IntroML

6 July 2022

IntroML

Welcome

The ML ⇄ Science Colaboratory

Plan for the day

Agenda

9:10	Round of introductions
Morning	**Core ML Concepts** **ML & software ⁄ learning paradigms ⁄ neural networks**
~12:30	**LUNCH BREAK**
Afternoon	**Machine Learning in Practice** **project pipeline: data, models & evaluation ⁄ ML in Science**
	Hands-on: Define your ML project **question ⁄ learning task ⁄ dataset ⁄ evaluation**
16:00	Closing – feedback round

Practical aspects

- Lunch beans curry/chicken: interested?
- Pauses 2x15’ + 60’ lunch break
- Internet → eduroam, share laptop
- Toilet → right side of the exit

?! Questions welcome at any time

Slides, links, notebook and feedback at
mlcolab.org/**introml02-participants**

Round of introductions

Tübingen is a great place to form a community of practice and mutual support around ML and science.

Let's get to know each other! We can share

- Name & where you work
- Expectations from ML related to your research (1 sentence)

The ML ⇌ Science Colaboratory

@mlcolab

At the Cluster ML: new perspectives in science

EBERHARD KARLS UNIVERSITÄT TÜBINGEN

«Establish machine learning across disciplines at the University of Tübingen»

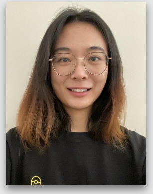
via ① cooperations — ② training — ③ scientific ML software

@sethaxen
Seth Axen

@elenasizana
Elena Sizana

@alpiges
Alexandra Gessner

@alvorithm
Álvaro Tejero



@HanqiZhou_Ivy
Hanqi Zhou

- **Part of the** Cluster ML in Science
- Scientists **like you**
  Astro, **atmospheric**, & **quantum physics**, environmental sciences, **neuroscience**, **genomics**, urban systems, int'l policy, **structural bio**…
- Let's work together!

Core Concepts in Machine Learning

Core Concepts in Machine Learning

What is ML?

What problems does it solve?

Games and the nature of intelligence

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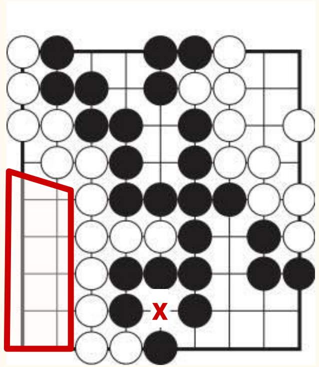
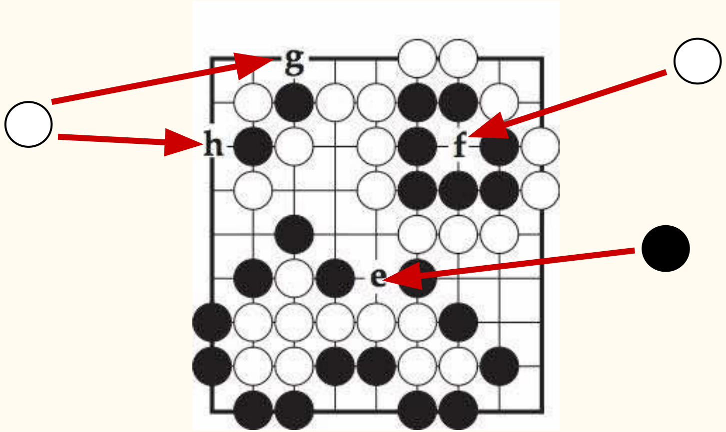
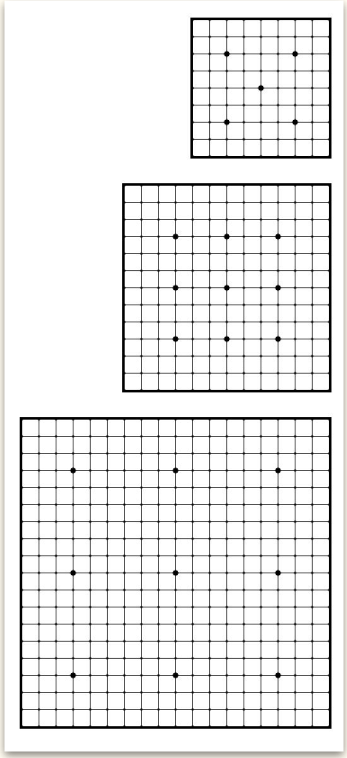


- form territories by surrounding empty areas
- capture by completely surrounding (*prisoners*) x

Points = crossings + prisoners





Real go is 19x19

British Go association

A surprising move

See also AlphaGo - The Movie

Definition of Machine Learning

Learning

Improving with experience at some task

- Improve over **task** T,
- with respect to **performance** measure M (**metric**)
- based on **experience** D (**data**)

e.g., Learn to play Go

- T: playing Go,
- M: points at the end of the game
- D: database of past games

AlphaGo: Deep-Learning powered (ML) Monte-Carlo Tree *Search*.

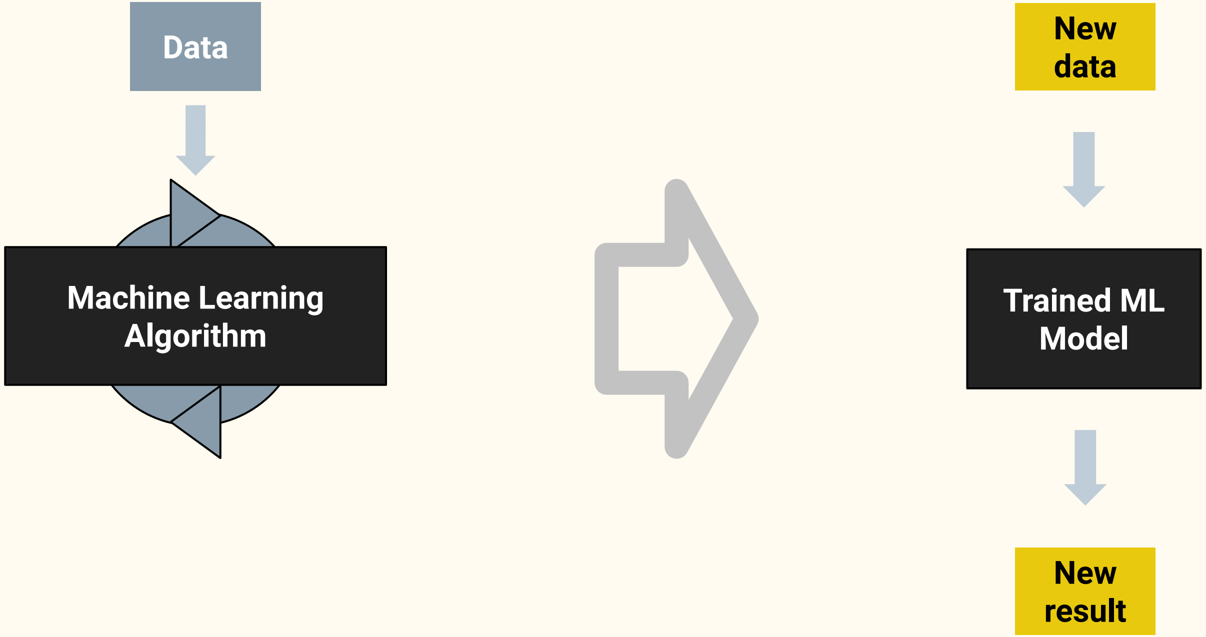
***Machine* learning**: the study of **algorithms** that allow computer programs to automatically improve **on a specific task** through **experience**

Mitchell, 1997

ML: Training and Deployment phases

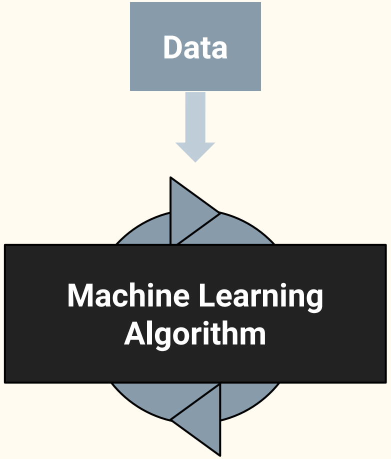
Preparation: training

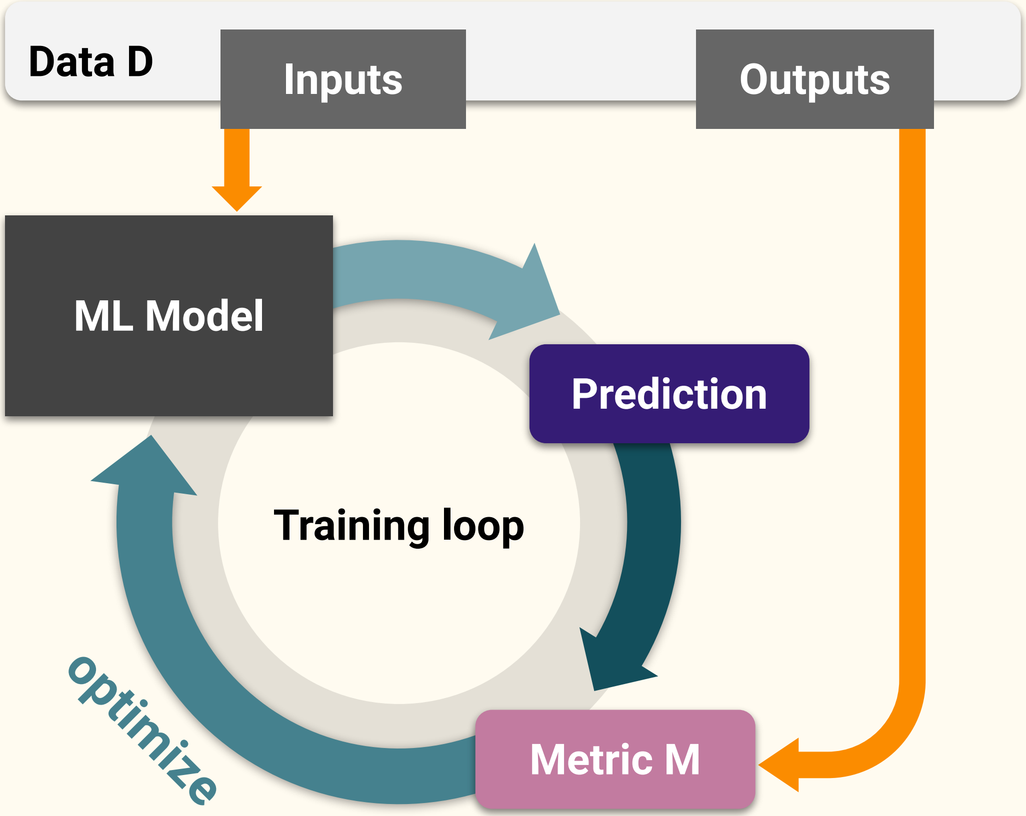
Use: deployment*



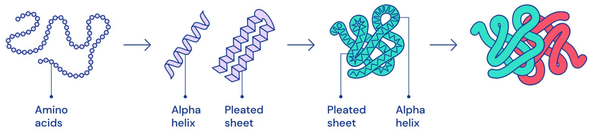
* or “inference”

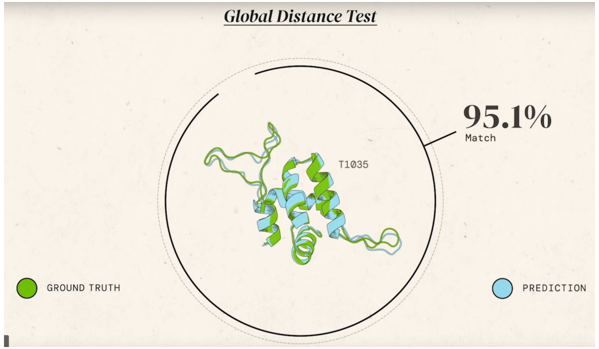
Inside the black box

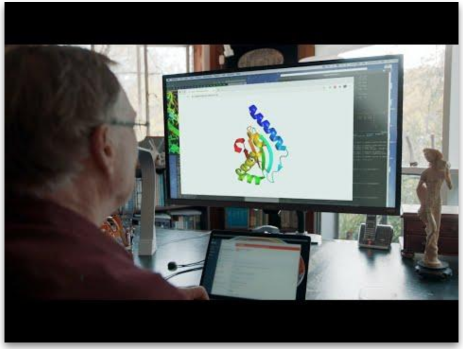




From proteins to planets, ML in science





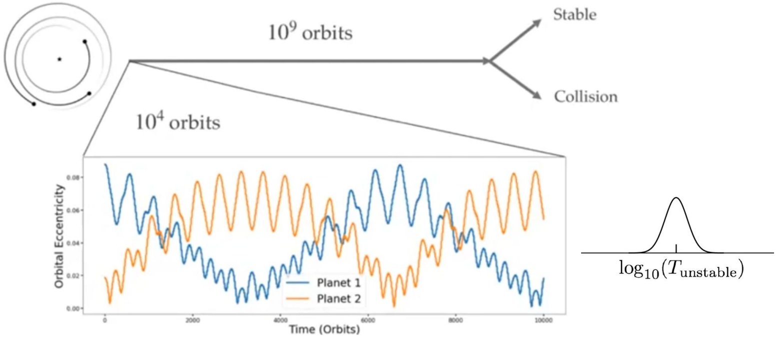


Protein structure prediction with transformers

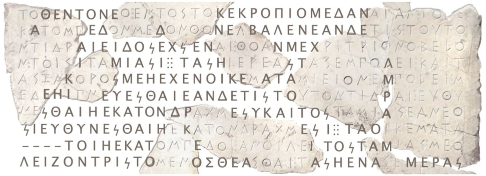
Senior et al. 2020, Jumper et al. 2021

Planetary stability with Bayesian neural networks

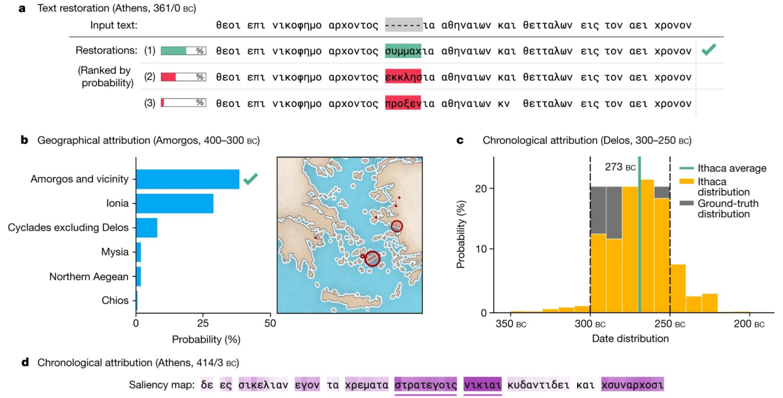
Cranmer, Tamayo et al. 2021



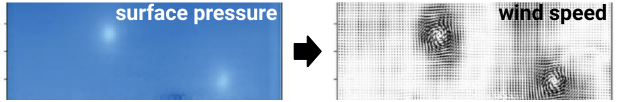
Ancient greeks and seasonal hurricanes



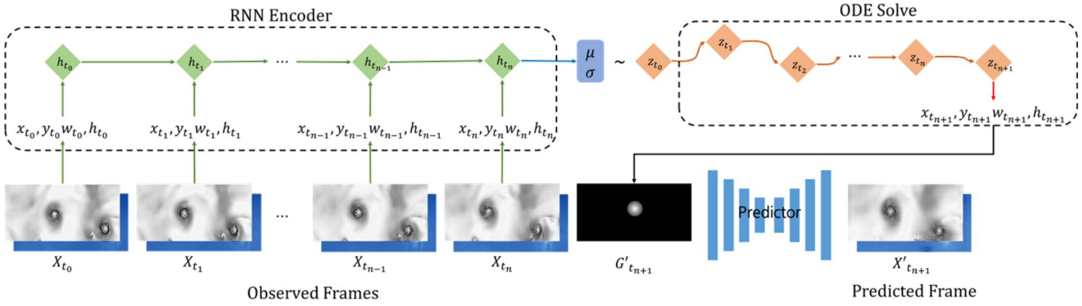
Text restoration and geochronological attribution with data augmentation



Assael, Sommerschield et al. 2022



Hurricane path forecast & speed field with nODEs & GANs

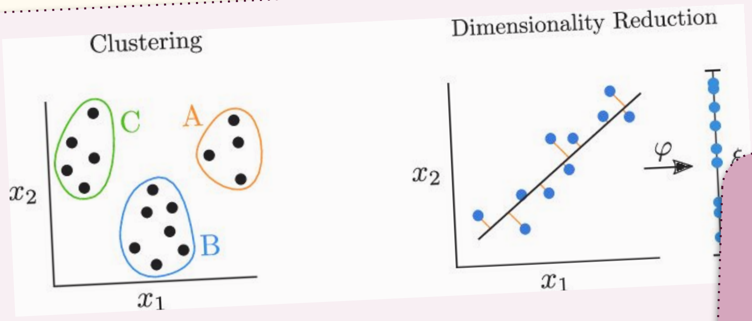


Park, Kim et al. 2020

Core Concepts in Machine Learning

Learning paradigms

Main Learning Paradigms

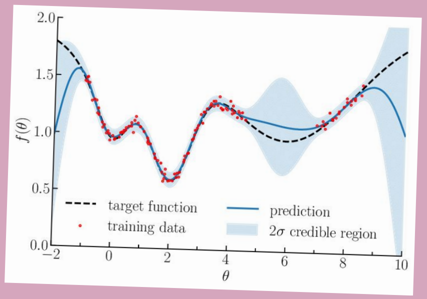


Unsupervised learning

Exploring structure

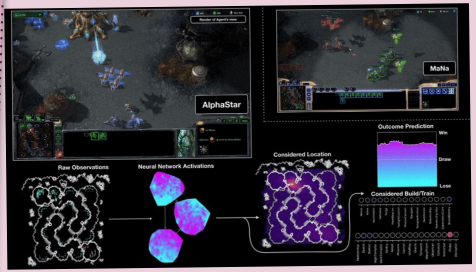
Supervised learning

Teaching to label



Reinforcement learning

Harnessing interaction

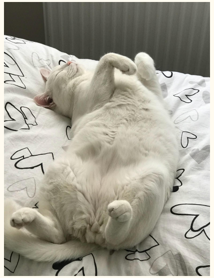
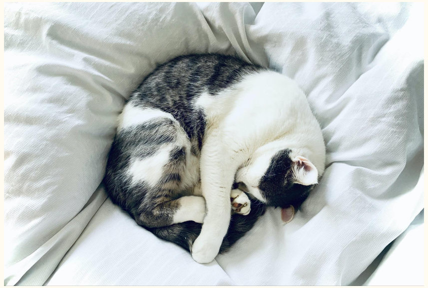
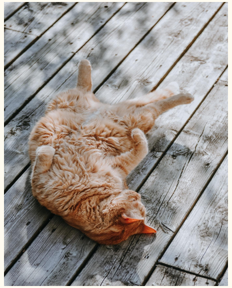


Figures DeepMind 2019, Leclerc 2018, jovian.ai 2021

Core Concepts in Machine Learning

Unsupervised learning

An example dataset

Instance

ID	R01	G01	B01…
1	215	198	180 …
2	61	61	51 …
3	219	227	227 …
4	47	43	37 …

Feature

Photo by Sarah Ball on Unsplash   Photo by Gökhan Konyalı on Unsplash   Photo by Ben Wicks on Unsplash   Photo by Jacalyn Beales on Unsplash

Finding structure in the data


Photo by Sarah Ball on Unsplash

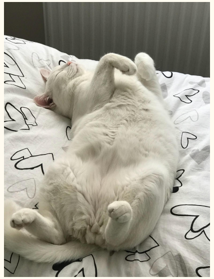


Photo by Gökhan Konyalı on Unsplash

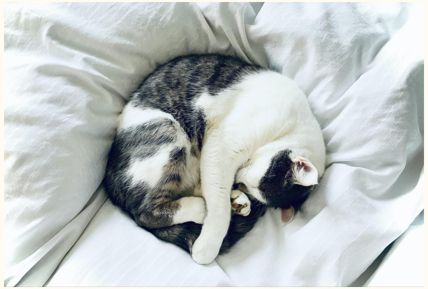


Photo by Ben Wicks on Unsplash

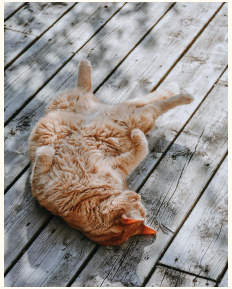
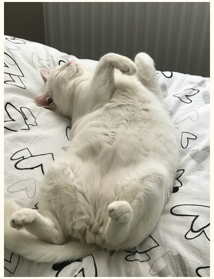
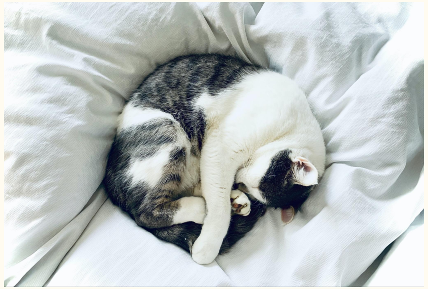


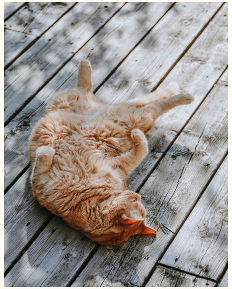
Photo by Jacalyn Beales on Unsplash

Task: group the images into any numbers of groups that you like

Finding structure in the data

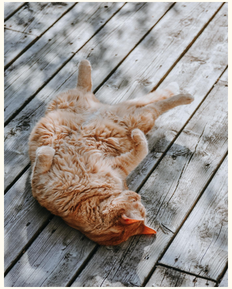
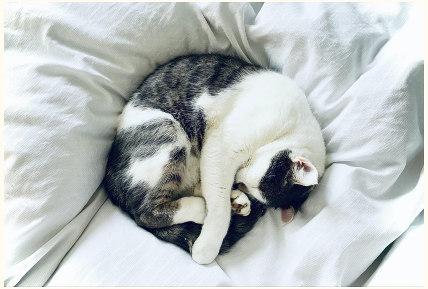
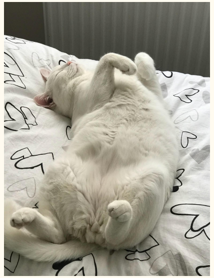






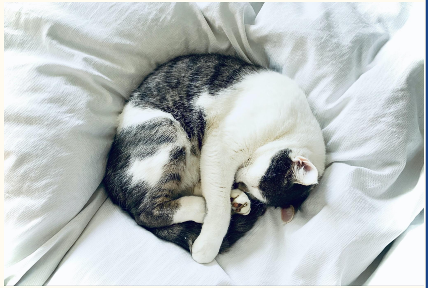
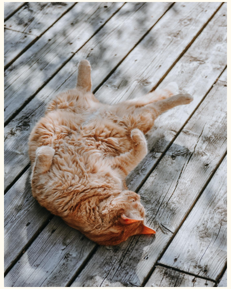
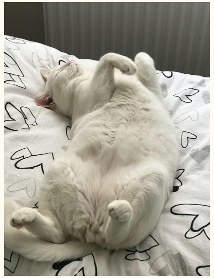
For example: 4 groups based on the breed of cat

Finding structure in the data

For example: 2 groups based on colors (orange or not orange)

Finding structure in the data

For example: 2 groups based on gesture

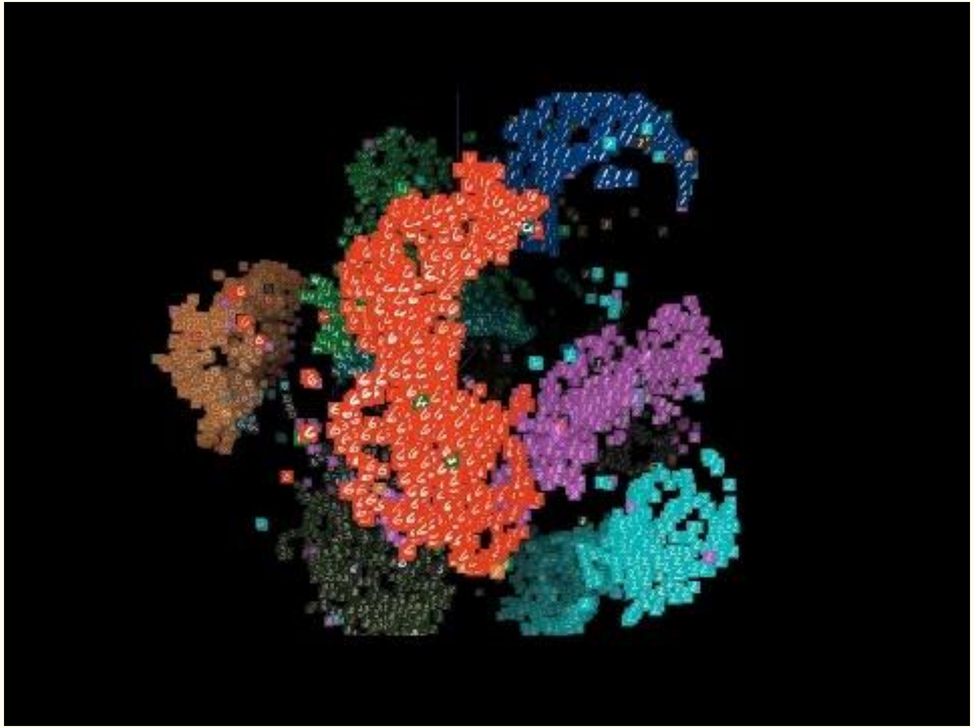
Unsupervised Learning

Goals

- Structure discovery
- Dimensionality reduction
- Community detection

Requirements

- Data (unlabeled)
- Some notion of similarity of data points



Supervised learning

Supervised Learning

Goal

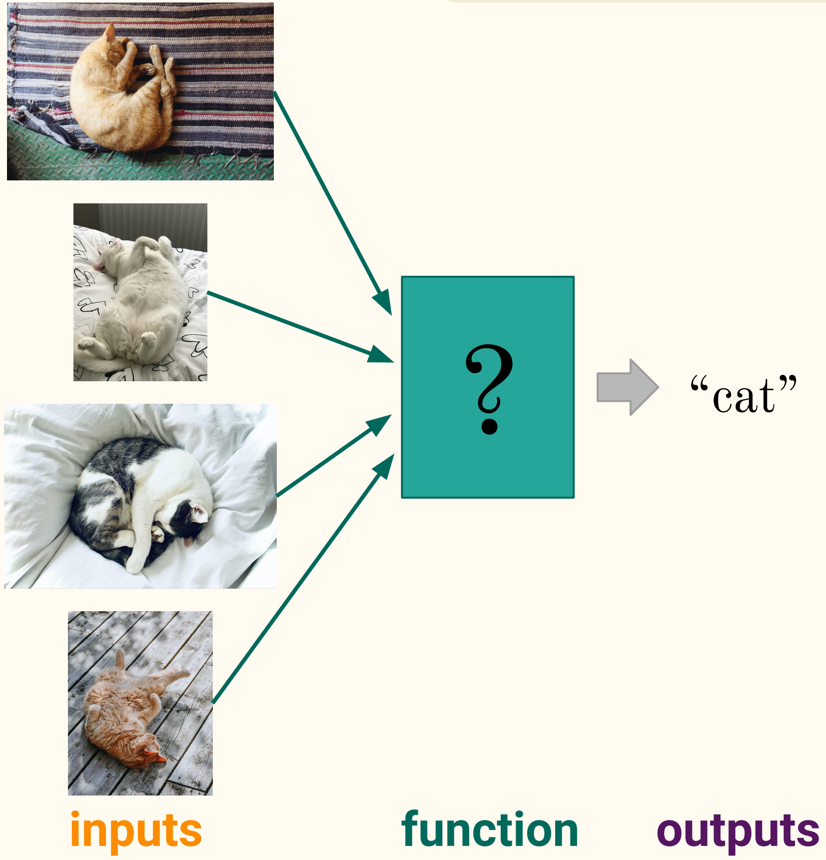
Learn a **function** to map **inputs** to **outputs**

Requirement

Dataset of inputs *and outputs* (“labels”)

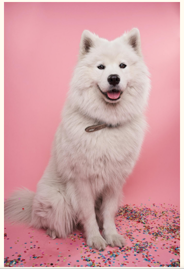
Modes

- Classification (category outputs)
- Regression (continuous outputs)

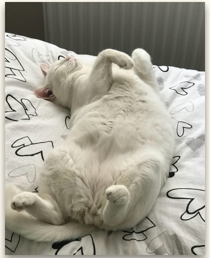


Supervised Learning: Classification

Cat



Dog



Cat

Dog

Category Label

ID	R01	G01	B01…	Type
1	184	187	187 …	Cat
2	218	157	164 …	Dog
3	61	61	51 …	Cat
4	236	236	236 …	Dog

Supervised Learning: Regression

47

0

2

-33

Continuous Label

ID	R01	G01	B01…	Head pose (degree)
1	116	98	81…	47
2	157	146	164 …	0
3	23	22	21…	2
4	137	130	129 …	-33

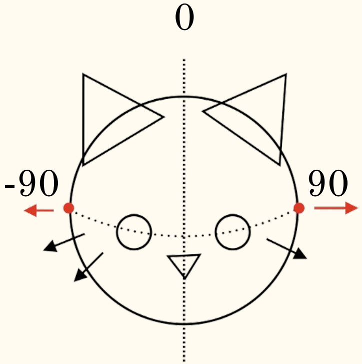


Photo by: cat-breeds-classifier

Reinforcement learning

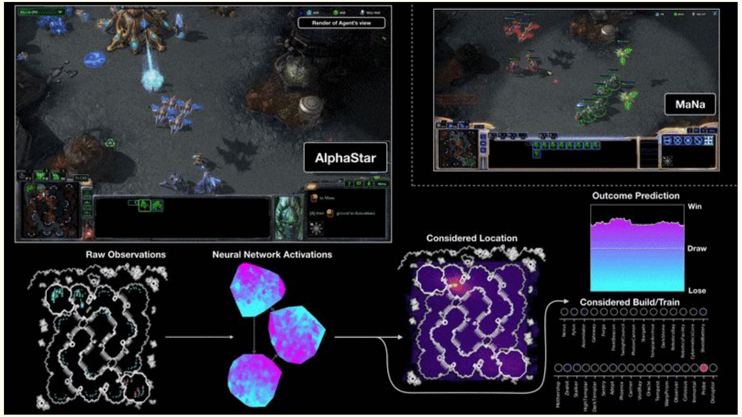
Reinforcement Learning

Goal

Train an agent to interact successfully with some environment

Requirements

- Agent interacting with an environment (real or simulated)
- Reward mechanism for actions taken



Reinforcement Learning

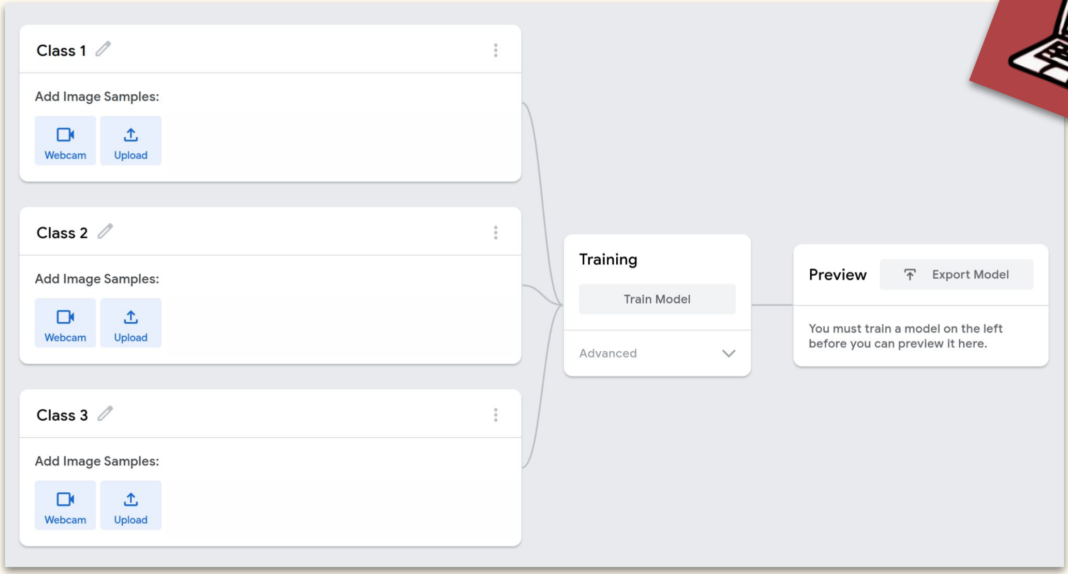
Reinforcement Learning

Core Concepts in Machine Learning

Supervised learning

One step at a time

Let’s train a supervised classifier



Navigate to:
https://teachablemachine.withgoogle.com/train/image

We’ve trained a supervised classifier

- Collect data
  image frames + labels
- Train*
  neural network
  * fine-tune
- Infer or predict
  class of new image

ML brings the senses to computers

HOW? Supervised Learning Tutorial

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Supervised learning: One step at a time

In this notebook, we slowly introduce supervised learning, along with basic machine learning concepts we encounter on the way.

The data

At regularly spaced 1-dimensional points x, we have generated fake, noisy 1-dimensional observations y. We assume that there is some true but unknown underlying process f, so that

$$y_i = f(x_i) + \text{noise}.$$

x_i is a single **raw feature**. y_i is an **output** or continuous **label**.

Interactive notebook downloadable at mlcolab.org/introml02-participants

Core Concepts in Machine Learning

Neural Networks

Layer upon layer upon layer

Building a neural network - terminology

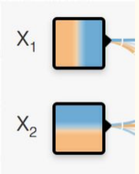
playground.tensorflow.org

DATA

Inputs: coordinates

X_1 horizontal

X_2 vertical



optional: *(hand-crafted)* **features**

X_1^2, X_2^2, X_1X_2, $\sin X_1$, $\sin X_2$ ← augment input

Outputs: Binary classes **orange (-1)** or **blue (+1)** → **TASK: CLASSIFICATION**

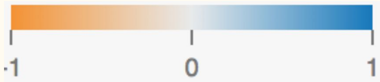
MODEL

Hidden layers = number of nestings in the NN; *here: fully connected*

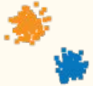
Neurons = units in each layer

} **architecture**

Model output: f(X_1, X_2, *features*(X_1, X_2))

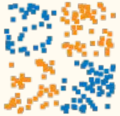


Neural network playground – Training



blobs

What is the simplest architecture you can find?



xor

What minimal architecture can you find using only X_1 and X_2?

Can you improve using features?

concentric

Does the default setting solve the problem?

Can you simplify the network using features?

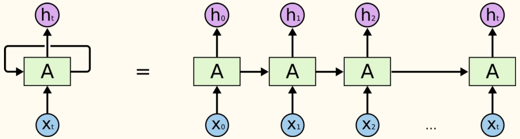
spiral

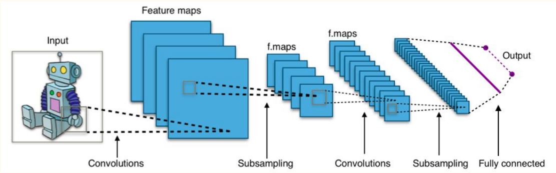
Use 1 layer and features
→ "feature engineering"

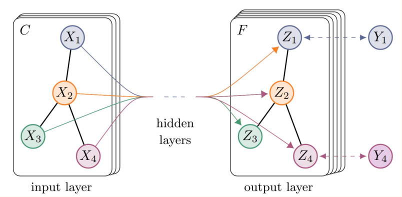
Construct a deep network, but only use X_1 and X_2

Task-specific architectures

Data	**Time series, sequences (1D)**	**Images (2D)**	**Networks**
e.g.	Text, speech, temperature, …	Microscopy, astronomical shots, density maps, ...	Social networks, molecular graphs, knowledge graphs, …
NN types	RNNs *(recurrent) NNs* Transformers	CNNs – *(convolutional) NNs*	GNNs – *graph NNs*







Machine Learning in Practice

The ML ⇌ Science Colaboratory

ML development cycle

From data to scientific results

Zooming out: the ML dev cycle

Let's talk about how to…

1. … define the task
2. … obtain data, and prepare it
3. … implement the model
4. … evaluate, interpret and report output

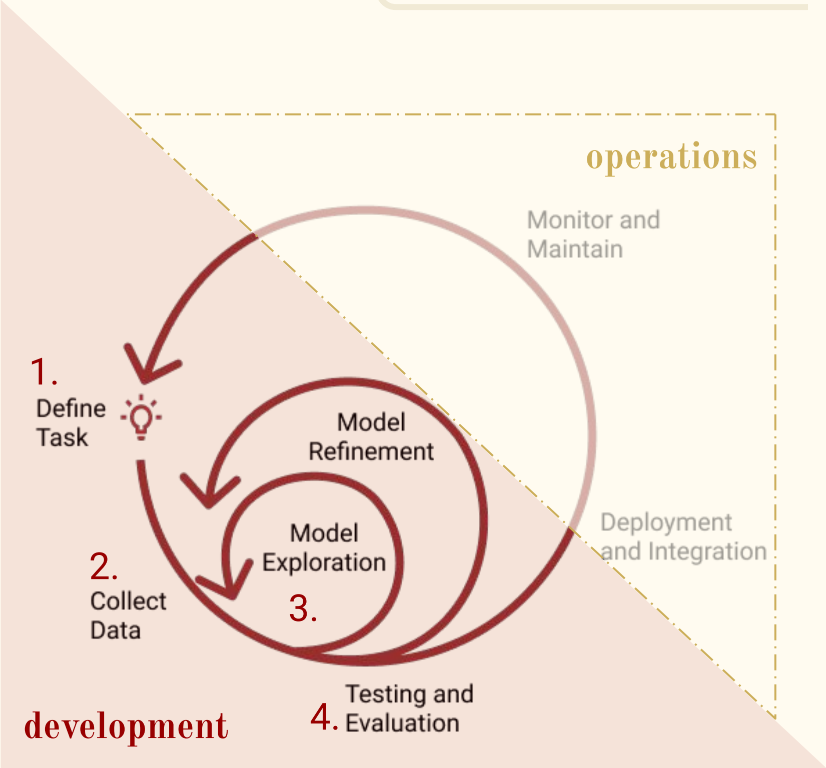


Figure based on Jordan 2018: organizing ML projects

1. Task: Feasibility & Impact of ML Project

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Do you know your data?

- All relevant regimes/conditions covered?
- Cost of additional (labeled) data?

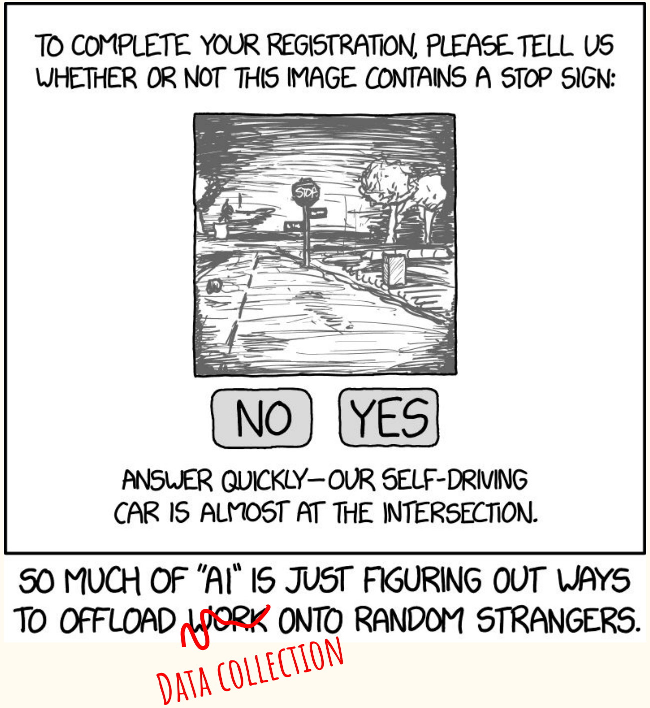
Model requirements, alternatives

- Are there pre-trained models?
- Does it need to be interpretable?
- Are there classical/hand-crafted models known to work well?

How to measure performance?

- Can performance be measured? How?
- Can humans do it? With what performance?
- Consequence of wrong predictions?
- Are there performance baselines? (using ML *or not*).

2. Data: How to get It



xkcd.com/1897

Strategies for data preparation (YOU!)

- **Complement** with public ancillary data
- **Reduce** via pretrained models
- **Augment** with synthetic or modified data ("Data augmentation")

Data sources

- Your own *sensor* data. Cheap!
- Your own *survey* data
- Public data sources

Data preparation : labeling

- Make it efficient: user interfaces
- Automatic labeling (active learning)
- 3rd party services: gamification

2. Data: Common Modalities

- Time series
- Images
- Relational (graph) data
- Tabular
- Video
- Georeferenced measurements
- Spectra
- A mix!

Data modalities provide knowledge that can be exploited, e.g.

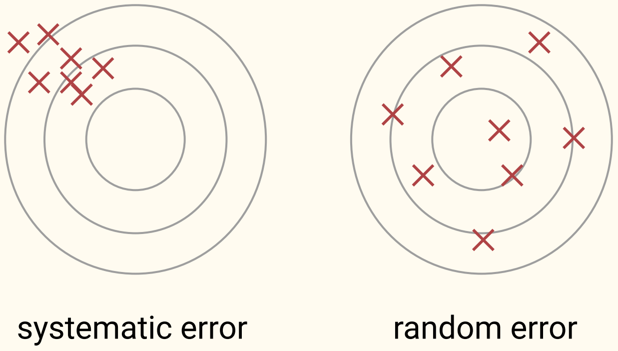
- The future depends on the past
- Close points are usually similar
- The curvature of the Earth matters

Icons from Icons8

2. Data: Pitfalls

Data might not represent the sampling distribution because of

- Systematic error (bias)
- Noise (i.e. “random” error)
- Sampling bias
- Independence across samples
- Missing data
- Multi-scale phenomena
- Censored data



2. Data: Processing

- Validation – verify **data quality**
- Aggregation
- Cleaning
- Transforming
- Reduction
- Summarization, Visualization

! As **domain expert**, you know a lot about your data that you might take for granted

Take home:

- Data processing assumes some model!
- Make data processing programmatic for reproducibility!
- **Never** overwrite **raw** data with **processed** data!

2. Data: Processing

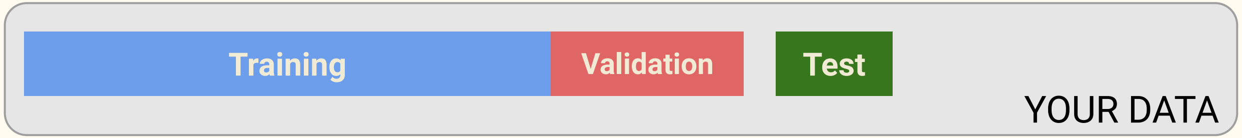
- Validation – verify **data quality**
  - Are data types correct and consistent?
  - Is data plausible / consistent?
  - Do data satisfy ranges and constraints?
  - Reasons for data imbalance?
- Aggregation
- Cleaning
  - Outlier detection/removal
  - Integrating data from different sources
- Transforming
  - Standardizing (shifting and scaling)
  - Smoothing/denoising
  - Imputation of missing data
  - Augmentation
- Reduction
  - Downscaling, feature selection
- Summarization, Visualization

! As domain expert, you know a lot about your data that you might take for granted

Take home:

- Data processing assumes some model!
- Make data processing programmatic for reproducibility!
- **Never** overwrite **raw** data with **processed** data!

3. Model: Training, Validating and Testing



- Training data to tune **parameters:** minimize loss function

- Validation data* to set ***hyper*parameters:** evaluate metrics
  *or *development set*

TRAINING

EVALUATE

- Test data 🔒 to estimate **generalization performance:** compare metrics <u>after</u> training with **baselines** (random or specific) and toplines (human performance). *Held out* of training.

3. Model: Implementation & Embodiments

- **"Classical ML"**
  - \+ stable, documented, interpretable
  - ○ CPU arrays (numpy, R)

  `R, sklearn, mlj`

- **Probabilistic programming**
  - \+ uncertainty quantification
  - \+ interpretable
  - – CPU mostly, expensive
  - – expert knowledge

  `PyMC, Pyro, Stan, turing`

- **Deep learning**
  - \+ expressive, versatile
  - – hard to interpret
  - ○ Training vs inference
    - ■ Resources & devices
  - ○ GPU

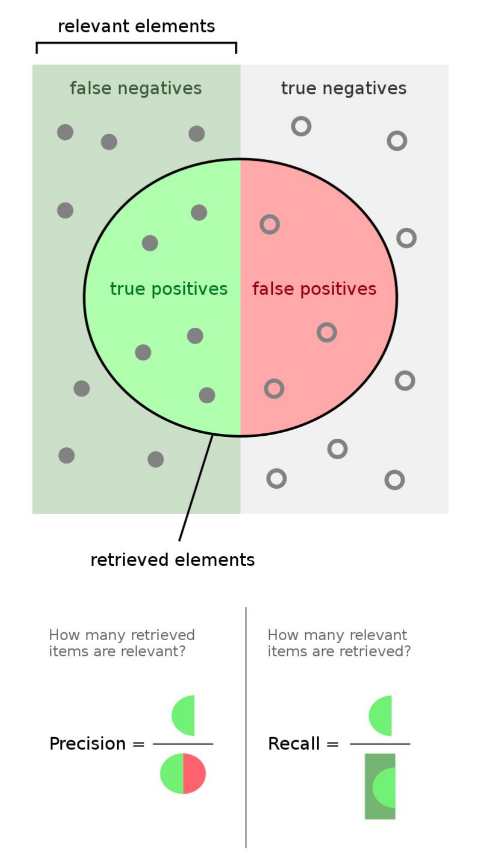
  `PyTorch, TensorFlow, jax, flux`

- **Pretrained**
  - ○ API serving (query only) or
  - ○ download-and-finetune (transfer learning)

  `Huggingface, GPT, ...`

4. Evaluation & Performance Metrics

- Use held-out test data ▯▯▯ ▮🔒 to report & compare models
  - *Benchmarks* are combinations of task + dataset used to drive development in ML
- You get what you optimize for…
  … but not all you care about we can optimize for
  → need **metrics**, not just loss
- Metrics for:
  - **Regression**: MSE (cf. poly regression), ...
  - **Classification**: precision, recall, F-score, …

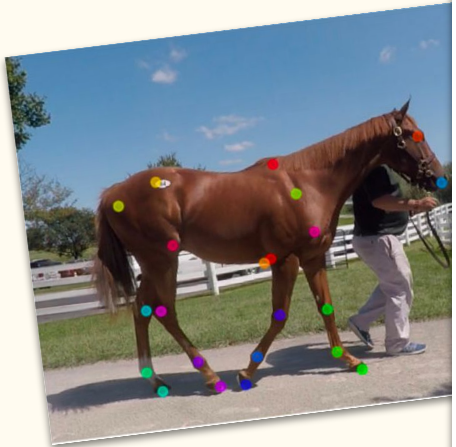


Machine Learning in Science

Learning from language, images, simulations…

Computer Vision (CV)

Data: images or videos



Pose estimation

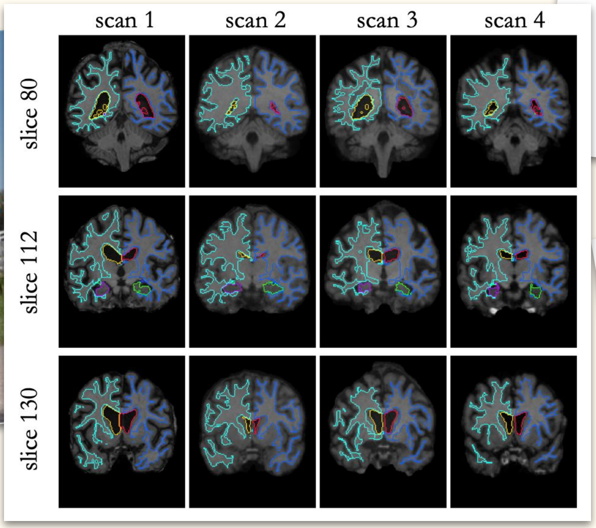
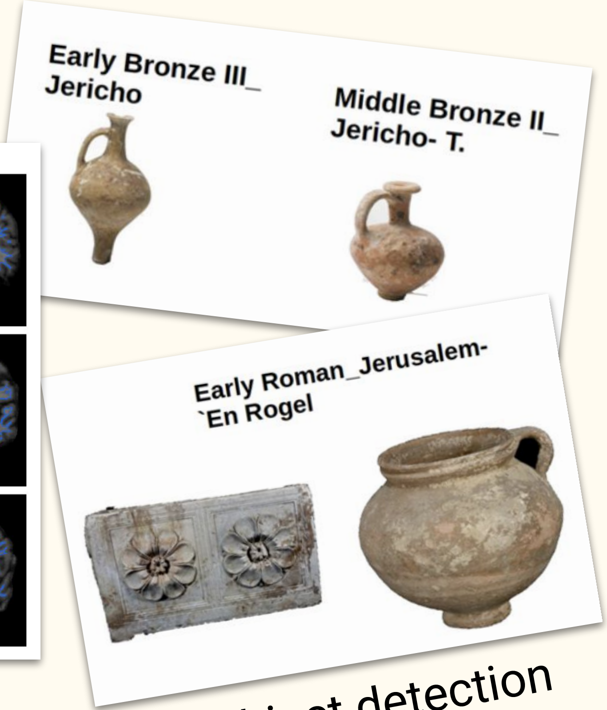


Image segmentation



Object detection

Balakrishnan, Zhao et al. 2019,
Nath, Mathis et al.2018, Resler, Yeshurun et al. 2021

CV: pose estimation without body markers

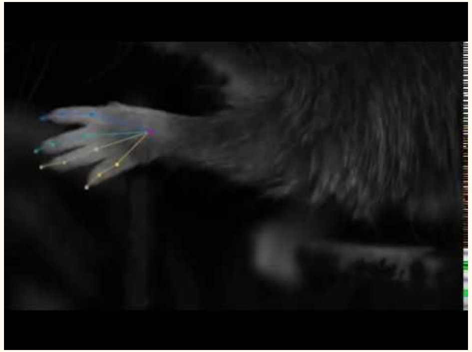
Hypothesis We can detect body parts of multiple animal species from unstaged video without body markers

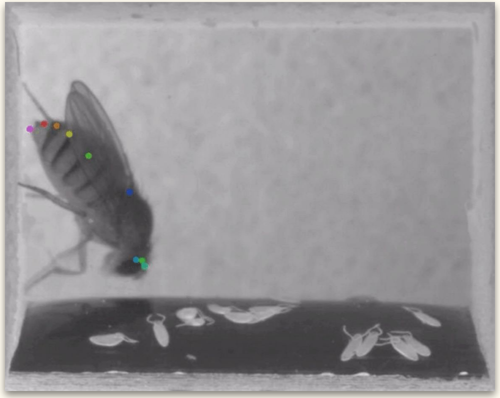
Dataset video frames with *labeled* positions of body parts

Task frame-based pose estimation

Evaluation distance *(RMSE)* between predicted and labeled positions

Model *pre-trained* ResNet with fully convolutional upsampling

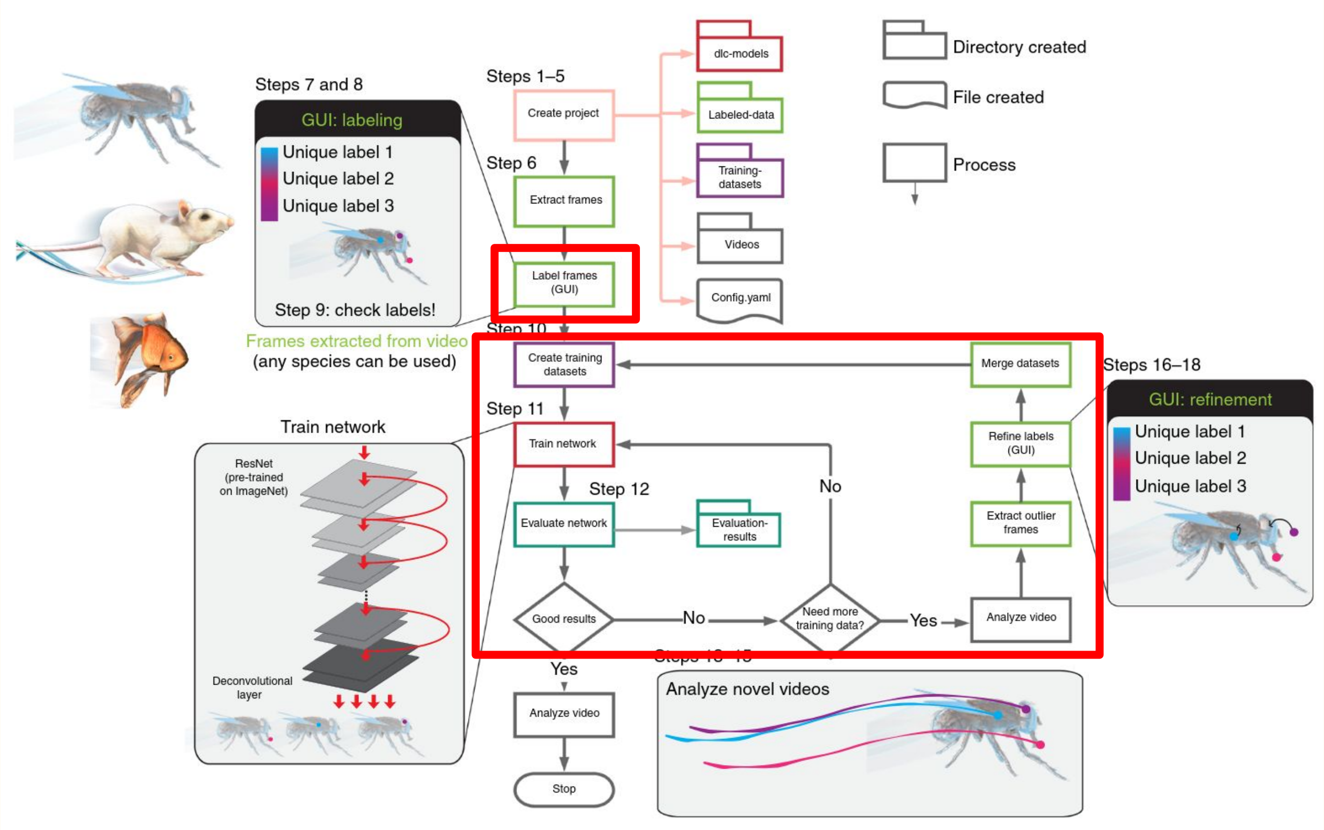




Fruit fly

Nath, Mathis et al.2018

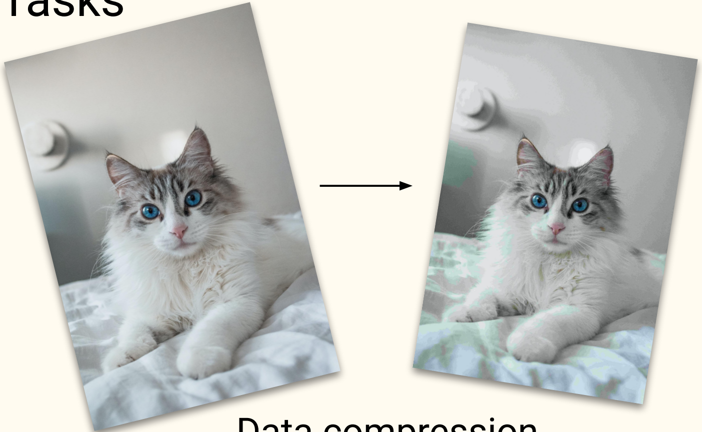
CV: pose estimation without body markers



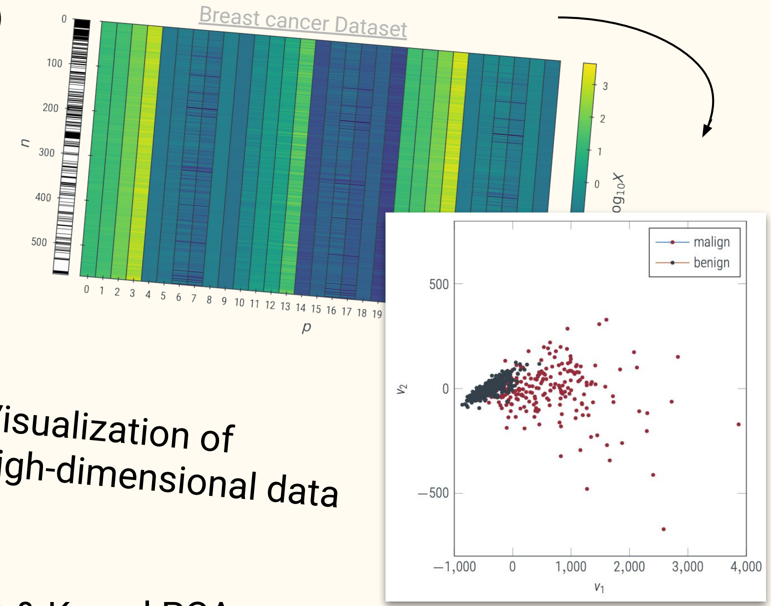
Nath, Mathis et al.2018

Dimensionality reduction

- Data
  - High-dimensional data (e.g. k space data)
- Tasks



Data compression



Visualization of high-dimensional data

- Models
  - Unsupervised models
    - Principal component analysis (PCA) & Kernel PCA
    - Autoencoders
    - t-SNE, UMAP (for visualization)
- NOTE: Often for pre-processing of the data

Cell-type prediction for single-cell transcriptomics

Hypothesis can identify similar cells via gene expression profiles

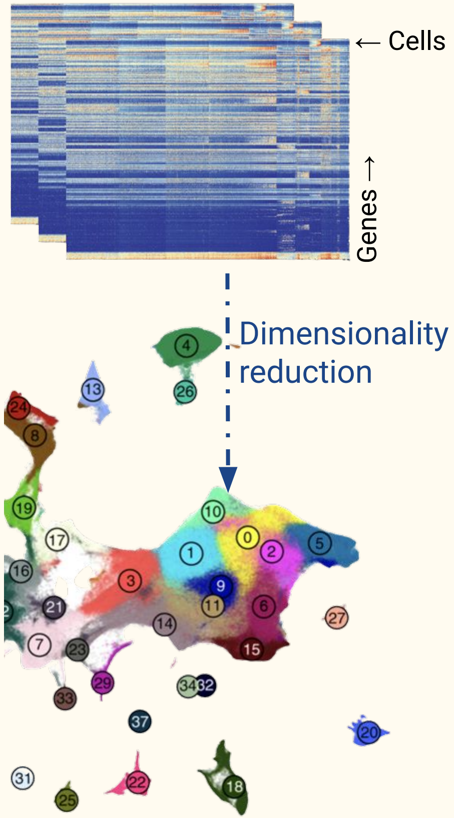
Dataset gene expression matrices (read counts per million)

Task *dimensionality reduction*

Evaluation % neighbor cells preserved in lower-dim space

Model *t-SNE* with PCA initialisation

Luecken,Theis et al.2019

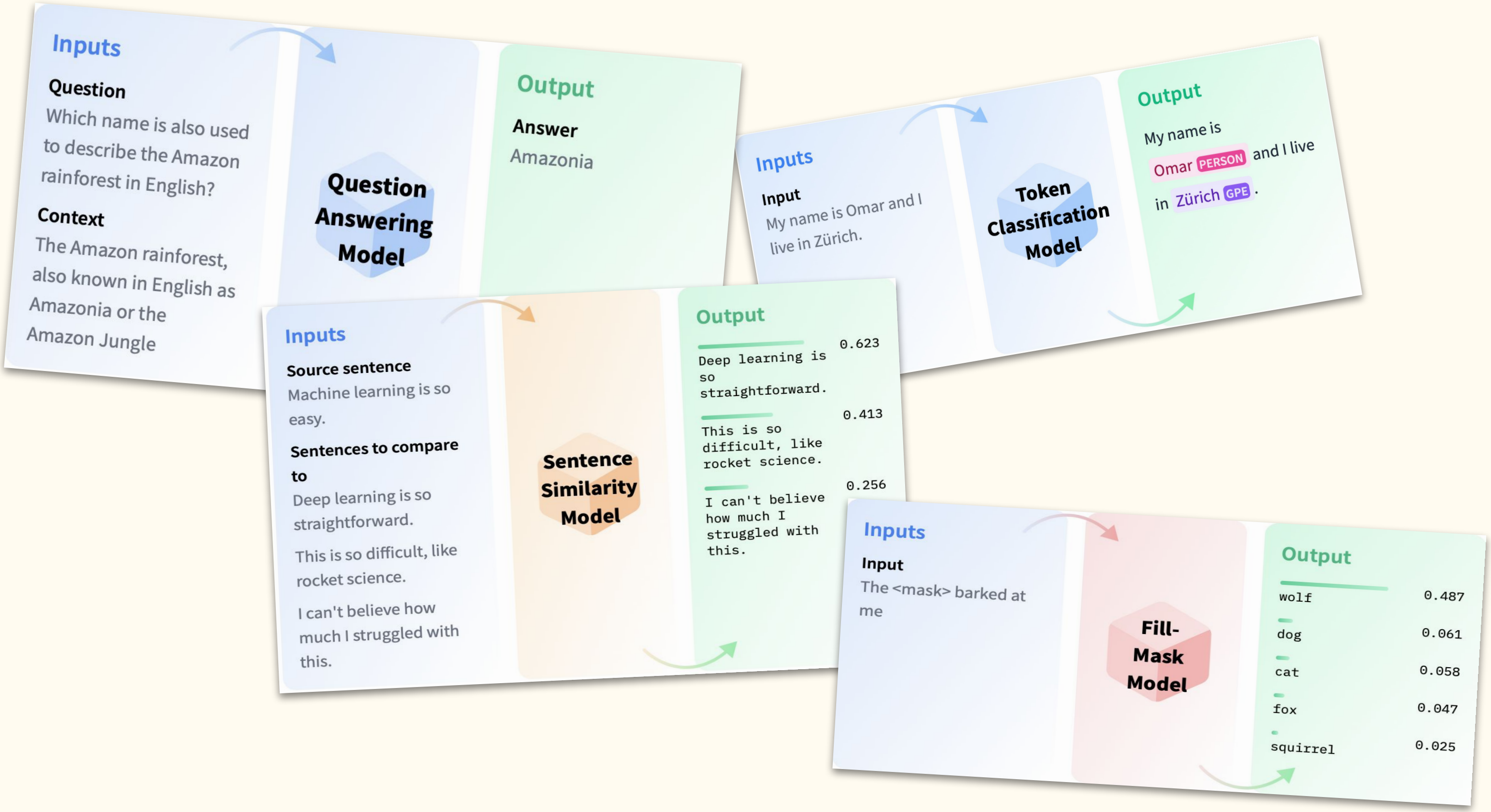


Kobak, Berens et al.2019

Natural Language Processing: tasks

huggingface.co: tasks

NLP: Tasks



huggingface

NLP: Author Attribution in Latin

Hypothesis rhythmic constructions in Latin help reveal author identity

Data *Samples*: ~37k prose fragments of 10 consecutive > 4-word sentences. *Labels*: Author class

Features: Syllabic length (SL): short ∪, long —, anceps *X* (ngrams), other "base features"

Arma vi|rumque ca|nō, Trō|iae quī| prīmus ab| ōrīs|| → — ∪ ∪| — ∪ ∪ | — —| — —| — ∪ ∪ | — *X*||

Task author attribution = fragment *classification*

comparing (base features **together with** SL) with just (base features)

Evaluation cross-entropy *loss* for training, *F*-score M/m *metric* for early stopping & feature importance

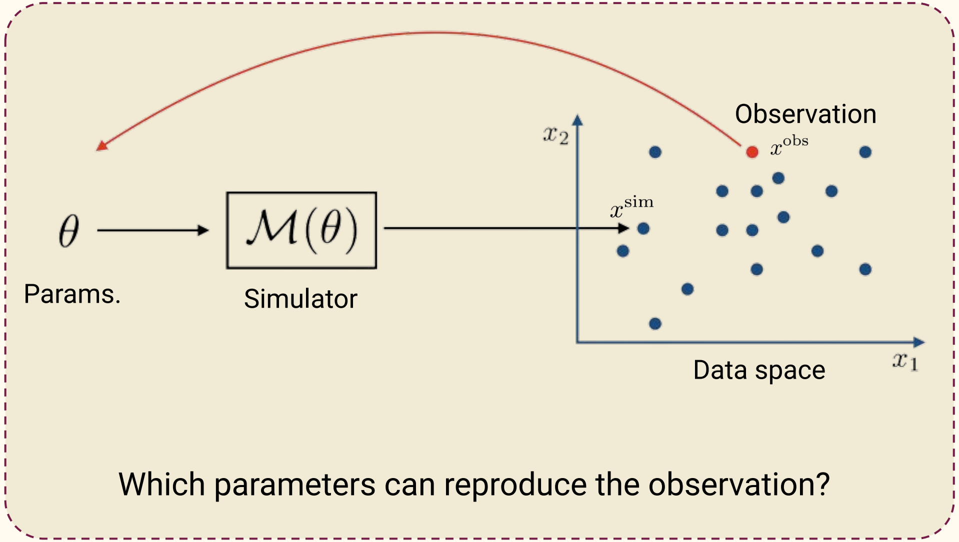
Model multi-channel NN (BF, SL, DVs), CharCNN 5 layers, avg proba decision

Corbara 2021 (preprint)

Simulation-based inference (SBI)

Tasks

- General inference in absence of likelihoods (losses)
- Particularly suited for black-box simulators $x^{sim} = \mathbf{M}(\theta)$.
- How can we learn a distribution over the parameters θ such that $\mathbf{M}(\theta) \approx x^{obs}$



Note

We have a full 3-day workshop on SBI

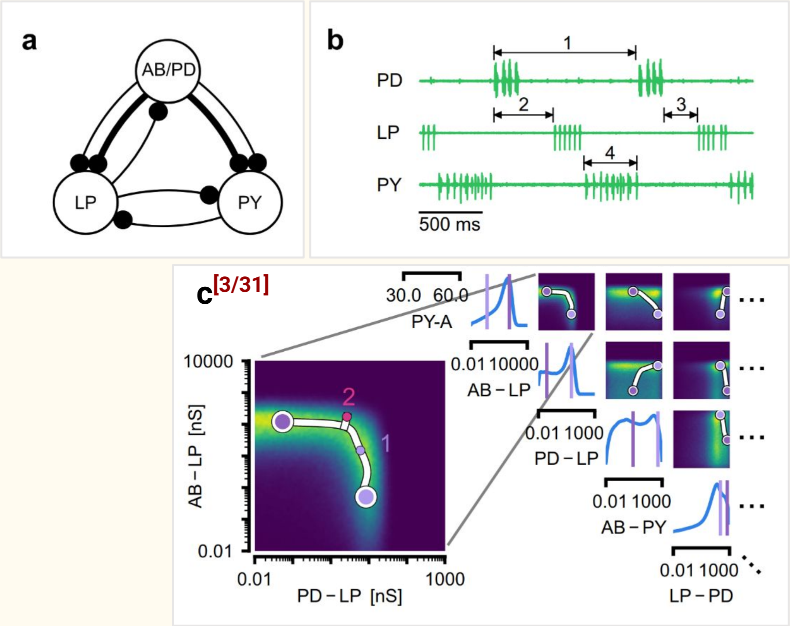
SBI: Stable Firing in the Pyloric Ganglia

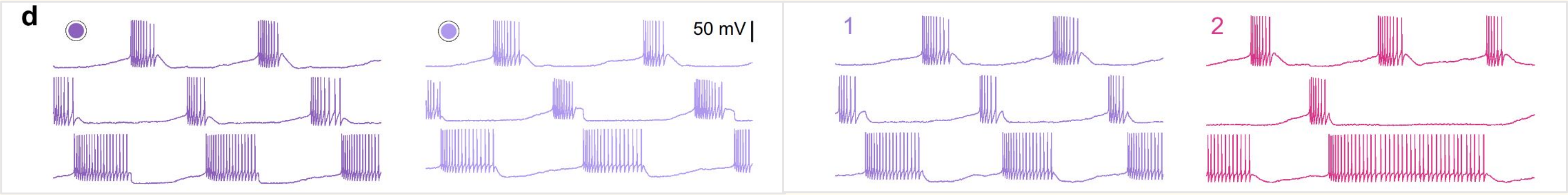
Hypothesis the pyloric rhythm is robust to changes in conductances θ.

Dataset summary features of cell-electrophysiological (x^{obs}), computer simulations of the same $x^{sim} = \mathbf{M}(\theta)$.

Task Bayesian solution for the inverse problem "θ=θ(x^{obs})"

Model normalizing flows (invertible NNs) as conditional density estimators





Gonçalves et al. 2020

Limitations of Today's ML for Science

- Inductive paradigm, limited by data
  - Bad at extrapolation
  - Building in inductive biases still a craft
- Compute intensive
- Correlational, mostly not causal
  - But can help you fit mechanistic models that are causal
- Interpretability (mostly post-hoc)
- Uncertainty quantification

Should I use ML for my problem?

Use ML when the problem…

- … has a simple objective,
- is too complex for explicit rules,
- is constantly changing,
- is perceptive, or
- is observable, but unstudied

Don't use if:

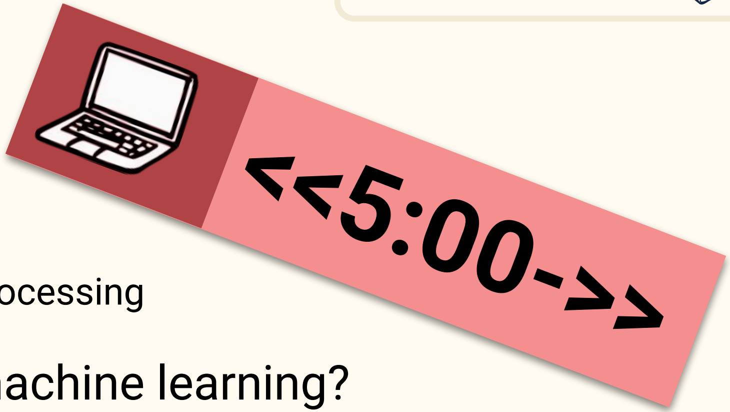
- there exist performant classical models
- every decision must be explainable
- errors are high-consequence,
- getting dense data is infeasible or costly…

Machine Learning in Science

Bring Your Science Problem

Task, data, metrics...

Checklist for group discussion



1. What is the scientific question?

2. **Data:** Describe your dataset:
   - data modalities, labels (if there are), size, state of processing

3. **Task:** Which part of the work might involve machine learning?
   - Identify the learning paradigm that applies to your problem (supervised, unsupervised, ...)

4. **Performance:** How could you measure `success’ in your problem?

5. Are there relevant baselines/toplines for performance?

The ML $\rightleftharpoons$ Science Colaboratory

Connecting ML with Science

Engaging with Us

EBERHARD KARLS UNIVERSITÄT TÜBINGEN

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NLP, probprog, dim red...

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In closing...

Thank you very much for attending our IntroML workshop!


Seth


Álvaro


Elena


Alex


Yutong

One last thing,

… we thrive on critical, constructive feedback

please visit **mlcolab.org/introml02-participants** and give us some!