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Submodularity in Machine Learning and Vision

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Network Inference



How to learn who influences whom?

Multiple object detection



How to locate multiple objects in an image?

Segmentation & MAP inference



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

What's common?

Formalization:

Optimize a set function F(S) under constraints







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



- will assume $F(\emptyset) = 0$ (w.l.o.g.)
- \bullet 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 $F: 2^V \to \mathbb{R}$
- Marginal gain: $\Delta_F(s \mid A) = F(\{s\} \cup A) F(A)$



new sensor s

Decreasing gains: submodularity

placement $A = \{1,2\}$ placement $B = \{1, ..., 5\}$ Romo **Big gain** Adding s do small gain lich new sensor s B S $F(A \cup s) - F(A)$ $F(B \cup s) - F(B)$ \geq $A \subseteq B$ $s \notin B$ $\Delta(s \mid A)$

Equivalent characterizations

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

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



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

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



How do I prove my problem is submodular?

Why is submodularity useful?

Example: Set cover



Node predicts values of positions with some radius $A \subseteq V : \qquad F(A) =$ "area covered by sensors placed at A"

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

Set cover is submodular



More complex model for sensing



Y_s: temperature at location s

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

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

 $Y_1,...,Y_m, X_1, ..., X_n$ random variables $F(A) = I(Y; X_A) = H(Y)-H(Y | X_A)$

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?



Closedness under linear combinations

 $F_1,...,F_m$ submodular functions on V and $\lambda_1,...,\lambda_m \ge 0$ 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

Submodularity ...





... or concavity?

Convex aspects



Concave aspects



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



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(F₁,F₂) not submodular in general!

Two faces of submodular functions



What to do with submodular functions



Here we focus on optimization & applications



Minimization and maximization not the same??

Submodular minimization



clustering

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



structured sparsity regularization



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

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



... is a function on binary vectors!

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

$$x = e_A$$

$$1 \quad a$$

$$1 \quad b$$

$$0 \quad c$$

$$0 \quad d$$

pseudo-boolean function

Submodularity and convexity



- 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

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

Lovász, 1982

The submodular polyhedron P_F

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

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

$$A = F(A)$$

$$\{\} = 0$$

$$\{a\} = -1$$

$$\{b\} = 2$$

$$\{a,b\} = 0$$

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!!! \bigotimes Computable in O(n log n) time $\bigotimes_{\text{[Edmonds '70]}}$

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



Submodular minimization

F(A)

 $\min_{A \subseteq V}$

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: $O(n^{4}T + n^{5}logM) \qquad [Iwata '03]$ $O(n^{6} + n^{5}T) \qquad [Orlin '09]$

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The minimum-norm-point algorithm



Empirical comparison



Minimum norm point algorithm: usually orders of magnitude faster

[Fujishige & Isotani '11]

Example I: Sparsity



 $y \approx Mx$

Want "representative" Want "simple" explanations dictionaries (e.g., use few columns of M)

Example I: Sparsity

pixels



large wavelet coefficients

dwideband 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

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

explain y with few columns of M: few x_i

discrete regularization on support S of x

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

relax to convex envelope

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



in nature: sparsity pattern often not random...

Structured sparsity





Structured sparsity



Structured sparsity



Sparsity-inducing norms through submodular functions [Bach NIPS 2010]

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



Optimization: submodular minimization

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:
$$\{y_1,\ldots,y_n\}\subseteq \mathbb{R}^d$$

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

Structured sparse dictionary learning [Bach et al, 2011]



Original images

Dictionary from NMF

Structured-sparse Dictionary (SSPCA)

Example II: MAP inference







$$\max_{\mathbf{x}\in\{0,1\}^n} \frac{P(\mathbf{x} \mid \mathbf{z}) \propto \exp(-E(\mathbf{x}; \mathbf{z}))}{\sum_{\substack{\text{labels} \\ \text{values}}}} \Leftrightarrow \min_{\mathbf{x}\in\{0,1\}^n} E(\mathbf{x}; \mathbf{z})$$

Example II: MAP inference





Recall: equivalence

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



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

if each E_{ij} is submodular ("attractive"): $E_{ij}(1,0) + E_{ij}(0,1) \geq E_{ij}(0,0) + E_{ij}(1,1)$ (a)

then F is a graph cut function.

MAP inference = Minimum cut: fast \bigcirc

Pairwise is not enough...



color + pairwise +



color + pairwise











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 \rightarrow submodular \odot

Can still be transformed into a graph cut instance!

Other special cases

- Symmetric: $F(S) = F(V \setminus S)$
 - Queyranne's algorithm: O(n³)
 [Queyranne, 1998]
- Concave of modular:

$$F(S) = \sum_{i} g_{i} \left(\sum_{s \in S} w(s) \right)$$

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

Sum of submodular functions, each bounded support

[Kolmogorov `12]

Submodular minimization



Submodular minimization

- unconstrained: $\min F(A)$ s.t. $A \subseteq V$
 - nontrivial algorithms, polynomial time
- constraints: e.g. $\min F(A)$ s.t. $|A| \ge k$
 - limited cases doable:
 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]

special case:

balanced

cut

Constraints

minimum...



ground set: edges in a graph



Constrained modular minimization

 $\min_{S \in \mathcal{C}} F(S)$

Constrained submodular minimization

Submodular ("cooperative") cut [Jegelka & Bilmes CVPR '11]

Graph cut









Efficient constrained optimization

Idea: minimize a series of modular surrogate functions

only need to solve sum-of-weights problems

Provides certain approximation guarantees



spanning tree



cut

efficient



matching



[Jegelka & Bilmes `11, Iyer et al. ICML `13, see also Krause et al '06] ₆₄

Outline

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





Outlook and pointers

Submodular maximization



summarization

Two faces of submodular functions



Submodular maximization



submodularity and concavity

Concave aspects

• submodularity: $A \subseteq B, \ s \notin B$: $F(A \cup s) - F(A) \ge F(B \cup s) - F(B)$



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-ε}) approximation)

maximum
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 $F(A_R) \ge 1/2 \max_A F(A)$

Cannot do better in general than ½ unless P = NP

Unconstrained vs. constraint maximization

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

 $\frac{\text{Option 1:}}{\underset{A}{\max} F(A) - C(A)}$ s.t. $A \subseteq V$

"Scalarization"

Option 2:

$$\max_{A} F(A)$$

s.t. $C(A) \le B$

"Constrained maximization"

Can get 1/2 approx... if F(A)-C(A) ≥ 0 for all sets A Positiveness is a strong requirement ⓒ

What is possible?

Optimization



Monotonicity



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

Adding sensors can only help

Cardinality constrained maximization

Given: finite set V, monotone submodular F

Want:

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

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!

Greedy algorithm:

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

For i = 1 to k
 $s^* \leftarrow \arg \max F(\mathcal{A} \cup \{s\})$
 $\mathcal{A} \leftarrow \mathcal{A} \cup \{s^*\}$



How well can this simple heuristic do?

Performance of greedy



One reason submodularity is useful

Theorem [Nemhauser, Fisher & Wolsey '78]
For monotonic submodular functions,
Greedy algorithm gives constant factor approximation
$$F(A_{greedy}) \ge (1-1/e) F(A_{opt})$$

~63%

- 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...



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 = {s₁,...,s_i}
- pick $s_{i+1} = argmax_s F(A_i U \{s\}) F(A_i)$

I.e., maximize "marginal benefit" \otimes (s | A_i)

 \otimes (s | A_i) = F(A_i U {s})-F(A_i)

Key observation: Submodularity implies

$$i \leq j \implies \bigotimes(s \mid A_i) \ge \bigotimes(s \mid A_j)$$

 $s \bowtie$

Marginal benefits can never increase!

"Lazy" greedy algorithm [Minoux '78]

Lazy greedy algorithm:

- First iteration as usual
- Keep an ordered list of marginal benefits ⊗ from previous iteration
- Re-evaluate ⊗ only for top element
- If ⊗ 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]



30x speedup

700x speedup

Multiple object detection [Barinova et al.'12]



x_j = index of hypothesis explaining x_j





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

Illustrations courtesy of Pushmeet Kohli

Multiple object detection [Barinova et al.'12]



x_j = index of hypothesis explaining x_i

> submodular maximization

Voting elements

Illustrations courtesy of Pushmeet Kohli



Inference



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

Results for pedestrians detection



Blue = Hough transform + non-maximum suppression Light-blue = greedy detection

submodularity for detection also in [Blaschko'11]

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: engadge engadge achine Learning Cheory Slashdof Slashdo STAPUNDIT.COM sisu sisu boinaboina® boinaboina®

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 observed cascades

→ Log likelihood monotonic submodular in selected edges $F(E) = \sum_{i} \log \max_{\text{tree } T \subseteq E} P(C_i \mid T)$ ₉₃

Evaluation: Synthetic networks



- 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

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



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



Water distribution networks [J WRPM '08]



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)

(s g) Greedy works well Need **non-greedy** algorithms

 Survey on "Submodular Function Maximization" [Krause & Golovin '12] on submodularity.org

Two-faces of submodular functions



	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



- (1-1/e) for max. w card. const.
- 1/(p+1) for p-indep. systems
- for min-cost-cover log Q
- for min-sum-cover

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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
 - Multilinear extension and applications
 - 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! ③