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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

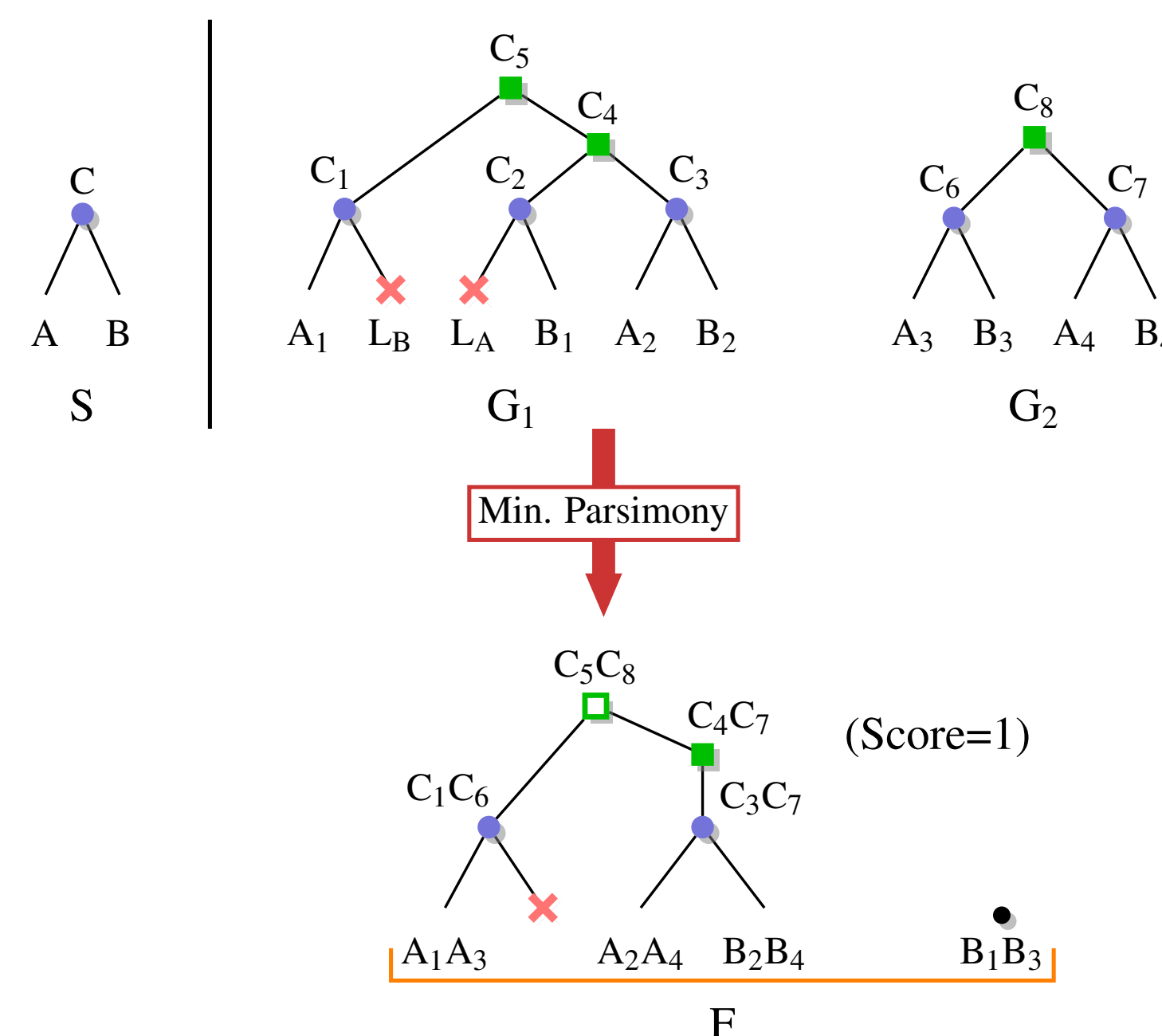
### Input:

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

### Output:

- Max-parsimony adjacency forest

**Parsimony:** #adjacencies gains/breaks



## Results: DeClone

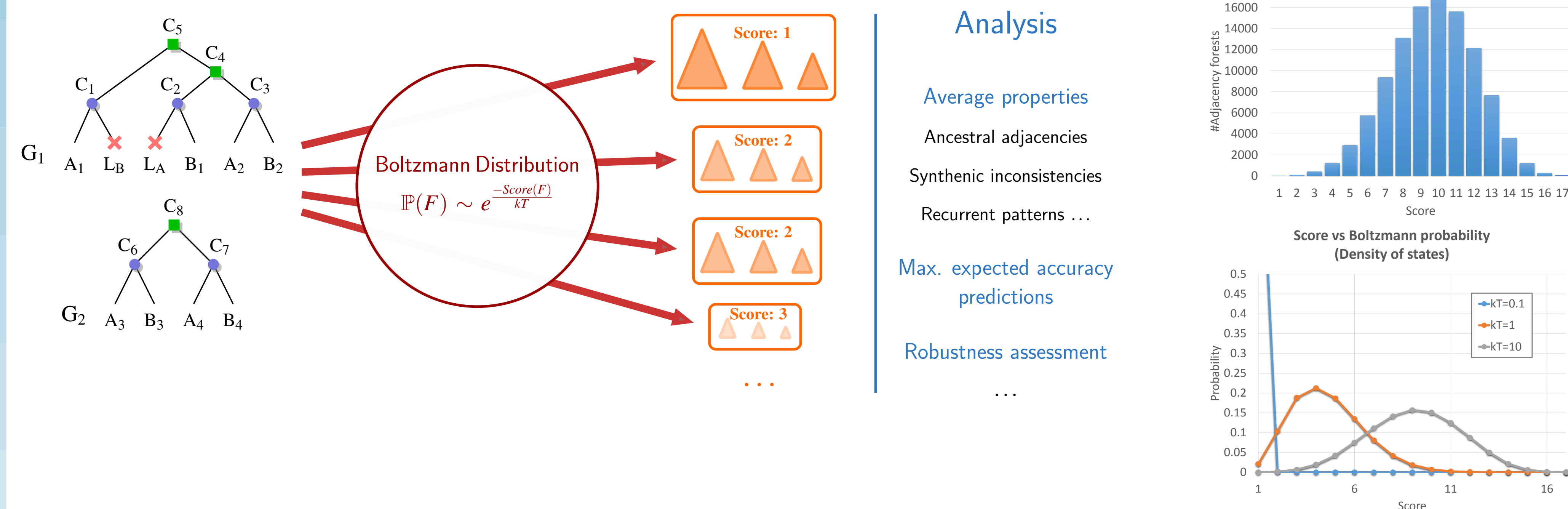
We describe **DeClone**, an extension of DeCo, using **Advanced Dynamic Programming** techniques, that allows the **sampling** of adjacency forests under the **Boltzmann distribution**, as well as the computation of **probabilities** of presence/absence of ancestral gene adjacencies, again under the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

### Dynamic programming algorithm (excerpt):

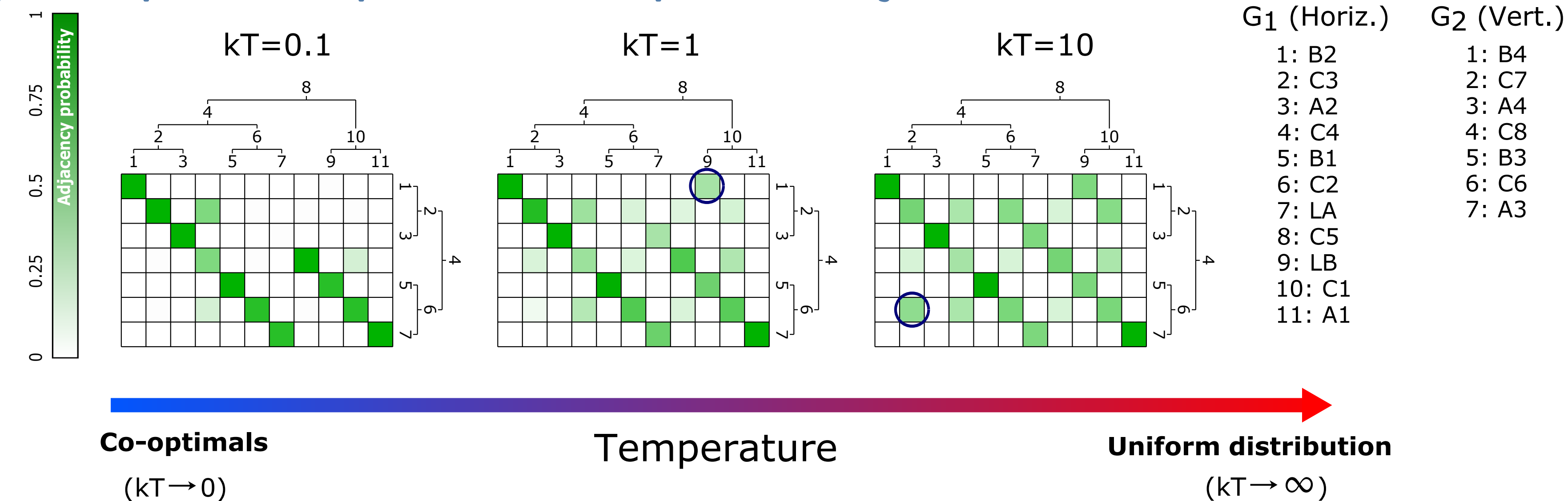
$$c_1(v^1, v^2) = \min \begin{cases} c_1(ca(v^1), cb(v^2)) + c_1(cb(v^1), ca(v^2)) \\ c_1(ca(v^1), cb(v^2)) + c_0(cb(v^1), ca(v^2)) + Break \\ c_0(ca(v^1), cb(v^2)) + c_1(cb(v^1), ca(v^2)) + Break \\ c_0(ca(v^1), cb(v^2)) + c_0(cb(v^1), ca(v^2)) + 2Break \\ c_1(ca(v^1), ca(v^2)) + c_1(cb(v^1), cb(v^2))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

## DeCo+Advanced Dynamic Programming=DeClone

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



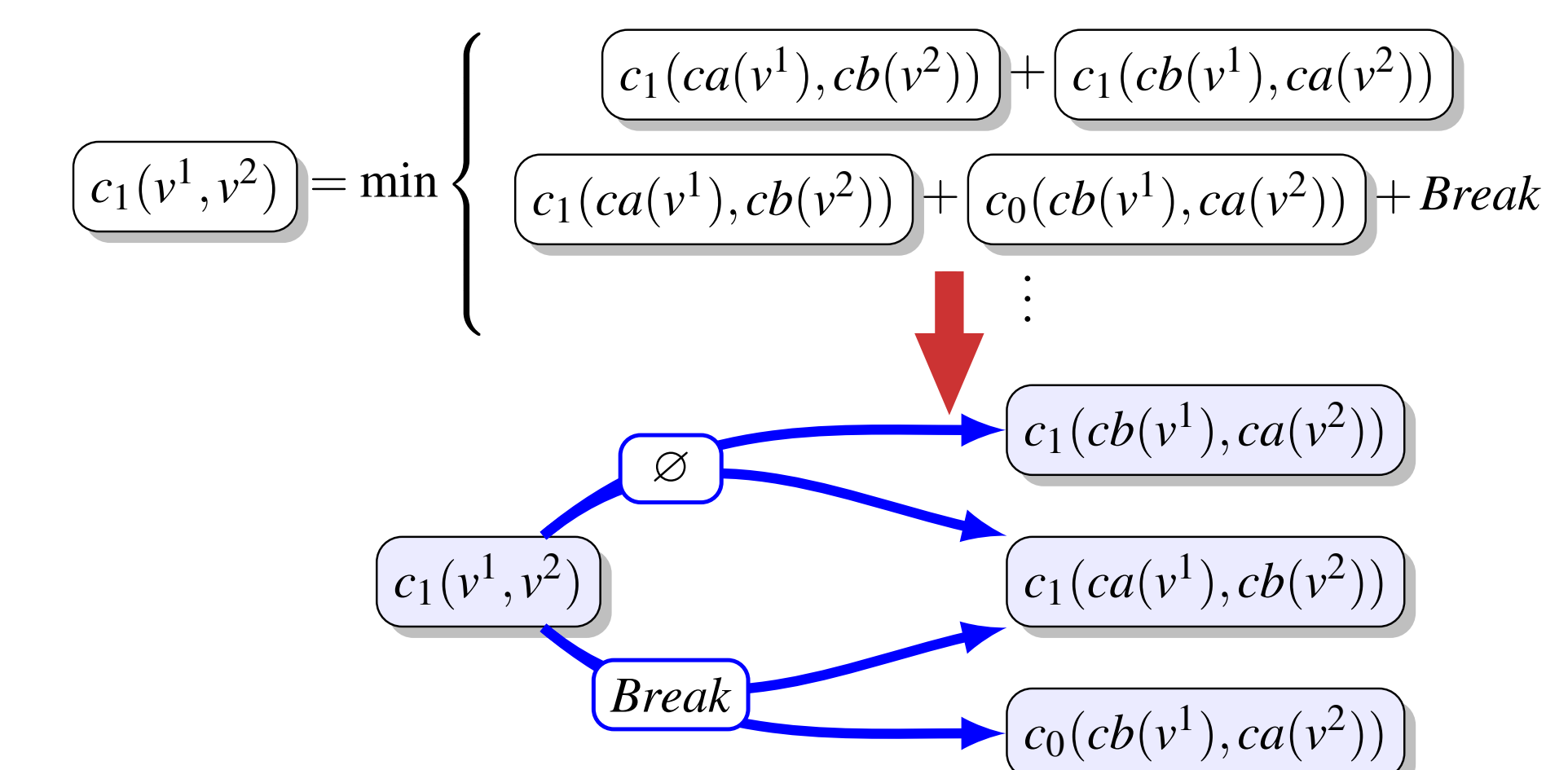
### Impact of pseudo-temperature $kT$ on predicted adjacencies



## 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.
$\geq 0.3$	118,687	110,180	10,351
$\geq 0.4$	117,639	106,973	8,330
$\geq 0.5$	116,231	103,479	6,677
$\geq 0.6$	114,538	99,720	5,113
$\geq 0.7$	112,564	96,039	4,092
$\geq 0.8$	110,086	91,821	3,276
$\geq 0.9$	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.