

Submodular Functions and Machine Learning

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Set functions



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

$$F \left(\begin{array}{c} & & \\ & &$$

We will assume:

•
$$F(\emptyset) = 0$$

• black box "oracle" to evaluate F

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

Diminishing marginal gains



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Submodularity



diminishing marginal costs

Submodular set functions

В

• e

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

+• e

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

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



Roadmap

- Submodular set functions
 - definition & basic properties
 - links to convexity
 - special polyhedra
- Minimizing submodular functions
 - general and special cases
 - constraints
- Maximizing submodular functions

Convex relaxation





$\min_{S \subseteq \mathcal{V}} F(S) = \min_{x \in \{0,1\}^n} F(x) = \min_{x \in [0,1]^n} f(x)$

1. relaxation: convex optimization (non-smooth)

2. relaxation is exact!

→ submodular minimization in polynomial time! (Grötschel, Lovász, Schrijver 1981)

Lovász extension



if *F* is submodular, this is equivalent to:

$$f(x) = \max_{y \in \mathcal{B}_F} y^\top x$$



Theorem (Lovász, 1983) Lovász extension is convex \Leftrightarrow F is submodular.



 \Leftarrow done.

$$f(1_A + 1_B) \leq f(1_A) + f(1_B)$$

= $f(1_{A \cup B} + 1_{A \cap B}) = F(A) + F(B)$

 $= F(A \cup B) + F(A \cap B)$

Submodular minimization

convex optimization

- ellipsoid method (Grötschel-Lovasz-Schrijver 81)
- subgradient method
- minimum-norm point / Fujishige-Wolfe algorithm

combinatorial methods

- first polynomial-time: (Schrijver 00, Iwata-Fleischer-Fujishige 01)
- currently fastest:

 $O(n^4T + n^5\log M)$ (Iwata 03)

 $O(n^6 + n^5 T) \qquad \qquad \text{(Orlin 09)}$

ult: $O(n^2 T \log nM + n^3 \log^c nM)$ $O(n^3 T \log^2 n + n^4 \log^c n)$ (Lee-Sidford-Wong 15)

Recall: convex relaxation

Lovász extension

$$\min_{x \in [0,1]^n} f(x)$$

$$= \max_{y \in \mathcal{B}_F} \left(\sum_{i=1}^n \min\{y_i, 0\} \right)$$

optimal discrete solution:

 $S^* = \{ i \mid x_i^* > 0 \}$

 $= \{ \, i \mid y_i^* < 0 \, \}$

+ + 0 0

Proximal problem

 $\min_{x \in [0, \mathbf{\hat{x}}]^n} f(x) + \frac{1}{2} \|x\|^2$

why? solves $\min_{S \subseteq \mathcal{V}} F(S) + \alpha |S| \quad \text{ for all } \alpha$

- Let S^{α} be the largest minimizer of $\left.F(S)+\alpha|S|\right.$
- can show: if $\alpha < \beta$, then $S^{\alpha} \supseteq S^{\beta}$ \rightarrow chain $\emptyset \subset S^{\alpha_1} \subset S^{\alpha_2} \subset \dots \mathcal{V}$
- "encode" in vector u :

$$\{e \mid u_e \ge \alpha\} = S^{\alpha}$$

$$u = \arg\min_{x} f(x) + \frac{1}{2} ||x||^2$$



3 equivalent problems

convex dual problem

$$\{e \mid y_e^* \le -\alpha\} =$$

$$S^{\alpha} = \{ e \mid \boldsymbol{x}_{e}^{*} \geq \alpha \}$$

thresholding

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$$\boldsymbol{x_e^*} = \sup\{\alpha \mid e \in S^\alpha\}$$

divide-and-conquer

Minimum-norm-point algorithm

Fujishige '91, Fujishige & Isotani '11

proximal problem dual: minimum norm problem $\min f(x) + \frac{1}{2} ||x||^2$ $y^* = \arg\min_{y \in \mathcal{B}_F} \frac{1}{2} \|y\|^2$ $y^* = \begin{bmatrix} -1 & a \\ 1 & b \end{bmatrix}$ \mathcal{B}_F F(A)AØ a $\mathbf{2}$ -21 b $\{a,b\}$ 0

$$S^* = \{i \mid y_i^* \le 0\}$$

minimizes F !
$$S^* = \arg\min_{S \subseteq \mathcal{V}} F(S)$$

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Overview



Solving the min-norm problem

 $\min_{y \in \mathcal{B}_F} \quad \frac{1}{2} \|y\|^2$

- costly: testing membership in \mathcal{B}_F
- costly: projection onto \mathcal{B}_F
- easy: linear optimization over \mathcal{B}_F : greedy algorithm! \odot

- conditional gradient algorithm (Frank & Wolfe 1956)
- active set methods: Fujishige-Wolfe (Fujishige & Isotani 2011, Chakrabarty-Jain-Kothari 2014,...)



Empirically



Conditional gradient algorithm

min h(y) s.t. $y \in \mathcal{P}$

h convex, differentiable

P polyhedral

 $\begin{array}{l} y^0 \in \mathcal{P} \\ \text{for } t=0,1,\dots \text{ to } T \text{ do} \\ s^t = \operatorname{argmin}_{s \in \mathcal{P}} \left< \nabla h(y^t), s \right> \\ y^{t+1} = (1-\gamma)y^t + \gamma s^t \\ \text{end for} \end{array}$

step size? how many iterations?



Conditional gradient algorithm

min h(y) s.t. $y \in \mathcal{P}$

h convex, differentiable

P polyhedral

for
$$t = 0, 1, ...$$
 to T do
 $s^t = \operatorname{argmin}_{s \in \mathcal{P}} \langle \nabla h(y^t), s \rangle$
 $y^{t+1} = (1 - \gamma)y^t + \gamma s^t$
end for

1. fixed step size:

$$\gamma^t = \frac{2}{t+2}$$

2. line search:

$$\gamma^t = \arg\min_{\gamma \in [0,1]} h(y^t + \gamma(s^t - y^t))$$

3. re-optimization:

$$y^{t+1} = \operatorname{argmin}_{y \in \operatorname{conv}(s^0, \dots, s^t)} h(y)$$

How many iterations?

$$y^* = -x^*$$

dual problem
 $\max_{y \in \mathcal{B}_F} -\frac{1}{2} \|y\|^2$ primal problem
 $\min_x f(x) + \frac{1}{2} \|x\|^2$

always: primal value ≥ dual value
at optimum: primal value = dual value
→ bound the duality gap: primal - dual value

Theorem (Jaggi 2013)
After T iterations of the algorithm, there is an iterate y^{τ} with
 $gap(y^{\tau}) \leq \frac{16C}{T+2}$ For $h(y) = ||y||^2$, $C = diam(\mathcal{P})^2$ Exercise: how many
iterations for a
 $gap < \epsilon$?

Are we done yet?

want: $\min_{S \subseteq \mathcal{V}} F(S)$ ----->

$$S^t_\alpha = \{e \mid -y^t_e \geq \alpha\} \blacktriangleleft$$

 $\max_{y \in \mathcal{B}_F} -\frac{1}{2} \|y\|^2$

solve via conditional gradient & friends have convergence bound

How many iterations until $F(S^t) - F(S^*) \le \epsilon$?

Theorem (Bach 2013)

If $gap(y^{\tau}) \leq \epsilon'$ then there exists an α such that the discrete duality gap is bounded as

$$F(S_{\alpha}^{\tau}) - F(S^{*}) \le F(S_{\alpha}^{\tau}) - y_{-}^{\tau}(\mathcal{V}) \le \sqrt{2n\epsilon'}$$

Submodularity and convexity

- convex Lovasz extension
 - easy to compute: greedy algorithm (special polyhedra!)
- submodular minimization via convex optimization: duality results & fast algorithms for many applications $\min_{x \in [0,1]^n} f(x) \qquad \min_{x} f(x) + \frac{1}{2} ||x||^2$
- structured sparsity (Bach 2010)
- decomposition & parallel algorithms (J-Bach-Sra 2013, Nishihara-J-Jordan 2014)
- variational inference (Djolonga & Krause 2014)

Sparsity



observe (y_i, a_i^{\top}) , want to estimate w

- what if m << p? underdetermined!
- in general, no recovery possible:
 - → exploit additional structure, e.g.: w has only k non-zeros
- also: interpretability



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Sparsity



 $\underbrace{A \quad w}_{m \times p \ p \times 1}$



+









Structured sparse PCA



 $\hat{w} = \arg\min_{w} ||Aw - y||^2 + \lambda \Omega(w)$



Sparse reconstruction

$$\hat{w} = \arg \min_{w} ||Aw - y||^{2} + \lambda \Omega(w)$$
Assumption:
w is sparse
discrete regularization on support S of w
$$\Omega(w) = ||w||_{0} = |S|$$
relax to convex envelope
$$\Omega(w) = ||w||_{1}$$
Assumption:
w is sparse

sparsity pattern often not random...

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Structured sparsity

Assumption: support of w has structure



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express by set function!



Preference for trees



Set function: F(T) < F(S)if T is a tree and S not |S| = |T|
$$F(S) = \left| \bigcup_{s \in S} \operatorname{ancestors}(s) \right|$$

use as regularizer?

Sparsity

$$\hat{w} = \arg \min_{w} ||Aw - y||^{2} + \lambda \Omega(w)$$
• w sparse
discrete regularization on support S of w
submodular function
$$\Omega(w) = ||w||_{0} = |S|$$
relax to convex envelope
$$\Omega(w) = ||w||_{1}$$

$$\widehat{w}$$
Lovász extension
$$\Omega(w) = f(|w|)$$

Optimization: sequence of min-norm problems (submodular minimization)

(Bach2010) 28

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Norms from submodular functions

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

Proposition For monotone increasing *f*, f(|x|) is a norm. *(Exercise: show this)*

Special cases:
$$F(S) = |S| \Rightarrow f(|x|) = ||x||_1$$

 $F(S) = \min\{|S|, 1\} \Rightarrow f(|x|) = ||x||_\infty$
 $F(S) = \sum_{k=1}^{k} \min\{|S \cap G_j|, 1\} \Rightarrow f(|x|) = \sum_{k=1}^{k} ||x_{G_j}||$

j=1

 ∞

j=1

Special case

• minimize a sum of submodular functions

$$F(S) = \sum_{i=1}^{r} F_i(S) \min_{\substack{S \\ \text{"easy"}}} F_i(S)$$

- combinatorial algorithms (Kolmogorov 12, Fix-Joachims-Park-Zabih 13, Fix-Wang-Zabih 14)
- convex relaxations

Relaxation

$$F: 2^{\mathcal{V}} \to \mathbb{R} \equiv F: \{0, 1\}^n \to \mathbb{R} \qquad f: \mathbb{R}^n_+ \to \mathbb{R}$$

 convex Lovász extension: tight relaxation

$$\min_{S \subseteq \mathcal{V}S \subseteq \mathcal{V}_i} \mathbb{F}_i(S) = \min_{\substack{x \in [0,1]^n \\ \swarrow}} \underbrace{\sum_{i=1}^r f_i(x)}_{i=1} f_i(x) + \frac{1}{2} \|x\|^2$$



dual decomposition: parallel algorithms

(Komodakis-Paragios-Tziritas 11, Savchynskyy-Schmidt-Kappes-Schnörr 11, J-Bach-Sra 13)

Results: dual decomposition



(Jegelka, Bach, Sra 2013; Nishihara, Jegelka, Jordan 2014)

Submodularity and convexity

- convex Lovasz extension
 - easy to compute: greedy algorithm (special polyhedra!)
- submodular minimization via convex optimization: fast algorithms for many applications
- duality results
- structured sparsity (Bach 2010)
- decomposition & parallel algorithms
- variational inference (Djolonga & Krause 2014)



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Graph cuts



G = (V, E) edge weights w_{uv}

$$F(S) = \sum_{u \in S, v \notin S} w_{uv}$$

• Cut for one edge:



 $F(\{u\}) + F(\{v\}) \geq F(\{u,v\}) + F(\emptyset)$



• Graph cuts: faster algorithms than general submodular!

MAP inference





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

Phi
Attractive potentials



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

spatial coherence:

$$E_{ij}(x_i, x_j) = \begin{cases} \nu_{ij} > 0 & \text{if } x_i \neq x_j \\ 0 & \text{otherwise} \end{cases}$$

$$=\nu_{ij}(x_i-x_j)^2$$

 $= \operatorname{Cut}(1_S)$



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Quadratic functions and cuts

$$E_{ij}(x_i, x_j) = \nu_{ij}(x_i - x_j)^2 = \operatorname{Cut}(1_S)$$

what about the linear terms?

$$E_{ij}(x_i, x_j) + E_i(x_i) + E_j(x_j) - \alpha_j$$

make it an (s,t)-cut! Source s always selected

$$\alpha_i > 0$$

$$\alpha_j < 0$$



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Quadratic functions and cuts

$$E_{ij}(x_i, x_j) = \nu_{ij}(x_i - x_j)^2 = \text{Cut}(1_S)$$

linear terms:

$$E_{ij}(x_i, x_j) + \alpha_i x_i + \alpha_j x_j - \alpha_j$$

MAP inference = minimum cut 🙂

Is every such quadratic function a graph cut function?

any linear terms are fine $\, \odot \,$

quadratic terms? What if $\nu_{ij} < 0$?



Submodular functions and cuts

• Formally:

$$E(x) = \sum_{i} \alpha_{i} x_{i} + \sum_{ij} \nu_{ij} (x_{i} - x_{j})^{2}$$
$$= \sum_{i} \alpha_{i} x_{i} + \sum_{ij} \nu_{ij} x_{i}^{2} + \nu_{ij} x_{j}^{2} - 2\nu_{ij} x_{i} x_{j}$$
$$= \sum_{i} \beta_{i} x_{i} + \sum_{ij} -2\nu_{ij} x_{i} x_{j}$$

Every quadratic pseudo-boolean function with non-positive second-order coefficients is a graph cut function.

Equivalent condition: E(x) is submodular.

Quadratic submodular functions

$$E(x) = \beta_i x_i + \beta_j x_j + \nu'_{ij} x_j x_j$$

check submodularity: $V = \{ (i), (j) \}$

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

$$S = \{i\}, T = \{j\}: \qquad (i) \qquad (j) \qquad (j) \qquad (i) \qquad (i$$

$$E(1,0) + E(0,1) \geq E(0,0) + E(1,1)$$

$$\beta_i + \beta_j \geq 0 + \beta_i + \beta_j + \nu'_{ij}$$

E(x) submodular $\Leftrightarrow \nu'_{ij} \leq 0$

Submodular polynomials & cuts

$$\sum_{i} \beta_{i} x_{i} + \sum_{ij} \nu_{ij} x_{i} x_{j} + \sum_{ijk} \nu_{ijk} x_{i} x_{j} x_{k} + \dots$$

- What if my function has degree > 2 ?
- If $\nu_S \leq 0$ for all ν_S then E(x) is submodular and can be written as a graph cut
- In general:



Submodular functions generalize graph cuts!



Submodular functions generalize graph cuts!

• symmetric submodular functions:

 $F(S) = F(\mathcal{V} \setminus S)$

 special algorithm for minimizing symmetric submodular functions in O(n³) time (Queyranne, 1998) generalization of a min-cut algorithm!



• semi-supervised learning (Guillory & Bilmes 2011, Hein et al 2013)



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Constraints?

e.g. min
$$F(S)$$
 s.t. $|S| = k$

generally: min F(S) s.t. $S \in \mathcal{C}$

- In most cases, this is NP-hard and cannot even be approximated within a constant factor ☺
- What to do? approximation

$$\widehat{S} \in \mathcal{C} \qquad \text{and} \qquad F(\widehat{S}) \leq \alpha \; F(S^*)$$
 approximate solution

Recall: MAP and cuts



binary labeling: $x = 1_A$ pairwise random field: $E(x) = \operatorname{Cut}(A)$

What's the problem?





minimum cut: prefer short cut = short object boundary

What's wrong?

we get ...



local coherence = short cut





ideally ...



Plif

homogeneous cut global dependencies!



not homogeneous

Cooperative cuts



local coherence homogeneous cut = short cut global dependencies! cooperative graph cut cost of a cut $C \subseteq \mathcal{E}$: cost of a cut $C \subseteq \mathcal{E}$: submodular function F(C)euges are independent edges are not independent cut weight

= energy

Homogeneity via group sparsity

sum of weights: use few edges



submodular cost function: use few types of edges Mii



One type (13 edges) Many types (6 edges)

$$F(\operatorname{Cut}) = \sum_{\operatorname{type} k} F_k(\operatorname{Cut})$$



Results



Quantitatively: up to 70% reduction in error!

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Results







Cooperative cut





Plif

Similarly: contour completion RF



(a)



(c)

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geometric edge groups:

- straight lines
- parabolas

Minimum cut?

• find a minimum cut with cost function: $C \subseteq \mathcal{E}$



normally:

$$\operatorname{Cost}(C) = \sum_{e \in C} w(e)$$
now:
 $\operatorname{Cost}(C) = F(C)$

 $\min F(S)$ s.t. constraints on S

Constrained optimization

- 2 strategies:
- convex relaxation using the Lovasz extension
- approximate the submodular function

$$S^* = \arg\min_{S \in \mathcal{C}} F(S) \longrightarrow \widehat{S} = \arg\min_{S \in \mathcal{C}} \widehat{F}(S)$$

Approximation of *F*

• recall: for $x = 1_S$ and F increasing

$$F(S) = f(x) = \max_{y \in \mathcal{P}_F} y^\top x$$

approximate polyhedron by ellipsoid

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$$\begin{array}{l}
\mathcal{E}_{F} \\
\mathcal{F}_{F} \\
\mathcal{P}_{F} \\
\mathcal{F}_{F} \\
\mathcal{F$$

How good is this?

$$\widehat{F}(S) = \max_{y \in \mathcal{E}_F} y^\top x \qquad \qquad \widehat{S} = \arg\min_{S \in \mathcal{C}} \widehat{F}(S)$$

• One can show that for all S:

$$F(S) \leq \widehat{F}(S) \leq \alpha F(S) \qquad \alpha$$

It follows that:

 $F(\widehat{S}) \leq \widehat{F}(\widehat{S}) \leq \widehat{F}(S^*) \leq \alpha F(S^*)$

 $= O(\sqrt{n \log n})$

A practical approximation

idea: submodularity = discrete concavity



fast: only need to solve linear optimization problem!

(Jegelka & Bilmes 2011; lyer, Jegelka, Bilmes 2013)

Does it work?



- often works well in practice
- theory: approximation guarantees depending on curvature of F

(lyer et al 2013)

• special cases: exact solution (Kohli et al 2013)

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Setup



- 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



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

Kempe, Kleinberg & Tardos 2003

Summarization

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





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Summarization

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

• Coverage / relevance

• Diversity

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

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



(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)

Many more functions are possible ...
→Learn a weighted combination: via "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 $B = A \cup \{a\}$.

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

marginal gain



Maximizing monotone functions

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





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

Voting elements

Hypotheses

Illustrations courtesy of Pushmeet Kohli

73 (Barinova et al.'10)

Object detection



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...

empirically:



sensor placement

Mii



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?

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