Machine Learning Foundations
Data Structures & Algorithms

Computer Science
Techniques for Developing the
Most Efficient Data Models

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jonkrohn.com/talks

github.com/jonkrohn/ML-foundations

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Data Structures & Algorithms

Slides: jonkrohn.com/talks

Code: github.com/jonkrohn/ML-foundations

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The Pomodoro Technique

Rounds of:

- 25 minutes of work
- with 5 minute breaks

Questions best handled at breaks, so save questions until then.

When people ask questions that have already been answered, do me a favor and let them know, politely providing response if appropriate.

Except during breaks, I recommend attending to this lecture only as topics are not discrete: Later material builds on earlier material.

POLL

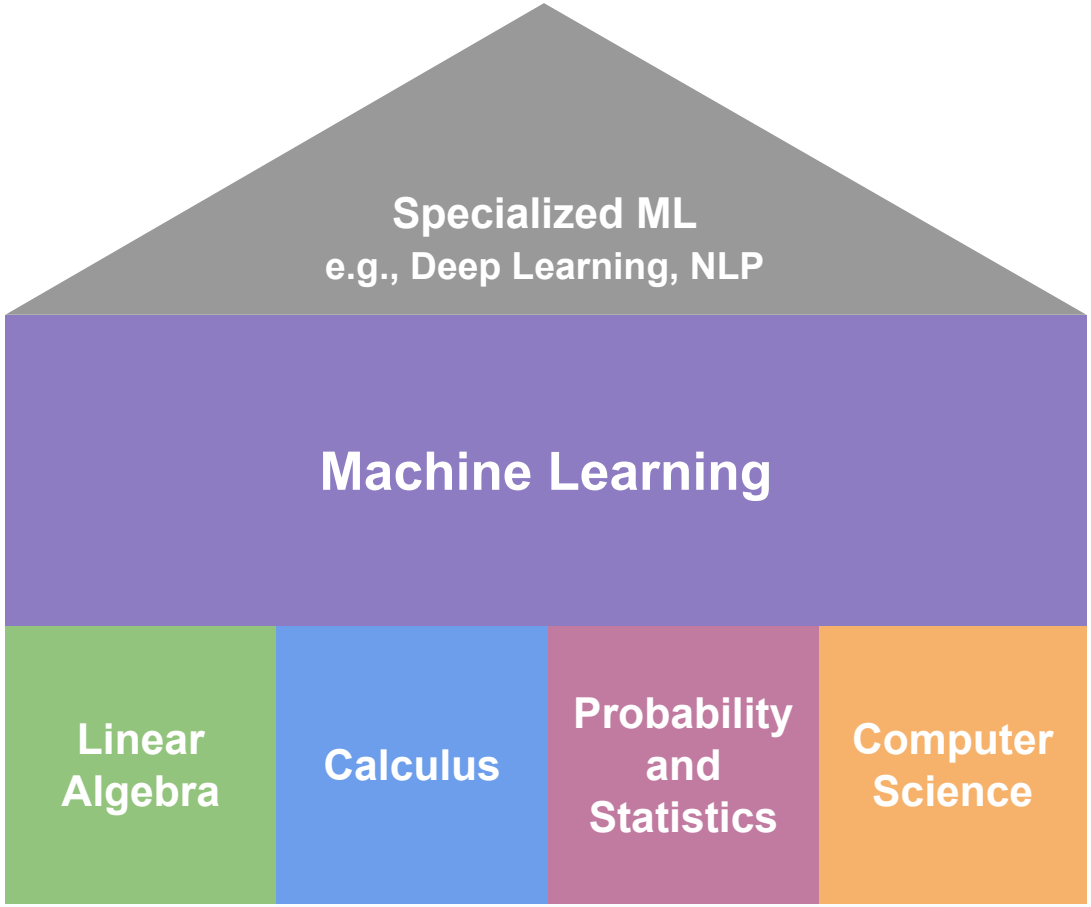
What is your level of familiarity with data structures and algorithms?

- Little to no formal exposure
- Some understanding of the theory
- Deep understanding of the theory

POLL

What is your level of familiarity with Machine Learning?

- Little to no exposure, or exposure to theory only
- Experience applying machine learning with code
- Experience applying machine learning with code and some understanding of the underlying theory
- Experience applying machine learning with code and strong understanding of the underlying theory


Specialized ML
e.g., Deep Learning, NLP
Machine Learning
Linear Algebra
Calculus
Probability and Statistics
Computer Science
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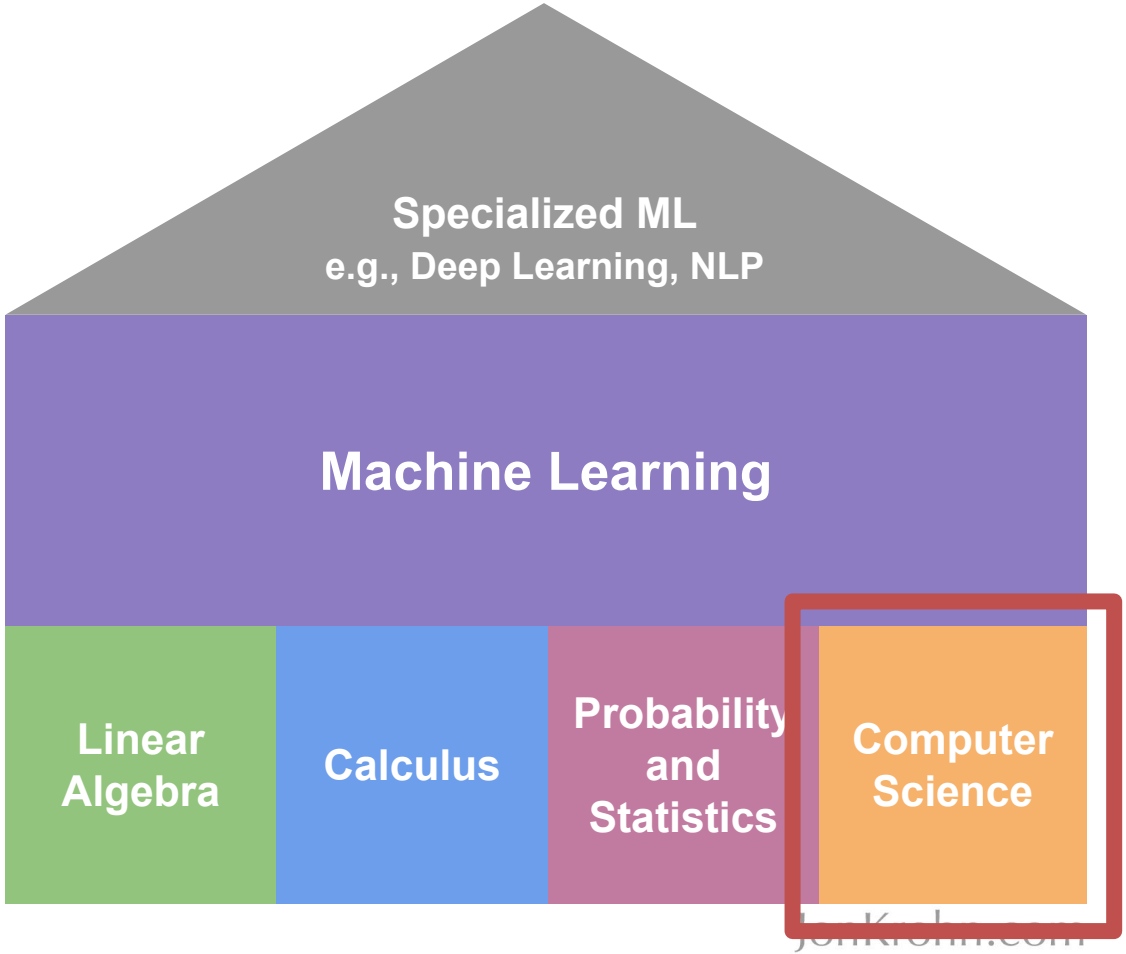

Specialized ML
e.g., Deep Learning, NLP
Machine Learning
Linear Algebra
Calculus
Probability and Statistics
Computer Science

ML Foundations Series

Algorithms & Data Structures **builds upon** and is **foundational for**:

1. Intro to Linear Algebra *(arrays/tensors)*
2. Linear Algebra II: Matrix Operations
3. Calculus I: Limits & Derivatives *(graphs)*
4. Calculus II: Partial Derivatives & Integrals *(ROC AUC)*
5. Probability & Information Theory *(random sampling)*
6. Intro to Statistics
7. **Algorithms & Data Structures**
8. Optimization

Data Structures & Algorithms

1. Intro to Data Structures and Algorithms
2. Lists and Dictionaries
3. Trees and Graphs

Data Structures & Algorithms

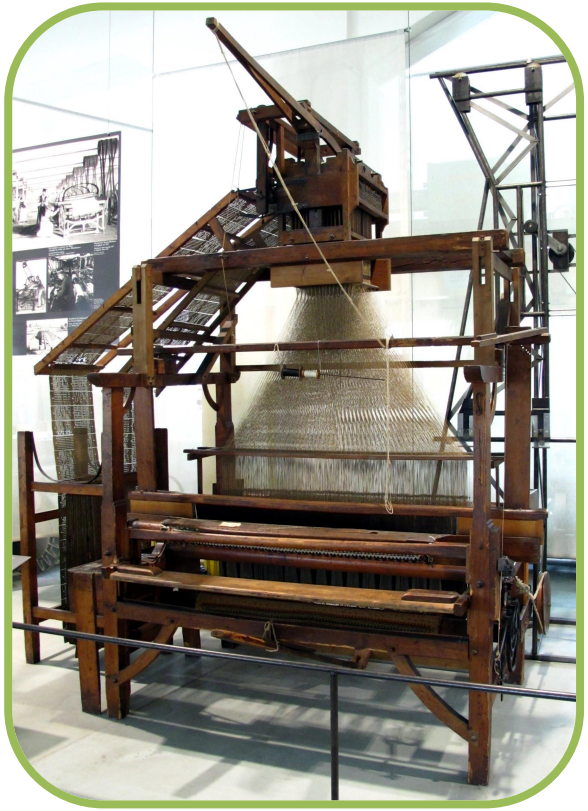
1. **Intro to Data Structures and Algorithms**
2. Lists and Dictionaries
3. Trees and Graphs

Segment 1: Intro to DSA

- A Brief History of Data
- A Brief History of Algorithms
- Applications of DSA to ML
- “Big O” Notation for Time and Space Complexity

Brief History of Data

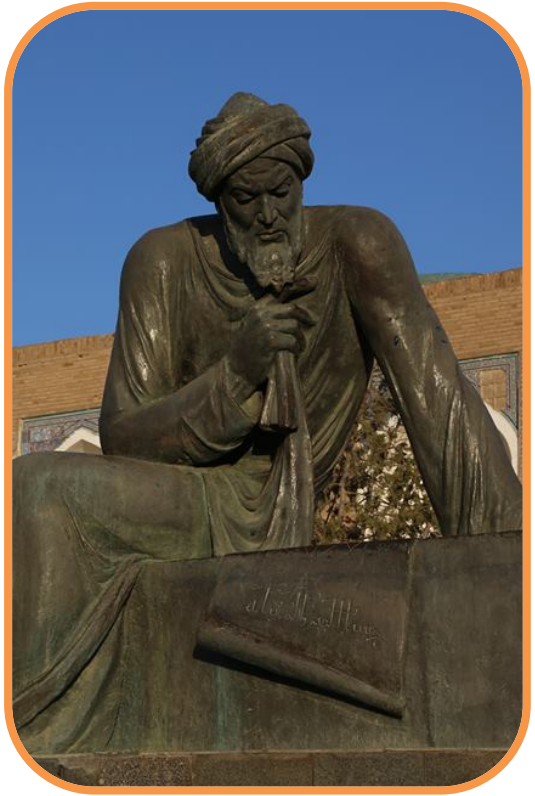
- **Data** are units of information
  - 18th c. from Latin *datum*, “something given”
- 4b-year-old **RNA** (Earth is 4.5b) → DNA
- 7500 BCE **Mesopotamia**: clay accounting tokens
- 3400-3100 BCE **Sumeria**: written clay records
- Punch cards / punched tape
  - Since 1725: **used in mechanical looms**
  - 1950s to 1970s: common in computing
- 1946: “Data” term in computing
- 1954: “Data processing” term
- Today: hard disk drives, optical discs, mag. tape
- **Data structures**: lists, dictionaries, objects, etc.



commons.wikimedia.org/wiki/File:DMM_29263ab_Jacquardwebstuhl.jpg

Brief History of Algorithms

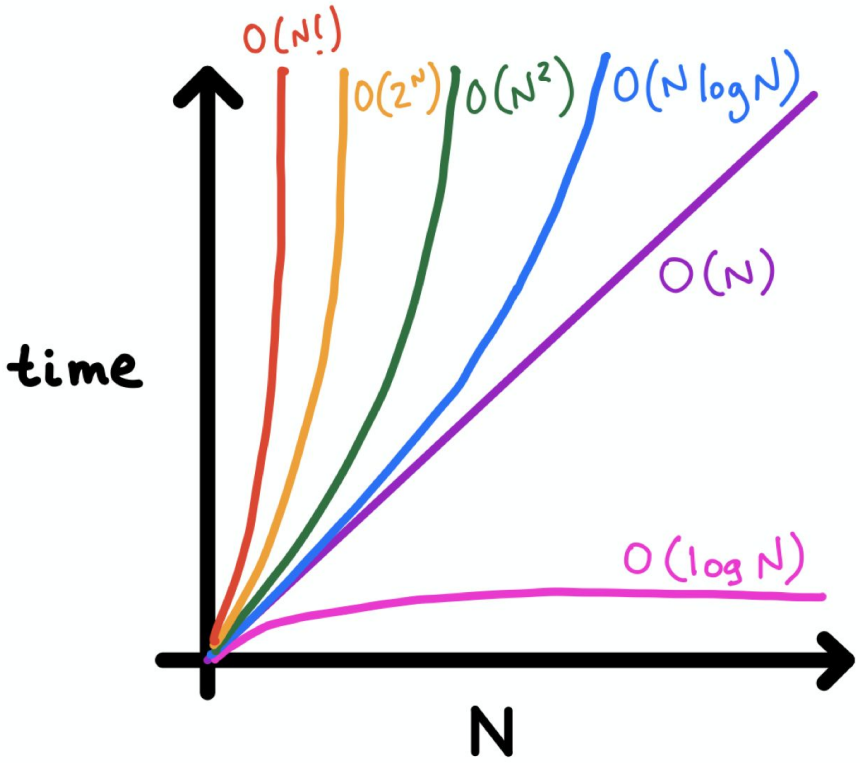
- Unambiguous instructions for solving problem or performing computation
- From initial state (e.g., input) go thru finite well-defined states ‘til final state (e.g., with output)
- Can incorporate random probabilities so not necessarily deterministic, e.g., SGD, MCMC
- Arithmetic algos (e.g., for division) are ancient:
  - Babylonians (2500 BCE), Egyptians (1500 BCE)
  - Greeks’ sieve of Eratosthenes, Euclidean algo
- 9th c. CE: Arab cryptographic algos
  - Word from **Muḥammad ibn Mūsā al-Khwārizmī**
- 1930s: Modern concept formalized
  - Gödel, Turing, many others



Applications of DSA to ML

- Ensure you're using the correct data structure for the situation
- Be thoughtful about time/space complexity considerations
  - Model training
  - Model deployment in production
  - Software 2.0: ML/DL algos typically have constant time/space complexity, assuming fixed batch size
- Conceptualize and implement ML models as graphs
  - TensorFlow
  - PyTorch
  - "Knowledge graphs"

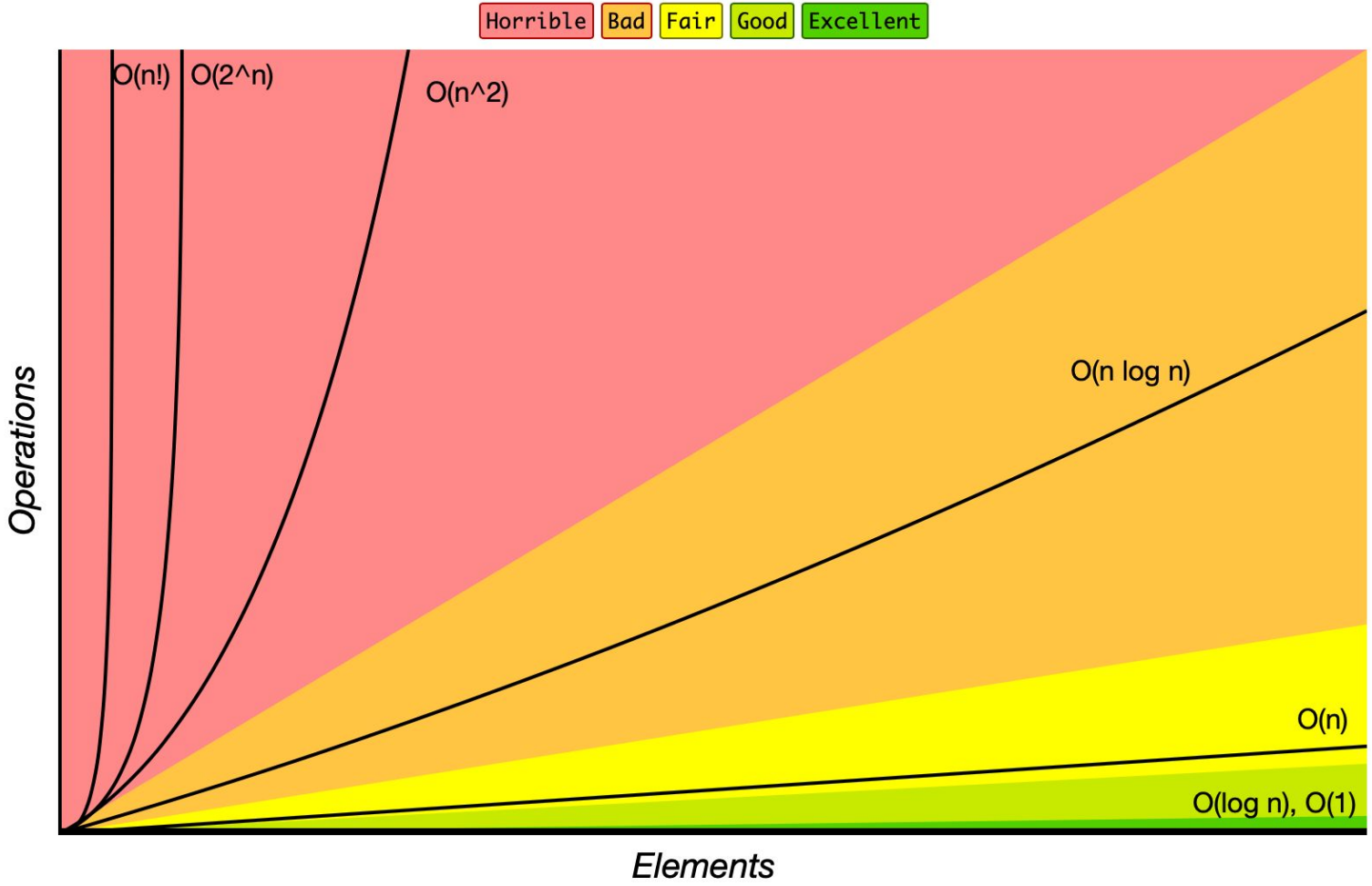
“Big O” (Order of Complexity) Notation



Hands-on code demo: `7-algos-and-data-structures.ipynb`

Common Runtimes

Big O	Nickname	Example(s)
O(1)	constant	first item in list; is list length odd or even
O(n)	linear	search linearly through list; print every item in list
O(n^2)	polynomial	loop nested within loop; bubble sort
O(log n)	logarithmic	binary search
O(2^n)	exponential	count combinations of list elements
O(n log n)		mergesort; quick sort
O(n!)	factorial	generate all permutations of a list; simple Traveling Salesman solution



bigocheatsheet.com

Best vs Worst Case

- Variance in Big O possible based on data
- E.g., for quick sort:
  - Best case is $O(n)$ if all items are equal
  - Worst case is $O(n^2)$ if "pivot" is always largest item
  - Expected case (a.k.a. average case) is $O(n \log n)$

Further Big O Detail

- Given n, can then select appropriate algo based on Big O
- Can equally be applied to space complexity
- Drop constants: $O(2n) \rightarrow O(n)$
- Retain only dominant term: $O(n^2 + n) \rightarrow O(n^2)$
- May involve multiple variables, e.g.: $O(n^2 + m)$, $O(nm)$

Exercise: Estimate the Google Colab runtime of the `element_multiplier()` method with a list of length of a million.

Data Structures & Algorithms

1. Intro to Data Structures and Algorithms
2. **Lists and Dictionaries**
3. Trees and Graphs

Segment 2: Lists and Dictionaries

- List-Based Data Structures
- Searching and Sorting
- Set-Based Data Structures
- Hashing

Lists

- An *ordered* **collection** of items
- Can specify item by its index
- List-based data structures:
  - Arrays
  - Linked lists
  - Stacks
  - Queues
  - Deques

Hands-on code demo

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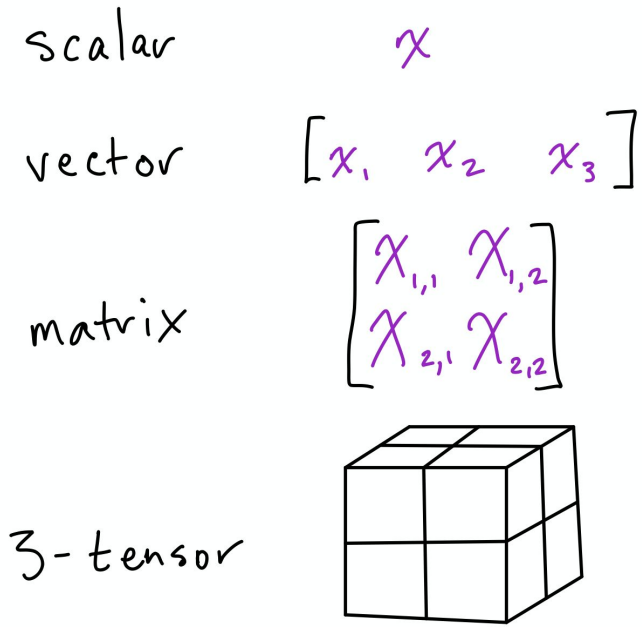
Arrays

- **Lists** we can apply math operations on
- Used extensively in *ML Foundations*
- Most important data structure in ML; commonly used for:
  - Tensors
  - Holding data for training models (e.g., input from HDF5, CSV)
  - Preprocessing data
  - Receiving model outputs
  - Calculating summary metrics
  - Plotting
- Typically, all elements are same type
  - Most often numeric in ML



Hands-on code demo

Linked Lists

- Similar to (vector) array, but elements aren't indexed
  - Instead, elements in linked lists (called *nodes* or *units*) store which element in list is next (nodes are "linked")
- Makes adding or removing elements anywhere in the list computationally efficient (O(1))
  - Note, however, that accessing elements is O(n) in worst case
- Not a built-in Python data structure
- Not especially common in ML; could be used for parsing lists with undefined length then converted to array before input into ML model

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Doubly-Linked Lists

- Nodes store which is next *and which precedes it*
- Enables traversal in either direction
- Same time complexities as singly-linked

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Stacks

- Behave like real-world stacks
  - I.e., LIFO: "*Last in, first out*"
- E.g., imagine stacking a deck of cards:
  - Put (*push*) one card on table
  - Stack (*push*) another on top, then push a third
  - To access cards, top card is retrieved (*pop*-ped) first
  - Last to pop is card placed on table first
- Push and pop are both O(1)
- Useful anytime most recent items will be needed before earlier ones
  - E.g., social media newsfeed
- Rare to use directly in ML
  - Could be used under hood to implement programming languages

Hands-on code demo

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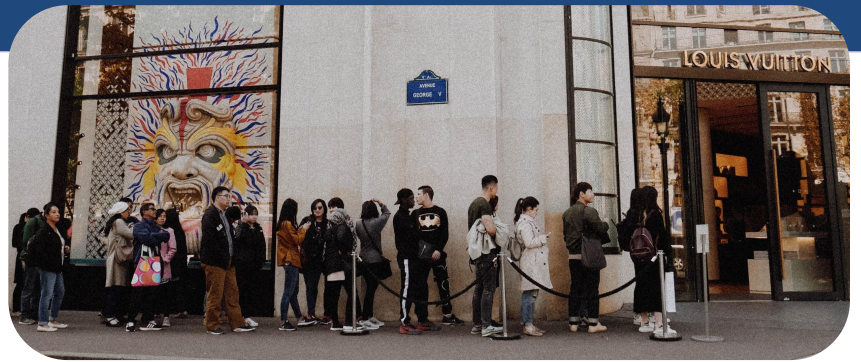
Queues



- Behave like real-world queues (“lines” in U.S./Canada)
  - I.e., FIFO: “*First in, first out*”
- **Head**: first/oldest element
- **Tail**: last/newest
- *Enqueue*: add element to tail
- *Dequeue*: remove element from head
- *Peek*: access head element but leave it in queue

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Deques

- *Double-ended queue*
- Can enqueue or dequeue *from either end*
- In other words, a generalized:
  - stack (enqueue and dequeue from same end)
  - *or* queue (enqueue and dequeue from opposing ends)

Hands-on code demo:

jonkrohn.com/DQN

unsplash.com/photos/sLtmudkaL9M

Searching & Sorting

- Will not typically write search/sort algos in ML
- Exemplary to demo:
  - Time complexity
  - Space complexity
  - Typical time/space tradeoff
- Helpful for any ML pipelines, incl.:
  - Data capture
  - Preprocessing
  - Training
  - Deployment

Hands-on code demo: `7-algos-and-data-structures.ipynb`

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Maps

- Have *key-value structure*
  - **Key** (name) indicates where **value** is
  - ...like real-world map shows where place is
- A.k.a. **dictionary** (e.g., in Python)
  - ...like how name shows where definition is
- Used frequently in NLP: integer index of words

Hands-on code demo:

jonkrohn.com/film-classifier

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Sets

- *Unordered* collection of items
  - Akin to having a bag of stuff
- No elements can be duplicated
- **Maps** are a **set**-type data structure
  - The keys are a formal set
    - *No duplicate keys*

Hands-on code demo: `7-algos-and-data-structures.ipynb`

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Hashing

- **Hash functions** enable set searching in constant time, O(1) !!!
- This contrasts starkly with:
  - List-based structures (or unhashed sets), where search is linear time O(*n*)
  - Or, at best, O(log *n*) with binary search of pre-sorted list
- *Well, that's crazy pants… how does it work?*

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Hashing

- Ultimate trick is that *indexed* data structures (e.g., with *sequential* integers) have O(1) time search/retrieval
- So, what we need is a way to convert dictionary values into an index…
- *This* is what hash functions do:
  - Input some value
  - Output a *hash value*
    - Used as indices of *hash table*

Hands-on code demo

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Hashing in ML

- Integer-string maps in NLP
- Efficiently loading large training data set
- Any production data access
  - Use instead of arrays
  - E.g., cached, pre-computed features

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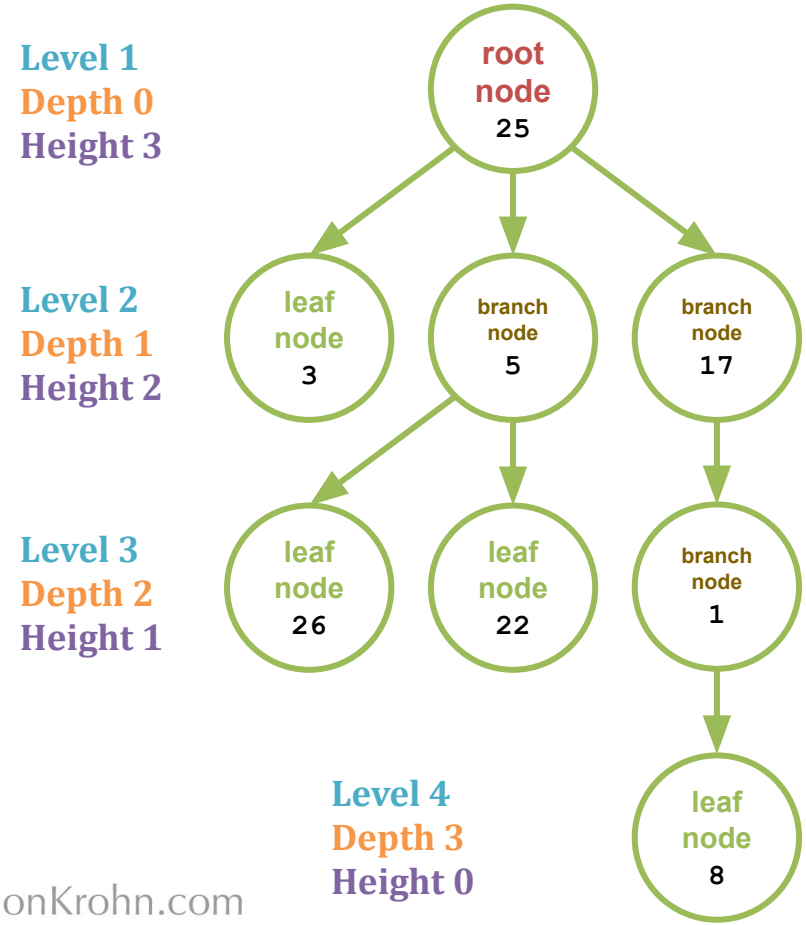
Data Structures & Algorithms

1. Intro to Data Structures and Algorithms
2. Lists and Dictionaries
3. **Trees and Graphs**

Segment 3: Trees and Graphs

- Trees
  - General Terminology
  - Decision Trees
  - Random Forests
  - Gradient-Boosting (XGBoost)
- Graphs
  - General Terminology
  - Directed vs Undirected Graphs
  - Directed Acyclic Graphs
- Resources for Further Study

Trees



- Extension of linked list
- Start at *root node*
- Add *branch* (aka *internal*) *nodes*
- All nodes must be connected
- Each *child* node has one *parent*
- Childless nodes: *leaf* or *external*
- No cyclic connections
- Tree "height" = n_{levels} - 1 (i.e., root)

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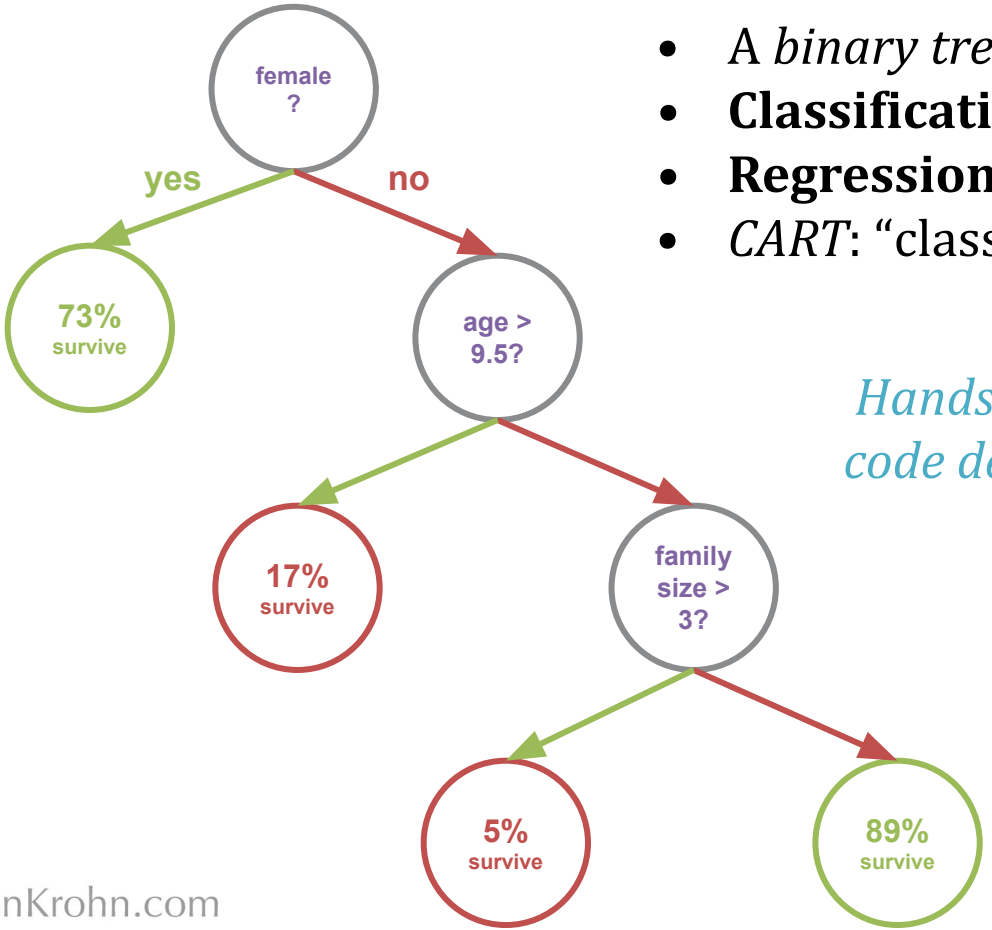
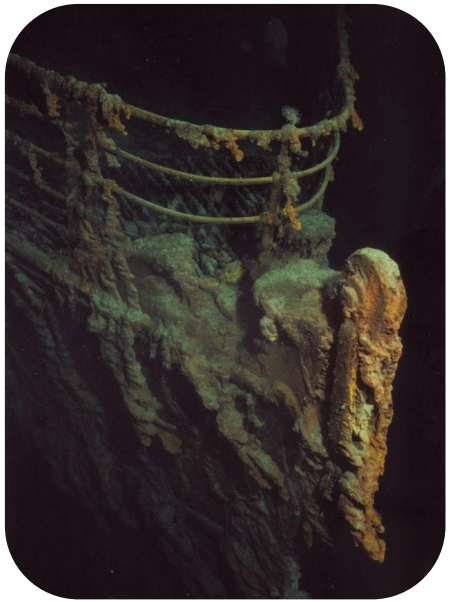
Decision Trees



- A *binary tree* ("max. 2 child nodes per parent")
- **Classification tree**: predict categorical outcome
- **Regression tree**: predict continuous outcome
- *CART*: "classification and regression trees"

Hands-on code demo



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Random Forests

- Ensembles tend to outperform any single model
  - Less prone to overfitting relative to single decision tree
- Repeat this stochastic process, e.g., 100 times:
  - Use sampling with replacement to "bootstrap aggregate" (*bag*) a "new" sample of training data
  - Fit a decision tree; when splitting each node:
    - Use all of the features or,
    - Randomly subset the feature set
- Averaging diverse trees together tends to:
  - Reduce variance
  - Cancel out errors

Hands-on code demo

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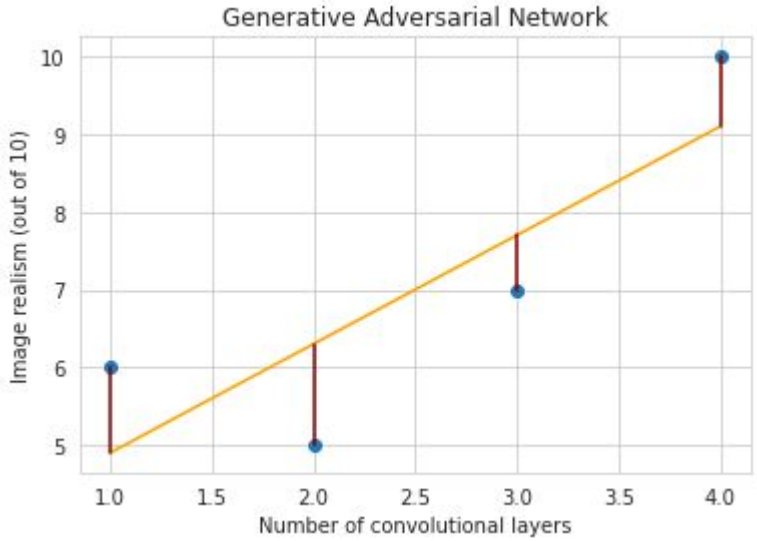
Gradient-Boosted Decision Trees



- Also an ensemble method
- However, trees are *not* independent
- 1st tree is a regular ol' decision tree
- 2nd tree trained on 1st's residuals (errors)
- 3rd tree trained on 2nd's residuals
- …
- Repeat until no more improvements
- Alongside deep learning, a common competition-winning approach

Hands-on code demo

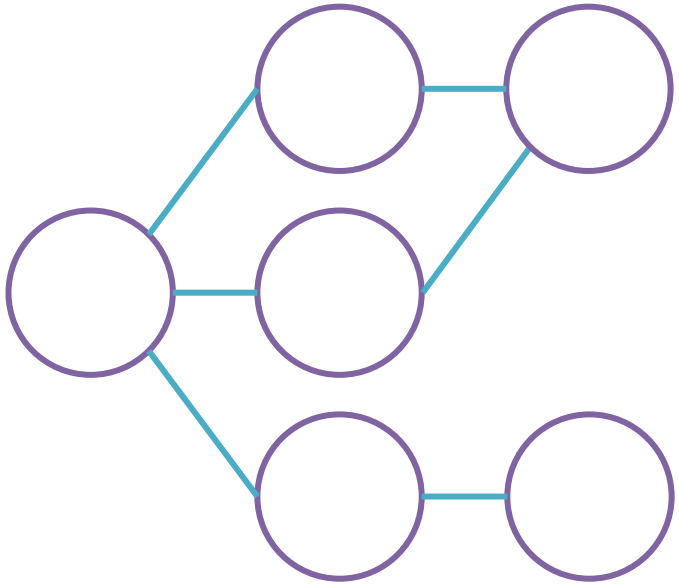
Other Tree Concepts

(Largely irrelevant to ML, so a quick skim only)

- More considerations during search relative to 1D data structure
  - Generally search has O(n) time complexity
- Likewise, data deletion or insertion have extra considerations, e.g.:
  - Handling children after deleting parent node
- **Binary search tree** (BST):
  - Binary tree wherein larger values are to the right of smaller ones
  - Typically much quicker O(log n) search
    - Except in O(n) worst case (i.e., *unbalanced*, a high level:node ratio)
  - "Self-balancing" BSTs automatically structured for O(log n) traversal
    - Used for ***k*-nearest neighbor** clustering algos
- **Heaps**: in "max heaps", parent has value > childrens'; opposite in min heap
  - ~Reduced time complexity, e.g., average O(n/2) search for binary heap

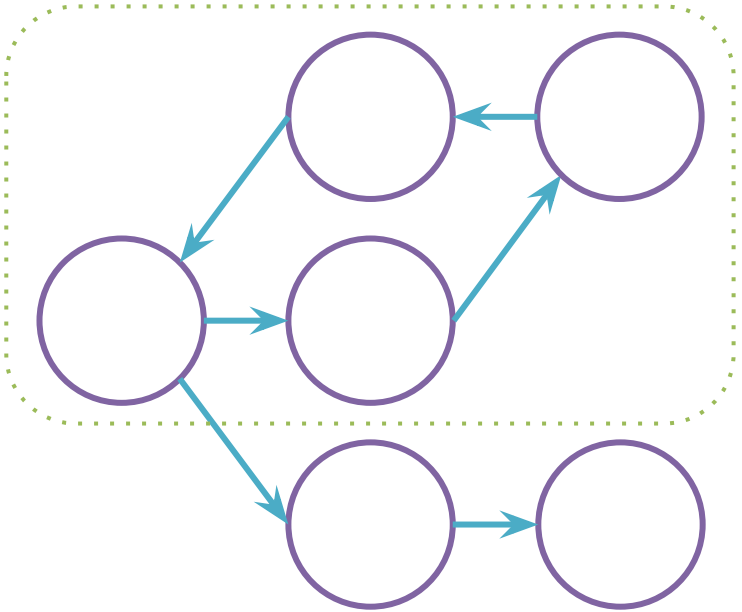
Graphs (a.k.a. Networks)

- **Nodes** (or *vertices*) are connected by **edges**
- Edges aren't necessarily "directed"
- Nodes typically store data, but edges can too
  - E.g., social network: Jane and Sal have met 25 times
- No general limitation on # of edges per node
- Generally, no particular root note
- Trees, however, are a specific type of graph



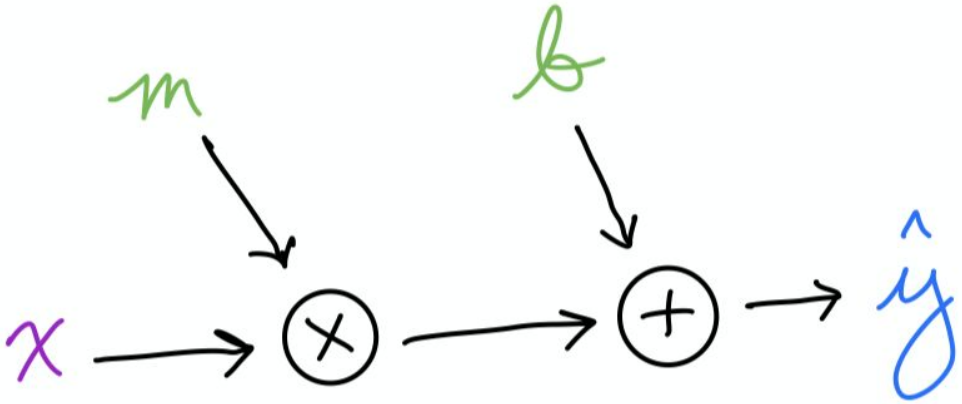
Directed Graphs

- **Edges** have direction
- Can convey temporal sequence through nodes
  - E.g., specifying a calculation or algo
- Can have **cycles**
  - ...which can lead to infinite loops



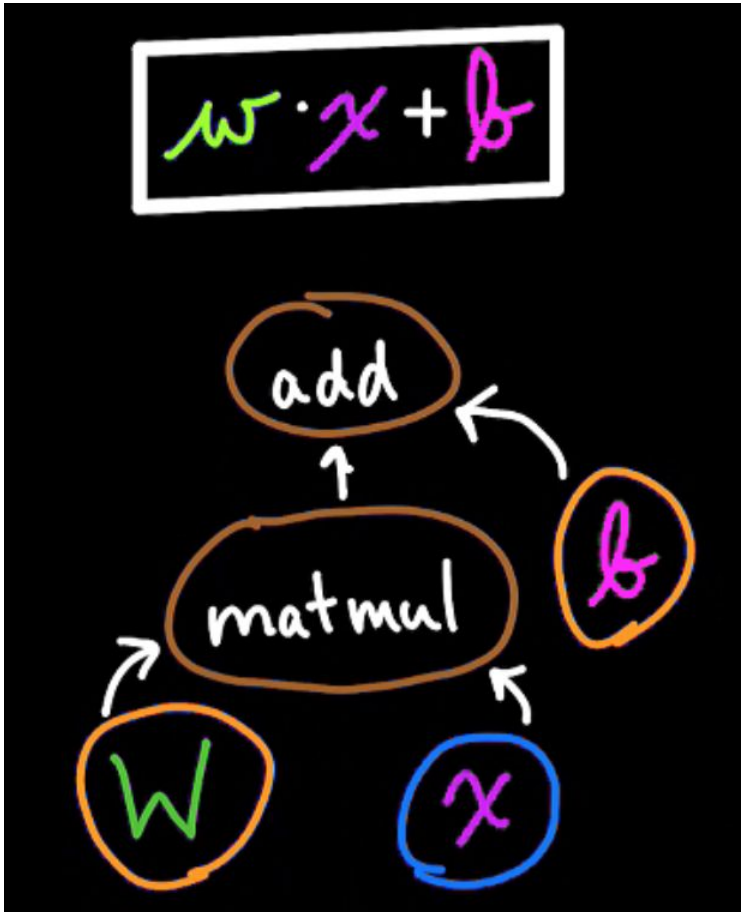
Directed *Acyclic* Graphs (DAGs)

- Directed graph with no cycles
- Line equation $y = mx + b$ as DAG (from *Calc I* and *Calc II*)
  - Nodes are input, output, parameters, or operations
  - Edges are tensors (but non-operation nodes can be too)



Hands-on code demo: `single-point-regression-gradient.ipynb`

Dense Neuron Layer DAG



- Operation
- Placeholder tensor input
- Variable tensor input

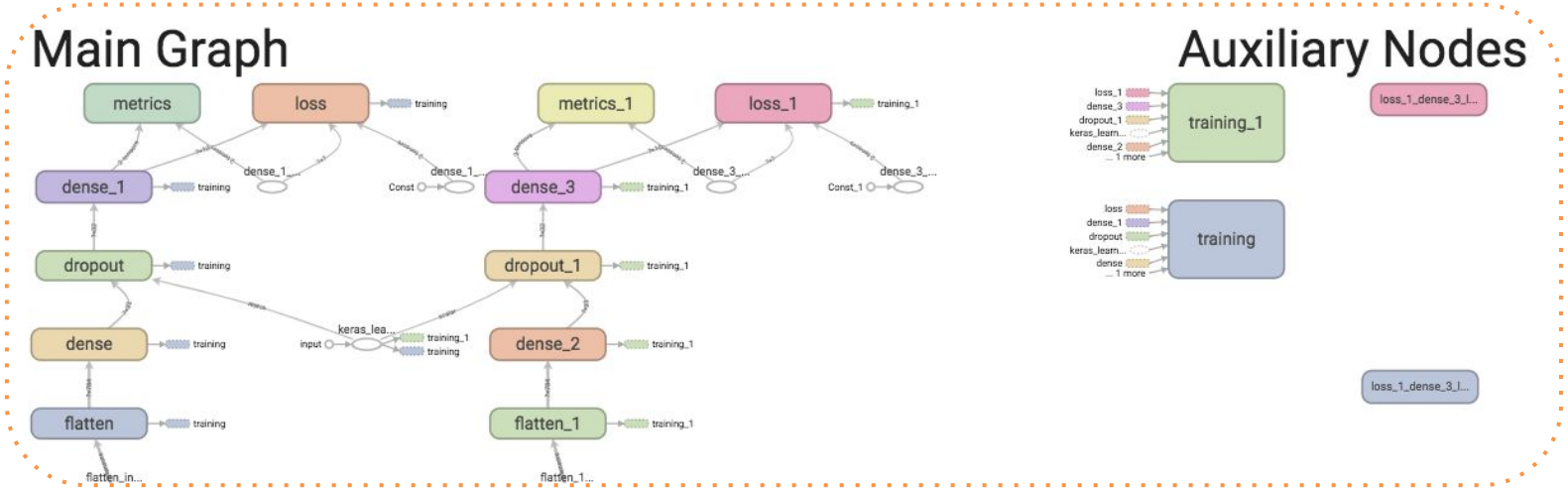
Hands-on code demos:

`jonkrohn.com/neurTF1`

`jonkrohn.com/deepTF1`

TensorBoard

- Compatible with TensorFlow: tensorflow.org/tensorboard
- ...and PyTorch: pytorch.org/tutorials/recipes/recipes/tensorboard_with_pytorch.html
- Detail on Graphs: tensorflow.org/tensorboard/graphs



Other Graph Concepts

(Largely irrelevant to ML, so a quick skim only)

Connectivity

- A graph can have subgraphs that are unconnected
- Two graphs can have the same number of nodes
  - One with more edges has relatively greater connectivity

Graph traversal

- *Depth-first search*: follow a given path as far as it will go
- *Breadth-first search*: priority is traversing adjacent nodes

Bonus: What about Pandas??

- Critical data structures in Python ML
- Not a traditional CS data structures
- **DataFrame**
  - 2D matrix array
  - Columns of independent types
- **Series**: 1D vector array
- Lots of:
  - Convenient data methods
  - Optimization

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Resources for Further Study

- Udacity *Data Structures & Algorithms in Python* course
  - Free
  - Clear, concise videos
  - Python exercises with interactive testing
- Sedgewick & Wayne (2011) *Algorithms* (4th ed.)
  - Free, standalone website to accompany textbook
    - Wonderful visualizations of theory
    - Note: Accompanying code's in Java
- Bhargava (2016) *Grokking Algorithms*
- Classic DSA computer science problems:
  - Shortest Path
  - Traveling Salesman
  - Knapsack

Next (Final) Subject: *Optimization*

- Ties the preceding seven subjects together
- How we descend gradients of cost w.r.t. model parameters
  - Granular, matrix-level operations
  - Quickly, abstractly with auto-differentiation libraries, e.g.:
    - PyTorch
    - TensorFlow
- “Fancy” optimizers common in deep learning, e.g.:
  - RMSProp
  - Adam
  - Nadam

POLL *with Multiple Answers Possible*

What other topics interest you most?

- Linear Algebra
- Calculus
- Probability Theory
- Statistics
- More Computer Science (e.g., algorithms, data structures)
- Machine Learning Basics
- Advanced Machine Learning, incl. Deep Learning
- Something Else

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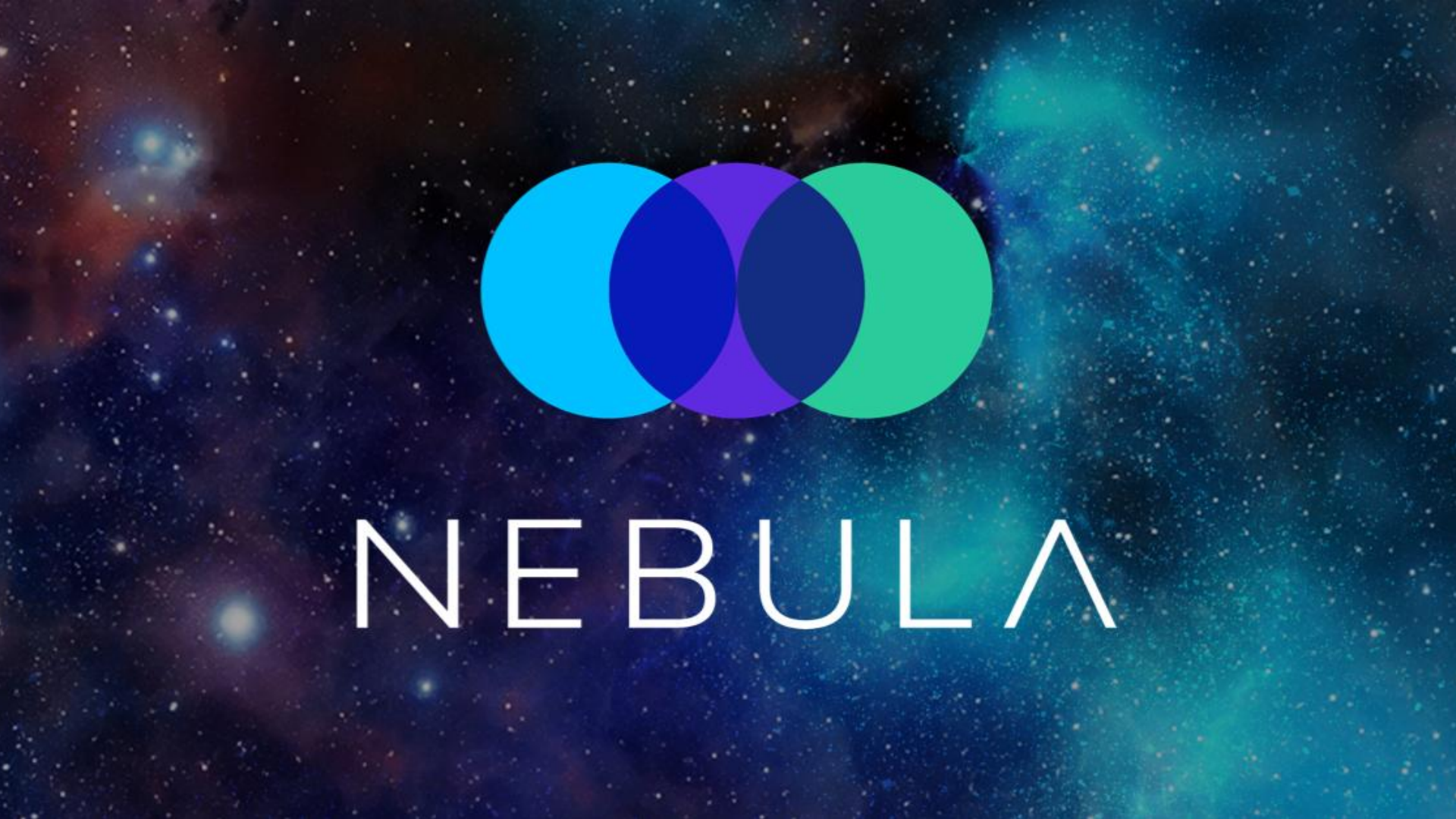
NEBULA

PLACEHOLDER
FOR:

5-Minute Timer

PLACEHOLDER
FOR:

10-Minute Timer

PLACEHOLDER
FOR:

15-Minute Timer