ETH Eidgenössische Technische Hochschule Zürich Swiss Federal Institute of Technology Zurich



Tutorial on Submodularity in Machine Learning and Computer Vision



Stefanie Jegelka Andreas Krause

Semantic Segmentation



How can we map pixels to objects?

Document Summarization



How can we select representative sentences?

Network inference



How can we learn who influences whom?

What's common?

- Can be formalized as optimizing a set function F(S) under constraints
- Generally very hard
- Structure helps: We'll see that if F(S) is submodular,
 - can solve maximization and minimization problems with strong guarantees
 - can solve learning problems involving submodular functions
- You'll learn about theory and applications

Outline

- What is submodularity?
 - Properties of submodular functions
- Optimization
 - Minimization
 - Maximization
- Learning
- Learning for Optimization

Running example: Sensor placement



Want to place sensors to monitor temperature

Set functions

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



- Will always assume F({}) = 0 (w.l.o.g.)
- Assume black-box that can evaluate F for any input A
 - Approximate (noisy) evaluation of F is ok

Example: Sensor placement

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 gains

• 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

Submodularity: Decreasing marginal gains

Placement A = $\{1,2\}$

Placement $B = \{1, \dots, 5\}$



Alternative characterizations

Set function F on V is called submodular if

 $\forall A, B \subseteq V : F(A) + F(B) \ge F(A \cup B) + F(A \cap B)$



• Equivalent diminishing returns characterization:

$$\forall A \subseteq B \subseteq V, s \notin B:$$

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

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

$$\Delta(s \mid B)$$

+

Questions

How do I prove my problem is submodular?

Why is submodularity useful?

Example: Set cover



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

Formally: W finite set, 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



15

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

Uncertainty
about temperature Y
after sensing



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



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

Example: Submodularity of info-gain

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

• F(A) is NOT always submodular

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



Proof: Submodularity of information gain

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

Variables X independent given Y

 Δ (s | A) = F(A U {s})-F(A) monotonically nonincreasing \Leftrightarrow F submodular \odot

Example: costs



Example: costs



breakfast??





$$= t_1 + 1 + t_2 + 2$$

= #shops + #items

submodular?



Shared fixed costs



Another example: Cut functions



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

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

Cut function is submodular!

Why are cut functions submodular?





S	F _{ab} (S)
{}	0
{a}	W
{b}	W
{a,b}	0

Submodular if $w \ge 0!$



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:

 $F_1,...,F_m$ submodular, $\lambda_i > 0 \rightarrow \sum_i \lambda_i F_i(A)$ submodular

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



Convex aspects

- Submodularity as discrete analogue of convexity
 - Convex extension
 - Efficient minimization
 - Duality



However, this is only one half of the story...

Concave aspects

• Marginal gain $\Delta_F(s \mid A) = F(\{s\} \cup A) - F(A)$

• Submodular:

 $\forall A \subseteq B, s \notin B : \quad F(A \cup \{s\}) - F(A) \ge F(B \cup \{s\}) - F(B)$

• Concave:

 $\forall a < b, s > 0$ $f(a+s) - f(a) \ge f(b+s) - f(b)$



Submodularity and Concavity

Suppose $g: N \rightarrow R$ and F(A) = g(|A|)Then F(A) submodular *if and only if* g is concave !



Maximum of submodular functions

Suppose $F_1(A)$ and $F_2(A)$ submodular. Is $F(A) = max(F_1(A), F_2(A))$ submodular?



max(F₁, F₂) 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(F₁,F₂) not submodular in general!

Two faces of submodular functions



What to do with submodular functions



Optimization



Minimization and maximization not the same??
Submodular minimization



Submodular minimization



Submodular function minimization



Submodular function minimization

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

polynomial-time?

submodularity and convexity

Set functions and energy functions

Can view any set function

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

equivalently as function on binary vectors:

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

where |V|=n



Submodularity and Convexity

• Extension:

• minimum of F is a minimum of f

➔ submodular minimization reduces to convex min

The submodular polyhedron P_F

43

Evaluating the Lovász extension







- Subgradient
- Separation oracle
- Central for optimization

Example Lovasz extension



Submodular function minimization



T = time for evaluating F

"efficient" ...?

The submodular polyhedron P_F

A more practical alternative? [Fujishige '91, Fujishige et al '11]



Runtime finite but worst-case complexity open

{a,b}

0

Empirical comparison [Fujishige et al '06]



Image segmentation



$$p(x|y) \propto \exp(-E(x;y))$$





MAP inference = energy minimization

Set functions and energy functions

Can view any set function

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

equivalently as function on binary vectors:

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

where |V|=n

Conversely: a function on binary variables is a set function!

 $x = e_{A}$

0

а

b

С

d

Α

а

b

С

d

Set functions & probabilistic models

Maximum a posteriori:
 observations y: infer binary labels x

maximize

$$p(x \mid y) \propto \exp(-E(x; y))$$



$$\iff \min_{x \in \{0,1\}^n} E(x; y)$$

minimize

if F is submodular: polynomial-time ③



$$F(\mathbf{A}) := E(\mathbf{e}_{\mathbf{A}}; y)$$

Example: 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(T) < F(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 $\min \|y - Mx\|^2 + \lambda \Omega(x)$ \mathcal{X} explain y with few prior knowledge: patterns of nonzeros columns of M: few x_i 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

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]

More applications ...







Corpus training set extraction

...

Special cases

Minimizing general submodular functions: poly-time, but not very scalable

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

🤍 ...

Graph cuts

$$\operatorname{Cut}(S) = \sum_{\boldsymbol{u} \in S, \boldsymbol{v} \notin S} w(\boldsymbol{u}, \boldsymbol{v})$$

Given *F*, can we build a graph so that *F*(*S*) = *Cut*(*S*)?



Solving a Min-(*s*,*t*)-cut: efficient

general case: O(mn) ^[Orlin`12] special cases: linear-time

MAP inference as graph cut



Minimum energy = minimum cut!

Which functions can be minimized as cuts?

Functions of order two:

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

Need regularity:

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

→ Each pairwise term must be submodular

[Queyranne, Picard&Ratliff,...]

But ...



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

Pⁿ potentials





66

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?

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

• 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]

General strategy:

reduce to pairwise case by adding auxiliary variables possibly many extra nodes in the graph

Fast approximate minimization

- Not all submodular functions are graph cuts
- Avoid adding too many extra nodes

- parametric maxflow
 [Fujishige & Iwata`99]
- approximate by a series of graph cuts
 [Jegelka, Lin & Bilmes `11]



Other special cases

- Symmetric:
 - Queyranne's algorithm: O(n³)

$$F(S) = F(V \setminus S)$$

[Queyranne, 1998]

Concave of modular:

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

[Kolmogorov `12, Stobbe & Krause `10, Kohli et al, `09]

Sum of submodular functions, each bounded support

[Kolmogorov `12]

Submodular minimization



Submodular Minimization

- Polynomial time
- Empirically better: minimum-norm point algorithm
- Provably better: special cases (graph cuts, concave, ...)

What if we have constraints?

Hint: graph cuts are submodular functions...

limited cases doable:

- odd/even cardinality
- inclusion/exclusion of a set
- ring family

...

General case: NP-hard polynomial lower bounds
Limitations of graph cuts



instead: prefer congruous boundary → look at entire cut at once

Graph cut as edge selection



now: prefer congruous cuts



minimize sum



s.t. C is a cut

minimize submodular function

F(C)

s.t. C is a cut



Rewarding co-occurrence of edges

sum of weights: use few edges



submodular cost function: use few groups S_i of edges



One group(13 edges)Many groups(6 edges)

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



Optimization? efficient iterative algorithm

Results











SFM & Combinatorial Constraints



Submodular Minimization

- Convex Lovász extension
- (High-order) polynomial time
- Empirically better: minimum-norm point algorithm
- Provably better: special cases

 Applications: MAP inference, combinatorial regularizers, clustering, ...



Optimization



Optimization



Submodular function maximization



Two faces of submodular functions



Reminder: Diminishing returns



Maximizing submodular functions

Minimizing convex functions: Polynomial time solvable! Minimizing submodular functions: Polynomial time solvable!

Maximizing convex functions: NP hard! Maximizing submodular functions: NP hard! J But can get approximation guarantees ©

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

Maximizing positive submodular functions

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

Theorem

There is an efficient algorithm, that, given a positive submodular function F, F({})=0, returns set A_{LS} such that $F(A_{LS}) \ge 1/2 \max_A F(A)$

- picking a random set gives ¼ approximation (½ approximation if F is symmetric!)
- we cannot get better than ½ approximation unless P = NP

Optimization



Scalarization vs. constrained maximization

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



Can get 1/2 approx... if $F(A)-C(A) \ge 0$ for all sets A

Positiveness is a strong requirement ⊗

Monotonicity

Placement A = $\{1,2\}$





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

Constrained maximization

Given: <u>finite set V of locations</u>

• Want:
$$\begin{array}{c|c} \mathcal{A}^* \subseteq \mathcal{V} & \text{such that} \\ \mathcal{A}^* = \operatorname*{argmax}_{|\mathcal{A}| \leq k} F(\mathcal{A}) \\ |\mathcal{A}| \leq k \end{array}$$

Typically NP-hard!



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]

All algorithms worst-case exponential!

Greedy algorithm

Given: <u>finite set V of locations</u>

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

Typically 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



93

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!
- For information gain: Guarantees best possible unless P = NP! [Krause & Guestrin '05]

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" $\Delta(s | A_i)$

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

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]

Μ

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]



Object detection [Barinova et al.'10]



Object detection



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?

Inferring diffusion networks [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 observed cascades

→ Log likelihood monotonic submodular in selected edges $F(E) = \sum_{i} \log \max_{\text{tree } T \subseteq E} P(C_i \mid T)$ 104

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

Diffusion Network (small part)



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**

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

Relevance Diversity

Relevance of a summary

$$F(S) = R(S) + \lambda D(S) \xrightarrow{\alpha C_i(V)}$$

$$R(S) = \sum_i \min\{C_i(S), \alpha C_i(V)\}$$
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.
$$r_j = \frac{1}{N} \sum w_{i,j}$$

 P_1 3 1 P_3 P_2

Clustering of sentences in document

Similarity between i and j

Can be made query-specific; multi-resolution; etc.

i

Empirical results [Lin & Bilmes '11]

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

Best F1 score on benchmark corpus DUC-07!



Can all be reduced to monotonic submodular maximization

More complex constraints

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

• Can one handle more complex constraints?

Example: Camera network

- Ground set $V = \{1_a, 1_b, \dots, 5_a, 5_b\}$ Configuration: $S = \{v^1, \dots, v^k\}$ Sensing quality model $F: 2^V \to \mathbb{R}$
- Configuration is feasible if no camera is pointed in two directions at once



Matroids

Abstract notion of feasibility: independence

S is independent if ...



• S independent \rightarrow $T \subseteq S$ also independent

Matroids

Abstract notion of feasibility: independence

S is independent 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

Example: Camera network

- Ground set $V = \{1_a, 1_b, \dots, 5_a, 5_b\}$ Configuration: $S = \{v^1, \dots, v^k\}$ Sensing quality model $F: 2^V \to \mathbb{R}$
- Configuration is feasible if no camera is pointed in two directions at once

This is a partition matroid: $P_1 = \{1_a, 1_b\}, \dots, P_5 = \{5_a, 5_b\}$ Independence: $|S \cap P_i| \le 1$



Greedy algorithm for matroids:

• Given: finite set V

• Want:
$$\mathcal{A}^* \subseteq \mathcal{V}$$
 such that
 $\mathcal{A}^* = \underset{A \text{ independent}}{\operatorname{argmax}} F(A)$

Greedy algorithm:
Start with
$$\mathcal{A} = \emptyset$$

While $\exists s : A \cup \{s\}$ indep.
 $s^* \leftarrow \operatorname{argmax} F(A \cup \{s\})$

*
$$\leftarrow \underset{s: A \cup \{s\} \text{ indep.}}{\operatorname{argmax}} F(A \cup \{s\}$$

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



Maximization over matroids

Theorem [Nemhauser, Fisher & Wolsey '78]
For monotonic submodular functions,
Greedy algorithm gives constant factor approximation
$$F(A_{greedy}) \ge \frac{1}{2} F(A_{opt})$$

- Greedy gives 1/(p+1) over intersection of p matroids
 - Can model rankings with p=2!
- Can get also obtain (1-1/e) for arbitrary matroids [Vondrak et al '08] using continuous greedy algorithm

Non-constant cost functions

- For each s ∈ V, let c(s)>0 be its cost (e.g., length of sentence; feature acquisition costs, ...)
- Cost of a set $C(A) = \sum_{s \in A} c(s)$
- Want to solve

 $A^* = \operatorname{argmax} F(A) \text{ s.t. } C(A) \leq B$

Cost-benefit optimization [Wolsey '82, Sviridenko '04, Krause et al '05]



Note: Can also get

- (1-1/e) approximation in time O(n⁴) [Sviridenko '04]
- (1-1/e) approximation for multiple linear constraints [Kulik '09]
- 0.38/k approximation for k matroid and m linear constraints [Chekuri et al '11]

Summary: More complex constraints

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

Often the (best) algorithms are non-greedy

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, ...)



		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, still useful algorithms

What to do with submodular functions



What to do with submodular functions



Example 1: Valuation Functions



 For combinatorial auctions, show bidders various subsets of items, see their bids

Can we learn a bidder's utility function from few bids?

Example 2: Graph Evolution



- Want to track changes in a graph
- Instead of storing entire graph at each time step, store some measurements
- # of measurements << # of edges in graph</p>

Random Graph Cut #1



- Choose a random partition of vertices
- Count total # of edges across partition

Random Graph Cut #2



- Choose another random partition of vertices
- Count total # of edges across partition

Symmetric Graph Cut Function



f(A) = sum of weights of edges between A and VA

- V = set of vertices
- One-to-one correspondence of graphs and cut functions

Can we learn a graph from the value of few cuts? [E.g., graph sketching, computational biology, ...]

General Problem: Learning Set Functions

Base Set VSet function $f: 2^V \to \mathbb{R}$



• Wish to learn f from:

- Small measurement collection $\mathcal{M} = \{A_1, \ldots, A_m\}$
- Function values

 $f(A_1),\ldots,f(A_m)$

Approximating submodular functions [Goemans, Harvey, Kleinberg, Mirrokni, '08]

Pick m sets, A₁ ... A_m, get to see F(A₁), ..., F(A_m)

• From this, want to approximate F by \hat{F} s.t.

$$\hat{F}(A) \leq F(A) \leq \alpha \hat{F}(A)$$
 for all A

Theorem: Even if

- F is monotonic
- we can pick polynomially many A_i, chosen adaptively,

cannot approximate better than $\alpha = n^{\frac{1}{2}} / \log(n)$ unless one looks at exponentially many sets A_i

But can efficiently obtain $\alpha = n^{\frac{1}{2}} \log(n)$

Learning submodular functions [Balcan, Harvey STOC '11]

- Sample m sets $A_1 \dots A_m$, from dist. D; see $F(A_1)$, ..., $F(A_m)$
- From this, want to generalize well
- \hat{F} is $(\alpha, \varepsilon, \delta)$ -PMAC iff with prob. 1- δ it holds that $P_{A \sim \mathcal{D}} \left[\hat{F}(A) \leq F(A) \leq \alpha \hat{F}(A) \right] \geq 1 - \varepsilon$

Theorem: cannot approximate better than $\alpha = n^{1/3} / \log(n)$ unless one looks at exponentially many samples A_i

But can efficiently obtain $\alpha = n^{\frac{1}{2}}$

What if we have structure?

- To learn effectively, need additional assumptions beyond submodularity.
- Sparsity in Fourier domain [Stobbe & Krause '12]

$$f(A) = \sum_{B \in 2^V} (-1)^{|A \cap B|} \hat{f}(B)$$

Sparsity: Most coefficients ≈0

- "Submodular" compressive sensing
- Cuts and many other functions sparse in Fourier domain!
- Also can learn XOS valuations [Balcan et al '12]

Compressive sensing with set functions [Stobbe & Krause '12]

Theorem: Suppose number of random measurements is proportional to the sparsity times log factors

 $m = O(k \log^4(p))$

Then we can recover ${\bf \hat{f}}~$ by solving:

$$\min ||\mathbf{x}||_1 \text{ s.t. } \mathbf{f}_{\mathcal{M}} = \mathbf{\Phi}_{\mathcal{M}} \mathbf{x}$$

Random Hadamard-Walsh basis functions satisfy RIP w.h.p Can also handle noisy observations Many more details [see paper]

Graph Evolution Results

- Tracking evolution of 128-vertex subgraph using random cuts
- Δ = number of differences
 between graphs



- Autonomous Systems Graph (from SNAP)
- \bullet For low error, observing $m\approx 8\Delta$ random cuts suffices

What to do with submodular functions



Learning to optimize

- Have seen how to
 - optimize submodular functions
 - learn submodular functions

What if we only want to learn *enough* to optimize?

Learning to optimize submodular functions

- Structured prediction with submodular functions
 - Learn function parameters to achieve target minimizer
 - Application: MAP inference; summarization
- Online submodular optimization
 - Learn to pick a sequence of sets to maximize a sequence of (unknown) submodular functions
 - Application: Building algorithm portfolios
- Adaptive submodular optimization
 - Gradually build up a set, taking into account feedback
 - Application: Sequential experimental design

Structured Prediction with SFs

• Given training data $\{(S_1, \mathbf{x}_1), \dots, (S_n, \mathbf{x}_n)\}$ and paramerized family of SFs F, can we find parameters θ such that

$$S_i \approx \arg\min_S F(S; \theta, \mathbf{x}_i)$$

With margin!



- Parameter learning in submodular MRFs [Taskar et al. '04]
 Minimization
- Learning mixtures of submodular shells [Lin & Bilmes '12]
 - ➔ Maximization
Learning to summarize [Lin & Bilmes'12]

Input:

- Collection of documents d_k and human summaries S_k
- Goal:

Learn parameterized submodular relevance & diversity

$$F(S; d_k) = \sum_i \alpha_i R_i(S; d_k) + \sum_j \beta_j D_j(S; d_k)$$

Relevance & Paivænsitærsinstantiædelafor each document k

$$\bullet$$
 Want to achieve that $~S_k \approx \mathop{\mathrm{argmax}}_{S:|S| \leq B} F(S;d_k)~$ for all k

 Can efficiently find solution with bounded generalization error!

Learning mixtures for summarization

DUC-07	R	\mathbf{F}
Toutanova et al. [53]	11.89	11.89
Haghighi and Vanderwende [16]	11.80	-
Celikyilmaz and Hakkani-tür [4]	11.40	-
Lin and Bilmes [28]	12.38	12.33
Best system in DUC-07 (peer 15)	12.45	12.29
Submodular Shell Mixture	12.51	12.40

Training data: Documents with human summaries

Learning to optimize submodular functions

- Structured prediction with submodular functions
 - Learn function parameters to achieve target minimizer
 - Application: MAP inference; summarization

Online submodular optimization

- Learn to pick a sequence of sets to maximize a sequence of (unknown) submodular functions
- Application: Building algorithm portfolios

Adaptive submodular optimization

- Gradually build up a set, taking into account feedback
- Application: Sequential experimental design

Online maximization of submodular functions [Streeter, Golovin NIPS '08]



Can get 'no-regret' over 'omniscient' greedy algorithm

Application: Learning to solve SAT quickly [Streeter, Golovin, Smith]

• Hybridization via *Task-Switching Schedules*

Example Schedule S	Heuristic #1
2 sec 4 sec 6 sec 2 sec 10 sec	Heuristic #2
	Heuristic #3
Time	Heuristic #4

• Need to learn which schedules work well!

Hybridizing Solvers [Streeter & Golovin '08]

- V = {run heuristic h for t seconds : h in H, t >0}
- $f_i(S) = Pr[schedule S completes job f in time limit].$
 - This is a submodular function! 🙂
- Task: Select {S_i : i =1, 2, ..., T} online to maximize # instances solved
- This is an online submodular maximization problem! ③
- Online greedy algorithm achieves no-(1-1/e)-regret

Example Schedule

[Streeter, Golovin, Smith, AAAI '07 & CSP '08]



SAT 2007 Competition Data

Number of benchmark instances solved within the time limit.

Category	Offline greedy	Online greedy	Parallel schedule	Top solver
Industrial	147	149	132	139
Random	350	347	302	257
Hand-crafted	114	107	95	98

The CADE ATP System Competition (2008)

Percentage of benchmark instances solved within the time limit.

Category	MetaProver	2nd best	3rd best
FNT	74%	70%	70%
SAT	100%	97.5%	96.3%

Other results on online submodular optimization

- Online submodular maximization
 - No (1-1/e) regret for ranking (partition matroids) [Streeter, Golovin, Krause 2009]
 - Distributed implementation [Golovin, Faulkner, Krause '2010]
 - Improved bounds for bandits with linear combinations of SFs [Yue, Guestrin, NIPS 2011]
- Online submodular coverage
 - Min-cost / Min-sum submodular cover [Streeter & Golovin NIPS 2008]
 - Guillory & Bilmes [NIPS 2011]
- Online Submodular Minimization
 - Unconstrained [Hazan & Kale NIPS 2009]
 - Constrained [Jegelka & Bilmes ICML 2011]

What to do with submodular functions



Learning to optimize submodular functions

- Structured prediction with submodular functions
 - Learn function parameters to achieve target minimizer
 - Application: MAP inference; summarization
- Online submodular optimization
 - Learn to pick a sequence of sets to maximize a sequence of (unknown) submodular functions
 - Application: Building algorithm portfolios
- Adaptive submodular optimization
 - Gradually build up a set, taking into account feedback
 - Application: Sequential experimental design

Adaptive Sensing / Diagnosis



Want to effectively diagnose while minimizing cost of testing! Classical submodularity does not apply 😕

Can we generalize submodularity for sequential decision making?

Adaptive selection in diagnosis

- Prior over diseases P(Y)
- Deterministic test outcomes P(X_v | Y)
- Each test eliminates hypotheses y





Problem Statement

Given:

- Items (tests, experiments, actions, ...) V={1,...,n}
- Associated with random variables $X_1, ..., X_n$ taking values in O • Objective: $f: 2^V \times O^V \to \mathbb{R}$
- Policy π maps observation $\mathbf{x}_{\mathbf{A}}$ to next item

Value of policy TT:
$$F(\pi) = \sum_{\mathbf{x}_V} P(\mathbf{x}_V) f(\pi(\mathbf{x}_V), \mathbf{x}_V)$$

Tests run by T
if world in state \mathbf{x}_V
NP-hard (also hard to approximate!)

Adaptive greedy algorithm

- Suppose we've seen $X_A = x_{A.}$
- Conditional expected benefit of adding item s:

$$\Delta(s \mid \mathbf{x}_A) = \mathbb{E}\left[f(A \cup \{s\}, \mathbf{x}_V) - f(A, \mathbf{x}_V) \mid \mathbf{x}_A\right]$$
Adaptive Greedy algorithm efit if world in state \mathbf{x}_V

Start with
$$A = \emptyset$$
For i = 1:k• Pick $s_k \in \operatorname{argmax} \Delta(s \mid \mathbf{x}_A)$ • Observe $X_{s_k} = x_{s_k}$ • Set $A \leftarrow A \cup \{s_k\}$

Conditional on observations $\mathbf{x}_{\mathbf{A}}$

When does this adaptive greedy algorithm work??

Adaptive submodularity [Golovin & Krause, JAIR 2011]

 $\begin{array}{l} \text{Adaptive monotonicity:} \\ \Delta(s \mid \mathbf{x}_{A}) \geq 0 \\ \text{Adaptive submodularity:} \\ \Delta(s \mid \mathbf{x}_{A}) \geq \Delta(s \mid \mathbf{x}_{B}) \end{array} \text{ whenever } \mathbf{x}_{A} \preceq \mathbf{x}_{B} \end{array}$

Theorem: If f is adaptive submodular and adaptive monotone w.r.t. to distribution P, then $F(\pi_{greedy}) \ge (1-1/e) F(\pi_{opt})$

Many other results about submodular set functions can also be "lifted" to the adaptive setting!

From sets to policies

Submodularity

Adaptive submodularity

Applies to: set functions

$$\Delta_F(s \mid A) = F(A \cup \{s\}) - F(A)$$
$$\Delta_F(s \mid A) \ge 0$$
$$A \subseteq B \Rightarrow \Delta_F(s \mid A) \ge \Delta_F(s \mid B)$$

 $\max_{A} F(A)$

Greedy algorithm provides

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

policies, value functions

$$\Delta_F(s \mid \mathbf{x}_A) = \mathbb{E} \Big[f(A \cup \{s\}, \mathbf{x}_V) - f(A, \mathbf{x}_V) \mid \mathbf{x}_A \Big]$$
$$\Delta_F(s \mid \mathbf{x}_A) \ge 0$$
$$\mathbf{x}_A \preceq \mathbf{x}_B \Rightarrow \Delta_F(s \mid \mathbf{x}_A) \ge \Delta_F(s \mid \mathbf{x}_B)$$

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

Greedy policy provides

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

Optimal Diagnosis

- Prior over diseases P(Y)
- Deterministic test outcomes $P(X_v | Y)$
- How should we test to eliminate all incorrect hypotheses?

$$\Delta(t \mid x_A) = \mathbb{E}\begin{bmatrix} \text{mass ruled c} \\ \text{by } t \text{ if we} \\ \text{know } x_A \end{bmatrix}$$

"Generalized binary search" Equivalent to max. infogain



 X_{2}

OD is Adaptive Submodular



 $b_0 \ge b_1, \ g_0 \ge g_1$ Not hard to show that $\Delta(s \mid \{\}) \ge \Delta(s \mid \mathbf{x}_{v,w})$

Theoretical guarantees



Result requires that tests are *exact* (no noise)!

What if there is noise? [w Daniel Golovin, Deb Ray, NIPS '10]

- Prior over diseases P(Y)
- Noisy test outcomes P(X_v | Y)
- How should we test to learn about y (infer MAP)?
- Existing approaches:
 - Generalized binary search?
 - Maximize information gain?
 - Maximize value of information?



Not adaptive submodular!

Theorem: All these approaches can have cost **more than n/log n** times the optimal cost!

→ Is there an adaptive submodular criterion??

Theoretical guarantees [with Daniel Golovin, Deb Ray, NIPS '10]

Theorem: Equivalence class edge-cutting (EC²) is adaptive monotone and adaptive submodular. Suppose $P(\mathbf{x}_V, h) \in \{0\} \cup [\delta, 1]$ for all \mathbf{x}_V, h Then it holds that

$$\operatorname{Cost}(\pi_{\operatorname{Greedy}}) \leq \mathcal{O}\left(\log \frac{1}{\delta}\right) \operatorname{Cost}(\pi^*)$$

First approximation guarantees for **nonmyopic VOI** in general graphical models!

Example: The Iowa Gambling Task [with Colin Camerer, Deb Ray]



Various competing theories on how people make decisions under uncertainty

- Maximize expected utility? [von Neumann & Morgenstern '47]
- Constant relative risk aversion? [Pratt '64]
- Portfolio optimization? [Hanoch & Levy '70]
- (Normalized) Prospect theory? [Kahnemann & Tversky '79]

How should we design tests to distinguish theories?

Iowa Gambling as BED

Every possible test $X_s = (g_{s,1}, g_{s,2})$ is a pair of gambles

Theories parameterized by $\boldsymbol{\theta}$

Each theory predicts utility for every gamble U(g,y,θ)



$$P(X_{s} = 1 \mid y, \theta) = \frac{1}{1 + \exp(U(g_{s,1}, y, \theta) - U(g_{s,2}, y, \theta))}$$

Simulation Results



Experimental Study [with Colin Camerer, Deb Ray]



- Strongest support for PT, with some heterogeneity
- Unexpectedly no support for CRRA
- Submodularity enables real-time performance!

Interactive submodular coverage

- Alternative formalization of adaptive optimization [Guillory & Bilmes, ICML '10]
 - Addresses the worst case setting
- Applications to (noisy) active learning, viral marketing [Guillory & Bilmes, ICML '11]

Other directions

- Game theory
 - Equilibria in cooperative (supermodular) games / fair allocations
 - Price of anarchy in non-cooperative games
 - Incentive compatible submodular optimization
- New algorithms for submodular maximization
 - Robust submodular optimization
- Generalizations of submodular functions
 - L#-convex / discrete convex analysis
 - XOS/Subadditive functions
- Efficient minimization of subclasses

Further resources

- submodularity.org
 - References
 - Matlab Toolbox for Submodular Optimization
- discml.cc
 - NIPS Workshops on Discrete Optimization in Machine Learning
 - Videos of invited talks on videolectures.net







Submit to DISCML 2012! ^(C)

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
- Can handle complex constraints
- Can learn to optimize (online, adaptive, ...)