Randomized Self-assembly for Approximate Shapes

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Abstract. In this paper we design tile self-assembly systems which assemble arbitrarily close approximations to target squares with arbitrarily high probability. This is in contrast to previous work which has only considered deterministic assemblies of a single shape. Our technique takes advantage of the ability to assign tile concentrations to each tile type of a self-assembly system. Such an assignment yields a probability distribution over the set of possible assembled shapes. We show that by considering the assembly of close approximations to target shapes with high probability, as opposed to exact deterministic assembly, we are able to achieve significant reductions in tile complexity. In fact, we restrict ourselves to constant sized tile systems, encoding all information about the target shape into the tile concentration assignment. In practice, this offers a potentially useful tradeoff, as large libraries of particles may be infeasible or require substantial effort to create, while the replication of existing particles to adjust relative concentration may be much easier.

To illustrate our technique we focus on the assembly of $n \times n$ squares, a special case class of shapes whose study has proven fruitful in the development of new self-assembly systems.

Keywords: Self-Assembly, Randomized Algorithms, Approximation Algorithms.

1 Introduction

Self-assembly is the process by which simple objects autonomously assemble into complexes. This phenomenon is common in nature and is the mechanism behind many natural occurrences such as crystal growth. Current research is particularly interested in understanding and harnessing the power of self-assembly for the purpose of massive fabrication of nanoscale devices such as computer circuits. In particular, researchers have identified DNA molecules as a promising medium in which to design controlled self-assembly systems for nanomanufacturing and biologically based computing.
The leading theoretical model for self-assembly is the tile assembly model introduced by Winfree [15]. The tile assembly model extends the theory of Wang tilings of the plane [14] by adding a natural mechanism for growth. Informally, particles of a self-assembly system are modeled by four-sided Wang tiles, each with a type of glue assigned to each side. The tiles float about in the plane and stick together when they bump if the affinity between touching glues is strong enough. In this way, the particles or tiles of the system self-assemble into a complex pattern or shape. The goal is then as follows: Given a target shape or pattern, design a system of tiles that will assemble into the target. The quality or efficiency of the system is then measured by how few distinct tile types are used. This measurement is motivated by the fact that each distinct type of tile must be manufactured if the system is to be implemented.

The tile model of self-assembly is primarily motivated by a DNA based implementation. Double and triple crossover DNA molecules have been designed that can act as four-sided building blocks (tiles) for DNA self-assembly [7,9]. Experimental work has been done to show the effectiveness of using these tiles to assemble DNA crystals and perform DNA computation [10,11,16,17].

Traditional work in this field has taken the approach of encoding information about the target shape into the tile types of the system [12,1,2,3,13]. In particular, Rothemund et al. [12] and Adleman et al. [1] show how the assembly of $n \times n$ squares can be assembled using $\Theta(\log n / \log \log n)$ distinct tile types. However, the design of large sets of distinct tile types can be problematic. Many mediums of self-assembly may have small practical limitations on the number of glues or tiles that can be manufactured. Even in the most promising scenario of DNA self-assembly in which glues and tiles are encoded with long strands of DNA, there is an associated computational complexity with the design of large sets of DNA glues, as well as the likely need to redesign DNA tile structure for increasingly large tile sets.

In contrast, recent work has been done examining the possibility of encoding the complexity of the target shape outside of the particles in the system entirely. In [8], we showed that there exists a constant sized tile set that can effectively be programmed to assemble any $n \times n$ square with affecting a short sequence of temperatures in the system. Further, Demaine et. al. [6] showed how constant size tile sets can build arbitrary shapes by mixing intermediate self-assembly batches together in a sequence of stages. However, with these techniques the complexity of the target shape is contained within a sequence of laboratory steps, rather than within the system of particles itself.

In this paper we take a new approach. We do encode the complexity of the target shape within the particles of the system entirely. But, we avoid the problems of encoding complexity into the distinct tile types of the system. Rather, we encode the complexity into the relative concentrations of tiles in the system. While completely encoding the complexity of the target shape into the particles of the system, we use only a $O(1)$ size set of distinct tiles. In many instances, in particular in the case of DNA, design of distinct, new particles or tiles is much more difficult than creating a large number of copies of a given particle.