

## **Submodularity in Data Science**

Andreas Krause Data Science Summer School

### Acknowledgments

• Based on earlier tutorials with Stefanie Jegelka

#### **Set functions**



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

$$F\left( \bigvee F \left( \bigcup f \right) = F \right)$$

We will assume:

•  $F(\emptyset) = 0$ 

ETH

• black box "oracle" to evaluate F

cost/loss of picking items together, or utility, or probability, ...



 $\mathcal{V} = \text{ variables to observe } F(S) = \text{``information''}$ 

 $\mathcal{V} =$  seed nodes F(S) = "spread"

 $\mathcal{V} = \text{ images (sentences, ...)}$ F(S) = "representation"



maximize coverage, spread, diversity  $\max_S F(S)$ 

Dictionary learning, matrix approximation, object detection,...



 $\mathcal{V} = \text{ data points}$ F(S) = "coherence/separation"



F(S) = "coherence/matching"

 $\mathcal{V} = \text{ coordinates (variables)}$ F(S) = "coherence"



maximize coherence, smoothness  $\min_S F(S)$ 

### Convex functions (Lovász, 1983)

- "occur in many models in economy, engineering and other sciences", "often the only nontrivial property that can be stated in general"
- preserved under many operations and transformations: larger effective range of results
- sufficient structure for a "mathematically beautiful and practically useful theory"
- efficient minimization

"It is less apparent, but we claim and hope to prove to a certain extent, that a similar role is played in discrete optimization by *submodular set-functions*" [...] they share the above four properties.



- 1. What is Submodularity? Examples, connections
- 2. Submodular minimization
- 3. Submodular maximization
- 4. Advanced Topics

TOMORROW

submodularity in deep learning, probabilistic inference, active learning, bandits, ...

## **Diminishing gains**

#### placement A = {1,2}



#### placement B = {1,2,3,4}



Big gain

small gain

for all  $A \subseteq B$ and s not in B



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

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# **Diminishing costs: economies of scale**



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

extra cost: one drink  $\geq \quad F(B \cup s) - F(B)$ 

extra cost: free refill ©

#### **Submodular set functions**



• Union-Intersection: for all  $S, T \subseteq \mathcal{V}$ 

### **Example: modular function**

each element  $e \in \mathcal{V}$  has a weight w(e)

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

#### $A \subset B$

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$$F(A \cup e) - F(A) = w(e) = F(B \cup e) - F(B) = w(e)$$

submodular and supermodular!

### **Example: coverage**

 $\mathcal{V}$  = all possible sensor locations





# **Example: Diversity in recommender systems (FLID)**

[Tschiatschek, Djolonga, K, AISTATS 2016]



$$D(S) = \sum_{d=1}^{k} \left[ \max_{i \in S} W_{i,d} \right]$$

13

### **Example: sensing**



- $\mathcal{V}$  = random variables we can possibly observe
- Utility to have sensors in locations A:

$$F(A) = H(\mathbf{Y}) - H(\mathbf{Y} | \mathbf{X}_A) = I(\mathbf{Y}; \mathbf{X}_A)$$
  
Uncertainty  
about temperature Y  
before sensing  
$$I(\mathbf{Y}; \mathbf{X}_A) = I(\mathbf{Y}; \mathbf{X}_A)$$
  
about temperature Y  
after sensing

### **Example: entropy**

 $X_1, \ldots, X_n$  discrete random variables  $F(S) = H(X_S) =$  joint entropy of variables indexed by S  $A \subset B$  $H(X_{A \cup e}) - H(X_A) = H(X_e | X_A)$  $\geq H(X_e|X_B)$  "information never hurts"  $=H(X_{B\cup e})-H(X_B)$ 

#### discrete entropy is submodular!

# Submodularity and independence

 $X_1, \ldots, X_n$  discrete random variables

 $X_i, i \in S$  statistically independent  $\Leftrightarrow$  H is modular/linear on S  $H(X_S) = \sum_{e \in S} H(X_e)$ 

Similarly: linear independence



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vectors in S linearly independent ⇔ F is modular/linear on S: F(S) = |S|



- cut of one edge is submodular!
- large graph: sum of edges

sum of submodular functions is submodular

### **Closedness properties**

 $F_1,...,F_m$  submodular functions on V and  $\lambda_1,...,\lambda_m > 0$ 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! ③

### **Other closedness properties**

- Restriction: F(S) submodular on V, W subset of V Then  $F'(S) = F(S \cap W)$  is submodular



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- 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





discrete convexity ....

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... or concavity?

#### **Convex aspects**

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#### **Concave aspects**

• submodularity:





### 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



# Application: higher-order potentials

Pixels in a superpixel should have the same label





concave function of cardinality  $\rightarrow$  submodular  $\odot$ 

#### **Deep Submodular Functions**



(Dolhansky & Bilmes 16)

# Submodularity more generally

• Lattices and continuous functions

$$f(x) + f(y) \ge f(x \lor y) + f(x \land y)$$

subclass: diminishing returns (DR) – submodular fn's



(Milgrom-Shannon 94; Topkis 98; Murota 03; Kapralov-Post-Vondrak 10; Soma et al 2014-16; Bach 2015; Ene & Nguyen 2016; Bian-Mirzasoleiman-Buhmann-Krause 16)

### **Origins and history**



nonconvex optimization lattice / continuous submodularity many optimization & duality results generalize

#### probability measures

log-supermodular (→positive assoc.) log-submodular (←negative assoc.) sampling, mode, approx. partition function

#### submodular set functions

convexity: minimization *max. coherence*  dim. returns: maximization *max. diversity* 

#### many examples:

- linear/modular functions
- entropy
- mutual information
- rank functions

- coverage
- diffusion in networks
- volume
- graph cut ...

### **Submodular minimization**

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

#### "maximize coherence"



# Idea: relaxation $\min_{x \in \{0,1\}^n} F(x) \longrightarrow \min_{x \in [0,1]^n} f(x)$

#### Lovász extension

• expectation:

$$f(x) = \mathbb{E}_{\theta \sim x}[F(S_{\theta})]$$

- sample threshold  $\theta \in [0,1]$  uniformly
- $S_{\theta} = \{e \mid x_e \ge \theta\}$



$$f(x) = \mathbb{E}_{\theta}[F(S_{\theta})]$$



#### **Alternative characterization**

$$f(x) = \mathbb{E}_{\theta \sim x}[F(S_{\theta})]$$

#### if *F* is submodular, this is equivalent to:

$$f(x) = \max_{y \in \mathcal{B}_F} y^\top x$$



**Theorem** (*Edmonds* 1971, *Lovász* 1983) Lovász extension is convex  $\Leftrightarrow$  *F* is submodular.

## Submodular polyhedra

submodular polyhedron:

A

Ø

ab

 $\{a,b\}$ 

F(A)

0

 $\mathbf{2}$ 

0

-1

$$\mathcal{P}_{F} = \left\{ y \in \mathbb{R}^{n} \mid \sum_{a \in A} y_{a} \leq F(A) \text{ for all } A \subseteq \mathcal{V} \right\}$$
  
base polytope:  
$$2$$
$$\mathcal{B}_{F} = \left\{ y \in \mathcal{P}_{F} \mid \sum_{a \in \mathcal{V}} y_{a} = F(\mathcal{V}) \right\}$$
  
$$1$$
$$\mathcal{P}_{F}$$
  
$$4$$
$$\mathbf{y}_{a}$$
  
Examples:  
$$\text{ probability simplex} \\ \text{ spanning tree polytope}$$

- spanning tree polytope
- permutahedron

= - - -

 $\mathcal{P}_F$ 

-1

#### **Base polytopes**


# The magic of base polytopes

$$f(x) = \max_{y \in \mathcal{B}_F} y^{\top} x = \max_{y \in \mathcal{B}_F} \sum_i y_i x_i$$

- Linear optimization over the base polytope? exponentially many constraints (one for each subset)
- Edmonds 1971: greedy works ☺
- 1. sort cost vector  $x_{\pi(1)} \ge x_{\pi(2)} \ge \dots$

2. gives sets 
$$S_i = \{\pi(1), ..., \pi(i)\}$$

3. Set 
$$y_{\pi(i)} = F(S_i) - F(S_{i-1})$$

#### Implications: can compute

- Lovász extension
- subgradients of Lovász extension

### **Putting things together**



1. relaxation: convex optimization computable subgradients

← many ways to do Step 1

2. relaxation is exact! pick elements with positive coordinates  $S^* = \{e \mid x_e^* > 0\}$ 

**Submodular minimization in polynomial time!** (Grötschel, Lovász, Schrijver 1981)

# **Submodular minimization**

#### convex optimization

- ellipsoid method (Grötschel-Lovasz-Schrijver 81)
- subgradient method ... (..., Chakrabarty-Lee-Sidford-Wong 16)
- minimum-norm point / Fujishige-Wolfe algorithm (different relaxation) (Fujishige-Isotani 11)

#### combinatorial methods

- first polynomial-time: (Schrijver 00, Iwata-Fleischer-Fujishige-01)
- $O(n^4T + n^5 \log M)$  (Iwata 03)  $O(n^6 + n^5T)$  (Orlin 09)

Latest:

 $O(n^{2}T \log nM + n^{3} \log^{c} nM)$   $O(n^{3}T \log^{2} n + n^{4} \log^{c} n) \qquad \text{(Lee-Sidford-Wong 15)}$ 

### **Different relaxation**

$$\min_{x} f(x) + \frac{1}{2} \|x\|^2$$

solves  $\min_{S \subseteq \mathcal{V}} F(S) + \alpha |S| \quad \text{ for all } \alpha$ 

threshold optimal solution  $x^*$  at lpha

• dual problem: minimum norm point of base polytope



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### Minimum norm point

 $\min_{y\in\mathcal{B}_F} \|y\|^2$ 

$$s^t \in \arg\max_{s \in \mathcal{B}_f} \langle -\nabla g(y^t), s \rangle$$



### **Empirically**



(Figure from Bach, 2012)

# Submodularity and convexity

- convex Lovász extension
  - easy to compute: greedy algorithm (special polyhedra!)
- submodular minimization via convex optimization: exact
- duality results
- structured sparsity (Bach 10)
- decomposition & parallel algorithms (Komodakis-Paragios-Tziritas 11, Stobbe-Krause 10, Jegelka-Bach-Sra 13, Nishihara-Jegelka-Jordan 14, Ene-Nguyen 15)
- variational inference (Djolonga-Krause 14)
- ...

### Structured sparsity and submodularity

y = Mx + noise



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





### **Sparsity**



Optimization: submodular minimization (min-norm)

# Submodular min: special cases

- **"Graph-representable": reduction to minimum cut** (Billionet & Minoux 85, Kolmogorov-Zabih 04, Freedman & Drineas 05, Živný 09, Živný & Jeavons 10, ...)
- Decomposable functions <sup>1</sup>

$$F(S) = \sum_{i} F_i(S)$$

(Stobbe-Krause 10, Komodakis-Paragios-Tziritas 11, Kolmogorov 12, Jegelka-Bach-Sra 13, Nishihara-Jegelka-Jordan 14, Ene-Nguyen 15, Fix-Joachims-Park-Zabih 13, Fix-Wang-Zabih 14)

• Symmetric functions  $F(S) = F(\mathcal{V} \setminus S)$ (Queyranne 98)  $O(n^3)$  nonconvex optimization lattice / continuous submodularity many optimization & duality results generalize

#### probability measures

log-supermodular (→positive assoc.) log-submodular (←negative assoc.) sampling, mode, approx. partition function

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## **Submodular Maximization**



- ground set  ${\cal V}$
- submodular function  $F: 2^{\mathcal{V}} \to \mathbb{R}$

$$\max F(S)$$

Often s.t. to some constraints

Survey: Krause & Golovin (2014) "Submodular Function Maximization"

# Application: Information Gathering







- where put sensors?
- which experiments?
- which labels?

F(S) = "information"

(Krause & Guestrin '05, Hoi-Jin-Zhu-Lyu '06, Das & Kempe '08, ...)

# **Application: Data Summarization**



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- which text, images, videos?
- which data points for training?



F(S) = "relevance, diversity, ..."

(El-Arini et al '09, Yue & Guestrin '09, Gomes & Krause'10, Lin & Bilmes '11, ...)

#### More maximization ...



(Gomez Rodriguez et al 2012)

#### ETH

#### Monotonicity

#### if $S \subseteq T$ then $F(S) \leq F(T)$



## **Maximizing monotone functions**

if 
$$A \subseteq B$$
 then  $F(A) \leq F(B)$ 



• NP-hard

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• Approximation: Greedy algorithms

## **Maximizing monotone functions**

$$\max_{S} F(S) \text{ s.t. } |S| \le k$$

#### Greedy algorithm:

$$S_0 = \emptyset$$
  
for  $i = 0, ..., k-1$   
$$e^* = \arg \max_{e \in \mathcal{V} \setminus S_i} F(S_i \cup \{e\})$$
$$S_{i+1} = S_i \cup \{e^*\}$$



How "good" is 
$$S_k$$
 ?

# How good is greedy? in practice...

empirically:







## How good is greedy? ... in theory

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$$\max_{S} F(S) \text{ s.t. } |S| \le k$$

Theorem (Nemhauser, Wolsey, Fisher '78) F monotone submodular,  $S_k$  solution of greedy. Then  $F(S_k) \geq \left(1 - \frac{1}{e}\right) F(S^*)$ 

in general, no poly-time algorithm can do better than that!

#### **Proof Sketch**



#### Appliction: Network Inference [Gomez Rodriguez, Leskovec, Krause ACM TKDE 2012]



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

→ Formulate as optimization problem

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

## **Estimation problem**



- Many influence trees T consistent with data
- For cascade  $C_i$ , model  $P(C_i | T)$
- Find sparse graph that maximizes likelihood for all  ${}^{\bullet}$ observed cascades
- Log likelihood monotonic submodular in selected edges  $F(E) = \sum \log \max_{\text{tree } T \subseteq E} P(C_i \mid T)$



- 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

#### Questions

- What if I have more complex constraints?
- Greedy takes O(nk) time. What if n, k are large?
- What if my function is not monotone?

# More complex constraints: budget

$$\max F(S) \text{ s.t. } \sum_{e \in S} c(e) \le B$$

- 1. run greedy:  $S_{\rm gr}$
- 2. run a modified greedy:  $\mathit{S}_{\rm mod}$

$$e^* = \arg\max_{e} \frac{F(S_i \cup \{e\}) - F(S_i)}{c(e)}$$

3. pick better of  $S_{gr}$ ,  $S_{mod}$  $\Rightarrow$  approximation factor:  $1 - \frac{1}{\sqrt{e}}$ 

even better but less fast: partial enumeration (Sviridenko, '04) or filtering (Badanidiyuru & Vondrák '14)

(Leskovec-Krause-Guestrin-Faloutsos-VanBriesen-Glance '07)

#### **Relax: Discrete to continuous**



#### Algorithm:

- 1. approximately maximize  $f_M$  over  $\mathcal{P} = \operatorname{conv}(\mathcal{I})$
- 2. round to discrete set

(Vondrák '08; Calinescu-Chekuri-Pal-Vondrák '11; Kulik-Shachnai-Tamir'11)

#### **Multilinear extension**

 ${\mathcal X}$ 

0.5

1.0

0.5

0.2

0.2

sample item e with probability  $x_e$ 

$$f_M(x) = \mathbb{E}_{S \sim x} [F(S)] \qquad p(1) =$$
$$= \sum_{S \subseteq \mathcal{V}} F(S) \prod_{e \in S} x_e \prod_{e \notin S} (1 - x_e) \qquad p(2) =$$
$$p(3) =$$

#### **Compare: Multilinear vs. Lovász ext.**



- convex
- computable in O(n log n)
- Submodular minimization



- concave in certain directions, convex in others
- approximate by sampling
- Submodular maximization

### **Illustration of Continuous Greedy**



### **Continuous submodular maximization**

- Continuous Greedy (~Frank Wolfe) "works" for any
  - downward closed solvable polytope *P* (Calinescu-Chekuri-Pál-Vondrák'11)

- monotone continuous "DR-submodular" function (beyond multilinear extension) (Bian-Mirzasoleiman-Buhmann-Krause'16)
  Non-convex optimization with guarantees
- "works" means (1-1/e) approx. for continuous problem
- Rounding strategy depends on constraints
  - Pipage rounding for matroids (Ageev, Sviridenko '04)
  - Contention resolution for more general *P* (Chekuri-Vondrák-Zenklusen'11)

#### Questions

- What if I have more complex constraints?
  - budget constraints
  - Downward closed constraints (matroids, p-systems, knapsacks, their intersections, ...)
- Greedy takes O(nk) time. What if n, k are large?
- What if my function is not monotone?

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#### Scaling up the greedy algorithm [Minoux '78]

In round i+1,

- have picked  $A_i = \{s_1, \dots, s_i\}$
- pick  $s_{i+1} = argmax_s F(A_i \cup \{s\})-F(A_i)$
- I.e., maximize "marginal benefit"  $\Delta(s | A_i)$

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

Key observation: Submodularity implies

$$i \leq j \implies \Delta(s \mid A_i) \geq \Delta(s \mid A_j)$$



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<sub>i</sub> from previous iteration
- Re-evaluate Δ<sub>i</sub> only for top element
- If Δ<sub>i</sub> stays on top, use it, otherwise re-sort



Note: Very easy to compute online bounds, lazy evaluations, etc. [Leskovec, Krause et al. '07]
### Lazier than lazy greedy



$$\max_{S} F(S) \text{ s.t. } |S| \le k$$

- for i=1...k:
- randomly pick set *T* of size  $\frac{n}{k} \log \frac{1}{\epsilon}$
- find best a element in T and add

$$a_{i} = \arg\max_{a \in T} F(a|S_{i-1})$$
$$S_{i} \leftarrow S_{i-1} \cup \{a_{i}\}$$

(Mirzasoleiman et al 2014)





faster

# **Distributed greedy algorithms**



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greedy is sequential. pick in parallel??

pick *k* elements on each machine.

combine and run greedy again.

## GREEDI



(Mirzasoleiman-Karbasi-Sarkar-Krause'13, da Ponte Barbosa-Ene-Nguyen-Ward'15)

#### **Empirical Performance**





(Mirzasoleiman-Karbasi-Sarkar-Krause '13)

## Questions

- What if I have more complex constraints?
  - budget constraints
  - Downward closed solvable polytopes
- Greedy takes O(nk) time. What if n, k are large?
  - Lazy greedy, lazier than lazy greedy (Minoux'78, Mirzasoleiman-Badanidiyuru-Karbasi-Vondrák-Krause'15)
  - filtering / streaming / multi-stage (Badanidiyuru & Vondrák 2014; Badanidiyuru-Mirzasoleiman-Karbasi-Krause'14, Wei-lyer-Bilmes'14)
  - Distributed (Mirzasoleiman-Karbasi-Sarkar-Krause'13, Kumar-Moseley-Vassilivitskii-Vattani'13)
- What if my function is not monotone?

#### **Non-monotone functions**



### Greedy can fail ...





coverage: 100

-60

cost:

= - - -



for *i*=1, ..., *n* //add or remove?

- gain of adding (to A):  $\Delta_+ = [F(A \cup a_i) F(A)]_+$
- gain of removing (from B):  $\Delta_{-} = [F(B \setminus a) F(B)]_{+}$

add with probability

$$\mathbb{P}(\text{add}) = \frac{\Delta_+}{\Delta_+ + \Delta_-} = 40\%$$



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Start: 
$$A = \emptyset, \ B = \mathcal{V}$$

for *i*=1, ..., *n* //add or remove?

add with probability

$$\mathbb{P}(\text{add}) = \frac{\Delta_+}{\Delta_+ + \Delta_-}$$

add to A or remove from B





ETH



### **Double greedy**

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

**Theorem** (Buchbinder, Feldman, Naor, Schwartz '12)

F submodular,  $S_g$  solution of double greedy. Then

$$\mathbb{E}[F(S_g)] \ge \frac{1}{2}F(S^*)$$

optimal solution

# **Non-monotone maximization**

- Generally inapproximable unless F is nonnegative
- Unconstrained maximization:
  - Local search (Feige-Mirrokni-Vondrák'07)
  - Double greedy: Optimal <sup>1</sup>/<sub>2</sub> approximation

(Buchbinder-Feldman-Naor-Schwartz'12)

- Constrained maximization:
  - Cardinality constraints: randomized greedy (Buchbinder-Feldman-Naor-Schwartz'14)
  - Filtering based algorithms (Mirzasoleiman-Badanidiyuru-Karbasi'16)
  - More general constraints: Continuous local search via multilinear extension (Chekuri–Vondrák-Zenklusen'11)
- Distributed algorithms? yes!
  - divide-and-conquer as before (de Ponte Barbosa-Ene-Nguyen-Ward '15)
  - concurrency control / Hogwild (Pan-Jegelka-Gonzalez-Bradley-Jordan '14)

## Submodular maximization: summary

- Many applications: diverse, informative subsets
- NP-hard, but variants of greedy / local search work
- Distinguish monotone / non-monotone
- Can handle several types of constraints
- Scalable algorithms for solving massive problems

### **Summary: Submodular Optimization**

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Minimization	Maximization
Unconstrained SFMin tractable, constrained SFMin generally hard	SFMax generally hard distinguish montone & non-monotone
Combinatorial and continuous algorithms	Greedy-like and continuous algorithms
Convex Lovász extension	Nonconvex multilinear extension
Faster algorithms for special cases	Fast distributed/ streaming algorithms