FMM Data Structures

Nail Gumerov &
Ramani Duraiswami
UMIACS
[gumerov][ramani]@umiacs.umd.edu

Content

Reference:

N.A. Gumerov, R. Duraiswami & E.A. Borovikov

Data Structures, Optimal Choice of Parameters, and Complexity Results for Generalized Multilevel Fast Multipole Methods in *d* Dimensions

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AVAILABLE ONLINE VIA http://www.umiacs.umd.edu/~gumerov
http://www.umiacs.umd.edu/~ramani

Introduction

FMM Data Structures

- Since the complexity of FMM should not exceed $O(N^2)$ (at $M \sim N$), data organization should be provided for efficient numbering, search, and operations with these data.
- Some naive approaches can utilize search algorithms that result in $O(N^2)$ complexity of the FMM (and so they kill the idea of the FMM).
- In d-dimensions $O(N \log N)$ complexity for operations with data can be achieved.

FMM Data Structures (2)

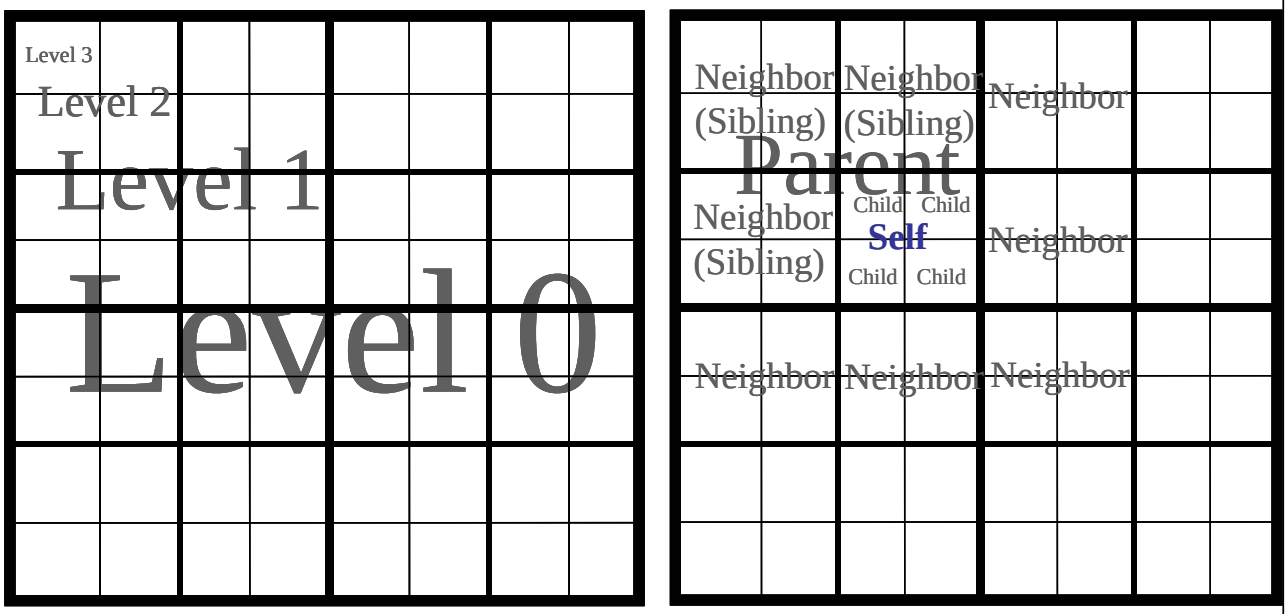
- Approaches include:
  - Data preprocessing
    - Sorting
    - Building lists (such as neighbor lists): requires memory, potentially can be avoided;
    - Building and storage of trees: requires memory, potentially can be avoided;
  - Operations with data during the FMM algorithm execution:
    - Operations on data sets;
    - Search procedures.
- Preferable algorithms:
  - Avoid unnecessary memory usage;
  - Use fast (constant and logarithmic) search procedures;
  - Employ bitwise operations;
  - Can be parallelized.
- Tradeoff Between Memory and Speed

Space Subdivision with 2^d-Trees

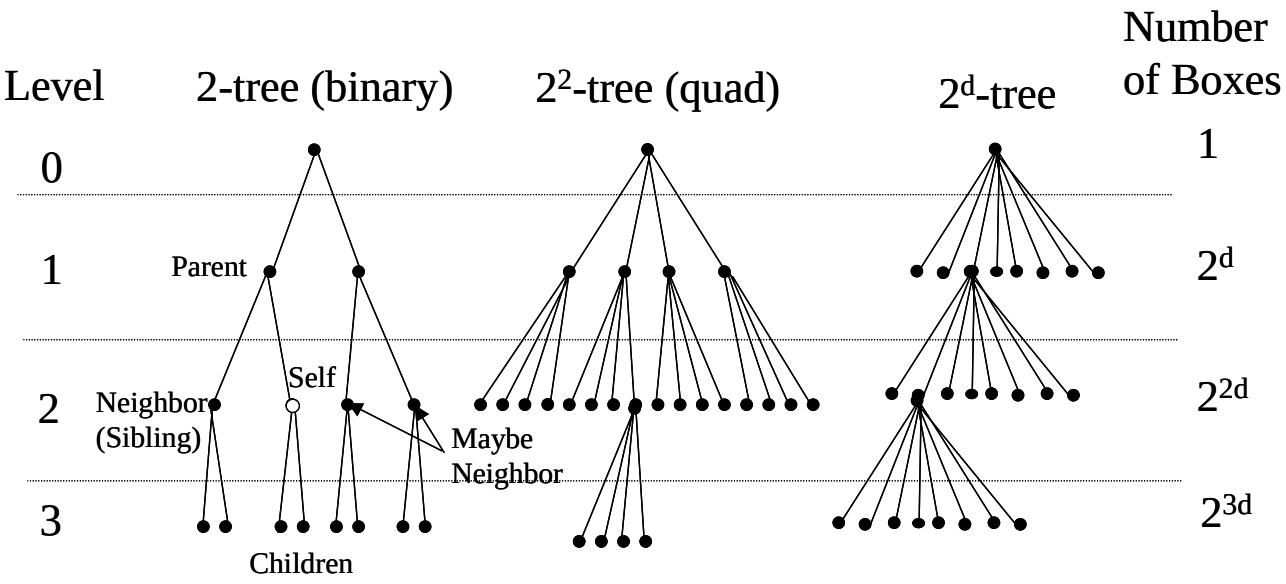
Historically:

- Binary trees (1D), Quadtrees (2D), Octrees (3D);
- We will consider a concept of 2^d-tree.
  - d=1 – binary;
  - d=2 – quadtree;
  - d=3 – octree;
  - d=4 – hexatree;
  - and so on..

Hierarchy in 2^d-tree

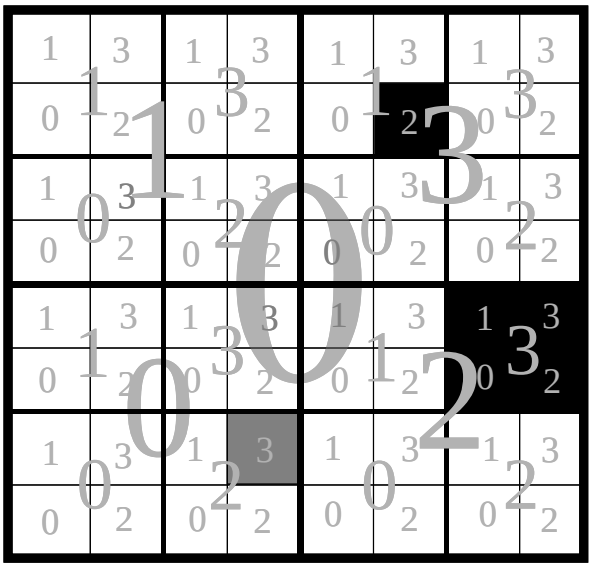


2^d-trees



Hierarchical Indexing

Hierarchical Indexing in 2^d-trees. Index at the Level.



Indexing in quad-tree

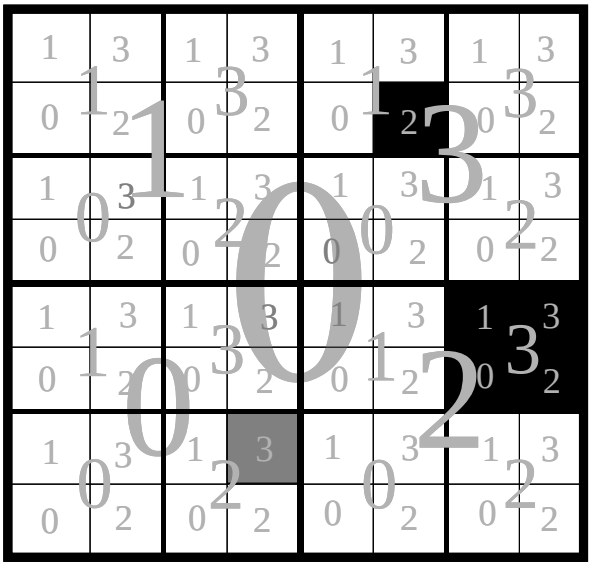
The large black box has the indexing string (2,3). So its index is $23_4=11_{10}$.

The small black box has the indexing string (3,1,2). So its index is $312_4=54_{10}$.

In general: Index (Number) at level l is:

$$Number = \left(2^d\right)^{l-1} \bullet N_1 + \left(2^d\right)^{l-2} \bullet N_2 + \ldots + 2^d \bullet N_{l-1} + N_l.$$

Universal Index (Number)



The large black box has the indexing string (2,3). So its index is $23_4=11_{10}$ at level 2

The small gray box has the indexing string (0,2,3). So its index is $23_4=11_{10}$ at level 3.

In general: Universal index is a pair:

$$UniversalNumber = (Number, l)$$

This index at this level

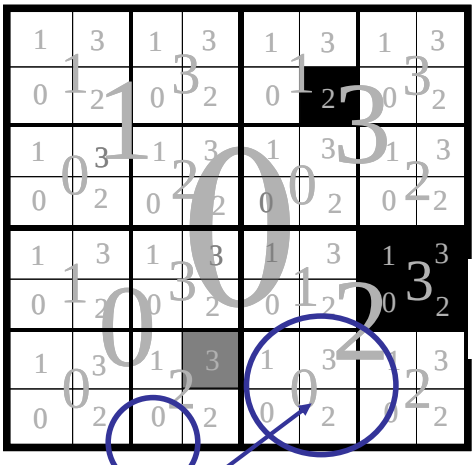
Parent Index

Parent's indexing string:

$$Parent(N_1, N_2, ..., N_{l-1}, N_l) = (N_1, N_2, ..., N_{l-1}).$$

Parent's index:

$$Parent(Number) = \left(2^d\right)^{l-2} \bullet N_1 + \left(2^d\right)^{l-3} \bullet N_2 + ... + N_{l-1}.$$



Parent index does not depend on the level of the box! E.g. in the quad-tree at any level

$$Parent(11_{10}) = Parent(23_4) = 2_4 = 2_{10}.$$

Parent's universal index:

$$Parent((Number, l)) = (Parent(Number), l-1).$$

Algorithm to find the parent number:

$$Parent(Number) = \left[Number/2^d\right]$$

For box #23 (gray or black) the parent box index is 2

Children Indexes

Children indexing strings:

$$Children(N_1,N_2,...,N_{l-1},N_l) = \{(N_1,N_2,...,N_{l-1},N_l,N_{l+1})\}, \quad N_{l+1} = 0,...,2^d - 1.$$

Children indexes:

$$Children(Number) = \left\{ \left(2^d\right)^l \bullet N_1 + \left(2^d\right)^{l-1} \bullet N_2 + ... + \left(2^d\right) \bullet N_l + N_{l+1} \right\}, \quad N_{l+1} = 0,...,2^d - 1.$$

Children indexes do not depend on the level of the box! E.g. in the quad-tree at any level:

$$Children(11_{10}) = Children(23_4) = \{230_4, 231_4, 232_4, 233_4\} = \{44_{10}, 45_{10}, 46_{10}, 47_{10}\}$$

Children universal indexes:

$$Children((Number, l)) = (Children(Number), l+1).$$

Algorithm to find the children numbers:

$$Children(Number) = \{2^d \bullet Number + j\}, \quad j = 0,...,2^d - 1,$$

A couple of examples:

Problem: Using the above numbering system and decimal numbers find parent box number for box #5981 in oct-tree.

Solution: Find the integer part of division of this number by 8. [5981/8] = 747.

Answer: #747.

Problem: Using the above numbering system and decimal numbers find children box numbers for box #100 in oct-tree.

Solution: Multiply this number by 8 and add numbers from 0 to 7.

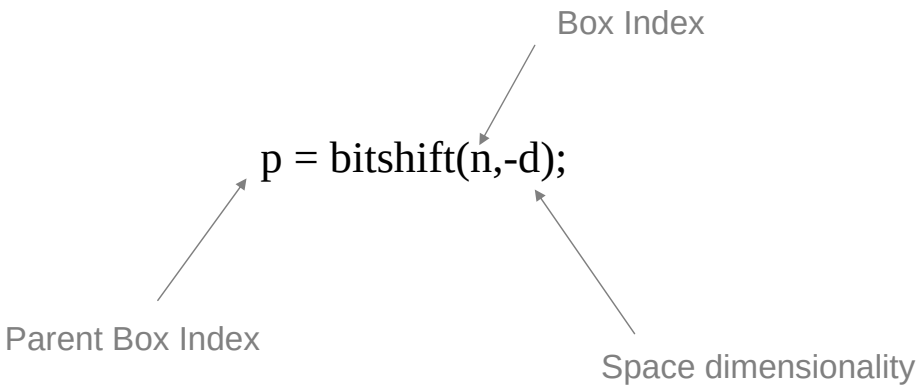
Answer: ##800, 801, 802, 803, 804, 805, 806, 807.

Can it be even faster?

YES!
USE BITSHIFT PROCEDURES!

(HINT: Multiplication and division by 2^d
are equivalent to d-bit shift.)

Matlab Program for Parent Finding



Binary Ordering

All $\bar{x} \in [0,1]$ naturally ordered and can be represented in decimal system as

$$\bar{x} = (0.a_1 a_2 a_3 \ldots)_{10}, \quad a_j = 0,\ldots,9; \quad j = 1,2,\ldots$$

Note that the point $\bar{x} = 1$ can be written not only $\bar{x} = 1.0000\ldots$, but also as

$$\bar{x} = 1 = (0.999999\ldots.)_{10}$$

We also can represent any point $\bar{x} \in [0,1]$ in binary system as

$$\bar{x} = (0.b_1 b_2 b_3 \ldots)_2, \quad b_j = 0,1; \quad j = 1,2,\ldots$$

By the same reasons as for decimal system the point $\bar{x} = 1$ can be written as

$$\bar{x} = 1 = (0.111111\ldots.)_2.$$

Finding the index of the box containing a given point

Level	Box Size (dec)	Box Size (bin)
0	1	1
1	0.5	0.1
2	0.25	0.01
3	0.125	0.001
...	...	...

Level 1:

$$(0.0b_1b_2b_3...)_2 \in Box((0)), \quad (0.1b_1b_2b_3...)_2 \in Box((1)), \quad \forall b_j = 0,1; \quad j = 1,2,...,$$

Level 2:

$$(0.00b_1b_2b_3...)_2 \in Box((0,0)), \quad (0.01b_1b_2b_3...)_2 \in Box((0,1)),$$
$$(0.10b_1b_2b_3...)_2 \in Box((1,0)), \quad (0.11b_1b_2b_3...)_2 \in Box((1,1)),$$
$$\forall b_j = 0,1; \quad j = 1,2,...,$$

Level l:

$$(0.N_1N_2...N_lb_1b_2b_3...)_2 \in Box((N_1,N_2,...,N_l)), \quad \forall b_j = 0,1; \quad j = 1,2,...$$

We use indexing strings !

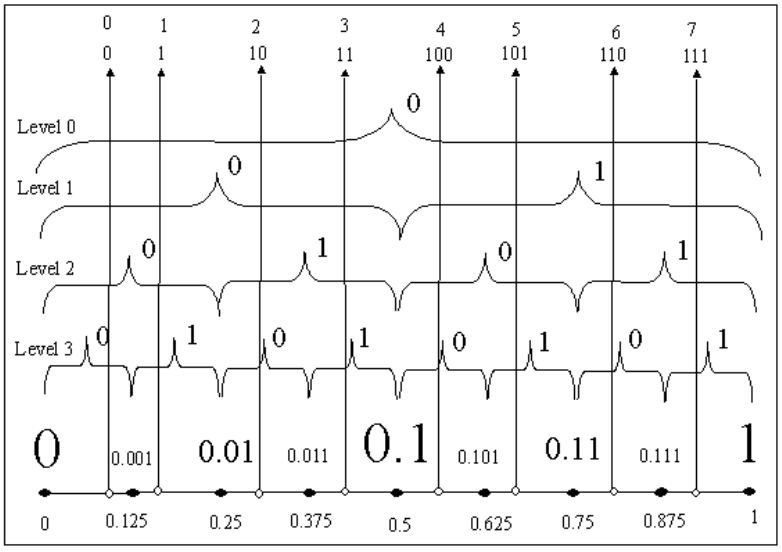
Finding the index of the box containing a given point (2)

$$(0.N_1N_2...N_lb_1b_2b_3...)_2 \rightarrow (N_1N_2...N_l.b_1b_2b_3...)_2; \quad N_1N_2...N_l = [(N_1N_2...N_l.b_1b_2b_3...)_2].$$

$$(Number, l) = \left[2^l \cdot \bar{x}\right].$$

This is an algorithm for finding of the box index at level l (!).

Faster method: Use bit shift and take prefix.



Finding the center of a given box.

For box number *Number* at level l the left boundary can be found by l –bit shift:

$$Number = (N_1 N_2 ... N_l)_2 \rightarrow (0.N_1 N_2 ... N_l)_2,$$

Add 1 as an extra digit (half of the box size), so we have for the center of the box at level l :

$$\bar{x}_c(Number, l) = (0.N_1 N_2 ... N_l 1)_2.$$

This procedure also can be written in the form that does not depend on the counting system:

$$\bar{x}_c(Number, l) = 2^{-l} \cdot Number + 2^{-l-1} = 2^{-l} \cdot (Number + 2^{-1}).$$

since addition of one at position $l+1$ after the point in the binary system is the same as addition of 2^{-l-1}.

Problem: Find the center of box #31 (decimal) at level 5 of the binary tree.

Solution: We have $\bar{x}_c(31,5) = 2^{-5} \cdot (31 + 0.5) = 0.984375$.

Answer: 0.984375.

This is the algorithm!

Neighbor finding

Due to all boxes are indexed consequently:

Neighbor((Number,level))=Number±1

If the neighbor number at level l equal 2^l or -1 we drop this box from the neighbor list.

Problem: Find all neighbors of box #31 (decimal) at level 5 of the binary tree.

Solution: The neighbors should have numbers $31 - 1 = 30$ and $31 + 1 = 32$. However, $32 = 2^5$, which exceeds the number allowed for this level. Thus, only box #30 is the neighbor.

Answer: #30.

Spatial Ordering Using Bit Interleaving

Bit Interleaving

Coordinates of a point $\bar{\mathbf{x}} = (\bar{x}_1, ..., \bar{x}_d)$ in the d-dimensional unit cube can be represented in binary form

$$\bar{x}_k = (0.b_{k1}b_{k2}b_{k3}...)_2, \quad b_{kj} = 0,1; \quad j = 1,2,..., \quad k = 1,...,d.$$

Instead of having d numbers characterizing each point we can form a single binary number that represent the same point by ordered mixing of the digits in the above binary representation (this is also called *bit interleaving*), so we can write:

$$\bar{\mathbf{x}} = (0.b_{11}b_{21}...b_{d1}b_{12}b_{22}...b_{d2}...b_{1j}b_{2j}...b_{dj}...)_2.$$

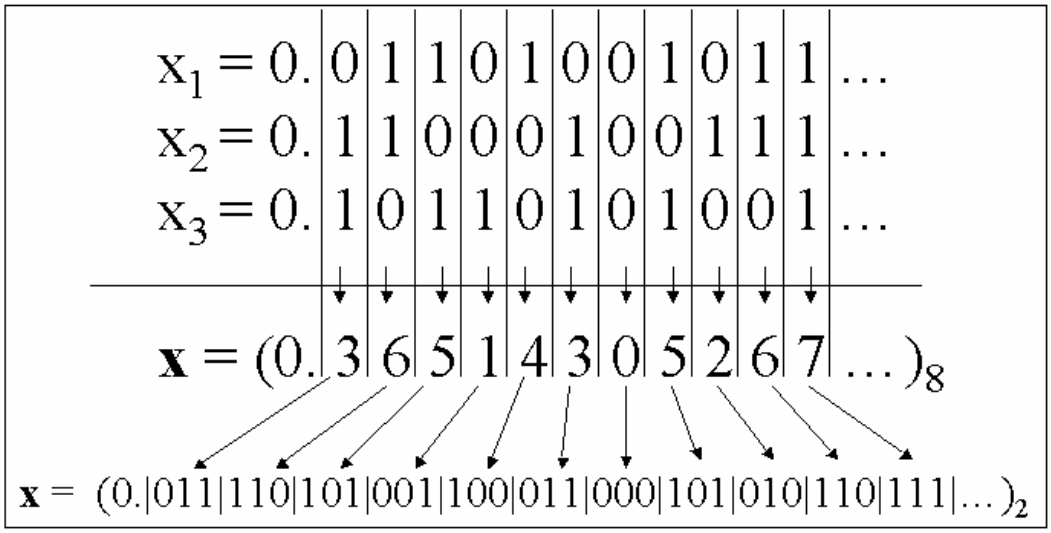
This number can be rewritten in the system with base 2^d:

$$\bar{\mathbf{x}} = (0.N_1N_2N_3...N_j...)_{2^d}, \quad N_j = (b_{1j}b_{2j}...b_{dj})_2, \quad j = 1,2,..., \quad N_j = 0,...,2^d - 1.$$

This maps $\mathbf{R}^d \rightarrow \mathbf{R}$, where coordinates are ordered naturally!

Example of Bit Interleaving.

Consider 3-dimensional space, and an octree.

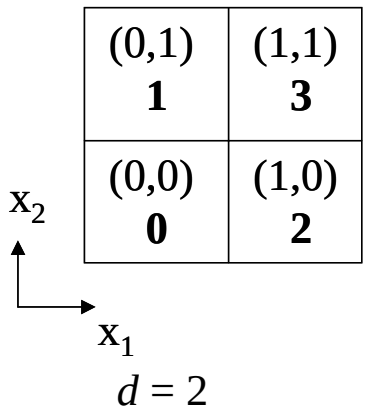


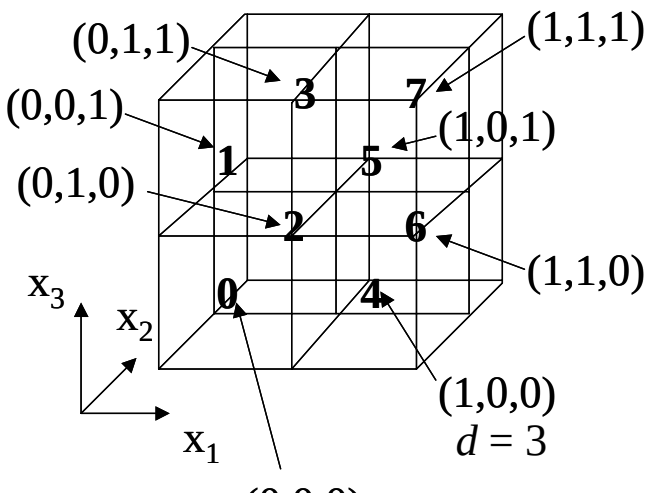
Convention for Children Ordering.

Any binary string of length d can be converted into a a single number (binary or in some other counting system, e.g. with the base 2^d):

$$(b_1, b_2, \ldots, b_d) \rightarrow (b_1 b_2 \ldots b_d)_2 = N_{2^d}.$$

This provides natural numbering of 2^d children of the box.





Finding the index of the box containing a given point.

Level 1:

$$\bar{\mathbf{x}} = (0.b_{11}b_{21}...b_{d1}b_{12}b_{22}...b_{d2}...b_{1j}b_{2j}...b_{dj}...)_2 \in Box((b_{11}b_{21}...b_{d1})_2) = Box((N_1)_{2^d}),$$

Let us use 2^d-based counting system. Then we can find the box containing a given point at Level l :

$$(0.N_1N_2...N_lc_1c_2c_3...)_{2^d} \in Box((N_1,N_2,...,N_l)_{2^d}), \quad \forall c_j = 0,...,2^d-1; \quad j = 1,2,...$$

Therefore to find the number of the box at level l to which the given point belongs we need simply shift the 2^d number representing this point by l positions and take the integer part of this number:

$$(0.N_1N_2...N_lc_1c_2c_3...)_{2^d} \to (N_1N_2...N_l.c_1c_2c_3...)_{2^d}; \quad N_1N_2...N_l = [(N_1N_2...N_l.b_1b_2b_3...)_{2^d}].$$

Finding the index of the box containing a given point. Algorithm and Example.

This procedure also can be performed in binary system by $d \cdot l$ bit shift:

$$(0.b_{11}b_{21}...b_{d1}b_{12}b_{22}...b_{d2}...b_{1l}b_{2l}...b_{dl}b...)_2 \to (b_{11}b_{21}...b_{d1}b_{12}b_{22}...b_{d2}...b_{1l}b_{2l}...b_{dl}.b...)_2;$$
$$Number = (b_{11}b_{21}...b_{d1}b_{12}b_{22}...b_{d2}...b_{1l}b_{2l}...b_{dl})_2.$$

In arbitrary counting system:

$$(Number, l) = \left[2^{dl} \cdot \bar{\mathbf{x}}\right].$$

Problem: Find decimal numbers of boxes at levels 3 and 5 of the oct-tree containing point $\bar{\mathbf{x}} = (0.7681, 0.0459, 0.3912)$.

Solution: First we convert the coordinates of the point to binary format, where we can keep only 5 digits after the point (maximum level is 5), so $\bar{\mathbf{x}} = (0.11000, 0.00001, 0.01100)_2$. Second, we form a single mixed number $\bar{\mathbf{x}} = 0.100101001000010_2$. Performing $3 \cdot 3 = 9$ bit shift and taking integer part we have $(Number, 3) = 100101001_2 = 297$. Performing $3 \cdot 5 = 15$ bit shift we obtain $(Number, 5) = 100101001000010_2 = 19010$.

Answer: #297 and #19010.

Bit Deinterleaving

Convert the box number at level l into binary form

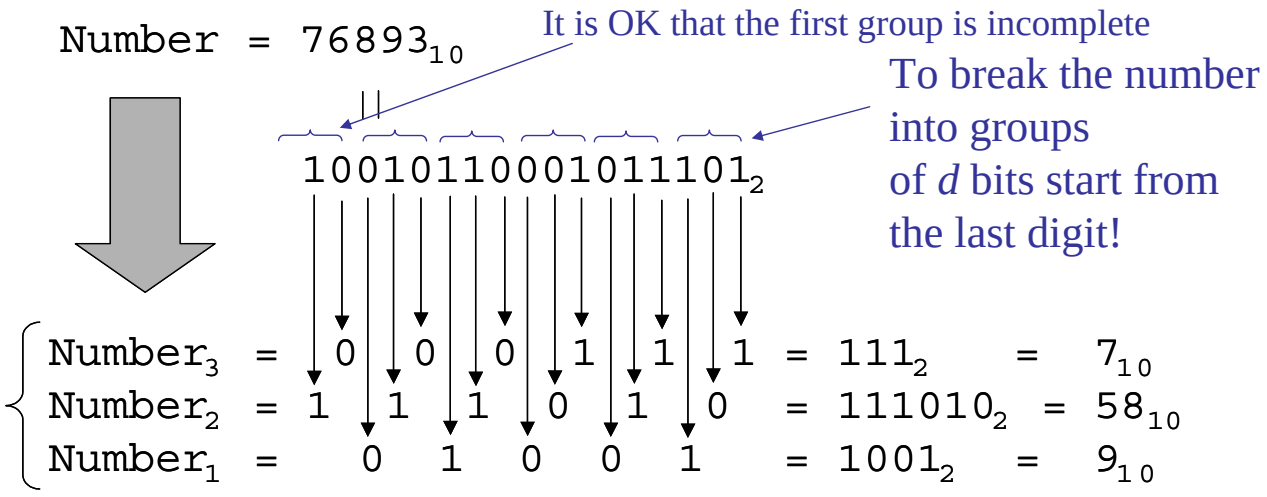
$$Number = (b_{11}b_{21}...b_{d1}b_{12}b_{22}...b_{d2}...b_{1l}b_{2l}...b_{dl})_2.$$

Then we decompose this number to d numbers that will represent d coordinates:

$$Number_1 = (b_{11}b_{12}...b_{1l})_2.$$
$$Number_2 = (b_{21}b_{22}...b_{2l})_2.$$
$$...$$
$$Number_d = (b_{d1}b_{d2}...b_{dl})_2.$$

.

Bit deinterleving (2). Example.



Finding the center of a given box.

Coordinates of the box center in binary form are

$$\bar{x}_{k,c}(Number, l) = (0.b_{k1}b_{k2}...b_{kl}1)_2, \quad k = 1,...,d.$$

or in the form that does not depend on the counting system:

$$\bar{x}_{k,c}(Number, l) = 2^{-l} \cdot Number_k + 2^{-l-1} = 2^{-l} \cdot \left(Number_k + \frac{1}{2}\right), \quad k = 1,...,d.$$

Problem: Find the center of box #533 (decimal) at level 5 of the oct-tree.

Solution: Converting this number to the bit string we have $533_{10} = 1000010101_2$. Retrieving the digits of three components from the last digit of this number we obtain: $Number_3 = 1001_2 = 9_{10}$, $Number_2 = 10_2 = 2_{10}$, $Number_1 = 1_2 = 1_{10}$. We have then $\bar{x}_{1,c}(533,5) = 2^{-5} \cdot (1 + 0.5) = 0.04875$, $\bar{x}_{2,c}(533,5) = 2^{-5} \cdot (2 + 0.5) = 0.078125$, $\bar{x}_{3,c}(533,5) = 2^{-5} \cdot (9 + 0.5) = 0.296875$.

Answer: $\bar{\mathbf{x}}_c = (0.04875, 0.078125, 0.296875)$.

Neighbor Finding

Step 1: Deinterleaving:

$$Number \rightarrow \{Number_1, ..., Number_d\}$$

Step 2: Shift of the coordinate numbers

$$Number_k^+ = Number_k + 1, \quad Number_k^- = Number_k - 1, \quad k = 1,...,d,$$

and formation of sets:

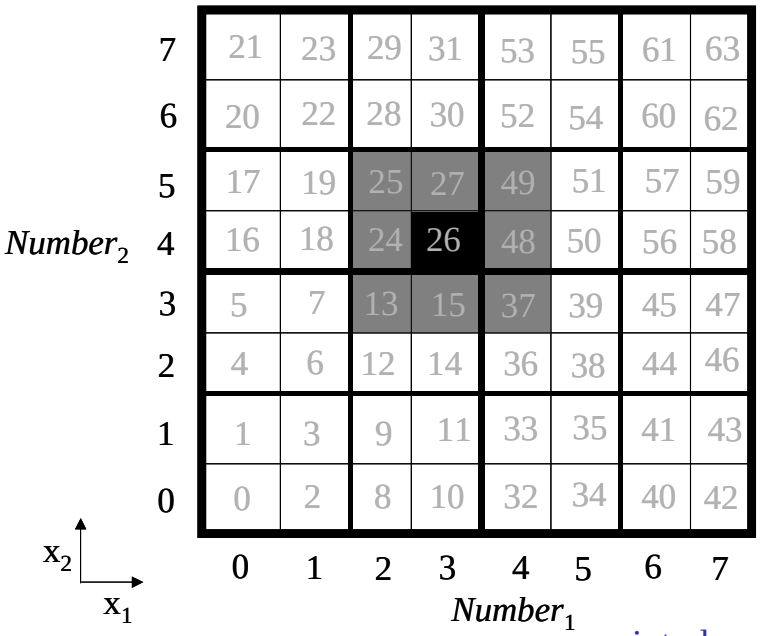
$$s_k = \begin{cases} \{Number_k^-, Number_k, Number_k^+\}, & Number_k \neq 0, 2^l - 1 \\ \{Number_k, Number_k^+\}, & Number_k = 0. \\ \{Number_k^-, Number_k\}, & Number_k = 2^l - 1. \end{cases} \qquad k = 1,...,d.$$

The set of neighbor generating numbers is then

$$n = (n_1, ..., n_d), \quad n_k \in s_k, \quad k = 1,...,d.$$

where each n_k can be any element of s_k , except of the case when all $n_k = Number_k$ simultaneously for all $k = 1,...,d$, since this case corresponds to the box itself.

Example of Neighbor Finding



$26_{10} = 11010_2$

deinterleaving

$(11,100)_2 = (3,4)_{10}$

generation of neighbors

(2,3) ,(2,4),(2,5),(3,3),
(3,5),(4,3),(4,4),(4,5)
=
(10,11),(10,100),(10,101),
(11,11),(11,101),(100,11),
(100,100),(100,101)

interleaving

1101,11000,11001,1111,11011,100101,110000,110001
= 13, 24, 25, 15, 27, 37, 48, 49

Spatial Data Structuring

Definitions

Data Collection.

Scaling and mapping finite d-dimensional data into a unit d-dimensional cube yields in a *collection* C of N points distributed inside such a cube:

$$\mathsf{C} = \{\bar{\mathbf{x}}_1, \bar{\mathbf{x}}_2, ..., \bar{\mathbf{x}}_N\}, \quad \bar{\mathbf{x}}_i \in [0,1) \times [0,1) \times ... \times [0,1) \subset \mathsf{R}^d, \quad i = 1, ..., N.$$

Data Set.

We call a collection $\mathsf{C} = \{\bar{\mathbf{x}}_1, \bar{\mathbf{x}}_2, ..., \bar{\mathbf{x}}_N\}$ "*data set*", if $\forall i \neq j$, $dist(\bar{\mathbf{x}}_i, \bar{\mathbf{x}}_j) \neq 0$, where $dist(\bar{\mathbf{x}}_i, \bar{\mathbf{x}}_j)$ denotes distance between $\bar{\mathbf{x}}_i$ and $\bar{\mathbf{x}}_j$.

Non-Separable (Multi-entry) Data Collection.

We call a collection $\mathsf{C} = \{\bar{\mathbf{x}}_1, \bar{\mathbf{x}}_2, ..., \bar{\mathbf{x}}_N\}$ "*non-separable data collection*", if $\exists i \neq j$, $dist(\bar{\mathbf{x}}_i, \bar{\mathbf{x}}_j) = 0$.

(By this definition a non-separable data collection cannot be uniquely ordered using distance function $dist(\bar{\mathbf{x}}_i, \bar{\mathbf{x}}_j)$).

Threshold Level

We call level $L_{th}(\mathsf{C})$ "*threshold level*" of data collection C if the maximum number of data points in a box for any level of subdivision $L > L_{th}(\mathsf{C})$ is the same as for $L_{th}(\mathsf{C})$ and differs from $L_{th}(\mathsf{C})$ for any $L < L_{th}(\mathsf{C})$.

Note: in case if C is a data set of power $N \geqslant 2$, then at level $L_{th}(\mathsf{C})$ we will have maximum one data point per box, and at $L < L_{th}(\mathsf{C})$ there exists at least 1 box containing 2 or more data points.

Spatial Data Sorting

Consider data collection **C**. Each point can be then indexed (or numbered):

$$\mathbf{v} = (v_1, v_2, ..., v_N), \quad v_i = Number(\bar{\mathbf{x}}_i, L), \quad i = 1, ..., N,$$

where *Number* can be determined using the algorithm described in the previous sections.

The array **v** then can be sorted for $O(N \log N)$ operations:

$$(v_1, v_2, ..., v_N) \rightarrow (v_{i_1}, v_{i_2}, ..., v_{i_N}), \quad v_{i_1} \leqslant v_{i_2} \leqslant ... \leqslant v_{i_N}.$$

using standart sorting algorithms. These algorithms also return the permutation index (other terminology can be permutation vector or pointer vector) of length N :

$$\mathbf{ind} = (i_1, i_2, ..., i_N),$$

that can be stored in the memory. In terms of memory usage the array **v** should not be rewritten and stored again, since **ind** is a pointer and

$$\mathbf{v}(i) = v_i, \quad \mathbf{ind}(j) = i_j, \quad \mathbf{v}(\mathbf{ind}(j)) = \mathbf{v}(i_j) = v_{ij}, \quad i,j = 1, ..., N,$$

so

$$\mathbf{v}(\mathbf{ind}) = (v_{i_1}, v_{i_2}, ..., v_{i_N}).$$

Spatial Data Sorting (2)

- Before sorting represent your data with maximum number of bits available (or intended to use). This corresponds to maximum level $L_{\text{available}}$ available (say [$L_{\text{available}} = BitMax/d$].
- In the hierarchical 2^d-tree space subdivision the sorted list will remain sorted at any level $L < L_{\text{available}}$. So the data ordering is required only one time.

After data sorting we need to find the maximum level of space subdivision that will be employed

In Multilevel FMM two following conditions can be mainly considered:

- At level L_{max} each box contains not more than s points (s is called clustering or grouping parameter)
- At level L_{max} the neighborhood of each box contains not more than q points.

The threshold level determination algorithm in $O(N)$ time

```
i = 0, m = s,
while m < N
  i = i + 1, m = m + 1;
  a = Interleaved(v(ind(i));
  b = Interleaved(v(ind(m));
  j = Bit_max + 1
  while a ≠ b
    j = j − 1;
    a = Parent(a);
    b = Parent(b);
    l_max = max(l_max, j);
  end;
end;
```

s is the clustering parameter

Binary Search in Sorted List

- Operation of getting non-empty boxes at any level L (say neighbors) can be performed with O(log$N$) complexity for any fixed d.
  - It consists of obtaining a small list of all neighbor boxes with O(1) complexity and
  - Binary search of each neighbor in the sorted list at level L is an $O(Ld)$ operation.
  - For small L *and* d this is almost $O(1)$ procedure.

Operations on Sets

Difference: $\mathbb{C} = \mathbb{A} \backslash \mathbb{B}$
Intersection: $\mathbb{C} = \mathbb{A} \cap \mathbb{B}$
Union: $\mathbb{C} = \mathbb{A} \cup \mathbb{B}$

Let $Pow(\mathbb{A}) = N, \quad Pow(\mathbb{B}) = M, \quad N \geqslant M,$

Then the complexity for sorted input/output:

$$\mathbb{A} \backslash \mathbb{B} : N$$
$$\mathbb{A} \cap \mathbb{B} : \min(N, M \log N)$$
$$\mathbb{A} \cup \mathbb{B} : N$$

Operations

$$Neighbors(\mathbb{W}; n, l) = NeighborsAll(n, l) \cap \mathbb{W}, \quad \mathbb{W} = \mathbb{X}, \mathbb{Y},$$
$$Children(\mathbb{W}; n, l) = ChildrenAll(n, l) \cap \mathbb{W}, \quad \mathbb{W} = \mathbb{X}, \mathbb{Y}.$$

are $O(\log N)$ operations for minimum memory requirements and $O(1)$ for sufficiently large memory.