Annotated-skeleton Biased Motion Planning for Faster Relevant Region Discovery

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Abstract. Motion planning algorithms often leverage topological information about the environment to improve planner performance. However, these methods often focus only on the environment’s connectivity while ignoring other properties such as obstacle clearance, terrain conditions and resource accessibility. We present a method that augments a skeleton representing the workspace topology with such information to guide a sampling-based motion planner to rapidly discover regions most relevant to the problem at hand. Our approach decouples guidance and planning, making it possible for basic planning algorithms to find desired paths earlier in the planning process. We demonstrate the efficacy of our approach in both robotics problems and applications in drug design. Our method is able to produce desirable paths quickly with no change to the underlying planner.

Keywords: Motion and Path Planning, Topology Guidance, Computational Biology

1 Introduction

Motion planning, finding a valid path for a movable object from one state to another, has applications in many domains including robotics, computer-aided design, and computational biology [14]. Problems in these applications are usually defined with conditions on the quality of the solution. For example, path safety is paramount to robot navigation, availability of recharging stations is important for mission completion in robotics, and energy feasibility is critical in protein-ligand binding simulations. While motion planning algorithms can successfully handle complex motion planning problems, balancing fast computation and additional path quality conditions is a challenge.
To address the fast computation part, one can take advantage of topological information when solving problems whose workspace and configuration space are closely related. In such scenarios, the workspace topology knowledge can be used to identify regions of the environment and their connectivity, to be explored by the planner \cite{5,21,22,6}. This guidance can increase the speed of planning process. In applications that require a certain quality of the path however, the planner, even guided topologically, can spend time exploring parts of the environment that are not relevant to the needed solution.

Prior research in path quality often focuses on one metric. Planning methods like medial axis planning \cite{17,26} push every configuration sampled to the medial axis. This provides paths with high clearance from obstacles, which is helpful in scenarios like the one mentioned above, where path safety is needed for navigation. However, metric-specific methods like medial axis planning cannot be as easily generalized for other metrics like region priority.

In this work, we present annotated-skeleton biased planning, a method that embeds environment information in a topological skeleton to guide sampling-based motion planning algorithms. Given a biasing metric, the method annotates the workspace skeleton with its related information, and the planner explores the environment along the skeleton, biasing towards the specified requirement.

We combine workspace guidance and environment-specific information to steer planning. Our method presents an advantage over metric-specific planning algorithms that are biased towards a single metric, by separating planning from biasing, making it possible to use any underlying planner to achieve the specified path quality requirements.

This method is tested on robotics environments and protein-ligand binding applications using different biases like path safety and binding energy to demonstrate its generality and flexibility. The method is compared to a skeleton guided planner and achieves the desired planning behavior with a negligible time trade-off.

### 2 Related Work

As the environment gets more complex or as the degrees of freedom of the movable object increase, exact motion planning solutions become intractable \cite{20}, hence the popularity of sampling-based algorithms that use randomness and heuristics to solve high-dimensional complex problems. Sampling-based algorithms can be subdivided into two categories, namely, the tree-based rapidly exploring random trees (RRT) \cite{16} and the graph-based probabilistic roadmaps (PRM) \cite{11}. Typically, RRT-based algorithms optimize speed and are easily applied to robotics problems with nonholonomic constraints, while PRM-based algorithms optimize connectivity and can be applied to multi-query problems. Rapidly exploring random graphs (RRG) \cite{9} are a hybrid of both algorithms that combines their strengths. There have been variants of heuristics applied to these algorithms to improve planning in specific conditions.
2.1 Topology-Guided Planning

Topological guidance involves using the workspace structure to direct how sampling-based planners explore the environment. Some motion planning approaches use the workspace decomposition for planning, especially to target narrow passages. For example, Vonasek et al. [24] use Voronoi diagrams to guide an RRT through a protein environment and discover possible protein tunnels that could connect to a binding site.

Several topology-guided planners use workspace skeletons, which are graphs that capture the topological features of the environment. One such planner is Dynamic Region-biased RRT (DR-RRT) [5]. This strategy guides the planner to sample only from particular regions based on the workspace topology. A skeleton, or graph that maps the essence of the free workspace topology, directs region selection. These regions are created, sampled based on their previous exploration success rate, and then destroyed as the planner explores new regions.

Topological guidance has been used for online planning [21, 22], and in control problems for planning with dynamic environments with interactions [8]. Ha et al [6] recently defined H-signatures to find optimal paths in cluttered environments.

2.2 Property-Specific Planning

Property-specific planners guide the planning process with objective-based functions that depend on certain environment features. Such planners target specific environment characteristics relevant to the path requirements. For example, medial axis based algorithms [17,26] aim to build a roadmap along the medial axis of the environment, which results in paths with maximized obstacle clearance. On the other hand, obstacle based algorithms [12,27] increase chances of finding shortest paths through narrow passages by building a roadmap close to obstacle surfaces. Although medial axis and obstacle based algorithms successfully return a roadmap with the desired properties, they can be computationally expensive because the planner has to interact with the workspace to guide planning. In addition, these methods and others [25,7] that are property-specific are not capable of handling other priorities.

3 Methodology

The annotated-skeleton biased planning algorithm annotates the workspace skeleton with biasing metric information and then guides the planner based on this information to increase chances of finding desirable paths faster. In the following sections we explain how the skeleton is constructed and annotated with environment properties and how regions of the environment are dynamically selected to bias the discovery of regions following a given metric. Algorithm 1 outlines the annotated-skeleton biased approach, and Figure 1 illustrates a simple example of a planner guided by a clearance-based annotated skeleton.
Fig. 1: Example execution of the annotated-skeleton biased method: (a) Workspace Skeleton annotated with clearance value (red $\rightarrow$ lowest clearance, yellow $\rightarrow$ medium clearance, green $\rightarrow$ highest clearance). The query is shown as S for start and G for goal. (b) Region selection based on maximum clearance-bias. A region over a shorter edge is preferred to a longer one in poor conditions. (c) Exploration process where the passage on the right is explored first. (d) Extracted maximum-clearance path. Shorter less safe alternative is shown in dashed line.
3.1 Constructing and Annotating the Skeleton

Given a motion planning problem and some biasing metric, we first construct a skeleton through the free workspace. A workspace skeleton is a unit-dimensional curve fully contained inside the environment free space such that the free space can be collapsed into the skeleton in a continuous way [3]. There are different ways of constructing the workspace skeleton, and for our purpose, we are usually most interested in a medially centered structure so that we can accurately extract local properties of the environment. For that reason, we construct a Medial Axis [4] in 2D environments and use a Mean Curvature Skeleton [23] in 3D environments.

We annotate the skeleton with environment properties by saving for each edge the bottleneck w.r.t. each property. This is so that we can get the property value that can inform us on the highest cost to incur in the region represented by the edge. If we are interested in path safety in relation to obstacle clearance for example, we save the lowest obstacle clearance of the skeleton edge. In a similar way, for the protein-ligand binding application, where we need to guide the planner towards high volume and low energy regions, we save the highest energy along the edge in addition to the lowest obstacle clearance value. A clearance-annotated skeleton can be seen in Figure 1a. It is color-coded from highest to lowest clearance, starting with green to yellow and ending with red.

The annotated skeleton is robot-independent and can be reused in the same workspace with different types of robots. We demonstrate this in the protein-ligand application by using a set of ligand probes, commonly used in protein-ligand binding site prediction research [15], to compute van der Waals attraction forces at different protein locations along the mean curvature skeleton edges.

3.2 Growing the Roadmap with Biasing

In this phase we grow a sampling-based roadmap that explores environment regions that are most relevant to the biasing metric. We start by finding the closest skeleton vertex to the start configuration as shown in Line 4 of the algorithm. We then spark a spherical sampling regions along each outgoing edge of the vertex. These regions have a fixed radius equivalent to the size of the robot.

The following steps from Line 6 to 18 are repeated until the problem is solved. A sampling region is selected from the set of active regions based on the annotation of the skeleton edge along which the region is defined. The selection is done in three steps shown in Algorithm 2. Each active region is weighted based on the skeleton edge annotation. The relative edge length is used as a scaling factor to take into consideration how much time it would take to traverse the edge. As illustrated in Figure 1b factoring the relative length of the edge into the selection process allows the planner to make a choice between two equally poorly qualified regions based on the expected duration of the poor conditions.

The roadmap is extended towards the selected region using an RRT Extend step. Depending on the problem, GrowRoadmap() builds a tree or a graph. In applications where we are interested in increasing the quality of the returned
Algorithm 1 Annotated-skeleton biased planner

**Input:** Environment $env$, Start $s$, Goal $g$, Bias Metric $\mu$

**Output:** Path $P$

1: $WS \leftarrow \text{GetWorkspaceSkeleton}(env)$
2: $AS \leftarrow \text{AnnotateSkeleton}(env, WS, env.Properties)$
3: Initialize $R$ to $\phi$
4: $v \leftarrow \text{GetInitialVertex}(start, AS)$
5: $\{A_r\} \leftarrow \text{CreateActiveRegions}(v)$
6: while $\neg$done
7:     $r \leftarrow \text{SelectRegion}(\{A_r\}, \mu)$
8:     if $r ==$ NULL
9:         $r \leftarrow env.GetBoundary()$
10:     end if
11:     $R \leftarrow \text{GrowRoadmap}(r, \mu)$
12:     $\text{AdvanceRegion}(r)$
13:     if $\text{RegionReachedEndOfEdge}(G, r)$
14:         $v \leftarrow \text{GetNextVertex}(r)$
15:         $\{A_r\} \leftarrow \{A_r\} \setminus r$
16:         $\{A_r\} \leftarrow \text{CreateActiveRegions}(v)$
17:     end if
18: end while
19: $P \leftarrow \text{Query}(R, s, g)$
20: return $P$

path, such as the protein-ligand binding application, we increase connections and build an RRG.

These steps increase the chance of the first sequence of explored regions to contain a path that satisfies the given conditions. At each iteration, the algorithm greedily attempts to expand the roadmap towards regions with a higher probability of satisfying the query conditions.

After the roadmap is constructed, it is queried to find the paths to the goal using a graph search algorithm. The quality of the extracted path is dependent in part on the density of the roadmap. This in turn is dependent in part on the sampling region size as well as the step size for the RRT extension or the PRM local planner move. To save computation time, we use fixed-size spherical sampling regions defined based on the size of the robot, and in the Query step in Line 19 of Algorithm 1 we find homotopic paths to the extracted one using smoothing algorithms.

### 3.3 Probabilistic Completeness

Given that the workspace skeleton represents the free space, a skeleton-guided planner with unlimited resources, operating in a region of radius $r$ big enough to cover the whole environment is probabilistically complete. For that reason, as proposed by Denny et al.

[1] we keep a probability $p > 0$ of selecting the full environment as an active sampling region in order to conserve completeness.
Algorithm 2 SelectRegion

**Input:** active regions set \( \{R\} \), biasing metric \( \mu \)

**Output:** active region \( r \)

1: \( r \leftarrow NULL \)
2: for each \( r_i \in \{R\} \)
3: \( a \leftarrow r_i.\text{GetSkeletonEdge().GetMetric}(\mu) \)
4: \( l \leftarrow r_i.\text{GetSkeletonEdge().GetLength}() \)
5: \( \text{region\_weights.push\_back(Weight(a/l/minL))} \)
6: end for
7: \( r \leftarrow \text{min\_arg(region\_weights)} \)
8: return \( r \)

In addition, to the theoretical completeness, the method is experimentally faster than traditional unguided planning methods. This can be explained by two properties of topological guidance: First, the workspace skeleton indicates the connectivity of the free space, making it possible to find narrow passages as easily as wide areas are found. Second, region sizes are conservatively set so that they contain a valid configuration of the robot while minimizing chances of covering obstacle space. This is done by using a medially centered skeleton and a spherical region of radius \( r = \text{robot.Length} \).

Annotating the skeleton with information relevant to the problem similarly indicates regions that are important to the solution, giving the planner a higher chance of visiting them earlier.

4 Experiments

We used robotics and computational biology examples to study the effect of using an annotated skeleton to guide a planner through different definitions of quality. In robotics environments, we used maximum clearance to bias towards safer regions. In protein environments, we used two different metrics: maximum clearance to find high volume protein tunnels and minimum energy to find low energy tunnels.

Our experiments test the ability of using a general planner to achieve different specific planning behaviors, which is impossible to do with any one specialized planner.

4.1 Environments studied

We studied two robotics examples and two protein variants to study protein-ligand binding.

Robotics Environments To analyze the general applicability of our method, we tested 2D and 3D robotics environment with robots of varying constraints. Both environments have more than one possible path to solve the query. We
explicitly made the most desirable path different from the easily discoverable one to test the ability of the planner to find the desired path.

We define success as the ability to return paths relevant to the query conditions. After planning, we analyzed paths checking the ones that went through a sequence of regions that maximizes clearance.

- **3D Boxes** (Fig 2): This is a 6 DOF rigid body robot in an environment with three boxes. This 3D example was used to test the efficiency of mean curvature skeleton guidance.
- **Hallways** (Fig 3): A 3 DOF nonholonomic iRobot Create is tested in a planar environment with hallways of different widths. Safe navigation is important in this environment to allow a margin of error when the path found is deployed on a physical system.

**Protein-Ligand Binding** A protein is a large molecular structure made from a chain of amino acids, involved in several essential metabolic reactions. It reacts with a drug molecule called a ligand to activate or inhibit its functionality, through a process called protein-ligand binding. This process is conditioned by geometric and energetic compatibility between the protein’s molecules and the ligand. Molecules involved in the binding process form the protein’s binding site. A large number of proteins have their binding sites buried inside the cavity of the protein and accessible from the outside through protein tunnels. Molecules that line up those tunnels often regulate the binding site’s accessibility, further increasing the protein’s selectivity [10].

The protein configuration data is procured from the Protein Data Bank (PDB) [19] and a geometric structure can be constructed using a software called CHIMERA [18]. We model the ligand as a 3D rotational multi-linkage robot with a torsional joint degree of freedom per linkage.

Given a protein geometry as an environment, we use motion planning to find possible tunnels inside the protein. The start configuration is generated by sampling a valid configuration of the ligand with maximum contact with the protein binding site molecules. Using the workspace skeleton for guidance, we explore tunnels that connect the binding site to the outside surface. An annotated skeleton can help explore regions inside the protein that are likely to contain viable tunnels. These are regions with low energy cost and high obstacle clearance.

After planning, we analyze paths found by classifying them using a scoring function to evaluate tunnel accessibility. The scoring function takes into consideration the tunnel volume, energy minima, and bottlenecks.

We studied haloalkane dehalogenase (DhaA) protein (Figure 4a). It is used in the degradation of soil pollutants like tri-chloropropane (TCP). DhaA binds with TCP and the velocity of that reaction depends on the accessibility of DhaA’s binding site. To increase its reactivity, biochemists have engineered DhaA mutants that are more accessible to the ligand. We used motion planning to compare the native structure (wild type) and one of its mutants, DhaA31. The success
ratio was determined by the number of tunnels discovered compared to the experimentally known number of tunnels for the protein-ligand pair.

- **DhaA**: The active site of DhaA is connected to the protein surface by two major access tunnels, although three more tunnels have been predicted through molecular modeling [12].

- **DhaA31**: To increase its activity towards TCP, certain residues were modified, which reduced the size of the binding pocket to fit the ligand and leave little space to the solvent. This was reported to increase DhaA’s activity towards TCP. Two tunnels are documented for this protein [13].

### 4.2 Experimental Setup

We run three types of strategies and analyze the planner’s performance in terms of speed and ability to satisfy path requirements, and the role that guidance plays in that:

- **MA-RRT/MA-RRG**: Medial axis RRT/RRG without topological guidance. This is an example of a specialized planner, expected to find paths near the medial axis of the environment, maximizing obstacle clearance.

- **DR-RRT/DR-RRG**: Dynamic Region-biased RRT/RRG with topological guidance without environment property annotation. It is expected to improve planning speed by guiding the planner away from workspace regions occupied by obstacles.

- **AB-RRT/AB-RRG**: Our method, Annotated-skeleton Biased RRT/RRG guided by an annotated workspace skeleton.

The robotics environments were run with 40 seeds each while the protein experiments were run with 10 seeds. MA-RRG is not reported in the protein environments because it could not solve the problem within the time limit of four minutes.

### 4.3 Results and Discussion

Table 1 shows the running times for the robotics environments. In the skeleton construction phase, we observed that the overhead added by the annotation was less than 0.01 seconds. Note that MA-RRT does not rely on a workspace skeleton and incurs the cost of computing a medial axis during run time.

Figures 2 and 3 show distinct paths returned by each planner. In both environments, AB-RRT with maximum clearance bias, returned 100% of its paths passing through the higher clearance regions of the environment, while DR-RRT and MA-RRT fluctuated between trials.

In the Boxes environment, DR-RRT and MA-RRT returned paths that went through the first first sequence of regions encountered between the start and the goal. In the Walls environment, the skeleton guided methods took about the same time to solve the query. However, AB-RRT returned paths with higher clearance, which are more likely for the iRobot Create to execute successfully
compared to the shorter paths returned by the other two strategies. MA-RRT succeeded to return paths through the safe regions 18% of the time, but it took more than 10 times longer than it took the guided planners.

Table 1: Running time (seconds) in robotics environments averaged over 40 runs. Total planning time reported includes skeleton annotation time.

| Strategy | 3D Boxes | Walls |
|----------|----------|-------|
|          | Time   | Success rate (%) | Time   | Success rate (%) |
|----------|--------|-----------------|--------|-----------------|
| Skeleton Planning | avg | σ | avg | σ | avg | σ | avg | σ |
| MA-RRT   | 0.94   | 0.36            | 0      | 1.99            | 0.01 | 18 |
| DR-RRT   | 0.22   | 0.01            | 0.66   | 0.004           | 0.001 | 0.043 | 0.017 | 0 |
| AB-RRT   | 0.23   | 0.02            | 0.72   | 0.005           | 0.001 | 0.047 | 0.020 | 100 |

(a) AB-RRT  
(b) DR-RRT  
(c) MA-RRT

Fig. 2: Five extracted paths from 40 random runs in the Boxes environment.

Table 2 and Figure 4 show the running time and path profiles for DhaA and its variant DhaA31. Across the board, DhaA31 paths were found in less time compared to the wild type case. Running time correlates with binding site accessibility, signaling that the easier a tunnel is to plan through, the easier it could be for the ligand to traverse it.

In DhaA wild type, AB-RRG with energy bias returned predicted paths in less time than DR-RRG, showing the advantage of biasing in problems with com-
Fig. 3: Five extracted paths from 40 random runs in the Walls environment.

plex geometry. Moreover, AB-RRG with energy bias returned all five expected tunnels in less time than it took DR-RRG to discover two. Figure 4b shows that high clearance is not always correlated with low energy. This is motivation for our future plan to study how multiple metrics can be combined to find an optimal path balancing them.

In DhaA31, AB-RRG with clearance bias did not find any paths in the limited time set of 3 minutes. This is in agreement with the fact that DhaA31 was modified by reducing its access tunnels volume to increase stability of the reaction with TCP. Figure 4c shows that AB-RRG correctly identified a path through the energetically favorable tunnel. Using AB-RRG, we are able to identify both tunnels present in the protein and get an intuition on which protein variant is more accessible by looking at the time it took to identify those tunnels.
These results show that motion planning algorithms can be reliably used to study the accessibility of protein binding sites. Moreover, the guidance of a skeleton annotated with energy information allows fast discovery of relevant tunnels.

Table 2: Running time (seconds) in protein environments averaged over 10 runs. Success rate = Tunnels discovered / Tunnels expected.

| Strategy | Bias | DhaA | DhaA31 |
|----------|------|------|--------|
|          |      | Time | Success | Time | Success |
|          | avg  | σ    | avg     | std  | (%)     |
|          | avg  | σ    | avg     | σ    | (%)     |
| DR-RRG   |       | 27.5 | 0.5     | 239.7| 14.7    |
|          | energy | 40   | 30.5    | 0.3  | 202.3   | 24.5   | 50     |
| AB-RRG   | clearance | 27.8 | 0.2     | 177.9| 0.3     |
|          | energy | 40   | 32.6    | 0.5  | 180.0   | 0.0    |
|          |       | 27.8 | 0.2     | 176.0| 0.0     |
|          | energy | 100  | 32.6    | 0.5  | 150.4   | 16.3   | 100    |

5 Conclusion

We presented an annotated-skeleton biased planning strategy to find environment-informed guided paths for motion planning problems. By separating biasing from the planning process, we were able to use different planning strategies to solve a variety of problems. We showed the merit of the AB-RRT method in robotics problems where obstacle clearance is important. For protein-ligand binding problems, we used AB-RRG to assess the accessibility of protein binding sites and find feasible paths through protein tunnels. In the future, we plan to study how multiple metrics can be combined to dynamically discover relevant regions to a specific query. We also plan to use the annotated skeleton in dynamic environments where the topology of the problem stays the same and a planner needs guidance based on changes in the environment.
Annotated Skeleton Biased Planning

(a) DhaA protein and its 5 tunnels

(b) DhaA

(c) DhaA31

Fig. 4: Best paths found by DR-RRG and AB-RRG in DhaA and DhaA31.
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