

# Submodular Functions and Machine Learning

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#### Resources

- submodularity.org
- people.csail.mit.edu/stefje/mlss/literature.pdf
   references for the lectures, pointers to surveys, papers, books
- discml.cc talks on submodularity in machine learning



#### Setup



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

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max F(S)

### **Submodularity**



diminishing marginal costs

### Roadmap

- Submodular set functions
  - links to convexity
  - special polyhedra
- Minimizing submodular functions
  - general and special cases
  - constraints
- Maximizing submodular functions
  - monotone & non-monotone
  - repulsive point processes

### **Maximizing Influence**

F(S) =expected # infected nodes



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

Kempe, Kleinberg & Tardos 2003

#### **Informative Subsets**







- where put sensors?
- which experiments?
- summarization

F(S) = "information"

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### **Summarization**

- videos, text, pictures ...
- would like: relevance, reliability, diversity







#### Monotonicity

llii.

#### 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
- 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 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)

(Leskovec et al 2007)

### **Example: 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

(partition) matroid constraint!



#### Matroids (semi-formally)

S is independent ( = feasible) if ...



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

### Matroids

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

### **Example: 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

(partition) matroid constraint:

$$P_1 = \{1_a, 1_b\}, \dots, P_5 = \{5_a, 5_b\}$$

require:

$$|S \cap P_i| \le 1$$



## **Greedy algorithm for matroids**

$$S = \emptyset$$
  
While  $\exists e : S \cup e \text{ independent}$   

$$S \leftarrow S \cup \underset{e:S \cup e \text{ indep.}}{\operatorname{argmax}} F(S \cup e)$$

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

better approximation (1-1/e): relaxation



### Submodular welfare



• assign set  $S_i$  to person i to maximize

$$\sum_{i=1}^{k} F_i(S_i)$$

- $\mathcal{V} =$  all possible assignments
- partition matroid: assign each item only once

#### **Relaxation?**

- concave analog of Lovasz extension: not in polynomial time

   S
- multi-linear extension: probability distribution from x sample element e with probability  $x_e$

$$f_{M}(x) = \sum_{S \subseteq \mathcal{V}} F(S) \prod_{e \in S} x_{e} \prod_{e \notin S} (1 - x_{e})$$

$$= \mathbb{E}_{S \sim x} [F(S)] \qquad p(1) = 0.5 \qquad \mathbf{x}$$

$$p(2) = 1.0 \qquad \mathbf{0}$$

$$p(3) = 0.5 \qquad \mathbf{0}$$

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#### Multilinear extension



- 1. concave in positive directions:  $f_M(x + \lambda d)$  concave function of  $\lambda$  if  $d \succeq 0$ .
- 2. convex in swap directions:  $f_M(x+\lambda d)$  convex function of  $\lambda$  if  $d = 1_i - 1_i$

Optimization: continuous greedy move in directions  $v = \arg \max_{v \in P} v^{\top} \nabla f_M(x^t)$ 

### **Relaxation: algorithm**

- 1. approximately maximize  $f_M$  (Frank-Wolfe like algorithm)
- 2. round (pipage rounding)

#### Lovász extension as expectation



- sample a threshold  $\theta$  uniformly between 0 and 1
- Pick

$$S^{\theta} = \{ i \mid x_i \ge \theta \}$$

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$$f_L(x) = \mathbb{E}_{S \sim \theta} [F(S)]$$
$$= \alpha_i F(S_i)$$



#### Multilinear relaxation vs. Lovász ext.





- concave in positive directions, convex in others
- approximate by sampling

- convex
- computable in O(n log n)

#### Multilinear relaxation vs. Lovász ext.



### 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



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

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)

#### Performance



#### even more data ... distributed greedy algorithm?

### **Distributed greedy algorithms**



greedy is sequential. pick in parallel??

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pick *k* elements on each machine.

combine and run greedy again.

#### **Distributed greedy algorithms**



pick in parallel from *m* machines

Is this useful?

(Mirzasoleiman et al 2013)

#### **Distributed Greedy**



In practice, performs often quite well.

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

#### Distributed greedy algorithms



- each machine:  $\alpha$ -approximation algorithm
- level 2:  $\beta$  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)

#### **Distributed greedy algorithms**



(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
  - distributed
- What if my function is not monotone?
#### **Non-monotone functions**



## **Picking at random**

- Let F be a non-monotone nonnegative submodular function. Pick set S uniformly at random from  ${\mathcal V}$ 

Pr(include i) = 1/2 for all i

• Then

 $\mathbb{E}[F(S)] \ge \frac{1}{4}F(S^*)$ 

• If F is symmetric:

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

## **Picking at random**

• Can we do this for constrained (monotone) maximization?

 $\max_{|S| \le k} F(S)$ 

- Example:  $F(S) = |S \cap R| + \epsilon \cdot \min\{|S \cap B|, 1\} \qquad |R| = k$  $F(S^*) = F(R) = k$
- Pick k elements at random: will hit very few red ones

$$\mathbb{E}[F(S)] < \Big(\frac{k+\epsilon}{n}\Big)F(S^*)$$

#### **Non-monotone maximization**

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

#### Can we do better than completely random?

$$\mathbb{E}[F(S)] \ge \frac{1}{4}F(S^*)$$

#### Greedy can fail ...



#### **Greedy can fail ...**

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

luir.





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

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

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





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









#### **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

- 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 with constant approximation factors (monotone and non-monotone)

## Adaptive/sequential settings

Sequential diagnosis:



- learning a policy: model updated after observation
- submodularity does not apply directly
- suitable generalization: adaptive submodularity greedy results generalize <sup>(i)</sup>

## Roadmap

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#### **Diversity and distributions**



Point process: distribution over sets Phir

P(S)

### **Diversity priors**





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

"spread out"

#### **Point processes – examples**

• independent coin flips

$$P(Y = S) = \prod_{i \in S} p_i \prod_{j \notin S} (1 - p_j)$$

• if  $S \cap T = \emptyset$ then  $Y \cap S$  and  $Y \cap T$  are independent



#### **Point processes – examples**



$$P(x|z) \propto P(z|x) P(x) \qquad x \in \{0,1\}^n$$

$$|abels pixel \\ values | x = \left\{ -\left(\sum_i \beta_i x_i + \sum_{ij} \nu_{ij} x_i x_j\right) \right\}$$

our examples: spatial coherence, "attractive" --- positive correlations

### **Repulsion?**

in a graphical model:

- computationally hard
- dependencies between all elements → fully connected



## **Determinantal point processes**



- normalized similarity matrix K
- sample *Y*:

 $P(S \subseteq Y) = \det(K_S)$ 

$$P(e_i \in Y) = K_{ii}$$

$$P(e_i, e_j \in Y) = K_{ii}K_{jj} - K_{ij}^2$$

$$= P(e_i \in Y)P(e_j \in Y) - K_{ij}^2$$
repulsion

 $F(S) = \log \det(K_S)$  is submodular

#### **DPP** sample



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

similarities:

$$\sigma^2 = 35$$

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#### **DPP sample – larger bandwidth**



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

 $\sigma^2 = 135$ 

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#### **DPPs**

- definitions
- computing marginals
- sampling
- computing the mode (MAP)

## **Determinantal Point Processes**

- Macchi 1975: "fermion processes"
- Borodin & Olshanski 2000: "determinantal PP"

#### 2 Definitions:

- marginal kernel K:
  - positive semidefinite
  - eigenvalues in [0,1]:  $0 \leq K \leq 1$
- L-ensemble: (Borodin & Rains, 2005)
  - positive semidefinite L
  - normalization constant:

$$\sum_{S \subseteq \mathcal{V}} \det(L_S) = \det(L + I_n)$$

$$P(S \subseteq Y) = \det(K_S)$$

$$P(Y=T) \propto \det(L_T)$$

## **2** Definitions

#### Marginal kernel

- $P(S \subseteq Y) = \det(K_S)$
- $0 \leq K \leq 1$ •
- *K* from L:

$$K = L(L+I)^{-1}$$

$$K = \sum_{k=1}^{n} \frac{\lambda_k}{1 + \lambda_k} v_k v_k^{\top}$$

#### L-ensemble

$$P(Y=T) \propto \det(L_T)$$

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• 
$$0 \leq L$$

• *L* from *K*:  

$$L = K(I - K)^{-1}$$

$$L = \sum_{k=1}^{n} \lambda_k v_k v_k^{\top}$$

## **Geometric view**

- data points  $x_1, \ldots, x_n$  : feature vectors in  $\mathbb{R}^d$
- L-ensemble:  $L_{ij} = x_i^\top x_j$
- Then  $P_L(S) \propto \det(L_S) = \operatorname{Vol}^2(\{x_i\}_{i \in S})$



What happens if dimension d < number of points n?

# "Everything" is simple ③

• normalization

$$\sum_{S \subseteq \mathcal{V}} \det(L_S) = \det(L + I_n)$$

• marginal probabilities: from marginal kernel

$$K = L(L+I)^{-1}$$

• conditioning:

.

$$P(Y = A \cup B \mid A \subseteq Y) = \frac{\det(L_{A \cup B})}{\det(L + I_{\mathcal{V} \setminus A})}$$

also a DPP (Borodin & Rains, 2005)

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### How many points in the sample?

- L has eigenvalues  $\lambda_1, \lambda_2, \ldots, \lambda_n$
- cardinality |Y| of sample: Poisson Binomial flip n coins,  $p_k(head) = \frac{\lambda_k}{\lambda_k+1}$  - how many heads?

$$\mathbb{E}[|Y|] = \sum_{k=1}^{n} \frac{\lambda_k}{\lambda_k + 1} = \operatorname{trace}(K)$$

Can we sample efficiently?

## Sampling: main idea

• Every DPP is a mixture of "elementary" DPPs

$$P_L(Y) = \sum_T \pi_T P^T(Y) \qquad = \frac{1}{Z} \sum_{T \subseteq \{1,\dots,n\}} \prod_{k \in T} \lambda_k P^T(Y)$$

- 1. Sample a component  $P^T$  with probability  $\pi_T$
- 2. Sample Y from  $P^T$
- *L* has n eigenvectors
- $T \subseteq \{1, \ldots, n\}$  indexes a set of eigenvectors

• 
$$\pi_T = \prod_{k \in T} \frac{\lambda_k}{\det(L+I)}$$

# Sampling Y

n

k=1

- compute eigendecomposition  $L = \sum \lambda_k v_k v_k^{ op}$
- 1. sample eigenvectors:  $V = \emptyset$ add  $v_k$  to V with probability  $\frac{\lambda_k}{\lambda_k + 1}$
- 2. sample |V| points:



→ recall: Bernoulli process,

$$\mathbb{E}[|Y|] = \sum_{k=1}^{n} \frac{\lambda_k}{\lambda_k + 1}$$

(Hough et al 2006)

# **Elementary DPP** $P^A(Y)$

- "elementary" DPP: all eigenvalues of K are 0 or 1.
- pick a set A of eigenvectors  $v_k$  of our L

$$K^A = \sum_{k \in A} v_k v_k^\top$$



- eigenvalues:  $\underbrace{1, 1, \dots, 1}_{|A| \text{ times}}, \underbrace{0, 0, \dots, 0}_{n-|A|}$
- sample from this DPP: |Y| = |A| a.s.

- Why?

$$\mathbb{E}[|Y|] = |A| \qquad \text{for } |Y| > |A|:$$
$$P_K(Y) = \det(K_Y^A) = 0$$

# Sampling Y

- compute eigendecomposition  $L = \sum \lambda_k v_k v_k^{ op}$
- 1. sample eigenvectors:  $V = \emptyset$ add  $v_k$  to V with probability  $\frac{\lambda_k}{\lambda_k+1}$
- 2. sample |V| points:  $Y = \emptyset$



n





(Hough et al 2006)

#### Sampling



from: (Kulesza & Taskar, FTML)

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## Finding the mode

$$P(Y=T) \propto \det(L_T)$$



• submodular maximization problem!

#### The simplest DPP

$$K = \begin{bmatrix} p_1 & 0 & 0 & 0 \\ 0 & p_2 & 0 & 0 \\ 0 & 0 & p_3 & 0 \\ 0 & 0 & 0 & p_4 \end{bmatrix}$$

$$P(Y = S) = \prod_{i \in S} p_i \prod_{j \notin S} (1 - p_j)$$
## **Example: random spanning trees**



 sample a spanning tree uniformly at random

• probability of a set of edges  $S \subseteq \mathcal{E}$  occurring together?

 $\Pr(S \subseteq T)$ 

 negative correlation: This is a DPP!

 $\Pr(S \subseteq T) \leq \prod_{e \in S} \Pr(e \in T)$ 

feature vector for edge e = (u, v)

$$b_e = \begin{bmatrix} 0 \\ 1 \\ 0 \\ -1 \\ 0 \end{bmatrix} \leftarrow \mathbf{v} \qquad x_e = \mathcal{L}^{\dagger/2} b_e$$

### **Application: pose estimation**





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## **Application: pose estimation**

$$L_{ij} = x_i^{\top} x_j = q_i \phi_i^{\top} \phi_j q_j \qquad Q_{ij} = \phi_i^{\top} \phi_j$$
  
quality score normalized feature vector  
$$\det(L_S) = \left(\prod_{i \in S} q_i^2\right) \det(Q_S)$$

- quality model: part detectors for likelihood of body part at location / orientation
- similarity model: location
- data: 73 still frames from TV shows, each 3+ people

(Kulesza&Taskar 2010)

#### **Pose estimation**







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(Kulesza & Taskar 10)

# Summary

- Submodular set functions
  - links to convexity
  - special polyhedra
- Minimizing submodular functions
  - general and special cases: polynomial-time
  - constraints: NP-hard, approximations
- Maximizing submodular functions
  - monotone & non-monotone: NP-hard, constant-factor approximations
  - determinantal point processes

## 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