Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

Submodularity in Machine Learning

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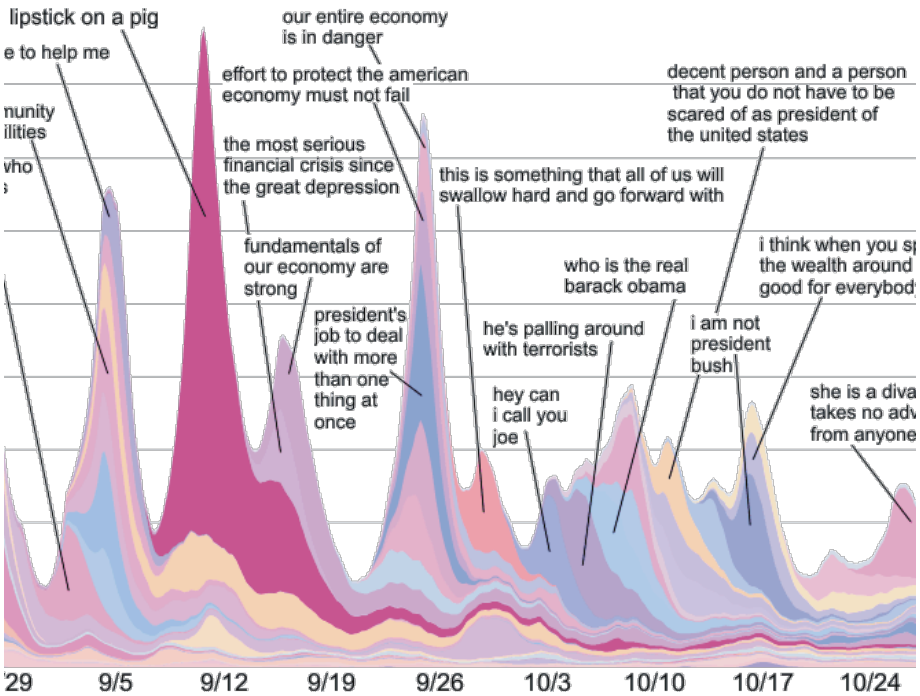
Machine Learning Summer School 2013
Tübingen

Network Inference

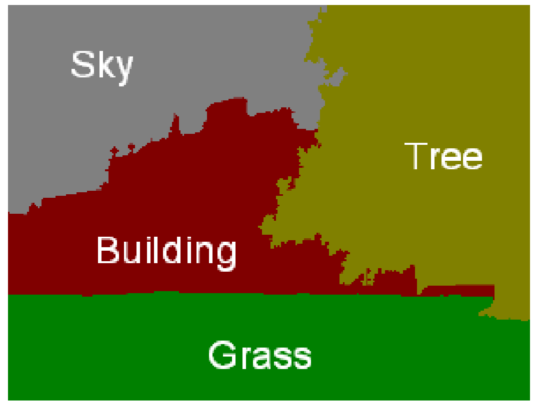


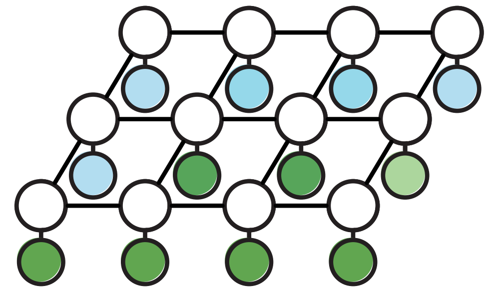
How to learn who influences whom?

Summarizing Documents

How to select representative sentences?

MAP inference





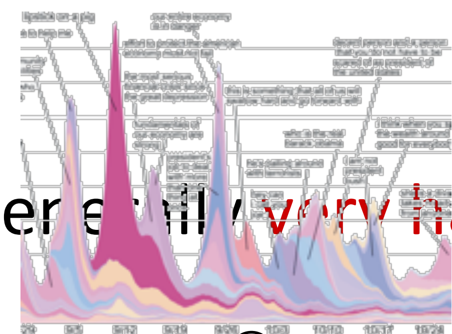
$$\max_x \; p(x \mid z)$$

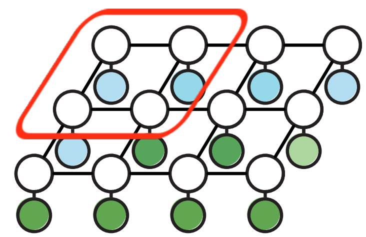
How find the MAP labeling in discrete graphical models *efficiently*?

What’s common?

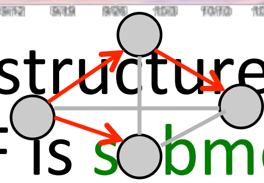
- Formalization:

  Optimize a set function F(S) under constraints





- generally very hard
- but: structure helps!
  … if F is submodular, we can …



  - solve optimization problems with strong guarantees
  - solve complex structured learning problems

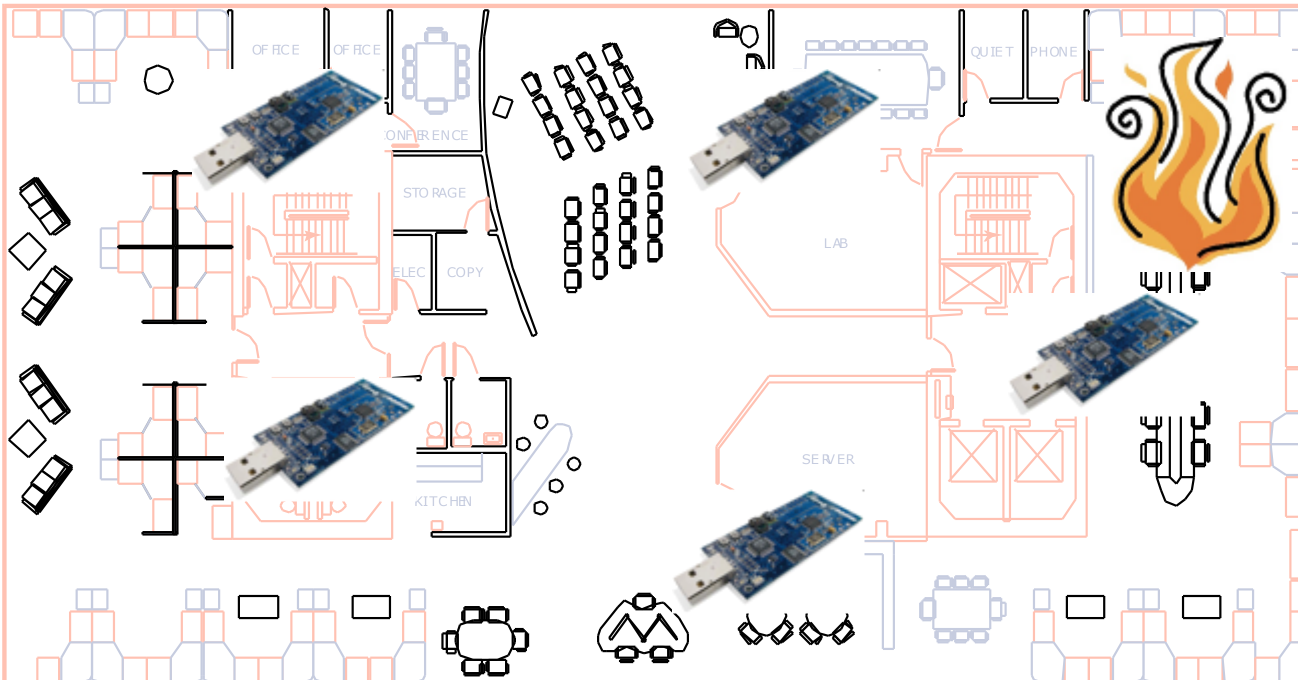
Outline

- What is submodularity?
- Optimization
  - Minimization
  - Maximization
- Applications
- Outlook and pointers

submodularity.org

slides, code, references, workshops, …

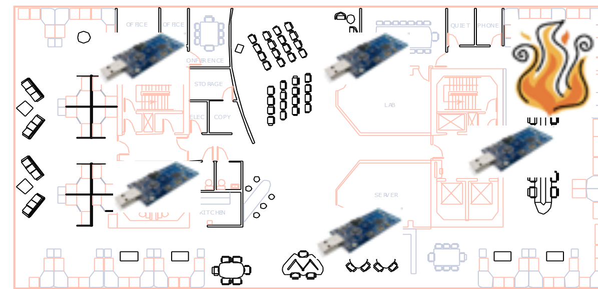
Example: placing sensors



Place sensors to monitor temperature

Set functions

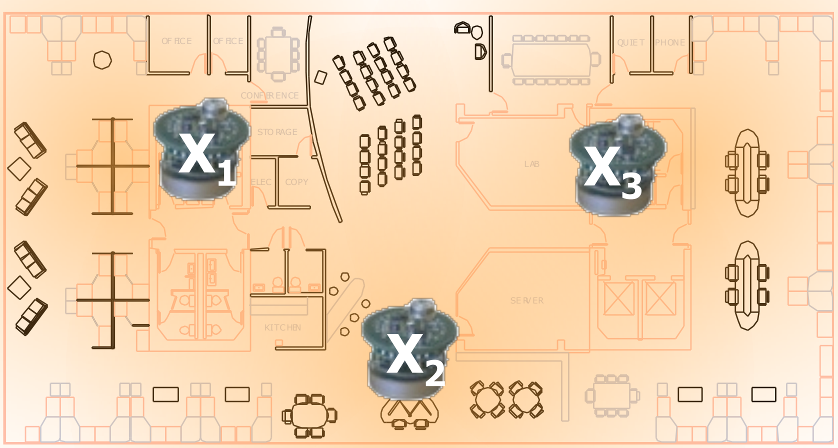
- finite ground set $V = \{1, 2, \ldots, n\}$
- set function $F : 2^V \to \mathbb{R}$



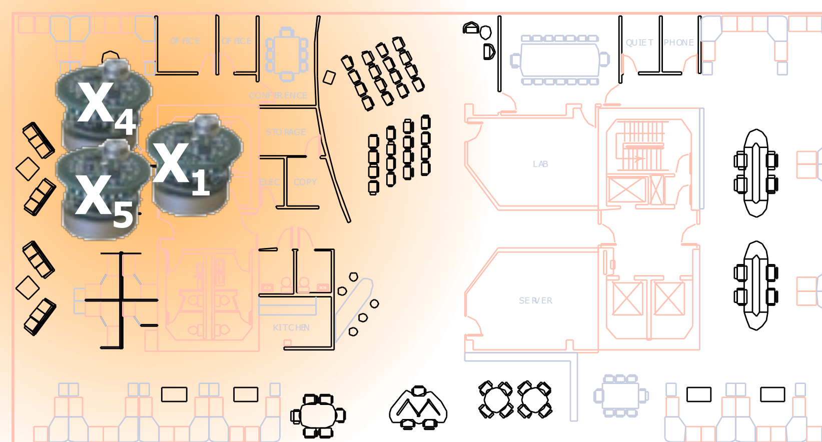
- will assume $F(\emptyset) = 0$ (w.l.o.g.)
- assume black box that can evaluate $F(A)$ for any $A \subseteq V$

Example: placing sensors

Utility $F(A)$ of having sensors at subset A of all locations



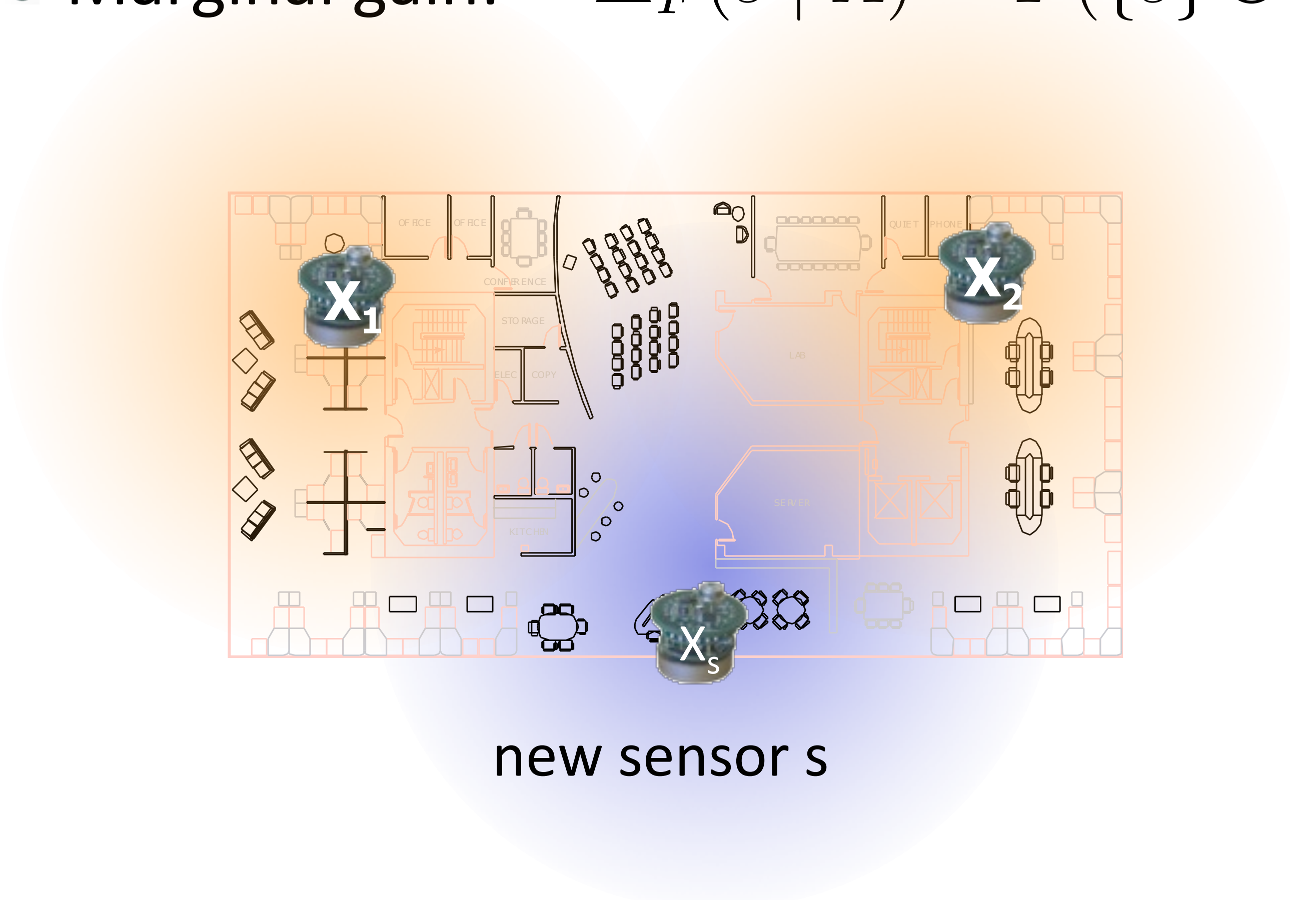
A={1,2,3}: Very informative
High value F(A)



A={1,4,5}: Redundant info
Low value F(A)

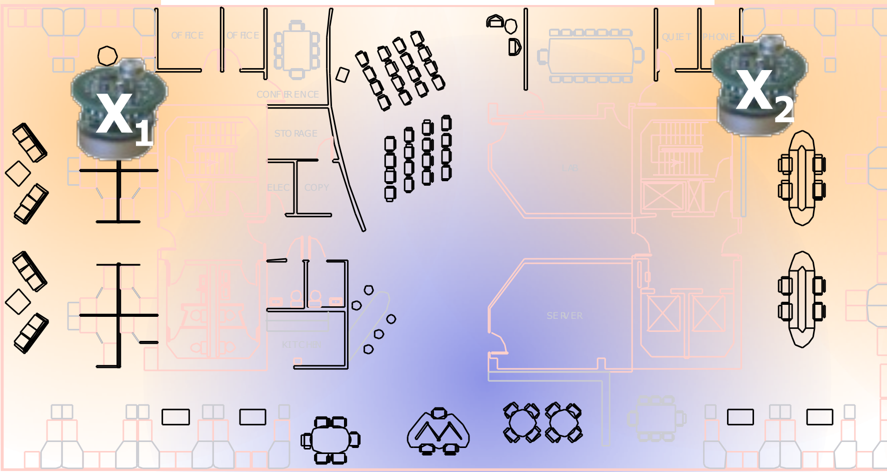
Marginal gain

- Given set function $F : 2^V \rightarrow \mathbb{R}$
- Marginal gain: $\Delta_F(s \mid A) = F(\{s\} \cup A) - F(A)$

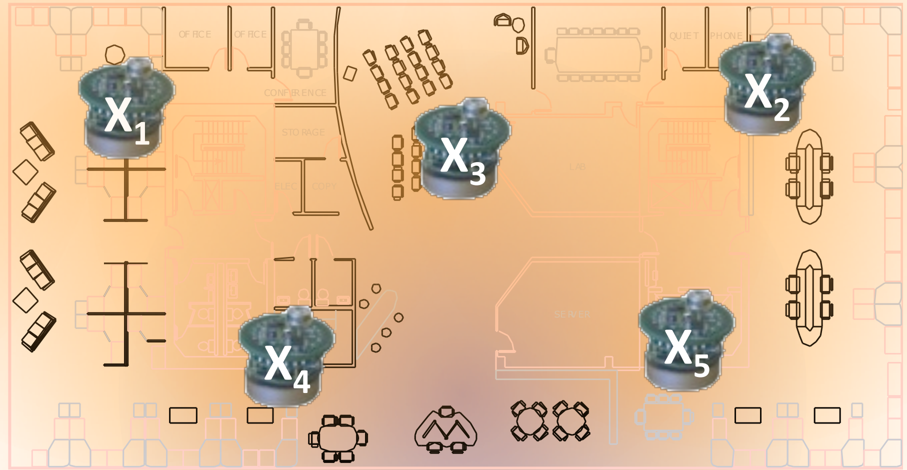


Decreasing gains: submodularity

placement A = {1,2}



placement B = {1,...,5}

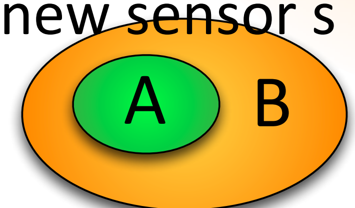


Big gain

new sensor s

small gain

+ • s



+ • s

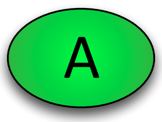
$$A \subseteq B$$
$$s \notin B$$

$$F(A \cup s) - F(A)$$

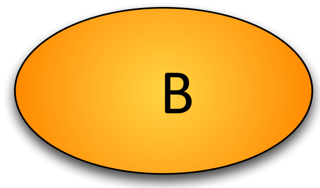
$$\Delta(s \mid A)$$

Equivalent characterizations

- Diminishing returns: for all $A \subseteq B$ and $s \notin B$



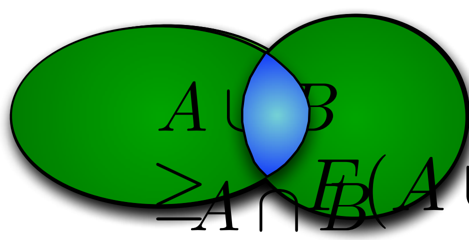
+ • s



+ • s

$$F(A \cup s) - F(A) \quad \geq \quad F(B \cup s) - F(B)$$

- Union-Intersection: for all $A, B \subseteq V$



$$F(A) + F(B) \geq F(A \cup B) + F(A \cap B)$$

Submodular, modular & supermodular

A set function F is called

- supermodular if -F is submodular
- modular if F is both submodular and supermodular. Such functions can be written as

$$F(A) = \sum_{i \in A} w_i$$

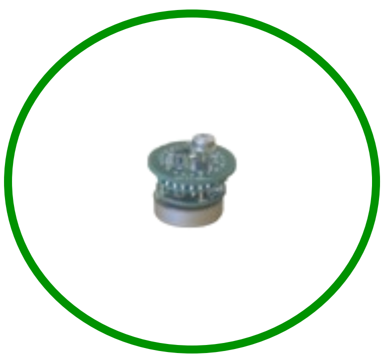
Questions

How do I prove my problem is submodular?

Why is submodularity useful?

Example: Set cover

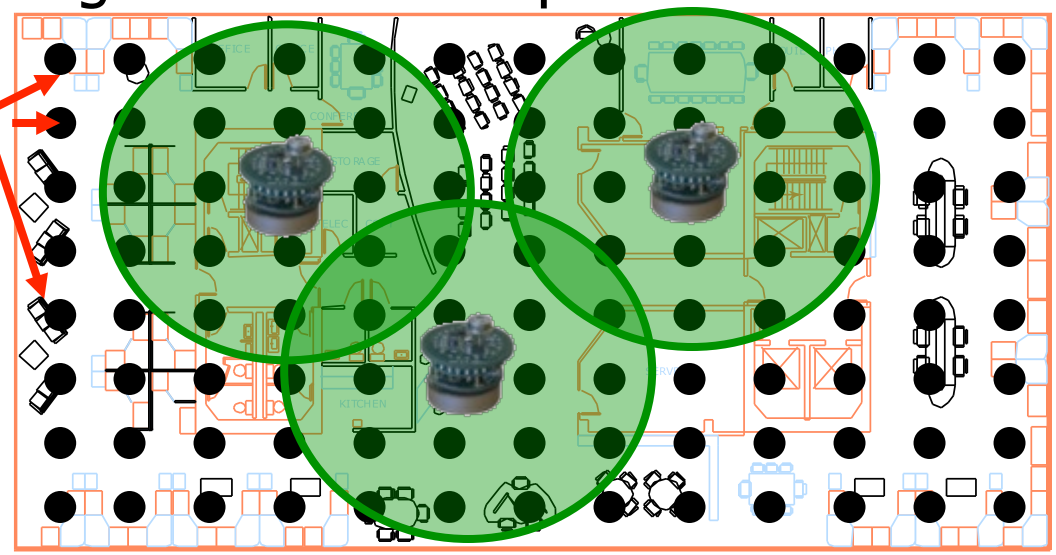
place sensors in building



Node predicts values of positions with some radius

goal: cover floorplan with discs

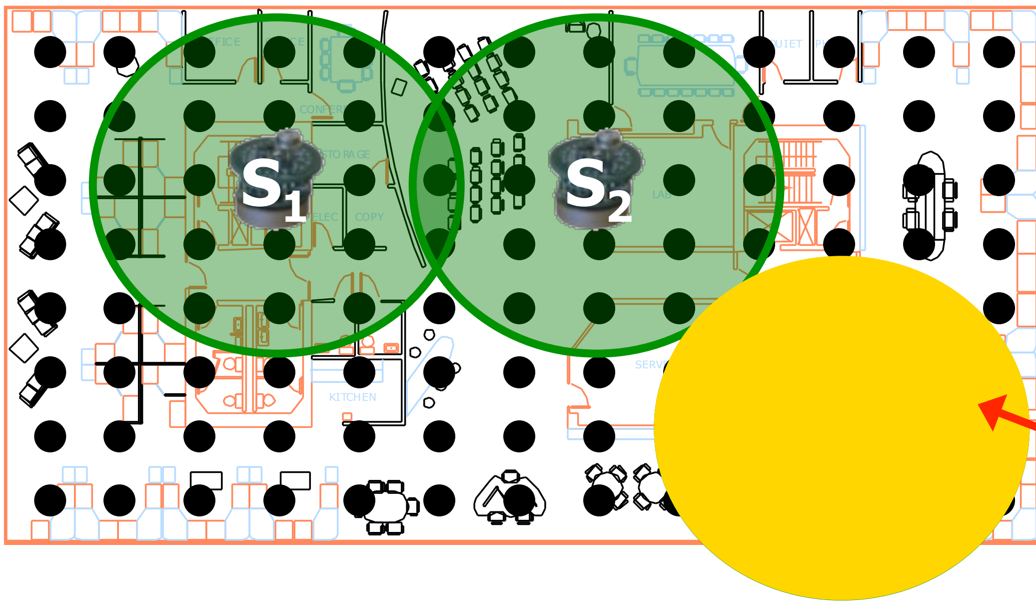
Possible locations V



$A \subseteq V$: $F(A) =$
"area covered by sensors placed at A"

Formally:
Finite set W, collection of n subsets $S_i \subseteq W$
For $A \subseteq V$ define $F(A) = |\bigcup_{i \in A} S_i|$

Set cover is submodular

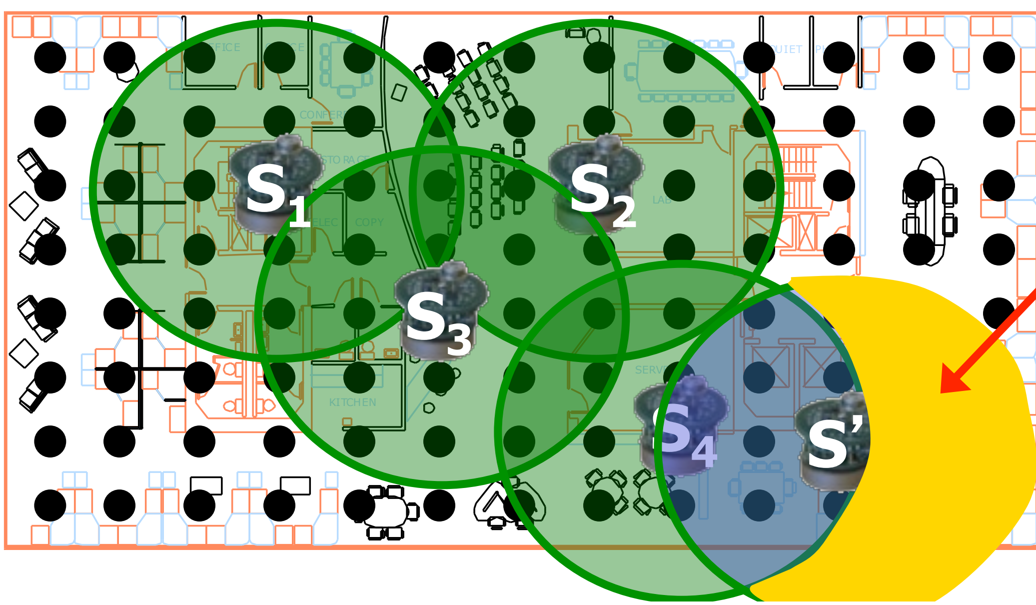


$A=\{s_1,s_2\}$

$F(A \cup \{s'\}) - F(A)$

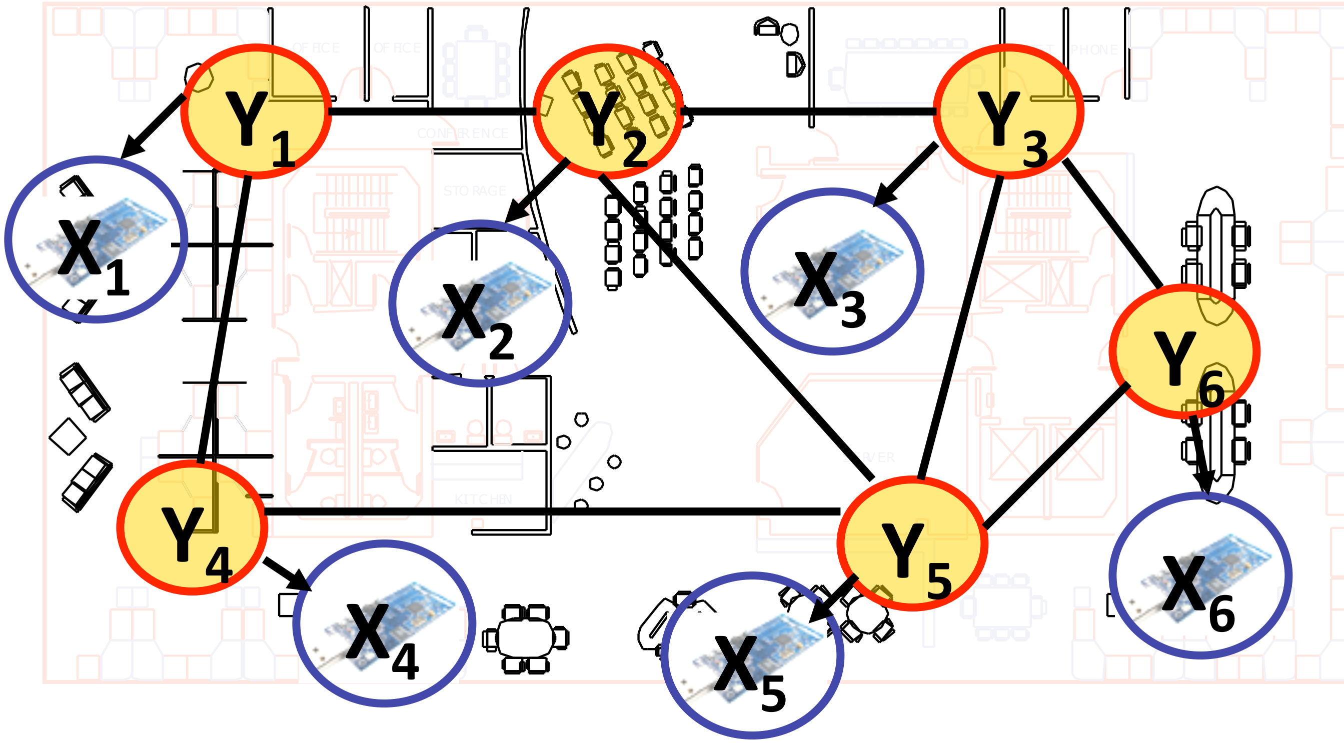
$\geq$

$F(B \cup \{s'\}) - F(B)$



$B = \{s_1,s_2,s_3,s_4\}$

More complex model for sensing



Y_s: temperature at location s

X_s: sensor value at location s

$X_s = Y_s + \text{noise}$

Joint probability distribution

$$P(X_1,\ldots,X_n,Y_1,\ldots,Y_n) = \underbrace{P(Y_1,\ldots,Y_n)}_{\textbf{Prior}}\ \underbrace{P(X_1,\ldots,X_n \mid Y_1,\ldots,Y_n)}_{\textbf{Likelihood}}$$

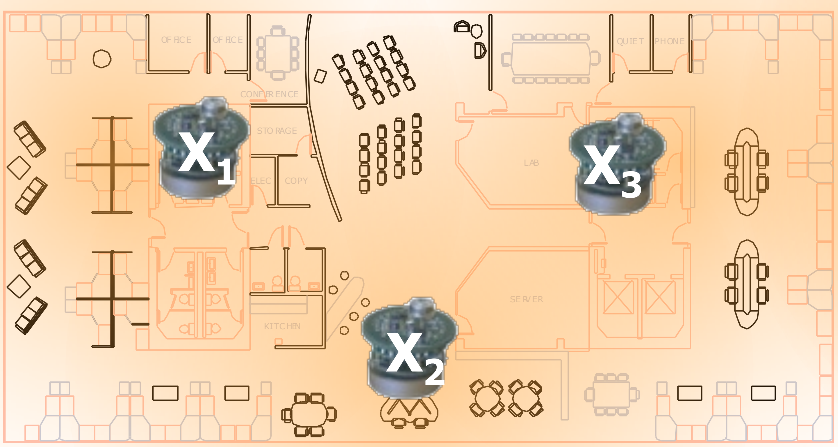
Example: Sensor placement

Utility of having sensors at subset A of all locations

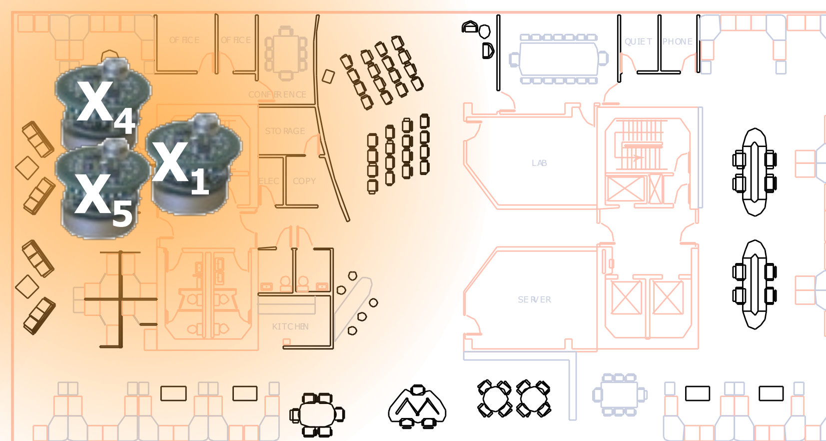
$$F(A) = H(\mathbf{Y}) - H(\mathbf{Y} \mid \mathbf{X}_A)$$

Uncertainty
about temperature Y
before sensing

Uncertainty
about temperature Y
after sensing



A={1,2,3}: High value F(A)



A={1,4,5}: Low value F(A)

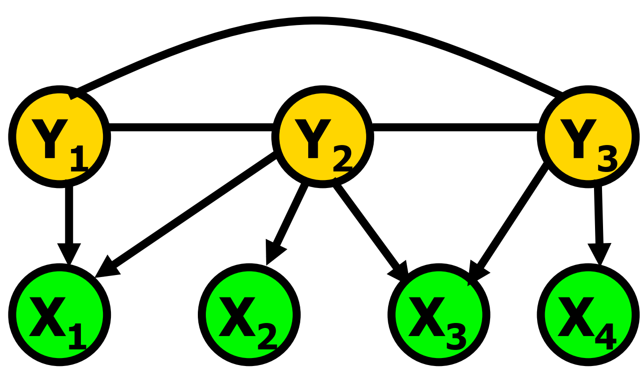
Submodularity of Information Gain

$Y_1,\ldots,Y_m$, X_1, …, X_n discrete RVs

$F(A) = I(Y; X_A) = H(Y)\text{-}H(Y \mid X_A)$

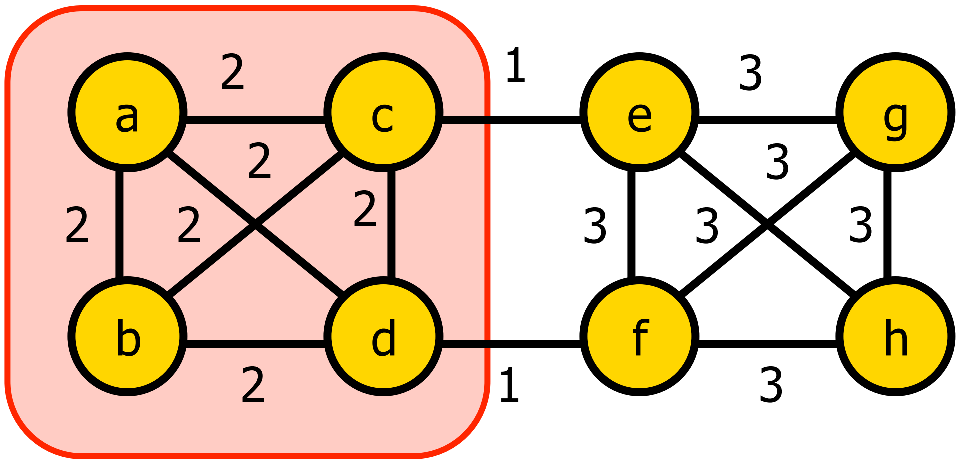
- F(A) is NOT always submodular

If X_i are all conditionally independent given Y,
then F(A) is submodular! [Krause & Guestrin `05]



Proof:
"information never hurts"

Another example: Cut functions



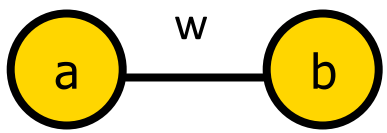
V={a,b,c,d,e,f,g,h}

$$F(A) = \sum_{s \in A, t \notin A} w_{s,t}$$

–

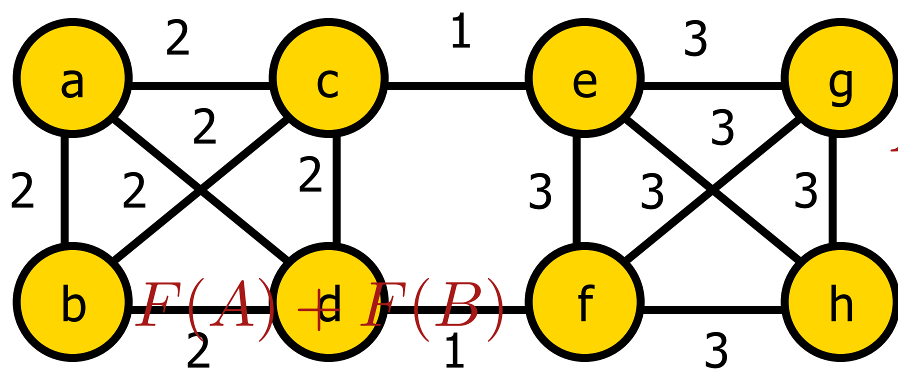
Cut function is submodular!

Why are cut functions submodular?



	S	F_{ab}(S)
$A \cap B$	{}	0
A	{a}	w
B	{b}	w
$A \cup B$	{a,b}	0

Submodular if w ≥ 0!



$$F(A) + F(B) \geq F(A \cap B) + F(A \cup B)$$

$$F(S) = \sum_{(i,j)\in E} \underbrace{F_{i,j}(S \cap \{i,j\})}_{}$$

Cut function in subgraph {i,j}

➔ Submodular!

Closedness properties

$F_1,\ldots,F_m$ submodular functions on V and $\lambda_1,\ldots,\lambda_m \geq 0$

Then: $F(A) = \sum_i \lambda_i F_i(A)$ is submodular

Submodularity closed under nonnegative linear combinations!

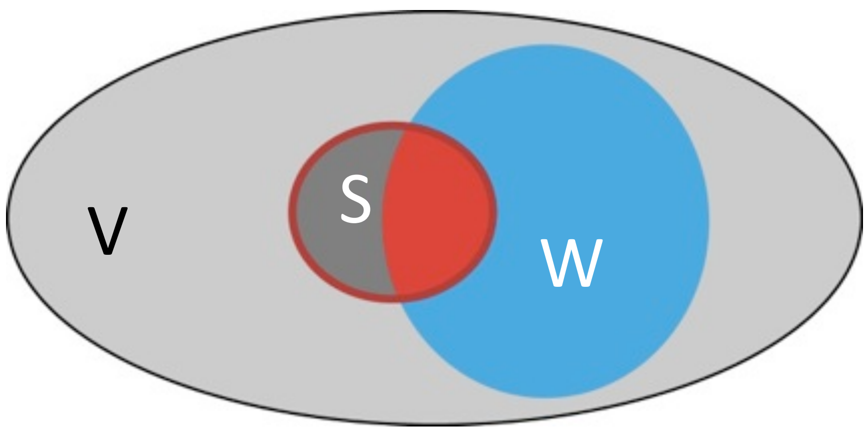
Extremely useful fact:

- $F_\theta(A)$ submodular $\Rightarrow$ $\sum_\theta P(\theta) F_\theta(A)$ submodular!
- Multicriterion optimization
- A basic proof technique! ☺

Other closedness properties

- Restriction: F(S) submodular on V, W subset of V

  Then $F'(S) = F(S \cap W)$ is submodular



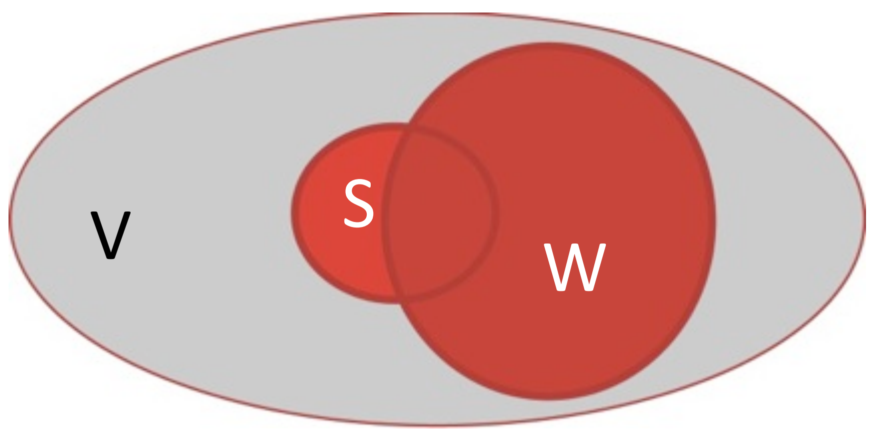
Other closedness properties

- Restriction: F(S) submodular on V, W subset of V

  Then $F'(S) = F(S \cap W)$ is submodular

- Conditioning: F(S) submodular on V, W subset of V

  Then $F'(S) = F(S \cup W)$ is submodular



Other closedness properties

- Restriction: F(S) submodular on V, W subset of V

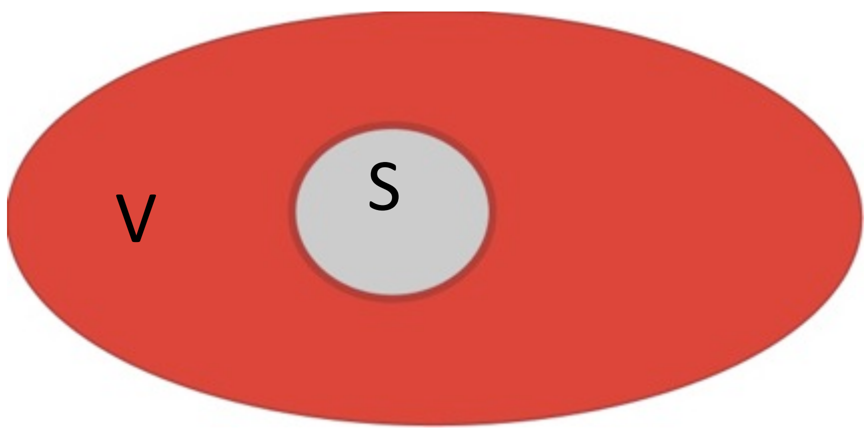
  Then $F'(S) = F(S \cap W)$ is submodular

- Conditioning: F(S) submodular on V, W subset of V

  Then $F'(S) = F(S \cup W)$ is submodular

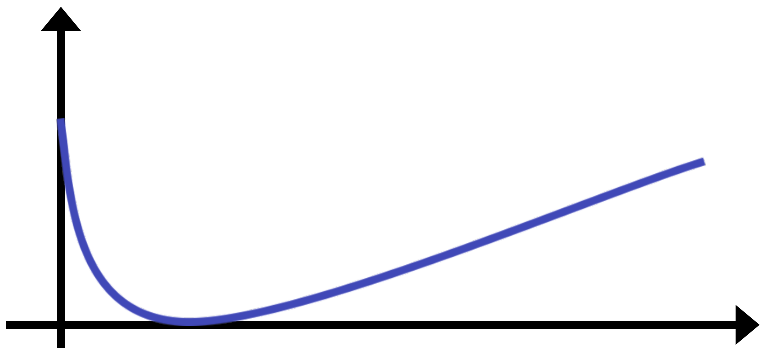
- Reflection: F(S) submodular on V

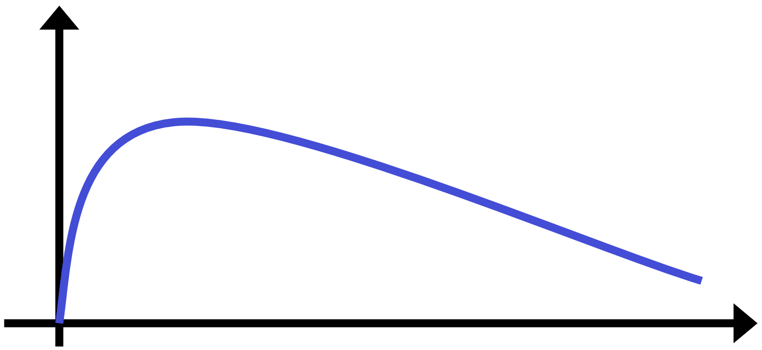
  Then $F'(S) = F(V \setminus S)$ is submodular



Submodularity …

discrete convexity ….

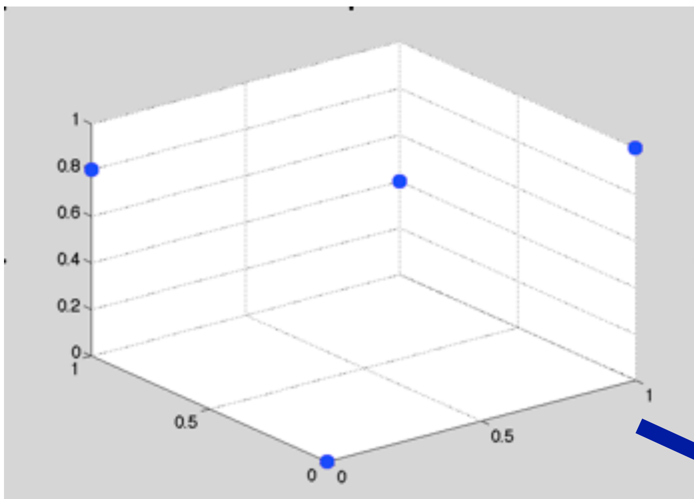


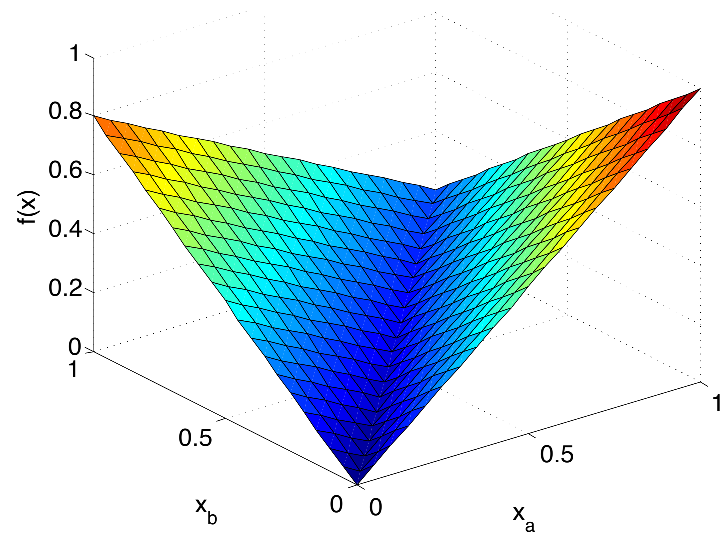


… or concavity?

Convex aspects

- convex extension
  - duality
  - efficient minimization





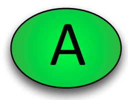
But this is only half of the story…

Concave aspects

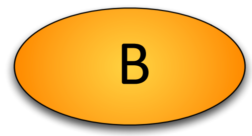
- submodularity:

$A \subseteq B, \;\; s \notin B:$

$$F(A \cup s) - F(A) \quad \geq \quad F(B \cup s) - F(B)$$



+ • s

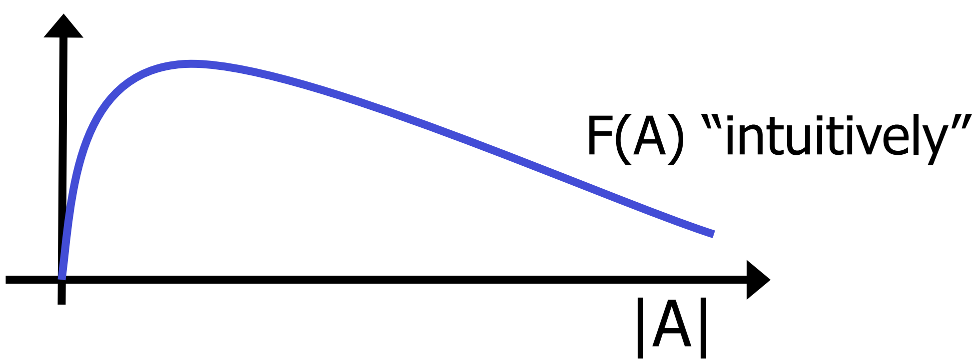


+ • s

- concavity:

$a \leq b, \;\; s > 0:$

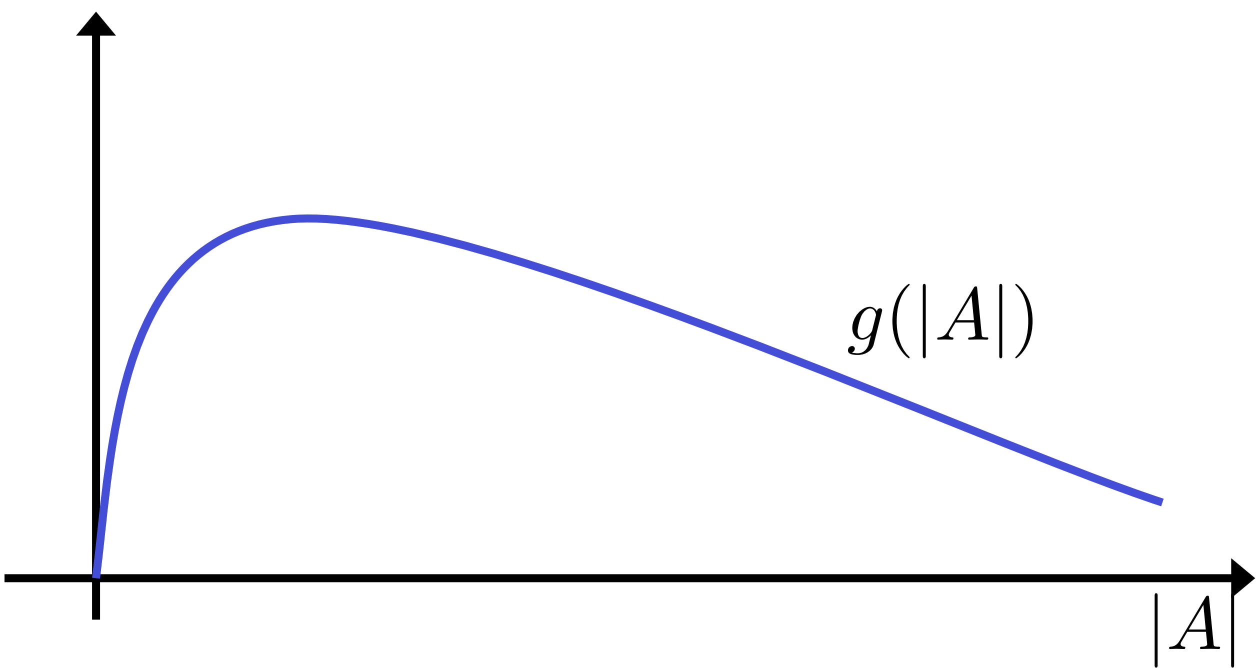
$$f(a+s) - f(a) \quad \geq \quad f(b+s) - f(b)$$



Submodularity and concavity

- suppose $g : \mathbb{N} \to \mathbb{R}$ and $F(A) = g(|A|)$

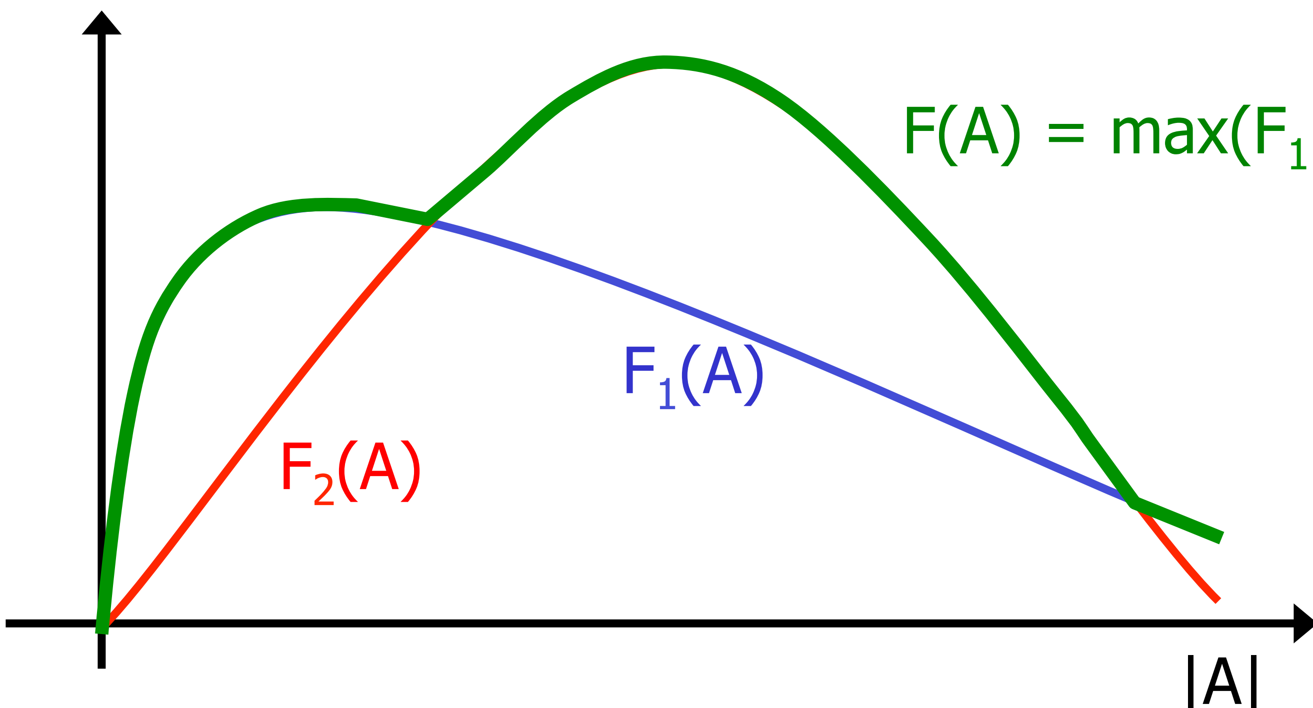
$F(A)$ submodular *if and only if* ... g is concave



Maximum of submodular functions

- $F_1(A), F_2(A)$ submodular. What about

$$F(A) = \max\{\, F_1(A), F_2(A) \,\} \quad ?$$



max(F_1,F_2) not submodular in general!

Minimum of submodular functions

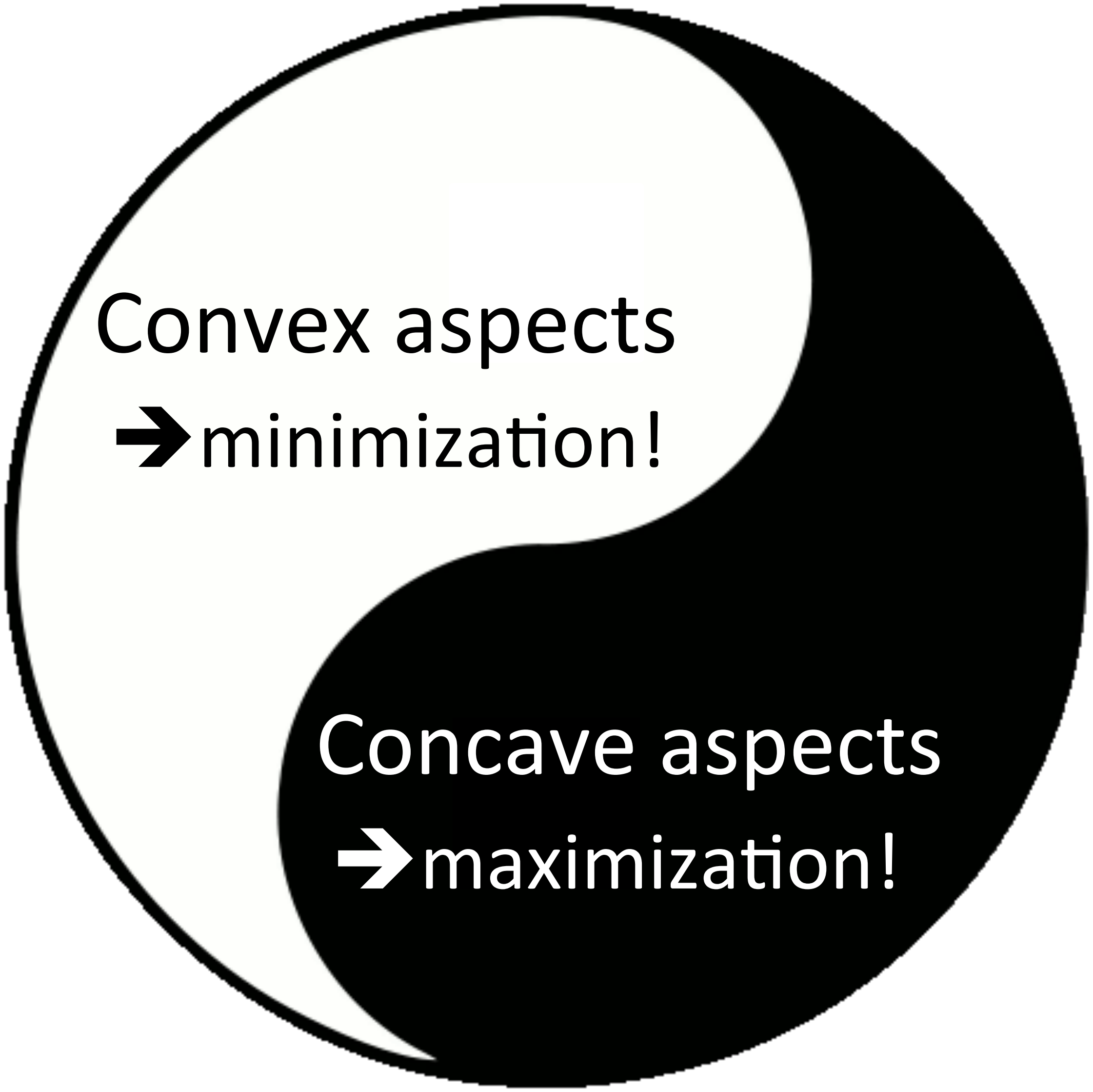
Well, maybe $F(A) = \min(F_1(A),F_2(A))$ instead?

	$F_1(A)$	$F_2(A)$
{}	0	0
{a}	1	0
{b}	0	1
{a,b}	1	1

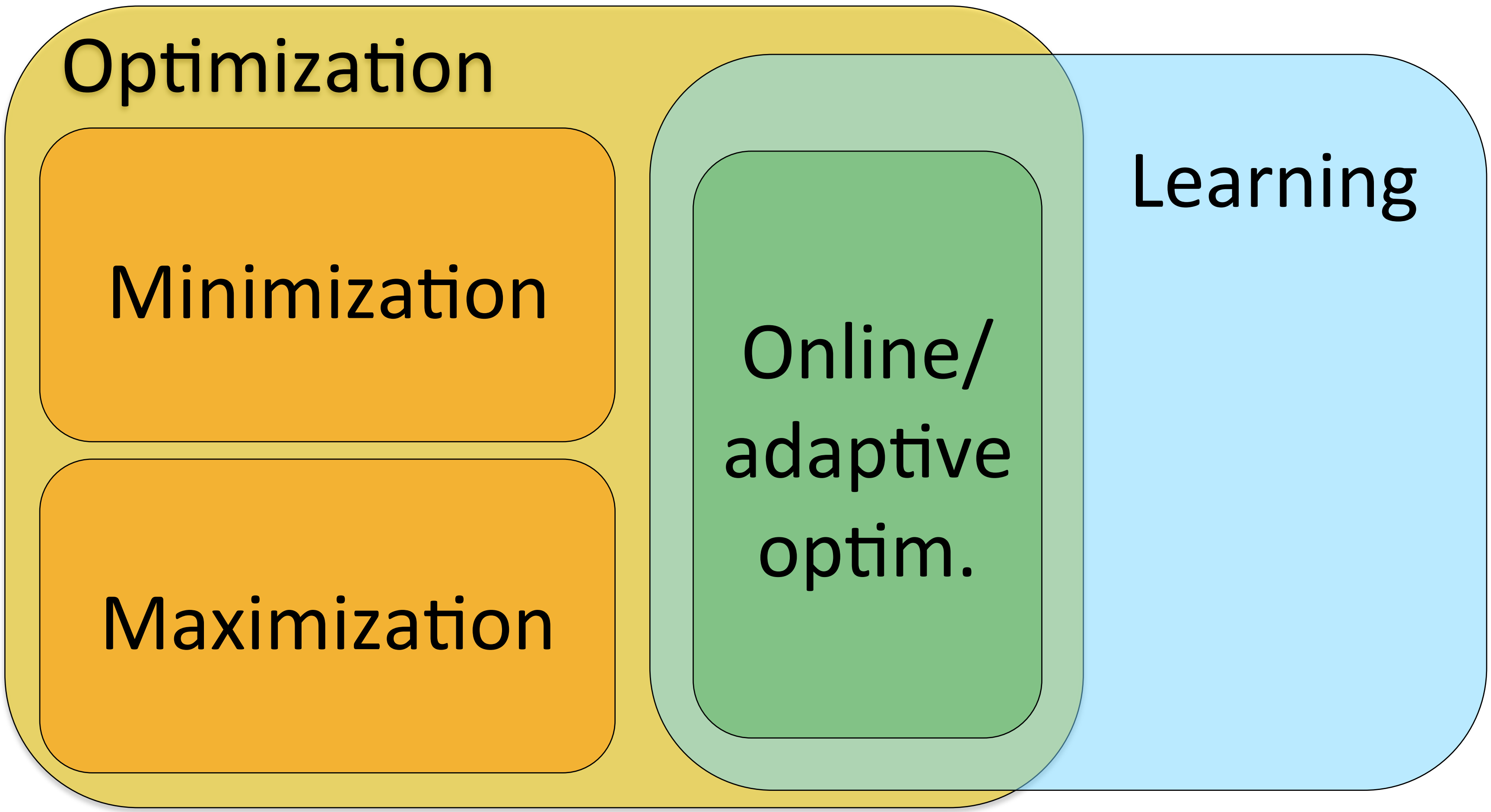
$$F(\{b\}) - F(\{\}) = 0$$
$$<$$
$$F(\{a,b\}) - F(\{a\}) = 1$$

$\min(F_1,F_2)$ not submodular in general!

Two faces of submodular functions



What to do with submodular functions



Here we focus on optimization & applications

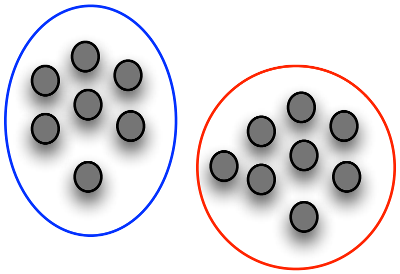
Optimization

Minimization

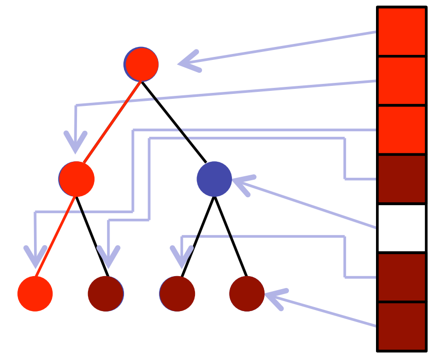
Maximization

Minimization and maximization not the same??

Submodular minimization

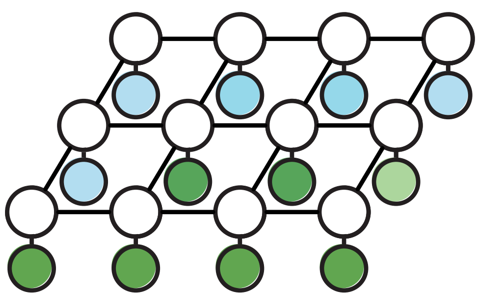


clustering

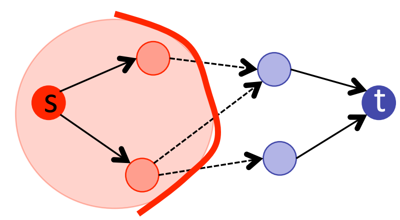


structured sparsity regularization

$$\min_{S \subseteq V} F(S)$$



MAP inference



minimum cut

Submodular minimization

$$\min_{S \subseteq V} F(S)$$

➔ submodularity and convexity

Set functions and energy functions

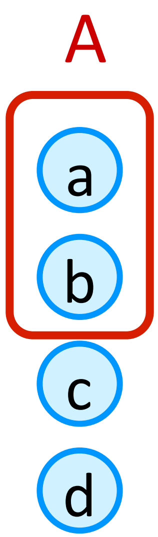
any set function

with $|V| = n$

... is a function on binary vectors!

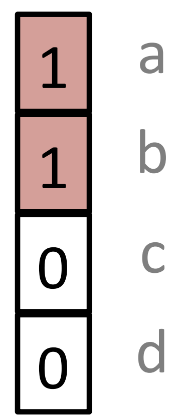
$$F : 2^V \to \mathbb{R}$$

$$F : \{0,1\}^n \to \mathbb{R}$$



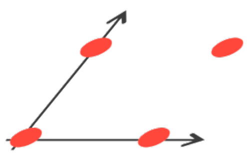
$\hat{=}$

$$x = e_A$$



pseudo-boolean function

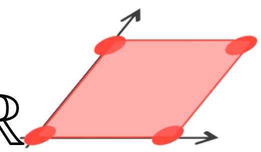
Submodularity and convexity



extension

$$f : [0,1]^n \to \mathbb{R}$$

$$F : \{0,1\}^n \to \mathbb{R}$$



Lovász extension

$$f(x) = \max_{y \in P_F} x \cdot y$$

convex

Lovász, 1982

- minimum of *f* is a minimum of F
- submodular minimization as convex minimization: polynomial time!

Grötschel, Lovász, Schrijver 1981

Submodularity and convexity

extension

$F : \{0,1\}^n \to \mathbb{R}$ $\longrightarrow$ $f : [0,1]^n \to \mathbb{R}$

Lovász extension

$$f(x) = \max_{y \in P_F} x \cdot y$$

convex

Lovász, 1982

- minimum of *f* is a minimum of F
- submodular minimization as convex minimization: polynomial time!

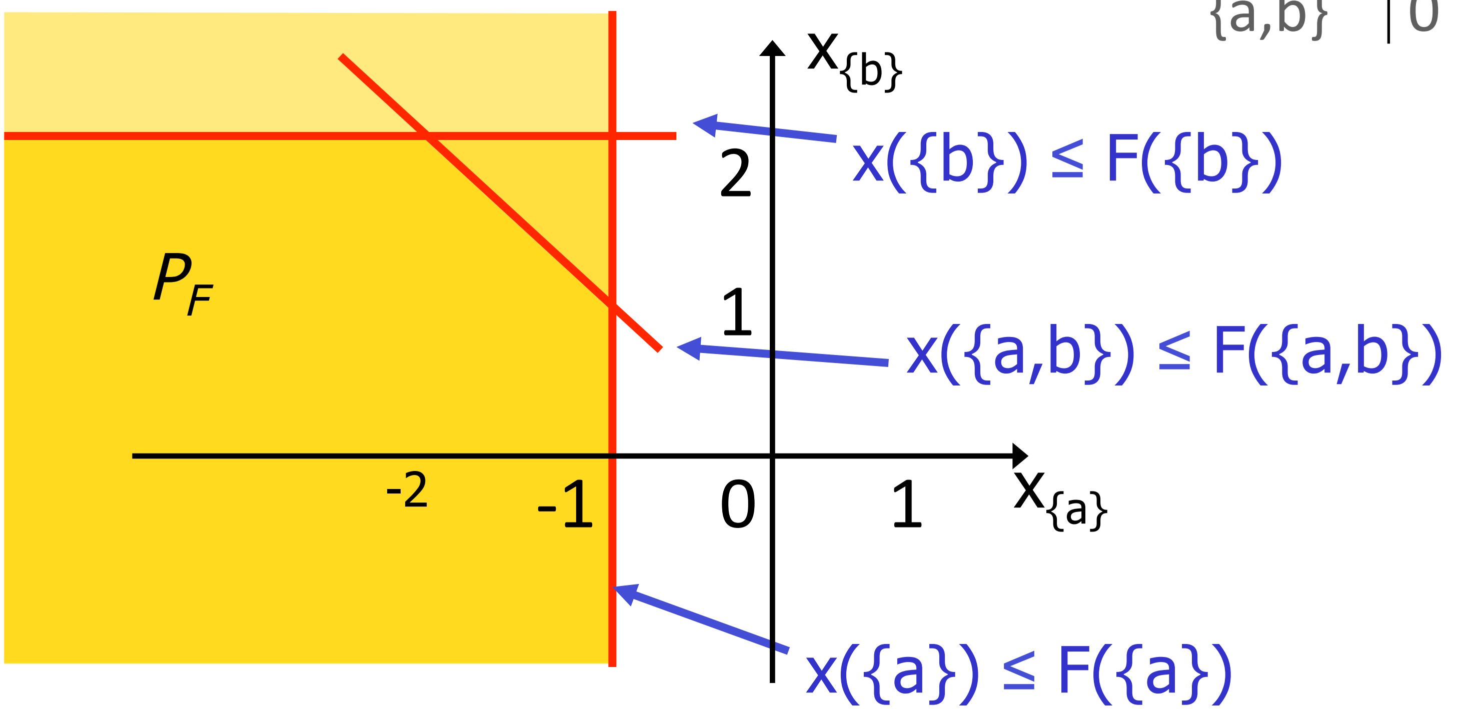
The submodular polyhedron P_F

$$P_F = \{x \in \mathbb{R}^n : x(A) \leq F(A) \text{ for all } A \subseteq V\}$$

$$x(A) = \sum_{i \in A} x_i$$

Example: V = {a,b}

A	F(A)
{}	0
{a}	-1
{b}	2
{a,b}	0



Evaluating the Lovász extension

$$P_F = \{x \in \mathbb{R}^n : x(A) \le F(A) \text{ for all } A \subseteq V\}$$

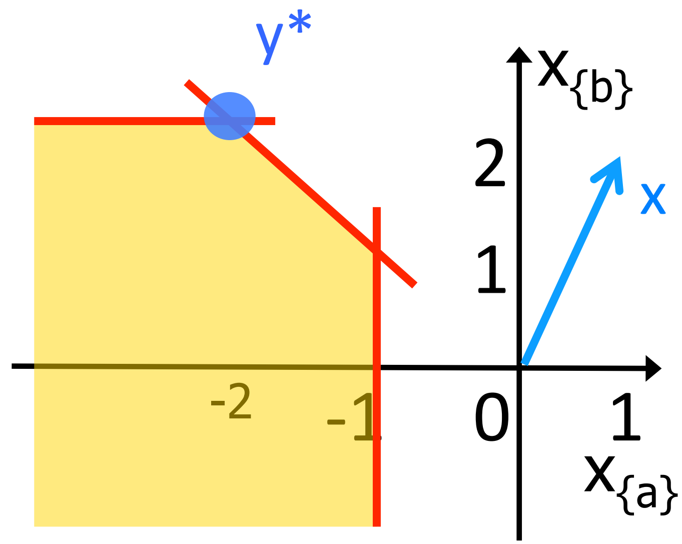
Linear maximization over P_F

$$f(x) = \max_{y \in P_F} x \cdot y$$

Exponentially many constraints!!! ☹

Computable in O(n log n) time ☺

[Edmonds '70]

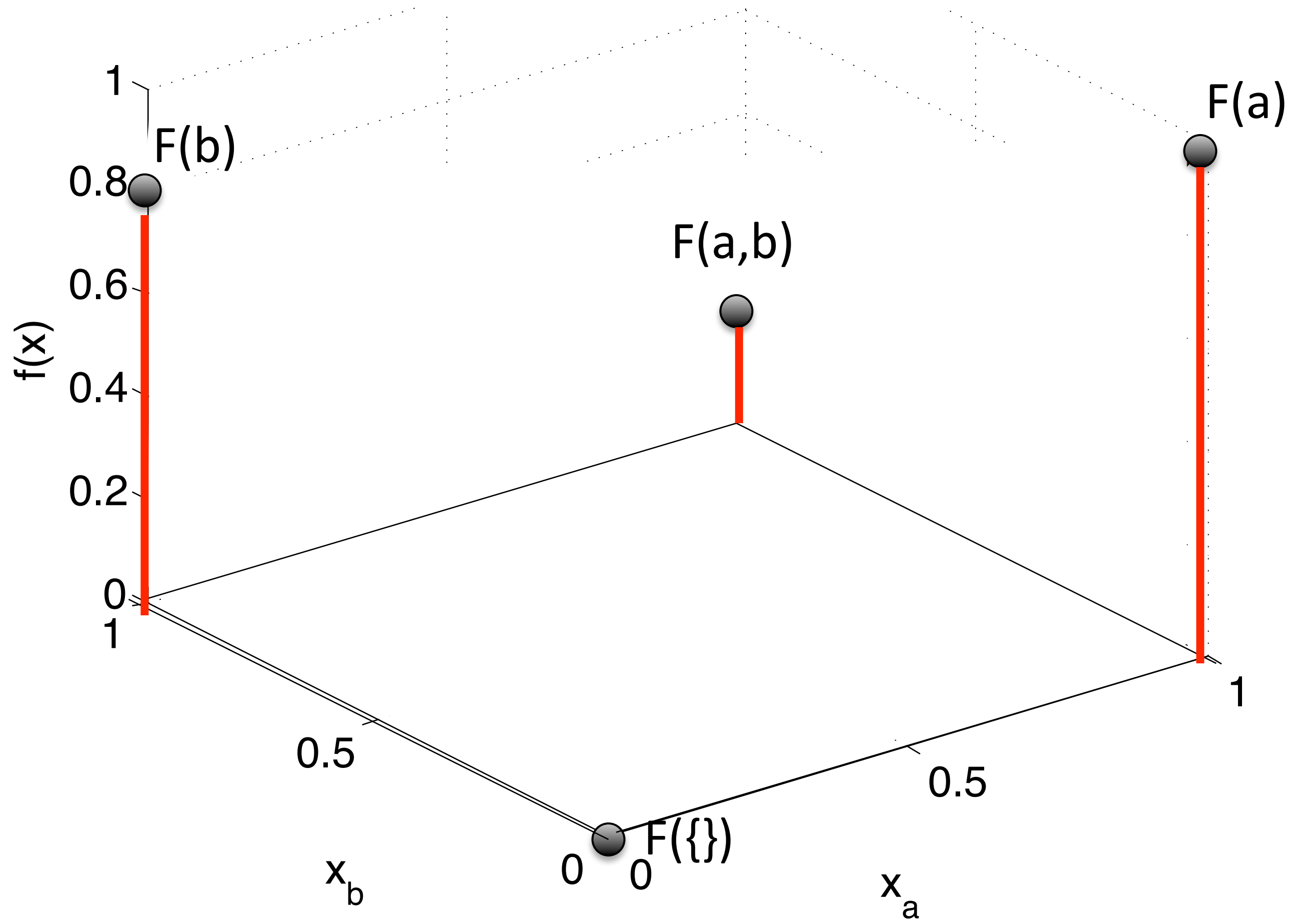


greedy algorithm:

- sort x
- order defines sets $S_i = \{1, \ldots, i\}$
- $y_i = F(S_i) - F(S_{i-1})$

- Subgradient
- Separation oracle

Lovász extension: example



A	F(A)
{}	0
{a}	1
{b}	.8
{a,b}	.2

Submodular minimization

$$\min_{A \subseteq V} F(A)$$

minimize convex extension

- ellipsoid algorithm
  [Grötschel et al. `81]
- subgradient method, smoothing [Stobbe & Krause `10]
- duality: minimum norm point algorithm
  [Fujishige & Isotani '11]

combinatorial algorithms

- Fulkerson prize
  Iwata, Fujishige, Fleischer '01 & Schrijver '00
- state of the art:
  $O(n^4T + n^5 \log M)$ [Iwata '03]
  $O(n^6 + n^5T)$ [Orlin '09]

T = time for evaluating *F*

The minimum-norm-point algorithm

Example: V = {a,b}

Lovász extension

Regularized problem

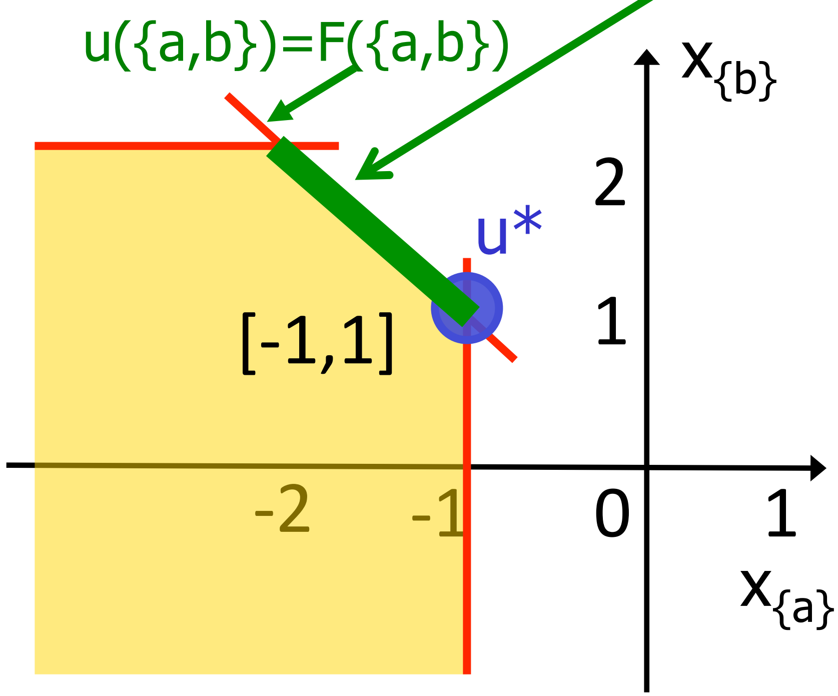
A	F(A)
{}	0
{a}	-1
{b}	2
{a,b}	0

$$\min_{x\in[0,1]^n} f(x) + \frac{1}{2}\|x\|^2$$

dual: minimum norm problem

$$u^* = \arg\min_{u\in B_F} \frac{1}{2}\|u\|^2$$

Base polytope B_F



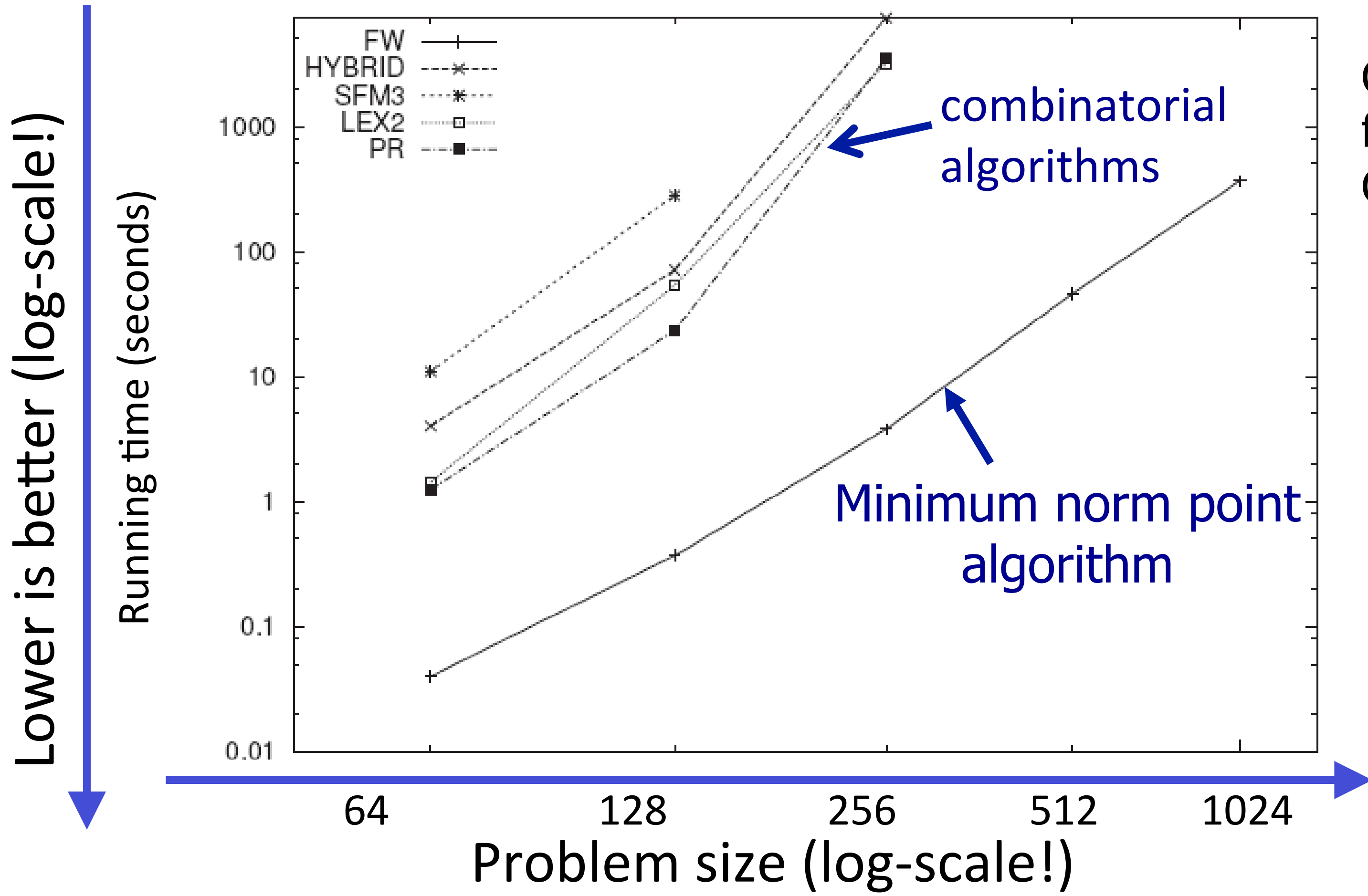
$$A^* = \{i \mid u^*(i) \le 0\}$$

minimizes *F*:

$$A^* = \arg\min_{A\subseteq V} F(A)$$

Fujishige '91, Fujishige & Isotani '11

Empirical comparison



Cut functions from DIMACS Challenge

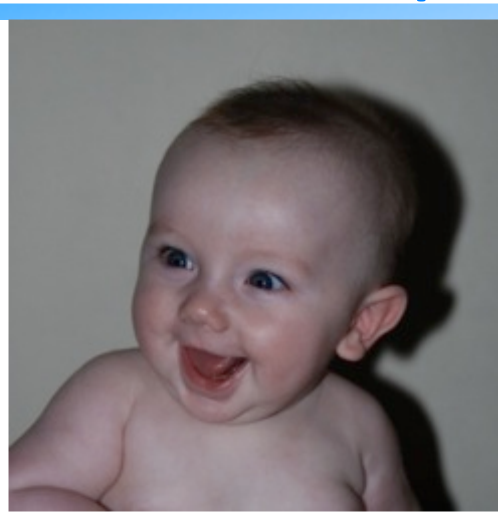
Minimum norm point algorithm: usually orders of magnitude faster

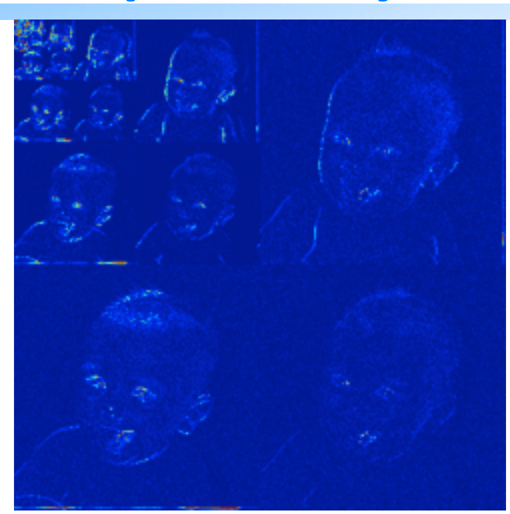
[Fujishige & Isotani ’11]

Example I: Sparsity

d

pixels



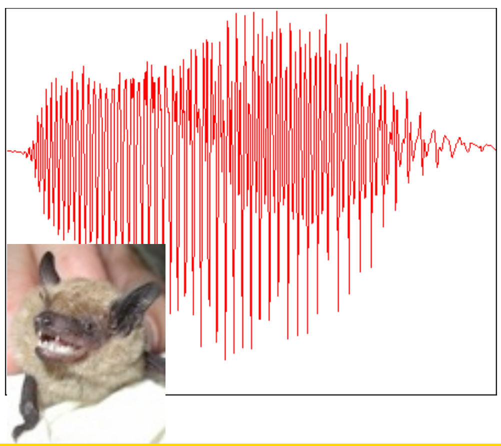


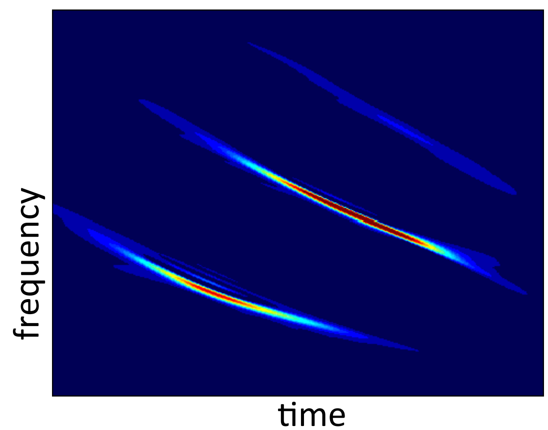
$k \ll d$

large
wavelet
coefficients

d

wideband
signal
samples





$k \ll d$

large
Gabor (TF)
coefficients

Many natural signals sparse in suitable basis.
Can exploit for learning/regularization/compressive sensing...

Sparse reconstruction

$$\min_{x} \|y - Mx\|^2 \quad + \lambda\Omega(x)$$

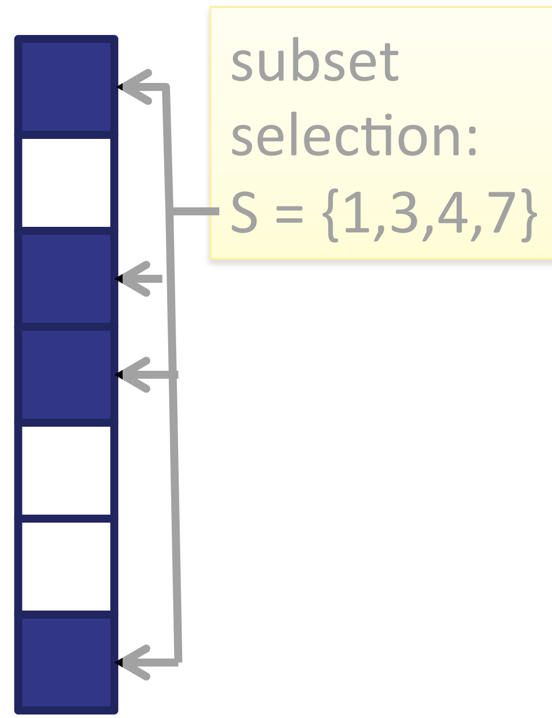
- explain *y* with few columns of *M*: few x_i

discrete regularization on support *S* of *x*

$$\Omega(x) = \|x\|_0 \quad = |S|$$

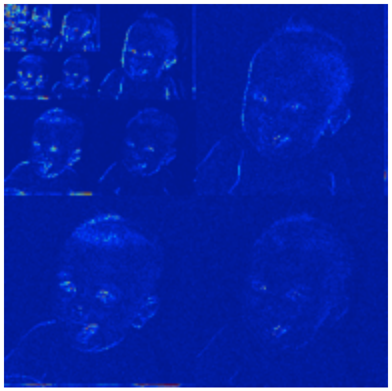
relax to convex envelope

$$\Omega(x) = \|x\|_1$$

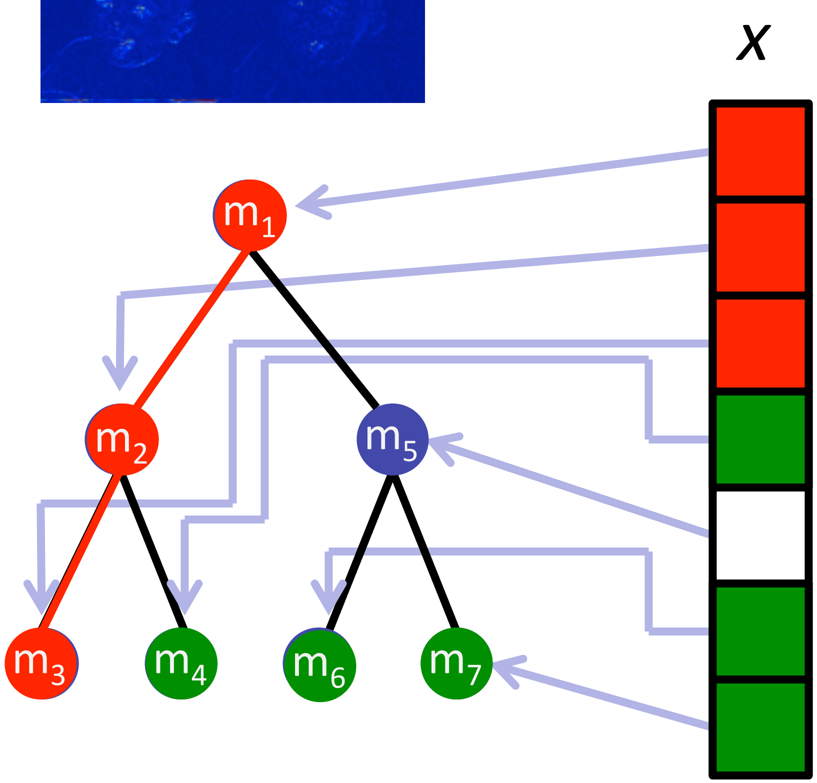


in nature: sparsity pattern often not random…

Structured sparsity



Incorporate tree preference in regularizer?



Set function:

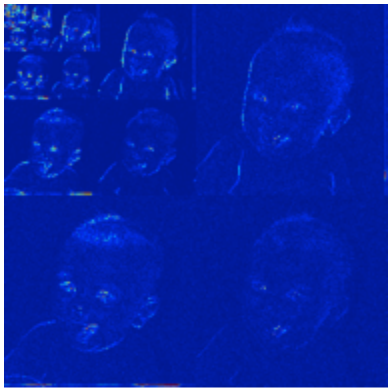
$$F(T) < F(S)$$

if T is a tree and S not

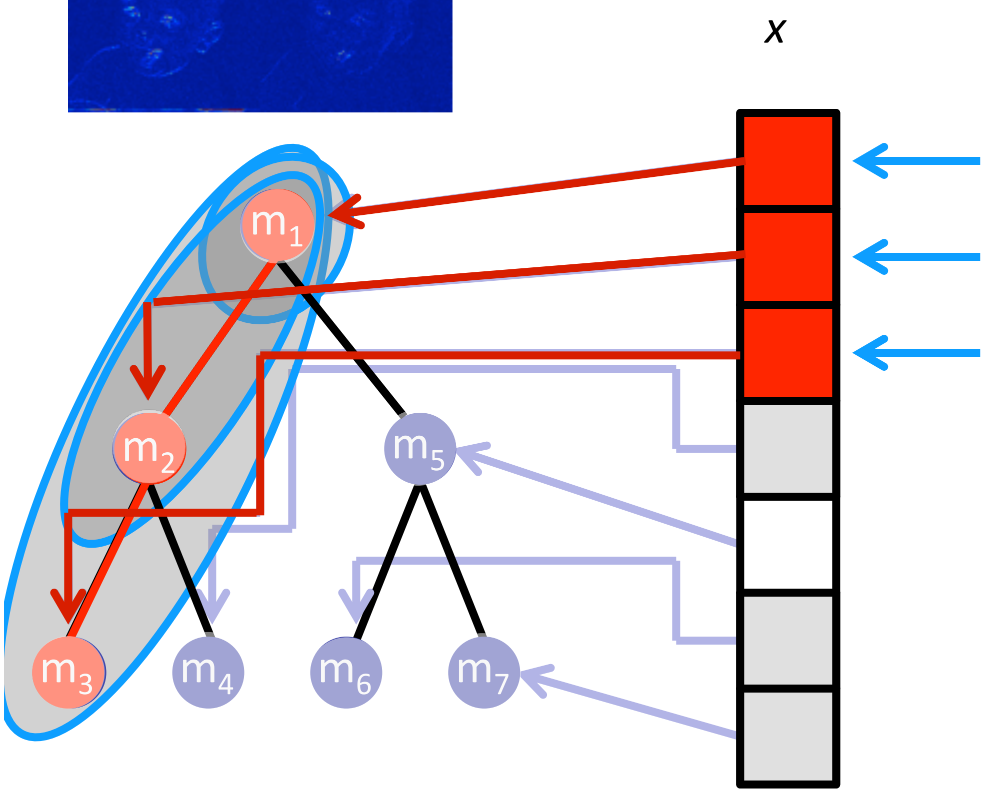
$|S| = |T|$

$$F(S) = \left| \bigcup_{s \in S} \text{ancestors}(s) \right|$$

Structured sparsity



Incorporate tree preference in regularizer?



Set function:

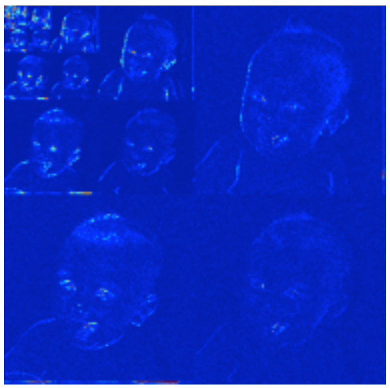
$$F(T) < F(S)$$

If T is a tree and S not, $|S| = |T|$

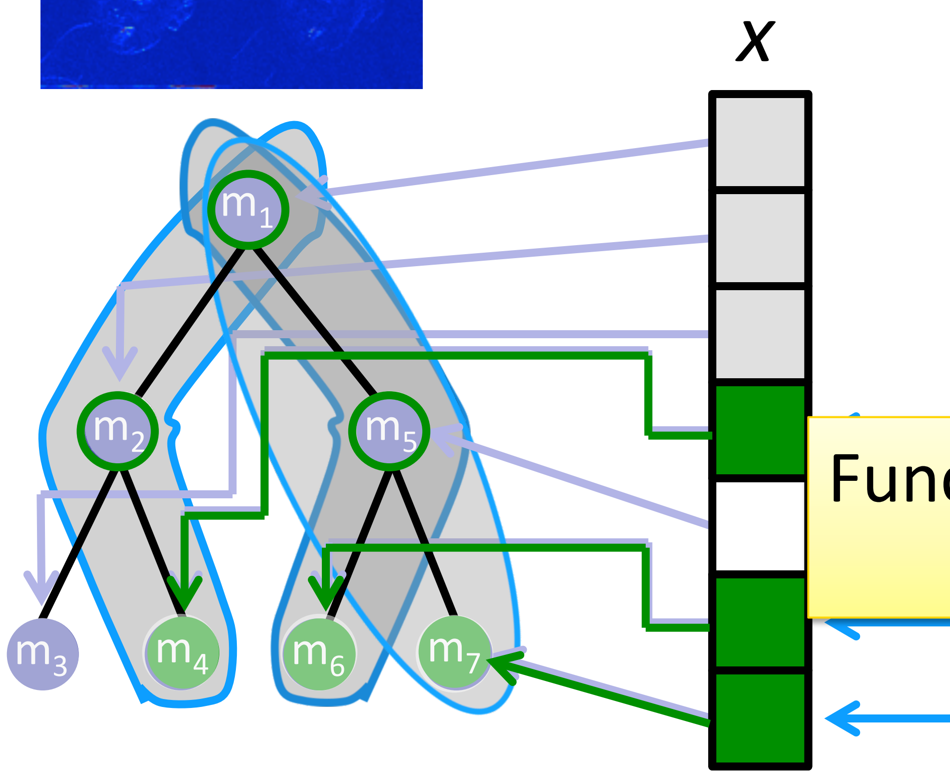
$$F(S) = \left| \bigcup_{s \in S} \text{ancestors}(s) \right|$$

$$F(T) = 3$$

Structured sparsity



Incorporate tree preference in regularizer?



Set function:

$$F(T) < F(S)$$

If T is a tree and S not, $|S| = |T|$

Function F is …

submodular! ☺

$$F(T) = 3$$

Sparsity

$$\min_x \|y - Mx\|^2 \quad +\lambda\Omega(x)$$

- explain *y* with few columns of *M*: few x_i
- prior knowledge: patterns of nonzeros

discrete regularization on support *S* of *x*

$$\Omega(x) = \|x\|_0 \quad = |S|$$

- submodular function

$$\Omega(x) = F(S)$$

relax to convex envelope

$$\Omega(x) = \|x\|_1$$

➔ Lovász extension

$$\Omega(x) = f(|x|)$$

- Optimization: submodular minimization

[Bach`10]

Further connections: Dictionary Selection

$$\min_{x} \|y - Mx\|^2 + \lambda\Omega(x)$$

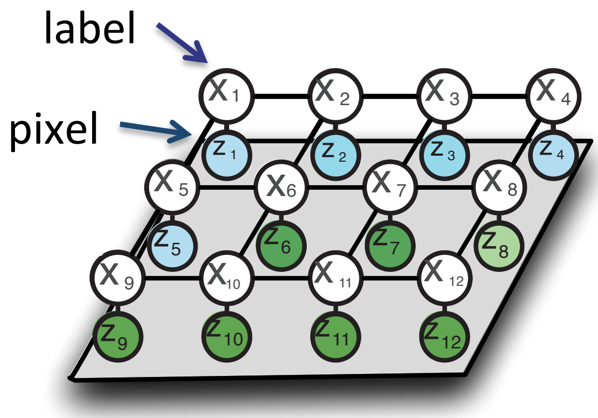
Where does the dictionary M come from?

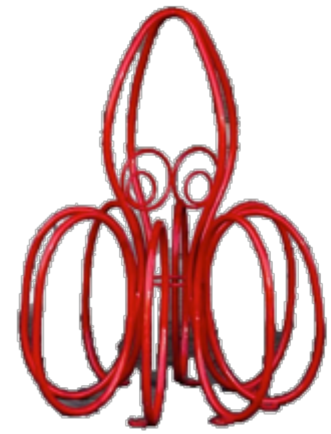
Want to learn it from data: $\{y_1, \ldots, y_n\} \subseteq \mathbb{R}^d$

Selecting a dictionary with near-max. variance reduction
⇔ Maximization of approximately submodular function

[Krause & Cevher '10; Das & Kempe '11]

Example II: MAP inference





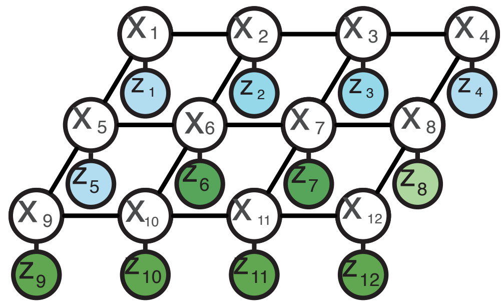
$$\max_{\mathbf{x}\in\{0,1\}^n} \quad P(\mathbf{x} \mid \mathbf{z}) \propto \exp(-E(\mathbf{x};\mathbf{z}))$$

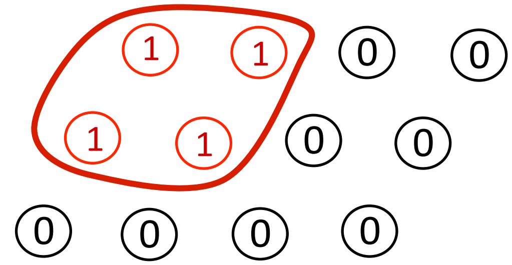
labels

pixel values

$$\Leftrightarrow \quad \min_{\mathbf{x}\in\{0,1\}^n} \quad E(\mathbf{x};\mathbf{z})$$

Example II: MAP inference

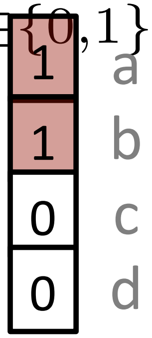




$$\max_{\mathbf{x}\in\{0,1\}^n} P(\mathbf{x} \mid \mathbf{z}) \propto \exp(-E(\mathbf{x};\mathbf{z}))$$

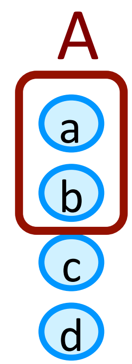
Recall: equivalence

function on binary vectors | set function



$x = e_A$

$$E(e_A;\mathbf{z}) \quad = \quad F(A)$$



if F is submodular, then $\Leftrightarrow \quad \min_{\mathbf{x}\in\{0,1\}^n} E(\mathbf{x};\mathbf{z})$

MAP inference = submodular minimization!

polynomial-time

Special cases

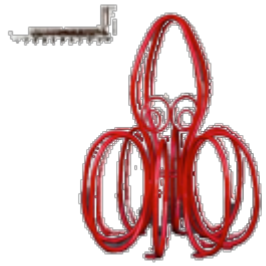
Minimizing general submodular functions:

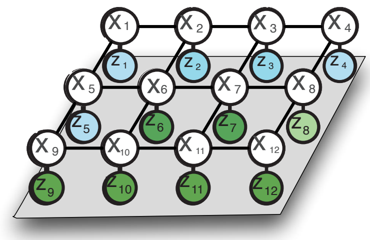
poly-time, but not very scalable

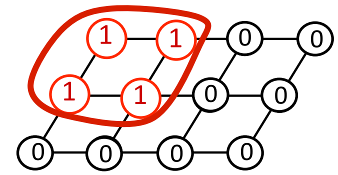
Special structure → faster algorithms

- Symmetric functions
- Graph cuts
- Concave functions
- Sums of functions with bounded support
- ...

MAP inference







$$\min_{\mathbf{x}\in\{0,1\}^n} E(\mathbf{x};\mathbf{z}) = \sum_i E_i(x_i) + \sum_{ij} E_{ij}(x_i, x_j) \quad \equiv \min_{A\subseteq V} F(A)$$

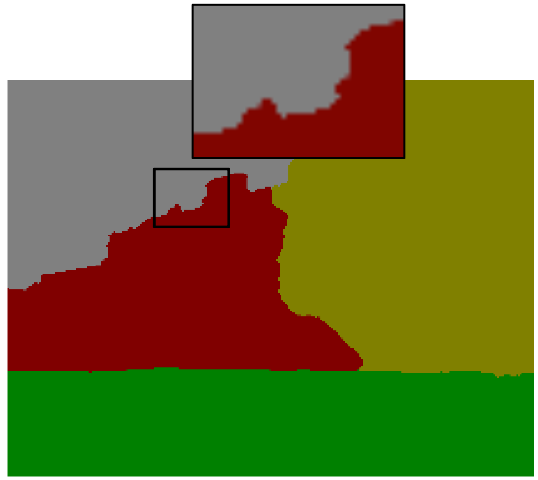
if each E_{ij} is submodular ("attractive"):

$$\underbrace{E_{ij}(1,0)}_{a} + \underbrace{E_{ij}(0,1)}_{b} \;\geq\; E_{ij}(0,0) + \underbrace{E_{ij}(1,1)}_{a\,b}$$

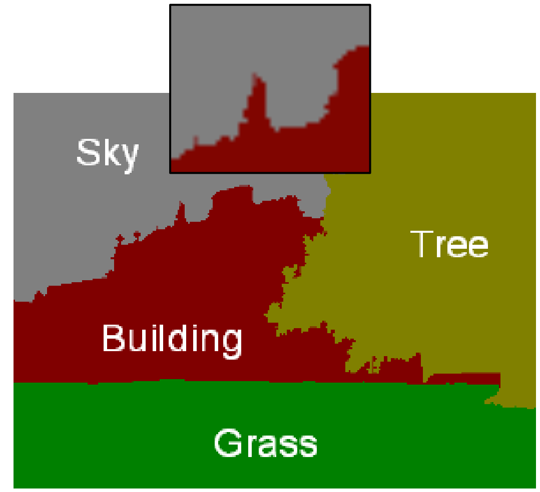
then F is a graph cut function.

$\boxed{\text{MAP inference = Minimum cut: fast ☺}}$

Pairwise is not enough…



color + pairwise



color + pairwise +

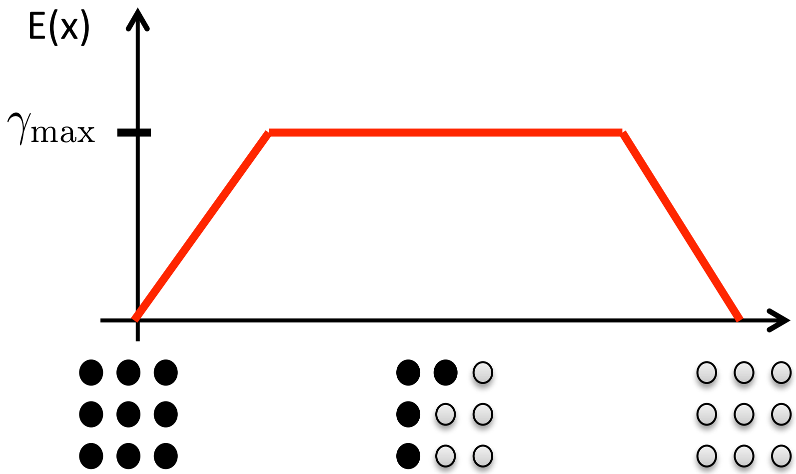
$$E(x) = \sum_i E_i(x_i) + \sum_{ij} E_{ij}(x_i, x_j)$$

Pixels in one tile should have the same label

[Kohli et al.`09]

Enforcing label consistency

Pixels in a superpixel should have the same label



concave function of cardinality ➔ submodular ☺

Can still be transformed into a graph cut instance!

Other special cases

- Symmetric: $F(S) = F(V \setminus S)$
  - Queyranne's algorithm: O(n^3) [Queyranne, 1998]

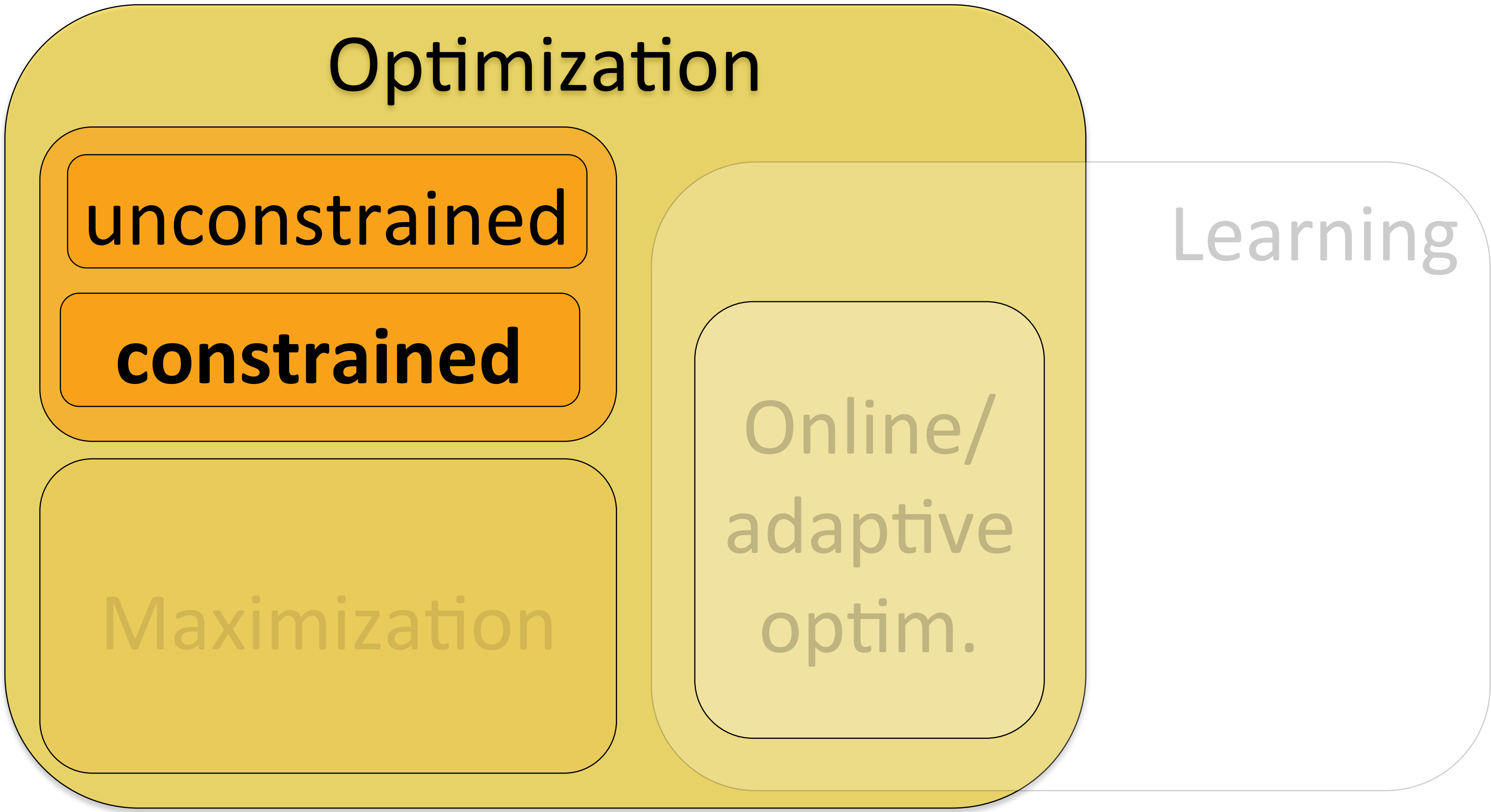
- Concave of modular: $F(S) = \sum_i g_i\Big(\sum_{s \in S} w(s)\Big)$

  [Stobbe & Krause `10, Kohli et al, `09]

- Sum of submodular functions, each bounded support

  [Kolmogorov `12]

Submodular minimization



Submodular minimization

- unconstrained: $\min \; F(A) \quad \text{s.t. } A \subseteq V$
  - nontrivial algorithms, polynomial time

special case: balanced cut

- constraints: e.g. $\min \; F(A) \quad \text{s.t. } |A| \geq k$
  - limited cases doable: $\ldots$
    odd/even cardinality, inclusion/exclusion of a set

General case: NP hard

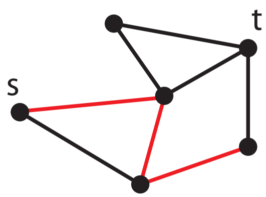
- hard to approximate within polynomial factors!
- But: special cases often still work well

[Lower bounds: Goel et al.`09, Iwata & Nagano `09, Jegelka & Bilmes `11]

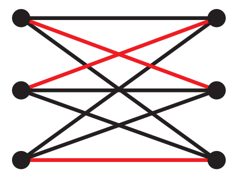
Constraints

minimum…

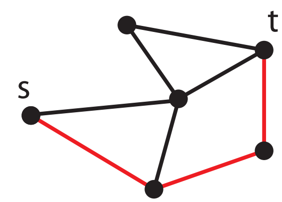
cut



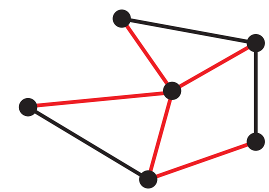
matching



path



spanning tree



ground set: edges in a graph

$$\min_{S\in\mathcal{C}} \sum_{e\in S} w(e) \quad \longrightarrow \quad \min_{S\in\mathcal{C}} F(S)$$

Submodular ("cooperative") cut

[Jegelka & Bilmes '11]

Graph cut | Cooperative cut






Efficient constrained optimization

minimize a series of surrogate functions

1. compute linear upper bound $\widehat{F}^i(S^i) = F(S^i)$

$$\hat{F}^i(S) = \sum_{e \in S} w^i(S)$$

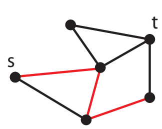
2. Solve easy sum-of-weights problem:

$$S^i = \arg\min_{S \in \mathcal{C}} \hat{F}^i(S)$$

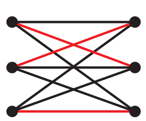
and repeat.

- efficient
- only need to solve sum-of-weights problems
- Provides certain approximation guarantees

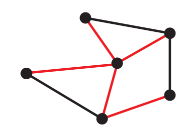
cut



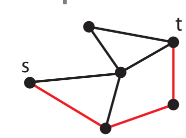
matching



spanning tree



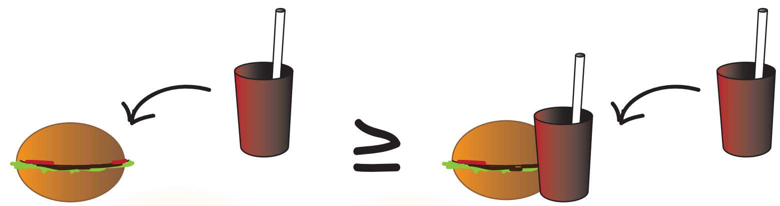
path

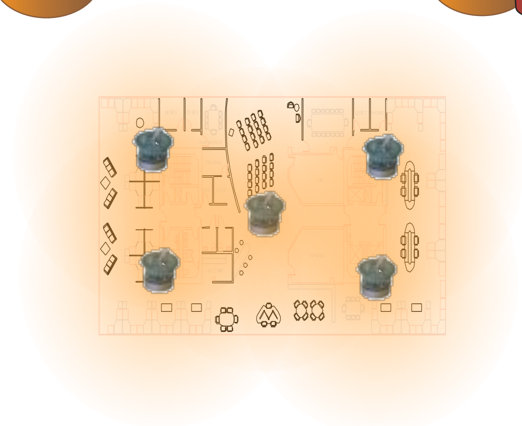


[Jegelka & Bilmes `11, Iyer et al. ICML `13]

Outline

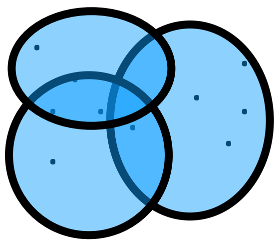
- What is submodularity?
- Optimization
  - Minimize costs
  - **Maximize utility**



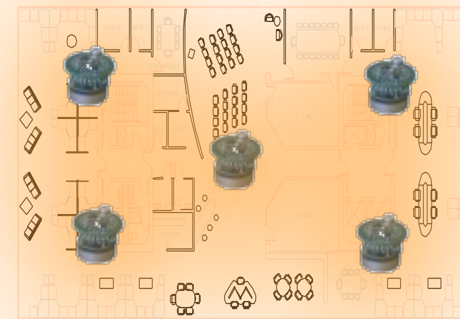


- Applications
- Outlook and pointers

Submodular maximization



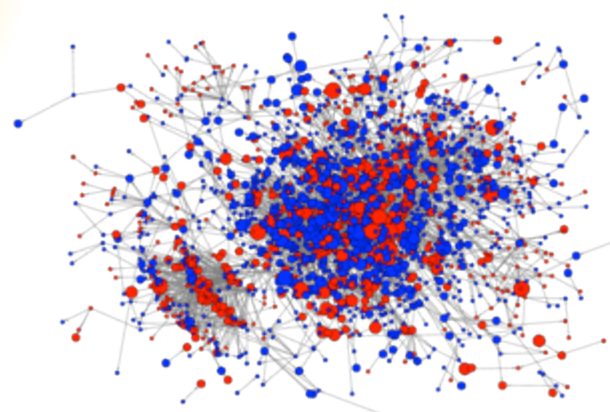
covering



sensing

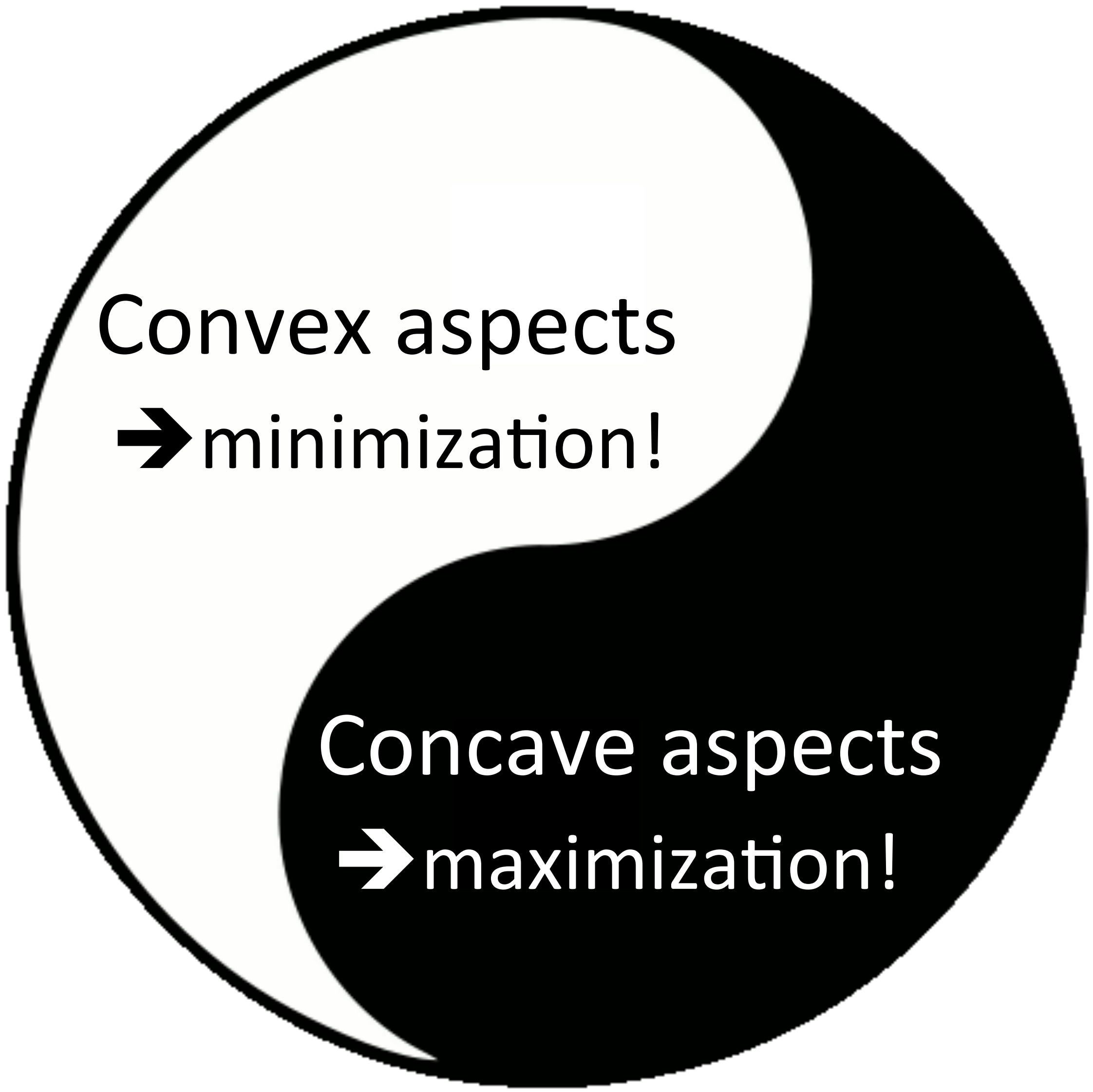
$$\max_{S \subseteq V} F(S)$$

summarization



network inference

Two faces of submodular functions



Submodular maximization

$$\max_{S \subseteq V} F(S)$$

➔ submodularity and concavity

Concave aspects

- submodularity:

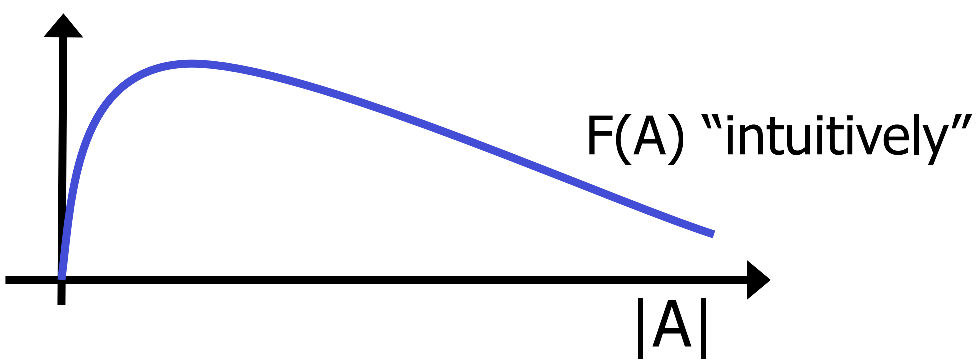
$$A \subseteq B, \;\; s \notin B:$$

$$F(A \cup s) - F(A) \quad \geq \quad F(B \cup s) - F(B)$$

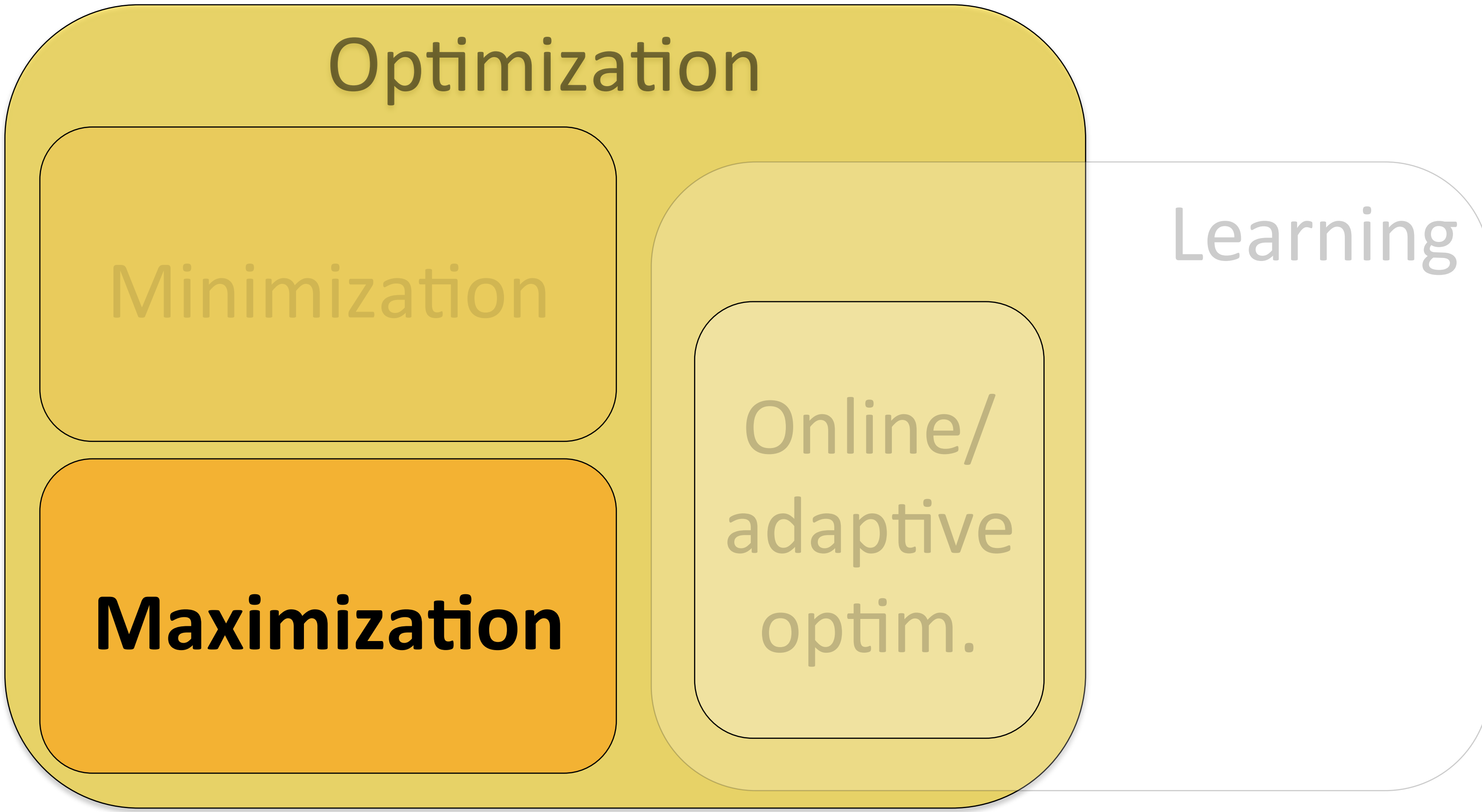
- concavity:

$$a \leq b, \;\; s > 0:$$

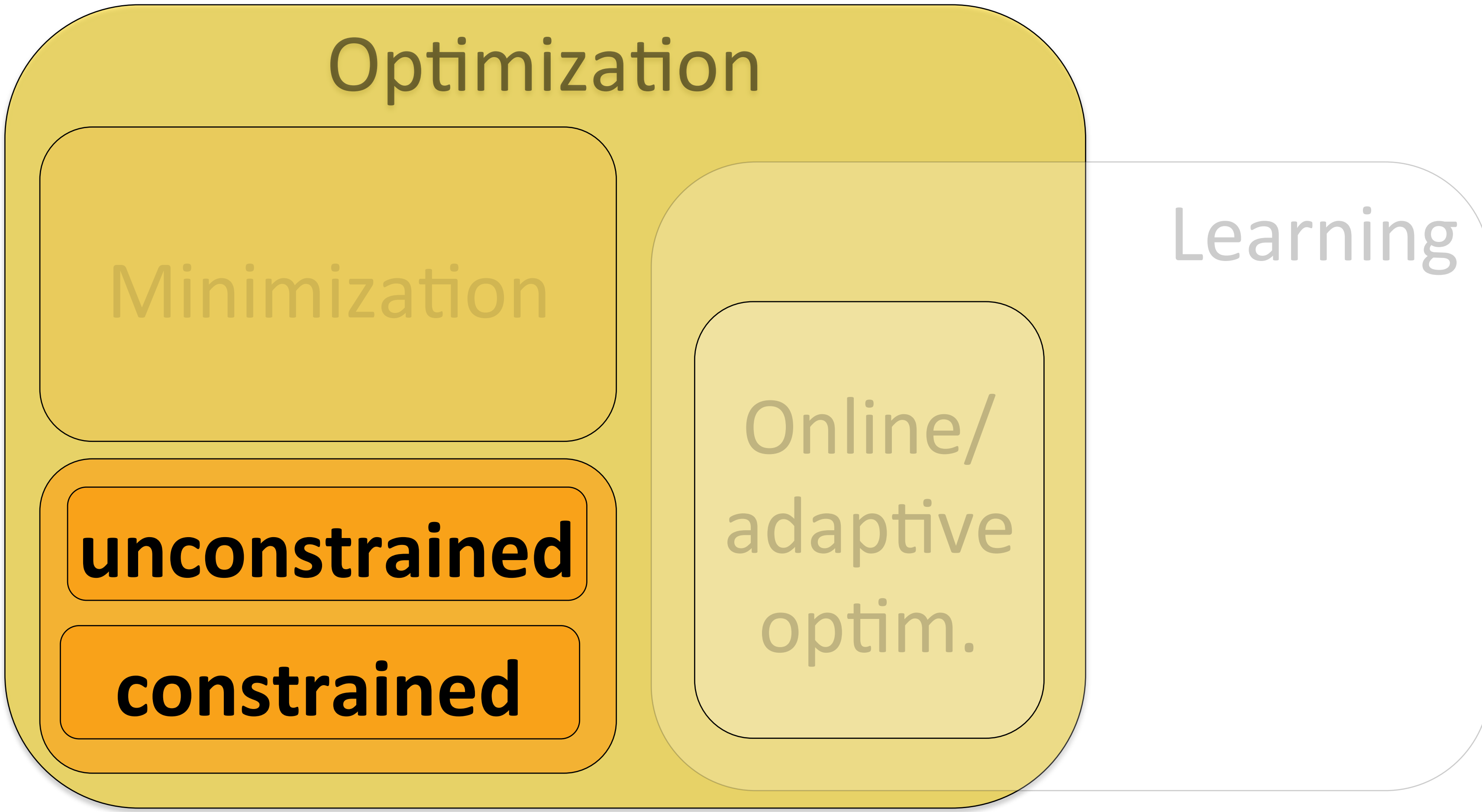
$$f(a+s) - f(a) \qquad \geq \qquad f(b+s) - f(b)$$



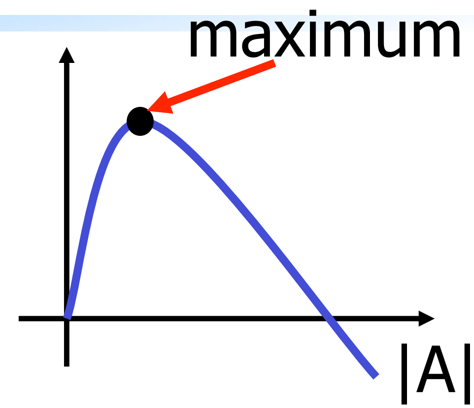
Optimization



Optimization



Maximizing submodular functions



- Suppose we want for submodular F

$$A^* = \arg\max_A F(A) \text{ s.t. } A \subseteq V$$

- Example:
  - F(A) = U(A) – C(A) where U(A) is submodular utility, and C(A) is supermodular cost function

- In general: NP hard. Moreover:
- If F(A) can take negative values:
  As hard to approximate as maximum independent set (i.e., NP hard to get $O(n^{1-\varepsilon})$ approximation)

Exact maximization of SFs

- Mixed integer programming
  - Series of mixed integer programs [Nemhauser et al ‘81]
  - Constraint generation [Kawahara et al ‘09]
- Branch-and-bound
  - „Data-Correcting Algorithm“ [Goldengorin et al ’99]

Useful for small/moderate problems

All algorithms worst-case exponential!

Maximizing positive submodular functions

[Feige, Mirrokni, Vondrak '09; Buchbinder, Feldman, Naor, Schwartz '12]

Theorem

Given a nonnegative submodular function F,
RandomizedUSM returns set A_R such that

$$F(A_R) \geq 1/2 \ \max_A F(A)$$

- Cannot do better in general than ½ unless P = NP

Unconstrained vs. constraint maximization

Given monotone utility F(A) and cost C(A), optimize:

<u>Option 1:</u>

$$\boxed{\max_A F(A) - C(A) \quad \text{s.t. } A \subseteq V}$$

"Scalarization"

Can get 1/2 approx…

if F(A)-C(A) ≥ 0

for all sets A

<u>Option 2:</u>

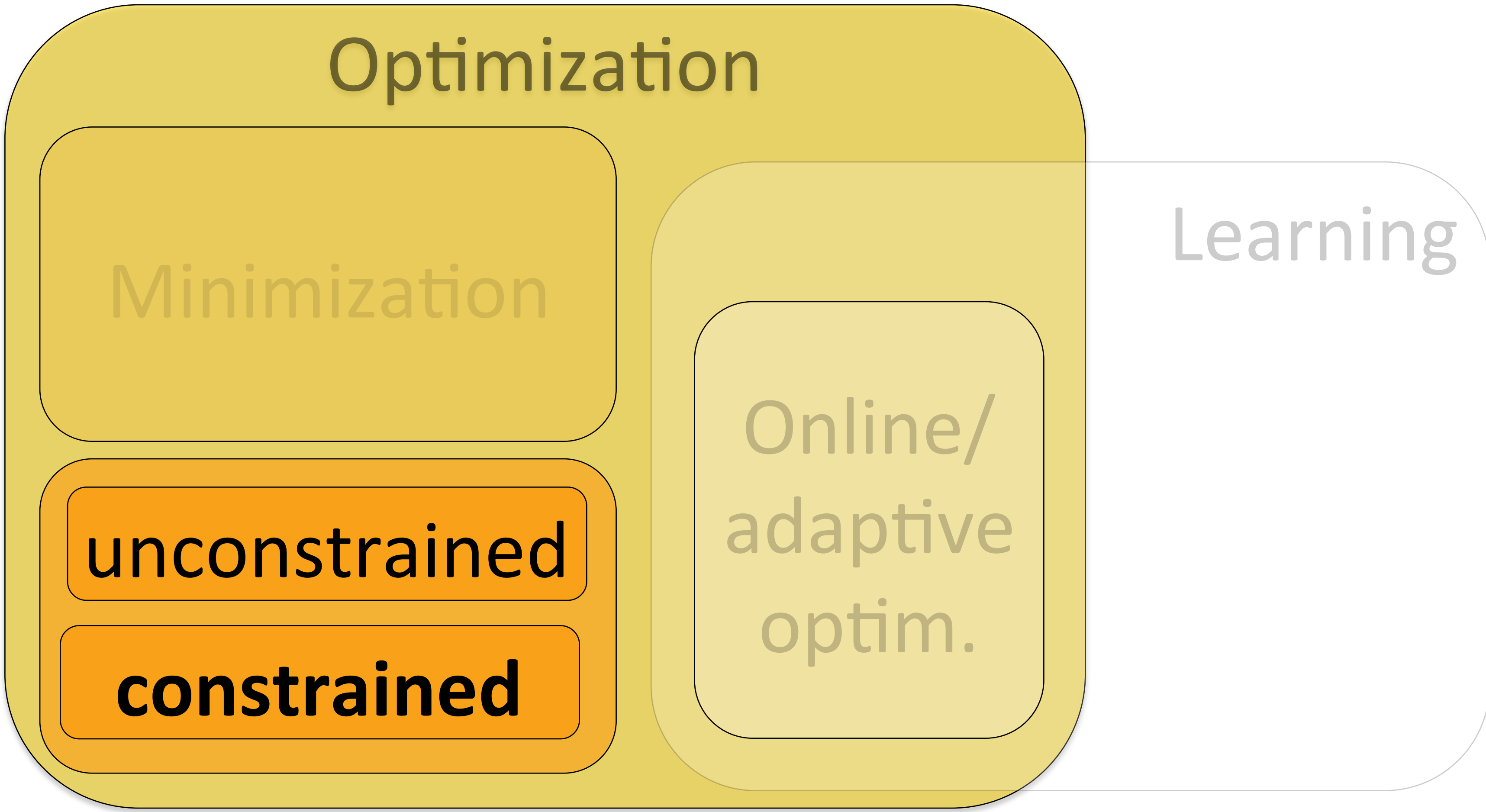
$$\boxed{\max_A F(A) \quad \text{s.t. } C(A) \leq B}$$

"Constrained maximization"

What is possible?

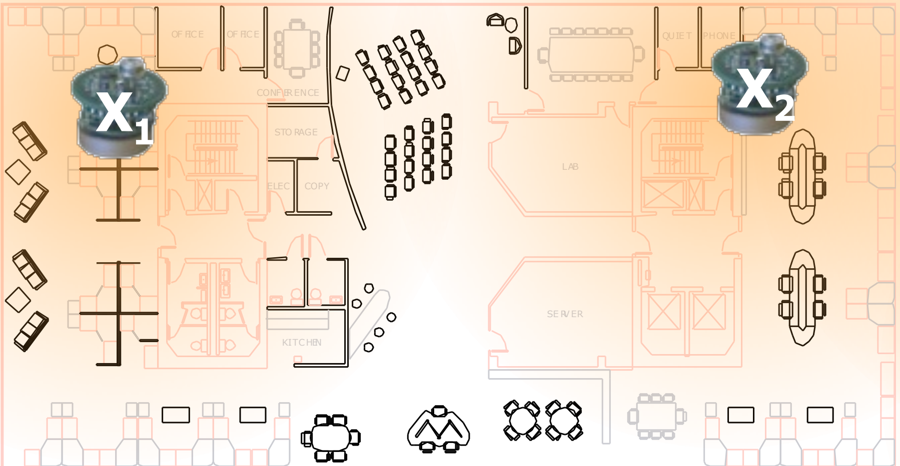
Positiveness is a strong requirement ☹

Optimization

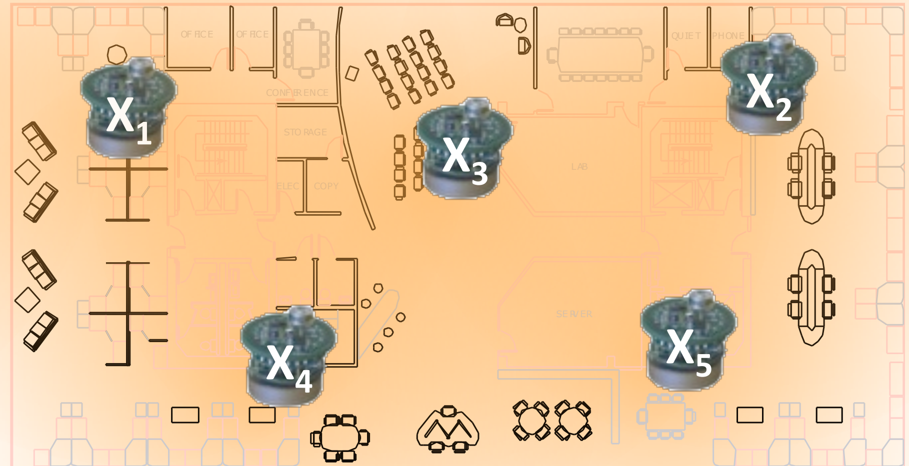


Monotonicity

Placement A = {1,2}



Placement B = {1,…,5}



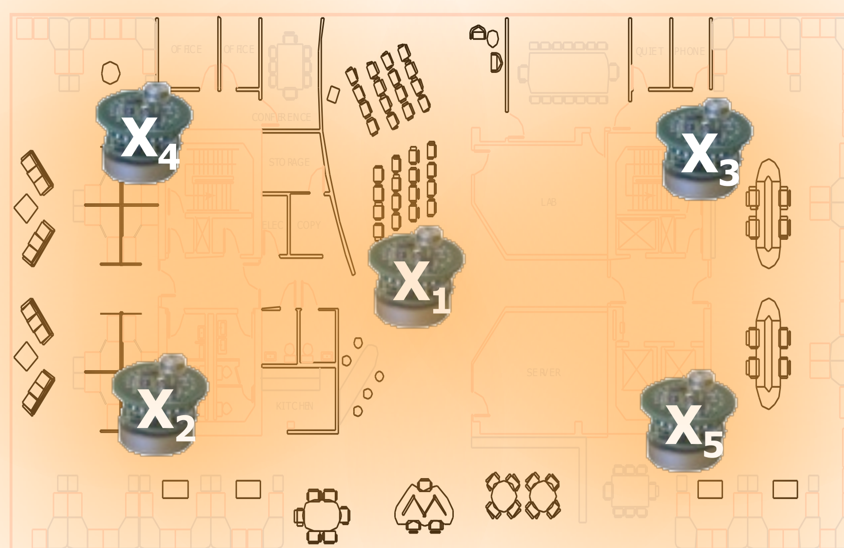
F is monotonic: $$\forall A, s : \underbrace{F(A \cup \{s\}) - F(A)}_{\Delta(s \mid A) \geq 0} \geq 0$$

Adding sensors can only help

Cardinality constrained maximization

- **Given**: finite set V, monotone submodular F
- **Want**: $\mathcal{A}^* \subseteq \mathcal{V}$ such that
$$\mathcal{A}^* = \operatorname*{argmax}_{|\mathcal{A}| \le k} F(\mathcal{A})$$

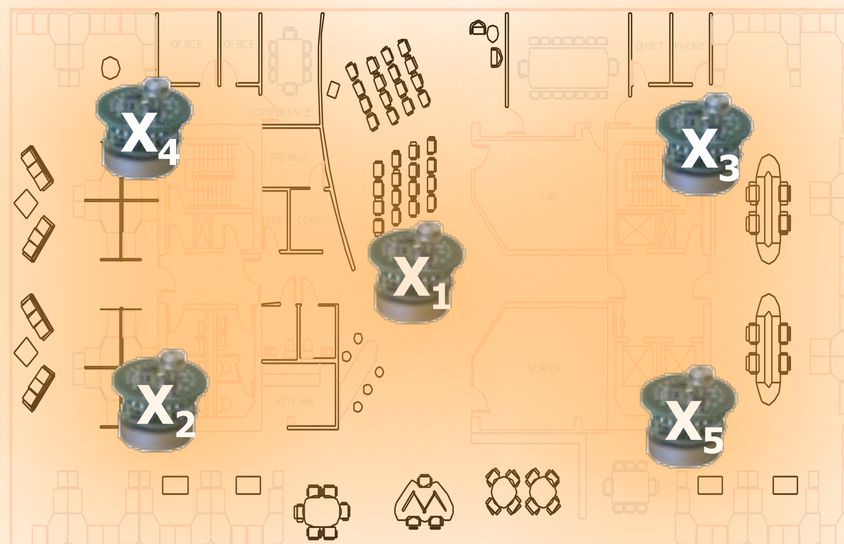
NP-hard!



Greedy algorithm

- **Given**: finite set V, monotone submodular F
- **Want**: $\mathcal{A}^* \subseteq \mathcal{V}$ such that

$$\mathcal{A}^* = \operatorname*{argmax}_{|\mathcal{A}| \leq k} F(\mathcal{A})$$



NP-hard!

<u>Greedy algorithm:</u>

Start with $\mathcal{A} = \emptyset$

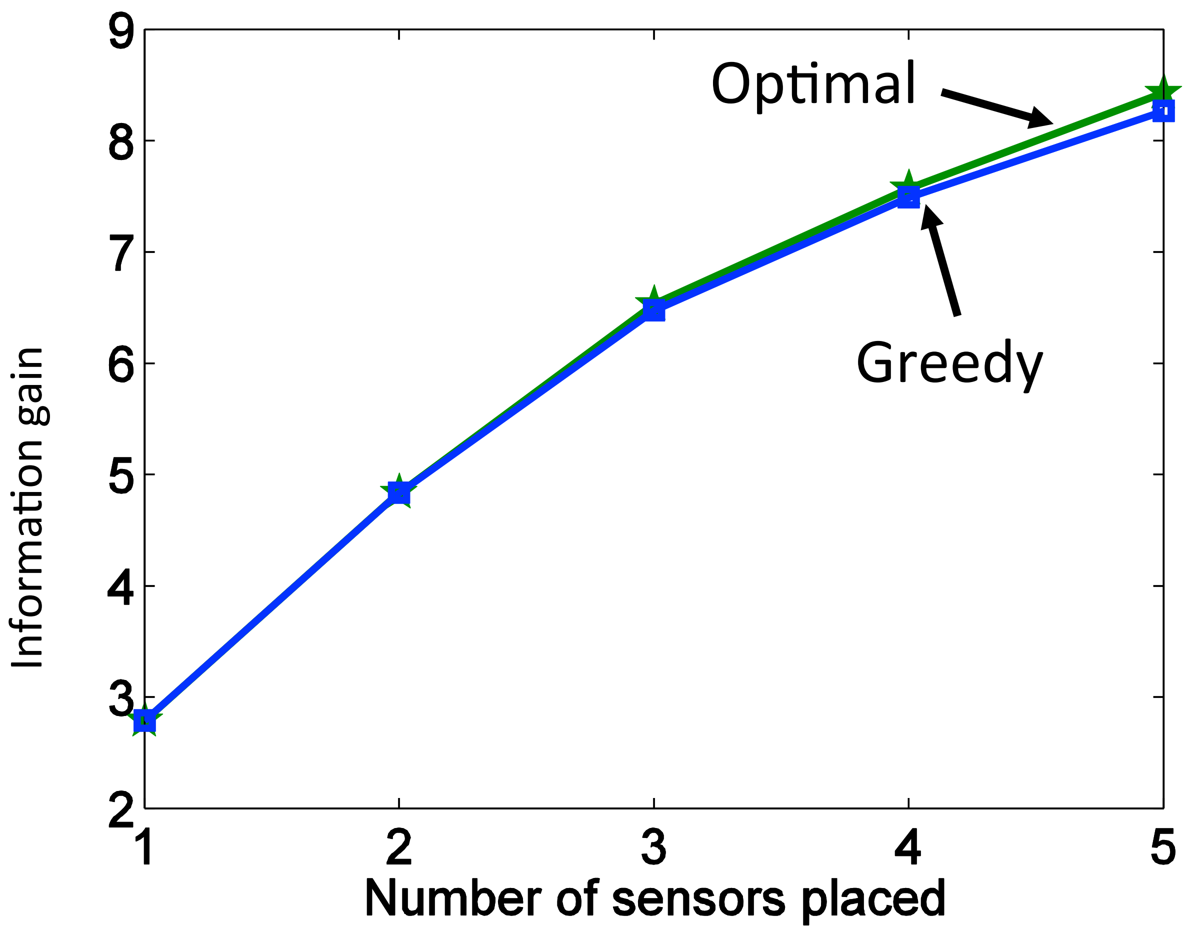
For i = 1 to k

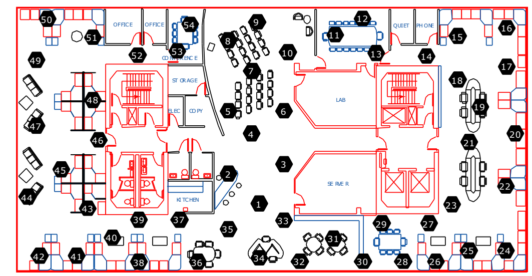
$$s^* \leftarrow \arg\max_s F(\mathcal{A} \cup \{s\})$$

$$\mathcal{A} \leftarrow \mathcal{A} \cup \{s^*\}$$

How well can this simple heuristic do?

Performance of greedy





Temperature data
from sensor network

Greedy empirically close to optimal. Why?

One reason submodularity is useful

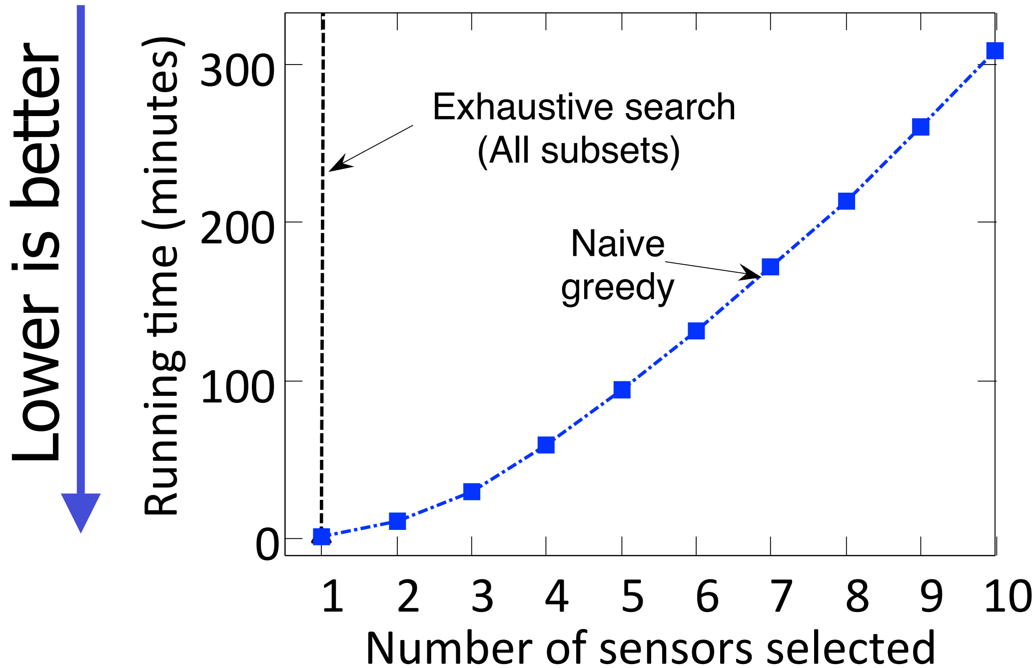
Theorem [Nemhauser, Fisher & Wolsey '78]

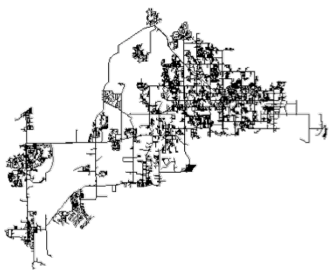
For monotonic submodular functions,
Greedy algorithm gives constant factor approximation

$$F(A_{greedy}) \geq \underbrace{(1-1/e)}_{\sim 63\%} F(A_{opt})$$

- Greedy algorithm gives near-optimal solution!
- In general, need to evaluate exponentially many sets to do better!
  [Nemhauser & Wolsey '78]
- Also many special cases are hard (set cover, mutual information, …)

Even greedy can be slow…





Sensor placement

Placing 10 sensors takes 5 hours on highly optimized implementation

Scaling up the greedy algorithm [Minoux '78]

In round i+1,

- have picked $A_i = \{s_1,\ldots,s_i\}$
- pick $s_{i+1} = \operatorname{argmax}_s F(A_i \cup \{s\})-F(A_i)$

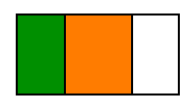
I.e., maximize "marginal benefit" $\Delta(s \mid A_i)$

$$\Delta(s \mid A_i) = F(A_i \cup \{s\})-F(A_i)$$

Key observation: Submodularity implies

$$i \leq j \quad \Rightarrow \quad \Delta(s \mid A_i) \;\geq\; \Delta(s \mid A_j)$$

$\Delta(s \mid A_i) \geq \Delta(s \mid A_{i+1})$

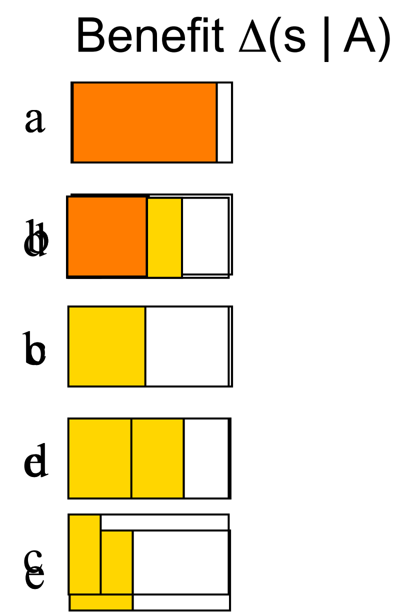
s


Marginal benefits can never increase!

“Lazy” greedy algorithm [Minoux ’78]

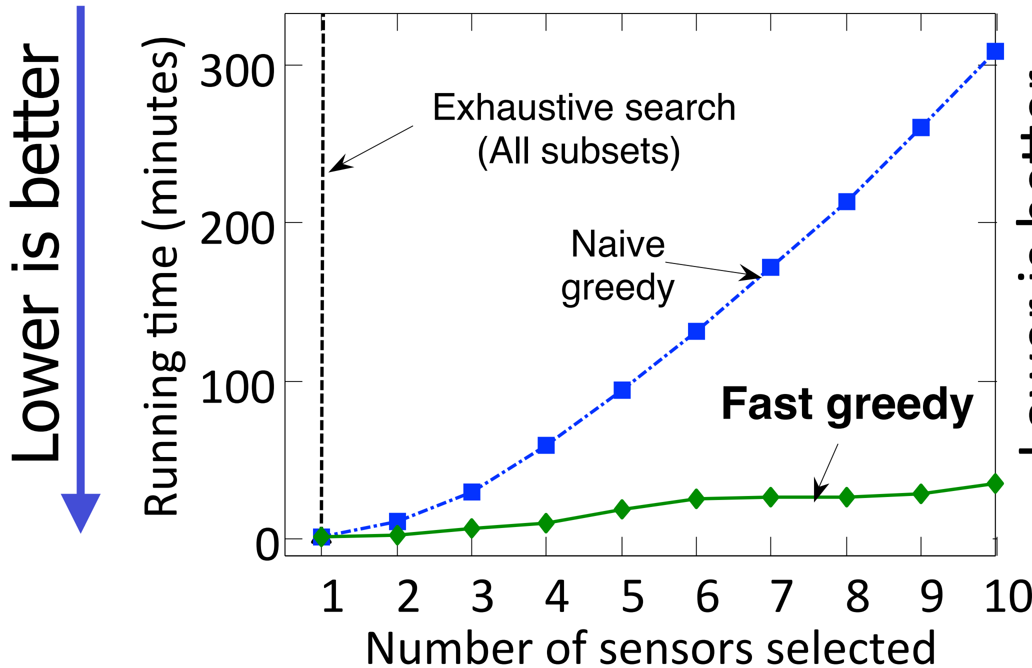
Lazy greedy algorithm:

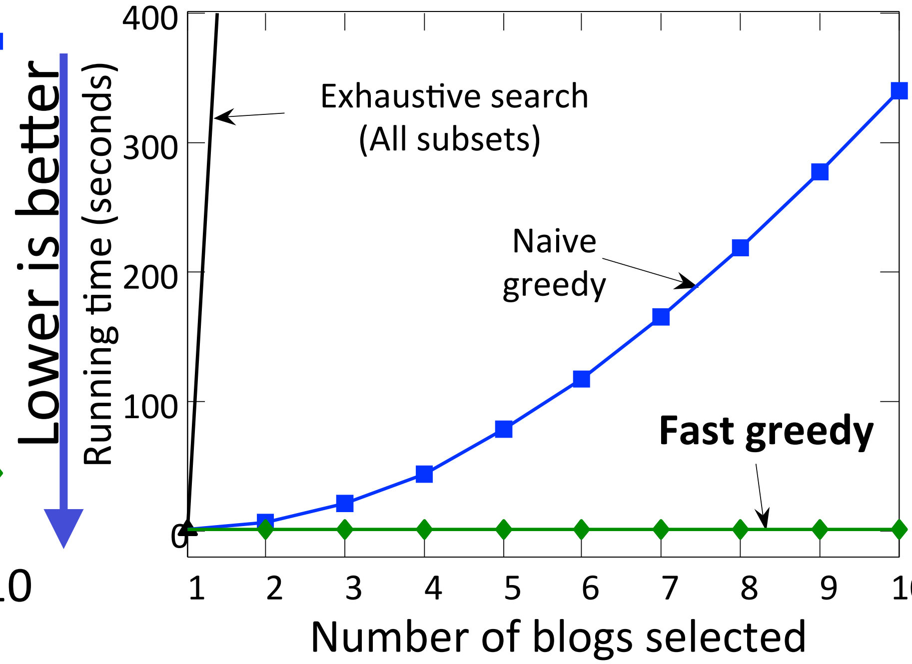
- First iteration as usual
- Keep an ordered list of marginal benefits Δ_i from previous iteration
- Re-evaluate Δ_i only for top element
- If Δ_i stays on top, use it, otherwise re-sort



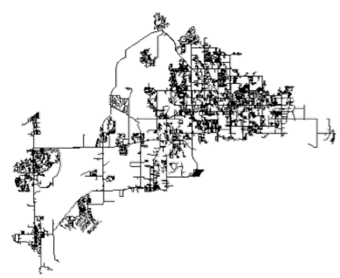
Note: Very easy to compute online bounds, lazy evaluations, etc. [Leskovec, Krause et al. ’07]

Empirical improvements [Leskovec, Krause et al'06]





Sensor placement

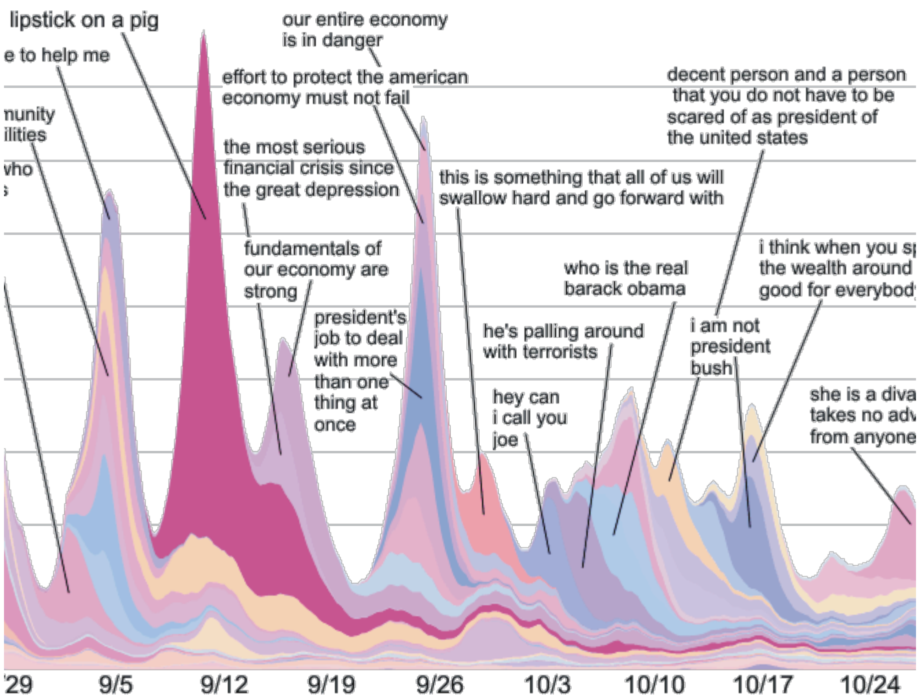


Blog selection

30x speedup

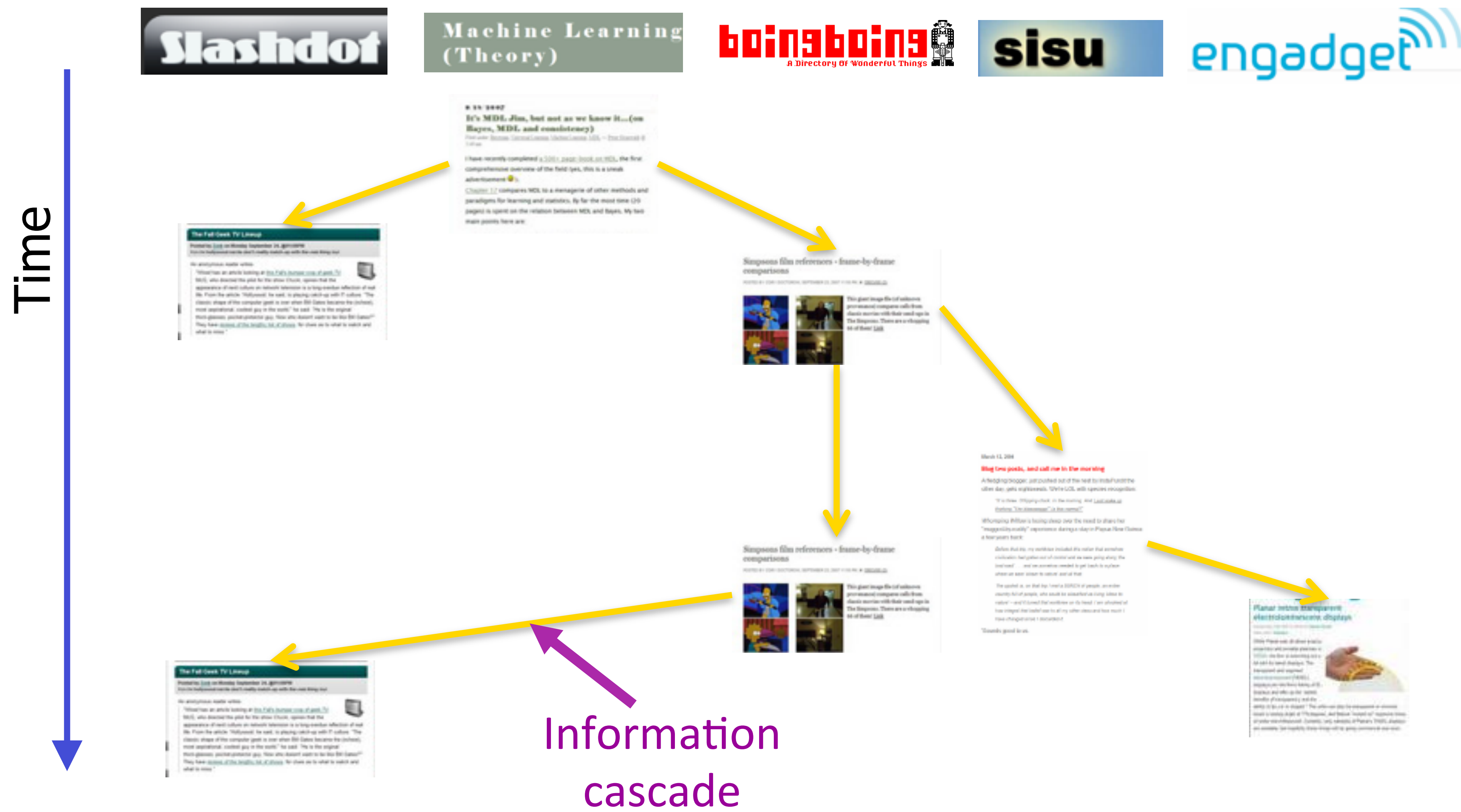
700x speedup

Network inference



How can we learn who influences whom?

Cascades in the Blogosphere



Inferring diffusion networks

[Gomez Rodriguez, Leskovec, Krause ACM TKDE 2012]

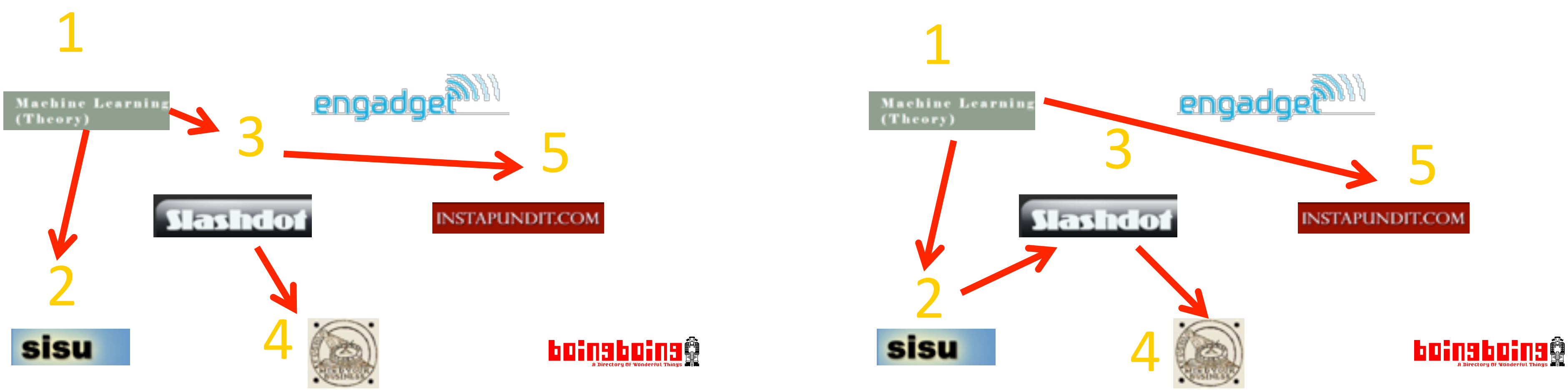
Given: Want:

Given traces of influence, wish to infer sparse directed network G=(V,E)

➔ Formulate as optimization problem

$$E^* = \arg \max_{|E| \leq k} F(E)$$

Estimation problem

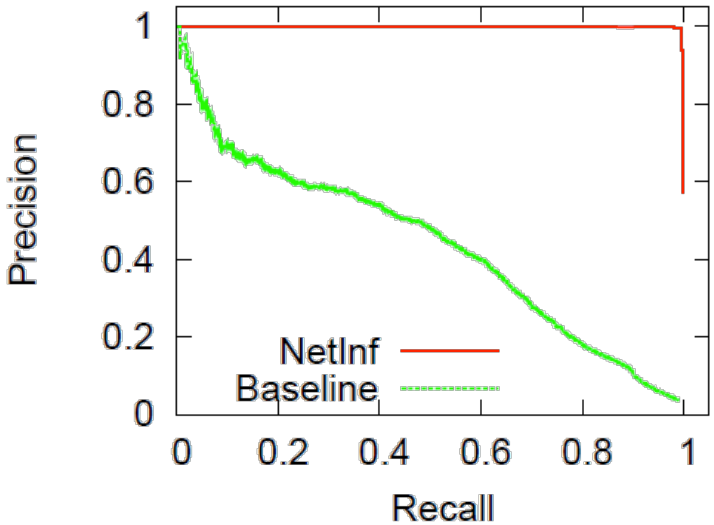


- Many influence trees T consistent with data
- For cascade C_i, model $P(C_i \mid T)$
- Find sparse graph that maximizes likelihood for all observed cascades

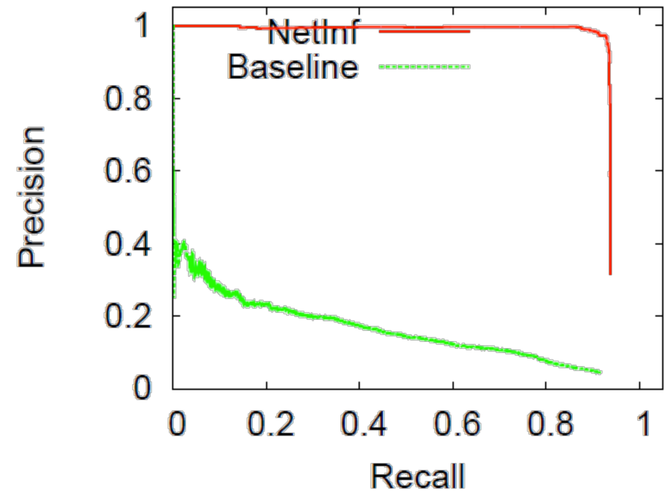
➔ Log likelihood monotonic submodular in selected edges

$$F(E) = \sum_i \log \max_{\text{tree } T \subseteq E} P(C_i \mid T)$$

Evaluation: Synthetic networks



1024 node hierarchical Kronecker exponential transmission model

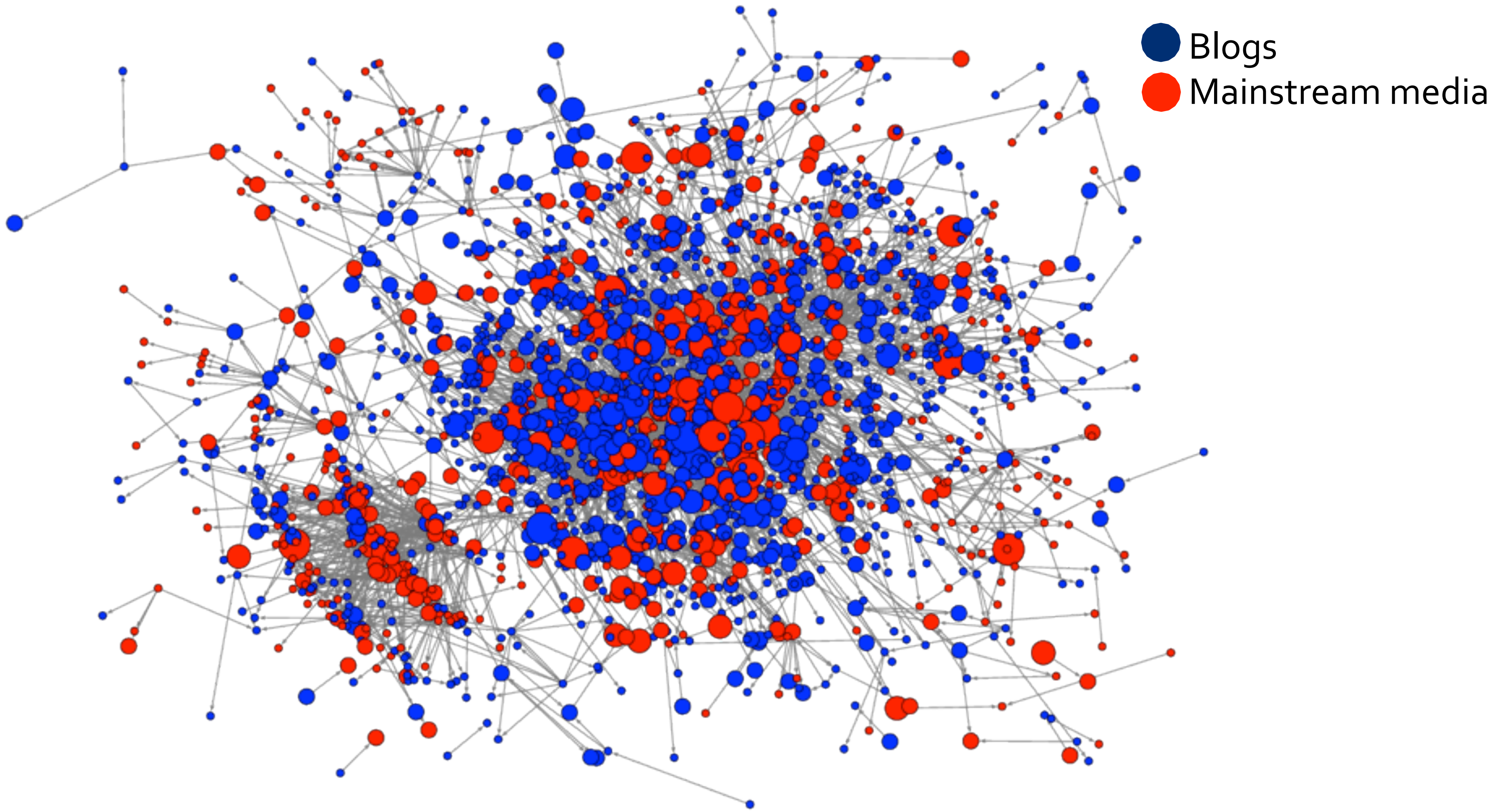


1000 node Forest Fire (α = 1.1) power law transmission model

- Performance does not depend on the network structure:
  - Synthetic Networks: Forest Fire, Kronecker, etc.
  - Transmission time distribution: Exponential, Power Law
- Break-even point of > 90%

Diffusion Network

[Gomez Rodriguez, Leskovec, Krause ACM TKDE 2012]



Actual network inferred from 172 million articles from 1 million news sources

Document summarization [Lin & Bilmes '11]

- Which sentences should we select that best summarize a document?

Marginal gain of a sentence

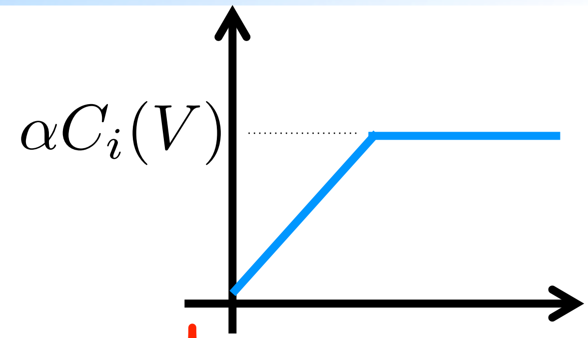
- Many natural notions of „document coverage“ are submodular [Lin & Bilmes ‘11]

Document summarization

$$F(S) = \underbrace{R(S)}_{\text{Relevance}} + \lambda \underbrace{D(S)}_{\text{Diversity}}$$

Relevance of a summary

$$F(S) = R(S) + \lambda D(S)$$



$$R(S) = \sum_i C_i(S)$$

How well is sentence i „covered“ by S

$$C_i(S) = \sum_{j \in S} w_{i,j}$$

Similarity between i and j

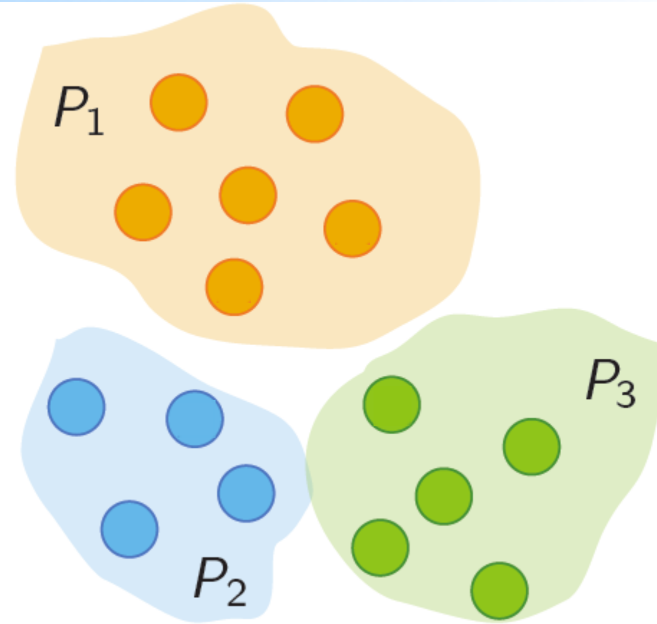
Diversity of a summary

$$D(S) = \sum_{i=1}^{K} \sqrt{\sum_{j \in P_i \cap S} r_j}$$

Relevance of sentence j to doc.

$$r_j = \frac{1}{N} \sum_i w_{i,j}$$

Similarity between i and j



Clustering of sentences in document

Empirical results [Lin & Bilmes '11]

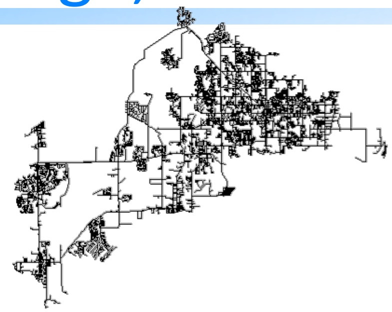
	R	F
$\mathcal{L}_1(S) + \lambda \mathcal{R}_Q(S)$	12.18	12.13
$\mathcal{L}_1(S) + \sum_{\kappa=1}^{3} \lambda_\kappa \mathcal{R}_{Q,\kappa}(S)$	**12.38**	$\boxed{\textbf{12.33}}$
Toutanova et al. (2007)	11.89	11.89
Haghighi and Vanderwende (2009)	11.80	-
Celikyilmaz and Hakkani-tür (2010)	11.40	-
Best system in DUC-07 (peer 15), using web search	**12.45**	12.29

Best F1 score on benchmark corpus DUC-07!

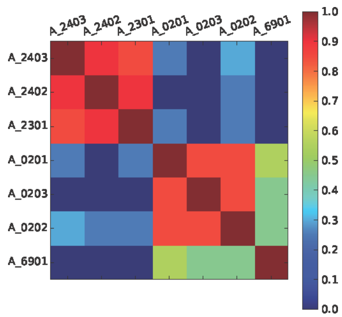
Can do even better using submodular structured prediction! [Lin & Bilmes '12]

Submodular Sensing Problems
[with Guestrin, Leskovec, Singh, Sukhatme, …]

Environmental monitoring
[UAI'05, JAIR '08, ICRA '10]



Water distribution networks
[J WRPM '08]



Experiment design
[NIPS '10, '11, PNAS'13]

Machine Learning (Theory)
Slashdot
boingboing
sisu
engadget

Recommending blogs & news
[KDD '07, '10]

Can all be reduced to monotonic submodular maximization

Maximization: More complex constraints

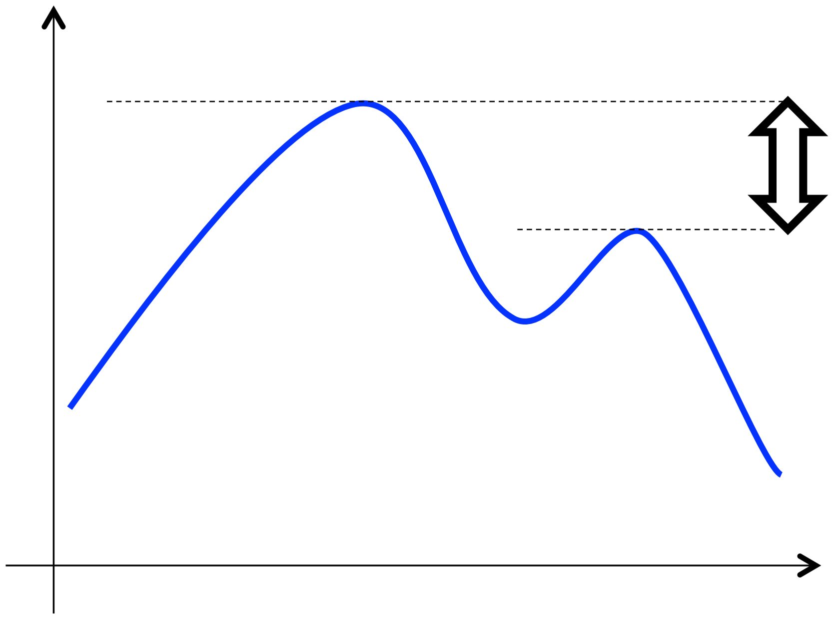
- Approximate submodular maximization possible under a variety of constraints:
  - (Multiple) matroid constraints
  - Knapsack (non-constant cost functions)
  - Multiple matroid and knapsack constraints
  - Path constraints (Submodular orienteering)
  - Connectedness (Submodular Steiner)
  - Robustness (minimax)
  - ...

Greedy works well

Need **non-greedy** algorithms

- Survey on „Submodular Function Maximization“ [Krause & Golovin '12] on submodularity.org

Key intuition for approx. maximization



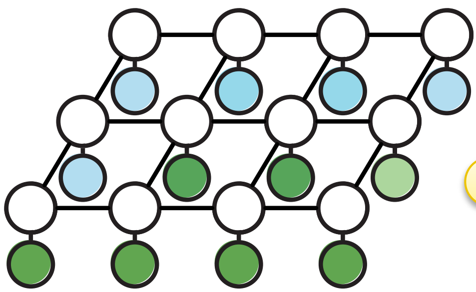
For submod. functions, local maxima can't be too bad

- E.g., all local maxima under cardinality constraints are within factor 2 of global maximum
- Key insight for more complex maximization
  ➔ Greedy, local search, simulated annealing
  for (non-monotone, constrained, ...)

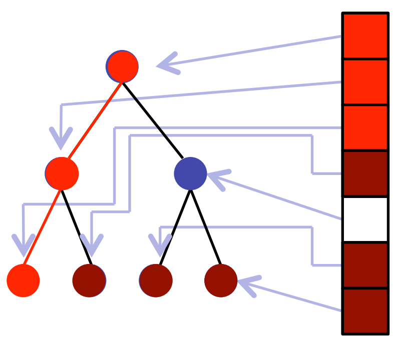
Two-faces of submodular functions

Cuts,
clustering,
similarity

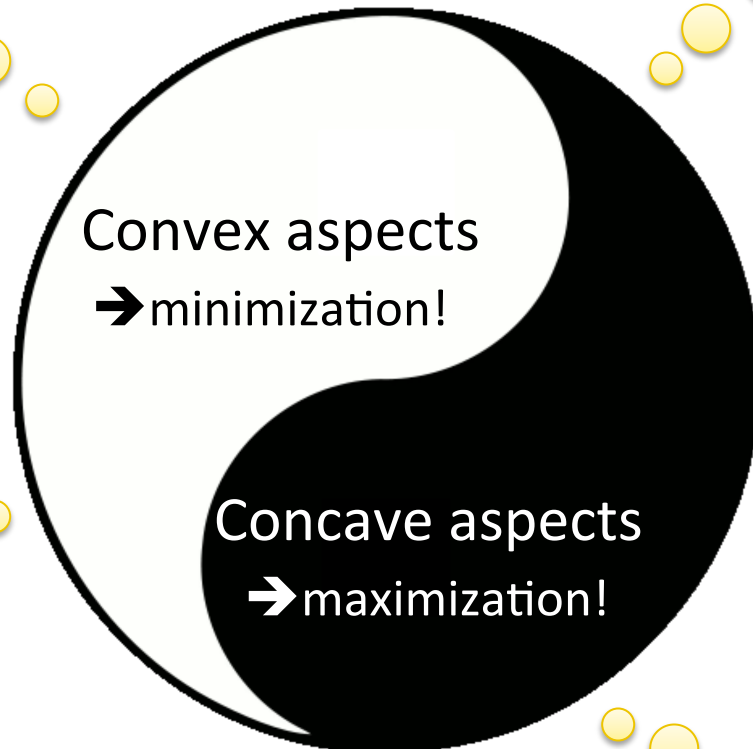
Coverage,
diversity



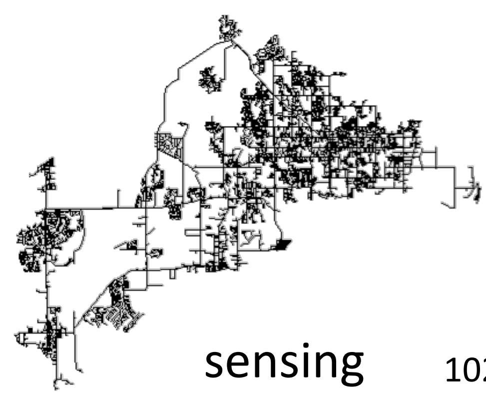
MAP inference



structured sparsity
regularization



summarization



sensing

	Maximization	Minimization
Unconstrained	NP-hard, but well-approximable (if nonnegative)	Polynomial time! Generally inefficent (n^6), but can exploit special cases (cuts; symmetry; decomposable; ...)
Constrained	NP-hard but well-approximable „Greedy-(like)“ for cardinality, matroid constraints; Non-greedy for more complex (e.g., connectivity) constraints	NP-hard; hard to approximate in general, still useful algorithms

Further topics in submodularity & ML

- Learning submodular functions
  - **Goal**: learn a submodular function from few samples
  - **Applications**: Preference elicitation, graph sketching, ...
  - Generally very hard
  - Possible under special structure (e.g., sparsity)
- Online submodular optimization
  - **Goal**: Repeatedly solve submodular optimization problems
  - **Applications**: Recommender systems
  - No regret algorithms for online submodular min & max
- Active learning with submodular functions
  - **Goal**: Adaptive select elements given feedback
  - **Applications**: Active learning, experimental design
  - *Adaptive submodularity* generalizes SFs to policies

Other directions

- Game theory
  - Equilibria in cooperative (supermodular) games / fair allocations
  - Price of anarchy in non-cooperative games
  - Incentive compatible submodular optimization
- Generalizations of submodular functions
  - L#-convex / discrete convex analysis
  - XOS/Subadditive functions
- More optimization algorithms
  - Robust submodular maximization
  - Maximization and minimization under complex constraints
  - Submodular-supermodular procedure / semigradient methods

Further resources

- submodularity.org
  - Tutorial Slides
  - Annotated bibliography
  - Matlab Toolbox for Submodular Optimization
  - Links to workshops and related meetings
- discml.cc
  - NIPS Workshops on Discrete Optimization in Machine Learning
  - Videos of invited talks on videolectures.net

...

Conclusions

- Discrete optimization abundant in applications
- Fortunately, some of those have structure: submodularity
- Submodularity can be exploited to develop efficient, scalable algorithms with strong guarantees
- Many exciting research directions! ☺