Representation Policy Iteration

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Abstract

This paper addresses a fundamental issue central to approximation methods for solving large Markov decision processes (MDPs): how to automatically learn the underlying representation for value function approximation? A novel theoretically rigorous framework is proposed that automatically generates geometrically customized orthonormal sets of basis functions, which can be used with any approximate MDP solver like least-squares policy iteration (LSPI). The key innovation is a coordinate-free representation of value functions, using the theory of smooth functions on a Riemannian manifold. Hodge theory yields a constructive method for generating basis functions for approximating value functions based on the theory of smooth functions on a Riemannian manifold. This approach allows applying powerful mathematical tools for basis function generation by exploiting the properties of the self-adjoint Laplace operator on Riemannian manifolds.

1 Introduction

This paper presents a unified framework for learning representation and behavior, integrating policy learning using the framework of Markov decision processes [16] with automated representation discovery using abstract harmonic analysis to build geometrically customized basis functions on graphs [4]. The resulting combined approach enables agents to learn representations that reflect both their past experience and the inherent large-scale geometry of the environment, as well as learn policies by using these customized basis functions to approximate value functions. The key innovation is a coordinate-free representation of value functions, using the Hilbert space of smooth functions on a Riemannian manifold. This approach allows applying powerful mathematical tools for basis function generation by exploiting the properties of the self-adjoint Laplace operator on Riemannian manifolds.

Markov decision processes (MDPs) are a well-studied model of acting under uncertainty studied in decision-theoretic planning [3] and reinforcement learning [19]. A finite MDP $M = \langle S, A, P^a_{s\rightarrow}, R^a_{s\rightarrow} \rangle$ is specified by a set of states $S$, a set of actions $A$, a transition model $P^a_{s\rightarrow}$ specifying the distribution over future states $s'$ when an action $a$ is performed in state $s$, and a corresponding reward model $R^a_{s\rightarrow}$, specifying a scalar cost or reward. Methods for solving MDPs have been studied for almost 50 years: exact methods such as value iteration and policy iteration represent value functions using a table [16]; approximate methods like least-squares policy iteration (LSPI) and linear programming methods project the exact value function onto a subspace spanned by a set of handcoded basis functions [6, 7, 8]. The proposed approach can be viewed as automatically generating subspaces for projecting the value function using the framework of harmonic analysis [1]. The framework for representation discovery is
based on spectral analysis of a self-adjoint symmetric random walk operator on graphs [4]. The proposed approach fundamentally differs from past work on basis function generation, for example tuning a pre-defined set of functions [13] or generating tabular basis functions for a linear programming based value function approximator using a greedy algorithm, based on the error in approximating a particular value function [15].

2 Overview of the Approach

The framework combines Samuel’s value function paradigm with Amarel’s representation learning paradigm [11]. The framework also provides a new formulation of task-independent RL, where agents learn global basis functions or proto-value functions [10]. In this paper, we present the framework as an enhancement of policy iteration, namely representation policy iteration (RPI), since it enables learning both policies and the underlying representations. The proposed framework uses spectral graph theory [4] to build basis representations for smooth (value) functions on graphs induced by Markov decision processes. Any policy in an MDP can be viewed as a Markov chain partitioning states into transient and recurrent states. The construction of basis functions is based on analyzing a symmetric operator (the graph Laplacian) which can be viewed as a reversible random walk on the state space. It is important to note that the set of basis functions learned from a reversible random walk is still useful in approximating value functions for any policy. Thus, the process of learning basis functions by spectral analysis of reversible random walks is an off-policy representation learning method, in the sense that the actual MDP dynamics under a specific policy may induce a non-reversible random walk. Reversible random walks greatly simplify spectral analysis since such random walks are similar to a symmetric operator on the state space.

For any graph \( G \), the “tabular” representation is the orthonormal set of basis functions \( \phi(i) = [0 \ldots i \ldots 0] \), one for each vertex (state) in the graph. Besides being inefficient, this representation does not exploit the topology of the specific graph. Intuitively, a representation should reflect the (irregular) topology of the state space under consideration. This problem also affects more efficient approximations, such as the polynomial basis functions where \( \phi(s) = [1 s \ldots s^k] \) for some fixed \( k \) [8]. While this encoding is sparse, it is numerically unstable for large graphs, dependent on the ordering of vertices, and once again, insensitive to the underlying state space geometry. Our approach addresses these shortcomings by building basis functions on graphs using harmonic analysis of the graph topology. First, we briefly review linear approximation methods for solving MDPs, in particular LSPI. LSPI and other linear approximation methods approximate the true action-value function \( Q^\pi(s, a) \) for a policy \( \pi \) using a set of handcoded basis functions \( \phi(s, a) \) that can be viewed as doing dimensionality reduction: the true action value function \( Q^\pi(s, a) \) is a vector in a high dimensional space \( \mathcal{R}^{S \times A} \), and using the basis functions amounts to reducing the dimension to \( \mathcal{R}^k \) where \( k \ll |S| \times |A| \). The approximated action value is thus

\[
\hat{Q}^\pi(s, a; w) = \sum_{j=1}^k \phi_j(s, a)w_j
\]

where the \( w_j \) are weights or parameters that can be determined using a least-squares method. Let \( Q^\pi \) be a real (column) vector \( \in \mathcal{R}^{S \times A} \). The column vector \( \phi(s, a) \) is a real vector of size \( k \) where each entry corresponds to the basis function \( \phi_j(s, a) \) evaluated at the state action pair \((s, a)\). The approximate action-value function can be written as \( Q^\pi = \Phi w^\pi \), where \( w^\pi \) is a real column vector of length \( k \) and \( \Phi \) is a real matrix with \( |S| \times |A| \) rows and \( k \) columns. Each row of \( \Phi \) specifies all the basis functions for a particular state action pair \((s, a)\), and each column represents the value of a particular basis function over all state action pairs. LSPI uses a least-squares fixed-point approximation \( T_\pi Q^\pi \approx Q^\pi \), where \( T_\pi \) is the Bellman backup operator. This latter approach yields the following solution for the coefficients:

\[
w^\pi = (\Phi^T (\Phi - \gamma P \Pi_\pi \Phi))^\dagger \Phi^T R
\]

where \( R \) is the reward vector (over all state action pairs), \( P \) is the transition matrix, and \( \Pi_\pi \) is a stochastic matrix of size \( |S| \times |S| \) for \( \Pi_\pi(s, (s, a)) = \pi(a; s) \). LSPI uses the LSTDQ (least-squares TD Q-learning) method as a subroutine for learning the state-action value function \( \hat{Q}^\pi \). The LSTDQ method solves the system of linear equations \( A w^\pi = b \) where

\[
A = \Phi^T \Delta_\mu (\Phi - \gamma P \Pi_\pi)
\]

Also, \( \mu \) is a probability distribution over \( S \times A \) that defines the projection of the true action value function onto the subspace spanned by the handcoded basis functions, and \( b = \Phi^T \Delta_\mu R \). Since \( A \) and \( b \) are unknown when learning, they are approximated from samples using the update equations

\[
\begin{align*}
\hat{A}^{t+1} &= \hat{A}^t + \phi(s_t, a_t)\phi(s_t, a_t) - \gamma \phi(s'_t, \pi(s'_t))
\hat{b}^{t+1} &= \hat{b}^t + \phi(s_t, a_t)r_t
\end{align*}
\]

where \((s_t, a_t, r_t, s'_t)\) is the \( t \)th sample of experience from a trajectory generated by the agent (using some random or guided policy), and \( \hat{A}^0 \) and \( \hat{b}^0 \) are set to 0.
and then returns the coefficients \( \tilde{w} \) by solving the system \( \tilde{A}w^\pi = \tilde{b} \). The overall LSPI method uses a policy iteration procedure, starting with a policy \( \pi \) defined by an initial weight vector \( w \), and then repeatedly invoking LSTDQ to find the updated weights \( w' \), and terminating when the difference \( ||w - w'|| \leq \epsilon \).

3 Representation Policy Iteration

With this brief overview of the framework and linear least-squares approximation methods such as LSPI, we can now introduce the Representation Policy Iteration framework, which interleaves representation learning and policy learning. For ease of exposition, we present the complete algorithm in Figure 1 in the context of LSPI and illustrate its behavior, before providing a detailed overview of the underlying theory. Also, much of this introductory paper will focus on explaining the theory of how representations can be learned by harmonic analysis of a given set of sample transitions. It is clear that if representations can be successfully learned from an experience sample, then representation learning can easily be interleaved with policy learning by generating a new sample of transitions from executing the current policy. A detailed algorithmic analysis of fully interleaved policy and representation learning is beyond the scope of this introductory paper.

Steps 1 and 3b automatically build customized basis functions given an experience sample, where the basis functions reflect large-scale geometry of the approximated manifold, and provide a theoretically guaranteed orthonormal set for approximating any smooth function on the approximated manifold.

3.1 Abstract Harmonic Analysis

Temporarily setting aside the theory underlying RPI (see the sections below), we illustrate its performance on the classic chain example from [7, 8]. The chain MDP, originally studied in [7], is a sequential open chain of varying number of states, where there are two actions for moving left or right along the chain. The reward structure can vary, such as rewarding the two actions for moving left or right along the chain. The reward structure can vary, such as rewarding the two actions for moving left or right along the chain. The reward structure can vary, such as rewarding the two actions for moving left or right along the chain.

Figure 1: Representation Policy Iteration interleaves representation and policy learning.
can approximate any real-valued smooth function on the vertices of this graph. In the limit, Hodge theory (see below) guarantees that the approximation will be exact.

![Figure 2: Laplacian eigenfunctions for a 50 state open and closed chain MDP produced from a random walk of 10000 steps by learning the underlying graph and computing its combinatorial graph Laplacian.](image)

Figure 3 and Figure 4 show the results of running the Representation Policy Iteration (RPI) algorithm on a 50 state chain graph, using the display format from [8]. Here, being in states 10 and 41 earns the agent rewards of +1 and there is no reward otherwise. The optimal policy is to go right in states 1 through 9 and 26 through 41 and left in states 11 through 25 and 42 through 50. The number of samples initially collected was set at 10,000. The discount factor was set at $\gamma = 0.8$. By increasing the number of desired basis functions, it is possible to get very accurate approximation, although as Figure 4 shows, even a crude approximation using 5 basis functions is sufficient to learn a close to optimal policy. Using 20 basis functions, the learned policy is exact. A detailed comparison with hand-coded polynomial and RBF encoding techniques studied earlier with LSPI is given in Section 6.

4 Spectral Graph Theory

We provide a brief theoretical overview of spectral graph theory and Riemannian manifolds. While these subfields have been applied to semi-supervised learning [2], clustering [14], and image segmentation [18], their use for representation learning and value function approximation in MDPs and RL is novel, which unlike supervised learning or classification requires approximating arbitrary real-valued functions. The graph Laplacian [4] can be used to construct a set of orthonormal basis functions $\phi_1^G(s), \ldots, \phi_k^G(s)$ that in the limit are guaranteed to exactly capture any smooth real-valued function on $G$. The graph Laplacian is a special case of the Laplacian on a Riemannian manifold, and this result generalizes to all connected oriented Riemannian manifolds [17]. But, let us first focus on the simple case of (connected) undirected graphs. Let $d_v$ denote the degree of vertex $v$. The random walk operator on a graph is given by $D^{-1}A$, where $D$ is the diagonal matrix whose entries are given by the vertex degrees, or row sums of the adjacency matrix $A$. The random walk operator is not symmetric, but it is closely related to a symmetric graph Laplacian operator as follows. The combinatorial Laplacian $L$ is defined as $D - A$, and acts on a function $f$ as

$$Lf(x) = \sum_{y \sim x} (f(x) - f(y))$$

where $y \sim x$ means $y$ is adjacent to $x$. It is easy to show that the combinatorial Laplacian is essentially the discrete case of the well-known Laplacian partial differential equation on a graph. The nor-
The Rayleigh quotient for higher-order basis functions is similar: each function is perpendicular to the subspace spanned by previous functions. A further property of Laplacian eigenfunctions is that they transparently reflect the nonlinear geometry of state spaces (see experiments below). To formally explain this, we briefly review spectral geometry. The Cheeger constant $h_G$ of a graph $G$ is defined as

$$h_G(S) = \min_{S \subseteq \tilde{S}} \frac{|E(S, \tilde{S})|}{\min(\text{vol } S, \text{vol } \tilde{S})}$$

Figure 4: The policies learned at each iteration using Representation Policy Iteration on a 50 node chain graph, for 5 basis functions (top four panels), and 20 basis functions (bottom nine panels) in row major order. Even using 5 basis functions results in a close to optimal policy. The light (blue) color denotes the left action and the dark (red) denotes going right. The top half of each plot is exact, and the bottom is approximate.

It can be shown that $\mathcal{L}$ is a symmetric self-adjoint operator, and its spectrum (eigenvalues) lie in the interval $(0, 2)$. If $G$ is a constant degree $k$ graph, then it follows that $\mathcal{L} = I - \frac{1}{k}A$, where $A$ is the adjacency matrix of $G$. For a general graph $G$, $\mathcal{L} = D^{-\frac{1}{2}}LD^{-\frac{1}{2}} = I - D^{-\frac{1}{2}}AD^{-\frac{1}{2}}$. Note that this implies that $D^{-1}A = D^{-\frac{1}{2}}(I - \mathcal{L})D^\frac{1}{2}$. In other words, the random walk operator $D^{-1}A$ is similar to $I - \mathcal{L}$ in that both have the same eigenvalues, but the eigenfunctions of the random walk operator are the eigenfunctions of $I - \mathcal{L}$ scaled by $D^{-\frac{1}{2}}$. The Laplacian $\mathcal{L}$ is an operator on the space of functions defined on the graph $g : V \rightarrow \mathcal{R}$, where $V$ is the vertex set of $G$, and $u \sim v$ means $u$ and $v$ are neighbors:

$$\mathcal{L}(u,v) = \begin{cases} 
1 & \text{if } u = v \text{ and } d_u \neq 0 \\
-\frac{1}{\sqrt{d_u d_v}} & \text{if } u \text{ and } v \text{ are adjacent} \\
0 & \text{otherwise}
\end{cases}$$

The Rayleigh quotient provides a variational characterization of eigenvalues using projections of arbitrary function $g : V \rightarrow \mathcal{R}$ onto the subspace $\mathcal{L}g$. The quotient gives the eigenvalues and the functions satisfying orthonormality are the eigenfunctions (here $\langle f,g \rangle = \sum_u f(u)g(u)$ denotes the inner product on graph $G$):

$$\frac{\langle g,\mathcal{L}g \rangle}{\langle g,g \rangle} = \frac{\langle g,D^{-\frac{1}{2}}LD^{-\frac{1}{2}}g \rangle}{\langle g,g \rangle} = \frac{\sum_{u,v}(f(u) - f(v))^2}{\sum_u f^2(u)d_u}$$

where $f \equiv D^{-\frac{1}{2}}g$. The first eigenvalue is $\lambda_0 = 0$, and is associated with the constant function $f(u) = 1$, which means the first eigenfunction $g_0(u) = \sqrt{D}$ 1. The first eigenfunction (associated with eigenvalue 0) of the combinatorial Laplacian is the constant function 1. The second eigenfunction is the infimum over all functions $g : V \rightarrow \mathcal{R}$ that are perpendicular to $g_0(u)$, which gives us a formula to compute the first non-zero eigenvalue $\lambda_1$, namely

$$\lambda_1 = \inf_{g \perp g_0} \frac{\sum_{u,v}(f(u) - f(v))^2}{\sum_u f^2(u)d_u}$$

Theorem 1 [4]: Define $\lambda_1$ to be the first (non-zero) eigenvalue of the Laplace-Beltrami operator $\mathcal{L}$ on a
5 Hodge Theory

In this section we briefly discuss how the graph Laplacian can be generalized to the setting of Riemannian manifolds [17]. Manifolds are locally Euclidean sets, defining a bijection (one-to-one, onto mapping) from an open set containing any element \( p \in \mathcal{M} \) to the \( n \)-dimensional Euclidean space. Smooth manifolds in addition require that the homeomorphism mapping any point \( p \) to its coordinates \((\rho_1(p),\ldots,\rho_n(p))\) be a differentiable function with a differentiable inverse. Given two coordinate functions \( p(p) \) and \( \xi(p) \), which are individually called charts, the induced mapping \( \psi : \rho \circ \xi^{-1} : \mathcal{R}^n \to \mathcal{R}^n \) must have continuous partial derivatives of all orders. Riemannian manifolds are smooth manifolds where the Riemann metric defines the notion of length. Given any element \( p \in \mathcal{M} \), the tangent space \( T_p(\mathcal{M}) \) is an \( n \)-dimensional vector space that is isomorphic to \( \mathcal{R}^n \). More formally, a Riemannian manifold is a smooth manifold \( \mathcal{M} \) with a family of smoothly varying positive definite inner products \( g_p, p \in \mathcal{M} \) where \( g_p : T_p(\mathcal{M}) \times T_p(\mathcal{M}) \to \mathcal{R} \). For the Euclidean space \( \mathcal{R}^n \), the tangent space \( T_p(\mathcal{M}) \) is clearly isomorphic to \( \mathcal{R}^n \) itself. Consequently, the Riemannian inner product is simply \( g(x,y) = \langle x,y \rangle_{\mathcal{R}^n} = \sum_i x_i y_i \), which remains the same over the entire space.

Hodge’s theorem states that any smooth function on a compact manifold has a discrete spectrum [17]. We are interested in those functions \( f \) that are eigenfunctions of \( \Delta \), the Laplace-Beltrami operator. On the manifold \( \mathcal{R}^n \), the Laplace-Beltrami operator is simply \( \mathcal{L} = -\sum_i \frac{\partial^2}{\partial x_i^2} \) (the sign is a convention). Eigenfunctions give us back the function itself, scaled by an eigenvalue. If the domain is the unit circle, the trigonometric functions \( \sin(\theta) \) and \( \cos(\theta) \) form eigenfunctions, which leads to Fourier analysis, the most well-known example of harmonic analysis. Abstract harmonic analysis generalizes Fourier methods to orthogonal decompositions of smooth functions on arbitrary Riemannian manifolds. The smoothness functional for an arbitrary real-valued function on the manifold \( f : \mathcal{M} \to \mathcal{R} \) is given by

\[
S(f) \equiv \int_\mathcal{M} |\nabla f|^2 \, d\mu = \int_\mathcal{M} \nabla f \nabla f \, d\mu = \langle \Delta f, f \rangle_{L^2(\mathcal{M})}
\]

where \( \nabla f \) is the gradient vector field of \( f \). For \( \mathcal{R}^n \), the gradient vector field is \( \nabla f = \sum_i \frac{\partial f}{\partial x_i} \). For a Riemannian manifold \( (\mathcal{M},g) \), where the Riemannian metric \( g \) is used to define distances on manifolds, the Laplace-Beltrami operator is given by

\[
\Delta = -\frac{1}{\sqrt{\det g}} \sum_{ij} \partial_i \left( \sqrt{\det g} \, g^{ij} \partial_j \right)
\]

where \( g \) is the Riemannian metric, \( \det g \) is the measure of volume on the manifold, and \( \partial_i \) denotes differentiation with respect to the \( i \)-th coordinate function. This general form is invariant to reparameterization, and reduces to the expression for \( \Delta \) given earlier for Euclidean spaces \( \mathcal{R}^n \) where \( G = I \) and \( \det G = 1 \).

**Theorem 2 (Hodge [17]):** Let \( (\mathcal{M},g) \) be a compact connected oriented Riemannian manifold. There exists an orthonormal basis for all smooth (square-integrable) functions \( L^2(\mathcal{M},g) \) consisting of eigenfunctions of the Laplacian. All the eigenvalues are positive, except that zero is an eigenvalue with multiplicity 1.

Hodge’s theorem guarantees that a smooth function \( f \in L^2(\mathcal{M}) \) can be expressed as \( f(x) = \sum_{i=0}^{\infty} a_i e_i(x) \) where \( e_i \) are the eigenfunctions of \( \Delta \), i.e. \( \Delta e_i = \lambda_i e_i \). The smoothness \( S(e_i) = \langle \Delta e_i, e_i \rangle_{L^2(\mathcal{M})} = \lambda_i \). This theorem shows that the eigenfunctions of the Laplace-Beltrami operator can be used to approximate any value function on a manifold. We now turn to describe some experimental results.

6 Experiments

Figure 5 shows a sample state value function output by RPI for a 100 state grid world MDP partitioned into two room. Here, an initial random walk of 9144 steps was used to learn an undirected graph, from which 20 basis functions were extracted by computing the normalized Laplacian. A constant reward of −1 was

![Figure 5: The state value function produced during a run of RPI in a two room gridworld with 100 states.](image-url)
provided at each step, and the goal is to reach the diagonally opposite corner in the far room (hidden from view). Note how the nonlinear geometry of the environment is transparently reflected in the approximation produced by RPI. Figure 6 gives an example of the eigenfunctions of the Laplacian for a grid world MDP consisting of five rooms, each of dimension $21 \times 20$ connected by a single door in the middle of the boundary walls separating each room. The smoothness of each basis function depends on its spectral ranking: low-order functions are geodesically smooth: within each room, they are smooth, but discontinuous across rooms to capture the geometric invariant of the walls separating the rooms. Higher order functions provide harmonic functions for reconstructing value functions within a room. These properties makes Laplacian basis functions well-suited to value function approximation. Figure 7 shows how Laplacian eigenfunctions capture the presence of a centrally placed obstacle in a square grid. Finally, Figure 8 shows how eigenfunctions can efficiently approximate a given value function in a four room grid world (here, the goal is to get to the diagonally opposite corner of the last room).

Next, we provide a detailed control learning experiment comparing the learned basis functions using RPI with using two handcoded basis functions in LSPI, polynomial encoding and radial-basis functions (RBF) (see Table 1). Following [8], +1 rewards are given in states 10 and 41 only in this 50 state chain. Each row reflects the performance of either RPI using learned basis functions or LSPI with a handcoded basis function (values in parentheses indicate the number of basis functions used for each architecture). Each result is the average of five experiments on a sample of 10,000 transitions. The two numbers reported are average steps to convergence and the average error in the learned policy (number of incorrect actions). The results show the automatically learned Laplacian basis functions in RPI provide a more stable performance at both the low end (5 basis functions) and at the higher end with $k = 25$ basis functions. As the number of basis functions are increased, RPI takes longer to converge, but learns a more accurate policy. LSPI with RBF is unstable at the low end, converging to a very poor policy for 6 basis functions. LSPI with a 5 degree polynomial approximator works reasonably well, but its performance noticeably degrades at higher de-
degrees, converging to a very poor policy in one step for $k = 15$ and $k = 25$.

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<tr>
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<td>LSPI Poly (25)</td>
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Table 1: This table compares the performance of RPI using automatically learned basis functions with LSPI combined with two handcoded basis functions on a 50 state chain graph problem. See text for explanation.

7 Discussion

Further development of RPI is continuing on several fronts, including incremental variants, extensions to factored MDPs, and scaling to large states and action spaces. The basis functions used in this paper are global Fourier eigenfunctions. A related approach from harmonic analysis is to use multiscale wavelets, which are based not on differential equations, but dilation equations. Diffusion wavelets [5] are a general multiresolution model of diffusion processes on manifolds and graphs. A detailed study of Fourier eigenfunctions and diffusion wavelets with RPI for value function approximation has been completed [12]. The left inverse of the Laplacian is called the Green’s function and closely relates to the solution of the Bellman equation. We have also developed a novel fast policy evaluation method by using diffusion wavelets to compactly represent powers of the transition matrix [9]. In large graphs the learned basis functions can be computed from samples of the complete graph using Nyström approximations and other low-rank methods.

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