Title
Navigation between states in ecological communities by taking shortcuts, with application to control

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Controlling ecological state transitions

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Author contributions
BB conceived the project, wrote the initial implementation, and carried out statistical analyses and visualizations. ML strengthened the implementation and concepts, and carried out the final pathfinding analyses. CT and ZS provided conceptual input. All authors contributed to writing.

Data availability
Algorithms are implemented in Julia. Statistical analyses and data visualization are implemented in R. All data used in this study are drawn from previously published studies. Algorithms and pre-formatted public datasets are available at https://github.com/michaelhlim/CoexistenceControl.jl. Statistical analysis and visualization code are available at https://github.com/bblonder/CoexistenceControl-Pathfinding-Analysis. Both can be used to replicate the study and will be archived upon acceptance at Zenodo or another similar public repository.

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Abstract

Many community ecology problems can be framed in terms of controlling the transition from an initial state to a desired state. However, it is often unclear what action sequence (if any) would yield the desired state. Here we develop a simple approach for navigating to desired states, applicable when the costs and outcomes of actions are known. We find lowest-cost action sequences (adding a species, removing a species, changing the environment, waiting) via A* search on a state diagram. Lowest-cost sequences usually are indirect and leverage waiting for natural transitions caused by competitive exclusion. In tests on simulated and empirical data across taxa, our approach provides ~50% probability of substantial cost improvement relative to nominal approaches. As an example, numerous successes are predicted in gut microbial communities for removing the pathogen *Clostridium difficile*. This work thus provides a conceptual foundation for efficient state transitions in species-rich communities.
Introduction

Management (control) problems involve observing an ecological community in an initial state, then taking a set of actions to yield a desired state. Control problems are often solved by expert knowledge or direct interventions. Such interventions may succeed but with high cost and side effects. Theory-based approaches to ecological control may instead help identify alternate control policies that are faster, more effective, or have fewer side effects. The challenge is to identify sequences of actions (perturbations to state variables, parameters, or the environment) that yield the desired state at lowest cost. However, there are potentially near-infinite numbers of action sequences to consider, making it challenging in theory and practice to discover useful solutions.

In ecology, control has typically been considered in the context of fisheries, forestry, agriculture, and other natural resource challenges (Krausman et al. 2013; Boettiger et al. 2015; Palmer et al. 2016; Lapeyrolerie et al. 2021), and also in microbial systems (Costello et al. 2012; Mueller & Sachs 2015; García-Jiménez et al. 2018; Angulo et al. 2019; Jones et al. 2020). These problems are unified by a relatively low number of state variables, and focus on limited types of actions (e.g. harvesting (Chakraborty et al. 2011)). Applications have focused on analytic approaches for simplified models and low-richness communities (Liu & Rohlf 1998; Jiang & Lu 2007). More recently the problem has been explored for the dynamics of higher-richness communities (Angulo et al. 2019; Jones et al. 2020; Brias & Munch 2021; Blonder et al. in preparation). Prior work has been limited by focusing on community dynamics. This forward simulation is computationally intensive and has precluded use in highly species-rich communities (Brias & Munch 2021).
We instead propose an alternate and complementary approach to control of community states, motivated by three ideas. First, many ecological management problems can be simplified to coexistence outcomes (Maynard et al. 2020; Blonder & Godoy in preparation). Obtaining an outcome (desired state) may be more important than the intermediate trajectory. Second, simple discrete actions, such as adding or removing a species, or changing some action of the environment, may be more realistic to implement than precisely timed or measured actions, including actions that continually change over time. Third, desired states should be restricted to coexistence outcomes that can be maintained without active intervention, for reasons of practicality. These ideas match the constraints of many real-world problems and can substantially reduce the mathematical and computational complexity of the problem.

We develop an approach for controlling coexistence outcomes based on pathfinding between initial and desired states. The central hypothesis is that it should be possible to leverage the internal dynamics of a community to take shortcuts between states. For example, to remove an infectious gut species ‘A’, one typically introduces an antibiotic that affects ‘A’ but also unfortunately removes ‘B’ and ‘C’ as collateral damage. Instead, it might be possible to introduce ‘F’, which in turn affects ‘E’ and in turn ‘D’, which then outcompetes ‘A’, with no negative impacts on ‘B’ and ‘C’.

First, we show how to enumerate a state diagram characterizing all of the possible transitions between all possible combinations of states. Using this state diagram we then show how to find optimal action sequences using pathfinding algorithms. Second, we implement the approach using the generalized Lotka-Volterra (GLV) model via simulated and empirical parameter sets. Action sets include adding or removing species, changing the environment, or waiting (doing nothing).
Materials and Methods

The state diagram approach

There is a set of \( n \) species comprising a regional pool, of which any subset may co-occur locally in the community. The state of the community at any time, \( \{X(t)\} \in \mathbb{R}^n \), is defined as the vector of abundances of each species \( X \) at a time \( t \). There is a set of environments defined by \( E(t) \in M \), with cardinality \( |M| = m \). There is some dynamical model that predicts temporal changes in the state as a function of variables, which may include \( X \) and \( E \), \( \frac{dX(t)}{dt} = f(X(t), E(t),...) \). Based on this dynamical model, there may be some set of fixed points where \( \frac{dX(t)}{dt} = 0 \), \( \Xi = \{X^*\} \), with cardinality \( \xi \), given the value of \( E \) and any other variables. Each of these fixed points may be feasible (i.e. all species present occur at non-negative abundances; \( X^* \in \mathbb{R}^n_{\geq 0} \)) and/or stable (for every small \( \epsilon > 0 \) there exists a \( \delta > 0 \) such that if \( \left| X(t_0) - X^* \right| < \delta \) then \( \left| X(t) - X^* \right| < \epsilon \) for \( t \to \infty \)).

We next identify all fixed points \( \Xi \) that could occur in the model, for all combinations of species being present or absent in the community (i.e. the empty community, all species occurring alone, all pairs, all triplets, etc.). These fixed points can be identified by exploring every subspace of the state space, then re-calculating the dynamical model nullclines. This requires \( 2^n \) iterations (for all combinations of presences/absences); for each iteration, there may be any number (including zero) of fixed points identified.

We consider four types of actions: adding a species at a sufficient abundance that a shift to a different fixed point occurs, regardless of the current state; removing a species completely,
changing the environment to an adjacent value (e.g. hotter or colder), and waiting. We then predict the outcome of each action for each state, based on the dynamical model.

In considering these actions, we make the assumptions that (1) any state eventually reaches a fixed point as $t \to \infty$; (2) the time required to reach a fixed point is small relative to the time available for an action sequence; (3) an action can be taken instantaneously relative to the dynamics, i.e., multiple actions could be taken before the state reaches a fixed point; (4) the magnitude of an addition or removal does not influence the fixed point reached; and (5) each wait action has a deterministic effect. Many of these restrictive assumptions could be successfully relaxed but we proceed this way for maximum clarity of presentation (see Discussion).

With this information for fixed points and the outcomes of actions at each fixed point, we can construct a directed graph called the ‘state diagram’ (Figure 2). The vertices are the fixed points (in each environment) and the edges are the actions, where the head is the state after the action and the tail is the state before the action. Each vertex has attributes for stability+feasibility. Each edge has an attribute for the action’s cost. Action sequences are sets of adjacent edges. The full graph includes approximately $\xi \times m$ vertices (all fixed points across all environments) and $\xi \times m \times (n + 3)$ edges ($n$ additions or removals, 2 environmental changes, 1 wait action).

Vertices that are stable+feasible in a given environment represent realistic desired states, while the opposite indicates states that cannot be reached except by continuous effort. ‘Natural transitions’ are edges connecting unstable vertices to stable vertices, i.e. changes in state that occur spontaneously if the ‘wait’ action is selected. We omit edges for ‘wait’ actions that do not cause state transitions because they are not useful.
An ‘optimal solution’ is a set of edges connecting the initial and desired states whose summed cost is minimal (Figure 1b). That is, the problem reduces to solving a shortest path problem on a directed graph. A ‘nominal solution’ is a set of edges connecting the initial and desired states without natural transitions. There may be multiple nominal action sequences, corresponding to different ordering of the same actions, or of different actions.

We solve the minimal-cost problem between pairs of starting and desired states using the A* algorithm, which is a best-first search algorithm that expands local paths around the source vertex according to a combination of the cost of the path from the initial vertex to the current vertex plus the cost of a heuristic estimate of the cost from the current vertex to the desired vertex. We use an admissible heuristic that optimistically assumes that a single wait action is sufficient to cover all deletions needed to reach the goal vertex. A* does not require knowledge of the entire graph and is guaranteed to find a solution if one exists (Hart et al. 1968).

GLV implementation

We implemented the state diagram approach for the GLV model, which has been widely studied to explore questions of species coexistence (Barabás et al. 2016; Saavedra et al. 2017). The GLV model is also empirically useful when environmental influences parameter values (Sharpless et al. 2022). The dynamical model is

\[ \frac{dX(t)}{dt} = \text{diag}(X(t))(r(E) + A(E)X(t)) \]

where \( E \) is assumed constant unless changed by an action. Here, \( r(E) \) is a \( n \times 1 \) vector indicating the intrinsic growth rates of each species, and \( A(E) \) is a \( n \times n \) matrix whose \( i,j \) entry representing the change in species \( i \)'s per-capita growth rate for a unit change in the density of species \( j \).
If A is non-singular, for each parameter combination, there is one non-trivial fixed point, determinable by nullcline analysis:

\[ X^* = - (A(E))^{-1} r(E). \]

The fixed point is then feasible if all \( X^*_i \geq 0 \). If the fixed point is not feasible, the state will shift to a subspace with some species absent (see below). If A is singular, there can be many fixed points corresponding to the null space of A, corresponding to cases where parameters are either linear combinations or there is partitioning in the interaction network (Angulo et al. 2019); here numerical simulation of trajectories can instead be used to identify fixed points.

The fixed point is locally stable if

\[ \max_i \left( \text{Re} \left( \lambda_i(E) \right) \right) < 0 \]

where \( \lambda_i(E) \) are the \( n \) eigenvalues of \( A(E) \). Note that the location of the fixed point, as well as the feasibility and stability properties, may all change when the environment changes.

To then calculate all the fixed points in \( \Xi \), the process can be iterated for all combinations of species. Because all GLV interactions are pairwise, cases where species \( j \) is absent can be handled by dropping row \( j \) and column \( j \) of the \( A \) matrix (i.e. obtaining the principal submatrix), and simultaneously dropping entry \( j \) of the \( r \) vector. Multiple entries can be dropped in cases where multiple species are absent. This is non-trivial, as the eigenvalues of a principal submatrix (which are closely related to the matrix inverse, and thus the location of the fixed point) are not necessarily the same as for the original matrix (Johnson & Robinson 1981). That is, combinations of species may behave differently from subsets of those combinations (Saavedra et al. 2017), a phenomenon also seen in models with higher-order interactions (Mayfield & Stouffer 2017). If A and all its principal submatrices are non-singular, then there is a single fixed point.
per iteration, yielding \( \xi = 2^n \) fixed points. If \( A \) is singular, there may be more or fewer fixed points to be considered.

All of the vertex and edge properties are determined based on the relevant values of \( A(E) \) and \( r(E) \). For natural transitions, we assume that infeasible fixed points transition to the fixed point for the sub-community comprising only the subset of species occurring at non-negative abundances.

**Simulation analysis**

We made GLV simulations that drew random parameter values for \( A(E) \) and \( r(E) \) for a range of \( n \) values and \( m = 1 \) (\( E \in \{0\} \)), 3 (\( E \in \{-1, 0, 1\} \)), or 5 discrete environments (\( E \in \{-2, -1, 0, 1, 2\} \)). We explore a scenario where environmental change increases or decreases the strength of some pairwise interactions and growth rates. We assume that the interaction coefficients are normally distributed for \( E = 0 \),

\[
A_{ij}(E) \sim \text{If else}\left[i = j, -1, N(\mu_r, \sigma_r)\right]
\]

where \( \mu_A \) and \( \sigma_A \) are constant parameters setting the overall distribution of coefficients. Setting the diagonal entries to -1 standardizes the scale of competition among species. For \( E \neq 0 \),

\[
A_{ij}(E) \sim A_{ij}(E - 1) \times \text{If else}\left[U(0, 1) < \alpha, 1, \beta\right] \quad \text{if } E > 0,
\]

\[
A_{ij}(E) \sim A_{ij}(E + 1) \times \text{If else}\left[U(0, 1) < \alpha, 1, 1/\beta\right] \quad \text{otherwise},
\]

where \( \alpha \) is a constant parameter whose values indicate how likely it is that environmental change impacts species interactions, and \( \beta \) determines how large those impacts are. In the ‘hotter’ or ‘colder’ environments, a fraction \( \alpha \) of the entries become larger or smaller by a ratio \( \beta \) than they would be otherwise.
We also assume that the intrinsic growth rates are similarly distributed,

\[ r_i(E) \sim N(\mu_r, \sigma_r) \quad \text{if } E = 0, \]

\[ r_i(E) \sim r_i(E - 1) \times \text{if else}[U(0, 1) < \alpha, 1, \beta] \quad \text{if } E > 0, \]

\[ r_i(E) \sim r_i(E + 1) \times \text{if else}[U(0, 1) < \alpha, 1, 1/\beta] \quad \text{otherwise,} \]

where \( \mu_r \) and \( \sigma_r \) are constant parameters.

We explored three scenarios \((n=5 \ m=3, \ n=10 \ m=1, \ \text{and} \ n=15 \ m=1)\). As \( n \) increases, coexistence becomes increasingly rarer in GLV models with randomly distributed parameters (May 1973; Goh & Jennings 1977; Serván et al. 2018). We therefore picked values of \( \mu_A, \sigma_A, \mu_r, \)

and \( \sigma_r \) that would yield state diagrams in which a mean of ~25% of fixed points were stable+feasible (Figure S1). This approach allows comparison of performance under similar conditions. Parameter values were found using cross-entropy (De Boer et al. 2005) (Table S1).

**Empirical analysis**

We also considered situations where estimates of parameter values for \( A \) and \( r \) have been made by fitting generalized Lotka Volterra models to empirical data. We used four datasets: (1; ‘Human gut’) a \( n=12 \ m=1 \) synthetic human gut microbial community (Venturelli et al. 2018), (2; ‘Mouse gut’) a \( n=11 \ m=1 \) mouse gut microbial community including the pathogen Clostridium difficile (Stein et al. 2013) based on data from (Buffie et al. 2012), (3; ‘Ciliate’) a \( n=5 \ m=1, \ 3, \ \text{or} \ 5 \) protozoan ciliate community (Maynard et al. 2020) based on data for 19 °C; 15, 19, 23°C; and 15, 17, 19, 21, and 23 °C growth from (Pennekamp et al. 2018), and (4; ‘Protist’) a \( n=11, \ m=1 \) protist and rotifer community based on A values from (Carrara et al. 2015) and \( r \) values from
(Carrara et al. 2012) and supplemented by additional r values for two missing taxa (pers. comm. F. Altermatt, May 7, 2021).

**Statistical analysis**

We assumed that additions had a cost of 1, that removals had a cost of 3, environmental change had a cost of 5, and waiting had a cost of 0.1. This reflects a scenario in which it is easier to introduce a species than eradicate it, environmental manipulations are costly, and where costs are invariant across contexts.

For each pair of feasible+stable starting and target states in each dataset, we calculated the optimal solution and a nominal solution. Because multiple nominal solutions may exist, we select one comprising sequential removals, then sequential additions.

We calculated the 'proportional cost improvement' (PCI) of optimal control as the difference between the cost of the nominal and the optimal path, divided by the cost of the nominal path. Larger values of PCI indicate the value of the pathfinding approach. For each dataset, we reported the probability of a PCI exceeding 10%, the mean PCI, and the fraction of states that are feasible+stable. Summaries are provided in Table 1.

To determine whether some target states are more easily reached than others, we identified the 50 cases that had the highest PCI within each dataset. We then hierarchically clustered and visualized the target states.

To additionally explore the impact of different factors on performance, we built random forest models, where PCI was the dependent variable, and predictor variables included dataset name, the species pool richness (n), the number of environments (m), the fraction of states that are feasible+stable in the dataset, the change in richness between starting and target state, the
Jaccard similarity between the starting and target state, and the change in mean \( r \) and \( A \) values between the starting and target state. Because a small number of \( r \) and \( A \) values took extreme values in the empirical parameter sets, we removed values outside of the range (-10,10) \((\text{Figure S2})\). Random forests were fitted using \texttt{mtry}=3 and \texttt{ntrees}=500 in the \texttt{ranger} package (version 0.13.1) in R.

For the ‘mouse gut’ dataset, we also determined the prevalence of \( \text{PCI} > 0 \) in scenarios whose initial states had the pathogenic \textit{C. difficile} present and whose desired states did not.

**Results**

**Cost improvement**

The optimal approach usually yielded lower-cost action sequences than the nominal approach \((\text{Figure 3, Table 1})\). The probability of a proportional cost improvement (PCI) greater than 10\% for a randomly selected pair of initial and desired states was between 29\% - 88\% for all datasets, except the ciliate \((m=3)\) dataset, which had a probability of 16\%.

The mean PCI ranged from 8-39\% across all datasets, except the ciliate \((m=3)\) datasets, which had a value of 4\%. PCI standard deviations ranged from 10\% - 32\% across datasets.

**Target states**

Within each dataset, the states with the highest PCI were more likely to correspond to some target states than others \((\text{Figure 4})\). For example, in the human gut datasets, singlets involving ER were common, as were pairs involving BU and FP. In the mouse gut dataset, triplets involving uncLac, Bar, and Oth were common, as were pairs of Bla and undEnt. In the protist
dataset, singlets involving Dex, Pau, and Cyc, were common, as were pairs of Chi and Eug, or Eug and Col, or Cyc and Eup. The combinations described here represent target states that are easiest to reach. Taxa names are given in Table S2.

In contrast, the ciliate dataset had high-PCI states whose composition depended on the number of environments being considered. In $m=1$ environment, pairs of DE and SP or LO and PA were common, as were all singlets. However in $m=3$ and $m=5$ environments, DE was always absent and other triplets were common; quadruplets sometimes appeared in $m=3$ environments.

Patterns in the simulated datasets were more random, consistent with the random assignment of parameter values to species labels. However, the apparent appearance of pattern in the $n=5 m=3$ simulation indicates that some caution is warranted in interpreting low richness datasets.

Factors explaining performance

The random forest model of PCI explained 55% of the variation in the out-of-bag estimate, and there was substantial variation in PCI directly ascribed to the dataset. Thus, the factors explored provided a partial but incomplete explanation for why some pairs of initial and desired states had high PCI. The best explanation is that some parts of the state diagram have more natural transitions than others - but enumerating such natural transitions is equivalent to running the pathfinding algorithm, so it is instead of interest to identify easily-measured heuristics that might predict PCI and give biological insight into the distribution and frequency of natural transitions.
PCI increased strongly when the net richness change was negative. This reflects the high cost benefit of natural transitions that lead to species loss. Additionally, PCI decreased strongly with net Jaccard similarity. This reflects the greater difficulty of transitioning to a very different state, where there may not be available natural transitions to provide shortcuts. PCI also increased with no change in mean $A$, and with increases in mean $r$. This likely reflects the greater probability of natural transitions when competitive exclusion is more common. Finally, PCI also decreased when the overall fraction of feasible+stable states increased. This also reflects the probability of natural transitions being lower when more states are feasible+stable. The number of species or environments in the dataset did not have a clear effect on PCI.

**Illustrative examples**

In a mouse gut example ([Figure 6a](#)), a high PCI can be obtained in a transition involving a shift from an initial state containing the undesired and hard-to-remove pathogen *C. difficile* to one that does not. The optimal solution involves adding two desired species, then waiting for a natural transition that competitively excludes *C. difficile*. In contrast, the nominal solution involves three high-cost targeted removals (including *C. difficile*) and two additions.

In a ciliate example ([Figure 6b](#)), a high PCI can be obtained in a transition from an initial state to a target state with different species composition. The optimal solution adds a species, then changes the environment, then adds another species. Then after waiting, the state then shifts via natural transition to the desired state. In contrast, the nominal solution requires two high-cost removals, two additions, and an environmental change.
Clodif removals

We also further investigated the mouse gut dataset, focusing on transitions between initial states in which Clodif pathogen was present and desired states in which it was not. Of these 57,753 transitions, we found that 43,548 (75%) involved Clodif being lost by waiting for a natural transition (i.e. through competitive exclusion). Additionally, these cases had a mean PCI of 53%, compared to a PCI of 24% for those in which Clodif was lost through direct removal. Thus, natural transitions provide a potentially effective way to remove undesired and persistent pathogens that obviates the usage of antibiotics.

Discussion

This study highlights four phenomena relevant to ecological state transitions. First, indirect action sequences often outperform direct action sequences. These solutions sometimes yielded substantial cost reductions, suggesting that direct approaches to control like antibiotic use or clearcutting have viable alternatives. Second, these indirect action sequences are more successful because they leverage instability in the underlying community dynamics. Temporarily reaching infeasible or unstable fixed points is necessary for taking shortcuts through the state diagram. In the GLV model, these instabilities arise from competitive exclusion driving natural transitions. In other dynamical models, different instabilities may occur, including those that lead to gains not just losses of species. Third, the ordering of action sequences is critical. Actions taken when a community is in the wrong state, or taken at the wrong time, may appear to have no effect - while taking the same action at the right state or the right time may have a large effect. Fourth, this approach to control does not require that the dynamical model is known - instead, only states and state transitions are needed. Together, these principles indicate that there are likely key
opportunities for leveraging the intrinsic dynamics of a community, even when they are unknown, to solve control problems.

If the GLV model has direct empirical value, then our approach also offers specific and quantitative predictions of action sequences that will reach desired target states, e.g. ones with higher or lower richness, or with pathogenic species like *C. difficile* absent. However, these predictions must be validated in real experiments. Elsewhere, control policies for microbial communities have been proposed (García-Jiménez *et al.* 2018; Angulo *et al.* 2019; Jones *et al.* 2020), but experimental tests similarly have been absent. To date, very few optimal control studies in ecology have ever attempted validation, e.g. (Desharnais *et al.* 2001).

**Open questions and applications**

Navigation between states may be easier or harder in certain assemblages, or within certain dynamical models. We do not yet know which states can be easily reached or why. Conversely, there may be sets of states that are ‘holes’, i.e. forbidden and/or infeasible (Angulo *et al.* 2021) to reach. Integrating this work with structural coexistence concepts (Saavedra *et al.* 2017) may be useful for understanding why certain community states might be unreachable. It may also be the case that navigation algorithms should avoid certain states when proposing action sequences (e.g. if they are unethical to create, or if their creation would have negative ecological consequences). These additional constraints may strongly influence reachability of desired states and require further algorithm development (Cornelius *et al.* 2013; Bansal & Tomlin 2020).
There are also open questions about the prevalence of natural transitions within a dynamical model, as well as the identity of the states connecting these transitions. Structural coexistence and related ideas may ultimately help unravel the properties of state diagrams (Grilli et al. 2017; Saavedra et al. 2017). State diagrams and natural transitions may also help clarify the role of priority effects in order-dependent community assembly from regional pools (Fukami 2015). This is because species additions and removals in certain contexts may create unstable states that then naturally transition to other stable states. In random communities, order-dependent assembly decreases in frequency when regional pool richness is higher (Serván et al. 2018), but less is known for other models and non-random parameters.

The state diagram approach could also be useful for assembling synthetic communities, e.g. in microbial bioreactor applications (Baranwal et al. 2021; Clark et al. 2021). This problem maps onto the navigation problem, because the desired state is a certain stable+feasible community and the initial state is an empty community. Our approach could potentially identify action sequences to achieve these goals when direct assembly of all species in the desired state is not possible or cost-effective.

Relaxing limiting assumptions

We made the assumption that the costs of each action are constant by type. In reality, removing species A might be more costly than removing species B, either because the time or effort required is high or may depend on whether species C is also present, or the costs of different actions may also not be known in advance. This assumption could be relaxed in future real applications, where the local context would determine costs.
We also assumed that in the GLV model that the algebraically calculated fixed point would always be reached for each combination of species, and that the outcome of actions was always one of these fixed points. This assumption could be relaxed if the magnitude of the addition (or equivalently, the size of an incomplete removal) influenced the fixed point reached, which would in turn increase the number of edges in the state diagram (e.g. instead of a single ‘add X’ action, one could have ‘add 10 of X’, ‘add 20 of X’, etc.) and outcomes could be calculated via forward simulation. There also may be multiple fixed points for a given set of species presences and absences, representing multiple basins of attraction (Jones et al. 2020), which would increase the number of fixed points. Similarly, if the dynamical model was stochastic, then edges in the state diagram could be given probability weights to allow for uncertainty in the outcomes of actions.

We also assumed that the environment cannot change except due to an action. Extrinsically driven environmental variation could result in changes to the identity and number of vertices and edges on the state diagram. These cases could be handled by other pathfinding algorithms (Browne et al. 2012) or by model predictive control if the dynamical model is known (Agachi et al. 2016).

Waiting actions were assumed to lead to transitions ‘down’ to lower richness states, as natural transitions in the GLV model can only cause species loss. This assumption could be relaxed in models with stochasticity or immigration, where waiting could result in spontaneous transitions ‘up’ to higher richness too.
We also assumed that all trajectories eventually reach fixed points, i.e. not other types of attractors like limit cycles. However, the approach still generalizes: if ‘states’ and ‘actions’ can still be defined, then a state diagram can still be constructed - that is, a limit cycle can itself be treated as a state.

**Extensions to the navigation approach**

The pathfinding algorithms are applicable regardless of the identity of vertices and edges in the state diagram. Indeed, knowledge of these vertices and edges is the only information required to apply the pathfinding algorithm; detailed knowledge of the dynamical model itself is not actually necessary.

The pathfinding problem does not even require full enumeration of the state diagram, if quasi-optimal solutions are acceptable. Such solutions can be found through local search, which only requires enumeration of a smaller set of states that are transiently reached, plus a slightly larger set of states that are explored and discarded. Approximate algorithms such as Monte Carlo Tree Search (MCTS) (Browne et al. 2012) can be used for larger problems by focusing computation only on promising state and action sequences. Moreover, MCTS can handle stochastic transitions, as well as uncertainty in observations of states when the problem is formulated as a partially observable Markov decision process (Katt et al. 2017; Sunberg & Kochenderfer 2018). A last advantage is that they allow definition of more complex multi-state targets through an arbitrary reward function - for example, any state that has a richness above a certain value, or that does not include a certain species, or that has a certain trait composition.
There is also potential for applying approximate algorithms in ecological cases where little is known about the properties of states, or of natural transitions, and the dynamical model is wholly unknown. In these cases, it is likely expensive (time and money) to evaluate each state or transition. Thus, these approximate algorithms solve the meta-optimization problem of finding an algorithm that minimizes empirical evaluation of states and transitions.

There is also potential to solve the limited-knowledge problem by developing methods which simultaneously learn the rules for classifying the properties of states (e.g. predicting stability and feasibility) and transitions (predicting whether natural transitions will occur), and also learn the rules for optimal control (transitions among states). Such approaches might be especially successful under conditions where models are too complex for their full parameter sets to be estimated. Model-free reinforcement learning could potentially solve both problems, while the first problem might be solved by classification algorithms (Kong et al. 2020; Maynard et al. 2020; Blonder & Godoy in preparation).

**Conclusion**

We have proposed a pathfinding approach for controlling coexistence in ecological communities. We showed that optimal action sequences leverage natural transitions that can be found using graph search without knowledge of a dynamical model. The approach may be useful in a wide range of contexts if empirical validations are successful.
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Figure 1. A hypothetical example of transitions between an initial four-species community ‘abcd’ and a desired one-species community ‘d’. Gray boxes indicate species compositions. Actions are indicated as: species additions (orange +), species removals (red -), waiting for a natural transition (blue >). (a) In this example, a nominal solution involves three removals (of species ‘a’ then ‘b’ then ‘c’) to each state ‘d’. (b). In contrast, an optimal solution based on pathfinding on a state diagram involves one addition (species ‘e’), and one wait for a natural transition to reach state ‘d’. The solution is optimal under the condition that removals are costly and additions and waits are not.
Figure 2. Example state diagram for the fixed points in a GLV model with $n=6$ species, $m=1$ environment, with $\mu_A = -0.7$ and $\mu_r = 1.7$. Each of the $2^6=64$ states are shown as rectangles with labels indicating species composition (e.g. ‘ade’ indicates species a, d, and e are present), and vertically arranged by increasing richness. Stable and feasible states are shown in white; other states are shown in gray. Red arrows indicate species removal actions; orange arrows indicate species addition actions; blue arrows indicate waiting actions (for natural transitions).
Figure 3. Histogram of proportional cost improvements for optimal paths relative to nominal paths for all transitions within each dataset. Note the y axis is sqrt-transformed.
Figure 4. Most frequent target states among the action sequences with the highest proportional cost improvement within each dataset. Species present in the target state are shown in green; absent, in gray. Columns indicate species and rows indicate target states. Taxa names are provided in Table S2.
Figure 5. Partial dependence plots indicating the effect of each predictor on proportional cost improvement. Lines indicate variation among datasets.
Figure 6. Comparison of the optimal and nominal paths for (A) an efficient removal of the pathogen Clodif in the mouse gut in one environment, and (B) an efficient state shift between two different ciliate communities in three environments. X-axis indicates the sequences of actions; the top subpanel indicates the cumulative costs, while the bottom subpanel indicates the states and actions for either the optimal path (left) or the nominal path (right). Actions are indicated as: species additions (orange +), species removals (red -), environmental change (green =), waiting for a natural transition (blue >). Gray boxes indicate species abbreviations (see Table S2). File S1 provides additional visualizations for other cases.
Table 1. Summary of dataset properties. PCI is proportional cost improvement.

| Dataset name          | Number of species (n) | Number of environments (m) | Proportion of states feasible+stable | Prob(PCI > 0.1) | PCI (mean) | PCI (sd) |
|-----------------------|-----------------------|----------------------------|--------------------------------------|----------------|------------|----------|
| Mouse gut             | 11                    | 1                          | 0.24                                 | 0.8            | 0.37       | 0.23     |
| Human gut             | 12                    | 1                          | 0.05                                 | 0.81           | 0.39       | 0.24     |
| Ciliate (m=1)         | 5                     | 1                          | 0.25                                 | 0.29           | 0.2        | 0.32     |
| Ciliate (m=3)         | 5                     | 3                          | 0.9                                  | 0.16           | 0.04       | 0.1      |
| Ciliate (m=5)         | 5                     | 5                          | 0.74                                 | 0.34           | 0.08       | 0.13     |
| Protist               | 11                    | 1                          | 0.02                                 | 0.68           | 0.36       | 0.29     |
| Simulated (n=5 m=3)   | 5                     | 3                          | 0.24                                 | 0.36           | 0.13       | 0.21     |
| Simulated (n=10 m=1)  | 10                    | 1                          | 0.21                                 | 0.74           | 0.33       | 0.24     |
| Simulated (n=15 m=1)  | 15                    | 1                          | 0.24                                 | 0.88           | 0.39       | 0.2      |
Supporting Information
File S1. PDF of visualizations (as in Figure 6) for 20 selected transitions from each of the 9 datasets. Transitions are randomly sampled from cases with optimal path length >1, and proportional cost improvement > 0.1.
Table S1. Parameters used in normal distributions for generating the $r$ and $A$ parameters in simulated datasets. The hyperparameters for the cross-entropy method used to arrive at these parameters are the following: 90 parameter samples, 20 simulation evaluations per parameter sample, 30 elite samples, and at most 30 cross-entropy iterations.

| Dataset name               | $\mu_A$  | $\sigma_A$ | $\mu_r$  | $\sigma_r$  |
|----------------------------|----------|------------|----------|-------------|
| Simulated ($n=10 \ m=1$)  | -0.3495734 | 0.31748953 | 2.09004577 | 0.34374938  |
| Simulated ($n=15 \ m=1$)  | -0.074988  | 0.2853568  | 2.22670281 | 0.31981157  |
| Simulated ($n=5 \ m=3$)   | -0.9244721 | 0.30508806 | 1.92884143 | 0.44384383  |
**Table S2.** Taxon names within each dataset.

| Dataset     | Taxon ID | Abbreviation | Full name               |
|-------------|----------|--------------|-------------------------|
| Mouse gut   | 1        | Bar          | *Barnesiella*           |
| Mouse gut   | 2        | undLac       | und. Lachnospiraceae    |
| Mouse gut   | 3        | uncLac       | uncl. Lachnospiraceae   |
| Mouse gut   | 4        | Oth          | Other                   |
| Mouse gut   | 5        | Bla          | *Blautia*               |
| Mouse gut   | 6        | undMol       | und. uncl. Mollicutes   |
| Mouse gut   | 7        | Akk          | *Akkermansia*           |
| Mouse gut   | 8        | Cop          | *Coprobacillus*         |
| Mouse gut   | 9        | Clodif       | *Clostridium difficile* |
| Mouse gut   | 10       | Ent          | *Enterococcus*          |
| Mouse gut   | 11       | undEnt       | und. Enterobacteriaceae |
| Human gut   | 1        | BH           | *Blautia hydrogenotrophica* |
| Human gut   | 2        | CA           | *Collinsella aerofaciens* |
| Human gut   | 3        | BU           | *Bacteroides uniformis* |
| Human gut   | 4        | PC           | *Prevotella copri*      |
| Human gut   | 5        | BO           | *Bacteroides ovatus*    |
| Human gut   | 6        | BV           | *Bacteroides vulgatus*  |
| Human gut   | 7        | BT           | *Bacteroides thetaiotaomicron* |
| Human gut   | 8        | EL           | *Eggerthella lenta*     |
| Human gut   | 9        | FP           | *Faecalibacterium prausnitzii* |
| Human gut   | 10       | CH           | *Clostridium hiranonis* |
| Human gut   | 11       | DP           | *Desulfovibrio piger*   |
| Human gut   | 12       | ER           | *Eubacterium rectale*   |
| Ciliate (m=1)| 1      | CO           | *Colpidium striatum*    |
| Ciliate (m=1)| 2      | DE           | *Dexiostoma campylum*   |
| Ciliate (m=1) | 3 | LO | Loxocephalus sp. |
|---------------|---|----|-----------------|
| Ciliate (m=1) | 4 | PA | Paramecium caudatum |
| Ciliate (m=1) | 5 | SP | Spirostomum teres |
| Ciliate (m=3) | 1 | CO | Colpidium striatum |
| Ciliate (m=3) | 2 | DE | Dexiostoma campylum |
| Ciliate (m=3) | 3 | LO | Loxocephalus sp. |
| Ciliate (m=3) | 4 | PA | Paramecium caudatum |
| Ciliate (m=3) | 5 | SP | Spirostomum teres |
| Ciliate (m=5) | 1 | CO | Colpidium striatum |
| Ciliate (m=5) | 2 | DE | Dexiostoma campylum |
| Ciliate (m=5) | 3 | LO | Loxocephalus sp. |
| Ciliate (m=5) | 4 | PA | Paramecium caudatum |
| Ciliate (m=5) | 5 | SP | Spirostomum teres |
| Protist       | 1 | Chi| Chilomonas sp.  |
| Protist       | 2 | Cyc| Cyclidium sp.  |
| Protist       | 3 | Tet| Tetrahymena sp.|
| Protist       | 4 | Dex| Dexiostoma sp. |
| Protist       | 5 | Col| Colpidium sp.  |
| Protist       | 6 | Pau| Paramecium aurelia |
| Protist       | 7 | Cep| Cephalodella sp.|
| Protist       | 8 | Spi| Spirostomum sp. |
| Protist       | 9 | Eug| Euglena gracilis |
| Protist       | 10| Eup| Euplotes aediculatus |
| Protist       | 11| Pbu| Paramecium bursaria |
| Simulated (n=5 m=3) | 1 | 1 | - |
| Simulated (n=5 m=3) | 2 | 2 | - |
| Simulated (n=5 m=3) | 3 | 3 | - |
| Simulated (n=5 m=3) | 4   | 4   |   |
|---------------------|-----|-----|---|
| Simulated (n=5 m=3) | 5   | 5   |   |
| Simulated (n=10 m=1) | 1   | 1   |   |
| Simulated (n=10 m=1) | 2   | 2   |   |
| Simulated (n=10 m=1) | 3   | 3   |   |
| Simulated (n=10 m=1) | 4   | 4   |   |
| Simulated (n=10 m=1) | 5   | 5   |   |
| Simulated (n=10 m=1) | 6   | 6   |   |
| Simulated (n=10 m=1) | 7   | 7   |   |
| Simulated (n=10 m=1) | 8   | 8   |   |
| Simulated (n=10 m=1) | 9   | 9   |   |
| Simulated (n=10 m=1) | 10  | 10  |   |
| Simulated (n=15 m=1) | 1   | 1   |   |
| Simulated (n=15 m=1) | 2   | 2   |   |
| Simulated (n=15 m=1) | 3   | 3   |   |
| Simulated (n=15 m=1) | 4   | 4   |   |
| Simulated (n=15 m=1) | 5   | 5   |   |
| Simulated (n=15 m=1) | 6   | 6   |   |
| Simulated (n=15 m=1) | 7   | 7   |   |
| Simulated (n=15 m=1) | 8   | 8   |   |
| Simulated (n=15 m=1) | 9   | 9   |   |
| Simulated (n=15 m=1) | 10  | 10  |   |
| Simulated (n=15 m=1) | 11  | 11  |   |
| Simulated (n=15 m=1) | 12  | 12  |   |
| Simulated (n=15 m=1) | 13  | 13  |   |
| Simulated (n=15 m=1) | 14  | 14  |   |
| Simulated (n=15 m=1) | 15  | 15  |   |
**Figure S1.** Fraction of states that are feasible+stable in simulated datasets when using the GLV parameters presented in **Table S1.** Density plots show distributions over 100 replicate draws.
Figure S2. Distribution of predictors used in random forest models. Density plots are shown after trimming $r$ and A values.