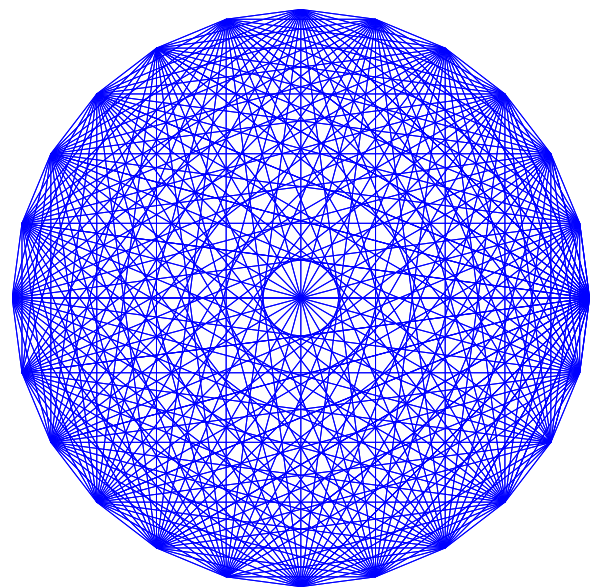


# Tractability of Interpretability via Selection of Group-Sparse Models

A tale of NP-hard problems claimed to be solved by convex relaxations...

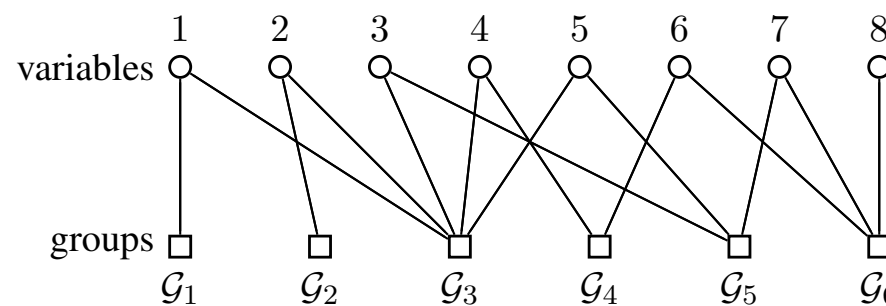
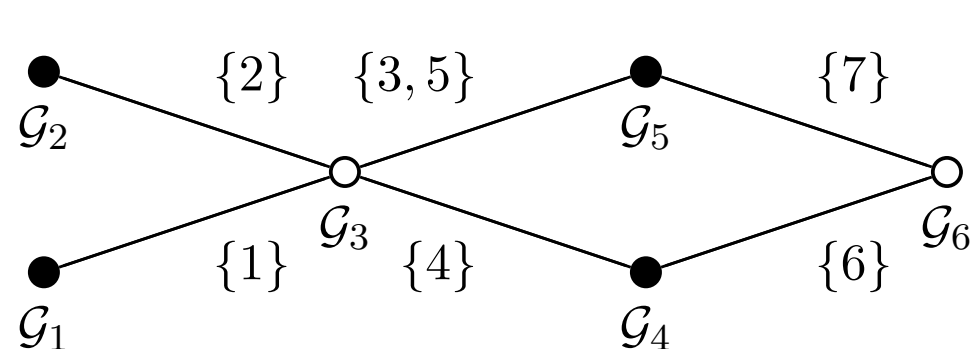


**Luca Baldassarre**

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*Ecole Polytechnique Federale de Lausanne*

[volkan.cevher@epfl.ch](mailto:volkan.cevher@epfl.ch)



joint work with

**Nirav Bhan**

**Volkan Cevher**

**Siddhartha Satpathi**

# A natural generalization of sparsity

$\iota(x)$  **sparse**

0	$x_1$
0	$x_2$
1	$x_3$
0	$x_4$
1	$x_5$
0	$x_6$
1	$x_7$
0	$x_8$

$x =$

**support indicator vector:**

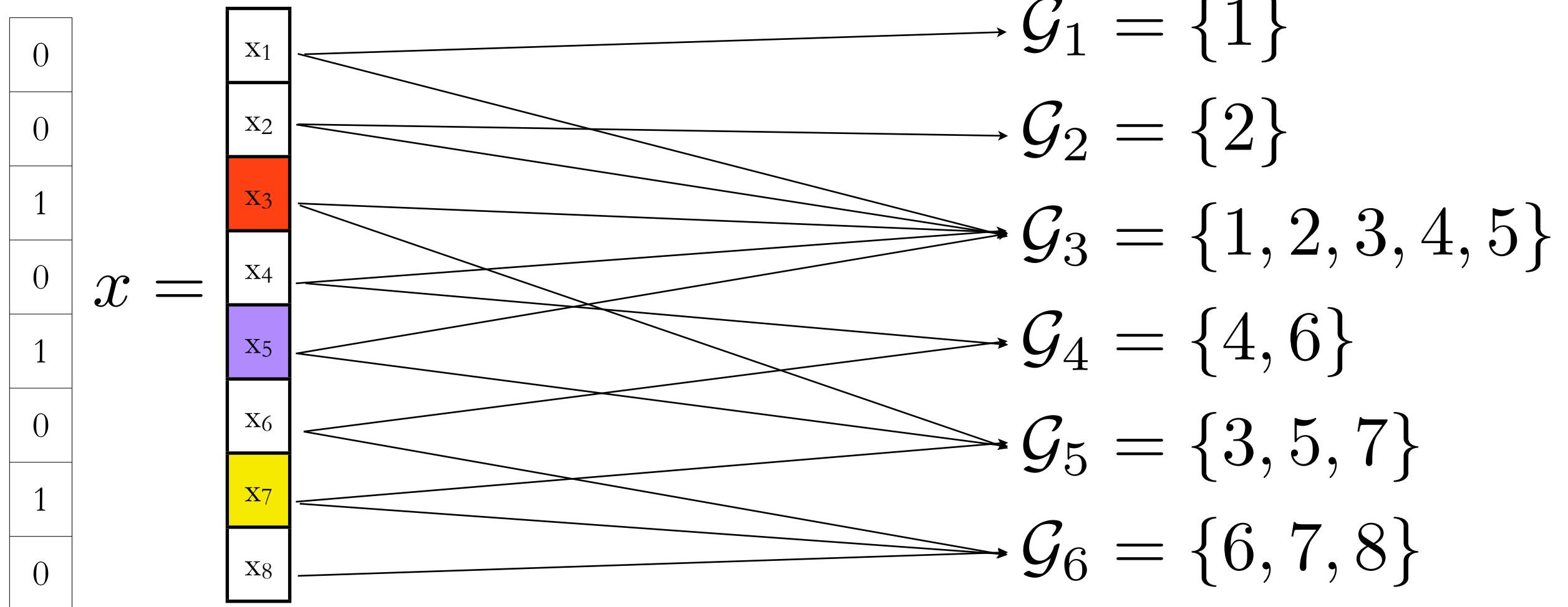
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$$x \in \mathbb{R}^N$$

$$\sum_i \iota(x)_i := K \ll N$$

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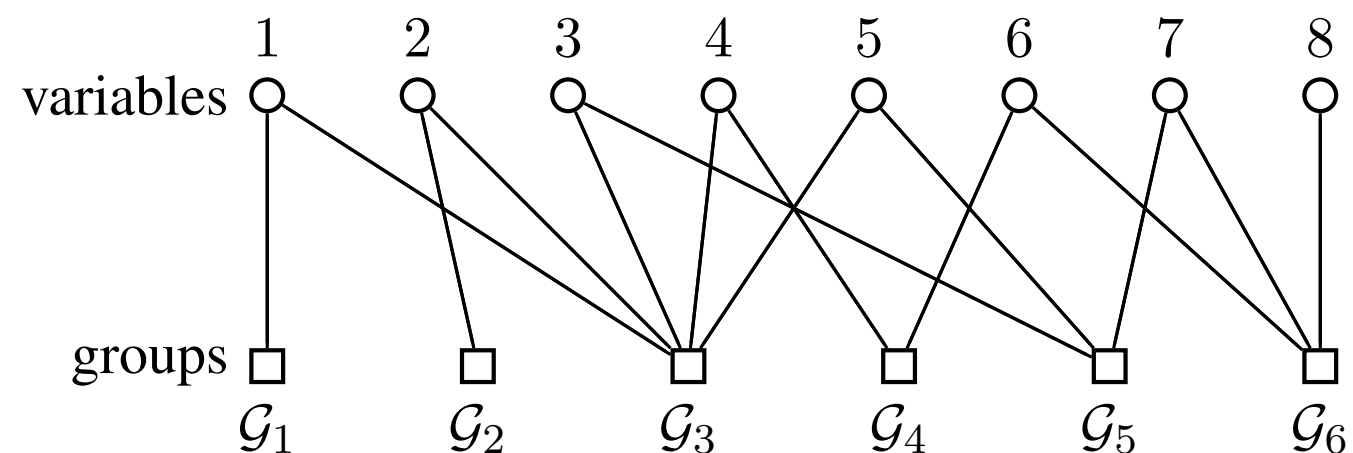
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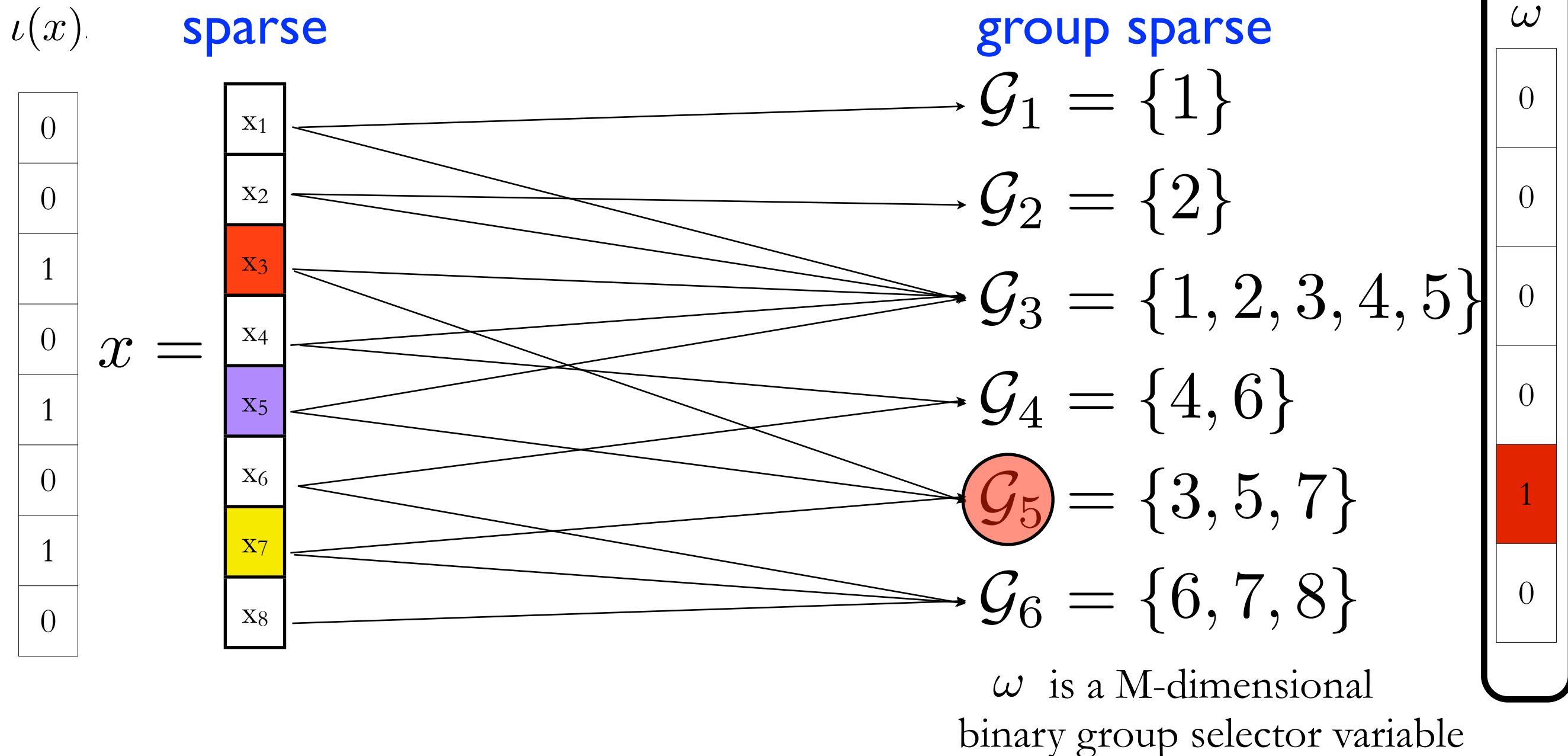
$$x \in \mathbb{R}^N$$

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**Group-structure:** a collection of groups of variables



# A natural generalization of sparsity



## Goal:

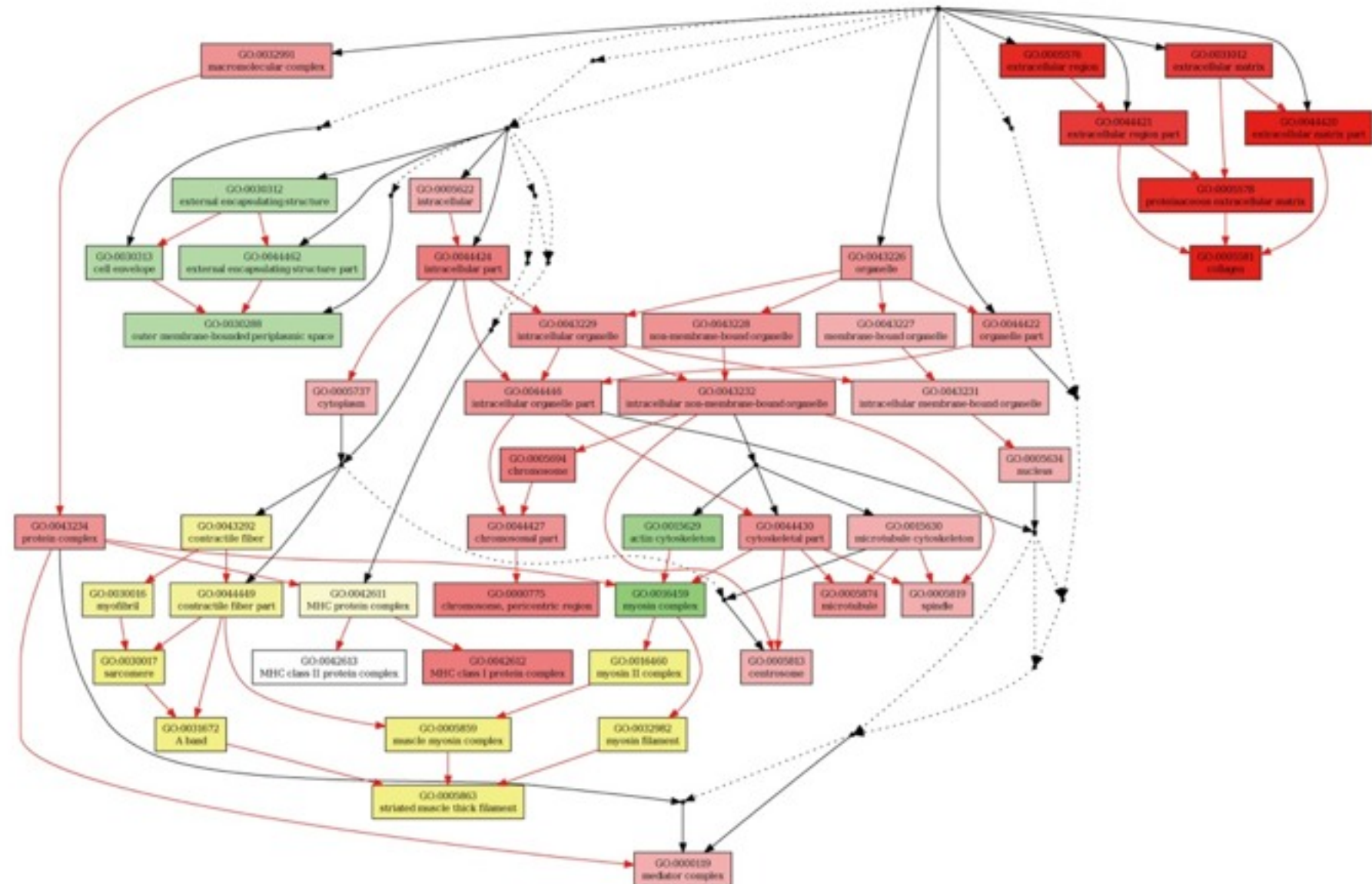
Given a signal  $x \in \mathbb{R}^N$ , we want to find an approximation  $\hat{x}$  whose support is contained in the union of **a few active groups** from the group-structure

# Group-based interpretations

Group models are ubiquitous.

## Examples:

- Genetic Pathways in Microarray data analysis

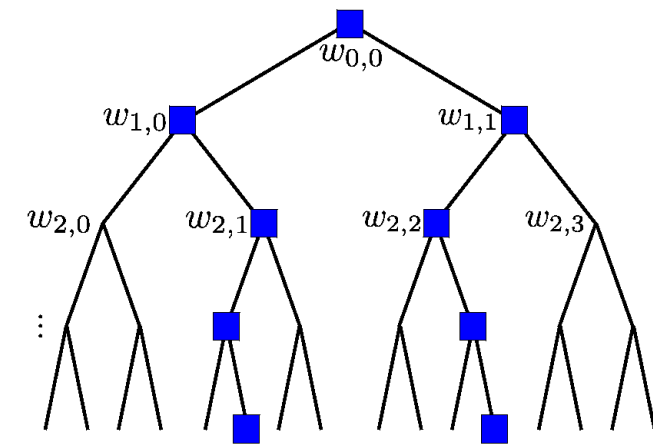
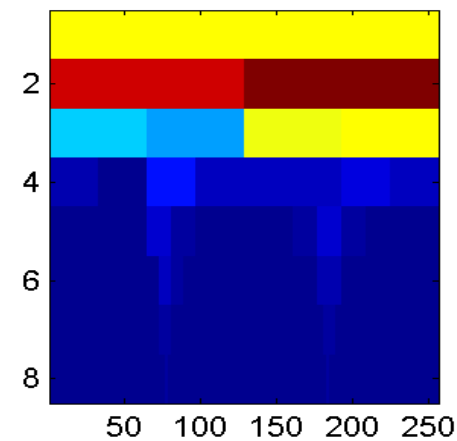
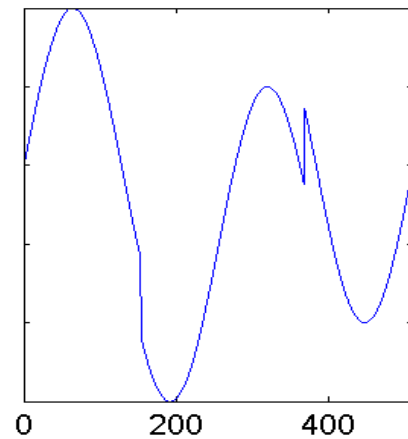
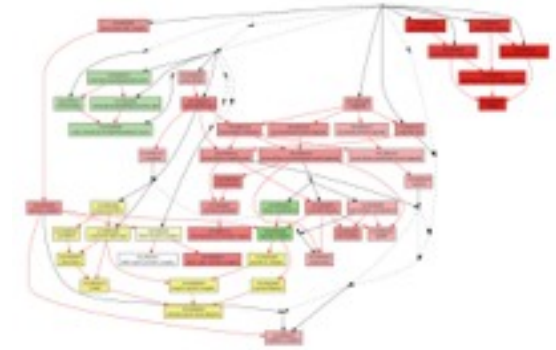


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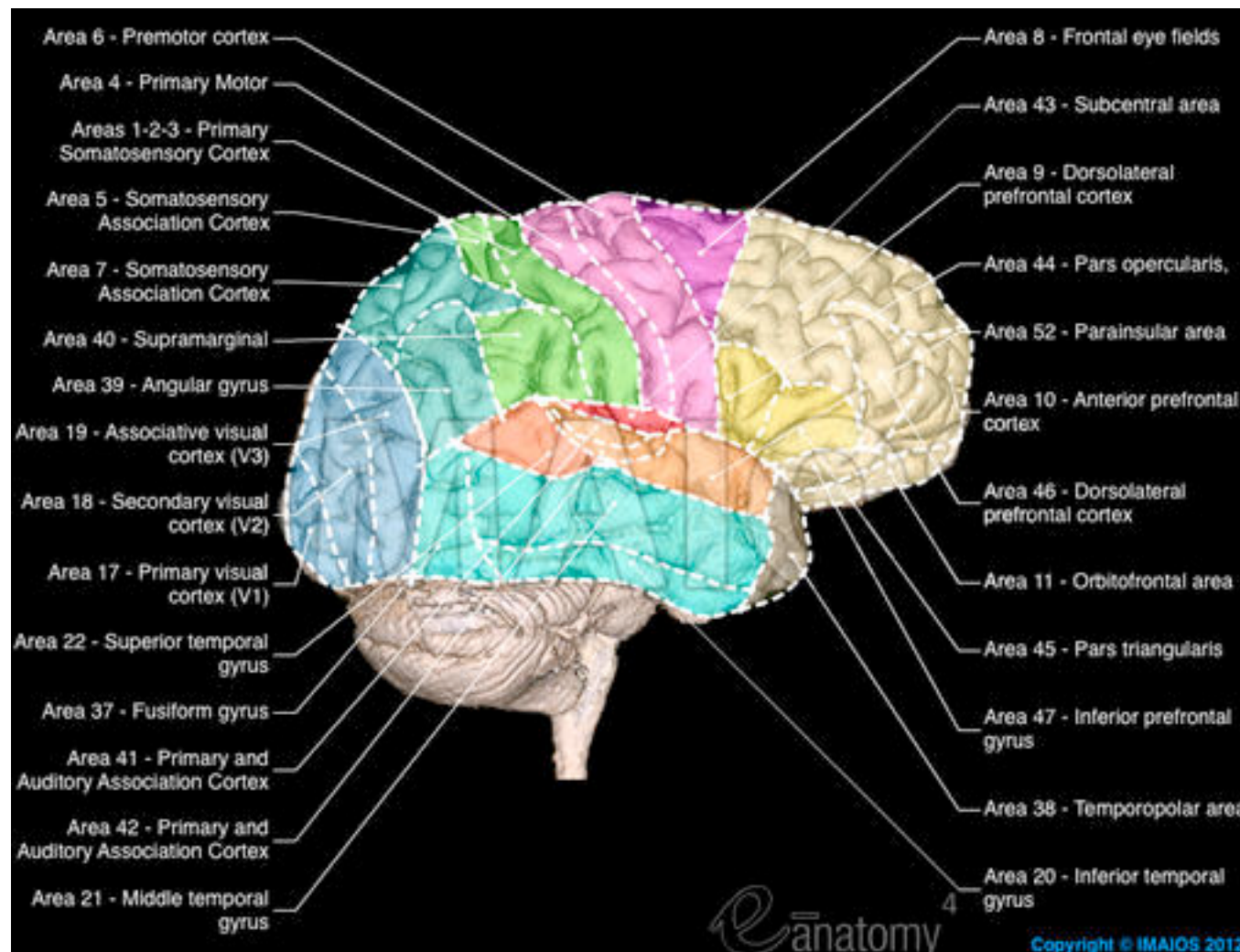
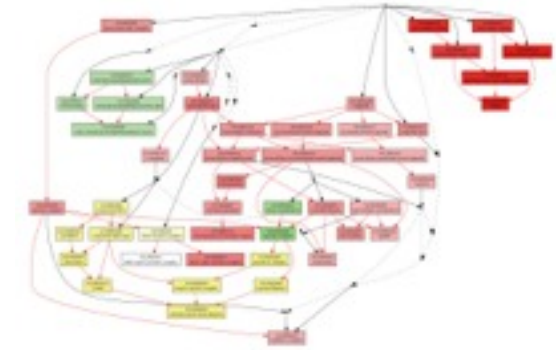
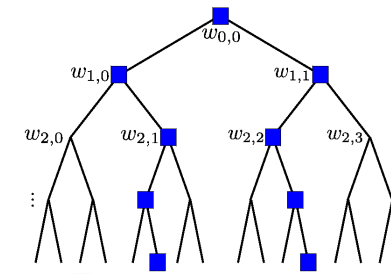
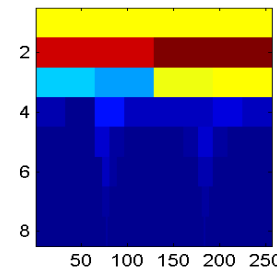
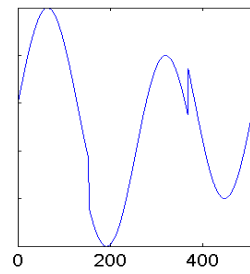




# Group-based interpretations

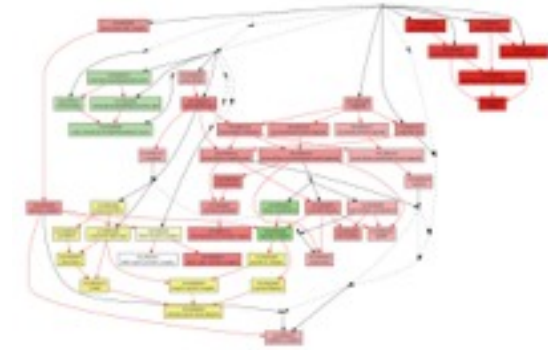
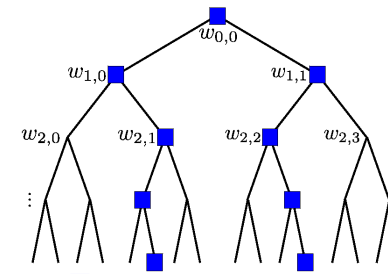
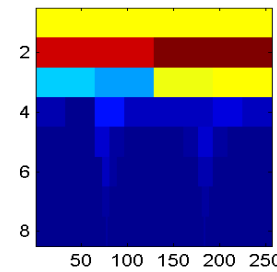
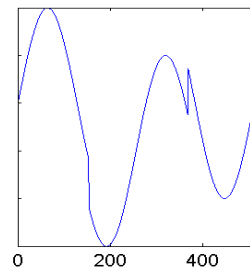
Group models are ubiquitous.  
**Examples:**

- Genetic Pathways in Microarray data analysis
- Wavelet models in image processing
- Brain regions in neuroimaging



# Group-based interpretations

Group models are ubiquitous.  
**Examples:**



- Genetic Pathways in Microarray data analysis
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Group models are motivated by **interpretability**.

- Which are the pathways that lead to correct diagnosis of cancer?
- Which coefficients capture most of the energy in the image?
- Which brain regions decode external stimuli?



# Outline

---

1. Definitions and graph-based representation of group structures.
2. **NP-hardness** of the group-sparse decompositions.
3. Special group-structures that allow tractable decompositions.
4. Relaxations:
  - I. *Discrete relaxations* & **totally unimodular** constraints.
  - II. Convex relaxations & their deficiencies.
5. Generalizations:       group model + sparsity
6. Conclusions

# Definitions I $x \in \mathbb{R}^N$

Ground set:  $\mathcal{N} = \{1, \dots, N\}$

Group structure: a collection of subsets of the ground set

$$\mathfrak{G} = \{\mathcal{G}_1, \dots, \mathcal{G}_M\} \quad \mathcal{G}_j \subseteq \mathcal{N}, \quad \forall j = 1, \dots, M$$

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Binary matrix encoding the group structure

$$\mathbf{A}_{ij}^{\mathfrak{G}} = \begin{cases} 1 & \text{if } i \in \mathcal{G}_j \\ 0 & \text{otherwise} \end{cases}$$

Example:

$$\mathcal{G}_1 = \{1\}$$

$$\mathcal{G}_4 = \{4, 6\}$$

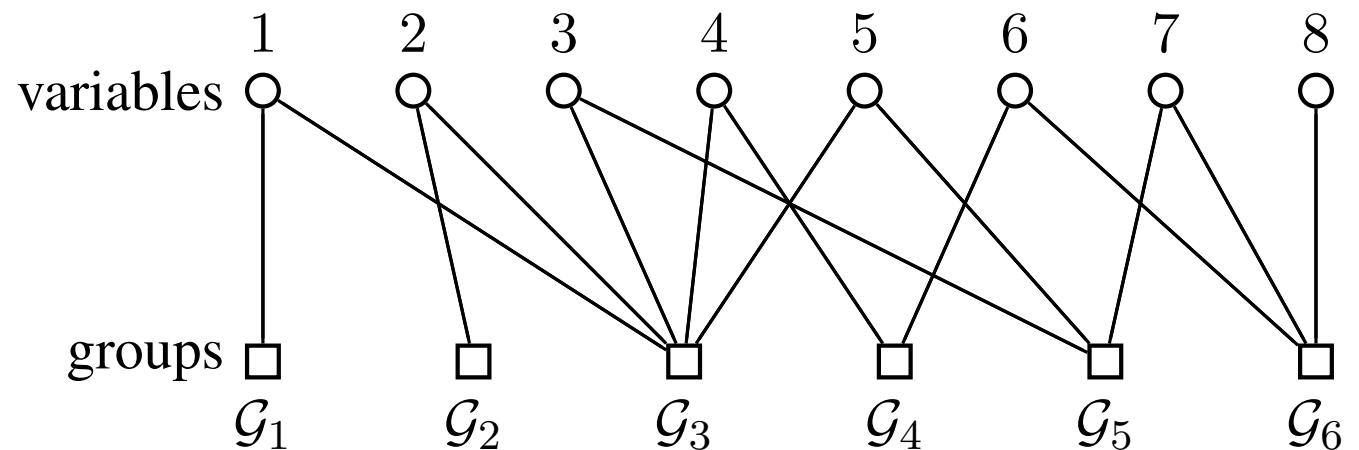
$$\mathcal{G}_2 = \{2\}$$

$$\mathcal{G}_5 = \{3, 5, 7\}$$

$$\mathcal{G}_3 = \{1, 2, 3, 4, 5\}$$

$$\mathcal{G}_6 = \{6, 7, 8\}$$

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & \color{red}{1} & 0 & \color{red}{1} & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$



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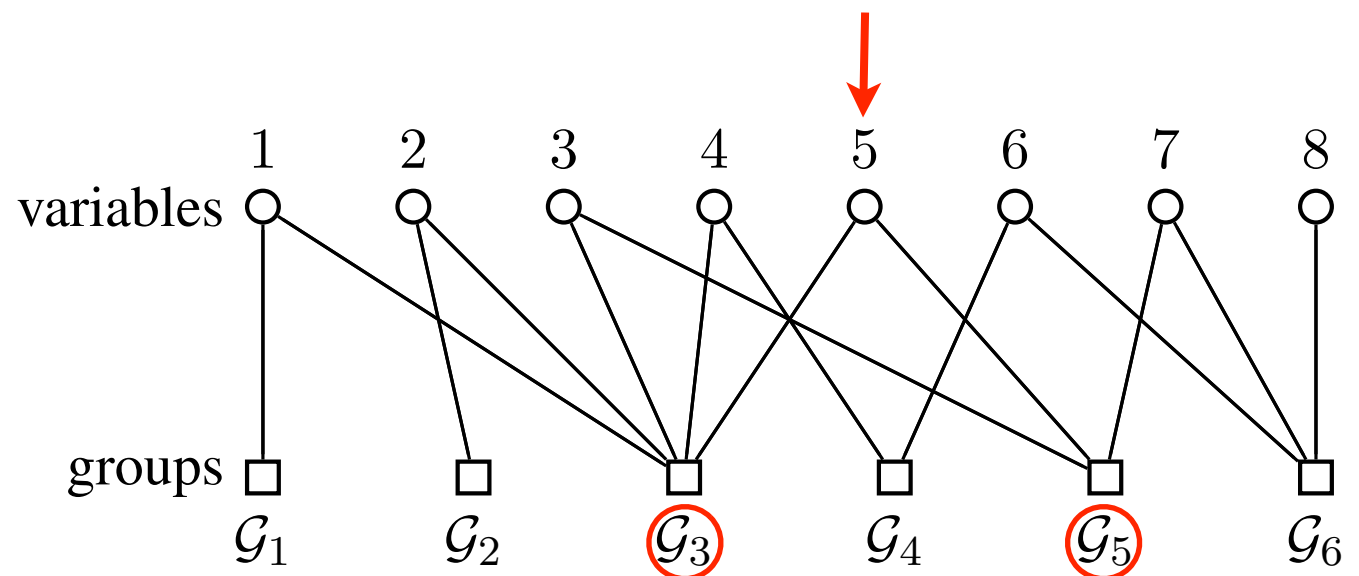
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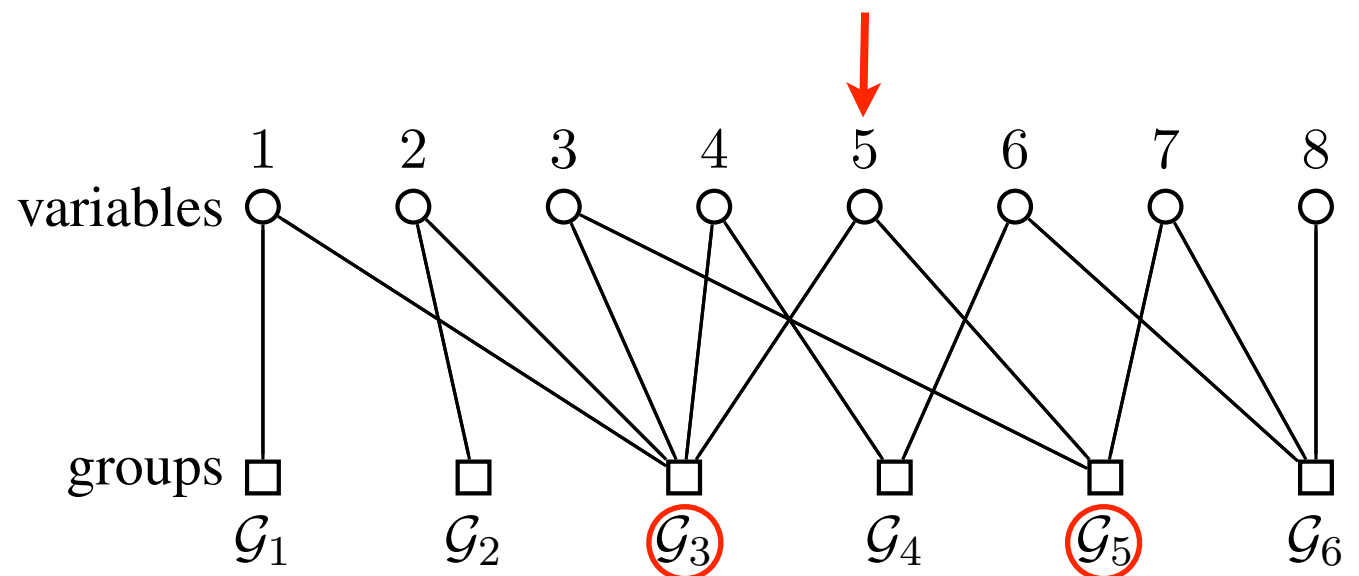
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Usage: group cover

$$\mathbf{A}^{\mathfrak{G}} \omega \geq \iota(x)$$

support indicator vector:

$$\iota(x)_i = \begin{cases} 1 & \text{if } x_i \neq 0 \\ 0 & \text{otherwise} \end{cases}$$

$\omega$  is a M-dimensional binary group selector variable



# Definitions II

Group cover:  $S(x) \subseteq \mathfrak{G}$  s.t.  $\text{supp}(x) \subseteq \bigcup_{\mathcal{G} \in S} \mathcal{G}$

G-group cover:  $S^G(x) \subseteq \mathfrak{G}$  s.t.  $|S| \leq G$ ,  $\text{supp}(x) \subseteq \bigcup_{\mathcal{G} \in S} \mathcal{G}$  Might not exist!

Minimal group-cover:  $\mathcal{M}(x)$  smallest group cover Might not be unique!

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$$\hat{\omega} \in \underset{\omega}{\text{argmin}} \left\{ \sum \omega_j : \mathbf{A}^{\mathfrak{G}} \omega \geq \iota(x) \right\}$$

# Signal approximation with the group- $\ell_0$ “norm”

$$\|x\|_{\mathfrak{G},0} := \min_{\omega \in \mathbb{B}^M} \left\{ \sum_{j=1}^M \omega_j : A^{\mathfrak{G}} \omega \geq \iota(x) \right\}$$

$x$  is **G-group sparse** if  $\|x\|_{\mathfrak{G},0} \leq G$

**G-group sparse approximation** of a signal  $\hat{x} \in \operatorname{argmin}_{z \in \mathbb{R}^N} \{ \|x - z\|_2^2 : \|z\|_{\mathfrak{G},0} \leq G \}$

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$$\hat{x}_I = x_I, \quad \hat{x}_{I^c} = 0$$

$$S^G(\hat{x}) \in \operatorname{argmax}_{\substack{S \subseteq \mathfrak{G} \\ |S| \leq G}} \left\{ \sum_{i \in I} x_i^2 : I = \bigcup_{\mathcal{G} \in S} \mathcal{G} \right\}$$

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**Weighted Maximum Coverage** problem

$$S^G(\hat{x}) = \{ \mathcal{G}_j \in \mathfrak{G} : \omega_j^G = 1 \}$$

$$(\omega^G, y^G) \in \operatorname{argmax}_{\omega \in \mathbb{B}^M, y \in \mathbb{B}^N} \left\{ \sum_{i=1}^N y_i x_i^2 : A^{\mathfrak{G}} \omega \geq y, \sum_{j=1}^M \omega_j \leq G \right\}$$

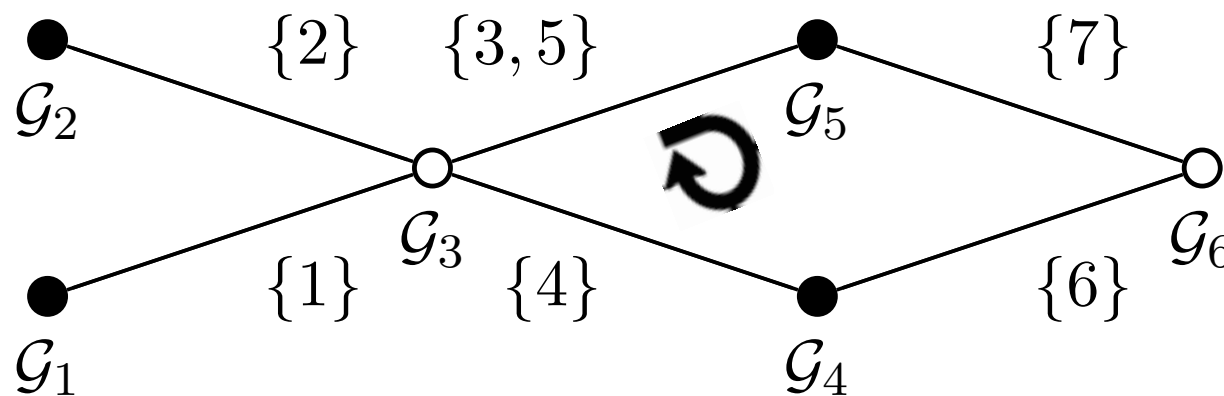
NP-HARD!



# Tractability of Interpretability I

Weighted Maximum Coverage

$$\max_{\omega \in \mathbb{B}^M, y \in \mathbb{B}^N} \left\{ \sum_{i=1}^N y_i x_i^2 : A^{\mathfrak{G}} \omega \geq y, \sum_{j=1}^M \omega_j \leq G \right\}$$



NP-HARD!

# Tractability of Interpretability I

## Weighted Maximum Coverage

$$\max_{\omega \in \mathbb{B}^M, y \in \mathbb{B}^N} \left\{ \sum_{i=1}^N y_i x_i^2 : A^{\mathfrak{G}} \omega \geq y, \sum_{j=1}^M \omega_j \leq G \right\}$$

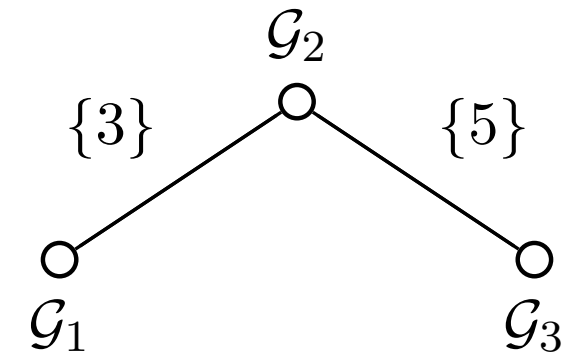
Solve with **Dynamic Programming** for **loopless pairwise overlapping groups**

- Only pairwise overlaps
- No loops

$$\mathcal{G}_1 = \{1, 2, 3\}$$

$$\mathcal{G}_2 = \{3, 4, 5\}$$

$$\mathcal{G}_3 = \{5, 6, 7\}$$



The DP is polynomial-time  $O(GM^2)$

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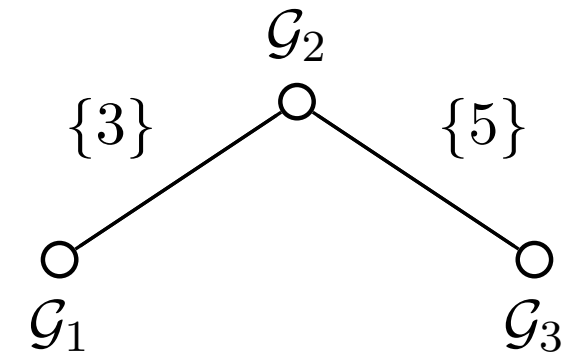
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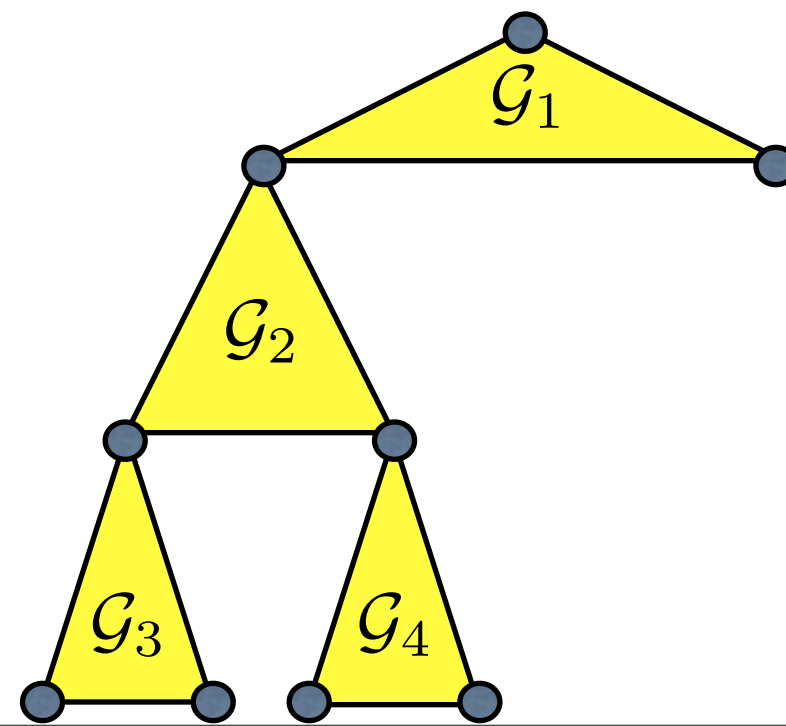
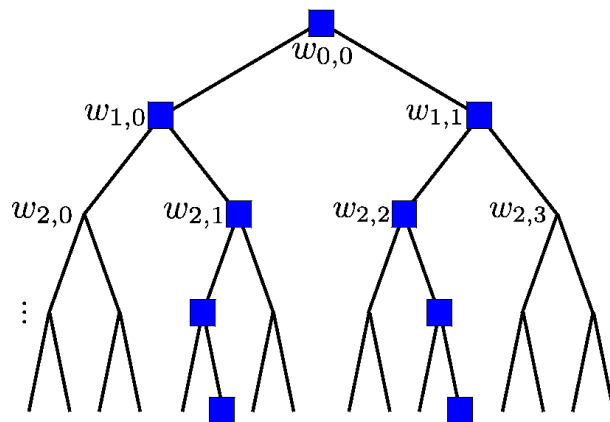
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The DP is polynomial-time  $O(GM^2)$

Example: a new wavelet **family** model  
(where no child is left behind)



# Tractability of Interpretability II

**Weighted Maximum Coverage**

$$\max_{\omega \in \mathbb{B}^M, y \in \mathbb{B}^N} \left\{ \sum_{i=1}^N y_i x_i^2 : A^{\mathfrak{G}} \omega \geq y, \sum_{j=1}^M \omega_j \leq G \right\}$$

**Discrete relaxation:  
linear program**

$$\max_{\omega \in \mathbb{B}^M, y \in \mathbb{B}^N} \left\{ \sum_{i=1}^N y_i x_i^2 - \lambda \sum_{j=1}^M \omega_j : A^{\mathfrak{G}} \omega \geq y \right\}$$

# Tractability of Interpretability II

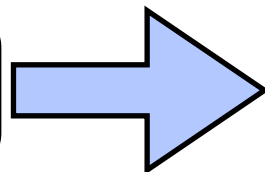
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if  $A^{\mathfrak{G}}$  is Totally Unimodular



Polynomial-time solvers

**\*TU: every square submatrix has determinant  $\pm 1$  or 0**



# Tractability of Interpretability II

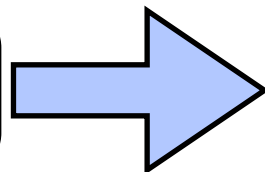
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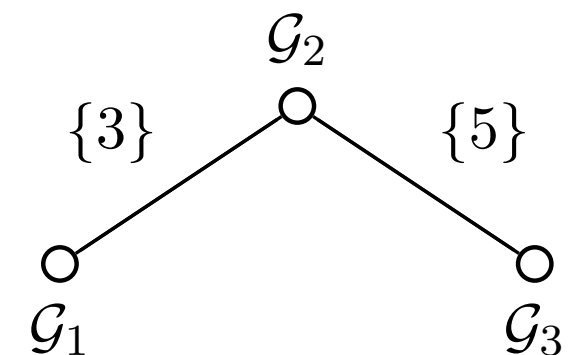
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**\*TU: every square submatrix has determinant  $\pm 1$  or 0**

**Theorem:** Any loopless group model is TU!



# Tractability of Interpretability II

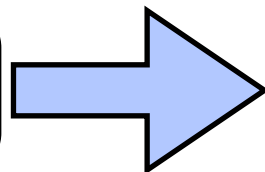
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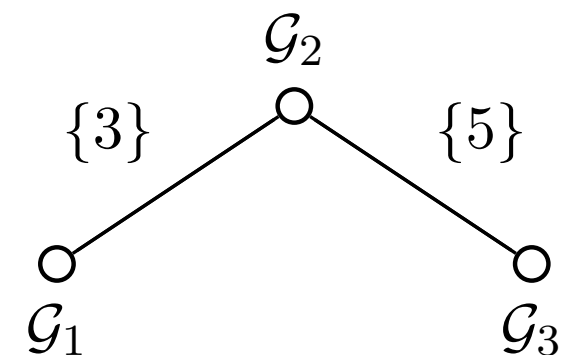
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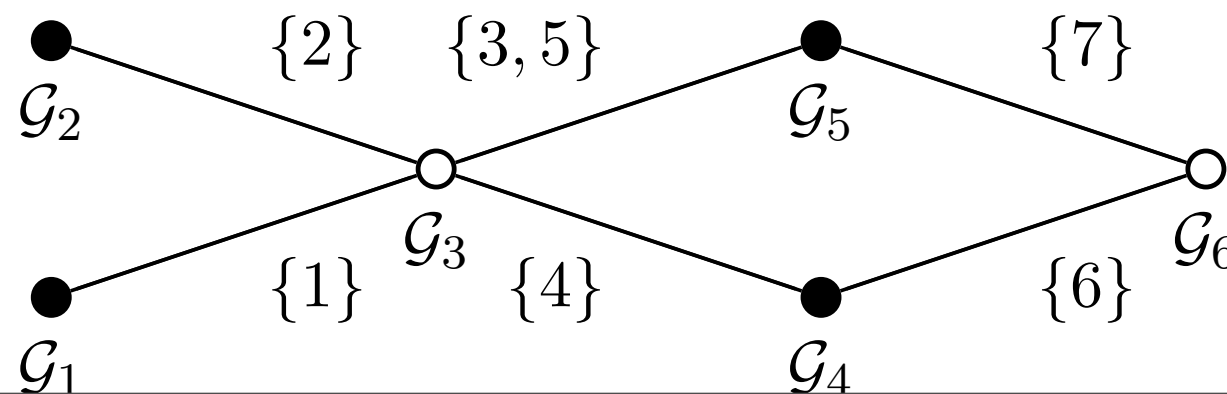
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**Theorem:** Any loopless group model is TU!



**Theorem:** Any bipartite group model is TU!



# Example: Approximation via wavelet trees

**Pareto frontier** of **WMC**:

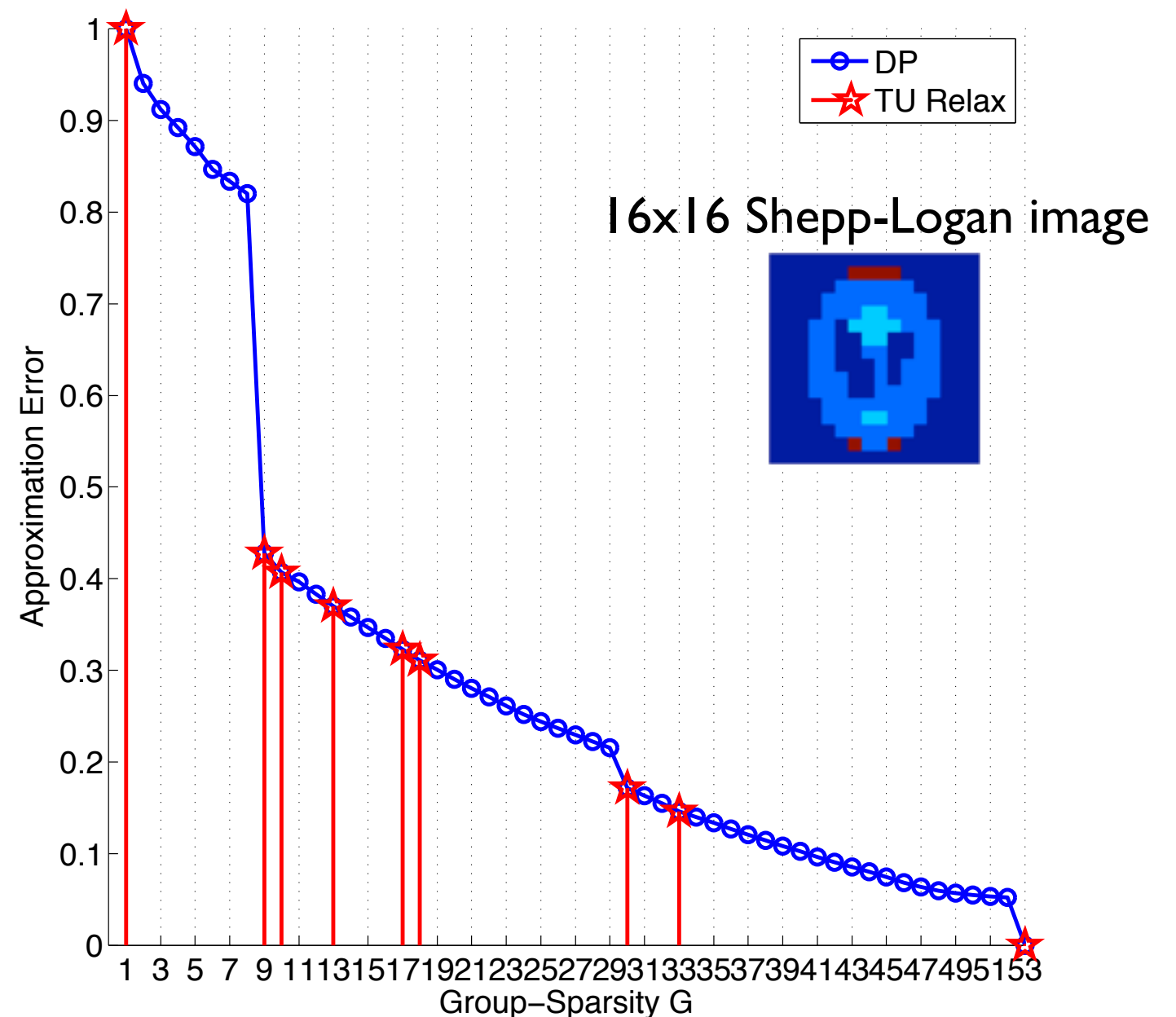
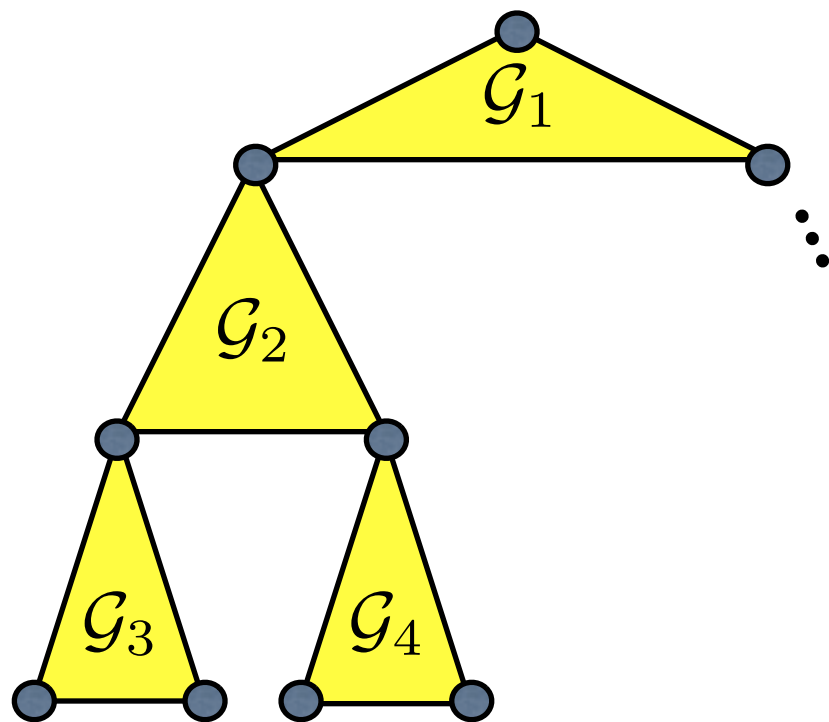
set of optimal values as parameter  $G$  is varied

$$\mathcal{P} = \left\{ G, \sum_i x_i^2 y_i \right\}_{G=1}^M$$

**Theorem:** The discrete relaxation finds only the solutions in the intersection between  $\mathcal{P}$  and the **boundary of the convex hull** of  $\mathcal{P}$

## Methods:

1. Dynamic Programming (DP)
2. Discrete relaxation with TU constraints (TU)



# Existing convex relaxations: the fine print

## Latent Group Lasso Norm for overlapping groups

promotes sparsity at the group level via decompositions [Obozinski et al., 2011]

$$\|x\|_{\mathfrak{G}, \{1,2\}} := \inf_{\substack{\mathbf{v}^1, \dots, \mathbf{v}^M \in \mathbb{R}^N \\ \forall j, \text{supp}(\mathbf{v}^j) = \mathcal{G}_j}} \left\{ \sum_{j=1}^M d_j \|\mathbf{v}^j\|_2 : \sum_{j=1}^M \mathbf{v}^j = x \right\} \quad (*)$$

The group cover  $\check{\mathcal{S}}(x)$  is defined by the non-zero terms in any **optimal decomposition**:

$$\check{\mathcal{S}}(x) := \{ \mathcal{G}_j \in \mathfrak{G} : \exists \mathbf{v} \in \mathcal{V}(x) \text{ s.t. } \mathbf{v}_j \neq 0 \} \quad \mathcal{V}(x) \text{ is the set of solutions of } (*)$$

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**Group-sparse approximation:**  $\hat{x} = \underset{z \in \mathbb{R}^N}{\operatorname{argmin}} \left\{ \|x - z\|_2^2 : \|z\|_{\mathfrak{G},\{1,2\}} \leq \lambda \right\}$

Group-support recovery guarantees are given with respect to  $\check{\mathcal{S}}(x)$  and not to the underlying discrete problem (WMC).



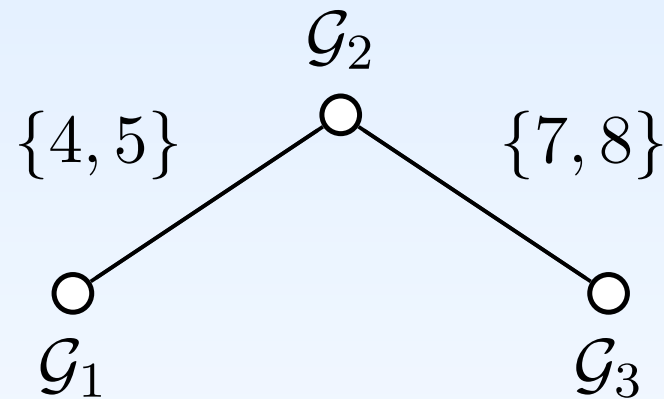
# To be (consistent), or not to be

$$\mathcal{N} = \{1, \dots, 11\}$$

$$\mathcal{G}_1 = \{1, \dots, 5\}$$

$$\mathcal{G}_2 = \{4, \dots, 8\}$$

$$\mathcal{G}_3 = \{7, \dots, 11\}$$



Loopless pairwise  
overlapping groups

$$x = [0 \ 0 \ \overbrace{1 \ 1 \ 1}^{\mathcal{G}_1} \ 0 \ \underbrace{1 \ 1 \ 1}_{\mathcal{G}_2} \ 0 \ 0]^\top$$

Minimal Group Cover:  $\mathcal{M}(x) = \{\mathcal{G}_1, \mathcal{G}_3\}$

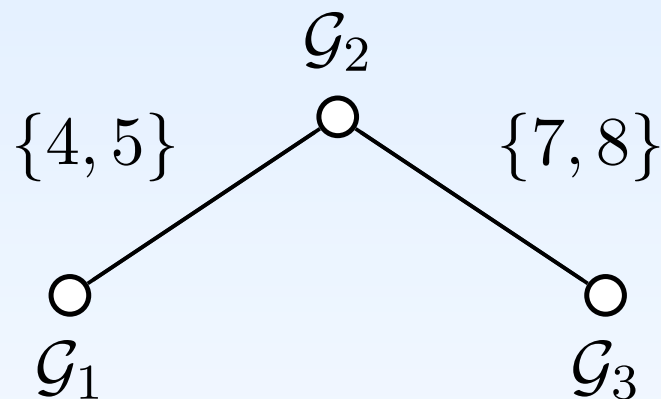
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Minimal Group Cover:  $\mathcal{M}(x) = \{\mathcal{G}_1, \mathcal{G}_3\}$

DP solution:  $S^G(\hat{x}) = \{\mathcal{G}_1, \mathcal{G}_3\}$  for  $G = 2$

Discrete relaxation solution:  $S^\lambda(\hat{x}) = \{\mathcal{G}_1, \mathcal{G}_3\}$  for  $0 < \lambda \leq 2$

Convex relaxation solution:  $\check{S}(x) = \emptyset$  with  $d_j = \text{constant}$

$\check{S}(x) = \{\mathcal{G}_1, \mathcal{G}_3\}$  with  $d_1 = d_3 = 1$  and  $d_2 > \frac{2}{\sqrt{3}}$

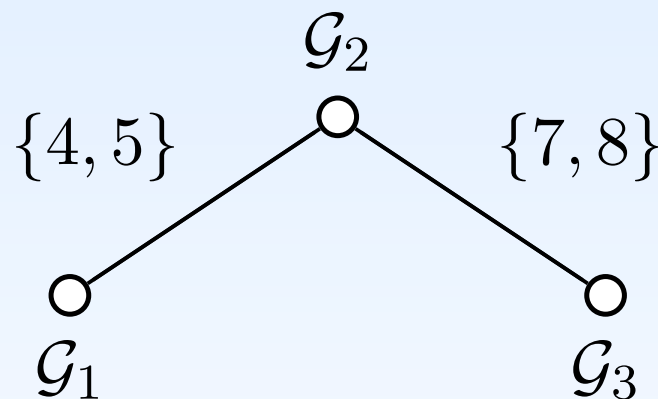
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Need to know **beforehand** which groups are irrelevant!

# Two important generalizations

I. Introduce **sparsity budget**  $K$ .

- Allow **individual elements** within a group to be selected.
- Discrete problem (still **NP-HARD** in general)

## Generalized Weighted Maximum Coverage

$$\begin{array}{ll} \text{maximize} & \sum_{i=1}^N y_i x_i^2 \\ \omega \in \mathbb{B}^M, y \in \mathbb{B}^N & \\ \text{subject to} & A^{\mathfrak{G}} \omega \geq y \\ & \sum_{j=1}^M \omega_j \leq G \\ & \sum_{i=1}^N y_i \leq K \end{array}$$

- **Dynamic Program for loopless:  $O(K^2 M^2 G)$  - *can be improved for regular models***

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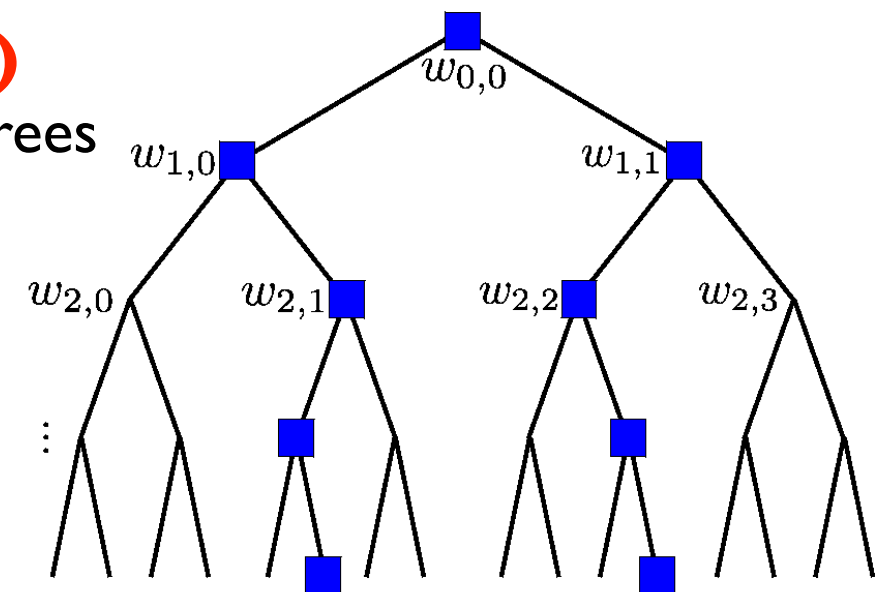
- **Dynamic Program for loopless:  $O(K^2 M^2 G)$  - can be improved for regular models**

2. Introduce **hierarchical constraints** to be encoded in the Generalized WMC.

- **Polynomial-time** Dynamic Program.
- **Hierarchical constraints are TU.**

**$O(KDN)$**   
for regular trees

$$\max_{\omega \in \mathbb{B}^M, y \in \mathbb{B}^N} \left\{ \sum_{i=1}^N y_i x_i^2 - \lambda_G \sum_{j=1}^M \omega_j - \lambda_K \sum_{i=1}^N y_i : A^{\mathfrak{G}} \omega \geq y \right\}$$



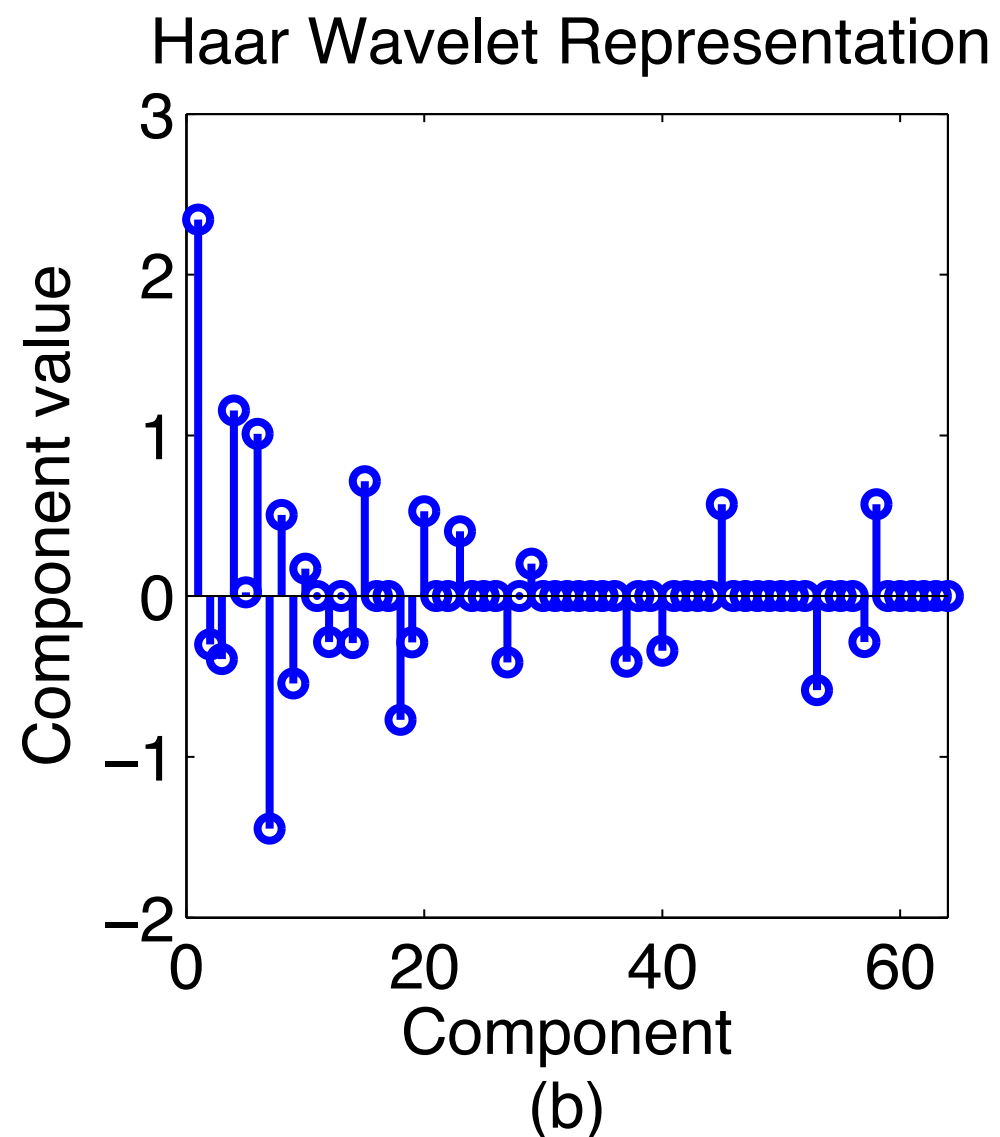
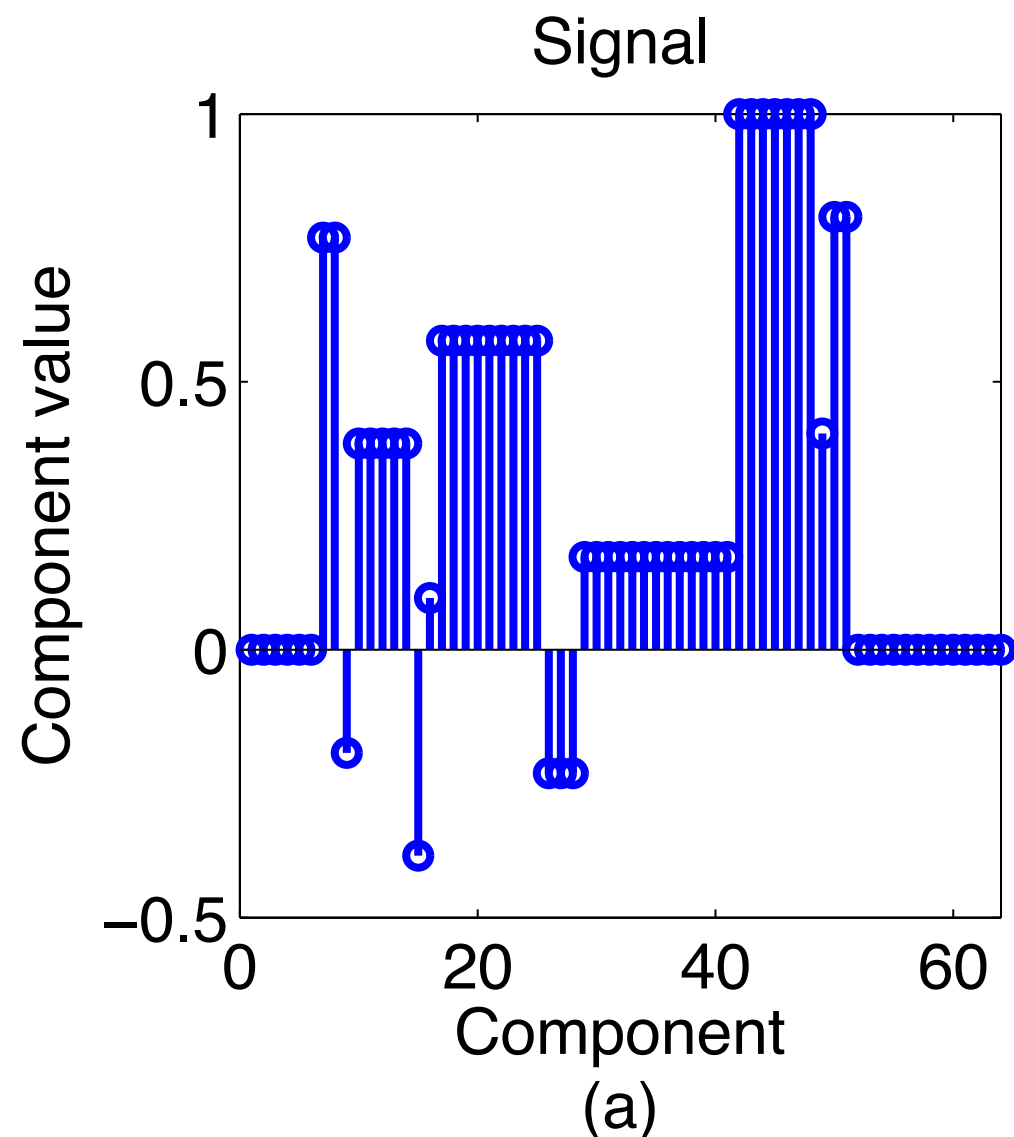
# Example: Approximation via wavelet trees

**Pareto frontier** of **WMC**:

set of optimal values as parameter K is varied

$$\mathcal{P} = \left\{ K, \sum_i x_i^2 y_i \right\}_{K=1}^N$$

- **Block signal** of size  $N = 64$
- Sparse representation in **Haar wavelet** coefficients that satisfy **hierarchical constraints**



# Example: Approximation via wavelet trees

## Pareto frontier of WMC:

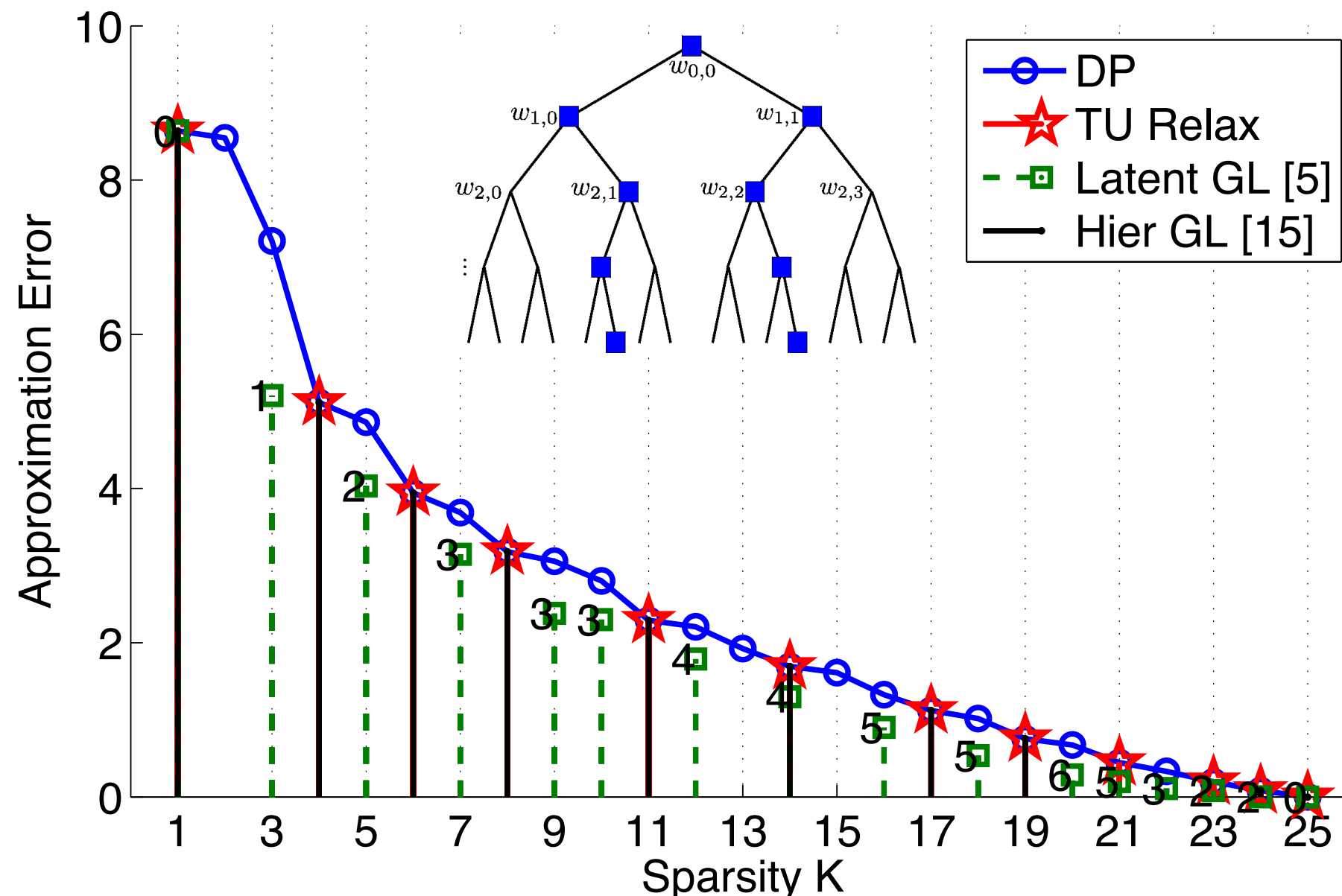
set of optimal values as parameter K is varied

$$\mathcal{P} = \left\{ K, \sum_i x_i^2 y_i \right\}_{K=1}^N$$

- Block signal of size  $N = 64$
- Sparse representation in Haar wavelet coefficients that satisfy hierarchical constraints

## Methods:

1. Dynamic Programming (DP)
2. Discrete relaxation with TU constraints (TU)
3. Latent Group Lasso with groups given as all father-child pairs: **not all constraints are satisfied** [Rao et al., 2012]
4. Hierarchical group lasso [Jenatton et al., 2009]



# Conclusions

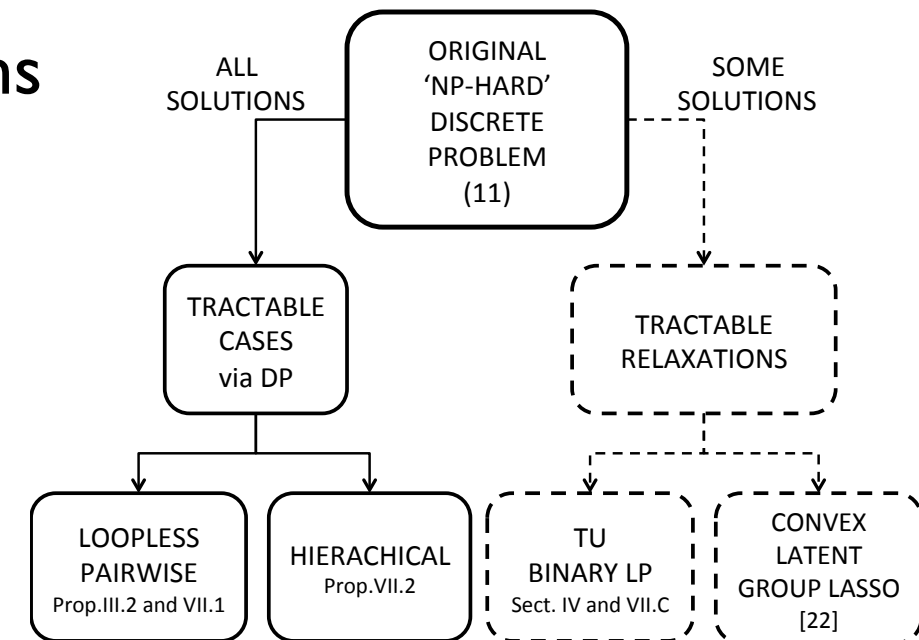
- Group sparse problems  $\Leftrightarrow$  **NP-Hard** in general (GWMC)

- Deceiving consistency results via convex relaxations

- **Tractable group-based interpretations**

- Loopless & hierarchical models with sparsity

- Totally Unimodular group structures



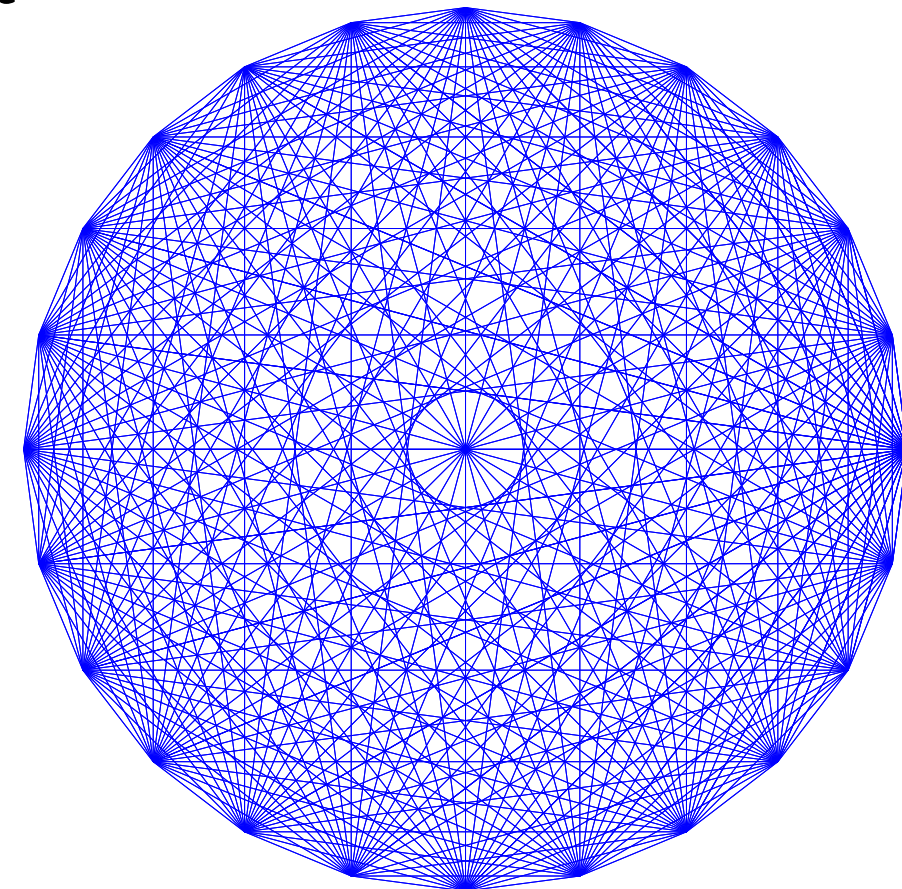
- Pareto Frontier of solutions can be radically different

- Dynamic Programming solutions (full frontier)

- Linear Programming relaxations (convex hull)

- Convex relaxations (sometimes! convex hull)

- ➔ Depressing problem: **breast cancer dataset**  
group-graph of the top 25 pathways from  
the Molecular Signature Database





# References

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- Subramanian, A. et al., *Gene set enrichment analysis: a knowledge-based approach for interpreting genome-wide expression profiles*, PNAS, 2005.
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