# Algorithms and Bioinformatics

## Part II — Comparative Genomics

### II.3 — More on FPT Algorithms
### (some of them in Bioinformatics)

Laurent Bulteau

# Dynamic Programming

- Not specific to FPT, but often used in this context
- aka. "table-filling"
- Enumerate polynomialy many subproblems, solve each one by combining results from other (sub-)subproblems
- Other point of view: write a simple recursive program, use a cache to store and re-use intermediate results

## Maximum Agreement Subtree

**Input:** Two trees $T_1$, $T_2$, with leaf labels

**Output:** Subtrees $T'_1$ of $T_1$ and $T'_2$ of $T_2$, with max. number of leaves, such that $T'_1 = T'_2$ up to degree-2 vertex contraction.

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12. Give the recursive relation in the Dynamic Programming algorithm of Maximum Agreement Subtrees.

# Color Coding

- General use: find size-$k$ subsets with specific properties in a large set of elements
- Randomized technique, can be de-randomized
- Best-known use case: find a length-$k$ simple path in a graph

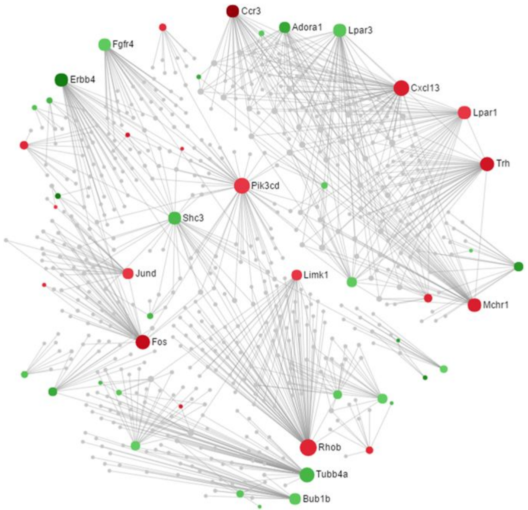
### Minimum Weight Path

**Input:** A (directed) graph $G = (V, E)$, edge weights $w : E \to \mathbb{N}$, integer $k$
**Param.:** $k$
**Output:** A length-$k$ simple path of $G$ with maximum weight

- NP-hard...
- Motivation: find *signaling pathways* in protein-protein interaction networks

# Color Coding

## PPI Network




A Protein-Protein Interaction Network. [1]

[1] credits: Fan et al., Nature Scientific Reports 8:351, 2018

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## Principle

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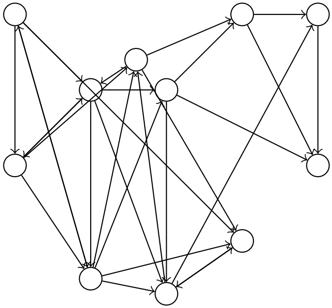
- Plus: you know in which order the colors are visited!
- Exactly how we get this information we shall see later: for now just assume we know this.

# Color Coding

## With color order



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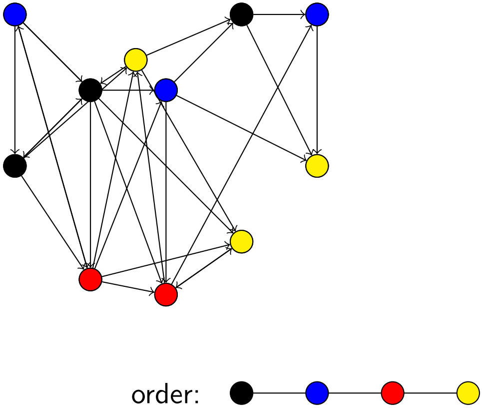

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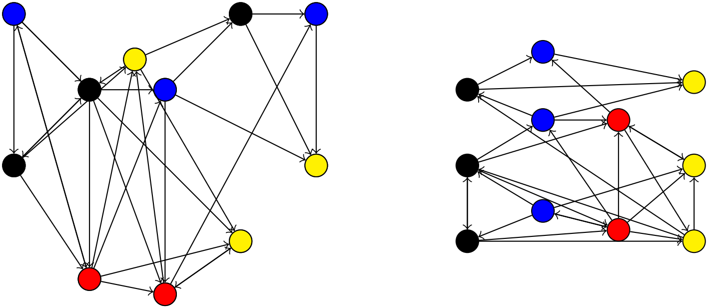
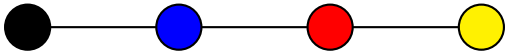


order: 

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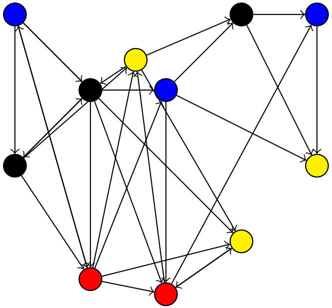

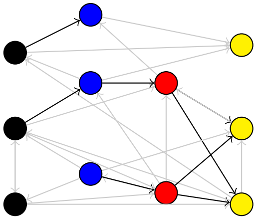

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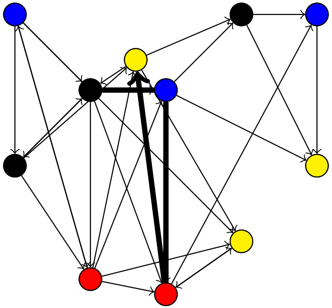

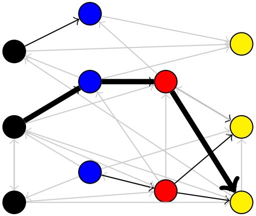

# Color Coding

## Dynamic Programming with color order

### Dynamic programming table

For each $u \in V$, what is the maximum weight of a color-consistent path up to $u$? $\rightarrow W[u]$ ($n$ entries)

### Filling the table

If $u$ has color-rank $i$,

$$W[u] = \max_{v \text{ of rank } i-1} (W[v] + w(v \rightarrow u))$$

Border cases:

$$W[u] = 0 \text{ if } u \text{ has rank } 0$$

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## Dynamic Programming without color order

### Dynamic programming table

For each $u \in V$, and each subset $X \subseteq [k]$ of colors, what is the maximum weight of a path ending in $u$ using once each color in $X$? $\rightarrow W'[u, X]$ ($2^k n$ entries)

### Filling the table

$$W'[u, X] = \max_v W'[v, X \backslash] + w(v \rightarrow u)$$

Border cases:

$$W'[u, X] = 0 \text{ if } X = \{col(u)\}$$

Running time: $O(2^k n^2))$

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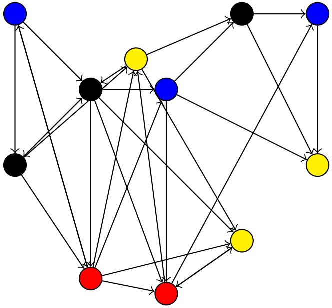

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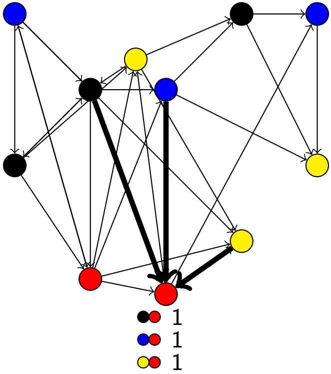

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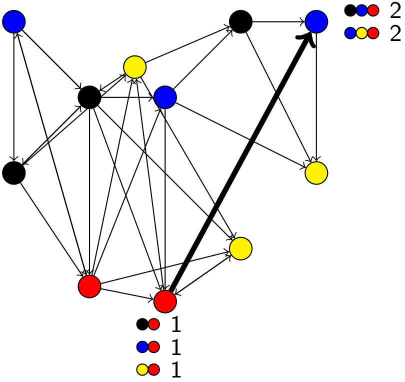

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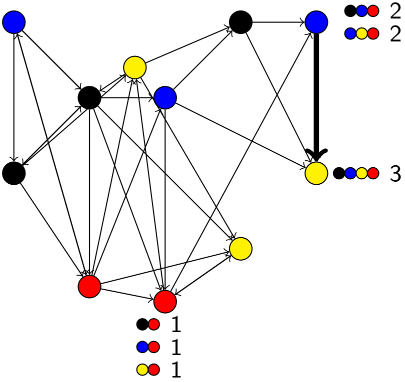

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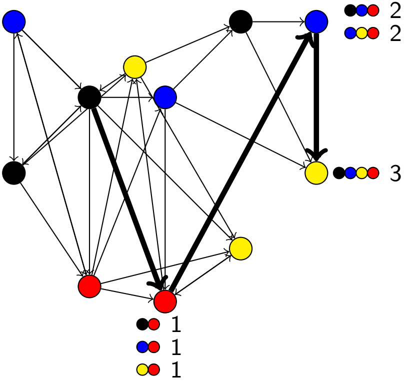

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- Draw $C.e^k$ random colorings of the graph.
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Anyway: Two algorithms in one; let the user choose.

# Practice

13. Give an FPT algorithm based on color-coding for the problem below. Bonus: show that it is NP-complete.

### CHEAP SUBTREE

**Input:** A complete binary tree $T$ with a set $L$ of leaves,
a graph $G = (V, E)$,
a cost function $c : V \times L \to \mathbb{N}$

**Param.:** $k = |L|$

**Output:** A subset $V' \subseteq V$ such that:
- $G[V']$ is isomorphic to $T$,
- the total cost of the mapping betwen $V$ and $L$ is minimal.

14. Same question:

### POLYCHROME MATCHING

**Input:** A graph $G$ with an $r$-edge coloring

**Param.:** $r$

**Output:** A maximum-size set of independent edges of $G$ with pairwise-distinct colors.

# Practice

15. Same question:

DISJOINT $r$-SUBSETS

**Input:** Size-$r$ subsets $X_1, \ldots X_m$ of $[n]$, integer $k$
**Param.:** $k + r$
**Output:** $k$ pairwise disjoint subsets $X_{i_1}, \ldots X_{i_k}$

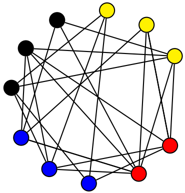
# Color Coding

## Final remarks

- Color coding cannot help W[1]-hard problems.

**MULTI-COLOR CLIQUE**

**Input:** A $k$-partite graph $G = (V, E)$, with $V = V_1 \uplus \cdots \uplus V_k$
**Param.:** $k$
**Output:** A size-$k$ clique $K$, such that $|K \cap V_i| = 1$ for all $i$.



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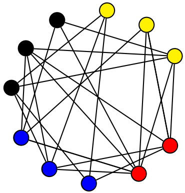

- Use more colors in randomized algorithms: optimal close to $1.3k$ for Minimum Weight Path (fewer trials, but longer dynamic programming)

# Iterative Compression

## Principle

- Other "heavy" approach, mostly for graphs
- Idea:
  - Start with an empty graph and an empty solution
  - Add vertices (or edges) one by one
  - Each time: update the solution
  - If the solution is too large: compress it by one
- Core algorithm: Given a graph, a target solution size of $k$, and a solution of size $k+1$, find a solution of size $k$ (if any).

# Iterative Compression

## Vertex Cover

- Start with empty graph, empty solution ($X$)
- Add vertex $v$ (and connecting edges) to $G$ and to $X$
- If $|X| = k + 1$:
  - Partition $X$ into $K$ ("Keep") and $D$ ("Discard")
  - Create $X' = K \cup N(D)$. If $|X'| \leq k$, continue with next vertex.
  - Try with every $2^{k+1}$ branches: reject if no good $X'$.
- Total running time: $O(2^k n^2)$

# Iterative Compression

## Odd Cycle Transversal

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**Input:** A graph $G = (V, E)$, an integer $k$
**Param.:** $k$
**Output:** A subset $X$ of $G$ such that $G[V \setminus X]$ is bipartite.

- Start with empty graph, empty solution ($X$)
- Add vertex $v$ (and connecting edges) to $G$ and to $X$
- If $|X| = k + 1$:
  - Partition $X$ into 3 parts $(K, L, R)$
  - Create $X'$ using Min-Cut. If $|X'| \leq k$, continue with next vertex.
  - Try with every $3^{k+1}$ branches: reject if no good $X'$.

16. Fill-in the missing steps of the Iterative Compression algorithm of Odd Cycle Transversal.