DataJoint User Manual

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DataJoint contributors

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This is a detailed manual for active users of DataJoint in MATLAB.

This documentation can be read sequentially from start to end or used as reference for specific topics.

For a guided introduction to DataJoint, please explore our tutorials at http://tutorials.datajoint.io

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CHAPTER

ONE

INTRODUCTION

1.1 Data Pipelines

1.1.1 What is a data pipeline?

A scientific **data pipeline** is a collection of processes and systems for organizing the data, computations, and workflows used by a research group as they jointly perform complex sequences of data acquisition, processing, and analysis.

A variety of tools can be used for supporting shared data pipelines:

Data repositories Research teams set up a shared **data repository**. This minimal data management tool allows depositing and retrieving data and managing user access. For example, this may include a collection of files with standard naming conventions organized into folders and sub-folders. Or a data repository might reside on the cloud, for example in a collection of S3 buckets. This image of data management – where files are warehoused and retrieved from a hierarchically-organized system of folders – is an approach that is likely familiar to most scientists.

Database systems Databases are a form of data repository providing additional capabilities:

- 1) Defining, communicating, and enforcing structure in the stored data.
- Maintaining data integrity: correct identification of data and consistent cross-references, dependencies, and groupings among the data.
- 3) Supporting queries that retrieve various cross-sections and transformation of the deposited data.

Most scientists have some familiarity with these concepts, for example the notion of maintaining consistency between data and the metadata that describes it, or applying a filter to an Excel spreadsheet to retrieve specific subsets of information. However, usually the more advanced concepts involved in building and using relational databases fall under the specific expertise of data scientists.

Data pipelines Data pipeline frameworks may include all the features of a database system along with additional functionality:

- 1) Integrating computations to perform analyses and manage intermediate results in a principled way.
- 2) Supporting distributed computations without conflict.
- 3) Defining, communicating, and enforcing **workflow**, making clear the sequence of steps that must be performed for data entry, acquisition, and processing.

Again, the informal notion of an analysis "workflow" will be familiar to most scientists, along with the logistical difficulties associated with managing a workflow that is shared by multiple scientists within or across labs.

Therefore, a full-featured data pipeline framework may also be described as a scientific workflow system.

Data Pipeline workflow computation Database structure (schema) data integrity (identity, references, groups) queries Data Repository deposit & retrieve access control

Fig. 1: Major features of data management frameworks: data repositories, databases, and data pipelines.

1.1.2 What is DataJoint?

DataJoint is a free open-source framework for creating scientific data pipelines directly from MATLAB or Python (or any mixture of the two). The data are stored in a language-independent way that allows interoperability between MATLAB and Python, with additional languages in the works. DataJoint pipelines become the central tool in the operations of data-intensive labs or consortia as they organize participants with different roles and skills around a common framework.

In DataJoint, a data pipeline is a sequence of steps (more generally, a directed acyclic graph) with integrated data storage at each step. The pipeline may have some nodes requiring manual data entry or import from external sources, some that read from raw data files, and some that perform computations on data stored in other database nodes. In a typical scenario, experimenters and acquisition instruments feed data into nodes at the head of the pipeline, while downstream nodes perform automated computations for data processing and analysis.

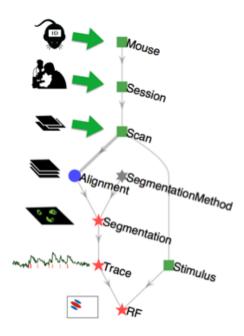


Fig. 2: For example, this is the pipeline for a simple mouse experiment involving calcium imaging in mice.

In this example, the experimenter first enters information about a mouse, then enters information about each imaging session in that mouse, and then each scan performed in each imaging session. Next the automated portion of the pipeline takes over to import the raw imaging data, perform image alignment to compensate for motion, image segmentation to identify cells in the images, and extraction of calcium traces. Finally, the receptive field (RF) computation is performed by relating the calcium signals to the visual stimulus information.

1.1.3 How DataJoint works

DataJoint enables data scientists to build and operate scientific data pipelines.



Fig. 3: Conceptual overview of DataJoint operation.

DataJoint provides a simple and powerful data model, which is detailed more formally in Yatsenko D, Walker EY, Tolias AS (2018). DataJoint: A Simpler Relational Data Model.. Put most generally, a "data model" defines how to

1.1. Data Pipelines 5

think about data and the operations that can be performed on them. DataJoint's model is a refinement of the relational data model: all nodes in the pipeline are simple tables storing data, tables are related by their shared attributes, and query operations can combine the contents of multiple tables. DataJoint enforces specific constraints on the relationships between tables that help maintain data integrity and enable flexible access. DataJoint uses a succinct data definition language, a powerful data query language, and expressive visualizations of the pipeline. A well-defined and principled approach to data organization and computation enables teams of scientists to work together efficiently. The data become immediately available to all participants with appropriate access privileges. Some of the "participants" may be computational agents that perform processing and analysis, and so DataJoint features a built-in distributed job management process to allow distributing analysis between any number of computers.

From a practical point of view, the back-end data architecture may vary depending on project requirements. Typically, the data architecture includes a relational database server (e.g. MySQL) and a bulk data storage system (e.g. AWS S3 or a filesystem). However, users need not interact with the database directly, but via MATLAB or Python objects that are each associated with an individual table in the database. One of the main advantages of this approach is that DataJoint clearly separates the data model facing the user from the data architecture implementing data management and computing. DataJoint works well in combination with good code sharing (e.g. with git) and environment sharing (e.g. with Docker)

DataJoint is designed for quick prototyping and continuous exploration as experimental designs change or evolve. New analysis methods can be added or removed at any time, and the structure of the workflow itself can change over time, for example as new data acquisition methods are developed.

With DataJoint, data sharing and publishing is no longer a separate step at the end of the project. Instead data sharing is an inherent feature of the process: to share data with other collaborators or to publish the data to the world, one only needs to set the access privileges.

1.1.4 Real-life example

The Mesoscale Activity Project (MAP) is a collaborative project between four neuroscience labs. MAP uses DataJoint for data acquisition, processing, analysis, interfaces, and external sharing.

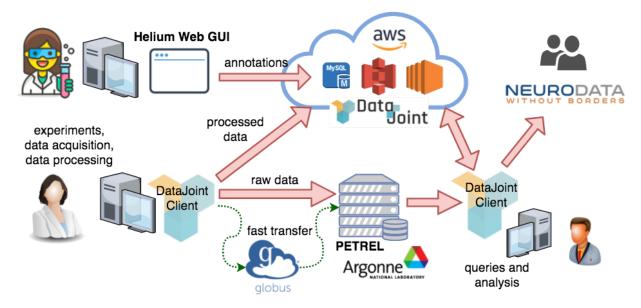


Fig. 4: The DataJoint pipeline for the MAP project.

The pipeline is hosted in the cloud through Amazon Web Services (AWS). MAP data scientists at the Janelia Research Campus and Baylor College of Medicine defined the data pipeline. Experimental scientists enter manual data directly

into the pipeline using the Helium web interface. The raw data are preprocessed using the DataJoint client libraries in MATLAB and Python; the preprocessed data are ingested into the pipeline while the bulky and raw data are shared using Globus transfer through the PETREL storage servers provided by the Argonne National Lab. Data are made immediately available for exploration and analysis to collaborating labs, and the analysis results are also immediately shared. Analysis data may be visualized through web interfaces. Intermediate results may be exported into the NWB format for sharing with external groups.

1.1.5 Summary of DataJoint features

- 1. A free, open-source framework for scientific data pipelines and workflow management
- 2. Data hosting in cloud or in-house
- 3. MySQL, filesystems, S3, and Globus for data management
- 4. Define, visualize, and query data pipelines from MATLAB or Python
- 5. Enter and view data through GUIs
- 6. Concurrent access by multiple users and computational agents
- 7. Data integrity: identification, dependencies, groupings
- 8. Automated distributed computation

1.2 Teamwork

1.2.1 Data management in a science project

Science labs organize their projects as a sequence of activities of experiment design, data acquisition, and processing and analysis.

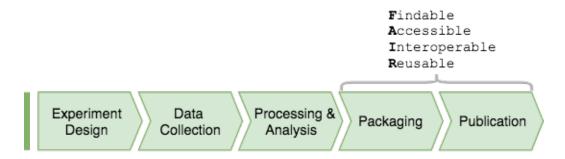


Fig. 5: Workflow and dataflow in a common findings-centered approach to data science in a science lab.

Many labs lack a uniform data management strategy that would span longitudinally across the entire project lifecycle as well as laterally across different projects.

Prior to publishing their findings, the research team may need to publish the data to support their findings. Without a data management system, this requires custom repackaging of the data to conform to the FAIR principles for scientific data management.

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1.2.2 Data-centric project organization

DataJoint is designed to support a data-centric approach to large science projects in which data are viewed as a principal output of the research project and are managed systematically throughout in a single framework through the entire process.

This approach requires formulating a general data science plan and upfront investment for setting up resources and processes and training the teams. The team uses DataJoint to build data pipelines to support multiple projects.

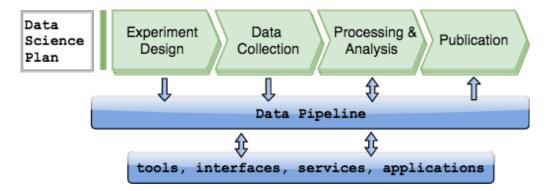


Fig. 6: Workflow and dataflow in a data pipeline-centered approach.

Data pipelines support project data across their entire lifecycle, including the following functions

- experiment design
- · animal colony management
- electronic lab book: manual data entry during experiments through graphical user interfaces.
- acquisition from instrumentation in the course of experiments
- ingest from raw acquired data
- computations for data analysis
- visualization of analysis results
- export for sharing and publishing

Through all these activities, all these data are made accessible to all authorized participants and distributed computations can be done in parallel without compromising data integrity.

1.2.3 Team roles

The adoption of a uniform data management framework allows separation of roles and division of labor among team members, leading to greater efficiency and better scaling.

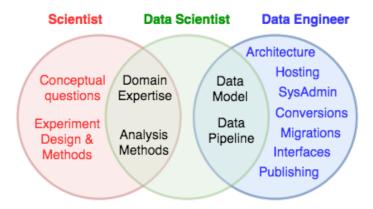


Fig. 7: Distinct responsibilities of data science and data engineering.

Scientists

design and conduct experiments, collecting data. They interact with the data pipeline through graphical user interfaces designed by others. They understand what analysis is used to test their hypotheses.

Data scientists

have the domain expertise and select and implement the processing and analysis methods for experimental data. Data scientists are in charge of defining and managing the data pipeline using DataJoint's data model, but they may not know the details of the underlying architecture. They interact with the pipeline using client programming interfaces directly from languages such as MATLAB and Python.

The bulk of this manual is written for working data scientists, except for System Administration.

Data engineers

work with the data scientists to support the data pipeline. They rely on their understanding of the DataJoint data model to configure and administer the required IT resources such as database servers, data storage servers, networks, cloud instances, Globus endpoints, etc. Data engineers can provide general solutions such as web hosting, data publishing, interfaces, exports and imports.

The System Administration section of this tutorial contains materials helpful in accomplishing these tasks.

DataJoint is designed to delineate a clean boundary between **data science** and **data engineering**. This allows data scientists to use the same uniform data model for data pipelines backed by a variety of information technologies. This delineation also enables economies of scale as a single data engineering team can support a wide spectrum of science projects.

1.3 Input and Output

1.3.1 Where is my data?

New users often ask this question thinking of passive **data repositories** – collections of files and folders and a separate collection of metadata – information about how the files were collected and what they contain. Let's address metadata first, since the answer there is easy: Everything goes in the database! Any information about the experiment that would normally be stored in a lab notebook, in an Excel spreadsheet, or in a Word document is entered into tables in the database. These tables can accommodate numbers, strings, dates, or numerical arrays. The entry of metadata can be manual, or it can be an automated part of data acquisition (in this case the acquisition software itself is modified to enter information directly into the database).

Depending on their size and contents, raw data files can be stored in a number of ways. In the simplest and most common scenario, raw data continue to be stored in either a local filesystem or in the cloud as collections of files and folders. The paths to these files are entered in the database (again, either manually or by automated processes). This is the point at which the notion of a **data pipeline** begins. Below these "manual tables" that contain metadata and file paths are a series of tables that load raw data from these files, process it in some way, and insert derived or summarized data directly into the database. For example, in an imaging application, the very large raw .TIFF stacks would reside on the filesystem, but the extracted fluorescent trace timeseries for each cell in the image would be stored as a numerical array directly in the database. Or the raw video used for animal tracking might be stored in a standard video format on the filesystem, but the computed X/Y positions of the animal would be stored in the database. Storing these intermediate computations in the database makes them easily available for downstream analyses and queries.

1.3.2 Do I have to manually enter all my data into the database?

No! While some of the data will be manually entered (the same way that it would be manually recorded in a lab notebook), the advantage of DataJoint is that standard downstream processing steps can be run automatically on all new data with a single command. This is where the notion of a **data pipeline** comes into play. When the workflow of cleaning and processing the data, extracting important features, and performing basic analyses is all implemented in a DataJoint pipeline, minimal effort is required to analyze newly-collected data. Depending on the size of the raw files and the complexity of analysis, useful results may be available in a matter of minutes or hours. Because these results are stored in the database, they can be made available to anyone who is given access credentials for additional downstream analyses.

1.3.3 Won't the database get too big if all my data are there?

Typically, this is not a problem. If you find that your database is getting larger than a few dozen TB, DataJoint provides transparent solutions for storing very large chunks of data (larger than the 4 GB that can be natively stored as a LONGBLOB in MySQL). However, in many scenarios even long time series or images can be stored directly in the database with little effect on performance.

1.3.4 Why not just process the data and save them back to a file?

There are two main advantages to storing results in the database. The first is data integrity. Because the relationships between data are enforced by the structure of the database, DataJoint ensures that the metadata in the upstream nodes always correctly describes the computed results downstream in the pipeline. If a specific experimental session is deleted, for example, all the data extracted from that session are automatically removed as well, so there is no chance of "orphaned" data. Likewise, the database ensures that computations are atomic. This means that any computation performed on a dataset is performed in an all-or-none fashion. Either all of the data are processed and inserted, or none at all. This ensures that there are no incomplete data. Neither of these important features of data integrity can be guaranteed by a file system.

The second advantage of storing intermediate results in a data pipeline is flexible access. Accessing arbitrarily complex subsets of the data can be achieved with DataJoint's flexible query language. When data are stored in files, collecting the desired data requires trawling through the file hierarchy, finding and loading the files of interest, and selecting the interesting parts of the data.

This brings us to the final important question:

1.3.5 How do I get my data out?

This is the fun part. See *Queries* for details of the DataJoint query language directly from MATLAB and Python.

1.3.6 Interfaces

Multiple interfaces may be used to get the data into and out of the pipeline.

Some labs use third-party GUI applications such as HeidiSQL and Navicat, for example. These applications allow entering and editing data in tables similarly to spreadsheets.

The Helium Application (https://mattbdean.github.io/Helium/ and https://github.com/mattbdean/Helium) is web application for browsing DataJoint pipelines and entering new data. Matt Dean develops and maintains Helium under the direction of members of Karel Svoboda's lab at Janelia Research Campus and Vathes LLC.

Data may also be imported or synchronized into a DataJoint pipeline from exising LIMS (laboratory information management systems). For example, the International Brain Lab synchronizes data from an Alyx database. For implementation details, see https://github.com/int-brain-lab/IBL-pipeline.

Other labs (e.g. Sinz Lab) have developed GUI interfaces using the Flask web framework in Python.

GUIs, Google Docs integration, LIMS integration, Slack integration, etc.

. progress: 2.0 100% Dimitri

1.4 Publishing Data

DataJoint is a framework for building data pipelines that support rigorous flow of structured data between experimenters, data scientists, and computing agents *during* data acquisition and processing within a centralized project. Publishing final datasets for the outside world may require additional steps and conversion.

1.4.1 Provide access to a DataJoint server

One approach for publishing data is to grant public access to an existing pipeline. Then public users will be able to query the data pipelines using DataJoint's query language and output interfaces just like any other users of the pipeline. For security, this may require synchronizing the data onto a separate read-only public server.

1.4.2 Containerizing as a DataJoint pipeline

Containerization platforms such as docker allow convenient distribution of environments including database services and data. It is convenient to publish DataJoint pipelines as a docker container that deploys the populated DataJoint pipeline. One example of publishing a DataJoint pipeline as a docker container is > Sinz, F., Ecker, A.S., Fahey, P., Walker, E., Cobos, E., Froudarakis, E., Yatsenko, D., Pitkow, Z., Reimer, J. and Tolias, A., 2018. Stimulus domain transfer in recurrent models for large scale cortical population prediction on video. In Advances in Neural Information Processing Systems (pp. 7198-7209). https://www.biorxiv.org/content/early/2018/10/25/452672

The code and the data can be found at https://github.com/sinzlab/Sinz2018_NIPS

1.4. Publishing Data

1.4.3 Exporting into a collection of files

Another option for publishing and archiving data is to export the data from the DataJoint pipeline into a collection of files. DataJoint provides features for exporting and importing sections of the pipeline. Several ongoing projects are implementing the capability to export from DataJoint pipelines into Neurodata Without Borders files.

1.5 Progress

Dimitri Yatsenko began development of DataJoint in Andreas S.Tolias' lab in the Neuroscience Department at Baylor College of Medicine in the fall of 2009. Initially implemented as a thin MySQL API in MATLAB, it defined the major principles of the DataJoint model.

Many students and postdocs in the lab as well as collaborators and early adopters have contributed to the project. Jacob Reimer and Emmanouil Froudarakis became early adopters in Andreas Tolias' Lab and propelled development. Alexander S. Ecker, Philipp Berens, Andreas Hoenselaar, and R. James Cotton contributed to the formulation of the overall requirements for the data model and critical reviews of DataJoint development.

Outside the Tolias lab, the first labs to adopt DataJoint (approx. 2010) were the labs of Athanassios G. Siapas at CalTech, Laura Busse and Steffen Katzner at the University of Tübingen.

In 2015, the Python implementation gained momentum with Edgar Y. Walker and Fabian Sinz joining as principal contributors.

In 2016, Andreas Tolias Lab joined the MICrONS project, using DataJoint to process volumes of neurophysiology and neuroanatomical data shared across large teams.

In 2016, Vathes LLC was founded to provide support to groups using DataJoint.

In 2017, DARPA awarded a small-business innovation research grant to Vathes LLC (Contract D17PC00162) to further develop and publicize the DataJoint framework.

In June 2018, the Princeton Neuroscience Institute, under the leadership of Prof. Carlos Brody, began funding a project to generate a detailed DataJoint user manual.

1.6 License

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1.7 FAQs

1.7.1 How do I use GUIs with DataJoint?

It is common to enter data during experiments using a graphical user interface.

1.7.2 Does DataJoint support other programming languages?

DataJoint was originally developed to support MATLAB, followed by Python. DataJoint's data model and data representation are largely language independent, which means that any language with a DataJoint client can work with a data pipeline defined in any other language. DataJoint clients for other programming languages will be implemented based on demand. All languages must comply to the same data model and computation approach as defined in DataJoint: a simpler relational data model.

1.7.3 Is DataJoint another ORM?

Programmers are familiar with object-relational mappings (ORM) in various programming languages. Python in particular has several popular ORMs such as SQLAlchemy and Django ORM. The purpose of ORMs is to allow representations and manipulations of objects from the host programming language as data in a relational database. ORMs allow making objects persistent between program executions. ORMs create a bridge or a **mapping** between the object model used by the host language and the relational model allowed by the database. The result is always a compromise, usually toward the object model. ORMs usually forgo key concepts, features, and capabilities of the relational model for the sake of convenient programming constructs in the language.

In contrast, DataJoint implements a data model that is a refinement of the relational data model and that adheres to it faithfully without compromising its principles. DataJoint supports data integrity (entity integrity, referential integrity, and group integrity) and provides a fully capable relational query language. DataJoint remains absolutely data-centric, with the primary focus on the structure and integrity of the data pipeline. Other ORMs are more application-centric, primarily focusing on the application design while the database plays a secondary role supporting the application with object persistence and sharing.

1.7.4 How can I use DataJoint with a LIMS?

Lab Information Management Systems (LIMS)

1.7.5 What is the difference between DataJoint and Alyx?

Alyx is an experiment management database application developed in Kenneth Harris' lab at UCL.

Alyx is an application with a fixed pipeline design with a nice graphical user interface. In contrast, DataJoint is a general-purpose library for designing and building data processing pipelines.

Alyx is geared towards ease of data entry and tracking for a specific workflow (e.g. mouse colony information and some pre-specified experiments) and data types. DataJoint could be used as a more general purposes tool to design, implement, and execute processing on such workflows/pipelines from scratch, and DataJoint focuses on flexibility, data integrity, and ease of data analysis. The purposes are partly overlapping and complementary. The International Brain Lab project is developing a bridge from Alyx to DataJoint, hosted as an open-source project. It implements a DataJoint schema that replicates the major features of the Alyx application and a synchronization script from an existing Alyx database to its DataJoint counterpart.

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1.8 Release Notes

1.8.1 3.4.1 – December 18, 2020

- Bugfix: Error on accessing unmanaged Imported/Computed tables (#336) PR #338
- Bugfix: Certain characters in attribute comment not escaped properly (#210, #335) PR #338
- Bugfix: dj.config.load(...) after initial MATLAB boot throws invalid input error. PR #338

1.8.2 3.4.0 - December 11, 2020

- Minor: Add dj.config to be compatible with dj-python and removed dj.set (#186) #188
- Minor: Add UUID DataJoint datatype (#180) PR #194
- Minor: Add file external storage (#143) PR #197
- Minor: Add S3 external storage (#88) PR #207
- Minor: Improve dependency version compatibility handling (#228) PR #285
- Minor: Add unique and nullable options for foreign keys (#110) PR #303
- Minor: Add non-interactive option for dj.new (#69) #317
- Minor: Add dj.kill_quick (#251) PR #314
- Minor: Log connection ID, user in jobs table (#87, #275) PR #314
- Bugfix: Handle empty password (#250) PR #279, #292
- Bugfix: Disable GUI password if running headless (#278) PR #280, #292
- Bugfix: Add order_by option to dj.kill output (#229) PR #248, #292
- Bugfix: erd function missing from package (#307) PR #310
- Bugfix: Error on extremely short table names (#311) PR #317
- Bugfix: Incorrect return when fetchn of an external field (#269) PR #274
- Bugfix: MATLAB crashes randomly on insert 8-byte string (#255) PR #257
- Bugfix: Errors thrown when seeing unsupported DataJoint types (#254) PR #265
- Bugfix: Fix SQL argument growth condition on blobs (#217) PR #220
- Tests: Add R2016b tests (#233) PR #235
- Tests: Convert testing framework from TravisCI to GitHub Actions (#320) PR #317
- Tests: Increase test coverage

1.8.3 3.3.2 - October 15, 2020

- Bugfix: Add blob validation for insert/update regarding sparse matrices which are not yet supported (#238) PR #241
- Bugfix: Modify update to allow nullable updates for strings/date (#211) PR #213
- Bugfix: createSchema had some issues with MySQL8 PR #213
- Update tests
- Docs: Update example related to virtual class (#199) PR #261
- Docs: Fix typos (#150, #151) PR #263, PR #262
- Upgrade packaging and installation to utilize MATLAB Toolbox i.e. DataJoint.mltbx PR #285

1.8.4 3.3.1 – October 31, 2019

- Ability to create schema without GUI PR #155
- Support secure connections with TLS (aka SSL) (#103) PR #157, mym-PR #11, #12, #13
- Allow GUI-based password entry to avoid cleartext password from being captured in MATLAB log PR #159
- Add detailed error message if DJ012 Python-native blobs detected (#170) mYm-PR #16
- Add support for PAM connections via MariaDB's Dialog plugin (#168, #169) mYm-PR #14, #15
- Minor improvements to reuse of connection if applicable PR #166, #167
- Bugfixes (#152)

1.8.5 3.2.2 - February 5, 2019

Previous release notes TBD

1.8. Release Notes

CHAPTER

TWO

SERVER ADMINISTRATION

2.1 Database Server Hosting

Let's say a person, a lab, or a multi-lab consortium decide to use DataJoint as their data pipeline platform. What IT resources and support will be required?

DataJoint uses a MySQL-compatible database server such as MySQL, MariaDB, Percona Server, or Amazon Aurora to store the structured data used for all relational operations. Large blocks of data associated with these records such as multidimensional numeric arrays (signals, images, scans, movies, etc) can be stored within the database or stored in additionally configured *bulk storage*.

The first decisions you need to make are where this server will be hosted and how it will be administered. The server may be hosted on your personal computer, on a dedicated machine in your lab, or in a cloud-based database service.

2.1.1 Cloud hosting

Increasingly, many teams make use of cloud-hosted database services, which allow great flexibility and easy administration of the database server. A cloud hosting option will be provided through https://hub.datajoint.io. The hub simplifies the setup for labs that wish to host their data pipelines in the cloud and allows sharing pipelines between multiple groups and locations. Being an open-source solution, other cloud services such as Amazon RDS can also be used in this role, albeit with less DataJoint-centric customization.

2.1.2 Self hosting

In the most basic configuration, the relational database software and DataJoint are installed onto a single computer which is used by an individual user. To support a small group of users, a larger computer can be used instead and configured for remote access. As the number of users grows, individual workstations can be installed with the DataJoint software and used to connect to a larger and more specialized centrally located database server machine.

For even larger groups or multi-site collaborations, multiple database servers may be configured in a replicated fashion to support larger workloads and simultaneous multi-site access. The following section provides some basic guidelines for these configurations here and in the subsequent sections of the documentation.

2.1.3 General server / hardware support requirements

The following table lists some likely scenarios for DataJoint database server deployments and some reasonable estimates of the required computer hardware. The required IT/systems support needed to ensure smooth operations in the absence of local database expertise is also listed.

Table 1: IT infrastructures

Usage Scenario	DataJoint Database Com-	Required IT Support	
	puter		
Single User	Personal Laptop or Worksta-	Self-Supported or Ad-Hoc General	
	tion	IT Support	
Small Group (e.g. 2-10 Users)	Workstation or Small Server	Ad-Hoc General or Experienced IT	
		Support	
Medium Group (e.g. 10-30 Users)	Small to Medium Server	Ad-Hoc/Part Time Experienced or	
		Specialized IT Support	
Large Group/Department (e.g. 30-50+	Medium/Large Server or	Part Time/Dedicated Experienced	
Users)	Multi-Server Replication	or Specialized IT Support	
Multi-Location Collaboration (30+ users,	Large Server, Advanced	Dedicated Specialized IT Support	
Geographically Distributed)	Replication		

2.2 Relational Database Server

2.2.1 Hardware considerations

As in any computer system, CPU, RAM memory, disk storage, and network speed are important components of performance. The relational database component of DataJoint is no exception to this rule. This section discusses the various factors relating to selecting a server for your DataJoint pipelines.

CPU

CPU speed and parallelism (number of cores/threads) will impact the speed of queries and the number of simultaneous queries which can be efficiently supported by the system. It is a good rule of thumb to have enough cores to support the number of active users and background tasks you expect to have running during a typical 'busy' day of usage. For example, a team of 10 people might want to have 8 cores to support a few active queries and background tasks.

RAM

The amount of RAM will impact the amount of DataJoint data kept in memory, allowing for faster querying of data since the data can be searched and returned to the user without needing to access the slower disk drives. It is a good idea to get enough memory to fully store the more important and frequently accessed portions of your dataset with room to spare, especially if in-database blob storage is used instead of external *bulk storage*.

Disk

The disk storage for a DataJoint database server should have fast random access, ideally with flash-based storage to eliminate the rotational delay of mechanical hard drives.

Networking

When network connections are used, network speed and latency are important to ensure that large query results can be quickly transferred across the network and that delays due to data entry/query round-trip have minimal impact on the runtime of the program.

General recommendations

DataJoint datasets can consist of many thousands or even millions of records. Generally speaking one would want to make sure that the relational database system has sufficient CPU speed and parallelism to support a typical number of concurrent users and to execute searches quickly. The system should have enough RAM to store the primary key values of commonly used tables and operating system caches. Disk storage should be fast enough to support quick loading of and searching through the data. Lastly, network bandwidth must be sufficient to support transferring user records quickly.

2.2.2 Large-scale installations

Database replication may be beneficial if system downtime or precise database responsiveness is a concern Replication can allow for easier coordination of maintenance activities, faster recovery in the event of system problems, and distribution of the database workload across server machines to increase throughput and responsiveness.

Master-slave replication

Master/slave replication allows for creation of a read-only database copy which is updated in real time. This copy can be used for backup or queries which are not time sensitive. It can also be upgraded with read-write usage in the event that the main database fails.

Multi-master replication

Multi-master replication configurations allow for all replicas to be used in a read/write fashion, with the workload being distributed among all machines. However, multi-master replication is also more complicated, requiring frontend machines to distribute the workload, similar performance characteristics on all replicas to prevent bottlenecks, and redundant network connections to ensure the replicated machines are always in sync.

2.2.3 Recommendations

It is usually best to go with the simplest solution which can suit the requirements of the installation, adjusting workloads where possible and adding complexity only as needs dictate.

Resource requirements of course depend on the data collection and processing needs of the given pipeline, but there are general size guidelines that can inform any system configuration decisions. A reasonably powerful workstation or small server should support the needs of a small group (2-10 users). A medium or large server should support the needs of a larger user community (10-30 users). A replicated or distributed setup of 2 or more medium or large servers may be required in larger cases. These requirements can be reduced through the use of external or cloud storage, which is discussed in the subsequent section.

Table 2: Recommendations

Usage Scenario	DataJoint Database	Hardware Recommendation	
	Computer		
Single User	Personal Laptop or	4 Cores, 8-16GB or more of RAM, SSD or better storage	
	Workstation		
Small Group (e.g. 2-10	Workstation or Small	8 or more Cores, 16GB or more of RAM, SSD or better	
Users)	Server	storage	
Medium Group (e.g. 10-30	Small to Medium	8-16 or more Cores, 32GB or more of RAM, SSD/RAID	
Users)	Server	or better storage	
Large Group/Department	Medium/Large	16-32 or more Cores, 64GB or more of RAM, SSD Raid	
(e.g. 30-50+ Users)	Server or Multi-	storage, multiple machines	
	Server Replication		
Multi-Location Collaboration	Large Server, Ad-	16-32 or more Cores, 64GB or more of RAM, SSD Raid	
(30+ users, Geographically	vanced Replication	storage, multiple machines; potentially multiple machines	
Distributed)		in multiple locations	

2.2.4 Docker

A Docker image is available for a MySQL server configured to work with DataJoint: https://github.com/datajoint/mysql-docker.

2.3 User Management

Create user accounts on the MySQL server. For example, if your username is alice, the SQL code for this step is:

```
CREATE USER 'alice'@'%' IDENTIFIED BY 'alices-secret-password';
```

Existing users can be listed using the following SQL:

```
SELECT user, host from mysql.user;
```

Teams that use DataJoint typically divide their data into schemas grouped together by common prefixes. For example, a lab may have a collection of schemas that begin with common_. Some common processing may be organized into several schemas that begin with pipeline_. Typically each user has all privileges to schemas that begin with her username.

For example, alice may have privileges to select and insert data from the common schemas (but not create new tables), and have all privileges to the pipeline schemas.

Then the SQL code to grant her privileges might look like:

```
GRANT SELECT, INSERT ON `common\_%`.* TO 'alice'@'%';
GRANT ALL PRIVILEGES ON `pipeline\_%`.* TO 'alice'@'%';
GRANT ALL PRIVILEGES ON `alice\_%`.* TO 'alice'@'%';
```

To note, the ALL PRIVILEGES option allows the user to create and remove databases without administrator intervention.

Once created, a user's privileges can be listed using the SHOW GRANTS statement.

```
SHOW GRANTS FOR 'alice'@'%';
```

2.3.1 Grouping with Wildcards

Depending on the complexity of your installation, using additional wildcards to group access rules together might make managing user access rules simpler. For example, the following equivalent convention:

```
GRANT ALL PRIVILEGES ON `user_alice\_%`.* TO 'alice'@'%';
```

Could then facilitate using a rule like:

```
GRANT SELECT ON `user\_%\_%`.* TO 'bob'@'%';
```

to enable bob to query all other users tables using the user_username_database convention without needing to explicitly give him access to alice_%, charlie_%, and so on.

This convention can be further expanded to create notions of groups and protected schemas for background processing, etc. For example:

```
GRANT ALL PRIVILEGES ON `group\_shared\_%`.* TO 'alice'@'%';

GRANT ALL PRIVILEGES ON `group\_wonderland\_%`.* TO 'alice'@'%';

GRANT ALL PRIVILEGES ON `group\_wonderland\_%`.* TO 'alice'@'%';
```

could allow both bob an alice to read/write into the group_shared databases, but in the case of the group_wonderland databases, read write access is restricted to alice.

2.4 Bulk Storage Systems

2.4.1 Why External Bulk Storage?

DataJoint supports the storage of large data objects associated with relational records externally from the MySQL Database itself. This is significant and useful for a number of reasons.

Cost

One of these is that the high-performance storage commonly used in database systems is more expensive than that used in more typical commodity storage, and so storing the smaller identifying information typically used in queries on fast, relational database storage and storing the larger bulk data used for analysis or processing on lower cost commodity storage can allow for large savings in storage expense.

Flexibility

Storing bulk data separately also facilitates more flexibility in usage, since the bulk data can managed using separate maintenance processes than that in the relational storage.

For example, larger relational databases may require many hours to be restored in the event of system failures. If the relational portion of the data is stored separately, with the larger bulk data stored on another storage system, this downtime can be reduced to a matter of minutes. Similarly, due to the lower cost of bulk commodity storage, more emphasis can be put into redundancy of this data and backups to help protect the non-relational data.

Performance

Storing the non-relational bulk data separately can have system performance impacts by removing data transfer, disk I/O, and memory load from the database server and shifting these to the bulk storage system. Additionally, datajoint supports caching of bulk data records which can allow for faster processing of records which already have been retrieved in previous queries.

Data Sharing

DataJoint provides pluggable support for different external bulk storage backends, which can provide benefits for data sharing by publishing bulk data to S3-Protocol compatible data shares both in the cloud and on locally managed systems and other common tools for data sharing, such as Globus, etc.

2.4.2 Bulk Storage Scenarios

Typical bulk storage considerations relate to the cost of the storage backend per unit of storage, the amount of data which will be stored, the desired focus of the shared data (system performance, data flexibility, data sharing), and data access. Some common scenarios are given in the following table:

Scenario	Storage Solu- tion	System Requirements	Notes	
Local Object	Local External	Local Hard Drive	Used to Speed Access to other Storage	
Cache	Storage			
LAN Object	Network Exter-	Local Network Share	Used to Speed Access to other storage, reduce	
Cache	nal Storage		Cloud/Network Costs/Overhead	
Local Object	Local/Network	Local/Network Storage	Used to store objects externally from the	
Store	External Stor-		database	
	age			
Local S3-	Local S3-	Network S3-Server	Used to host S3-Compatible services locally	
Compatible	Compatible		(e.g. minio) for internal use or to lower cloud	
Store	Server		costs	
Cloud S3-	Cloud Provider	Internet Connectivity	Used to reduce/remove requirement for external	
Compatible			storage management, data sharing	
Storage				
Globus Stor-	Globus End-	Local/Local Network	Used for institutional data transfer or publish-	
age	point	Storage, Internet Connectivity	ing.	

2.4.3 Bulk Storage Considerations

Although external bulk storage provides a variety of advantages for storage cost and data sharing, it also uses slightly different data input/retrieval semantics and as such has different performance characteristics.

Performance Characteristics

In the direct database connection scenario, entire result sets are either added or retrieved from the database in a single stream action. In the case of external storage, individual record components are retrieved in a set of sequential actions per record, each one subject to the network round trip to the given storage medium. As such, tables using many small records may be ill suited to external storage usage in the absence of a caching mechanism. While some of these impacts may be addressed by code changes in a future release of DataJoint, to some extent, the impact is directly related from needing to coordinate the activities of the database data stream with the external storage system, and so cannot be avoided.

Network Traffic

Some of the external storage solutions mentioned above incur cost both at a data volume and transfer bandwidth level. The number of users querying the database, data access, and use of caches should be considered in these cases to reduce this cost if applicable.

Data Coherency

When storing all data directly in the relational data store, it is relatively easy to ensure that all data in the database is consistent in the event of system issues such as crash recoveries, since MySQL's relational storage engine manages this for you. When using external storage however, it is important to ensure that any data recoveries of the database system are paired with a matching point-in-time of the external storage system. While DataJoint does use hashing to help facilitate a guarantee that external files are uniquely named throughout their lifecycle, the pairing of a given relational dataset against a given filesystem state is loosely coupled, and so an incorrect pairing could result in processing failures or other issues.

2.5 External Store

DataJoint organizes most of its data in a relational database. Relational databases excel at representing relationships between entities and storing structured data. However, relational databases are not particularly well-suited for storing large continuous chunks of data such as images, signals, and movies. An attribute of type <code>longblob</code> can contain an object up to 4 GiB in size (after compression) but storing many such large objects may hamper the performance of queries on the entire table. A good rule of thumb is that objects over 10 MiB in size should not be put in the relational database. In addition, storing data in cloud-hosted relational databases (e.g. AWS RDS) may be more expensive than in cloud-hosted simple storage systems (e.g. AWS S3).

DataJoint allows the use of *external* storage to store large data objects within its relational framework but outside of the main database.

Defining an externally-stored attribute is used using the notation blob@storename (see also: *definition syntax*) and works the same way as a longblob attribute from the users perspective. However, its data are stored in an external storage system rather than in the relational database.

Various systems can play the role of external storage, including a shared file system accessible to all team members with access to these objects or a cloud storage solutions such as AWS S3.

For example, the following table stores motion-aligned two-photon movies.

```
# Motion aligned movies
-> twophoton.Scan
---
aligned_movie : blob@external # motion-aligned movie in 'external' store
```

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All *insert* and *fetch* operations work identically for *external* attributes as they do for *blob* attributes, with the same serialization protocol. Similar to *blobs*, *external* attributes cannot be used in restriction conditions.

Multiple external storage configurations may be used simultaneously with the **@storename** portion of the attribute definition determining the storage location.

```
# Motion aligned movies
-> twophoton.Scan
---
aligned_movie : blob@external-raw # motion-aligned movie in 'external-raw' store
```

2.5.1 Principles of operation

External storage is organized to emulate individual attribute values in the relational database. DataJoint organizes external storage to preserve the same data integrity principles as in relational storage.

 The external storage locations are specified in the DataJoint connection configuration with one specification for each store.

Note: External storage is not yet implemented in MATLAB. The feature will be added in an upcoming release: https://github.com/datajoint/datajoint-matlab/issues/143

- 2. Each schema corresponds to a dedicated folder at the storage location with the same name as the database schema.
- 3. Stored objects are identified by the SHA-256 hashes (in web-safe base-64 ASCII) of their serialized contents. This scheme allows for the same object—used multiple times in the same schema—to be stored only once.
- 4. In the external-raw storage, the objects are saved as files with the hash as the filename.
- 5. In the external storage, external files are stored in a directory layout corresponding to the hash of the filename. By default, this corresponds to the first 2 characters of the hash, followed by the second 2 characters of the hash, followed by the actual file.
- Each database schema has an auxiliary table named ~external_<storename> for each configured external store.

It is automatically created the first time external storage is used. The primary key of ~external_<storename> is the hash of the data (for blobs and attachments) or of the relative paths to the files for filepath-based storage. Other attributes are the count of references by tables in the schema, the size of the object in bytes, and the timestamp of the last event (creation, update, or deletion).

Below are sample entries in ~external_<storename>.

Table 3: ~external_raw

HASH	size	filepath	contents_ha	timestamp
1GEqtEU6JY	1039536788	NULL	NULL	2017-06-07 23:14:01
VZio1ga25v				

The fields *filepath* and *contents_hash* relate to the *filepath* datatype, which will be discussed separately.

7. Attributes of type @<storename> are declared as renamed *foreign keys* referencing the ~external_<storename> table (but are not shown as such to the user).

- 8. The *insert* operation encodes and hashes the blob data. If an external object is not present in storage for the same hash, the object is saved and if the save operation is successful, corresponding entities in table ~external_<storename> for that store are created.
- 9. The *delete* operation first deletes the foreign key reference in the target table. The external table entry and actual external object is not actually deleted at this time (*soft-delete*).
- 10. The *fetch* operation uses the hash values to find the data.

In order to prevent excessive network overhead, a special external store named cache can be configured. If the cache is enabled, the fetch operation need not access ~external_<storename> directly. Instead fetch will retrieve the cached object without downloading directly from the *real* external store.

- 11. Cleanup is performed regularly when the database is in light use or off-line.
- 12. DataJoint never removes objects from the local cache folder. The cache folder may just be periodically emptied entirely or based on file access date. If dedicated cache folders are maintained for each schema, then a special procedure will be provided to remove all objects that are no longer listed in ~external_<storename>.

Data removal from external storage is separated from the delete operations to ensure that data are not lost in race conditions between inserts and deletes of the same objects, especially in cases of transactional processing or in processes that are likely to get terminated. The cleanup steps are performed in a separate process when the risks of race conditions are minimal. The process performing the cleanups must be isolated to prevent interruptions resulting in loss of data integrity.

2.5.2 Configuration

The following steps must be performed to enable external storage:

1. Assign external location settings for each storage as shown in the *Step 1* example above.

Use dj.config for configuration.

- protocol [s3, file] Specifies whether s3 or file external storage is desired.
- endpoint [s3] Specifies the remote endpoint to the external data for all schemas as well as the target port.
- bucket [s3] Specifies the appropriate s3 bucket organization.
- location [s3, file] Specifies the subdirectory within the root or bucket of store to preserve data. External objects are thus stored remotely with the following path structure: <bucket (if applicable)>/<location>/<schema_name>/<subfolding_strategy>/<object>.
- access_key [s3] Specifies the access key credentials for accessing the external location.
- secret_key [s3] Specifies the secret key credentials for accessing the external location.
- secure [s3] Optional specification to establish secure external storage connection with TLS (aka SSL, HTTPS). Defaults to False.
- 2. Optionally, for each schema specify the cache folder for local fetch cache.

Note: The cache folder is not yet implemented in MATLAB. The feature will be added in an upcoming release: https://github.com/datajoint/datajoint-matlab/issues/143

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2.5.3 Cleanup

Deletion of records containing externally stored blobs is a *soft-delete* which only removes the database-side records from the database. To cleanup the external tracking table or the actual external files, a separate process is provided as follows.

Note: External storage is not yet implemented in MATLAB. The feature will be added in an upcoming release: https://github.com/datajoint/datajoint-matlab/issues/143

2.5.4 Migration between DataJoint v0.11 and v0.12

Note: Please read carefully if you have used external storage in DataJoint v0.11!

The initial implementation of external storage was reworked for DataJoint v0.12. These changes are backward-incompatible with DataJoint v0.11 so care should be taken when upgrading. This section outlines some details of the change and a general process for upgrading to a format compatible with DataJoint v0.12 when a schema rebuild is not desired.

The primary changes to the external data implementation are:

- The external object tracking mechanism was modified. Tracking tables were extended for additional external datatypes and split into per-store tables to improve database performance in schemas with many external objects.
- The external storage format was modified to use a nested subfolder structure (*folding*) to improve performance and interoperability with some filesystems that have limitations or performance problems when storing large numbers of files in single directories.

Depending on the circumstances, the simplest way to migrate data to v0.12 may be to drop and repopulate the affected schemas. This will construct the schema and storage structure in the v0.12 format and save the need for database migration. When recreation is not possible or is not preferred to upgrade to DataJoint v0.12, the following process should be followed:

- 1) Stop write activity to all schemas using external storage.
- 2) Perform a full backup of your database(s).
- 3) Upgrade your DataJoint installation to v0.12
- 4) Adjust your external storage configuration (in *datajoint.config*) to the new v0.12 configuration format (see above).
- 5) Migrate external tracking tables for each schema to use the new format. For instance in Python:

```
>>> import datajoint.migrate as migrate
>>> db_schema_name='schema_1'
>>> external_store='raw'
>>> migrate.migrate_dj011_external_blob_storage_to_dj012(db_schema_name, external_store)
6) Verify pipeline functionality after this process has completed. For instance in Python:
```

```
>>> x = myschema.TableWithExternal.fetch('external_field', limit=1)[0]
```

Note: This migration function is provided on a best-effort basis, and will convert the external tracking tables into a format which is compatible with DataJoint v0.12. While we have attempted to ensure correctness of the process,

all use-cases have not been heavily tested. Please be sure to fully back-up your data and be prepared to investigate problems with the migration, should they occur.

Please note:

- The migration only migrates the tracking table format and does not modify the backing file structure to support *folding*. The DataJoint v0.12 logic is able to work with this format, but to take advantage of the new backend storage, manual adjustment of the tracking table and files, or a full rebuild of the schema should be performed.
- Additional care to ensure all clients are using v0.12 should be taken after the upgrade. Legacy clients may incorrectly create data in the old format which would then need to be combined or otherwise reconciled with the data in v0.12 format. You might wish to take the opportunity to version-pin your installations so that future changes requiring controlled upgrades can be coordinated on a system wide basis.

2.6 Backups and Recovery

Backing up your DataJoint installation is critical to ensuring that your work is safe and can be continued in the event of system failures, and several mechanisms are available to use.

Much like your live installation, your backup will consist of two portions:

- Backup of the Relational Data
- Backup of optional external bulk storage

This section primarily deals with backup of the relational data since most of the optional bulk storage options use "regular" flat-files for storage and can be backed up via any "normal" disk backup regime.

There are many options to backup MySQL; subsequent sections discuss a few options.

2.6.1 Cloud hosted backups

In the case of cloud-hosted options, many cloud vendors provide automated backup of your data, and some facility for downloading such backups externally. Due to the wide variety of cloud-specific options, discussion of these options falls outside of the scope of this documentation. However, since the cloud server is also a MySQL server, other options listed here may work for your situation.

2.6.2 Disk-based backup

The simplest option for many cases is to perform a disk-level backup of your MySQL installation using standard disk backup tools. It should be noted that all database activity should be stopped for the duration of the backup to prevent errors with the backed up data. This can be done in one of two ways:

- Stopping the MySQL server program
- Using database locks

These methods are required since MySQL data operations can be ongoing in the background even when no user activity is ongoing. To use a database lock to perform a backup, the following commands can be used as the MySQL administrator:

```
FLUSH TABLES WITH READ LOCK; UNLOCK TABLES;
```

The backup should be performed between the issuing of these two commands, ensuring the database data is consistent on disk when it is backed up.

2.6.3 MySQLDump

Disk based backups may not be feasible for every installation, or a database may require constant activity such that stopping it for backups is not feasible. In such cases, the simplest option is MySQLDump, a command line tool that prints the contents of your database contents in SQL form.

This tool is generally acceptable for most cases and is especially well suited for smaller installations due to its simplicity and ease of use.

For larger installations, the lower speed of MySQLDump can be a limitation, since it has to convert the database contents to and from SQL rather than dealing with the database files directly. Additionally, since backups are performed within a transaction, the backup will be valid up to the time the backup began rather than to its completion, which can make ensuring that the latest data are fully backed up more difficult as the time it takes to run a backup grows.

2.6.4 Percona XTraBackup

The Percona xtrabackup tool provides near-realtime backup capability of a MySQL installation, with extended support for replicated databases, and is a good tool for backing up larger databases.

However, this tool requires local disk access as well as reasonably fast backup media, since it builds an ongoing transaction log in real time to ensure that backups are valid up to the point of their completion. This strategy fails if it cannot keep up with the write speed of the database. Further, the backups it generates are in binary format and include incomplete database transactions, which require careful attention to detail when restoring.

As such, this solution is recommended only for advanced use cases or larger databases where limitations of the other solutions may apply.

2.6.5 Locking and DDL issues

One important thing to note is that at the time of writing, MySQL's transactional system is not data definition language aware, meaning that changes to table structures occurring during some backup schemes can result in corrupted backup copies. If schema changes will be occurring during your backup window, it is a good idea to ensure that appropriate locking mechanisms are used to prevent these changes during critical steps of the backup process.

However, on busy installations which cannot be stopped, the use of locks in many backup utilities may cause issues if your programs expect to write data to the database during the backup window.

In such cases it might make sense to review the given backup tools for locking related options or to use other mechanisms such as replicas or alternate backup tools to prevent interaction of the database.

2.6.6 Replication and snapshots for backup

Larger databases consisting of many Terabytes of data may take many hours or even days to backup and restore, and so downtime resulting from system failure can create major impacts to ongoing work.

While not backup tools per-se, use of MySQL master-slave replication and disk snapshots can be useful to assist in reducing the downtime resulting from a full database outage.

Replicas can be configured so that one copy of the data is immediately online in the event of server crash. When a server fails in this case, users and programs simply restart and point to the new server before resuming work.

Replicas can also reduce the system load generated by regular backup procedures, since they can be backed up instead of the main server. Additionally they can allow more flexibility in a given backup scheme, such as allowing for disk snapshots on a busy system that would not otherwise be able to be stopped. A replica copy can be stopped temporarily and then resumed while a disk snapshot or other backup operation occurs.

CHAPTER

THREE

CLIENT SETUP

3.1 Install and Connect

- 1. Download the DataJoint MATLAB Toolbox from the MATLAB Central FileExchange.
- 2. Open DataJoint.mltbx and follow installation instructions.
- 3. After installation, verify from MATLAB that you have the latest version of DataJoint (3.0.0 or above):

```
>> dj.version
DataJoint version 3.0.0
```

4. At the MATLAB command prompt, assign the environment variables with the database credentials. For example, if you are connection to the server alicelab.datajoint.io with username alice and password haha not my real password, execute the following commands:

```
setenv DJ_USER alice
setenv DJ_HOST alicelab.datajoint.io
setenv DJ_PASS 'haha not my real password'
```

You will need to execute these commands at the beginning of each DataJoint work session. To automate this process, you might like to use the startup.m script.

However, be careful not to share this file or commit it to a public directory (a common mistake), as it contains a your login credentials in plain text. If you are not sure, it is better not to set DJ_PASS, in which case DataJoint will prompt to enter the password when connecting to the database.

To change the database password, use the following command

```
>> dj.setPassword('my#cool!new*psswrd')
```

And update your credentials in your startup script for the next session.

3.2 Other Configuration Settings

If you are not using DataJoint on your own, or are setting up a DataJoint system for other users, some additional configuration options may be required to support *TLS* or *external storage*.

3.2.1 TLS Configuration

Starting with v0.12 (Python) and v3.3.1 (MATLAB), DataJoint will by default use TLS if it is available. TLS can be forced on or off with the boolean use_tls in MATLAB, or dj.config['database.use_tls'] in Python.

3.3 DataJoint Python Windows Install Guide

This document outlines the steps necessary to install DataJoint on Windows for use in connecting to a remote server hosting a DataJoint database. Some limited discussion of installing MySQL is discussed in *MySQL for Windows*, but is not covered in-depth since this is an uncommon usage scenario and not strictly required to connect to DataJoint pipelines.

3.3.1 Quick steps

Quick install steps for advanced users are as follows:

- Install latest Python 3.x and ensure it is in PATH (3.6.3 current at time of writing)
- pip install datajoint

For ERD drawing support:

- Install Graphviz for Windows and ensure it is in PATH (64 bit builds currently tested; URL below.)
- pip install pydotplus matplotlib

Detailed instructions follow.

3.3.2 Step 1: install Python

Python for Windows is available from:

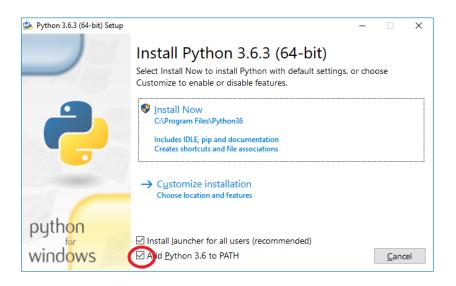
https://www.python.org/downloads/windows

The latest 64 bit 3.x version, currently 3.6.3, is available from the Python site.

From here run the installer to install Python.

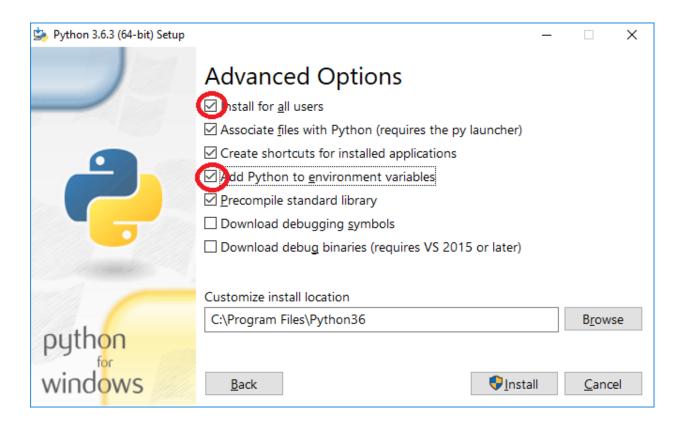
For a single-user machine, the regular installation process is sufficient - be sure to select the option:

Add Python to PATH option:



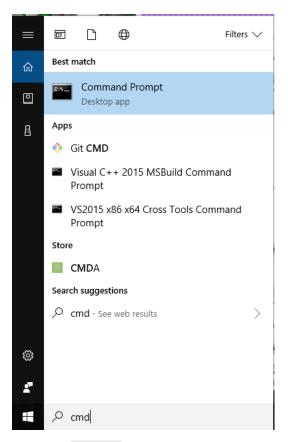
For a shared machine, run the installer as administrator (right-click, run as administrator) and select the advanced installation. Be sure to select options as follows:





3.3.3 Step 2: verify installation

To verify the Python installation and make sure that your system is ready to install DataJoint, open a command window by entering cmd into the Windows search bar:



From here python and the Python package manager pip can be verified by running python -V and pip -V, respectively:

```
Microsoft Windows [Version 10.0.15063]
(c) 2017 Microsoft Corporation. All rights reserved.

C:\Users\ctmsf>pip -V
pip 9.0.1 from c:\users\ctmsf\appdata\local\programs\python\python36\lib\site-packages (python 3.6)

C:\Users\ctmsf>python -V
Python 3.6.3

C:\Users\ctmsf>
```

If you receive the error message that either pip or python is not a recognized command, please uninstall Python and ensure that the option to add Python to the PATH variable was properly configured.

3.3.4 Step 3: install DataJoint

DataJoint (and other Python modules) can be easily installed using the pip Python package manager which is installed as a part of Python and was verified in the previous step.

To install DataJoint simply run pip install datajoint:

```
Microsoft Windows [Version 10.0.15963]
(c) 2017 Microsoft Corporation. All rights reserved.

C:\Users\ctmsf>pip install datajoint

✓
```

This will proceed to install DataJoint, along with several other required packages from the PIP repository. When finished, a summary of the activity should be presented:

```
Command Prompt
100% | Collecting s3transfer<0.2.0,>=0.1.10 (from boto3->datajoint Downloading s3transfer-0.1.11-py2.py3-none-any.whl (54kB) | 61kB 739kB/s
                                                                                           (from boto3->datajoint)
  ollecting parso=
                                                                          jedi>=0.10->ipython->datajoint)
                                                                                                 any.whl (89kB)
         100% |
                                                                                                           92kB 601kB/s
  ollecting ip
                                                                                       raitlets>=4.2->ipython->datajoint)
 Downloading ipython_genutis-0.2.0-py2.py3-none-any.whl
Collecting six (from traitlets>=4.2->ipython->datajoint)
Downloading six-1.11.0-py2.py3-none-any.whl
Collecting wcwidth (from prompt-toolkit<2.0.0,>=1.0.4->ipython->datajoint)
Downloading wcwidth-0.1.7-py2.py3-none-any.whl
Collecting python-dateutil<3.0.0,>=2.1 (from botocore<1.8.0,>=1.7.0->boto3->datajoint)
Downloading python_dateutil-2.6.1-py2.py3-none-any.whl (194kB)
                                                                                                        | 194kB 411kB/s
  ollecting docutils>=0.10 (from botocore<1.8.0,>=1.7
Downloading docutils-0.14-py3-none-any.whl (543kB)
                                                                 (from botocore<1.8.0,>=1.7.0->boto3->datajoint)
        100% |
                                                                                                      552kB 364kB/s
Installing collected packages: pyparsing, pymysql, decorator, networkx, pygments, parso, jedi, simplegeneric, pickleshar e, ipython-genutils, six, traitlets, wcwidth, prompt-toolkit, colorama, ipython, numpy, pydotplus, jmespath, python-date util, docutils, botocore, s3transfer, boto3, datajoint

Running setup.py install for simplegeneric ... done

Running setup.py install for pydotplus ... done

Successfully installed boto3-1.4.7 botocore-1.7.43 colorama-0.3.9 datajoint-0.8.2 decorator-4.1.2 docutils-0.14 ipython-
6.2.1 ipython-genutils-0.2.0 jedi-0.11.0 jmespath-0.9.3 networkx-1.11 numpy-1.13.3 parso-0.1.0 pickleshare-0.7.4 prompt-
toolkit-1.0.15 pydotplus-2.0.2 pygments-2.2.0 pymysql-0.7.11 pyparsing-2.2.0 python-dateutil-2.6.1 s3transfer-0.1.11 sim
plegeneric-0.8.1 six-1.11.0 traitlets-4.3.2 wcwidth-0.1.7
  :\Users\ctmsf>
```

Note: You can find out more about the packages installed here and many other freely available open source packages via pypi, the Python package index site.

3.3.5 (Optional) step 4: install packages for ERD support

To draw ERD diagrams of your DataJoint schema, the following additional steps should be followed.

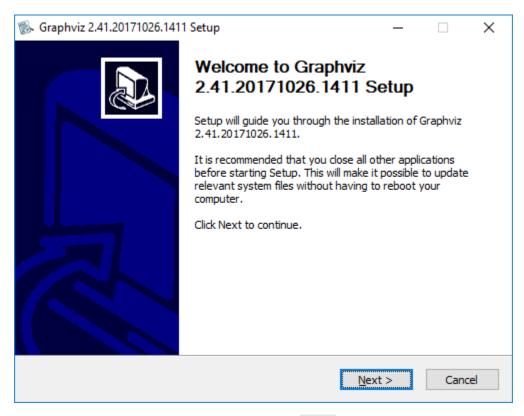
Install Graphviz

DataJoint currently utilizes Graphviz to generate the ERD visualizations. Although a Windows version of Graphviz is available from the main site, it is an older and out of date 32-bit version. The recommended pre-release builds of the 64 bit version are available here:

https://ci.appveyor.com/project/ellson/graphviz-pl238

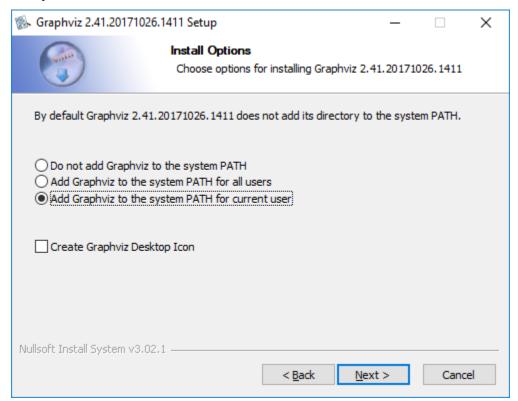
More specifically, the build artifacts from the Win64; Configuration: Release are recommended, available here.

This is a regular Windows installer executable, and will present a dialog when starting:

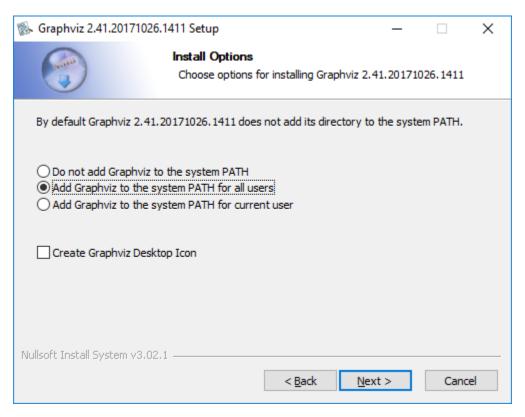


It is important that an option to place Graphviz in the PATH be selected.

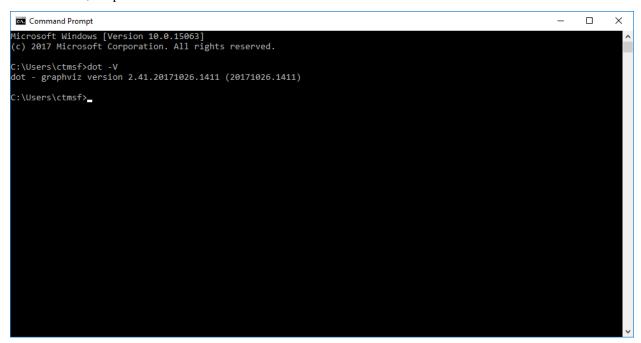
For a personal installation:



To install system wide:



Once installed, Graphviz can be verified from a fresh command window as follows:

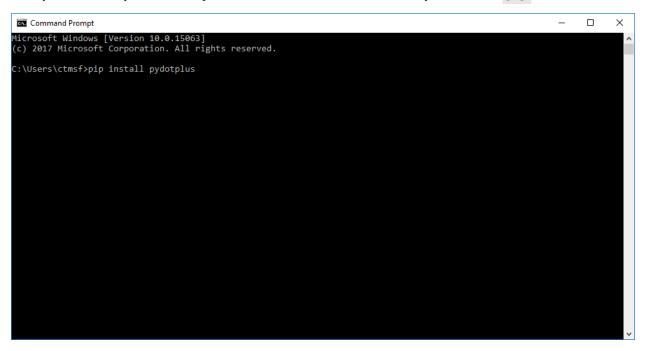


If you receive the error message that the dot program is not a recognized command, please uninstall Graphviz and ensure that the option to add Python to the PATH variable was properly configured.

Important: in some cases, running the dot -c command in a command prompt is required to properly initialize the Graphviz installation.

Install PyDotPlus

The PyDotPlus library links the Graphviz installation to DataJoint and is easily installed via pip:



Install Matplotlib

The Matplotlib library provides useful plotting utilities which are also used by DataJoint's ERD drawing facility. The package is easily installed via pip:

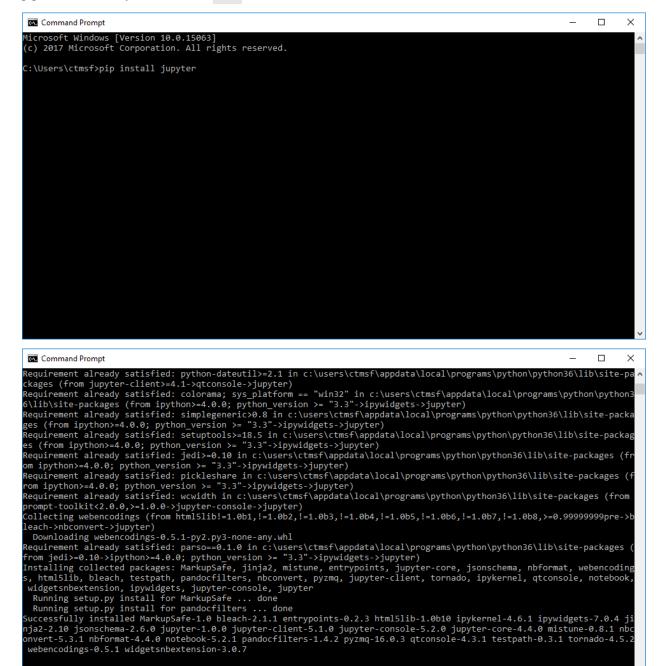
```
Command Prompt
                                                                                                                                                              ×
 Microsoft Windows [Version 10.0.15063]
(c) 2017 Microsoft Corporation. All rights reserved.
 C:\Users\ctmsf>pip install matplotlib
 Collecting matplotlib
Using cached matplotlib-2.1.0-cp36-cp36m-win_amd64.whl
 Requirement already satisfied: six>=1.10 in c:\users\ctmsf\appdata\local\programs\python\python36\lib\site-packages (fro
 n matplotlib)
 Requirement already satisfied: numpy>=1.7.1 in c:\users\ctmsf\appdata\local\programs\python\python36\lib\site-packages
  rom matplotlib)
 Requirement already satisfied: pytz in c:\users\ctmsf\appdata\local\programs\python\python36\lib\site-packages (from mat
 plotlib)
Requirement already satisfied: python-dateutil>=2.0 in c:\users\ctmsf\appdata\local\programs\python\python36\lib\site-packages (from matplotlib)
Requirement already satisfied: cycler>=0.10 in c:\users\ctmsf\appdata\local\programs\python\python36\lib\site-packages (
 from matplotlib)
Requirement already satisfied: pyparsing!=2.0.4,!=2.1.2,!=2.1.6,>=2.0.1 in c:\users\ctmsf\appdata\local\programs\python\
python36\lib\site-packages (from matplotlib)
Installing collected packages: matplotlib
Successfully installed matplotlib-2.1.0
 :\Users\ctmsf>_
```

3.3.6 (Optional) step 5: install Jupyter Notebook

As described on the jupyter.org website:

'The Jupyter Notebook is an open-source web application that allows you to create and share documents that contain live code, equations, visualizations and narrative text.'

Although not a part of DataJoint, Jupyter Notebook can be a very useful tool for building and interacting with DataJoint pipelines. It is easily installed from pip as well:



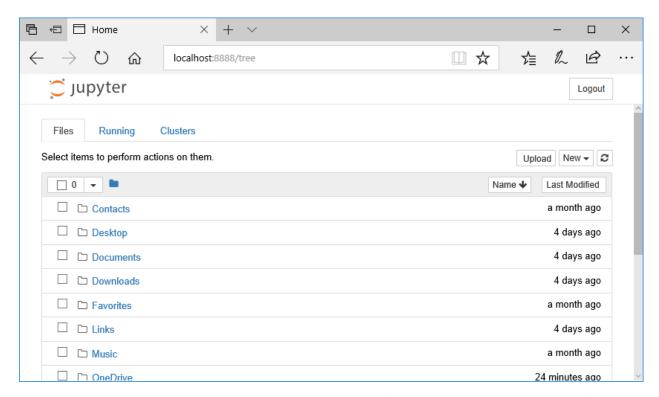
Once installed, Jupyter Notebook can be started via the jupyter notebook command, which should now be on your path:

By default Jupyter Notebook will start a local private webserver session from the directory where it was started and start a web browser session connected to the session.

```
Microsoft Windows [Version 10.0.15063]
(c) 2017 Microsoft Corporation. All rights reserved.

C:\Users\ctmsf>jupyter notebook
[I 66:15:24.697 NotebookApp] Serving notebooks from local directory: C:\Users\ctmsf
[I 66:15:24.697 NotebookApp] The Jupyter Notebook is running at:
[I 66:15:24.697 NotebookApp] The Jupyter Notebook is running at:
[I 66:15:24.697 NotebookApp] Use Control-C to stop this server and shut down all kernels (twice to skip confirmation).
[C 66:15:24.697 NotebookApp] Use Control-C to stop this server and shut down all kernels (twice to skip confirmation).
[C 66:15:24.697 NotebookApp]

Copy/paste this URL into your browser when you connect for the first time, to login with a token:
    http://localhost:8888/?token=29abf4278c6741c2c66205e1a91b09bc01219c24cf693557
[I 66:15:27.026 NotebookApp] Accepting one-time-token-authenticated connection from ::1
```



You now should be able to use the notebook viewer to navigate the filesystem and to create new project folders and interactive Jupyter/Python/DataJoint notebooks.

3.3.7 Git for Windows

The Git version control system is not a part of DataJoint but is recommended for interacting with the broader Python/Git/GitHub sharing ecosystem.

The Git for Windows installer is available from https://git-scm.com/download/win.



The default settings should be sufficient and correct in most cases.

3.3.8 MySQL for Windows

For hosting pipelines locally, the MySQL server package is required.

MySQL for windows can be installed via the installers available from the MySQL website. Please note that although DataJoint should be fully compatible with a Windows MySQL server installation, this mode of operation is not tested by the DataJoint team.

CHAPTER

FOUR

CONCEPTS

4.1 Data Model

4.1.1 What is a data model?

A **data model** refers to a conceptual framework for thinking about data and about operations on data. A data model defines the mental toolbox of the data scientist; it has less to do with the architecture of the data systems, although architectures are often intertwined with data models.

Among the most familiar data models are those based on files and folders: data of any kind are lumped together into binary strings called **files**, files are collected into folders, and folders can be nested within other folders to create a folder hierarchy.

Another family of data models are various **tabular models**. For example, items in CSV files are listed in rows, and the attributes of each item are stored in columns. Various **spreadsheet** models allow forming dependencies between cells and groups of cells, including complex calculations.

The **object data model** is common in programming, where data are represented as objects in memory with properties and methods for transformations of such data.

4.1.2 Relational data model

The **relational model** is a way of thinking about data as sets and operations on sets. Formalized almost a half-century ago (Codd, 1969), the relational data model provides the most rigorous approach to structured data storage and the most precise approach to data querying. The model is defined by the principles of data representation, domain constraints, uniqueness constraints, referential constraints, and declarative queries as summarized below.

Core principles of the relational data model

Data representation. Data are represented and manipulated in the form of relations. A relation is a set (i.e. an unordered collection) of entities of values for each of the respective named attributes of the relation. Base relations represent stored data while derived relations are formed from base relations through query expressions. A collection of base relations with their attributes, domain constraints, uniqueness constraints, and referential constraints is called a schema.

Domain constraints. Attribute values are drawn from corresponding attribute domains, i.e. predefined sets of values. Attribute domains may not include relations, which keeps the data model flat, i.e. free of nested structures.

Uniqueness constraints. Entities within relations are addressed by values of their attributes. To identify and relate data elements, uniqueness constraints are imposed on subsets of attributes. Such subsets are then referred to as keys. One key in a relation is designated as the primary key used for referencing its elements.

Referential constraints. Associations among data are established by means of referential constraints with the help of foreign keys. A referential constraint on relation A referencing relation B allows only those entities in A whose foreign key attributes match the key attributes of an entity in B.

Declarative queries. Data queries are formulated through declarative, as opposed to imperative, specifications of sought results. This means that query expressions convey the logic for the result rather than the procedure for obtaining it. Formal languages for query expressions include relational algebra, relational calculus, and SQL.

The relational model has many advantages over both hierarchical file systems and tabular models for maintaining data integrity and providing flexible access to interesting subsets of the data.

Popular implementations of the relational data model rely on the Structured Query Language (SQL). SQL comprises distinct sublanguages for schema definition, data manipulation, and data queries. SQL thoroughly dominates in the space of relational databases and is often conflated with the relational data model in casual discourse. Various terminologies are used to describe related concepts from the relational data model. Similar to spreadsheets, relations are often visualized as tables with *attributes* corresponding to *columns* and *entities* corresponding to *rows*. In particular, SQL uses the terms *table*, *column*, and *row*.

4.1.3 DataJoint is a refinement of the relational data model

DataJoint is a conceptual refinement of the relational data model offering a more expressive and rigorous framework for database programming (Yatsenko et al., 2018). The DataJoint model facilitates clear conceptual modeling, efficient schema design, and precise and flexible data queries. The model has emerged over a decade of continuous development of complex data pipelines for neuroscience experiments (Yatsenko et al., 2015). DataJoint has allowed researchers with no prior knowledge of databases to collaborate effectively on common data pipelines sustaining data integrity and supporting flexible access. DataJoint is currently implemented as client libraries in MATLAB and Python. These libraries work by transpiling DataJoint queries into SQL before passing them on to conventional relational database systems that serve as the backend, in combination with bulk storage systems for storing large contiguous data objects.

DataJoint comprises:

- a schema definition language
- a data manipulation language
- a data *query* language
- a diagramming notation for visualizing relationships between modeled entities

The key refinement of DataJoint over other relational data models and their implementations is DataJoint's support of *entity normalization*.

4.2 Terminology

DataJoint introduces a principled data model, which is described in detail in Yatsenko et al., 2018. This data model is a conceptual refinement of the Relational Data Model and also draws on the Entity-Relationship Model (ERM).

The Relational Data Model was inspired by the concepts of relations in Set Theory. When the formal relational data model was formulated, it introduced additional terminology (e.g. *relation, attribute, tuple, domain*). Practical programming languages such as SQL do not precisely follow the relational data model and introduce other terms to approximate relational concepts (e.g. *table, column, row, datatype*). Subsequent data models (e.g. ERM) refined the relational data model and introduced their own terminology to describe analogous concepts (e.g. *entity set, relationship set, attribute set*). As a result, similar concepts may be described using different sets of terminologies, depending on the context and the speaker's background.

For example, what is known as a **relation** in the formal relational model is called a **table** in SQL; the analogous concept in ERM and DataJoint is called an **entity set**.

The DataJoint documentation follows the terminology defined in Yatsenko et al, 2018, except *entity set* is replaced with the more colloquial *table* or *query result* in most cases.

The table below summarizes the terms used for similar concepts across the related data models.

Relational **ERM** SQL DataJoint (formal) This manual relation table entity set table entity set tuple entity row entity entity domain value set datatype datatype datatype attribute attribute column attribute attribute attribute value attribute value field value attribute value attribute value primary key primary key primary key primary key primary key foreign key foreign key foreign key foreign key foreign key schema schema schema or database schema schema SELECT statement relational expresdata query query expression query expression sion

Table 1: Data model terminology

4.2.1 DataJoint: databases, schemas, packages, and modules

A database is collection of tables on the database server. DataJoint users do not interact with it directly.

A DataJoint schema is

- a database on the database server containing tables with data and
- a collection of classes (in MATLAB or Python) associated with the database, one class for each table.

In MATLAB, the collection of classes is organized as a **package**, i.e. a file folder starting with a +.

In Python, the collection of classes is any set of classes decorated with the appropriate schema object. Very commonly classes for tables in one database are organized as a distinct Python module. Thus, typical DataJoint projects have one module per database. However, this organization is up to the user's discretion.

4.2.2 Base tables

Base tables are tables stored in the database, and are often referred to simply as *tables* in DataJoint. Base tables are distinguished from **derived tables**, which result from relational *operators*.

4.2.3 Relvars and relation values

Early versions of the DataJoint documentation referred to the relation objects as **relvars** https://en.wikipedia.org/wiki/Relvar. This term emphasizes the fact that relational variables and expressions do not contain actual data but are rather symbolic representations of data to be retrieved from the database. The specific value of a relvar would then be referred to as the **relation value**. The value of a relvar can change with changes in the state of the database.

The more recent iteration of the documentation has grown less pedantic and more often uses the term table instead.

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4.2.4 Metadata

The vocabulary of DataJoint does not include this term.

In data science, the term **metadata** commonly means "data about the data" rather than the data themselves. For example, metadata could include data sizes, timestamps, data types, indexes, keywords.

In contrast, neuroscientists often use the term to refer to conditions and annotations about experiments. This distinction arose when such information was stored separately from experimental recordings, such as in physical notebooks. Such "metadata" are used to search and to classify the data and are in fact an integral part of the *actual* data.

In DataJoint, all data other than blobs can be used in searches and categorization. These fields may originate from manual annotations, preprocessing, or analyses just as easily as from recordings or behavioral performance. Since "metadata" in the neuroscience sense are not distinguished from any other data in a pipeline, DataJoint avoids the term entirely. Instead, DataJoint differentiates data into *data tiers*.

4.3 Entity Normalization

DataJoint uses a uniform way of representing any data. It does so in the form of **entity sets**, unordered collections of entities of the same type. The term **entity normalization** describes the commitment to represent all data as well-formed entity sets. Entity normalization is a conceptual refinement of the *relational data model* and is the central principle of the DataJoint model (Yatsenko et al., 2018). Entity normalization leads to clear and logical database designs and to easily comprehensible data queries.

Entity sets are a type of **relation** (from the *relational data model*) and are often visualized as **tables**. Hence the terms **relation**, **entity set**, and **table** can be used interchangeably when entity normalization is assumed.

4.3.1 Criteria of a well-formed entity set

- 1. All elements of an entity set belong to the same well-defined and readily identified **entity type** from the model world.
- 2. All attributes of an entity set are applicable directly to each of its elements, although some attribute values may be missing (set to null).
- 3. All elements of an entity set must be distinguishable form each other by the same primary key.
- 4. Primary key attribute values cannot be missing, i.e. set to null.
- 5. All elements of an entity set participate in the same types of relationships with other entity sets.

4.3.2 Entity normalization in schema design

Entity normalization applies to schema design in that the designer is responsible for the identification of the essential entity types in their model world and of the dependencies among the entity types.

The term entity normalization may also apply to a procedure for refactoring a schema design that does not meet the above criteria into one that does. In some cases, this may require breaking up some entity sets into multiple entity sets, which may cause some entities to be represented across multiple entity sets. In other cases, this may require converting attributes into their own entity sets. Technically speaking, entity normalization entails compliance with the Boyce-Codd normal form while lacking the representational power for the applicability of more complex normal forms (Kent, 1983). Adherence to entity normalization prevents redundancies in storage and data manipulation anomalies. The same criteria originally motivated the formulation of the classical relational normal forms.

4.3.3 Entity normalization in data gueries

Entity normalization applies to data queries as well. DataJoint's *query operators* are designed to preserve the entity normalization of their inputs. For example, the outputs of operators *restriction*, *proj*, and *aggr* retain the same entity type as the (first) input. The *join* operator produces a new entity type comprising the pairing of the entity types of its inputs. *Universal sets* explicitly introduce virtual entity sets when necessary to accomplish a query.

4.3.4 Examples of poor normalization

Design choices lacking entity normalization may lead to data inconsistencies or anomalies. Below are several examples of poorly normalized designs and their normalized alternatives.

Indirect attributes

All attributes should apply to the entity itself. Avoid attributes that actually apply to one of the entity's other attributes. For example, consider the table Author with attributes author_name, institution, and institution_address. The attribute institution_address should really be held in a separate Institution table that Author depends on.

Repeated attributes

Avoid tables with repeated attributes of the same category. A better solution is to create a separate table that depends on the first (often a *part table*), with multiple individual entities rather than repeated attributes. For example, consider the table Protocol that includes the attributes equipment1, ``equipment2, and equipment3. A better design would be to create a ProtocolEquipment table that links each entity in Protocol with multiple entities in Equipment through *dependencies*.

Attributes that do not apply to all entities

All attributes should be relevant to every entity in a table. Attributes that apply only to a subset of entities in a table likely belong in a separate table containing only that subset of entities. For example, a table Protocol should include the attribute stimulus only if all experiment protocols include stimulation. If the not all entities in Protocol involve stimulation, then the stimulus attribute should be moved to a part table that has Protocol as its master. Only protocols using stimulation will have an entry in this part table.

Transient attributes

Attributes should be relevant to all entities in a table at all times. Attributes that do not apply to all entities should be moved to another dependent table containing only the appropriate entities. This principle also applies to attributes that have not yet become meaningful for some entities or that will not remain meaningful indefinitely. For example, consider the table <code>Mouse</code> with attributes <code>birth_date</code> and <code>death_date</code>, where <code>death_date</code> is set to <code>NULL</code> for living mice. Since the <code>death_date</code> attribute is not meaningful for mice that are still living, the proper design would include a separate table <code>DeceasedMouse</code> that depends on <code>Mouse</code>. <code>DeceasedMouse</code> would only contain entities for dead mice, which improves integrity and averts the need for <code>updates</code>.

4.4 Data Integrity

The term **data integrity** describes guarantees made by the data management process that prevent errors and corruption in data due to technical failures and human errors arising in the course of continuous use by multiple agents. DataJoint pipelines respect the following forms of data integrity: **entity integrity**, **referential integrity**, and **group integrity** as described in more detail below.

4.4.1 Entity integrity

In a proper relational design, each table represents a collection of discrete real-world entities of some kind. **Entity integrity** is the guarantee made by the data management process that entities from the real world are reliably and uniquely represented in the database system. Entity integrity states that the data management process must prevent duplicate representations or misidentification of entities. DataJoint enforces entity integrity through the use of *primary keys*.

Entity integrity breaks down when a process allows data pertaining to the same real-world entity to be entered into the database system multiple times. For example, a school database system may use unique ID numbers to distinguish students. Suppose the system automatically generates an ID number each time a student record is entered into the database without checking whether a record already exists for that student. Such a system violates entity integrity, because the same student may be assigned multiple ID numbers. The ID numbers succeed in uniquely identifying each student record but fail to do so for the actual students.

Note that a database cannot guarantee or enforce entity integrity by itself. Entity integrity is a property of the entire data management process as a whole, including institutional practices and user actions in addition to database configurations.

4.4.2 Referential integrity

Referential integrity is the guarantee made by the data management process that related data across the database remain present, correctly associated, and mutually consistent. Guaranteeing referential integrity means enforcing the constraint that no entity can exist in the database without all the other entities on which it depends. Referential integrity cannot exist without entity integrity: references to entity cannot be validated if the identity of the entity itself is not guaranteed.

Referential integrity fails when a data management process allows new data to be entered that refers to other data missing from the database. For example, assume that each electrophysiology recording must refer to the mouse subject used during data collection. Perhaps an experimenter attempts to insert ephys data into the database that refers to a nonexistent mouse, due to a misspelling. A system guaranteeing referential integrity, such as DataJoint, will refuse the erroneous data.

Enforcement of referential integrity does not stop with data ingest. *Deleting* data in DataJoint also deletes any dependent downstream data. Such cascading deletions are necessary to maintain referential integrity. Consider the deletion of a mouse subject without the deletion of the experimental sessions involving that mouse. A database that allows such deletion will break referential integrity, as the experimental sessions for the removed mouse depend on missing data. Any data management process that allows data to be deleted with no consideration of dependent data cannot maintain referential integrity.

Updating data already present in a database system also jeopardizes referential integrity. For this reason, the DataJoint workflow does not include updates to entities once they have been ingested into a pipeline. Allowing updates to upstream entities would break the referential integrity of any dependent data downstream. For example, permitting a user to change the name of a mouse subject would invalidate any experimental sessions that used that mouse, presuming the mouse name was part of the primary key. The proper way to change data in DataJoint is to delete the existing entities and to insert corrected ones, preserving referential integrity.

4.4.3 Group integrity

Group integrity denotes the guarantee made by the data management process that entities composed of multiple parts always appear in their complete form. Group integrity in DataJoint is formalized through *master-part* relationships. The master-part relationship has important implications for dependencies, because a downstream entity depending on a master entity set may be considered to depend on the parts as well.

4.4.4 Relationships

In DataJoint, the term **relationship** is used rather generally to describe the effects of particular configurations of *dependencies* between multiple entity sets. It is often useful to classify relationships as one-to-one, many-to-one, one-to-many, and many-to-many.

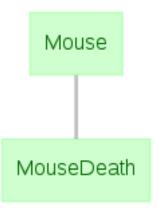
In a **one-to-one relationship**, each entity in a downstream table has exactly one corresponding entity in the upstream table. A dependency of an entity set containing the death dates of mice on an entity set describing the mice themselves would obviously be a one-to-one relationship, as in the example below.

+test/Mouse.m

```
%{
mouse_name : varchar(64)
---
mouse_dob : datetime
%}
classdef Mouse < dj.Manual
end</pre>
```

+test/MouseDeath.m

```
%{
    -> test.Mouse
    ---
    death_date : datetime
%}
classdef MouseDeath < dj.Manual
end</pre>
```



In a **one-to-many relationship**, multiple entities in a downstream table may depend on the same entity in the upstream table. The example below shows a table containing individual channel data from multi-channel recordings,

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representing a one-to-many relationship.

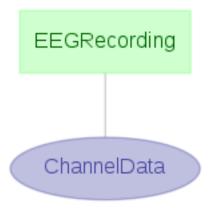
+test/EEGRecording.m

```
%{
    -> test.Session
    eeg_recording_id : int
    ---
    eeg_system : varchar(64)
    num_channels : int
%}
classdef EEGRecording < dj.Manual
end</pre>
```

+test/ChannelData.m

```
%{
    -> test.EEGRecording
    channel_idx : int
    ---
    channel_data : longblob
%}

classdef ChannelData < dj.Imported
end</pre>
```



In a **many-to-one relationship**, each entity in a table is associated with multiple entities from another table. Many-to-one relationships between two tables are usually established using a separate membership table. The example below includes a table of mouse subjects, a table of subject groups, and a membership *part table* listing the subjects in each group. A many-to-one relationship exists between the Mouse table and the SubjectGroup table, with is expressed through entities in GroupMember.

+test/Mouse.m

50

```
%{
mouse_name : varchar(64)
---
mouse_dob : datetime
%}
```

(continues on next page)

(continued from previous page)

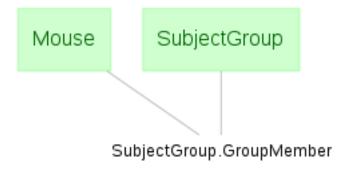
```
classdef Mouse < dj.Manual
end
```

+test/SubjectGroup.m

```
%{
group_number : int
---
group_name : varchar(64)
%}
classdef SubjectGroup < dj.Manual
end</pre>
```

+test/SubjectGroupGroupMember.m

```
%{
-> test.SubjectGroup
-> test.Mouse
%}
classdef SubjectGroupGroupMember < dj.Part
end</pre>
```



In a **many-to-many relationship**, multiple entities in one table may each relate to multiple entities in another upstream table. Many-to-many relationships between two tables are usually established using a separate association table. Each entity in the association table links one entity from each of the two upstream tables it depends on. The below example of a many-to-many relationship contains a table of recording modalities and a table of multimodal recording sessions. Entities in a third table represent the modes used for each session.

+test/RecordingModality.m

```
%{
modality : varchar(64)
%}
classdef RecordingModality < dj.Lookup
end</pre>
```

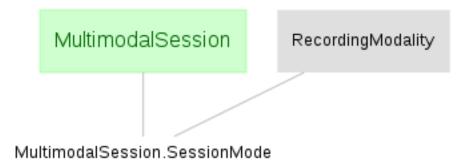
+test/MultimodalSession.m

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```
%{
-> test.Session
modes : int
%}
classdef MultimodalSession < dj.Manual
end</pre>
```

+test/MultimodalSessionSessionMode.m

```
%{
-> test.MultimodalSession
-> test.RecordingModality
%}
classdef MultimodalSessionSessionMode < dj.Part
end</pre>
```



The types of relationships between entity sets are expressed in the *ERD* of a schema.

CHAPTER

FIVE

DATA DEFINITION

5.1 Creating Schemas

5.1.1 Schemas

On the database server, related tables are grouped into a named collection called a **schema**. This grouping organizes the data and allows control of user access. A database server may contain multiple schemas each containing a subset of the tables. A single pipeline may comprise multiple schemas. Tables are defined within a schema, so a schema must be created before the creation of any tables.

A schema can be created either automatically using the dj.createSchema script or manually. While dj.createSchema simplifies the process, the manual approach yields a better understanding of what actually takes place, so both approaches are listed below.

Manual

Step 1. Create the database schema

Use the following command to create a new schema on the database server:

```
query(dj.conn, 'CREATE SCHEMA `alice_experiment`')
```

Note that you must have create privileges for the schema name pattern (as described in *Database Server Hosting*). It is a common practice to grant all privileges to users for schemas that begin with the username, in addition to some shared schemas. Thus the user alice would be able to perform any work in any schema that begins with alice.

Step 2. Create the MATLAB package

DataJoint organizes schemas as MATLAB packages. If you are not familiar with packages, please review:

- How to work with MATLAB packages
- How to manage MATLAB's search paths

In your project directory, create the package folder, which must begin with a + sign. For example, for the schema called experiment, you would create the folder +experiment. Make sure that your project directory (the parent directory of your package folder) is added to the MATLAB search path.

Step 3. Associate the package with the database schema

This step tells DataJoint that all classes in the package folder +experiment will work with tables in the database schema alice_experiment. Each package corresponds to exactly one schema. In some special cases, multiple packages may all relate to a single database schema, but in most cases there will be a one-to-one relationship between packages and schemas.

In the +experiment folder, create the file getSchema.m with the following contents:

```
function obj = getSchema
persistent OBJ
if isempty(OBJ)
    OBJ = dj.Schema(dj.conn, 'experiment', 'alice_experiment');
end
obj = OBJ;
end
```

This function returns a persistent object of type dj.Schema, establishing the link between the experiment package in MATLAB and the schema alice_experiment on the database server.

Automatic

Alternatively, you can execute

```
>> dj.createSchema
```

This automated script will walk you through the steps 1–3 above and will create the schema, the package folder, and the getSchema function in that folder.

5.1.2 Working with existing data

See the chapter *Work with Existing Pipelines* for how to work with data in existing pipelines, including accessing a pipeline from one language when the pipeline was developed using another.

5.2 Creating Tables

5.2.1 Classes represent tables

To make it easy to work with tables in MATLAB and Python, DataJoint programs create a separate class for each table. Computer programmers refer to this concept as object-relational mapping. For example, the class experiment.Subject in the DataJoint client language may correspond to the table called subject on the database server. Users never need to see the database directly; they only interact with data in the database by creating and interacting with DataJoint classes.

Data tiers

The table class must inherit from one of the following superclasses to indicate its data tier: dj.Lookup, dj.Manual, dj.Imported, dj.Computed, or dj.Part. See *Data Tiers* and *Master-Part Relationship*.

5.2.2 Defining a table

DataJoint provides the interactive script dj.new for creating a new table. It will prompt to enter the new table's class name in the form package.ClassName. This will create the file +package/ClassName.m.

For example, define the table experiment.Person

```
>> dj.new
Enter <package>.<ClassName>: experiment.Person

Choose table tier:
   L=lookup
   M=manual
   I=imported
   C=computed
   P=part
   (L/M/I/C/P) > M
```

This will create the file +experiment/Person.m with the following contents:

```
%{
# my newest table
# add primary key here
-----
# add additional attributes
%}
classdef Person < dj.Manual
end</pre>
```

While dj.new adds a little bit of convenience, some users may create the classes from scratch manually.

Each newly created class must inherit from the DataJoint class corresponding to the correct *data tier*: dj.Lookup, dj.Manual, dj.Imported or dj.Computed.

The most important part of the table definition is the comment preceding the **classdef**. DataJoint will parse this comment to define the table.

The class will become usable after you edit this comment as described in *Table Definition*.

5.2.3 Valid class names

Note that in both MATLAB and Python, the class names must follow the CamelCase compound word notation:

- start with a capital letter and
- contain only alphanumerical characters (no underscores).

Examples of valid class names:

```
TwoPhotonScan , Scan2P , Ephys , MembraneVoltage
Invalid class names:
```

Two_photon_Scan , twoPhotonScan , 2PhotonScan , membranePotential , membrane_potential

5.2. Creating Tables 55

5.3 Table Definition

DataJoint models data as sets of **entities** with shared **attributes**, often visualized as tables with rows and columns. Each row represents a single entity and the values of all of its attributes. Each column represents a single attribute with a name and a datatype, applicable to entity in the table. Unlike rows in a spreadsheet, entities in DataJoint don't have names or numbers: they can only be identified by the values of their attributes. Defining a table means defining the names and datatypes of the attributes as well as the constraints to be applied to those attributes. Both MATLAB and Python use the same syntax define tables.

For example, the following code in defines the table User, that contains users of the database:

The table definition is contained in the first block comment in the class definition file. Note that although it looks like a mere comment, the table definition is parsed by DataJoint. This solution is thought to be convenient since MATLAB does not provide convenient syntax for multiline strings.

```
%{
# database users
username : varchar(20)  # unique user name
---
first_name : varchar(30)
last_name : varchar(30)
role : enum('admin', 'contributor', 'viewer')
%}
classdef User < dj.Manual
end</pre>
```

This defines the class User that creates the table in the database and provides all its data manipulation functionality.

5.3.1 Table creation on the database server

Users do not need to do anything special to have the table created in the database. The table is created upon the first attempt to use the class for manipulating its data (e.g. inserting or fetching entities).

5.3.2 Changing the definition of an existing table

Once the table is created in the database, the definition string has no further effect. In other words, changing the definition string in the class of an existing table will not actually update the table definition. To change the table definition, one must first *drop* the existing table. This means that all the data will be lost, and the new definition will be applied to create the new empty table.

Therefore, in the initial phases of designing a DataJoint pipeline, it is common to experiment with variations of the design before populating it with substantial amounts of data.

It is possible to modify a table without dropping it. This topic is covered separately.

5.3.3 Reverse-engineering the table definition

DataJoint objects provide the describe method, which displays the table definition used to define the table when it was created in the database. This definition may differ from the definition string of the class if the definition string has been edited after creation of the table.

Examples

```
s = describe(lab.User)
```

Furthermore, DataJoint provides the syncDef method to update the classdef file definition string for the table with the definition in the actual table:

```
syncDef(lab.User) % updates the table definition in file +lab/User.m
```

5.4 Definition Syntax

The table definition consists of one or more lines. Each line can be one of the following:

- The optional first line starting with a # provides a description of the table's purpose. It may also be thought of as the table's long title.
- A new attribute definition in any of the following forms (see *Datatypes* for valid datatypes):

- The divider --- (at least three hyphens) separating primary key attributes above from secondary attributes below.
- A foreign key in the format -> ReferencedTable . (See *Dependencies*.)

For example, the table for Persons may have the following definition:

```
# Persons in the lab
username : varchar(16) # username in the database
---
full_name : varchar(255)
start_date : date # date when joined the lab
```

This will define the table with attributes username, full_name, and start_date, in which username is the primary key.

5.4.1 Attribute names

Attribute names must be in lowercase and must start with a letter. They can only contain alphanumerical characters and underscores. The attribute name cannot exceed 64 characters.

```
Valid attribute names first_name, two_photon_scan, scan_2p, two_photon_scan_
```

```
Invalid attribute names firstName, first name, 2photon_scan, two-photon_scan, TwoPhotonScan
```

Ideally, attribute names should be unique across all tables that are likely to be used in queries together. For example, tables often have attributes representing the start times of sessions, recordings, etc. Such attributes must be uniquely named in each table, such as session_start_time or recording_start_time.

5.4.2 Default values

Secondary attributes can be given default values. A default value will be used for an attribute if no other value is given at the time the entity is *inserted* into the table. Generally, default values are numerical values or character strings. Default values for dates must be given as strings as well, contained within quotes (with the exception of CURRENT_TIMESTAMP). Note that default values can only be used when inserting as a mapping. Primary key attributes cannot have default values (with the exceptions of auto_increment and CURRENT_TIMESTAMP attributes; see *Primary Key*).

An attribute with a default value of NULL is called a **nullable attribute**. A nullable attribute can be thought of as applying to all entities in a table but having an optional *value* that may be absent in some entities. Nullable attributes should *not* be used to indicate that an attribute is inapplicable to some entities in a table (see *Entity Normalization*). Nullable attributes should be used sparingly to indicate optional rather than inapplicable attributes that still apply to all entities in the table. NULL is a special literal value and does not need to be enclosed in quotes.

Here are some examples of attributes with default values:

```
failures = 0 : int
due_date = "2020-05-31" : date
additional_comments = NULL : varchar(256)
```

5.5 Data Tiers

DataJoint assigns all tables to one of the following data tiers that differentiate how the data originate.

Tier	Superclass	Description
Lookup	dj.Lookup	Small tables containing general facts and settings of the data pipeline; not specific to any experiment or dataset.
Manual	dj.Manual	Data entered from outside the pipeline, either by hand or with external helper scripts.
Imported	dj.Imported	Data ingested automatically inside the pipeline but requiring access to data outside the pipeline.
Computed	dj.Computed	Data computed automatically entirely inside the pipeline.

Table 1: Table tiers

Table data tiers indicate to database administrators how valuable the data are. Manual data are the most valuable, as re-entry may be tedious or impossible. Computed data are safe to delete, as the data can always be recomputed from within DataJoint. Imported data are safer than manual data but less safe than computed data because of dependency on external data sources. With these considerations, database administrators may opt not to back up computed data, for example, or to back up imported data less frequently than manual data.

The data tier of a table is specified by the superclass of its class. For example, the User class in *Table Definition* uses the dj.Manual superclass. Therefore, the corresponding User table on the database would be of the Manual tier. Furthermore, the classes for **imported** and **computed** tables have additional capabilities for automated processing as described in *Auto-populate*.

5.5.1 Internal conventions for naming tables

On the server side, DataJoint uses a naming scheme to generate a table name corresponding to a given class. The naming scheme includes prefixes specifying each table's data tier.

First, the name of the class is converted from CamelCase to snake_case (separation by underscores). Then the name is prefixed according to the data tier.

- Manual tables have no prefix.
- Lookup tables are prefixed with #.
- Imported tables are prefixed with _, a single underscore.
- Computed tables are prefixed with ___, two underscores.

For example:

The table for the class StructuralScan subclassing dj.Manual will be named structural_scan.

The table for the class SpatialFilter subclassing dj.Lookup will be named #spatial_filter.

Again, the internal table names including prefixes are used only on the server side. These are never visible to the user, and DataJoint users do not need to know these conventions However, database administrators may use these naming patterns to set backup policies or to restrict access based on data tiers.

5.5.2 Part tables

Part tables do not have their own tier. Instead, they share the same tier as their master table. The prefix for part tables also differs from the other tiers. They are prefixed by the name of their master table, separated by two underscores.

For example, the table for the class Channel(dj.Part) with the master Ephys(dj.Imported) will be named _ephys__channel.

5.6 Datatypes

DataJoint supports the following datatypes. To conserve database resources, use the smallest and most restrictive datatype sufficient for your data. This also ensures that only valid data are entered into the pipeline.

5.6.1 Most common datatypes

- tinyint: an 8-bit integer number, ranging from -128 to 127.
- tinyint unsigned: an 8-bit positive integer number, ranging from 0 to 255.
- smallint: a 16-bit integer number, ranging from -32,768 to 32,767.
- smallint unsigned: a 16-bit positive integer, ranging from 0 to 65,535.
- int: a 32-bit integer number, ranging from -2,147,483,648 to 2,147,483,647.
- int unsigned: a 32-bit positive integer, ranging from 0 to 4,294,967,295.
- enum: one of several explicitly enumerated values specified as strings. Use this datatype instead of text strings to avoid spelling variations and to save storage space. For example, the datatype for an anesthesia attribute could be enum("urethane", "isoflurane", "fentanyl"). Do not use enums in primary keys due to the difficulty of changing their definitions consistently in multiple tables.

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- date: date as 'YYYY-MM-DD'.
- time: time as 'HH:MM:SS'.
- datetime: Date and time to the second as 'YYYY-MM-DD HH:MM:SS'
- timestamp: Date and time to the second as 'YYYY-MM-DD HH:MM:SS'. The default value may be set to CURRENT_TIMESTAMP. Unlike datetime, a timestamp value will be adjusted to the local time zone.
- char(N): a character string up to N characters (but always takes the entire N bytes to store).
- varchar(N): a text string of arbitrary length up to N characters that takes M+1 or M+2 bytes of storage, where M is the actual length of each stored string.
- float: a single-precision floating-point number. Takes 4 bytes. Single precision is sufficient for many measurements.
- double: a double-precision floating-point number. Takes 8 bytes. Because equality comparisons are error-prone, neither float nor double should be used in primary keys.
- decimal(N,F): a fixed-point number with N total decimal digits and F fractional digits. This datatype is well suited to represent numbers whose magnitude is well defined and does not warrant the use of floating-point representation or requires precise decimal representations (e.g. dollars and cents). Because of its well-defined precision, decimal values can be used in equality comparison and be included in primary keys.
- longblob: arbitrary numeric array (e.g. matrix, image, structure), up to 4 GiB in size. Numeric arrays are compatible between MATLAB and Python (NumPy). The longblob and other blob datatypes can be configured to store data *externally* by using the blob@store syntax.

5.6.2 Less common (but supported) datatypes

- decimal(N,F) unsigned: same as decimal, but limited to nonnegative values.
- mediumint a 24-bit integer number, ranging from -8,388,608 to 8,388,607.
- mediumint unsigned: a 24-bit positive integer, ranging from 0 to 16,777,216.
- mediumblob: arbitrary numeric array, up to 16 MiB
- blob : arbitrary numeric array, up to 64 KiB
- tinyblob: arbitrary numeric array, up to 256 bytes (actually smaller due to header info).

5.6.3 Special DataJoint-only datatypes

These types abstract certain kinds of non-database data to facillitate use together with DataJoint.

- attach: a *file attachment* similar to email attachments facillitating sending/receiving an opaque data file to/from a DataJoint pipeline.
- filepath@store : a filepath used to link non-DataJoint managed files into a DataJoint pipeline.

5.6.4 Datatypes not (yet) supported

- binary
- text
- longtext
- bit

For additional information about these datatypes, see http://dev.mysql.com/doc/refman/5.6/en/data-types.html

5.7 External Data

5.7.1 File Attachment Datatype

Note: External storage is not yet implemented in MATLAB. The feature will be added in an upcoming release: https://github.com/datajoint/datajoint-matlab/issues/143

Configuration & Usage

Corresponding to issue #480, the attach attribute type allows users to *attach* files into DataJoint schemas as DataJoint-managed files. This is in contrast to traditional *blobs* which are encodings of programming language data structures such as arrays.

The functionality is modeled after email attachments, where users *attach* a file along with a message and message recipients have access to a copy of that file upon retrieval of the message.

For DataJoint attrack attributes, DataJoint will copy the input file into a DataJoint store, hash the file contents, and track the input file name. Subsequent fetch operations will transfer a copy of the file to the local directory of the Python process and return a pointer to it's location for subsequent client usage. This allows arbitrary files to be *uploaded* or *attached* to a DataJoint schema for later use in processing. File integrity is preserved by checksum comparison against the attachment data and verifying the contents during retrieval.

For example, given a localattach store:

```
dj.config['stores'] = {
   'localattach': {
     'protocol': 'file',
     'location': '/data/attach'
   }
}
```

A ScanAttachment table can be created:

```
@schema
class ScanAttachment(dj.Manual):
    definition = """
    -> Session
    ---
    scan_image:    attach@localattach # attached image scans
    """
```

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Files can be added using an insert pointing to the source file:

```
>>> ScanAttachment.insert1((0, '/input/image0.tif'))
```

And then retrieved to the current directory using fetch:

```
>>> s0 = (ScanAttachment & {'session_id': 0}).fetch1()
>>> s0
{'session_id': 0, 'scan_image': './image0.tif'}
>>> fh = open(s0['scan_image'], 'rb')
>>> fh
<_io.BufferedReader name='./image0.tif')</pre>
```

5.7.2 Filepath Datatype

Note: External storage is not yet implemented in MATLAB. The feature will be added in an upcoming release: https://github.com/datajoint/datajoint-matlab/issues/143

Note: Filepath Datatype is available as a preview feature in DataJoint Python v0.12. This means that the feature is required to be explicitly enabled. To do so, make sure to set the environment variable FILEPATH_FEATURE_SWITCH=TRUE prior to use.

Configuration & Usage

Corresponding to issue #481, the filepath attribute type links DataJoint records to files already managed outside of DataJoint. This can aid in sharing data with other systems such as allowing an image viewer application to directly use files from a DataJoint pipeline, or to allow downstream tables to reference data which reside outside of DataJoint pipelines.

To define a table using the **filepath** datatype, an existing DataJoint *store* should be created and then referenced in the new table definition. For example, given a simple store:

```
dj.config['stores'] = {
   'data': {
     'protocol': 'file',
     'location': '/data',
     'stage': '/data'
}
```

we can define an ScanImages table as follows:

```
@schema
class ScanImages(dj.Manual):
    definition = """
    -> Session
    image_id:    int
    ---
    image_path:    filepath@data
    """
```

This table can now be used for tracking paths within the /data local directory. For example:

```
>>> ScanImages.insert1((0, 0, '/data/images/image_0.tif'))
>>> (ScanImages() & {'session_id': 0}).fetch1(as_dict=True)
{'session_id': 0, 'image_id': 0, 'image_path': '/data/images/image_0.tif'}
```

As can be seen from the example, unlike *blob* records, file paths are managed as path locations to the underlying file.

Integrity Notes

Unlike other data in DataJoint, data in filepath records are deliberately intended for shared use outside of DataJoint. To help ensure integrity of filepath records, DataJoint will record a checksum of the file data on insert, and will verify this checksum on fetch. However, since the underlying file data may be shared with other applications, special care should be taken to ensure records stored in filepath attributes are not modified outside of the pipeline, or, if they are, that records in the pipeline are updated accordingly. A safe method of changing filepath data is as follows:

1) Delete the filepath database record.

This will ensure that any downstream records in the pipeline depending on the filepath record are purged from the database.

- 2) Modify filepath data.
- 3) Re-insert corresponding the filepath record.

This will add the record back to DataJoint with an updated file checksum.

4) Compute any downstream dependencies, if needed.

This will ensure that downstream results dependent on the filepath record are updated to reflect the newer filepath contents.

5.8 Primary Key

5.8.1 Primary keys in DataJoint

Entities in tables are neither named nor numbered. DataJoint does not answer questions of the type "What is the 10th element of this table?" Instead, entities are distinguished by the values of their attributes. Furthermore, the entire entity is not required for identification. In each table, a subset of its attributes are designated to be the **primary key**. Attributes in the primary key alone are sufficient to differentiate any entity from any other within the table.

Each table must have exactly one primary key: a subset of its attributes that uniquely identify each entity in the table. The database uses the primary key to prevent duplicate entries, to relate data across tables, and to accelerate data queries. The choice of the primary key will determine how you identify entities. Therefore, make the primary key **short**, **expressive**, and **persistent**.

For example, mice in our lab are assigned unique IDs. The mouse ID number animal_id of type smallint can serve as the primary key for the table Mice. An experiment performed on a mouse may be identified in the table Experiments by two attributes: animal_id and experiment_number.

DataJoint takes the concept of primary keys somewhat more seriously than other models and query languages. Even **table expressions**, i.e. those tables produced through operations on other tables, have a well-defined primary key. All operators on tables are designed in such a way that the results always have a well-defined primary key.

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In all representations of tables in DataJoint, the primary key attributes are always listed before other attributes and highlighted for emphasis (e.g. in a **bold** font or marked with an asterisk *)

5.8.2 Defining a primary key

In table declarations, the primary key attributes always come first and are separated from the other attributes with a line containing at least three hyphens. For example, the following is the definition of a table containing database users where username is the primary key.

```
# database users
username : varchar(20)  # unique user name
---
first_name : varchar(30)
last_name : varchar(30)
role : enum('admin', 'contributor', 'viewer')
```

5.8.3 Entity integrity

The primary key defines and enforces the desired property of databases known as *entity integrity*. **Entity integrity** ensures that there is a one-to-one and unambiguous mapping between real-world entities and their representations in the database system. The data management process must prevent any duplication or misidentification of entities.

To enforce entity integrity, DataJoint implements several rules: * Every table must have a primary key. * Primary key attributes cannot have default values (with the exception of below). * Operators on tables are defined with respect to the primary key and preserve a primary key in their results.

5.8.4 Datatypes in primary keys

All integer types, dates, timestamps, and short character strings make good primary key attributes. Character strings are somewhat less suitable because they can be long and because they may have invisible trailing spaces. Floating-point numbers should be avoided because rounding errors may lead to misidentification of entities. Enums are okay as long as they do not need to be modified after *dependencies* are already created referencing the table. Finally, DataJoint does not support blob types in primary keys.

The primary key may be composite, i.e. comprising several attributes. In DataJoint, hierarchical designs often produce tables whose primary keys comprise many attributes.

5.8.5 Choosing primary key attributes

A primary key comprising real-world attributes is a good choice when such real-world attributes are already properly and permanently assigned. Whatever characteristics are used to uniquely identify the actual entities can be used to identify their representations in the database.

If there are no attributes that could readily serve as a primary key, an artificial attribute may be created solely for the purpose of distinguishing entities. In such cases, the primary key created for management in the database must also be used to uniquely identify the entities themselves. If the primary key resides only in the database while entities remain indistinguishable in the real world, then the process cannot ensure entity integrity. When a primary key is created as part of data management rather than based on real-world attributes, an institutional process must ensure the uniqueness and permanence of such an identifier.

For example, the U.S. government assigns every worker an identifying attribute, the social security number. However, the government must go to great lengths to ensure that this primary key is assigned exactly once, by checking against

other less convenient candidate keys (i.e. the combination of name, parents' names, date of birth, place of birth, etc.). Just like the SSN, well managed primary keys tend to get institutionalized and find multiple uses.

Your lab must maintain a system for uniquely identifying important entities. For example, experiment subjects and experiment protocols must have unique IDs. Use these as the primary keys in the corresponding tables in your DataJoint databases.

Using hashes as primary keys

Some tables include too many attributes in their primary keys. For example, the stimulus condition in a psychophysics experiment may have a dozen parameters such that a change in any one of them makes a different valid stimulus condition. In such a case, all the attributes would need to be included in the primary key to ensure entity integrity. However, long primary keys make it difficult to reference individual entities. To be most useful, primary keys need to be relatively short.

This problem is effectively solved through the use of a hash of all the identifying attributes as the primary key. For example, MD5 or SHA-1 hash algorithms can be used for this purpose. To keep their representations human-readable, they may be encoded in base-64 ASCII. For example, the 128-bit MD5 hash can be represented by 21 base-64 ASCII characters, but for many applications, taking the first 8 to 12 characters is sufficient to avoid collisions.

auto_increment

Some entities are created by the very action of being entered into the database. The action of entering them into the database gives them their identity. It is impossible to duplicate them since entering the same thing twice still means creating two distinct entities.

In such cases, the use of an auto-incremented primary key is warranted. These are declared by adding the word auto_increment after the data type in the declaration. The datatype must be an integer. Then the database will assign incrementing numbers at each insert.

The example definition below defines an auto-incremented primary key

```
# log entries
entry_id : smallint auto_increment
---
entry_text : varchar(4000)
entry_time = CURRENT_TIMESTAMP : timestamp(3) # automatic timestamp with millisecond precision
```

DataJoint passes auto_increment behavior to the underlying MySQL and therefore it has the same limitation: it can only be used for tables with a single attribute in the primary key.

If you need to auto-increment an attribute in a composite primary key, you will need to do so programmatically within a transaction to avoid collisions.

For example, let's say that you want to auto-increment scan_idx in a table called Scan whose primary key is (animal_id, session, scan_idx). You must already have the values for animal_id and session in the dictionary key. Then you can do the following:

```
key.scah_idx = fetch1(Scan & key, 'next=max(scan_idx)+1')
```

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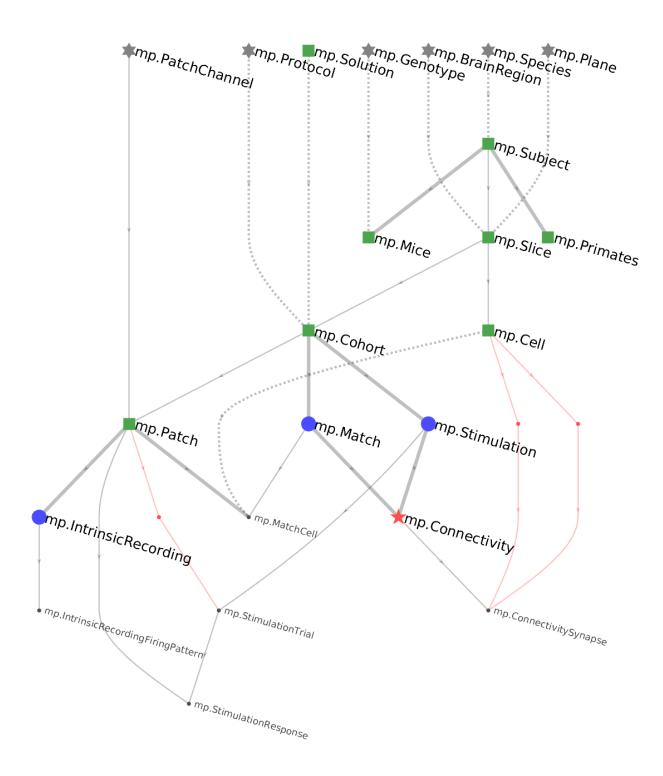
5.9 Dependencies

5.9.1 Understanding dependencies

A schema contains collections of tables of related data. Accordingly, entities in one table often derive some of their meaning or context from entities in other tables. A **foreign key** defines a **dependency** of entities in one table on entities in another within a schema. In more complex designs, dependencies can even exist between entities in tables from different schemas. Dependencies play a functional role in DataJoint and do not simply label the structure of a pipeline. Dependencies provide entities in one table with access to data in another table and establish certain constraints on entities containing a foreign key.

A DataJoint pipeline, including the dependency relationships established by foreign keys, can be visualized as a graph with nodes and edges. The diagram of such a graph is called the **entity relationship diagram** or *ERD*. The nodes of the graph are tables and the edges connecting them are foreign keys. The edges are directed and the overall graph is a **directed acyclic graph**, a graph with no loops.

For example, the ERD below is the pipeline for multipatching experiments



The graph defines the direction of the workflow. The tables at the top of the flow need to be populated first, followed by those tables one step below and so forth until the last table is populated at the bottom of the pipeline. The top of the pipeline tends to be dominated by lookup tables (gray stars) and manual tables (green squares). The middle has many imported tables (blue triangles), and the bottom has computed tables (red stars).

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5.9.2 Defining a dependency

Foreign keys are defined with arrows -> in the *table definition*, pointing to another table.

A foreign key may be defined as part of the *Primary Key*.

In the ERD, foreign keys from the primary key are shown as solid lines. This means that the primary key of the referenced table becomes part of the primary key of the new table. A foreign key outside the primary key is indicated by dashed line in the ERD.

For example, the following definition for the table mp.Slice has three foreign keys, including one within the primary key.

```
# brain slice
-> mp.Subject
               : smallint
                                # slice number within subject
slice_id
-> mp.BrainRegion
-> mp.Plane
slice_date
                : date
                                       # date of the slicing (not patching)
thickness
                 : smallint unsigned
                                       # slice thickness in microns
experimenter
               : varchar(20)
                                        # person who performed this experiment
```

You can examine the resulting table heading with

```
show(mp.BrainSlice)
```

The heading of mp.Slice may look something like

```
subject_id
               : char(8)
                                # experiment subject id
slice id
               : smallint
                                # slice number within subject
brain_region
                   : varchar(12)
                                        # abbreviated name for brain region
                   : varchar(12)
                                        # plane of section
plane
slice_date
                   : date
                                        # date of the slicing (not patching)
thickness
                   : smallint unsigned # slice thickness in microns
experimenter
                   : varchar(20)
                                        # person who performed this experiment
```

This displayed heading reflects the actual attributes in the table. The foreign keys have been replaced by the primary key attributes of the referenced tables, including their data types and comments.

5.9.3 How dependencies work

The foreign key -> A in the definition of table B has the following effects:

- 1. The primary key attributes of A are made part of B 's definition.
- 2. A referential constraint is created in B with reference to A.
- 3. If one does not already exist, an index is created to speed up searches in B for matches to A. (The reverse search is already fast because it uses the primary key of A.)

A referential constraint means that an entity in B cannot exist without a matching entity in A. Matching means attributes in B that correspond to the primary key of A must have the same values. An attempt to insert an entity into B that does not have a matching counterpart in A will fail. Conversely, deleting an entity from A that has matching entities in B will result in the deletion of those matching entities and so forth, recursively, downstream in the pipeline.

When B references A with a foreign key, one can say that B depends on A. In DataJoint terms, B is the dependent table and A is the referenced table with respect to the foreign key from B to A.

Note: Note to those already familiar with the theory of relational databases: The usage of the words "depends" and "dependency" here should not be confused with the unrelated concept of *functional dependencies* that is used to define normal forms.

5.9.4 Referential integrity

Dependencies enforce the desired property of databases known as **referential integrity**. Referential integrity is the guarantee made by the data management process that related data across the database remain present, correctly associated, and mutually consistent. Guaranteeing referential integrity means enforcing the constraint that no entity can exist in the database without all the other entities on which it depends. An entity in table B depends on an entity in table A when they belong to them or are computed from them.

5.9.5 Dependencies with renamed attributes

In most cases, a dependency includes the primary key attributes of the referenced table as they appear in its table definition. Sometimes it can be helpful to choose a new name for a foreign key attribute that better fits the context of the dependent table. DataJoint provides the following *projection* syntax to rename the primary key attributes when they are included in the new table.

The dependency

```
-> Table.project(new_attr='old_attr')
```

renames the primary key attribute old_attr of Table as new_attr before integrating it into the table definition. Any additional primary key attributes will retain their original names. For example, the table Experiment may depend on table User but rename the user attribute into operator as follows:

```
-> User.proj(operator='user')
```

In the above example, an entity in the dependent table depends on exactly one entity in the referenced table. Sometimes entities may depend on multiple entities from the same table. Such a design requires a way to distinguish between dependent attributes having the same name in the reference table. For example, a table for Synapse may reference the table Cell twice as presynaptic and postsynaptic. The table definition may appear as

```
# synapse between two cells
-> Cell.proj(presynaptic='cell_id')
-> Cell.proj(postsynaptic='cell_id')
---
connection_strength : double # (pA) peak synaptic current
```

If the primary key of Cell is (animal_id, slice_id, cell_id), then the primary key of Synapse resulting from the above definition will be (animal_id, slice_id, presynaptic, postsynaptic). Projection always returns all of the primary key attributes of a table, so animal_id and slice_id are included, with their original names.

Note that the design of the Synapse table above imposes the constraint that the synapse can only be found between cells in the same animal and in the same slice.

Allowing representation of synapses between cells from different slices requires the renaming of slice_id as well: .. code-block:: text

5.9. Dependencies 69

synapse between two cells -> Cell(presynaptic_slice='slice_id', presynaptic_cell='cell_id') -> Cell(postsynaptic_slice='slice_id', postsynaptic_cell='cell_id') — connection_strength : double # (pA) peak synaptic current

In this case, the primary key of Synapse will be (animal_id, presynaptic_slice, presynaptic_cell, postsynaptic_slice, postsynaptic_cell). This primary key still imposes the constraint that synapses can only form between cells within the same animal but now allows connecting cells across different slices.

In the ERD, renamed foreign keys are shown as red lines with an additional dot node in the middle to indicate that a renaming took place.

5.9.6 Foreign key options

Note: Foreign key options are currently in development.

Foreign keys allow the additional options nullable and unique, which can be inserted in square brackets following the arrow.

For example, in the following table definition

```
rig_id : char(4) # experimental rig
---
-> Person
```

each rig belongs to a person, but the table definition does not prevent one person owning multiple rigs. With the unique option, a person may only appear once in the entire table, which means that no one person can own more than one rig.

```
rig_id : char(4) # experimental rig
---
-> [unique] Person
```

With the nullable option, a rig may not belong to anyone, in which case the foreign key attributes for Person are set to NULL:

```
rig_id : char(4) # experimental rig
---
-> [nullable] Person
```

Finally with both *unique* and *nullable*, a rig may or may not be owned by anyone and each person may own up to one rig.

```
rig_id : char(4) # experimental rig
---
-> [unique, nullable] Person
```

Foreign keys made from the primary key cannot be nullable but may be unique.

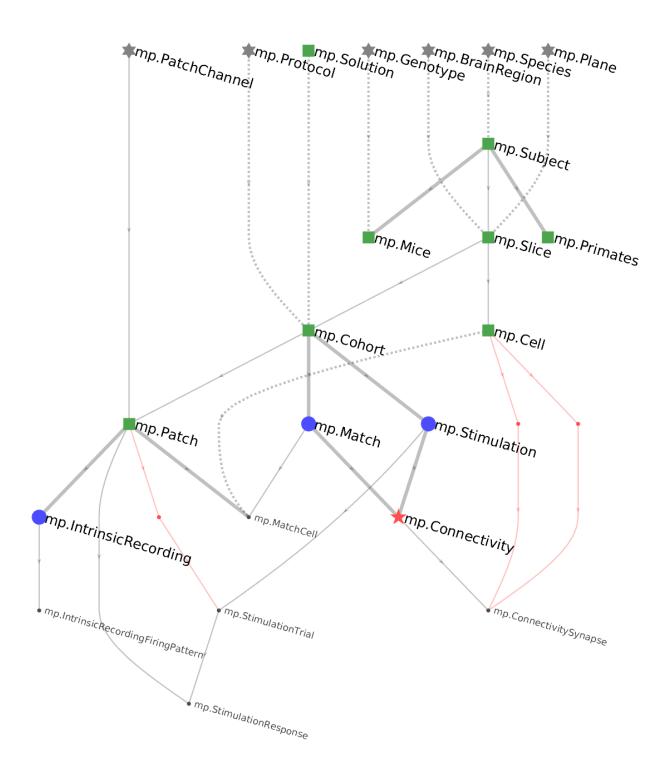
5.10 ERD

ERD stands for **entity relationship diagram**. Objects of type dj.ERD allow visualizing portions of the data pipeline in graphical form. Tables are depicted as nodes and *dependencies* as directed edges between them. The *draw* method plots the graph.

5.10.1 Diagram notation

Consider the following ERD

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DataJoint uses the following conventions:

- Tables are indicated as nodes in the graph. The corresponding class name is indicated by each node.
- *Data tiers* are indicated as colors and symbols: Lookup=gray asterisk, Manual=green square, Imported=blue circle, Computed=red star, Part=black dot. The names of *part tables* are indicated in a smaller font.
- Dependencies are indicated as edges in the graph and always directed downward, forming a directed acyclic

graph.

- Foreign keys contained within the primary key are indicated as solid lines. This means that the referenced table becomes part of the primary key of the dependent table.
- Foreign keys that are outside the primary key are indicated by dashed lines.
- If the primary key of the dependent table has no other attributes besides the foreign key, the foreign key is a thick solid line, indicating a 1:{0,1} relationship.
- Foreign keys made without renaming the foreign key attributes are in black whereas foreign keys that rename the attributes are indicated in red.

5.10.2 Diagramming an entire schema

The schema object for a package can be obtained using its getSchema function. (See Creating Schemas.)

DataJoint provides shortcuts to plot ERD of a table neighborhood or a schema using the erd command:

```
% plot the ERD of the stimulus schema
erd stimulus

% plot the neighborhood of the stimulus.Trial table
erd stimulus.Trial

% plot the stimulus and experiment schemas and the neighborhood of preprocess.Sync
erd stimulus experiment preprocess.Sync
```

Initializing with a single table

A *dj.ERD* object can be initialized with a single table.

```
draw(dj.ERD(seq.Genome))
```

A single node makes a rather boring graph but ERDs can be added together or subtracted from each other using graph algebra.

Adding ERDs together

However two graphs can be added, resulting in new graph containing the union of the sets of nodes from the two original graphs. The corresponding foreign keys will be automatically

```
% plot the ERD with tables Genome and Species from package +seq.
draw(dj.ERD(seq.Genome) + dj.ERD(seq.Species))
```

5.10. ERD 73

Expanding ERDs upstream and downstream

Adding a number to an ERD object adds nodes downstream in the pipeline while subtracting a number from ERD object adds nodes upstream in the pipeline.

Examples:

```
% Plot all the tables directly downstream from ``seq.Genome``:
draw(dj.ERD(seq.Genome)+1)
```

```
% Plot all the tables directly upstream from ``seq.Genome``:
draw(dj.ERD(seq.Genome)-1)
```

```
% Plot the local neighborhood of ``seq.Genome``
draw(dj.ERD(seq.Genome)+1-1+1-1)
```

5.11 Manual Tables

Manual tables are populated during experiments through a variety of interfaces. Not all manual information is entered by typing. Automated software can enter it directly into the database. What makes a manual table manual is that it does not perform any computations within the DataJoint pipeline.

The following code defines three manual tables Animal, Session, and Scan:

File +experiment/Animal.m

```
%{
    # information about animal
    animal_id : int # animal id assigned by the lab
---
-> experiment.Species
    date_of_birth=null : date # YYYY-MM-DD optional
    sex=" : enum('M', 'F', ") # leave empty if unspecified
%}
classdef Animal < dj.Manual
end</pre>
```

File +experiment/Session.m

```
# Experiment Session
-> experiment.Animal
session : smallint # session number for the animal
---
session_date : date # YYYY-MM-DD
-> experiment.User
-> experiment.Anesthesia
-> experiment.Rig
%}
classdef Session < dj.Manual
end</pre>
```

File +experiment/Scan.m

```
# Two-photon imaging scan
-> experiment.Session
scan : smallint # scan number within the session
---
-> experiment.Lens
laser_wavelength : decimal(5,1) # um
laser_power : decimal(4,1) # mW
%}
classdef Scan < dj.Manual
end</pre>
```

5.12 Lookup Tables

Lookup tables contain basic facts that are not specific to an experiment and are fairly persistent. Their contents are typically small. In GUIs, lookup tables are often used for drop-down menus or radio buttons. In computed tables, they are often used to specify alternative methods for computations. Lookup tables are commonly populated from their contents property. In an *ERD* they are shown in gray. The decision of which tables are lookup tables and which are manual can be somewhat arbitrary.

The table below is declared as a lookup table with its contents property provided to generate entities.

File +lab/User.m

5.13 **Drop**

The drop method completely removes a table from the database, including its definition. It also removes all dependent tables, recursively. DataJoint will first display the tables being dropped and the number of entities in each before prompting the user for confirmation to proceed.

The drop method is often used during initial design to allow altered table definitions to take effect.

```
% drop the Person table from the lab schema drop(lab.Person)
```

5.12. Lookup Tables 75

5.13.1 Dropping part tables

A *part table* is usually removed as a consequence of calling drop on its master table.

Note: This rule is currently not enforced in MATLAB, but calling drop directly on a part table will produce an error in the future. See issue #125 on datajoint-matlab for more information.

CHAPTER

SIX

WORK WITH EXISTING PIPELINES

6.1 Loading Classes

6.1.1 Creating a virtual class

To facilitate working with existing pipelines, DataJoint MATLAB creates a TableAccessor property in each schema object. The TableAccessor property, a *virtual class generator*, is available as schema.v, and allows listing and querying of the tables defined on the server without needing to create the MATLAB table definitions locally. For example, creating a scratch experiment schema package and querying an existing my_experiment.Session table on the server can be done as follows:

```
dj.createSchema('experiment', '/scratch', 'my_experiment')
addpath('/scratch')
experiment_schema = experiment.getSchema();
experiment_schema.v.Session() & 'session_id=1234';
```

Note: You can view the available tables in a schema by using tab completion on the schema.v property.

CHAPTER

SEVEN

DATA MANIPULATION

7.1 Manipulation

Data **manipulation** operations change the state of the data stored in the database without modifying the structure of the stored data. These operations include *insert*, *delete*, and *update*.

Data manipulation operations in DataJoint respect the *integrity* constraints.

7.2 Insert

The insert method of DataJoint table objects inserts entities into the table.

The insert method inserts any number of entities in the form of a structure array with field names corresponding to the attribute names.

For example

```
s.username = 'alice';
s.first_name = 'Alice';
s.last_name = 'Cooper';
insert(lab.Person, s)
```

Quick entry of multiple entities takes advantage of MATLAB's cell array notation:

```
insert(lab.Person, {
    'alice' 'Alice' 'Cooper'
    'bob' 'Bob' 'Dylan'
    'carol' 'Carol' 'Douglas'
})
```

In this case, the values must match the order of the attributes in the table.

The optional parameter command can be either 'IGNORE' or 'REPLACE'. Duplicates, unmatched attributes, or missing required attributes will cause insert errors, unless command is specified.

7.2.1 Batched inserts

Inserting a set of entities in a single insert differs from inserting the same set of entities one-by-one in a for loop in two ways:

- 1. Network overhead is reduced. Network overhead can be tens of milliseconds per query. Inserting 1000 entities in a single insert call may save a few seconds over inserting them individually.
- 2. The insert is performed as an all-or-nothing transaction. If even one insert fails because it violates any constraint, then none of the entities in the set are inserted.

However, inserting too many entities in a single query may run against buffer size or packet size limits of the database server. Due to these limitations, performing inserts of very large numbers of entities should be broken up into moderately sized batches, such as a few hundred at a time.

7.2.2 Server-side inserts

Data inserted into a table often come from other tables already present on the database server. In such cases, data can be *fetched* from the first table and then inserted into another table, but this results in transfers back and forth between the database and the local system. Instead, data can be inserted from one table into another without transfers between the database and the local system using *queries*.

In the example below, a new schema has been created in preparation for phase two of a project. Experimental protocols from the first phase of the project will be reused in the second phase. Since the entities are already present on the database in the Protocol table of the phase_one schema, we can perform a server-side insert into phase_two.Protocol without fetching a local copy.

```
% Server-side inserts are faster...
phase_two.Protocol.insert(phase_one.Protocol)

% ...than fetching before inserting
protocols = phase_one.Protocol.fetch();
phase_two.Protocol.insert(protocols)
```

7.3 Delete

The del method deletes entities from a table and all dependent entries in dependent tables.

Delete is often used in conjunction with the *restriction* operator to define the subset of entities to delete. Delete is performed as an atomic transaction so that partial deletes never occur.

7.3.1 Examples

Delete the entire contents of the table tuning. VonMises and all its dependents:

```
% delete all entries from tuning.VonMises
del(tuning.VonMises)

% delete entries from tuning.VonMises for mouse 1010
del(tuning.VonMises & 'mouse=1010')

% delete entries from tuning.VonMises except mouse 1010
del(tuning.VonMises - 'mouse=1010')
```

7.3.2 Deleting from part tables

Entities in a part table are usually removed as a consequence of deleting the master table.

Note: This rule is currently not enforced in MATLAB, but calling del directly on a part table will produce an error in the future. See issue #193 on datajoint-matlab for more information.

7.4 Cautious Update

In database programming, the **update** operation refers to modifying the values of individual attributes in an entity within a table without replacing the entire entity. Such an in-place update mechanism is not part of DataJoint's data manipulation model, because it circumvents data *dependency constraints*.

This is not to say that data cannot be changed once they are part of a pipeline. In DataJoint, data are changed by replacing entire entities rather than by updating the values of their attributes. The process of deleting existing entities and inserting new entities with corrected values ensures the *integrity* of the data throughout the pipeline.

This approach applies specifically to automated tables (see *Auto-populate*). However, manual tables are often edited outside DataJoint through other interfaces. It is up to the user's discretion to allow updates in manual tables, and the user must be cognizant of the fact that updates will not trigger re-computation of dependent data.

7.5 Transactions

In some cases, a sequence of several operations must be performed as a single operation: interrupting the sequence of such operations halfway would leave the data in an invalid state. While the sequence is in progress, other processes accessing the database will not see the partial results until the transaction is complete. The sequence make include *data queries* and *manipulations*.

In such cases, the sequence of operations may be enclosed in a transaction.

Transactions are formed using the methods startTransaction, cancelTransaction, and commitTransaction of a connection object. A connection object may obtained from any table object.

For example, the following code inserts matching entries for the master table Session and its part table SessionExperimenter.

```
% get the connection object
session = Session
connection = session.conn

% insert Session and Session.Experimenter entries in a transaction
connection.startTransaction
try
    key.subject_id = animal_id;
    key.session_time = session_time;

session_entry = key;
    session_entry.brain_region = region;
    insert(Session, session_entry)

experimenter_entry = key;
    experimenter_entry.experimenter = username;
```

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```
insert(SessionExperimenter, experiment_entry)
  connection.commitTransaction
catch
  connection.cancelTransaction
end
```

Here, to external observers, both inserts will take effect together only upon exiting from the try-catch block or will not have any effect at all. For example, if the second insert fails due to an error, the first insert will be rolled back.

CHAPTER

EIGHT

QUERIES

8.1 Query Objects

Data queries retrieve data from the database. A data query is performed with the help of a **query object**, which is a symbolic representation of the query that does not in itself contain any actual data. The simplest query object is an instance of a **table class**, representing the contents of an entire table.

For example, if experiment. Session is a DataJoint table class, you can create a query object to retrieve its entire contents as follows:

```
query = experiment.Session;
```

More generally, a query object may be formed as a **query expression** constructed by applying *operators* to other query objects.

For example, the following query retrieves information about all experiments and scans for mouse 102 (excluding experiments with no scans):

```
query = experiment.Session * experiment.Scan & 'animal_id = 102';
```

You can preview the contents of the query in Python, Jupyter Notebook, or MATLAB by simply displaying the object. In the image below, the object <code>query</code> is first defined as a restriction of the table <code>EEG</code> by values of the attribute <code>eeg_sample_rate</code> greater than 1000 Hz. Displaying the object gives a preview of the entities that will be returned by <code>query</code>. Note that this preview only lists a few of the entities that will be returned. Also, the preview does not contain any data for attributes of datatype <code>blob</code>.

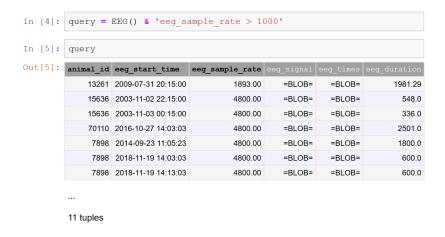


Fig. 1: Defining a query object and previewing the entities returned by the query.

Once the desired query object is formed, the query can be executed using its *fetch* methods. To **fetch** means to transfer the data represented by the query object from the database server into the workspace of the host language.

```
s = query.fetch()
```

Here fetching from the query object produces the struct array s of the queried data.

8.1.1 Checking for returned entities

The preview of the query object shown above displayed only a few of the entities returned by the query but also displayed the total number of entities that would be returned. It can be useful to know the number of entities returned by a query, or even whether a query will return any entities at all, without having to fetch all the data themselves.

The exists method applied to a query object evaluates to true if the query returns any entities and to false if the query result is empty.

The count method applied to a query object determines the number of entities returned by the query.

```
% number of ephys sessions since the start of 2018.
n = count(ephys.Session & 'session_date >= "2018-01-01"')
```

8.1.2 Normalization in queries

Query objects adhere to entity *entity normalization* just like the stored tables do. The result of a query is a well-defined entity set with an readily identifiable entity class and designated primary attributes that jointly distinguish any two entities from each other. The query *operators* are designed to keep the result normalized even in complex query expressions.

8.2 Example Schema

The example schema below contains data for a university enrollment system. Information about students, departments, courses, etc. are organized in multiple tables.

Warning: Empty primary keys, such as in the CurrentTerm table, are not yet supported by DataJoint. This feature will become available in a future release. See Issue #127 for more information.

File +university/Student.m

```
%{
 student_id
               : int unsigned # university ID
               : varchar(40)
 first_name
 last_name
               : varchar(40)
                : enum('F', 'M', 'U')
 date_of_birth : date
 home_address
                : varchar(200) # street address
 home_city
                : varchar(30)
 home_state
                : char(2) # two-letter abbreviation
 home_zipcode : char(10)
 home_phone : varchar(14)
```

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```
classdef Student < dj.Manual
end</pre>
```

File +university/Department.m

File +university/StudentMajor.m

```
%{
    -> university.Student
    ---
    -> university.Department
    declare_date : date # when student declared her major
%}
classdef StudentMajor < dj.Manual
end</pre>
```

File +university/Course.m

```
%{
    -> university.Department
    course : int unsigned # course number, e.g. 1010
    ---
    course_name : varchar(200) # e.g. "Cell Biology"
    credits : decimal(3,1) # number of credits earned by completing the course
%}
classdef Course < dj.Manual
end</pre>
```

File +university/Term.m

```
%{
   term_year : year
   term : enum('Spring', 'Summer', 'Fall')
%}
classdef Term < dj.Manual
end</pre>
```

File +university/Section.m

```
%{
    -> university.Course
    -> university.Term
    section : char(1)
    ---
    room : varchar(12) # building and room code
%}
```

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```
classdef Section < dj.Manual
end</pre>
```

File +university/CurrentTerm.m

```
%{
    ---
    -> university.Term
%}
classdef CurrentTerm < dj.Manual
end</pre>
```

File +university/Enroll.m

```
%{
    -> university.Section
    -> university.Student
%}
classdef Enroll < dj.Manual
end</pre>
```

File +university/LetterGrade.m

```
%{
    grade : char(2)
    ---
    points : decimal(3,2)
%}
classdef LetterGrade < dj.Manual
end</pre>
```

File +university/Grade.m

```
%{
    -> university.Enroll
    ---
    -> university.LetterGrade
%}
classdef Grade < dj.Manual
end</pre>
```

8.2.1 Example schema ERD

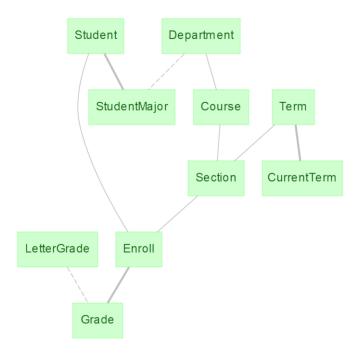


Fig. 2: Example schema for a university database. Tables contain data on students, departments, courses, etc.

8.3 Fetch

Data queries in DataJoint comprise two distinct steps:

- 1. Construct the query object to represent the required data using tables and operators.
- 2. Fetch the data from query into the workspace of the host language described in this section.

Note that entities returned by **fetch** methods are not guaranteed to be sorted in any particular order unless specifically requested. Furthermore, the order is not guaranteed to be the same in any two queries, and the contents of two identical queries may change between two sequential invocations unless they are wrapped in a transaction. Therefore, if you wish to fetch matching pairs of attributes, do so in one **fetch** call.

The examples below are based on the *example schema* for this part of the documentation.

DataJoint for MATLAB provides three distinct fetch methods: fetch, fetch1, and fetchn. The three methods differ by the type and number of their returned variables.

query.fetch returns the result in the form of an $n \times 1$ struct array where n is the number of records matching the query expression.

query.fetch1 and query.fetchn split the result into separate output arguments, one for each attribute of the query.

The types of the variables returned by fetch1 and fetchn depend on the *datatypes* of the attributes. query.fetchn will enclose any attributes of char and blob types in cell arrays whereas query.fetch1 will unpack them.

MATLAB has two alternative forms of invoking a method on an object: using the dot notation or passing the object as the first argument. The following two notations produce an equivalent result:

8.3. Fetch 87

```
result = query.fetch(query, 'attr1')
result = fetch(query, 'attr1')
```

However, the dot syntax only works when the query object is already assigned to a variable. The second syntax is more commonly used to avoid extra variables.

For example, the two methods below are equivalent although the second method creates an extra variable.

```
# Method 1
result = fetch(university.Student, '*');

# Method 2
query = university.Student;
result = query.fetch()
```

8.3.1 Fetch the primary key

Without any arguments, the **fetch** method retrieves the primary key values of the table in the form of a single column **struct**. The attribute names become the fieldnames of the **struct**.

```
keys = query.fetch;
keys = fetch(university.Student & university.StudentMajor);
```

Note that MATLAB allows calling functions without the parentheses ().

8.3.2 Fetch entire query

With a single-quoted asterisk ('*') as the input argument, the fetch command retrieves the entire result as a struct array.

```
data = query.fetch('*');
data = fetch(university.Student & university.StudentMajor, '*');
```

In some cases, the amount of data returned by fetch can be quite large. When query is a table object rather than a query expression, query.sizeOnDisk() reports the estimated size of the entire table. It can be used to assess whether running query.fetch('*') would be wise. Please note that it is only currently possible to query the size of entire tables stored directly in the database.

8.3.3 As separate variables

The fetch1 and fetchn methods are used to retrieve each attribute into a separate variable. DataJoint needs two different methods to tell MATLAB whether the result should be in array or scalar form; for numerical fields it does not matter (because scalars are still matrices in MATLAB) but non-uniform collections of values must be enclosed in cell arrays.

query.fetch1 is used when query contains exactly one entity, otherwise fetch1 will raise an error.

query.fetchn returns an arbitrary number of elements with character arrays and blobs returned in the form of cell arrays, even when query happens to contain a single entity.

```
% when tab has exactly one entity:
[name, img] = query.fetch1('name', 'image');

% when tab has any number of entities:
[names, imgs] = query.fetchn('name', 'image');
```

8.3.4 Obtaining the primary key along with individual values

It is often convenient to know the primary key values corresponding to attribute values retrieved by fetchn. This can be done by adding a special input argument indicating the request and another output argument to receive the key values:

```
% retrieve names, images, and corresponding primary key values:
[names, imgs, keys] = query.fetchn('name', 'image', 'KEY');
```

The resulting value of keys will be a column array of type struct. This mechanism is only implemented for fetchn.

8.3.5 Rename and calculate

In DataJoint for MATLAB, all **fetch** methods have all the same capability as the *proj* operator. For example, renaming an attribute can be accomplished using the syntax below.

```
[names, BMIs] = query.fetchn('name', 'weight/height/height -> bmi');
```

See *Proj* for an in-depth description of projection.

8.3.6 Sorting and limiting the results

To sort the result, add the additional ORDER BY argument in fetch and fetchn methods as the last argument.

```
% retrieve field ``course_name`` from courses
% in the biology department, sorted by course number
notes = fetchn(university.Course & 'dept="BIOL"', 'course_name', ...
'ORDER BY course');
```

The ORDER BY argument is passed directly to SQL and follows the same syntax as the ORDER BY clause

Similarly, the LIMIT and OFFSET clauses can be used to limit the result to a subset of entities. For example, to return the most advanced courses, one could do the following:

```
s = fetch(university.Course, '*', 'ORDER BY course DESC LIMIT 5')
```

The limit clause is passed directly to SQL and follows the same rules

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8.4 Iteration

The DataJoint model primarily handles data as sets, in the form of tables. However, it can sometimes be useful to access or to perform actions such as visualization upon individual entities sequentially. In DataJoint this is accomplished through iteration.

In the simple example below, iteration is used to display the names and values of the primary key attributes of each entity in the simple table or table expression tab.

```
for key = tab.fetch()'
    disp(key)
end
```

Note that the results returned by fetch must be transposed. MATLAB iterates across columns, so the single column struct returned by fetch must be transposed into a single row.

8.5 Operators

Data queries have the form of expressions using operators to derive the desired table. The expressions themselves do not contain any data. They represent the desired data symbolically.

Once a query is formed, the *fetch* methods are used to bring the data into the local workspace. Since the expressions are only symbolic representations, repeated **fetch** calls may yield different results as the state of the database is modified.

DataJoint implements a complete algebra of operators on tables:

operator	notation	meaning
restric-	A & cond	The subset of entities from table A that meet condition cond
tion		
restric-	A - cond	The subset of entities from table A that do not meet condition cond
tion		
join	A * B	Combines all matching information from A and B
proj	A.proj()	Selects and renames attributes from A or computes new attributes
aggr	A.aggr(B,)	Same as projection but allows computations based on matching information in
		В
union	A + B	All unique entities from both A and B

8.5.1 Principles of relational algebra

DataJoint's algebra improves upon the classical relational algebra and upon other query languages to simplify and enhance the construction and interpretation of precise and efficient data queries.

- 1. **Entity integrity**: Data are represented and manipulated in the form of tables representing *well-formed entity sets*. This applies to the inputs and outputs of query operators. The output of a query operator is an entity set with a well-defined entity type, a primary key, unique attribute names, etc.
- 2. **Algebraic closure**: All operators operate on entity sets and yield entity sets. Thus query expressions may be used as operands in other expressions or may be assigned to variables to be used in other expressions.
- 3. **Attributes are identified by names**: All attributes have explicit names. This includes results of queries. Operators use attribute names to determine how to perform the operation. The order of the attributes is not significant.

8.5.2 Matching entities

Binary operators in DataJoint are based on the concept of **matching entities**; this phrase will be used throughout the documentation.

Two entities **match** when they have no common attributes or when their common attributes contain the same values.

Here **common attributes** are those that have the same names in both entities. It is usually assumed that the common attributes are of compatible datatypes to allow equality comparisons.

Another way to phrase the same definition is

Two entities match when they have no common attributes whose values differ.

It may be conceptually convenient to imagine that all tables always have an additional invisible attribute, omega whose domain comprises only one value, 1. Then the definition of matching entities is simplified:

Two entities match when their common attributes contain the same values.

Matching entities can be **merged** into a single entity without any conflicts of attribute names and values.

Examples

This is a matching pair of entities:



and so is this one:



but these entities do not match:



8.5.3 Join compatibility

All binary operators with other tables as their two operands require that the operands be **join-compatible**, which means that:

- 1. All common attributes in both operands (attributes with the same name) must be part of either the primary key or a foreign key.
- 2. All common attributes in the two relations must be of a compatible datatype for equality comparisons.

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These restrictions are introduced both for performance reasons and for conceptual reasons. For performance, they encourage queries that rely on indexes. For conceptual reasons, they encourage database design in which entities in different tables are related to each other by the use of primary keys and foreign keys.

8.6 Restriction

8.6.1 Restriction operators & and -

The restriction operator A & cond selects the subset of entities from A that meet the condition A. The exclusion operator A - A cond selects the complement of restriction, i.e. the subset of entities from A that do not meet the condition A cond A cond A that do not meet the condition A cond A c

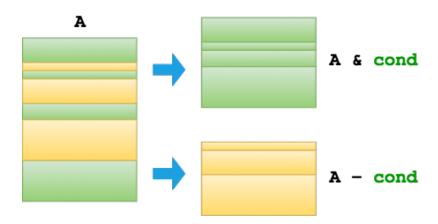


Fig. 3: Restriction and exclusion.

The condition **cond** may be one of the following:

- another table
- a mapping, or struct
- an expression in a character string
- a collection of conditions as a struct or cell array
- a Boolean expression (true or false)
- a query expression

As the restriction and exclusion operators are complementary, queries can be constructed using both operators that will return the same results. For example, the queries A & cond and A - Not (cond) will return the same entities.

8.6.2 Restriction by a table

When restricting table A with another table, written A & B, the two tables must be **join-compatible** (see *Join compatibility*). The result will contain all entities from A for which there exist a matching entity in B. Exclusion of table A with table B, or A - B, will contain all entities from A for which there are no matching entities in B.

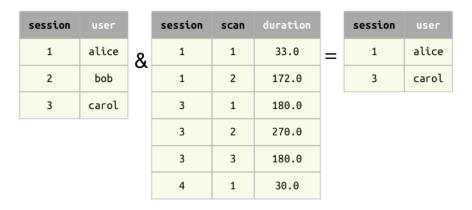


Fig. 4: Restriction by another table.

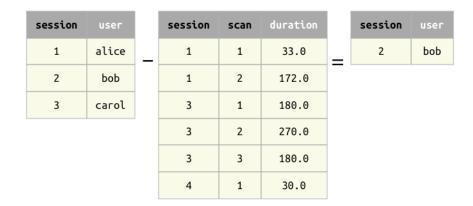


Fig. 5: Exclusion by another table.

Restriction by a table with no common attributes

Restriction of table A with another table B having none of the same attributes as A will simply return all entities in A, unless B is empty as described below. Exclusion of table A with B having no common attributes will return no entities, unless B is empty as described below.

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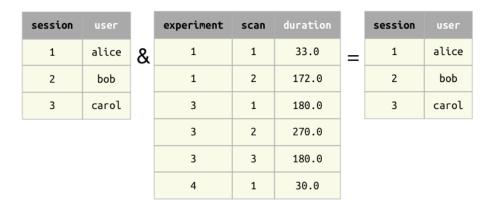


Fig. 6: Restriction by a table having no common attributes.



Fig. 7: Exclusion by a table having no common attributes.

Restriction by an empty table

Restriction of table A with an empty table will return no entities regardless of whether there are any matching attributes. Exclusion of table A with an empty table will return all entities in A.



Fig. 8: Restriction by an empty table.

session	user		experiment	scan	duration		session	user
1	alice	_				=	1	alice
2	bob						2	bob
3	carol						3	carol

Fig. 9: Exclusion by an empty table.

8.6.3 Restriction by a mapping

A key-value mapping may be used as an operand in restriction. For each key that is an attribute in A, the paired value is treated as part of an equality condition. Any key-value pairs without corresponding attributes in A are ignored.

Restriction by an empty mapping or by a mapping with no keys matching the attributes in A will return all the entities in A. Exclusion by an empty mapping or by a mapping with no matches will return no entities.

For example, let's say that table Session has the attribute session_date of *datatype* datetime. You are interested in sessions from January 1st, 2018, so you write the following restriction query using a mapping.

```
ephys.Session & struct('session_dat', '2018-01-01')
```

Our mapping contains a typo omitting the final e from session_date, so no keys in our mapping will match any attribute in Session. As such, our query will return all of the entities of Session.

8.6.4 Restriction by a string

Restriction can be performed when cond is an explicit condition on attribute values, expressed as a string. Such conditions may include arithmetic operations, functions, range tests, etc. Restriction of table A by a string containing an attribute not found in table A produces an error.

```
% All the sessions performed by Alice
ephys.Session & 'user = "Alice"'

% All the experiments at least one minute long
ephys.Experiment & 'duration >= 60'
```

8.6.5 Restriction by a collection

Warning: This section documents future intended behavior in MATLAB, which is contrary to current behavior. DataJoint for MATLAB has an open issue tracking this change.

A collection can be a cell array or structure array. Cell arrays can contain collections of arbitrary restriction conditions. Structure arrays are limited to collections of mappings, each having the same attributes.

```
% a cell aray:
cond_cell = {'first_name = "Aaron"', 'last_name = "Aaronson"'}
% a structure array:
(continues on next page)
```

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(continued from previous page)

```
cond_struct = struct('first_name', 'Aaron', 'last_name', 'Paul')
cond_struct(2) = struct('first_name', 'Rosie', 'last_name', 'Aaronson')
```

When cond is a collection of conditions, the conditions are applied by logical disjunction (logical OR). Thus, restriction of table A by a collection will return all entities in A that meet *any* of the conditions in the collection. For example, if you restrict the Student table by a collection containing two conditions, one for a first and one for a last name, your query will return any students with a matching first name *or* a matching last name.

```
university.Student() & {'first_name = "Aaron"', 'last_name = "Aaronson"'}

STUDENT_ID first_name last_name sex date_of_birth home_address home_city home_state home_zipcode home_phone

1.1236e+05 'Rosie' 'Aaronson' 'F' '1988-10-24' '3 Ring Road' 'Algoe' 'NY' '12776' '2228477'
1.2346e+05 'Aaron' 'Aaronson' 'M' '1980-02-12' '1 Drive Way' 'Derry' 'ME' '04401' '5553437'
2.6343e+05 'Aaron' 'Paul' 'M' '1992-04-30' '123 Peppermint Tree' 'Houston' 'TX' '77401' '7135246'
3 tuples (0.449 s)
```

Fig. 10: Restriction by a collection, returning any entities matching any condition in the collection.

Restriction by an empty collection returns no entities. Exclusion of table A by an empty collection returns all the entities of A.

8.6.6 Restriction by a Boolean expression

```
A & true and A - false are equivalent to A.

A & false and A - true are empty.
```

8.6.7 Restriction by a query

Restriction by a query object is a generalization of restriction by a table (which is also a query object), because DataJoint queries always produce well-defined entity sets, as described in *entity normalization*. As such, restriction by queries follows the same behavior as restriction by tables described above.

The example below creates a query object corresponding to all the sessions performed by the user Alice. The **Experiment** table is then restricted by the query object, returning all the experiments that are part of sessions performed by Alice.

```
query = ephys.Session & 'user = "Alice"'
ephys.Experiment & query
```

8.7 Join

8.7.1 Join operator *

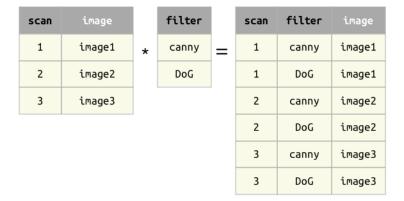
The Join operator A * B combines the matching information in A and B. The result contains all matching combinations of entities from both arguments.

Principles of joins

- 1. The operands A and B must be join-compatible.
- 2. The primary key of the result is the union of the primary keys of the operands.

Examples of joins

Example 1: When the operands have no common attributes, the result is the cross product – all combinations of entities.



Example 2: When the operands have common attributes, only entities with matching values are kept.

session	user		session	scan	duration		session	scan	user	duration
1	alice	*	1	1	33.0	_	1	1	alice	33.0
2	bob		1	2	172.0	_	1	2	alice	172.0
3	carol		3	1	180.0		3	1	carol	180.0
			3	2	270.0		3	2	carol	270.0
			3	3	180.0		3	3	carol	180.0
			4	1	30.0					

Example 3: Joining on secondary attribute.

id	signal	filter		filter	low	high		id	filter	signal	low	high
1	signal1	1	*	1	3.0	120	=	1	1	signal1	3.0	120
2	signal2	2		2	1.0	600		2	2	signal2	1.0	600
3	signal3	3						4	1	signal4	1.0	120
4	signal4	1										

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Properties of join

- 1. When A and B have the same attributes, the join A * B becomes equivalent to the set intersection A \cap B. Hence, DataJoint does not need a separate intersection operator.
- 2. Commutativity: A * B is equivalent to B * A.
- 3. Associativity: (A * B) * C is equivalent to A * (B * C).

8.8 Proj

The **proj** operator represents **projection** and is used to select attributes (columns) from a table, to rename them, or to create new calculated attributes.

8.8.1 Simple projection

The simple projection selects a subset of attributes of the original table. However, the primary key attributes are always included.

Using the *example schema*, let table department have attributes **dept**, *dept_name*, *dept_address*, and *dept_phone*. The primary key attribute is in bold.

Then department.proj() will have attribute dept.

```
department.proj('dept') will have attribute dept.
```

department.proj('dept_name', 'dept_phone') will have attributes dept, dept_name, and dept_phone.

8.8.2 Renaming

In addition to selecting attributes, **proj** can rename them. Any attribute can be renamed, including primary key attributes.

Renaming is done using a string: tab('old_attr->new_attr').

For example, let table tab have attributes **mouse**, **session**, *session_date*, *stimulus*, and *behavior*. The primary key attributes are in bold.

Then

```
tab.proj('mouse->animal', 'stimulus')
```

will have attributes animal, session, and stimulus.

Renaming is often used to control the outcome of a *join*. For example, let tab have attributes **slice**, and **cell**. Then tab * tab will simply yield tab . However,

```
tab * tab.proj('cell->other')
```

yields all ordered pairs of all cells in each slice.

8.8.3 Calculations

In addition to selecting or renaming attributes, proj can compute new attributes from existing ones.

For example, let tab have attributes mouse, scan, surface_z, and scan_z. To obtain the new attribute depth computed as scan_z - surface_z and then to restrict to depth > 500:

```
tab.proj('scan_z-surface_z -> depth') & 'depth > 500'
```

Calculations are passed to SQL and are not parsed by DataJoint. For available functions, you may refer to the MySQL documentation.

8.9 Aggr

Aggregation, performed with the aggr operator, is a special form of proj with the additional feature of allowing aggregation calculations on another table. It has the form tab.aggr(other, ...) where other is another table. Without the argument other, aggr and proj are exactly equivalent. Aggregation allows adding calculated attributes to each entity in tab based on aggregation functions over attributes in the *matching* entities of other.

Aggregation functions include count, sum, min, max, avg, median, percentile, stdev, var, and others. Aggregation functions can only be used in the definitions of new attributes within the aggregator.

As with proj, the output of aggr has the same entity class, the same primary key, and the same number of elements as tab. Primary key attributes are always included in the output and may be renamed, just like in proj.

8.9.1 Examples

```
% Number of students in each course section
university.Section.aggr(university.Enroll, 'count(*)->n')
% Average grade in each course
university.Course.aggr(university.Grade * university.LetterGrade, 'avg(points)->avg_grade')
```

8.10 Union

The union operator is not yet implemented – this page serves as the specification for the upcoming implementation. Union is rarely needed in practice.

8.10.1 Union operator +

The result of the union operator A + B contains all the entities from both operands. *Entity normalization* requires that the operands in a union both belong to the same entity type with the same primary key using homologous attributes. In the absence of any secondary attributes, the result of a union is the simple set union.

When secondary attributes are present, they must have the same names and datatypes in both operands. The two operands must also be **disjoint**, without any duplicate primary key values across both inputs. These requirements prevent ambiguity of attribute values and preserve entity identity.

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Principles of union

- 1. As in all operators, the order of the attributes in the operands is not significant.
- 2. Operands A and B must have the same primary key attributes. Otherwise, an error will be raised.
- 3. Operands A and B may not have any common non-key attributes. Otherwise, an error will be raised.
- 4. The result A + B will have the same primary key as A and B.
- 5. The result A + B will have all the non-key attributes from both A and B.
- 6. For entities that are found in both A and B (based on the primary key), the secondary attributes will be filled from the corresponding entities in A and B.
- 7. For entities that are only found in either A or B, the other operand's secondary attributes will filled with null values.

Examples of union

Example 1: Note that the order of the attributes does not matter.

slice	cell		cell	slice		slice	cell
1	1		1	1		1	1
1	2	+	1	3	=	1	2
2	6		2	3		2	6
						3	1
						3	2

Example 2: Non-key attributes are combined from both tables and filled with NULLs when missing.

scan	response		scan	latency		scan	response	latency
1	6	+	1	8	_	1	6	8
2	7		3	8		2	6	NULL
3	6		4	8		3	6	8
						4	NULL	8

Properties of union

```
1. Commutative: A + B is equivalent to B + A.
```

```
2. Associative: (A + B) + C is equivalent to A + (B + C).
```

8.11 Universal Sets

All *query operators* are designed to preserve the entity types of their inputs. However, some queries require creating a new entity type that is not represented by any stored tables. This means that a new entity type must be explicitly defined as part of the query. Universal sets fulfill this role.

Universal sets are used in DataJoint to define virtual tables with arbitrary primary key structures for use in query expressions. A universal set, defined using class dj.U, denotes the set of all possible entities with given attributes of any possible datatype. Universal sets allow query expressions using virtual tables when no suitable base table exists. Attributes of universal sets are allowed to be matched to any namesake attributes, even those that do not come from the same initial source.

For example, you may like to query the university database for the complete list of students' home cities, along with the number of students from each city. The *schema* for the university database does not have a table for cities and states. A virtual table can fill the role of the nonexistent base table, allowing queries that would not be possible otherwise.

Note: dj.U is not yet implemented in MATLAB. The feature will be added in an upcoming release: https://github.com/datajoint/datajoint-matlab/issues/144

```
% All home cities of students
dj.U('home_city', 'home_state') & university.Student

% Total number of students from each city
aggr(dj.U('home_city', 'home_state'), university.Student, 'count(*)->n')

% Total number of students from each state
aggr(U('home_state'), university.Student, 'count(*)->n')

% Total number of students in the database
aggr(U(), university.Student, 'count(*)->n')
```

The result of aggregation on a universal set is restricted to the entities with matches in the aggregated table, such as Student in the example above. In other words, X.aggr(A, ...) is interpreted as (X & A).aggr(A, ...) for universal set X. All attributes of a universal set are considered primary.

Universal sets should be used sparingly when no suitable base tables already exist. In some cases, defining a new base table can make queries clearer and more semantically constrained.

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CHAPTER

NINE

COMPUTATION

9.1 Auto-populate

Auto-populated tables are used to define, execute, and coordinate computations in a DataJoint pipeline.

Tables in the initial portions of the pipeline are populated from outside the pipeline. In subsequent steps, computations are performed automatically by the DataJoint pipeline in auto-populated tables.

Computed tables belong to one of the two auto-populated *data tiers*: dj.Imported and dj.Computed. DataJoint does not enforce the distinction between imported and computed tables: the difference is purely semantic, a convention for developers to follow. If populating a table requires access to external files such as raw storage that is not part of the database, the table is designated as **imported**. Otherwise it is **computed**.

Auto-populated tables are defined and queried exactly as other tables. (See *Manual Tables*.) Their data definition follows the same *definition syntax*.

9.1.1 Make

For auto-populated tables, data should never be entered using *insert* directly. Instead these tables must define the callback method make(self, key). The insert method then can only be called on self inside this callback method.

Imagine that there is a table test.Image that contains 2D grayscale images in its image attribute. Let us define the computed table, test.FilteredImage that filters the image in some way and saves the result in its filtered_image attribute.

The class will be defined as follows.

```
%{
# Filtered image
-> test.Image
---
filtered_image : longblob
%}

classdef FilteredImage < dj.Computed
   methods(Access=protected)
   function make(self, key)
        img = fetch1(test.Image & key, 'image');
        key.filtered_image = myfilter(img);
        self.insert(key)
   end</pre>
```

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end **end**

Note: Currently matlab uses makeTuples rather than make. This will be fixed in an upcoming release: https://github.com/datajoint/datajoint-matlab/issues/141

The make method receives one argument: the struct key containing the primary key value of an element of *key source* to be worked on.

The make method received one argument: the key of type struct in MATLAB and dict in Python. The key represents the partially filled entity, usually already containing the *primary key* attributes of the key source.

The make callback does three things:

- 1. Fetches data from tables upstream in the pipeline using the key for restriction.
- 2. Computes and adds any missing attributes to the fields already in key.
- 3. Inserts the entire entity into self.

make may populate multiple entities in one call when key does not specify the entire primary key of the populated table.

9.1.2 Populate

The inherited populate method of dj.Imported and dj.Computed automatically calls make for every key for which the auto-populated table is missing data.

The FilteredImage table can be populated as

populate(test.FilteredImage)

Note that it is not necessary to specify which data needs to be computed. DataJoint will call make, one-by-one, for every key in Image for which FilteredImage has not yet been computed.

Chains of auto-populated tables form computational pipelines in DataJoint.

9.1.3 Populate options

Behavior of the populate method depends on the number of output arguments requested in the function call. When no output arguments are requested, errors will halt population. With two output arguments (failedKeys and errors), populate will catch any encountered errors and return them along with the offending keys.

9.1.4 Progress

```
{%
  # the job reservation table
 table_name : varchar(255)
                                         # className of the table
                 : char(32)
                                         # key hash
 key_hash
                   : enum('reserved', 'error', 'ignore') # if tuple is missing, the job is available
  status
 key=null
                    : blob
                                           # structure containing the key
 error_message="" : varchar(1023)
                                           # error message returned if failed
 error_stack=null : blob
                                           # error stack if failed
 host="" : varchar(255)  # system hostname
pid=0 : int unsigned  # system process id
  timestamp=CURRENT_TIMESTAMP : timestamp # automatic timestamp
```

A job is considered to be available when package>. Jobs contains no matching entry.

For each make call, parpopulate sets the job status to reserved. When the job is completed, the record is removed. If the job results in error, the job record is left in place with the status set to error and the error message and error stacks saved. Consequently, jobs that ended in error during the last execution will not be attempted again until you delete the corresponding entities from package>.Jobs.

The primary key of the jobs table comprises the name of the class and a 32-character hash of the job's primary key. However, the key is saved in a separate field for error debugging purposes.

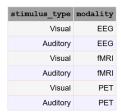
9.2 Key Source

9.2.1 Default key source

Key source refers to the set of primary key values over which *autopopulate* iterates, calling the make method at each iteration. Each key from the key source is passed to the table's make call. By default, the key source for a table is the *join* of its primary *dependencies*.

For example, consider a schema with three tables. The Stimulus table contains one attribute stimulus_type with one of two values, "Visual" or "Auditory". The Modality table contains one attribute modality with one of three values, "EEG", "fMRI", and "PET". The Protocol table has primary dependencies on both the Stimulus and Modality tables.

The key source for Protocol will then be all six combinations of stimulus_type and modality as shown in the figure below.



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9.2.2 Custom key source

A custom key source can be configured by setting the keySource property within a table's classdef block, using MATLAB's dependent properties syntax.

Any *query object* can be used as the key source. In most cases the new key source will be some alteration of the default key source. Custom key sources often involve restriction to limit the key source to only relevant entities. Other designs may involve using only one of a table's primary dependencies.

In the example below, the EEG table depends on the Recording table that lists all recording sessions. However, the populate method of EEG should only ingest recordings where the recording_type is EEG. Setting a custom key source prevents the populate call from iterating over recordings of the wrong type.

A custom key source can be configured by setting the keySource property within a table's classdef block, using MATLAB's dependent properties syntax.

9.3 Master-Part Relationship

Often an entity in one table is inseparably associated with a group of entities in another, forming a **master-part** relationship. The master-part relationship ensures that all parts of a complex representation appear together or not at all. This has become one of the most powerful data integrity principles in DataJoint.

As an example, imagine segmenting an image to identify regions of interest. The resulting segmentation is inseparable from the ROIs that it produces. In this case, the two tables might be called Segmentation and Segmentation.ROI.

In MATLAB, the master and part tables are declared in a separate classdef file. The name of the part table must begin with the name of the master table. The part table must declare the property master containing an object of the master.

+test/Segmentation.m

```
# image segmentation
-> test.Image
%}
classdef Segmentation < dj.Computed
   methods(Access=protected)
     function make(self, key)
        self.insert(key)
        make(test.SegmentationRoi, key)
   end
end
end</pre>
```

+test/SegmentationROI.m

```
%{
# Region of interest resulting from segmentation
-> test.Segmentation
roi : smallint # roi number
---
roi_pixels : longblob # indices of pixels
roi_weights : longblob # weights of pixels
%}
```

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```
classdef SegmentationROI < dj.Part</pre>
    properties(SetAccess=protected)
        master = test.Segmentation
    end
    methods
        function make(self, key)
            image = fetch1(test.Image & key, 'image');
            [roi_pixels, roi_weighs] = mylib.segment(image);
            for roi=1:length(roi_pixels)
                entity = key;
                entity.roi_pixels = roi_pixels{roi};
                entity.roi_weights = roi_weights{roi};
                self.insert(entity)
            end
        end
    end
end
```

9.3.1 Populating

Master-part relationships can form in any data tier, but DataJoint observes them more strictly for auto-populated tables. To populate both the master Segmentation and the part Segmentation.ROI, it is sufficient to call the populate method of the master:

```
populate(Segmentation)
```

Note that the entities in the master and the matching entities in the part are inserted within a single make call of the master, which means that they are a processed inside a single transactions: either all are inserted and committed or the entire transaction is rolled back. This ensures that partial results never appear in the database.

For example, imagine that a segmentation is performed, but an error occurs halfway through inserting the results. If this situation were allowed to persist, then it might appear that 20 ROIs were detected where 45 had actually been found.

9.3.2 Deleting

To delete from a master-part pair, one should never delete from the part tables directly. The only valid method to delete from a part table is to delete the master. This has been an unenforced rule, but upcoming versions of DataJoint will prohibit direct deletes from the master table. DataJoint's *delete* operation is also enclosed in a transaction.

Together, the rules of master-part relationships ensure a key aspect of data integrity: results of computations involving multiple components and steps appear in their entirety or not at all.

9.3.3 Multiple parts

The master-part relationship cannot be chained or nested. DataJoint does not allow part tables of other part tables per se. However, it is common to have a master table with multiple part tables that depend on each other. For example:

+test/ArrayResponse.m

```
%{
    -> Probe
array: int
%}
classdef ArrayResponse < dj.Computed
    methods(Access=protected)
    function make(self, key)
        self.insert(key)
        make(test.ArrayResponseElectrodeResponse, key)
    end
end
end</pre>
```

+test/ArrayResponseElectrodeResponse.m

```
%{
    -> test.ArrayResponse
electrode : int % electrode number on the probe
%}
classdef ArrayResponseElectrodeResponse < dj.Part
    methods(SetAccess=protected)
        function make(self, key)
            self.insert(key)
        end
end
end</pre>
```

+test/ArrayResponseChannelResponse.m

```
%{
    -> test.ArrayResponseElectrodeResponse
    channel: int
    ---
    response: longblob % response of a channel
%}
classdef ArrayResponseChannelResponse < dj.Part
    methods(SetAccess=protected)
        function make(self, key)
            self.insert(key)
        end
    end
end</pre>
```

Conceptually, one or more channels belongs to an electrode, and one or more electrodes belong to an array. This example assumes that information about an array's response (which consists ultimately of the responses of multiple electrodes each consisting of multiple channel responses) including it's electrodes and channels are entered together.

9.4 Transactions in Make

Each call of the *make* method is enclosed in a transaction. DataJoint users do not need to explicitly manage transactions but must be aware of their use.

Transactions produce two effects:

First, the state of the database appears stable within the make call throughout the transaction: two executions of the same query will yield identical results within the same make call.

Second, any changes to the database (inserts) produced by the make method will not become visible to other processes until the make call completes execution. If the make method raises an exception, all changes made so far will be discarded and will never become visible to other processes.

Transactions are particularly important in maintaining *group integrity* with *master-part relationships*. The make call of a master table first inserts the master entity and then inserts all the matching part entities in the part tables. None of the entities become visible to other processes until the entire make call completes, at which point they all become visible.

9.5 Distributed Computing

9.5.1 Job reservations

Running populate on the same table on multiple computers will causes them to attempt to compute the same data all at once. This will not corrupt the data since DataJoint will reject any duplication. One solution could be to cause the different computing nodes to populate the tables in random order. This would reduce some collisions but not completely prevent them.

To allow efficient distributed computing, DataJoint provides a built-in job reservation process. When dj.Computed tables are auto-populated using job reservation, a record of each ongoing computation is kept in a schema-wide jobs table, which is used internally by DataJoint to coordinate the auto-population effort among multiple computing processes.

Job reservations are activated by replacing populate calls with identical parpopulate calls.

With job management enabled, the make method of each table class will also consult the jobs table for reserved jobs as part of determining the next record to compute and will create an entry in the jobs table as part of the attempt to compute the resulting record for that key. If the operation is a success, the record is removed. In the event of failure, the job reservation entry is updated to indicate the details of failure. Using this simple mechanism, multiple processes can participate in the auto-population effort without duplicating computational effort, and any errors encountered during the course of the computation can be individually inspected to determine the cause of the issue.

As part of DataJoint, the jobs table can be queried using native DataJoint syntax. For example, to list the jobs currently being run:

The above output shows that a record for the JobResults table is currently reserved for computation, along with various related details of the reservation, such as the MySQL connection ID, client user and host, process ID on the remote system, timestamp, and the key for the record that the job is using for its computation. Since DataJoint table keys can be of varying types, the key is stored in a binary format to allow the table to store arbitrary types of record key data. The subsequent sections will discuss querying the jobs table for key data.

As mentioned above, jobs encountering errors during computation will leave their record reservations in place, and update the reservation record with details of the error.

By leaving the job reservation record in place, the error can be inspected, and if necessary the corresponding dj.Computed update logic can be corrected. From there the jobs entry can be cleared, and the computation can then be resumed. In the meantime, the presence of the job reservation will prevent this particular record from being processed during subsequent auto-population calls. Inspecting the job record for failure details can proceed much like any other DataJoint query.

After any system or code errors have been resolved, the table can simply be cleaned of errors and the computation rerun.

In some cases, it may be preferable to inspect the jobs table records using populate keys. Since job keys are hashed and stored as a blob in the jobs table to support the varying types of keys, we need to query using the key hash instead of simply using the raw key data.

9.5.2 Managing connections

The DataJoint method dj.kill allows for viewing and termination of database connections. Restrictive conditions can be used to identify specific connections. Restrictions are specified as strings and can involve any of the attributes of information_schema.processlist: ID, USER, HOST, DB, COMMAND, TIME, STATE, and INFO.

Examples:

```
dj.kill('HOST LIKE "%compute%"') lists only connections from hosts containing "compute". dj.kill('TIME > 600') lists only connections older than 10 minutes.
```

A list of connections meeting the restriction conditions (if present) are presented to the user, along with the option to kill processes.

For example, to sort the output by hostname in descending order:

```
dj.kill('', dj.conn, 'host desc');
       USER
                                COMMAND
                                          TIME
                                                 STATE
                                                         INFO
                                                                 TIME MS
                                                                           ROWS_SENT
                                                                                       ROWS_EXAMINED
              localhost:38772 Sleep
                                           94
                                                                            0
                                                                                        0
 35
                                                                  94040
       cat
                                                                                         0
  36
              localhost:36543 Sleep
                                           68
                                                                  68421
                                                                            1
       cat
process to kill ('q'-quit, 'a'-all) > q
```

COMMUNITY

10.1 Publications

The following are some of the studies that used DataJoint for building their data pipelines.

- 1. Rosón, M. R., Bauer, Y., Kotkat, A. H., Berens, P., Euler, T., & Busse, L. (2019). Mouse dLGN receives functional input from a diverse population of retinal ganglion cells with limited convergence. Neuron, 102(2), 462-476.
- Ecker, A. S., Sinz, F. H., Froudarakis, E., Fahey, P. G., Cadena, S. A., Walker, E. Y., ... & Bethge, M. (2018). A rotation-equivariant convolutional neural network model of primary visual cortex. arXiv preprint arXiv:1809.10504.
- 3. Chettih, S. N., & Harvey, C. D. (2019). Single-neuron perturbations reveal feature-specific competition in V1. Nature, 567(7748), 334.
- 4. Denfield, G. H., Ecker, A. S., Shinn, T. J., Bethge, M., & Tolias, A. S. (2018). Attentional fluctuations induce shared variability in macaque primary visual cortex. Nature communications, 9(1), 2654.
- 5. Shan, Kevin Q., Evgueniy V. Lubenov, and Athanassios G. Siapas. "Model-based spike sorting with a mixture of drifting t-distributions." Journal of neuroscience methods 288 (2017): 82-98.
- Reimer, J., McGinley, M. J., Liu, Y., Rodenkirch, C., Wang, Q., McCormick, D. A., & Tolias, A. S. (2016). Pupil fluctuations track rapid changes in adrenergic and cholinergic activity in cortex. Nature communications, 7, 13289.
- 7. Franke, K., Berens, P., Schubert, T., Bethge, M., Euler, T., & Baden, T. (2017). Inhibition decorrelates visual feature representations in the inner retina. Nature, 542(7642), 439.
- 8. Cadwell, Cathryn R., et al. "Electrophysiological, transcriptomic and morphologic profiling of single neurons using Patch-seq." Nature biotechnology 34.2 (2016): 199.
- 9. Shan, K. Q., Lubenov, E. V., Papadopoulou, M., & Siapas, A. G. (2016). Spatial tuning and brain state account for dorsal hippocampal CA1 activity in a non-spatial learning task. Elife, 5, e14321.
- 10. Jiang, X., Shen, S., Cadwell, C. R., Berens, P., Sinz, F., Ecker, A. S., ... & Tolias, A. S. (2015). Principles of connectivity among morphologically defined cell types in adult neocortex. Science, 350(6264), aac9462.
- 11. Yatsenko, D., Josić, K., Ecker, A. S., Froudarakis, E., Cotton, R. J., & Tolias, A. S. (2015). Improved estimation and interpretation of correlations in neural circuits. PLoS computational biology, 11(3), e1004083.
- 12. Reimer, J., Froudarakis, E., Cadwell, C. R., Yatsenko, D., Denfield, G. H., & Tolias, A. S. (2014). Pupil fluctuations track fast switching of cortical states during quiet wakefulness. Neuron, 84(2), 355-362.
- 13. Erisken, S., Vaiceliunaite, A., Jurjut, O., Fiorini, M., Katzner, S., & Busse, L. (2014). Effects of locomotion extend throughout the mouse early visual system. Current Biology, 24(24), 2899-2907.

- 14. Froudarakis, E., Berens, P., Ecker, A. S., Cotton, R. J., Sinz, F. H., Yatsenko, D., ... & Tolias, A. S. (2014). Population code in mouse V1 facilitates readout of natural scenes through increased sparseness. Nature neuroscience, 17(6), 851.
- 15. Ecker, A. S., Berens, P., Cotton, R. J., Subramaniyan, M., Denfield, G. H., Cadwell, C. R., ... & Tolias, A. S. (2014). State dependence of noise correlations in macaque primary visual cortex. Neuron, 82(1), 235-248.
- Cotton, R. J., Froudarakis, E., Storer, P., Saggau, P., & Tolias, A. S. (2013). Three-dimensional mapping of microcircuit correlation structure. Frontiers in neural circuits, 7, 151.
- 17. Vaiceliunaite, A., Erisken, S., Franzen, F., Katzner, S., & Busse, L. (2013). Spatial integration in mouse primary visual cortex. Journal of neurophysiology, 110(4), 964-972.

10.2 Contribute

Thank you for your interest in contributing!

To help keep everyone in alignment and coordinated in the community effort, we've created this document. It serves as the contribution guideline that outlines how open-source software development is to be conducted. Any software development that makes reference to this document can be assumed to adopt the policies outlined below. We've structured the guideline in a FAQ (frequently asked questions) format to make it easier to digest. Feel free to review the questions below to determine any specific policy.

The principal maintainer of DataJoint and associated tools is the DataJoint Neuro team (Vathes Inc.). The pronouns "we" and "us" in this guideline refer to the principal maintainers. We invite reviews and contributions of the open-source software. We compiled these guidelines to make this work clear and efficient.

10.2.1 1) Which issue should I contribute towards?

There are three primary things to consider when looking to contribute.

- Availability: An indication of whether anyone is currently working on a fix for the given issue. Availability is indicated by who is assigned. Issues that are unassigned mean that there is no one yet working on resolving the issue and the issue is available for someone to work on. If an issue has been assigned, then any additional work on that issue should be coordinated with the assignee.
- **Specification**: In order for issues to be properly addressed, the requirements of satisfying and closing the issue should be clear. If it is not, a label will be added as unspecified. This could be due to more debug info being necessary, more details on intended behavior, or perhaps that further discussion is required to determine a good solution. Feel free to help us arrive at a proper specification.
- **Priority**: As a community, we work on a concerted effort to bring about the realization of the milestones. We utilize milestones as a planning tool to help focus a group of changes around a release. To determine the priority of issues, simply have a look at the next milestone that is expected to arrive. Therefore, each milestone following this can be understood as lower in priority respectively. Bear in mind that much like a hurricane forecast, the execution plan is much more likely to be accurate the closer to today's date as opposed to milestones further out. Extremely low priority issues are assigned to the **Backburner** milestone. Since **Backburner** does not have a target date, this indicates that its issues may be deferred indefinitely. Occasionally the maintainers will move issues from **Backburner** as it makes sense to address them within a release. Also, issues unassigned to a milestone can be understood as new issues which have not been triaged.

After considering the above, you may comment on the issue you'd like to help fix and a maintainer will assign it to you.

10.2.2 2) What is the proper etiquette for proposing changes as contribution?

What is generally expected from new contributions are the following:

- Any proposed contributor changes should be introduced in the form of a pull request (PR) from their fork.
- Proper branch target specified. The following is generally the available branches that can be targeted:
 - main or master: Represents the single source of truth and the latest in completed development.
 - pre: Represents the source at the point of the last stable release.

For larger more involved changes, a maintainer may determine it best to create a feature-specific branch and adjust the PR accordingly.

- A summary description that describes the overall intent behind the PR.
- Proper links to the issue(s) that the PR serves to resolve.
- Newly introduced changes must pass any required checks. Typically as it relates to tests, this means:
 - 1. No syntax errors
 - 2. No integration errors
 - 3. No style errors e.g. PEP8, etc.
 - 4. Similar or better code coverage
- Additional documentation to reflect new feature or behavior introduced.
- Necessary updates to the changelog following Keep a Changelog convention.
- A contributor should not approve or merge their own PR.
- Reviewer suggestions or feedback should not be directly committed to a branch on a contributor's fork. A less
 intrusive way to collaborate would be for the reviewer to PR to the contributor's fork/branch that is associated
 with the main PR currently in review.

Maintainers will also ensure that PR's have the appropriate assignment for reviewer, milestone, and project.

10.2.3 3) How can I track the progress of an issue that has been assigned?

Since milestones represent the development plan, projects represent the actual execution. Projects are typically fixed-time sprints (1-2 weeks). A 'workable' number of issues that have been assigned to developers and assigned to the next milestone are selected and tracked in each project to provide greater granularity in the week-to-week progress. Automation is included observing the Automated kanban with reviews template. Maintainers will adjust the project assignment to reflect the order in which to resolve the milestone issues.

10.2.4 4) What is the release process? How do I know when my merged contribution will officially make it into a release?

Releases follow the standard definition of semantic versioning. Meaning:

MAJOR . MINOR . PATCH

- 1. MAJOR version when you make incompatible API changes,
- 2. MINOR version when you add functionality in a backwards compatible manner, and
- 3. PATCH version when you make backwards compatible bug fixes.

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Each release requires tagging the commit appropriately and is then issued in the normal medium for release e.g. PyPi, NPM, YARN, GitHub Release, etc.

Minor releases are triggered when all the issues assigned to a milestone are resolved and closed. Patch releases are triggered periodically from main or master after a reasonable number of PR merges have come in.

10.2.5 5) I am not yet too comfortable contributing but would like to engage the community. What is the policy on community engagement?

In order to follow the appropriate process and setting, please reference the following flow for your desired mode of engagement:

5a) Generally, how do I perform ?

If the documentation does not provide clear enough instruction, please see StackOverflow posts related to the datajoint tag or ask a new question tagging it appropriately. You may refer to our datajoint tag wiki for more details on its proper use.

5b) I just encountered this error, how can I resolve it?

Please see StackOverflow posts related to the datajoint tag or ask a new question tagging it appropriately. You may refer to our datajoint tag wiki for more details on its proper use.

5c) I just encountered this error and I am sure it is a bug, how do I report it?

Please file it under the issue tracker associated with the open-source software.

5d) I have an idea or new feature request, how do I submit it?

Please file it under the issue tracker associated with the open-source software.

5e) I am curious why the maintainers choose to ______? i.e. questions that are 'opinionated' in nature with answers that some might disagree.

Please join the community on the DataJoint Slack and ask on the most relevant channel. There, you may engage directly with the maintainers for proper discourse.

5f) What is the timeline or roadmap for the release of certain supported features?

Please refer to milestones and projects associated with the open-source software.

5g) I need urgent help best suited for live debugging, how can I reach out directly?

Please join the community on the DataJoint Slack and ask on the most relevant channel. Please bear in mind that as open-source community software, availability of the maintainers might be limited.

10.3 Engagements

DataJoint was originally developed by working systems neuroscientists at Andreas Tolias' Lab at Baylor College of Medicine to meet the needs of their own research.

Below is a partial list of known DataJoint users. Please let us know if you would like to add another lab or make a correction.

10.3.1 Multi-lab collaboratives

- 1. International Brain Laboratory
- 2. Mesoscale Activity Project
- 3. IARPA MICrONS
- 4. Princeton U19 Project
- 5. UCSD U19 Project "Reverse Engineering the Brain Stem Circuits That Govern Exploratory Behavior"

10.3.2 Invidiual Labs

- 1. Tolias Lab (Andreas Tolias), Baylor College of Medicine
- 2. Siapas Lab (Athanassios G. Siapas), California Institute of Technology
- 3. Svoboda Lab (Karel Svoboda), Janelia Research Campus
- 4. Li Lab (Nuo Li), Baylor College of Medicine
- 5. Busse Lab (Laura Busse), Ludwig-Maximilians-Universität München, München, Germany
- 6. Katzner Lab (Steffen Katzner), Ludwig-Maximilians-Universität München, München, Germany
- 7. Sinz Lab (Fabian Sinz), Wilhelm Schickard Institute for Computer Science, Cyber Valley Initiative, University Tübingen
- 8. Berens Lab (Philipp Berens), Werner Reichardt Centre for Integrative Neuroscience, Tübingen, Germany
- 9. Euler Lab (Thomas Euler), Werner Reichardt Centre for Integrative Neuroscience, Tübingen, Germany
- 10. Bethge Lab (Matthias Bethge), Werner Reichardt Centre for Integrative Neuroscience, Tübingen, Germany
- 11. Shcheglovitov Lab (Alex Shcheglovitov) University of Utah
- 12. Moser Group (May-Britt Moser and Edvard Moser), Kavli Institute for Systems Neuroscience and Centre for Neural Computation, Norwegian University of Science and Technology (NTNU), Trondheim, Norway
- 13. Seung Lab (Sebastian Seung), Princeton University
- 14. Mouse Motor Lab (Mackenzie Mathis), Rowland Institute at Harvard University
- 15. Harvey Lab (Christopher Harvey), Harvard Medical School
- 16. Angelaki Lab (Dora Angelaki), New York University

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- 17. Smirnakis Lab (Stelios Smirnakis), Harvard Medical School
- 18. McGinley Lab (Matthew McGinley), Baylor College of Medicine
- 19. Reimer Lab (Jacob Reimer), Baylor College of Medicine
- 20. Wang Lab (Fan Wang), Duke University
- 21. Applied Physics Laboratory, Johns Hopkins University