

## Notes 25: Largest Simplex Problem

### 1. LARGEST SIMPLEX

**Problem 1.1.** Maximum Volume Simplex (MVS)

**Input:**  $n + 1$  vectors  $v_1, \dots, v_{n+1} \in \mathbb{R}^d$  in  $d$ -dimension

**Goal:** Choose subset  $S \in \binom{[n+1]}{d+1}$  of the given vectors whose simplex  $\{v_i\}_{i \in S}$  has largest volume

In recommendation systems in machine learning, if each vector represents features of articles, largest volume may mean diversity of topics.

**Problem 1.2.** Maximum subdeterminant (MSD)

**Input:**  $n$ -by- $n$  positive-semidefinite matrix  $X$  of rank  $d$

**Goal:**  $d$ -by- $d$  principal submatrix  $X_{S,S}$  of  $X$  maximizing  $\det(X_{S,S})$ , where  $S \in \binom{[n]}{d}$

The first problem reduces to the second by the following algorithm:

Reduction

For every  $i \in [n + 1]$  (Try to include  $v_i$  in the solution)  
 Set  $u_j = v_j - v_i$  (Shift all vectors so that  $v_i$  is at the origin)  
 Set Gram matrix  $X_{jk} = \langle u_j, u_k \rangle$  for  $j, k \in [n + 1] \setminus \{i\}$   
 Solve MSD on  $X$  to find  $S \subseteq [n + 1] \setminus \{i\}$  with  $|S| = d$   
 A candidate solution is  $S \cup \{i\}$   
 Output the candidate solution with the maximum volume

Given  $d$  vectors  $u_1, \dots, u_d$  in  $\mathbb{R}^d$ ,

$$\text{vol}(\text{simplex}(0, u_1, \dots, u_d)) = \frac{1}{d!} \text{vol}(\text{parallelepiped}(u_1, \dots, u_d)) = \frac{1}{d!} \det(U),$$

where  $U$  is the matrix with column vectors  $u_1, \dots, u_d$ .

When  $X = U^T U$  is the Gram matrix of  $u_1, \dots, u_d$ ,

$$\det(X) = \det(U^T U) = \det(U)^2.$$

Finding  $S \in \binom{[n+1] \setminus \{i\}}{d}$  of maximum  $\det(X_{S,S})$  means maximizing  $\text{vol}(\text{simplex}(v_i, v_S))$ .

### 2. NIKOLOV'S ALGORITHM

Nikolov's algorithm for MSD has approximation factor  $e^{-d+o(d)}$ .

It is based on the convex program:

$$\begin{aligned} \max \log \det \left( \sum_{i \in [n]} c_i u_i u_i^\top \right) \\ \sum_{i \in [n]} c_i = d \\ c_i \geq 0 \quad \text{for } i \in [n] \end{aligned}$$

$\log \det(X)$  is concave in  $X$  ( $\det$  is log-concave in  $X$ ).

A solution to the program is fractional solution to MSD: When  $c = \mathbb{1}_S$ ,

$$\det \sum_{i \in [n]} c_i u_i u_i^\top = \det \sum_{i \in S} u_i u_i^\top = \det(U_S U_S^\top) = \det(U_S)^2,$$

where  $U_S$  is the matrix with column vectors  $\{u_i\}_{i \in S}$ .

Therefore the program is a relaxation of MSD.

## 3. LÖWNER ELLIPSOID

Dual program to the above program:

$$\begin{aligned} \min \quad & -\log \det(W) \\ & u_i^\top W u_i \leq 1 \quad \text{for } i \in [n] \\ & W \succ 0 \end{aligned}$$

One can check that strong duality holds and there is no duality gap (e.g. Slater's condition is satisfied).

What we call the dual program here was historically the primal program for MSD.

Let  $X$  be the Gram matrix of  $u_1, \dots, u_n \in \mathbb{R}^d$ .

Löwner ellipsoid of  $u_1, \dots, u_n$  is the smallest volume ellipsoid containing every  $u_i$ .

The dual program finds the Löwner ellipsoid (centered at the origin) of  $u_1, \dots, u_n$ .

An ellipsoid is the image of the unit ball  $\mathbb{B}^d = \{x \in \mathbb{R}^d \mid \|x\| \leq 1\}$  under an affine map:

$$E = \{Ax + b \mid \|x\| \leq 1\},$$

where  $A$  is a linear map on  $\mathbb{R}^d$  and  $b \in \mathbb{R}^d$  is the center of the ellipsoid.

Equivalently,

$$\begin{aligned} b + y \in E & \iff y = Ax \text{ for some } \|x\| \leq 1 \\ & \iff \|A^{-1}y\|^2 = y^\top (A^{-1})^\top A^{-1}y \leq 1 \quad \text{if } A \text{ is invertible.} \end{aligned}$$

$A$  is invertible if and only if  $E$  is full dimensional.

$W$  in the dual program plays the role of  $(A^\top A)^{-1} = (A^{-1})^\top A^{-1}$ .

**Claim 3.1.** *An ellipsoid centered at the origin has orthogonal principal semi-axes  $y_1, \dots, y_d$ , so that*

$$E = \left\{ \sum_{i \in [d]} x_i y_i \mid \|x\| \leq 1 \right\}.$$

*Proof.* Spectral theorem applied to the symmetric matrix  $A^\top A$  yields the decomposition

$$A^\top A = \sum_{i \in [d]} \lambda_i v_i v_i^\top$$

where  $\lambda_i$  are eigenvalues and  $v_i$  are orthonormal eigenvectors. All eigenvalues are nonnegative, since eigenvalues of  $A^\top A$  are squared singular values of  $A$ .

Let  $y_i = \sqrt{\lambda_i} v_i$ .

Then the semi-axes  $y_i$  are orthogonal, because  $\langle y_i, y_j \rangle = \sqrt{\lambda_i \lambda_j} \langle v_i, v_j \rangle$ .

Also,

$$y \in E \iff y = Ax \text{ for some } \|x\| \leq 1 \iff y \in \text{range } A \text{ and } y^\top (A^\top A)^+ y \leq 1.$$

$y$  is in the range (column-space) of  $A$  if and only if it is in the range of  $A^\top A$ , because the right-singular vectors of  $A$  are the eigenvectors of  $A^\top A$ .

Therefore  $y = \sum_{i \in [d]} z_i y_i$  for some  $z \in \mathbb{R}^d$ . And

$$y^\top (A^\top A)^+ y = \left( \sum_i z_i y_i^\top \right) \left( \sum_{i: \lambda_i \neq 0} \frac{1}{\lambda_i} v_i v_i^\top \right) \left( \sum_i z_i y_i \right) = \sum_i z_i^2.$$

Therefore  $y \in E$  if and only if the sum of coefficients squared is at most 1.  $\square$

From the above proof,  $\det(A^\top A) = \prod_{i \in [d]} \lambda_i = \text{vol}(E)^2 / \text{vol}(\mathbb{B}^d)^2 \propto \text{vol}(E)^2$ .

Therefore  $1/\det W$  (dual objective exponentiated) is proportional to  $\text{vol}(E)^2$ , since  $1/\det W = \det(W^{-1}) = \det(A^\top A)$ .

## 4. NIKOLOV'S ROUNDING

## Rounding

Solve the primal convex program

Let  $p_i = c_i/d$  for  $i \in [n]$

Sample  $i \in [n]$  with probability  $p_i$  independently with replacement for  $d$  times to get  $S$

The primal constraints mean  $p_i$ 's are the probability mass of a distribution over  $[n]$

**Proposition 4.1.**

$$\mathbb{E}[\det(U_S)^2] = d! \det \sum_{i \in [n]} p_i u_i u_i^\top.$$

The proof requires the following classical result from linear algebra.

**Lemma 4.2** (Cauchy–Binet). *For any  $d$ -by- $n$  matrix  $U$ ,*

$$\det(UU^\top) = \sum_{S \in \binom{[n]}{d}} \det(U_S)^2.$$

*Proof of Proposition 4.1.* When choosing  $S$  with replacement, if any element in  $S$  repeats, then  $\det(U_S)^2 = 0$ .

If there are no repeated elements, then  $S$  can be chosen in  $d!$  ways, each with probability  $\prod_{i \in S} p_i$ . Therefore

$$\mathbb{E}[\det(U_S)^2] = d! \sum_{S \in \binom{[n]}{d}} \prod_{i \in S} p_i \det(U_S)^2 = d! \sum_{S \in \binom{[n]}{d}} \det((UP^{1/2})_S)^2$$

where  $P = \text{Diag}(p_1, \dots, p_n)$  is the diagonal matrix with  $p_i$  on the diagonal.

By Cauchy–Binet, the sum of determinants equals  $\det(UPU^\top)$ . And that is  $\det \sum_{i \in [n]} p_i u_i u_i^\top$ .  $\square$

Since  $p_i = c_i/d$ ,

$$\det \sum_{i \in [n]} p_i u_i u_i^\top = \frac{1}{d^d} \det \sum_{i \in [n]} c_i u_i u_i^\top.$$

The determinant on the right is the primal objective (exponentiated).

In expectation, Nikolov's algorithm outputs a principal submatrix  $X_{S,S}$  with determinant  $d!/d^d$  times the primal objective value (exponentiated).

Standard (Stirling's) approximation gives

$$\frac{d!}{d^d} \sim \sqrt{2\pi d} e^{-d} = e^{-d+o(d)}.$$