

Submodular Functions – Part I

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Set functions





We will assume:

•
$$F(\emptyset) = 0$$

• black box "oracle" to evaluate F

cost of buying items together, or utility, or probability, ... l liit

Discrete Labeling





F(S) =coherence + likelihood

Summarization



F(S) = relevance + diversity or coverage

Informative Subsets







- where put sensors?
- which experiments?
- summarization

F(S) = "information"

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Sparsity









Formalization

Formalization:
 Optimize a set function F(S) (under constraints)



- generally very hard ⊗
- submodularity helps: efficient optimization & inference with guarantees!
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Roadmap

- Submodular set functions
 - what is this? where does it occur? how recognize?
- Maximizing submodular functions: diversity, repulsion, concavity greed is not too bad
- Minimizing submodular functions: coherence, regularization, convexity the magic of "discrete analog of convex"
- Other questions around submodularity & ML

more reading & papers: <u>http://people.csail.mit.edu/stefje/mlss/literature.pdf</u>

Sensing



V = all possible locations F(S) = information gained from locations in S

Marginal gain

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



new sensor s

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Diminishing marginal gains



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Submodularity



diminishing marginal costs

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Submodular set functions

• Diminishing gains: for all $A \subseteq B$



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



The big picture



Examples

- each element e has a weight w(e)

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



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$A \subset B$

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

linear / modular function F and -F always submodular!

Examples



sensing: F(S) = information gained from locations S

Example: cover



More complex model for sensing



Y_s: temperature at location s

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X_s: sensor value at location s

 $X_s = Y_s + noise$

Joint probability distribution $P(X_1,...,X_n,Y_1,...,Y_n) = P(Y_1,...,Y_n) P(X_1,...,X_n | Y_1,...,Y_n)$ Prior Likelihood

Sensor placement

Utility of having sensors at subset A of all locations

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

Uncertainty about temperature Y **before** sensing Uncertainty about temperature Y after sensing



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



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Information gain

 $X_1, \ldots X_n, Y_1, \ldots, Y_m$ discrete random variables

$$F(A) = I(Y; X_A) = H(X_A) - H(X_A|Y)$$
modular!
$$= \sum_{i \in A} H(X_i|Y)$$

if all X_i, X_j conditionally independent given Ythen *F* is submodular!



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Entropy

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 X_1, \ldots, X_n discrete random variables: $X_e \in \{1, \ldots, m\}$ $F(S) = H(X_S) =$ joint entropy of variables indexed by S $H(X_e) = \sum P(X_e = x) \log P(X_e = x)$ $x \in \{1, ..., m\}$ $A \subset B, e \notin B$ $F(A \cup e) - F(A) \ge F(B \cup e) - F(B)??$ $H(X_{A\cup e}) - H(X_A) = H(X_e|X_A)$ $\leq H(X_e|X_B)$ "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



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

Maximizing Influence

F(S) =expected # infected nodes



 $F(S \cup s) - F(S) \ge F(T \cup s) - F(T)$

(Kempe, Kleinberg & Tardos 2003)

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Graph cuts



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

Useful property: sum of submodular functions is submodular

Sets and boolean vectors

any set function with |V| = n.

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

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



subset selection = binary labeling!

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Attractive potentials





$$\max_{\mathbf{x}\in\{0,1\}^n} \begin{array}{c|c} P(\mathbf{x} \mid \mathbf{z}) \propto \exp(-E(\mathbf{x}; \mathbf{z})) \\ & & & & \\ \text{labels pixel} \\ & & \text{values} \end{array} \Leftrightarrow \min_{\mathbf{x}\in\{0,1\}^n} E(\mathbf{x}; \mathbf{z}) \end{array}$$

Attractive potentials



$$E(\mathbf{x};\mathbf{z}) = \sum_{i} E_{i}(x_{i}) + \sum_{ij} E_{ij}(x_{i}, x_{j})$$

spatial coherence:

$$E_{ij}(1,0) + E_{ij}(0,1) \ge E_{ij}(0,0) + E_{ij}(1,1)$$

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$$S = \{i\} \qquad T = \{j\} \qquad S \cap T = \emptyset \qquad S \cup T$$

 $F(S) + F(T) \geq F(S \cup T) + F(S \cap T)$

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Diversity priors





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$P(S \mid \text{data}) \propto P(S) P(\text{data} \mid S)$

"spread out"

Determinantal point processes



- similarity matrix L $L_{ij} = x_i^\top x_j$
- sample set *Y*:

$$P(Y = S) \propto \det(L_S)$$
$$= \operatorname{Vol}(\{x_i\}_{i \in S})^2$$



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DPP sample



similarities:

$$s_{ij} = \exp(-\frac{1}{2\sigma^2} ||x_i - x_j||^2)$$

$$\sigma^2 = 35$$

 $\mathbb{P}[\mathbf{i}]$

608967736170200863904377144677

Submodularity: many examples

- linear/modular functions
- graph cut function
- coverage
- propagation/diffusion in networks
- entropy
- rank functions
- information gain
- log P(S|data) [repulsion] or -log P(S|data) [coherence]



Closedness properties

F(S) submodular on V. The following are submodular:

• Restriction: $F'(S) = F(S \cap W)$



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Closedness properties

 ${\cal F}(S)$ submodular on V. The following are submodular:

- Restriction: $F'(S) = F(S \cap W)$
- Conditioning: $F'(S) = F(S \cup W)$



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Closedness properties

F(S) submodular on V. The following are submodular:

- **Restriction:** $F'(S) = F(S \cap W)$
- Conditioning: $F'(S) = F(S \cup W)$
- Reflection: $F'(S) = F(V \setminus S)$





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Submodularity ...







... or concavity?

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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.

Convex aspects



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Concave aspects

• submodularity: $A \subseteq B, \ s \notin B :$ $F(A \cup s) - F(A) \geq F(B \cup s) - F(B)$ • concavity: $a < b, \ s > 0 :$

$$f(a+s) - f(a) \ge f(b+s) - f(b)$$



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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



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Max / min

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• Maximum of convex functions is convex



Maximum of submodular functions

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





 $\max\{F_1, F_2\}$ not submodular in general!

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Max / min

Plif

• Minimum of concave functions is concave



Minimum of submodular functions

What about $F(A) = \min\{F_1(A), F_2(A)\}$?

 $\begin{array}{cccc}
0 & 0 & 1 & 0 \\
F(A) + F(B) \geq F(A \cup B) + F(A \cap B)?
\end{array}$

		F ₁ (A)	F ₂ (A)	
$A \cap B$	{}	0	0	$A \cap B$
A	{a}	1	0	A
В	{b}	0	1	В
$A \cup B$	{a,b}	1	1	$A\cup B$

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

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Submodular optimization



- Maximizing submodular functions: diversity, repulsion, concavity greed is not too bad
- Minimizing submodular functions: coherence, regularization, convexity magic with polytopes, and "discrete analog of convex"

Submodular Maximization



- ground set ${\cal V}$
- (scoring) function $F: 2^{\mathcal{V}} \to \mathbb{R}_+$

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 $\max F(S)$

Informative Subsets







- where put sensors?
- which experiments?
- summarization

F(S) = "information"

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Maximizing Influence

F(S) =expected # infected nodes



Kempe, Kleinberg & Tardos 2003

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Summarization

- videos, text, pictures ...
- would like:

relevance, reliability, diversity







Summarization

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

• Coverage / relevance

• Diversity

$$R(S) = \sum_{a \in \mathcal{V}} \max_{b \in S} s_{a,b}$$

$$D(S) = \sum_{j=1}^{m} \sqrt{|S \cap P_j|}$$

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(Simon et al 2007, Lin & Bilmes 2011&2012, Tschiatschek et al 2014, Kim et al 2014, Gygli et al 2015, ...)

Diversity

• Diversity

$$D(S) = \sum_{j=1}^{m} \sqrt{|S \cap P_j|}$$

Another diversity function ...

$$D(S) = -\sum_{a,b\in S} s_{a,b}$$





decreasing

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Summarization: results

	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	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

(Lin & Bilmes 2011)

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Many more functions are possible ...
→Learn a weighted combination: structured prediction works even better!

(Lin & Bilmes 2012, Tschiatschek et al 2014, Gygli et al 2015, Xu et al 2015,...)

More maximization ...



co-segmentation by maximizing anisotropic diffusion (Kim et al 2011)



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environmental monitoring (Krause, ...)

max F(S)

weakly supervised object detection (Song et al 2014)





recommendations (Yue & Guestrin)



inferring networks (Gomez Rodriguez et al 2012)

Monotonicity

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



Monotonicity – how check?

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

Let $B = A \cup \{a\}$.

$$\underbrace{F(A \cup \{a\}) - F(A)}_{F(A)} \ge 0.$$

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marginal gain



Maximizing monotone functions

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

$\max F(S)$

- NP-hard
- approximation: greedy algorithms

Maximizing monotone functions

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

• greedy algorithm:

$$S_{0} = \emptyset$$

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



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How "good" is
$$S_k$$
 ?

Pedestrian detection



 $x_i = index of hypothesis$ explaining x_i





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 $y_i = 1$: object i present $y_i = 0$: object i not present

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Voting elements

Hypotheses

Illustrations courtesy of Pushmeet Kohli

(Barinova et al.'10)

Pedestrian detection



 x_i = index of hypothesis explaining x_i



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Inference

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Datasets from [Andriluka et al. CVPR 2008] (with strongly occluded pedestrians added)

Using the Hough forest trained in [Gall&Lempitsky CVPR09]

Illustrations courtesy of Pushmeet Kohli

How good is greedy? in practice...





sensor placement

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How good is greedy? ... in theory

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

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

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

Questions

- What if I have more complex constraints?
 - budget constraints
 - matroid 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: S_{mod}

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

- 3. pick better of $S_{\rm gr}$, $S_{\rm mod}$
- ➔ approximation factor:

$$\frac{1}{2}\left(1-\frac{1}{e}\right)$$

even better but less fast: partial enumeration (Sviridenko, 2004) or filtering (Badanidiyuru & Vondrák 2014)

40 Line

(Leskovec et al 2007)

Other constraints: Camera network

- Ground set: $V = \{1_a, 1_b, \dots, 5_a, 5_b\}$
- Sensing quality model: $F: 2^V \to \mathbb{R}$
- Configuration (subset) is feasible if no camera is pointed in two directions at once
- Constraints:
- $P_1 = \{1_a, 1_b\}, \dots, P_5 = \{5_a, 5_b\}$ require: $|S \cap P_i| \le 1$



Generalization of Greedy algorithm

$$S = \emptyset$$

While $\exists e : S \cup e \text{ feasible}$

$$e^* \leftarrow \operatorname{argmax} \{F(S \cup e) \mid S \cup e \text{ feasible}\}$$

$$S \leftarrow S \cup e^*$$

Theorem (Nemhauser, Wolsey, Fisher 78) For monotone submodular functions: $F(S_{\text{greedy}}) \geq \frac{1}{2}F(S^*)$

Does this always work?

No. But works for matroid constraints.



Matroids: examples

set S is independent (= feasible) if ...





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Matroids

set S is independent (= feasible) if ...



- S independent \rightarrow $T \subseteq$ S also independent
- Exchange property: S, U independent, |S| > |U|
 → some e ∈ S can be added to U: U ∪ e independent
- All maximal independent sets have the same size

Generalization of Greedy algorithm

$$S = \emptyset$$
While $\exists e : S \cup e$ feasible
$$e^* \leftarrow \operatorname{argmax} \{F(S \cup e) \mid S \cup e \text{ feasible}\}$$

$$S \leftarrow S \cup e^*$$

Theorem (*Nemhauser, Wolsey, Fisher 78*) For monotone submodular functions:

 $F(S_{\text{greedy}}) \geq \frac{1}{2}F(S^*)$

- Works for matroid constraints
- Is this the best possible?

Can do a bit better with relaxation: (1-1/e)



Relax: Discrete to continuous



Algorithm:

1. approximately maximize f_M

(like Frank-Wolfe algorithm – next lecture)

2. round to discrete set (pipage rounding)

(Calinescu-Chekuri-Pal-Vondrak 2011)

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Multilinear extension

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• sample item e with probability x_e

```
f_M(x) = \mathbb{E}_{S \sim x} \left[ F(S) \right]
                   =\sum_{S\subseteq\mathcal{V}}F(S)\prod_{e\in S}x_e\prod_{e\notin S}(1-x_e)
                                                                                                                              \mathcal{X}
                                                                                                       p(1) = 0.5 *

p(2) = 1.0 

p(3) = 0.5 

0.2 *
                                                                                                                             0.2
```

Questions

- What if I have more complex constraints?
 - budget constraints
 - matroid constraints
- Greedy takes O(nk) time. What if n, k are large?
 - faster sequential algorithms
 - filtering
 - parallel / distributed
- What if my function is not monotone?
Making greedy faster: stochastic



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

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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)

Performance



even more data ... distributed greedy algorithm?

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greedy is sequential. pick in parallel??

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pick *k* elements on each machine.

combine and run greedy again.



pick in parallel from *m* machines

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Is this useful?

Distributed Greedy



In practice, performs often quite well.

- special structure: Improved guarantees if F is Lipschitz or a sum of many terms
- 2. randomization

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- each machine: α -approximation algorithm
- level 2: β approximation algorithm
- → overall approximation factor: $\mathbb{E}[F(\widehat{S})] \geq \frac{\alpha\beta}{\alpha+\beta}F(S^*)$

(Mirzasoleiman et al 2013, de Ponte Barbosa et al 2015, see also Mirrokni, Zadimoghaddam 2015)

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(Mirzasoleiman et al 2013, de Ponte Barbosa et al 2015, see also Mirrokni, Zadimoghaddam 2015)

Questions

- What if I have more complex constraints?
 - matroid constraints
 - budget constraints
- Greedy takes O(nk) time. What if n, k are large?
 - stochastic
 - parallel / distributed
 - filtering, structured, ...
- What if my function is not monotone?

Non-monotone functions

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Greedy can fail ...



Greedy can fail ...

$$F(A) = \left| \bigcup_{a \in A} \operatorname{area}(a) \right| - \sum_{a \in A} c(a)$$

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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

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Double greedy

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

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

F submodular, S_g solution of double greedy. Then

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

Non-monotone maximization

- alternatives to double greedy? local search (Feige et al 2007)
- constraints?
 possible, but different algorithms
- distributed algorithms? yes!
 - divide-and-conquer as before (de Ponte Barbosa et al 2015)
 - concurrency control / Hogwild (Pan et al 2014)

Submodular maximization: summary

- many applications: diverse, informative subsets
- NP-hard, but greedy or local search
- distinguish monotone / non-monotone
- several constraints possible (monotone and non-monotone)

Submodularity and machine learning

distributions over labels, sets log-submodular/ supermodular probability e.g. "attractive" graphical models, determinantal point processes

> submodularity & machine learning!

(convex) regularization submodularity: "discrete convexity" e.g. combinatorial sparse estimation diffusion processes, covering, rank, connectivity, entropy, economies of scale, summarization, ... submodular phenomena