a classical algorithm from Reinforcement Learning (RL) [31], guided by a novel analysis by Amortila et al. [2].

5.1 Background

In the standard reinforcement learning setting, an agent (the learning algorithm) repeatedly interacts with the environment, a Markov Decision Process (MDP) with *state* space S. At each step, the agent chooses an *action* from a set \mathcal{A} . The MDP draws a numeric *reward* according to a function $\mathcal{R} : S \times \mathcal{A} \to \text{Dist}([0, R])$, and transitions to a new random state drawn from a *transition* function $\mathcal{P} : S \times \mathcal{A} \to \text{Dist}(S)$. The current state of the process is known to the learner–imagine the current position of a chessboard–but the exact reward and transition functions (\mathcal{R}, \mathcal{P}) are not known. Given black-box access to \mathcal{R} and S, the goal of the learner is to find a policy map $\pi : S \to \mathcal{A}$ that maximizes the learner's expected reward when interacting with the unknown MDP over an infinite time horizon; estimated rewards in the future are reduced by a discount factor $\gamma \in [0, 1)$ for each step into the future.

For many approaches to learning the optimal policy, an important requirement is estimating the *value function* $V : S \rightarrow [0, R]$ of the MDP, i.e., the expected reward at each state if the agent were to repeatedly act according to some given policy π . *Temporal difference (TD)* learning is one approach to estimating the value function [31]. In brief, a TD learner maintains an estimate of Vand loops through states in S. At each state s, the learner selects an action $a \sim \pi(s)$, draws a reward $r \sim \mathcal{R}(s, a)$, and draws a transition $s' \sim \mathcal{R}(s, a)$. Then, the estimate V(s) is updated by incorporating the observed reward r and the estimated value V(s') of the new state.

Figure 3b shows one simple approach, known as TD(0). We assume that the program takes only one argument *V*, the initial estimate of the value function. All other parameters are assumed to be fixed: the current policy π , the reward and transition functions \mathcal{R} and \mathcal{P} , the discount factor γ , the step size $\alpha \in (0, 1)$ —higher α allows *V* to evolve faster–and the number of iterations *N*.

5.2 Verifying convergence for TD0

Since the true value function is not known, the initial estimate V chosen with little information. A natural question is: does the algorithm converge to the same distribution no matter how V is initialized? If so, how fast does convergence happen, as a function of the number of iterations N? To answer these questions, we will verify that **TD0** is contractive on V. More specifically, we will show the bound

$$\widetilde{rpe}(\mathrm{TD0}(V), \|V\langle 1\rangle - V\langle 2\rangle\|_{\infty}) \le k^N \cdot \|V\langle 1\rangle - V\langle 2\rangle\|_{\infty},$$
(2)

where $k \triangleq (1 - \alpha + \alpha \gamma) < 1$. Before we describe the verification, we unpack the guarantee. First, the ∞ -norms are defined by $||V\langle 1\rangle - V\langle 2\rangle||_{\infty} \triangleq \max_{i < |S|} |V\langle 1\rangle[i] - V\langle 2\rangle[i]|$. By Theorem 4, Eq. (2) implies that for any inputs V_1 and V_2 , there exists a coupling μ of the output distributions μ_1 and μ_2 from **TD0**($V\langle 1\rangle$) and **TD0**($V\langle 2\rangle$), such that:

$$k^{N} \cdot \|V_{1} - V_{2}\|_{\infty} \geq \mathbb{E}_{(s_{1}, s_{2}) \sim \mu}[\|s_{1}(V) - s_{2}(V)\|_{\infty}]$$

$$\geq \max_{i < |S|} \mathbb{E}_{(s_{1}, s_{2}) \sim \mu}[|s_{1}(V[i]) - s_{2}(V[i])|]$$

$$\geq \max_{i < |S|} \left| \mathbb{E}_{(s_{1}, s_{2}) \sim \mu}[s_{1}(V[i]) - s_{2}(V[i])] \right|$$

$$= \max_{i < |S|} \left| \mathbb{E}_{s_{1} \sim \mu_{1}}[s_{1}(V[i])] - \mathbb{E}_{s_{2} \sim \mu_{2}}[s_{2}(V[i])] \right|$$
 (by Theorem 2)

In words, the right-hand side of the final line is the maximum difference between the average estimates of V[i] in the two outputs, taking the maximum over all indices *i*. Since k < 1, both sides tend to zero exponentially quickly from any pair of starting states V_1 and V_2 .

Inner loop. We start by analyzing the inner loop w_{in} . We first show that

$$\widetilde{rpe}(w_{in}, \|W\langle 1\rangle - W\langle 2\rangle\|_{\infty}) \le I_{in}$$

for the invariant I_{in} :

$$\begin{split} I_{in} &\triangleq [i\langle 1 \rangle \neq i\langle 2 \rangle] \cdot \infty \\ &+ [i\langle 1 \rangle = i\langle 2 \rangle] \cdot \max_{l < |S|} ([l < i\langle 1 \rangle] \cdot |W\langle 1 \rangle [l] - W\langle 2 \rangle [l]| + [i\langle 1 \rangle \leq l] \cdot k \cdot ||V\langle 1 \rangle - V\langle 2 \rangle ||_{\infty}). \end{split}$$

Let c_{in} be the body, and c_{samp} be the three sampling statements. Applying INV, it suffices to show:

$$[i\langle 1\rangle < |\mathcal{S}| \land i\langle 2\rangle < |\mathcal{S}|] \cdot \widetilde{ppe}(c_{in}, I_{in}) + [i\langle 1\rangle \ge |\mathcal{S}| \land i\langle 2\rangle \ge |\mathcal{S}|] \cdot ||W\langle 1\rangle - W\langle 2\rangle||_{\infty} + [i\langle 1\rangle \ne i\langle 2\rangle] \cdot \infty \le I_{in}$$

The main case is bounding $\widetilde{rpe}(c_{in}, I_{in})$; the other cases are simpler. We describe the overall idea here, deferring details to Appendix F. To bound the relational pre-expectation for the three sampling instructions, we apply the sampling rule SAMP. Since the relational pre-expectation is computed in reverse order, we must choose a coupling for sampling *j* first, then choose a coupling for sampling *r*, and then finally choose a coupling for sampling *a*. We aim to take the identity coupling in each case, ensuring $j\langle 1 \rangle = j\langle 2 \rangle$, $r\langle 1 \rangle = r\langle 2 \rangle$, and $a\langle 1 \rangle = a\langle 2 \rangle$, but there is a small problem: we can only take the identity coupling when samples are taken from the same distributions, e.g., $\mathcal{R}(i\langle 1 \rangle, a\langle 1 \rangle) = \mathcal{R}(i\langle 2 \rangle, a\langle 2 \rangle)$. The invariant assumes $i\langle 1 \rangle = i\langle 2 \rangle$, but we can only ensure $a\langle 1 \rangle = a\langle 2 \rangle$ after we have specified the couplings for *j* and *r*. Accordingly, our coupling functions for SAMP will be of the following form: if $a\langle 1 \rangle = a\langle 2 \rangle$ then we take the identity coupling, otherwise we take the trivial (independent) coupling.

Outer loop. We now turn to the analysis of the outer loop. Consider the invariant:

$$I_{out} \triangleq [n\langle 1 \rangle \neq n\langle 2 \rangle] \cdot \infty + [n\langle 1 \rangle = n\langle 2 \rangle] \cdot k^{(N \ominus n\langle 1 \rangle)} ||V\langle 1 \rangle - V\langle 2 \rangle||_{\infty},$$

where $N \ominus n$ denotes max(N-n, 0). We compute:

$$\begin{split} \widetilde{rpe}(i \leftarrow 0; w_{in}; V \leftarrow W; n \leftarrow n+1, \mathcal{I}_{out}) \\ &= \widetilde{rpe}(i \leftarrow 0; w_{in}, [n\langle 1 \rangle \neq n\langle 2 \rangle] \cdot \infty + [n\langle 1 \rangle = n\langle 2 \rangle] \cdot k^{(N \ominus (n\langle 1 \rangle + 1))} \|W\langle 1 \rangle - W\langle 2 \rangle\|_{\infty}) \\ &\leq \widetilde{rpe}(i \leftarrow 0, [n\langle 1 \rangle \neq n\langle 2 \rangle] \cdot \infty + [n\langle 1 \rangle = n\langle 2 \rangle] \cdot k^{(N \ominus (n\langle 1 \rangle + 1))} \cdot \mathcal{I}_{in}) \\ &\leq [n\langle 1 \rangle \neq n\langle 2 \rangle] \cdot \infty + [n\langle 1 \rangle = n\langle 2 \rangle] \cdot k \cdot k^{(N \ominus (n\langle 1 \rangle + 1))} \|V\langle 1 \rangle - V\langle 2 \rangle\|_{\infty} = \mathcal{I}_{out} \end{split}$$

where the last step holds because $I_{in} = k \cdot ||V\langle 1\rangle - V\langle 2\rangle||_{\infty}$ when i = 0. This establishes the outer invariant. Computing the pre-expectation of the first initialization, we conclude:

 $\widetilde{rpe}(\mathbf{TD0}(V), \|V\langle 1\rangle - V\langle 2\rangle\|_{\infty}) \le k^N \cdot \|V\langle 1\rangle - V\langle 2\rangle\|_{\infty} .$

6 EXAMPLE: RANDOM WALKS AND CARD SHUFFLES

In this section, we verify more challenging examples of probabilistic convergence from the theory of Markov chains, formalizing arguments by Aldous [1] in his seminal work introducing the coupling method. Our use of relational pre-expectations is similar in spirit to the previous section, but there are two key differences: (1) we aim to prove convergence under Total Variation (TV) distance, which is the standard notion of distance in this field, and (2) our arguments will require selecting more complex couplings, instead of just the identity coupling.

6.1 Preliminaries: Card shuffling and Markov chain mixing

Distributions that are easy to describe can be surprisingly difficult to sample from. For instance, consider the uniform distribution over all permutations of a deck of playing cards. It is not clear how to sample from this distribution—i.e., perform a *perfect shuffle*—but we can implement a card shuffle algorithm that executes a sequence of simple randomized steps (e.g. swapping pairs of cards) and hope that after a small number steps, we will produce a shuffle that is close to uniform.

Abstracting a bit, card shuffling algorithms are a representative example of random walks for approximating complex distributions. This is a technique with a long history, combining elements of probability theory with statistical physics; and it is the basis of many heuristic algorithms used today, e.g., Markov Chain Monte Carlo (MCMC). From a theoretical perspective, the central question is: *how fast do these processes converge to their target distribution*? How many steps do we need to get within ϵ distance of the uniform distribution on shuffles?

Random walks and card shuffling algorithms are classical examples of *Markov chains*. A finite, discrete-time Markov chain is defined by a finite state space Σ and a transition function $P: \Sigma \to \text{Dist}(\Sigma)$. Given an initial state σ , the associated Markov process $\{X_k^\sigma\}_{k \in \mathbb{N}}$ is a sequence of distributions such that $X_0^\sigma = \delta(\sigma)$ and $X_{k+1}^\sigma(\tau') = \sum_{\tau} X_k^\sigma(\tau) \cdot P(\tau, \tau')$. For example, the state space Σ could be the set of all permutations of a deck of cards, and the transition function τ could describe randomly splitting the deck and interleaving the halves.

Consider the TV distance v(k) between two state distributions after running k steps from two states σ , τ , i.e., $v(k) \triangleq \max_{\sigma,\tau} TV(X_k^{\sigma}, X_k^{\tau})$. If v(k) tends to 0, then there exists a unique *stationary* distribution η such that $\eta(\sigma) \cdot P(\sigma, \sigma') = \eta(\sigma')$; typically, η will be the target distribution we are trying to sample from. Furthermore, v(k) provides an upper bound on the distance between the state distribution after k steps to the stationary distribution η :

$$\max_{\sigma} TV(X_t^{\sigma}, \eta) \le v(k) \; .$$

While it is usually not possible to derive v(k) exactly, we can upper-bound v(k) by constructing couplings of $(X_t^{\sigma}, X_t^{\tau})$ and applying Theorems 1 and 3. In this way, we can prove bounds on the number of steps needed to get within some distance of the target distribution.

6.2 Warmup: Hypercube walk

We start off with a (rather naive) random walk for sampling N uniformly random bits, which serves as a toy version of the more complex random walks we will see later. Our *position* is a string of Nbits (which can be regarded as a vertex of an N-dimensional *hypercube*). On every iteration of the walk we uniformly sample from $\{0, ..., N\}$. Note that there are N + 1 possible draws, but only Ncoordinates: if we sample 0, then we do not move, otherwise we reverse the sampled coordinate i in

the current position. We will show that starting from any two positions, the process *mixes rapidly*, i.e. starting from any position we will quickly reach the uniform distribution over positions.

Let $e(i) = (0, ..., 1, ..., 0) \in \{0, 1\}^N$ be the position where all coordinates are set to zero except for coordinate *i*, which is set to one. We also write \oplus for xor applied coordinate-wise. We can model *K* steps of the random walk with the following simple PWHILE program:

$$\begin{aligned} \mathbf{hWalk}(pos, N, K) \\ k \leftarrow 0; \\ \mathbf{while} \ k < K \ \mathbf{do} \\ i \xleftarrow{s} U([N+1]); \\ \mathbf{if} \ i \neq 0 \ \mathbf{then} \ pos \leftarrow pos \oplus e(i); \\ k \leftarrow k+1 \end{aligned}$$

Consider two program runs, started at pos(1) and pos(2) respectively. Let d_H be normalized Hamming distance between the two positions:

$$d_H \triangleq rac{1}{N} \sum_{i=1}^N [pos\langle 1 \rangle [i] \neq pos\langle 2 \rangle [i]] \; .$$

That is, d_H equals the fraction of coordinates where pos(1) and pos(2) differ. Let $C(pos(1), pos(2)) \subseteq [N]$ be the set of differing coordinates. We specify a coupling on U([N+1]) by giving a bijection on [N+1]. There are three cases:

- (1) $d_H \ge 2/N$: Let $C(pos(1), pos(2)) = \{i_0, \ldots, i_{m-1}\}$. Take the bijection that behaves like the identity on $[N+1] \setminus C(pos(1), pos(2))$ and that, for all $0 \le n \le m$, maps i_n to i_{n+1} , where we set $i_m = i_0$.
- (2) $d_H = 1/N$: Take the bijection exchanging the differing coordinate and 0.
- (3) $d_H = 0$: Take the identity bijection.

The coupling captures the following intuition. When $d_H \ge 2/N$, the distance decreases by 2/N if we select a differing coordinate; otherwise, it remains unchanged. Likewise when $d_H = 1/N$, if we select the differing coordinate or 0, then the distance decreases by 1/N (to 0); otherwise, the distance remains unchanged.

We can analyze the program **hWalk** using our relational pre-expectation calculus. Let the target relational expectation be d_H . The main step in the reasoning is to select a relational invariant for the loop. We define:

$$I \triangleq [k\langle 1 \rangle \neq k\langle 2 \rangle] \cdot \infty + [k\langle 1 \rangle = k\langle 2 \rangle] \cdot d_H \cdot \left(\frac{N-1}{N+1}\right)^{K \ominus k\langle 1 \rangle}$$

Then, we can verify for the loop while k < K do *bd* of program hWalk that

$$\begin{split} & [(k\langle 1\rangle < K\langle 1\rangle) \land (k\langle 2\rangle < K\langle 2\rangle)] \cdot \widetilde{rpe}(bd, I) \\ + & [(k\langle 1\rangle \ge K\langle 1\rangle) \land (k\langle 2\rangle \ge K\langle 2\rangle)] \cdot d_H \\ + & [(k\langle 1\rangle < K\langle 1\rangle) \ne (k\langle 2\rangle < K\langle 2\rangle)] \cdot \infty \qquad \leq \quad I, \end{split}$$

and conclude by the loop rule (Theorem 7):

$$\widetilde{rpe}($$
while $k < K \text{ do } bd, d_H) \leq I$.

The main step here is showing that

$$\left[(k\langle 1 \rangle < K\langle 1 \rangle) \land (k\langle 2 \rangle < K\langle 2 \rangle) \right] \cdot \widetilde{rpe}(bd, I) \leq \left[(k\langle 1 \rangle < K\langle 1 \rangle) \land (k\langle 2 \rangle < K\langle 2 \rangle) \right] \cdot I ,$$

where we use the fact that the coupling described above makes d_H decrease.

rTrans(deck, N, K)rTop(deck, N, K)riffle(deck, N, K) $k \leftarrow 0$: $k \leftarrow 0;$ $k \leftarrow 0;$ while k < K do while k < K do while k < K do $p \notin U([N]);$ $p \notin U([N]); p' \notin U([N]);$ $b \notin U(\{0,1\}^N);$ $deck \leftarrow shiftR(deck, p);$ $c \leftarrow deck[p]; c' \leftarrow deck[p'];$ $top \leftarrow deck(\bar{b});$ $k \leftarrow k + 1;$ $deck[p] \leftarrow c'; deck[p'] \leftarrow c;$ *bot* \leftarrow *deck*(*b*); $k \leftarrow k + 1;$ $deck \leftarrow cat(top, bot);$ $k \leftarrow k + 1;$

Fig. 4. Shuffling algorithms

Pushing the invariant past the initialization instruction $k \leftarrow 0$ yields:

$$\widetilde{rpe}(\mathbf{hWalk}(pos, N, K), d_H) \le \widetilde{rpe}(k \leftarrow 0, \mathcal{I}) = \left(\frac{N-1}{N+1}\right)^K$$

Since the distance d_H takes distance at least 1/N on pairs of distinct positions, by Theorem 3 the TV distance between the distributions over positions satisfies

$$\begin{aligned} \upsilon(K,N) &= \max_{p_1,p_2 \in \{0,1\}^N} TV(\llbracket \mathbf{hWalk} \rrbracket(p_1,N,K), \llbracket \mathbf{hWalk} \rrbracket(p_2,N,K)) \\ &\leq N \left(1 - \frac{2}{N+1}\right)^K. \end{aligned}$$

Plugging in specific values gives concrete bounds between the two output distributions. Let $\rho > 1$. To achieve a bound of $O(1/\rho)$ on the right hand side, we need to take $K \ge (1/2)N \log(N\rho)$. The inequality above also gives useful asymptotic information; if we set $\rho = N$, and take $K \ge N \log N$, the right-hand side is asymptotically bounded by O(1/N) for large N. We can show that this converges to the uniform distribution over vectors. We provide more details in Section 7. In summary, we have shown the following:

THEOREM 9. Let $K = N \log N$. For any initial position pos,

$$TV\left(\mathbf{hWalk}(pos, N, K), U(\{0, 1\})^N)\right) \in O(1/N)$$
.

6.3 Random-to-top shuffle

For our shuffling examples, we will need some notation. We view a permutation *deck* as a map from positions in $p \in [N]$ to names of cards in $c \in C$; deck[p] denotes the card at position p, while $deck^{-1}(c)$ denotes the position corresponding to card c. Summation over an empty set of indices is treated as zero, while the product over an empty set of indices is treated as one. We outline the arguments here; further details are provided in Appendix F.

For our first card shuffling algorithm we consider the *random-to-top* shuffle. In each iteration, it selects a random position in the deck and moves the card at that position to the top.² We model this shuffle with program **rTop** in Figure 4. For a given input deck of size N, the program repeats K times the process of selecting a random card and moving it to the top. The operation shiftR(*deck*, *j*) takes the block *deck*[0], . . . , *deck*[*j*] and cycles it one position to the right (thus moving *deck*[*j*] to the top), leaving the rest of the deck intact.

 $^{^{2}}$ This algorithm is the time-reversed version of the *top-to-random* shuffle, where the top card is moved to a random position. It is known that a Markov chain's convergence behavior is equivalent to that of its reversed process [1].

We are interested in bounding the distance between the stationary distribution—which in this case is the uniform distribution—and the output distribution after K iterations. We will start with two decks of size N that are both permutations of [N]. As in the hypercube example, we bound the pre-expectation of the normalized Hamming distance:

$$d_{H} \triangleq rac{1}{N} \sum_{i=0}^{N-1} [deck\langle 1
angle[i]
eq deck\langle 2
angle[i]] \,.$$

Note that d_H takes distance at least 1/N on pairs of distinct permutations. If we can show that the pre-expectation of d_H is not too big, then we can apply Theorem 3 to conclude that the final distributions over permutations have a close TV distance. It will be convenient to work with an auxiliary distance:

$$d_M \triangleq (1/N) \cdot \left(N - \max_i \left(\forall j < i.deck \langle 1 \rangle [j] = deck \langle 2 \rangle [j] \right) \right)$$

The idea is that the coupling chooses identical cards on both decks and moves them to the top. This will form a block of matched cards on the top of both decks. Intuitively, d_M measures the fraction of the deck that is not part of this top block. The target distance d_H is upper-bounded by d_M , since d_M counts all cards outside the first block as different. Bounds on d_H follow from bounds on d_M . To bound the pre-expectation of d_M , we take the invariant:

$$I \triangleq [k\langle 1 \rangle \neq k\langle 2 \rangle] \cdot \infty + [k\langle 1 \rangle = k\langle 2 \rangle] \cdot d_M \cdot \left(\frac{N-1}{N}\right)^{K \ominus k\langle 1 \rangle}$$

We can check that it satisfies the inequality

$$[k\langle 1 \rangle < K \land k \langle 2 \rangle < K] \cdot \widetilde{pe}(bd, I) + [k\langle 1 \rangle \ge K \land k \langle 2 \rangle \ge K] \cdot d_H + [(k\langle 1 \rangle < K) \neq (k\langle 2 \rangle < K)] \cdot \infty \le I,$$

where bd is the loop body. The main case is to show the inequality for the first term when both loop guards are true: we need to bound the pre-expectation of I with respect to bd. We can bound

$$\widetilde{rpe}(bd, I) \le d_M \cdot \left(\frac{N-1}{N}\right)^{K \ominus k \langle 1 \rangle}$$

by applying the sampling rule (Proposition 6) with the coupling function M that selects the same card in both decks:

$$M(s_1, s_2)(p_1, p_2) \triangleq \begin{cases} 1/N & : \llbracket deck \rrbracket s_1[p_1] = \llbracket deck \rrbracket s_2[p_2] \\ 0 & : \text{ otherwise.} \end{cases}$$

The idea is that if we pick two cards in the first matched block, which happens with probability $(1-d_M)$, then the distance will remain the same. Otherwise, we will create at least one new matched pair in the first block and the distance will decrease by 1/N. Hence, we can apply the loop rule (Theorem 7) to conclude:

$$\widetilde{rpe}($$
while $k < K$ do $bd, d_H) \leq I$

Computing the pre-expectation of I with respect to the first instruction, we have

$$\widetilde{rpe}(\mathbf{rTop}(deck, N, K), d_H) \le \left(\frac{N-1}{N}\right)^K$$

noting that the distance d_M between the initial decks is at most 1. Since d_H assigns pairs of distinct decks a distance at least 1/N, Theorem 3 implies that the TV distance between the distributions

over decks satisfies:

$$v(K,N) = \max_{d_1, d_2 \in [N]} TV(\llbracket \mathbf{rTop} \rrbracket(d_1, N, K), \llbracket \mathbf{rTop} \rrbracket(d_2, N, K)) \le N \left(\frac{N-1}{N}\right)^K$$

v

For example, if we choose *K* to be $N \log(N\rho)$, then the distance between permutation distributions is bounded by $O(1/\rho)$ for large *N* and $\rho > 1$. By setting $\rho = N$, we have shown the following:

THEOREM 10. Let $K = 2N \log N$, and Perm([N]) be the set of permutations over N. For any initial permutation of deck,

$$TV(\mathbf{rTop}(deck, N, K), U(Perm([N]))) \in O(1/N).$$

6.4 Random transpositions shuffle

Our next shuffle (**rTrans** in Figure 4) repeatedly selects two positions uniformly at random and swaps the cards, allowing for the possibility of swapping a card with itself. As before, let d_H be the normalized Hamming distance between the two decks. We aim to bound $\tilde{rpe}(\mathbf{rTrans}, d_H)$. As before, the key of the proof is finding an invariant for the loop. We take:

$$I \triangleq [k\langle 1 \rangle \neq k\langle 2 \rangle] \cdot \infty + [k\langle 1 \rangle = k\langle 2 \rangle] \cdot d_H \cdot \left(1 - \frac{1}{N^2}\right)^{K \ominus k\langle 1 \rangle}$$

There are two samplings in the loop body, so we need to provide two couplings. For the first sampling p, we use the identity coupling. For the second sampling p', we couple using the bijection induced by the two decks $deck\langle 1 \rangle$ and $deck\langle 2 \rangle$, i.e., the coupling matches every position $p'\langle 1 \rangle$ with the unique position $p'\langle 2 \rangle$ such that $deck[p']\langle 1 \rangle = deck[p']\langle 2 \rangle$. There are three cases: (1) if cards at $p\langle 1 \rangle, p\langle 2 \rangle$ are already matched, d_H remains unchanged; (2) if positions $p'\langle 1 \rangle, p'\langle 2 \rangle$ are equal, d_H remains unchanged; otherwise (3) d_H decreases by 1. This is enough to show that the invariant decreases. We can conclude:

$$\widetilde{rpe}(\mathbf{rTrans}(deck, N, K), d_H) \le \left(1 - \frac{1}{N^2}\right)^K$$

using the fact that d_H between the inputs is at most 1. Since d_H takes value of at least 1/N for pairs of distinct decks, by Theorem 3

$$v(K,N) = \max_{d_1,d_2 \in [N]} TV([[\mathbf{rTrans}]](d_1,N,K), [[\mathbf{rTrans}]](d_2,N,K)) \le N\left(1 - \frac{1}{N^2}\right)^K$$

so the distance between the deck distribution and the uniform distribution decreases as *K* increases. If we take $K \ge N^2 \log(N\rho)$, then the right-hand side is bounded asymptotically by $O(1/\rho)$ for large *N*. By setting $\rho = N$, we conclude:

THEOREM 11. Let $K = 2N^2 \log N$, and Perm([N]) be the set of permutations over N. For any initial permutation of deck,

$$TV(\mathbf{rTrans}(deck, N, K), U(Perm([N]))) \in O(1/N)$$

REMARK. Aldous' [1] bound is slightly sharper: the TV distance between output distributions is bounded by O(1/N) asymptotically already for $K \ge CN^2$ for some constant C. This discrepancy appears because our proofs are carried out compositionally, while Aldous uses a global analysis. However, it is possible that a clever choice of coupling or loop invariant could let us match Aldous' bound.

6.5 Uniform riffle shuffle

In this example we will analyze the uniform riffle shuffle, which is a more realistic model of how cards are shuffled by humans. The shuffle begins by dividing the deck in approximately two halves, and then merges the two halves in an approximately alternating manner. The reversed process, program **riffle** on Figure 4 which we analyze, takes a deck, samples a uniform random bit for each card, and then places all cards labeled with 0 on top of the deck without altering their relative order. After repeating this process *k* times, for every card *i* we have sampled a string of bits $(b_{i,0}, \ldots, b_{i,k-1})$, and card *i* is on top of card *j* if, for some *m*, $b_{i,k} = b_{j,k}, b_{i,k-1} = b_{j,k-1}, \ldots, b_{i,m} = b_{j,m}$ and $b_{i,m-1} < b_{j,m-1}$.

The vector *b* holds *N* bits, indexed by position; \overline{b} negates each entry. We use shorthands for partitioning: deck(b) and $deck(\overline{b})$ represent the sub-permutations from taking all positions where *b* is 0 and 1, respectively. Finally, cat concatenates two permutations.

We will take the coupling that always samples the same bit for the same card on both sides: $b(deck^{-1}(c))\langle 1 \rangle = b(deck^{-1}(c))\langle 2 \rangle$ for every $c \in C$. It is not hard to see that this coupling will eventually make the decks match. However, choosing an appropriate distance takes more care, since the Hamming distance may not always decrease under this coupling. For reasons of space, we leave the details of verification to Appendix G. We can show the following:

THEOREM 12. Let $K = 3 \log N$, and Perm([N]) be the set of permutations over N. For any initial permutation of deck,

 $TV(riffle(deck, N, K), Unif\{Perm([N])\}) \in O(1/N).$

7 EXTENSIONS: PROVING LOWER BOUNDS AND UNIFORMITY

In this section, we describe two extensions to our random walk examples from Section 6: proving that the limit distribution is uniform, and proving lower bounds on the TV distance.

7.1 Convergence to uniform distribution

In Section 6, we showed that the Markov chains correspond to each example converge to a stationary distribution, but we did not shown that this distribution is the uniform distribution over states—if we had made an error in the implementation, the probabilistic program may converge to the wrong distribution. We can use our relational pre-expectation calculus along with Theorem 2 to show that the limit distribution is indeed uniform.

We illustrate the technique for the random-to-top shuffle, but the idea is applicable to all our examples. Consider any two permutations of the deck R_1 , R_2 , and the unary expectations

$$S_1(deck) \triangleq [deck = R_1]$$
 and $S_2(deck) \triangleq [deck = R_2].$

To show that the shuffle converges to uniform, we need to show that the expected values of S_1 and S_2 converge to the same value. Recall that Theorem 2 states that for any initial states s_1 , s_2 ,

$$\left|\mathbb{E}_{\llbracket \mathbf{rTop} \rrbracket s_1}[S_1] - \mathbb{E}_{\llbracket \mathbf{rTop} \rrbracket s_2}[S_2]\right| \le |S_1 - S_2|^{\#} \left(\llbracket \mathbf{rTop} \rrbracket s_1, \llbracket \mathbf{rTop} \rrbracket s_2\right)$$

so it suffices to show that the right hand side converges to zero.

Computing the weakest pre-expectation of $|S_1 - S_2|$ directly is difficult, so we define an alternative distance. We can see R_1 and R_2 as defining a relation (actually, a permutation π over [N]) of pairs $(R_1[i], R_2[i])$ of cards that are at the same positions. We let *d* be the distance defined by:

$$d(deck\langle 1\rangle, deck\langle 2\rangle) \triangleq \sum_{i=0}^{N-1} [(deck\langle 1\rangle[i], deck\langle 2\rangle[i]) \notin \pi].$$

$$\begin{split} & wpe(\mathbf{skip}, \mathcal{E}) \triangleq \mathcal{E} \\ & wpe(x \leftarrow e, \mathcal{E}) \triangleq \mathcal{E}\{e/x\} \\ & wpe(x \leftarrow d, \mathcal{E}) \triangleq \lambda_{\mathcal{S}}.\mathbb{E}_{x \sim d}[\mathcal{E}\{e/x\}] \\ & wpe(c; c', \mathcal{E}) \triangleq wpe(c, wpe(c', \mathcal{E})) \\ \end{split}$$

$$wpe(\text{if } e \text{ then } c \text{ else } c', \mathcal{E}) \triangleq [e] \cdot wpe(c, \mathcal{E}) + [\neg e] \cdot wpe(c', \mathcal{E}) \\ & wpe(\text{while } e \text{ do } c, \mathcal{E}) \triangleq [\text{fp}X.[e] \cdot wpe(c, X) + [\neg e] \cdot \mathcal{E} \end{split}$$

Fig. 5. Definition of the weakest pre-expectation operator $wpe(c, \mathcal{E})$

We can show that $|S_1(deck\langle 1\rangle) - S_2(deck\langle 2\rangle)| \le d(deck\langle 1\rangle, deck\langle 2\rangle)$, since *d* takes non-negative integer values, and whenever d = 0, then S_1 and S_2 can only be true simultaneously. So it suffices to show that the right-hand side converges to zero. This bound can also be established by our pre-expectation calculus in much the same way as in our proof for the random-to-top shuffle, but we use a different coupling. After sampling $p\langle 1\rangle$ on the first execution we just need to pick the $p\langle 2\rangle$ on the second such that $(deck\langle 1\rangle[p\langle 1\rangle], deck\langle 2\rangle[p\langle 2\rangle]) \in \pi$. This makes *d* decrease any time a new match is formed, and once a match is formed and moved to the top, it is never undone. By starting from the same permutation $deck\langle 1\rangle = deck\langle 2\rangle$, this analysis shows that the rate of convergence—this time to the *uniform* distribution—is the same as in our previous analysis of random-to-top: *d* converges to 0 at rate $(1 - 1/N)^K$.

7.2 Proving lower bounds

Previously, we verified upper bounds of the Total Variation distance by using the Kantorovich distance. It is also interesting to compute *lower bounds* on the TV distance, describing how far apart the distributions must be. We consider how to verify these bounds using the *wpe* calculus of McIver and Morgan [25], summarized in Figure 5. We will need an alternative definition of the TV distance expressed in terms of expected values rather than sets:

PROPOSITION 13. Let $\mu_1, \mu_2 \in \text{Dist}(X)$. Then,

$$\sup_{f: X \to [0,1]} |\mathbb{E}_{\mu_1}[f] - \mathbb{E}_{\mu_2}[f]| = \sup_{S \subseteq X} |\mu_1(S) - \mu_2(S)| = TV(\mu_1, \mu_2) .$$

Thus, it suffices to pick any $f: X \to [0, 1]$ and compute its expected values wr.t. μ_1 and μ_2 to get *a* lower bound on $TV(\mu_1, \mu_2)$. This is performed with the *wpe* operator, which takes a program *c* and an *expectation* \mathcal{F} : **State** $\to [0, \infty]$ and computes:

$$wpe(c, \mathcal{F}) = \lambda s.\mathbb{E}_{x \sim [c]s}[\mathcal{F}(c)]$$

Computing lower bounds using *wpe* poses some technical challenges. First, we need to find some expectation f that will achieve a lower bound that is as large as possible. Second, as we are computing a difference of two expected values, we need to be able to compute exact pre-expectations—standard invariant rules for *wpe* only produce *upper bounds* on the expectation. Overcoming the first problem requires ingenuity, but the second problem can be addressed by using a technical result of Kaminski et al. [21]. We start by defining upper and lower invariants.

DEFINITION 3. A family of unary expectations $\{I_n\}_{n \in \mathbb{N}}$ is an upper ω -invariant of the loop while b do c with respect to the expectation \mathcal{F} if

$$[\neg b] \cdot \mathcal{F} \leq I_0$$
 and $[b] \cdot wpe(c, I_n) + [\neg b] \cdot \mathcal{F} \leq I_{n+1}$.

The definition of lower ω -invariant is analogous, reversing the two inequalities.

These invariants can be used to compute exact weakest pre-expectations of loops.

THEOREM 14 (KAMINSKI ET AL. [21, THEOREM 5]). Let I_n and J_n be an upper and a lower ω -invariant of while b do c with respect to \mathcal{F} , respectively. If the limits $\lim_{n\to\infty} I_n$ and $\lim_{n\to\infty} J_n$ exist, then

$$\lim_{n\to\infty} J_n \leq wpe(\text{while } b \text{ do } c, \mathcal{F}) \leq \lim_{n\to\infty} I_n .$$

When the limits coincide, the weakest pre-expectation is determined exactly.

We illustrate our technique on the example from Section 6.2. Let w_H be the expression denoting the normalized Hamming weight of a vector, i.e. $w_H \triangleq (1/N) \sum_{i=0}^{N} pos[i]$. We can use the expected value of w_H to compute a lower bound for the *TV* distance between two runs of **hWalk**. We will compute this expected value by using the usual (unary) pre-expectation calculus. To compute *exact* weakest preconditions, we need to find upper and lower invariants. We consider the following ω -invariant $I_n \triangleq [K - n \le k](\mathcal{B}_k + \mathcal{A}_k \cdot w_H)$, where

$$\mathcal{A}_k \triangleq \left(\frac{N-1}{N+1}
ight)^{K \ominus k} \quad ext{and} \quad \mathcal{B}_k \triangleq rac{1}{N+1} \cdot \sum_{i=0}^{K-k-1} \left(rac{N-1}{N+1}
ight)^i \; .$$

We can check that I_n is both an upper and a lower ω -invariant, therefore the weakest pre-expectation for the loop is exactly $\lim_{n\to\infty} I_n = \mathcal{B}_k + \mathcal{A}_k \cdot w_H$. After computing its pre-expectation with respect to the first assignment, we get:

$$wpe(\mathbf{hWalk}, w_H) = \mathcal{B}_0 + \mathcal{A}_0 \cdot w_H$$

Now, let $W(p) \triangleq (1/N) \sum_{i=0}^{N} p[i]$, and let s_1, s_2 be any two initial states such that $s_1(N) = s_2(N)$ and $s_1(K) = s_2(K)$. By Proposition 13, we can lower bound the TV distance as follows:

$$TV(\llbracket\mathbf{hWalk}\rrbracket(s_1(pos),N,K), \llbracket\mathbf{hWalk}\rrbracket(s_2(pos),N,K)) \ge |wpe(\mathbf{hWalk},w_H)(s_1) - wpe(\mathbf{hWalk},w_H)(s_2)|$$
$$= \left(\frac{N-1}{N+1}\right)^K |W(s_1(pos)) - W(s_2(pos))|.$$

By selecting the initial positions appropriately—essentially, picking worst-case inputs—we can derive useful lower bounds on the Total Variation distance between output distributions. For instance, taking $s_1(pos)$ to be the all-zeros vector and $s_2(pos)$ to be the all-ones vector gives:

$$TV(\llbracket\mathbf{hWalk}\rrbracket(s_1(pos), N, K), \llbracket\mathbf{hWalk}\rrbracket(s_2(pos), N, K)) \geq \left(\frac{N-1}{N+1}\right)^K$$

Using standard algebraic bounds, the right-hand side (and the TV distance between the two output distributions) is at least $\rho > 0$ when $K < (N/2) \log \rho$.

Verifying precise lower bounds is highly challenging—for many simple examples of randomized processes, exact lower bounds are not known. Nonetheless, efforts in this direction could provide useful, complementary information when analyzing probabilistic programs.

8 EXTENSIONS: RULES FOR ASYNCHRONOUS REASONING

Our relational pre-expectation operator $\widetilde{rpe}(c, \mathcal{E})$ can often derive useful upper bounds on the Kantorovich distance $rpe(c, \mathcal{E})$, but it gives a trivial bound of infinity when the program c can take different branches on the two inputs. In this section, we develop techniques to give more useful bounds in the asynchronous case.

8.1 Asynchronous rules for bounding the Kantorovich distance

Our asynchronous bounds will use one-sided relational operators $wpe\langle 1 \rangle (c, \mathcal{E})$ (resp. $wpe\langle 2 \rangle (c, \mathcal{E})$) that transform relational expectations by holding the left (right) state constant and then computing the unary weakest pre-expectation $wpe(c, \mathcal{E})$. We use the following soundness lemma for the left version of the operator, the one for the right version being analogous.

LEMMA 1. Let c be a PWHILE program that is almost surely terminating, i.e., wpe(c, 1) = 1. Then, for all $s_1, s_2, \mathbb{E}_{s'_1 \sim [c] s_1}[\mathcal{E}(s'_1, s_2)] \leq wpe(1)(c, \mathcal{E})(s_1, s_2).$

Now we can present our asynchronous rules.

THEOREM 15. Let c be a program that is almost surely terminating. Then:

$$rpe(\text{if } e \text{ then } c \text{ else }, \mathcal{E}) \leq [e\langle 1 \rangle \land e\langle 2 \rangle] \cdot \widetilde{rpe}(c, \mathcal{E}) + [e\langle 1 \rangle \land \neg e\langle 2 \rangle] \cdot wpe\langle 1 \rangle (c, \mathcal{E}) \\ + [\neg e\langle 1 \rangle \land e\langle 2 \rangle] \cdot wpe\langle 2 \rangle (c, \mathcal{E}) + [\neg e\langle 1 \rangle \land \neg e\langle 2 \rangle] \cdot \mathcal{E}$$

Let while e do c be an almost surely terminating loop, $\rho_i(s)$ be the probability that the loop does not terminate after executing the body at most i times starting from state s, and:

 $M_i(\mathcal{E}, s_1, s_2) = \max\{\mathcal{E}(t_1, t_2) \mid t_1 \in supp([\![c_i]\!]s_1), t_2 \in supp([\![c_i]\!]s_2)\}$

where c_i is the first *i* iterations of the loop. If ρ_i and M_i satisfy:

 $\lim_{i \to \infty} (\rho_i(s_1) + \rho_i(s_2)) \cdot M_i(\mathcal{E}, s_1, s_2) = 0$

for any two states (s_1, s_2) , and if I is an invariant satisfying

$$\begin{split} & [e\langle 1\rangle \wedge e\langle 2\rangle] \cdot \widetilde{rpe}(c, I) + [e\langle 1\rangle \wedge \neg e\langle 2\rangle] \cdot wpe\langle 1\rangle(c, I) \\ & + [\neg e\langle 1\rangle \wedge e\langle 2\rangle] \cdot wpe\langle 2\rangle(c, I) + [\neg e\langle 1\rangle \wedge \neg e\langle 2\rangle] \cdot \mathcal{E} \leq I , \end{split}$$

then rpe(while *e* do *c*, \mathcal{E}) $\leq \mathcal{I}$.

PROOF SKETCH. The soundness of the conditional rule follows a similar argument as soundness for the definition of \widetilde{rpe} for conditionals, using Lemma 1 for the asynchronous cases. The soundness of the loop rule is more intricate, but it follows the same strategy as in Theorem 7: we define a loop characteristic function based on the conditional rule (now asynchronous), show that the least fixed-point lies above *rpe*, and finally show that the invariant rule implies that \mathcal{I} is a pre-fixed-point, so it must be above the fixed point.

We detail the full proof in Appendix J.

8.2 Example: Bounding the distance between binomial distributions

Consider the following program, which simulates a binomial distribution:

$$binom(N)$$

 $n \leftarrow 0;$
 $k \leftarrow 0;$
while $n < N$ do
 $b \notin Bern(p);$
if b then $k \leftarrow k + 1;$
 $n \leftarrow n + 1;$

We treat $p \in [0, 1]$ as a fixed constant. We will compare the distribution on the output *k* starting from two inputs. Since the loops will run for different numbers of iterations if $N\langle 1 \rangle \neq N\langle 2 \rangle$, we will employ our asynchronous rule. We take the following invariant:

$$I \triangleq |k\langle 1\rangle - k\langle 2\rangle + p \cdot (N\langle 1\rangle \ominus n\langle 1\rangle) - p \cdot (N\langle 2\rangle \ominus n\langle 2\rangle)|,$$

We will show the following invariant bound:

$$\begin{split} & [(n <)\langle 1 \rangle \land (n < N)\langle 2 \rangle] \cdot \widetilde{\textit{rpe}}(c, \mathcal{I}) + [(n < N)\langle 1 \rangle \land (n \ge N)\langle 2 \rangle] \cdot \textit{wpe}\langle 1 \rangle (c, \mathcal{I}) \\ & + [(n \ge N)\langle 1 \rangle \land (n < N)\langle 2 \rangle] \cdot \textit{wpe}\langle 2 \rangle (c, \mathcal{I}) + [(n \ge N)\langle 1 \rangle \land (n \ge N)\langle 2 \rangle] \cdot \mathcal{E} \le \mathcal{I} \end{split}$$

In the synchronous case, we can establish the invariant by applying SAMP with the identity coupling; the inner conditional can also be analyzed synchronously. In the asynchronous case, computing the unary weakest pre-expectation establishes the invariant. Thus, the asynchronous loop rule (Theorem 15) gives:

$$rpe(w, |k\langle 1 \rangle - k\langle 2 \rangle|) \le I$$

where *w* is the loop. Applying the assignment rule, we conclude:

 $rpe(binom(N), |k\langle 1 \rangle - k\langle 2 \rangle|) \le p \cdot |N\langle 1 \rangle - N\langle 2 \rangle|.$

By Theorem 2, this bound implies that the expected values of the output k differ by at most $p \cdot |N\langle 1\rangle - N\langle 2\rangle|$ across the two runs.

9 RELATED WORK

Proving expected sensitivity of probabilistic programs. We have shown that the quantitative logic **E**PRHL [7] can be embedded into the framework of this paper (cf. Section 3.4), so we focus on other work. Wang et al. [33] propose an alternative method based on martingales for proving the expected sensitivity of probabilistic programs. Their technique focuses on computing the expected sensitivity when the (expected) number of iterations for a loop may be different across two related executions (i.e., loops may be *asynchronous*); this is similar to our asynchronous rules from Section 8. However, Wang et al. [33] also frame their target property in a slightly weaker way, showing that programs are Lipschitz continuous for *some* finite Lipschitz constant. In contrast, our method establishes bounds on this constant, which is an important aspect in many applications (e.g., it determines the rate of convergence for Markov chains). We are also able to handle the broader class of expected sensitivity properties arising from Kantorovich metrics, subsuming the notion considered by Wang et al. [33] where the output distance is the absolute difference between two expected values.

Formal reasoning for probabilistic programs. Logics for probabilistic programs has been an active research area since the 1980s. Seminal work by Kozen [22] defines a probabilistic propositional dynamic logic for reasoning about probabilistic programs, using real-valued functions rather than boolean assertions. Morgan et al. [25] define a weakest pre-expectation calculus for a programming language with (demonic) non-determinism and probabilities. Extensions of this calculus with recursion and conditioning have been considered [26, 27]. Kaminski et al. [21] define a similar calculus for bounding expected run-times of probabilistic programs. These works do not prove relational properties of programs, and are unsuitable for verifying sensitivity.

Continuity in programs and process calculi. Formal reasoning about the continuity of deterministic programs has received some attention. Chaudhuri et al. [12, 13] were the first to give a sound, compositional framework for verifying that a program is continuous. Reed and Pierce [30] gave a type system that can verify Lipschitz continuity of functional programs (see also [4, 5, 14, 35]). Recently, Huang et al. [20] proposed the tool PSense which can perform sensitivity analysis of probabilistic programs. Their technique relies on symbolic computation using the symbolic verifier PSI and Mathematica, and supports, e.g., the Total Variation distance and the expectation distance. PSense cannot reason, however, about general Kantorovich distances, or unbounded loops.

Finally, in the process-algebra setting, compositional reasoning about metrics has received some attention. Gebler et al. [15] used uniform continuity to reason about the distance between recursive processes in a compositional way, while Gebler and Tini [16] recently defined specification formats

that can check uniform continuity syntactically. A more general framework for reasoning about metrics has been given by Bacci et al. [6], who presented an algebraic axiomatization of Markov processes in quantitative equational logic. Their framework supports reasoning about various metrics, including the Kantorovich metric.

10 CONCLUSION

We defined a pre-expectation calculus to compute upper bounds for Kantorovich metrics, and applied it to prove convergence of reinforcement learning and card shuffling algorithms, algorithmic stability of SGD, and uniformity of limit distributions. Our calculus provides theoretical foundations for reasoning about quantitative relational properties of probabilistic programs.

There are several natural directions for future work. One possible extension is to lift the requirement that programs terminate with equal probability on pairs of executions, possibly by leveraging alternative notions of the Kantorovich metric that accommodate distributions of different weight [29]. Other directions include developing a relational version of quantitative separation logic [9], and use it for proving relational properties of probabilistic heap-manipulating programs.

We also explored methods for proving lower bounds of convergence speed. In general, we are not aware of many works that prove lower bounds using program logics, with some notable exceptions [19]. Developing more tools and techniques for reasoning about these fascinating properties is an interesting avenue for future work.

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A BACKGROUND: REAL ANALYSIS

The following are standard convergence results in real analysis, see for instance [34]. In all of them we consider a sequence of relational expectations \mathcal{E}_n : State × State $\rightarrow \mathbb{R}_{\geq 0}^{\infty}$ and a distribution μ : Dist(State × State).

LEMMA 2 (FATOU'S LEMMA). Let \mathcal{E}_n be a monotone increasing sequence of relational expectations. Then,

$$\mathbb{E}_{\mu}[\lim_{n\to\infty}\mathcal{E}_n]\leq \lim_{n\to\infty}\mathbb{E}_{\mu}[\mathcal{E}_n].$$

Fatou's Lemma also holds when \mathcal{E}_n is not a monotone sequence (replacing the limit by a limit inferior), but the monotone version suffices for our purposes.

Now we present a result that will be useful in showing convergence of couplings. A similar result can be found in the monograph Villani [32, Theorem 5.19].

THEOREM 16 (CONVERGENCE OF COUPLINGS). Let v_i and ρ_i denote two sequences of sub-distributions with countable support over X, converging pointwise to v and ρ respectively. Let $\mu_i \in \Gamma(v_i, \rho_i)$ be a sequence of couplings of v_i and ρ_i . Then there exists a subsequence μ'_i of μ_i that converges to a coupling $\mu \in \Gamma(v, \rho)$.

PROOF. The proof proceeds in two steps. First we show that there exists a convergent subsequence of couplings. By the Bolzano-Weierstrass theorem, [0, 1] is *sequentially compact*, i.e., every sequence in [0, 1] has a subsequence that converges in [0, 1]. Moreover, countable products preserve sequential compactness. Since every v_i and ρ_i have countable support, so does every μ_i , so we can consider the sequence $\{\mu_i\}_{i \in \mathbb{N}}$ as a sequence over $[0, 1]^S$ where $S = \bigcup_i \text{supp}(\mu_i)$. Since this is a sequentially compact space, we can extract a subsequence $\{\mu'_i\}_{i \in \mathbb{N}}$ that converges pointwise to some distribution, call it $\mu \in \text{Dist}(X \times X)$; let $\{v'_i\}_{i \in \mathbb{N}}$ and $\{\rho'_i\}_{i \in \mathbb{N}}$ be the corresponding subsequences of $\{v_i\}_{i \in \mathbb{N}}$ and $\{\rho_i\}_{i \in \mathbb{N}}$ such that $\mu'_i \in \Gamma(v'_i, \rho'_i)$. Since they are subsequences of convergent sequences, these were convergent, $\{v'_i\}_{i \in \mathbb{N}}$ converges to v and $\{\rho'_i\}_{i \in \mathbb{N}}$ converges to ρ .

The main task is showing that μ is indeed a coupling of ν and ρ , i.e., $\mu \in \Gamma(\nu, \rho)$. We consider the first marginal condition. Let $\epsilon > 0$ be any positive number. Since ρ is a distribution over a countable set, there exists a finite set $S(\epsilon)$ such that $\sum_{x_2 \notin S(\epsilon)} \rho(x_2) < \epsilon$. We first show that:

$$\lim_{i \to \infty} \sum_{x_2 \notin S(\epsilon/2)} \rho_i(x_2) = 0.$$
(3)

Since $\{\rho'_i\}_i$ converges pointwise to ρ , it also converges in L_1 . So, there exists a finite number $N(\epsilon)$ such that for all $i > N(\epsilon)$, we have:

$$\sum_{x_2\in X} |\rho_i'(x_2) - \rho(x_2)| < \epsilon.$$

Thus for all $i > N(\epsilon/2)$, we have:

$$\sum_{x_2 \notin S(\epsilon/2)} \rho'_i(x_2) = \sum_{x_2 \notin S(\epsilon/2)} (\rho'_i(x_2) - \rho(x_2)) + \sum_{x_2 \notin S(\epsilon/2)} \rho(x_2)$$

$$\leq \sum_{x_2 \in X} |\rho'_i(x_2) - \rho(x_2)| + \epsilon/2$$

$$\leq \epsilon.$$

$$|v(x_{1}) - (\pi_{1}(\mu))(x_{1})| = |v(x_{1}) - \sum_{x_{2} \in X} \lim_{i \to \infty} \mu_{i}(x_{1}, x_{2})|$$

$$\leq |v(x_{1}) - \sum_{x_{2} \in S(\epsilon)} \lim_{i \to \infty} \mu_{i}(x_{1}, x_{2})| + \sum_{x_{2} \notin S(\epsilon)} \lim_{i \to \infty} \mu_{i}(x_{1}, x_{2}) \quad \text{(triangle ineq.)}$$

$$= |\nu(x_1) - \lim_{i \to \infty} \sum_{x_2 \in S(\epsilon)} \mu_i(x_1, x_2)| + \sum_{x_2 \notin S(\epsilon)} \lim_{i \to \infty} \mu_i(x_1, x_2)$$
 (S(\epsilon) finite)

$$\leq |\nu(x_1) - \lim_{i \to \infty} \sum_{x_2 \in S(\epsilon)} \mu_i(x_1, x_2)| + \sum_{x_2 \notin S(\epsilon)} \lim_{i \to \infty} \rho_i(x_2) \qquad (\pi_2(\mu_i) = \rho_i)$$

$$\leq |\nu(x_1) - \lim_{i \to \infty} \sum_{x_2 \in S(\epsilon)} \mu_i(x_1, x_2)| + \sum_{x_2 \notin S(\epsilon)} \rho(x_2)$$
 (limit ρ)

$$\leq |v(x_1) - \lim_{i \to \infty} \sum_{x_2 \in S(\epsilon)} \mu_i(x_1, x_2)| + \epsilon \qquad (\text{def. } S(\epsilon))$$

$$= |v(x_1) - \lim_{i \to \infty} v_i(x_1) + \lim_{i \to \infty} \sum_{x_2 \notin S(\epsilon)} \mu_i(x_1, x_2) | + \epsilon \qquad (\pi_1(\mu_i) = v_i)$$

$$= |\lim_{i \to \infty} \sum_{x_2 \notin S(\epsilon)} \mu_i(x_1, x_2)| + \epsilon$$
 (limit ν)

$$\leq \lim_{i \to \infty} \sum_{x_2 \notin S(\epsilon)} \rho_i(x_2) + \epsilon = \epsilon.$$
 (by Eq. (3))

Since $\epsilon > 0$ and $x_1 \in X$ are arbitrary, this shows the first marginal condition $\nu = \pi_1(\mu)$. The second marginal condition follows similarly, and so $\mu \in \Gamma(\nu, \rho)$ as desired.

B PROGRAM SEMANTICS

A state $s \in$ **State** is a map from a finite set of variable names **Var** to a set of values **Val**. Given an expression *e*, we abuse the notation s(e) to denote the natural lifting of *s* to a map from expressions to values. Similarly, given an expression *d* denoting a distribution, we abuse the notation s(d) to denote the lifting of *s* to a map from distributions to distribution over values. Given $s \in$ **State**, $x \in$ **Var** and $v \in$ **Val**, we write $s\{v/x\}$ to denote the unique state such that $s\{v/x\}(y) = v$ if y = x and $s\{v/x\}(y) = s(y)$ otherwise.

The semantics [c] of a command *c* is a map from an input state in **State** to an output distribution in **Dist(State)**. This semantics is standard, and is defined by induction on the structure of the command:

$$\llbracket \mathbf{skip} \rrbracket s \triangleq \delta(s)$$

$$\llbracket x \leftarrow e \rrbracket s \triangleq \delta(s\{s(e)/x\})$$

$$\llbracket x \notin d \rrbracket s \triangleq \mathbb{E}_{v \sim s(d)}[s\{v/x\}]$$

$$\llbracket c; c' \rrbracket s \triangleq \mathbb{E}_{s' \sim \llbracket c \rrbracket s}[\llbracket c' \rrbracket s']$$

$$\llbracket \mathbf{if} \ e \ \mathbf{then} \ c \ \mathbf{else} \ c' \rrbracket s \triangleq [s(e)] \cdot \llbracket c \rrbracket s + [\neg s(e)] \cdot \llbracket c' \rrbracket \delta(s)$$

$$\llbracket \mathbf{while} \ e \ \mathbf{do} \ c \rrbracket s \triangleq \lim_{n \to \infty} \llbracket c_n \rrbracket s \quad \text{where} \ c_0 \triangleq \mathbf{abort} \ \mathbf{and} \ c_{i+1} \triangleq \mathbf{if} \ e \ \mathbf{then} \ c; c_i$$

We use a dummy **abort** command that denotes the constant zero sub-distribution to help define the semantics for loops. The limit exists and is a sub-distribution because for any initial state *s*, the sub-distributions $[c_i]$ s are monotone increasing in *i* under the pointwise order on sub-distributions,

i.e., $(\llbracket c_i \rrbracket s)(s') \leq (\llbracket c_j \rrbracket s)(s')$ for all states $s, s' \in$ State and all $i \leq j$, and $(\llbracket c_i \rrbracket s)(s')$ is bounded above by 1.

C SECTION 2: OMITTED PROOFS

THEOREM 1. For the direction " \leq ", it suffices to show that $|\mu_1(S) - \mu_2(S)| \leq \mathbb{E}_{\mu}[\mathcal{E}]$ for every $\mu \in \Gamma(\mu_1, \mu_2)$ and every $S \subseteq X$. By the property of marginals and monotonicity of probabilities, we have:

$$\begin{aligned} \left|\mu_1(S) - \mu_2(S)\right| &= \left|\mu(S \times X) - \mu(X \times S)\right| = \left|\mu(S \times (X \setminus S)) - \mu((X \setminus S) \times S)\right| \\ &\leq \max(\mu(S \times (X \setminus S)), \mu((X \setminus S) \times S)) \leq \mu(\{x_1, x_2) \mid x_1 \neq x_2\}) = \mathbb{E}_{\mu}[\mathcal{E}] . \end{aligned}$$

For the other direction, we construct a so-called optimal coupling. For every $x \in X$, let $\mu_0(x) = \min(\mu_1(x), \mu_2(x))$. The optimal coupling for (μ_1, μ_2) is defined by:

$$\mu(x_1, x_2) = \begin{cases} \mu_0(x_1) & : x_1 = x_2 \\ \frac{(\mu_1(x_1) - \mu_0(x_1)) \cdot (\mu_2(x_2) - \mu_0(x_2))}{TV(\mu_1, \mu_2)} & : x_1 \neq x_2 \end{cases}$$

where 0/0 := 0. One can check that μ is a coupling for (μ_1, μ_2) and that $\mu([x_1 \neq x_2]) = TV(\mu_1, \mu_2)$. \Box

THEOREM 2. It suffices to show $|\mathbb{E}_{\mu_1}[f_1] - \mathbb{E}_{\mu_2}[f_2]| \leq \mathbb{E}_{\mu}[\mathcal{E}]$ for every $\mu \in \Gamma(\mu_1, \mu_2)$, which follows from the marginal properties of couplings, linearity of expectation, and the fact that $|\mathbb{E}_{\mu}[f]| \leq \mathbb{E}_{\mu}[|f|]$:

$$\begin{aligned} \left| \mathbb{E}_{\mu_1}[f_1] - \mathbb{E}_{\mu_2}[f_2] \right| &= \left| \mathbb{E}_{\mu}[\lambda(x_1, x_2). \ f_1(x_1)] - \mathbb{E}_{\mu}[\lambda(x_1, x_2). \ f_2(x_2)] \right| \\ &= \left| \mathbb{E}_{\mu}[\lambda(x_1, x_2). \ f_1(x_1) - f_2(x_2)] \right| \leq \mathbb{E}_{\mu}[\lambda(x_1, x_2). \ \left| f_1(x_1) - f_2(x_2) \right| \right] = \mathbb{E}_{\mu}[\mathcal{E}] . \end{aligned}$$

THEOREM 3. The proof follows from Theorem 1 and from the observations that $(\rho \cdot \mathcal{E})^{\#} = \rho \cdot \mathcal{E}^{\#}$ and that $\mathcal{E} \leq \mathcal{E}'$ implies $\mathcal{E}^{\#} \leq \mathcal{E}'^{\#}$, taking the pointwise order in both cases.

D SOUNDNESS AND CONTINUITY: OMITTED PROOFS

The syntactic relational pre-expectation transformer is a monotonic operator.

LEMMA 3 (MONOTONICITY OF $\widetilde{rpe}(c, -)$). Let \mathcal{E} be a relational expectation and let c be a program. Then $\widetilde{rpe}(c, -)$ and $\Phi_{\mathcal{E},c}(-)$ are monotonic, i.e. for any two relational expectations $\mathcal{E}_1, \mathcal{E}_2$ such that $\mathcal{E}_1 \leq \mathcal{E}_2$, we have $\widetilde{rpe}(c, \mathcal{E}_1) \leq \widetilde{rpe}(c, \mathcal{E}_2)$ and $\Phi_{\mathcal{E},c}(\mathcal{E}_1) \leq \Phi_{\mathcal{E},c}(\mathcal{E}_2)$.

PROOF. The latter result is a corollary from the former. By definition,

$$\Phi_{\mathcal{E},c,e}(\mathcal{E}_1) = [e\langle 1 \rangle \land e\langle 2 \rangle] \cdot \widetilde{rpe}(c,\mathcal{E}_1) + [\neg e\langle 1 \rangle \land \neg e\langle 2 \rangle] \cdot \mathcal{E} + [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot \infty$$

and

$$\Phi_{\mathcal{E},c,e}(\mathcal{E}_2) = [e\langle 1 \rangle \land e\langle 2 \rangle] \cdot \widetilde{rpe}(c,\mathcal{E}_2) + [\neg e\langle 1 \rangle \land \neg e\langle 2 \rangle] \cdot \mathcal{E} + [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot \infty$$

So given $\widetilde{rpe}(c, \mathcal{E}_1) \leq \widetilde{rpe}(c, \mathcal{E}_2)$ we can conclude $\Phi_{\mathcal{E}, c, e}(\mathcal{E}_1) \leq \Phi_{\mathcal{E}, c, e}(\mathcal{E}_2)$.

The former result is proven by induction on *c*:

• skip. Then

$$\widetilde{rpe}(skip, \mathcal{E}_1) = \mathcal{E}_1 \leq \mathcal{E}_2 = \widetilde{rpe}(skip, \mathcal{E}_2)$$

• $x \leftarrow e$. Then

$$\widetilde{rpe}(x \leftarrow e, \mathcal{E}_1) = \mathcal{E}_1\{e\langle 1 \rangle, e\langle 2 \rangle / x \langle 1 \rangle, x \langle 2 \rangle\}$$

and

$$\widetilde{rpe}(x \leftarrow e, \mathcal{E}_2) = \mathcal{E}_2\{e\langle 1 \rangle, e\langle 2 \rangle / x\langle 1 \rangle, x\langle 2 \rangle\}$$

Consider a pair of states s_1 , s_2 then:

$$\mathcal{E}_1\{e\langle 1\rangle, e\langle 2\rangle/x\langle 1\rangle, x\langle 2\rangle\}(s_1, s_2) = \mathcal{E}_1(s_1\{s_1(e)/x\})(s_2\{s_2(e)/x\})$$
$$\leq \mathcal{E}_2(s_1\{s_1(e)/x\})(s_2\{s_2(e)/x\})$$
$$= \mathcal{E}_2\{e\langle 1\rangle, e\langle 2\rangle/x\langle 1\rangle, x\langle 2\rangle\}(s_1, s_2)$$

• $x \notin d$. Then,

$$\widetilde{rpe}(x \stackrel{s}{\leftarrow} d, \mathcal{E}_1) = \inf_{\mu \in \Gamma(\mu_1, \mu_2)} \mathbb{E}_{\mu}[\mathcal{E}_1]$$

and

$$\widetilde{rpe}(x \xleftarrow{} d, \mathcal{E}_2) = \inf_{\mu \in \Gamma(\mu_1, \mu_2)} \mathbb{E}_{\mu}[\mathcal{E}_2]$$

Let $\mu \in \Gamma(\mu_1, \mu_2)$ be an arbitrary coupling. By monotonicity of the expectation, then $\mathbb{E}_{\mu}[\mathcal{E}_1] \leq \mathbb{E}_{\mu}[\mathcal{E}_2]$, and therefore the infimum for \mathcal{E}_1 is less or equal than the one for \mathcal{E}_2 .

• *c*; *c*′. By the induction hypothesis,

$$\widetilde{rpe}(c;c',\mathcal{E}_1) = \widetilde{rpe}(c,\widetilde{rpe}(c',\mathcal{E}_1)) \le \widetilde{rpe}(c,\widetilde{rpe}(c',\mathcal{E}_2)) = \widetilde{rpe}(c;c',\mathcal{E}_2)$$

Note that the inequality needs two applications of the I.H., one to show that $\widetilde{rpe}(c', \mathcal{E}_1) \leq \widetilde{rpe}(c', \mathcal{E}_2)$ and another one to show $\widetilde{rpe}(c, \widetilde{rpe}(c', \mathcal{E}_1)) \leq \widetilde{rpe}(c, \widetilde{rpe}(c', \mathcal{E}_2))$.

• if *e* then *c* else *c'*. By the induction hypothesis (applied at *c* and *c'*),

$$\widetilde{rpe}(\text{if } e \text{ then } c \text{ else } c', \mathcal{E}_1) = [e\langle 1 \rangle \land e\langle 2 \rangle] \cdot \widetilde{rpe}(c, \mathcal{E}_1) + [\neg e\langle 1 \rangle \land \neg e\langle 2 \rangle] \cdot \widetilde{rpe}(c', \mathcal{E}_1) + [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot \infty$$
$$\leq [e\langle 1 \rangle \land e\langle 2 \rangle] \cdot \widetilde{rpe}(c, \mathcal{E}_2) + [\neg e\langle 1 \rangle \land \neg e\langle 2 \rangle] \cdot \widetilde{rpe}(c', \mathcal{E}_2) + [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot \infty$$
$$= \widetilde{rpe}(\text{if } e \text{ then } c \text{ else } c', \mathcal{E}_2)$$

• while e do c. Then,

 $\widetilde{rpe}(\text{while } e \text{ do } c, \mathcal{E}_1) = \text{lfp}X.[e\langle 1 \rangle \land e\langle 2 \rangle] \cdot \widetilde{rpe}(c, X) + [\neg e\langle 1 \rangle \land \neg e\langle 2 \rangle] \cdot \mathcal{E}_1 + [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot \infty$ $\widetilde{rpe}(\text{while } e \text{ do } c, \mathcal{E}_2) = \text{lfp}X.[e\langle 1 \rangle \land e\langle 2 \rangle] \cdot \widetilde{rpe}(c, X) + [\neg e\langle 1 \rangle \land \neg e\langle 2 \rangle] \cdot \mathcal{E}_2 + [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot \infty$

Existence of the least fixed points is guaranteed by monotonicity of the functionals, which follows from the inductive hypothesis applied to *c*. Suppose X_2 is the least fixpoint of the second expression. We will show that it is a pre-fixpoint of the first expression.

$$[e\langle 1 \rangle \land e\langle 2 \rangle] \cdot \widetilde{rpe}(c, X_2) + [\neg e\langle 1 \rangle \land \neg e\langle 2 \rangle] \cdot \mathcal{E}_1 + [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot \infty$$

$$\leq [e\langle 1 \rangle \land e\langle 2 \rangle] \cdot \widetilde{rpe}(c, X_2) + [\neg e\langle 1 \rangle \land \neg e\langle 2 \rangle] \cdot \mathcal{E}_2 + [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot \infty$$

$$= X_2$$

By Knaster-Tarski, the least fixed point of a monotonically increasing operator is the greatest lower bound of the set of pre-fixpoints. From this we conclude $\widetilde{rpe}(\mathbf{while } e \mathbf{ do } c, \mathcal{E}_1) \leq X_2$. \Box

We need a lemma about the existence of a coupling realizing the minimum Kantorovich distance.

LEMMA 4. Let $\mu_1, \mu_2 \in \text{Dist}(\text{State})$ be two subdistributions of finite support with the same weight, and let $\mathcal{E}: \text{State} \times \text{State} \to \mathbb{R}_{\geq 0}^{\infty}$ be a relational expectation. There exists a coupling $\mu \in \Gamma(\mu_1, \mu_2)$ realizing the minimum Kantorovich distance:

$$\mathbb{E}_{\mu}[\mathcal{E}] = \inf_{\mu \in \Gamma(\mu_1, \mu_2)} \mathbb{E}_{\mu}[\mathcal{E}] = \mathcal{E}^{\#}(\mu_1, \mu_2) .$$

This is an extremely simple case of standard existence results in the theory of optimal transport (see, e.g., Theorem 4.1 in Villani's monograph [32]). We include a proof to keep the exposition self-contained.

PROOF. Let $d^* = \inf_{\mu \in \Gamma(\mu_1, \mu_2)} \mathbb{E}_{\mu}[\mathcal{E}]$ be the infimum distance. If $d^* = \infty$ then the product coupling realizes the distance. Otherwise, suppose that the infimum d^* is finite. By the definition of infimum, there exists a sequence of couplings $\mu^{(1)}, \mu^{(2)}, \dots \in \Gamma(\mu_1, \mu_2)$ such that

$$\lim_{k\to\infty}\mathbb{E}_{\mu^{(k)}}[\mathcal{E}]=d^*.$$

Without loss of generality, we may assume that for each k the distance $\mathbb{E}_{\mu^{(k)}}[\mathcal{E}]$ is finite as well. Let $S = \bigcup_k \operatorname{supp}(\mu^{(k)})$ be the union of the supports of all $\mu^{(k)}$. Since μ_1, μ_2 have countable support, S is countable. Since all the expected distances are finite, in fact all pairs of states $(s_1, s_2) \in S$ have $\mathcal{E}(s_1, s_2) < \infty$. By Theorem 16 we can find a subsequence of $\mu^{(k)}$ that is converging pointwise; define:

$$\mu(s_1, s_2) = \lim_{k \to \infty} \mu^{(k)}(s_1, s_2)$$

for every $s_1, s_2 \in$ **State**, where the limit is taken over the subsequence (so it exists). Then μ is indeed a coupling in $\Gamma(\mu_1, \mu_2)$. To show that μ realizes the infimum distance, we derive:

$$\begin{split} \mathbb{E}_{\mu}[\mathcal{E}] &= \sum_{(s_{1},s_{2})\in S} \mathcal{E}(s_{1},s_{2}) \cdot \mu(s_{1},s_{2}) \\ &= \sum_{(s_{1},s_{2})\in S} \mathcal{E}(s_{1},s_{2}) \cdot \lim_{k \to \infty} \mu^{(k)}(s_{1},s_{2}) \\ &\leq \sum_{(s_{1},s_{2})\in S} \lim_{k \to \infty} \mathcal{E}(s_{1},s_{2}) \cdot \mu^{(k)}(s_{1},s_{2}) \\ &\leq \lim_{k \to \infty} \sum_{(s_{1},s_{2})\in S} \mathcal{E}(s_{1},s_{2}) \cdot \mu^{(k)}(s_{1},s_{2}) \\ &= \lim_{k \to \infty} \mathbb{E}_{\mu^{(k)}}[\mathcal{E}] \\ &= d^{*}. \end{split}$$

The first inequality is because \mathcal{E} may take value infinity; the second inequality is by Fatou's lemma.

Continuity proceeds in two steps. We first need a lemma about continuity of the Kantorovich distance. While it seems challenging to establish this lemma for distributions with infinite support, we establish it for distributions with finite support.

LEMMA 5. Let $\mu_1, \mu_2 \in \text{Dist}(\text{State})$ be two distributions with finite support, and let \mathcal{E}_n : State \times State $\rightarrow \mathbb{R}^{\infty}_{\geq 0}$ be a monotonically increasing chain of relational expectations converging pointwise to \mathcal{E} : State $\rightarrow \mathbb{R}^{\infty}_{\geq 0}$. Then:

$$\inf_{\mu\in\Gamma(\mu_1,\mu_2)}\mathbb{E}_{\mu}[\mathcal{E}] = \inf_{\mu\in\Gamma(\mu_1,\mu_2)}\mathbb{E}_{\mu}[\lim_{n\to\infty}\mathcal{E}_n] = \lim_{n\to\infty}\inf_{\mu\in\Gamma(\mu_1,\mu_2)}\mathbb{E}_{\mu}[\mathcal{E}_n].$$

PROOF. If μ_1, μ_2 have different weights, then both infimums are infinity and we are done. It is not hard to show that

$$\lim_{n\to\infty}\inf_{\mu\in\Gamma(\mu_1,\mu_2)}\mathbb{E}_{\mu}[\mathcal{E}_n]\leq\inf_{\mu\in\Gamma(\mu_1,\mu_2)}\mathbb{E}_{\mu}[\mathcal{E}],$$

since $\mathcal{E}_n \leq \mathcal{E}$ and the coupling realizing the infimum (which exists by Lemma 4) is a valid coupling in each of the limit terms.

Showing the other direction is more involved. Define the finite relations

$$R_{<\infty} = \{(s_1, s_2) \mid \mathcal{E}(s_1, s_2) < \infty\} \cap (\operatorname{supp}(\mu_1) \times \operatorname{supp}(\mu_2))$$
$$R_{\infty} = (\operatorname{supp}(\mu_1) \times \operatorname{supp}(\mu_2)) \setminus R_{<\infty}.$$

We first consider the case where

$$\inf_{\mu\in\Gamma(\mu_1,\mu_2)}\mathbb{E}_{\mu}[\mathcal{E}]=\infty.$$

This means that every coupling must put weight on $R_{<\infty}$. To see this fact, note that the following infimum is realized by some coupling μ^* :

$$\inf_{\mu\in\Gamma(\mu_1,\mu_2)}\mathbb{E}_{\mu}[R_{\infty}].$$

If $\mu^*(R_\infty) = 0$, then μ^* does not place any mass on points where \mathcal{E} is infinity. Since μ^* has finite support, this means that $\mathbb{E}_{\mu^*}[\mathcal{E}]$ would be finite, a contradiction. So, we have:

$$\inf_{\mu\in\Gamma(\mu_1,\mu_2)}\mathbb{E}_{\mu}[R_{\infty}] = \inf_{\mu\in\Gamma(\mu_1,\mu_2)}\mathbb{E}_{\mu}[R_{\infty}] \ge \rho > 0.$$

for some constant ρ . Now, let M be any real number greater than ρ , and take N large enough so that for every $(s_1, s_2) \in R_{\infty}$, we have $\mathcal{E}_n(s_1, s_2) > M/\rho$ for all n > N. Such an N must exist since R_{∞} is finite, and $\mathcal{E}_n(s_1, s_2)$ is tending to infinity for $(s_1, s_2) \in R_{\infty}$. We now have

$$\inf_{\mu \in \Gamma(\mu_1, \mu_2)} \mathbb{E}_{\mu}[\mathcal{E}_n] \ge \inf_{\mu \in \Gamma(\mu_1, \mu_2)} \mathbb{E}_{\mu}[[R_{\infty}] \cdot \mathcal{E}_n] \ge (M/\rho) \cdot \rho \ge M$$

for all n > N. Since this is true for *M* arbitrarily large, we must have

$$\lim_{n\to\infty}\inf_{\mu\in\Gamma(\mu_1,\mu_2)}\mathbb{E}_{\mu}[\mathcal{E}_n]=\infty\geq\inf_{\mu\in\Gamma(\mu_1,\mu_2)}\mathbb{E}_{\mu}[\mathcal{E}]$$

as claimed.

Otherwise, suppose that the infimum is equal to $w^* < \infty$. Let $M = \sup_{(s_1, s_2) \in \mathbb{R}_{<\infty}} \mathcal{E}(s_1, s_2)$ be the largest finite value assigned by \mathcal{E} . Since $\mathcal{E}_n(s_1, s_2)$ tends to infinity for all $(s_1, s_2) \in \mathbb{R}_{\infty}$ and \mathbb{R}_{∞} is finite, we may take a subsequence \mathcal{E}'_n such that $\mathcal{E}'_n(s_1, s_2) \ge n$ for all $(s_1, s_2) \in \mathbb{R}_{\infty}$. Let v'_i be a coupling realizing the infimum

$$\inf_{\mu\in\Gamma(\mu_1,\mu_2)}\mathbb{E}_{\mu}[\mathcal{E}'_i].$$

Since this infimum is less than w^* , we have $v'_i(s_1, s_2) < w^*/n$ for every $(s_1, s_2) \in R_{\infty}$. Since each v'_i has finite support and takes values in [0, 1], by the Bolzano-Weierstrass theorem there exists a subsequence v''_i converging pointwise to v^* ; we write \mathcal{E}''_i for the corresponding expectations. Note that $v''_i \in \Gamma(\mu_1, \mu_2)$ is a coupling, and $v''_i(R_{\infty}) = 0$.

Now let $\epsilon > 0$. Let *N* be such that for all n > N and $(s_1, s_2) \in R_{<\infty}$, we have $|\nu''_n(s_1, s_2) - \nu^*(s_1, s_2)| < \epsilon/M$; such an *N* exists since the distributions have finite support. Then since $\mathcal{E}''_n(s_1, s_2) \leq \mathcal{E}(s_1, s_2) \leq M$ for all $(s_1, s_2 \in R_{<\infty}$, and $\nu^*(s_1, s_2) = 0$ for all $(s_1, s_2) \in R_{\infty}$, we have

$$\mathbb{E}_{\nu^*}[\mathcal{E}_n''] < \inf_{\mu \in \Gamma(\mu_1, \mu_2)} \mathbb{E}_{\mu}[\mathcal{E}_n''] + \epsilon$$

for all n > N. The monotone convergence theorem implies:

$$\mathbb{E}_{\nu^*}[\mathcal{E}] = \lim_{n \to \infty} \mathbb{E}_{\nu^*}[\mathcal{E}''_n] \le \lim_{n \to \infty} \inf_{\mu \in \Gamma(\mu_1, \mu_2)} \mathbb{E}_{\mu}[\mathcal{E}''_n] + \epsilon.$$

On the other hand, we have the bound

$$\inf_{\mu\in\Gamma(\mu_1,\mu_2)}\mathbb{E}_{\mu}[\mathcal{E}]\leq\mathbb{E}_{\nu^*}[\mathcal{E}]$$

Since both bounds hold for all ϵ , we can conclude:

$$\inf_{\mu\in\Gamma(\mu_1,\mu_2)} \mathbb{E}_{\mu}[\mathcal{E}] \leq \lim_{n\to\infty} \inf_{\mu\in\Gamma(\mu_1,\mu_2)} \mathbb{E}_{\mu}[\mathcal{E}''_n] = \lim_{n\to\infty} \inf_{\mu\in\Gamma(\mu_1,\mu_2)} \mathbb{E}_{\mu}[\mathcal{E}_n].$$

Now, we can prove continuity of relational pre-expectations, provided that programs sample from distributions with *finite* support. Note that such programs can still produce distributions with infinite support, for instance by sampling in a loop.

THEOREM (CONTINUITY). Let c be a program where all primitive distributions have finite support, and let \mathcal{E}_n : State \times State $\rightarrow \mathbb{R}_{\geq 0}^{\infty}$ be a monotonically increasing chain of relational expectations converging pointwise to \mathcal{E} : State \times State $\rightarrow \mathbb{R}_{\geq 0}^{\infty}$. Then,

$$\widetilde{rpe}(c, \mathcal{E}) = \sup_{n \in \mathbb{N}} \widetilde{rpe}(c, \mathcal{E}_n).$$

PROOF OF THEOREM 5. By induction on the structure of the program.

• skip. Then,

$$\widetilde{rpe}(skip, \mathcal{E}) = \mathcal{E} = \sup_{n \in \mathbb{N}} \mathcal{E}_n = \sup_{n \in \mathbb{N}} \widetilde{rpe}(skip, \mathcal{E}_n)$$

• $x \leftarrow e$. Then,

$$\widetilde{rpe}(x \leftarrow e, \mathcal{E}) = \mathcal{E}\{e\langle 1 \rangle, e\langle 2 \rangle / x \langle 1 \rangle, x \langle 2 \rangle\}$$

= $\sup_{n \in \mathbb{N}} \mathcal{E}_n\{e\langle 1 \rangle, e\langle 2 \rangle / x \langle 1 \rangle, x \langle 2 \rangle\}$ (subst. continuous)
= $\sup_{n \in \mathbb{N}} \widetilde{rpe}(x \leftarrow e, \mathcal{E}_n)$

• $x \notin d$. Let s_1, s_2 be any two states. By assumption, $[\![d]\!]s_1$ and $[\![d]\!]s_2$ have finite support, so $\mu_1 = [\![x \notin d]\!]s_1$ and $\mu_2 = [\![x \notin d]\!]s_2$ also have finite support. By Lemma 5 applied to μ_1, μ_2 , we have

$$\widetilde{rpe}(x \xleftarrow{} d, \mathcal{E})(s_1, s_2) = \inf_{\mu \in \Gamma(\mu_1, \mu_2)} \mathbb{E}_{\mu}[\mathcal{E}] = \lim_{n \in \mathbb{N}} \inf_{\mu \in \Gamma(\mu_1, \mu_2)} \mathbb{E}_{\mu}[\mathcal{E}_n] = \lim_{n \in \mathbb{N}} \widetilde{rpe}(x \xleftarrow{} d, \mathcal{E}_n)(s_1, s_2).$$

By monotonicity, the sup and the lim coincide.

• *c*; *c*′. Then,

$$\widetilde{rpe}(c; c', \mathcal{E}) = \widetilde{rpe}(c, \widetilde{rpe}(c', \mathcal{E}))$$

= $\widetilde{rpe}(c, \sup_{n \in \mathbb{N}} \widetilde{rpe}(c', \mathcal{E}_n))$ (induction)

$$= \sup_{n \in \mathbb{N}} \widetilde{rpe}(c, \widetilde{rpe}(c', \mathcal{E}_n))$$
(induction)
$$= \sup_{n \in \mathbb{N}} \widetilde{rpe}(c; c', \mathcal{E}_n)$$
(definition)

$$= \sup_{n \in \mathbb{N}} \widetilde{rpe}(c; c', \mathcal{E}_n)$$
 (definition)

• if *e* then *c* else *c*'. Then,

$$\widetilde{rpe}($$
if *e* then *c* else *c'*, $\mathcal{E})$

$$= [e\langle 1 \rangle \wedge e\langle 2 \rangle] \cdot \widetilde{rpe}(c, \mathcal{E}) + [\neg e\langle 1 \rangle \wedge \neg e\langle 2 \rangle] \cdot \widetilde{rpe}(c', \mathcal{E}) + [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot \infty$$

$$= [e\langle 1 \rangle \wedge e\langle 2 \rangle] \cdot \sup_{n \in \mathbb{N}} \widetilde{rpe}(c, \mathcal{E}_n) + [\neg e\langle 1 \rangle \wedge \neg e\langle 2 \rangle] \cdot \sup_{n \in \mathbb{N}} \widetilde{rpe}(c', \mathcal{E}_n) + [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot \infty$$

(induction)

$$= \sup_{n \in \mathbb{N}} ([e\langle 1 \rangle \land e\langle 2 \rangle] \cdot \widetilde{rpe}(c, \mathcal{E}_n) + [\neg e\langle 1 \rangle \land \neg e\langle 2 \rangle] \cdot \widetilde{rpe}(c', \mathcal{E}_n) + [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot \infty)$$

=
$$\sup_{n \in \mathbb{N}} \widetilde{rpe}(\text{if } e \text{ then } c \text{ else } c', \mathcal{E}_n)$$
(definition)

• while e do c. Then,

$$\widetilde{rpe}(\text{while } e \text{ do } c, \mathcal{E}) = \operatorname{lfp} X.\Phi_{c,\mathcal{E}}(X)$$

where $\Phi_{c,\mathcal{E}}(X) \triangleq [e\langle 1 \rangle \wedge e\langle 2 \rangle] \cdot \widetilde{rpe}(c,X) + [\neg e\langle 1 \rangle \wedge \neg e\langle 2 \rangle] \cdot \mathcal{E} + [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot \infty$

We claim that:

$$\widetilde{rpe}(\text{while } e \text{ do } c, \mathcal{E}) = \text{lfp}X.\Phi_{c,\sup_{n \in \mathbb{N}} \mathcal{E}_n}(X)$$
$$= \text{lfp}X.\sup_{n \in \mathbb{N}} \Phi_{c,\mathcal{E}_n}(X)$$
(1)

$$= \sup_{n \in \mathbb{N}} \operatorname{lfp} X.\Phi_{c, \mathcal{E}_n}(X) \tag{2}$$

$$= \sup_{n \in \mathbb{N}} \widetilde{rpe}(\text{while } e \text{ do } c, \mathcal{E}_n)$$
 (definition)

Equality (1) follows from:

$$\begin{split} \mathsf{lfp} X. \Phi_{c, \sup_{n \in \mathbb{N}} \mathcal{E}_n}(X) &= \mathsf{lfp} X. [e\langle 1 \rangle \land e\langle 2 \rangle] \cdot \widetilde{rpe}(c, X) + [\neg e\langle 1 \rangle \land \neg e\langle 2 \rangle] \cdot \sup_{n \in \mathbb{N}} \mathcal{E}_n + [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot \infty \\ &= \mathsf{lfp} X. \sup_{n \in \mathbb{N}} ([e\langle 1 \rangle \land e\langle 2 \rangle] \cdot \widetilde{rpe}(c, X) + [\neg e\langle 1 \rangle \land \neg e\langle 2 \rangle] \cdot \mathcal{E}_n + [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot \infty) \end{split}$$

To show (2) we note that—by the Knaster-Tarski fixpoint theorem and the fact that $\Phi_{c, \mathcal{E}_n}(X)$ is monotonic—lfp is itself a supremum (over the ordinals), namely

$$\operatorname{lfpX.} \sup_{n \in \mathbb{N}} \Phi_{c, \mathcal{E}_n}(X) = \sup_{m} \sup_{n \in \mathbb{N}} \Phi^m_{c, \mathcal{E}_n}(0).$$

Hence, the two suprema can be swapped.

We are now ready to show soundness (Theorem 4).

THEOREM (SOUNDNESS). Let c be a program, and suppose that $\mathcal{E}: \text{State} \times \text{State} \to \mathbb{R}_{\geq 0}^{\infty}$ is a relational expectation. Then

$$pe(c, \mathcal{E}) \leq \widetilde{rpe}(c, \mathcal{E})$$

Equivalently, if $\widetilde{rpe}(c, \mathcal{E})(s_1, s_2)$ is finite for input states $s_1, s_2 \in$ State then there exists a coupling $\mu_{s_1, s_2} \in \Gamma(\llbracket c \rrbracket s_1, \llbracket c \rrbracket s_2)$ such that

$$\mathbb{E}_{\mu_{s_1,s_2}}[\mathcal{E}] \leq \widetilde{rpe}(c,\mathcal{E})(s_1,s_2)$$

PROOF. Given $v \in X$, we write $\delta(v)$ for the point distribution centered at v, and given $\mu \in \text{Dist}(X)$ and $f: X \to \text{Dist}(X)$, we write $\mathbb{E}_{\mu}[f]$ for the distribution bind. Throughout, let $(s_1, s_2) \in \text{State} \times \text{State}$ be two initial states. We prove the second, equivalent formulation by induction on the structure of c. Suppose that $\widetilde{rpe}(c, \mathcal{E})(s_1, s_2)$ is finite.

• skip. Take the coupling $\delta(s_1, s_2)$. Then

$$\mathbb{E}_{\delta(s_1, s_2)}[\mathcal{E}] = \mathcal{E}(s_1, s_2) = \widetilde{rpe}(\mathbf{skip}, \mathcal{E})(s_1, s_2)$$

- $x \leftarrow e$. Analogous to skip, but taking the coupling $\delta(s'_1, s'_2)$, where $s'_i = s_i[x \mapsto [\![e]\!]s_i]$.
- $x \notin d$. Let F: State \rightarrow Dist(State) be defined as $F = [x \notin d]$. $F(s_1)$ and $F(s_2)$ must have equal weights for $\widetilde{rpe}(x \notin d, \mathcal{E})(s_1, s_2)$ to be finite and evidently $F(s_1)$ and $F(s_2)$ both have countable support, so Lemma 4 implies that there exists a coupling $\mu \in \Gamma([x \notin d] s_1, [x \notin d] s_2)$ such that

$$\mathbb{E}_{\mu}[\mathcal{E}] = \mathcal{E}^{\#}(\llbracket x \stackrel{s}{\leftarrow} d \rrbracket s_1, \llbracket x \stackrel{s}{\leftarrow} d \rrbracket s_2) = \widetilde{rpe}(x \stackrel{s}{\leftarrow} d, \mathcal{E}).$$

• *c*; *c'*. By induction, there exists a coupling $\mu_{s_1, s_2} \in \Gamma(\llbracket c \rrbracket s_1, \llbracket c \rrbracket s_2)$ such that

$$\mathbb{E}_{\mu_{s_1,s_2}}[\widetilde{rpe}(c',\mathcal{E})] \leq \widetilde{rpe}(c;c',\mathcal{E})(s_1,s_2) < \infty.$$

As a consequence, $\widetilde{rpe}(c', \mathcal{E})(s'_1, s'_2)$ must be finite for all pairs $(s'_1, s'_2) \in \operatorname{supp}(\mu_{s_1, s_2}) \triangleq S$. Again by induction, for all $(s'_1, s'_2) \in S$ there exists a coupling $\mu'_{s'_1, s'_2} \in \Gamma(\llbracket c' \rrbracket s'_1, \llbracket c' \rrbracket s'_2)$ such that

$$\mathbb{E}_{\mu'_{s'_1,s'_2}}[\mathcal{E}] \leq \widetilde{rpe}(c',\mathcal{E})(s'_1,s'_2) < \infty.$$

35

Define the following joint distribution:

$$\mu_{s_1,s_2}^*(x_1,x_2) = \mathbb{E}_{(y_1,y_2) \sim \mu_{s_1,s_2}}[\mu_{y_1,y_2}'(x_1,x_2)].$$

By a routine calculation, it is not hard to show that μ^* is indeed a coupling in $\Gamma(\llbracket c; c' \rrbracket s_1, \llbracket c; c' \rrbracket s_2)$. Let's for instance compute the first marginal (the second marginal is analogous):

$$\pi_{1}(\mu_{s_{1},s_{2}}^{*})(x_{1}) = \sum_{x_{2}\in\text{State}} \mu_{s_{1},s_{2}}^{*}(x_{1},x_{2})$$

$$= \sum_{x_{2}\in\text{State}} \mathbb{E}_{(y_{1},y_{2})\sim\mu_{s_{1},s_{2}}}[\mu_{y_{1},y_{2}}^{'}(x_{1},x_{2})]$$

$$= \mathbb{E}_{(y_{1},y_{2})\sim\mu_{s_{1},s_{2}}}[\sum_{x_{2}\in\text{State}} \mu_{y_{1},y_{2}}^{'}(x_{1},x_{2})]$$

$$= \mathbb{E}_{(y_{1},y_{2})\sim\mu_{s_{1},s_{2}}}[([[c']]y_{1})(x_{1})]$$

$$= \sum_{y_{1}\in\text{State}} \sum_{y_{2}\in\text{State}} ([[c']]y_{1})(x_{1}) \cdot \mu_{s_{1},s_{2}}(y_{1},y_{2})$$

$$= \left(\sum_{y_{1}\in\text{State}} ([[c']]y_{1})(x_{1})\right) \cdot \left(\sum_{y_{2}\in\text{State}} \mu_{s_{1},s_{2}}(y_{1},y_{2})\right)$$

$$= \sum_{y_{1}\in\text{State}} ([[c']]y_{1})(x_{1}) \cdot ([[c]]s_{1})(y_{1})$$

$$= ([[c;c']]s_{1})(x_{1})$$

Combining inequalities and applying monotonicity of expectations yields

$$\mathbb{E}_{\mu^*_{s_1,s_2}}[\mathcal{E}] = \mathbb{E}_{\mu_{s_1,s_2}}[\mathbb{E}_{\mu'_{-,-}}[\mathcal{E}]] \le \mathbb{E}_{\mu_{s_1,s_2}}[\widetilde{rpe}(c',\mathcal{E})] \le \widetilde{rpe}(c;c',\mathcal{E})(s_1,s_2).$$

• if *e* then *c* else *c'*. Note that *e* cannot be different between s_1 and s_2 , otherwise

 $\widetilde{rpe}($ if *e* then *c* else *c'*, $\mathcal{E})(s_1, s_2)$

is infinite. Thus, there are two possible cases: either *e* is true in both s_1 , s_2 , or *e* is false in both s_1 , s_2 . In the first case, we have:

[[if *e* then *c* else
$$c'$$
] $s_i = [[c]]s_i$

By induction, there exists a coupling $\mu_t(s_1, s_2) \in \Gamma(\llbracket c \rrbracket s_1, \llbracket c \rrbracket s_2)$ such that

$$\mathbb{E}_{\mu_t(s_1,s_2)}[\mathcal{E}] \leq \widetilde{rpe}(c,\mathcal{E})(s_1,s_2) = \widetilde{rpe}(\text{if } e \text{ then } c \text{ else } c',\mathcal{E})(s_1,s_2)$$

since the right-hand side is finite by assumption. Similarly, if *e* is false in both s_1 and s_2 , by induction there exists a coupling $\mu_f(s_1, s_2) \in \Gamma(\llbracket c' \rrbracket s_1, \llbracket c' \rrbracket s_2)$ such that

$$\mathbb{E}_{\mu_f(s_1,s_2)}[\mathcal{E}] \le \widetilde{rpe}(c',\mathcal{E})(s_1,s_2) = \widetilde{rpe}(\text{if } e \text{ then } c \text{ else } c',\mathcal{E})(s_1,s_2)$$

since the right-hand side is finite by assumption. Thus, we can define the desired coupling by case analysis:

$$\mu(s_1, s_2) \triangleq \begin{cases} \mu_t(s_1, s_2) &: \llbracket e \rrbracket s_1 = \llbracket e \rrbracket s_2 = tt \\ \mu_f(s_1, s_2) &: \llbracket e \rrbracket s_1 = \llbracket e \rrbracket s_2 = ff \\ &: \llbracket e \rrbracket s_1 \neq \llbracket e \rrbracket s_2 \quad \text{(impossible)} \end{cases}$$

• while *e* do *c*. By induction on *c*, for any pair of states s'_1, s'_2 and any expectation \mathcal{E}_c such that $\widetilde{rpe}(c, \mathcal{E}_c)(s'_1, s'_2)$ is finite, there exists a coupling $v_{s_1, s_2} \in \Gamma(\llbracket c \rrbracket s_1, \llbracket c \rrbracket s_2)$ such that

$$\mathbb{E}_{\nu_{s_1,s_2}}[\mathcal{E}_c] \leq \mathcal{E}_c(s_1',s_2').$$

Now, let's consider the loop. We define the following loop approximants:

$$c_0 \triangleq$$
while *tt* do skip

$$c_{i+1} \triangleq$$
 if *e* then *c*; c_i else skip

Each approximant executes at most *i* iterations of the loop; the zero-th approximant returns the zero distribution and does not execute any iterations of the loop body. By definition, the relational pre-expectation of \mathcal{E} with respect to c_0 is:

$$\widetilde{rpe}(c_0, \mathcal{E}) = \operatorname{lfp} X.\Phi_{\mathcal{E}, \operatorname{skip}}(X),$$

where the characteristic functional of a loop while *e* do *c* is defined as:

$$\Phi_{\mathcal{E},c}(X) \triangleq [e\langle 1 \rangle \land e\langle 2 \rangle] \cdot \widetilde{rpe}(c,X) + [\neg e\langle 1 \rangle \land \neg e\langle 2 \rangle] \cdot \mathcal{E} + [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot$$

It is easy to show that the constant zero relational expectation is a fixed point for the loop c_0 , and evidently it must be the least fixed point. So, $\widetilde{rpe}(c_0, \mathcal{E}) = 0$. Let

$$\mathcal{E}_0 \triangleq \widetilde{rpe}(c_0, \mathcal{E}) = 0$$

$$\mathcal{E}_{i+1} \triangleq \widetilde{rpe}(c_{i+1}, \mathcal{E}) = [e\langle 1 \rangle \land e\langle 2 \rangle] \cdot \widetilde{rpe}(c, \mathcal{E}_i) + [\neg e\langle 1 \rangle \land \neg e\langle 2 \rangle] \cdot \mathcal{E} + \cdot [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot \infty$$

By induction and definition of relational pre-expectation, $\mathcal{E}_i = \Phi^i_{\mathcal{E},c}(0)$. Furthermore, by monotonicity (Lemma 3) $\Phi^i_{\mathcal{E},c}(0)$ is a monotone increasing sequence in *i*. We now need two small lemmas.

LEMMA 6. For every $j \in \mathbb{N}$, program *c*, and relational expectation \mathcal{E} , we have:

$$\Phi_{\mathcal{E},c}^{J}(0) \leq \operatorname{lfp} X.\Phi_{\mathcal{E},c}(X) = \widetilde{rpe}(\text{while } e \text{ do } c, \mathcal{E}).$$

PROOF. By induction on *j*. The base case j = 0 is clear, and the inductive step follows by monotonicity (Lemma 3):

$$\Phi_{\mathcal{E},c}^{j+1}(0) = \Phi_{\mathcal{E},c}(\Phi_{\mathcal{E},c}^{i}(0)) \le \Phi_{\mathcal{E},c}(\mathsf{lfp}X.\Phi_{\mathcal{E},c}(X)) = \mathsf{lfp}X.\Phi_{\mathcal{E},c}(X).$$

Now, let (s_1, s_2) be two given input states such that $\widetilde{rpe}($ while e do $c, \mathcal{E})(s_1, s_2) < \infty$. As an immediate consequence, $\Phi^i_{\mathcal{E}, c}(0)(s_1, s_2)$ must be finite for all i, so $\mathcal{E}_i(s_1, s_2)$ are all finite.

LEMMA 7. For all $j \in \mathbb{N}$ and $(s'_1, s'_2) \in$ State × State, if $\mathcal{E}_j(s'_1, s'_2) < \infty$ then there exists a coupling $\mu_{j,s'_1,s'_2} \in \Gamma(\llbracket c_j \rrbracket s'_1, \llbracket c_j \rrbracket s'_2)$ such that

$$\mathbb{E}_{\mu_{j,s_1',s_2'}}[\mathcal{E}] \leq \mathcal{E}_j(s_1',s_2') < \infty.$$

PROOF. By induction on *j*. The base case j = 0 is clear, taking the null coupling that assigns probability zero to every pair of states. For the inductive step, we have

$$\mathcal{E}_{j+1} = [e\langle 1 \rangle \land e\langle 2 \rangle] \cdot \widetilde{rpe}(c, \mathcal{E}_j) + [\neg e\langle 1 \rangle \land \neg e\langle 2 \rangle] \cdot \mathcal{E} + [e\langle 1 \rangle \neq e\langle 2 \rangle] \cdot \infty.$$

Note that *e* must be equal in s'_1 and s'_2 , since $\mathcal{E}_{j+1}(s'_1, s'_2)$ is finite. There are two cases. If *e* is false in s'_1 and s'_2 , then $[\![c_{j+1}]\!]s'_1 = \delta(s'_1)$ and $[\![c_{j+1}]\!]s'_2 = \delta(s'_2)$. We can define the coupling $\mu_{s'_1,s'_2} = \delta(s'_1,s'_2) \in \Gamma([\![c_{j+1}]\!]s'_1, [\![c_{j+1}]\!]s'_2)$ and we are done, since

$$\mathbb{E}_{\mu_{s'_1,s'_2}}[\mathcal{E}] = \mathcal{E}(s'_1,s'_2) = \mathcal{E}_{j+1}(s'_1,s'_2).$$

Otherwise, suppose that *e* is true in s'_1 and s'_2 . Since $\mathcal{E}_{j+1}(s'_1, s'_2) < \infty$, we must have $\widetilde{pe}(c, \mathcal{E}_j)(s'_1, s'_2) < \infty$ as well. Hence by the (outer) induction on the structure of the program, there exists a coupling $v_{s'_1, s'_2} \in \Gamma(\llbracket c \rrbracket s'_1, \llbracket c \rrbracket s'_2)$ such that

$$\mathbb{E}_{\nu_{s_1',s_2'}}[\mathcal{E}_j] \le \mathcal{E}_j(s_1',s_2') < \infty$$

As a result, for all states $(t_1, t_2) \in \text{supp}(v_{s'_1, s'_2})$, we must have $\mathcal{E}_j(t_1, t_2)$ finite as well. By the (inner) induction hypothesis on j, there is a coupling $\mu_{j, t_1, t_2} \in \Gamma(\llbracket c_j \rrbracket t_1, \llbracket c_j \rrbracket t_2)$ such that

$$\mathbb{E}_{\mu_{j,t_1,t_2}}[\mathcal{E}] \le \mathcal{E}_j(t_1,t_2) < \infty$$

Now, we can define the coupling for the (j + 1)-th approximants:

$$\mu_{j+1,s_1',s_2'} \triangleq \mathbb{E}_{\nu_{s_1',s_2'}}[\mu_{j,-,-}]$$

We first check the distance condition. By definition, we have:

$$\begin{split} \mathbb{E}_{\mu_{j+1,s_1',s_2'}}[\mathcal{E}] &= \mathbb{E}_{(t_1,t_2) \sim \nu_{s_1',s_2'}}[\mathbb{E}_{\mu_{j,t_1,t_2}}[\mathcal{E}]] \\ &\leq \mathbb{E}_{(t_1,t_2) \sim \nu_{s_1',s_2'}}[\mathcal{E}_j(t_1,t_2)] \\ &\leq \mathcal{E}_j(s_1',s_2') \\ &\leq \mathcal{E}_{j+1}(s_1',s_2') \end{split}$$

The marginal condition is not hard to show, using the marginal properties of $v_{s'_1,s'_2}$ and μ_{j,t_1,t_2} combined with the definition of approximants: since *e* is true in s'_1 and s'_2 , we have $[\![c_{j+1}]\!]s'_1 = [\![c;c_j]\!]s'_1$ and $[\![c_{j+1}]\!]s'_2 = [\![c;c_j]\!]s'_2$. The proof follows the case for sequential composition. \Box

Since $\mathcal{E}_i(s_1, s_2) < \infty$ by assumption, we may apply Lemma 7 with input states s_1, s_2 and expectations \mathcal{E}_i to produce a sequence of couplings $\mu_{i,s_1,s_2} \in \Gamma(\llbracket c_i \rrbracket s_1, \llbracket c_i \rrbracket s_2)$ such that

$$\mathbb{E}_{\mu_{i,s_1,s_2}}[\mathcal{E}] \leq \mathcal{E}_i(s_1,s_2) = \widetilde{rpe}(c_i,\mathcal{E}) = \Phi^i_{\mathcal{E},c}(0) < \infty.$$

By Theorem 16, from the sequence μ_{i,s_1,s_2} we can extract a subsequence μ'_{i,s_1,s_2} (and a corresponding subsequence c'_i of c_i) that converges monotonically to a coupling satisfying

$$\tilde{\mu}_{s_1,s_2} \in \Gamma(\lim_{i\to\infty} \llbracket c'_i \rrbracket s_1, \lim_{i\to\infty} \llbracket c'_i \rrbracket s_2) = \Gamma(\llbracket \mathbf{while} \ e \ \mathbf{do} \ c \rrbracket s_1, \llbracket \mathbf{while} \ e \ \mathbf{do} \ c \rrbracket s_2),$$

by the definition of semantics for loops. All that remains to show is:

$$\mathbb{E}_{(s_1',s_2')\sim\tilde{\mu}_{s_1,s_2}}[\mathcal{E}(s_1',s_2')] \leq \widetilde{rpe}(\text{while } e \text{ do } c,\mathcal{E})(s_1,s_2).$$

We can compute:

$$\mathbb{E}_{(s'_{1},s'_{2})\sim\tilde{\mu}_{s_{1},s_{2}}}[\mathcal{E}(s'_{1},s'_{2})] = \sum_{(s'_{1},s'_{2})\in\text{State}\times\text{State}} \mathcal{E}(s'_{1},s'_{2}) \cdot \lim_{i\to\infty} \mu'_{i,s_{1},s_{2}}(s'_{1},s'_{2})$$

$$\leq \sum_{(s'_{1},s'_{2})\in\text{State}\times\text{State}} \lim_{i\to\infty} \mathcal{E}(s'_{1},s'_{2}) \cdot \mu'_{i,s_{1},s_{2}}(s'_{1},s'_{2}) \qquad (\mathcal{E} \text{ may be }\infty)$$

$$\leq \lim_{i\to\infty} \sum_{(s'_{1},s'_{2})\in\text{State}\times\text{State}} \mathcal{E}(s'_{1},s'_{2}) \cdot \mu'_{i,s_{1},s_{2}}(s'_{1},s'_{2}) \qquad (by \text{ Fatou's lemma})$$

$$\leq \lim_{i\to\infty} (\widetilde{rpe}(c'_{i},\mathcal{E})(s_{1},s_{2})) \qquad (by \text{ construction})$$

$$= (\lim_{i\to\infty} \widetilde{rpe}(c'_{i},\mathcal{E}))(s_{1},s_{2}) \qquad (definition)$$

$$= \lim_{i\to\infty} (\Phi^{i} = (0))(s_{1},s_{2}) \qquad (subsequence)$$

$$= \lim_{i \to \infty} (\Psi_{\mathcal{E}, c}(0))(s_1, s_2)$$
 (subsequence)

$$\leq (\text{lfp}X.\Phi_{\mathcal{E},c}(X))(s_1, s_2) \qquad (\text{Lemma 6})$$

$$= rpe(\textbf{while } e \textbf{ do } c, \mathcal{E})(s_1, s_2).$$
 (definition)

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PROOF OF THEOREM 8. We adopt the convention that $f(\infty) \triangleq \infty$, even if f is constant. The proof is by induction on the derivation.

Case Assn: By definition, we have:

$$\widetilde{rpe}(x \leftarrow e, \mathcal{E} + [\neg Q] \cdot \infty) = \mathrm{id}(\mathcal{E}\{e\langle 1 \rangle, e\langle 2 \rangle / x \langle 1 \rangle, x \langle 2 \rangle\}) + [\neg Q\{e\langle 1 \rangle, e\langle 2 \rangle / x \langle 1 \rangle, x \langle 2 \rangle\}] \cdot \infty$$

Case RAND^{*}: By the proof rule for sampling (Proposition 6) taking the coupling function given by the bijection coupling $M(s_1, s_2) = M_h$, we have:

$$\begin{split} \widetilde{rpe}(x \notin [D], \mathcal{E} + [\neg Q] \cdot \infty) &\leq \mathbb{E}_{v \sim \llbracket [D] \rrbracket} [\mathcal{E}\{v, h(v)/x\langle 1 \rangle, x\langle 2 \rangle\} + [\neg Q\{v, h(v)/x\langle 1 \rangle, x\langle 2 \rangle\}] \cdot \infty] \\ &\leq \mathbb{E}_{v \sim \llbracket [D] \rrbracket} [\mathcal{E}\{v, h(v)/x\langle 1 \rangle, x\langle 2 \rangle\}] + [\forall v \in D. \ \neg Q\{v, h(v)/x\langle 1 \rangle, x\langle 2 \rangle\}] \cdot \infty \end{split}$$

where the second inequality is because each element $v \in D$ has positive probability under [[D]], so if $\neg Q\{v, h(v)/x\langle 1 \rangle, x\langle 2 \rangle\}$ for some $v \in D$ then both sides are infinite. **Case SEq:** By induction, we have:

$$\widetilde{rpe}(c', \mathcal{E}'' + [\neg R] \cdot \infty) \le f'(\mathcal{E}') + [\neg Q] \cdot \infty$$
(induction)
$$\widetilde{rpe}(c, \mathcal{E}' + [\neg Q] \cdot \infty) \le f(\mathcal{E}) + [\neg P] \cdot \infty$$
(induction)

Then, we can conclude:

$$\widetilde{rpe}(c; c', \mathcal{E}'' + [\neg R] \cdot \infty) = \widetilde{rpe}(c, \widetilde{rpe}(c', \mathcal{E}'' + [\neg R] \cdot \infty))$$
(definition)
$$= \widetilde{rpe}(c, f'(\mathcal{E}') + [\neg Q] \cdot \infty)$$
(monotonicity)
$$\leq f'(\widetilde{rpe}(c, \mathcal{E}' + [\neg Q] \cdot \infty))$$
(affine)
$$\leq f'(f(\mathcal{E}) + [\neg P] \cdot \infty)$$
(monotonicity)
$$= f' \circ f(\mathcal{E}) + [\neg P] \cdot \infty$$

Case COND: By induction, we have:

$$\widetilde{rpe}(c, \mathcal{E}' + [\neg Q] \cdot \infty) \le f(\mathcal{E}') + [\neg (P \land e\langle 1 \rangle)] \cdot \infty$$
(induction)
$$\widetilde{rpe}(c', \mathcal{E}' + [\neg Q] \cdot \infty) \le f(\mathcal{E}') + [\neg (P \land \neg e\langle 1 \rangle)] \cdot \infty$$
(induction)

$$\begin{split} \operatorname{Assn} & \overline{+ \{Q[e_1(1), e_2(2)/x_1(1), x_2(2)\}; \mathcal{E}[e_1(1), e_2(2)/x_1(1), x_2(2)]\} x_1 \leftarrow e_1 \sim_{\operatorname{id}} x_2 \leftarrow e_2 \{Q; \mathcal{E}\}} \\ \operatorname{RanD}^* & \frac{h: D \to D \text{ bijection}}{+ \{\forall v \in D. Q[v, h(v)/x_1(1), x_2(2)]; \mathbb{E}_{v \sim [D]}[\mathcal{E}[v, h(v)/x(1), x(2)]]\} x_1} \overset{\leftarrow}{\leftarrow} [D] \sim_{\operatorname{id}} x_2 \overset{\leftarrow}{\leftarrow} [D] \{Q; \mathcal{E}\}} \\ & \operatorname{Seq} & \frac{+ \{P; \mathcal{E}\} c_1 \sim_f c_2 \{Q; \mathcal{E}'\} - + \{Q; \mathcal{E}'\} c_1' \sim_{f'} c_2' \{R; \mathcal{E}''\}}{+ \{P; \mathcal{E}\} c_1; c_1' \sim_{f' \circ f} c_2; c_2' \{R; \mathcal{E}''\}} \\ & \operatorname{Conv} & \frac{+ \{P \land e_1(1); \mathcal{E}\} c_1' \sim_f c_2 \{Q; \mathcal{E}'\} - + \{P \land e_1(1) = e_2(2)\}}{+ \{P; \mathcal{E}\} \text{ if } e_1 \text{ then } c_1 \text{ else } c_1' \sim_f f e_2 (P \land v(1) = e_2(2) (Q; \mathcal{E}')\}} \\ & \operatorname{White} & \frac{+ \{P \land v(1) = k; \mathcal{E}_k\} c_1 \sim_{f_k} c_2 \{P \land v(1) = k - 1; \mathcal{E}_{k-1}\}}{= P \to e_1(1) = e_2(1) \land (v(1) \leq 0 \leftrightarrow \neg e_1(1))} \\ \\ & \operatorname{White} & \frac{+ \{P \land v(1) = n; \mathcal{E}_n\} \text{ while } e_1 \text{ do } c_1 \sim_{f_1 \circ \cdots \circ f_n} \text{ while } e_2 \text{ do } c_2 \{P \land v(1) = 0; \mathcal{E}_0\}} \\ \\ & \operatorname{Conseq} & \frac{+ \{P; \mathcal{E}\} c_1 \sim_f c_2 \{Q; \mathcal{E}'\} - + \{P' \land P' \land f(\mathcal{E}) \leq f'(\mathcal{E}'')\} \land Q \to Q' \land (\mathcal{E}''' \leq \mathcal{E}')}{+ \{P'; \mathcal{E}''\} c_1 \sim_{f'} c_2 \{Q; \mathcal{E}'\}} \\ \\ & \operatorname{Case} & \frac{+ \{P \land R; \mathcal{E}\} c_1 \sim_f c_2 \{Q; \mathcal{E}'\} - + \{P \land \neg R; \mathcal{E}\} c_1 \sim_f c_2 \{Q; \mathcal{E}'\}}{+ \{P; \mathcal{E}\} c_1 \sim_f c_2 \{Q; \mathcal{E}'\}} \\ \\ & \operatorname{Frame-D} & \frac{+ \{P; \mathcal{E}\} c_1 \sim_f c_2 \{Q; \mathcal{E}'\} - f(z) \{Q; \mathcal{E}'\} - + \{P \land \neg R; \mathcal{E}\} c_1 \sim_f c_2 \{Q; \mathcal{E}'\}}{+ \{P; \mathcal{E} + \mathcal{E}''\} c_1 \sim_f c_2 \{Q; \mathcal{E}' + \mathcal{E}''\}} \\ \end{array}$$



Then, we have:

Case WHILE: Let *n* be any natural number. For any natural number $0 < m \le n$, we write $f^{(m)} = f_1 \circ \cdots \circ f_m$ and we define $f^{(0)} = \text{id}$. We will show:

 $\widetilde{rpe}(\text{while } e \text{ do } c, \mathcal{E}_0 + [\neg (P \land v \langle 1 \rangle = 0)] \cdot \infty) \leq f^{(n)}(\mathcal{E}_n) + [\neg (P \land v \langle 1 \rangle = n)] \cdot \infty$

We take the following loop invariant:

$$I_n \triangleq \sum_{j=0}^n ([P \land v \langle 1 \rangle = j] \cdot f^{(j)}(\mathcal{E}_j)) + [\neg (P \land v \langle 1 \rangle \le n)] \cdot \infty$$

We claim that:

$$\begin{split} \left[e\langle 1\rangle \wedge e\langle 2\rangle\right] \cdot \widetilde{rpe}(c, I_n) + \left[\neg e\langle 1\rangle \wedge \neg e\langle 2\rangle\right] \cdot \left(\mathcal{E}_0 + \left[\neg (P \wedge \upsilon \langle 1\rangle = 0)\right] \cdot \infty\right) + \left[e\langle 1\rangle \neq e\langle 2\rangle\right] \cdot \infty \leq I_n. \\ \text{Both sides are infinite if } e\langle 1\rangle \neq e\langle 2\rangle, \text{ or } \neg (P \wedge \upsilon \langle 1\rangle \leq n), \text{ or } \neg e\langle 1\rangle \wedge \neg e\langle 2\rangle \wedge \upsilon \neq 0. \text{ So, it} \end{split}$$

suffices to prove:

$$[P \land e \langle 1 \rangle \land e \langle 2 \rangle \land \upsilon \langle 1 \rangle \leq n] \cdot \widetilde{rpe}(c, I_n) + [P \land \neg e \langle 1 \rangle \land \neg e \langle 2 \rangle] \cdot \mathcal{E}_0 \leq [P \land \upsilon \langle 1 \rangle \leq n] \cdot I_n = \sum_{j=0}^n [P \land \upsilon \langle 1 \rangle = j] \cdot f^{(j)}(\mathcal{E}_j) \cdot \mathcal{E}_0$$

If $P \wedge \neg e(1) \wedge \neg e(2)$ holds, then v(1) = 0 holds by assumption. So by definition of I_n :

$$[P \wedge \neg e\langle 1 \rangle \wedge \neg e\langle 2 \rangle] \cdot \mathcal{E}_0 = [P \wedge v\langle 1 \rangle = 0] \cdot f^{(0)}(\mathcal{E}_0) \leq \mathcal{I}_n.$$

If $P \wedge e\langle 1 \rangle \wedge e\langle 2 \rangle \wedge v\langle 1 \rangle \leq n$ holds, then suppose that $v\langle 1 \rangle = k$ with $0 < k \leq n$. We have: $[P \wedge e\langle 1 \rangle \wedge e\langle 2 \rangle \wedge v\langle 1 \rangle = k] \cdot \widetilde{rpe}(c, I_n)$ $\leq [P \wedge e\langle 1 \rangle \wedge e\langle 2 \rangle \wedge v\langle 1 \rangle = k] \cdot \widetilde{rpe}(c, \sum_{j=0}^{n} [P \wedge v\langle 1 \rangle = j] \cdot f^{(j)}(\mathcal{E}_j) + [\neg (P \wedge v\langle 1 \rangle = k - 1)] \cdot \infty)$ (boolean alg.)

$$= [P \land e\langle 1 \rangle \land e\langle 2 \rangle \land v\langle 1 \rangle = k] \cdot \widetilde{rpe}(c, [P \land v\langle 1 \rangle = k-1] \cdot f^{(k-1)}(\mathcal{E}_{k-1}) + [\neg (P \land v\langle 1 \rangle = k-1)] \cdot \infty)$$

(boolean alg.)

$$\leq [P \land e\langle 1 \rangle \land e\langle 2 \rangle \land v\langle 1 \rangle = k] \cdot f^{(k-1)}(\widetilde{rpe}(c, \mathcal{E}_{k-1} + [\neg (P \land v\langle 1 \rangle = k-1)] \cdot \infty))$$
(affine)
$$\leq [P \land e\langle 1 \rangle \land e\langle 2 \rangle \land v\langle 1 \rangle = k] \cdot f^{(k-1)}(f_k(\mathcal{E}_k) + [\neg (P \land v\langle 1 \rangle = k)] \cdot \infty)$$
(induction)
$$= [P \land e\langle 1 \rangle \land e\langle 2 \rangle \land v\langle 1 \rangle = k] \cdot f^{(k)}(\mathcal{E}_k)$$
(boolean alg.)
$$\leq [P \land e\langle 1 \rangle \land e\langle 2 \rangle \land v\langle 1 \rangle = k] \cdot I_n$$
(definition)

Above, we have used the induction hypothesis:

$$\widetilde{rpe}(c, \mathcal{E}_{k-1} + [\neg (P \land v \langle 1 \rangle = k - 1)] \cdot \infty) \le f_k(\mathcal{E}_k) + [\neg (P \land v \langle 1 \rangle = k)] \cdot \infty.$$

By the loop rule, we can conclude:

$$\widetilde{rpe}($$
while e do $c, \mathcal{E} + [\neg (P \land v \langle 1 \rangle = 0)] \cdot \infty) \leq I_n \leq f^{(n)}(\mathcal{E}_n) + [\neg (P \land v \langle 1 \rangle = n)] \cdot \infty.$
Case Conseq: By induction, we have:

$$\widetilde{rpe}(c, \mathcal{E}''' + [\neg Q'] \cdot \infty) = \widetilde{rpe}(c, [Q] \cdot \mathcal{E}''' + [\neg Q'] \cdot \infty)$$
(boolean alg.)

$$\leq \widetilde{rpe}(c, \mathcal{E}' + [\neg Q'] \cdot \infty)$$
(monotonicity)

$$\leq f(\mathcal{E}) + [\neg P] \cdot \infty$$
(induction)

$$\leq f(\mathcal{E}) + [\neg P'] \cdot \infty$$
(assumption)

$$= [P'] \cdot f(\mathcal{E}) + [\neg P'] \cdot \infty$$
(boolean alg.)

$$\leq [P'] \cdot f'(\mathcal{E}'') + [\neg P'] \cdot \infty$$
(assumption)

$$\leq f'(\mathcal{E}'') + [\neg P'] \cdot \infty$$

Case CASE: By induction, we have:

$$\widetilde{rpe}(c, \mathcal{E}' + [\neg Q] \cdot \infty) \le f(\mathcal{E}') + [\neg (P \land R)] \cdot \infty$$
 (induction)
$$\widetilde{rpe}(c, \mathcal{E}' + [\neg Q] \cdot \infty) \le f(\mathcal{E}') + [\neg (P \land R)] \cdot \infty$$
 (induction)

$$rpe(c, \mathcal{E}' + [\neg Q] \cdot \infty) \le f(\mathcal{E}') + [\neg (P \land \neg R)] \cdot \infty$$
 (induction)

Thus, we have:

$$\widetilde{rpe}(c, \mathcal{E}' + [\neg Q] \cdot \infty) \le f(\mathcal{E}') + \min([\neg (P \land R)], [\neg (P \land \neg R)]) \cdot \infty$$
(induction)
$$\le f(\mathcal{E}') + [\neg P] \cdot \infty$$
(boolean alg.)

Case FRAME-D: We have:

$$\begin{split} \widetilde{rpe}(c, \mathcal{E}' + \mathcal{E}'' + [\neg Q] \cdot \infty) &\leq \widetilde{rpe}(c, \mathcal{E}' + [\neg Q] \cdot \infty) + \mathcal{E}'' \qquad (\text{frame}) \\ &\leq f(\mathcal{E}) + [\neg P] \cdot \infty + \mathcal{E}'' \qquad (\text{induction}) \\ &\leq f(\mathcal{E} + \mathcal{E}'') + [\neg P] \cdot \infty \qquad (f \text{ expanding}) \end{split}$$

F CONVERGENCE OF TD(0): OMITTED DETAILS

We start by analyzing the inner loop w_{in} . We first show that

$$\widetilde{rpe}(w_{in}, \|W\langle 1\rangle - W\langle 2\rangle\|_{\infty}) \le I_{in}$$

for the invariant I_{in} :

$$\begin{split} I_{in} &\triangleq [i\langle 1 \rangle \neq i\langle 2 \rangle] \cdot \infty \\ &+ [i\langle 1 \rangle = i\langle 2 \rangle] \cdot \max_{l < |S|} ([l < i\langle 1 \rangle] \cdot |W\langle 1 \rangle [l] - W\langle 2 \rangle [l]| + [i\langle 1 \rangle \leq l] \cdot k \cdot ||V\langle 1 \rangle - V\langle 2 \rangle ||_{\infty}). \end{split}$$

Let c_{in} be the body, and c_{samp} be the three sampling statements. Applying INV, it suffices to show: $[i\langle 1 \rangle < |S| \land i\langle 2 \rangle < |S|] \cdot \widetilde{rpe}(c_{in}, \mathcal{I}_{in}) + [i\langle 1 \rangle \ge |S| \land i\langle 2 \rangle \ge |S|] \cdot ||W\langle 1 \rangle - W\langle 2 \rangle ||_{\infty} + [i\langle 1 \rangle \neq i\langle 2 \rangle] \cdot \infty \le \mathcal{I}_{in}$ We describe how to bound the key part of the invariant, $\widetilde{rpe}(c_{in}, \mathcal{I}_{in})$ in the first term; the other cases are simpler. Computing the pre-expectation for the last two instructions gives us

$$\widetilde{rpe}(c_{in}, I_{in}) \leq \widetilde{rpe}(c_{samp}, [i\langle 1 \rangle = i\langle 2 \rangle] \cdot \mathcal{J}),$$

where \mathcal{J} is the following relational expectation:

$$\max_{l < |S|} \left(\begin{array}{c} [l < i\langle 1 \rangle] \cdot |W\langle 1 \rangle [l] - W\langle 2 \rangle [l] | \\ +[l = i\langle 1 \rangle] \cdot |(1 - \alpha) \cdot (V[i]\langle 1 \rangle - V[i]\langle 2 \rangle) + \alpha \cdot (r\langle 1 \rangle - r\langle 2 \rangle + \gamma \cdot (V[j]\langle 1 \rangle - V[j]\langle 2 \rangle)) | \\ +[i\langle 1 \rangle + 1 \le l] \cdot k \cdot ||V\langle 1 \rangle - V\langle 2 \rangle ||_{\infty} \end{array} \right).$$

By taking an appropriate coupling, we will show that $\widetilde{rpe}(c_{samp}, \mathcal{J})$ is at most \mathcal{I}_{in} . For sampling j, we take the coupling function where if $a\langle 1 \rangle = a\langle 2 \rangle$, then we take the identity coupling ensuring $j\langle 1 \rangle = j\langle 2 \rangle$, otherwise we take the product coupling. We take the same coupling for sampling r. Finally for sampling a, we take the identity coupling ensuring $a\langle 1 \rangle = a\langle 2 \rangle$. When $i\langle 1 \rangle = i\langle 2 \rangle$, $j\langle 1 \rangle = j\langle 2 \rangle$, and $r\langle 1 \rangle = r\langle 2 \rangle$. By applying rule SAMP, we can upper-bound $\widetilde{rpe}(c_{in}, \mathcal{I}_{in})$ by $[i\langle 1 \rangle = i\langle 2 \rangle = i]$ times:

$$\rho(v_a, v_r, v_j, i) \cdot \max_{l < |S|} \begin{pmatrix} [l < i] \cdot |W\langle 1\rangle[l] - W\langle 2\rangle[l]| \\ +[l = i] \cdot |(1 - \alpha) \cdot (V[i]\langle 1\rangle - V[i]\langle 2\rangle) + \alpha \cdot (\gamma \cdot (V\langle 1\rangle[v_j] - V\langle 2\rangle[v_j]))| \\ +[i + 1 \le l] \cdot k \cdot ||V\langle 1\rangle - V\langle 2\rangle||_{\infty} \end{pmatrix}$$

$$(4)$$

taking a sum over triples $(v_a, v_r, v_j) \in \mathcal{A} \times \mathcal{R} \times \mathcal{S}$ and $\rho(v_a, v_r, v_j, i)$ is the probability of drawing v_a, v_r, v_j in current state *i*; note that for any fixed $i < |\mathcal{S}|$, the coefficients sum to 1.

$$pgd(w_0, \alpha, 1):$$

$$w \leftarrow w_0;$$

$$t \leftarrow 1;$$
while $t < T$ do
$$g \leftarrow \nabla \ell(z, -)(w);$$

$$w \leftarrow \Pi_{\Omega}(w - \alpha_t \cdot g);$$

$$t \leftarrow t + 1;$$

T

. 17

Fig. 7. Projected Gradient Descent (PGD)

Now for any l < |S| and any input states, at most one of the three summands in the max is non-zero. We can bound the first and last summands:

$$[l < i] \cdot |W\langle 1\rangle[l] - W\langle 2\rangle[l]| \le I_{in} \qquad (\text{since } l < i)$$

$$[i+1 \le l] \cdot k \cdot ||V\langle 1\rangle - V\langle 2\rangle||_{\infty} \le I_{in} \qquad (\text{since } i \le l)$$

For the second summand, we have:

$$\begin{split} |l = i] \cdot |(1 - \alpha) \cdot (V\langle 1\rangle[i] - V\langle 2\rangle[i]) + \alpha \gamma \cdot (V\langle 1\rangle[v_j] - V\langle 2\rangle[v_j])| \\ \leq [l = i] \cdot |(1 - \alpha) \cdot ||V\langle 1\rangle - V\langle 2\rangle||_{\infty} + \alpha \gamma \cdot ||V\langle 1\rangle - V\langle 2\rangle||_{\infty}| \\ \leq [l = i] \cdot k \cdot ||V\langle 1\rangle - V\langle 2\rangle||_{\infty} \\ \leq I_{in} , \qquad (\text{since } i \leq l) \end{split}$$

Putting everything together, we have:

$$\widetilde{rpe}(c_{in}, I_{in}) \leq [i\langle 1 \rangle = i\langle 2 \rangle = i] \cdot \sum_{v_a, v_r, v_j} (\text{Eq. (4)})$$
$$\leq [i\langle 1 \rangle = i\langle 2 \rangle = i] \cdot \sum_{v_a, v_r, v_j} \rho(v_a, v_r, v_j, i) \cdot I_{in}$$
$$= I_{in},$$

establishing the inner invariant.

G VERIFYING ROBUSTNESS OF PROJECTED GRADIENT DESCENT (PGD)

This example is inspired by an analysis by Miller and Hardt [24]. Let $\Omega \subseteq \mathbb{R}^d$ be a compact and convex set of feasible parameters, and let $\Pi_{\Omega} : \mathbb{R}^d \to \Omega$ be the Euclidean projection sending a point from \mathbb{R}^d to the closest point in Ω under the Euclidean distance. Given a loss function ℓ , initial parameters w_0 , and a sequence of step sizes $\{\alpha_t\}_t$, the program **pgd** in Figure 7 runs projected gradient descent for *T* iterations.

Consider running this algorithm with two different loss functions $\ell \langle 1 \rangle$ and $\ell \langle 2 \rangle$, satisfying the following conditions:

(1) Gradients are close. For any parameter $w \in \mathbb{R}^d$,

$$\|\nabla \ell \langle 1 \rangle(z, -)(w) - \nabla \ell \langle 2 \rangle(z, -)(w)\| \le \gamma.$$

(2) Gradient of loss function is Lipschitz. For any two parameters $w, w' \in \mathbb{R}^d$,

 $\|\nabla \ell \langle 1 \rangle(z, -)(w) - \nabla \ell \langle 1 \rangle(z, -)(w')\| \le \beta \|w - w'\|.$

Taking the step sizes $\alpha_t \leq \alpha/t$, we can bound the distance between final weights $||w\langle 1\rangle - w\langle 2\rangle||$ from running projected gradient descent on the loss functions $\ell\langle 1\rangle$ and $\ell\langle 2\rangle$ by showing the following bound on the relational pre-expectation, which matches the analysis of Miller and Hardt [24]:

$$\widetilde{rpe}(\mathbf{pgd}(w_0, \alpha, T), \|w\langle 1\rangle - w\langle 2\rangle\|) \le \alpha \gamma T^{\alpha\beta+1}$$

Intuitively, this property means that small changes to the loss function in PGD do not lead to large changes in the learned parameters.

To start the proof, we take the following loop invariant:

$$I \triangleq [t\langle 1 \rangle \neq t\langle 2 \rangle] \cdot \infty$$

+ $[t\langle 1 \rangle = t\langle 2 \rangle] \cdot ||w\langle 1 \rangle - w\langle 2 \rangle|| \prod_{j=t\langle 1 \rangle}^{T} (1 + \alpha_j \beta)$
+ $[t\langle 1 \rangle = t\langle 2 \rangle] \cdot \sum_{s=t\langle 1 \rangle}^{T} \alpha_s \gamma \prod_{j=s+1}^{T} \exp(1 + \alpha_j \beta)$

To apply the loop rule, we need to check

$$[(t < T)\langle 1 \rangle \land (t < T)\langle 2 \rangle] \widetilde{rpe}(c, I) + [(t \ge T)\langle 1 \rangle \land (t \ge T)\langle 2 \rangle] \mathcal{E} + [(t < T)\langle 1 \rangle \neq (t < T)\langle 2 \rangle] \cdot \infty \le I.$$

The main case is when both loop guards are true and when both loop counters are equal. Taking the relational pre-expectation for the loop body in this case, we have:

$$\begin{split} \widetilde{ppe}(c,I) &= \\ &= \|\Pi_{\Omega}(w - \alpha_t \cdot \nabla \ell(z,-)(w))\langle 1 \rangle - \Pi_{\Omega}(w - \alpha_t \cdot \nabla \ell(z,-)(w))\langle 2 \rangle \| \prod_{j=t\langle 1\rangle+1}^{T} (1 + \alpha_j \beta) + \sum_{s=t\langle 1\rangle+1}^{T} \alpha_s \gamma \prod_{j=s+1}^{T} (1 + \alpha_j \beta) \\ &\leq (\|w\langle 1\rangle - w\langle 2\rangle\| + \alpha_t \|\nabla \ell(z,-)(w)\langle 1\rangle - \nabla \ell(z,-)(w)\langle 2\rangle\|) \prod_{j=t\langle 1\rangle+1}^{T} (1 + \alpha_j \beta) + \sum_{s=t\langle 1\rangle+1}^{T} \alpha_s \gamma \prod_{j=s+1}^{T} (1 + \alpha_j \beta) \\ &\leq (\|w\langle 1\rangle - w\langle 2\rangle\| + \alpha_t \beta \|w\langle 1\rangle - w\langle 2\rangle\| + \alpha_t \gamma) \prod_{j=t\langle 1\rangle+1}^{T} (1 + \alpha_j \beta) + \sum_{s=t\langle 1\rangle+1}^{T} \alpha_s \gamma \prod_{j=s+1}^{T} (1 + \alpha_j \beta) \\ &\leq (\|w\langle 1\rangle - w\langle 2\rangle\| + \alpha_t \beta \|w\langle 1\rangle - w\langle 2\rangle\| + \alpha_t \gamma) \prod_{j=t\langle 1\rangle+1}^{T} (1 + \alpha_j \beta) + \sum_{s=t\langle 1\rangle+1}^{T} \alpha_s \gamma \prod_{j=s+1}^{T} (1 + \alpha_j \beta) \\ &= I \end{split}$$

Pushing the invariant past the initial assignment instructions and taking the same step sizes $\alpha_t \leq \alpha/t$ as Miller and Hardt [24], we conclude:

$$\widetilde{rpe}(\operatorname{pgd}(w_0, \alpha, T), ||w\langle 1\rangle - w\langle 2\rangle||) \leq \sum_{s=1}^{T} \alpha_s \gamma \prod_{j=s+1}^{T} (1 + \alpha_j \beta)$$

$$\leq \sum_{s=1}^{T} \alpha_s \gamma \prod_{j=s+1}^{T} \exp(\alpha_j \beta)$$

$$\leq \sum_{s=1}^{T} \frac{\alpha\gamma}{s} \prod_{j=s+1}^{T} \exp\left(\frac{\alpha\beta}{j}\right)$$

$$= \sum_{s=1}^{T} \frac{\alpha\gamma}{s} \exp\left(\alpha\beta \sum_{j=s+1}^{T} \frac{1}{j}\right)$$

$$\leq \sum_{s=1}^{T} \frac{\alpha\gamma}{s} \exp\left(\alpha\beta \log(T/s)\right)$$

$$\leq \alpha\gamma T^{\alpha\beta} \sum_{s=1}^{T} \frac{1}{s^{\alpha\beta+1}}$$

$$\leq \alpha\gamma T^{\alpha\beta+1}.$$

H RANDOM-TO-TOP: OMITTED DETAILS

Axioms. We assume a few axioms about the shift operation. Let a_1, a_2 be two decks and J such that $\forall i.(0 \le i \le J) \Rightarrow a_1[i] = a_2[i]$. Then,

• If $j \leq J$ and $a'_i = \text{shiftR}(a_i, j)$, then $\forall i . (0 \leq i \leq J) \Rightarrow a'_1[i] = a'_2[i]$

• If $j_1, j_2 > J$, $a'_i = \text{shiftR}(a_i, j_i)$, and $a_1[j_1] = a_2[j_2]$, then $\forall i.(0 \le i \le J + 1) \Rightarrow a'_1[i] = a'_2[i]$

Additionally, if *a* is a permutation of [N], then, for all i < N, so is shift R(a, i).

Establishing the invariant. Let $C \triangleq (N - 1)/N$. Recall the loop invariant:

$$\mathcal{I} \triangleq [k\langle 1 \rangle \neq k\langle 2 \rangle] \cdot \infty + [k\langle 1 \rangle = k\langle 2 \rangle] \cdot d_M \cdot C^{\max(0, K - k\langle 1 \rangle)}$$

We check that it satisfies the loop rule:

$$[k\langle 1 \rangle < K \land k\langle 2 \rangle < K] \cdot \widetilde{rpe}(c, \mathcal{I}) + [k\langle 1 \rangle \ge K \land k\langle 2 \rangle \ge K] \cdot F + [(k\langle 1 \rangle < K) \neq (k\langle 2 \rangle < K)] \cdot \infty \le \mathcal{I},$$

If $[k\langle 1 \rangle \neq k\langle 2 \rangle] \infty$ then the right-hand side of the inequality is ∞ , and it is satisfied. Otherwise, if $[k\langle 1 \rangle \geq K \land k\langle 2 \rangle \geq K]$ then we need to check that, indeed,

$$F \le d_M \cdot C^{\max(0, K - k\langle 1 \rangle)} = d_M$$

Finally, if $[k\langle 1 \rangle < K \land k\langle 2 \rangle < K]$, we compute the pre-expectation of the loop body with respect to \mathcal{I} . Let \mathcal{I}' be the pre-expectation of the loop body without the sampling, i.e.,

$$\mathcal{I}' \triangleq [k\langle 1 \rangle + 1 \neq k\langle 2 \rangle + 1] \cdot \infty + [k\langle 1 \rangle + 1 = k\langle 2 \rangle + 1] \cdot (1/N) \cdot \left(N - \max_{i} \left(\forall j < i.a' \langle 1 \rangle [j] = a' \langle 2 \rangle [j] \right) \cdot C^{\max(0, K - k \langle 1 \rangle - 1)} \right)$$

where $a'\langle 1 \rangle = \text{shiftR}(a\langle 1 \rangle, y\langle 1 \rangle)$ and $a'\langle 2 \rangle = \text{shiftR}(a\langle 2 \rangle, y\langle 2 \rangle)$. In the following, let *l'* denote $\max_i (\forall j < ia' \langle 1 \rangle [j] = a' \langle 2 \rangle [j])$. We pick a coupling induced by a bijection π such that, for all *z*,

 $a\langle 1\rangle[z\langle 1\rangle] = a\langle 2\rangle[\pi(z\langle 1\rangle)]$. The pre-expectation induced by this assignment is:

$$\mathcal{I}^{\prime\prime} \triangleq [k\langle 1\rangle + 1 \neq k\langle 2\rangle + 1] \cdot \infty + [k\langle 1\rangle + 1 = k\langle 2\rangle + 1] \cdot (1/N) \cdot \left(N - \max_{i}(\forall j < i.a^{\prime\prime}\langle 1\rangle[j] = a^{\prime\prime}\langle 2\rangle[j]) \cdot C^{\max(0,K-k\langle 1\rangle - 1)}\right)$$

where $a''\langle 1 \rangle = \text{shiftR}(a\langle 1 \rangle, y)$ and $a'\langle 2 \rangle = \text{shiftR}(a\langle 2 \rangle, \pi(y))$.

Now we have to compute the expected value of I'' when we sample y uniformly from U([N]). There are two cases. If y < l', then $\pi(y) = y$, and $a\langle 1 \rangle [y] = a\langle 2 \rangle [y]$, and

$$\max_{i} (\forall j < i.a'' \langle 1 \rangle [j] = a'' \langle 2 \rangle [j]) = \max_{i} (\forall j < i.a \langle 1 \rangle [j] = a \langle 2 \rangle [j])$$

where we use the first axiom of shift R. The probability of this happening is precisely $l'/N = 1 - d_M$. In the other case, by the second axiom of shift R

$$\max_{i} (\forall j < i.a'' \langle 1 \rangle [j] = a'' \langle 2 \rangle [j]) + 1 \le \max_{i} (\forall j < i.a \langle 1 \rangle [j] = a \langle 2 \rangle [j])$$

This case happens with probability d_M . The inequality arises from the fact that we may have matches below l'. From the expression above we derive:

$$(1/N)\left(N - \max_{i}(\forall j < i.a''\langle 1\rangle[j] = a''\langle 2\rangle[j])\right) \le (1/N)\left(N - \max_{i}(\forall j < i.a\langle 1\rangle[j] = a\langle 2\rangle[j]) - 1\right)$$
$$= d_M - 1/N$$

Using this inequality, we can bound the pre-expectation of the loop invariant (simplifying under the assumptions $[k\langle 1 \rangle \ge K \land k\langle 2 \rangle \ge K]$ and $[k\langle 1 \rangle = k\langle 2 \rangle]$):

$$\mathbb{E}_{y \notin U([N])}[\mathcal{I}''] \leq (1 - d_M) \cdot d_M \cdot C^{K - k \langle 1 \rangle - 1} + d_M \cdot (d_M - 1/N) \cdot C^{K - k \langle 1 \rangle - 1}$$
$$= C^{K - \langle 1 \rangle - 1} \cdot d_M \cdot ((1 - d_M) + (d_M - 1/N))$$
$$= C^{K - \langle 1 \rangle - 1} \cdot d_M \cdot C$$
$$= C^{K - \langle 1 \rangle} \cdot d_M = \mathcal{I}$$

This finishes the proof of the premise of the loop rule. Note that we did not explicitly compute the pre-expectation of the loop invariant, we just found an upper bound which is enough to apply the loop rule.

I UNIFORM RIFFLE: OMITTED DETAILS

Axioms. We use some axioms about permutations, filtering, and concatenation.

• Let $perm(a_1, a_2)$ be the predicate that a_1 and a_2 are permutations of *C*. Then if we split a deck into two pieces and concatenate them, the result is a permutation of the original. Formally, for any bit-vector *b* we have:

 $\operatorname{perm}(a, \operatorname{cat}(a(\bar{b}), a(b)))$

• Let a_1, a_2 be permutations, b_1, b_2 be bitstrings, and a'_1, a'_2 be

$$a_i' = \operatorname{cat}(a_i(b_i), a_i(b_i)).$$

Then if b_1, b_2 match cards in a_1, a_2 , i.e., $b_1 \circ a_1^{-1} = b_2 \circ a_2^{-1}$, then we can bound the size of blocks in the block decomposition of a'_1, a'_2 as:

 $\forall c \in [C]. \ |BD(a_1',a_2')(c)| \leq \bar{b}(a_1^{-1}(c))(\bar{b}(BD(a_1,a_2)(c))) + b(a_1^{-1}(c))(b(BD(a_1,a_2)(c)))$

where we write b(P) and $\bar{b}(P)$ to mean the total number of ones in *b* and \bar{b} at the positions *P*.

• Summing the previous bound over all cards gives:

$$\sum_{c \in C} |BD(a_1', a_2')(c)| \le \sum_{[c] \in BD(a_1, a_2)} \bar{b}(BD(a_1, a_2)(c))^2 + b(BD(a_1, a_2)(c))^2$$

where the right-hand side sums over the equivalence classes of cards/positions induced by the block decomposition.

Defining the distance. Defining the distance between decks requires some care. Consider the following distance based on positions:

$$d_P(\textit{deck}_1,\textit{deck}_2) riangleq (1/N^2) \sum_{c \in C} |\textit{deck}_1^{-1}(c) - \textit{deck}_2^{-1}(c)|$$

This distance measures the total difference between the positions of each card in $deck_1$ and its counterpart in $deck_2$, normalized to be in [0, 1]; and $d_P = 0$ holds only when $deck_1 = deck_2$. However, it is not easy to directly show that this distance is monotonically decreasing in expectation—indeed, some terms in the sum may actually increase. Instead, we define an upper bound d_c on $|deck_1^{-1}(c) - deck_2^{-1}(c)|$ for every card. The sum $d_M \triangleq 1/N^2 \sum_{c \in C} d_c$ will be an upper bound of d_P , and d_M decreases monotonically to zero.

We will define d_c in terms of a few concepts from the theory of permutations. Given two decks $deck_1$, $deck_2$ and a permutation π on positions taking $deck_1$ to $deck_2$, there is a unique *cyclical* decomposition of π , i.e., we can partition the positions into P_1, \ldots, P_k such that π moves positions in P_i as a single cycle. We define a *block* decomposition of π to be a partition of the positions B_1, \ldots, B_j such that each block is contiguous, and π acts as a permutation on each B_i . A block decomposition is *minimal* if no block can be further decomposed; it is not hard to show that a minimal block decomposition must be unique. When $deck_1$, $deck_2$ are permutations, we write $BD(deck_1, deck_2)$ for the block decomposition induced by two decks $deck_1$ and $deck_2$. Finally, to define the distance, for every card $c \in C$ we let:

$$d_c \triangleq |BD(deck_1, deck_2)(c)| - 1$$

where $|BD(deck_1, deck_2)(c)|$ is the size of the block containing card *c* in $deck_1$ and $deck_2$; both positions must be in the same block. The size of each block is at least 1, and if the distance d_c is zero then *c* must be at the same position in $deck_1$ and $deck_2$. It is not hard to show that the size of the *c*'s block is at least the difference in *c*'s position across $deck_1$ and $deck_2$:

$$|deck_1^{-1}(c) - deck_2^{-1}(c)| \le d_c$$

so $d_c = 0$ implies that *c* is at the same position in $deck_1$ and a_2 . (However, the reverse implication may not hold.) As a result, we can upper bound our target distance

$$d_P \leq \frac{1}{N^2} \sum_{c \in C} d_c = d_M.$$

Now, we turn to the loop. Let Φ be the binary invariant

$$\Phi \triangleq \mathsf{perm}(deck\langle 1 \rangle, deck\langle 2 \rangle) \land k\langle 1 \rangle = k\langle 2 \rangle \land (b \circ deck^{-1})\langle 1 \rangle = (b \circ deck^{-1})\langle 2 \rangle$$

and take the following invariant expectation:

$$I = [\neg \Phi] \cdot \infty + [\Phi] \cdot d_M \cdot (1/2)^{(K-k\langle 1 \rangle)_+}$$

We want to verify that:

$$\begin{array}{l} [(k < K)\langle 1 \rangle \land (k < K)\langle 2 \rangle] \cdot \overrightarrow{rpe}(bd, I) \\ + \quad [(k \ge K)\langle 1 \rangle \land (k \ge K)\langle 2 \rangle] \cdot d_P \\ + \quad [(k < K)\langle 1 \rangle \neq (k < K)\langle 2 \rangle] \cdot \infty \qquad \leq \quad I, \end{array}$$

where *bd* is the loop body. The cases $[(k \ge K)\langle 1 \rangle \land (k \ge K)\langle 2 \rangle]$ and $[(k < K)\langle 1 \rangle \neq (k < K)\langle 2 \rangle]$ are almost immediate. The main case is when $[(k < K)\langle 1 \rangle \land (k < K)\langle 2 \rangle]$. Focusing on the case where Φ holds (otherwise there is nothing to show), this boils down to:

$$\mathbb{E}_{b}[d_{M}(\operatorname{cat}(\operatorname{deck}(\bar{b}),\operatorname{deck}(b))\langle 1\rangle,\operatorname{cat}(\operatorname{deck}(\bar{b}),\operatorname{deck}(b))\langle 2\rangle)] \leq \frac{1}{2}d_{M}$$

i.e., each iteration of the loop halves the invariant, where the expected value is taken over $b\langle 1 \rangle \sim \{0,1\}^N$ and $b\langle 2 \rangle$ is coupled so that $(b \circ deck^{-1})\langle 1 \rangle = (b \circ deck^{-1})\langle 2 \rangle$. Above, we write $d_M(x_1, x_2)$ as shorthand for $d_M[x_1, x_2/deck\langle 1 \rangle, deck\langle 2 \rangle]$.

The inequality follows from the permutation axioms, and from the mean and variance of the binomial distribution—for $deck_1$, $deck_2$ fixed, $\bar{b}(BD(deck_1, deck_2))$ and $b(BD(deck_1, deck_2))$ each follow the binomial distribution with $|BD(deck_1, deck_2)(c)|$ trials and parameter 1/2. This completes the proof for the body of the loop. Finally, we push the invariant past the initialization of the procedure, and we have the bound:

$$\widetilde{rpe}(\mathbf{riffle}(deck, N, K), d_P) \le [\neg \Phi] + [\Phi] \cdot d_M \cdot (1/2)^K \le [\neg \Phi] + [\Phi] \cdot (1/2)^K$$

since the initial distance d_M is at most 1. Given that d_P assigns different decks a distance of at least $1/N^2$, Theorem 3 implies that the TV distance between the deck distributions is at most

$$v(K,N) = \max_{d_1,d_2 \in [N]} TV([[riffle]](d_1,N,K), [[riffle]](d_2,N,K)) \le N^2 \left(\frac{1}{2}\right)^K,$$

so the distributions converge to one another and to the uniform distribution exponentially quick. If we take $K \ge \log_2(N^2\rho)$, v(K) is asymptotically bounded by $O(1/\rho)$ for large *N*. When setting $\rho = N$, we establish the following guarantee.

THEOREM 17. Let $K = 3 \log N$, and Perm([N]) be the set of permutations over N. For any initial permutation of deck,

$$TV(riffle(deck, N, K), Unif\{Perm([N])\}) \in O(1/N)$$

Establishing the invariant. Recall that we need to show:

$$\mathbb{E}_{b}[d_{M}(\operatorname{cat}(\operatorname{deck}(\bar{b}),\operatorname{deck}(b))\langle 1\rangle,\operatorname{cat}(\operatorname{deck}(\bar{b}),\operatorname{deck}(b))\langle 2\rangle)] \leq \frac{1}{2}d_{M}(\operatorname{deck}\langle 1\rangle,\operatorname{deck}\langle 2\rangle),$$

i.e., each iteration of the loop halves the invariant, where the expected value is taken over $b\langle 1 \rangle \sim \{0,1\}^N$ and $b\langle 2 \rangle$ is coupled so that $(b \circ deck^{-1})\langle 1 \rangle = (b \circ deck^{-1})\langle 2 \rangle$. Writing $a_1, a_2 = deck\langle 1 \rangle, \langle 2 \rangle$, and $a'_1, a'_2 = \operatorname{cat}(deck(\bar{b}), deck(b))\langle 1 \rangle, \langle 2 \rangle$, and $b_1, b_2 = b\langle 1 \rangle, \langle 2 \rangle$, the permutation axioms give:

$$\begin{split} \mathbb{E}_{b} \left[d_{M}(a_{1}', a_{2}') \right] &= \frac{1}{N^{2}} \sum_{c \in C} \mathbb{E}_{b} \left[|BD(a_{1}', a_{2}')(c)| - 1 \right] \\ &\leq \frac{1}{N^{2}} \sum_{[c] \in BD(a_{1}, a_{2})} \mathbb{E}_{b} [\bar{b}(BD(a_{1}, a_{2})(c))^{2}] + \mathbb{E}_{b} [b(BD(a_{1}, a_{2})(c))^{2}] - |BD(a_{1}, a_{2})(c)| \\ &= \frac{1}{2N^{2}} \sum_{[c] \in BD(a_{1}, a_{2})} |BD(a_{1}, a_{2})(c)|^{2} - |BD(a_{1}, a_{2})(c)| \\ &= \frac{1}{2N^{2}} \sum_{c \in C} (|BD(a_{1}, a_{2})(c)| - 1) \\ &= \frac{1}{2} d_{M}(a_{1}, a_{2}). \end{split}$$

J ASYNCHRONOUS RULES: OMITTED DETAILS

We prove soundness of the asynchronous rules.

PROOF OF THEOREM 15. We start with the rule for conditionals. Let *c* be a program that is almost surely terminating, let \mathcal{E} be a relational pre-expectation, and let $s_1, s_2 \in$ State be two states. If $s_1(e) = s_2(e)$, then the bound follows from soundness of synchronous case (Theorem 4):

$$rpe(\text{if } e \text{ then } c, \mathcal{E})(s_1, s_2) \leq \widetilde{rpe}(\text{if } e \text{ then } c, \mathcal{E})(s_1, s_2)$$
$$= ([e\langle 1 \rangle \land e\langle 2 \rangle] \cdot \widetilde{rpe}(c, \mathcal{E}) + [\neg e\langle 1 \rangle \land \neg e\langle 2 \rangle] \cdot \mathcal{E})(s_1, s_2).$$

Otherwise if *e* is true in s_1 and false in s_2 , then:

$$rpe(\text{if } e \text{ then } c, \mathcal{E})(s_1, s_2) = \inf_{\mu \in \Gamma(\llbracket c \rrbracket s_1, \delta(s_2))} \mathbb{E}_{\mu}[\mathcal{E}] \le wpe\langle 1 \rangle(c, \mathcal{E})(s_1, s_2)$$

by Lemma 1. The case where *e* is false in s_1 and true in s_2 is almost identical.

Next, we consider the asynchronous rule for loops. Let **while** *e* **do** *c* be almost surely terminating. We define a sequence of loop approximants:

$$c_0 \triangleq \mathbf{skip}$$

 $c_{i+1} \triangleq (\mathbf{if} \ e \ \mathbf{then} \ c); c_i$

When the loop is almost surely terminating, we have the following equivalence:

$$\llbracket \mathbf{while} \ e \ \mathbf{do} \ c \rrbracket s = \lim_{i \to \infty} (\llbracket c_i \rrbracket s)$$

for any input state *s*, and the limit of distributions exists.

Our overall argument proceeds much like the proof for the synchronous case. We first show that the least-fixed point of a characteristic function of the loop is an upper bound on pre-expectation. Then, we argue that the asynchronous loop rule shows that I is a fixed point with respect to the characteristic function, so it must also be an upper bound. We work with the following characteristic function:

$$\Psi_{\mathcal{E},c}(\mathcal{E}') \triangleq [e\langle 1 \rangle \land e\langle 2 \rangle] \cdot \widetilde{rpe}(c, \mathcal{E}') + [\neg e\langle 1 \rangle \land \neg e\langle 2 \rangle] \cdot \mathcal{E} \\ + [e\langle 1 \rangle \land \neg e\langle 2 \rangle] \cdot wpe\langle 1 \rangle (c, \mathcal{E}') + [\neg e\langle 1 \rangle \land e\langle 2 \rangle] \cdot wpe\langle 2 \rangle (c, \mathcal{E}').$$

By Lemma 3 and monotonicity of the weakest pre-expectation operator, the operator $\Psi_{\mathcal{E},c}$ is monotone. Thus, the least fixed-point exists:

$$\mathcal{L}_{\mathcal{E},c} = \mathsf{lfp}X.\,\Psi_{\mathcal{E},c}(X).$$

We can inductively define:

$$\begin{split} \mathcal{E}_{0} &\triangleq \left[\neg e\langle 1 \rangle \land \neg \langle 2 \rangle \right] \cdot \mathcal{E} \\ \mathcal{E}_{i+1} &\triangleq \left[e\langle 1 \rangle \land e\langle 2 \rangle \right] \cdot \widetilde{rpe}(c, \mathcal{E}_{i}) + \left[\neg e\langle 1 \rangle \land \neg e\langle 2 \rangle \right] \cdot \mathcal{E} \\ &+ \left[e\langle 1 \rangle \land \neg e\langle 2 \rangle \right] \cdot wpe\langle 1 \rangle (c, \mathcal{E}_{i}) + \left[\neg e\langle 1 \rangle \land e\langle 2 \rangle \right] \cdot wpe\langle 2 \rangle (c, \mathcal{E}_{i}). \end{split}$$

By definition $\mathcal{E}_i = \Psi_{\mathcal{E},c}^i(\mathcal{E}_0)$, and by monotonicity \mathcal{E}_i is a monotone increasing sequence. Furthermore, for any expectation \mathcal{E}' we have $\mathcal{E}_0 \leq \Psi_{\mathcal{E},c}(\mathcal{E}')$, hence $\mathcal{E}_0 \leq \mathcal{L}_{\mathcal{E},c}$. By monotonicity of $\Psi_{\mathcal{E},c}$, we have $\mathcal{E}_i \leq \mathcal{L}_{\mathcal{E},c}$ for every *i*.

We now prove an analogue of Lemma 7.

LEMMA 8. For all $j \in \mathbb{N}$ and $(s'_1, s'_2) \in$ State × State, there exists $\mu_{j, s'_1, s'_2} \in \Gamma(\llbracket c_j \rrbracket s'_1, \llbracket c_j \rrbracket s'_2)$ such that $\mathbb{E}_{\mu_{j, s'_1, s'_2}}[\mathcal{E}] \leq \mathcal{E}_j(s'_1, s'_2) + (\rho_j(s'_1) + \rho_j(s'_2)) \cdot M_j(\mathcal{E}, s'_1, s'_2)$

where $\rho_i(s)$ is the probability of e being true in $[c_i]s$, and:

 $M_{j}(\mathcal{E}, s_{1}', s_{2}') = \max\{\mathcal{E}(t_{1}, t_{2}) \mid t_{1} \in supp(\llbracket c_{j} \rrbracket s_{1}'), t_{2} \in supp(\llbracket c_{j} \rrbracket s_{2}')\}.$

PROOF. By induction on *j*. The base case j = 0 is clear, taking the coupling $\delta(s'_1, s'_2)$. For the inductive step, we have

$$\mathcal{E}_{j+1} \triangleq [e\langle 1 \rangle \wedge e\langle 2 \rangle] \cdot \widetilde{rpe}(c, \mathcal{E}_j) + [\neg e\langle 1 \rangle \wedge \neg e\langle 2 \rangle] \cdot \mathcal{E} + [e\langle 1 \rangle \wedge \neg e\langle 2 \rangle] \cdot wpe\langle 1 \rangle (c, \mathcal{E}_j) + [\neg e\langle 1 \rangle \wedge e\langle 2 \rangle] \cdot wpe\langle 2 \rangle (c, \mathcal{E}_j).$$
(5)

There are four cases.

Case: $s'_1(e) = ff$ **and** $s'_2(e) = ff$. In this case, $[\![c_{j+1}]\!]s'_1 = \delta(s'_1)$ and $[\![c_{j+1}]\!]s'_2 = \delta(s'_2)$. We can define the coupling $\mu_{s'_1,s'_2} = \delta(s'_1,s'_2) \in \Gamma([\![c_{j+1}]\!]s'_1, [\![c_{j+1}]\!]s'_2)$ and we are done, since

$$\mathbb{E}_{\mu_{s'_1,s'_2}}[\mathcal{E}] = \mathcal{E}(s'_1, s'_2) = \mathcal{E}_{j+1}(s'_1, s'_2).$$

Case: $s'_1(e) = tt$ and $s'_2(e) = tt$. In this case, $[c_{j+1}]s'_1 = [c; c_j]s'_1$ and $[c_{j+1}]s'_2 = [c; c_j]s'_2$. If $\mathcal{E}_{j+1}(s'_1, s'_2)$ is infinite we are done, so suppose that it is finite. By Theorem 4, there exists a coupling $v_{s'_1, s'_2} \in \Gamma([c]s'_1, [c]]s'_2)$ such that

$$\mathbb{E}_{\nu_{s'_1,s'_2}}[\mathcal{E}_j] \le \mathcal{E}_j(s'_1,s'_2)$$

By the induction hypothesis, there is a coupling $\mu_{j,t_1,t_2} \in \Gamma(\llbracket c_j \rrbracket t_1, \llbracket c_j \rrbracket t_2)$ such that

$$\mathbb{E}_{\mu_{j,t_1,t_2}}[\mathcal{E}] \le \mathcal{E}_j(t_1,t_2) + (\rho_j(t_1) + \rho_j(t_2)) \cdot M_j(\mathcal{E},t_1,t_2).$$

Now, we can define the coupling for the (j + 1)-th approximants:

$$\mu_{j+1,s_1',s_2'} \triangleq \mathbb{E}_{\nu_{s_1',s_2'}}[\mu_{j,-,-}]$$

We first check the distance condition. By definition, we have:

$$\begin{split} \mathbb{E}_{\mu_{j+1,s_1',s_2'}}[\mathcal{E}] &= \mathbb{E}_{(t_1,t_2) \sim \nu_{s_1',s_2'}}[\mathbb{E}_{\mu_{j,t_1,t_2}}[\mathcal{E}]] \\ &\leq \mathbb{E}_{(t_1,t_2) \sim \nu_{s_1',s_2'}}[\mathcal{E}_j(t_1,t_2) + (\rho_j(t_1) + \rho_j(t_2)) \cdot M_j(\mathcal{E},t_1,t_2)] \\ &\leq \mathcal{E}_j(s_1',s_2') + (\rho_{j+1}(s_1') + \rho_{j+1}(s_2')) \cdot M_{j+1}(\mathcal{E},s_1',s_2') \\ &\leq \mathcal{E}_{j+1}(s_1',s_2') + (\rho_{j+1}(s_1') + \rho_{j+1}(s_2')) \cdot M_{j+1}(\mathcal{E},s_1',s_2'). \end{split}$$

The marginal condition is not hard to show, using the marginal properties of $v_{s'_1,s'_2}$ and μ_{j,t_1,t_2} combined with the definition of approximants: since e is true in s'_1 and s'_2 , we have $[c_{j+1}]s'_1 = [c; c_j]s'_1$ and $[c_{j+1}]s'_2 = [c; c_j]s'_2$. The proof follows the case for sequential composition. **Case:** $s'_1(e) = tt$ **and** $s'_2(e) = ff$. In this case, $[c_{j+1}]s'_1 = [c; c_j]s'_1$ and $[c_{j+1}]s'_2 = [skip]s'_2$. By Lemma 1,

there exists a coupling $v_{s'_1,s'_2} \in \Gamma(\llbracket c \rrbracket s'_1, \llbracket skip \rrbracket s'_2)$ such that

$$\mathbb{E}_{v_{s'_1,s'_2}}[\mathcal{E}_j] \le wpe\langle 1 \rangle(c, \mathcal{E})(s'_1, s'_2) = \mathcal{E}_j(s'_1, s'_2).$$

By the induction hypothesis, there is a coupling $\mu_{j,t_1,t_2} \in \Gamma(\llbracket c_j \rrbracket t_1, \llbracket c_j \rrbracket t_2)$ such that

$$\mathbb{E}_{\mu_{j,t_1,t_2}}[\mathcal{E}] \le \mathcal{E}_j(t_1, t_2) + (\rho_j(t_1) + \rho_j(t_2)) \cdot M_j(\mathcal{E}, t_1, t_2).$$

Now, we can define the coupling for the (j + 1)-th approximants:

$$\mu_{j+1,s_1',s_2'} \triangleq \mathbb{E}_{\nu_{s_1',s_2'}}[\mu_{j,-,-}]$$

The distance and marginal conditions follow as in the previous case.

Case: $s'_1(e) = ff$ and $s'_2(e) = tt$. In this case, $[c_{j+1}]s'_1 = [skip]s'_1$ and $[c_{j+1}]s'_2 = [c; c_j]s'_2$. By Lemma 1, there exists a coupling $v_{s'_1, s'_2} \in \Gamma([skip]s'_1, [c]]s'_2)$ such that

$$\mathbb{E}_{v_{s_1',s_2'}}[\mathcal{E}_j] \leq wpe\langle 2 \rangle(c, \mathcal{E})(s_1',s_2') = \mathcal{E}_j(s_1',s_2').$$

By the induction hypothesis, there is a coupling $\mu_{j,t_1,t_2} \in \Gamma(\llbracket c_j \rrbracket t_1, \llbracket c_j \rrbracket t_2)$ such that

$$\mathbb{E}_{\mu_{j,t_1,t_2}}[\mathcal{E}] \le \mathcal{E}_j(t_1,t_2) + (\rho_j(t_1) + \rho_j(t_2)) \cdot M_j(\mathcal{E},t_1,t_2).$$

Now, we can define the coupling for the (j + 1)-th approximants:

$$\mu_{j+1,s_1',s_2'} \triangleq \mathbb{E}_{\nu_{s_1',s_2'}}[\mu_{j,-,-}]$$

The distance and marginal conditions follow as in the previous case.

Thus, we may apply Lemma 8 with input states s_1, s_2 and expectations \mathcal{E}_i to produce a sequence of couplings $\mu_{i,s_1,s_2} \in \Gamma(\llbracket c_i \rrbracket s_1, \llbracket c_i \rrbracket s_2)$ such that

$$\mathbb{E}_{\mu_{i,s_{1},s_{2}}}[\mathcal{E}] \leq \mathcal{E}_{i}(s_{1},s_{2}) + (\rho_{i}(s_{1}) + \rho_{i}(s_{2})) \cdot M_{i}(\mathcal{E},s_{1},s_{2})$$

= $\Psi^{i}_{\mathcal{E},c}(\mathcal{E}_{0})(s_{1},s_{2}) + (\rho_{i}(s_{1}) + \rho_{i}(s_{2})) \cdot M_{i}(\mathcal{E},s_{1},s_{2}).$

By Theorem 16, we can extract a subsequence μ'_{i,s_1,s_2} (with a corresponding subsequence c'_i of c_i) from the sequence μ_{i,s_1,s_2} that converges monotonically to a coupling satisfying

$$\tilde{\mu}_{s_1,s_2} \in \Gamma(\lim_{i\to\infty} \llbracket c'_i \rrbracket s_1, \lim_{i\to\infty} \llbracket c'_i \rrbracket s_2) = \Gamma(\llbracket \mathbf{while} \ e \ \mathbf{do} \ c \rrbracket s_1, \llbracket \mathbf{while} \ e \ \mathbf{do} \ c \rrbracket s_2),$$

where the equality holds because the loop is almost surely terminating. All that remains to show is:

$$\mathbb{E}_{(s_1',s_2')\sim\tilde{\mu}_{s_1,s_2}}[\mathcal{E}(s_1',s_2')] \leq \widetilde{rpe}(\text{while } e \text{ do } c,\mathcal{E})(s_1,s_2).$$

We can compute:

$$\mathbb{E}_{(s_{1}',s_{2}')\sim\tilde{\mu}_{s_{1},s_{2}}}[\mathcal{E}(s_{1}',s_{2}')] = \sum_{(s_{1}',s_{2}')\in\text{State}\times\text{State}} \mathcal{E}(s_{1}',s_{2}') \cdot \lim_{i\to\infty} \mu_{i,s_{1},s_{2}}'(s_{1}',s_{2}')$$

$$\leq \sum_{(s_{1}',s_{2}')\in\text{State}\times\text{State}} \lim_{i\to\infty} \mathcal{E}(s_{1}',s_{2}') \cdot \mu_{i,s_{1},s_{2}}'(s_{1}',s_{2}') \qquad (\mathcal{E} \text{ may be } \infty)$$

$$\leq \lim_{i\to\infty} \sum_{(s_{1}',s_{2}')\in\text{State}\times\text{State}} \mathcal{E}(s_{1}',s_{2}') \cdot \mu_{i,s_{1},s_{2}}'(s_{1}',s_{2}') \qquad (by \text{ Fatou's lemma})$$

$$= (\lim_{i\to\infty} \Psi_{\mathcal{E},c}^{i}(\mathcal{E}_{0}))(s_{1},s_{2}) + \lim_{i\to\infty} (\rho_{i}'(s_{1}) + \rho_{i}'(s_{2})) \cdot M_{i}'(\mathcal{E},s_{1},s_{2}) \qquad (subsequence)$$

$$\leq \mathcal{L}_{\mathcal{E},c}(s_{1},s_{2}). \qquad (bounded assumption)$$

Finally, the premise of the asynchronous loop rule implies that $\Psi_{\mathcal{E},c}(\mathcal{I}) \leq \mathcal{I}$, i.e., \mathcal{I} is a pre-fixedpoint of $\Psi_{\mathcal{E},c}$. Since $\mathcal{L}_{\mathcal{E},c}$ is the least fixed point, we have:

$$rpe(\text{while } e \text{ do } c, \mathcal{E})(s_1, s_2) \leq \mathbb{E}_{(s_1', s_2') \sim \tilde{\mu}_{s_1, s_2}}[\mathcal{E}(s_1', s_2')] \leq \mathcal{L}_{\mathcal{E}, c}(s_1, s_2) \leq I(s_1, s_2).$$