Research Statement

Chinwe Ekenna
http://parasol.tamu.edu/~cekenna/

Overview

My principal research interests lie in planning the motions of movable objects such as proteins and robots. Motion planning as shown in Figure involves moving an object from a start to a goal configuration. Motion planning arises in many application domains such as robotics, computer animation (digital actors), intelligent CAD (virtual prototyping and training) and even computational biology (protein folding and drug design).

Interestingly, a single class of planners, called probabilistic roadmap methods (PRMs) are one of the state of the art motion planning techniques that have proven effective in all these domains.

Probabilistic Roadmap Methods (PRMs) sample robot configurations (nodes) and connect them via viable local paths (edges) to form a graph (roadmap) containing feasible trajectories then query the produced roadmap to find a solution path from its start to goal configuration. Environments where robots are expected to navigate in are most often heterogeneous e.g. a house or a factory. These robots also have different complexity ranging from rigid bodies to highly articulated linkages with many degrees of freedom and so a single PRM method can not successfully solve all of these scenarios. This could be due to specialization to robots and environments of interest or PRM algorithms that solve simple robot problems (few degrees of freedom or in homogeneous environments). Focusing research to areas of importance has however limited the use of these different PRM methods.

My research is geared towards using machine learning techniques to intelligently combine and use any existing PRM method. I studied which learning techniques to use and at what stage of the roadmap construction to use them. This affords us the opportunity to use all available PRM method irrespective of the problem scenario. My work removes the overhead of deciding what PRM method to use for a given input problem. I have successfully applied this method to study the motion path both for robots and protein folding simulations.

In expanding my research program, I am interested in biological problems where my research can have direct and critical impact on the study of diseases and also study robots with higher degree of freedom (more complexity) e.g., humanoid robots.
Probabilistic Roadmap Planning

Motion planning problems consist of finding collision-free paths between a given start and goal position for an object. To simplify these computationally hard problems, most algorithms assume that the start and goal are known by the agent. Probabilistic Roadmap Methods (PRMs) are a category of algorithms that solve motion planning problems in two phases. During the sampling stage, valid configurations of the robot in the environment are generated, and during the connection stage those sampled nodes are connected together with edges to construct a roadmap that is used to find the valid path.

There are certain motion planning problems, e.g., planning for deformable robots, manipulation planning and computational biology search problems, where the efficiency of the solution depends on applying the best method to the corresponding problem. However, it is hard to predict an optimal technique for every movable object or environment. Furthermore, heterogeneous environments such as shown in Figure 2, which comprise the majority of problems of interest in motion planning, would need more than one algorithm choice applied to different regions of the environment.

My research is geared towards investigations to determine the impact of applying learning during a roadmap construction using PRMs. I implemented a machine learning approach using the notion of cumulative reward on actions performed. These actions include how many successful edges or nodes were added to a roadmap using a learned method and what the cost overhead for such computation (time or collision recorded) was. My method was able to make improvements on the roadmap quality and solved query problems in less time than other non-learned scenarios.

I implemented 2 variants to this learning approach, the first variant rewards actions based on performance across the entire environment [4], and updated version learns and rewards performance based on local neighbor defined regions in the environment [7].

In further exploring this learning concept and machine learning as a whole, I plan to look into more machine learning techniques and come up with a novel learning algorithm that would reduce the amount of parameter tuning needed to achieve qualitative results.

Application to Protein Folding

Modeling the protein folding process is crucial in understanding not only how proteins fold and function, but also how they misfold triggering many devastating diseases (e.g., Mad Cow and Alzheimer’s).

Since the process is difficult to experimentally observe, computational methods are critical. Traditional computational approaches for generating folding trajectories such as molecular dynamics, Monte Carlo methods, and simulated annealing provide a single, detailed, high-quality folding pathway at a large computational expense. As such, they cannot be practically used to study global properties of the folding landscape or to produce multiple folding pathways. Statistical mechanical models have been applied to compute statistics related to the folding landscape.
While computationally more efficient, they do not produce individual pathway trajectories and are limited to studying global averages of the folding landscape.

We use the same (PRM) base code to simulate protein folding motions as we do for robot motion planning [1–3]. They construct a roadmap, or model, of the folding landscape by sampling conformations and connecting neighboring ones together with feasible transitions using a simple local planner. They can generate multiple folding pathways efficiently (e.g., a few hours on a desktop PC) enabling the study of both individual folding trajectories and global landscape properties.

In protein folding also, making good choices for each of the algorithmic steps remains difficult. We applied the similar machine learning reward concept to simulate protein motions but instead reward based on action that produces edges with less potential energy while still being an edge that would potentially simulate the folding pathways of the proteins [5, 6]. Figure 3 gives a description of the folding landscape of a sample protein using two connection methods if we applied our learning method to it. Our results indicates an improvement in the pathway quality and overall time needed to build a roadmap.

**Future Directions**

Motion Planning is a growing area that contributes to diverse areas such as bioinformatics, artificial intelligence and control. I plan to continue studying the usefulness of probabilistic motion planning and its applications to related problems in the areas of machine learning, optimization, and data mining. I plan to research other motion planning techniques that would further advance my research program. In particular, in bioinformatics, I plan to extend this research to include more complex proteins with real world implications in the study of diseases due to protein misfolding. I would like to explore more the relevance of local information discovered through sampling the folding landscape of proteins.

In robotics, I plan to expand my research to problems with dynamical environments, physical constraints and limited sensing capabilities. I plan to continue studying the application of planning metrics and machine learning for effective adaptive motion planning. There are many known planning methods including specialized heuristic-based roadmap methods, trees, and even some complete methods. It would be helpful to continue to explore how these methods can be used in concert in order to simplify and automate planning while taking advantage of each method’s strengths.

Figure 3: Two connection methods are used to build a roadmap on the protein’s energy landscape: $CM_A$ (yellow/light) and $CM_B$ (blue/dark).


References


