Databases in Biosciences

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Healthcare and life sciences data sources

Drug Research

Social Media

Patient Records

Gene Sequencing

Test Results

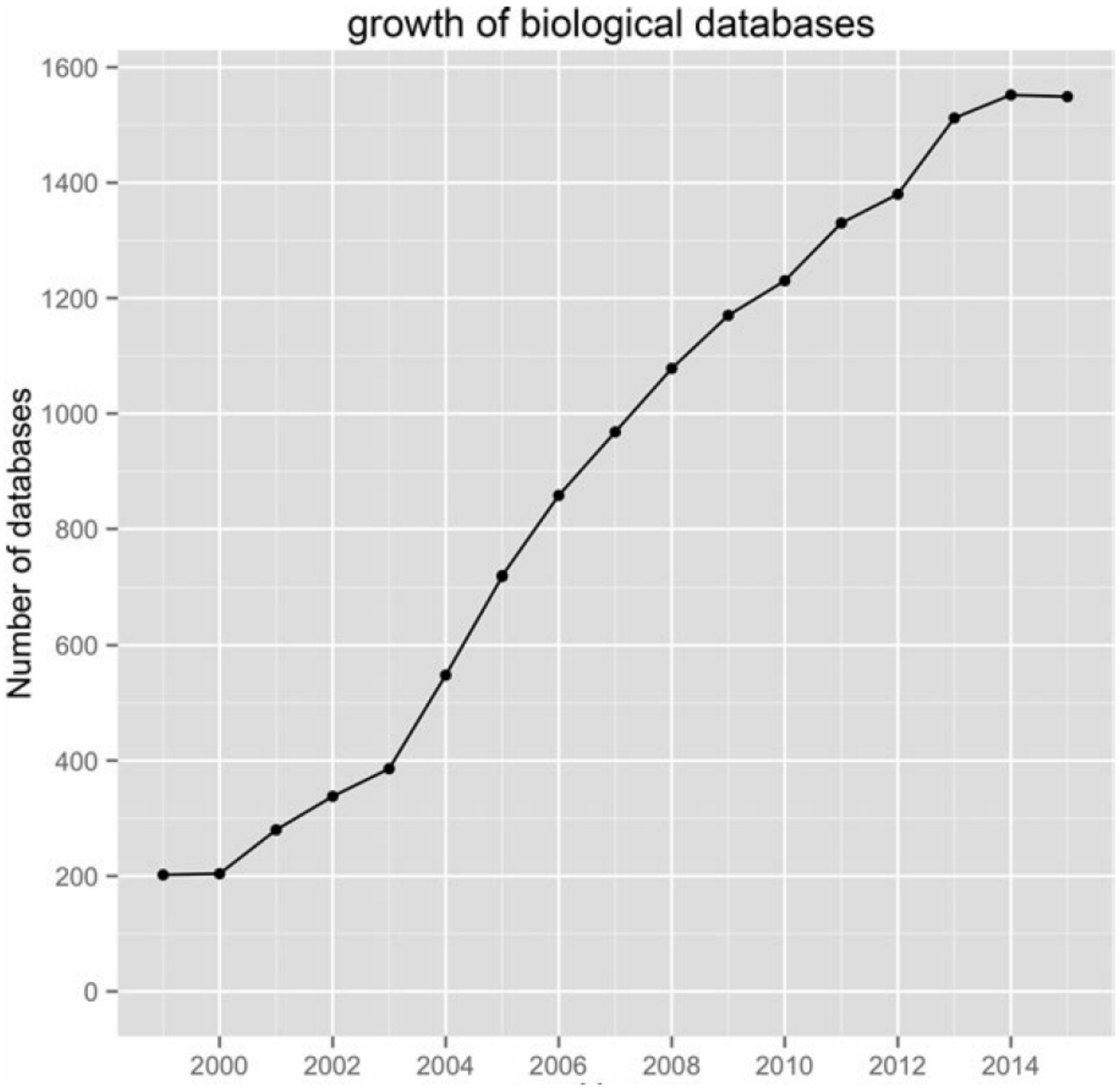
Claims

Home Monitoring

Mobile Apps

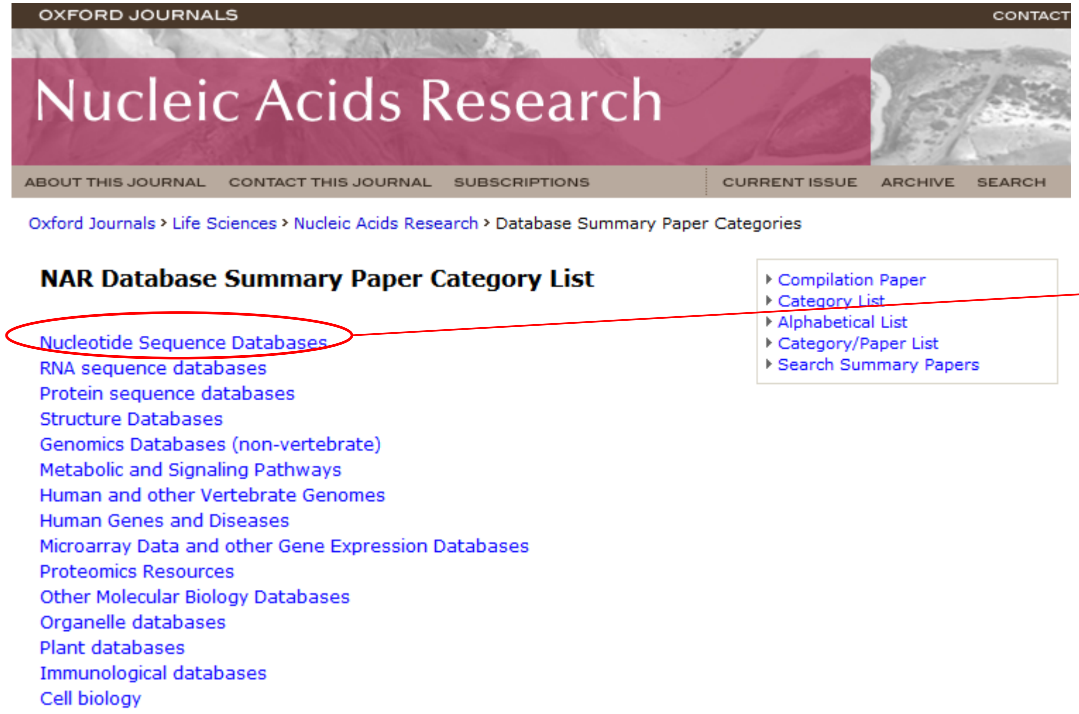
3Vs:

- Volume – high-throughput technologies
- Variety – diverse data types, different formats, structured vs. unstructured data
- Velocity – data streaming



growth of biological databases

It is now: nearly 2,000 databases in 2016!

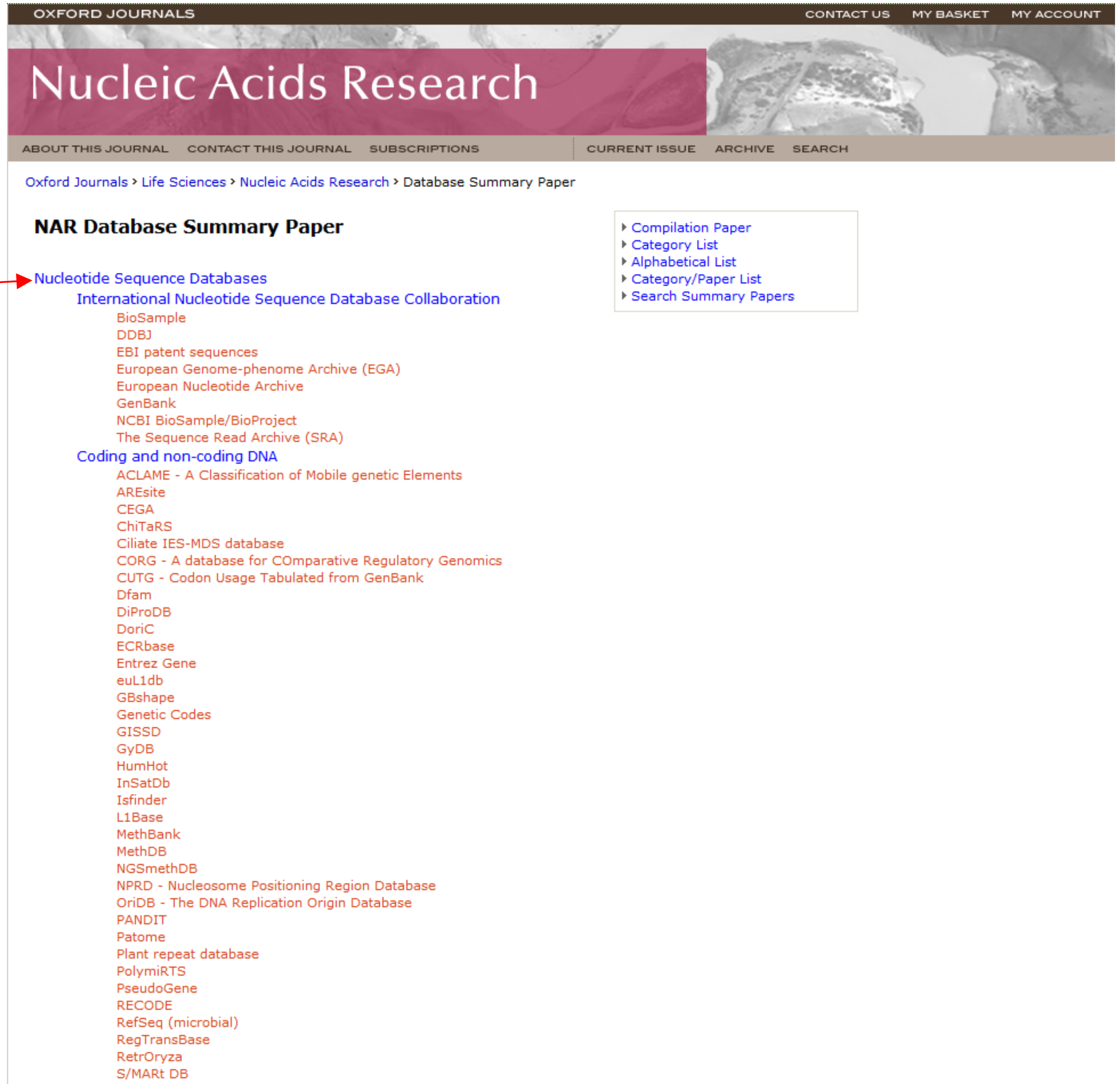


Oxford Journals > Life Sciences > Nucleic Acids Research > Database Summary Paper Categories

NAR Database Summary Paper Category List

- Compilation Paper
- Category List
- Alphabetical List
- Category/Paper List
- Search Summary Papers

Nucleotide Sequence Databases
RNA sequence databases
Protein sequence databases
Structure Databases
Genomics Databases (non-vertebrate)
Metabolic and Signaling Pathways
Human and other Vertebrate Genomes
Human Genes and Diseases
Microarray Data and other Gene Expression Databases
Proteomics Resources
Other Molecular Biology Databases
Organelle databases
Plant databases
Immunological databases
Cell biology



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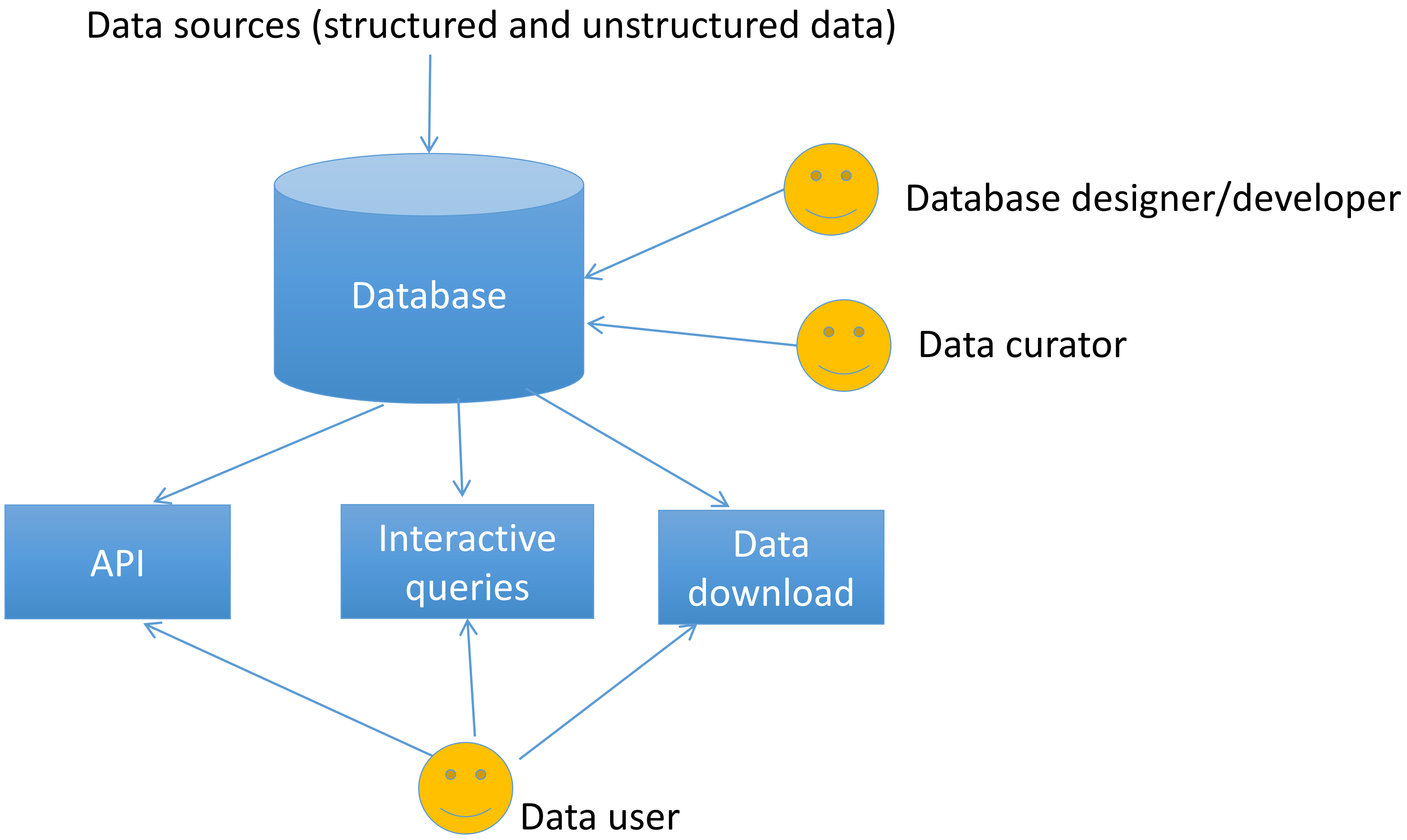
Nucleotide Sequence Databases
- International Nucleotide Sequence Database Collaboration
  - BioSample
  - DDBJ
  - EBI patent sequences
  - European Genome-phenome Archive (EGA)
  - European Nucleotide Archive
  - GenBank
  - NCBI BioSample/BioProject
  - The Sequence Read Archive (SRA)
- Coding and non-coding DNA
  - ACLAME - A Classification of Mobile genetic Elements
  - AREsite
  - CEGA
  - ChiTaRS
  - Ciliate IES-MDS database
  - CORG - A database for COmparative Regulatory Genomics
  - CUTG - Codon Usage Tabulated from GenBank
  - Dfam
  - DiProDB
  - DoriC
  - ECRbase
  - Entrez Gene
  - euL1db
  - GBshape
  - Genetic Codes
  - GISSD
  - GyDB
  - HumHot
  - InSatDb
  - Isfinder
  - L1Base
  - MethBank
  - MethDB
  - NGSmethDB
  - NPRD - Nucleosome Positioning Region Database
  - OriDB - The DNA Replication Origin Database
  - PANDIT
  - Patome
  - Plant repeat database
  - PolymiRTS
  - PseudoGene
  - RECODE
  - RefSeq (microbial)
  - RegTransBase
  - RetrOryza
  - S/MARt DB

Database ecosystem


Data sources (structured and unstructured data)
Database
Database designer/developer
Data curator
API
Interactive queries
Data download
Data user

What is a database?

- It’s not just a file
- It’s not just an Excel spreadsheet
- It’s an organized collection of related information that can easily be accessed, managed, and updated

Difference between Spreadsheet and Database

Spreadsheet	**Database**
Data analysis	Data management
Mathematical calculation	Structuring data and querying data to create subsets
Typically single user	Database management with multiple users
Formatting and chart display	Reports for data summarization
Limited in scale	Scalable

↓

Worksheet size:	1,048,576 rows by 16,384 columns
Column width:	255 characters
Total no. of characters that a cell can have:	32,767 characters

Some key database concepts

- **Data integrity** is the assurance that data are correct and consistent (data correctly reflects the real world)
- **Data redundancy** occurs if data are duplicated between files
- **Data dependency** defines linkage between data files and their order of entry
- **Data security** refers to data being protected so that only authorized personnel can access them
- **Data quality** defines how well the data fits its intended uses in operations, decision making and planning

Relational database (SQL database)

- The relational model was introduced by E.F. Codd in 1970, which is based on the mathematical set theory
- A relational database management system (RDBMS) is a computer application (software) of the relational data model (e.g., MS SQLServer, MySQL, Oracle, …)
- Relational databases have widely been used to manage data in different domains

Components of Relational Database

- A table (relation) represents some class of objects (e.g., patients, doctors, drugs, hospitals)
- Each table consists of columns (attributes) and rows (tuples).
    - Each column represents some attribute of the object represented by the table (e.g., patient id, patient name)
    - Each row corresponds to an instance of the object represented by the table (e.g., each row in the Patient table represents a patient who has a specific patient id and name.)

How to organize data into tables

Keys

- Primary key: Every table should have a primary key comprising a single or multiple columns that contain unique values. A primary key is the unique identifier of a table row (e.g., “sample id” is the primary key for the **Sample** table)
- Foreign key: it is a key taken from a different table. For example, in the **Experiment** table, the “sample id” is the foreign key to the **Sample** table.

Addition, Deletion and Modification Anomalies

Student ID	Name	Address	Subject
401	Adam	Noida	Biology
402	Alex	Panipat	Math
403	Stuart	Jammu	Math
404	Adam	Noida	Physics

Normalization

- Normalization is a *process* in which we systematically organize columns and tables to eliminate anomalies due to data redundancy
- It involves decomposing a (de-normalized) table into less redundant (smaller) tables without losing information
- The objective is to isolate data so that additions, deletions, modifications of data can be made in just one table and then propagated to other tables using foreign keys.
- Normalization is a trade-off between data redundancy and performance.
  - Normalizing a table reduces data redundancy but introduces the need for joins when all of the data is required for a report query.
- **Normal Form**: A set of tables free from a certain set of addition, deletion and modification anomalies.

Different Normal Forms

- **First normal form (1NF)**
- **Second normal form (2NF)**
- **Third normal form (3NF)**
- Boyce-Codd normal form (BCNF)
- Fourth normal form (4NF)
- Fifth normal form (5NF)
- Domain-Key normal form (DK/NF)
- …

First Normal Form

- Each column value must be a single value only.
- All values for a given column must be of the same data type.
- Each column name must be unique.
- The order of columns is insignificant
- The order of the rows is insignificant
- No two rows in a table can be identical.

First Normal Form Example

ID	Student	Age	Subject
401	Adam	15	Biology
404	Adam	15	Physics
402	Alex	14	Math
403	Stuart	17	Math

Second Normal Form

- A table is in second normal form (2NF) if it is in 1NF and if all of its non-key columns are dependent on all of the *key*.
  - A table is in second normal form if it is free from partial-key dependencies
- Tables that have a single column for a key are automatically in 2NF.
  - This is one reason why we often use artificial identifiers (non-composite keys) as keys.
- To achieve second normal form, we may need to split a table into multiple tables and match rows between tables using primary and foreign keys

Second Normal Form Example

Student	Age
Adam	15
Alex	14
Stuart	17

Student	Subject
Adam	Biology
Adam	Physics
Alex	Math
Stuart	Math

Third Normal Form

- Every non-primary key column must be dependent on primary key
- There should not be the case that a non-primary key column is determined by another non-primary (*transitive dependency*)
    - Student (ID, Name, DOB, City, State, Zip)
- *A table is in 3NF if the following are true:*
    - *it is in 2NF*
    - *All transitive dependencies (Zip->City)* are removed

Student (ID, Name, DOB, Zip)

Address (Zip, City, State)

Entity Relationship Diagram (ERD)

What is ERD

- It is a data model associated with a diagrammatic method (P. Chen 1976) used to conduct/view data modeling
- It describes the attributes of and the relationship between entities (data objects)
- DBA uses ERD to perform data modeling and explain the diagram to stakeholders

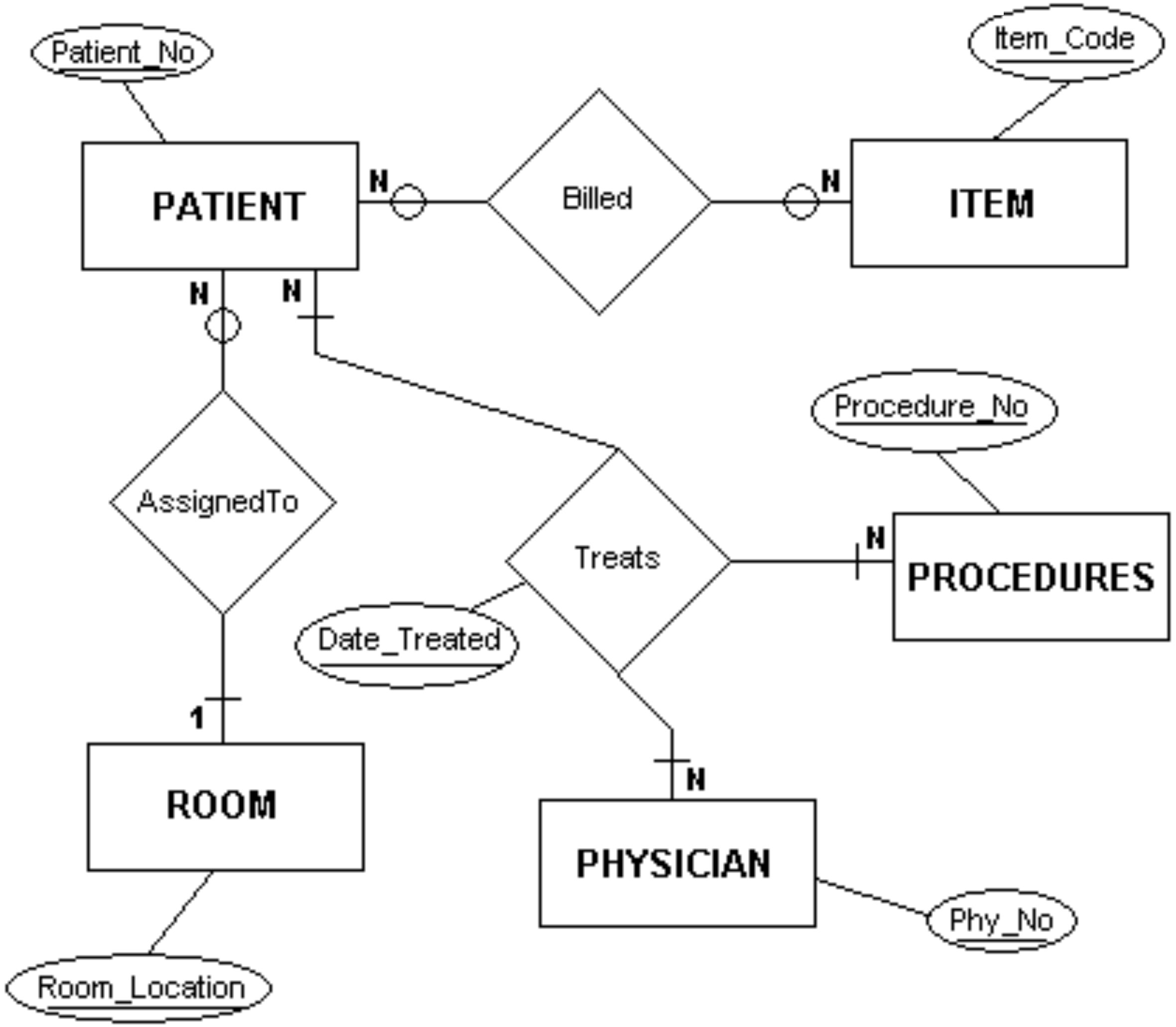
Primary Components of ERD

- **Entity** represents a collection of objects in the real world (e.g., person, place, event)
- **Attribute** is a named property or characteristic of an entity
- **Relationship** is an association between the instances of one or more entities

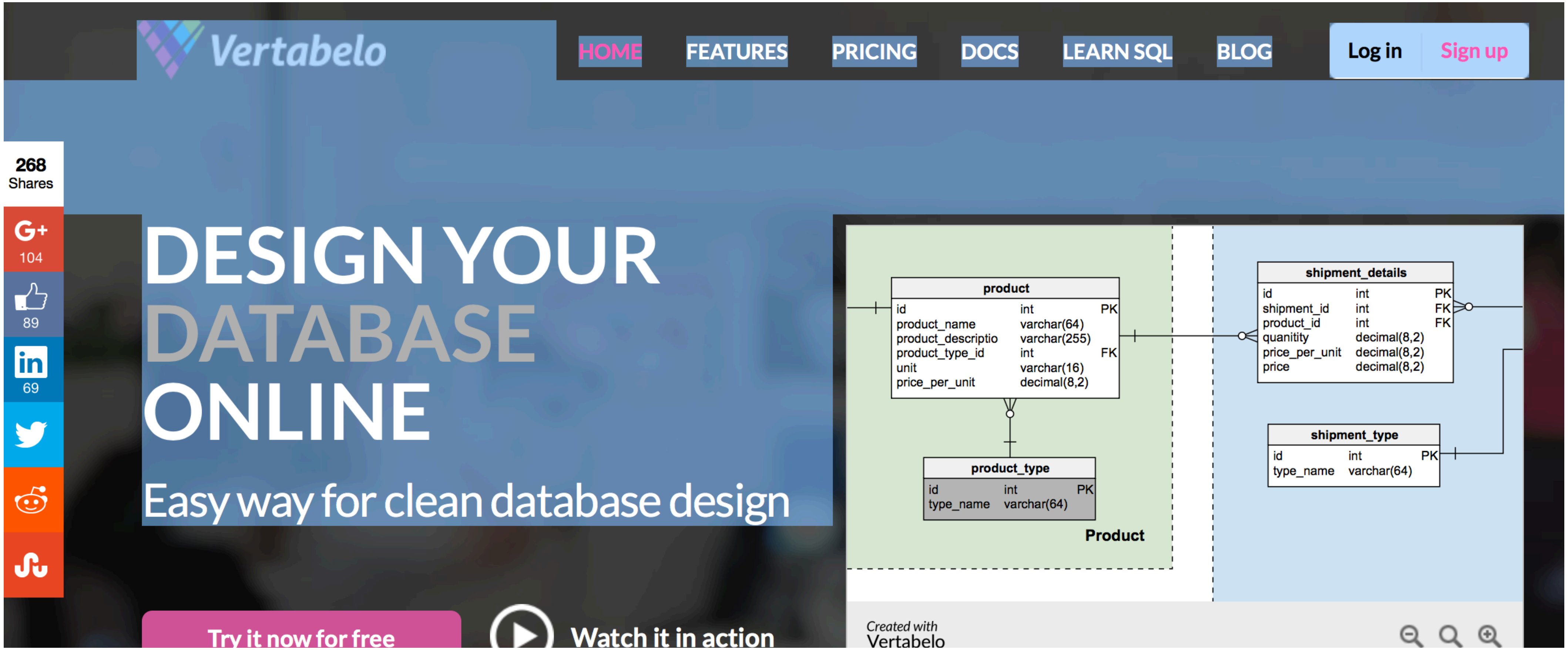
Relationship Cardinality

- It expresses the minimum and maximum number of occurrences of one entity for a single occurrence of the other
    - One-to-One (1:1)
    - One-to-Many (1:N)
    - Many-to-Many (M:N)

Example ERD (Hospital Database)



Vertabelo Demo



DESIGN YOUR DATABASE ONLINE

Easy way for clean database design

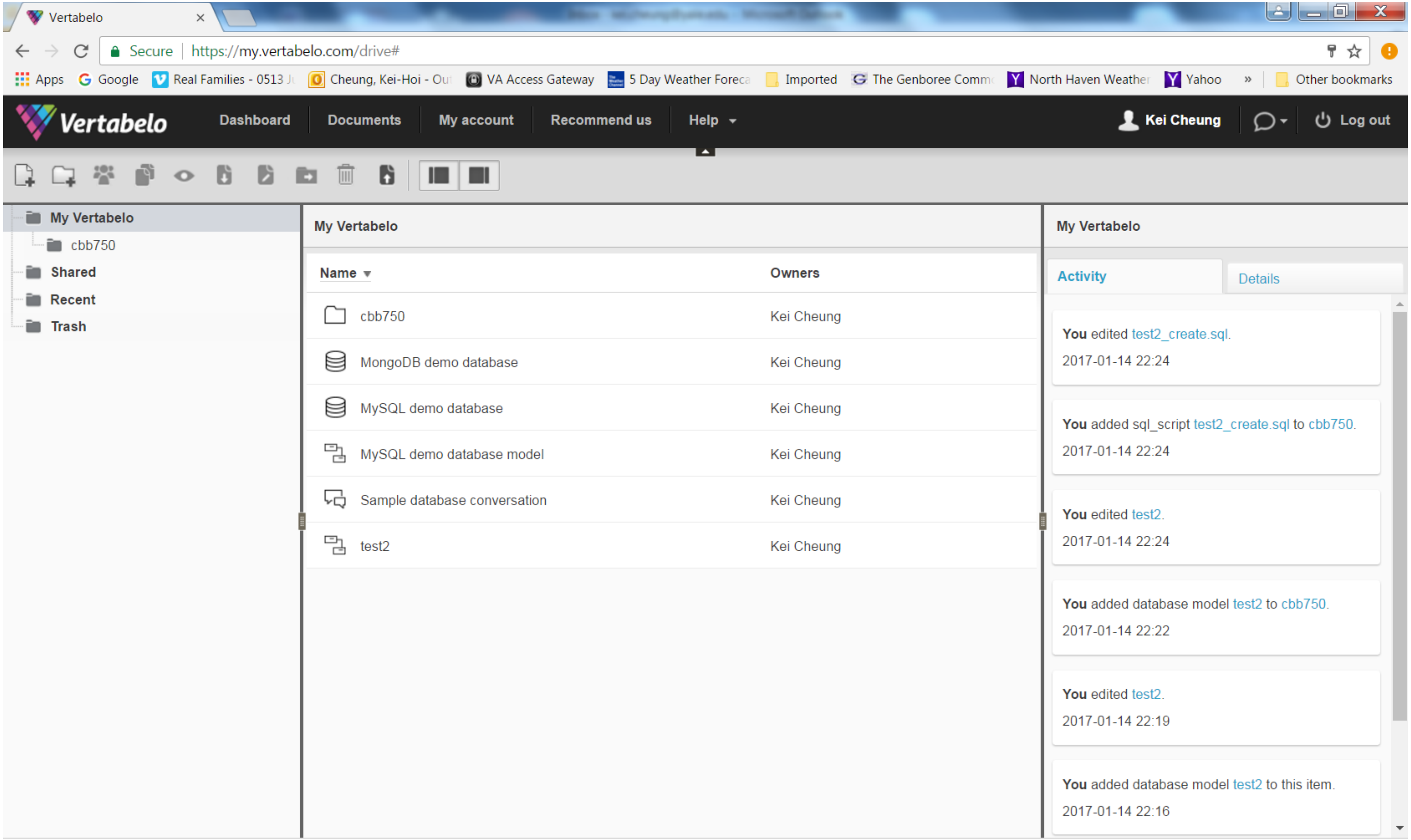
product		
id	int	PK
product_name	varchar(64)	
product_descriptio	varchar(255)	
product_type_id	int	FK
unit	varchar(16)	
price_per_unit	decimal(8,2)	

product_type		
id	int	PK
type_name	varchar(64)	

Product

shipment_details		
id	int	PK
shipment_id	int	FK
product_id	int	FK
quanitity	decimal(8,2)	
price_per_unit	decimal(8,2)	
price	decimal(8,2)	

shipment_type		
id	int	PK
type_name	varchar(64)	



My Vertabelo

Name ▾	Owners
cbb750	Kei Cheung
MongoDB demo database	Kei Cheung
MySQL demo database	Kei Cheung
MySQL demo database model	Kei Cheung
Sample database conversation	Kei Cheung
test2	Kei Cheung

My Vertabelo

You edited test2_create.sql.

2017-01-14 22:24

You added sql_script test2_create.sql to cbb750.

2017-01-14 22:24

You edited test2.

2017-01-14 22:24

You added database model test2 to cbb750.

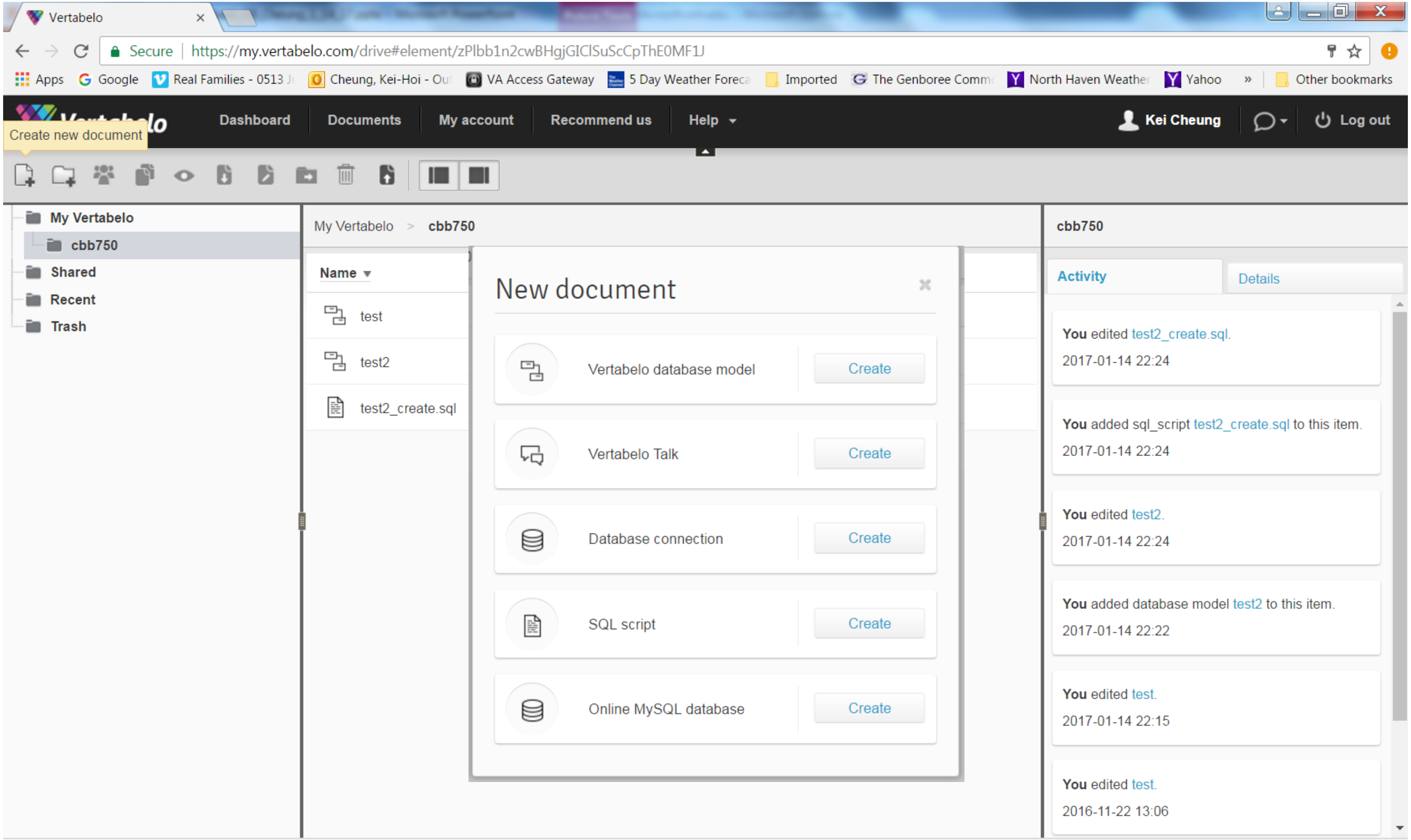
2017-01-14 22:22

You edited test2.

2017-01-14 22:19

You added database model test2 to this item.

2017-01-14 22:16



New document

Vertabelo database model	Create
Vertabelo Talk	Create
Database connection	Create
SQL script	Create
Online MySQL database	Create

You edited test2_create.sql.
2017-01-14 22:24

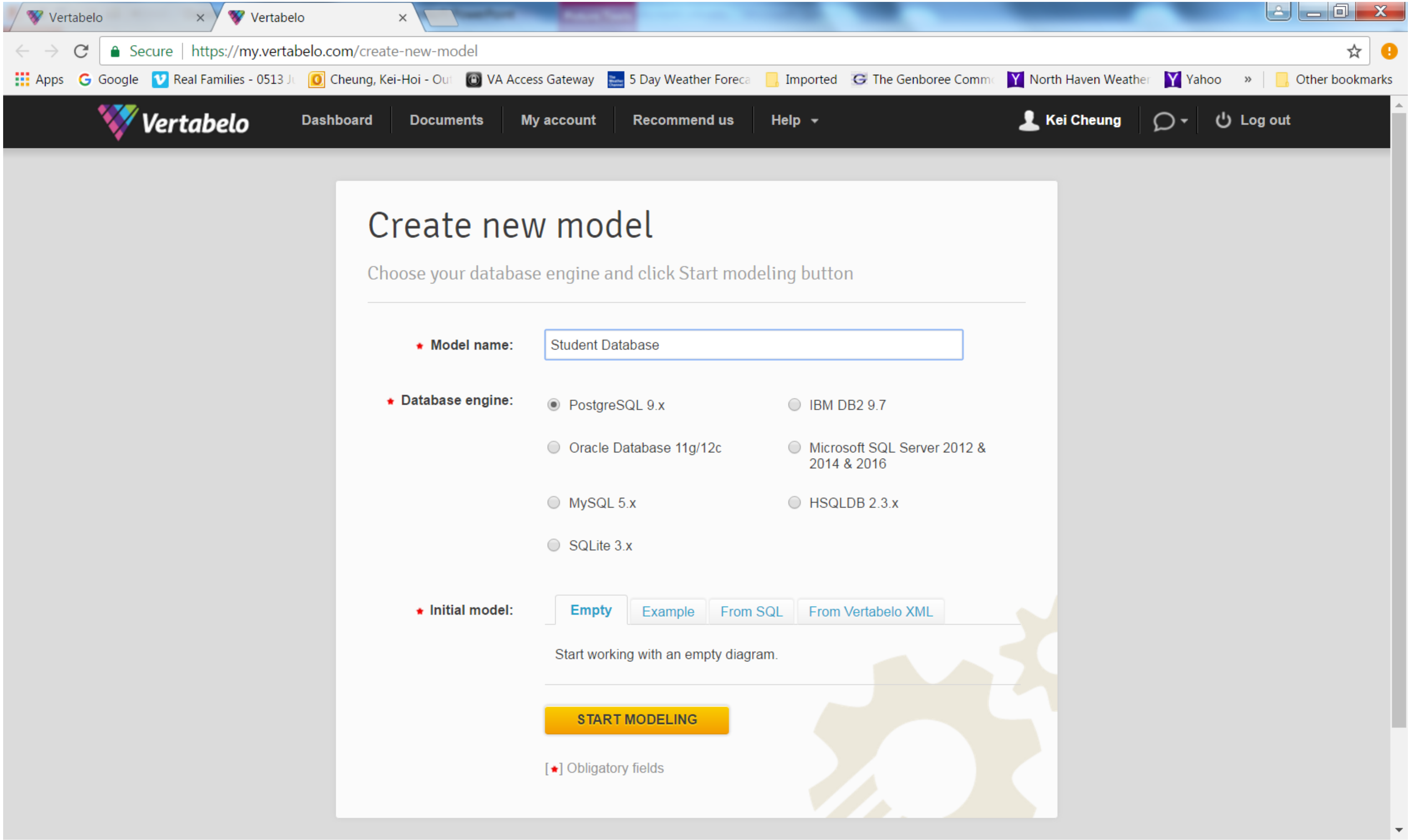
You added sql_script test2_create.sql to this item.
2017-01-14 22:24

You edited test2.
2017-01-14 22:24

You added database model test2 to this item.
2017-01-14 22:22

You edited test.
2017-01-14 22:15

You edited test.
2016-11-22 13:06



Create new model

Choose your database engine and click Start modeling button

* Model name: Student Database

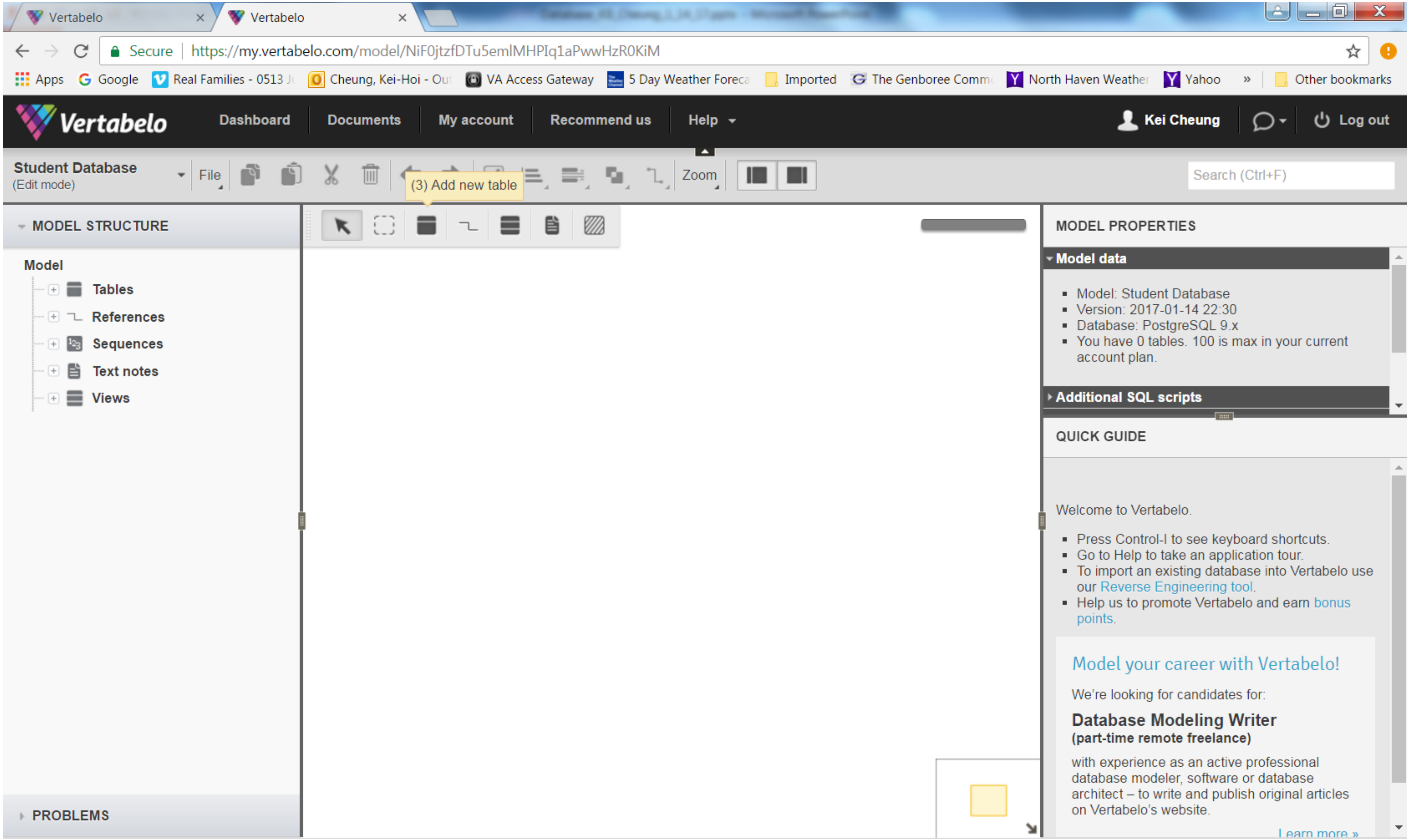
* Database engine:

● PostgreSQL 9.x
○ IBM DB2 9.7
○ Oracle Database 11g/12c
○ Microsoft SQL Server 2012 & 2014 & 2016
○ MySQL 5.x
○ HSQLDB 2.3.x
○ SQLite 3.x

* Initial model: [✓ Empty] Example From SQL From Vertabelo XML

Start working with an empty diagram.

[*] Obligatory fields



- Model: Student Database
- Version: 2017-01-14 22:30
- Database: PostgreSQL 9.x
- You have 0 tables. 100 is max in your current account plan.

Welcome to Vertabelo.

- Press Control-I to see keyboard shortcuts.
- Go to Help to take an application tour.
- To import an existing database into Vertabelo use our Reverse Engineering tool.
- Help us to promote Vertabelo and earn bonus points.

Model your career with Vertabelo!

We're looking for candidates for:

Database Modeling Writer
(part-time remote freelance)

with experience as an active professional database modeler, software or database architect – to write and publish original articles on Vertabelo's website.

Learn more »

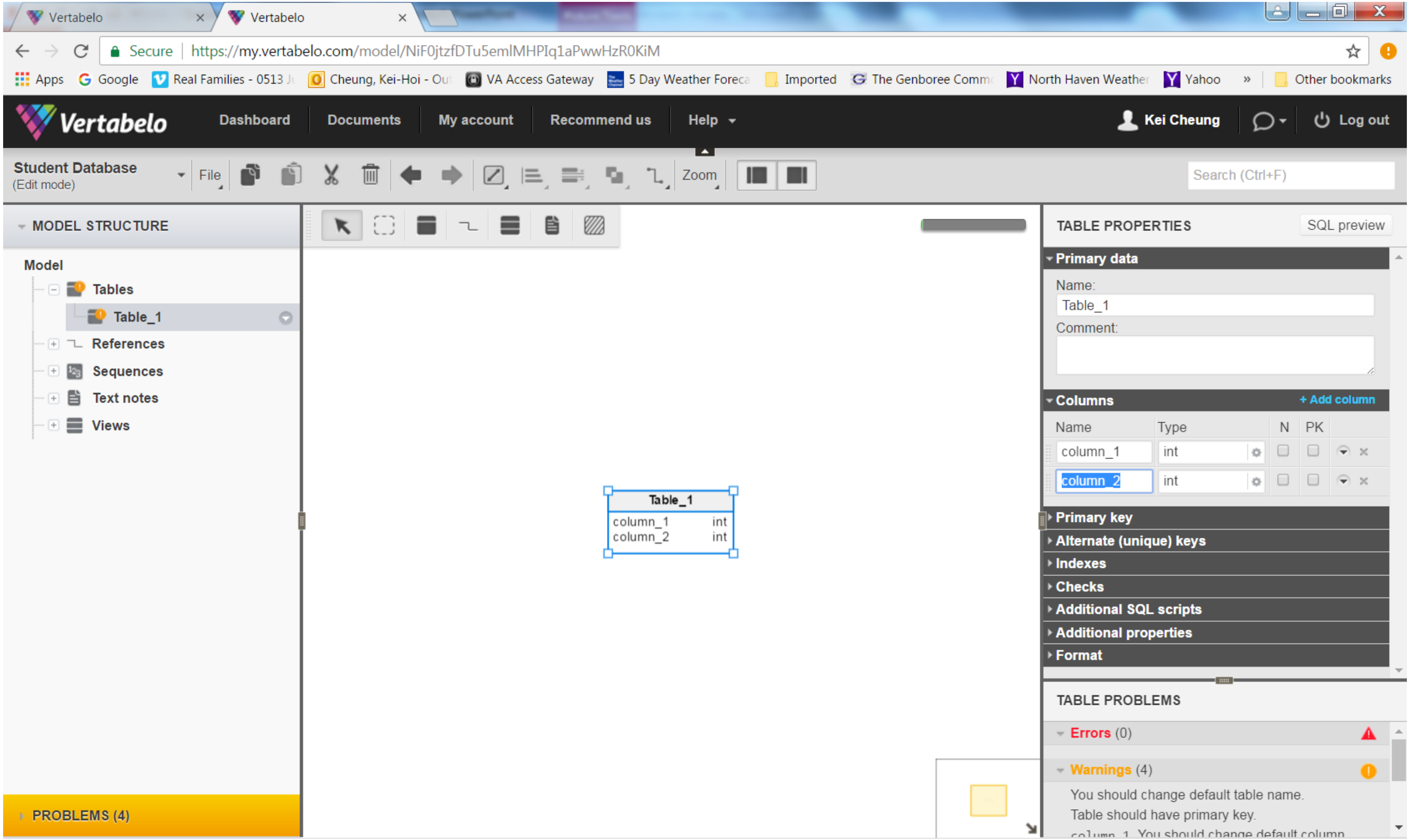


Table_1

column_1	int
column_2	int

Name: Table_1

Comment:

Name	Type	N	PK
column_1	int	□	□
column_2	int	□	□

You should change default table name.

Table should have primary key.

column_1 You should change default column

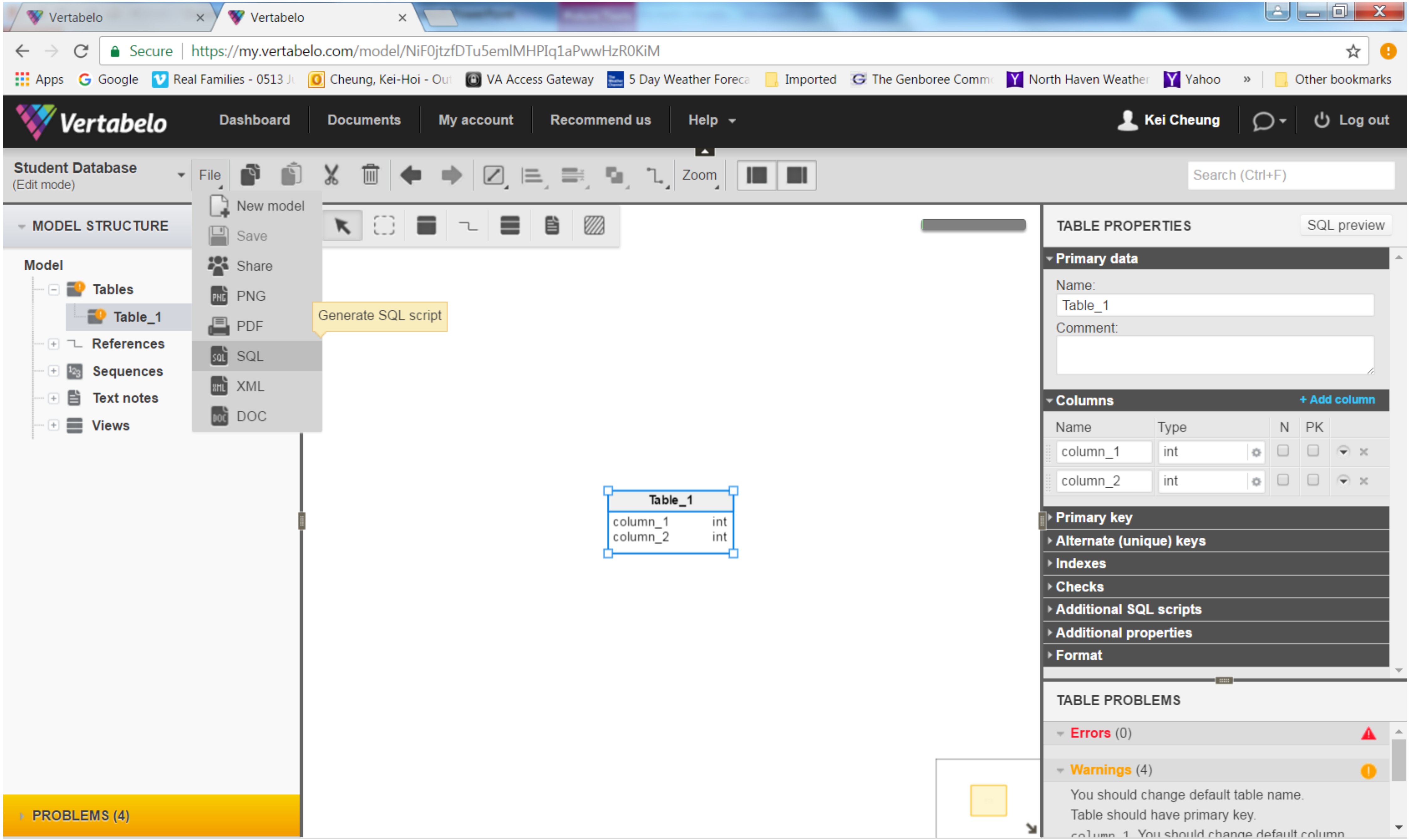


Table_1	
column_1	int
column_2	int

Name:
Table_1
Comment:

Name	Type	N	PK
column_1	int	□	□
column_2	int	□	□

You should change default table name.
Table should have primary key.
column_1 You should change default column

On-Line Transaction Processing (OLTP)

What is OLTP?

- It is a class of information systems (e.g., databases) that facilitate and manage transaction-oriented applications, typically for data entry and retrieval transactions
- A database that is based on a normalized relational model is considered an OLTP application. It supports the following transactions:
  - Insert new rows
  - Update existing rows
  - Delete rows
  - Select rows

Structured Query Language (SQL)

- It is a standard programming language for creating (CREATE) relational databases and tables as well as retrieving (SELECT), adding (INSERT), deleting (DELETE) and updating (UPDATE) data in a relational database
- It is compliant with ANSI and ISO standards

SQL Statement (CREATE DATABASE/TABLE)

```
CREATE DATABASE Patient_DB;

CREATE TABLE Patient_DB.Patient
(
        ID int,
        Name varchar (50),
        Address varchar (250),
        Age smallint
        Sex varchar (2)
);
```

INSERT Statement

```
INSERT INTO Patient_DB.Patient
(ID, Name, Address, Age, Sex)
VALUES (1, ‘John Doe’, ‘XYZ’, 40, ‘M’)
…
```

ID	Name	Address	Age	Sex
1	John Doe	XYZ	40	M
2	Jane Smith	ABC	34	F
3	Mary Queen	PQSRT	46	F
4	Mike Lee	DWQER	60	M

UPDATE Statement

```
UPDATE Patient_DB.Patient
SET AGE=41
WHERE ID=1
```

ID	Name	Address	Age	Sex
1	John Doe	XYZ	41	M
2	Jane Smith	ABC	34	F
3	Mary Queen	PQSRT	46	F
4	Mike Lee	DWQER	60	M

DELETE Statement

DELETE Patient_DB.Patient

WHERE Name='Mike Lee'

ID	Name	Address	Age	Sex
1	John Doe	XYZ	41	M
2	Jane Smith	ABC	34	F
3	Mary Queen	PQSRT	46	F

SELECT Statement

```
SELECT ID, Name, Age, Sex
FROM Patient_DB.Patient
WHERE Age>=40
ORDER BY Age
```

ID	Name	Address	Age	Sex
1	John Doe	XYZ	40	M
2	Jane Smith	ABC	34	F
3	Mary Queen	PQSRT	46	F
4	Mike Lee	DWQER	60	M

SELECT Statement (Aggregation)

```
SELECT Sex, avg(Age)
FROM Patient_DB.Patient
GROUP BY SEX
```

Results: M 50
F 40

ID	Name	Address	Age	Sex
1	John Doe	XYZ	40	M
2	Jane Smith	ABC	34	F
3	Mary Queen	PQSRT	46	F
4	Mike Lee	DWQER	60	M

SELECT Statement (JOIN)

```
SELECT A.*, B.Report_Text
FROM Patient_DB.Patient AS A
INNER JOIN Patient_DB.LabTest. AS B
ON A.ID = B.Patient_ID
```

ID	Name	Address	Age	Sex
1	John Doe	XYZ	40	M
2	Jane Smith	ABC	34	F
3	Mary Queen	PQSRT	46	F
4	Mike Lee	DWQER	60	M

Patient_ID	ID	Report_Text
1	1	……
1	2	…….

Other Types of SQL Statements

- TRUNCATE TABLE
- DROP TABLE
- CREATE VIEW
- CREATE INDEX (boost query performace)
  - Full-Text index (e.g., part of MS SQLServer)

From OLTP to OLAP (On-Line Analytical Processing)

OLAP Overview

- OLTP databases are tuned to small/medium size of data with relatively simple queries
- Some applications use fewer but more time-consuming analytic queries
- New architectures (data warehouses) have been developed to handle such analytic queries efficiently (De-normalization)

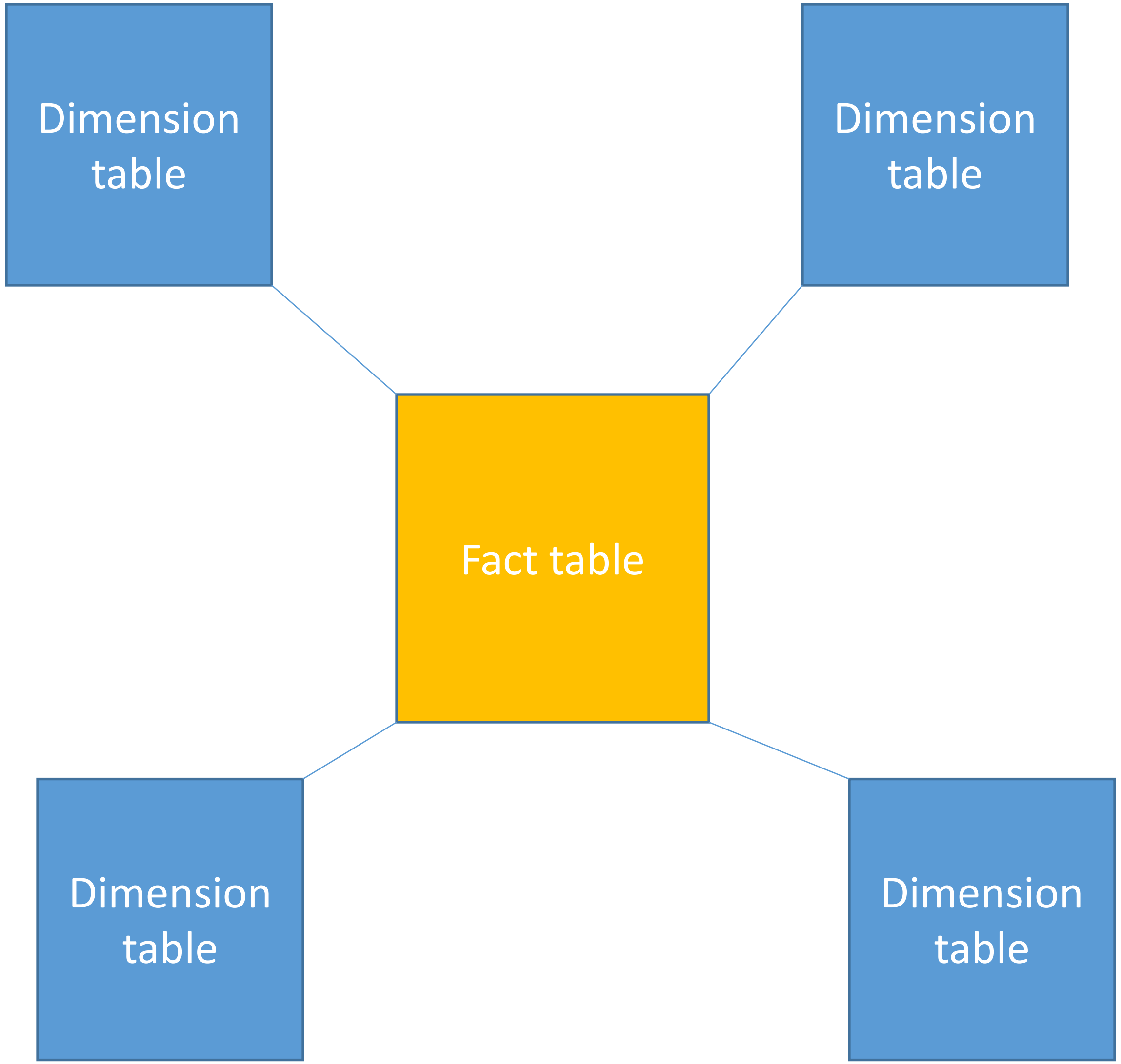
OLAP Example Queries

- Amazon analyzes purchases by its customers to identify products of likely interest to customers
- Analysts at Wal-Mart look for merchandise items with increasing sales in some region

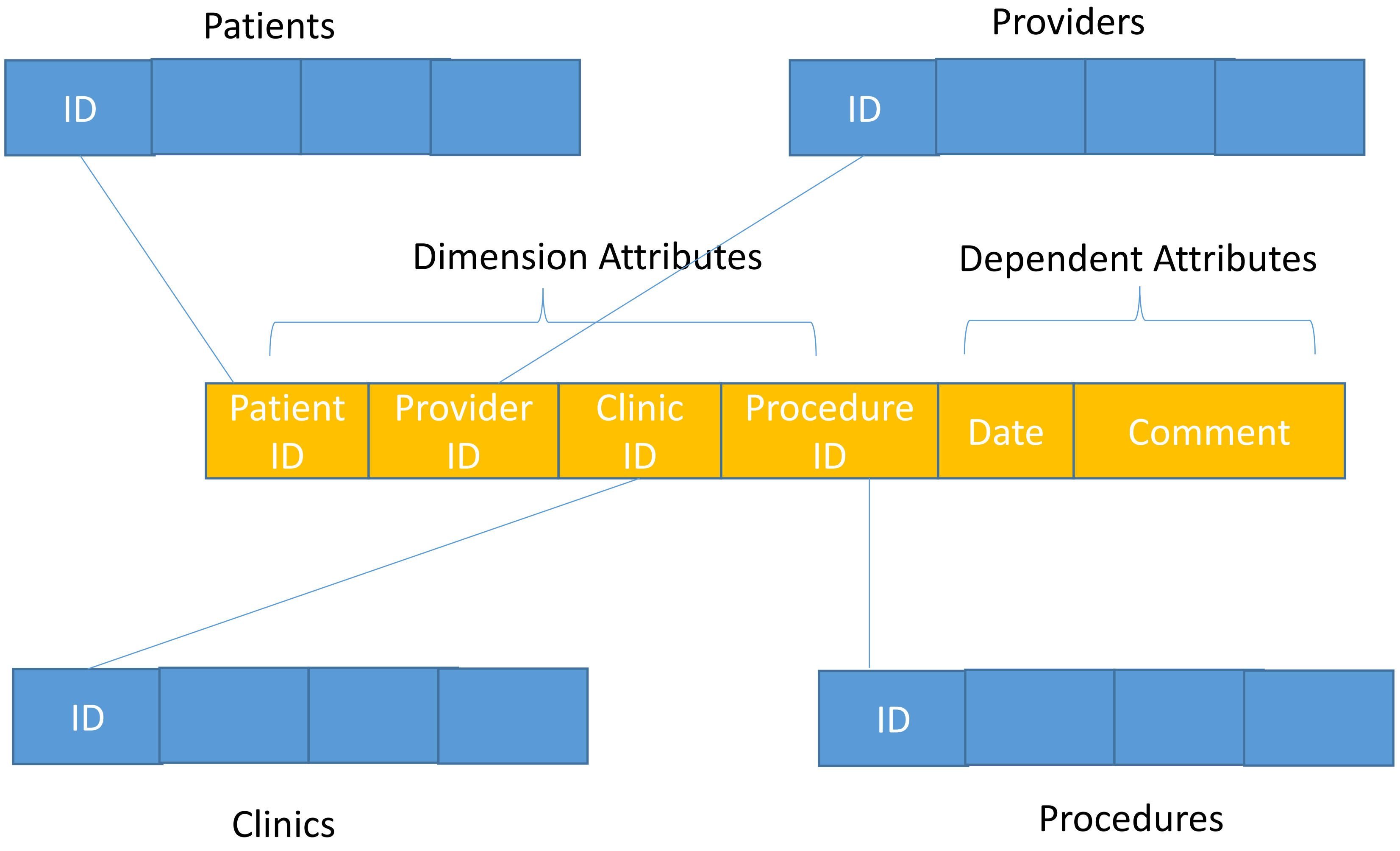
Data Warehouse

- The most common form of database integration
    - Copy source databases into a single database (data warehouse)
    - Update the data warehouse periodically (in batch mode)
    - Support analytic queries using a dimensional data model (vs. a normalized entity-relationship model)
- Example: VA CDW

Star Schema


Dimension table
Dimension table
Fact table
Dimension table
Dimension table

Star Schema Example



Example Queries

- Compare numbers of patient visits across different clinics for a given year
- Which are the top 10 most performed procedures among all clinics from 2010 to 2014

Beyond SQL

- NoSQL (graph databases like NEO4J, document databases like MongoDB)
- Semantic Web (standards for linked data and ontologies)

The End