

Zuker to Partition Function Variant: Example

$$W_{ij} = \min \begin{cases} W_{ij-1} \\ \min_{i \leq k < j-m} W_{ik-1} + V_{kj} \end{cases}$$

$$Z_{\mathcal{P}_{ij}} = Z_{\mathcal{P}_{ij-1}} + \sum_{i \leq k < j-m} Z_{\mathcal{P}_{ik-1}} \cdot Z_{\mathcal{P}'_{kj}}$$

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Decomposition by Zuker

$$W_{ij} = \min \begin{cases} W_{ij-1} \\ \min_{i \leq k < j-m} W_{ik-1} + V_{kj} \end{cases}$$

$$V_{ij} = \min \begin{cases} eH(i, j), \min_{i < i' < j' < j} V_{i'j'} + eSBI(i, j, i', j') \\ \min_{i < k < j} WM_{i+1k-1} + WM_{kj-1} + a \end{cases}$$

$$WM_{ij} = \min \begin{cases} WM_{ij-1} + c, WM_{i+1j} + c, V_{ij} + b \\ \min_{i < k < j} WM_{ik-1} + WM_{kj} \end{cases}$$

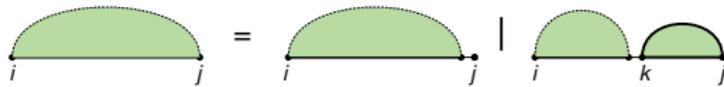
Remark

Combine energy function for stacking and interior loop:

$$eSBI(i, j, i', j') := \begin{cases} eS(i, j) & i' = i + 1 \wedge j' = j - 1 \\ eL(i, j, i', j') & \text{otherwise} \end{cases}$$

Decomposition by Zuker

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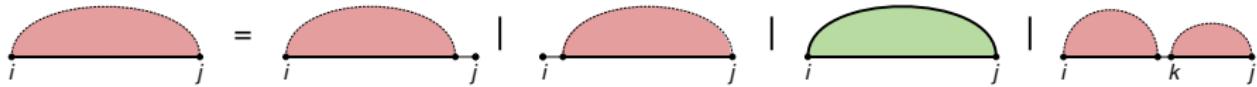
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Combine energy function for stacking and interior loop:

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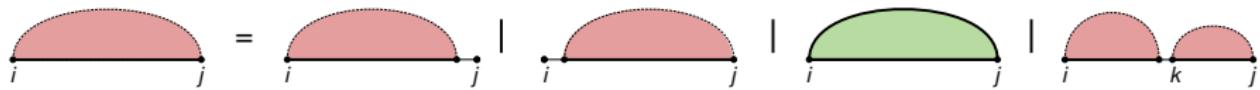
Decomposition of Structure Space by Zuker

$$\text{Diagram showing decomposition of a green semi-circle from vertex } i \text{ to } j \text{ into two parts: a green semi-circle from } i \text{ to } j \text{ and a green semi-circle from } i \text{ to } k \text{ followed by a green semi-circle from } k \text{ to } j.$$

$$\text{Diagram showing decomposition of a green semi-circle from vertex } i \text{ to } j \text{ into three parts: a black semi-circle from } i \text{ to } j, \text{ a green semi-circle from } i \text{ to } j' \text{ followed by a black semi-circle from } j' \text{ to } j, \text{ and a red semi-circle from } i \text{ to } k \text{ followed by a red semi-circle from } k \text{ to } j.$$

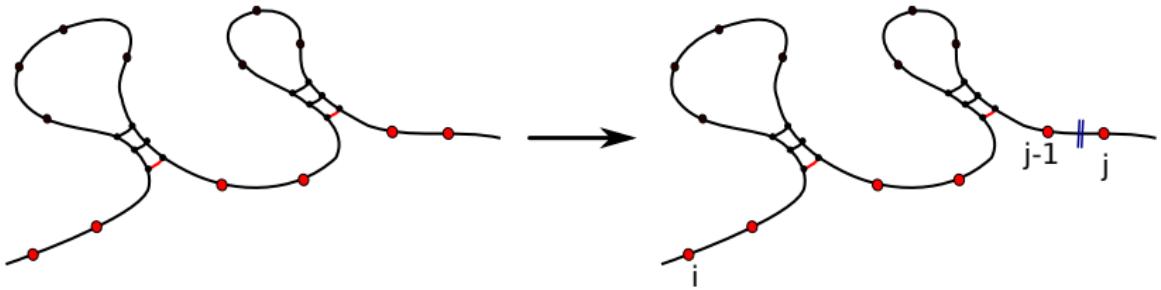
$$\text{Diagram showing decomposition of a red semi-circle from vertex } i \text{ to } j \text{ into four parts: a red semi-circle from } i \text{ to } j, \text{ a red semi-circle from } i \text{ to } j \text{ (repeated), a green semi-circle from } i \text{ to } j, \text{ and a red semi-circle from } i \text{ to } k \text{ followed by a red semi-circle from } k \text{ to } j.$$

Ambiguity Example



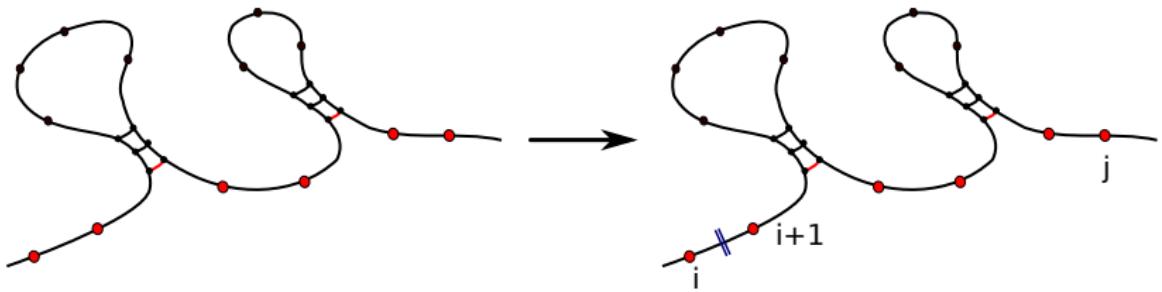
Ambiguity Example

$$\text{Diagram showing a shaded semi-circle from } i \text{ to } j \text{ equaling two parts: a semi-circle from } i \text{ to } j \text{ and a semi-circle from } i \text{ to } j \text{ plus a green semi-circle from } i \text{ to } j \text{ plus a semi-circle from } i \text{ to } k \text{ and another semi-circle from } k \text{ to } j.$$



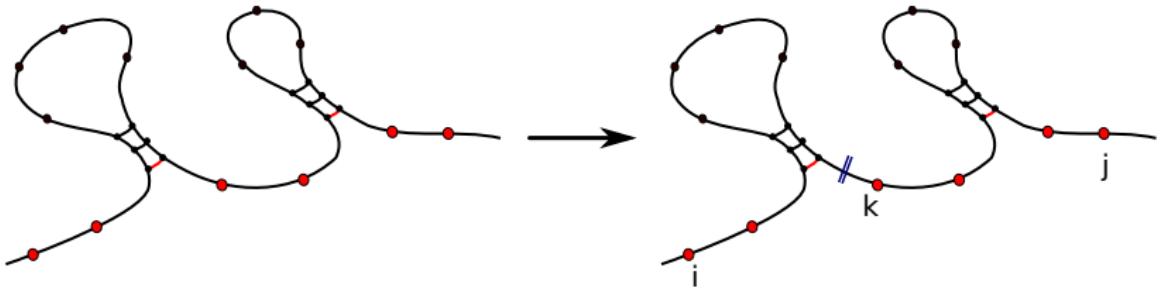
Ambiguity Example

$$\text{Diagram showing a shaded semi-circle from } i \text{ to } j \text{ equaling two parts: a semi-circle from } i \text{ to } j \text{ plus a semi-circle from } i \text{ to } j \text{ plus a semi-circle from } i \text{ to } k \text{ plus a semi-circle from } k \text{ to } j.$$



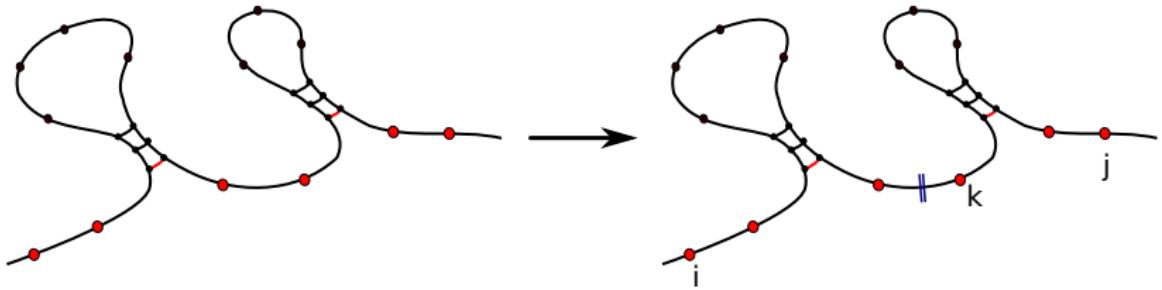
Ambiguity Example

$$\text{Diagram showing a shaded semi-circle from } i \text{ to } j \text{ equaling two parts: a semi-circle from } i \text{ to } j \text{ plus a semi-circle from } i \text{ to } j \text{ plus a semi-circle from } i \text{ to } k \text{ plus a semi-circle from } k \text{ to } j.$$



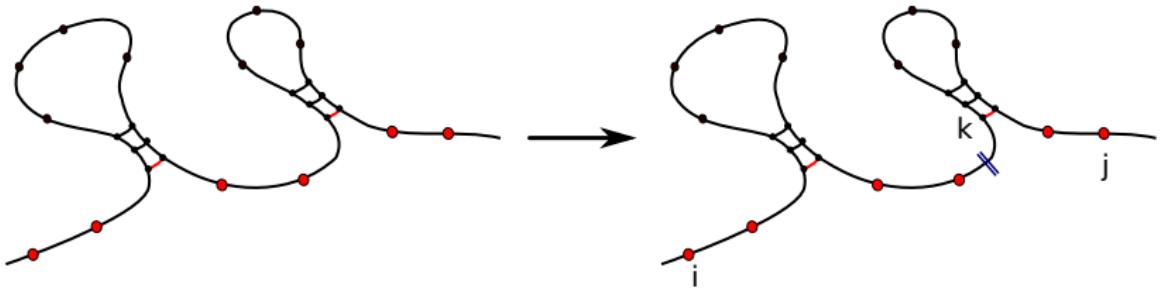
Ambiguity Example

$$\text{Diagram showing a shaded semi-circle from } i \text{ to } j \text{ equaling two separate terms:} \\ = \quad \text{Diagram showing a shaded semi-circle from } i \text{ to } j \quad | \quad \text{Diagram showing a shaded semi-circle from } i \text{ to } j \\ | \quad \text{Diagram showing a green shaded semi-circle from } i \text{ to } j \quad | \quad \text{Diagram showing two separate shaded semi-circles from } i \text{ to } k \text{ and } k \text{ to } j$$



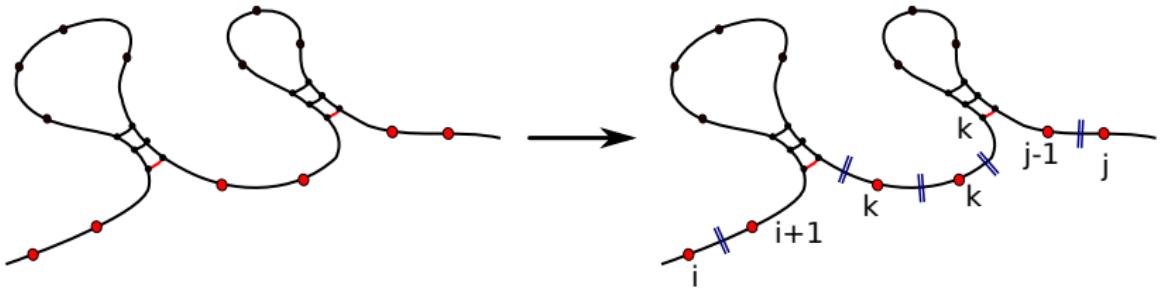
Ambiguity Example

$$\text{Diagram showing a decomposition of a shaded region from point } i \text{ to } j \text{ into two parts: a red semi-circle from } i \text{ to } j \text{ and a green semi-circle from } i \text{ to } j \text{ through point } k. The regions are separated by a vertical line. The red region is labeled with a red dot at its center, and the green region is labeled with a green dot at its center. The points } i \text{ and } j \text{ are marked on the horizontal axis.}$$

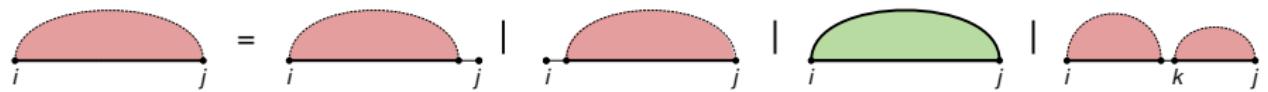


Ambiguity Example

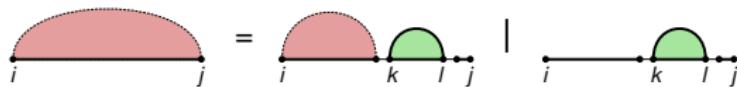
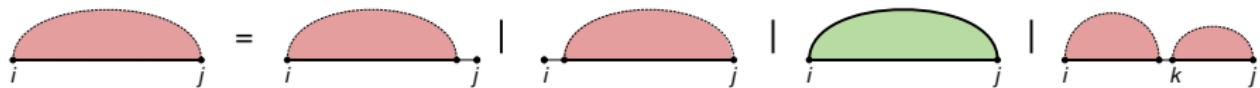
$$\text{Diagram showing a shaded semi-circle from } i \text{ to } j \text{ equaling two parts: a semi-circle from } i \text{ to } j \text{ plus a semi-circle from } i \text{ to } j \text{ plus a semi-circle from } i \text{ to } k \text{ plus a semi-circle from } k \text{ to } j.$$



Discarding Ambiguity



Discarding Ambiguity



Discarding Ambiguity

$$\text{Diagram } i \text{---} j = \text{Diagram } i \text{---} j \cdot \bullet | \text{Diagram } \bullet \text{---} j | \text{Diagram } i \text{---} j | \text{Diagram } i \text{---} k \cdot \bullet | \text{Diagram } i \text{---} k \text{---} j$$

$$\text{Diagram } i \text{---} j = \text{Diagram } i \text{---} k \cdot \bullet | \text{Diagram } i \text{---} k \text{---} l \cdot \bullet | \text{Diagram } i \text{---} k \text{---} l \text{---} j$$

$$\text{Diagram } i \text{---} j = \text{Diagram } i \text{---} k \cdot \bullet | \text{Diagram } i \text{---} k \text{---} l \cdot \bullet | \text{Diagram } i \text{---} k$$

$$\text{Diagram } i \text{---} j = \text{Diagram } i \text{---} j \cdot \bullet | \text{Diagram } i \text{---} j$$

Discarding Ambiguity

$$\text{Diagram showing a sum of two terms:} \\ \text{Term 1: A green semi-circle with endpoints } i \text{ and } j. \\ \text{Term 2: A sum of two terms separated by a vertical bar:} \\ \text{Sub-term 1: A green semi-circle with endpoints } i \text{ and } j' \text{ (where } j' > j\text{).} \\ \text{Sub-term 2: A red semi-circle with endpoints } i \text{ and } k \text{ (where } k > j'\text{).} \\ \text{The entire expression is preceded by an equals sign.}$$

Discarding Ambiguity



Unambiguous Decomposition: Summary

$$\text{Diagram: A green semi-circle from } i \text{ to } j \text{ is equal to a green semi-circle from } i \text{ to } j \text{ plus a green semi-circle from } i \text{ to } k \text{ plus a green semi-circle from } k \text{ to } j.$$

$$\text{Diagram: A green semi-circle from } i \text{ to } j \text{ is equal to a black semi-circle from } i \text{ to } j \text{ plus a green semi-circle from } i \text{ to } j' \text{ plus a red semi-circle from } i \text{ to } k \text{ plus a green semi-circle from } k \text{ to } j.$$

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$$\text{Diagram: A green semi-circle from } i \text{ to } j \text{ is equal to a green semi-circle from } i \text{ to } j-1 \text{ plus a green semi-circle from } i \text{ to } j.$$

McCaskill-Algorithm: Matrices

Given RNA sequence $S = S_1 \dots S_n$. As usual, \mathcal{P}_{ij} denotes the ij -subensemble of S .

- Matrix $Q = (Q_{ij})_{1 \leq i < j \leq n}$
- Matrix $Q^b = (Q_{ij}^b)_{1 \leq i < j \leq n}$
- Matrix $Q^m = (Q_{ij}^m)_{1 \leq i < j \leq n}$
- Matrix $Q^{m1} = (Q_{ij}^{m1})_{1 \leq i < j \leq n}$

McCaskill-Algorithm: Matrices

Given RNA sequence $S = S_1 \dots S_n$. As usual, \mathcal{P}_{ij} denotes the ij -subensemble of S .

- Matrix $Q = (Q_{ij})_{1 \leq i < j \leq n}$

$$Q_{ij} := Z_{\mathcal{P}_{ij}}$$

- Matrix $Q^b = (Q_{ij}^b)_{1 \leq i < j \leq n}$

$$Q_{ij}^b := Z_{\mathcal{P}_{ij}^b}, \text{ where } \mathcal{P}_{ij}^b := \{P \in \mathcal{P}_{ij} \mid (i, j) \in P\}$$

- Matrix $Q^m = (Q_{ij}^m)_{1 \leq i < j \leq n}$

$$Q_{ij}^m := Z_{\mathcal{P}_{ij}^m}^m, \text{ where } \mathcal{P}_{ij}^m := \{P \in \mathcal{P}_{ij} \mid P \text{ non-empty}\},$$

Z^m includes multiloop-contributions (for unpaired bases, inner base pairs), see earlier modification E^m .

- Matrix $Q^{m1} = (Q_{ij}^{m1})_{1 \leq i < j \leq n}$

$$Q_{ij}^{m1} := Z_{\mathcal{P}_{ij}^{m1}}^m,$$

where $\mathcal{P}_{ij}^{m1} := \{P \in \mathcal{P}_{ij} \mid \exists k : (i, k) \in P \wedge k+1, \dots, j \text{ unpaired in } P\}$.

Q-recursion

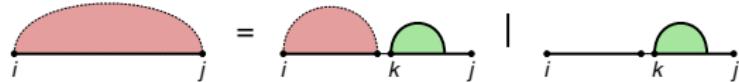
$$\text{Diagram illustrating } Q\text{-recursion:}$$

The diagram illustrates a mathematical concept called *Q*-recursion. It shows a single green semi-circle with endpoints labeled *i* and *j*. This is followed by an equals sign (=). To the right of the equals sign, there is a vertical line separating two distinct green semi-circles. The first semi-circle on the left has endpoints *i* and *j*, and the second semi-circle on the right also has endpoints *i* and *j*. This visual representation likely corresponds to a recursive definition or decomposition of a function or sequence.

Q^b -recursion

$$\text{Diagram showing } Q^b\text{-recursion:}$$

Q^m -recursion



Q^{m1} -recursion

$$\text{Diagram showing } Q^{m1}\text{-recursion:}$$
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McCaskill — Partition Function — Summary

$$Q_{ij} = 1 \quad (i \geq j - m)$$

$$Q_{ij} = Q_{ij-1} + \sum_{i \leq k < j-m} Q_{ik-1} \cdot Q_{kj}^b$$

$$Q_{ij}^b = 0 \quad (i \geq j - m)$$

$$\begin{aligned} Q_{ij}^b = & \exp(-\beta eH(i,j)) + \sum_{i < i' < j' < j} \exp(-\beta eSBI(i,j,i',j')) \cdot Q_{i'j'}^b \\ & + \sum_{i < k < j-m-1} Q_{i+1k-1}^m \cdot Q_{kj-1}^{m1} \cdot \exp(-\beta a) \end{aligned}$$

$$Q_{ij}^m = 0 \quad (i \geq j - m)$$

$$Q_{ij}^m = \sum_{i \leq k < j-m} (\exp(-\beta(k-i)c) + Q_{ik-1}^m) \cdot Q_{kj}^{m1}$$

$$Q_{ij}^{m1} = 0 \quad (i \geq j - m)$$

$$Q_{ij}^{m1} = \sum_{i+m < k \leq j} Q_{ik}^b \cdot \exp(-\beta b) \cdot \exp(-\beta(j-k)c)$$

McCaskill Remarks

- Partition function of the ensemble of S in $Z = Q_{1n}$
- Correctness due to disjoint (=unambiguous) and independent decomposition
- Complexity $O(n^2)$ space,
 $O(n^3)$ time (after bounding size of interior loops)
- Probabilities

- of a structure

$$\Pr[P|S] = Z^{-1} \exp(-\beta E(P)) \quad (\text{efficient!})$$

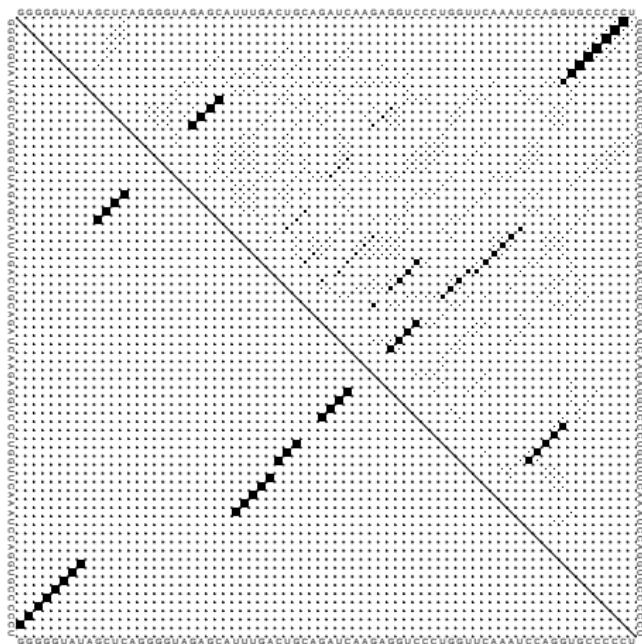
- of a structure set

$$\Pr[\mathcal{P}|S] = Z^{-1} \sum_{P \in \mathcal{P}} \exp(-\beta E(P)) \quad (\text{depends on } |\mathcal{P}|)$$

- of a base pair (i, j)

$$\Pr[(i, j)|S] = Z^{-1} \sum_{P \ni (i, j)} \exp(-\beta E(P)) \quad (?)$$

Base Pair Probabilities



$$\Pr[(i,j)|S] := \sum_{P \ni (i,j)} \Pr[P|S]$$