

We now present the theorems concerning the approximation algorithms. They all resemble the first such approximation algorithm in that almost all are linear-time algorithms and use a combination of global and local folding rules, although they differ in the underlying combinatorics used to achieve the close-to-optimal folding.

① Triangular Lattice:

Theorem

(Agarwala-Batzoglou-Dancik-Decatur-Farach-Hannenhalli-Skiena 1997)

There is a linear-time approximation algorithm that folds an arbitrary HP-protein sequence in the 2D triangular HP-model within $\frac{6}{11}$ (0.55) of optimal.

Theorem

(Agarwala-Batzoglou-Dancik-Decatur-Farach-Hannenhalli-Skiena 1997)

There is a linear-time approximation algorithm that folds an arbitrary HP-protein sequence in the 3D triangular HP-model within $\frac{44}{75}$ (0.59) of optimal.

Theorem (Batzoglou-Decatur 1996)

There is a linear-time approximation algorithm that folds an arbitrary HP-protein sequence in the 2D triangular HP-model within $\frac{1}{2}$ (0.5) of optimal.

Theorem (Batzoglou-Decatur 1996)

There is a linear-time approximation algorithm that folds an arbitrary HP-protein sequence in the 3D triangular HP-model within $\frac{3}{5}$ (0.6) of optimal.

2 2D Square Lattice:

Theorem (Hart-Istrail 1995)

There is a linear-time approximation algorithm that folds an arbitrary HP-protein sequence in the 2D square HP-model within $\frac{1}{4}$ (0.25) of optimal.

Theorem (Hart-Istrail 1995)

For every protein sequence S in the linear chain HP-model, consider the following:

- 1 $OPT_{2D}(S)$ = the maximal number of contacts of any fold of S on the 2D square lattice; $OPT_{3D}(S)$ = the maximal number of contacts of any fold of S on the 3D cubic lattice;

2

$$C_{2D}(S) = 2 \min\{\mathcal{O}(S), \mathcal{E}(S)\}$$

$$C_{3D}(S) = 4(\min\{\mathcal{O}(S), \mathcal{E}(S)\}) + 2$$

Then

- 1 $OPT_{2D}(s) \leq C_{2D}(S)$
- 2 $OPT_{3D}(s) \leq C_{3D}(S)$

Therefore, every 2D algorithm that constructs folds achieving a fraction of α of the $C_{2D}(S)$ contacts is an approximation algorithm with ratio α ; it is then guaranteed to achieve at least α of the optimal number of contacts. Similarly for the 3D case.

Theorem (Hart-Istrail 1995)

There is a linear-time approximation algorithm that folds an arbitrary HP-protein sequence in the 3D cubic HP-model within $\frac{3}{8}$ (0.38) of optimal.

Theorem (Newman 2002)

There is a linear-time approximation algorithm that folds an arbitrary HP-protein sequence in the 2D square HP-model within $\frac{1}{3}$ (0.33) of optimal.

Theorem (Newman 2002)

There exist HP-sequences S whose optimal fold in the 2D HP-model satisfies:

$$OPT_{2D}(S) \leq (1 + o(1)) \frac{C_{2D}(S)}{2}$$

Therefore, any algorithm that uses the bounding argument of Theorem 6 to obtain a mathematically guaranteed approximation ratio cannot approximate better than $\frac{1}{2}$ of optimal.

Theorem (Newman-Ruhl 2004)

There is a linear-time approximation algorithm that folds an arbitrary HP-protein sequence in the 3D square HP-model within 0.37501 of optimal (improving on $\frac{3}{8} = 0.3750$).

Theorem (Mauri-Pavesi-Piccolboni 1999)

There is a cubic-time approximation algorithm that folds an arbitrary HP-protein sequence in the 2D square lattice HP-model within $\frac{1}{4}$ (0.25) of optimal.

- ③ 2D Square and 3D Cubic Lattice with Diagonals (so-called Extended Lattices)

Theorem (Bokenhauer-Bongartz 2007)

There is a linear-time approximation algorithm that folds an arbitrary HP-protein sequence in the extended 2D cubic lattice HP-model within $\frac{15}{26}$ of optimal. There is a linear-time approximation algorithm that folds an arbitrary HP-protein sequence in the extended 3D cubic lattice HP-model within $\frac{5}{8}$ of optimal.