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Evolution of genes neighborhood within reconciled phylogenies: an ensemble approach

Cedric Chauve (SFU), Yann Ponty (CNRS/LIX/PIMS), João Paulo Pereira Zanetti (SFU/U. Campinas)



Background: DeCo

Reconstructing ancestral genome features is a classical comparative genomics problem, often addressed with dynamic programming (DP) algorithms. A DP algorithm, called **DeCo**, was recently introduced for computing **parsimonious** evolutionary scenarios for **gene adjacencies** in a **duplication-aware** framework, motivated by the reconstruction of **ancestral gene orders** [Bérard *et al.*, 2012].

DeCo

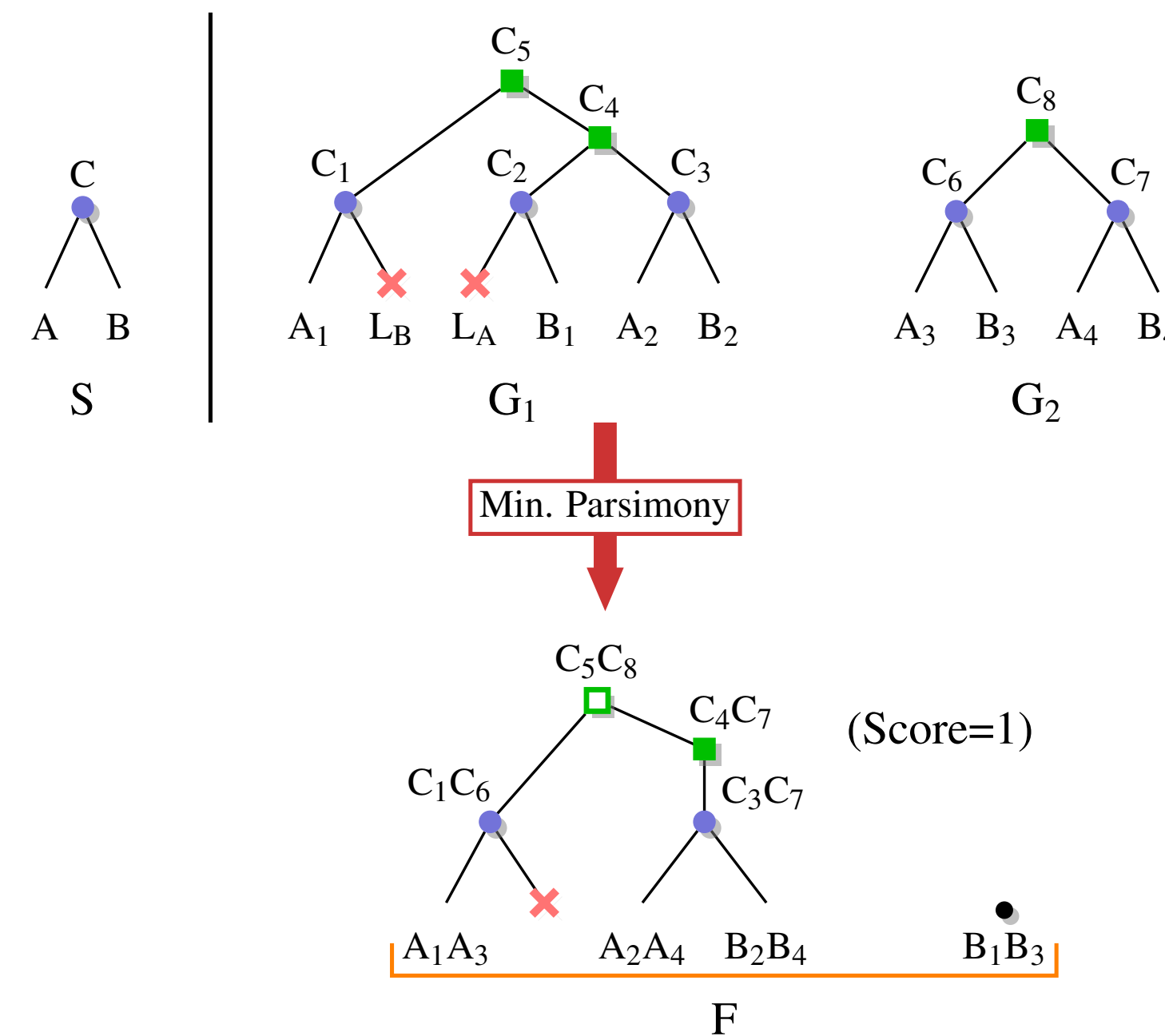
Input:

- Reconciled gene trees G_1 and G_2 ;
- Set of extant adjacencies.

Output:

- Max-parsimony adjacency forest

Parsimony: #adjacencies gains/breaks



Results: DeClone

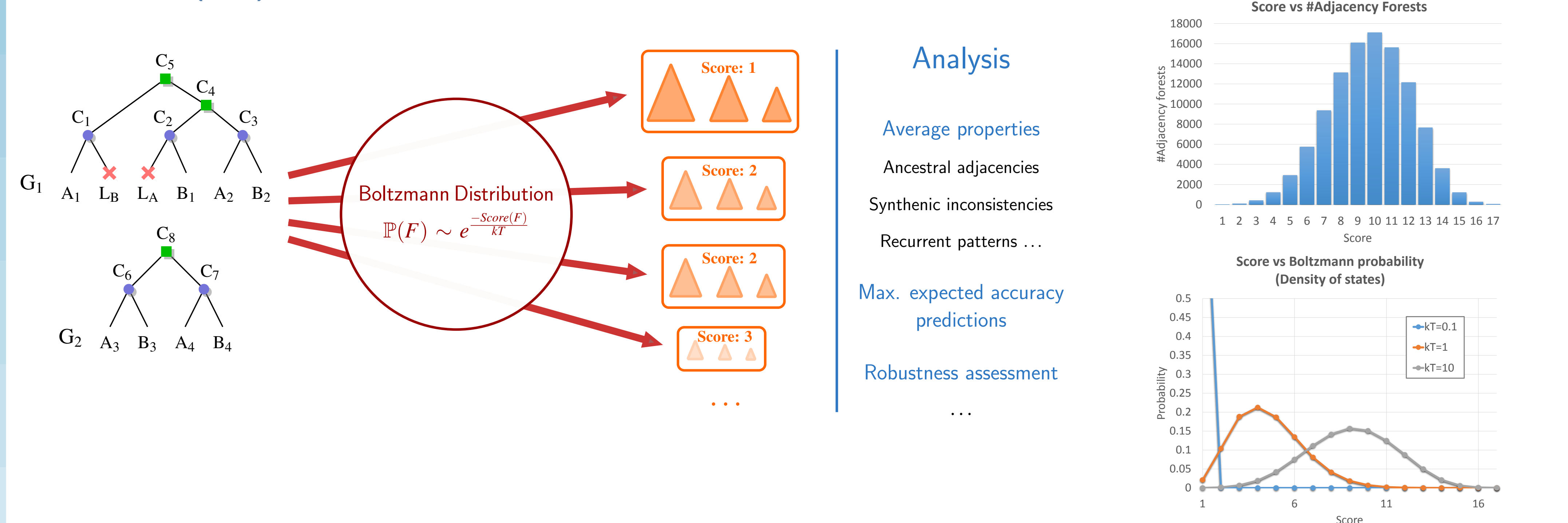
We describe **DeClone**, an extension of DeCo, using **Advanced Dynamic Programming** techniques, that allows the **sampling** of adjacency forests under the **Boltzmann distribution**, as well as the computation of **probabilities** of presence/absence of ancestral gene adjacencies, again under the Boltzmann distribution.

Dynamic programming algorithm (excerpt):

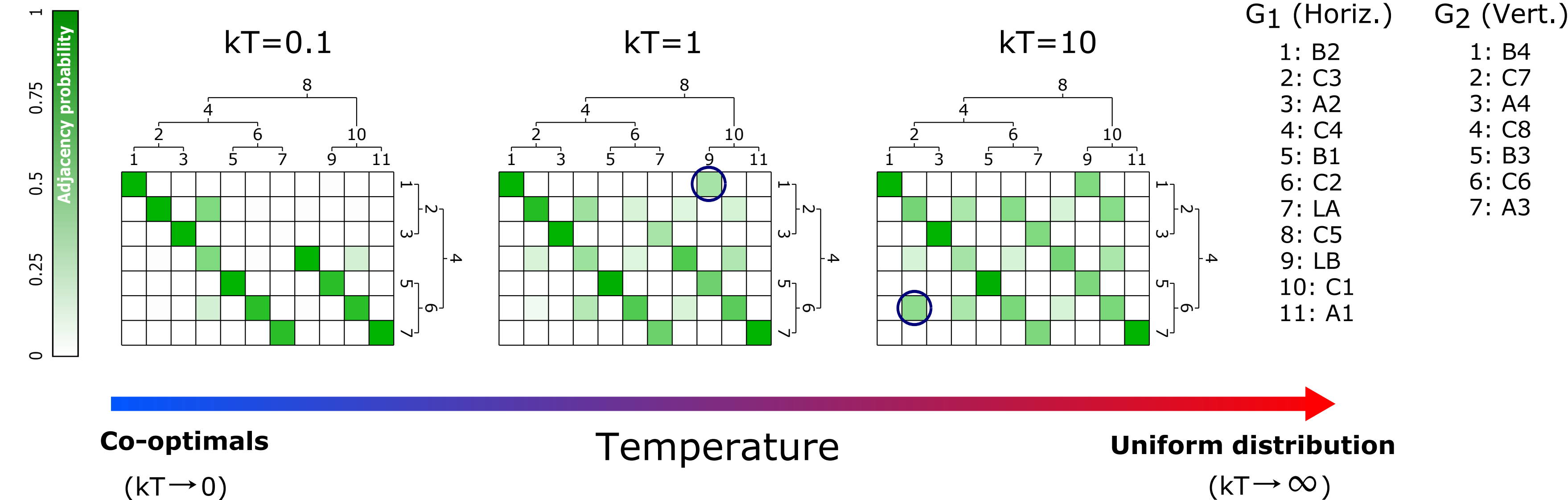
$$c_1(v^1, v^2) = \min \begin{cases} c_1(ca(v^1), cb(v^2)) + c_1(cb(v^1), ca(v^2)) \\ c_1(ca(v^1), cb(v^2)) + c_0(cb(v^1), ca(v^2)) + Break \\ c_0(ca(v^1), cb(v^2)) + c_1(cb(v^1), ca(v^2)) + Break \\ c_0(ca(v^1), cb(v^2)) + c_0(cb(v^1), ca(v^2)) + 2Break \\ c_1(ca(v^1), ca(v^2)) + c_1(cb(v^1), cb(v^2)) \\ c_1(ca(v^1), ca(v^2)) + c_0(cb(v^1), cb(v^2)) + Break \\ c_0(ca(v^1), ca(v^2)) + c_1(cb(v^1), cb(v^2)) + Break \\ c_0(ca(v^1), ca(v^2)) + c_0(cb(v^1), cb(v^2)) + 2Break \end{cases}$$

DeCo+Advanced Dynamic Programming=DeClone

The whole (sub)optimal space is modelled as a Boltzmann Ensemble Suboptimality vs combinatorics



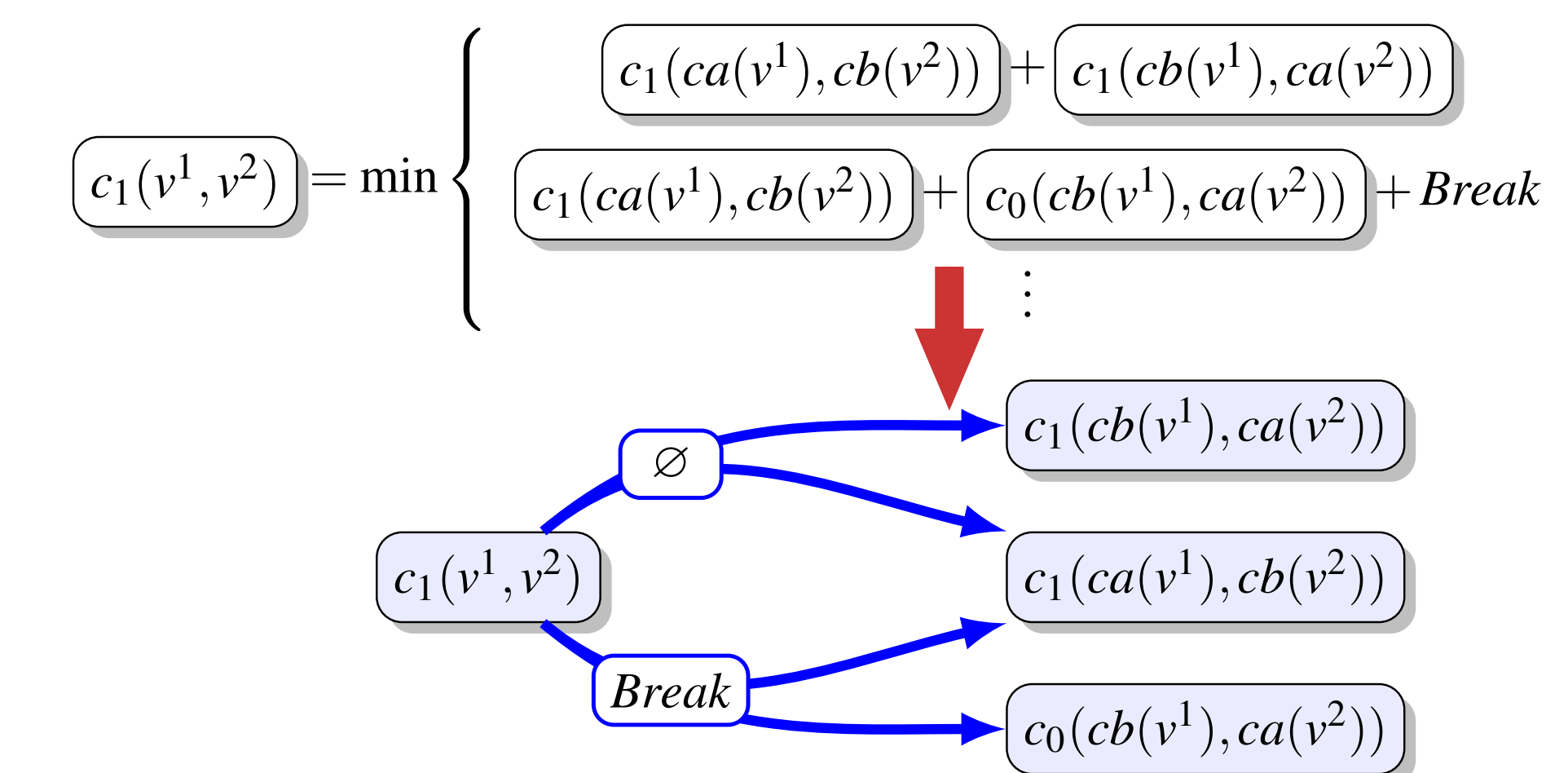
Impact of pseudo-temperature kT on predicted adjacencies



Algorithmic aspects

Algorithmic framework [Ponty/Saule, 2011]

Dyn. Prog. equations \rightarrow Weighted Hypergraphs



$$\text{DeCo: MaxPars}(q) = \min_{e=q \rightarrow (q_1, q_2, \dots)} w(e) + \sum_i \text{MaxPars}(q_i)$$

Claim: The DeCo DP scheme is **unambiguous** and **complete**

Algorithmic corollaries

- **Computing the partition function \mathcal{Z} in $\mathcal{O}(|G_1||G_2|)$**
Simple change of algebra ($\min, +, C$) \rightarrow ($\sum, \times, e^{-\frac{C}{kT}}$)
- **Boltzmann sampling of adjacency forests**
Each hyperedge chosen with probability proportional to its overall contribution to \mathcal{Z} .
- **Adjacency dot-plot:** $\mathcal{O}(|G_1||G_2|)$ inside/outside algorithm computes the probability of ancestral adjacencies.

Experiments

Data: 6,074 DeCo instances, with genes taken from 36 mammalian genomes from the Ensembl database in 2012. **Syntenic inconsistencies** with parsimonious scenarios concern 5,817, genes over 112,188 ancestral and extant adjacencies.

Methods: for each instance, we sampled 1,000 adjacency forests under a Boltzmann distribution that favours highly co-optimal scenarios.

Results:

Adj. freq.	Anc. genes	Anc. adj.	Synt. Inc.
≥ 0.3	118,687	110,180	10,351
≥ 0.4	117,639	106,973	8,330
≥ 0.5	116,231	103,479	6,677
≥ 0.6	114,538	99,720	5,113
≥ 0.7	112,564	96,039	4,092
≥ 0.8	110,086	91,821	3,276
≥ 0.9	107,564	87,790	2,710
$= 1$	100,443	79,078	1,348

Discussion

DeClone allows a controlled exploration of the space of all gene adjacency evolution scenarios: exhaustive enumeration, sampling, probabilities computation. Experiments show that exploring the whole solution space under a Boltzmann distribution biased toward co-optimal allows to reduce significantly the number of syntenic inconsistencies observed when a single arbitrary optimal scenario is considered.

References

- S. Bérard, *et al.*. 2012. Evolution of gene neighborhoods within reconciled phylogenies. *Bioinformatics*, 28(18):382–388.
- Y. Ponty and C. Saule. 2011. A Combinatorial Framework for Designing (Pseudoknotted) RNA Algorithms. *WABI 2011*, pp. 259–269.