

Part III - Case studies

Problems and Soft Constraints

Typical real problems include:

- **Hard** constraints (physical constraints)
- **Preferably satisfied** constraints (preferences, eg. deadlines)
- **Uncertain** constraints (errors, weathers...)

All such constraints \Rightarrow unfeasibility

No such constraint \Rightarrow many meaningless solutions

Usual approach: ad-hoc heuristic (but often efficient) handling.

RNA secondary structure prediction

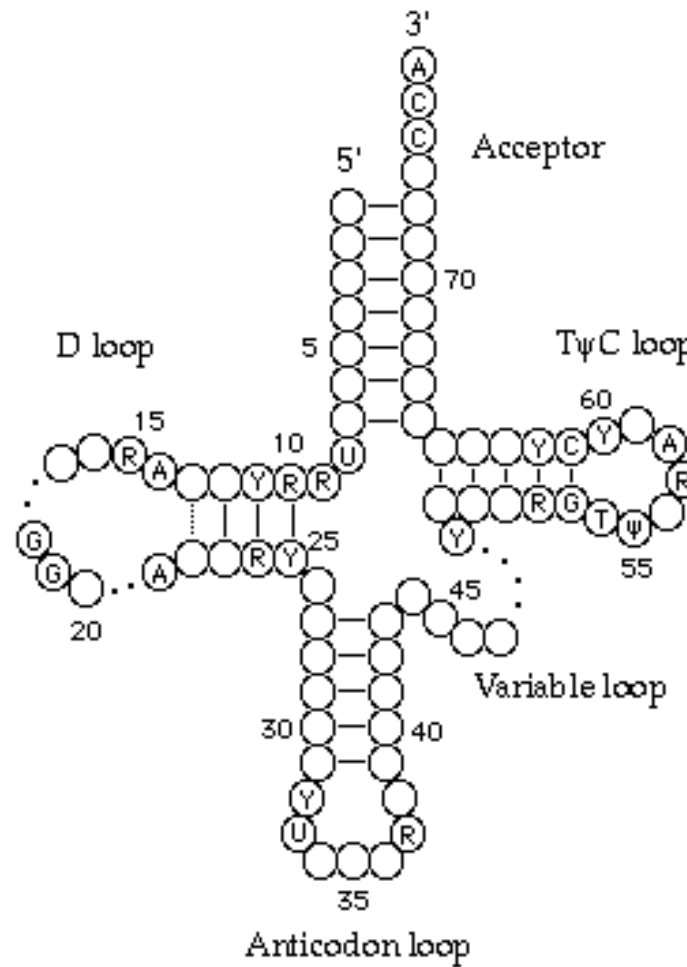
RNA is a single strand molecule composed of A,U,G,C. Functional RNA are **structured** (3d structure). Structure is related to function.

The structure is induced by **base pairing**: Watson-Crick (A-U,G-C) and Wobble (G-U).

Secondary structure: set of all Watson-Crick and Wobble base pairs.

Problem: determine the secondary structure of an RNA molecule from a single sequence.

A transfer RNA



RNA secondary structure prediction

Other sources of information:

- **thermodynamics.**

Zuker's algorithm: DP algorithm that finds an optimal secondary structure. Pb: thermodynamics is not precise enough.

McCaskill matrix: given an RNA sequence, computes the probability that a given base is paired to another given base (based on thermodynamics).

- **biological knowledge:** one may know/test that a given base is paired or not, is paired to a given other base.

A CSP model (C. Gaspin, 1995)

For a sequence of length $n = (b_1, \dots, b_n)$:

- one **variable** x_i per base
- **domains**: $d_i = \{1, \dots, n\}$. $b_i = i$ means b_i unpaired.
- **constraints**: Watson-Crick/Wobble only.

$$x_i = j \Leftrightarrow x_j = i$$

No pseudo-knot: for $i < j, k < l$, (j, l) is forbidden for x_i, x_k if $i < k < j < l$ or $k < i < l < j$.

Many other constraints...

Experimental knowledge: a base is unpaired, is paired, with a specific base...

Usually too many solutions. Need more information.

Exploiting thermodynamics

McCaskill matrix $P(i, j)$ probability that b_i is paired with b_j .

For algorithmic reasons (**satisfaction** problem):

- fix a threshold p .
- forbid all pairs $b_i = j$ such that $P(i, j) < p$.

Poor handling of probabilities, Choice of p ...

Enforce arc consistency, then solve as a Max-CSP with unary soft constraints (maximize the number of paired bases) using a maximal clique tree-search algorithm.

Satellite scheduling

- **var/dom**: a set S of pictures. Each picture can be taken at different time points.
- **binary constraints**: only three instruments are available and each picture requires some instruments with possible transition times for reconfiguration.
- **ternary constraints**: the data bus bandwidth is limited.
- **global constraint**: the local memory is limited.

Overconstrained: instantiate a subset of S which maximizes the sum of the weights of the pictures (and satisfies all constraints).

RDS (no global constraint)

val = # of pictures, * = optimality proof (within 30')

pb	n	e	FC	(cpu “)	RDS	(cpu “)
404	100	610	48	1800	49*	0.5
408	199	2032	3076	1800	3082*	14
412	300	4048	15078	1800	16102*	29
414	364	9744	21096	1800	22120*	86
503	105	403	8095	1800	9096*	2.5
505	240	2002	12088	1800	13100*	15
507	311	5421	12110	1800	15137*	55
509	348	8276	19104	1800	19125*	106

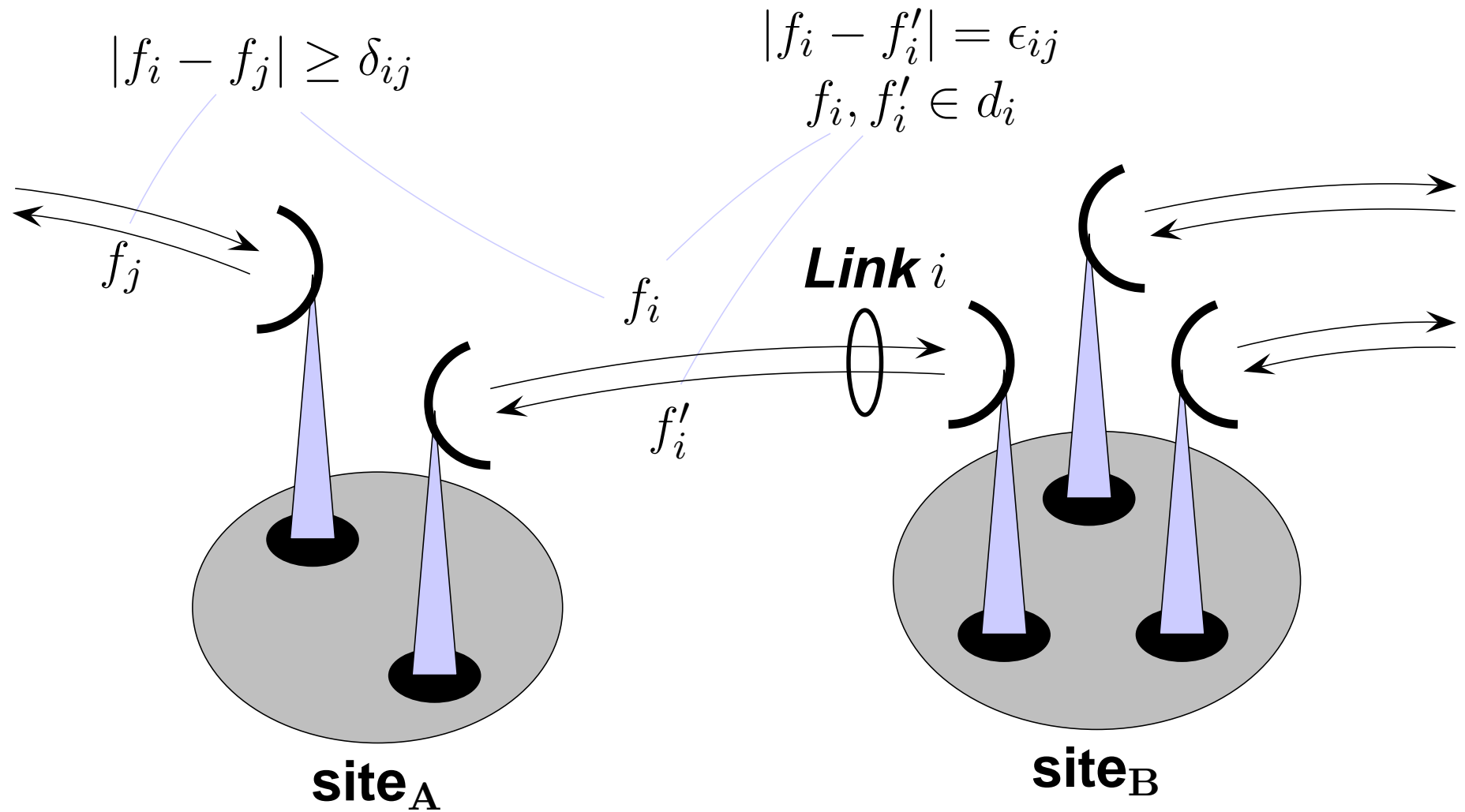
Satellite scheduling

Beyond RDS, these instances have been tackled by several approaches:

- **local search**: taboo search (M. Vasquez).
- **LP + column generation**: to provide global lower bounds
- **0/1 LP**: as a multidimensional Knapsack (MKP01), to provide global lower bounds (M. Vasquez).

The MKP01 model is solved to **optimality** by CPLEX 7.0 (with float tolerance problems) on most instances (including the global constraint). Cpu-time may reach $5 \cdot 10^4$ sec. on a modern Pentium machine.

Frequency assignment (CELAR)



- minimize the **maximum frequency** used (possibilistic CSP)
- minimize the **number of frequencies** used (optimisation/global soft constraint)
- minimize the **weighted constraint violation** (Max-CSP)

Several instances available: from 200 to 916 vars, from 1200 to more than 5000 binary constraints. Domains usually have more than 30 values.

FAP: results

Tackled in the CALMA project (1994) and then by individuals. Most problems solved to optimality...

Max-CSP problems are very hard (even for local search). No proof of optimality after CALMA.

- **1997**: graph decomposition + RDS proved optimality of Celar06 ($5 \cdot 10^6$ sec., Sparc 5). PFC-MRDAC ($2.6 \cdot 10^5$ sec, Sparc 2).
- **1999**: preprocessing (\approx soft AC) + dynamic programming (\approx bucket elimination) + a lot more: solves most instances to optimality (Arie Koster, PhD thesis).

Conclusion

Soft constraint technology is still in its infancy.

There is much to do:

- use existing frameworks to build **more realistic models** for existing problems, that may exploit recent algorithms (eg. bucket elimination, PFC-MRDAC...)
- improve **algorithms** for solving existing models in existing frameworks:
 - stronger preprocessing
 - global soft constraints
 - combination of bucket elimination, branching and local consistency or other preprocessing.

Existing implementations (we know...)

- **Con'Flex**: Conjunctive fuzzy CSP system with integer, symbolic and numerical constraints
(www.inra.fr/bia/T/conflex).
- **clp(FD,S)**: semi-ring CLP.
(pauillac.inria.fr/~georget/clp_fds/clp_fds.html).
- **LVCSP**: Common-Lisp library for Valued CSP with an emphasis on strictly monotonic operators
(<ftp.cert.fr/pub/lemaitre/LVCSP>).
- **Choco**: a claire library for CSP. Existing layers above Choco implements Weighted Max-CSP algorithms (part of LVCSP, (www.choco-constraints.net)).

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