Introduction to Workflows

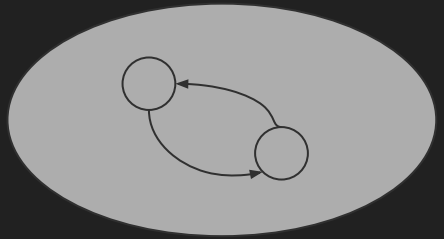
CMSE 890-402

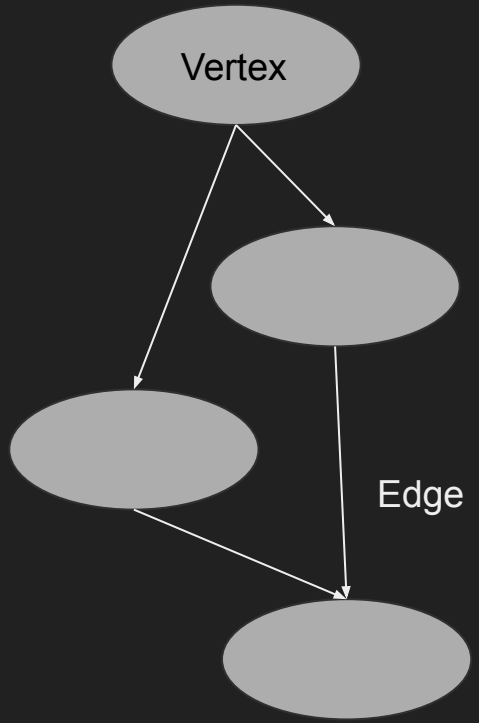
What is a workflow?

- Data In -> Process - > Result Out
- y = f(x) is a workflow!
- Recording data from an experiment and plotting it is a workflow
- Downloading data and changing its format is a workflow
- Workflows can be described as a *Directed Acyclic Graph*

Directed Acyclic Graph (DAG)

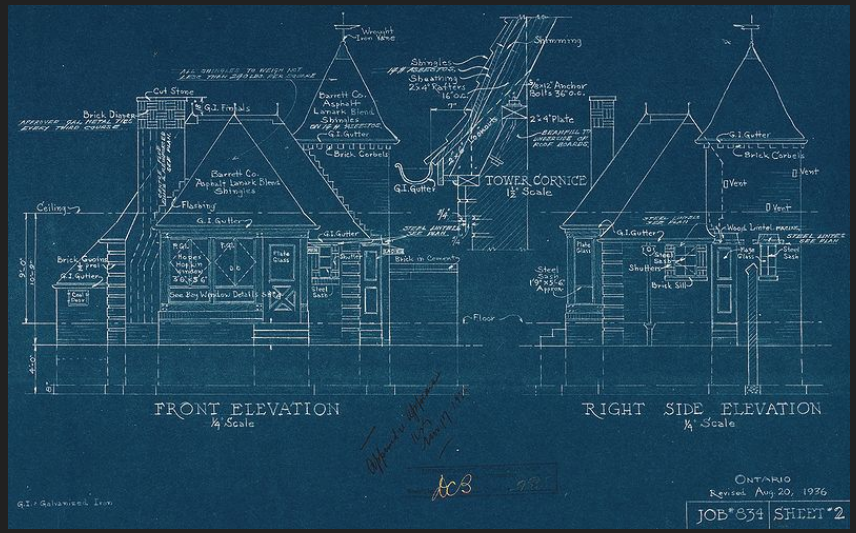
- Flowchart that goes in *one* direction
- Consists of *vertices* and *edges*
- Edges follow an *orientation*
- Edges do not return to a previous vertex (no *cycles*)
- Cycles can be encapsulated in a vertex (“condensation”)





Why workflows are important

- Describe the scientific process
- Break work into manageable steps
- Provide a blueprint for future work
- Track data sources



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Why automation matters

- Reliability
  - Not prone to human error
- Reproducibility
  - Does the same thing every time
- Sustainability
  - Does not need human interaction to complete
- Speed
  - Does not have to wait for a human to complete

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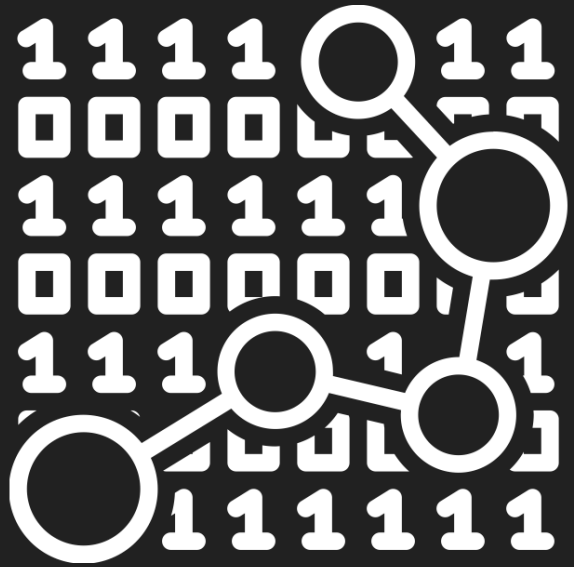
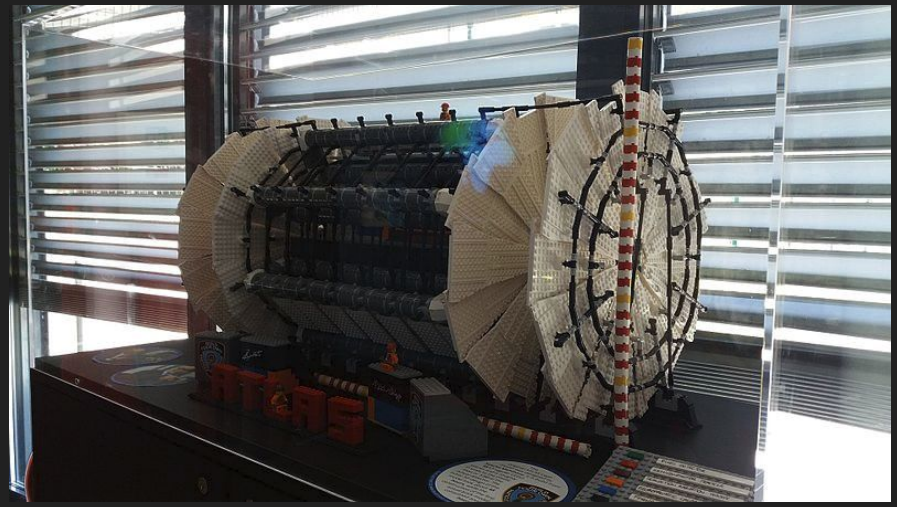
What computational workflows do

- Data processing!
  - Acquisition
  - Transformation
  - Reduction
  - Merging
  - Analysis
  - Presentation



Data Acquisition

- Experimental equipment
- Download from a server
- Result from a simulation
- Result from a previous workflow step



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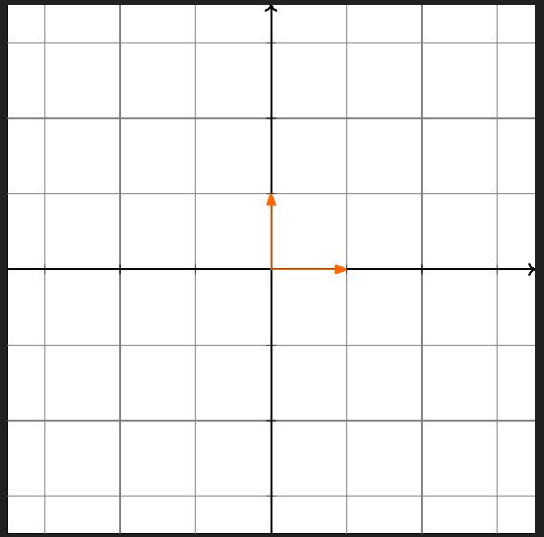
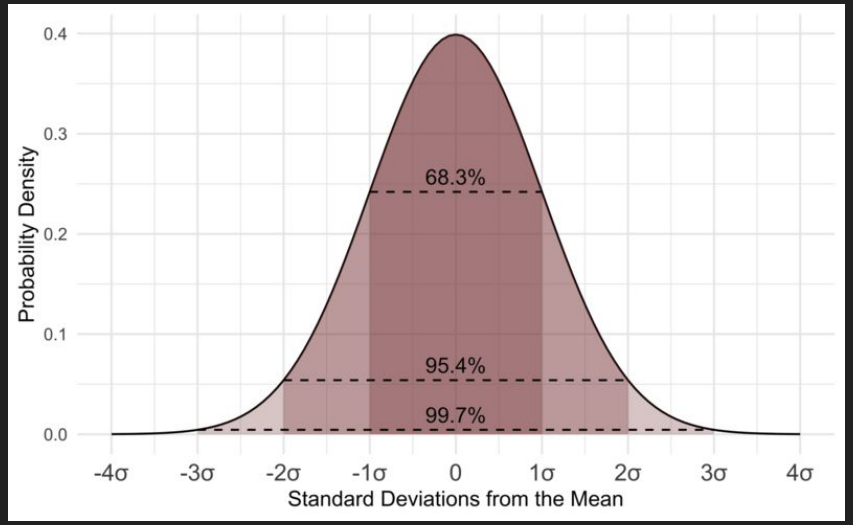
Data Transformation

- Rotate an image
- Convert a file format
- Transpose a table



Data Reduction

- Compute statistics from a column
- Extract individual frames from a video
- Cut out noise from audio
- Extract citations from text



Data Merging

- Add columns to a table
- Put tables into a database
- Collect images into a video
- Place text into a single document

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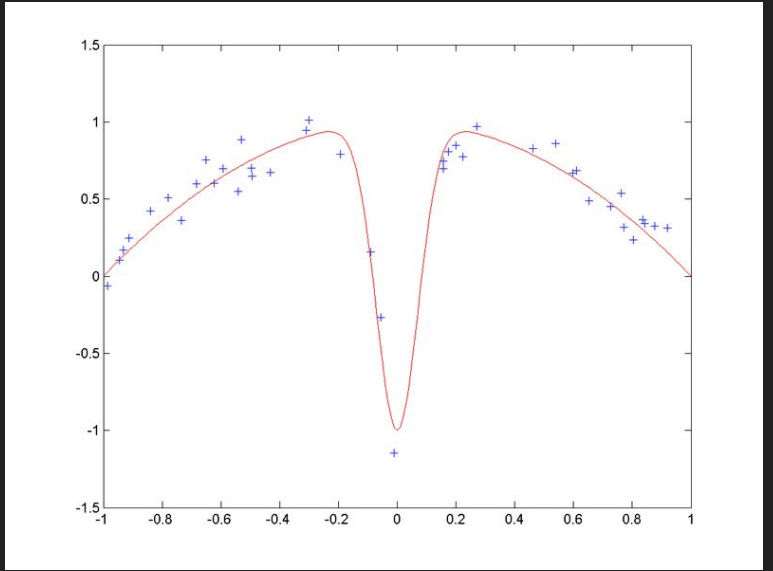
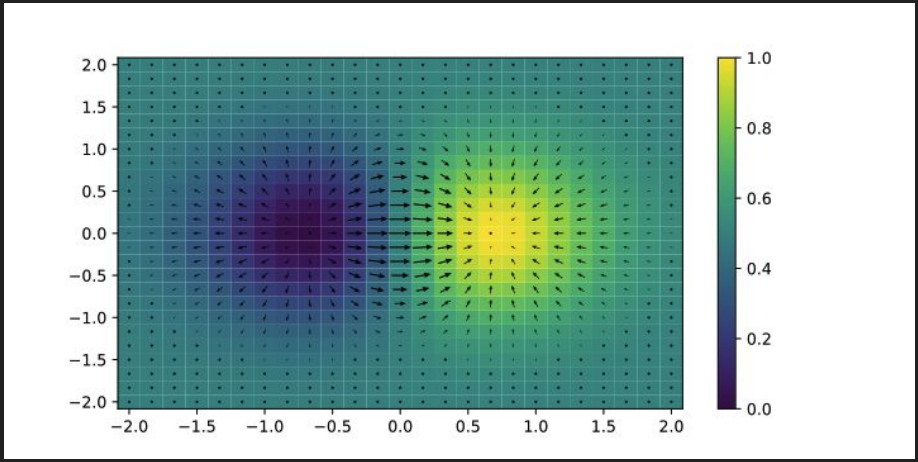
Data Analysis

- Compute statistics from multiple sources
- Extract interesting features
- Compare a model to an observation



Data Presentation

- Produce a plot from data
- Output a table in a human readable format
- Render an animation



How to build a computational workflow

1. Design: **The most difficult and important step**
    a. Break workflow into modules
    b. Connect modules together
2. Choose software description
    a. General scripting language (bash, Python etc.)
    b. Workflow description language (SnakeMake, NextFlow etc.)
3. Construct software description

Dataflow diagrams (DFDs)

- Created in the 1970s (*Structured Design*, Yourdan & Constantine)
- Common in business analysis
- Multiple systems of symbols
  - Yourdon and Coad
  - Yourdon and DeMarco
  - Gane and Sarson
- Four components:
  - External entity
  - Process
  - Data store
  - Data flow

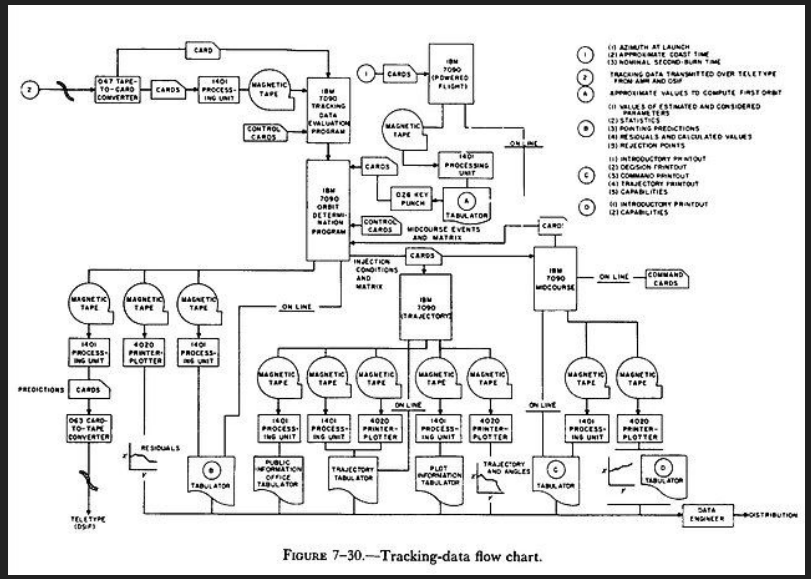


FIGURE 7–30.—Tracking-data flow chart.

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Symbols and Connectors

- Data flow connectors are DAG edges
- Symbols are DAG vertices
- DFDs do not have to be DAGs
  - But we are using them in this way
- Different sets of symbols can be used (but mean the same things)

Yourdon/Coad symbols (*Object Oriented Design*, Coad and Yourdon 1991)

Design a Dataflow Diagram for one of these projects

- Astronomy
- Genetics
- Linguistics
- **Use at least one of each symbol**
- **The DFD should consist of at least 5 vertices**
- **The DFD should follow the properties of a DAG**
  - One data flow direction
  - No cycles
- Online software option: https://www.smartdraw.com/data-flow-diagram/data-flow-diagram-software.htm

Astronomy feature detection

- Download multiple catalogs from different astronomy databases
- Merge the catalogs by object
- Plot data about the objects
- Detect important features on the plot
- Save the plot

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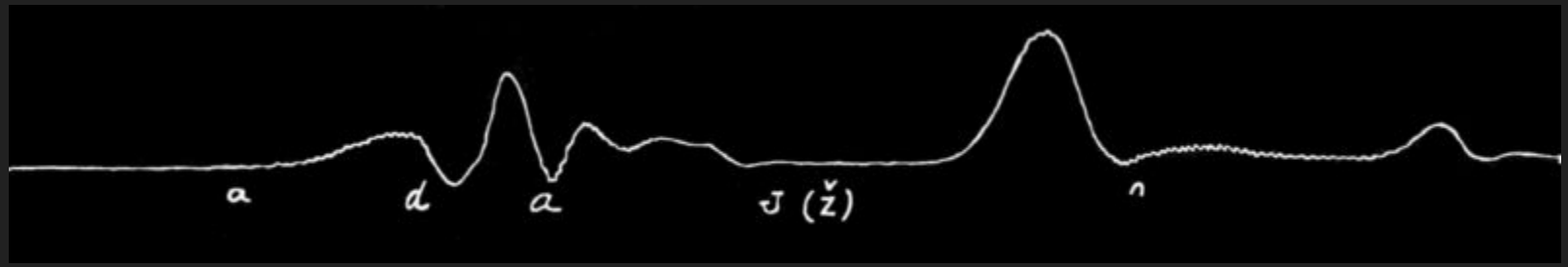
Genetics database matching

- Collect genetic data from genetics machines for multiple individuals
- Convert the data format
- Clean the data
- Match the data to an existing database
- Save the matched table

Audio linguistics study

- Obtain audio files from multiple recordings
- Validate audio files
- Process audio (e.g. remove noise)
- Extract linguistics information
- Save linguistics information



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Homework

- Finish and submit DFD
  - Save, photograph, or scan your DFD and email it to me (make sure it is legible!)
- Create a GitHub account if you have not already and email it/post in Teams

Pre-class 2:

- Complete the Git & GitHub fundamentals assignment
- Link will be emailed: https://classroom.github.com/a/x_9NcSvv