Submodularity in Machine Learning - New Directions -

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Network Inference



How learn who influences whom?

Summarizing Documents



How select representative sentences?

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 sobmodular, we can ...
 - solve optimization problems with strong guarantees
 - solve some learning problems









... and many new applications!

submodularity.org

slides, links, 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.)
- 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



Equivalent characterizations





 ${\scriptstyle \bullet}$ Union-Intersection: for all $~A,B\subseteq V$

$$F(A) + F(B) \xrightarrow{A \cup B} (A \cup B) + F(A \cap B)$$

Questions

How do I prove my problem is submodular?

Why is submodularity useful?

Example: Set cover



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

$$Y_1, ..., Y_m, X_1, ..., X_n \text{ discrete RVs}$$

 $F(A) = I(Y; X_A) = H(Y) - H(Y | X_A)$

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"

Example: costs



Example: costs



Shared fixed costs



Another example: Cut functions



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

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

Cut function is submodular!

Why are cut functions 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



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



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



What to do with submodular functions



Minimization and maximization not the same??

Submodular minimization



clustering

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



structured sparsity regularization



MAP inference



minimum cut

Submodular minimization



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 a
1 b
0 c
0 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



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

The submodular polyhedron P_F

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

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

$$A = F(A)$$

$$\{A = F(A)$$

$$\{A = F(A)$$

$$\{A = -1 \\ \{b\} = 2 \\ \{a,b\} = 0$$

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

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Evaluating the Lovász extension

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



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

 $\min_{A \subset V}$

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

The minimum-norm-point algorithm



The minimum-norm-point algorithm

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

2. $A^* = \{i \mid u^*(i) \le 0\}$
can we solve this??



yes! ☺
 recall: can solve
 linear optimization over P_F
 similar: optimization over B_F
 → can find u*
 (Frank-Wolfe algorithm)

Fujishige '91, Fujishige & Isotani '11

Empirical comparison



Minimum norm point algorithm: usually orders of magnitude faster

[Fujishige & Isotani '11]

Applications?

Example I: Sparsity



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



Set function: $F(\mathbf{T}) < F(\mathbf{S})$ if *T* is a tree and *S* not |S| = |T|

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

Structured sparsity



Structured sparsity



Sparsity $\min \|y - Mx\|^2 + \lambda \Omega(x)$ \boldsymbol{x} explain y with few prior knowledge: patterns columns of M: few x_i of nonzeros discrete regularization on support S of x submodular function $\Omega(x) = ||x||_0 = |S|$ $\Omega(x) = F(S)$ relax to convex envelope Lovász extension $\Omega(x) = \|x\|_1$ $\Omega(x) = f(|x|)$ **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: MAP inference



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

Example: MAP inference



Special cases

Minimizing general submodular functions:

poly-time, but not very scalable

- 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: $E_{ij}(1,0) + E_{ij}(0,1) \geq E_{ij}(0,0) + E_{ij}(1,1)$

then F is a graph cut function.

MAP inference = Minimum cut: fast

Pairwise is not enough...





color + pairwise

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



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

> 2 arguments: Graph cut ??

Higher-order functions as graph cuts?

$$\sum_{i} E_i(x_i) + \sum_{ij} E_{ij}(x_i, x_j) + \sum_{c} E_c(x_c)$$

General strategy: reduce to pairwise case by adding auxiliary variables

• works well for some particular $E_c(x_c)$

[Billionet & Minoux `85, Freedman & Drineas `05, Živný & Jeavons `10,...]

 necessary conditions complex and not all submodular functions equal such graph cuts [Živný et al. '09]

Fast approximate minimization

- Not all submodular functions can be optimized as graph cuts
- Even if they can: possibly many extra nodes in the graph 😕

Other options?

- minimum norm algorithm
- other special cases:
 - e.g. parametric maxflow

[Fujishige & Iwata`99]

Approximate! Every submodular function can be approximated by a series of graph cut functions [Jegelka, Lin & Bilmes `11] 10^4 minimum norm point algorithm $\approx O(n^4)$ 10^2 iterative approximate algorithm 10^{-2} $0(n^2)$ $0(n^2)$ 10^{-2} 10^{-

speech corpus selection [Lin&Bilmes `11]

Fast approximate minimization

- Not all submodular functions can be optimized as graph cuts
- Even if they can: possibly many extra nodes in the graph 😕

Approximate! 🙂

decompose:

- represent as much as possible exactly by a graph
- rest: approximate iteratively by changing edge weights

solve a series of cut problems

 10^4 minimum norm point algorithm $\approx O(n^4)$ 10^2 iterative approximate algorithm 10^4 $0(n^2)$ 10^{-2}

speech corpus selection [Lin&Bilmes `11]

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

special case: balanced cut

- 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]

Constraints

minimum...



ground set: edges in a graph



Recall: MAP and cuts



binary labeling: $x = e_A$ pairwise random field: $E(x) = \operatorname{Cut}(A)$

What's the problem?



minimum cut: prefer
short cut = short object boundary
MAP and cuts

Minimum cut





Minimum cooperative cut



implicit criterion: short cut = short boundary

minimize sum of edge weights

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

new criterion: boundary may be long if the boundary is homogeneous

minimize submodular function of edges



Reward co-occurrence of edges

sum of weights: use few edges



submodular cost function: use few groups S_i of edges

$$F(C) = \sum_{i} F_i(C \cap S_i)$$



25 edges, 1 type7 edges, 4 types

Results

Graph cut Cooperative cut

Optimization?

- not a standard graph cut
- MAP viewpoint:

global, non-submodular energy function

Constrained optimization



[Goel et al.`09, Iwata & Nagano `09, Goemans et al. `09, Jegelka & Bilmes `11, Iyer et al. ICML `13, Kohli et al `13...]

Efficient constrained optimization

minimize a series of surrogate functions

1. compute linear upper bound $\widehat{F}^{i}(S^{i}) = F(S^{i})$ $\widehat{F}^{i}(S) = \sum_{e \in S} w^{i}(S)$ 2. Solve easy sum-of-weights problem: $S^{i} = \arg\min_{S \in \mathcal{C}} \widehat{F}^{i}(S)$ and repeat.

only need to solve sum-of-weights problems

see Wed best student paper talk

unifying viewpoint of submodular min and max

spanning tree





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

cut

efficient



matching



Submodular min in practice

- Does a special algorithm apply?
 - symmetric function? graph cut? approximately?
- Continuous methods: convexity
 - minimum norm point algorithm
- Other techniques [not addressed here]
 - LP, column generation, ...
- Combinatorial algorithms: relatively high complexity
- Constraints: hard
 - majorize-minimize or relaxation

Outline

