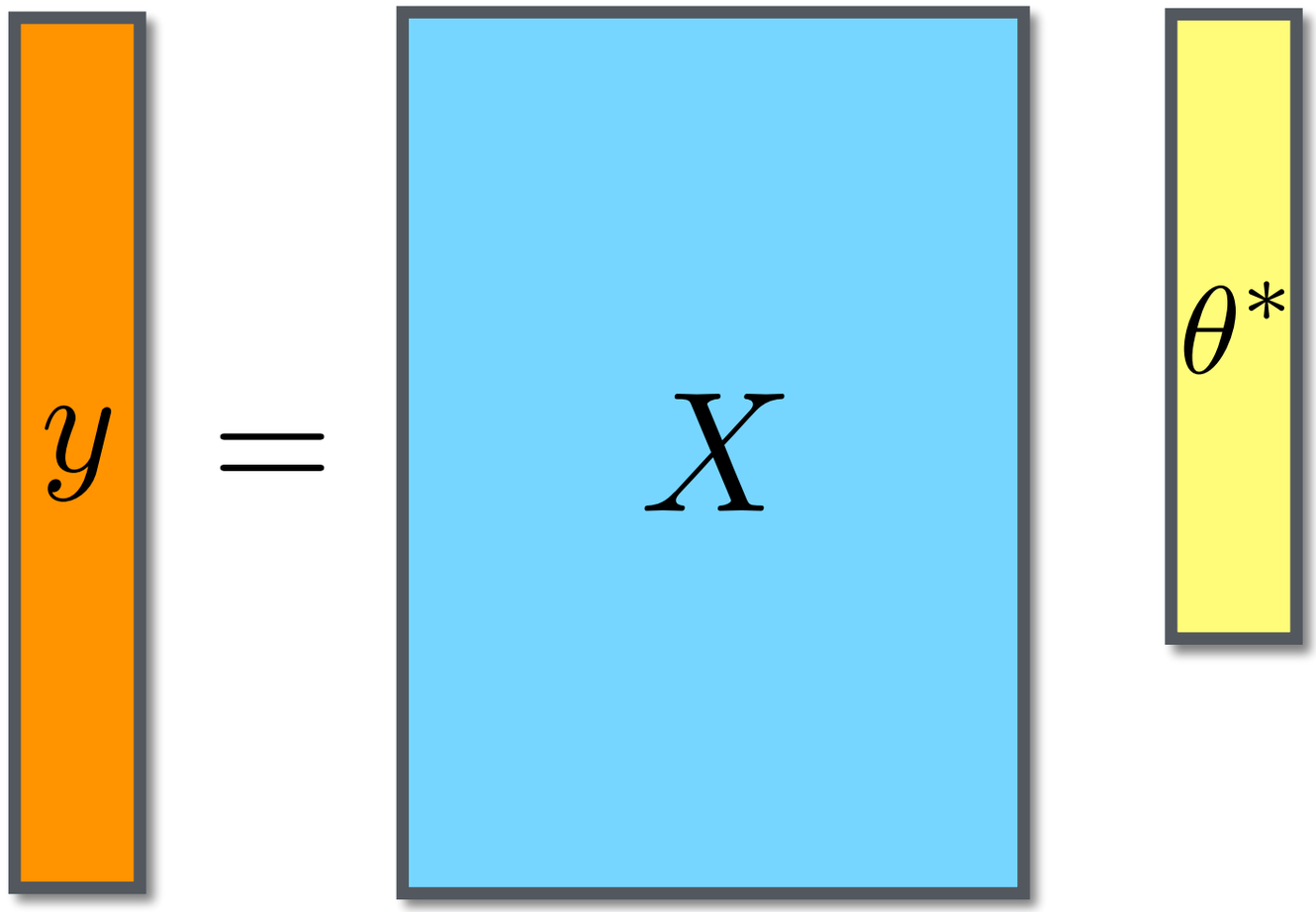
Linear Regression with Graph Constraints

Ludwig Schmidt
MIT → UC Berkeley

Based on joint works with Tobias Ehrenberger, Ernest Fraenkel, Chinmay Hegde, Piotr Indyk, Stefanie Jegelka, Alexander LeNail, Jonathan Li, and Karen Sachs.

Linear Regression



Given: data matrix X and observations y.

Goal: find the unknown θ*.

(also: predict y in the future)

Linear Regression

$$y = X \quad \theta^* \quad + \text{noise}$$

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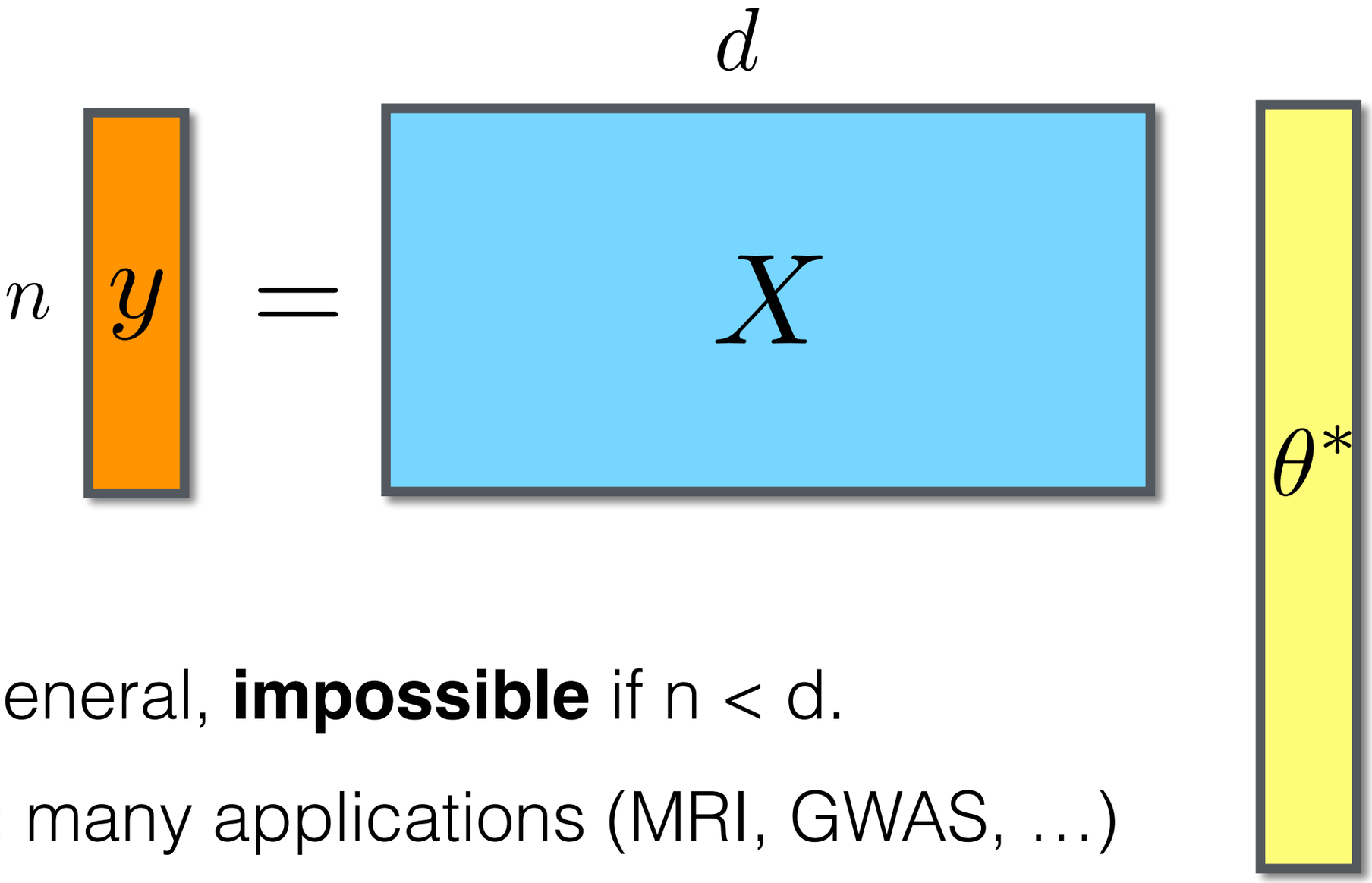
(also: predict y in the future)

Gauss, early 1800s

Constrained Linear Regression



In general, **impossible** if n < d.

But: many applications (MRI, GWAS, …)

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$$n \begin{bmatrix} y \end{bmatrix} = \overset{d}{\begin{bmatrix} X \end{bmatrix}} \begin{bmatrix} \theta^* \end{bmatrix}$$

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→ Use extra structure such as **sparsity**.

Solving Linear Regression with Constraints

	Standard Linear Regression	Sparse Linear Regression
Algorithm	$\arg\min_{\theta} \|y - X\theta\|_2^2$	
	Least Squares	

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	Least Squares	Lasso

Convex relaxation $\ell_0 \rightarrow \ell_1$

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Sample Complexity	$n = O(d)$	$n = O(s \log d)$

(d is the ambient dimension, s is the sparsity of the unknown vector)

Widely Used Methods

Rob Tibshirani

Popularized the Lasso

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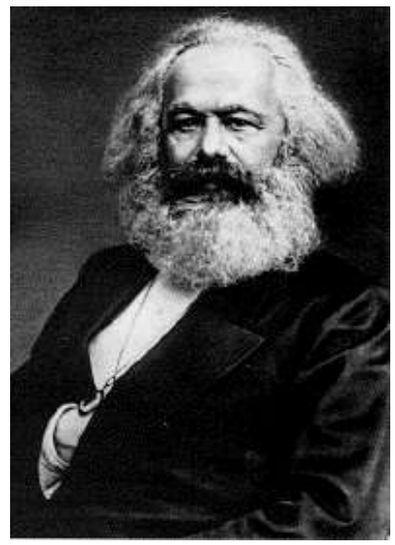

Karl Marx

Popularized Communism

Widely Used Methods

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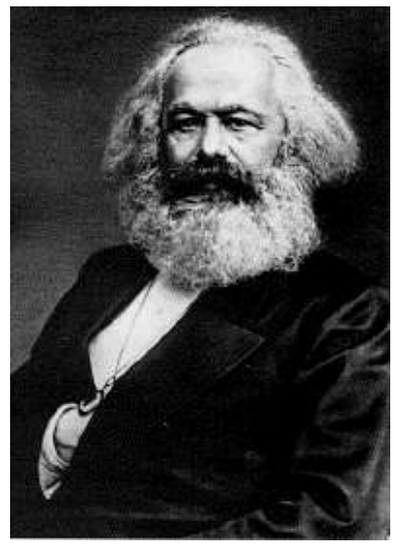

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What do they have in common?

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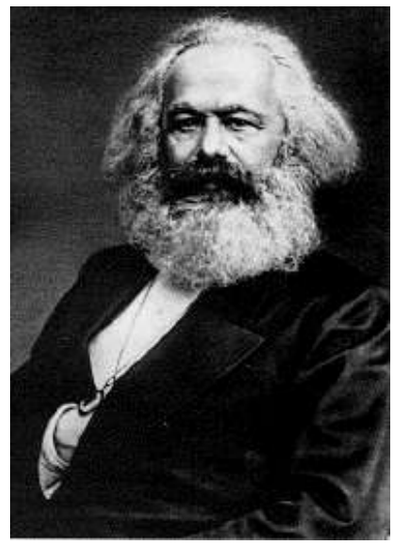
Google Scholar:
266,534 citations



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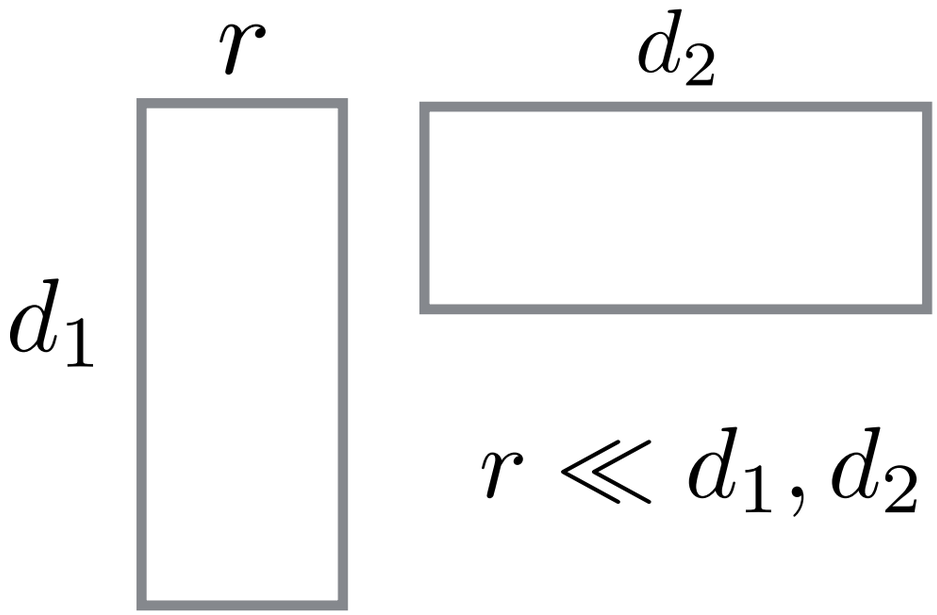
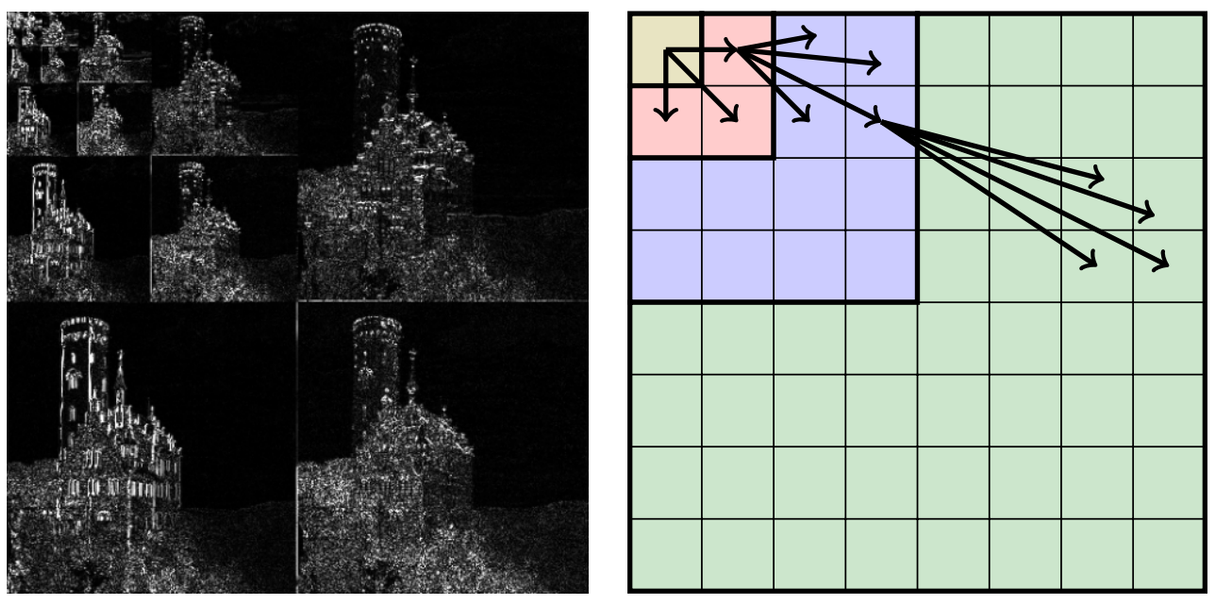
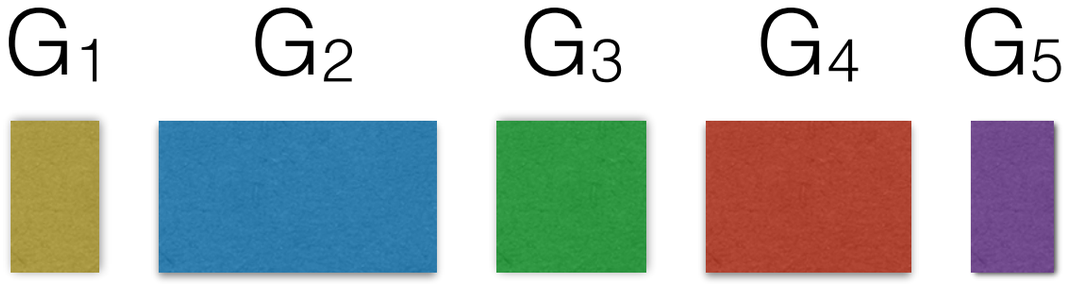
Wide Range of Constraints



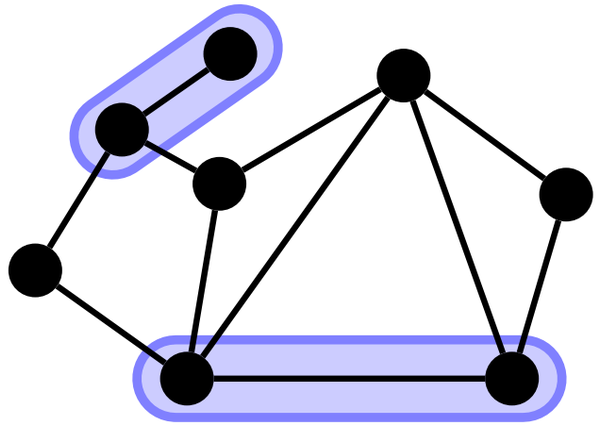
Low rank



Tree sparsity



Group sparsity



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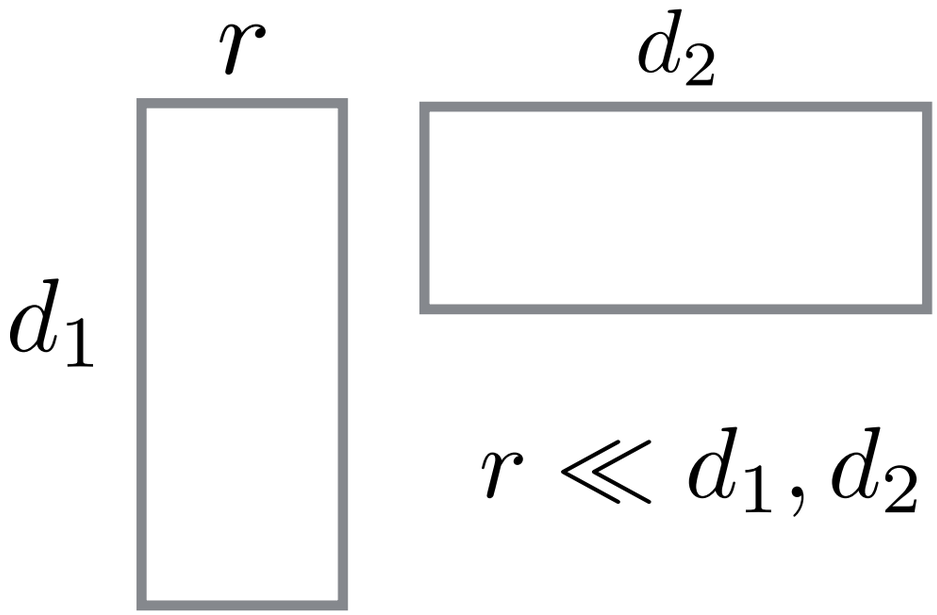

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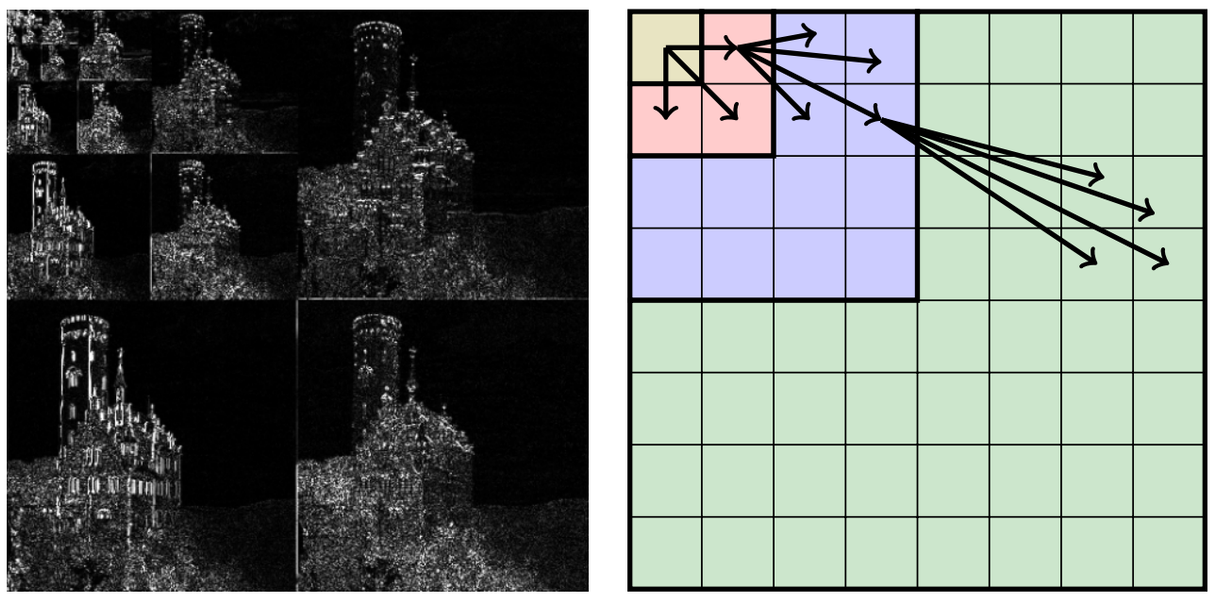

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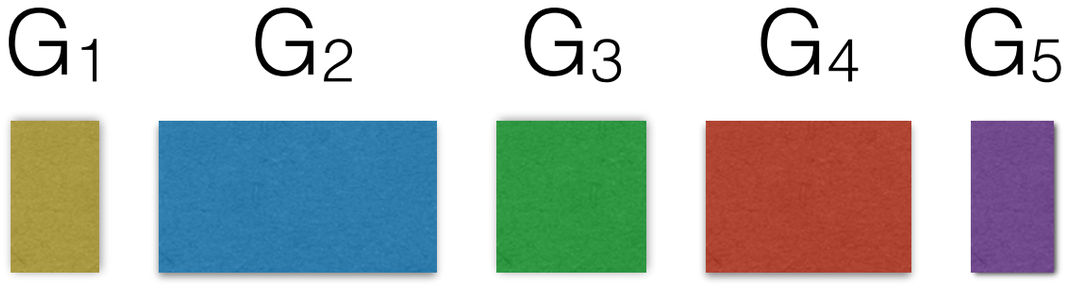

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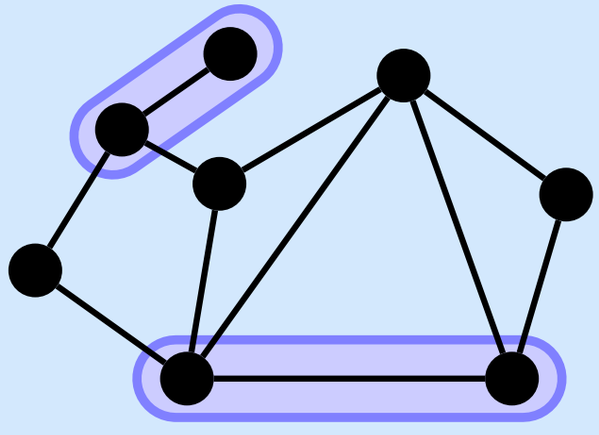
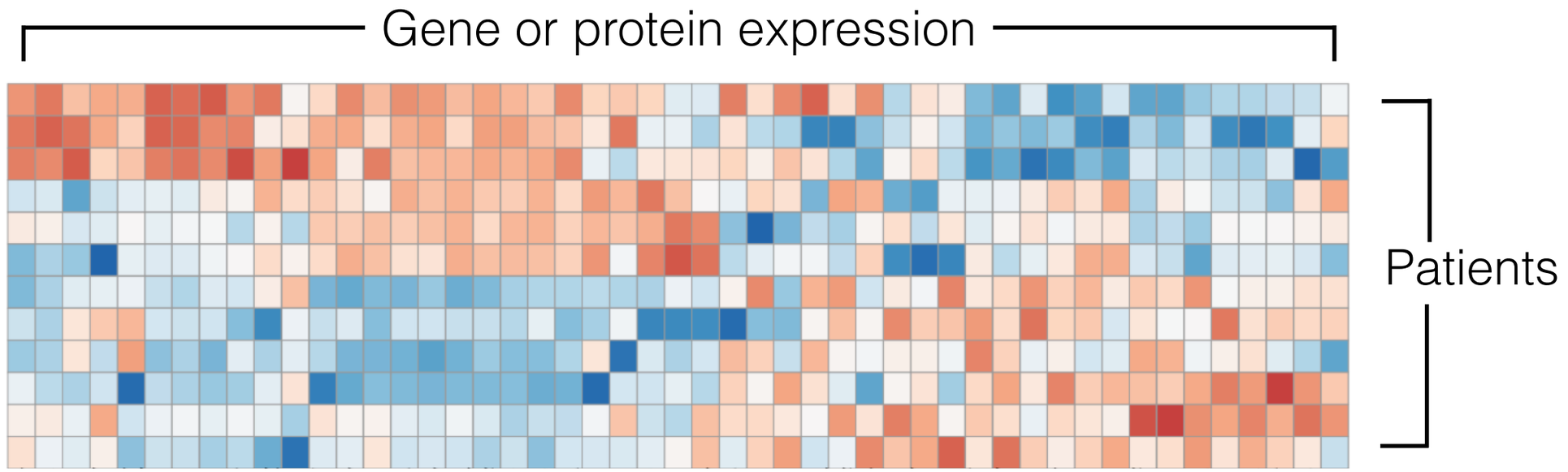


Graph sparsity

Example: Biological Network Data



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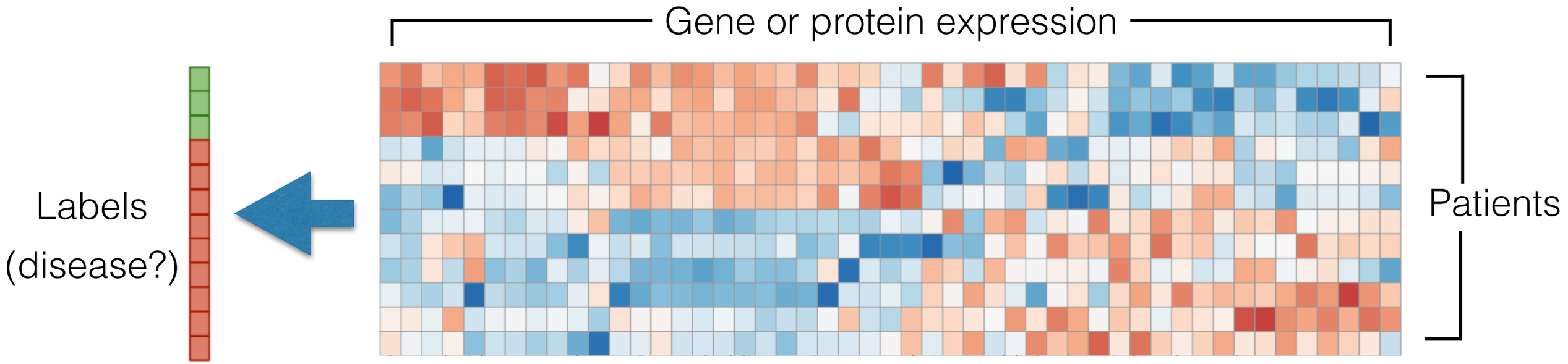

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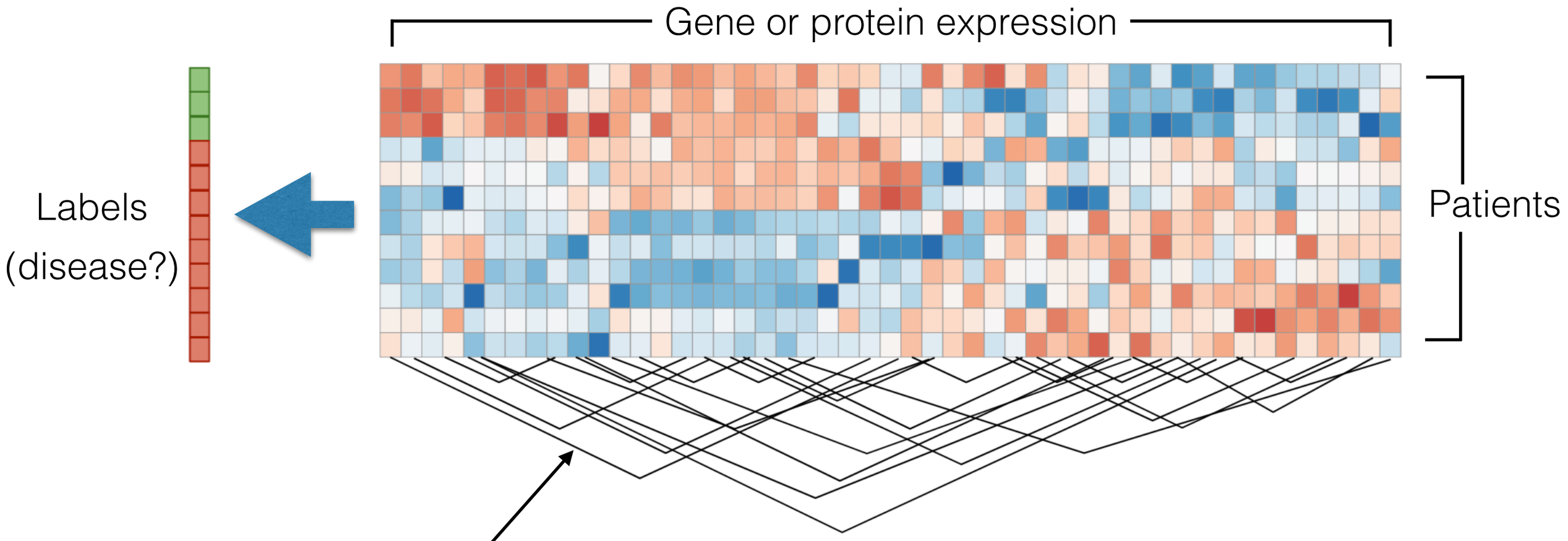

Some features
(genes / proteins)
are related.

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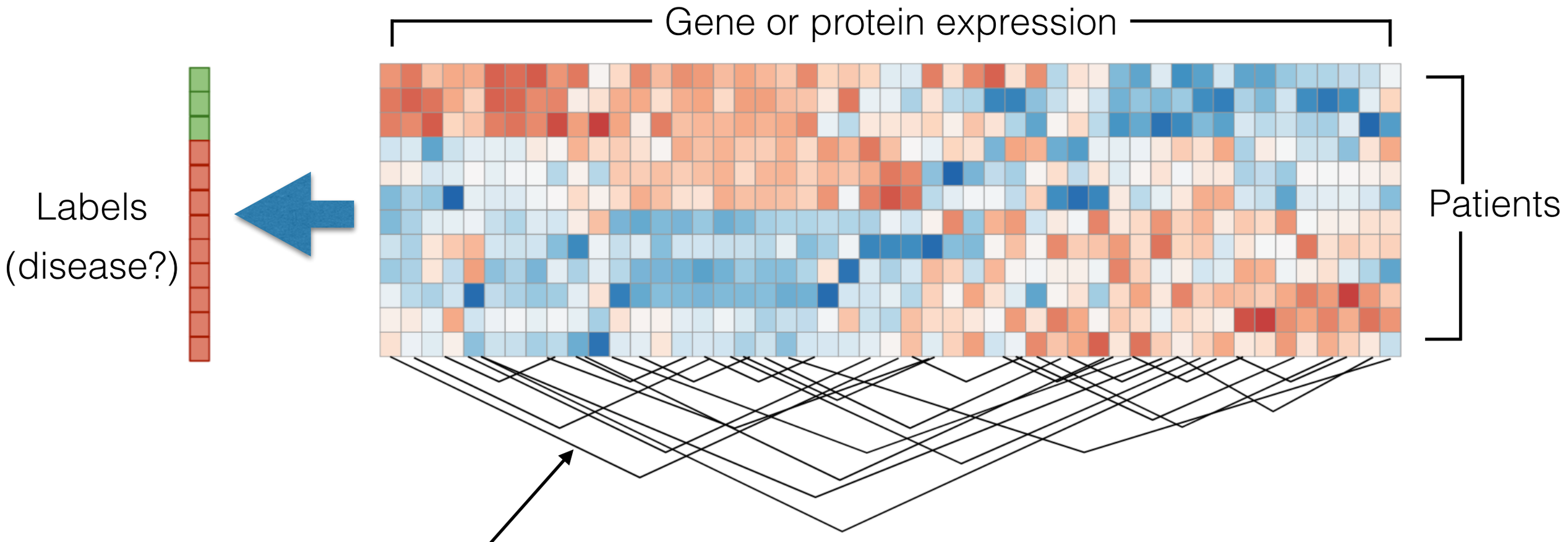
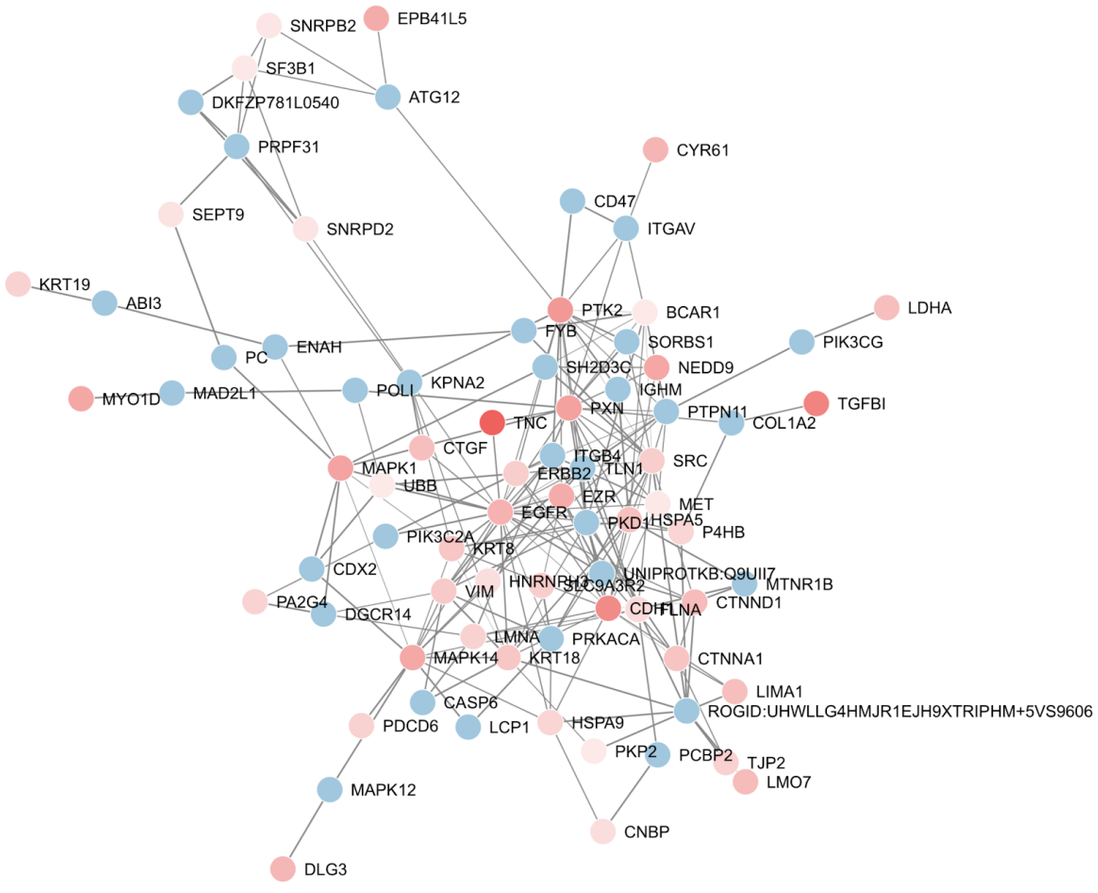


Goal: find the most relevant genes / proteins.

Graph Structure

Input



Every node corresponds to a feature (gene / protein).

Graph Structure

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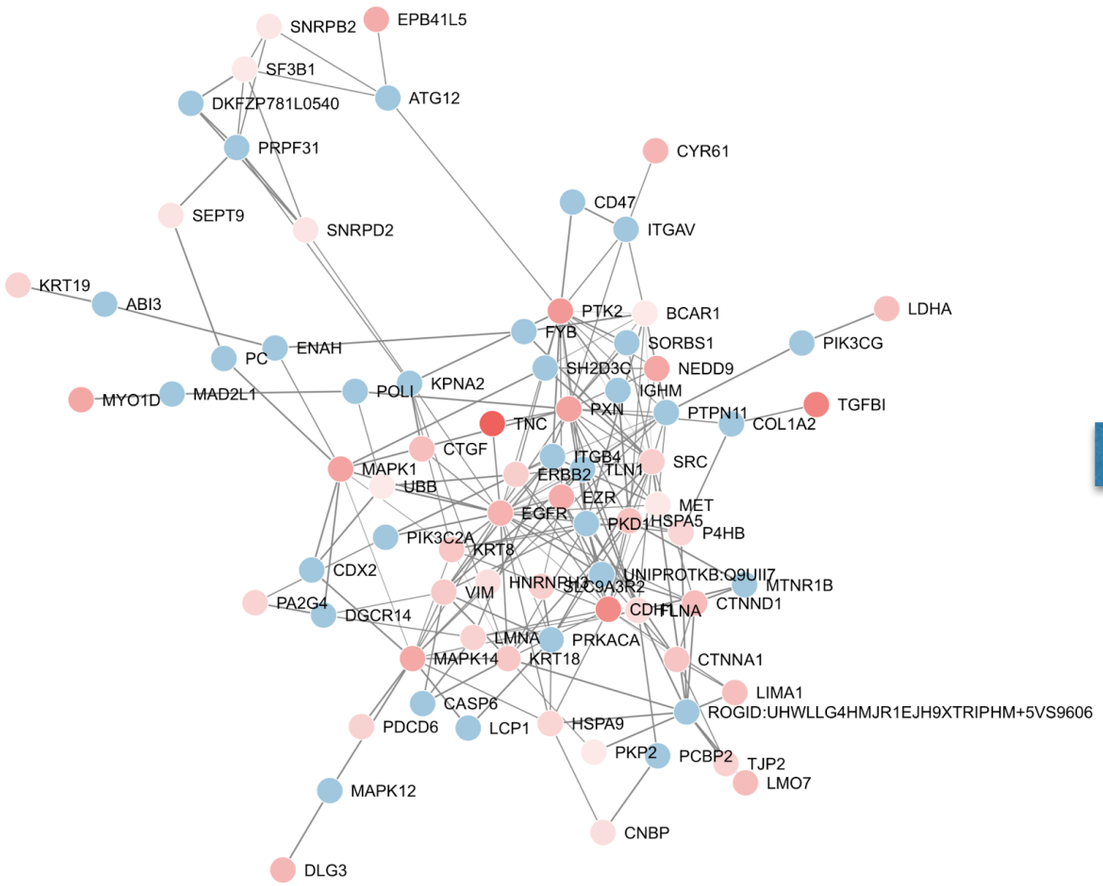

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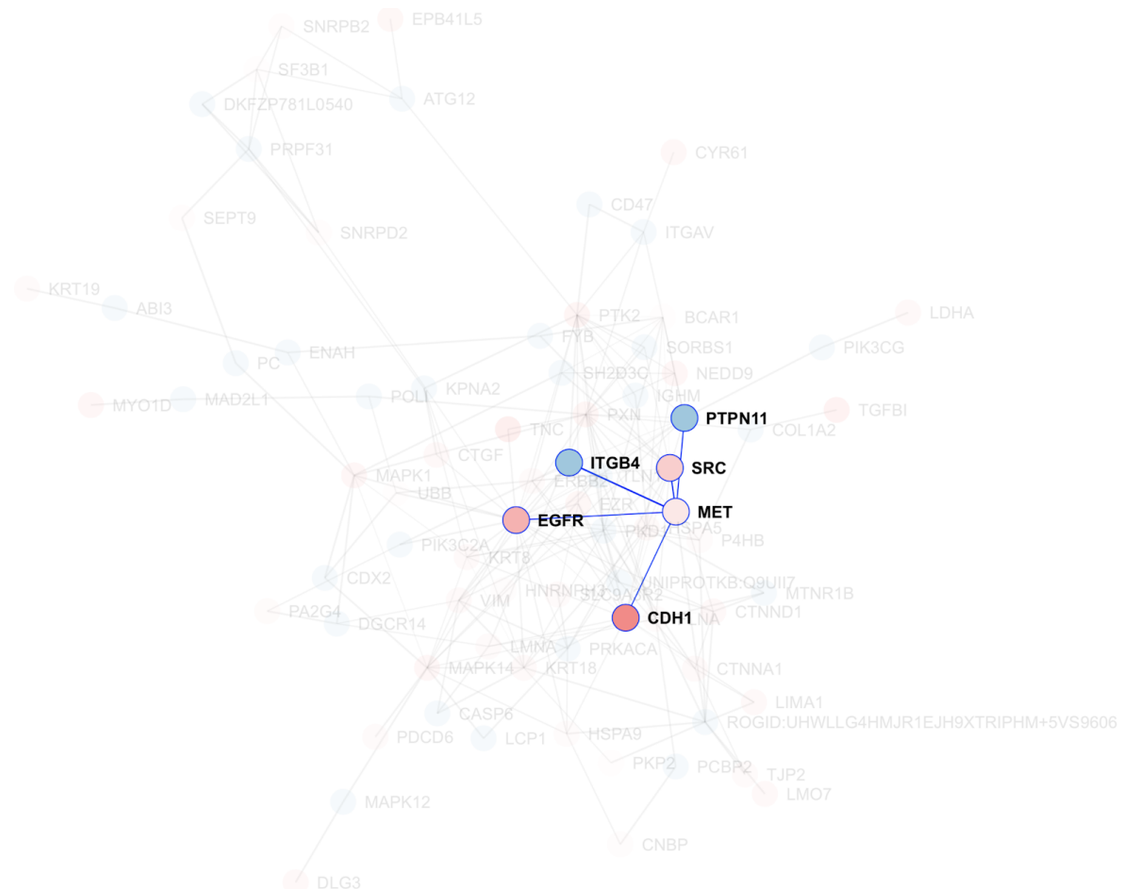
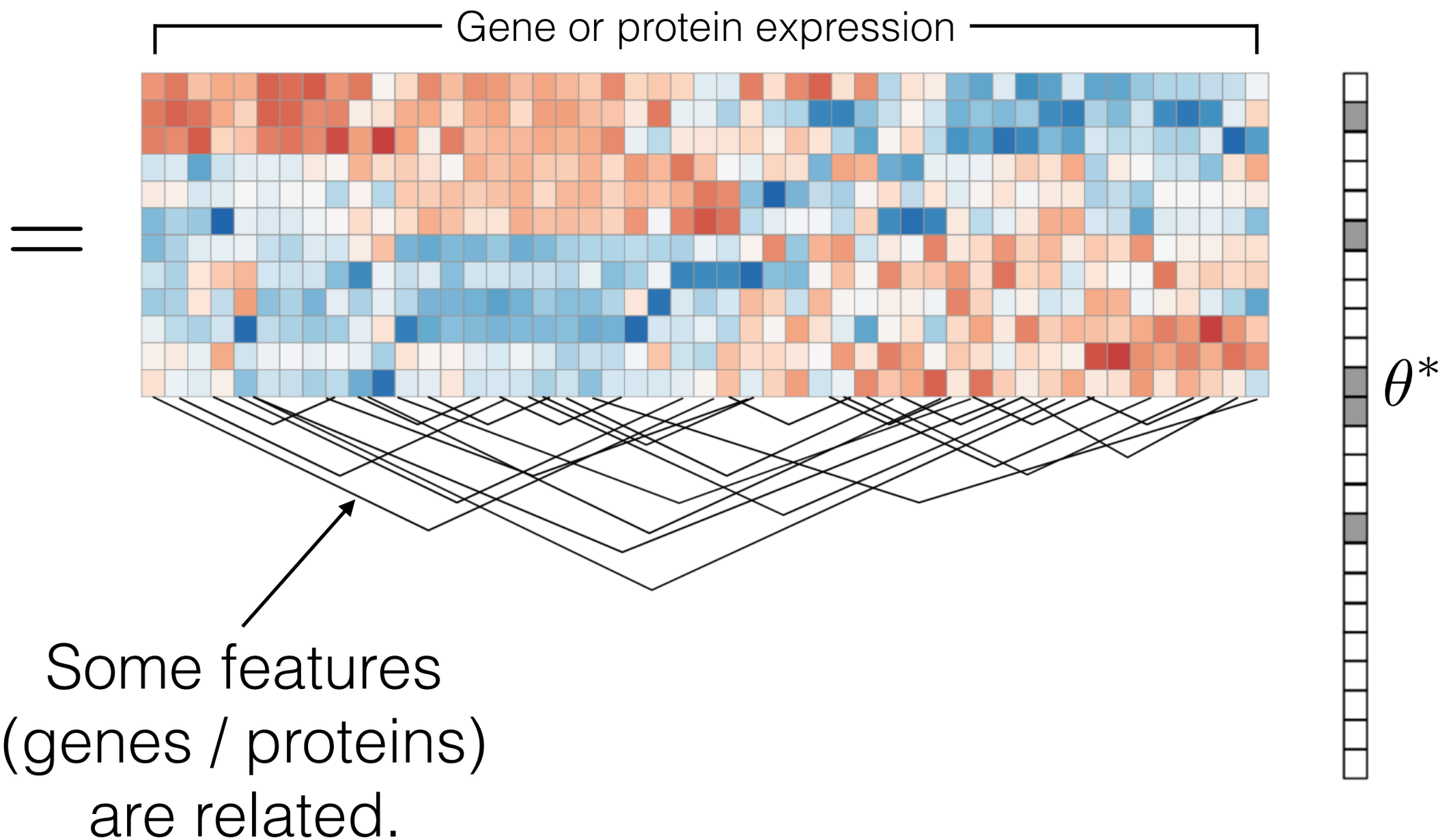


Every node corresponds to a feature (gene / protein).

Goal: Find one (or a few) **connected subgraph** with highly predictive features.

Linear Regression with Graph Constraint



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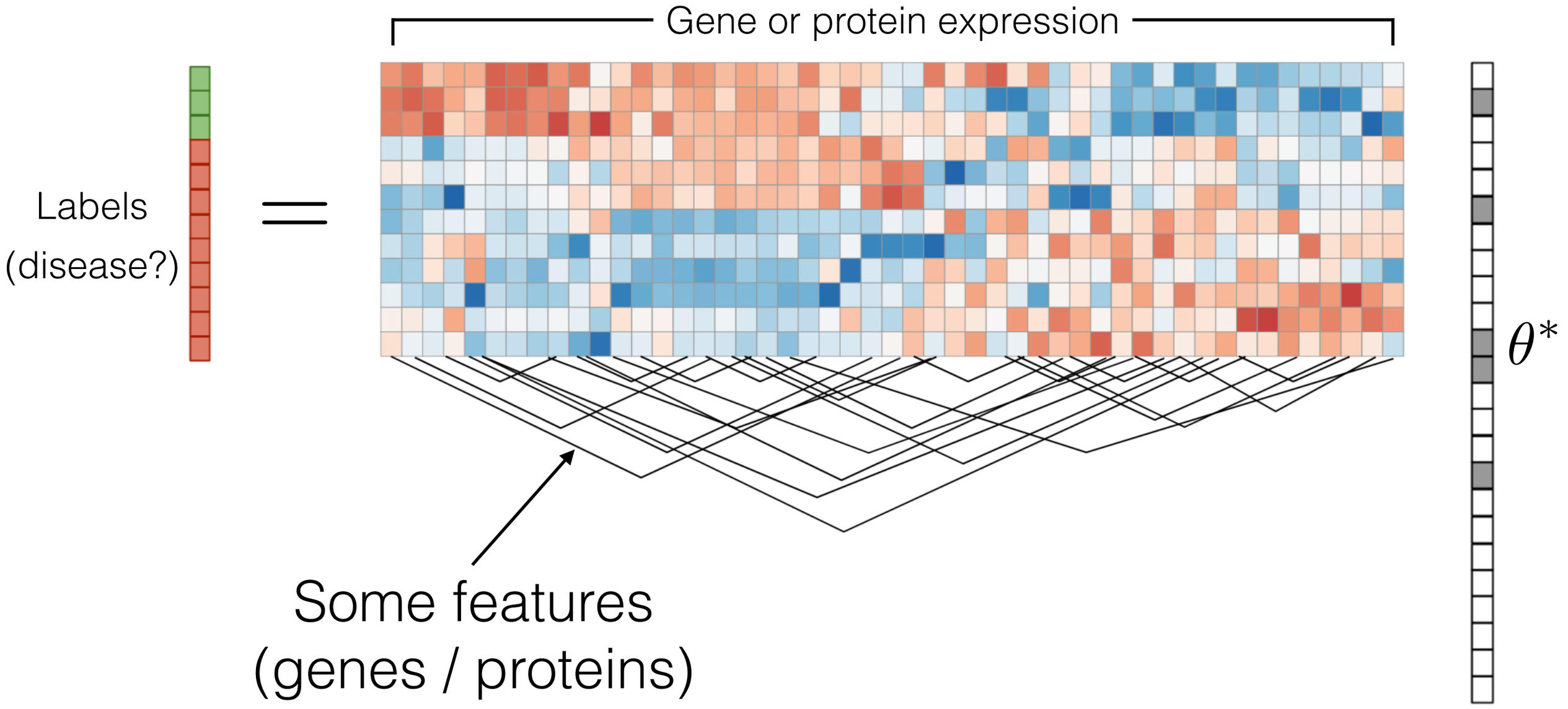

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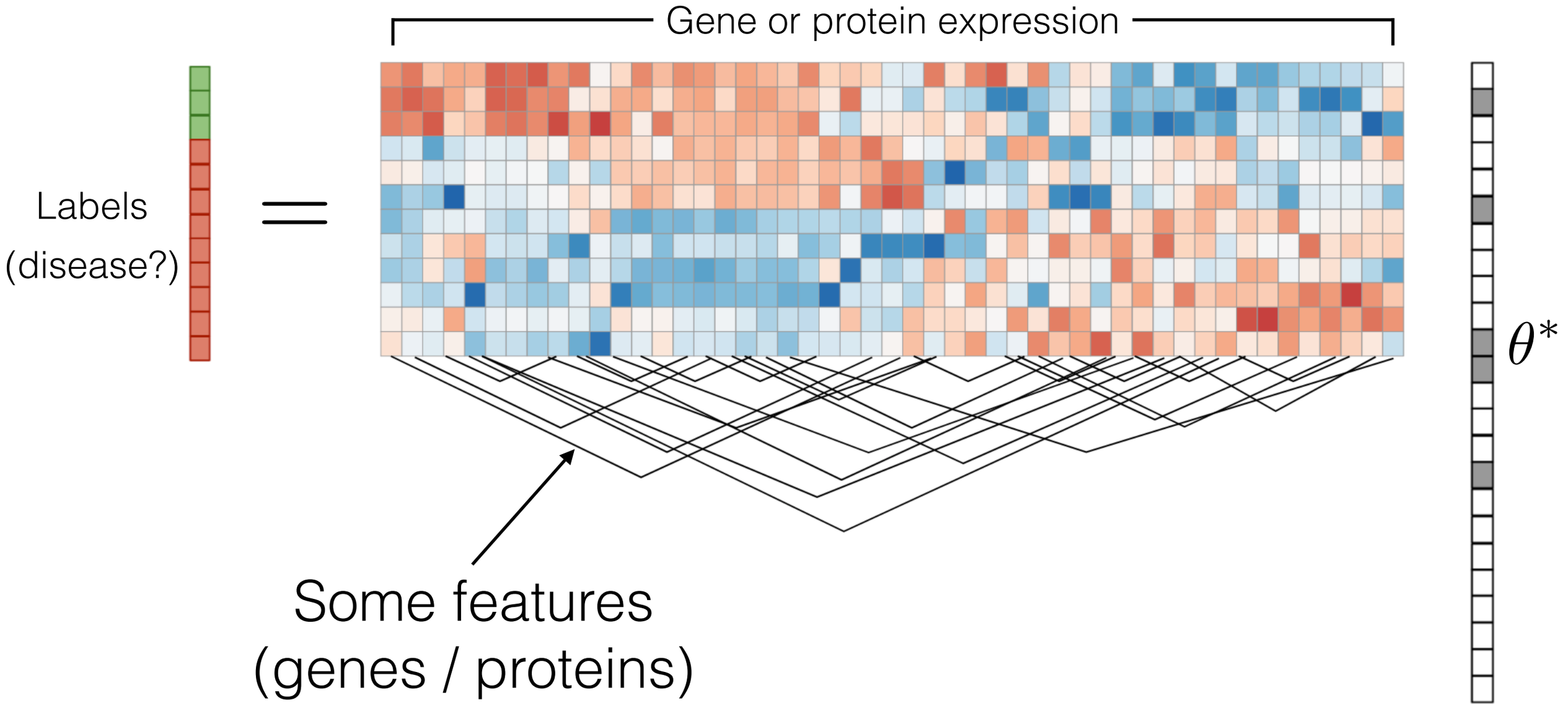

Goal: find a **graph**-sparse set of parameters θ*.

Solving Linear Regression with Constraints

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Algorithm	$\arg\min_{\|\theta\|_1 \leq \lambda} \|y - X\theta\|_2^2$	$\arg\min_{\theta \in \mathcal{C}} \|y - X\theta\|_2^2$

The set C is the set of graph-sparse vectors,
i.e., vectors with a sparsity pattern
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How can we solve this problem?

Projected Gradient Descent

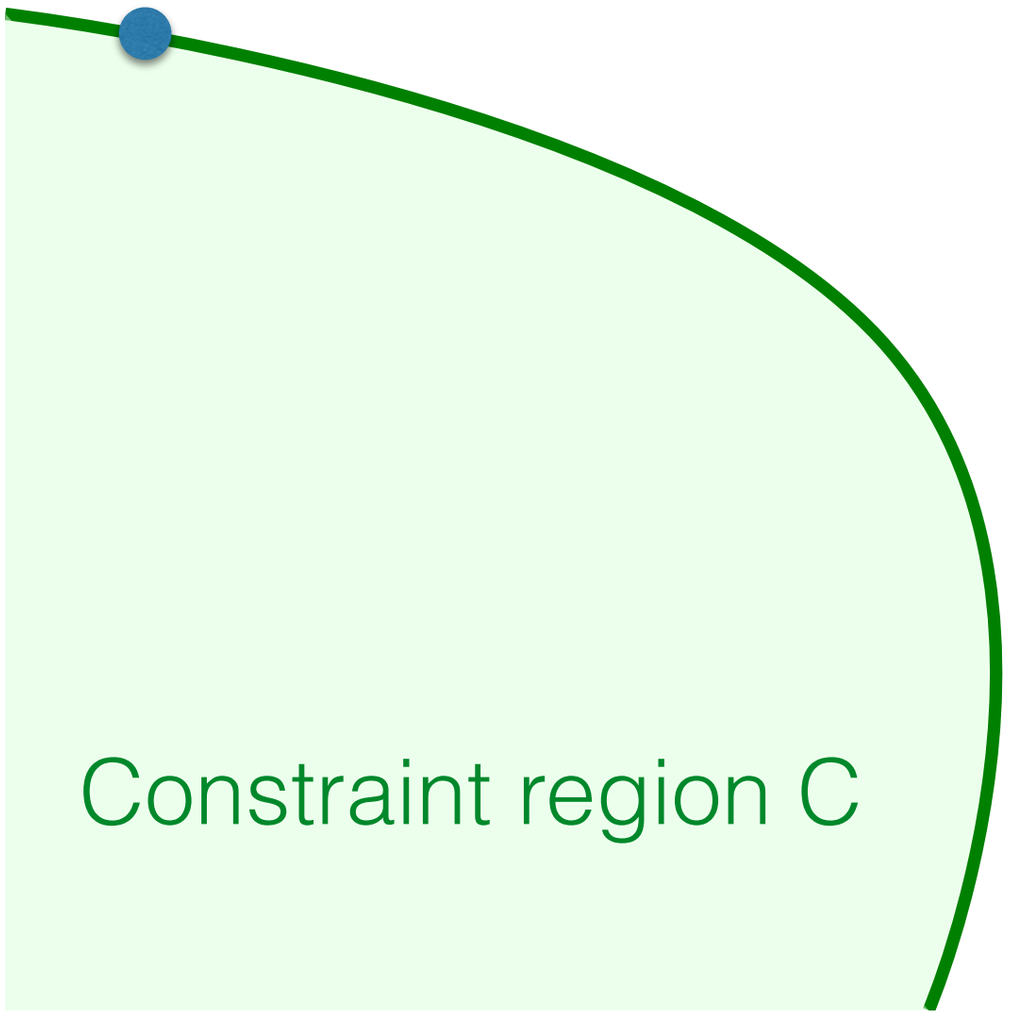
Repeat the following:

1. Compute gradient $\nabla f(\theta^i)$
2. Take a gradient step

$$\tilde{\theta}^{i+1} \leftarrow \theta^i + \eta \nabla f(\theta^i)$$

3. Project back to constraint set

$$\theta^{i+1} \leftarrow P_{\mathcal{C}}(\tilde{\theta}^{i+1})$$



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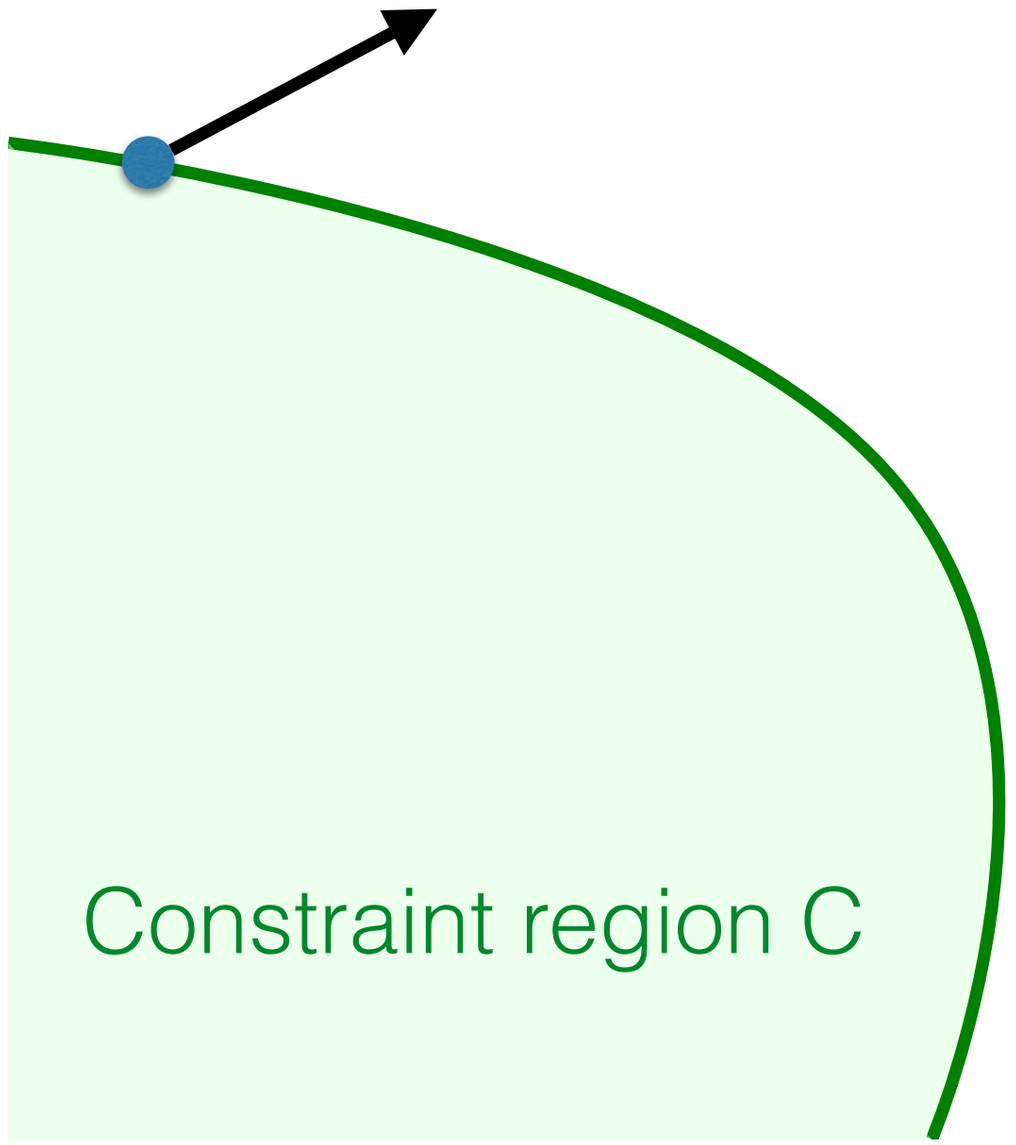

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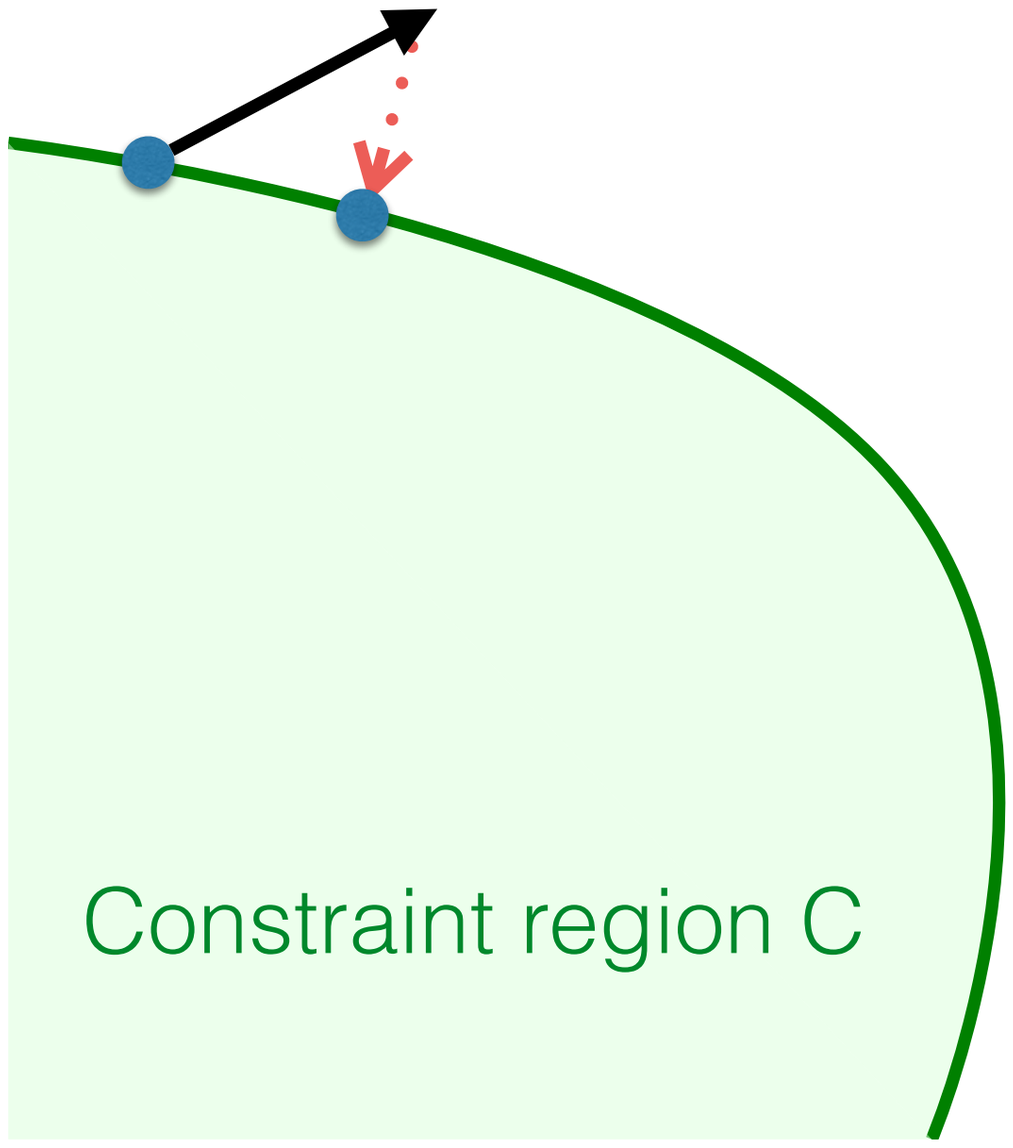

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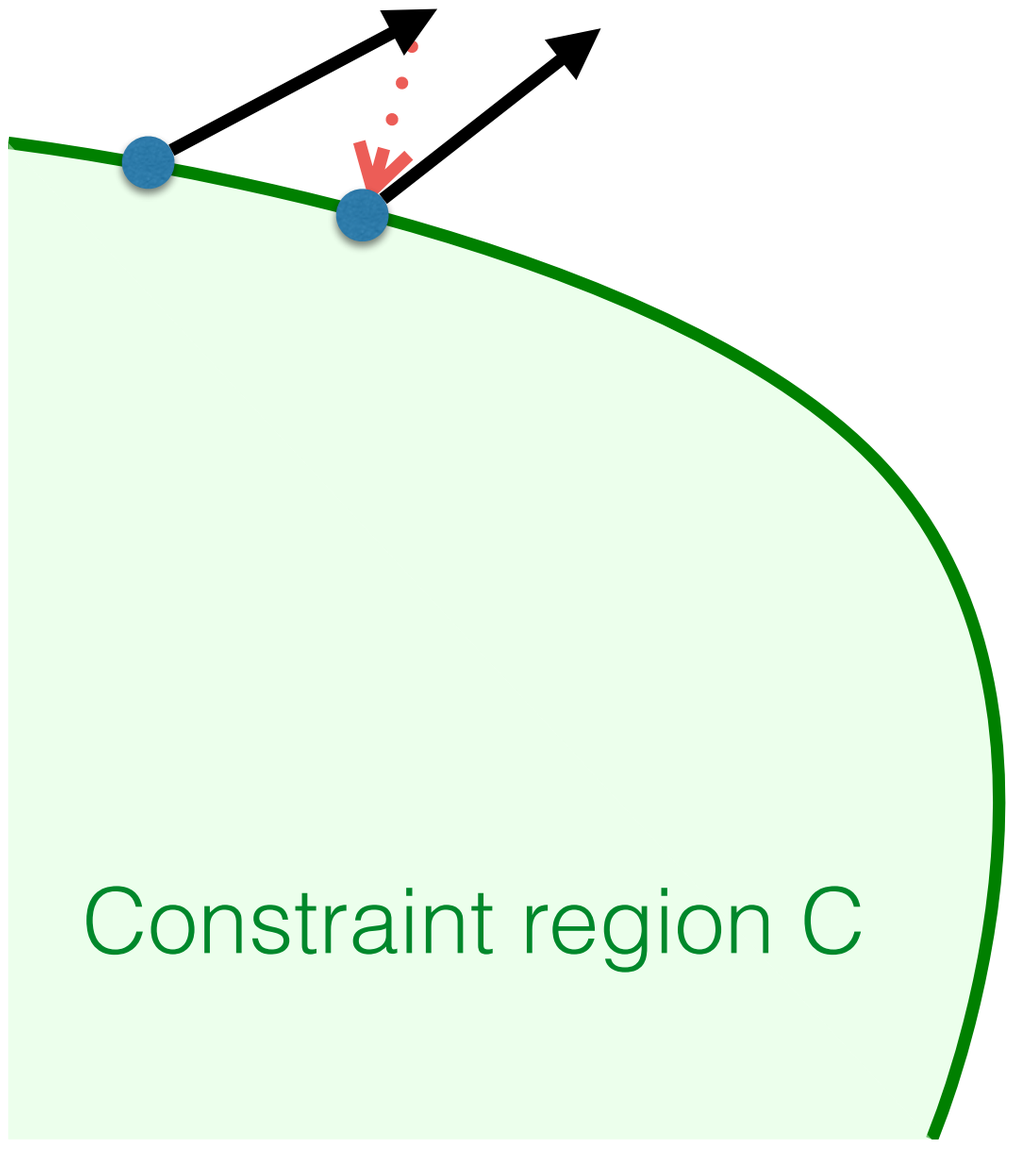

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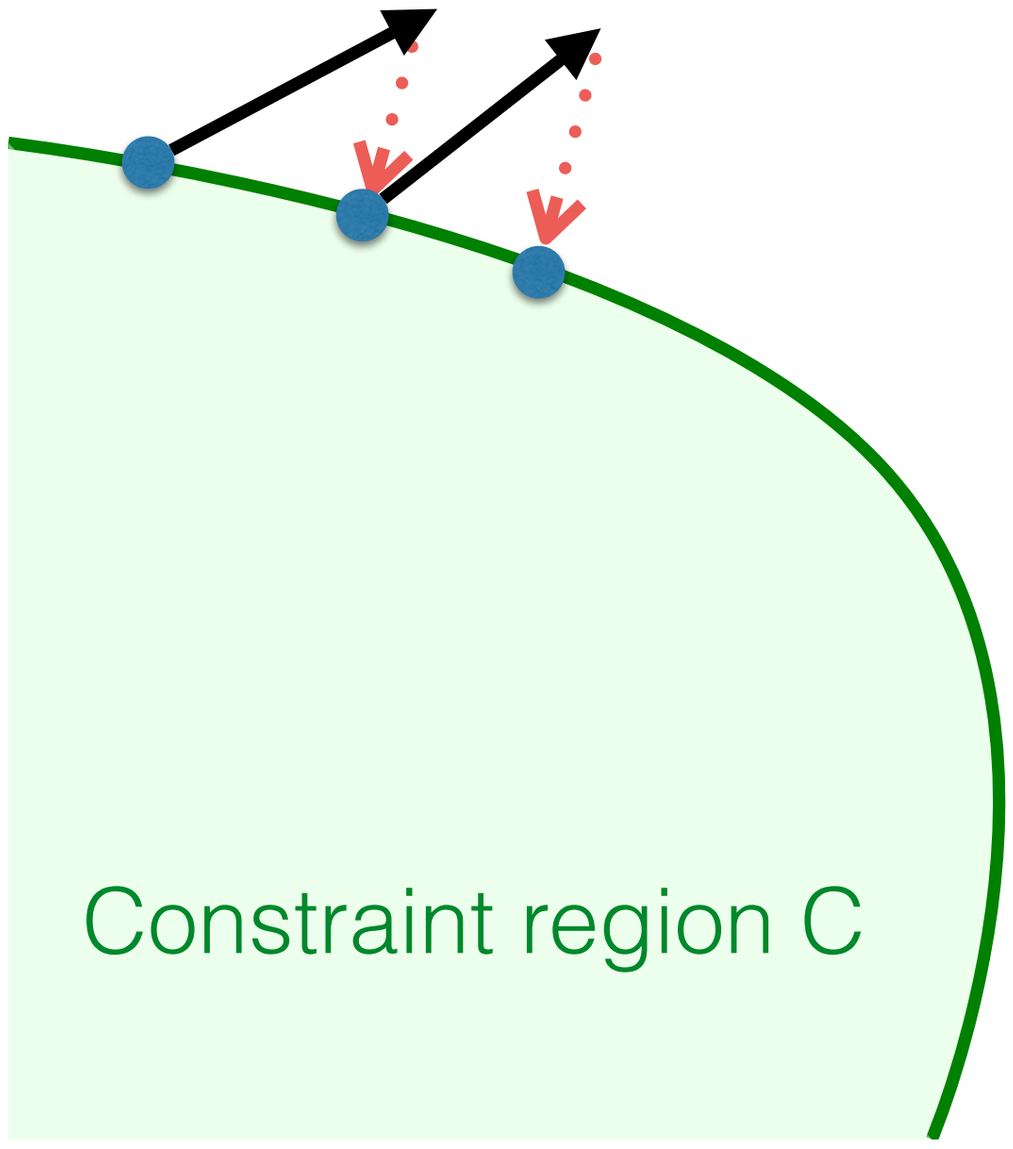

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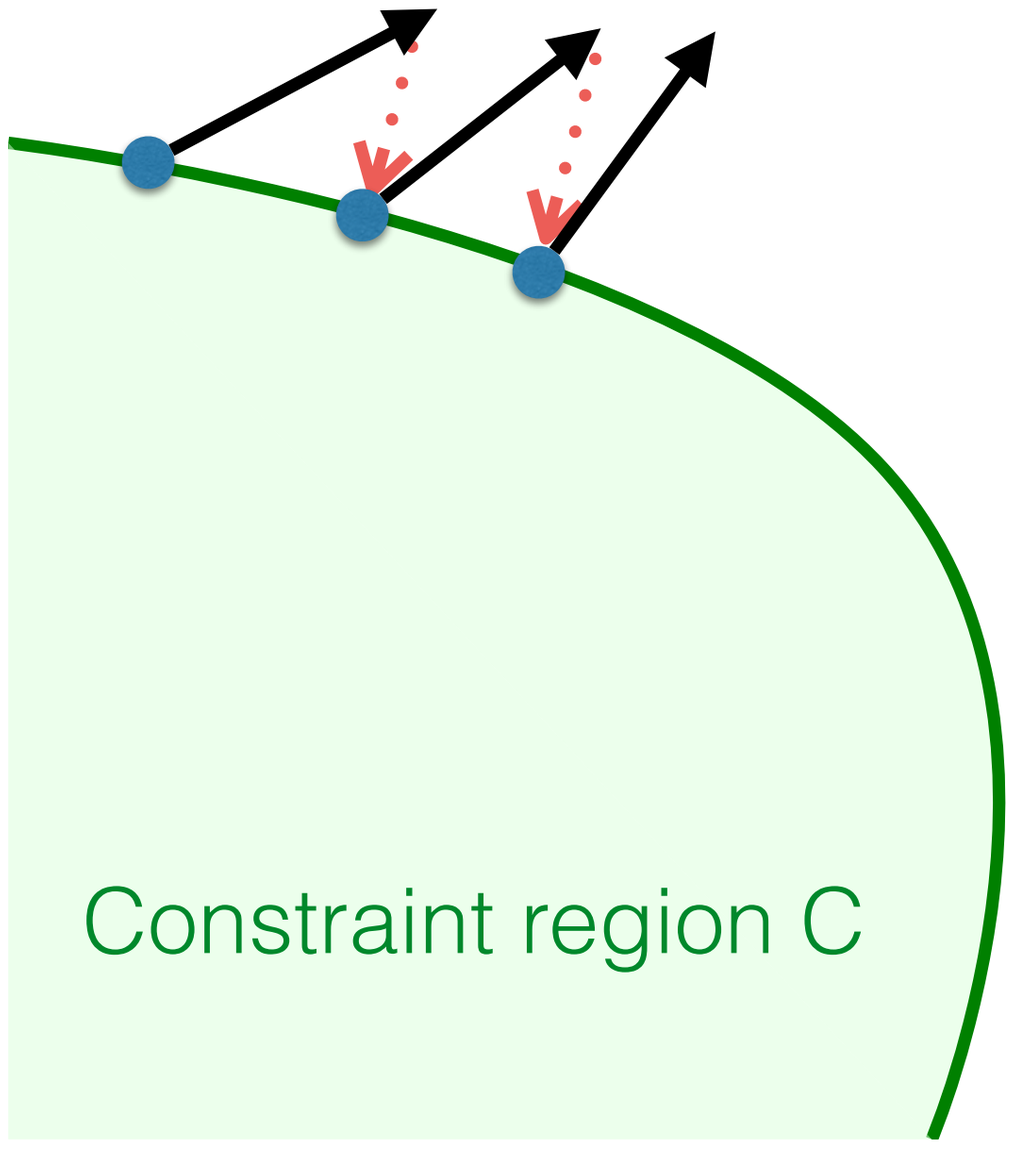

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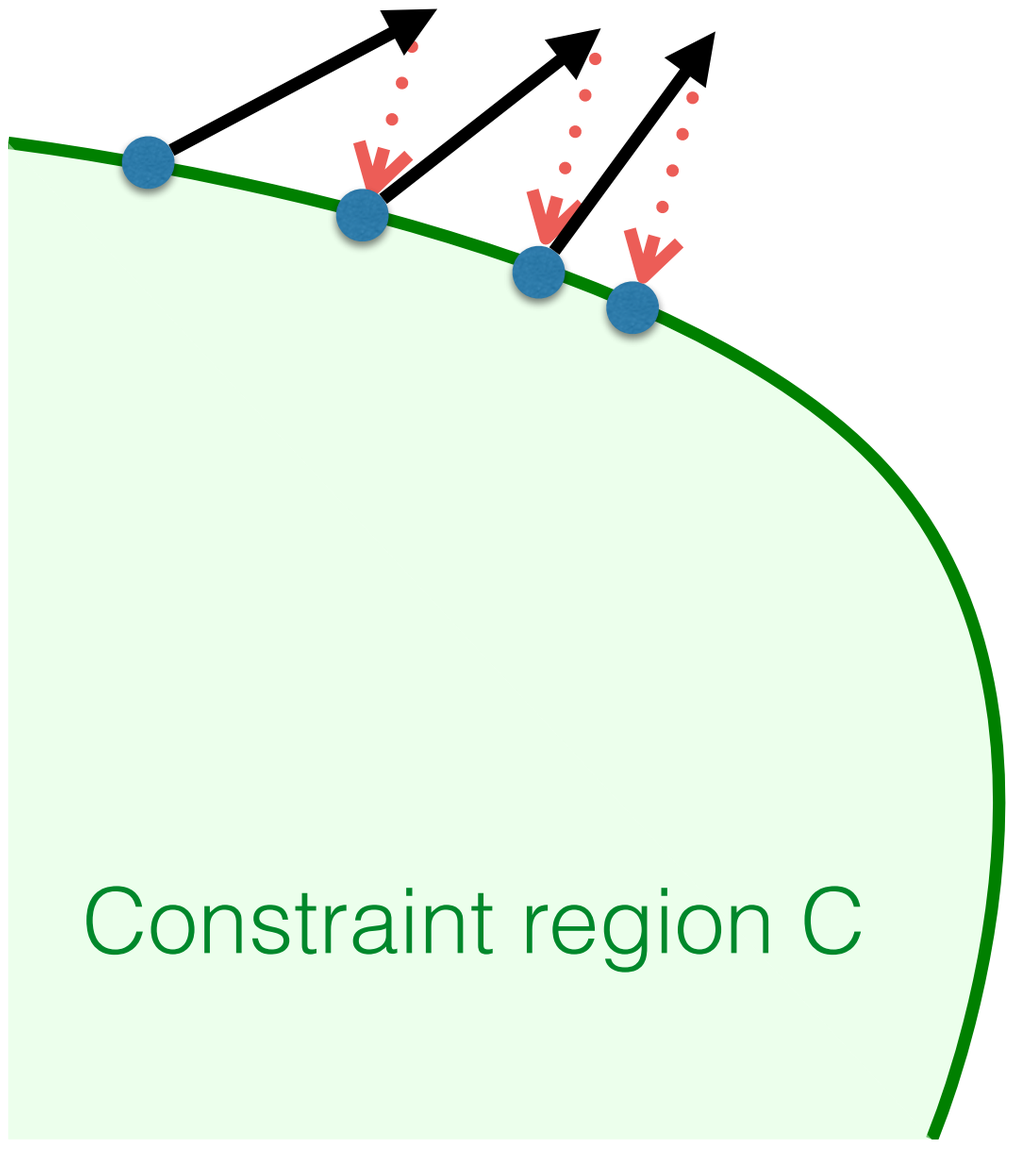

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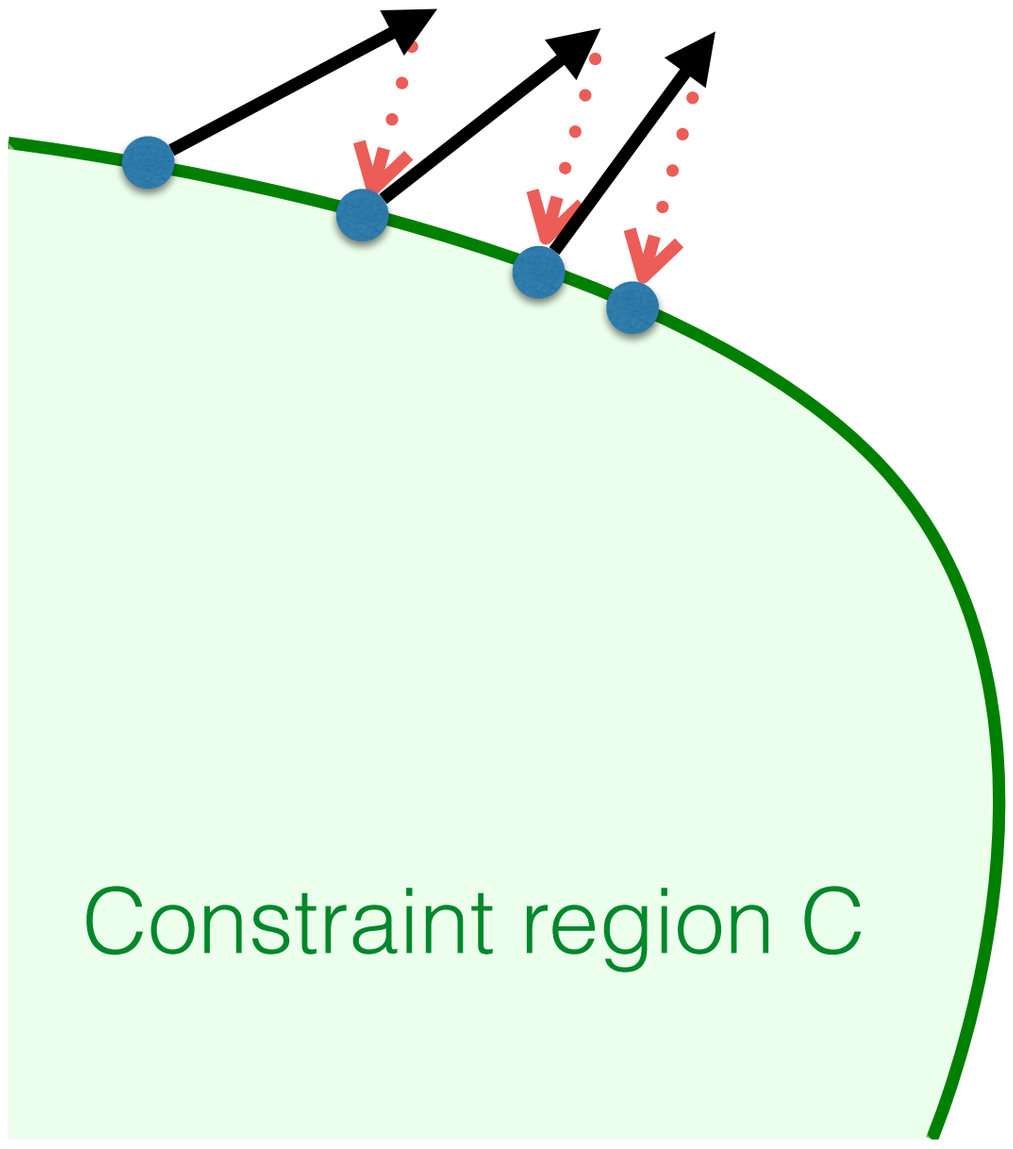
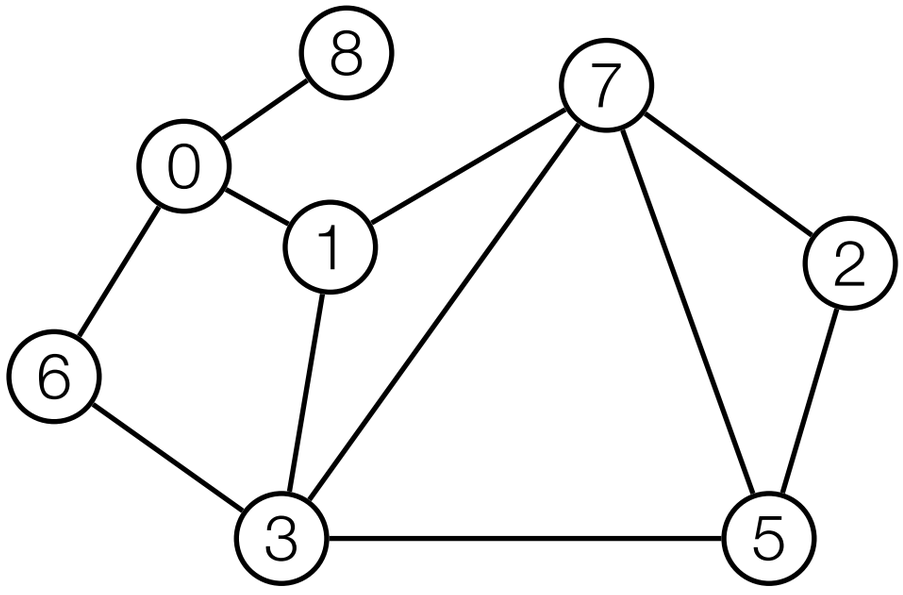
Computational bottleneck



Graph Sparsity Projection

Given a node-weighted graph, find a set of **g subtrees** with **total size s** so that the **sum of node weights** is maximized.

Example: g = 2, s = 3



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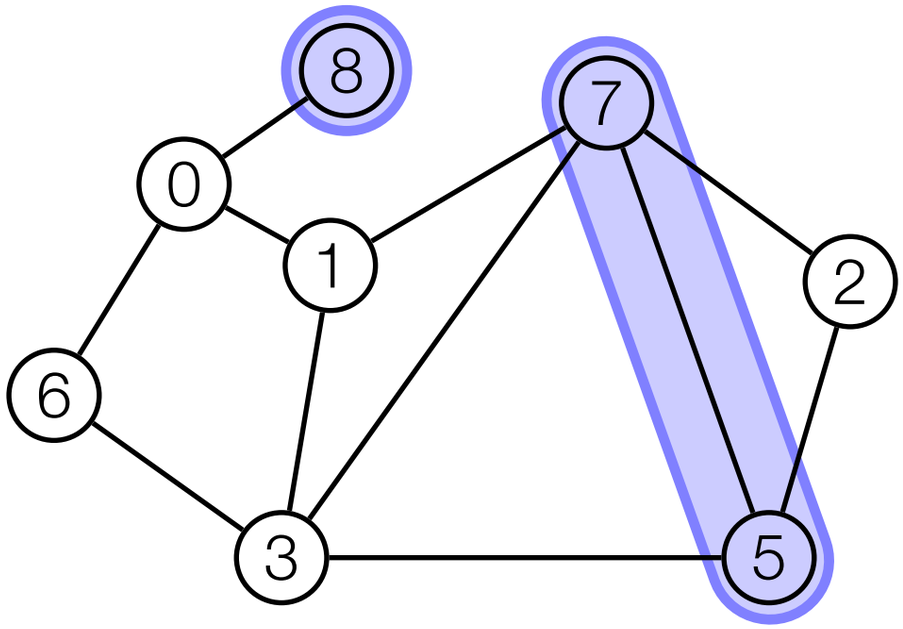

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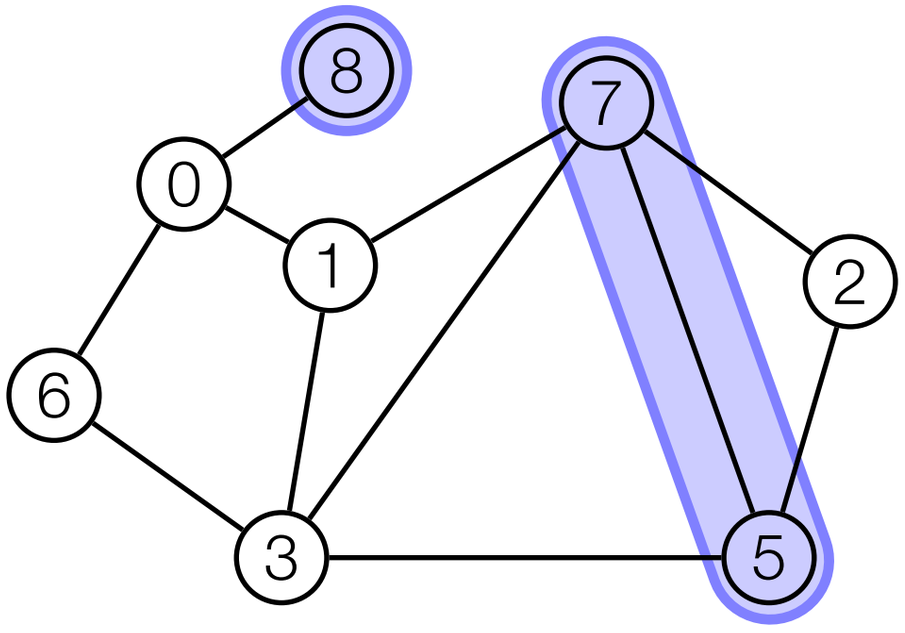

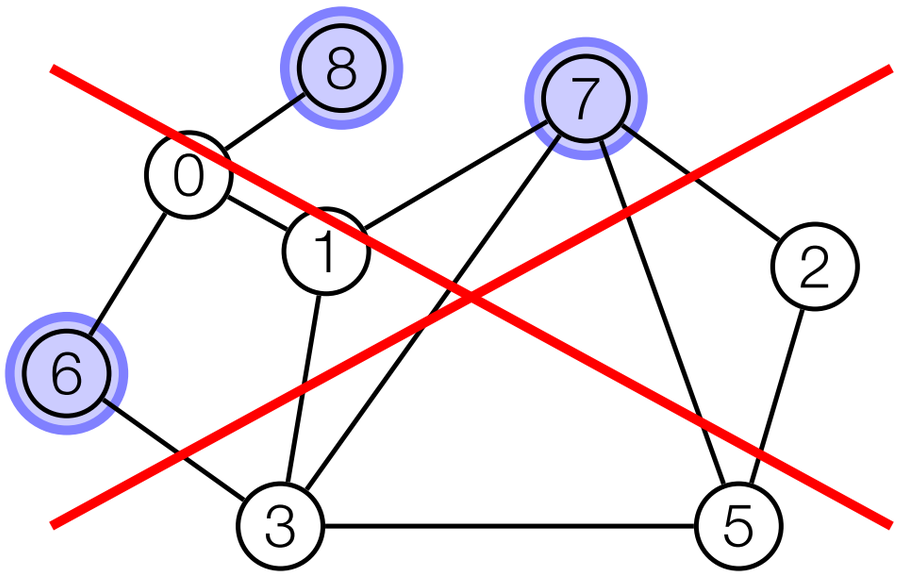

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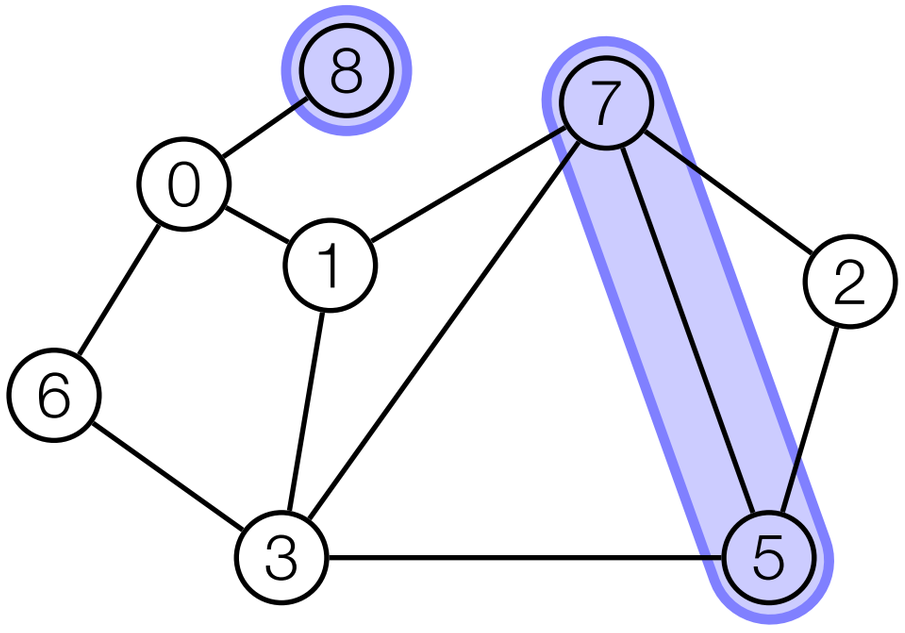

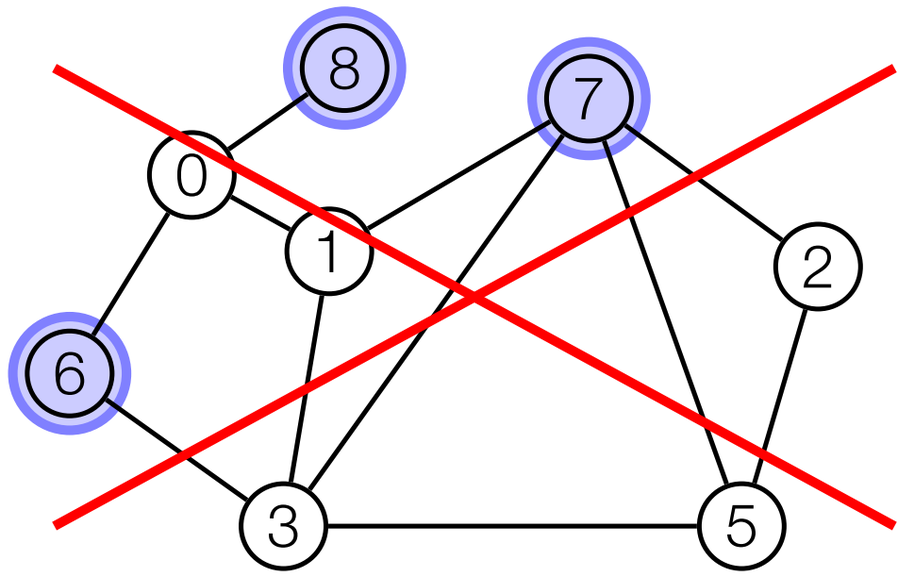

But: This problem is **NP-hard**.

How Can Approximation Help?

Natural relaxation: **“Tail” Approximation**

Given a point $p \in \mathbb{R}^d$, find a $q \in \mathcal{C}$ such that

$$\|p - q\|_2 \leq \min_{q' \in \mathcal{C}} \|p - q'\|_2$$

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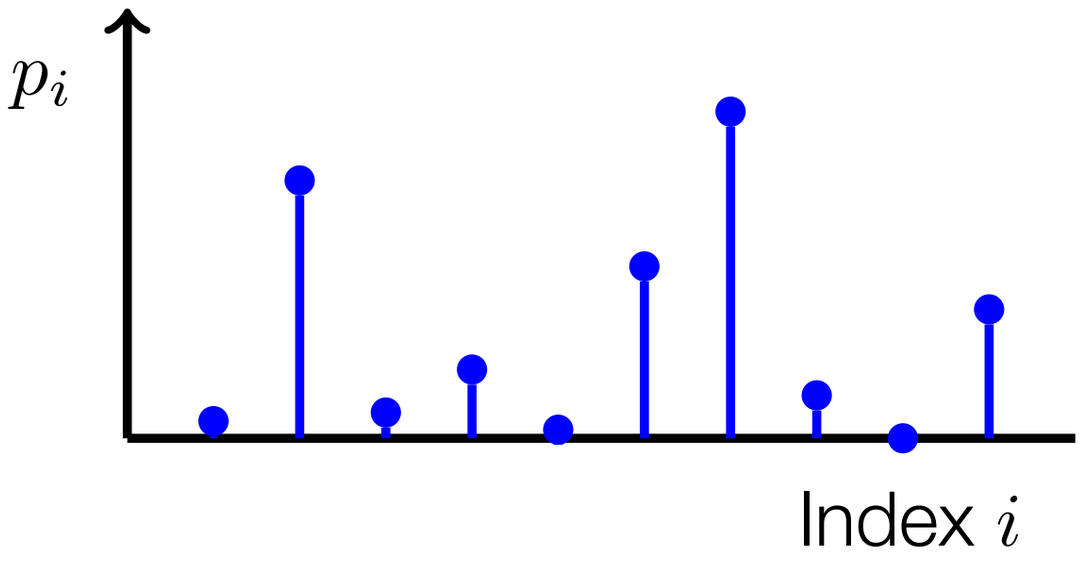

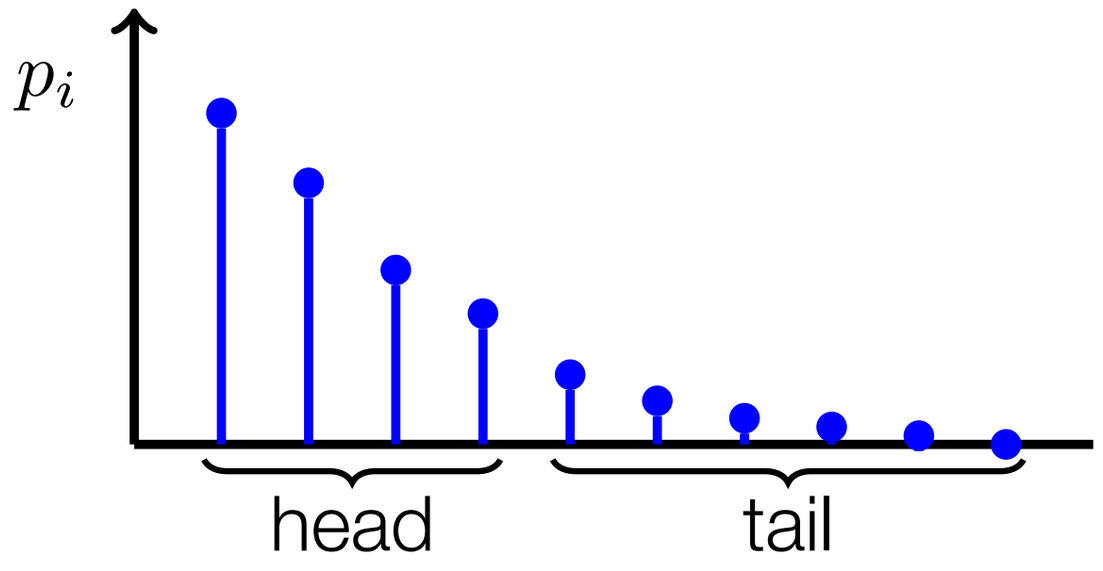

How Can Approximation Help?

Natural relaxation: **“Tail” Approximation**

Given a point $p \in \mathbb{R}^d$, find a $q \in \mathcal{C}$ such that

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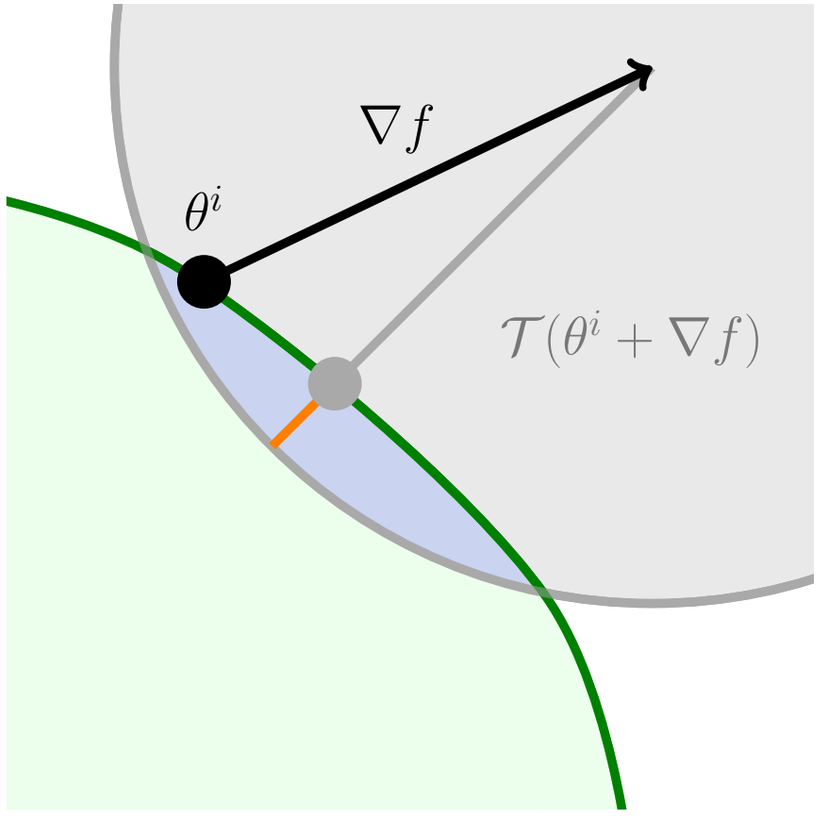
Gradient descent with tail approximation fails for any $c_T > 1$!



Simple Fix: More Approximation

Complementary guarantee: **“Head” Approximation**

Given a point $g \in \mathbb{R}^d$, find a $q \in \mathcal{C} \cap \mathbb{S}^{d-1}$ such that

$$\langle g, q \rangle \;\geq\; c_{\mathcal{H}} \cdot \max_{q' \in \mathcal{C} \cap \mathbb{S}^{d-1}} \langle g, q' \rangle \;.$$

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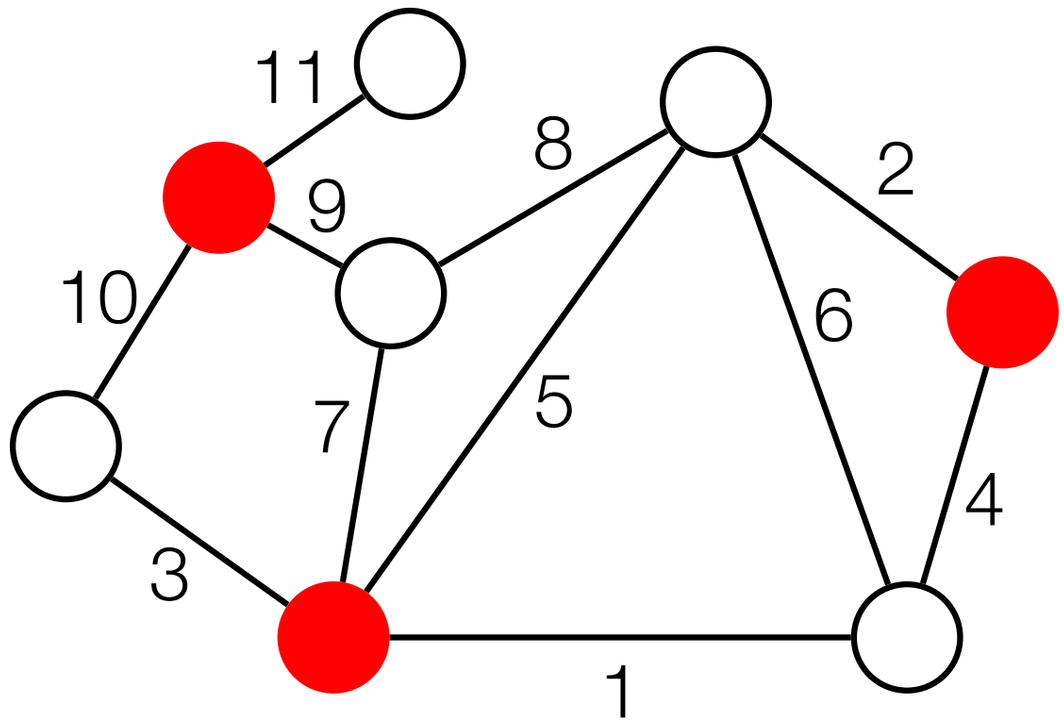
Head + Tail approximation combined provably succeeds.

- First analyzed in [Hegde-Indyk-Schmidt'14]
- Generalized in [Cohen-Hegde-Jegelka-Schmidt'??]

Prize-Collecting Steiner Tree

Generalization of the **Steiner tree** problem



Prize-Collecting Steiner Tree

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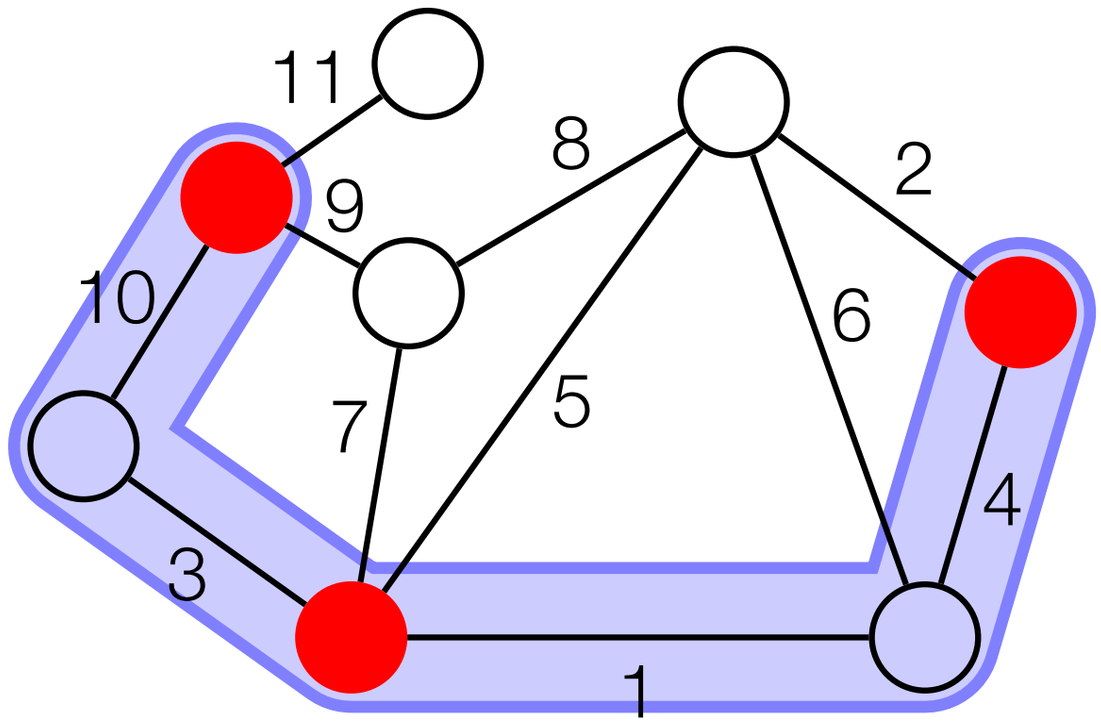
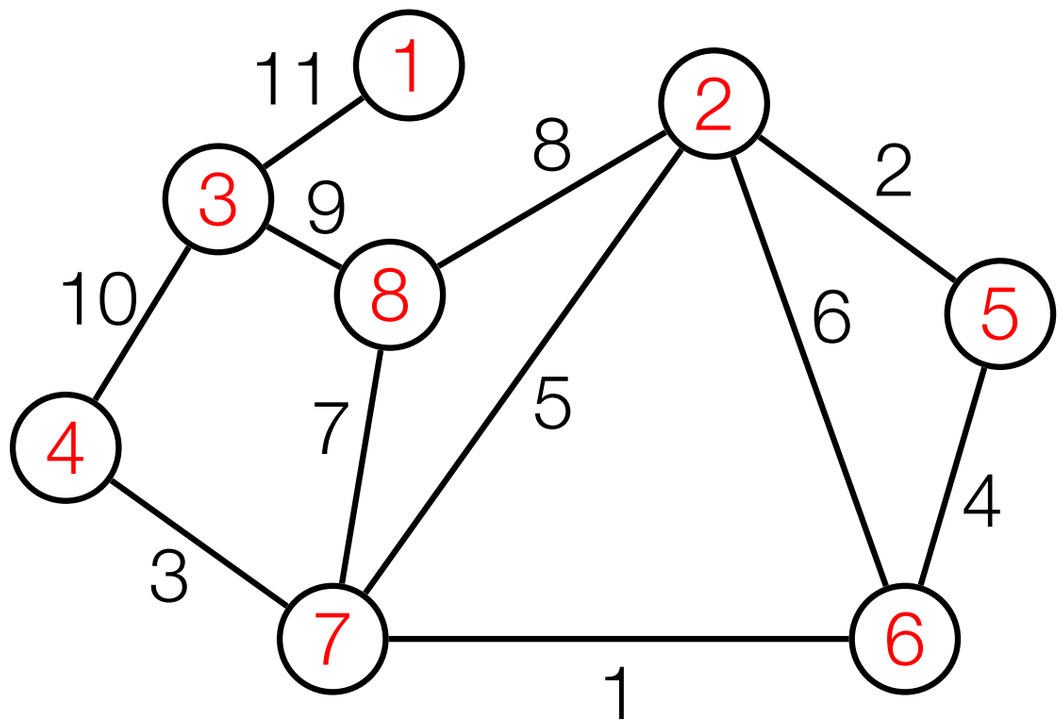


Prize-Collecting Steiner Tree

Generalization of the **Steiner tree** problem

Every node has a given prize π.



Goal: find a tree T minimizing $\sum_{v \notin V_T} \pi(v) + \sum_{e \in E_T} c(e)$

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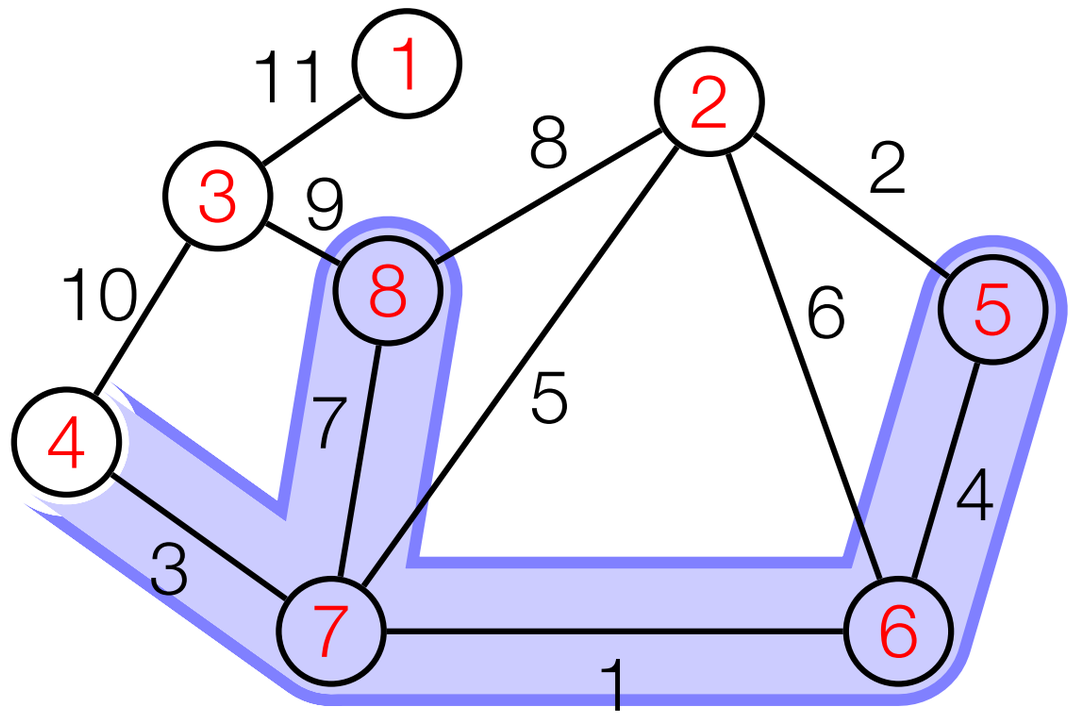

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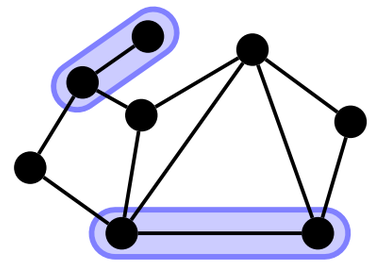
Connection to Graph Sparsity

Starting point: Goemans-Williamson approximation scheme

- Generalize to Steiner **forests**



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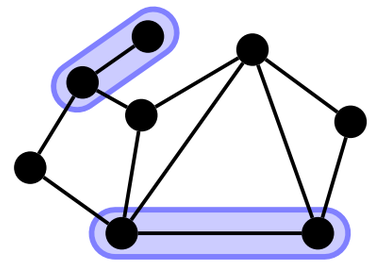
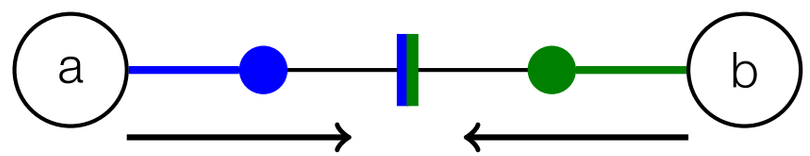


- Develop a **nearly-linear time** and **practical** algorithm



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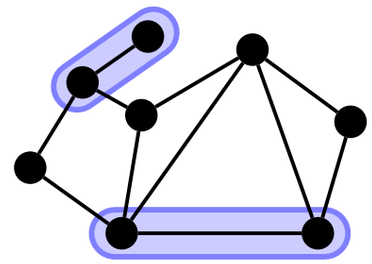

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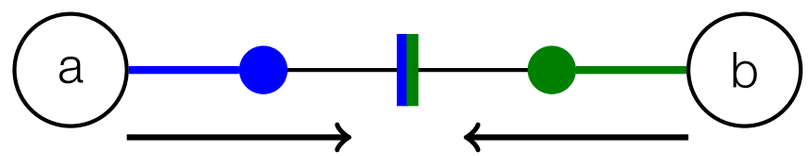

- **Reduce** graph sparsity projection to a sequence of PCSF instances

$$\sum_{v \notin V_T} \pi(v) + \lambda \cdot \sum_{e \in E_T} c(e)$$

Estimation Guarantee

Setup: $$y = X\theta^* + e$$

If X is a restricted isometry for graph-sparse vectors, projected gradient descent converges in $O(\log \|\theta^*\| / \|e\|)$ iterations and finds an estimate $\hat{\theta}$ such that:

$$\|\hat{\theta} - \theta^*\| \leq O(\|e\|)$$

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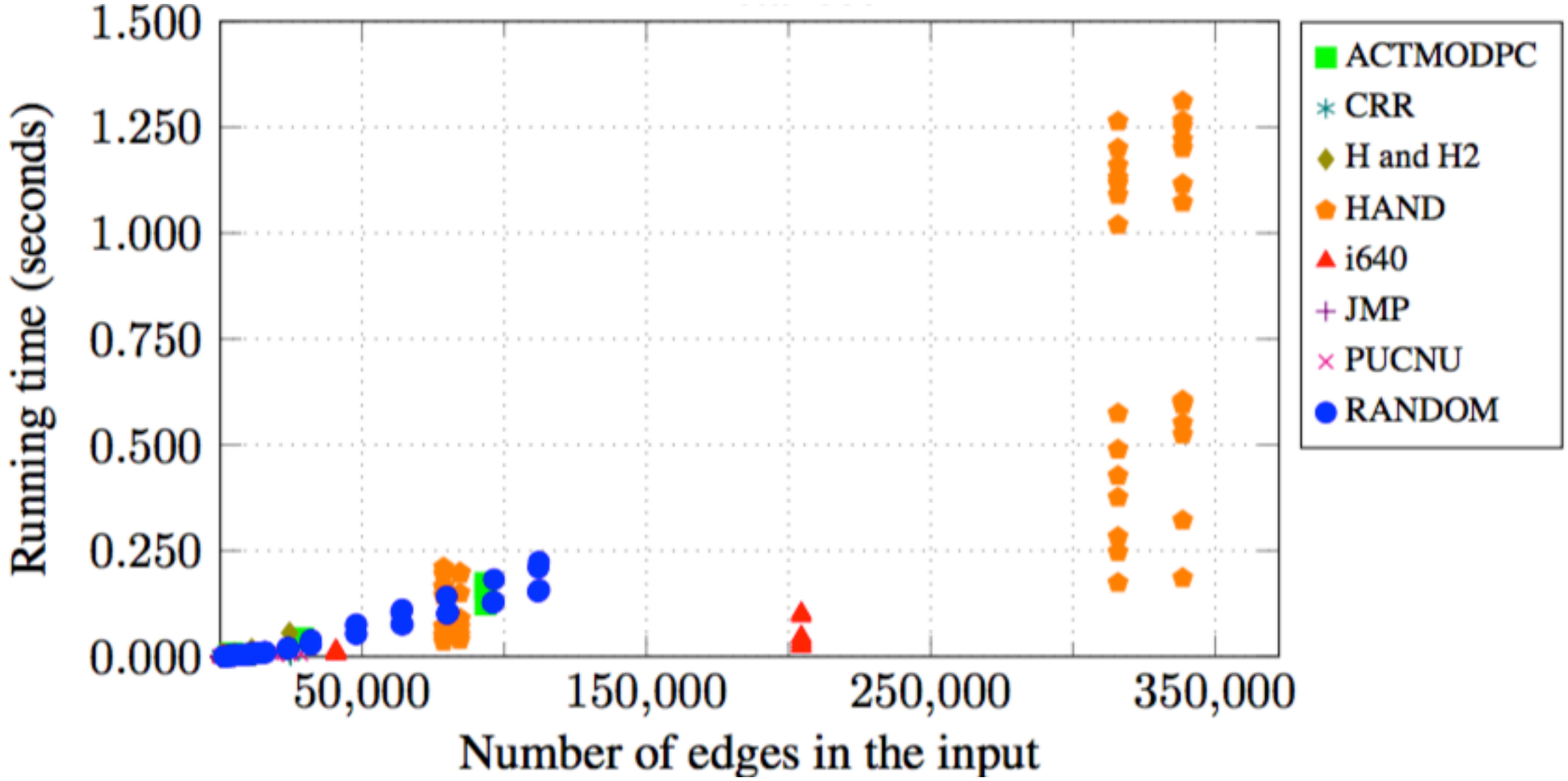
Same guarantee for approximate and exact projections.

Experiments: Prize Collecting Steiner Forest

Running time on instance of the 2014 DIMACS challenge.

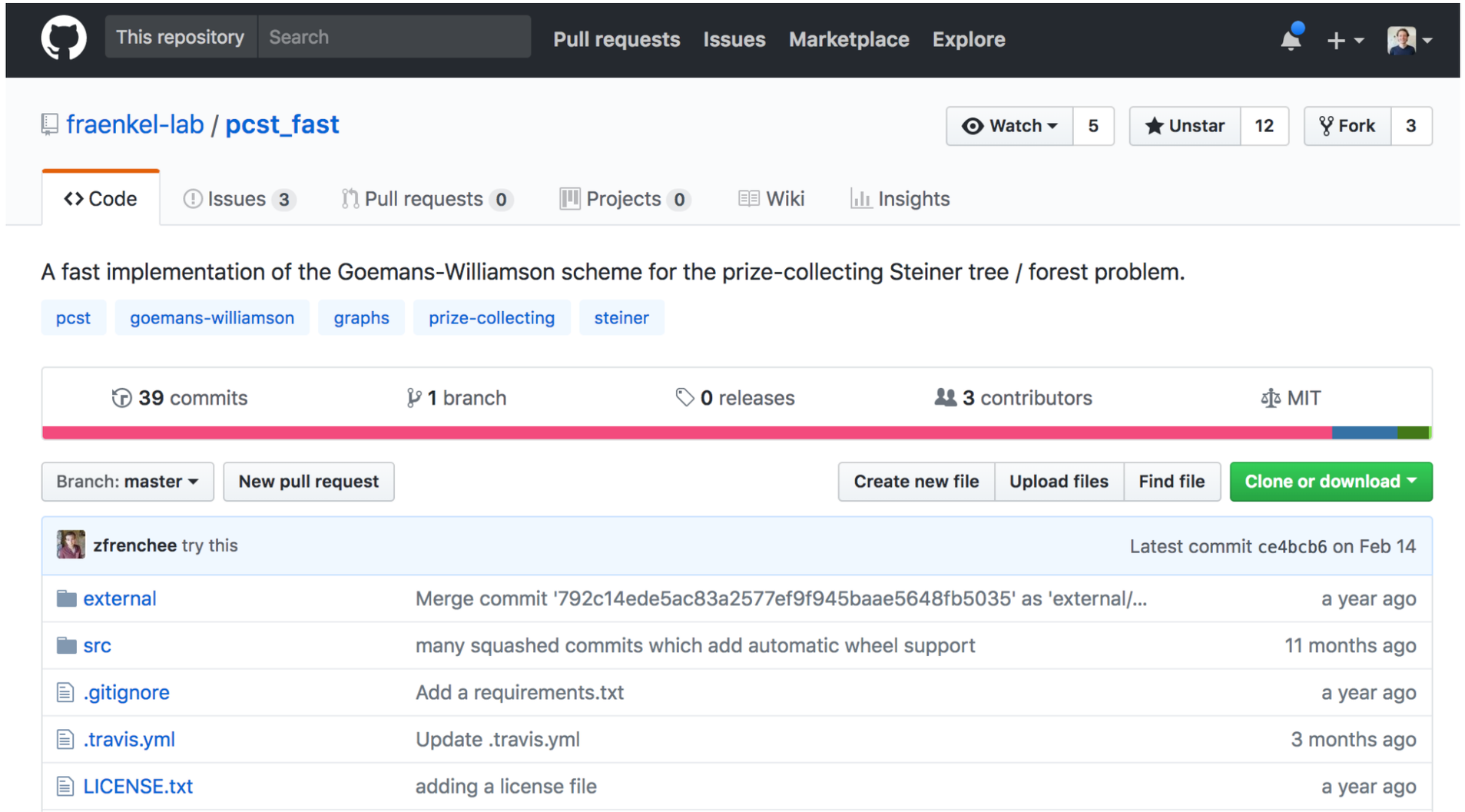


→ **Nearly-linear** scaling with number of edges.

Experiments: Prize collecting Steiner Forest

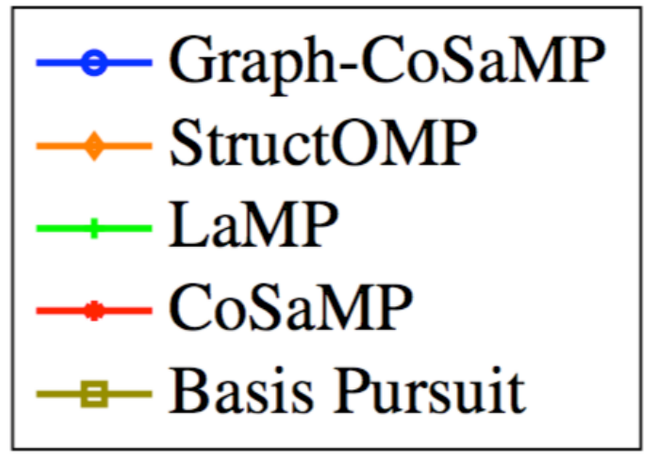
Algorithm	Solution value	Time
Hegde, Indyk, Schmidt	5601.8	**0.2**
mozartballs	5058.5	122.1
staynerd	**5057.4**	143.0
polito	5130.6	160.1
scipjack	5903.5	1052.3
Althaus-Blumenstock	5831.9	2113.5
KTS	5129.0	4842.1
heinz-dc	5695.5	6420.0

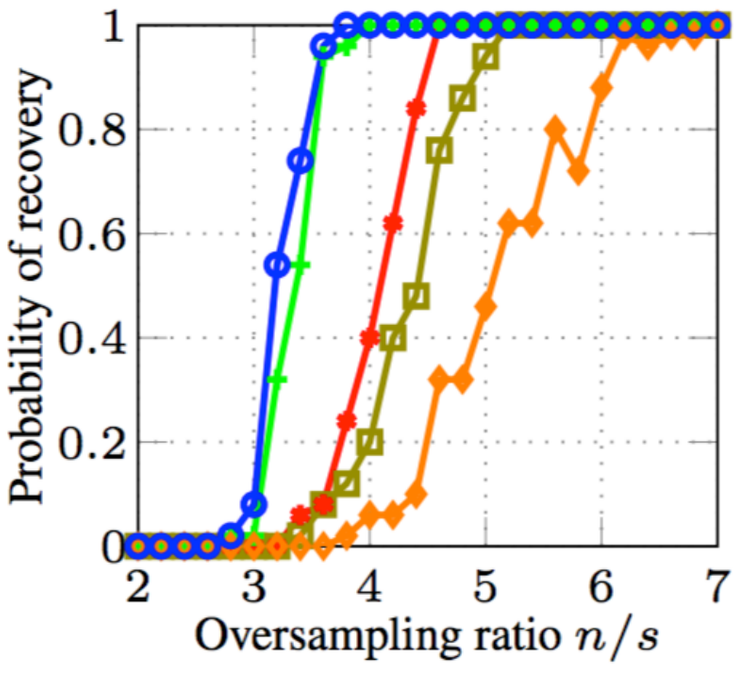
Code for PCSF

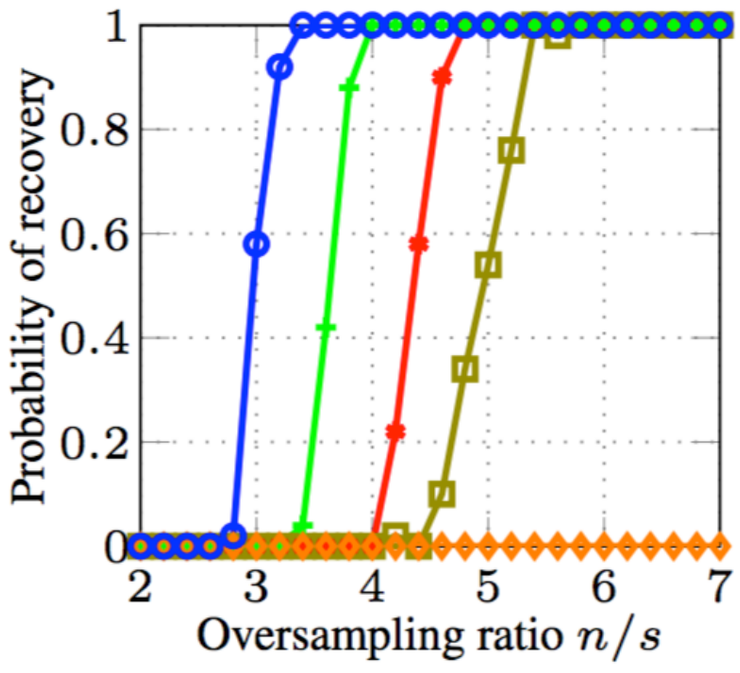


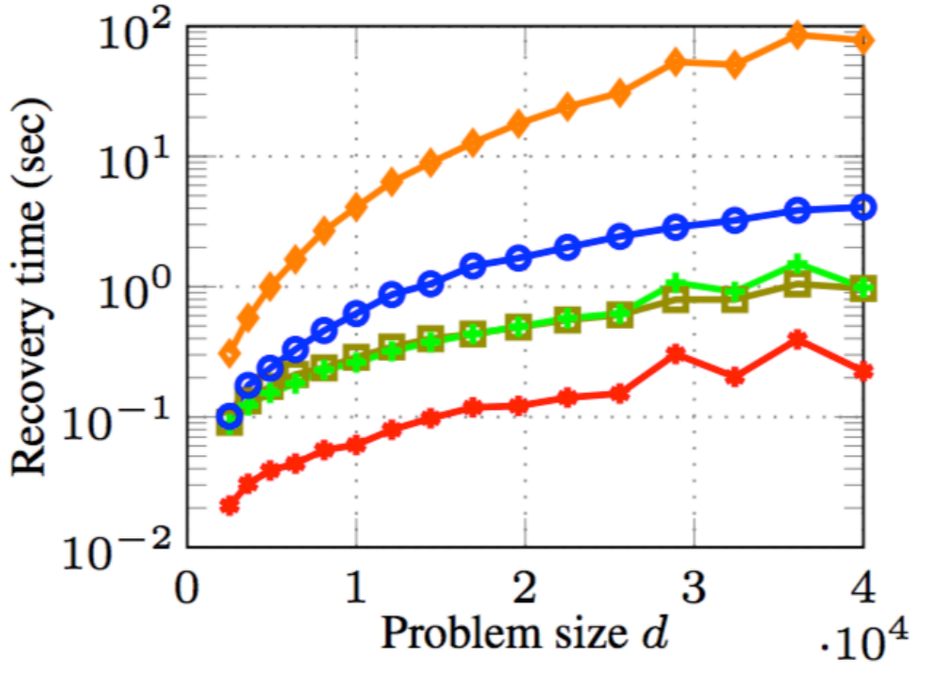
- C++ implementation with Python interface
- Has unit tests
- `pip install pcst_fast`

Compressive Sensing Experiments





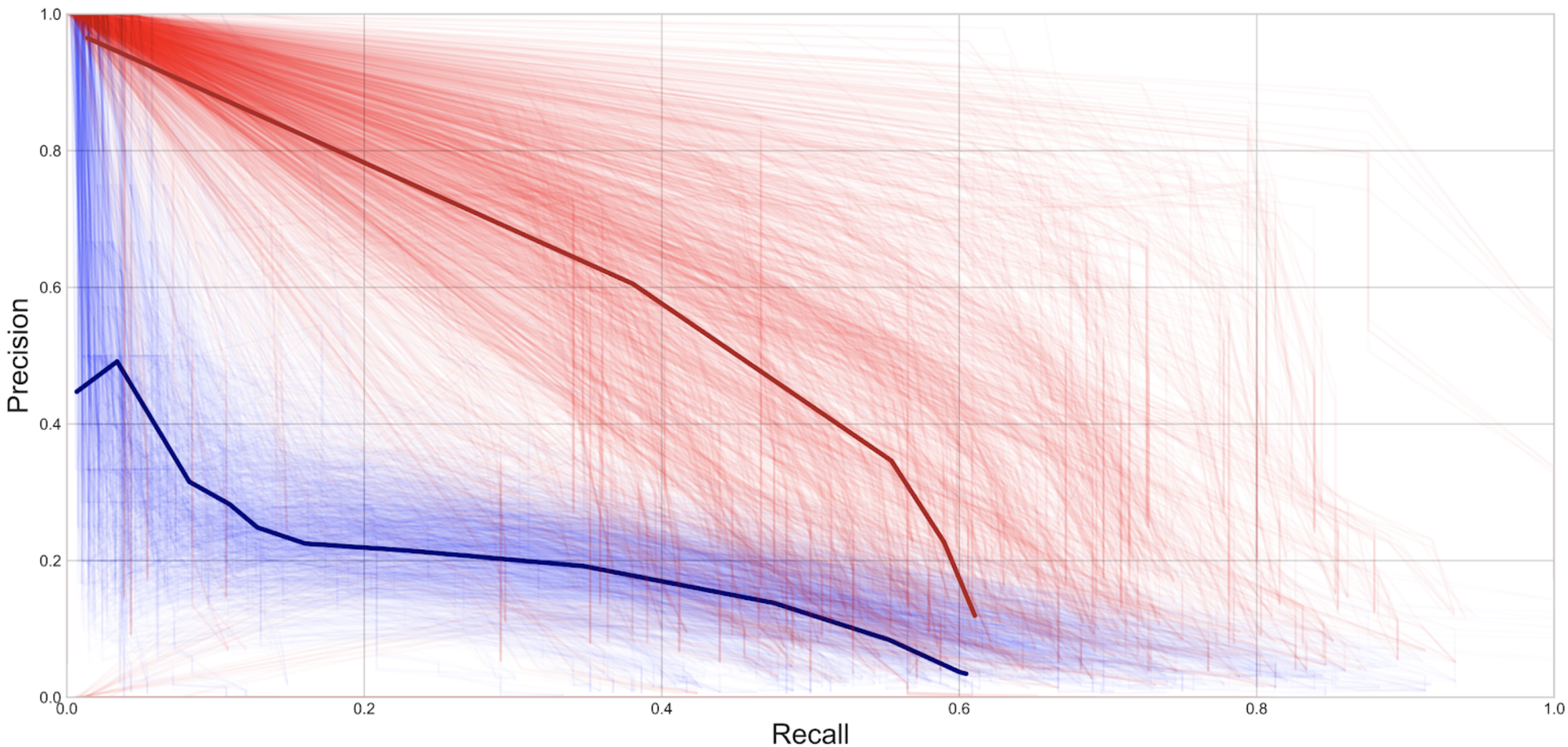




Graph-Sparse Linear Regression

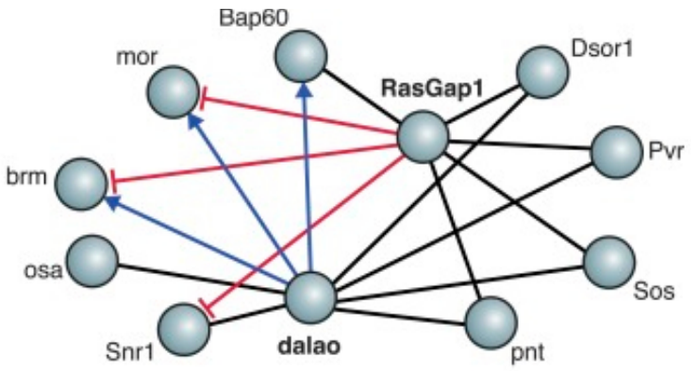
Support recovery on semi-synthetic data.

Graph-sparsity
Lasso



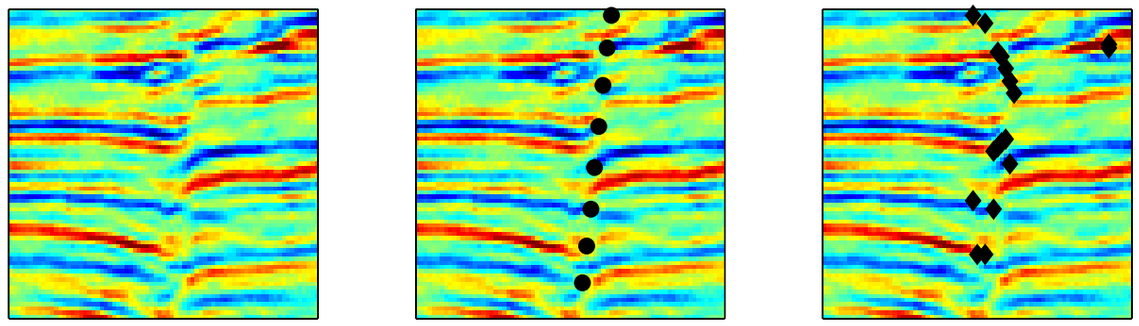
Code on github (but not production-ready yet).

Applications of PCSF



Omics Integrator

Outage Detection
in Power Networks



Computational Geophysics

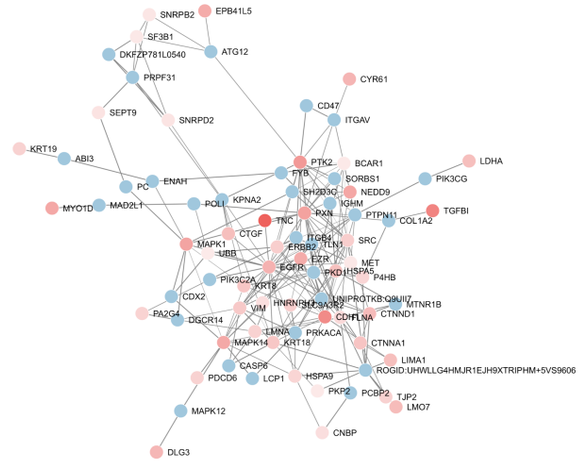
Event Detection
in Social Networks

Computational Biology

Conclusions

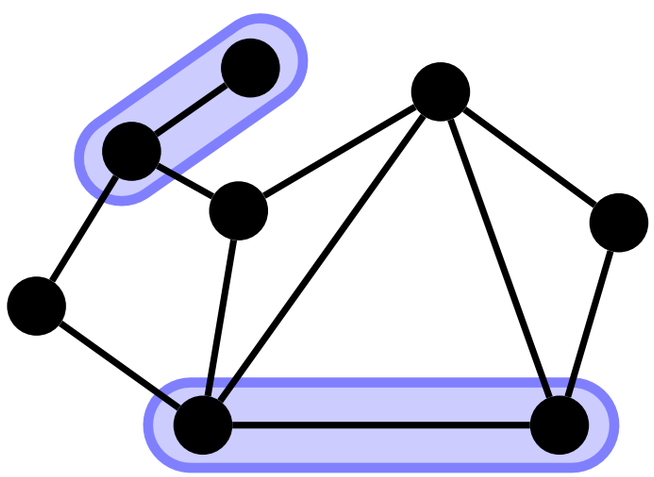
Linear regression with graph constraints

→ Find a predictive subgraph.



Fast, rigorous approximations for PCSF

→ Collect large node prizes for little edge cost.



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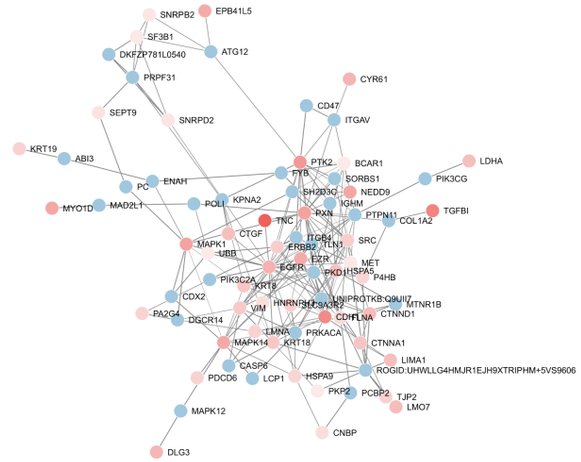

Fast, rigorous approximations for PCSF

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Future directions

- Applications?
- Other graph constraints in regression?