The substitution decomposition of matchings and RNA secondary structures

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Permutation Patterns 2018
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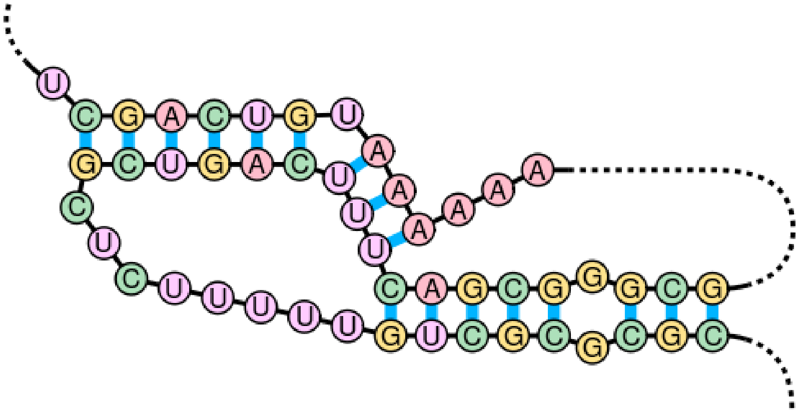
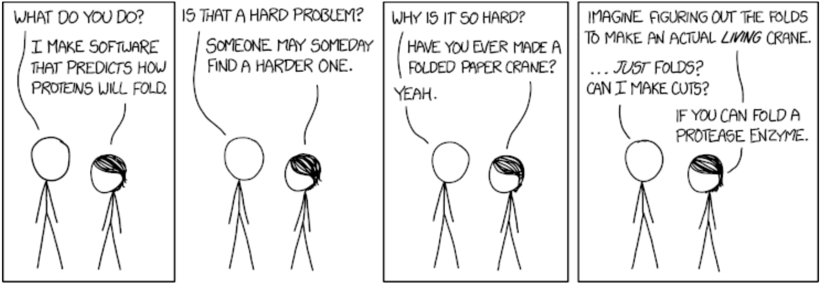
Predicting How RNA Folds

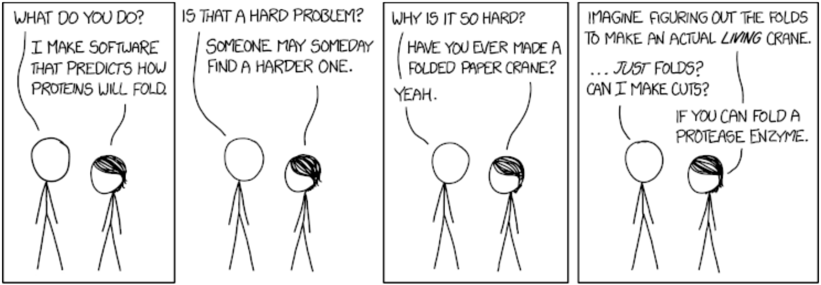


Problem: Given the primary structure, predict the secondary structure.

PREDICTING HOW RNA FOLDS



PREDICTING HOW RNA FOLDS



How about algorithms that only predict certain secondary structures?

There are *oodles* of them.

ORTHODOX STRUCTURES

For a long time biologists thought the edges of the corresponding matchings could not cross. Secondary structures without crossings are called *orthodox structures*.

We call those *non-crossing matchings*.

Counted by the Catalan numbers.

Crossings are called *pseudoknots*.

The D&P Family

Matchings which can be reduced to empty by consecutively deleting edges according to three rules. The edge (i, j) can be deleted if it is

- a directly adjacent edge, i.e., $j = i + 1$,
- a directly nested edge, i.e., there exists an edge (i', j') such that $i' = i + 1$ and $j' = j - 1$, or
- a "hairpin", i.e., there exists an edge (i', j') where either

$$j' = j + 1 = i' + 2 = i + 3 \text{ or } j = j' + 1 = i + 2 = i' + 3.$$

Dirks and Pierce. A partition function algorithm for nucleic acid secondary structure including pseudoknots. *J Comput. Chem. 24* (2003), 1664–1677.

THE D&P FAMILY

Counted by Saule et al. using the context-free language

$$
\begin{aligned}
S &\to dS\overline{d}S \mid P,\\
P &\to pSX\overline{p}S \mid \epsilon,\\
X &\to xSX\overline{x}S \mid ySY\overline{y}S,\\
Y &\to ySY\overline{y}S \mid \epsilon.
\end{aligned}
$$

Saule, Régnier, Steyaert, and Denise. Counting RNA pseudoknotted structures. *J. Comput. Biol. 18*, 10 (2011), 1339–1351.

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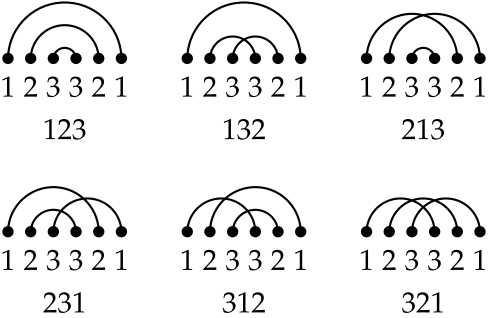
There is!

PP is a Special Case of MP

PP is a Special Case of MP (Learn more at MP2019 in Zürich)



We'll call these *permutational matchings* (following Jelínek for the term but Bloom and Elizalde for the "backwards" convention).

The permutational matchings are precisely those matchings that avoid .

Avoiding a Short Pattern

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- Av() — $n!$ enumeration, all of permutation patterns.

Note: Av() is isomorphic as a poset to Av(, ) — the smallest-yet example of "unbalanced Wilf-equivalence" (Burstein and Pantone).

The Substitution Decomposition

First famous use by Gallai in 1967. (Though the idea dates back to at least Fraïssé in 1953.)

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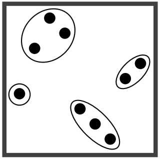
And also in the enumeration of permutation classes...

INTERVALS AND SIMPLE PERMUTATIONS



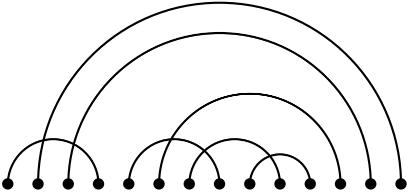
Ovals enclose the *intervals* of this permutation. A permutation is *simple* if all of its intervals are trivial (single entries or the whole permutation).

Albert and Atkinson (2005). *If a permutation class has only finitely many simple permutations then it...*

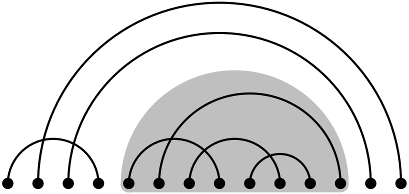
- *is defined by finitely many minimal forbidden permutations (finite basis),*
- *does not contain an infinite antichain, and*
- *has an algebraic generating function.*

Albert and Atkinson. Simple permutations and pattern restricted permutations. *Discrete Math. 300*, 1-3 (2005), 1–15.

Vertex Modules (analogues of intervals)



VERTEX MODULES (ANALOGUES OF INTERVALS)



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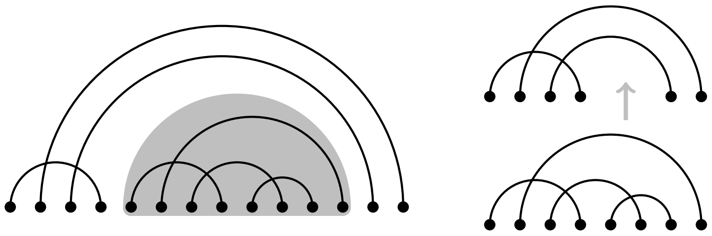
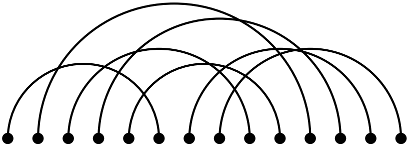
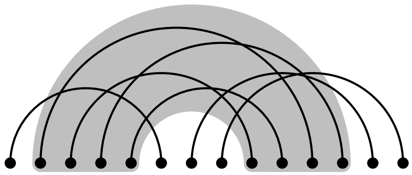


Matchings without vertex modules are *weakly indecomposable*.

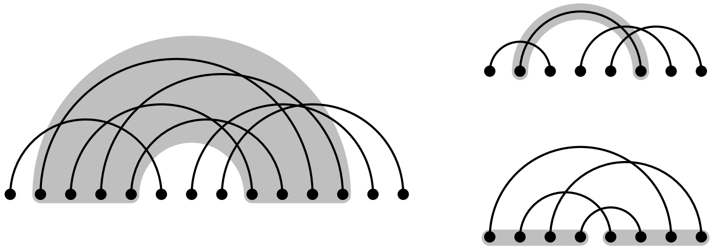
Edge Modules (also analogues of intervals?)



EDGE MODULES (ALSO ANALOGUES OF INTERVALS?)



Edge Modules (also analogues of intervals?)



- Note: we can only inflate an edge by a permutational matching.
- Matchings without vertex or edge modules are *strongly indecomposable*.

Counting Indecomposable Matchings

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Simple permutations of length 5:

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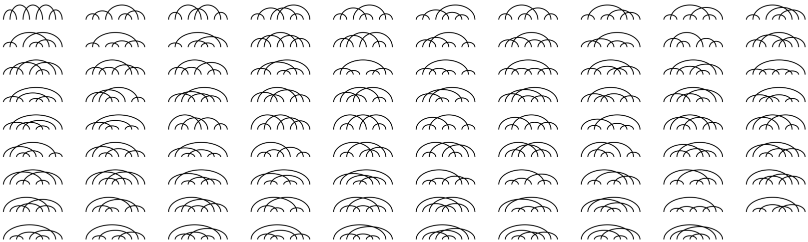
Strongly indecomposable matchings on 5 edges:



Building/Enumerating a Family

1. Identify the strongly indecomposable members of the family.
2. *Inflate* their edges to form the weakly indecomposable members.
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- *is defined by finitely many minimal forbidden matchings (finite basis),*
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(So the Albert–Atkinson Theorem holds in MP as well as PP.)

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Allowed edge inflations: Only , , , ...
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Strongly indecomposable matchings:  and  "hairpin".
Allowed edge inflations: Only , , , ... "ladders".
Allowed insertions: All.

Generating function f satisfies

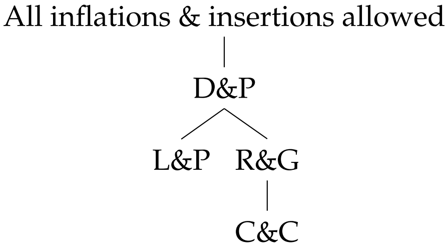
$$x^3f^6 - x^2f^5 + 2xf^3 - xf^2 - f + 1 = 0.$$

Sequence:

$$1, 3, 13, 65, 351, 1994, 11747, 71117, 439765, 2765775, \ldots$$

Given the description above, this is all completely routine.

Hairpin-Only Families



The L&P Family

Strongly indecomposable matchings: ∩ and ⋒ "hairpin".
Allowed edge inflations: Only ladders, ... "ladders".
Allowed insertions: *Only insert non-crossing matchings*.
Generating function f satisfies

$$(16x^3 - 8x^2 + x)f^2 + (-28x^2 + 15x - 2)f + (25x^2 - 14x + 2) = 0.$$

Sequence:

$$1, 3, 12, 51, 218, 926, 3902, 16323, 67866, 280746, \ldots$$

The same sequence arose in work of Klazar (2006), and the enumerative coincidence has been explained bijectively by Martinez and Riehl (2017).

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