Datascience

05 - Databases and SQL

Dávid Visontai
ELTE, Physics of Complex Systems Department
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Database server main operations

- Organized data storage in non-volatile memory
  - Data are indexed
- Execute queries
  - Optimize memory, IO and CPU during query execution
- Data modification
- Transaction processing
  - Long-running, concurrent execution of atomic operations
- Maintain data consistency
- Durable storage of data
  - Must survive partial system crash

The Types of Modern Databases

- Relational or non-relational

the popularity of non-relational databases is on the rise!

The choice depends on:

- Type of the data
- Structure of the data
- Data model
- Data store
- Use-case of your data

RDBMS

Relational databases emerged in the 70's to store data

- Originally for business applications

It is a collection of **tables** with **schema** that represents the fixed attributes and data types

Using **Structured Query Language** (SQL) statements RDBMS provide functionality for

- Reading
- Creating
- Updating
- Deleting data

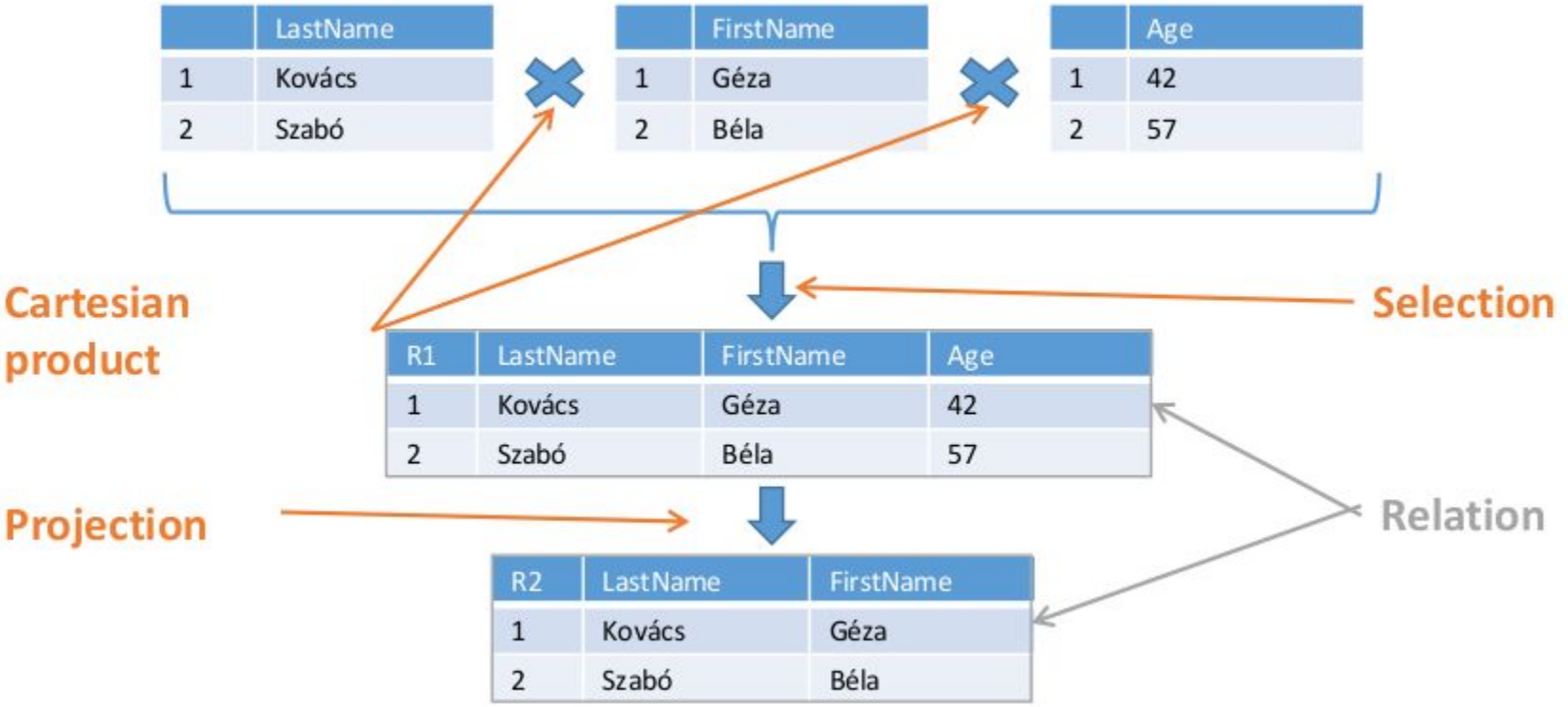
All RDBMS are **ACID-compliant**: **Atomicity, Consistency, Isolation,** and **Durability.**

Relational Data Model

- Set
  - One column of a table
  - Tuple of columns
- Operations
  - Cartesian product
  - Selection
  - Projection
  - Union, difference
- Schema
  - Constraints on which Cartesian products of the sets in what order can be taken
- Relation
  - Subset of a Cartesian product

Relational algebra

Tables with schema

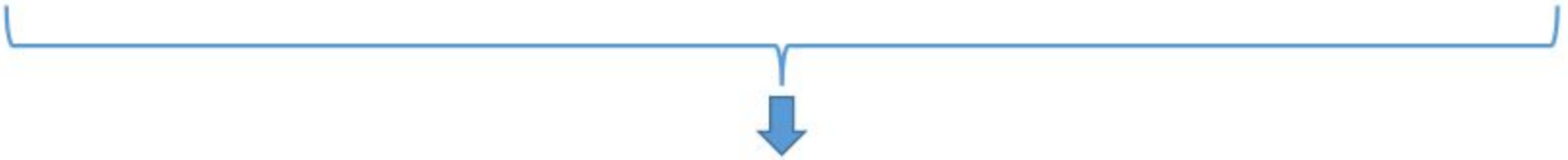


Relational algebra

Product of tables

ID	LastName	FirstName	Age
1	Kovács	Géza	42
2	Szabó	Béla	57

ID	Author	Title
1	1	Könyv 1
2	1	Könyv 2
3	2	Könyv 3



LastName	FirstName	Title
Kovács	Géza	Könyv 1
Kovács	Géza	Könyv 2
Szabó	Béla	Könyv 3

Logical data storage in SQL servers

- Tables are collections of data rows
- Table defines row format
- Data types
  - Fixed size: int, bigint, real, float, char(20), binary(250) etc.
  - Variable size: varchar(50), varbinary(250) etc.
  - BLOB (binary large object) text, ntext, varbinary(max), image etc. 2 GB maximum

Tables

- Table is the fundamental data storage entity of a database
  - Predefined set of columns
  - Any number of rows

Authors			
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- Column
  - Name
  - Data type: number, text, etc.
  - Variable/fix length for text
  - Constrains: unique, interval, auto increment etc.

- Row
  - Any number of rows in each table
  - Same data structure for each row

Constraints

- Primary Key
  - Unique identifier within a single table
  - Single column or combination of columns
- Foreign Key
  - A value in a column point to an ID in another table
- A single column or combination of columns
- Must be unique in the entire table
- Well-defined ordering
  - Multi-column: lexicographical ordering
  - Specify order direction for each column independently
  - Any two keys should be comparable: < or >
- Simplest key: incrementally generated integer ID

Authors

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Books

ID	Author	Title
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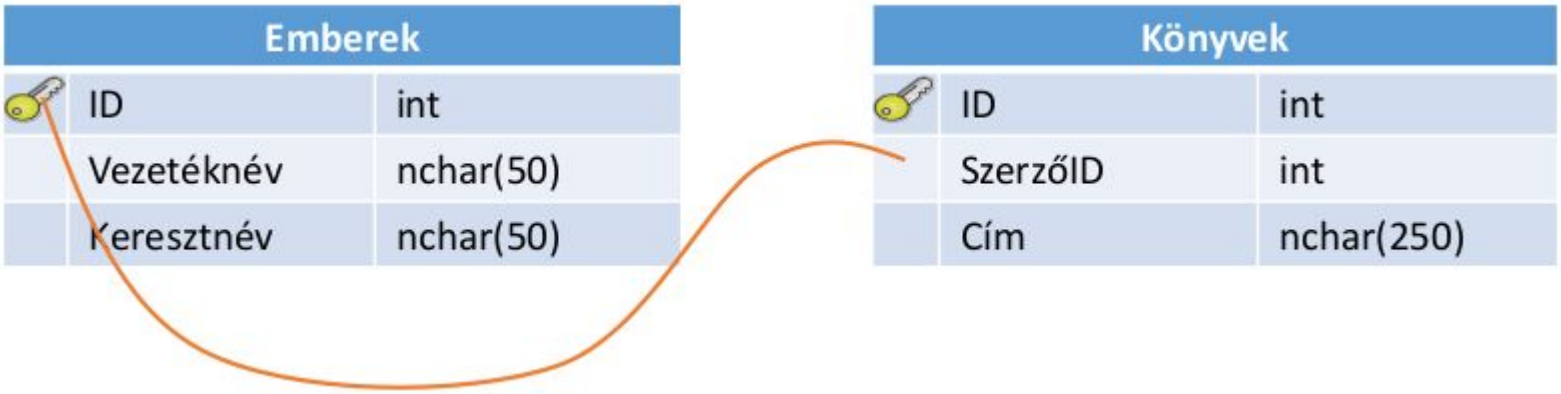
Primary key, foreign key



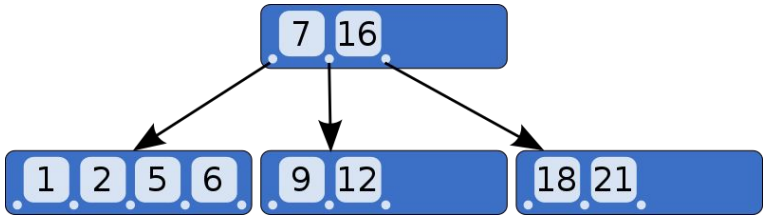
Indices

Indices allow logarithmic-time access to data

- A table can have only one clustered index
  - Determines the storage order for the entire table
  - Search and sort only by the primary key

B-tree and B+-tree

- Data structure to store ordered data
- Nodes: d data rows, d + 1 pointers
- Pointers point to additional rows



- When nodes are full, we split them into two
- Tree traversal using recursive algorithms
- Finding an item by key: o(logd)
- Tree can be scanned according to the ordering defined by the key (or in reverse order)
- Database servers: B+-tree
  a. only store keys in intermediate nodes
  b. Leaf nodes store actual data

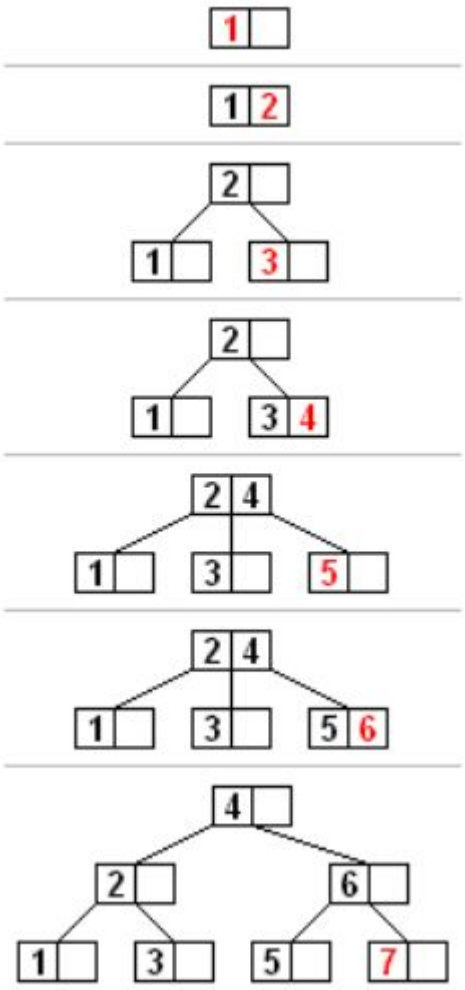
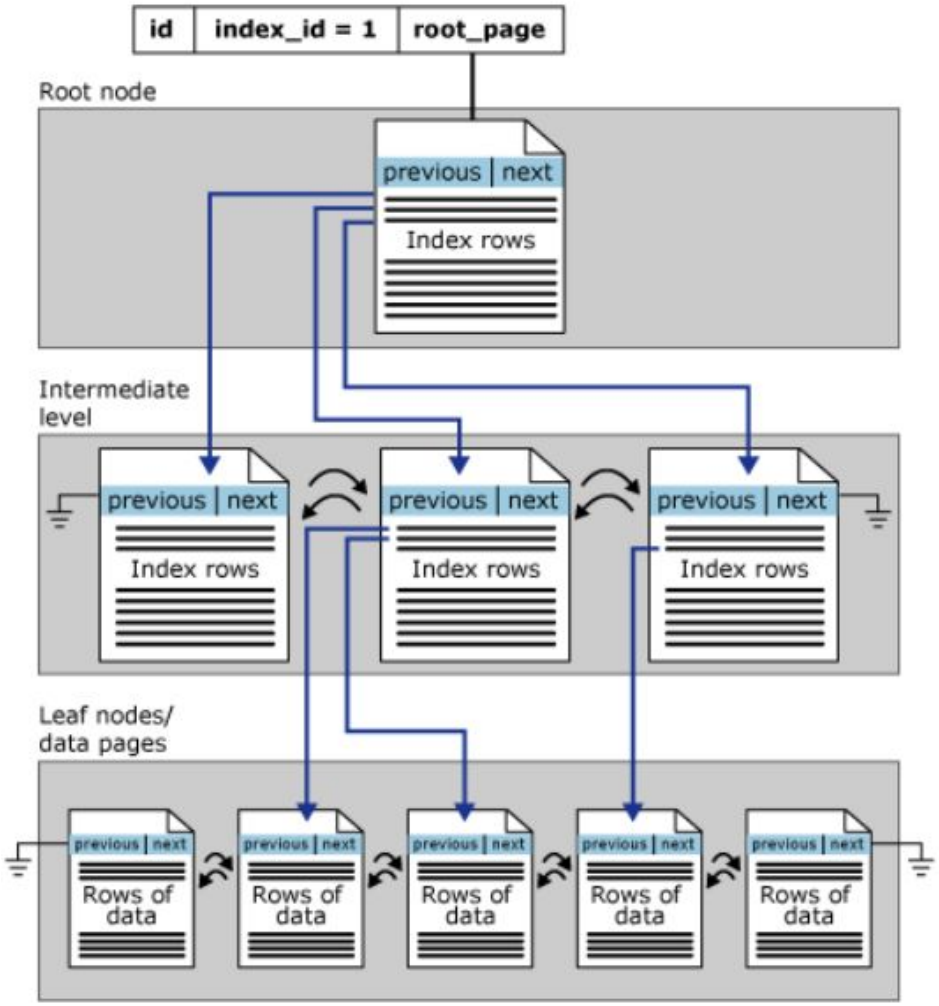


Table with clustered index

- Table stored as a B+-tree
- Tree node = data page
- Two page types
  - Index page
  - Leaf node page storing rows
- Pointers to prev/next page
  - Support sequential scan



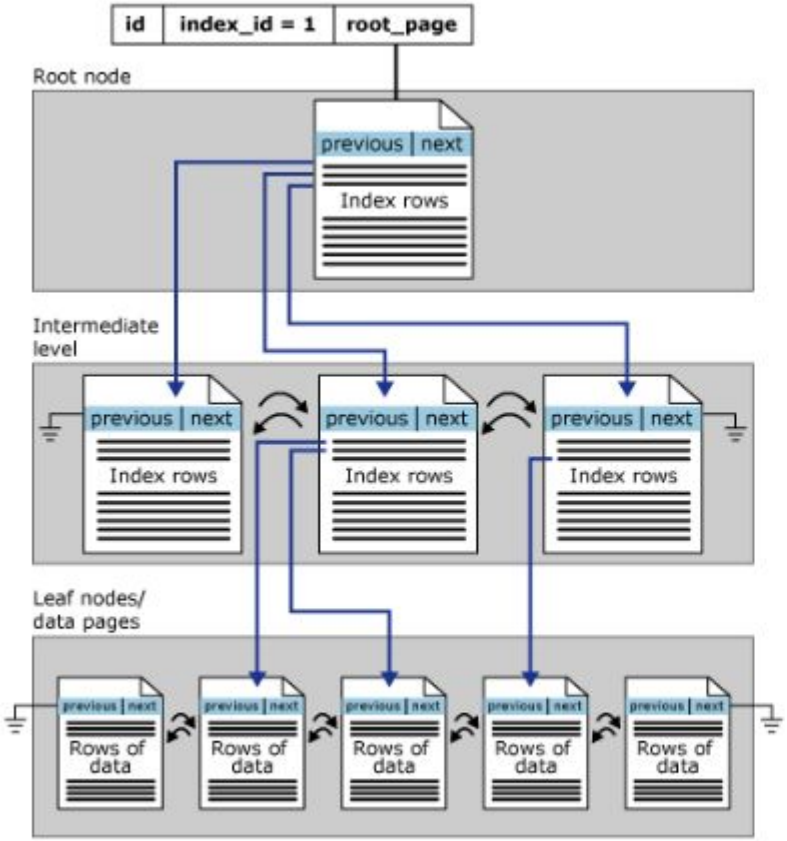
Advantage of clustered index

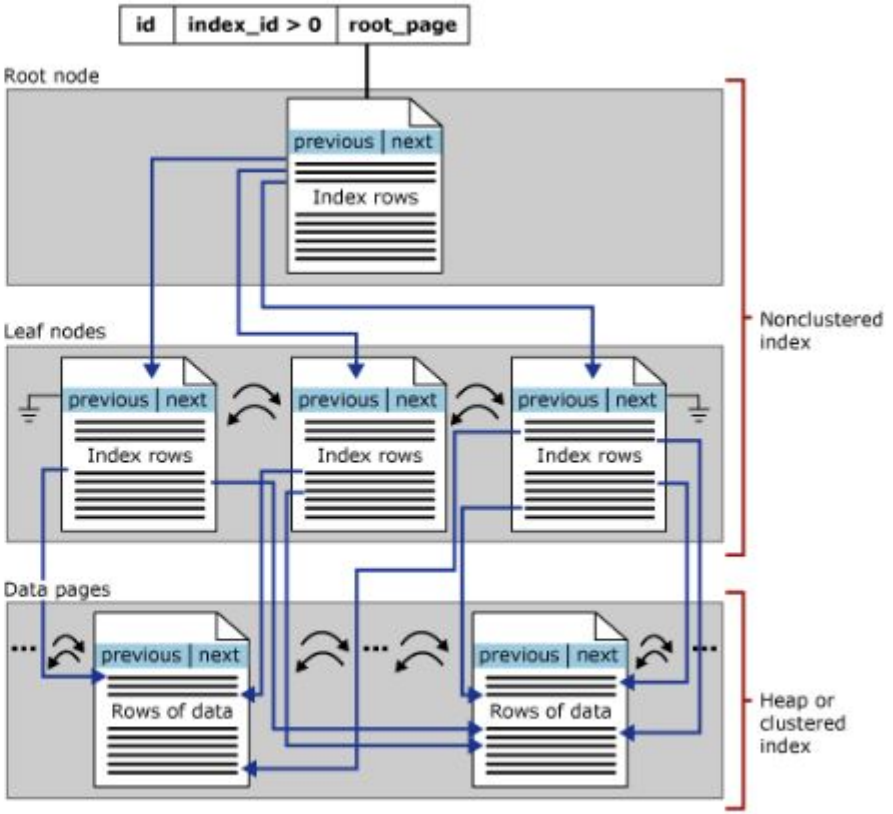
- Find row by key in n*log(n) time
  - SELECT * FROM t WHERE ID = 12
- Scan ID range very quickly
  - SELECT * FROM t WHERE ID BETWEEN 12 AND 36
- Read table in the order of the key (or in reverse)
  - Doesn’t require re-sorting!
  - SELECT * FROM t ORDER BY ID

Non-clustered indices

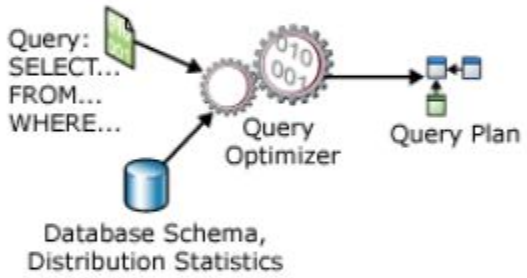
- What if we want to search by other columns?
- Additional data structure next to the table
- Built on one or more columns with given ordering
- Contains only indexed columns
- Pointers to data pages of the clustered index
- Can be unique
- Can implicitly contain non-indexed columns

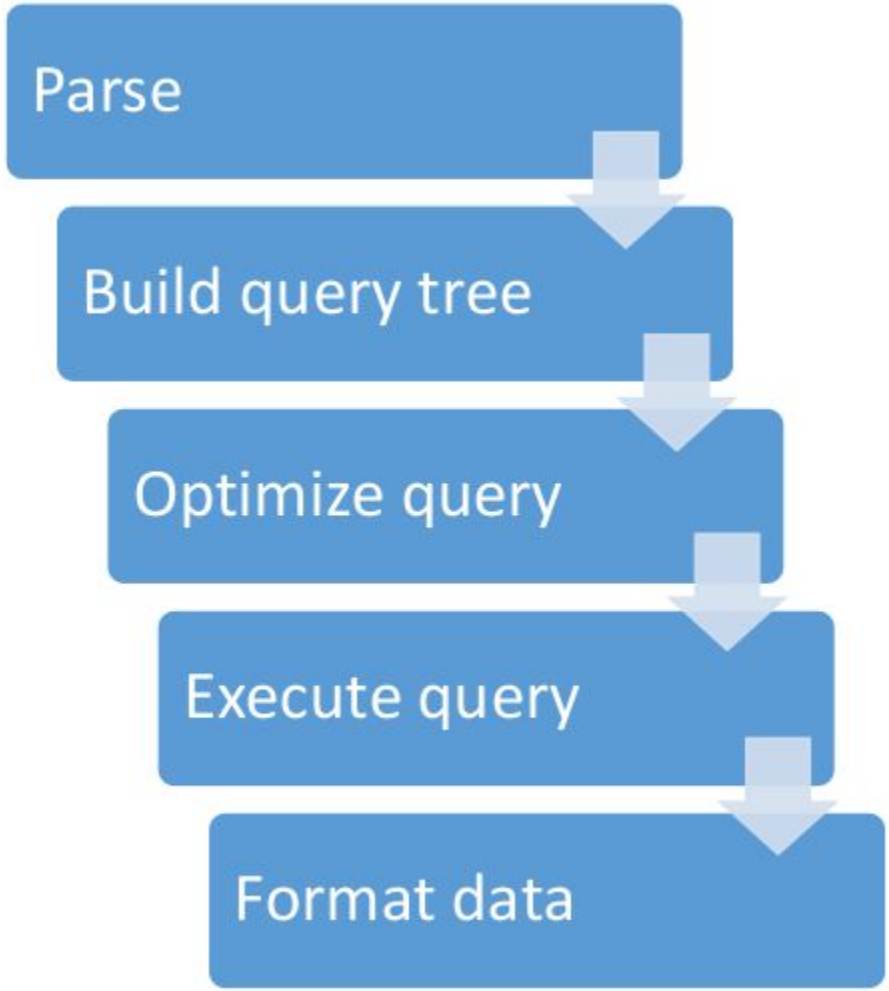
Clustered vs. Non clustered indices





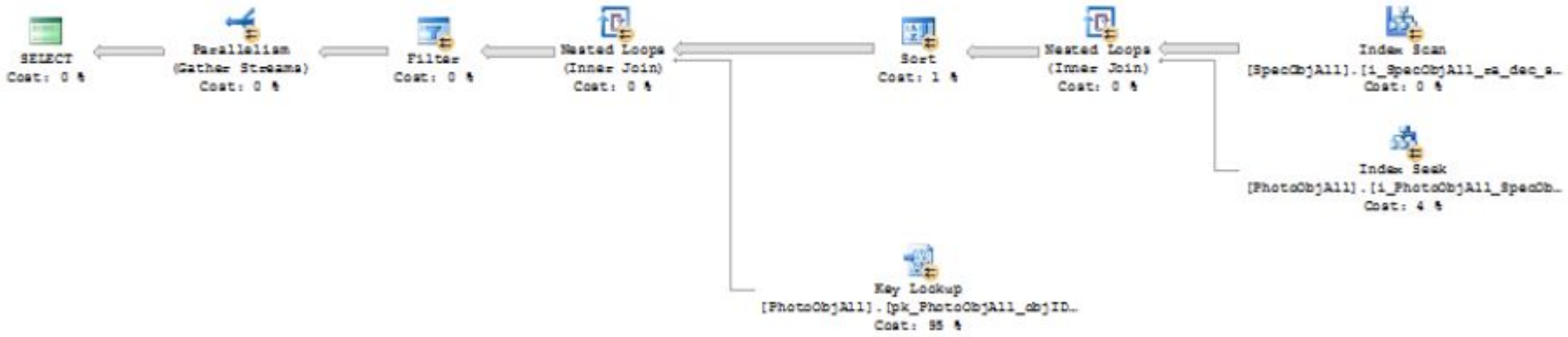
Steps of SQL query processing





Query plan example

```
SELECT s.SpecObjID, s.z
FROM   PhotoObjAll p
INNER JOIN SpecObjAll s
      ON p.SpecObjID = s.SpecObjID
WHERE p.dered_g < 17
```



You can also try http://retdb02.vo.elte.hu/basketball/

Physical operators: Table scan

- Table without any index
- Can be read only sequentially
- Have to read entire table
- No well-defined ordering
- Typical queries
  - SELECT * FROM t
  - SELECT * FROM t WHERE a = 2

Physical operators: Sort

- Table without ordering
- Output of another operator with wrong ordering
- Typical query
  - Table is not indexed by a

    > SELECT * FROM t ORDER BY a

- Have to sort rows
  - Quick sort with storage on disk
  - Algorithm optimized for large tables, still slow
- Sort happens in tempdb
  - Can be put on fast storage (SSD, NVME)

Physical operators: (Clustered) index scan

- Given a table t with an index on column c
- Column c contains unique values
- Scan range of key intervals

```
> SELECT c FROM t WHERE v BETWEEN 5 AND 10
```

- Order by index keys
  - Index defines an ordering
  - Different ordering always requires a sort

```
> SELECT c FROM t ORDER BY c
```

- Clustered index: contains all columns
- Non clustered index: only key and included columns
  - Querying other columns requires a bookmark lookup in clustered index
  - Results in random reads, slow

Physical operators: (Clustered) index seek

- Given a table t with index on column c
- Column c contains unique values
- Typical query

```
> SELECT c FROM t WHERE c = 12
```

- Finding a single row by ID
  - Table scan:o(N)
  - Index seek: o(log(N))
- If column c is not unique: index scan instead of seek
- Index seek mostly used for
  - Filtering by key
  - Joins on foreign keys (see later)

Physical operators: Bookmark (key) lookup

- Given a table t with non-clustered index on column c
- Query column d which is not part of the index

```
> SELECT d FROM t WHERE c BETWEEN 2 AND 10
```

- Rows found quickly using index on c
  - Index contains only pointers to the rows
  - Column d needs to be read from clustered index
  - Fetch row by primary key or bookmark (heap tables)

- Expensive operation, scans result in random IO

Logical join operations

- Relational algebra: a join is simply a subset of the Cartesian product of two tables

CROSS JOIN: entire Cartesian product

```
SELECT *
    FROM t1 CROSS JOIN t2
```

INNER JOIN: only rows satisfying join condition

```
SELECT *
    FROM t1 INNER JOIN t2 ON f(t1.c1, t2.c2)
```

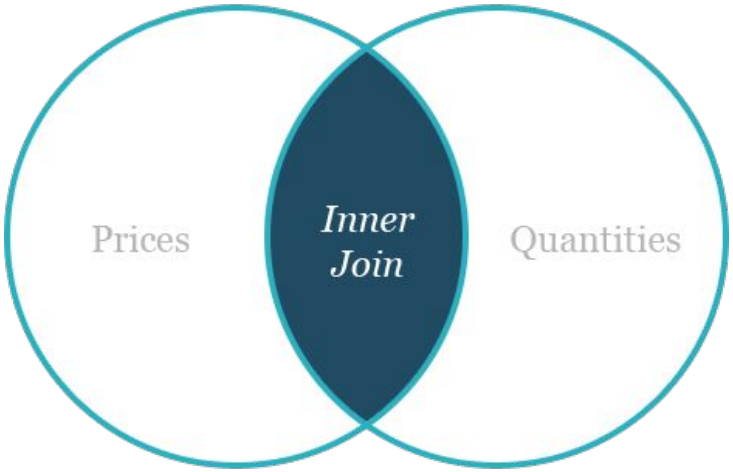


TABLE 1: PRICES

PRODUCT	PRICE
Potatoes	$3
Avocados	$4
Kiwis	$2
Onions	$1
Melons	$5
Oranges	$5
Tomatoes	$6

TABLE 2: QUANTITIES

PRODUCT	QUANTITY
Potatoes	45
Avocados	63
Kiwis	19
Onions	20
Melons	66
Broccoli	27
Squash	92

```
SELECT Prices.*, Quantities.Quantity
FROM Prices INNER JOIN Quantities
ON Prices.Product = Quantities.Product;
```

QUERY RESULT FOR INNER JOIN

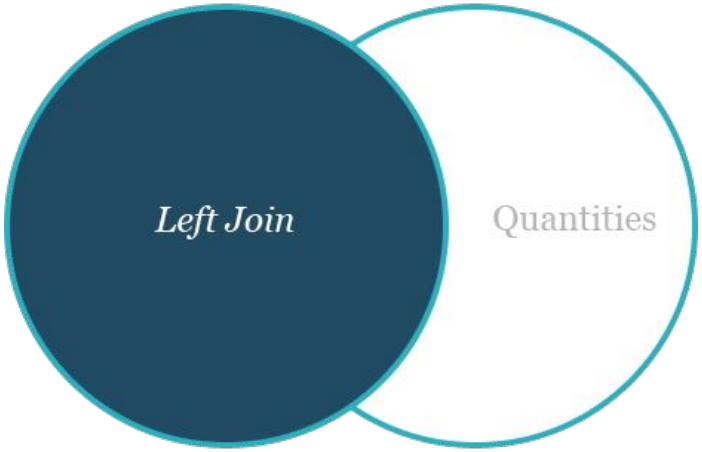
PRODUCT	PRICE	QUANTITY
Potatoes	$3	45
Avocados	$4	63
Kiwis	$2	19
Onions	$1	20
Melons	$5	66

Logical join operations

LEFT(RIGHT) OUTER JOIN

- Take all rows from left (right) table
- regardless if join condition is not satisfied
- Fill non-matches with NULL values

```
SELECT *
    FROM t1 LEFT OUTER JOIN t2 ON f(t1.c1, t2.c2)
```



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Broccoli	27
Squash	92

```
SELECT Prices.*, Quantities.Quantity
FROM Prices LEFT OUTER JOIN Quantities
ON Prices.Product = Quantities.Product;
```

QUERY RESULT FOR LEFT OUTER JOIN

PRODUCT	PRICE	QUANTITY
Potatoes	$3	45
Avocados	$4	63
Kiwis	$2	19
Onions	$1	20
Melons	$5	66
Oranges	$5	NULL
Tomatoes	$6	NULL

Additional logical join types

SEMI JOIN

- Only check if row exists in the other table

  > SELECT * FROM t1 WHERE t1.c1 IN (SELECT t2.c2 FROM t2)

ANTI JOIN

- Returns rows that are not in another table

  > SELECT * FROM t1

  WHERE t1.c1 NOT IN (SELECT t2.c2 FROM t2)

  > SELECT t1.*

  FROM t1 LEFT OUTER JOIN t2 ON f(t1.c1, t2.c2)

  WHERE t2.c2 IS NULL

Additional join types

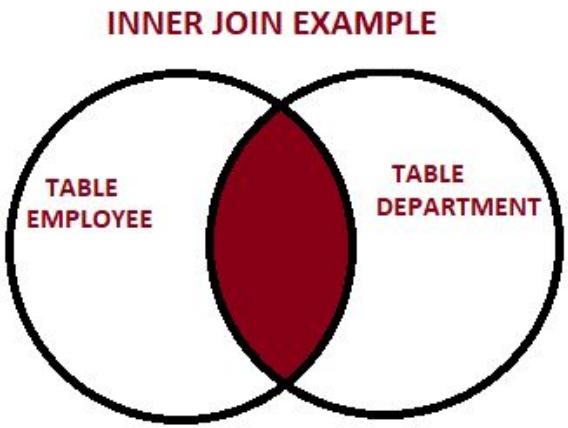
Range join

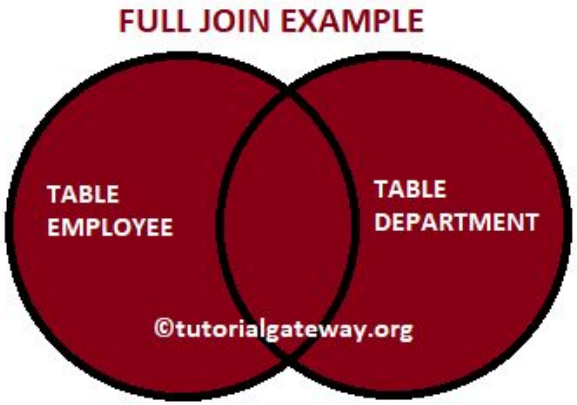
- If query restricts key not to a unique value but to a range
- Filter by interval

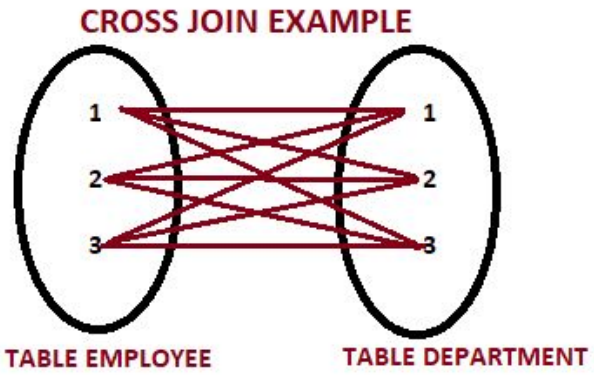
```
> SELECT *

    FROM t1 INNER JOIN t2

    t1.ID BETWEEN t2.start AND t2.end
```

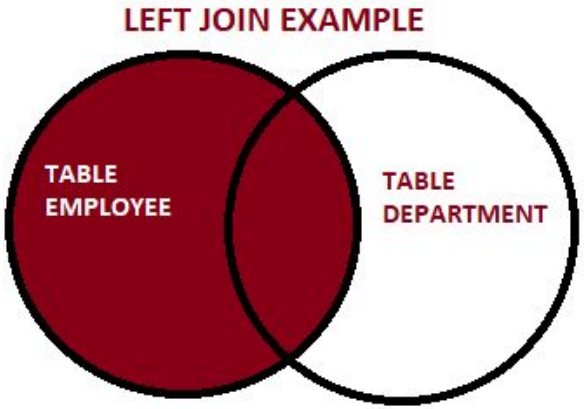
- Will be important for hierarchical spatial indices

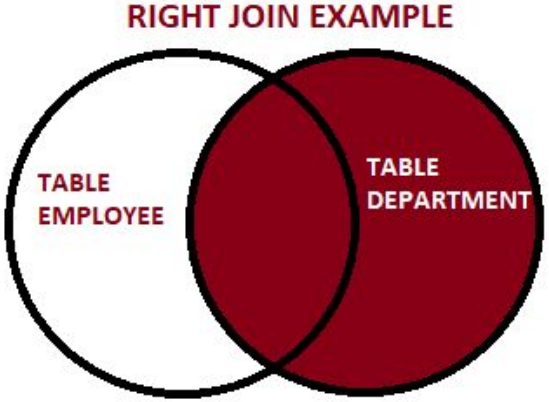
Join operations

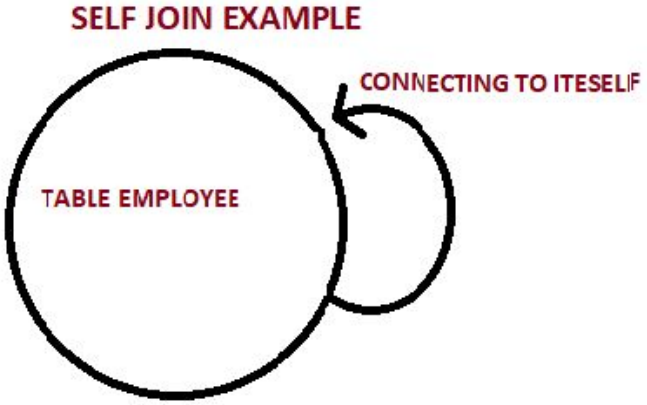












Aggregates

- COUNT(*), MIN, MAX, AVG, SUM, STDEV
- GROUP BY, HAVING
- User-defined aggregates
- Have to implement three functions
  - Accumulate: process next row
  - Merge: merge results from two threads
  - Terminate: calculate final result
- Aggregates must be computable with this simple model

An example: averaging

```
void Accumulate(avgstate a, double v)
{
        a.count ++;
        a.v += v;
}

void Merge(avgstate a, avgstate b)
{
        a.count += b.count;
        a.v += b.v;
}

double Terminate(avgstate a)
{
        return a.v / a.count;
}
```

Group by operations

- Hash match
  - If the table is small enough
  - Hash table stores status of each aggregate group
- Stream aggregate
  - Read table in the order of GROUP BY clause
  - Requires an appropriate index
  - Rows can be aggregated sequentially
  - No need to keep more than one aggregate group in memory

Employee

EmployeeID	Ename	DeptID	Salary
1001	John	2	4000
1002	Anna	1	3500
1003	James	1	2500
1004	David	2	5000
1005	Mark	2	3000
1006	Steve	3	4500
1007	Alice	3	3500

SELECT *DeptID, AVG(Salary)*
FROM *Employee*
GROUP BY *DeptID;*

GROUP BY Employee Table using DeptID

DeptID	AVG(Salary)
1	3000.00
2	4000.00
3	4250.00

Query optimization

The query optimization problem

- SQL language is declarative
  - We specify what we want in the results
  - Not how we want the results to be computed
- Information available to the server
  - The SQL query itself (WHERE, JOIN, GROUP BY, ORDER BY)
  - Database schema: tables, columns, keys, storage model
  - Non-clustered and clustered indices
  - Index statistics (histogram of key distribution)
  - Available memory, number of CPUs
- Server implements numerous phyisical operators
- SQL query can be processed many ways
  - Server enumerates possible query plans solving the same problem
  - Many query plans yield the same results
  - Tries to find the one with the shortest execution time

Manual query optimization

- Query optimization is a large area of research
- Server can only use information available to it
  - (Usually) doesn't build new indices automatically
  - Can sort a resultset, if necessary
- How can we help the server?
  - Try to collect all possible queries
  - Design indices to support possible queries
  - Define physical operators explicitly by query hints

Index selection

- Primary selection aspects
  - I**ndex contains all required columns** to answer the query
  - Included columns can help a lot here
  - **Index** must be **ordered** according to the query
  - Pick the smallest index, if there are multiple choices

- Determine I/O requirements
  - Required columns are listed in the SQL query
  - Need to estimate number of rows from index statistics
  - Sequential scan is cheap, random seek is expensive

Transaction

- Data modification consisting of multiple steps
- Many transactions are done concurrently

- **Atomicity**
  Transactions either finishes completely or nothing happens at all
- **Consistency**
  Transactions can take the database from consistent state to another consistent state only
- **Isolation**
  Concurrently running transactions might interfere with each other but only up to a certain, user-defined limit
- **Durability**
  Once a transaction is reported to be complete, it cannot be rolled back

Transaction

Transaction interference

- How many concurrent transactions can interfere with each other
- What state of the database is visible to a transaction
- Can changes made by a concurrent transaction be seen?
- What type of changes affect concurrent transactions?

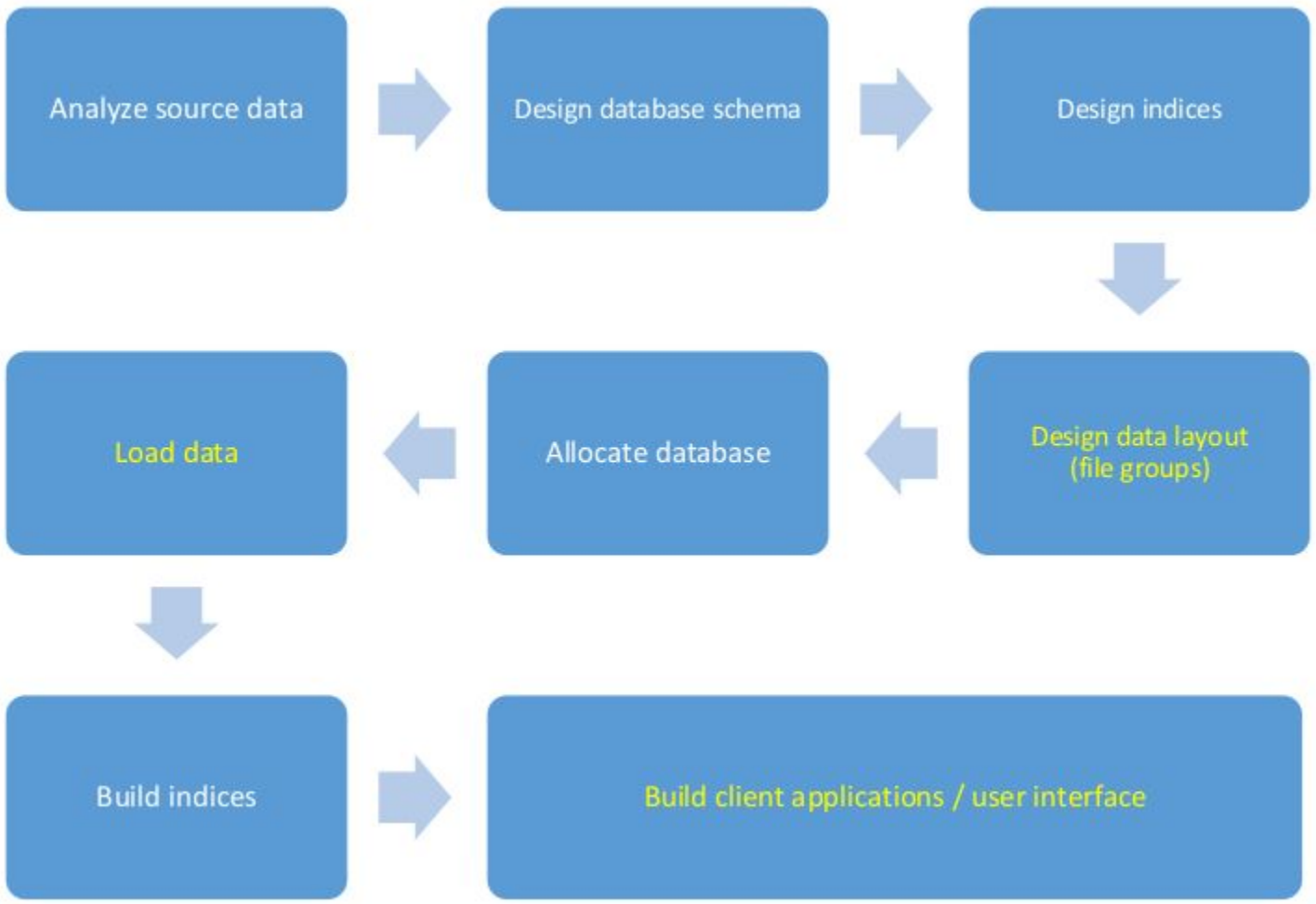
Transaction

Isolating transactions

- Goal: run many transactions in parallel but keep data integrity

- **Locking and Versioning**

Typical loading pipeline steps



Metadata

- Additional data belonging to tables and columns
- What is the data about?
  - Have to know exactly what all those numbers and strings mean
  - e.g. wavelength in vacuum or air?
  - Automatic conversion between unit systems?
  - Derived quantities? e.g. energy/wavelength/velocity
  - Measurement instructions: exact description of measuring process and calculations
  - Data quality information: Measurement errors, covariances
  - Provenance information: need to characterize veracity, reliability of data

- Need semantic information
  - Additional data about the data schema
  - Connect data model with reality

- Meta data need to be standardized for each field of science
  - Not only data format
  - Data models + meta data + ontology
  - Fundamental for easy sharing of complex data

- Display on web page of database

Meta data in databases

- Column name is not enough
- SQL Server
  - Supports extended properties (EP)
  - Every object of the schema can be tagged with EPs
  - EPs can be queries with standard SQL

- Include meta data in create table scripts
  - e.g. XML comments
  - Simple parser to process scripts and generate meta data

- Meta data on the user interface
  - Web site can automatically generate documentation from meta data

Data provenance

- Provenance: originally the history of an object, piece of art etc.

- Knowing the source of data is fundamental
  - How much data can be trusted
  - What if we just downloaded from the Internet
  - How measurement were made
  - How derived quantities were calculated

Data warehouse registry

- A data warehouse can contain hundreds of databases
- Need a thorough description of everything
  - Hardware: what machines where
  - Software configuration of machines
  - Databases: where what data in what format

- Where to direct a computation given its data and processing requirements
  - Minimize data movement

- Services available

Fundamental problems of databases in general

- Data is much bigger than the main memory
- Non-volatile storage is always much slower than the main memory and the CPU
- Sequential disk access is much faster than random
  - Store data in order, indexed
- Data processing algorithms
  - Optimize for sequential data access
  - Optimize memory for size, access pattern and NUMA
  - Fast or no transformation between in-memory and disk data formats

Goals with distributed databases

- Split large database among many servers: sharding
- Replicate data instead of back ups
  - Many options to achieve redundancy
- Mirror databases
  - Parallelize queries for higher IO throughput
  - Higher availability
  - Load balancing
- Regular data loading tasks
  - Dedicated load servers
  - Bulk insert, data validation, sorting
  - Faster to write storage

Data loading

Jim Gray's laws for data warehouse design

- Lots of data -> one server won't be enough
  - Scale out to multiple machines instead of scale up
  - Many machines instead of big iron
  - Easy management and expansion are very important
- Take computation to the data, not the data to the CPU
  - Moving data around takes much more time than processing
  - Try to solve problems within the database server, using SQL
  - Build servers with large storage and big CPUs
- What are the 20 most important queries you want to answer?
  - In a generic data warehouse, queries are not known beforehand
  - Users (scientists) come up with their own ideas
  - Optimize databases for the 20 queries
- Develop system gradually, from working version to working
  - Scientists want a working system as soon as possible
  - Don't rush forward and add unstable features

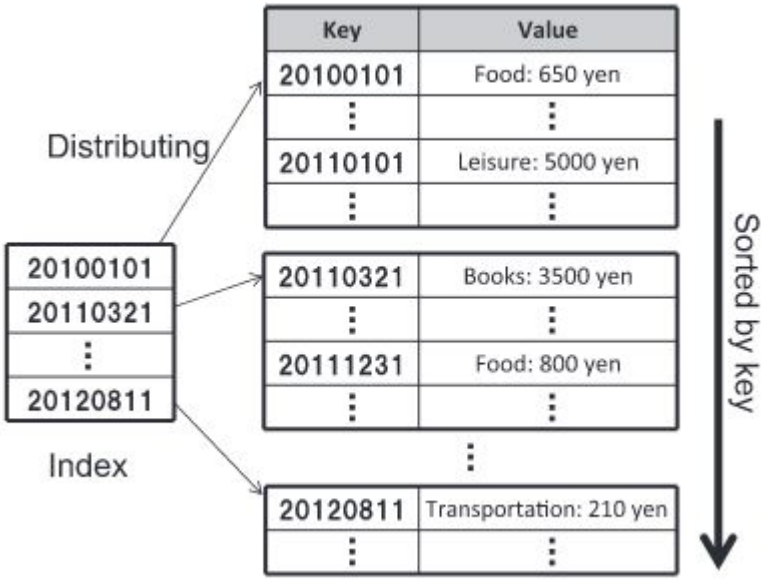
NoSQL / Non-relational databases

Alternative to RDBMS as web applications became increasingly complex

NoSQL databases can be schema agnostic, allowing unstructured and semi-structured data to be stored and manipulated.

Key-Value Stores, (Redis, Amazon DynamoDB)

- extremely simple
- store only key-value pairs
- provide basic functionality for retrieving the value associated with a known key.
- stored data is **not particularly complex**
- **speed** is of paramount importance.

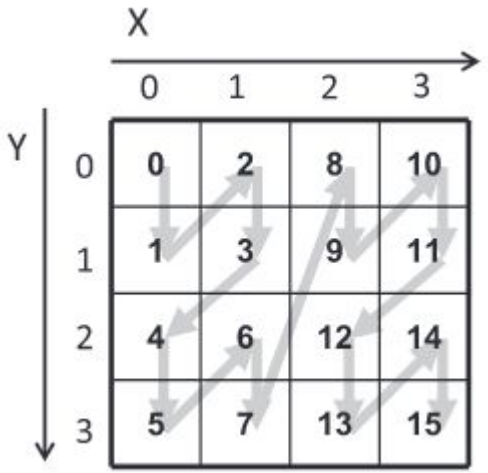


https://www.nec.com/en/global/techrep/journal/g12/n02/pdf/120216.pdf

NoSQL / Non-relational databases

Wide Column Stores (Cassandra, Scylla, HBase)

- schema-agnostic
- data in column families or table
  a multi-dimensional key-value store:
  e.g. latitude and longitude
- **Z-ordering**
- Space partitioning using the **Kd-tree method**
- scale well enough to manage
  petabytes of data within a distributed system.



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NoSQL / Non-relational databases

Document Stores (MongoDB, Couchbase)

- schema-free
- store data in JSON documents
- Key = document name
- Value = document
- Manage semi-structured data

A sample json:

```
{
"name": "notebook",
"qty": 50,
"rating": [ { "score": 8 }, { "score": 9 } ],
"size": { "height": 11, "width": 8.5, "unit": "in" },
"status": "A",
"tags": [ "college-ruled", "perforated"]
}
```

NoSQL / Non-relational databases

Graph Databases (Neo4J, Datastax Enterprise Graph)

- **data as a network** of related nodes/objects
  -> facilitates data visualizations and graph analytics
- node/object contains free-form data
  connected by relationships, grouped according to labels
- Analysis of the **relationships between heterogeneous data** points
- Fraud prevention, advanced enterprise operations, Facebook's friends graph.

NoSQL / Non-relational databases

Search Engines (Elasticsearch, Splunk, Solr)

- schema-free JSON documents -> similar to document stores
- unstructured or semi-structured data
- easily accessible via text-based searches with strings of varying complexity..

NoSQL / Non-relational databases

Advantages

- Since there are so many types and varied applications of NoSQL databases, it's hard to nail these down, but generally:
-
    - Schema-free data models are more flexible and easier to administer.
    - NoSQL databases are generally more horizontally scalable and fault-tolerant.
    - Data can easily be distributed across different nodes. To improve availability and/or partition tolerance, you can choose that data on some nodes be "eventually consistent".
-

Multidimensional data: few fundamental problems

- Cluster finding in point distributions
- Trajectories in space and time
  - Lagrangian mechanics
- Outlier detection
  - Find points with unusual properties
  - Fast generation of histograms
- • For analysis and visualization
- • Volume rendering methods
- • Correlation functions (pair and higher order)
- • Interactive visualization of large point clouds

Multidimensional data: few fundamental problems

- Find points in a given region of space
  - Region is given with analytic description
  - Equation of sphere, rectangle, polihedron etc.

- Find nearest neighbor of a query point
  - Find k nearest neighbors
  - Also for cluster finding
  - Point classification (machine learning)
  - Non-parametric regression, non-linear regression