

Advanced Topics in Data Sciences

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Lecture 2: Submodular Optimization

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Outline

▶ This lecture

1. Submodular Function Maximization
2. Performance of the Greedy Algorithm
3. Submodular Function Minimization
4. Lovász extension
5. Integer programming

Recommended Reading

- ▶ *Submodular function maximization*, Krause and Golovin, 2012
- ▶ *An analysis of approximations for maximizing submodular set functions*, Nemhauser, 1978
- ▶ *Submodular functions and convexity*, Lovász, 1983
- ▶ *Learning with submodular functions: A convex optimization perspective*, Francis Bach, 2013 (Sections 3 & 10).

- ▶ *Lecture 3: Convex analysis and complexity*, Mathematics of Data: From Theory to Computation, 2015.

Submodular optimization

Recall the definition of submodular functions:

Definition (Submodularity)

A function $f : 2^V \rightarrow \mathbb{R}$ is said to be:

- ▶ *submodular* if, for all $S \subseteq T \subseteq V$ and $e \in V \setminus T$, it holds $\Delta(e|S) \geq \Delta(e|T)$;
- ▶ *modular* if it always holds that $\Delta(e|S) = \Delta(e|T)$;

where

$$\Delta(e|S) = f(S \cup \{e\}) - f(S)$$

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Several problems in theoretical computer science, game theory, machine learning and learning-based CS (c.f., lecture 1) can be cast as a submodular optimization problem.

Problem (Submodular Optimization)

Given a submodular function $f : 2^V \rightarrow \mathbb{R}$,

$$\min_{S \in I} f(S) \quad (\text{SFMin}) \qquad \max_{S \in I} f(S) \quad (\text{SFMax})$$

Submodular optimization

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Given a submodular function $f : 2^V \rightarrow \mathbb{R}$,

$$\min_{S \in I} f(S)$$

(SFMin)

$$\max_{S \in I} f(S)$$

(SFMax)

In this lecture:

- ▶ For $I = 2^V$ (unconstrained), SFMin can be solved in polynomial time, while SFMax is NP-Hard¹.
- ▶ For $I = \{S : |S| \leq k\}$, and f *monotone*, SFMax admits a $(1 - \frac{1}{e})$ -approximation.
- ▶ For $I = 2^V$ or $I = \{S : |S| \leq k\}$, and f *modular*, SFMax/SFMin is easy to solve.
- ▶ For I defined by *totally unimodular* linear constraints, and f *modular*, SFMax/SFMin, which in this case is an integer program (IP), can be solved by linear programming (LP).

¹cannot be solved in polynomial time unless $P = NP$.

Unconstrained submodular maximization is NP hard

Given a graph $G(V, E)$, for any $S \subseteq V$, the *graph cut* function $f(S) = |\delta(S)|$ denotes the number of edges “cut” in the graph.

$$|\delta(S)| = |\{(u, v) \in E : u \in S, v \in V \setminus S\}|$$

Problem (Max cut)

Find $S \subseteq V$ such that the number of edges between S and the complementary subset is as large as possible.

$$\max_{S \subseteq V} |\delta(S)|$$

- ▶ Max Cut problem is *NP-Hard*.
- ▶ Graph cut function is *submodular*.
- ▶ Hence, SFMax is *NP-Hard*.

Unconstrained SFMax admits a *1/2-approximation* algorithm [2] which is *tight*; a $(1/2 + \epsilon)$ -approximation requires exponentially many oracle calls [5].

Modular function maximization

While *submodular* maximization is hard, *modular* maximization is extremely easy.

Unconstrained modular maximization

Given constants $c_1, \dots, c_n \in \mathbb{R}$,

$$\max_{S \subseteq V} f(S) := \sum_{i \in S} c_i$$

Optimal set S^* contains the indices i for which $c_i > 0$. This has complexity $O(n)$.

Cardinality Constrained modular maximization

$$\max_{|S| \leq k} \sum_{i \in S} c_i.$$

Optimal set S^* contains the indices i , among the k largest values of c_i , for which $c_i > 0$. This can be done by sorting, in $O(n \log n)$, or by Quickselect randomized algorithm in $\Theta(n)$ expected time [4].

Submodular maximization in Learning-based CS

LB-CS: Problem statement

Given a set of m *training signals* $\mathbf{x}_1, \dots, \mathbf{x}_m \in \mathbb{C}^p$, find an index set Ω of a given cardinality n such that a related *test signal* \mathbf{x} can reliably be recovered given the subsampled measurement vector $\mathbf{b} = \mathbf{P}_\Omega \Psi \mathbf{x}$.

Average energy criterion

$$\hat{\Omega} = \arg \max_{\Omega: |\Omega|=n} \frac{1}{m} \sum_{j=1}^m \sum_{i \in \Omega} |\langle \psi_i, \mathbf{x}_j \rangle|^2$$

This is a cardinality constrained modular maximization problem.

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This is a cardinality constrained modular maximization problem.

What about generalized case?

Generalized average energy criterion

$$\hat{\Omega} = \arg \max_{\Omega: |\Omega|=n} \frac{1}{m} \sum_{j=1}^m g \left(\sum_{i \in \Omega} |\langle \psi_i, \mathbf{x}_j \rangle|^2 \right).$$

where $g: \mathbb{R} \rightarrow \mathbb{R}$ be an increasing concave function with $g(0) = 0$. This is a cardinality constrained monotone submodular maximization problem.

Cardinality constrained submodular maximization

Cardinality constrained monotone submodular function maximization is also NP-hard.

$$S^* \in \arg \max_{|S| \leq k} f(S)$$

Greedy algorithm [9]

1. Initialize $S_0 = \emptyset$
2. For $i = 1, \dots, k$
 - ▶ Find $e_i = \arg \max_{e \in V \setminus S_{i-1}} \Delta(e|S_{i-1})$
 - ▶ Set $S_i = S_{i-1} \cup \{e_i\}$
3. Return S_k

Theorem (Approximation achieved by greedy algorithm [9])

For any monotone submodular function with $f(\emptyset) = 0$, after ℓ iterations of the greedy algorithm, it holds that

$$f(S_\ell) \geq (1 - e^{-\ell/k})f(S^*)$$

After k iterations, the greedy algorithm achieves a $(1 - 1/e)$ -*approximation*, which is *tight*; no algorithm requiring a *polynomial* number of oracle calls has a better performance [10].

Proof of greedy algorithm performance

We can assume w.l.o.g that $|S^*| = k$, since by monotonicity of f adding elements can only increase the function value. Let $S^* = \{e_1^*, e_2^*, \dots, e_k^*\}$, then for all $i < \ell$,

$$\begin{aligned} f(S^*) &\leq f(S^* \cup S_i) && \text{by monotonicity} \\ &= f(S_i) + \sum_{j=1}^k \Delta(e_j^* | S_i \cup \{e_1^*, e_2^*, \dots, e_{j-1}^*\}) && \text{by telescoping sums} \\ &\leq f(S_i) + \sum_{j=1}^k \Delta(e_j^* | S_i) && \text{by submodularity} \\ &\leq f(S_i) + \sum_{j=1}^k \Delta(e_i | S_i) && \text{by definition of the greedy updates} \\ &\leq f(S_i) + k(f(S_{i+1}) - f(S_i)) && |S^*| = k \end{aligned}$$

Proof of greedy algorithm performance

Let $\Delta f_i := f(S^*) - f(S_i)$. Then, $\Delta f_{i+1} \leq \left(1 - \frac{1}{k}\right) \Delta f_i, \forall i < \ell$.

$$\begin{aligned} f(S^*) - f(S_\ell) &\leq \left(1 - \frac{1}{k}\right)^\ell f(S^*) && (f(\emptyset) = 0) \\ &\leq e^{-\ell/k} f(S^*) && (1 - x \leq e^{-x}, \forall x \in \mathbb{R}) \end{aligned}$$

Rearranging terms yields $f(S_\ell) \geq (1 - e^{-\ell/k})f(S^*)$. □

- ▶ When $\ell = k$, the above approximation factor becomes $1 - 1/e \approx 0.63$
- ▶ Running the greedy algorithm for more than k iterations leads to a better approximation factor, but still with respect to the k -optimal solution. E.g., for $\ell = 5k$, $f(S_{5k}) \geq 0.9933 \max_{|S| \leq k} f(S)$

A related constrained submodular maximization problem

Two related questions:

- ▶ Given a fixed $k \in \mathbb{Z}$, if we choose k items greedily, how far away is $f(S_k)$ from the optimal function value $f(S_k^*)$ for sets of size k ?
- ▶ Given a fixed $z \in \mathbb{Z}$, $z \leq f(V)$, if we now run the greedy algorithm until we reach $f(S_\ell) \geq z$, how wasteful is the size of S_ℓ , compared to the minimum sized set achieving $f(S) \geq z$.

$$k^* = \min_{S \subseteq V} \{|S| : f(S) \geq z\} \quad (\text{Minimum submodular set cover})$$

Theorem ([15])

Given a normalized ($f(\emptyset) = 0$) monotone submodular integer-valued function f and a fixed $z \in \mathbb{Z}$, $z \leq f(V)$. Let ℓ be smallest integer such that $f(S_\ell) \geq z$. Then

$$\ell \leq \left(1 + \ln \max_{v \in V} f(\{v\})\right) k^*$$

Unconstrained submodular minimization

We abuse notation by treating any set function $f : 2^V \rightarrow \mathbb{R}$ as a function over $\{0, 1\}^n$ too, where $f(\mathbb{1}_S) = f(S)$. SFMin can then be equivalently written as:

$$\min_{s \in \{0, 1\}^n} f(s)$$

Relax and round approach:

- ▶ Relax integer constraints $\{0, 1\}^n$ to $[0, 1]^n$.
- ▶ Relax discrete objective f defined over $\{0, 1\}^n$ to a continuous *extension* f' defined over $[0, 1]^n$; i.e., $f'(s) = f(s), \forall s \in \{0, 1\}^n$.
- ▶ Choose a continuous function that can be minimized efficiently and is close to the original function f .

Definition (Convex closure)

Given any set function $f : \{0, 1\}^n \rightarrow \mathbb{R}$, we define $\forall x \in [0, 1]^n$ the convex closure of f as:

$$f^-(x) = \min_{\alpha \in [0, 1]^{2^n}} \left\{ \sum_{S \subseteq V} \alpha_S f(S) : x = \sum_{S \subseteq V} \alpha_S \mathbb{1}_S, \sum_{S \subseteq V} \alpha_S = 1, \alpha_S \geq 0 \right\}$$

Lovász extension

The convex closure $f^-(x) = f_L(x)$ where f_L is the Lovász extension of f iff f is a *submodular* function [14].

Definition (Lovász extension [7])

Given a normalized ($f(\emptyset) = 0$) set function $f : \{0, 1\}^n \rightarrow \mathbb{R}$, its Lovász extension $f_L : [0, 1]^n \rightarrow \mathbb{R}$ is defined $\forall s \in [0, 1]^n$ as follows:

$$f_L(s) = \sum_{k=1}^n s_{j_k} \left(f(\{j_1, \dots, j_k\}) - f(\{j_1, \dots, j_{k-1}\}) \right)$$

where $s_{j_1} \geq s_{j_2} \geq \dots \geq s_{j_n}$.

Observations:

1. f_L is an *extension* of f since $f_L(s) = f(s), \forall s \in \{0, 1\}^n$.
2. f_L can be computed efficiently in $O(n \log n)$.
3. For a fixed ordering of s , f_L is a *linear* function.
4. For modular functions, f_L is a *linear* function.
5. f_L is *positively homogenous*, i.e., $f_L(\alpha s) = \alpha f_L(s), \forall \alpha > 0$.
6. Let $h = f + g$, then $h_L = f_L + g_L$.
7. f_L is a *non-decreasing* function if f is monotone.
8. The Lovász extension has several equivalent definitions (c.f., [1]).

Lovász extension

Theorem ([7])

Given a set function f and its Lovász extension f_L , f_L is convex iff f is submodular.

Proof:

- ▶ If f is submodular, $f_L = f^-$ is convex.
- ▶ If f_L is convex, then:
 - ▶ The vector $\mathbb{1}_{A \cup B} + \mathbb{1}_{A \cap B} = \mathbb{1}_A + \mathbb{1}_B$ have entries equal to 2 on $A \cap B$, 1 on $A \Delta B = A \setminus B \cup B \setminus A$, and 0 outside of $A \cup B$.
 - ▶ By definition of LE:

$$\begin{aligned} f_L(\mathbb{1}_{A \cup B} + \mathbb{1}_{A \cap B}) &= 2(f(A \cap B) - f(\emptyset)) + 1(f(A \Delta B \cup A \cap B) - f(A \cap B)) \\ &= f(A \cap B) + f(A \cup B) \end{aligned}$$

- ▶ $f_L(\mathbb{1}_A) = f(A)$ and $f_L(\mathbb{1}_B) = f(B)$.
- ▶ $f_L(\mathbb{1}_{A \cup B} + \mathbb{1}_{A \cap B}) = f_L(\mathbb{1}_A + \mathbb{1}_B) \leq f_L(\mathbb{1}_A) + f_L(\mathbb{1}_B)$.
- ▶ It follows that $f(A \cap B) + f(A \cup B) \leq f(A) + f(B)$.

Examples of Lovász extensions

1. Let $f(S) = |S|$. f is a modular function. $f_L(s) = \mathbf{1}^T s$.
2. Let $f(S) = \mathbf{1}_{G \cap S \neq \emptyset}(S)$. f is a submodular function.

$$f_L(s) = s_{j_1} \mathbf{1}_{j_1 \in G} + s_{j_2} \mathbf{1}_{j_2 \in G, j_1 \notin G} + \cdots + s_{j_n} \mathbf{1}_{j_n \in G, V \setminus j_n \notin G} = \max_{k \in G} s_k,$$

where $s_{j_1} \geq s_{j_2} \geq \cdots \geq s_{j_n}$.

3. $f(S) = \sum_{G \in \mathfrak{G}} d_G \mathbf{1}_{G \cap S \neq \emptyset}(S)$, where $d_G > 0$. f is a submodular function.

$$f_L(s) = \sum_{G \in \mathfrak{G}} d_G \max_{k \in G} s_k.$$

Submodular functions can be minimized in polynomial time

Theorem (SFMin is equivalent to a convex problem)

Given a normalized submodular function f and its Lovász extension f_L ,

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

where any minimizer s^* of the LHS is a minimizer of the RHS, and any minimizer x^* of the RHS, has all its thresholded sets $\{x^* \geq \theta\}, \forall \theta \in (0, 1)$ as minimizers of the LHS.

Proof:

- ▶ Since $\{0, 1\}^n \subseteq [0, 1]^n$, then $f(s^*) \geq f_L(x^*)$.
- ▶ We use an equivalent definition of the Lovász extension [1]:

$$\begin{aligned} f_L(x^*) &= \sum_{k=1}^{n-1} (x_{j_k}^* - x_{j_{k+1}}^*) f(\{j_1, \dots, j_k\}) + x_{j_n}^* f(V) \\ &\geq \sum_{k=1}^{n-1} (x_{j_k}^* - x_{j_{k+1}}^*) f(s^*) + x_{j_n}^* f(s^*) && (x_{j_k} - x_{j_{k+1}} \geq 0) \\ &\geq x_{j_1} f(s^*) \\ &\geq f(s^*) && (\text{since } f(s^*) \leq f(\emptyset) = 0 \text{ and } x_{j_1} \leq 1) \end{aligned}$$

where $x_{j_1}^* \geq \dots \geq x_{j_n}^*$.

For the proof of the second claim, c.f., [1].

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The convex problem $\min_{x \in [0,1]^n} f_L(x)$ can be solved for e.g., by the following algorithms:

- ▶ Minimum norm point algorithm [3], $O((n^3 EO + n^3 \log n + n^4)F^2)$
- ▶ Frank Wolfe algorithm [1], $O((n^3 EO + n^3 \log n)F^2)$
- ▶ Combinatorial algorithms, e.g., [11], $O(n^5 EO + n^6)$
- ▶ Cutting plane method [6], $O(n^2 \log nF \cdot EO + n^3 \log^{O(1)} nF)$ and $O(n^3 \log^2 n \cdot EO + n^4 \log^{O(1)} n)$

where $F := \max_i \{ |f(\{i\})|, |f(V) - f(V \setminus i)| \}$ and EO is the running time of the evaluation oracle.

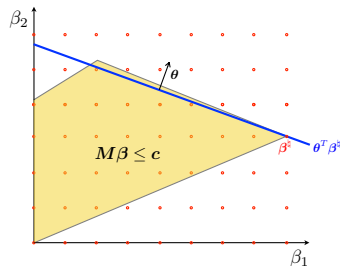
Integer linear programming

Integer linear program

Many important discrete optimization problems can be formulated as an integer linear program

$$\beta^{\text{opt}} \in \arg \max_{\beta \in \mathbb{Z}^m} \{\theta^T \beta : M\beta \leq c\} \quad (\text{IP})$$

NP-Hard (in general)



Convex Polyhedra

$$\mathcal{P} = \{\beta \mid M\beta \leq c\}$$

$$(\beta \in \mathbb{R}^m, c \in \mathbb{R}^m)$$

Polytope: A bounded polyhedron

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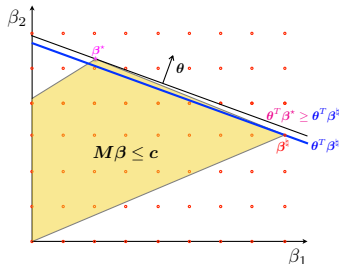
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Relaxation: Linear program

$$\beta^* \in \arg \max_{\beta \in \mathbb{R}^m} \{ \theta^T \beta : M\beta \leq c \} \quad (\text{LP})$$

Obtains an upperbound



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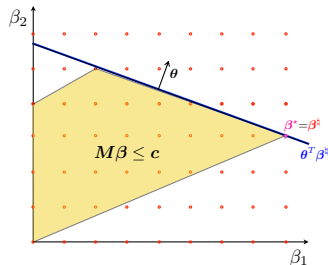
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Observation:

When every vertex of \mathcal{P} is integral,
LP has integer optimal solutions.

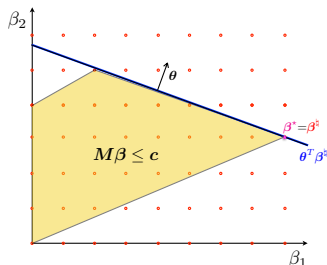
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Relaxation: Linear program

$$\beta^* \in \arg \max_{\beta \in \mathbb{R}^m} \{\theta^T \beta : M\beta \leq c\} \quad (\text{LP})$$

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$$\mathcal{P} = \{\beta \mid M\beta \leq c\}$$

Observation:

When every vertex of \mathcal{P} is integral,
LP has integer optimal solutions.

- ▶ Interior point method performs $\mathcal{O}\left(\sqrt{l} \log \frac{l}{\epsilon}\right)$ iterations ($l > m$) with up to $\mathcal{O}(m^2 l)$ operations, where ϵ is the absolute solution accuracy, and l is the number of constraints.

A sufficient condition: Total unimodularity

Definition (Total unimodularity)

A matrix $M \in \mathbb{R}^{l \times m}$ is totally unimodular (TU) iff the determinant of every square submatrix of M is 0, or ± 1 .

- ▶ Note that the entries of M are necessarily 0, ± 1 .
- ▶ Verifying if a matrix is TU can be done in polynomial time [13].

Theorem (TU Polyhedron is integral)

The polyhedron $\mathcal{P} = \{M\beta \leq c\}$ has *integer* vertices when M is TU and c is an integer vector.

Proof:

- ▶ Every vertex z is determined by a subsystem $M'z = c'$ where M' is matrix of full row rank.
- ▶ We can write $M' = [U, V]$ (up to some permutation of the coordinates), where $\det U = \pm 1$.
- ▶ z is then given by $z = \begin{bmatrix} U^{-1}c' \\ 0 \end{bmatrix}$
- ▶ Cramer's rule: $U^{-1} = \frac{\text{Adj}U}{\det U}$ where $\text{Adj}U$ is the adjugate matrix of U .

A sufficient condition: Total unimodularity

Definition (Equivalent definition of TU [12, 8])

A matrix M is TU iff for every subset J of its columns, there exists a partition J_1, J_2 of J such that

$$\left| \sum_{j \in J_1} M_{ij} - \sum_{j \in J_2} M_{ij} \right| \leq 1, \forall i = 1, \dots, l$$

Operations that preserve TU [8]: If M is TU then,

1. The transpose of M is TU.
2. (M, I) is TU.
3. Matrix after deleting a row (column) with at most one non-zero entry from M is TU.
4. Matrix after interchanging two rows (columns) in M is TU.
5. Matrix after multiplying a row (column) from M by (-1) is TU.
6. Matrix after duplicating rows (columns) of M is TU.
7. Matrix after applying a pivot operation on M is TU.

Examples of TU matrices

1. Given a directed graph, let T be its edge-node incidence matrix, i.e., $T_{\ell i} = 1$ and $T_{\ell j} = -1$ iff $e_{\ell} = (i, j)$ is an edge in the graph. Then, T is TU.
2. Given an undirected bipartite graph, let E be its edge-node incidence matrix, i.e., $T_{\ell i} = 1$ and $T_{\ell j} = 1$ iff $e_{\ell} = (i, j)$ is an edge in the graph. Then, E is TU.
3. Given an acyclic bipartite graph $G(U, V, E)$, where the degree of any node in U is at most 2. Let B be its biadjacency matrix, i.e., $B_{ij} = 1$ iff $i \in U, j \in V$ and $(i, j) \in E$. Then, B is TU.

Example of an integer program with TU constraints

Problem (k-sparse projection)

Recall $\|x\|_0 = |\text{supp}(x)|$ where $\text{supp}(x) = \{i : x_i \neq 0\}$. The projection of a vector $y \in \mathbb{R}^n$ over the set of k -sparse vectors is given by:

$$\min_{x \in \mathbb{R}^n} \{\|x - y\|_2^2 : \|x\|_0 \leq k\}$$

$$\begin{aligned} \min_{x \in \mathbb{R}^n} \{\|x - y\|_2^2 : \|x\|_0 \leq k\} &= \min_{|S| \leq k} \min_{x \in \mathbb{R}^n} \{\|x - y\|_2^2 : \text{supp}(x) = S\} \\ &= \min_{|S| \leq k} \min_{x \in \mathbb{R}^n} \left\{ \sum_{i \in S} (x_i - y_i)^2 + \sum_{i \notin S} y_i^2 : \text{supp}(x) = S \right\} \\ &= \min_{|S| \leq k} \left\{ \sum_{i \notin S} y_i^2 \right\} \\ &= \|y\|_2^2 - \max_{|S| \leq k} \left\{ \|y\|_2^2 - \sum_{i \in S} y_i^2 \right\} \\ &= \|y\|_2^2 - \max_{|S| \leq k} \left\{ \sum_{i \in S} y_i^2 \right\} \end{aligned}$$

Example of an integer program with TU constraints

We can view $\max_{|S| \leq k} \sum_{i \in S} y_i^2$ as an integer program over TU constraints:

$$\max_{s \in \{0,1\}} \left\{ \sum_{i=1}^n s_i y_i^2 : \mathbf{1}^T s \leq k \right\} = \max_{s \in [0,1]} \left\{ \sum_{i=1}^n s_i y_i^2 : \mathbf{1}^T s \leq k \right\}$$

Since matrix $\mathbf{1}^T$ is TU and $k \in \mathbb{Z}$.

References I

- [1] Francis Bach.
Learning with submodular functions: A convex optimization perspective.
arXiv preprint arXiv:1111.6453, 2011.
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