Chapter 5

Multivariate Interpolation

Definition 5.1. Let $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ denote N distinct points in $\mathbb{R}^{\mathrm{D}}$, and $\phi_1, \phi_2, \ldots, \phi_N$ denote N linearly independent continuous functions $\mathbb{R}^{\mathrm{D}} \mapsto \mathbb{R}$. The *multivariate interpolation problem* seeks $a_1, a_2, \ldots, a_N \in \mathbb{R}$ such that

$$\forall j = 1, 2, \ldots, N, \qquad \sum_{i=1}^{N} a_i \phi_i(\mathbf{x}_j) = f(\mathbf{x}_j), \tag{5.1}$$

where $f : \mathbb{R}^{\mathrm{D}} \to \mathbb{R}$ is a given function.

Definition 5.2. The *sites* $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_N$ of the multivariate interpolation problem are said to be *poised* with respect to the basis functions $\phi_1, \phi_2, \ldots, \phi_N$ iff the *sample matrix*

$$M = \begin{bmatrix} \phi_1(\mathbf{x}_1) & \phi_2(\mathbf{x}_1) & \cdots & \phi_N(\mathbf{x}_1) \\ \phi_1(\mathbf{x}_2) & \phi_2(\mathbf{x}_2) & \cdots & \phi_N(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{x}_N) & \phi_2(\mathbf{x}_N) & \cdots & \phi_N(\mathbf{x}_N) \end{bmatrix} \tag{5.2}$$

is non-singular.

Theorem 5.3. The multivariate interpolation problem has a unique solution if and only if its sites are poised.

Example 5.1. Suppose that the values of a function $f : \mathbb{R}^2 \to \mathbb{R}$ are known at the sites $(1, 0), (-1, 0), (0, 1)$, and $(0, -1)$. For the basis functions $1, x, y, xy$, the sample matrix

$$M = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 1 & 0 & -1 & 0 \end{bmatrix}$$

is clearly singular, and hence this multivariate interpolation problem does not admit a unique solution.

5.1 Rectangular grids

Theorem 5.4 (Lagrange formula for rectangular grids)**.** Given two subsets of $\mathbb{R}$ as $X = \{x_0, x_1, \ldots, x_m\}$ and $Y = \{y_0, y_1, \ldots, y_n\}$, the multivariate interpolation problem on the rectangular grid $X \times Y$ with the set of basis functions

$$\Phi = \{x^i y^j : i = 0, 1, \ldots, m;\ j = 0, 1, \ldots, n\} \tag{5.3}$$

is solved by the unique solution

$$p(x, y) = \sum_{i=0}^{m} \sum_{j=0}^{n} f(x_i, y_j) L_i(x) M_j(y), \tag{5.4}$$

where $L_i(x)$ and $M_j(y)$ are the elementary Lagrange interpolation polynomials defined in (3.9).

Proof. Define a *blending function*

$$\xi(x, y) = \sum_{i=0}^{m} f(x_i, y) L_i(x) \tag{5.5}$$

and apply Theorem 3.4 and Definition 3.8 dimension-by-dimension in a recursive manner. □

Corollary 5.5. The unique solution in Theorem 5.4 can also be expressed via divided differences as

$$p(x, y) = \sum_{i=0}^{m} \sum_{j=0}^{n} \pi_i(x) \pi_j(y) [x_0, \ldots, x_i][y_0, \ldots, y_j] f(x, y), \tag{5.6}$$

where π is defined in (3.10), and each divided difference acts on the function f with the other coordinate fixed.

Proof. Theorem 5.4 and Definition 3.11 yield (5.6). □

Example 5.2. Write down the unique interpolating polynomial for the following data

(x, y)	$(-1, -1)$	$(-1, 1)$	$(1, -1)$	$(1, 1)$
$f(x, y)$	1	5	-5	3

Proof. To apply (5.6), we calculate

$$\begin{aligned} [-1, 1]_x f(x, -1) &= \frac{-5 - 1}{1 + 1} = -3, \\ [-1, 1]_y f(-1, y) &= \frac{5 - 1}{1 + 1} = 2, \\ [-1, 1]_x f(x, 1) &= \frac{3 - 5}{1 + 1} = -1 \\ [-1, 1]_x [-1, 1]_y f(x, y) &= [-1, 1]_x \frac{f(x, 1) - f(x, -1)}{1 + 1} \\ &= \frac{-1 + 3}{1 + 1} = 1. \end{aligned}$$

It follows that the unique interpolating polynomial is

$$\begin{aligned} p(x,y) &= 1 - 3(x+1) + 2(y+1) + (x+1)(y+1) \\ &= 1 - 2x + 3y + xy. \end{aligned}$$

□

Lemma 5.6. For $k, \ell \in \mathbb{N}^+$, define

$$\left(\Delta_x^k \Delta_y^\ell\right) f(x,y) = \Delta_x^k(\Delta_y^\ell f(x,y)). \tag{5.7}$$

Then the two difference operators Δ_x^k and Δ_y^ℓ commute,

$$\Delta_x^k \Delta_y^\ell f(x,y) = \Delta_y^\ell \Delta_x^k f(x,y). \tag{5.8}$$

Proof. (5.8) follows from (5.7) and Definition 3.19. □

Corollary 5.7. Consider a rectangular grid with uniform spacing along each dimension,

$$\begin{aligned} &\forall i = 0,1,\ldots,m, \qquad x_i = x_0 + ih_x; \\ &\forall j = 0,1,\ldots,n, \qquad y_j = y_0 + jh_y. \end{aligned}$$

The unique solution in Theorem 5.4 can also be expressed via forward differences as

$$p(x_0 + sh_x, y_0 + th_y) = \sum_{i=0}^{m}\sum_{j=0}^{n}\binom{s}{i}\binom{t}{j}\Delta_x^i\Delta_y^j f(x_0,y_0), \tag{5.10}$$

where $\binom{s}{i}$ and $\binom{t}{j}$ are defined in (3.31).

Proof. (5.10) follows from Theorem 3.23, Lemma 5.6, and the structure of rectangular grids. □

5.2 Triangular grids

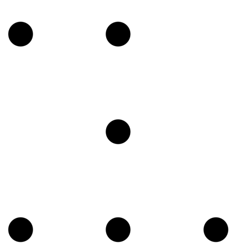
5.2.1 Triangular lattices in the plane

Definition 5.8. A *triangular lattice of degree n in two dimensions* is a set of isolated points in $\mathbb{R}^2$,

$$\mathcal{T}_2^n = \{(x_i, y_j) : i, j \geq 0, i + j \leq n\}, \tag{5.11}$$

where x_i's are $n+1$ distinct x-coordinates and y_j's are $n+1$ distinct y-coordinates.

Example 5.3. The constraints in (5.11) are not on the coordinates, but on their *indices*. Hence a triangular lattice might have a shape that does not look like a triangle.



For example, the above triangular lattice

$$\mathcal{T}_2^2 = \{(0,0),(0,2),(1,0),(1,1),(1,2),(2,0)\}$$

has distinct coordinates $x_0 = 1$, $x_1 = 0$, $x_2 = 2$ and $y_0 = 0$, $y_1 = 2$, $y_2 = 1$.

Theorem 5.9. A triangular lattice $\mathcal{T}_2^n$ is poised with respect to bivariate polynomials of degree no more than n

$$\Phi_2^n = \{1, x, y, x^2, xy, y^2, \ldots, x^n, x^{n-1}y, \ldots, xy^{n-1}, y^n\}; \tag{5.12}$$

the corresponding sample matrix M_2 satisfies

$$\det M_2 = C\psi_n(x)\psi_n(y), \tag{5.13}$$

where C is a nonzero constant and $\psi_n(x)$ is a polynomial in terms of the $n+1$ distinct coordinates x_i's,

$$\psi_n(x) := \prod_{i=1}^{n}\prod_{\ell=0}^{i-1}(x_i - x_\ell)^{n+1-i}. \tag{5.14}$$

Proof. For any fixed i, ℓ with $i > \ell$, replacing (x_i, y_j) with (x_ℓ, y_j) in $\mathcal{T}_2^n$ makes the corresponding sample matrix singular for each $j = 0, 1, \ldots, n-i$; furthermore, j cannot exceed $n - i$ because (5.11) dictates $i + j \leq n$. Therefore the number of this type of replacements is $n - i + 1$, and hence the exponent of $(x_i - x_\ell)$ in (5.14) is $n - i + 1$.

Now we vary ℓ while keeping i fixed. Since there are i indices less than i, the term $\prod_{\ell=0}^{i-1}(x_i - x_\ell)^{n+1-i}$ contributes to a total degree of $i(n+1-i)$ in terms of the $n+1$ coordinates $x_0, \ldots, x_n$. It follows that the total degree of $\psi_n(x)$ is

$$\sum_{i=1}^{n} i(n+1-i) = (n+1)\sum_{i=1}^{n} i - \sum_{i=1}^{n} i^2 = \frac{n(n+1)(n+2)}{6}, \tag{5.15}$$

where the second equality is proven by an easy induction.

Similarly, $\det M_2$ must contain a factor of $\psi_n(y)$, of which the total degree is also (5.15).

From the other viewpoint of Definition 0.146, the determinant of the sample matrix M_2 in Definition 5.2 is also a polynomial in terms of the variables $x_0, x_1, \ldots, x_n$ and $y_0, y_1, \ldots, y_n$, with each monomial being a product of all basis functions in (5.12) evaluated at some point (x_i, y_j). Hence the total degree of $\det M_2$ in the variables $x_0, x_1, \ldots, x_n$ and $y_0, y_1, \ldots, y_n$ is

$$\sum_{i=1}^{n} i(i+1) = \frac{n(n+1)(n+2)}{3}, \tag{5.16}$$

where i refers to the degree of a monomial and $i + 1$ the number of monomials of degree i, c.f. (5.12).

The proof is completed by the fact that if two complete polynomials have the same variables, the same total degree, and the same factors in terms of the same variables, then one is a constant multiple of the other. □

Corollary 5.10. A polynomial of the form

$$p_n(x,y) = \sum_{k=0}^{n}\sum_{r=0}^{k} c_{r,k-r}x^r y^{k-r} \tag{5.17}$$

uniquely interpolates any continuous function f on $\mathcal{T}_2^n$.

Proof. This follows from Theorems 5.9 and 5.4. □

Theorem 5.11. For any scalar function f whose domain includes $\mathcal{T}_2^n$, we have,

$$\forall m = 0, 1, \ldots, n, \quad f(x, y) = p_m(x, y) + r_m(x, y), \tag{5.18}$$

where the polynomial $p_m(x, y)$ interpolates $f(x, y)$ on $\mathcal{T}_2^m$ with $r_m(x, y)$ being the remainder,

$$p_m(x, y) = \begin{cases} [x_0][y_0]f = f(x_0, y_0), & m = 0; \\ p_{m-1}(x, y) + q_m(x, y), & m > 0, \end{cases} \tag{5.19a}$$

$$q_m(x, y) = \sum_{k=0}^{m} \pi_k(x)\pi_{m-k}(y)[x_0, \ldots, x_k][y_0, \ldots, y_{m-k}]f, \tag{5.19b}$$

$$\begin{aligned} r_m(x, y) = &\sum_{k=0}^{m} \pi_{k+1}(x)\pi_{m-k}(y)[x, x_0, \ldots, x_k][y_0, \ldots, y_{m-k}]f \\ &+ \pi_{m+1}(y)[x][y, y_0, \ldots, y_m]f. \end{aligned} \tag{5.19c}$$

Proof. The polynomial $p_m(x, y)$ clearly interpolates $f(x, y)$ on $\mathcal{T}_2^m$ because, for each $(x_i, y_j) \in \mathcal{T}_2^m$, all the $m + 2$ terms of $r_m(x, y)$ in (5.19c) are identically zero. The total degree of $p_m(x, y)$ is m while that of $r_m(x, y)$ is $m + 1$. It is easily verified that

$$f(x, y) = f(x_0, y_0) + (x - x_0)[x, x_0][y_0]f + (y - y_0)[x][y, y_0]f.$$

Hence (5.18) and (5.19) hold for the induction basis $m = 0$. Assume that (5.18) holds for $m \geq 0$. For the inductive step, we define

$$\begin{aligned} S_1 &= \sum_{k=0}^{m} \pi_{k+1}(x)\pi_{m-k}(y)[x_0, \ldots, x_{k+1}][y_0, \ldots, y_{m-k}]f, \\ S_2 &= \sum_{k=0}^{m} \pi_{k+2}(x)\pi_{m-k}(y)[x, x_0, \ldots, x_{k+1}][y_0, \ldots, y_{m-k}]f, \\ T_1 &= \pi_{m+1}(y)[x_0][y_0, \ldots, y_{m+1}]f, \\ T_2 &= \pi_1(x)\pi_{m+1}(y)[x, x_0][y_0, \ldots, y_{m+1}]f, \\ T_3 &= \pi_{m+2}(y)[x][y, y_0, \ldots, y_{m+1}]f. \end{aligned}$$

Utilizing (3.17), it is not difficult to prove

$$\begin{aligned} S_1 + T_1 &= q_{m+1}(x, y) = p_{m+1}(x, y) - p_m(x, y), \\ S_2 + T_2 + T_3 &= r_{m+1}(x, y), \\ r_m(x, y) &= r_{m+1}(x, y) + q_{m+1}(x, y). \end{aligned}$$

Hence we have

$$r_{m+1}(x, y) + p_{m+1}(x, y) = r_m(x, y) + p_m(x, y) = f(x, y),$$

which completes the inductive proof. □

Corollary 5.12. The interpolating polynomial on $\mathcal{T}_2^n$ in Theorem 5.11 can also be expressed as

$$p(x, y) = \sum_{m=0}^{n} \sum_{k=0}^{m} \pi_k(x)\pi_{m-k}(y)[x_0, \ldots, x_k][y_0, \ldots, y_{m-k}]f. \tag{5.20}$$

Proof. This follows directly from (5.19a) and (5.19b). □

The rest of this section concerns a special type of triangular grids.

Corollary 5.13. For the *principal lattice*

$$\mathcal{P}_2^n = \{(i, j) \in \mathbb{N}^2 : i + j \leq n\}, \tag{5.21}$$

the unique interpolating polynomial in Theorem 5.11 can be expressed as

$$p(x, y) = \sum_{m=0}^{n} \sum_{k=0}^{m} \binom{x}{k} \binom{y}{m-k} \Delta_x^k \Delta_y^{m-k} f(0, 0). \tag{5.22}$$

Proof. This follows from Corollary 5.12 and Theorem 3.22. □

Theorem 5.14 (Lagrange formula for principal lattices)**.** The unique interpolation polynomial on the principal lattice (5.21) can be expressed as

$$p_n(x, y) = \sum_{i,j} f(i, j)L_{i,j}(x, y), \tag{5.23}$$

where $(i, j) \in \mathcal{P}_2^n$ and the fundamental polynomial is

$$\begin{aligned} L_{i,j}(x, y) &= \prod_{s=0}^{i-1} \frac{x - s}{i - s} \prod_{s=0}^{j-1} \frac{y - s}{j - s} \prod_{s=i+j+1}^{n} \frac{x + y - s}{i + j - s} \\ &= \binom{x}{i} \binom{y}{j} \binom{n - x - y}{n - i - j}. \end{aligned} \tag{5.24}$$

Proof. Clearly we only need to show

$$L_{i,j}(x, y) = \begin{cases} 1 & \text{if } x = i, y = j; \\ 0 & \text{otherwise.} \end{cases}$$

It is trivial to verify $L_{i,j}(i, j) = 1$ in (5.24). As for the second clause, the following families of straight lines

- $x = 0, 1, \ldots, i - 1$,
- $y = 0, 1, \ldots, j - 1$,
- $x + y = i + j + 1, i + j + 2, \ldots, n$,

contains all sites of $\mathcal{P}_2^n \setminus \{(i, j)\}$, hence at least one factor in (5.24) is zero at any site. □

Example 5.4. The principal lattice $\mathcal{P}_2^2$ contains six sites and the corresponding interpolating polynomial is

$$\begin{aligned} p_2(x, y) = &\frac{1}{2}(x + y - 1)(x + y - 2)f(0, 0) + xyf(1, 1) \\ &- x(x + y - 2)f(1, 0) + \frac{1}{2}x(x - 1)f(2, 0) \\ &- y(x + y - 2)f(0, 1) + \frac{1}{2}y(y - 1)f(0, 2) \end{aligned}$$

The evaluation of $p_2(x, y)$ at the centroid of the triangle with vertices $(0, 0)$, $(2, 0)$, and $(0, 2)$ yields

$$p_2\left(\frac{2}{3}, \frac{2}{3}\right) = \frac{1}{3}(4\alpha - \beta),$$

where β is the mean of the values of f on the triangle vertices and α that on the other sites.

Theorem 5.15 (Neville-Aitken formula for principal lattices)**.** Define $p_0^{[i,j]} = f(i,j)$ and denote by $p_k^{[i,j]}(x,y)$ the unique interpolating polynomial of total degree k for the function $f(x,y)$ on the principal lattice

$$\mathcal{P}_k^{[i,j]} = \{(i+r, j+s) : r, s \geq 0,\ r+s \leq k\}. \tag{5.25}$$

Then, for $k \geq 0$ and $i, j \geq 0$, we have

$$\begin{aligned} p_{k+1}^{[i,j]}(x,y) = &\frac{i+j+k+1-x-y}{k+1} p_k^{[i,j]}(x,y) \\ &+ \frac{x-i}{k+1} p_k^{[i+1,j]}(x,y) + \frac{y-j}{k+1} p_k^{[i,j+1]}(x,y). \end{aligned} \tag{5.26}$$

Proof. The induction basis $k=0$ clearly holds because $\mathcal{P}_0^{[i,j]} = \{(i,j)\}$. Suppose $p_k^{[i,j]}(x,y)$ interpolates $f(x,y)$ on $\mathcal{P}_k^{[i,j]}$ for all $k \geq 0$ and all $i,j \in \mathbb{N}$. By (5.25), we have

$$\begin{aligned} \mathcal{I}_p :=& \mathcal{P}_k^{[i,j]} \cap \mathcal{P}_k^{[i+1,j]} \cap \mathcal{P}_k^{[i,j+1]} \\ =& \{(i+r, j+s) : r, s \geq 1, r+s \leq k\}. \end{aligned}$$

The induction hypothesis implies that, $\forall (\ell, m) \in \mathcal{I}_p$,

$$p_k^{[i,j]}(\ell,m) = p_k^{[i+1,j]}(\ell,m) = p_k^{[i,j+1]}(\ell,m) = f(\ell,m),$$

which, together with (5.26), yields

$$\forall (\ell,m) \in \mathcal{I}_p, \qquad p_{k+1}^{[i,j]}(\ell,m) = f(\ell,m).$$

Similarly, we have

$$\begin{aligned} \forall m-j = 1,2,\ldots,k,\ \ p_k^{[i,j]}(i,m) = p_k^{[i+1,j]}(i,m) = f(i,m), \\ \forall \ell-i = 1,2,\ldots,k,\ \ p_k^{[i,j]}(\ell,j) = p_k^{[i,j+1]}(\ell,j) = f(\ell,j). \end{aligned}$$

It follows from the above two equations and (5.26) that

$$\begin{aligned} \ell = i \Rightarrow\ \ p_{k+1}^{[i,j]}(\ell,y) = p_k^{[i,j]}(\ell,y) = f(\ell,y); \\ m = j \Rightarrow\ \ p_{k+1}^{[i,j]}(x,m) = p_k^{[i,j]}(x,m) = f(x,m). \end{aligned}$$

Hence $p_{k+1}^{[i,j]}(x,y)$ also interpolates $f(x,y)$ on $\mathcal{P}_{k+1}^{[i,j]} \setminus \mathcal{I}_p$ as any site in it satisfies $\ell = i$ or $m = j$. In summary, $p_{k+1}^{[i,j]}(x,y)$ interpolates $f(x,y)$ on $\mathcal{P}_k^{[i,j]}$.

The total degree of $p_k^{[i,j]}(x,y)$ being k can also be proved by an easy induction. □

Example 5.5. Use formula (5.26) to obtain the last equation in Example 5.4.

5.2.2 Triangular lattices in D dimensions

Notation 8. The first $n+1$ natural numbers is denoted by

$$\mathbb{Z}_n := \{0, 1, \ldots, n\} \tag{5.27}$$

and the first n positive integers by

$$\mathbb{Z}_n^+ := \{1, \ldots, n\}. \tag{5.28}$$

Definition 5.16. A subset $\mathcal{T}_{\mathrm{D}}^n$ of $\mathbb{R}^{\mathrm{D}}$ is called a *triangular lattice of degree* n *in* D *dimensions* if there exists $n+1$ coordinates for each of the D dimensions,

$$\begin{bmatrix} p_{1,0} & p_{1,1} & \cdots & p_{1,n} \\ p_{2,0} & p_{2,1} & \cdots & p_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ p_{\mathrm{D},0} & p_{\mathrm{D},1} & \cdots & p_{\mathrm{D},n} \end{bmatrix} \in \mathbb{R}^{\mathrm{D}\times(n+1)}, \tag{5.29}$$

such that

$$\mathcal{T}_{\mathrm{D}}^n = \left\{ (p_{1,k_1}, p_{2,k_2}, \ldots, p_{D,k_D}) \in \mathbb{R}^{\mathrm{D}} :\ k_i \in \mathbb{Z}_n;\ \sum_{i=1}^{\mathrm{D}} k_i \leq n \right\}, \tag{5.30}$$

where $p_{i,j}$ denotes the jth coordinate of the ith variable p_i.

Example 5.6. For $\mathrm{D} = 2$, Definition 5.16 reduces to Definition 5.8 since (5.30) simplifies to

$$\mathcal{T}_2^n = \{(p_{1,k_1}, p_{2,k_2}) :\ k_1, k_2 \geq 0;\ k_1 + k_2 \leq n\},$$

which is the same as (5.11).

Lemma 5.17. The cardinality of a triangular lattice is

$$\#\mathcal{T}_{\mathrm{D}}^n = \binom{n+\mathrm{D}}{\mathrm{D}} = \sum_{i=0}^{n} \#\mathcal{T}_{\mathrm{D}}^{=i} = \sum_{i=0}^{n} \binom{i+\mathrm{D}-1}{\mathrm{D}-1}, \tag{5.31}$$

where

$$\mathcal{T}_{\mathrm{D}}^{=m} := \left\{ (p_{1,k_1}, p_{2,k_2}, \ldots, p_{\mathrm{D},k_{\mathrm{D}}}) : k_i \geq 0; \sum_{i=1}^{\mathrm{D}} k_i = m \right\} \tag{5.32}$$

and its cardinality is

$$\#\mathcal{T}_{\mathrm{D}}^{=m} = \#\mathcal{T}_{\mathrm{D}}^{m} - \#\mathcal{T}_{\mathrm{D}}^{m-1} = \binom{m+\mathrm{D}-1}{\mathrm{D}-1}. \tag{5.33}$$

Proof. As the only nontrivial constraint on $\mathcal{T}_{\mathrm{D}}^n$ in (5.30), the sum of the D non-negative integers $i_1, \ldots, i_{\mathrm{D}}$ cannot exceed n. Hence $\#\mathcal{T}_{\mathrm{D}}^n$ equals the number of possibilities of placing n indistinguishable balls into $\mathrm{D}+1$ urns, with the first D urns corresponding to the D dimensions, respectively, and the last urn accounting for the deficit of $\sum_k i_k$ from n. This ball-urn problem is further equivalent to choosing D balls from $n+\mathrm{D}$ balls in a row because the chosen D balls divide the rest n balls into $\mathrm{D}+1$ consecutive arrays of balls, each of which corresponds to an urn. This proves the first equality in (5.31).

As for the second equality in (5.31), definitions (5.30) and (5.32) implies $\mathcal{T}_{\mathrm{D}}^n = \cup_{m=0}^n \mathcal{T}_{\mathrm{D}}^{=m}$ and that two subsets $\mathcal{T}_{\mathrm{D}}^{=m}$ and $\mathcal{T}_{\mathrm{D}}^{=n}$ are disjoint if and only if $m \neq n$.

An easy induction shows (5.33), which further implies the third equality in (5.31). □

Definition 5.18. The D*-variate polynomials of degree no more than* n form the set

$$\Phi_{\mathrm{D}}^n = \left\{ p_1^{e_1} p_2^{e_2} \ldots p_{\mathrm{D}}^{e_{\mathrm{D}}} : e_i \geq 0; \sum_{i=1}^{\mathrm{D}} e_i \leq n \right\}, \tag{5.34}$$

and the D*-variate polynomials of degree* m form the set

$$\Phi_{\mathrm{D}}^{=m} = \left\{ p_1^{e_1} p_2^{e_2} \ldots p_{\mathrm{D}}^{e_{\mathrm{D}}} : e_i \geq 0; \sum_{i=1}^{\mathrm{D}} e_i = m \right\}. \tag{5.35}$$

Lemma 5.19. The results on triangular lattices in Lemma 5.17 also hold for sets of multivariate polynomials. More precisely, (5.31) and (5.33) still hold when the symbol $\mathcal{T}$ is replaced with the symbol Φ.

Proof. This follows from a natural bijection between $\Phi_{\rm D}^n$ and $\mathcal{T}_{\rm D}^n$, the restriction of which is also a bijection between $\Phi_{\rm D}^{=n}$ and $\mathcal{T}_{\rm D}^{=n}$. $\square$

Lemma 5.20. For any positive integers D and n, we have

$$({\rm D}+1)\sum_{j=1}^{n} j\binom{n-j+{\rm D}}{{\rm D}} = \sum_{j=1}^{n} j\binom{j+{\rm D}}{{\rm D}}. \tag{5.36}$$

Proof. For $n=1$, both sides reduce to D+1. Suppose (5.36) holds. Then the inductive step also holds because

$$\begin{aligned}
&({\rm D}+1)\sum_{j=1}^{n+1} j\binom{n+1-j+{\rm D}}{{\rm D}}\\
=&({\rm D}+1)\sum_{i=0}^{n}(i+1)\binom{n-i+{\rm D}}{{\rm D}}\\
=&({\rm D}+1)\sum_{i=0}^{n} i\binom{n-i+{\rm D}}{{\rm D}} + ({\rm D}+1)\sum_{j=0}^{n}\binom{j+{\rm D}}{{\rm D}}\\
=&\sum_{j=1}^{n} j\binom{j+{\rm D}}{{\rm D}} + ({\rm D}+1)\binom{n+{\rm D}+1}{{\rm D}+1}\\
=&\sum_{j=1}^{n+1} j\binom{j+{\rm D}}{{\rm D}},
\end{aligned}$$

where the first two step follows from variable substitutions, the third step from the induction hypothesis and the well-known identity $\sum_{j=0}^{n}\binom{{\rm D}+j}{{\rm D}} = \binom{{\rm D}+n+1}{{\rm D}+1}$, and the last step from

$$\begin{aligned}
&({\rm D}+1)\binom{n+{\rm D}+1}{{\rm D}+1} = ({\rm D}+1)\frac{(n+{\rm D}+1)!}{({\rm D}+1)!n!}\\
=&(n+1)\frac{(n+{\rm D}+1)!}{{\rm D}!(n+1)!} = (n+1)\binom{n+{\rm D}+1}{{\rm D}}.
\end{aligned}$$ $\square$

Theorem 5.21. A triangular lattice $\mathcal{T}_{\rm D}^n$ is poised with respect to the D-variate polynomials of degree no more than n; the corresponding sample matrix $M_{\rm D}$ satisfies

$$\det M_{\rm D} = C\prod_{k=1}^{\rm D}\psi_n(p_k) \tag{5.37}$$

where C is a nonzero constant and $\psi_n(p_k)$ is a polynomial in terms of the $n+1$ distinct coordinates of the variable p_k,

$$\psi_n(p_k) := \prod_{i_k=1}^{n}\prod_{\ell=0}^{i_k-1}(p_{k,i_k}-p_{k,\ell})^{\alpha(i_k)}; \tag{5.38}$$

$$\alpha(i_k) := \binom{n-i_k+{\rm D}-1}{{\rm D}-1}. \tag{5.39}$$

Proof. We follow the steps in the proof of Theorem 5.9, with more complicated book-keeping on the combinatorics.

Consider the kth variable p_k. For any fixed i_k and ℓ with $i_k > \ell$, replacing the coordinate p_{k,i_k} with $p_{k,\ell}$ in a point

$$\mathbf{p}_k := (p_{1,i_1},\ldots,p_{k,i_k},\ldots,p_{{\rm D},i_{\rm D}}) \in \mathcal{T}_{\rm D}^n \tag{5.40}$$

makes the corresponding sample matrix $M_{\rm D}$ singular. Furthermore, when the coordinate index of the kth variable p_k is fixed at i_k in $\mathcal{T}_{\rm D}^n$, the cardinality of $\mathcal{T}_{\rm D}^n$ reduces to $\#\mathcal{T}_{{\rm D}-1}^{n-i_k}$, which, by Lemma 5.17, must equal $\alpha(i_k)$. In other words,

$$\#\{(p_{1,i_1},\ldots,p_{k,i_k},\ldots,p_{{\rm D},i_{\rm D}}) \in \mathcal{T}_{\rm D}^n : \ i_k \text{ is fixed}\}$$

equals the cardinality of a triangular lattice of degree $n-i_k$ in $\mathrm{D}-1$ dimensions because an index of i_k has been consumed from the total index n and one of the D dimensions has already been fixed. Therefore, the number of possible $\mathbf{p}_k$'s that admit the replacement of p_{k,i_k} with $p_{k,\ell}$ is $\alpha(i_k)$, and this justifies the exponent of $(p_{k,i_k}-p_{k,\ell})$ in (5.38).

Now we vary ℓ while keeping i_k fixed. Since there are i_k indices less than i_k, the term $\prod_{\ell=0}^{i_k-1}(p_{k,i_k}-p_{k,\ell})^{\alpha(i_k)}$ contributes to a total degree $i_k\alpha(i_k)$ in terms of the $n+1$ coordinates $p_{k,0},\ldots,p_{k,n}$. It follows that $\psi_n(p_k)$ must be a factor of $\det M_{\rm D}$ and the total degree of $\psi_n(p_k)$ is

$$\sum_{i_k=1}^{n} i_k\alpha(i_k) = \sum_{j=1}^{n} j\binom{n-j+{\rm D}-1}{{\rm D}-1}.$$

Similarly, $\det M_{\rm D}$ must contain a factor of $\psi_n(p_j)$ for each variable p_j, $j=1,\ldots,{\rm D}$. Hence the total degree of $\det M_{\rm D}$ is at least

$$\xi := {\rm D}\sum_{j=1}^{n} j\binom{n-j+{\rm D}-1}{{\rm D}-1}.$$

From the other viewpoint of Definition 0.146, the determinant of the sample matrix $M_{\rm D}$ is also a polynomial in terms of the coordinates $p_{1,0},p_{1,1},\ldots,p_{1,n}$, …, $p_{{\rm D},0},p_{{\rm D},1},\ldots,p_{{\rm D},n}$, with each monomial being a product of all basis functions in (5.34) evaluated at some point $(p_{1,i_1},p_{2,i_2},\ldots,p_{n,i_n})$. By Lemma 5.19 and (5.33), the total degree of $\det M_{\rm D}$ equals

$$\eta := \sum_{i=1}^{n} i\binom{i+{\rm D}-1}{{\rm D}-1},$$

where i refers to the degree of monomials in the subset $\Phi_{\rm D}^{=i}$ and $\binom{i+{\rm D}-1}{{\rm D}-1}$ the cardinality of $\Phi_{\rm D}^{=i}$.

Lemma 5.20 implies $\xi = \eta$. Hence the terms in $\prod_{k=1}^{\rm D}\psi_n(p_k)$ constitute all the non-constant factors of $\det M_{\rm D}$, which yields (5.37). $\square$

5.3 Poised-lattice generation (PLG)

5.3.1 Formulating the PLG problem

Notation 9. For a *fixed* coordinate system of $\mathbb{Z}_n^{\rm D}$, the *set of all triangular lattices of degree* n in $\mathbb{Z}_n^{\rm D}$ is denoted by

$$\mathcal{X} := \left\{\mathcal{T}_{\mathcal{D}}^n : \mathcal{T}_{\mathcal{D}}^n \subset \mathbb{Z}_n^{\rm D}\right\}, \tag{5.41}$$

where the D-dimensional cube of size $n+1$ is denoted by

$$\mathbb{Z}_n^{\rm D} := (\mathbb{Z}_n)^{\rm D} = \{0,1,\ldots,n\}^{\rm D}. \tag{5.42}$$

Definition 5.22. Given $K \subseteq \mathbb{Z}_n^{\mathrm{D}}$ and $\mathbf{q} \in K$, the *poised-lattice generation problem* seeks $\mathcal{T} \in \mathcal{X}$ such that $\mathbf{q} \in \mathcal{T}$ and $\mathcal{T} \subseteq K$.

5.3.2 A group action on triangular lattices

Definition 5.23. The *principal lattice* of degree n in $\mathbb{N}^{\mathrm{D}}$ is

$$\mathcal{P}_{\mathrm{D}}^n = \left\{ (j_1, \ldots, j_{\mathrm{D}}) \in \mathbb{N}^{\mathrm{D}} : \sum_{k=1}^{\mathrm{D}} j_k \le n \right\}. \tag{5.43}$$

Example 5.7. The principal lattice of degree 2 in two dimensions is

$$\mathcal{P}_2^2 = \{(0,0), (0,1), (0,2), (1,0), (1,1), (2,0)\}. \tag{5.44}$$

Definition 5.24. The *m-slice of a subset* $T \subseteq \mathbb{Z}_n^{\mathrm{D}}$ across the ith dimension is a subset of T defined as

$$L_{i,m}(T) = \{\mathbf{p} \in T : p_i = m\}. \tag{5.45}$$

Lemma 5.25. Any m-slice of a triangular lattice of degree n in D dimensions is a triangular lattice of degree $n - m$ in $\mathrm{D} - 1$ dimensions.

Proof. By Definition 5.16, the triangular lattice is

$$\mathcal{T}_{\mathrm{D}}^n = \left\{ (p_{1,j_1}, p_{2,j_2}, \ldots, p_{D,j_D}) : \ j_k \ge 0; \ \sum_{k=1}^{\mathrm{D}} j_k \le n \right\},$$

where each variable p_i has exactly $n + 1$ coordinates. By Definition 5.24, we have

$$\begin{aligned} L_{i,m}(\mathcal{T}) = \{ & (p_{1,j_1}, \ldots, p_{i-1,j_{i-1}}, m, p_{i+1,j_{i+1}}, \ldots, p_{D,j_D}) : \\ & j_k \ge 0; \ \sum_{k \neq i, k=1}^{\mathrm{D}} j_k \le n - m \}, \end{aligned}$$

which, by Definition 5.16, is a triangular lattice of degree $n - m$ in $\mathrm{D} - 1$ dimensions after renumbering the $n - m + 1$ coordinates for each dimension $k \neq i$. □

Definition 5.26. A D-*permutation of degree* n, written

$$A = (a_1, a_2, \ldots, a_{\mathrm{D}})^T,$$

is a map $A : \mathbb{Z}_n^{\mathrm{D}} \to \mathbb{Z}_n^{\mathrm{D}}$ defined as

$$A\mathbf{p} = (a_1(p_1), a_2(p_2), \cdots, a_{\mathrm{D}}(p_{\mathrm{D}}))^T, \tag{5.46}$$

where each $a_i : \mathbb{Z}_n \to \mathbb{Z}_n$ is a permutation.

Notation 10. Denote by G the *set of all* D*-permutations.*

Definition 5.27. The *multiplication of two* D*-permutations* is a binary operation $\cdot : G \times G \to G$ given by

$$A \cdot B = (a_1 \circ b_1, a_2 \circ b_2, \ldots, a_{\mathrm{D}} \circ b_{\mathrm{D}})^T \tag{5.47}$$

where "$\circ$" denotes function composition.

Definition 5.28. The *inverse of a* D*-permutation* A is a unitary operation $^{-1} : G \to G$ such that A^{-1} satisfies

$$A^{-1} \cdot A = A \cdot A^{-1} = E = (e_1, e_2, \ldots, e_{\mathrm{D}})^T, \tag{5.48}$$

where E denotes the distinguished D-permutation with each constituting permutation e_i as the identity map on $\mathbb{Z}_n$.

Lemma 5.29. The following algebra is a group,

$$(G, \cdot, ^{-1}, E). \tag{5.49}$$

Proof. It is straightforward to verify the conditions of a group from Definitions 5.26, 5.27, and 5.28. □

Lemma 5.30. For any $A \in G$, the map σ_A given by

$$\forall \mathcal{T} \in \mathcal{X}, \ \sigma_A(\mathcal{T}) = A\mathcal{T} := \{A\mathbf{p} : \mathbf{p} \in T\} \tag{5.50}$$

is a permutation of $\mathcal{X}$. In other words, D-permutations map triangular lattices to triangular lattices.

Proof. Since $\mathcal{T}$ is a triangular lattice, we know from Definition 5.16 that there exist $n + 1$ coordinates for each of the D dimensions such that *indices* of the D constituting coordinates of each point $\mathbf{p} \in \mathcal{T}$ add up to no more than n. The action of A upon $\mathcal{T}$ in (5.46) can be undone by applying A^{-1}; this means that for $A\mathcal{T}$ there exists a renumbering (specified by A^{-1}) of the coordinates along each axis such that $A\mathcal{T}$ is a triangular lattice. □

Lemma 5.31. The set of triangular lattices $\mathcal{X}$ is a G-set with its group action $G \times \mathcal{X} \to \mathcal{X}$ given by $\sigma_A(\mathcal{T})$ in (5.50).

Proof. By Lemma 5.30, $\bullet(A, \mathcal{T}) = \sigma_A(\mathcal{T})$ indeed has the signature $G \times \mathcal{X} \to \mathcal{X}$. By Definition (5.48), we have

$$\forall \mathcal{T} \in \mathcal{X}, \quad E\mathcal{T} = \mathcal{T}.$$

In addition, for any $A, B \in G$ and any $\mathcal{T} \in \mathcal{X}$, we have

$$\begin{aligned} (A \cdot B)\mathcal{T} &= \{(A \cdot B)\mathbf{p} : \mathbf{p} \in \mathcal{T}\} \\ &= \{((a_1 \circ b_1)(p_1), \ldots, (a_{\mathrm{D}} \circ b_{\mathrm{D}})(p_{\mathrm{D}}))^T : \mathbf{p} \in \mathcal{T}\} \\ &= \{(a_1(b_1(p_1)), \ldots, a_{\mathrm{D}}(b_{\mathrm{D}}(p_{\mathrm{D}})))^T : B\mathbf{p} \in \mathcal{T}\} \\ &= A(B\mathcal{T}), \end{aligned}$$

where the first step follows from (5.50), the second from (5.46) and (5.47), the third from Lemma 5.30, and the last from (5.50). The proof is completed by Definition 0.129. □

Definition 5.32. The *restoration of a triangular lattice* $\mathcal{T}_{\mathrm{D}}^n$ is a D-permutation $R_{\mathcal{T}} = (r_1, r_2, \ldots, r_{\mathrm{D}})^T$ such that

$$\begin{aligned} & \forall i = 1, 2, \ldots, \mathrm{D}, \ \forall m \in \mathbb{Z}_n, \\ & r_i(m) = \#\{j \in \mathbb{Z}_n : \#L_{i,j}(\mathcal{T}) > \#L_{i,m}(\mathcal{T})\}. \end{aligned} \tag{5.51}$$

Lemma 5.33. The restoration of a triangular lattice $\mathcal{T}_{\mathrm{D}}^n$ is a bijection that maps $\mathcal{T}_{\mathrm{D}}^n$ to the principal lattice $\mathcal{P}_{\mathrm{D}}^n$, i.e.

$$R_{\mathcal{T}_{\mathrm{D}}^n} \mathcal{T}_{\mathrm{D}}^n = \mathcal{P}_{\mathrm{D}}^n. \tag{5.52}$$

Proof. Lemma 5.25 and Lemma 5.17 imply that the slices of $\mathcal{T}$ along each axis have pairwise distinct cardinalities. By Definition 5.32, the cardinalities of rearranged slices along the ith dimension are not changed by any constituting permutations except r_i. By Lemma 5.30, $R_{\mathcal{T}}\mathcal{T}$ is also a triangular lattice. Furthermore, cardinalities of the m-slices of $R_{\mathcal{T}}\mathcal{T}$ decrease strictly monotonically as m increases. There is only one such triangular lattice, namely $\mathcal{P}_{\mathrm{D}}^n$ in (5.43). Finally, $R_{\mathcal{T}}$ is a bijection because each constituting permutation is a bijection. □

Definition 5.34. The *formation of a triangular lattice* $\mathcal{T}$ is the inverse of its restoration, i.e.,

$$A_{\mathcal{T}} = R_{\mathcal{T}}^{-1}. \tag{5.53}$$

Lemma 5.35. The formation of a triangular lattice $\mathcal{T}_{\mathrm{D}}^{n}$ is a bijection that maps the principal lattice $\mathcal{P}_{\mathrm{D}}^{n}$ to $\mathcal{T}_{\mathrm{D}}^{n}$,

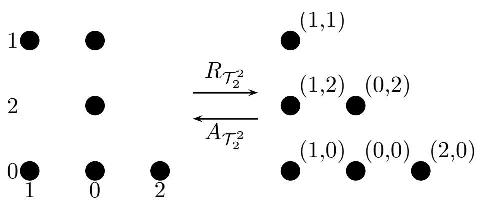
$$\mathcal{T}_{\mathrm{D}}^{n} = A_{\mathcal{T}_{\mathrm{D}}^{n}} \mathcal{P}_{\mathrm{D}}^{n}. \tag{5.54}$$

Proof. This follows directly from Definitions 5.32 and 5.34 and Lemma 5.33. □

Example 5.8. For the triangular lattice $\mathcal{T}_2^2$ in Example 5.3, its formation $A_{\mathcal{T}_2^2}$ equals its restoration $R_{\mathcal{T}_2^2}$,

$$\left\{ \begin{array}{l} r_1 : 0 \mapsto 1; 1 \mapsto 0; 2 \mapsto 2, \\ r_2 : 0 \mapsto 0; 1 \mapsto 2; 2 \mapsto 1. \end{array} \right. \tag{5.55}$$

The processes of restoration and formation are shown below.



On the left, the integers below the lattice are $r_1([0, 1, 2])$, i.e., the numbers of vertical slices with cardinalities larger than the current slice, and the integers to the left of the lattice are $r_2([0, 1, 2])$, i.e., the numbers of horizontal slices with cardinalities larger than the current slice. On the right, the multiindex close to a dot is the preimage of the dot under $R_{\mathcal{T}_2^2}$. The following table illustrates that the restoration is indeed a bijection.

$\mathbf{p} \in \mathcal{P}_2^2$	(0,0)	(0,1)	(0,2)	(1,0)	(1,1)	(2,0)
$\mathbf{p} \in \mathcal{T}_2^2$	(1,0)	(1,2)	(1,1)	(0,0)	(0,2)	(2,0)

Corollary 5.36. Denote by $S_{\mathcal{X}}$ the symmetric group on $\mathcal{X}$. The map $\phi : G \to S_{\mathcal{X}}$ defined by

$$\phi(A) = \sigma_A \tag{5.56}$$

is a monomorphism.

Proof. By Theorem 0.130 and Lemma 5.31, ϕ is a homomorphism. We still need to show that ϕ is injective. Suppose there exists $A \neq B$ in G such that $\phi(A) = \phi(B)$. Then

$$\forall \mathcal{T} \in \mathcal{X}, \ \sigma_A(\mathcal{T}) = A\mathcal{T} = B\mathcal{T} = \sigma_B(\mathcal{T}),$$

which implies $A^{-1}B = E$, a contradiction to $A \neq B$. □

Corollary 5.37. The PLG problem $(K, \mathbf{q})$ in Definition 5.22 is solved by a triangular lattice $\mathcal{T}$ if and only if its formation $A_{\mathcal{T}}$ satisfies

$$\exists \mathbf{p} \in \mathcal{P}_{\mathrm{D}}^{n}, \text{ s.t. } A_{\mathcal{T}}\mathbf{p} = \mathbf{q}; \tag{5.57a}$$

$$\forall \mathbf{p} \in \mathcal{P}_{\mathrm{D}}^{n}, \ A_{\mathcal{T}}\mathbf{p} \in K. \tag{5.57b}$$

Furthermore, all solutions to the PLG problems can be obtained by enumerating the formations.

Proof. The first sentence follows from Definition 5.22, Lemma 5.33, and Definition 5.34. By Lemma 5.35, any triangular lattice $\mathcal{T}$ determines a D-permutation, namely its formation, that generates $\mathcal{T}$ from the principal lattice. Hence all triangular lattices are generated by enumerating formations. □

5.3.3 Partitioning triangular lattices

Definition 5.38. A function $c : \mathbb{Z}_{\mathrm{D}}^{+} \to \mathbb{Z}_n$ is called a *column-pick map* for a multiindex $(\ell, m) \in \mathbb{Z}_{\mathrm{D}}^{+} \times \mathbb{Z}_n$ if

$$c(i) = \begin{cases} \leq m & \text{if } i < \ell; \\ m & \text{if } i = \ell; \\ < m & \text{if } i > \ell. \end{cases} \tag{5.58}$$

The set of all column-pick maps for a given multiindex (ℓ, m) is denoted by $C_{(\ell,m)}$.

Definition 5.39. The *test set* at $(\ell, m) \in \mathbb{Z}_{\mathrm{D}}^{+} \times \mathbb{Z}_n$ is a set of D-dimensional multiindices,

$$W_{(\ell,m)} = \left\{ (c(1), \ldots, c(\mathrm{D})) \in \mathbb{Z}_n^{\mathrm{D}} : c \in C_{(\ell,m)}; \sum_{i=1}^{\mathrm{D}} c(i) \leq n \right\}. \tag{5.59}$$

In particular, $W_{(\ell,m)} = \emptyset$ if $C_{(\ell,m)} = \emptyset$.

Lemma 5.40. Test sets form a partition of the principal lattice $\mathcal{P}_{\mathrm{D}}^{n}$. More precisely, we have

$$\bigcup_{\ell \in \mathbb{Z}_{\mathrm{D}}^{+}, m \in \mathbb{Z}_n} W_{(\ell,m)} = \mathcal{P}_{\mathrm{D}}^{n}; \tag{5.60a}$$

$$(\ell, m) \neq (i, j) \ \Leftrightarrow \ W_{(\ell,m)} \cap W_{(i,j)} = \emptyset. \tag{5.60b}$$

Proof. Suppose $\mathbf{p} \in W_{(\ell,m)}$ for some (ℓ, m). Then $\mathbf{p} \in \mathcal{P}_{\mathrm{D}}^{n}$ must hold because of the condition $\sum_{i=1}^{\mathrm{D}} c(i) \leq n$ in (5.59).

Conversely, let m be the largest coordinate of $\mathbf{p} \in \mathcal{P}_{\mathrm{D}}^{n}$ and ℓ be the largest dimension index of $\mathbf{p}$ such that $p_\ell = m$. Then (5.58) and (5.59) imply $\mathbf{p} \in W_{(\ell,m)}$.

Suppose for some $(i, j) \neq (\ell, m)$ we also have $\mathbf{p} \in W_{(i,j)}$. Since $\mathbf{p}$ has only one largest coordinate (that is assumed to be m), we must have $j = m$, which implies $i \neq \ell$. Because ℓ is the largest dimension index satisfying $c(\ell) = m$, we have $i < \ell$, which contradicts the third branch of (5.58). □

Example 5.9. The test-set partition of $\mathcal{P}_2^2$ in (5.44) is

$$W_{(1,1)} = \{(1,0)\}, \ W_{(1,2)} = \{(2,0)\},$$
$$W_{(2,0)} = \{(0,0)\}, \ W_{(2,1)} = \{(0,1),(1,1)\}, W_{(2,2)} = \{(0,2)\}.$$

5.3.4 Partitioning actions of D-permutations

Definition 5.41. A *partial function* from Y to Z is a function $Y' \to Z$ on some $Y' \subseteq Y$.

Definition 5.42. The (ℓ, m)*-partial* D*-permutation*, denoted by $A^{(\ell,m)}$, is a partial function on the test set $W_{(\ell,m)}$ that satisfies

$$\forall \mathbf{p} \in W_{(\ell,m)},\ A^{(\ell,m)}\mathbf{p} = A\mathbf{p}. \tag{5.61}$$

Definition 5.43. The *linear ordering of integer pairs* on a grid $\mathbb{Z}_{\mathrm{D}}^+ \times \mathbb{Z}_n$ is the column-wise ordering of the grid, i.e., the total ordering obtained by stacking all the columns of the grid into one column. More precisely, this ordering is a bijection s that maps a pair $(i,j) \in \mathbb{Z}_{\mathrm{D}}^+ \times \mathbb{Z}_n$ to a scalar index $k \in \mathbb{Z}_{\mathrm{D}(n+1)}^+$,

$$s(i,j) = i + j\mathrm{D}; \tag{5.62}$$

$$s^{-1}(k) = \left(1 + (k-1) \bmod \mathrm{D},\ \left\lfloor \frac{k-1}{\mathrm{D}} \right\rfloor\right), \tag{5.63}$$

where $\lfloor \cdot \rfloor : \mathbb{Q} \to \mathbb{N}$ is the floor operator.

Corollary 5.44. If $C_{(\ell,m)}$ is nonempty, any column-pick map $c \in C_{(\ell,m)}$ satisfies

$$\forall i \in \mathbb{Z}_{\mathrm{D}}^+,\ s(i, c(i)) \le s(\ell, m). \tag{5.64}$$

Proof. This follows from (5.58) and Definition 5.43. □

Notation 11. In matrix notation, a D-permutation is

$$A = \begin{bmatrix} a_1(0) & a_1(1) & \dots & a_1(n) \\ a_2(0) & a_2(1) & \dots & a_2(n) \\ \vdots & \vdots & \ddots & \vdots \\ a_{\mathrm{D}}(0) & a_{\mathrm{D}}(1) & \dots & a_{\mathrm{D}}(n) \end{bmatrix}, \tag{5.65}$$

which means that the (i,j)th-element of A is

$$A(i,j) = a_i(j). \tag{5.66}$$

Note that the row index i of the matrix starts from 1 while the column index j starts from 0. By Corollary 5.44, the matrix of a partial D-permutation is simply

$$A^{(\ell,m)}(i,j) = \begin{cases} A(i,j) & \text{if } s(i,j) \le s(\ell,m); \\ -1 & \text{otherwise,} \end{cases} \tag{5.67}$$

where s is defined in (5.62), and "-1" indicates undefined behavior. Since s is a bijection, it also makes sense to write

$$\forall t = s(\ell,m),\ A^{(t)} := A^{(\ell,m)}. \tag{5.68}$$

Lemma 5.45. A triangular lattice $\mathcal{T}_{\mathrm{D}}^n$ has the partition

$$\mathcal{T}_{\mathrm{D}}^n = \bigcup_{\ell \in \mathbb{Z}_{\mathrm{D}}^+, m \in \mathbb{Z}_n} A_{\mathcal{T}}^{(\ell,m)} W_{(\ell,m)}, \tag{5.69}$$

where the terms $A_{\mathcal{T}}^{(\ell,m)} W_{(\ell,m)}$ are pairwise disjoint.

Proof. By Lemma 5.40, Lemma 5.33, and (5.61), we have

$$\begin{aligned} \mathcal{T}_{\mathrm{D}}^n &= A_{\mathcal{T}} \mathcal{P}_{\mathrm{D}}^n = A_{\mathcal{T}} \bigcup_{(\ell,m)} W_{(\ell,m)} = \bigcup_{(\ell,m)} A_{\mathcal{T}} W_{(\ell,m)} \\ &= \bigcup_{(\ell,m)} A_{\mathcal{T}}^{(\ell,m)} W_{(\ell,m)}. \end{aligned}$$

The pairwise disjointness of the terms follows from (5.60b) and Lemma 5.35. □

Example 5.10. The triangular lattice in Example 5.3 is

$$\mathcal{T} = \{(0,0), (0,2), (1,0), (1,1), (1,2), (2,0)\} \tag{5.70}$$

and its formation is

$$A_{\mathcal{T}} = \begin{bmatrix} 1 & 0 & 2 \\ 0 & 2 & 1 \end{bmatrix}. \tag{5.71}$$

Following Examples 5.8 and 5.9, $\mathcal{T}$ is partitioned into

$$\begin{aligned} &A_{\mathcal{T}}^{(1,1)} W_{(1,1)} = \{(0,0)\},\ A_{\mathcal{T}}^{(1,2)} W_{(1,2)} = \{(2,0)\}, \\ &A_{\mathcal{T}}^{(2,0)} W_{(2,0)} = \{(1,0)\},\ A_{\mathcal{T}}^{(2,1)} W_{(2,1)} = \{(1,2), (0,2)\}, \\ &A_{\mathcal{T}}^{(2,2)} W_{(2,2)} = \{(1,1)\}. \end{aligned}$$

Theorem 5.46. The PLG problem $(K, \mathbf{q})$ in Definition 5.22 is solved by a triangular lattice $\mathcal{T} = A_{\mathcal{T}} \mathcal{P}_{\mathrm{D}}^n$ if and only if its formation $A_{\mathcal{T}}$ satisfies

$$\forall (\ell, m) \in \mathbb{Z}_{\mathrm{D}}^+ \times \mathbb{Z}_n,\ A_{\mathcal{T}}^{(\ell,m)} W_{(\ell,m)} \subset K; \tag{5.72a}$$

$$\exists \mathbf{p} \in \mathcal{P}_{\mathrm{D}}^n,\ \text{s.t. } A_{\mathcal{T}}\mathbf{p} = \mathbf{q}. \tag{5.72b}$$

Furthermore, an enumeration based on the partial D-permutations finds all solutions to the PLG problem.

Proof. This follows directly from Lemma 5.45 and Corollary 5.37. □

5.3.5 Depth-first search and backtracking

Definition 5.47. *Depth-first search (DFS)* is an algorithm for traversing a graph $G = (V, E)$; it starts at a given node $v \in V$ and explores as far as possible along each edge before backtracking. A recursive version is as follows.

Procedure DFS(G, v)

Input: A finite graph $G = (V, E)$ and a node $v \in V$

Preconditions: G is connected and initially all nodes in V are "undiscovered."

Side effects : all nodes in V are "discovered."

```
label v as "discovered"
for each edge (v, w) ∈ E do
    if w is not discovered then
        DFS(G, w)
    end
end
```

Definition 5.48 (Backtracking)**.** Denote by P a problem that admits an incremental assemblage of the solutions and hence a spanning-tree organization of the solution space. *Backtracking* is a generic algorithm that solves P by calling `BackTrack(`P, `root(`P`)`, $\{\}$`)`,

Procedure BackTrack(P, $\mathbf{r}$, T)

Input: $\mathbf{r}$ is a starting node in the solution space and T is a set of the solutions
Preconditions: Initially T is an empty set
Side effects : T contains all valid solutions

if *accept*$(P, \mathbf{r})$ **then**
  $T = T \cup \{\mathbf{r}\}$
  if *stopAfterAccept*$(P, \mathbf{r})$ **then return**
else if *reject*$(P, \mathbf{r})$ **then**
  return
end
$\mathbf{s} \leftarrow$ `first`$(P, \mathbf{r})$
while $\mathbf{s}$ *is not null* **do**
  BackTrack$(P, \mathbf{s}, T)$
  $\mathbf{s} \leftarrow$ `next`$(P, \mathbf{r}, \mathbf{s})$
end

where the details of P are given in the following user-defined subroutines,

- `root`(P): return the root node of the spanning tree of the solution space,
- `accept`$(P, \mathbf{r})$: return true if and only if $\mathbf{r}$ is already a solution; return false otherwise,
- `stopAfterAccept`$(P, \mathbf{r})$: return true if and only if the valid solution $\mathbf{r}$ can never be extended to another valid solution; return false otherwise,
- `reject`$(P, \mathbf{r})$: return true if and only if the partial candidate (or node) $\mathbf{r}$ can never be completed to a valid solution; return false otherwise,
- `first`$(P, \mathbf{r})$: return the first extension of $\mathbf{r}$ in the spanning tree if $\mathbf{r}$ is extendable; return null otherwise,
- `next`$(P, \mathbf{r}, \mathbf{s})$: return the next extension of $\mathbf{r}$ after $\mathbf{s}$ if $\mathbf{r}$ is still extendable; return null otherwise.

5.3.6 Backtracking for PLG

Definition 5.49. For a PLG problem $(K, \mathbf{q})$, the *test ordering* "$<$" of a subset $J_i \subseteq \mathbb{Z}_n$ along the ith dimension is a total order on J_i determined first by the cardinality of the slices, and then by breaking any tie with the distance to $\mathbf{q}$ along the ith dimension. More precisely, for any distinct $j, k \in J_i$, we say that k is *greater than* j, written $k > j$, or that j is *less than* k, written $j < k$, if and only if

$$\begin{aligned}&\big(\#L_{i,j}(K) < \#L_{i,k}(K)\big)\\ \vee&\big(\#L_{i,j}(K) = \#L_{i,k}(K) \quad\wedge\quad |j - q_i| > |k - q_i|\big),\end{aligned} \tag{5.73}$$

where q_i is the ith coordinate of $\mathbf{q}$. In particular, the element in J_i that is greater and less than all other elements in J_i is denoted by $\max J_i$ and $\min J_i$, respectively.

Definition 5.50 (Backtracking for PLG)**.** The following recursive algorithm finds all solutions to an PLG problem.

Input: the degree $n \in \mathbb{N}^+$, the dimensionality $\mathrm{D} \in \mathbb{N}^+$, the search domain $K \subseteq \mathbb{Z}_n^{\mathrm{D}}$, and the starting point $\mathbf{q} \in K$
Output: a set $\mathcal{U}$ of D-permutations
Postconditions: $\{A\mathcal{P}_{\mathrm{D}}^n : A \in \mathcal{U}\}$ is the set of all solutions of the PLG problem

$\mathcal{U} \leftarrow$ an empty set of D-permutations
$A^{(r)} \leftarrow$ `root`(n, D)
BackTrack $\big((K, \mathbf{q}), A^{(r)}, \mathcal{U}\big)$

where the procedures in Definition 5.48 are as follows.

- `root`(n, D): set $A^{(0)}$ to a D-by-$(n+1)$ matrix of constant -1 following Notation 11; return $A^{(0)}$.
- `accept`$((K, \mathbf{q}), A^{(t)})$: return false if $t < \mathrm{D}(n+1)$; otherwise return true if and only if
$$A^{(t)} W_{(\mathrm{D},n)} \subset K \text{ and } \mathbf{q} \in A^{(t)} \mathcal{P}_{\mathrm{D}}^n.$$
- `stopAfterAccept`$((K, \mathbf{q}), A^{(t)})$: return true.
- `reject`$((K, \mathbf{q}), A^{(t)})$: if $t = \mathrm{D}(n+1)$, return the negation of `accept`$((K, \mathbf{q}), A^{(t)})$; otherwise return the result if the logical statement
$$\exists \mathbf{p} \in W_{(\ell,m)} \text{ s.t. } A^{(t)}\mathbf{p} \notin K,$$
where $(\ell, m) = s^{-1}(t)$.
- `first`$((K, \mathbf{q}), A^{(t)})$: let $(\ell, m) = s^{-1}(t+1)$ and initialize
$$B^{(t+1)} \leftarrow A^{(t)},$$
$$J_\ell := \mathbb{Z}_n \setminus \Big\{B^{(t+1)}(\ell, j) : j = 0, 1, \ldots, m-1\Big\}. \tag{5.74}$$
Set $B^{(t+1)}(\ell, m) \leftarrow \max J_\ell$ as in Definition 5.49 and return $B^{(t+1)}$.
- `next`$((K, \mathbf{q}), A^{(t)}, B^{(t+1)})$: let $(\ell, m) = s^{-1}(t+1)$ and compute J_ℓ by (5.74). Return null if $B^{(t+1)}(\ell, m)$ equals $\min J_\ell$ as in Definition 5.49. Otherwise initialize $C^{(t+1)} \leftarrow B^{(t+1)}$, set $C^{(t+1)}(\ell, m)$ to be the element in J_ℓ that is *immediately* smaller than $B^{(t+1)}(\ell, m)$, and return $C^{(t+1)}$.

5.4 Programming assignments

A. Write a program to implement the recursive algorithm in Definition 5.50 and test your implement for $\mathrm{D} = 2, 3$ and $n = 2, 3, 4, 5$. In designing the tests $(K, \mathbf{q})$, use a simply connected polygon/polyhedron to derive K by declaring that any point covered by the polygon/polyhedron is not available. Display the generated poised lattices for both two and three dimensions.