Lecture 01

What are Machine Learning and Deep Learning? An Overview.

STAT 479: Deep Learning, Spring 2019

Sebastian Raschka

http://stat.wisc.edu/~sraschka/teaching/stat479-ss2019/

But first ...
a course overview

Main Topics

- History of neural networks and what makes deep learning different from “classic machine learning”
- Introduction to the concept of neural networks by connecting it to familiar concepts such as logistic regression and multinomial logistic regression
- Modeling and deriving non-convex loss function through computation graphs
- Introduction to automatic differentiation and PyTorch for efficient data manipulation using GPUs
- Convolutional neural networks for image analysis
- Tricks of the trade for neural network design and training
- 1D convolutions for sequence analysis
- Sequence analysis with recurrent neural networks
- Generative models to sample from input distributions
  - Autoencoders
  - Variational autoencoders
  - Generative Adversarial Networks

Course Material

- Field is relatively new and evolves quickly => No "good" textbook

- Main course material: Mainly slides
  + assigned reading (online references and papers)

- 3 lectures per week, so mainly slides instead of lecture notes (but I will make them more wordy compared to the FS2018 ML class)

Course Logistics

When

- Mon 11:00-11:50 am
- Wed 11:00-11:50 am
- Fri 11:00-11:50 am

Where

- Psychology 121

Instructors

- Instructor: Sebastian Raschka
- Teaching Assistant: Youran Qi

Office Hours

- Sebastian Raschka:
  - Wed 2:00-3:00 pm, Room MSC 1171
- Youran Qi:
  - TBD

Course Website

- Course Logistics
- Course Description
- Resources
- Grading
- Class Project
- Other Important Course Information
- Schedule
  - Topics Summary
  - Calendar

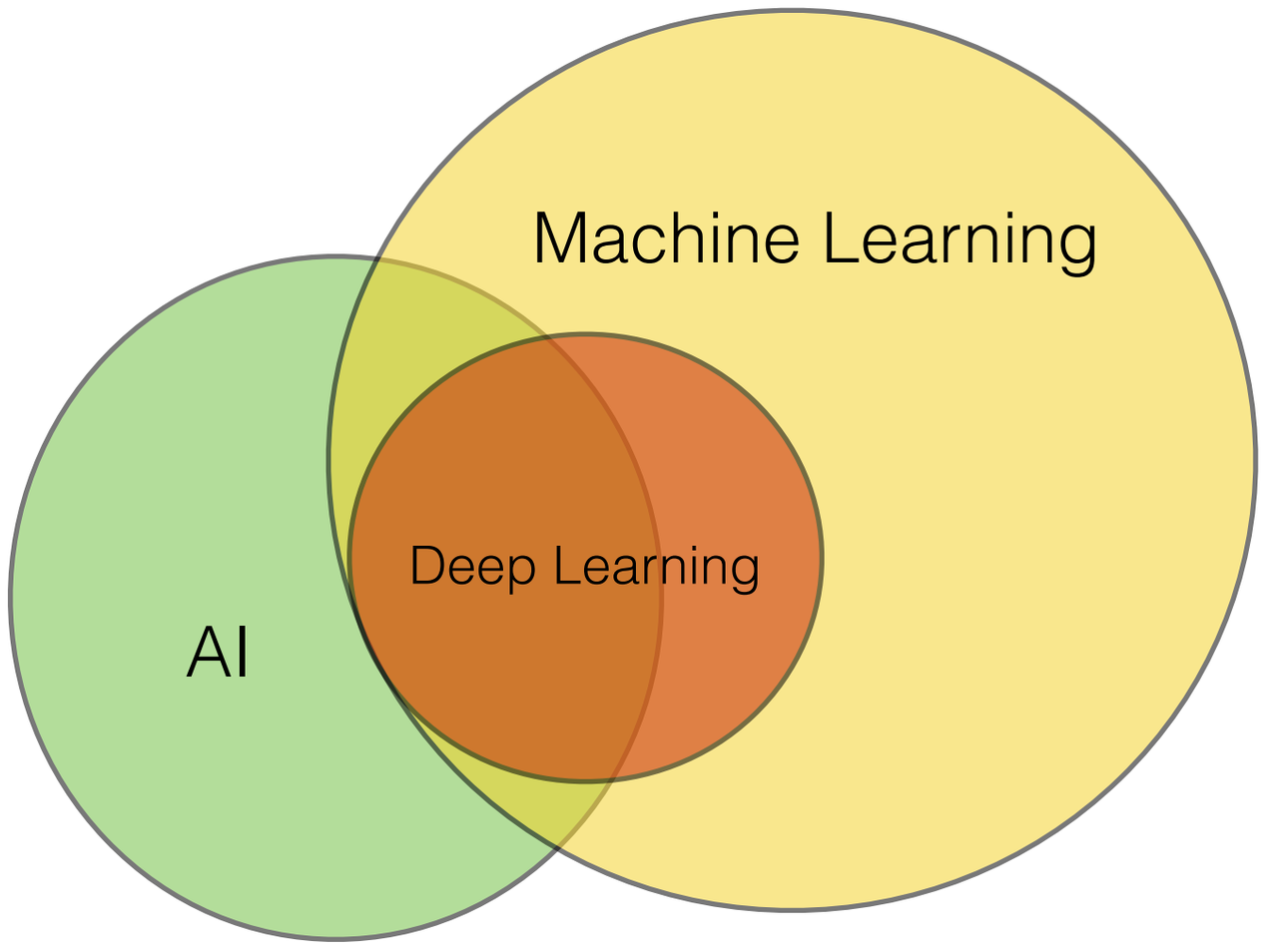
Please check regularly!

http://pages.stat.wisc.edu/~sraschka/teaching/stat479-ss2019/

What is Machine Learning?

A short overview before we jump into Deep Learning

The Connection Between Fields

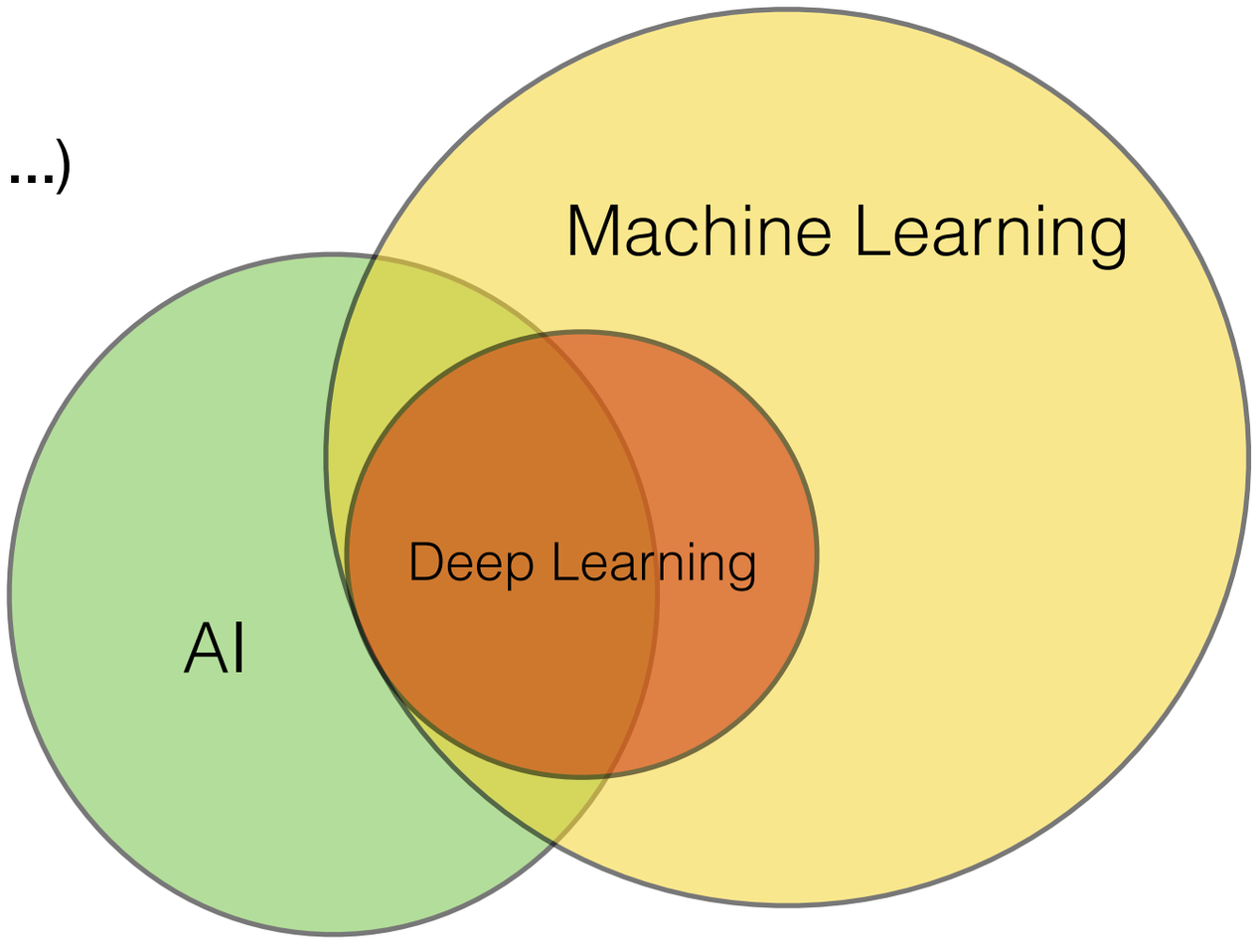


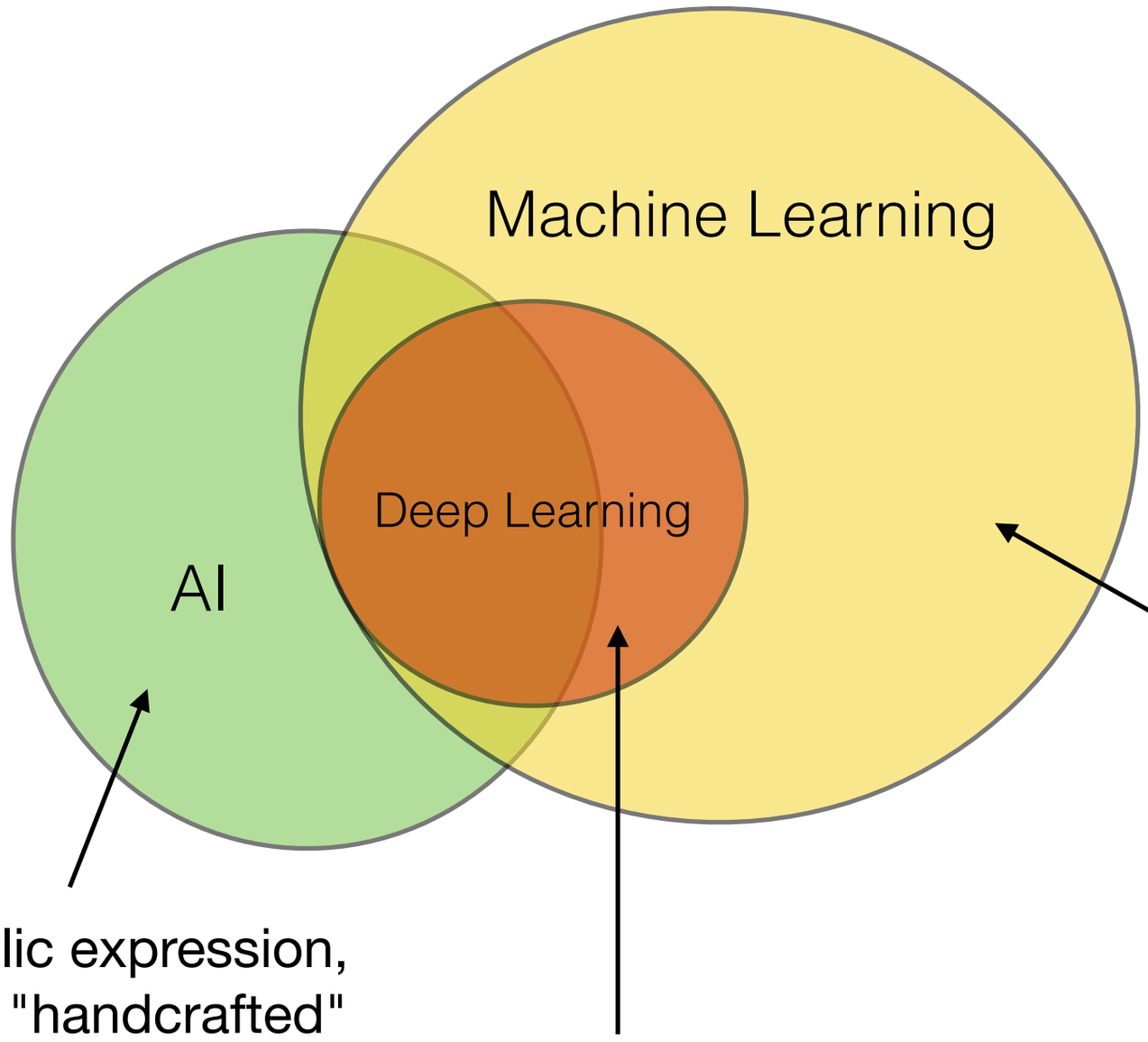
The Connection Between Fields

Artificial Intelligence (AI):
orig. subfield of computer science, solving tasks humans are good at (natural language, speech, image recognition, ...)

Artificial General Intelligence (AGI):
multi-purpose AI mimicking human intelligence across tasks

Narrow AI:
solving "a" task (playing a game, driving a car, ...)

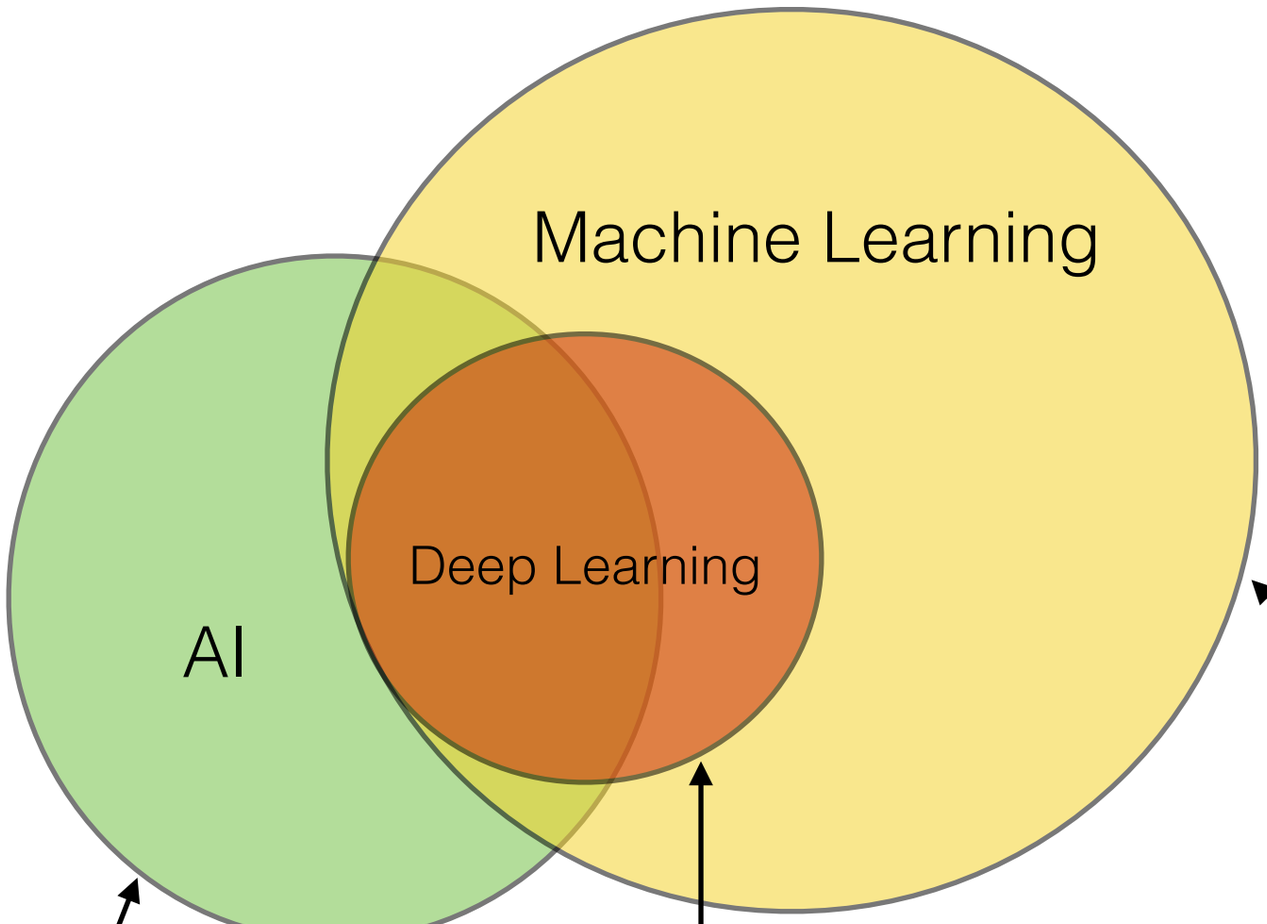




E.g., symbolic expression, logic rules / "handcrafted" nested if-else programming statements ...

Main focus of the course

E.g.,
generalized linear models, tree-based methods, "shallow" networks, SVM, nearest neighbors, ...



= a non-biological system
that is intelligent
through rules

= algorithms that parameterize multi-layers
neural networks that then learn
representations of data with multiple layers
of abstraction

= algorithms that learn
models/representations/
rules automatically
from data/examples

What is Machine Learning?

"Machine learning is the field of study that gives computers the ability to learn without being explicitly programmed"

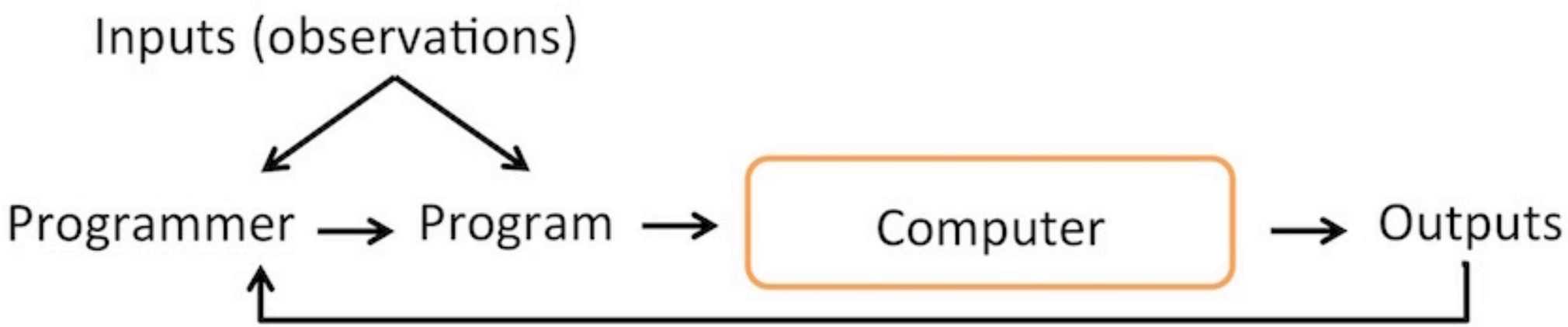
— Arthur L. Samuel, AI pioneer, 1959

[probably the first, and undoubtedly the most popular definition]

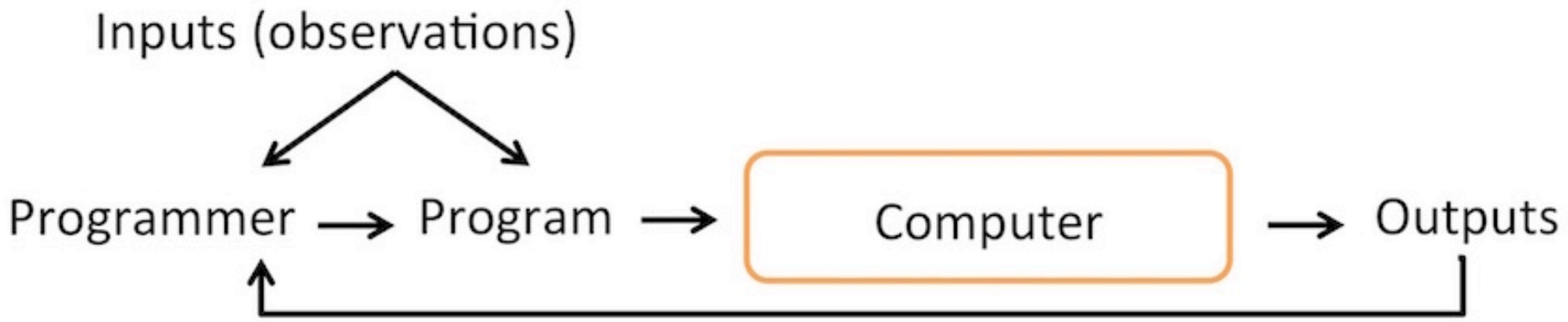
(This is likely not an original quote but a paraphrased version of Samuel's sentence "Programming computers to learn from experience should eventually eliminate the need for much of this detailed programming effort.")

Arthur L Samuel. "Some studies in machine learning using the game of checkers". In: *IBM Journal of research and development* 3.3 (1959), pp. 210–229.

The Traditional Programming Paradigm



The Traditional Programming Paradigm



Machine Learning is the field of study that gives computers the ability to learn without being explicitly programmed
– Arthur Samuel (1959)

Machine Learning

Some Applications of Machine Learning/Deep Learning

- Email spam detection
- Face detection and matching (e.g., iPhone X)
- Web search (e.g., DuckDuckGo, Bing, Google)
- Sports predictions
- Post office (e.g., sorting letters by zip codes)
- ATMs (e.g., reading checks)
- Credit card fraud
- Stock predictions

Some Applications of Machine Learning/Deep Learning

- Smart assistants (Apple Siri, Amazon Alexa, ...)
- Product recommendations (e.g., Netflix, Amazon)
- Self-driving cars (e.g., Uber, Tesla)
- Language translation (Google translate)
- Sentiment analysis
- Drug design
- Medical diagnoses
- ...

Categories of ML/DL

Supervised Learning

- Labeled data
- Direct feedback
- Predict outcome/future

Unsupervised Learning

- No labels/targets
- No feedback
- Find hidden structure in data

Reinforcement Learning

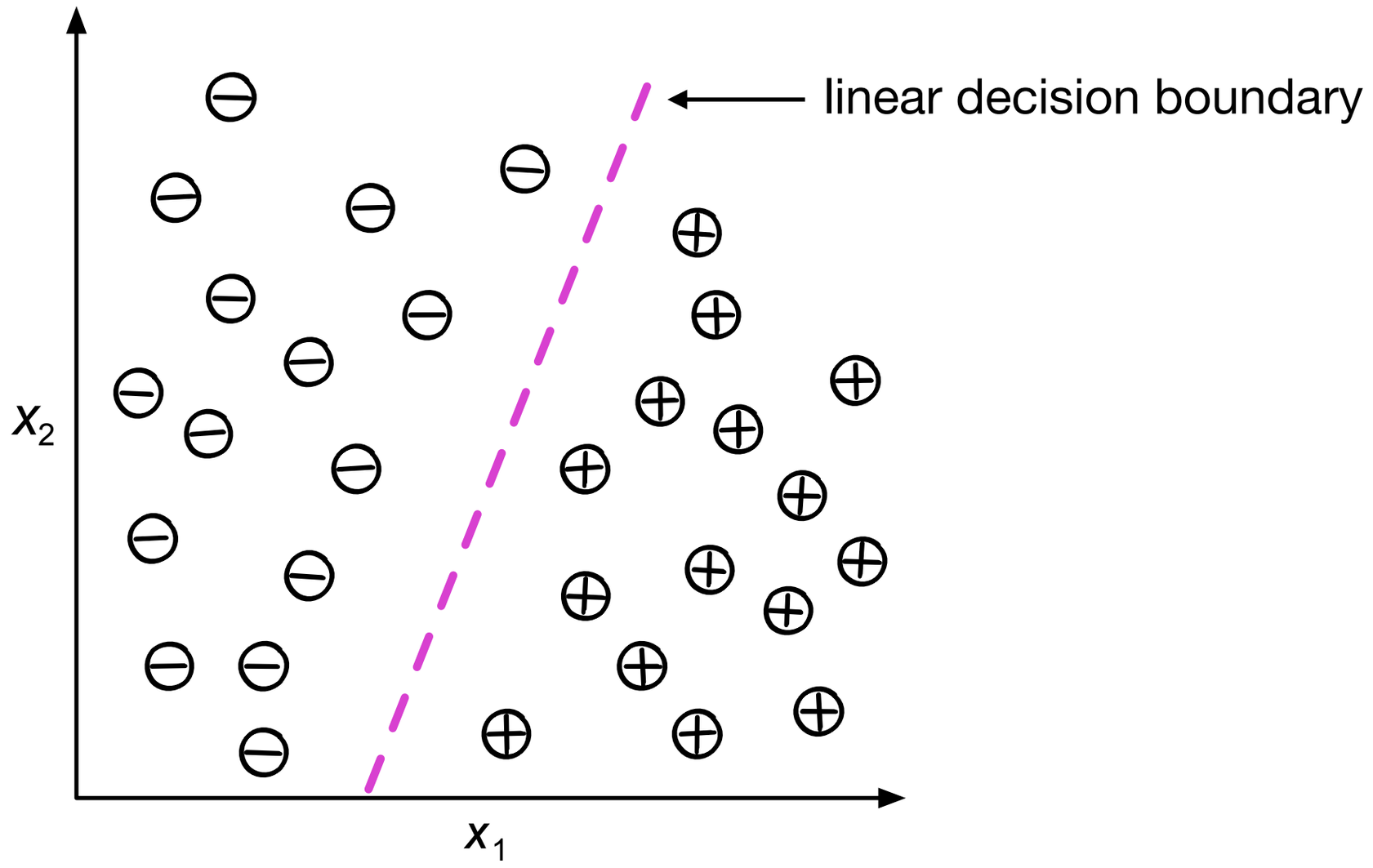
- Decision process
- Reward system
- Learn series of actions

Supervised Learning

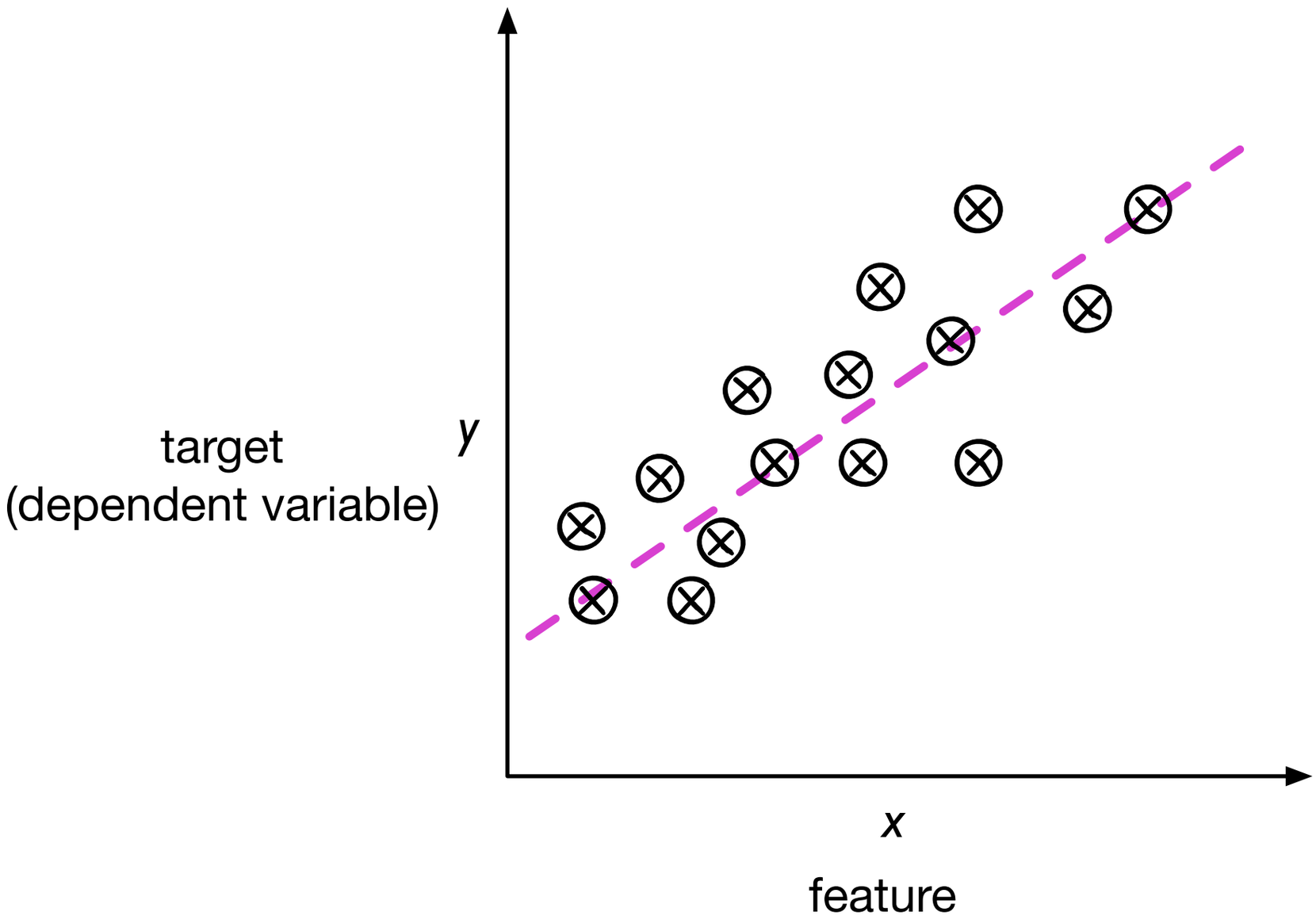
- Labeled data
- Direct feedback
- Predict outcome/future

Supervised Learning: Classification

Binary classification example with two *features* ("independent" variables, predictors)



Supervised Learning: Regression



Supervised Learning: Ordinal Regression

- Ordinal regression also called *ordinal classification* or *ranking* (although ranking is a bit different)

Order dependence like in metric regression, but no metric distance

discrete values like in classification, but order dependence

$$r_K \succ r_{K-1} \succ \ldots \succ r_1$$

E.g., movie ratings: *great* $\succ$ *good* $\succ$ *okay* $\succ$ *for genre fans* $\succ$ *bad*

Supervised Learning: Ordinal Regression

- Ranking: Correct order matters
  (0 loss if order is correct, e.g., rank a collection of movies by "goodness")

- Ordinal Regression: Correct label matters
  (E.g., age of a person in years; here, regard aging as a non-stationary process)

Excerpt from the UTKFace dataset
https://susanqq.github.io/UTKFace/

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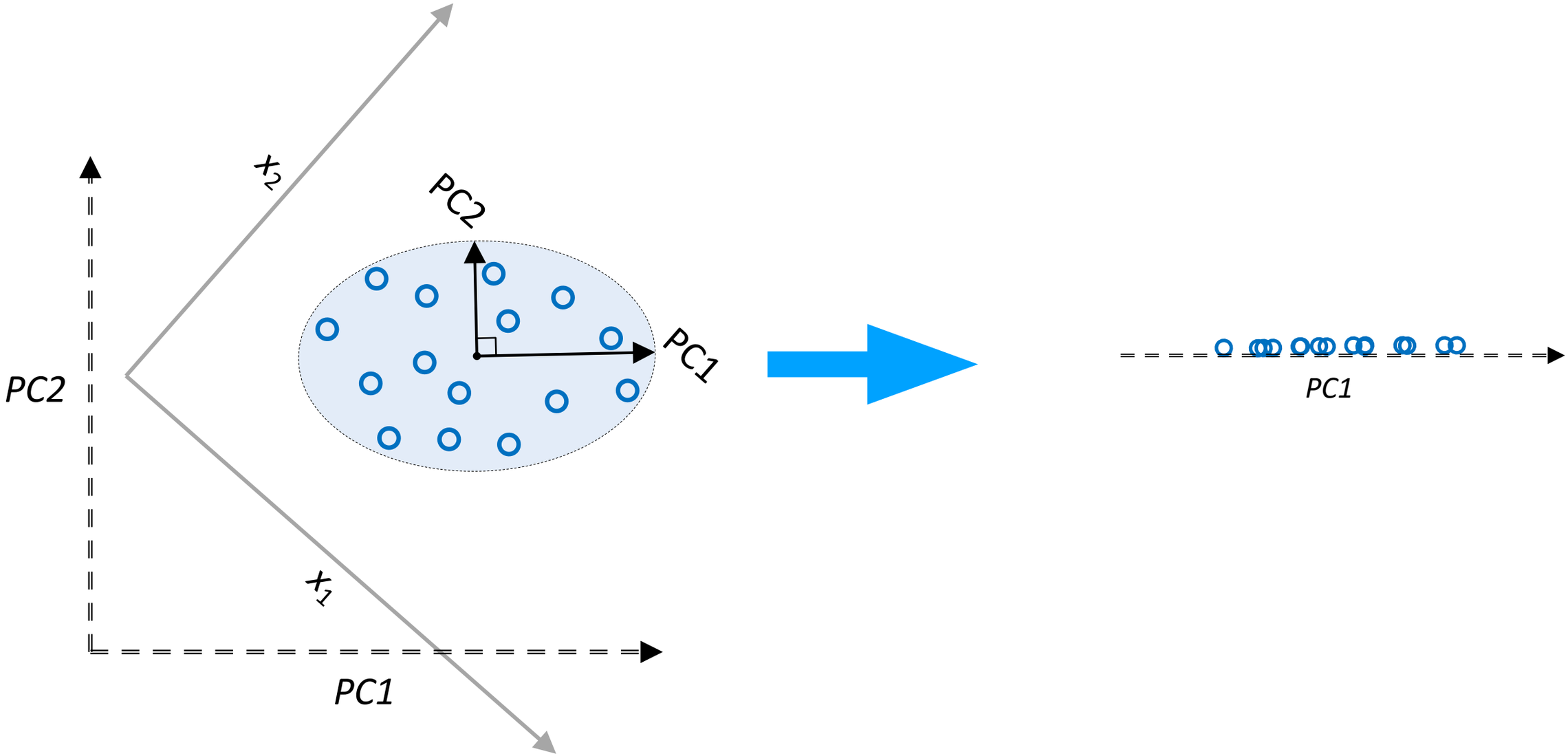
Unsupervised Learning

- No labels/targets
- No feedback
- Find hidden structure in data

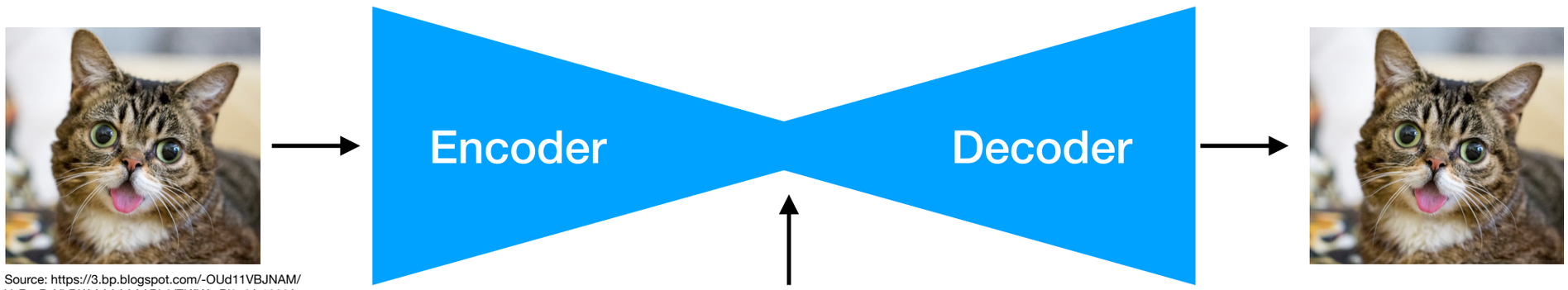
Unsupervised Learning: Representation Learning/Dimensionality Reduction

E.g., Principal Component Analysis



Unsupervised Learning: Representation Learning/Dimensionality Reduction

E.g., Autoencoders



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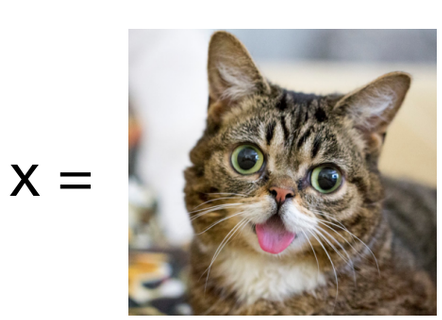
latent representation/
feature embedding

Reminder: Classification works like this



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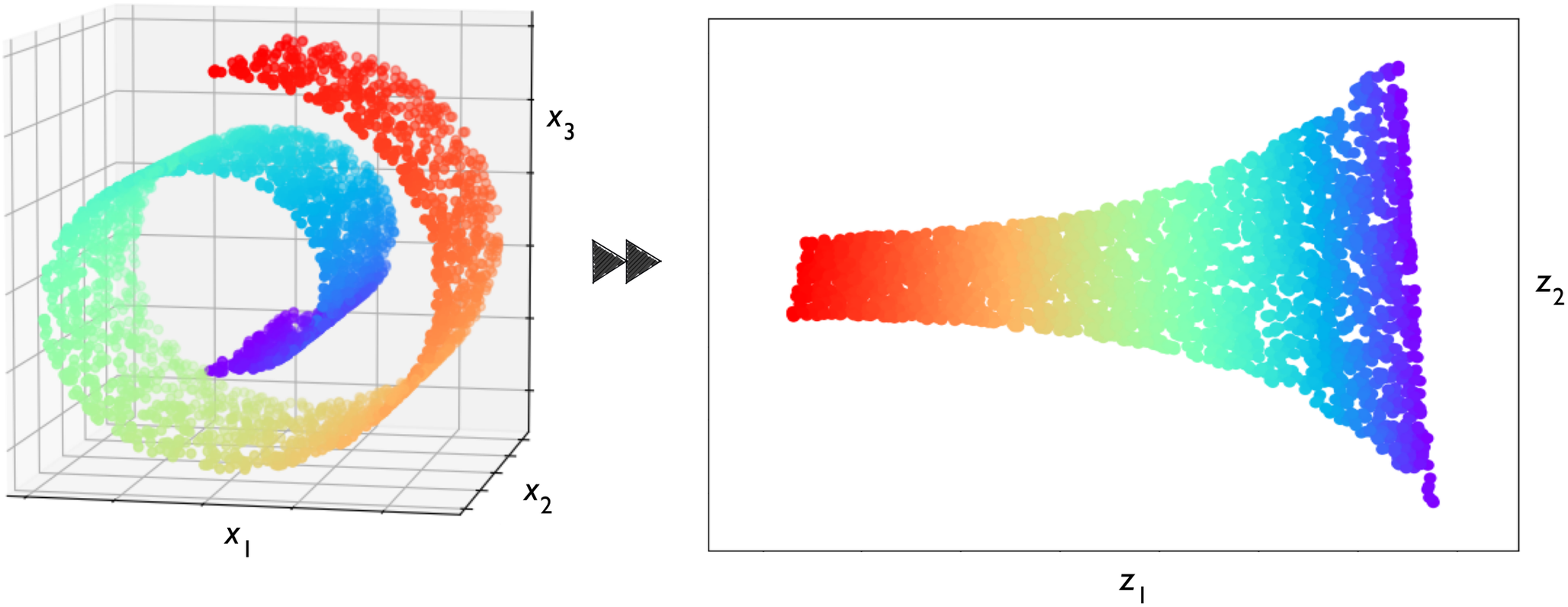
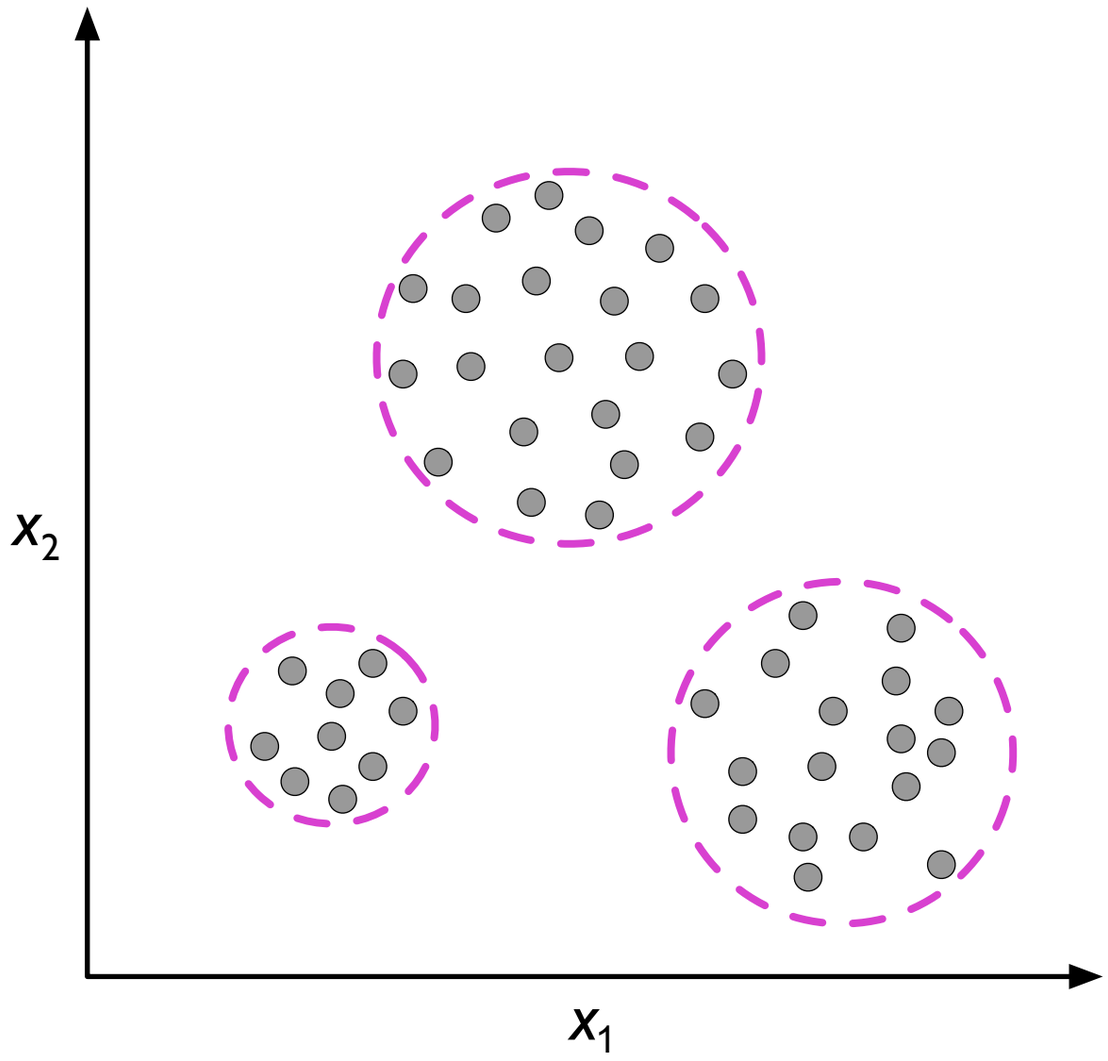
Unsupervised Learning: Representation Learning/Dimensionality Reduction



Example of manifold learning using kernel PCA

Unsupervised Learning: Clustering

Assigning group memberships to unlabelled examples (instances, data points)

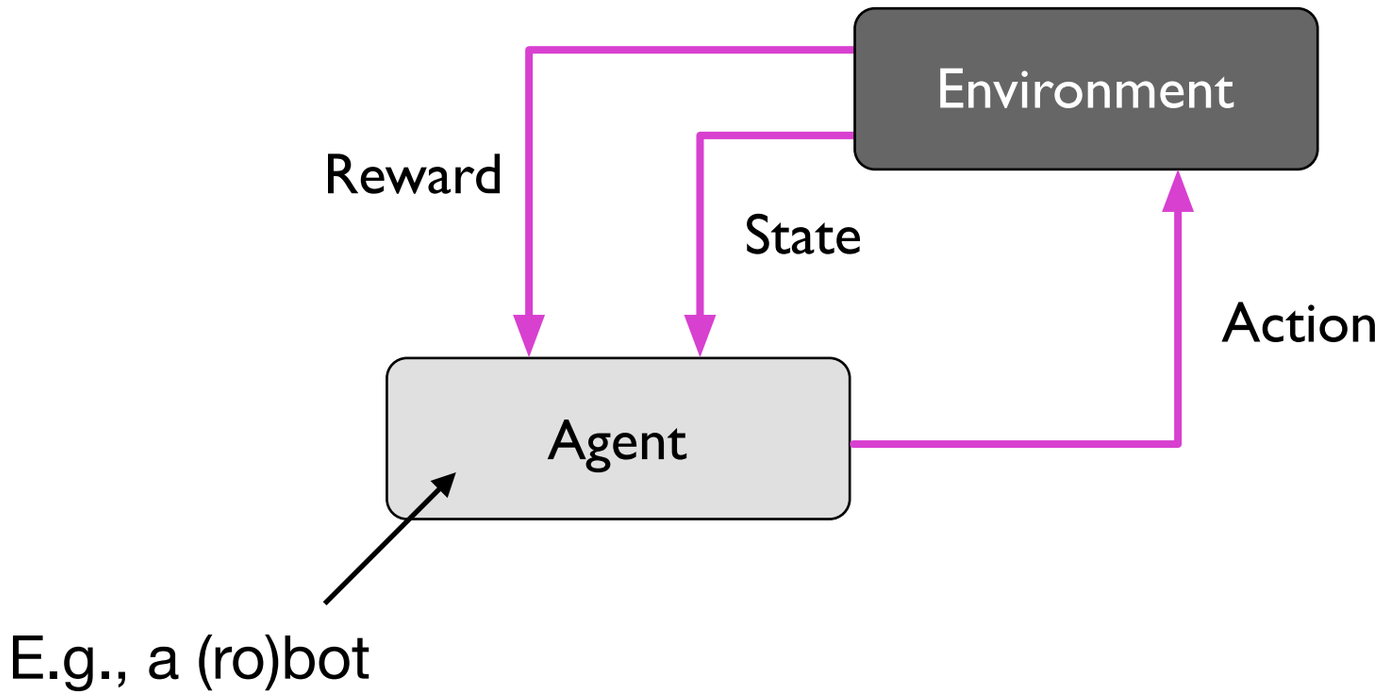


Semi-Supervised Learning

- mix between supervised and unsupervised learning
- some training examples contain outputs, but some do not
- use the labeled training subset to label the unlabeled portion of the training set, which we then also utilize for model training

Reinforcement Learning

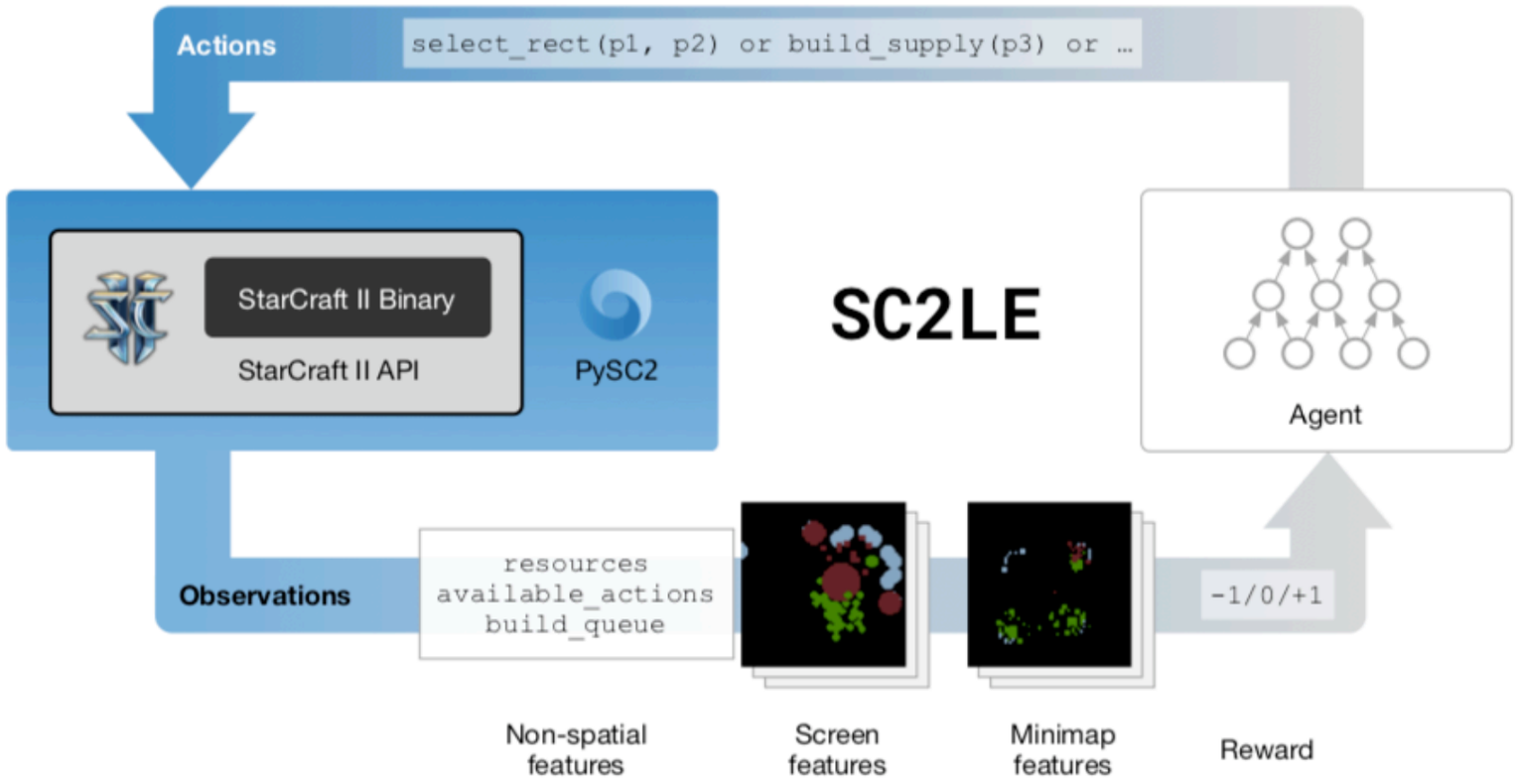
maximize the reward for a *series* of actions



(Probably won't cover this in this course)

Reinforcement Learning

Current state-of-the-art benchmark: StarCraft II



Vinyals, Oriol, Timo Ewalds, Sergey Bartunov, Petko Georgiev, Alexander Sasha Vezhnevets, Michelle Yeo, Alireza Makhzani et al. "Starcraft II: A new challenge for reinforcement learning." *arXiv preprint arXiv:1708.04782* (2017).

Machine Learning Jargon 1/2

- supervised learning:
  learn function to map input *x* (features) to output *y* (targets)

- structured data:
  databases, spreadsheets/csv files

- unstructured data:
  features like image pixels, audio signals, text sentences
  (previous to DL, extensive feature engineering required)

Supervised Learning (more formal notation)

"training examples"

Training set: $\mathscr{D} = \{\langle \mathbf{x}^{[i]}, y^{[i]} \rangle, i = 1, \ldots, n\},$

Unknown function: $f(\mathbf{x}) = y$

Hypothesis: $h(\mathbf{x}) = \hat{y}$ sometimes *t* or *o*

Classification

$h : \mathbb{R}^m \rightarrow \mathscr{Y}, \quad \mathscr{Y} = \{1, \ldots, k\}$

Regression

$h : \mathbb{R}^m \rightarrow \mathbb{R}$

Data Representation

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix}$$

Feature vector

Data Representation

$$\mathbf{x} = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_m \end{bmatrix}$$

Feature vector

$$\mathbf{X} = \begin{bmatrix} \mathbf{x}_1^T \\ \mathbf{x}_2^T \\ \vdots \\ \mathbf{x}_n^T \end{bmatrix}$$

Design Matrix

$$\mathbf{X} = \begin{bmatrix} x_1^{[1]} & x_2^{[1]} & \cdots & x_m^{[1]} \\ x_1^{[2]} & x_2^{[2]} & \cdots & x_m^{[2]} \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{[n]} & x_2^{[n]} & \cdots & x_m^{[n]} \end{bmatrix}$$

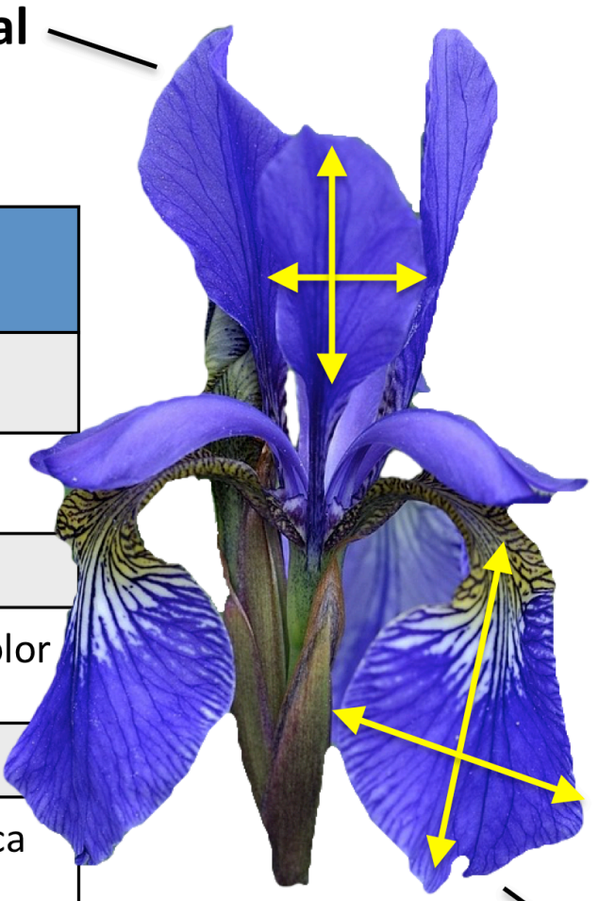
Design Matrix

Data Representation (structured data)

$m =$ ____

$n =$ ____

	Sepal length	Sepal width	Petal length	Petal width	
1	5.1	3.5	1.4	0.2	Setosa
2	4.9	3.0	1.4	0.2	Setosa
...					
50	6.4	3.5	4.5	1.2	Versicolor
...					
150	5.9	3.0	5.0	1.8	Virginica



Data Representation (unstructured data; images)

"traditional methods"

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686, 0.99215686, 0.99215686, 0.99215686, 0.99215686, 0.32941177, 0.14901961, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0
, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0
, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0, 0.0
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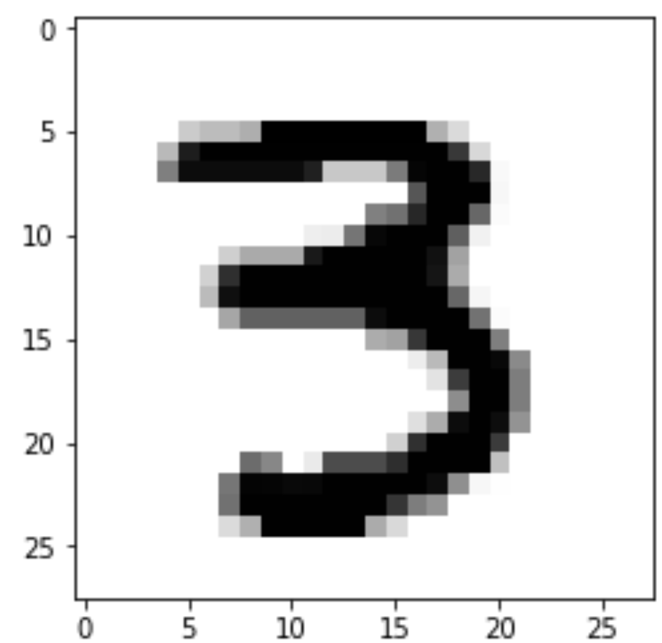

Data Representation (unstructured data; images)

Convolutional Neural Networks

```
Image batch dimensions: torch.Size([128, 1, 28, 28])
Image label dimensions: torch.Size([128])
```

← "NCHW" representation (more on that later)

```
print(images[0].size())
```

```
torch.Size([1, 28, 28])
```

```
images[0]
```

```
tensor([[[0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000,
          0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000,
          0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000,
          0.0000, 0.0000, 0.0000, 0.0000],
         [0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000,
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          0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000,
          0.0000, 0.0000, 0.0000, 0.0000],
         [0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000,
          0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000,
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          0.0000, 0.0000, 0.0000, 0.0000],

         [0.0000, 0.0000, 0.0000, 0.0000, 0.5020, 0.9529, 0.9529, 0.9529,
          0.9529, 0.9529, 0.9529, 0.8706, 0.2157, 0.2157, 0.2157, 0.5176,
          0.9804, 0.9922, 0.9922, 0.8392, 0.0235, 0.0000, 0.0000, 0.0000,
          0.0000, 0.0000, 0.0000, 0.0000],
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          0.8471, 0.9922, 0.9922, 0.5961, 0.0157, 0.0000, 0.0000, 0.0000,
          0.0000, 0.0000, 0.0000, 0.0000],
         [0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000, 0.0000,
          0.0000, 0.0000, 0.0000, 0.0667, 0.0745, 0.5412, 0.9725, 0.9922,
```
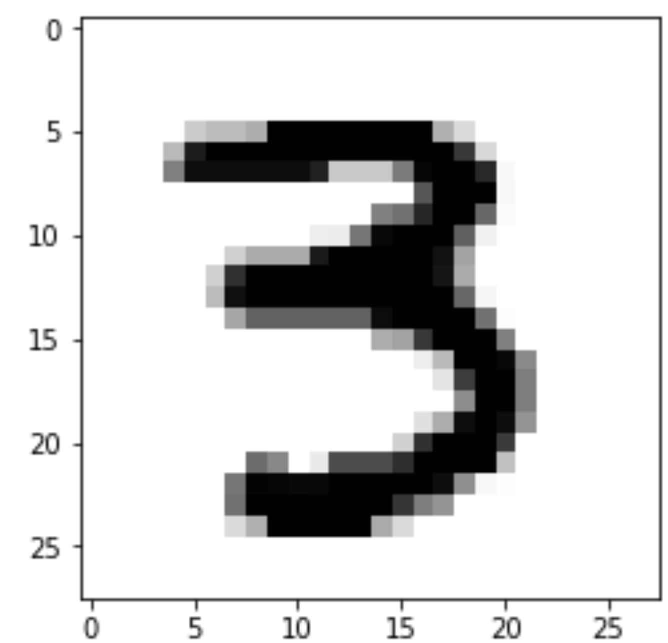



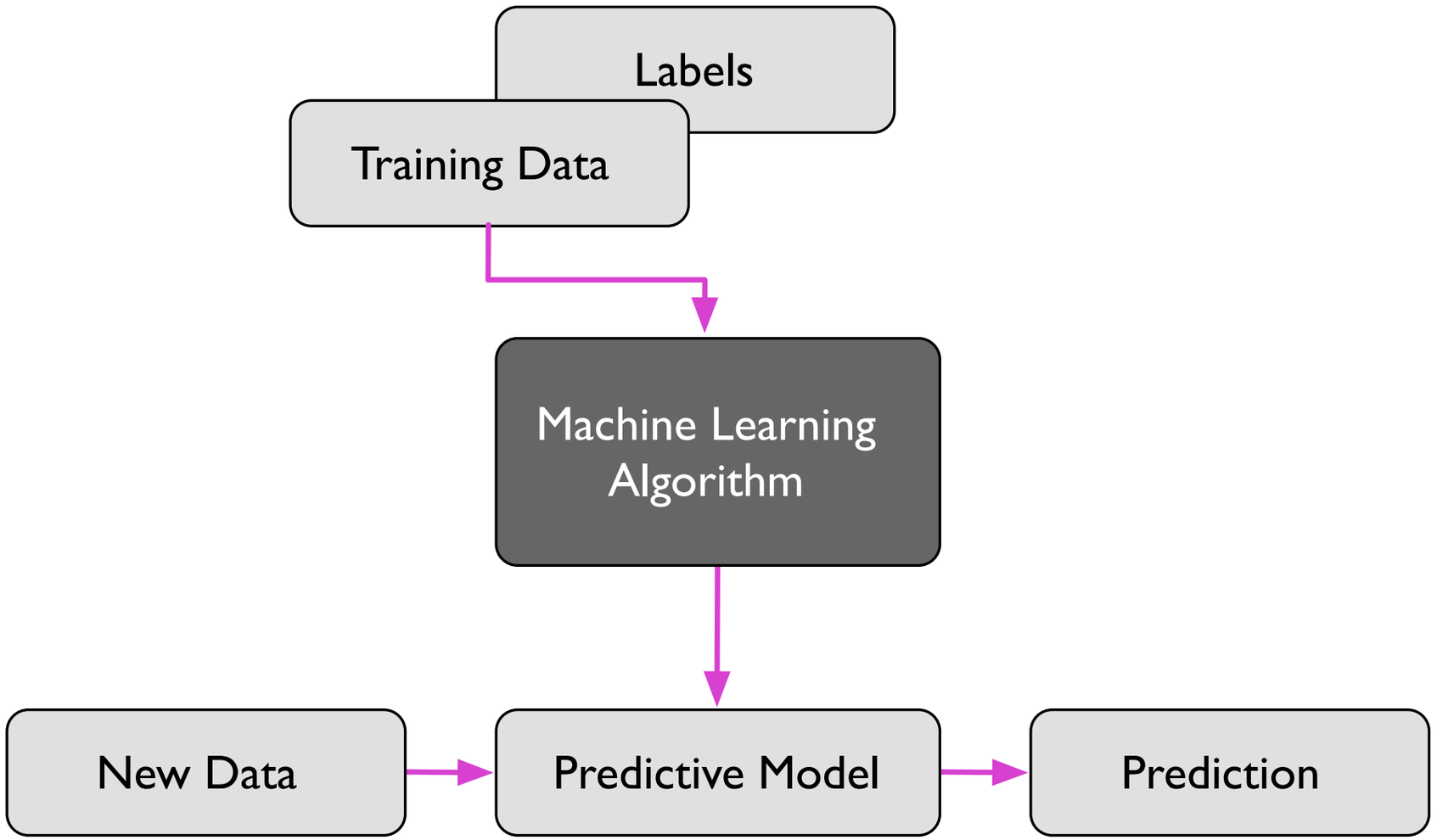
Machine Learning Jargon 2/2

- **Training example**, synonymous to
  observation, training record, training instance, training sample (in some contexts, sample refers to a collection of training examples)
- **Feature**, synonymous to
  predictor, variable, independent variable, input, attribute, covariate
- **Target**, synonymous to
  outcome, ground truth, output, response variable, dependent variable, (class) label (in classification)
- **Output / Prediction**, use this to distinguish from targets; here, means output from the model

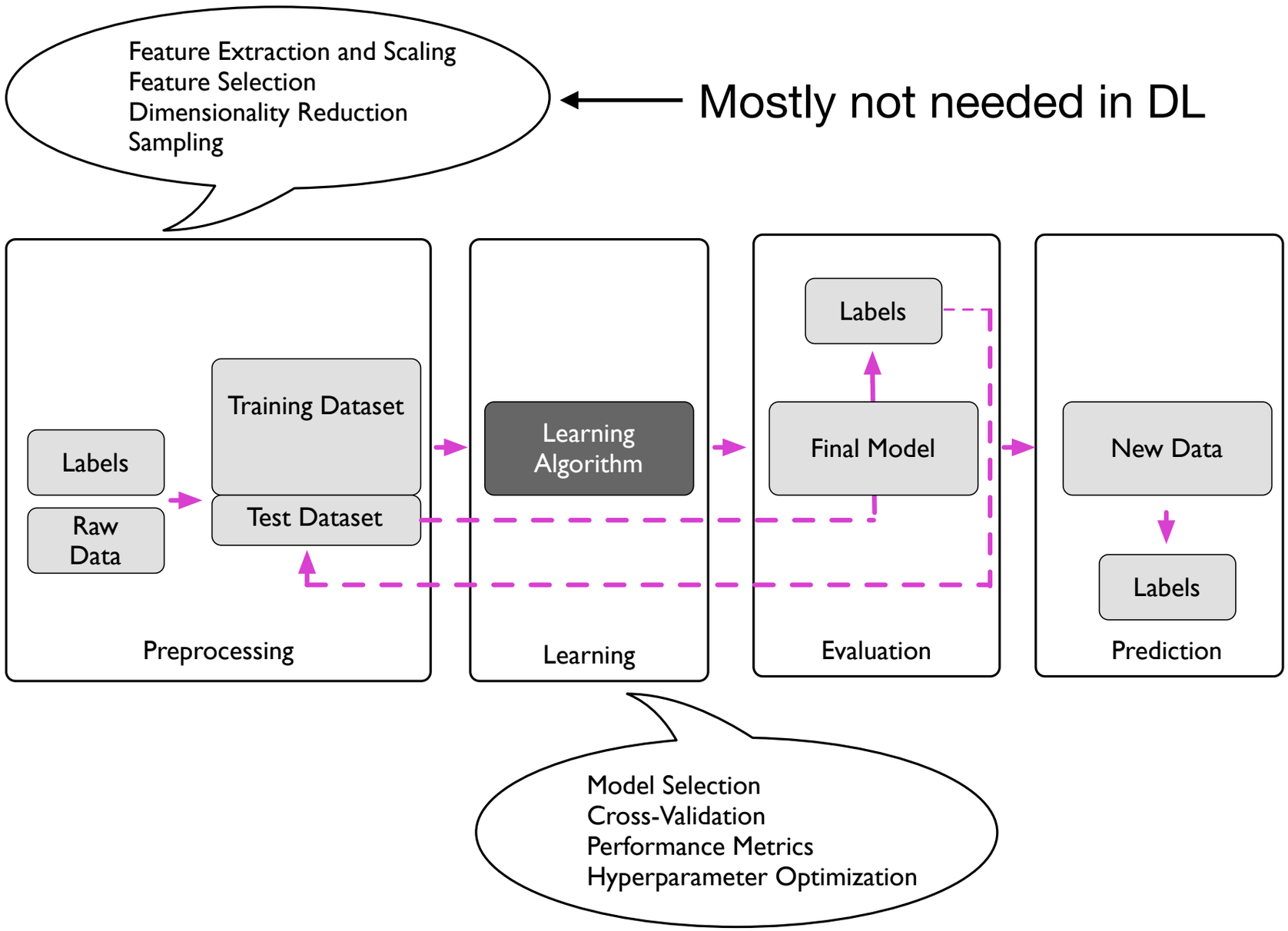
- use loss L for a single training example
- use cost C for the average loss over the training set
- use $\phi(\cdot)$, unless noted otherwise, for the activation function

(will make more sense later)

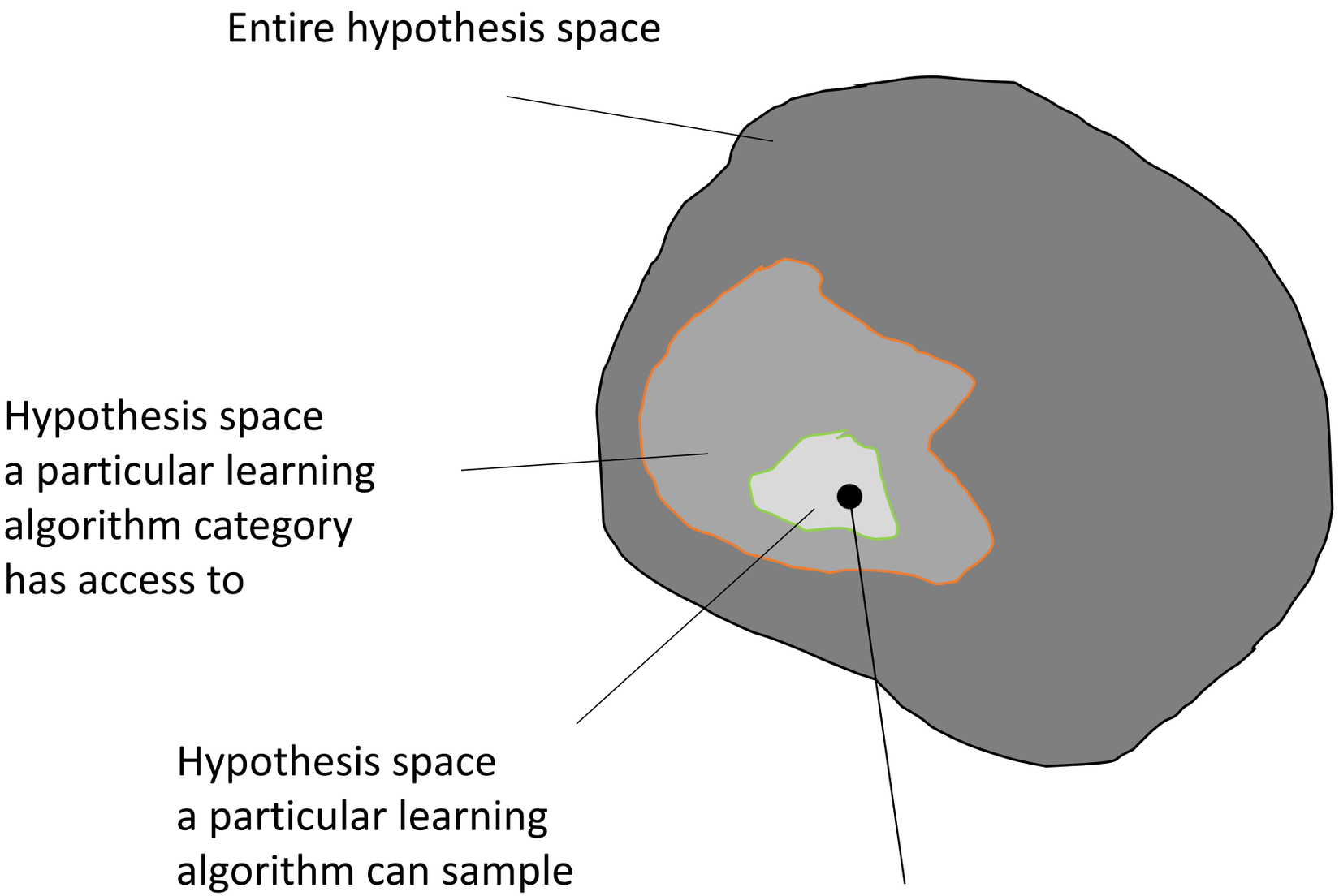
Supervised Learning Workflow



Supervised Learning Workflow (more detailed)



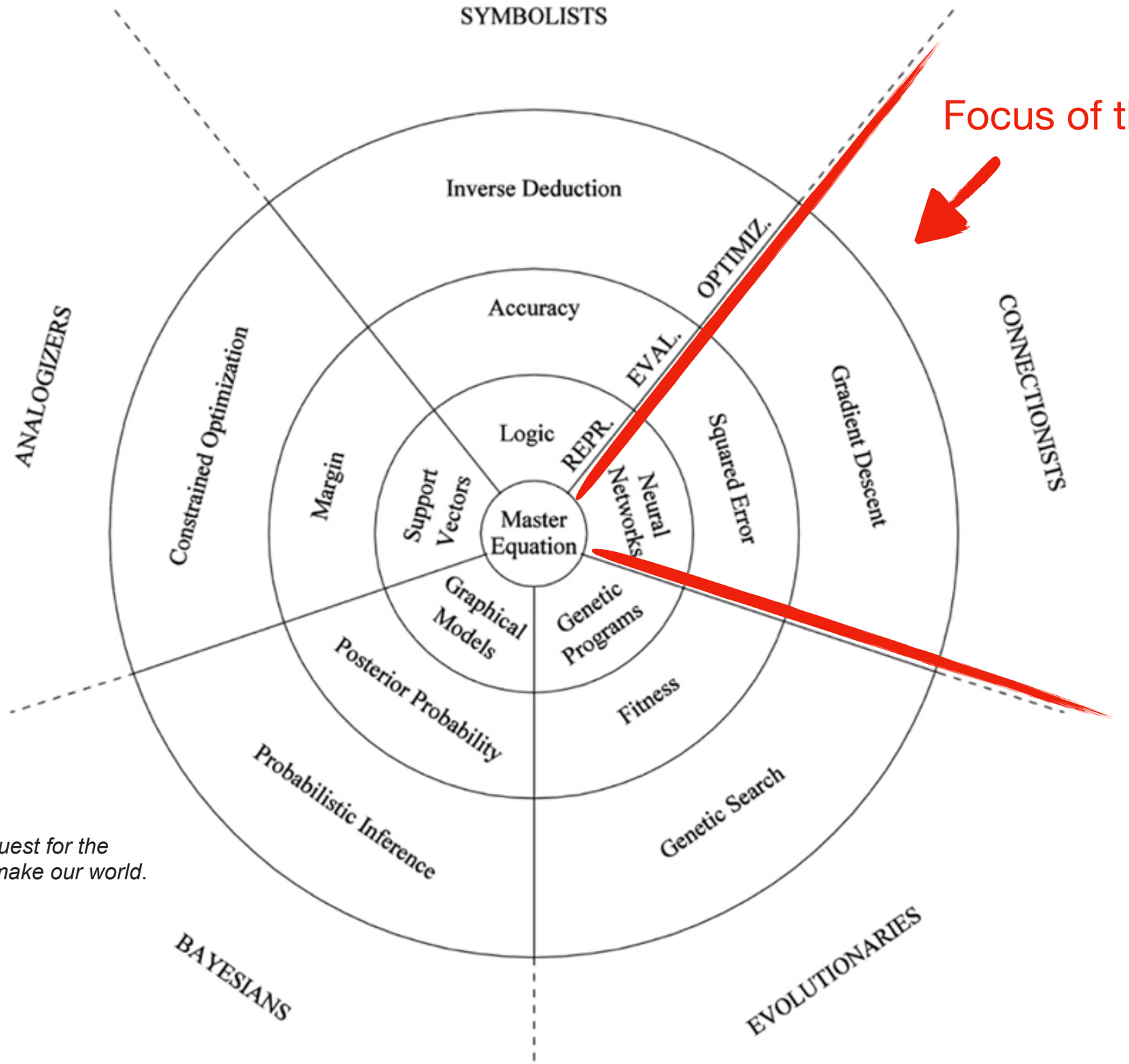
Hypothesis Space



5 Steps for Approaching an ML/DL Problem

1. Define the problem to be solved.
2. Collect (labeled) data.
3. Choose an algorithm class.
4. Choose an optimization metric for learning the model.
5. Choose a metric for evaluating the model.

Pedro Domingo's 5 Tribes of Machine Learning



Source: Domingos, Pedro.
The Master Algorithm: How the quest for the ultimate learning machine will remake our world.
Basic Books, 2015.

Learning = Representation + Evaluation + Optimization

(Pedro Domingos, *A Few Useful Things to Know about Machine Learning* https://homes.cs.washington.edu/~pedrod/papers/cacm12.pdf)

Objective Functions / Surrogate Risk/Loss

- Maximize the posterior probabilities (e.g., naive Bayes)
- Maximize a fitness function (genetic programming)
- Maximize the total reward/value function (reinforcement learning)
- Maximize information gain/minimize child node impurities (CART decision tree classification)
- Minimize a mean squared error cost (or loss) function (CART, decision tree regression, linear regression, adaptive linear neurons, ...)
- Maximize log-likelihood or minimize cross-entropy loss (or cost) function
- Minimize hinge loss (support vector machine)

Optimization Methods

- Combinatorial search, greedy search (e.g., decision trees)
- Unconstrained convex optimization (e.g., logistic regression)
- Constrained convex optimization (e.g., SVM)
- Nonconvex optimization, here: using backpropagation, chain rule, reverse autodiff. (e.g., neural networks)
- Constrained nonconvex optimization (e.g., semi-adversarial nets)

0/1 Loss, Misclassification Error

$$L(\hat{y}, y) = \begin{cases} 0 & \textbf{if } \hat{y} = y \\ 1 & \textbf{if } \hat{y} \neq y \end{cases}$$

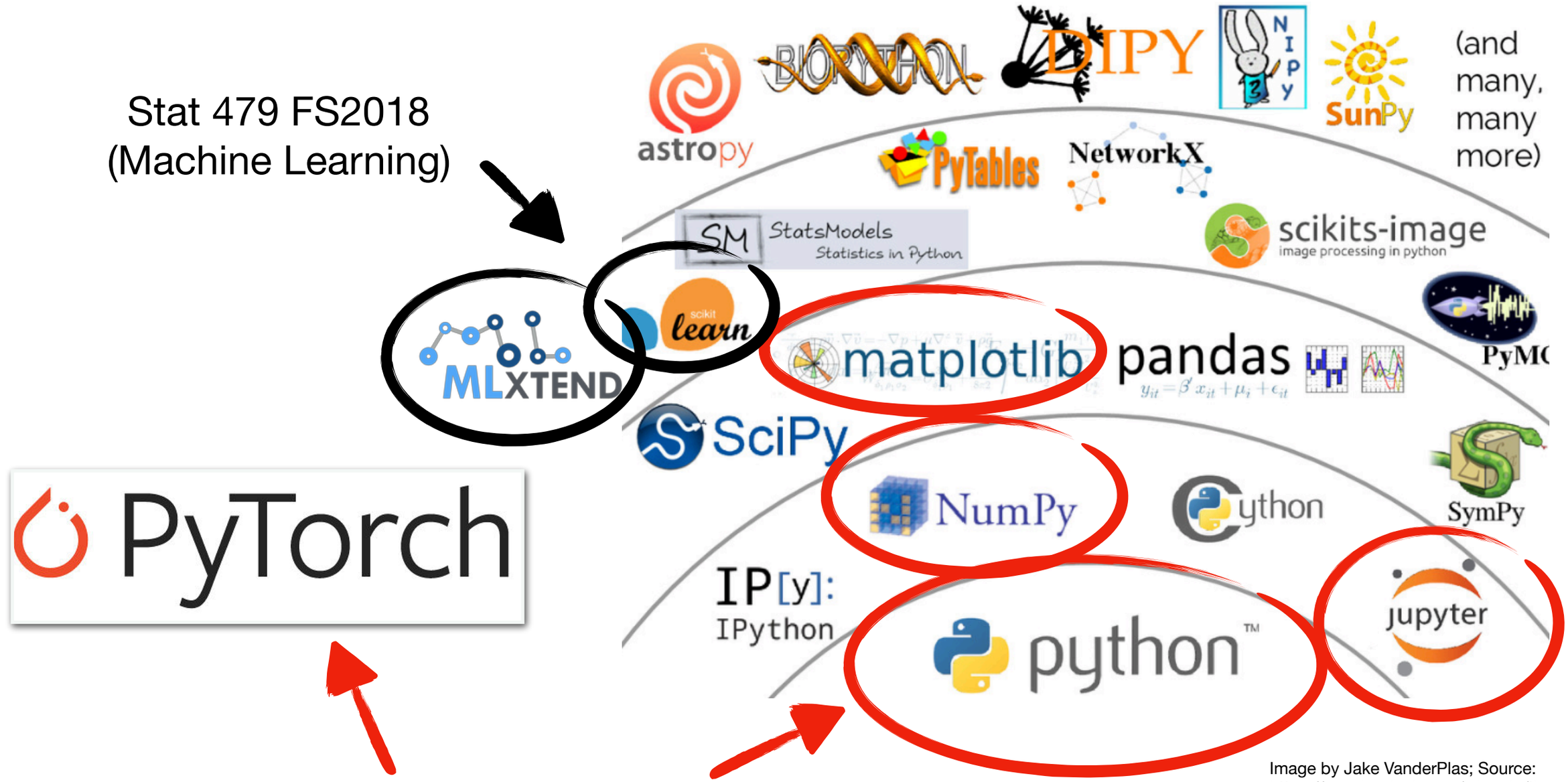
$$ERR_{\mathscr{D}}\textbf{test} = \frac{1}{n}\sum_{i=1}^{n} L\left(\hat{y}^{[i]}, y^{[i]}\right)$$

Other Performance Metrics

- Accuracy (1-Error)
- ROC AUC
- Precision
- Recall
- (Cross) Entropy
- Likelihood
- Squared Error/MSE
- L-norms
- Utility
- Fitness
- ...

Main Scientific Python Libraries

Stat 479 FS2018
(Machine Learning)



Main tools for this course

Image by Jake VanderPlas; Source: https://speakerdeck.com/jakevdp/the-state-of-the-stack-scipy-2015-keynote?slide=8)

Next Lecture:

A Brief Summary of the History of Neural Networks and Deep Learning

Reading Assignments

- Pedro Domingos, *A Few Useful Things to Know about Machine Learning* https://homes.cs.washington.edu/~pedrod/papers/cacm12.pdf

- STAT479 FS2018: Machine Learning, lecture notes 01: https://github.com/rasbt/stat479-machine-learning-fs18/blob/master/01_overview/01_ml-overview_notes.pdf

(exam questions also assume that you read the assigned reading materials)