New Algorithms for Approximate Minimization of the Difference Between Submodular Functions, with Applications

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Outline

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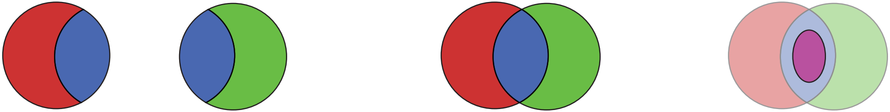
Submodular Functions

- A function $f : 2^V \to \mathbb{R}$ is submodular if for all $A, B \subseteq V$, $f(A) + f(B) \geq f(A \cup B) + f(A \cap B)$.
- Coverage of intersection of elements is less then common coverage.

$$f(A) + f(B) \quad \geq \quad f(A \cup B) \quad + \quad f(A \cap B)$$

$$= f(A_r) + 2f(C) + f(B_r) \qquad\qquad = f(A_r) + f(C) + f(B_r)$$



- Equivalently, diminishing returns: Let $A \subseteq B \subseteq V \setminus \{j\}$ then f is submodular iff

$$f(v|A) \triangleq f(A + v) - f(A) \geq f(B + v) - f(B) \triangleq f(v|B) \qquad (1)$$

- I.e., conditioning reduces valuation (like entropy).

Outline

Optimizing The Difference between Two Submodular Functions

- In this paper, we address the following problem. Given two submodular functions f and g, solve the optimization problem:

$$\min_{X \subseteq V} [f(X) - g(X)] \equiv \min_{X \subseteq V} [v(X)] \tag{2}$$

  with $v : 2^V \to \mathbb{R}$, $v = f - g$.
- A function r is said to be supermodular if $-r$ is submodular.

Applications

- Sensor placement with submodular costs. I.e., let V be a set of possible sensor locations, $f(A) = I(X_A; X_{V \setminus A})$ measures the quality of a subset A of placed sensors, and $c(A)$ the submodular cost. We have $\min_A f(A) - \lambda c(A)$.

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- Discriminatively structured graphical models, EAR measure $I(X_A; X_{V \setminus A}) - I(X_A; X_{V \setminus A} | C)$, and synergy in neuroscience.

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- Feature selection: a problem of maximizing $I(X_A; C) - \lambda c(A) = H(X_A) - [H(X_A|C) + \lambda c(A)]$, the difference between two submodular functions, where H is the entropy and c is a feature cost function.

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- Graphical Model Inference. Finding x that maximizes $p(x) \propto \exp(-v(x))$ where $x \in \{0, 1\}^n$ and v is a pseudo-Boolean function. When v is non-submodular, it can be represented as a difference between submodular functions.

Heuristics for General Set Function Optimization

Lemma (Narisimham & Bilmes, 2005)

Given any set function v, it can be expressed as $v(X) = f(X) - g(X), \forall X \subseteq V$ for some submodular functions f and g.

- We give a new proof that depends on computing $\alpha_v = \min_{X \subset Y \subseteq V \backslash j} v(j|X) - v(j|Y)$ which can be intractable for general v.
- However, we show that for those functions where α_v can be bounded efficiently, f and g can be computed efficiently.

Lemma

For a given set function v, if α_v or a lower bound can be found in polynomial time, a corresponding decomposition f and g can also be found in polynomial time.

Outline

Convex/Concave and Semigradients

- A convex function ϕ has a subgradient at any in-domain point y, namely there exists h_y such that

$$\phi(x) - \phi(y) \geq \langle h_y, x - y \rangle, \forall x. \quad (3)$$

- A concave ψ has a supergradient at any in-domain point y, namely there exists g_y such that

$$\psi(x) - \psi(y) \leq \langle g_y, x - y \rangle, \forall x. \quad (4)$$

- If a function has both a sub- and super-gradient at a point, then the function must be affine.

Submodular Subgradients

- For submodular function f, the subdifferential can be defined as:

$$\partial f(X) = \{x \in \mathbb{R}^V : \forall Y \subseteq V, x(Y) - x(X) \leq f(Y) - f(X)\} \quad (5)$$

- Extreme points of the sub-differential are easily computable via the greedy algorithm:

Theorem (Fujishige 2005, Theorem 6.11)

A point y is an extreme point of $\partial f(Y)$, iff there exists a chain $\emptyset = S_0 \subset S_1 \subset \cdots \subset S_n$ with $Y = S_j$ for some j, such that $y(S_i \setminus S_{i-1}) = y(S_i) - y(S_{i-1}) = f(S_i) - f(S_{i-1})$.

The Submodular Subgradients (Fujishige 2005)

- Let σ be a permutation of V and define $S_i^\sigma = \{\sigma(1), \sigma(2), \ldots, \sigma(i)\}$ as σ's chain containing Y, meaning $S_{|Y|}^\sigma = Y$ (we say that σ's chain contains Y).
- Then we can define a subgradient h_Y^f corresponding to f as:

$$h_{Y,\sigma}^f(\sigma(i)) = \begin{cases} f(S_1^\sigma) & \text{if } i = 1 \\ f(S_i^\sigma) - f(S_{i-1}^\sigma) & \text{otherwise} \end{cases}.$$

- We get a tight modular lower bound of f as follows:

$$h_{Y,\sigma}^f(X) \triangleq \sum_{x \in X} h_{Y,\sigma}^f(x) \leq f(X), \forall X \subseteq V.$$

Note, $h_{Y,\sigma}^f(Y) = f(Y)$.

Submodular/Supermodular Procedure

From Narisimham&Bilmes 2005.

Algorithm 1 The submodular-supermodular (SubSup) procedure

1: $X^0 = \emptyset$; $t \leftarrow 0$;
2: **while** not converged (i.e., $(X^{t+1} \neq X^t)$) **do**
3: Randomly choose a permutation σ^t whose chain contains the set X^t.
4: $X^{t+1} := \text{argmin}_X f(X) - h^g_{X^t,\sigma^t}(X)$
5: $t \leftarrow t + 1$
6: **end while**

Lemma

Algorithm 1 is guaranteed to decrease the objective function at every iteration. Further, the algorithm is guaranteed to converge to a local minima by checking at most $O(n)$ permutations at every iteration.

The Submodular Supergradients

- Can a submodular function also have a supergradient? We saw that in continuous case, simultaneous sub/super gradients meant linear.
- (Nemhauser, Wolsey, & Fisher 1978) established the following iff conditions for submodularity (if either hold, f is submodular):

$$f(Y) \leq f(X) - \sum_{j \in X \setminus Y} f(j|X \setminus j) + \sum_{j \in Y \setminus X} f(j|X \cap Y),$$
$$f(Y) \leq f(X) - \sum_{j \in X \setminus Y} f(j|(X \cup Y) \setminus j) + \sum_{j \in Y \setminus X} f(j|X)$$

Note that $f(A|B) \triangleq f(A \cup B) - f(B)$ is the gain of adding A in the context of B.

Submodular and Supergradients

- Using submodularity further, these can be relaxed to produce two tight modular upper bounds (Jegelka & Bilmes, 2011):

$$f(Y) \leq m^f_{X,1}(Y) \triangleq f(X) - \sum_{j \in X \setminus Y} f(j|X \setminus j) + \sum_{j \in Y \setminus X} f(j|\emptyset),$$
$$f(Y) \leq m^f_{X,2}(Y) \triangleq f(X) - \sum_{j \in X \setminus Y} f(j|V \setminus j) + \sum_{j \in Y \setminus X} f(j|X).$$

Hence, this yields two tight (at set X) modular upper bounds $m^f_{X,1}, m^f_{X,2}$ for any submodular function f.

Supermodular-Submodular (SupSub) Procedure

Algorithm 2 The supermodular-submodular (SupSub) procedure

1: $X^0 = \emptyset$; $t \leftarrow 0$;
2: **while** not converged (i.e., $(X^{t+1} \neq X^t)$) **do**
3: $\quad X^{t+1} := \text{argmin}_X \, m^f_{X^t}(X) - g(X)$
4: $\quad t \leftarrow t + 1$
5: **end while**

Theorem

The supermodular-submodular procedure (Algorithm 2) monotonically reduces the objective value at every iteration. Moreover, assuming a submodular maximization procedure in line 3 that reaches a local maxima of $m^f_{X^t}(X) - g(X)$, then if Algorithm 2 does not improve under both modular upper bounds then it reaches a local optima of v.

Supermodular-Submodular (SupSub) Procedure

- Each iteration requires submodular maximization, while this is NP-complete, it is easy to well approximate.
- Very recently, a fast randomized linear-time 1/2-approximation algorithm for submodular max was developed (FOCS 2012, "A Tight Linear Time (1/2)-Approximation for Unconstrained Submodular Maximization", Buchbinder, Feldman, Naor and Schwartz).
- The algorithm is extremely simple, and is essentially a randomized bi-directional greedy algorithm (very few iterations needed in practice).

Modular-Modular Procedure

Algorithm 3 Modular-Modular (ModMod) procedure

1: $X^0 = \emptyset$; $t \leftarrow 0$;
2: **while** not converged (i.e., $(X^{t+1} \neq X^t)$) **do**
3: Choose a permutation σ^t whose chain contains the set X^t.
4: $X^{t+1} := \text{argmin}_X \, m^f_{X^t}(X) - h^g_{X^t,\sigma^t}(X)$
5: $t \leftarrow t + 1$
6: **end while**

Theorem

Algorithm 3 monotonically decreases the function value at every iteration. If the function value does not increase on checking $O(n)$ different permutations with different elements at adjacent positions and with both modular upper bounds, then we have reached a local minima of v.

Modular-Modular Procedure

- Each iteration is very fast since only modular min.
- If $v >= 0$, then also applies to combinatorial constraints (trees, paths, matchings, cuts, etc.) since each iteration becomes standard combinatorial algorithm.
- In SubSup and ModMod the choice of the permutations is important since there are a combinatorial number of them (an problem left open from 2005).
- In the paper, we provide some heuristics which work well in practice.

Outline

1. Background
2. Optimizing $v(X) = f(X) - g(X)$ with f, g submodular
3. Procedures for minimizing $v(X)$
   - The Submodular Supermodular Procedure
   - The Supermodular Submodular Procedure
   - The Modular Modular Procedure
4. **Some Additional Theoretical Results**
5. Experiments

A P $\neq$ NP Hardness Result

- Given submodular functions f and g, the problem $\min_X [f(X) - g(X)]$ is inapproximable.

Theorem

Unless P = NP, there cannot exist any polynomial time approximation algorithm for $\min_X v(X)$ where $v(X) = [f(X) - g(X)]$ is a positive set function and f and g are given submodular functions. In particular, let n be the size of the problem instance, and $\alpha(n) > 0$ be any positive polynomial time computable function of n. If there exists a polynomial-time algorithm which is guaranteed to find a set $X' : f(X') - g(X') < \alpha(n) OPT$, where $OPT = \min_X v(X)$, then P = NP.

Information Theoretic Hardness

- We also have an information theoretic hardness result (i.e., one that is independent of the P $=$ NP question).

Theorem

For any $0 \leq \epsilon < 1$, there cannot exist any deterministic (or possibly randomized) algorithm for $\min_X [f(X) - g(X)]$ (where f and g are given submodular functions), that always finds a solution which is at most $\frac{1}{\epsilon}$ times the optimal, in fewer than $e^{\epsilon^2 n/8}$ queries.

Poly-time lower bounds on the optima

- On the more positive side, we do have lower bounds:

Theorem

Given submodular functions f and g, define $f'(X) \triangleq f(X) - \sum_{j \in X} f(j|V \backslash j)$, $g'(X) \triangleq g(X) - \sum_{j \in X} g(j|V \backslash j)$ *and* $k(X) = \sum_{j \in X} v(j|V \backslash j)$. *Then we have the following bounds:*

$$\min_X v(X) \geq \min_X f'(X) + k(X) - g'(V)$$

$$\min_X v(X) \geq f'(\emptyset) - g'(V) + \sum_{j \in V} \min(k(j), 0)$$

Computational bounds

This can be used to prove:

Theorem

The ϵ-approximate versions of algorithms 1, 2 and 3 have a worst case complexity of $O(\frac{\log(|M|/|m|)}{\epsilon} T)$, where $M = f'(\emptyset) + \sum_{j \in V} \min(v(j|V \backslash j), 0) - g'(V)$, $m = \min_k v(k)$ and $O(T)$ is the complexity of every iteration of the algorithm (which corresponds to respectively the submodular minimization, maximization, or modular minimization in algorithms 1, 2 and 3)..

Theoretical results - summary

- The problem $\min_X f(X) - g(X)$ for given submodular functions f and g is in general inapproximable.
- An information theoretic lower bound guarantees no sub-exponential time algorithm for exact minimization.
- Can provide poly-time lower bounds on the optimum, which can yield worst case additive approximation guarantees.
- Complexity results that our algorithms are polynomial time.
- And, again, the aforementioned local optima results of our new algorithms.

Outline

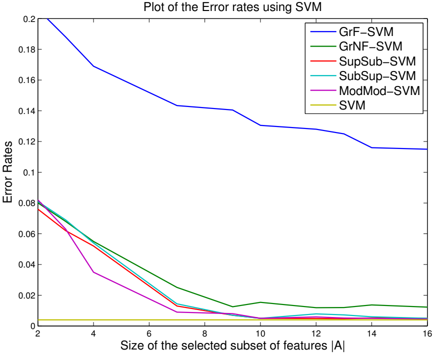
Experiments

- We consider features selection with objective $f(A) = I(X_A; C) = H(X_A) - H(X_A|C)$ (a difference between submodular functions) and **not** under the naïve Bayes model.
- We also consider two cost models, λ a tradeoff coefficient. Either
  1. modular cost model $c(A) = \lambda|A|$
  2. or submodular cost model using $c(A) = \lambda \sum_i \sqrt{m(A \cap S_i)}$ for a random partition of V and random weights m.
- We test two classifiers, a linear kernel SVM and a naïve Bayes (NB) classifier
- Data sets:
  1. Mushroom data (Iba, Wogulis, Langley, 1988), 8124 examples with 112 features.
  2. Adult data (Kohavi, 1996), 32,561 examples with 123 features.

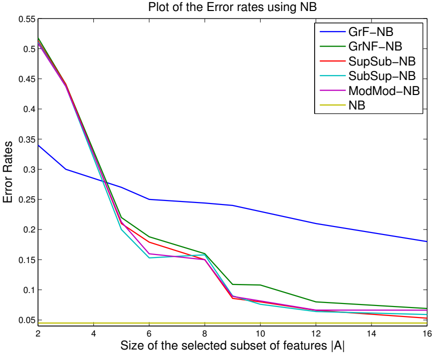
Feature Selection Algorithms Evaluated

- Feature selection algorithms evaluated.
  1. Greedy with factored MI (GrF) - simple greedy selection using conditional mutual information (CMI) with a NB assumption.
  2. Greedy with non-factored MI (GrNF) - greedy selection using CMI without assumptions.
  3. Submodular-Supermodular procedure (SubSup).
  4. Supermodular-Submodular procedure (SupSub).
  5. Modular-Modular procedure (ModMod)
- In SubSup and ModMod, we used the aforementioned smart permutation heuristic.
- ModMod and SubSup use exact minimization at each iteration, while SupSub use approximate minimization (via the new FOCS 2012 submodular maximization algoritm).

Mushroom Data - modular cost features



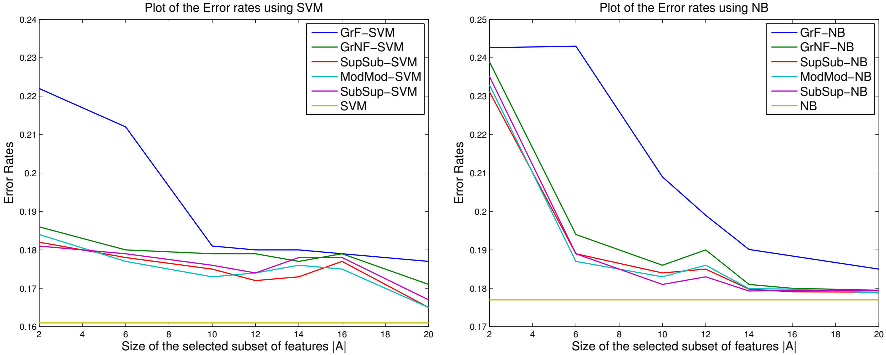
(a) SVM



(b) NB

Figure : Plot showing the accuracy rates vs. the number of features on the Mushroom data set.

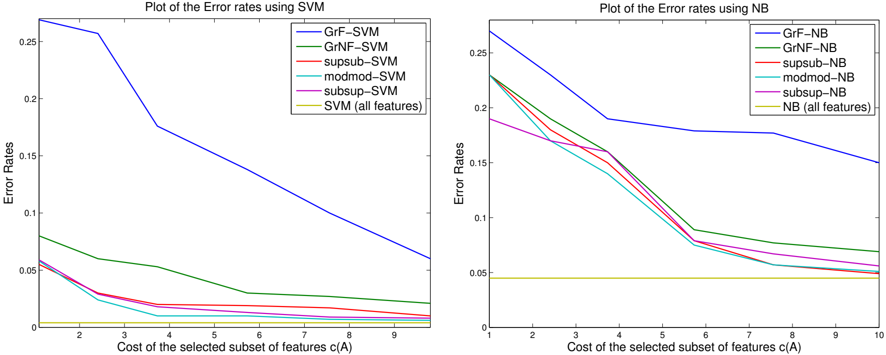
Adult Data - modular cost features



(a) SVM (b) NB

Figure : Plot showing the accuracy rates vs. the number of features on the Adult data set.

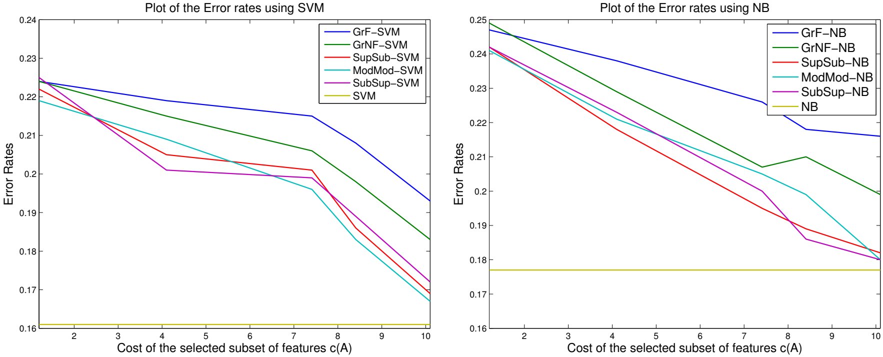
Mushroom Data - submodular cost features



(a) SVM (b) NB

Figure : Plot showing the accuracy rates vs. the cost of features for the Mushroom data set

Adult Data - submodular cost features



(a) SVM (b) NB

Figure : Plot showing the accuracy rates vs. the cost of features for the Adult data set

Experiments - Results Summarized

- Permutation heuristic is important for the performance of ModMod and SubSup.
- ModMod and SubSup do not show significant difference, but ModMod is must faster and scales very well.
- SubSup does not show appreciable benefit even though it uses exact submodular minimization at each iteration (and is slower).
- GrF and GrNF in general does not perform as well (with GrF worse than GrNF).
- More benefit to the $v = f - g$ approach under the submodular cost model than under the modular cost model.

Summary

- Applications of minimizing the difference between two submodular functions.
- New algorithms for minimizing the difference between two submodular functions.
- New theoretical hardness results and complexity bounds.
- Empirical experimental validation.