Tutorial: Evolutionary Submodular Optimisation



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GECCO '21 Companion, July 10-14, 2021, Lille, France © 2021 Copyright is held by the owner/author(s). Publication rights licensed to ACM. ACM ISBN 978-1-4503-8351-6/21/07...\$15.00 https://doi.org/10.1145/344972 6.3461433

Our task:

Given a function $f: X \to R$ and $D \subset X$ "set of feasible solutions"

Find $\arg \max_{x \in D} f(x)$

General purpose algorithms that can be applied without problem knowledge

Why General Purpose Algorithms?

- Algorithms are the heart of every nontrivial computer application.
- For many problems we know good or optimal algorithms
 - Sorting
 - Shortest paths
 - Minimum spanning trees
- What about a new or complex problems?
- Often there are no good problem specific algorithms.

Points that may rule out problem specific algorithms

- Problems that are rarely understood.
- Quality of solutions is determined by simulations.
- Problem falls into the black box scenario.

→ f(x)

• Not enough resources such as time, money, knowledge.

General purpose algorithms are often a good choice.

General purpose algorithms for

optimizing a function $f: X \to R$

- 1. Choose a representation for the elements in X.
- 2. Fix a function to evaluate the quality. (might be different from f)
- 3. Define operators that produce new elements.

Evolutionary algorithms (EAs)

- Evolutionary algorithms are general purpose algorithms.
- follow Darwin's principle (survival of the fittest).
- work with a set of solutions called population.
- parent population produces offspring population by variation operators (mutation, crossover).
- select individuals from the parents and children to create new parent population.
- Iterate the process until a "good solution" has been found.
- EAs are adaptive and often yield good solutions for complex, dynamic and/or stochastic problems

Motivation

- Want to understand a wide class of problems that evolutionary algorithms can solve or approximate well.
- Consider submodular functions which allow to model a wide range of important optimisation problems.
- Submodular functions can be considered as the discrete counterpart of convexity in the continuous domain (Lovasz, 1983).

Submodular Functions

- Let $X = \{x_1, ..., x_n\}$ be a ground set
- Submodular functions: A function f is submodular iff $f(A \cup B) + f(A \cap B) \le f(A) + f(B)$ for all $A, B \subseteq X$.
- Alternative definition of submodularity:

 $A\subseteq B\subseteq X \text{ and } x\in X\setminus B, \, f(B\cup\{x\})-f(B)\leq f(A\cup\{x\})-f(A).$

Maximizing submodular functions is NP-hard and also NP-hard to approximate.

Important subclasses:

Monotone functions: A function is monotone iff f(A) ≤ f(B) for all A ⊆ B.
We call f symmetric iff f(A) = f(X \ A) for all A ⊆ X.

Example: Sensor placement

Cover the largest possible area by selecting k sensors:



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Example Max Cut

- Given an undirected graph G=(V, E), find a partitioning of the vertices such that the number of edges crossing the two partitions is maximal.
- A is a set of nodes chosen for the first partition. Function f(A) counts the number of edges between A and V \ A.
- f is symmetric, submodular, but not monotone.

Matroids

A matroid is a pair (X, I) composed of a ground set X and a non-empty collection I of subsets of X satisfying (1) If $A \in I$ and $B \subseteq A$ then $B \in I$ and (2) If $A, B \in I$ and |A| > |B| then $B + x \in I$ for some $x \in A \setminus B$. The sets in I are called *independent*, the *rank* of a matroid is the size of any maximal independent set.

Example:

- For given graph G=(V,E), M=(E, F) where F is the set of all forests (subset of edges not containing cycles) is a matroid. Maximal independent sets are spanning trees (rank n-1).
- Given X all subsets of cardinality at most k build the uniform matroid.

Some Examples of Submodular Functions

- Linear functions: All linear functions $f: 2^X \to \mathbb{R}$ with $f(A) = \sum_{i \in A} w_i$ for some weights $w: X \to \mathbb{R}$ are submodular. If $w_i \ge 0$ for all $i \in X$, then f is also monotone.
- Cut: Given a graph G = (V, E) with nonnegative edge weights $w : E \to \mathbb{R}_{\geq 0}$. Let $\delta(S)$ be the set of all edges that contain both a vertex in S and $V \setminus S$. The cut function $w(\delta(S))$ is symmetric and submodular but not monotone.
- Coverage: Let the ground set be $X = \{1, 2, ..., n\}$. Given a universe U with n subsets $A_i \subseteq U$ for $i \in X$, and a non-negative weight function $w: U \to \mathbb{R}_{\geq 0}$. The coverage function $f: 2^X \to \mathbb{R}$ with $f(S) = |\bigcup_{i \in S} A_i|$ and the weighted coverage function f' with $f'(S) = w(\bigcup_{i \in S} A_i) = \sum_{u \in \bigcup_{i \in S} A_i} w(u)$ are monotone submodular.
- Rank of a matroid: The rank function $r(A) = \max\{|S|: S \subseteq A, S \in \mathcal{I}\}$ of a matroid (X, \mathcal{I}) is monotone submodular.

Submodular Optimisation

Research in this area can be characterized by the type of

- Functions to be optimized
 - Submodular / close to submodular
 - monotone / non-monotone
 - Additional function characteristics
- Types of constraints
 - Uniform, linear constraints
 - General cost constraints
 - Matroid / partition constraints.
 - Other types of constraints



GSEMO

• Given submodular function f, solutions are encoded as bitstrings of length n.

Al	gorithm 1: GSEMO Algorithm								
1 cl	hoose $x \in \{0,1\}^n$ uniformly at random								
2 d	2 determine $g(x)$								
3 F	3 $P \leftarrow \{x\}$								
4 r	epeat								
5	choose $x \in P$ uniformly at random								
6	create x' by flipping each bit x_i of x with probability $1/n$								
7	determine $g(x')$								
8	if x' is not strictly dominated by any other search point in P then								
9	include x' into P								
10	delete all other solutions $z \in P$ with $g(z) \leq g(x')$ from P								
11 u	11 until stop								

- Maximize bi-objective function g(x)=(z(x), |x|₀), where z(x)=f(x) iff x is feasible and z(x)=-1 otherwise
- Analyze expected time (number of fitness evaluations) to obtain good approximations

Monotone submodular functions under uniform constraint

A solution x is feasible iff its has at most k elements (1-bits), i.e.

 $F = \{x \mid x \in X \land |x|_1 \le k\}$

is the set of feasible solutions.

Result (Friedrich, Neumann (ECJ 2015)):

GSEMO achieves a (1-1/e)-approximation in expected time $O(n^2(k + \log n))$.

Proof Idea

- GSEMO obtains empty set in expected time O(n²log n).
- Afterwards mimics greedy approach (Nemhauser et al 1978) and obtains for each j, $0 \le j \le k$, a solution X_j with

$$f(X_j) \ge \left(1 - \left(1 - \frac{1}{k}\right)^{s}\right) \cdot f(\text{OPT}),$$

where f(OPT) is value of feasible optimal solution. Key induction argument:

- Assume that we already have $f(X_j) \ge \left(1 - \left(1 - \frac{1}{k}\right)^j\right) \cdot f(OPT), 0 \le j \le i$. Let δ_{i+1} be the increase in f that we obtain when choosing the solution $x \in P$ with $|x|_1 = i$ for mutation and inserting the element corresponding to the largest possible increase.

Due to monotonicity and submodularity, we have $f(OPT) \leq f(X_i \cup OPT) \leq f(X_i) + k\delta_{i+1}$ which implies $\delta_{i+1} \geq \frac{1}{k} \cdot (f(OPT) - f(X_i))$.

Gives X_{i+1} with $f(X_{i+1}) \ge f(X_i) + \frac{1}{k} (f(OPT) - f(X_i)) \ge \left(1 - \left(1 - \frac{1}{k}\right)^{i+1}\right) \cdot f(OPT).$

 X_k is (1-1/e)-approximation and obtained after O(n²k) steps.

Non-monotone symmetric under Matroid Constraints

Given k matroids $M_1, ..., M_k$ together with their independent systems $I_1, ..., I_k$, we consider the problem

 $\max\Big\{f(x) \mid x \in F := \bigcap_{j=1}^k I_j\Big\}.$

We assume that f is symmetric, submodular and nonnegative, but not necessarily monotone.

- For this setting, a local search capability is beneficial to obtain good approximations.
- In particular, dependent on the number of matroids, a local improvement in a neighborhood dependent on k can be obtained if the current solution is not of sufficient quality (Lee et al, STOC 2009).

Non-monotone symmetric under Matroid Constraints

Result (Friedrich, Neumann (ECJ 2015)):

GSEMO achieves a $\left(\frac{1}{(k+2)(1+\epsilon)}\right)$ -approximation in expected time $o\left(\frac{1}{\epsilon}n^{k+6}\log n\right)$. Proof idea:

- In expected time O(n²log n), GSEMO produces the search point 0ⁿ.
- Introducing the element with the largest gain gives a solution of quality at least OPT/n.
- Afterwards from the currently best feasible solution x, in expected time $O(n^{k+2})$ a solution y with $f(y) \ge (1 + \epsilon/n^4) \cdot f(x)$ can be produced if stated approximation guarantee has not yet been obtained.
- Total number of such local improvements required to obtain approximation is at most

$$\log_{(1+\frac{\epsilon}{n^4})} \frac{OPT}{OPT/n} = O\left(\frac{1}{\epsilon} n^4 \log n\right).$$

Remark: k=1 gives $(1/(3(1+\epsilon))$ -approximation for Max-Cut

Approximately Submodular Functions

Approximately submodular application

Sparse regression [Tropp, TIT'04]: given observation variables $V = \{v_1, ..., v_n\}$, a predictor variable z and a budget B, to find a subset $X \subseteq V$ such that $max_{X\subseteq V} \quad R_{z,X}^2 = \frac{\operatorname{Var}(z) - \operatorname{MSE}_{z,X}}{\operatorname{Var}(z)} \quad s.t. \quad |X| \leq B$ $\operatorname{Var}(z): \text{ variance of } z \qquad \operatorname{MSE}_{z,X}: \text{ mean squared error of predicting } z \\ \text{ by using observation variables in } X$ $R_{z,X}^2: \text{ squared multiple correlation, which is approximately submodular}$

Submodular ratio

Submodular [Nemhauser et al., MP'78]:

$$\forall X \subseteq Y \subseteq V, v \notin Y: f(X \cup \{v\}) - f(X) \ge f(Y \cup \{v\}) - f(Y);$$

or $\forall X \subseteq Y \subseteq V: f(Y) - f(X) \le \sum_{v \in Y \setminus X} f(X \cup \{v\}) - f(X)$
Submodular ratio [Das & Kempe, ICML'11; Zhang & Vorobeychi, AAAI'16]:
$$\alpha_f = \min_{X \subseteq Y, v \notin Y} \frac{f(X \cup \{v\}) - f(X)}{f(Y \cup \{v\}) - f(Y)}$$

$$\gamma_{U,k}(f) = \min_{X \subseteq U, Y: |Y| \le k, X \cap Y = \emptyset} \frac{\sum_{v \in Y} f(X \cup \{v\}) - f(X)}{f(X \cup Y) - f(X)} \quad (--)$$

Characterize to what extent a set function *f* satisfies the submodular property, i.e., the degree of approximate submodularity

For example, when f is monotone,

- $\alpha_f \in [0,1]$, the larger, more close to submodular
- *f* is submodular if and only if $\alpha_f = 1$

Submodular ratio

Submodular [Nemhauser et al., MP'78]:

$$\neg \neg \neg \forall X \subseteq Y \subseteq V, v \notin Y: f(X \cup \{v\}) - f(X) \ge f(Y \cup \{v\}) - f(Y);$$

or $\forall X \subseteq Y \subseteq V: f(Y) - f(X) \le \sum_{v \in Y \setminus X} f(X \cup \{v\}) - f(X)$
Submodular ratio [Das & Kempe, ICML'11; Zhang & Vorobeychi, AAAI'16]:
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$$\gamma_{U,k}(f) = \min_{X \subseteq U, Y: |Y| \le k, X \cap Y = \emptyset} \frac{\sum_{v \in Y} f(X \cup \{v\}) - f(X)}{f(X \cup Y) - f(X)}$$

Characterize to what extent a set function f satisfies the submodular property, i.e., the degree of approximate submodularity

For example, when *f* is monotone,

- $\forall U, k: \gamma_{U,k}(f) \in [0,1]$, the larger, more close to submodular
- *f* is submodular if and only if $\forall U, k: \gamma_{U,k}(f) = 1$

Submodular ratio

Submodular ratio [Das & Kempe, ICML/11; Zhang & Vorobeychi, AAAI'16] : characterize to what extent a general set function satisfies the submodular property

$$\begin{aligned} \alpha_f &= \min_{X \subseteq Y, v \notin Y} \frac{f(X \cup \{v\}) - f(X)}{f(Y \cup \{v\}) - f(Y)} \\ \gamma_{U,k}(f) &= \min_{X \subseteq U, Y: |Y| \le k, X \cap Y = \emptyset} \frac{\sum_{v \in Y} f(X \cup \{v\}) - f(X)}{f(X \cup Y) - f(X)} \end{aligned}$$

Lower bounds on submodular ratio for some concrete applications

- Sparse regression: $\gamma_{U,k}(f) \ge \lambda_{min}(\mathbb{C}, |U| + k)$ [Das & Kempe, ICML'11]
- Sparse support selection: $\gamma_{U,k}(f) \ge m/M$ [Elenberg et al., Annals of Statistics'18]
- Bayesian experimental design [Bian et al., ICML'17]:

$$\gamma_{U,k}(f) \ge \beta^2 / (\|V\|^2 (\beta^2 + \sigma^{-2} \|V\|^2))$$

• Determinantal function maximization [Qian et al., IJCAI'18]: $\alpha_f \ge (\lambda_n(A) - 1) / ((\lambda_1(A) - 1) \prod_{i=1}^{n-1} \lambda_i(A))$

Pareto optimization for approximately submodular f

The POSS algorithm [Qian, Yu and Zhou, NIPS'15]



Theoretical analysis

POSS can achieve the optimal approximation guarantee, previously obtained by the greedy algorithm

Theorem 1. For monotone approximately submodular maximization with a size constraint, POSS using $E[T] \le 2eB^2n$ finds a solution **x** with $|\mathbf{x}| \le B$ and



POSS can do better than the greedy algorithm in cases

Theorem 2. For the Exponential Decay subclass of sparse regression, POSS using $E[T] = O(B^2(n - B)n \log n)$ finds an optimal solution, while the greedy algorithm cannot

Experiments – sparse regression

the size constraint: B = 8

the number of iterations of POSS: $2eB^2n$

exhaustiv	re search		greedy a	algorithms	1	relaxation methods		
Data set	OPT	POSS	FR	FoBa	OMP	RFE	MCP	
housing	.7437±.0297	.7437±.0297	.7429±.0300•	.7423±.0301•	.7415±.0300•	.7388±.0304•	.7354±.0297•	
eunite2001	.8484±.0132	.8482±.0132	.8348±.0143•	.8442±.0144•	.8349±.0150•	.8424±.0153•	.8320±.0150•	
svmguide3	.2705±.0255	.2701±.0257	.2615±.0260•	.2601±.0279•	.2557±.0270•	.2136±.0325•	.2397±.0237•	
ionosphere	.5995±.0326	.5990±.0329	.5920±.0352•	.5929±.0346•	.5921±.0353•	.5832±.0415•	.5740±.0348•	
sonar	-	$.5365 \pm .0410$.5171±.0440•	.5138±.0432•	.5112±.0425•	.4321±.0636•	.4496±.0482•	
triazines	-	.4301±.0603	.4150±.0592•	.4107±.0600•	.4073±.0591•	.3615±.0712•	.3793±.0584•	
coil2000		$.0627 \pm .0076$.0624±.0076•	.0619±.0075•	.0619±.0075•	.0363±.0141•	.0570±.0075•	
mushrooms	1.21	.9912±.0020	.9909±.0021•	.9909±.0022•	.9909±.0022•	.6813±.1294•	.8652±.0474•	
clean1	-	.4368±.0300	.4169±.0299•	.4145±.0309•	.4132±.0315•	.1596±.0562•	.3563±.0364•	
w5a		.3376±.0267	.3319±.0247•	.3341±.0258•	.3313±.0246•	.3342±.0276•	.2694±.0385•	
gisette	-	$.7265 \pm .0098$.7001±.0116•	.6747±.0145•	.6731±.0134•	.5360±.0318•	.5709±.0123•	
farm-ads		$.4217 \pm .0100$.4196±.0101•	.4170±.0113•	.4170±.0113•	-	.3771±.0110•	
POSS: w	/in/tie/loss	-	12/0/0	12/0/0	12/0/0	11/0/0	12/0/0	

• denotes that POSS is significantly better by the *t*-test with confidence level 0.05

POSS is significantly better than all the compared algorithms on all data sets

Experiments – sparse regression

different size constraints: $B = 3 \rightarrow 8$



POSS tightly follows OPT, and has a clear advantage over the rest algorithms

Experiments – sparse regression

Running time comparison



POSS can be more efficient in practice

General cost constraints

Original problem



f(X): a monotone approximately submodular objective function

c(X): a monotone approximately submodular cost function

Pareto optimization for general cost constraints

The POMC algorithm [Qian, Shi, Yu and Tang, IJCAI'17]

	$max_{\boldsymbol{x}\in\{0,1\}^n} f(\boldsymbol{x}) s.t.$	$c(\boldsymbol{x}) \leq B$	original
Transformation:	$\hat{\Gamma}$		
	$min_{x \in \{0,1\}^n} (-f(x), c(x))$	(x))	bi-objective

Algorithm 2 POMC Algorithm		
Input: a monotone objective function f, a monotone approx-	Ir	itialization: put the special solution {0} ^{<i>n</i>}
imate cost function \hat{c} , and a budget B	ir	to the population P
Parameter: the number T of iterations	1	1 1
Output : a solution $x \in \{0, 1\}^n$ with $\hat{c}(x) \leq B$	/ _	
Process:	K	eproduction: pick a solution x randomly
1: Let $x = \{0\}^n$ and $P = \{x\}$.	fr	om P , and flip each bit of x with prob.
2: Let $t = 0$.	1	/n to produce a new solution
3: while $t < T$ do	/ /	in to produce a new solution
 Select x from P uniformly at random. 		
5: Generate x' by flipping each bit of x with prob. $1/n$.	T	Inducting: if the new solution \mathbf{x}' is not
6: if $\nexists z \in P$ such that $z \succ x'$ then	1	
7: $P = (P \setminus \{ \boldsymbol{z} \in P \mid \boldsymbol{x}' \succeq \boldsymbol{z} \}) \cup \{ \boldsymbol{x}' \}.$	a	ominated by any solution in P, put it
8: end if	ir	nto <i>P</i> and delete those solutions weakly
9: $t = t + 1$.	d	ominated by r'
10: end while	u	oniniated by x
11: return $\arg \max_{x \in P: \hat{c}(x) \leq B} f(x)$		
	' 🥆 C	Output: select the best feasible solution
		-

Theoretical analysis

POMC can achieve the best-known approximation guarantee, previously obtained by the generalized greedy algorithm

Theorem 3. For monotone approximately submodular maximization with a general cost constraint, POMC using $E[T] \leq enBP_{max}/\delta_c$ finds a solution **x** with $c(\mathbf{x}) \leq B$ and

$$f(\mathbf{x}) \ge \frac{\alpha_f}{2} \left(1 - \frac{1}{e^{\alpha_f}}\right) \cdot \text{OPT}$$

the best-known polynomial-time approximation ratio [Zhang & Vorobeychik, AAAI'16]

Proof



submodularity ratio

the optimal function value

Roughly speaking, the improvement on *f* by adding a specific item is proportional to the current distance to the optimum

Proof

Lemma 1. For any $(\widehat{x}) \subseteq V$, there exists one item $\widehat{v} \in V \setminus X$ such that $f(X \cup {\widehat{v}}) - f(X) \ge \alpha_f \frac{c(X \cup {\widehat{v}}) - c(X)}{B} (OPT - f(X))$ Main idea: a subset • consider a solution (\widehat{x}) with $c(\widehat{x}) \le i \in [0, B)$ and $f(\widehat{x}) \ge \left(1 - \left(1 - \alpha_f \frac{i}{Bk}\right)^k\right) \cdot OPT$ i = 0 $i + c(\widehat{x} \cup {\widehat{v}}) - c(\widehat{x}) \ge B$ initial solution $00 \dots 0$ $f(\widehat{x} \cup {\widehat{v}}) \ge \left(1 - \left(1 - \alpha_f \frac{i + c(\widehat{x} \cup {\widehat{v}}) - c(\widehat{x})}{B(k+1)}\right)^{k+1}\right) \cdot OPT$ i = 0 $f(\widehat{x} \cup {\widehat{v}}) \ge \left(1 - \left(1 - \alpha_f \frac{i + c(\widehat{x} \cup {\widehat{v}}) - c(\widehat{x})}{B(k+1)}\right)^{k+1}\right) \cdot OPT$ i = 0 $f(\widehat{x} \cup {\widehat{v}}) \ge \left(1 - \left(1 - \alpha_f \frac{B}{B(k+1)}\right)^{k+1}\right) \cdot OPT$ $\ge (1 - e^{-\alpha_f}) \cdot OPT$

Proof



Proof



Proof



Proof

Lemma 1. For any
$$\hat{x} \subseteq V$$
, there exists one item $\hat{v} \in V \setminus X$ such that
 $f(X \cup \{\hat{v}\}) - f(X) \ge \alpha_f \frac{c(X \cup \{\hat{v}\}) - c(X)}{B} (OPT - f(X))$
Main idea: a subset
• consider a solution \hat{x} with $c(x) \le i \in [0, B)$ and $f(x) \ge \left(1 - \left(1 - \alpha_f \frac{i}{Bk}\right)^k\right) \cdot OPT$
• in each iteration of POMC:
• select x from the population P the probability: $\frac{1}{|P|}$
• flip one specific 0-bit of x to 1-bit the probability: $\frac{1}{n}\left(1 - \frac{1}{n}\right)^{n-1} \ge \frac{1}{en}$
(i.e., add the specific item \hat{v} in Lemma 1)
• $c(x') \le i + c(x') - c(x)$ and $f(x') \ge \left(1 - \left(1 - \alpha_f \frac{i + c(x') - c(x)}{B(k+1)}\right)^{k+1}\right) \cdot OPT$
 $i \longrightarrow i + c(x') - c(x) \ge i + \delta_c$ the probability: $\frac{1}{|P|} \cdot \frac{1}{en}$
 $min\{c(x \cup \{v\}) - c(x) \mid v \notin x\}$

Proof

Lemma 1. For any
$$(x) \subseteq V$$
, there exists one item $\hat{v} \in V \setminus X$ such that
 $f(X \cup {\hat{v}}) - f(X) \ge \alpha_f \frac{c(X \cup {\hat{v}}) - c(X)}{B} (OPT - f(X))$
Main idea: a subset
• consider a solution (x) with $c(x) \le i \in [0, B)$ and $f(x) \ge \left(1 - \left(1 - \alpha_f \frac{i}{Bk}\right)^k\right) \cdot OPT$
• in each iteration of POMC:
 $i \longrightarrow i + \delta_c$ the probability: $\frac{1}{|P|} \cdot \frac{1}{en} \stackrel{|P| \le P_{max}}{\longrightarrow} \frac{1}{eP_{max}n}$
 $i \longrightarrow i + \delta_c$ the expected number of iterations: $eP_{max}n$
 $i = 0 \longrightarrow i + c(x \cup {\hat{v}}) - c(x) \ge B$
the expected number of iterations: $\frac{B}{\delta_c} \cdot eP_{max}n$

Theoretical analysis

POMC can achieve the best-known approximation guarantee, previously obtained by the generalized greedy algorithm

Theorem 3. [Qian, Shi, Yu and Tang, IJCAI'17] For monotone approximately submodular maximization with a general cost constraint, POMC using $E[T] \le enBP_{max}/\delta_c$ finds a solution **x** with $c(\mathbf{x}) \le B$ and

$$f(\mathbf{x}) \ge \frac{\alpha_f}{2} \left(1 - \frac{1}{e^{\alpha_f}}\right) \cdot \text{OPT}$$

the best-known polynomial-time approximation ratio [Zhang & Vorobeychik, AAAI'16]

By limiting the largest population size P_{max} , we get the EAMC algorithm whose running time is polynomial

Theorem 4. [Bian, Feng, Qian and Yu, AAAI'20] For monotone approximately submodular maximization with a general cost constraint, EAMC using $E[T] \le 2en^2(n+1)$ finds a solution \boldsymbol{x} with $c(\boldsymbol{x}) \le B$ and

$$f(\mathbf{x}) \ge \frac{\alpha_f}{2} \left(1 - \frac{1}{e^{\alpha_f}}\right) \cdot \text{OPT}$$

Experiments - sensor placement

• Sensor placement [Krause et al., JMLR'08]: select a subset of locations to install sensors such that the entropy is maximized

Formally stated: given *n* locations $V = \{v_1, ..., v_n\}$ and a budget *B*, let o_j denote the observation variable by installing a sensor at v_i , and then

 $max_{X\subseteq V} \quad H(\{o_j \mid v_j \in X\}) \quad s.t. \quad c(X) \le B$

- Constraints: cardinality $|X| \le B \in \{5, ..., 10\}$ and routing $c(X) \le B \in \{0.5, ..., 1\}$ the shortest walk to visit each node in *X* at least once
- Data sets: Berkeley (n = 55), Beijing (n = 36)
- For POMC on each data set with each *B* value, the run is repeated for 10 runs independently, and the average results are reported
- Compare POMC with the generalized greedy algorithm

Experiments – sensor placement



Experiments – influence maximization

• Influence maximization [Kempe et al., KDD'03]: select a subset of users from a social network such that the influence spread is maximized

Formally stated: given a directed graph $G = (V, E)$ with $ V = n$, edge
probabilities $p_{u,v}$ ((u, v) $\in E$) and a budget B , then
$max_{X\subseteq V}$ $f(X)$ s.t. $c(X) \leq B$
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The expected number of nodes activated by propagating from *X*





Experiments – influence maximization

• Influence maximization [Kempe et al., KDD'03]: select a subset of users from a social network such that the influence spread is maximized

Formally stated: given a directed graph G = (V, E) with |V| = n, edge probabilities $p_{u,v}$ ((u, v) $\in E$) and a budget B, then $max_{X \subseteq V}$ f(X) s.t. $c(X) \leq B$

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The expected number of nodes activated by propagating from X



POMC is always better

Pareto optimization vs. Greedy algorithm

(Generalized) Greedy algorithm:

· Generate a new solution by adding a single item

(i.e., single-bit forward search: $0 \rightarrow 1$)

Keep only one solution

Pareto optimization:

- Generate a new solution by flipping each bit with prob. 1/n
 - > single-bit forward search : 0 → 1
 - > backward search : $1 \rightarrow 0$
 - > multi-bit search : $00 \rightarrow 11$
- · Keep a set of non-dominated solutions due to bi-objective optimization

Pareto optimization may have a better ability of escaping from local optima

Dynamic Constraints

- Many real world optimization problems are dynamic and/or stochastic.
- Often the goal function to be optimized is fixed (reduce cost / maximize profit).
- Resources to achieve these goal are usually changing.

Example:

Trucks/trains may break down and/or be repaired. Algorithms have to react to such changes that effect the constraints of the given problem.

Now:

Study of (adaptive) greedy algorithms and Pareto optimization approaches for problems with dynamic constraints.

Problems with Dynamic Constraints

[V. Roostapour, A Neumann, F. Neumann, T. Friedrich: Pareto Optimization for Subset Selection with Dynamic Cost Constraints, AAAI'19]

Definitions

The Static Problem [C. Qian, J. Shi, Y. Yu, K. Tang, IJCAI'17]

Given a monotone objective function $f: 2^V \to \mathbb{R}^+$, the monotone cost function $c: 2^V \to \mathbb{R}^+$ and budget B, the aim is to find X such that

$$X = \arg \max_{Y \subseteq V} f(Y) \text{ s.t. } c(Y) \le B.$$

$$\phi = (\alpha_f/2)(1 - \frac{1}{e^{\alpha_f}})$$

The Dynamic Problem

[V. Roostapour, A. Neumann, F. Neumann, T. Friedrich, AAAI'19]

Let X be a ϕ -approximation for the static problem. The dynamic problem is given by a sequence of changes where in each change the current budget B changes to $B^* = B + d$, $d \in \mathbb{R}_{\geq -B}$. The goal is to compute a ϕ -approximation X' for each newly given budget B^* .



Greedy Algorithms

Approximation Adaptive Greedy

Consider n items

 $e_i = (c_i, f_i), 1 \le i \le n+1$

- Low profit items: $e_i = (1, \frac{1}{n}), 1 \le i \le n/2$
- High profit items: $e_i = (2, 1), n/2 + 1 \le i \le n$
- Special item:

 $e_{n+1} = (1,3)$

Linear objective and constraint function:

 $f_{inc}(X) = \sum_{e_i \in X} f_i$ $c_{inc}(X) = \sum_{e_i \in X} c_i$

Consider the following dynamic schedule:

• Start with B = 1 and increase B by 1 in each of n/2 steps.

Approximation Adaptive Greedy

Theorem 3. Given the dynamic knapsack problem (f_{inc}, c_{inc}) . Starting with B = 1 and increasing the bound n/2 times by 1, the adaptive greedy algorithm computes a solution that has approximation ratio O(1/n). [V. Roostapour, A. Neumann, T. Friedrich, AAAI'19]

Proof idea:

• For B=1, the special item $e_{n+1} = (1,3)$ is included.

- During n/2 steps increasing the budget by 1, all low profit items are included.
- For the obtained set S, we have

 $f(S) = 3 + (n/2) \cdot (1/n) = 7/2$ and c(S) = 1 + n/2

constraint bound.

- Optimal set S* consists of special item and n/4 high profit items and we have $f(S^*) = 3 + \frac{n}{4}$
- Approximation ratio (7/2)/(3+n/4) = O(1/n)

Pareto Optimization

Algorithm 3: POMC Algorithm										
input: Initial budget constraint B, time T										
1 $X \leftarrow \{0\}^n;$										
2 Compute $(f_1(X), f_2(X));$										
3 $P \leftarrow \{x\};$										
4 $t \leftarrow 0;$										
5 while $t < T$ do										
6 Select X from P uniformly at random;										
7 $X' \leftarrow$ flip each bit of X with probability $\frac{1}{n}$;										
8 Compute $(f_1(X'), f_2(X'));$										
9 if $\nexists Z \in P$ such that $Z \succ X'$ then										
10 $P \leftarrow (P \setminus \{Z \in P \mid X' \succeq Z\}) \cup \{X'\};$										
$11 \ \ t = t + 1;$										
12 return $\arg \max_{X \in P: \hat{c}(X) \leq B} f(x)$										

$$\begin{split} & \arg \max X \in \{0,1\}^n(f_1(X), f_2(X)) \\ & \text{where } f_1(X) = \begin{cases} -\infty, & \hat{c}(X) > B+1 \\ f(X), & \text{otherwise} \end{cases}, f_2(X) = -\hat{c}(X). \end{split}$$

Theoretical Results POMC

Theorem 5. Starting from $\{0\}^n$, POMC computes for any budget $b \in [0, B]$ a $\phi = (\alpha_f/2)(1 - 1/e^{\alpha_f})$ -approximate solution after $T = cnP_{max} \cdot \frac{B}{\delta_c}$ iterations with the constant probability, where $c \ge 8e + 1$ is a sufficiently large arbitrary constant.

Theorem 6. Let POMC has population P such that for every budget $b \in [0, B]$, there is a ϕ -approximation in P. After changing the budget to $B^* > B$, POMC has computed within $T = cnP_{max}\frac{d}{\delta_c}$ steps for every $b \in [0, B^*]$ a ϕ -approximation with probability $\Omega(1)$.

[V. Roostapour, A. Neumann, F. Neumann, T. Friedrich, AAAI'19]

Experiments

We consider the influence maximization problem in social networks. [Zhang & Vorobeychik, AAAI'16]

Two types of constraints:

- Routing constraint on routing cost for selected users
- Cardinality constraint on number of selected users



For both problems, we vary the constraint bound B over time.

• POMC has $\tau = 1000, 5000, 10000$ iterations after every change to recompute good solution.

Experimental results

Dynamic routing constraints

				ĭ							
1	Changes	GGA		AGGA		POM	$1C_{1000}$	POM	$1C_{5000}$	POMC10000	
		mean	st	mean	st	mean	st	mean	st	mean	st
	1-25	85.0349	12.88	81.5734	14.07	66.3992	17.95	77.8569	18.76	86.1057	17.22
	26-50	100.7344	22.16	96.1386	23.99	104.9102	15.50	117.6439	16.71	122.5604	15.54
	51-75	118.1568	30.82	110.4893	29.50	141.8249	5.64	155.2126	5.08	158.7228	5.20
	76-100	127.3422	31.14	115.2978	27.66	149.0259	3.36	159.9100	3.28	162.7353	3.65
	101-125	132.3502	29.62	116.9768	25.45	150.3415	3.17	160.1367	2.81	161.2852	2.68
	126-150	134.5256	27.69	118.6962	24.19	147.8998	7.36	154.7319	8.77	154.1470	7.43
	151-175	135.7651	25.89	119.4982	22.85	147.2478	4.68	153.1417	5.32	151.2966	3.17
	176-200	135.5133	24.41	119.1491	22.04	139.5072	8.08	143.6928	9.16	143.9832	8.67
<u>۱</u>											

Dynamic cardinality constraints

Changes	GGA	4	AGGA		POM	IC1000	POM	IC ₅₀₀₀	POMC10000		
	mean	st	mean	st	mean	st	mean	st	mean	st	
1-25	130.9410	14.71	130.6550	14.36	84.8898	24.32	114.8272	23.09	121.1330	19.72	
26-50	145.6766	20.70	145.0774	20.11	133.2130	14.69	155.4231	13.98	158.0245	14.34	
51-75	160.2780	26.86	159.6331	26.50	164.9157	3.84	184.3274	3.45	187.1952	3.68	
76-100	167.9512	26.84	167.3365	26.60	171.5600	1.89	189.4834	2.74	189.6107	2.78	
101-125	172.1483	25.45	171.6884	25.35	174.3528	2.11	188.2120	2.32	188.7572	2.46	
126-150	174.0582	23.77	173.6528	23.72	174.0404	5.88	183.0188	6.65	183.8033	6.47	
151-175	175.1998	22.23	174.8330	22.21	174.5846	4.03	181.3669	4.01	188.4192	3.60	
176-200	175.1023	20.94	174.7836	20.92	168.8791	8.05	173.8794	7.28	175.2773	7.23	

Summary

- Dynamic problems play a key role in the area of optimization.
- We have shown that an adaptive version of the generalized greedy algorithm only achieves arbitrary bad performance for simple submodular problems.
- The POMC Pareto optimization approach caters for dynamic changes by having for each possible budget b ≤ B a good approximation.
- POMC can recompute good approximations for all new possible budgets in the case of budget b ∈ [B, B*] increase from B to B* efficiently.
- Experiments on influence maximization in social networks show the advantage of POMC over greedy approaches.

Problems with Chance Constraints

[B. Doer, C. Doerr, A. Neumann, F. Neumann, A. M. Sutton: Optimization of Chance-Constrained Submodular Functions, AAAI'20]

Chance Constraints - Motivation

- Often problems involve stochastic components and constraints that can only be violated with a small probability.
- We investigate submodular problems with chance constraints and show that the adaptation of simple greedy algorithms asymptotically only looses a factor of 1-o(1) in terms of the worst case approximation obtained.

Chance Constraints

Let S be a potential solution to a given submodular problem, W(S) be its random weight and B be a given weight bound. We consider chance constraints of the form:

 $\Pr[W(S) > B] \le \alpha.$ small, e.g. 0.001

Weight bound can only be violated with a small probability.

Setting for Random Weights

- We consider two settings for random weights of a given set of items.
- Both settings assume that the weights of the items are chosen independent of each other.

Uniform independent and identically distributed (IID) weights:

$$W(s) \in [a - \delta, a + \delta] \ (\delta \leq a)$$

Uniform Weights with same dispersion

 $W(s) \in [a(s) - \delta, a(s) + \delta]$

Greedy Algorithms



Chance Constraints

- One of the difficulties lies in evaluating whether a given solution fulfills the chance constraint.
- Use surrogate functions such as Chernoff bounds and Chebyshev's inequality to determine whether a solution is feasible. [Chebyshev, MPA'67; Chernoff, AMS'52]
- These bounds don't allow for a precise calculation for the probability of a constraint violation.
- However, the give an upper bound and a solution is accepted if its upper bound is at most α .
- For our settings, we establish conditions based on the difference in expected weight and constraint B that show when a given solution is feasible.

Chance Constraint Conditions

Chernoff:

Lemma 1. Let $W(s) \in [a(s) - \delta, a(s) + \delta]$ be independently chosen uniformly at random. If

$$(B - E[W(X)]) \ge \sqrt{3\delta k \ln(1/\alpha)},$$

where
$$k = |X|$$
, then $\Pr[W(X) > B] \le \alpha$.

Chebyshev:

Lemma 2. Let X be a solution with expected weight E[W(X)] and variance Var[W(X)]. If

$$B - E[W(X)] \ge \sqrt{\frac{(1 - \alpha) \operatorname{Var}[W(X)]}{\alpha}}$$

then $\Pr[W(X) > B] \le \alpha$.

Uniform IID Weights

Algorithm 1: Greedy Algorithm (GA)

 $\begin{array}{l} \text{input: Set of elements } V, \text{ budget constraint } B, \text{ failure} \\ & \text{probability } \alpha. \\ 1 \quad S \leftarrow \emptyset; \\ 2 \quad V' \leftarrow V; \\ 3 \quad \text{repeat} \\ 4 \quad \left| \begin{array}{c} v^* \leftarrow \arg \max_{v \in V'} (f(S \cup \{v\}) - f(S)); \\ \text{if } \Pr[W(S \cup \{v^*\}) > B] \leq \alpha \text{ faen} \\ 6 \\ 6 \\ 1 \\ S \leftarrow S \cup \{v^*\}; \\ 7 \\ V' \leftarrow V' \setminus \{v^*\}; \\ 8 \quad \text{until } V' \leftarrow \emptyset; \\ 9 \quad \text{return } S; \end{array} \right|$

Theorem: If $B = \omega(1)$ then GA gives a (1-o(1))(1-1/e)- approximation for each monotone submodular function when using Chernoff or Chebyshev for the chance constraint evaluation.

Experiments

We consider the influence maximization problem in social

networks. [Zhang & Vorobeychik, AAA'16; Leskovec et al., SIGKDD'07; Kempe et al., SIGKDD'03; Kempe et al., TC'15]

- Given a graph G = (V,E) where nodes are users and and edge (u,v) have probability weights which determines how likely user u influences user v.
- Expected influence score is computed by propagation from the set of selected users. This is done through a simulation.
- In addition there is a constraint on the cost of selecting users.
- Goal: select a set of users that maximizes influence under the given constraint.
- Chance constraint settings: expected weights of 1 for IID case.

Experimental Results - Cost values





Experimental Results – Function values



Figure 1: Function value for budgets B = 20, 50, 100, 150 (from left to right) using Chebyshev's inequality (top) and Chernoff bound (bottom) for $\alpha = 0.1, 0.01, 0.001, 0.0001$ with all the expected weights 1.

Uniform Weights with same dispersion

Generalized Greedy Algorithm



Theorem: If $B = \omega(1)$ then GGA gives a (1/2-o(1))(1-1/e)approximation for each monotone submodular function when using Chernoff or Chebyshev for the chance constraint evaluation.

Experimental Results – Function values



Figure 3: Function values for budgets B = 100 (left) and B = 500 (right) using Chebyshev's inequality and Chernoff bound for $\alpha = 0.1, 0.01, 0.001, 0.0001$ with degree dependent random weights.

Expected weight 1+degree(v) for uniform with same dispersion case.



Figure 4: Maximal cost values for budget B = 100 (left) and B = 500 using Chebyshev's inequality (top) and Chernoff bound (bottom) for $\alpha = 0.1, 0.01, 0.001, 0.0001$ with degree dependent random weights.

Summary

- Optimization problems often involve stochastic components that effect the constraints of the problem.
- We presented a (first) study on submodular functions with chance constraints.
- We showed that simple greedy algorithms popular for dealing with monotone submodular functions can be easily adapted to the chance constrained case.
- In terms of approximation, we asymptotically only loose a factor of 1-o(1).
- Experimental results show the change in solution quality dependent on the uncertainty of the weights and the chance constraint violation probability.

Problems with Chance Constraints: Evolutionary Multi-Objective Algorithms

[A. Neumann and F. Neumann: Optimising Monotone Chance-Constrained Submodular Functions Using Evolutionary Multi-Objective Algorithms, PPSN'20]

Problem Definition

 We consider the performance of the Global Simple Evolutionary Multi-Objective Optimizer (GSEMO) and Nondominated Sorting Genetic Algorithm (NSGA-II) for the optimisation of chance constrained submodular functions.

[Doerr, B., Doerr, C., Neumann, A., Neumann, F., Sutton, A. M., AAAI'20; Xie, Neumann, A., Neumann, F., GECCO'20; Xie et al., GECCO 2019; Assimi et al., ECAI'20]

Use and evaluate Pr using Chernoff bounds or Chebyshev's inequality.

 $\Pr(W(X) > B) \le \hat{\Pr}(W(X) > B)$

• Uniform IID weights:

 $W(s) \in [a - \delta, a + \delta] \ (\delta \leq a).$

• Uniform weights with same dispersion:

$$W(s) \in [a(s) - \delta, a(s) + \delta].$$

Algorithm

Global Simple Evolutionary Multi-Objective Optimizer [Giel & Wegener, STACS'03]

Al	Algorithm 1: Global SEMO									
1 C	1 Choose $x \in \{0, 1\}^n$ uniformly at random;									
2 P	2 $P \leftarrow \{x\};$									
3 r	3 repeat									
4	Choose $x \in P$ uniformly at random;									
5	Create y by flipping each bit x_i of x with probability $\frac{1}{n}$;									
6	if $\not\exists w \in P : w \succ y$ then									
7	$\ \ S \leftarrow (P \cup \{y\}) \backslash \{z \in P \mid y \succcurlyeq z\};$									
8 u	8 until stop;									

Multi-Objective Formulation

[Motwani & Raghavan,'95; Doerr & Neumann, NCS '20; Xie, Harper, Assimi, Neumann, A., Neumann, F., GECCO'19]

Uniform IID Weights:

$$g(X) = (g_1(X), g_2(X))$$

 $g_1(X) = \begin{cases} E_W(X) - C & \text{if} \quad (C - E_W(X))/(\delta \cdot |X|) \ge 1\\ \hat{P}r(W(X) > C) & \text{if} \quad (E_W(X) < C) \land (C - E_W(X))/(\delta |X| < 1)\\ 1 + (E_W(X) - C) & \text{if} \quad E_W(X) \ge C \end{cases}$

$$g_2(X) = \begin{cases} f(X) \text{ if } g_1(X) \le \alpha \\ -1 \quad \text{if } \hat{Pr}(W(X) > C) > \alpha \end{cases}$$

Uniform Weights with the Same Dispersion:

 $\hat{g}(X) = (\hat{g}_1(X), g_2(X))$

$$\hat{g}_1(X) = E_W(X)$$

Theoretical Results

Uniform IID Weights:

Theorem: Let $k = \min\{n + 1, \lfloor C/a \rfloor\}$ and assume $\lfloor C/a \rfloor = \omega(1)$. Then the expected time until GSEMO has computed a (1-o(1))(1-1/e)-approximation for a given monotone submodular function under a chance constraint with uniform iid weights is O(nk(k + log n)).

Uniform Weights with the Same Dispersion:

Theorem: If $C/a_{max} = \omega(1)$ then GSEMO obtains a (1/2 - o(1))(1 - 1/e)-approximation for a given monotone submodular function under a chance constraint with uniform weights having the same dispersion in expected time $O(P_{max} \cdot n(C/a_{min} + \log n + \log(a_{max}/a_{min})))$.

[A. Neumann and F. Neumann, PPSN'20]

Experimental Results

C	α	δ	GA (1)	1) GSEMO (2)					NSGA-II (3)				
		-		mean	min	max	\mathbf{std}	stat	mean	min	max	\mathbf{std}	stat
20	0.1	0.5	51.51	55.75	54.44	56.85	0.5571	1 ⁽⁺)	55.66	54.06	56.47	0.5661	1 ⁽⁺⁾
20	0.1	1.0	46.80	50.65	49.53	51.68	0.5704	1(+)	50.54	49.61	52.01	0.6494	1(+)
50	0.1	0.5	90.55	94.54	93.41	95.61	0.5390	$1^{(+)},3^{(+)}$	92.90	90.75	94.82	1.0445	$1^{(+)}, 2^{(-)}$
30	0.1	1.0	85.71	88.63	86.66	90.68	0.9010	1 ⁽⁺⁾ , 3 ⁽⁺⁾	86.89	85.79	88.83	0.8479	$1^{(+)},2^{(-)}$
100	0.1	0.5	144.16	147.28	145.94	149.33	0.8830	$1^{(+)},3^{(+)}$	144.17	142.37	146.18	0.9902	2(-)
100	0.1	1.0	135.61	140.02	138.65	142.52	0.7362	1 ⁽⁺⁾ , 3 ⁽⁺⁾	136.58	134.80	138.21	0.9813	2(-)
20	0.001	0.5	48.19	50.64	49.10	51.74	0.6765	1(+)	50.33	49.16	51.25	0.5762	1(+)
20	0.001	1.0	39.50	44.53	43.63	45.55	0.4687	1(+)	44.06	42.18	45.39	0.7846	1(+)
50	0.001	0.5	75.71	80.65	78.92	82.19	0.7731	1(+)	80.58	79.29	81.63	0.6167	1(+)
30	0.001	1.0	64.49	69.79	68.89	71.74	0.6063	1(+)	69.96	68.90	71.05	0.6192	1(+)
100	0.001	0.5	116.05	130.19	128.59	131.51	0.7389	$1^{(+)},3^{(+)}$	127.50	125.38	129.74	0.9257	$1^{(+)},2^{(-)}$
100	0.001	1.0	96.18	108.95	107.26	109.93	0.6466	$1^{(+)},3^{(+)}$	107.91	106.67	110.17	0.7928	$1^{(+)},2^{(-)}$

Results for Influence Maximization with uniform chance constraints. [Kempe et al., SIGKDD '03]

Experimental Results

Results for Maximum Coverage with uniform chance constraints. [Feige, ACM'98, Khuller et al., IPL'99]

C	α	δ GA (1)			δ GA (1) GSEMO (2)				NSGA-II (3)				
Ū				mean	min	max	\mathbf{std}	stat	mean	min	max	\mathbf{std}	stat
10	0.1	0.5	448.00	458.80	451.00	461.00	3.3156	1 ⁽⁺⁾	457.97	449.00	461.00	4.1480	1 ⁽⁺⁾
10	0.1	1.0	376.00	383.33	379.00	384.00	1.7555	1(+)	382.90	379.00	384.00	2.0060	1(+)
15	0.1	0.5	559.00	559.33	555.00	562.00	2.0057	3(+)	557.23	551.00	561.00	2.4309	$1^{(-)}, 2^{(-)}$
15	0.1	1.0	503.00	507.80	503.00	509.00	1.1567	1(+)	507.23	502.00	509.00	1.8323	1(+)
	0.1	0.5	587.00	587.20	585.00	589.00	1.2149	3(+)	583.90	580.00	588.00	1.9360	$1^{(-)}, 2^{(-)}$
20	0.1	1.0	569.00	569.13	566.00	572.00	1.4559	3(+)	565.30	560.00	569.00	2.1520	$1^{(-)}, 2^{(-)}$
10	0.001	0.5	413.00	423.67	418.00	425.00	1.8815	1(+)	422.27	416.00	425.00	2.6121	1 ⁽⁺⁾
10	0.001	1.0	376.00	383.70	3 79.00	384.00	1.1492	1(+)	381.73	377.00	384.00	2.6514	1(+)
15	0.001	0.5	526.00	527.97	525.00	532.00	2.1573	1(+)	527.30	520.00	532.00	2.7436	
15	0.001	1.0	448.00	458.87	453.00	461.00	2.9564	1(+)	457.10	449.00	461.00	4.1469	1 ⁽⁺⁾
	0.001	0.5	568.00	568.87	565.00	572.00	1.5025	3(+)	564.60	560.00	570.00	2.7618	$1^{(-)}, 2^{(-)}$
20	0.001	1.0	526.00	528.03	525.00	530.00	1.8843	1(+)	527.07	522.00	530.00	2.2427	

Summary

- We presented a first runtime analysis of evolutionary algorithms for the optimisation of submodular functions with chance constraints.
- We showed that GSEMO using a multi-objective formulation of the problem based on tail inequalities is able to achieve the same approximation guarantee as recently studied greedy approaches.
- Experimental results show that GSEMO computes significantly better solutions than the greedy approach and often outperforms NSGA-II.

Summary

- Many real-world optimisation problems can be formulated in terms of optimising a submodular function under a given set of constraints.
- A wide range of state-of-the-art results for submodular problems have been obtained through evolutionary computing techniques.
- Bi-objective formulations of constrained submodular optimisation problems in terms of Pareto optimisation enable evolutionary algorithms to achieve
 - best theoretical performance guarantees and
 - state-of-the-art practical results

for a wide range of submodular optimisation problems.

• These approaches are also able to deal with dynamic and stochastic constraints in a very efficient way.

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