THE PATH TO DEEP LEARNING

Ștefan Máthé

BOSCH

Outline

- Math Refresher: Probability Theory
- The Challenge
- Machine Learning
- The Path to Deep Learning

MATH REFRESHER: PROBABILITY THEORY

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Quick Math Refresher
Uncertainty

- Sources of uncertainty
  - Stochastic universe
  - Incomplete observations
  - Incomplete modelling

- Approaches to measure uncertainty:
  - **Frequentist**: repeatable event outcomes
  - **Bayesian**: degree of believe

- **Random Variables**

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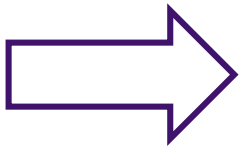

Governed by the same set of axioms

- **Random Variables**

Quick Math Refresher
Probabilities

- Probability Distributions
  - Probability Mass Function (PMF) ⇔ discrete variables
  - Probability Distribution Function (PDF) ⇔ continuous variables
- Joint Probability Distribution: $p(x, y)$
- Prior Probability Distribution: $p(x)$
- Conditional Probability Distribution: $p(y|x) = \frac{p(x,y)}{p(x)}$

Quick Math Refresher
Common Probability Distributions

- Binary Variables:
  - Bernoulli
  - Multinoulli
  - Multinomial
- Continuous Variables:
  - Gaussian
  - Dirac
  - Exponential
  - Laplace

$$\mathrm{P}(X = 1) = \theta$$
$$\mathrm{P}(X = 0) = 1 - \theta$$

Bernoulli

$$\mathrm{P}(X = i) = \theta_i, \forall i, 1 \leq i \leq k - 1$$
$$\mathrm{P}(X = 0) = 1 - \sum_{i=1}^{k-1} \theta_i$$

Multinoulli

$$p(X = x) = \frac{1}{\sqrt{2\pi\sigma}} e^{\frac{(x-\mu)^2}{2\sigma^2}}$$

Gaussian (1-dimensional)

$$p(X = \boldsymbol{x}) = \frac{1}{\sqrt{(2\pi)^n \det(\Sigma)}} e^{\frac{(\boldsymbol{x}-\boldsymbol{\mu})^\top \Sigma (\boldsymbol{x}-\boldsymbol{\mu})}{2\sigma^2}}$$

Gaussian (n-dimensional)

$$p(X = x) = \delta(x - \mu) \qquad \int_a^b \delta(x) = \begin{cases} 1 & a \leq x \leq b \\ 0 & \text{otherwise} \end{cases}$$

Dirac (1-dimensional)

Quick Math Refresher
Expectation and KL Divergence

- Expectation: “average” value of a function $f(x)$ when x is drawn from $p(x)$
  - For PDFs: $\mathbb{E}_{x\sim p(x)}[f(x)] = \int_x f(x)p(x)\mathrm{d}x$
  - For PMFs: $\mathbb{E}_{x\sim P(x)}[f(x)] = \sum_x f(x)P(x)\mathrm{d}x$

- KL Divergence: “distance” between two probability distributions

$$D_{KL}[P||Q] = \mathbb{E}_{x\sim P(x)}\left[\log\frac{P(x)}{Q(x)}\right]$$

  - Not a true distance (non-negative, but asymmetric and does not obey the triangle inequality)

THE CHALLENGE

The Challenge
Object Class Recognition: Easy or Hard?

Is this an image of a cat?

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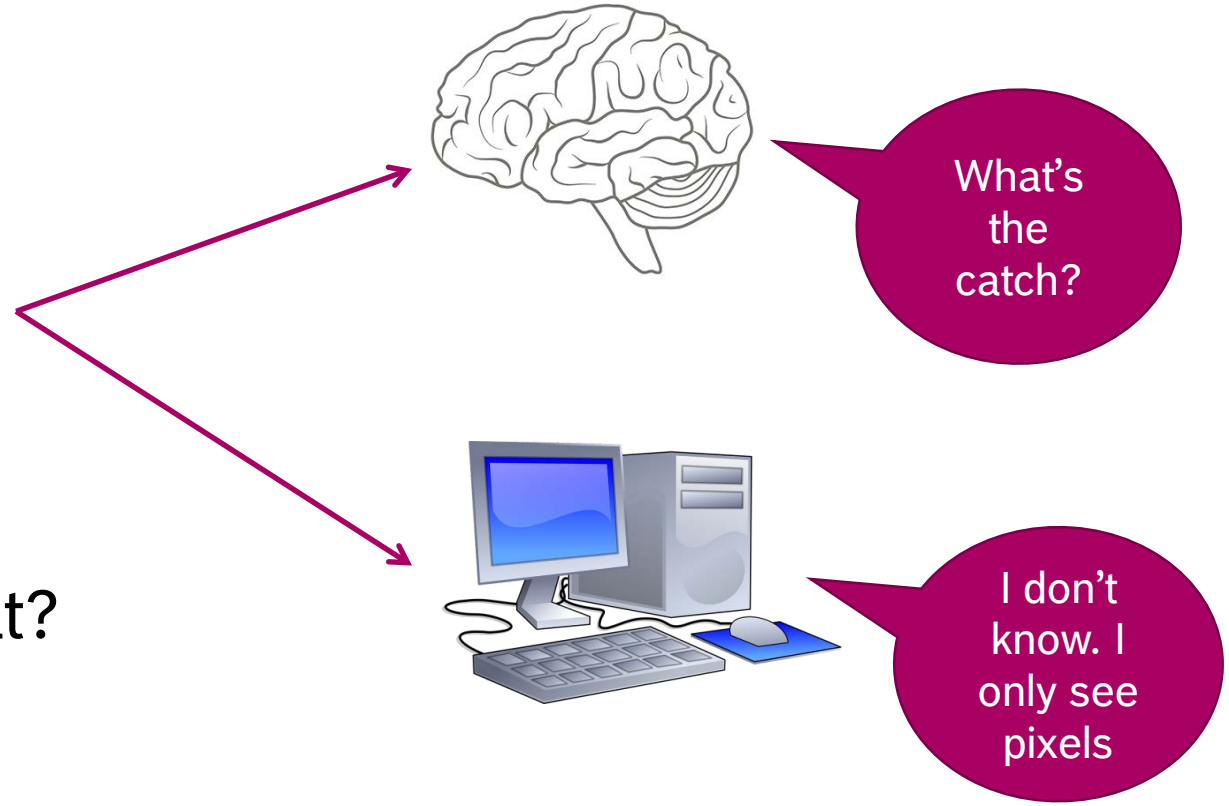

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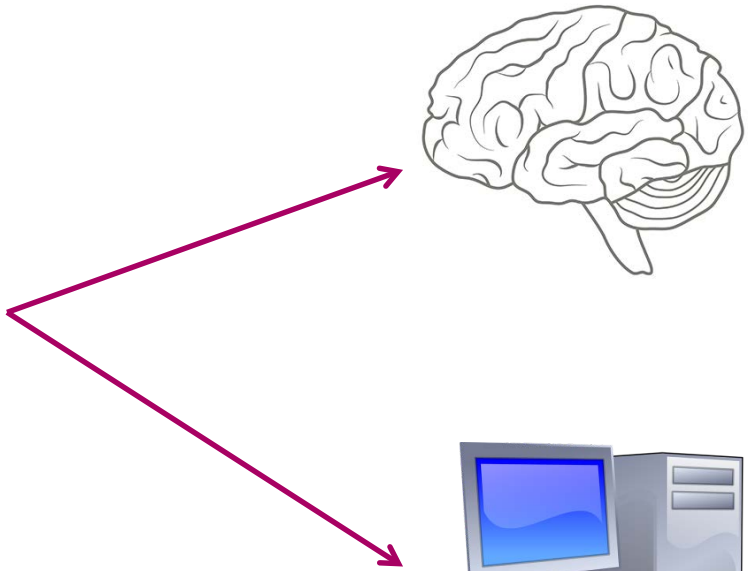

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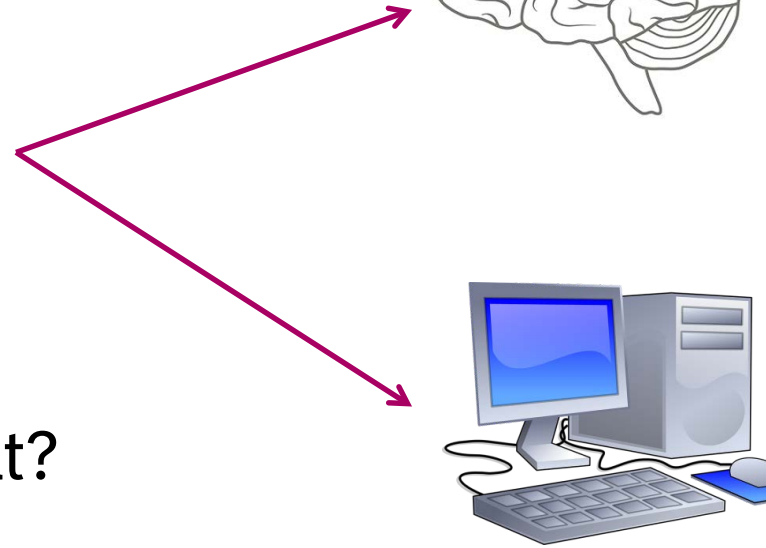
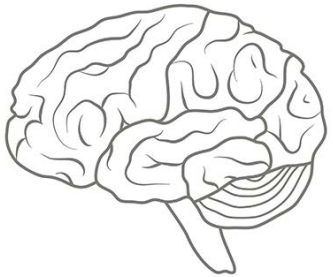




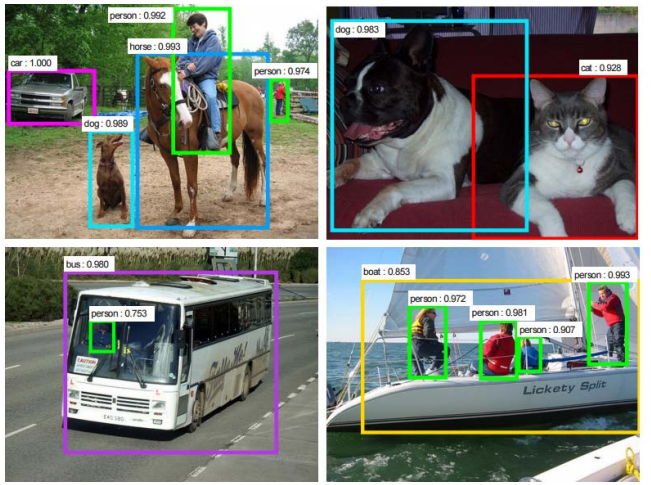
I don't have one. I look for a furry mammal with long pointy ears, etc.

Is this an image of a cat?

The Challenge
Problems with Inconspicuous Solutions

handwritten digit recognition

instance level segmentation



object detection

The Challenge
Humans vs. Thinking Machines

World of Humans	World of Thinking Machines: easy	World of Thinking Machines: hard
easy	**(not interesting)**	• **speech recognition** • **face recognition** • **car driving**
hard	• chess • go • question-answering (Quora)	• plant identification • cancer diagnosis

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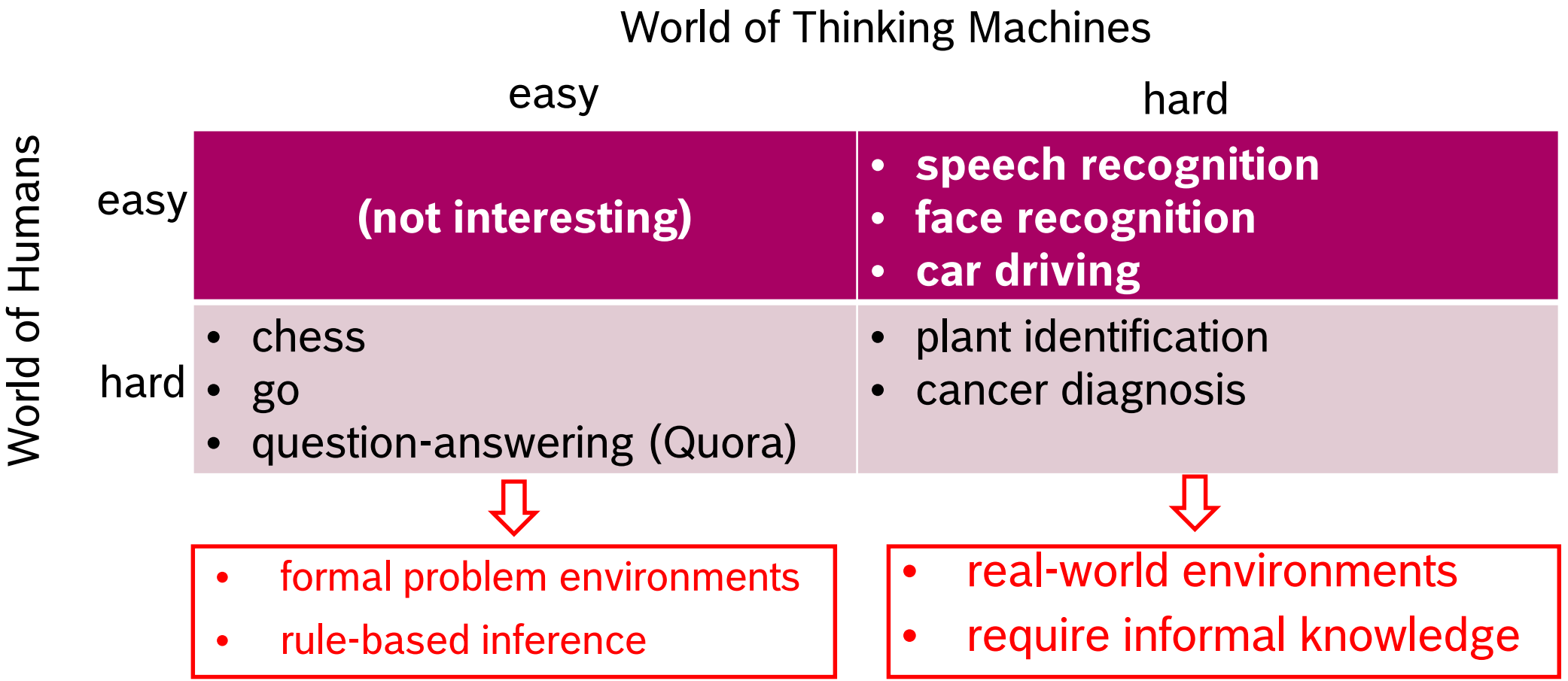
- formal problem environments
- rule-based inference

The Challenge
Humans vs. Thinking Machines

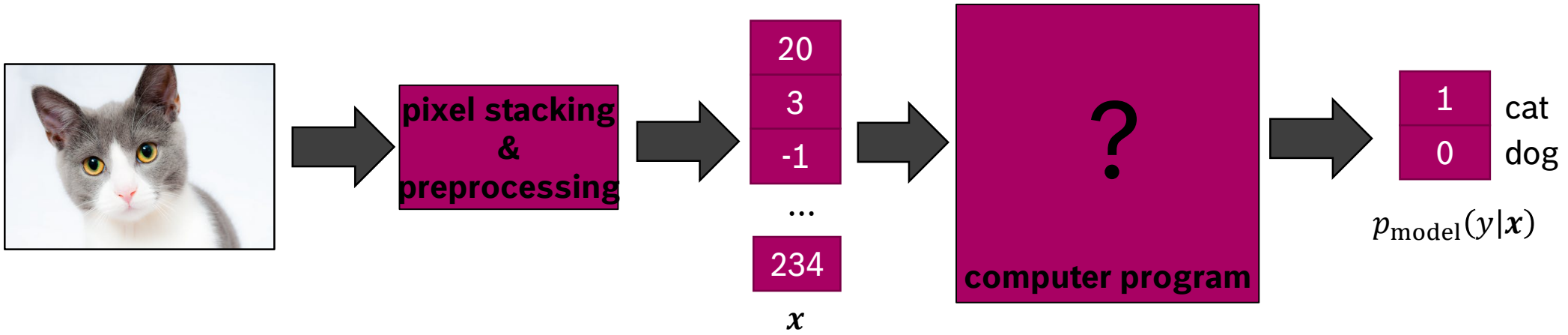


MACHINE LEARNING

BOSCH

Machine Learning
What do we want?

- A computer program
  - Input: a feature vector $\boldsymbol{x}$ obtained from the input image
  - Output: the probability $p_{\text{model}}(y|\boldsymbol{x})$ for each object class y



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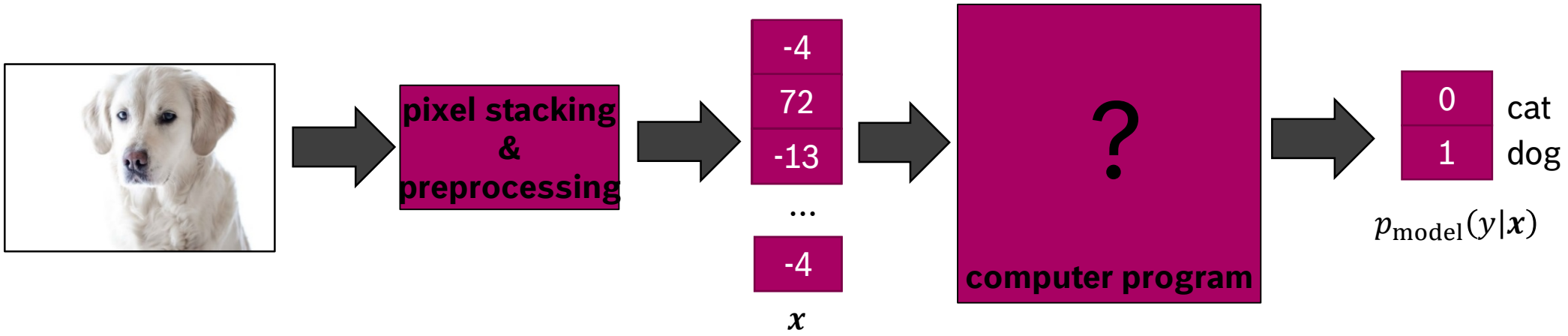

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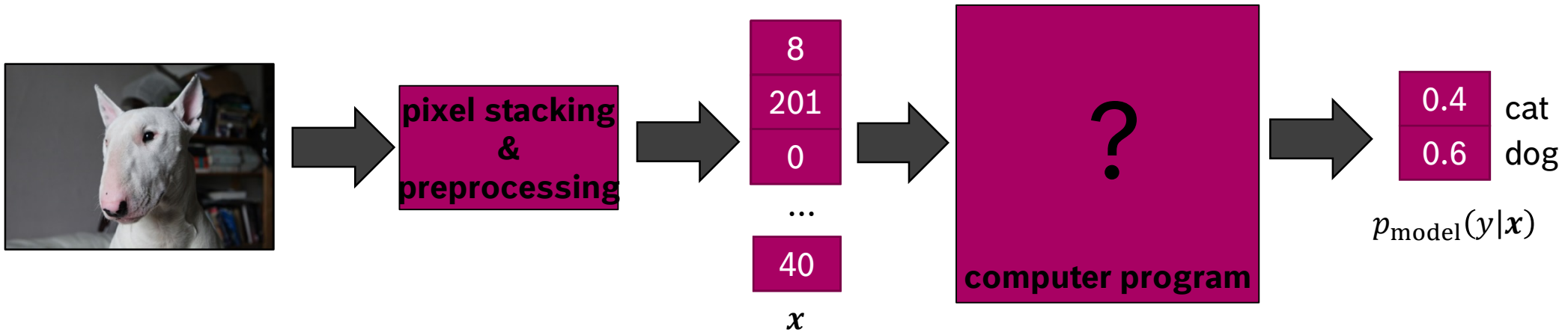


Machine Learning
What is a good solution?

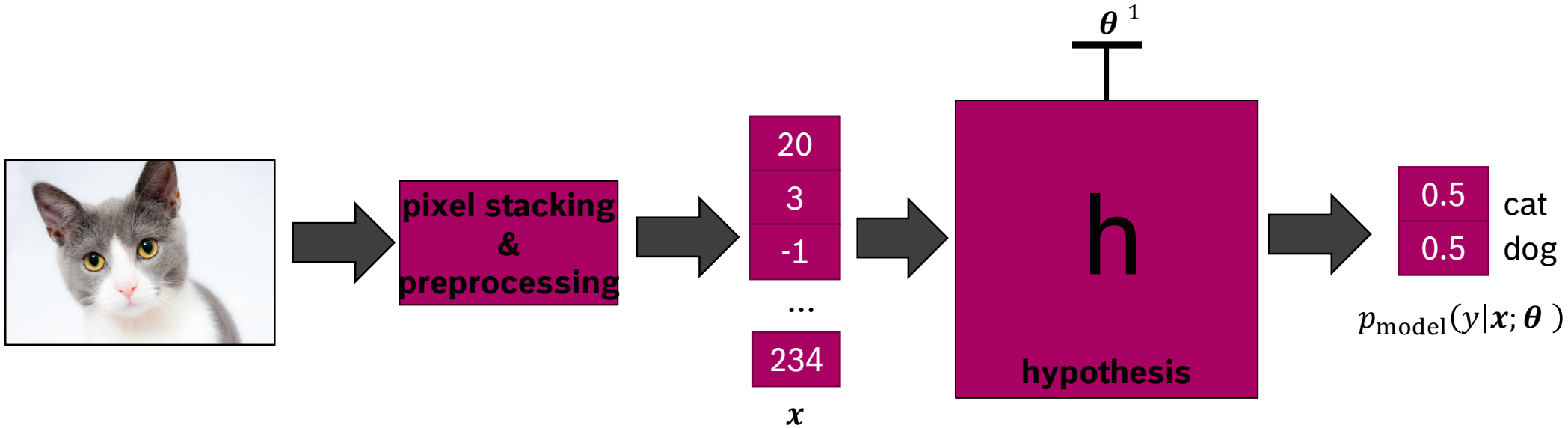
- Let $p_{\text{data}}(x, y)$ be the **true distribution** over features and labels
- Program output has a high **expected likelihood** on the true distribution:

$$\mathbb{E}_{\boldsymbol{x},y \sim p_{\text{data}}}[\log p_{\text{model}}(y|\boldsymbol{x})]$$

$p_{\text{data}}(x, y)$

Machine Learning
Parametric Hypothesis Space

- Consider a whole set H of possible programs H, called **hypothesis space**
- Assume each hypothesis is uniquely characterized by a **parameter vector $\boldsymbol{\theta}$**
- The parameter vector changes the behavior of our program



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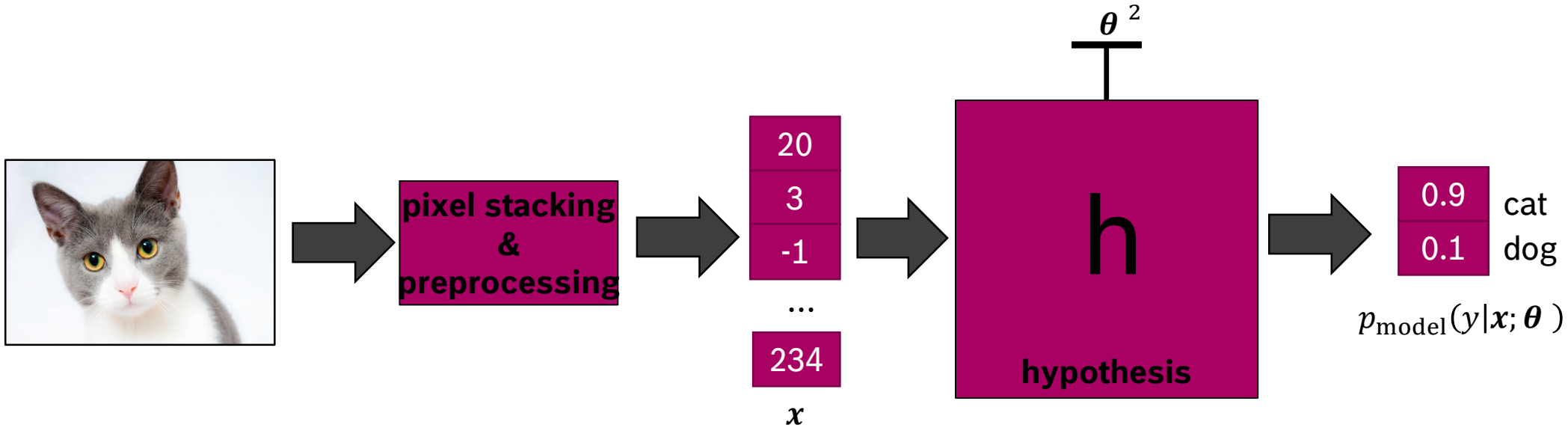

Machine Learning
The Ideal Setting

- Choose the hypothesis $\boldsymbol{\theta}^*$ that works best in the real world
- Formally: maximize the expected log likelihood on the true distribution

$$\boldsymbol{\theta}^* = \text{argmax}_{\boldsymbol{\theta}} \, \mathbb{E}_{x,y \sim p_{\text{data}}} [\log p_{\text{model}} (y|\boldsymbol{x}; \boldsymbol{\theta})]$$

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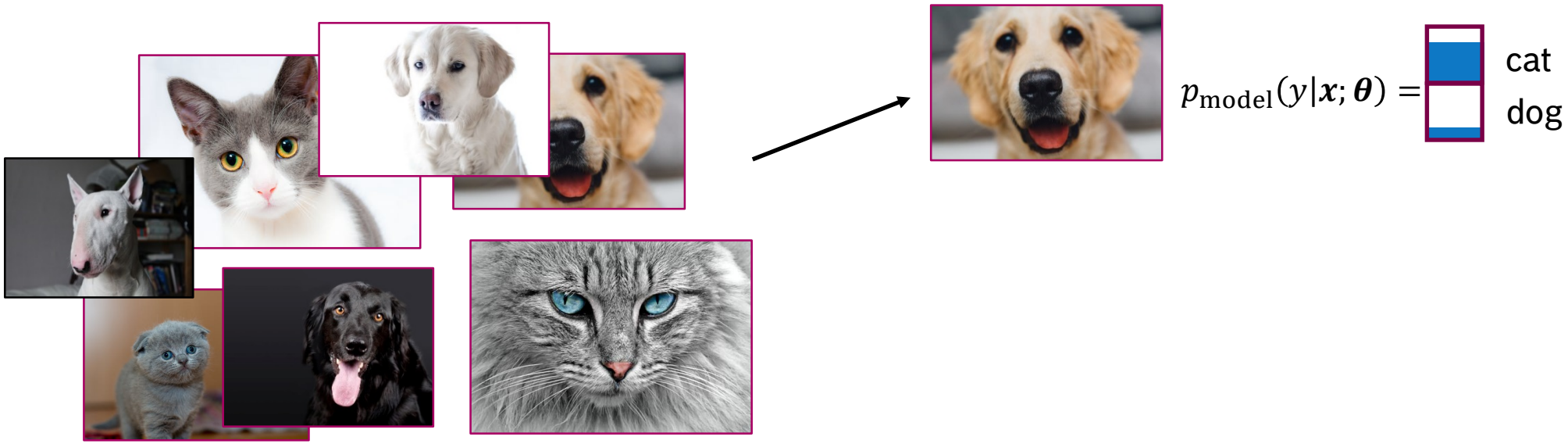

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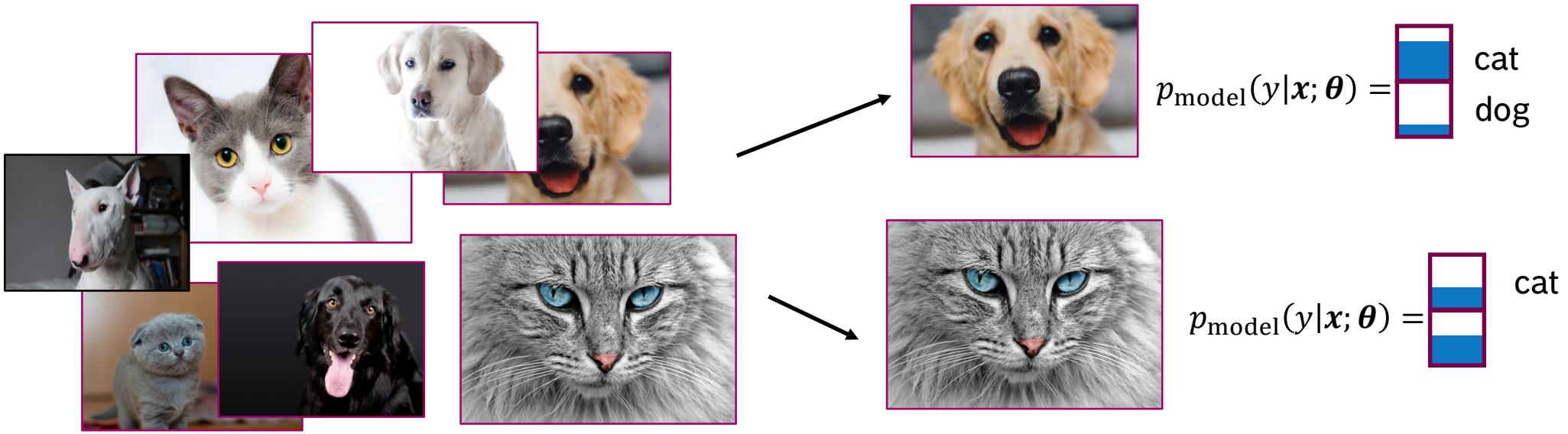

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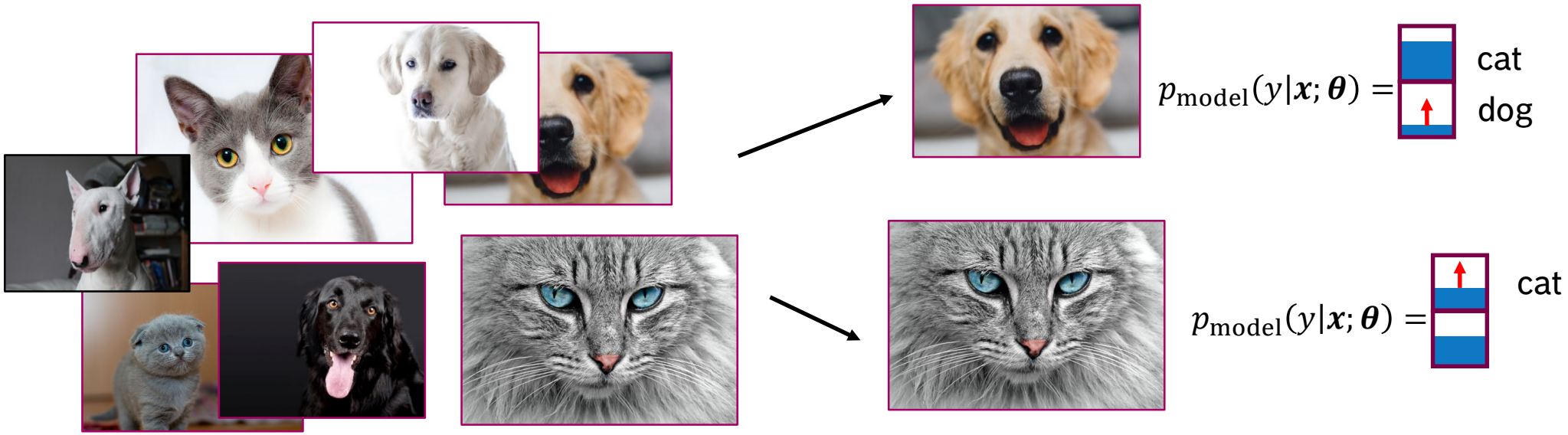

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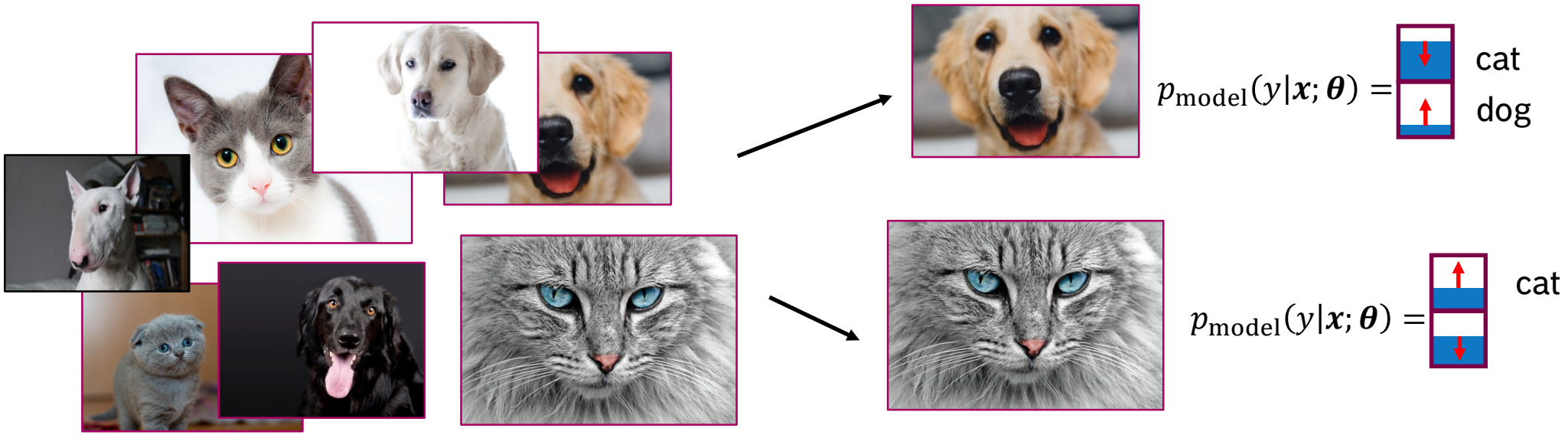
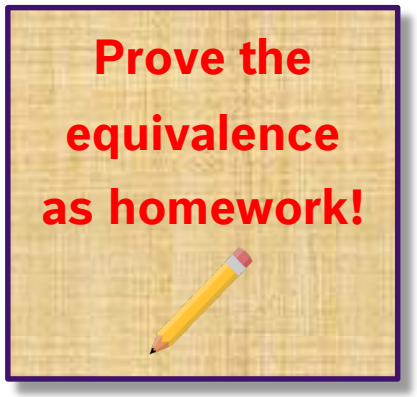


Machine Learning
Why Maximize the Log Likelihood?

- Numerical reasons
- Same as minimizing the divergence between the predicted and ground truth posteriors:

$$\boldsymbol{\theta}^* = \text{argmax}_{\boldsymbol{\theta}} \, \mathbb{E}_{x,y \sim p_{\text{data}}(x,y)} [\log p_{\text{model}}(y|\boldsymbol{x};\boldsymbol{\theta})]$$

$$\boldsymbol{\theta}^* = \text{argmin}_{\boldsymbol{\theta}} \, \mathbb{E}_{x \sim p_{\text{data}}(x)} \left[D_{\text{KL}} \left(p_{\text{data}}(y|\boldsymbol{x};\boldsymbol{\theta}) \,||\, p_{\text{model}}(y|\boldsymbol{x};\boldsymbol{\theta}) \right) \right]$$

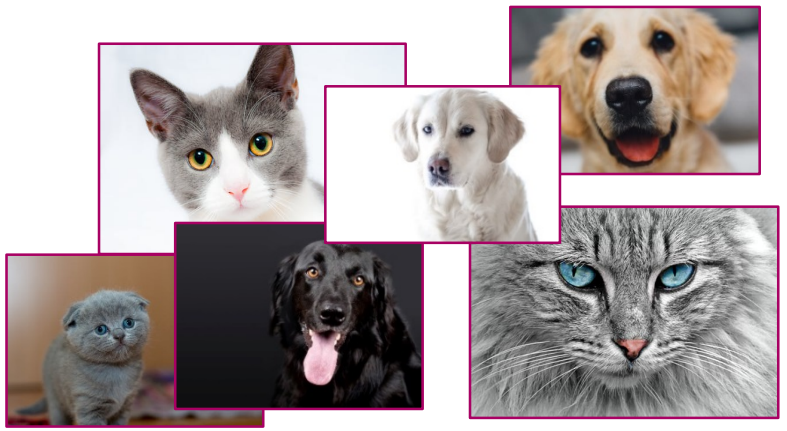


Machine Learning
Expectation Meets Reality

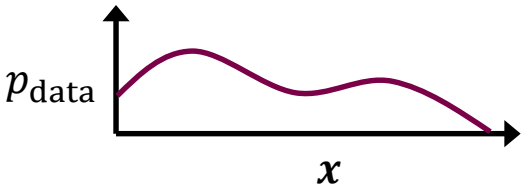
- But we do not have the true distribution!
- We only have a small **training set** drawn from the true distribution

$$\boldsymbol{x}_i, y_i \sim p_{\text{data}}(\boldsymbol{x}, y),\ i = \overline{1, n}$$

- The training set can be used to define the **empirical data distribution**:



$p_{\text{data}}(x, y)$



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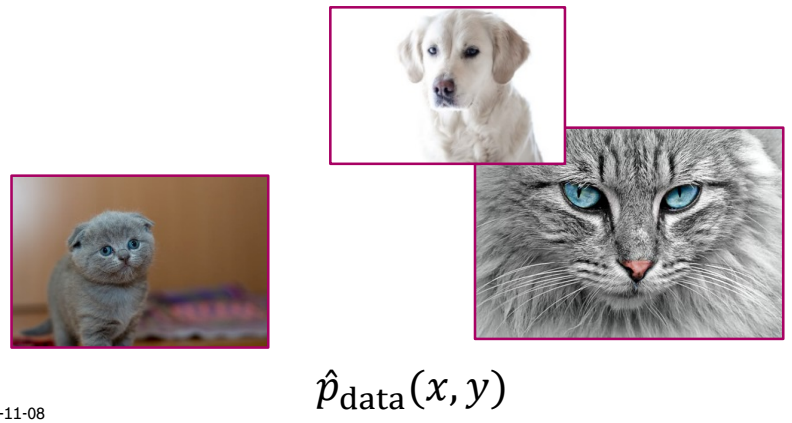

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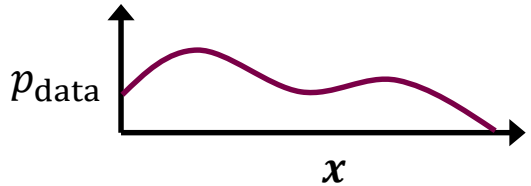

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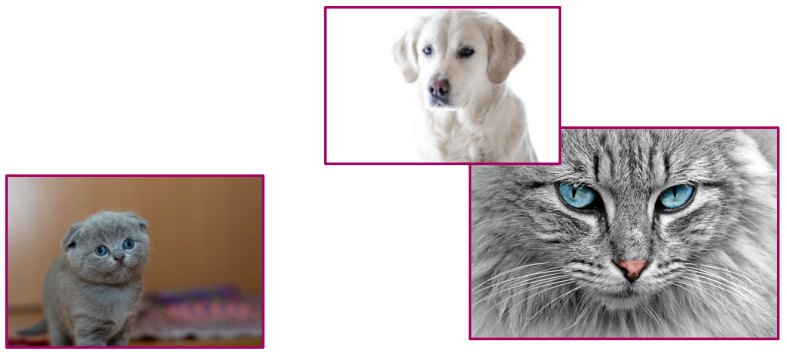

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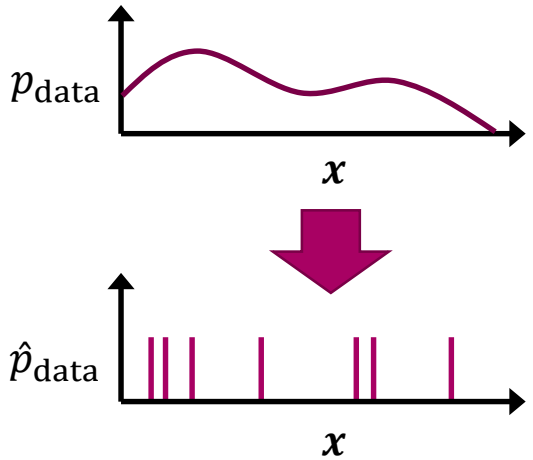

Machine Learning
The Compromise

- Solution: maximize the likelihood of the empirical data distribution
- Why would this work?

$p_{\text{data}}(x, y)$

$$\boldsymbol{\theta}^* = \text{argmax}_{\boldsymbol{\theta}} \, \mathbb{E}_{x,y \sim p_{\text{data}}} [\log p_{\text{model}} (y|\boldsymbol{x}; \boldsymbol{\theta})]$$

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$$\boldsymbol{\theta}^{\text{ML}} = \text{argmax}_{\boldsymbol{\theta}}\, \frac{1}{n} \sum_{\boldsymbol{i=1}}^{\boldsymbol{n}} \log p_{\text{model}}\,(y_i|\boldsymbol{x}_i; \boldsymbol{\theta})$$

Machine Learning
Justification: The IID Assumptions

- Look at the way we built our empirical distribution:

$$x_i, y_i \sim p_{\text{data}}(x, y),\ i = \overline{1, n}$$

- Assumption 1:
  - Data samples are drawn **independently** of each other
  - Why? Hypothesis always processes inputs from scratch.
- Assumption 2:
  - Training samples were **identically distributed**, i.e. drawn from the true distribution
  - Why? No learning unless training set is representative of the true world
- Are these assumptions enough?

Machine Learning
Justification: Maximum Likelihood Consistency

- An estimator is **consistent** if it converges given enough training data $(n \rightarrow \infty)$

- ML is **consistent** if:
  1. The hypothesis set contains the true model. For classifiers:

$$\exists \boldsymbol{\theta}, \forall \boldsymbol{x}, \forall y, p_{\text{data}}(y|\boldsymbol{x}) = \log p_{\text{model}}(y|\boldsymbol{x}; \boldsymbol{\theta})$$

  2. Each hypothesis is uniquely identified by $\boldsymbol{\theta}$

- In practice we never have enough data!

Machine Learning
The Loss Function

- Can also see ML as minimizing the **negative log likelihood** (NLL):

$$\boldsymbol{\theta}^{\mathrm{ML}} = \mathrm{argmin}_{\boldsymbol{\theta}} -\frac{1}{m}\sum_{\boldsymbol{i=1}}^{\boldsymbol{n}} \log p_{\mathrm{model}}\left(y_i|\boldsymbol{x}_i;\boldsymbol{\theta}\right)$$

- In general, we seek to minimize a **loss function** over the training set:

$$\boldsymbol{\theta}^{*} = \mathrm{argmin}_{\boldsymbol{\theta}}\, \mathcal{L}(\boldsymbol{\theta})$$

- NLL is a special case of loss function:

$$\mathcal{L}(\boldsymbol{\theta}) = -\frac{1}{m}\sum_{\boldsymbol{i=1}}^{\boldsymbol{n}} \log p_{\mathrm{model}}\left(y_i|\boldsymbol{x}_i;\boldsymbol{\theta}\right)$$

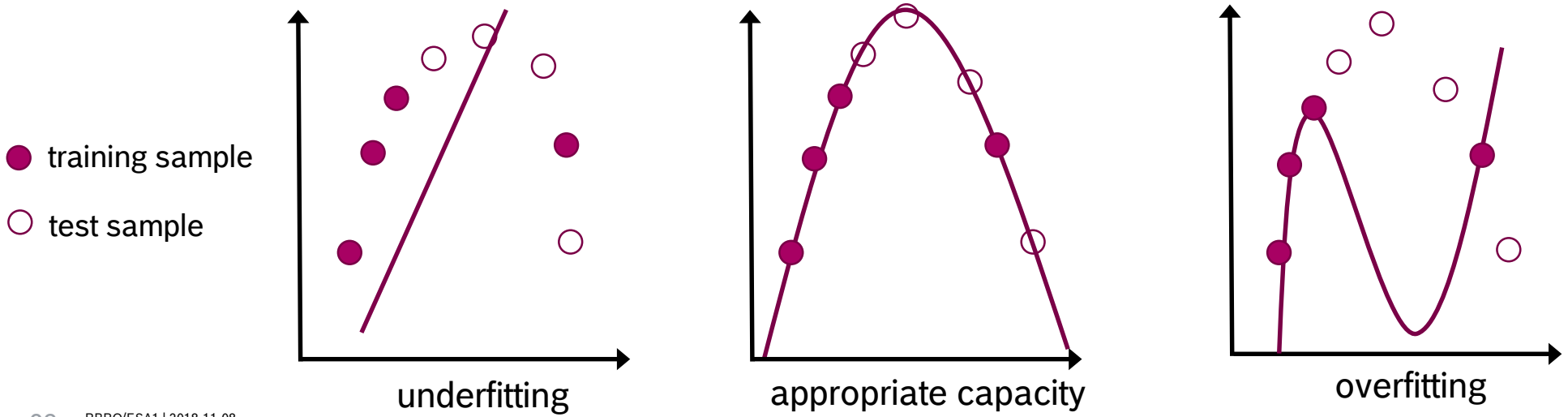
- The training loss is also called the **empirical risk**

Machine Learning
The Dangers of Failed Assumptions: Underfitting and Overfitting

- **Underfitting**: cannot find a model that fits the training data

  ⇔high loss on training data
- **Overfitting**: cannot find a model that generalizes on test (unseen) data

  ⇔ low training loss, high test loss



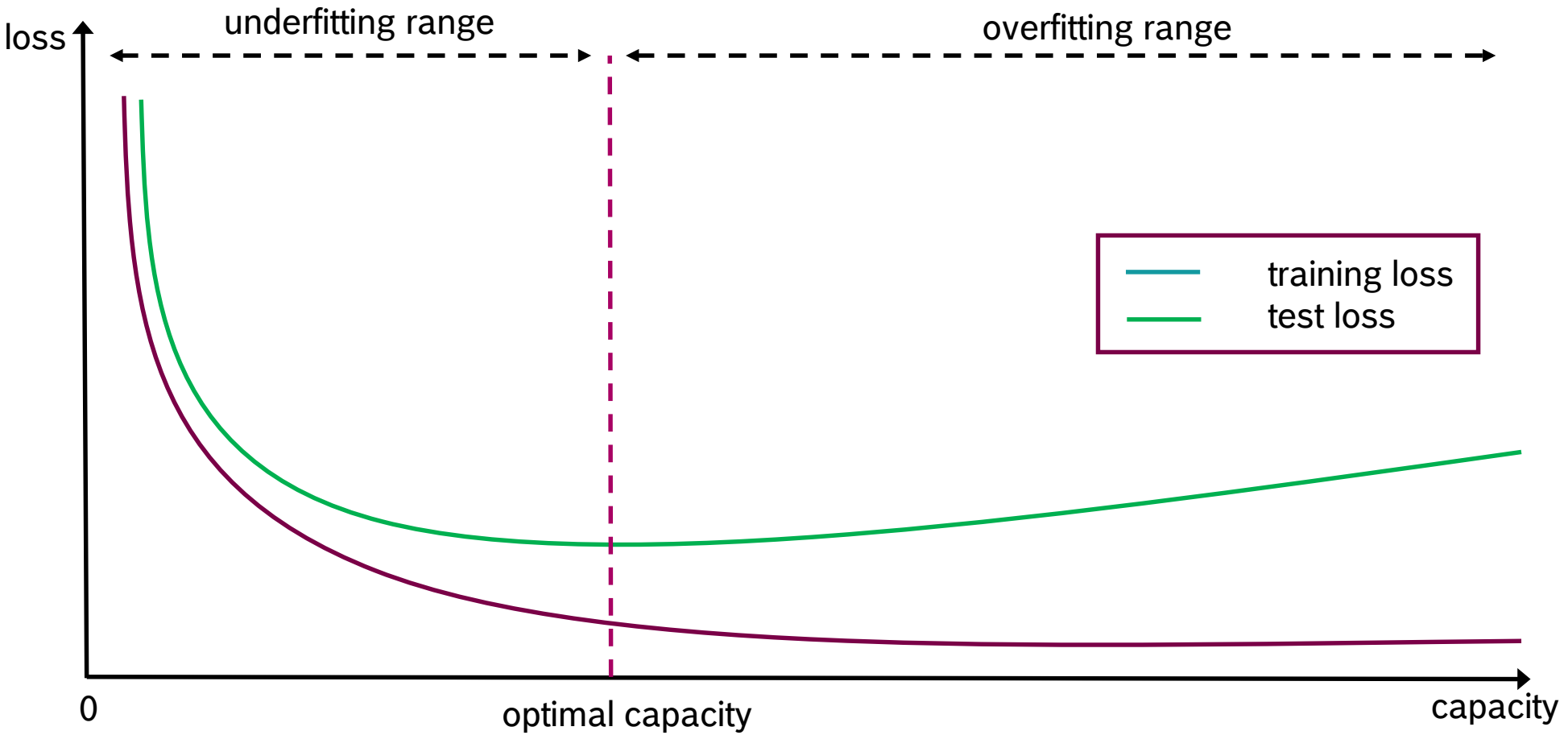
Machine Learning
Model Capacity

- **(Effective) capacity** = ability of the model to fit a wide variety of functions
- **Representational capacity** = ability of the hypothesis set to fit a wide variety of functions
- Due to imperfect optimizers:

$$\text{effective capacity} \leq \text{representational capacity}$$

- Underfitting ⇔effective capacity too low
- Overfitting ⇔effective capacity too high
- Formal definitions of capacity exist: Vapnik-Chervonenkis Dimension, Rademacher Complexity

Machine Learning
Capacity-Loss Relationship Curve



Machine Learning
Regularization (Capacity Control)

- Need to control model capacity:
  - via the optimization process (do not look for the optimal solution)
  - optimize a different objective that also looks at the parameters
  - restrict hypothesis set
- All of these methods introduce a bias:
  - Favor some hypotheses over others
  - Ockham's Razor principle: prefer simple explanations of the data
- There is no universally applicable bias:

The "no free lunch" theorem: ***Averaged over all data distributions, any two machine learning algorithms have the same accuracy (Wolpert, 1996)***

Machine Learning
Definition

- Machine learning can do much more than classification!

"A computer program is said to learn from experience E with respect to some class of tasks T and performance measure P , if its performance at tasks in T , as measured by P , improves with experience E." (Mitchell, 1997)

Machine Learning
The Task (T)

Task	Input	Output	Example Problem
classification	feature vector	discrete category	object recognition
regression	feature vector	real-valued quantity	image quality assessment
transcription	feature vector	sequence of symbols	transcribe text from image
translation	sequence of symbols	sequence of symbols	translate from English to German
synthesis	sequence of symbols feature vector	real-valued signal	speech synthesis style transfer
denoising	real-valued signal	real-valued signal	image restoration

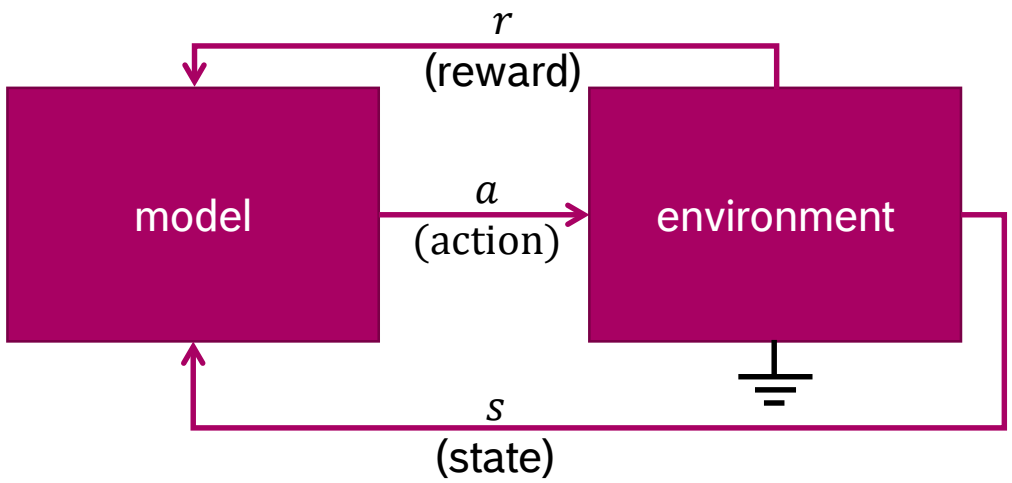
- The list above is far from exhaustive!

Machine Learning
The Experience (E)

supervised learning

unsupervised learning

semi supervised learning
(some labels may be missing)



reinforcement learning

Machine Learning
The Performance Measure (P)

- Very much task dependent

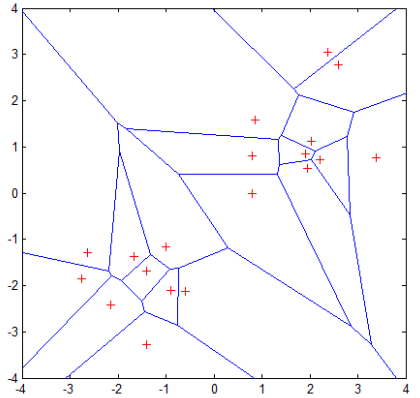
- For non-interactive methods: loss measured over the test set
  - Negative log likelihood (cross entropy)
  - 0-1 loss
  - Euclidean Loss
  - Hinge Loss
  - etc.

- For reinforcement learning: expected reward

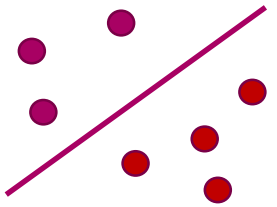
- Many losses correspond to probabilistic interpretations of model outputs (e.g. Euclidean Loss ⇔ Gaussian Output Distributions)

Machine Learning
Model Examples

- Shallow models
  - Non-parametric:
    - k-Nearest Neighbor (kNN) (Fixed & Hodges, 1951)
    - Kernel Density Estimation (Parzen, 1956; Rosenblatt,1962)
  - Parametric:
    - Linear Regression (Legendre, 1805)
    - Logistic Regression (David Cox, 1958)
    - ADALINE (Widrow & Hoff, 1960)
    - Support Vector Machines (SVM) (Vapnik & Chervonenkis, 1963)
    - Decision Trees (Morgan & Sonquist, 1963)
- Deep Models
  - Multilayer Perceptron (MLP) (Ivaknenko & Lapa, 1965)
  - Neocognitron (Fukushima, 1980)
  - Lenet-5 (Lecun et al., 1998)
  - AlexNet (Krizhevsky et al., 2012)
  - ResNet (He et al., 2015)



kNN decision surface



SVM decision surface

Machine Learning
Recap

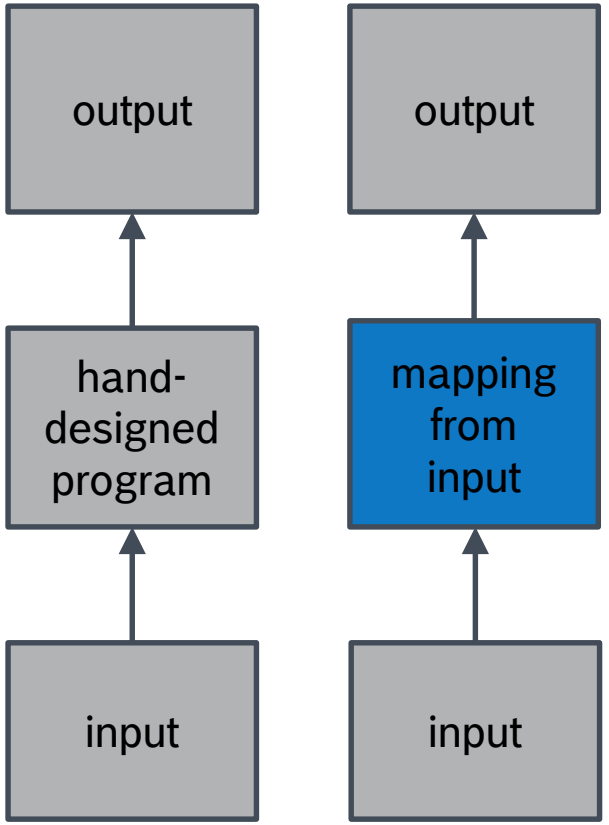
- Reformulated the inference problem as a machine learning problem
- Select the best hypothesis such that:
  - Fits the training data (seen)
  - Generalizes to the real world data (unseen)
- These are conflicting goals!
- The true challenges:
  - Controlling model capacity (underfitting, overfitting)
  - Introducing the right bias
  - Finding the hypothesis that fits the data (optimization problem)

THE PATH TO DEEP LEARNING

BOSCH

The Path to Deep Learning
Approaches to AI

- Rule Based Approaches
  - Hard-code informal knowledge in a formal language
  - Not very successful ☹
- Machine Learning Approaches
  - Acquire knowledge automatically from real-world data
  - Most promising to date ☺
  - But wait! What kind of knowledge? Can we learn a mapping from input to output?
  - We need to cover a large abstraction gap!



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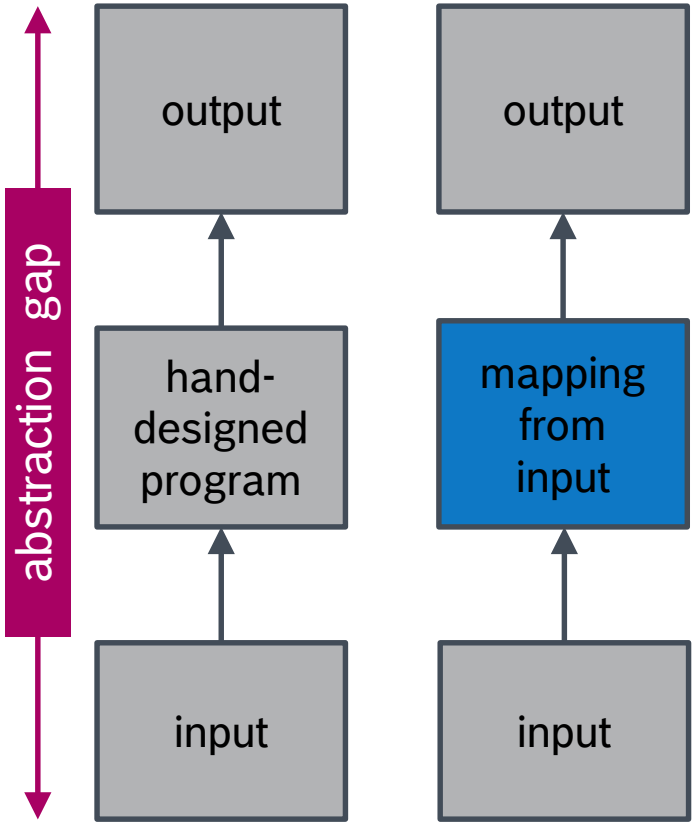


The Path To Deep Learning
Closing the Abstraction Gap is Difficult!

- Images are the complex result of multiple interacting **factors of variation**
- Need to separate what is relevant from what is not!

illumination

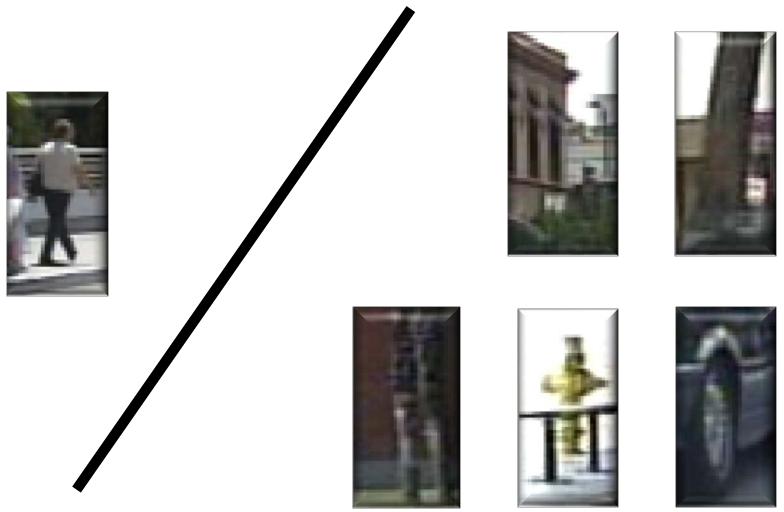
deformation

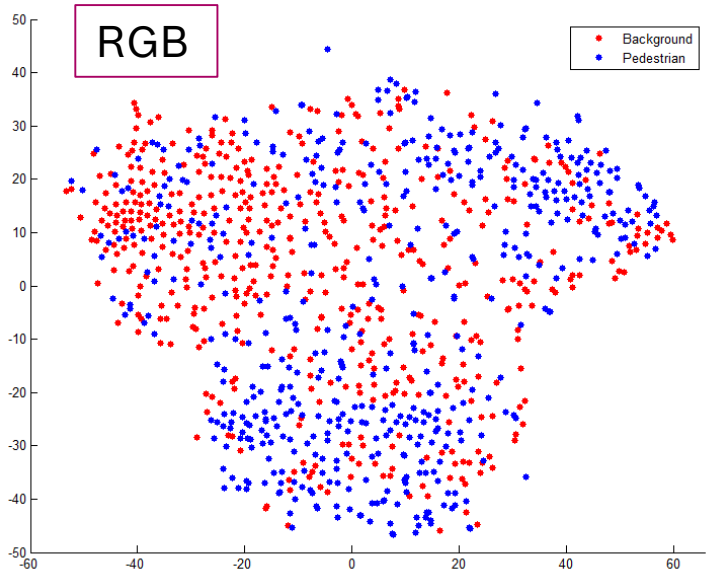
occlusion

Images taken from Fei-Fei, Karpathy & Johnson, Lecture Notes, 2016

The Path to Deep Learning
The Representation Problem

- We need **features**: relevant information extracted from the input
- How do we come up with good features?

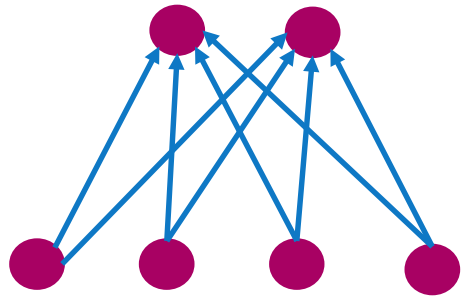




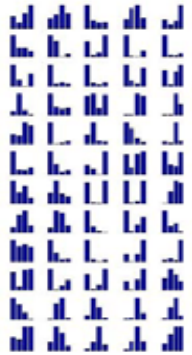
The Path to Deep Learning

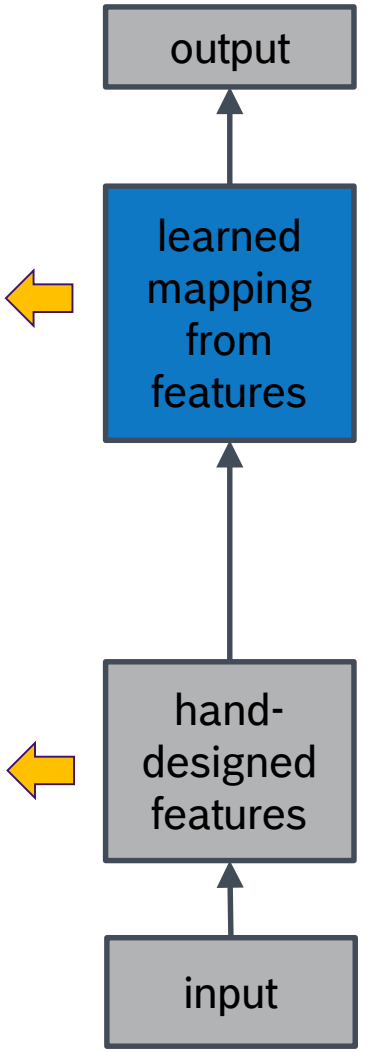
First Generation: Hand-Designed Representations

- Write a program to extract features!
- Examples:
  - **Edges (Canny)**
  - **Histograms of Gradients (HoGs)**
  - **Haar-like features**
  - **Aggregated Channel Features (ACF)**
- Pros:
  - better than rule-based systems
  - can inject human bias
- Cons:
  - still worse than human performance
  - large feature-output abstraction gap
  - hard to design good features
  - does not scale



HOGs





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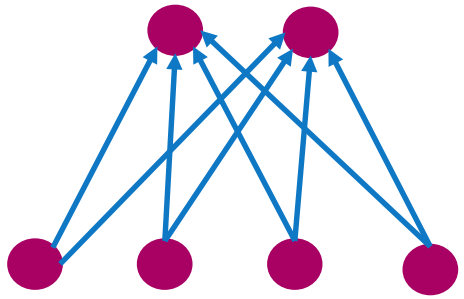
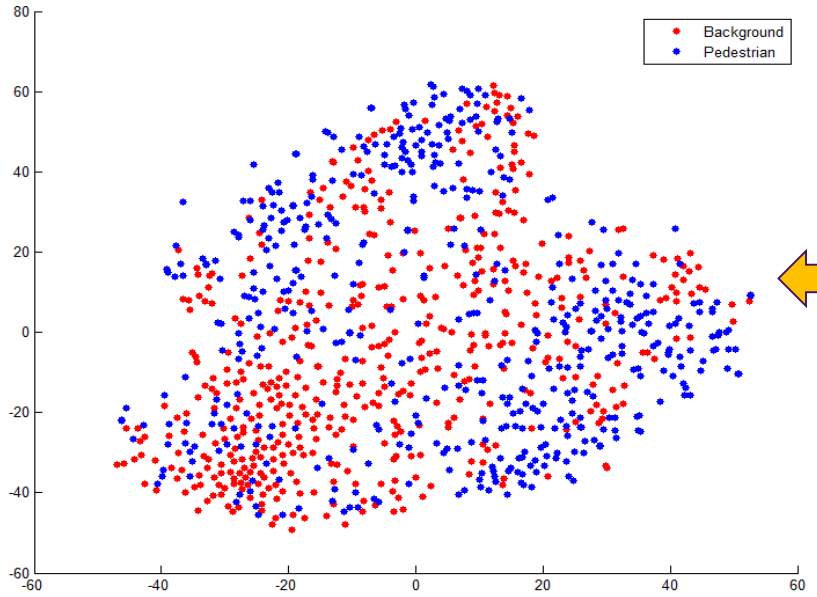
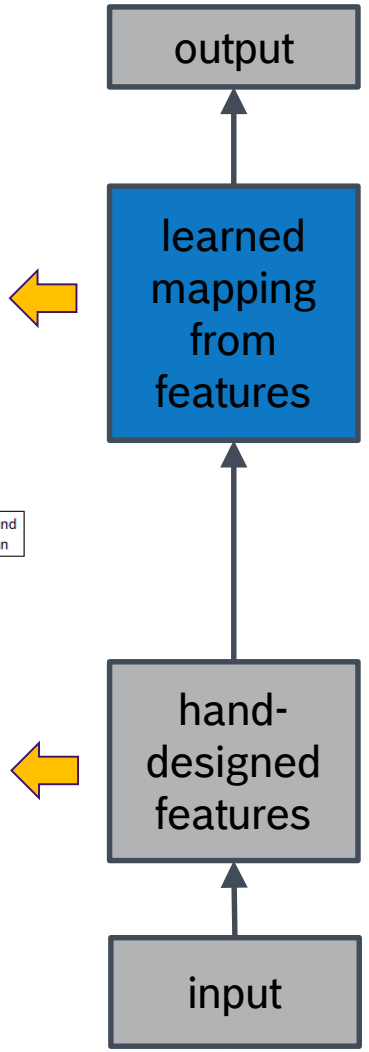
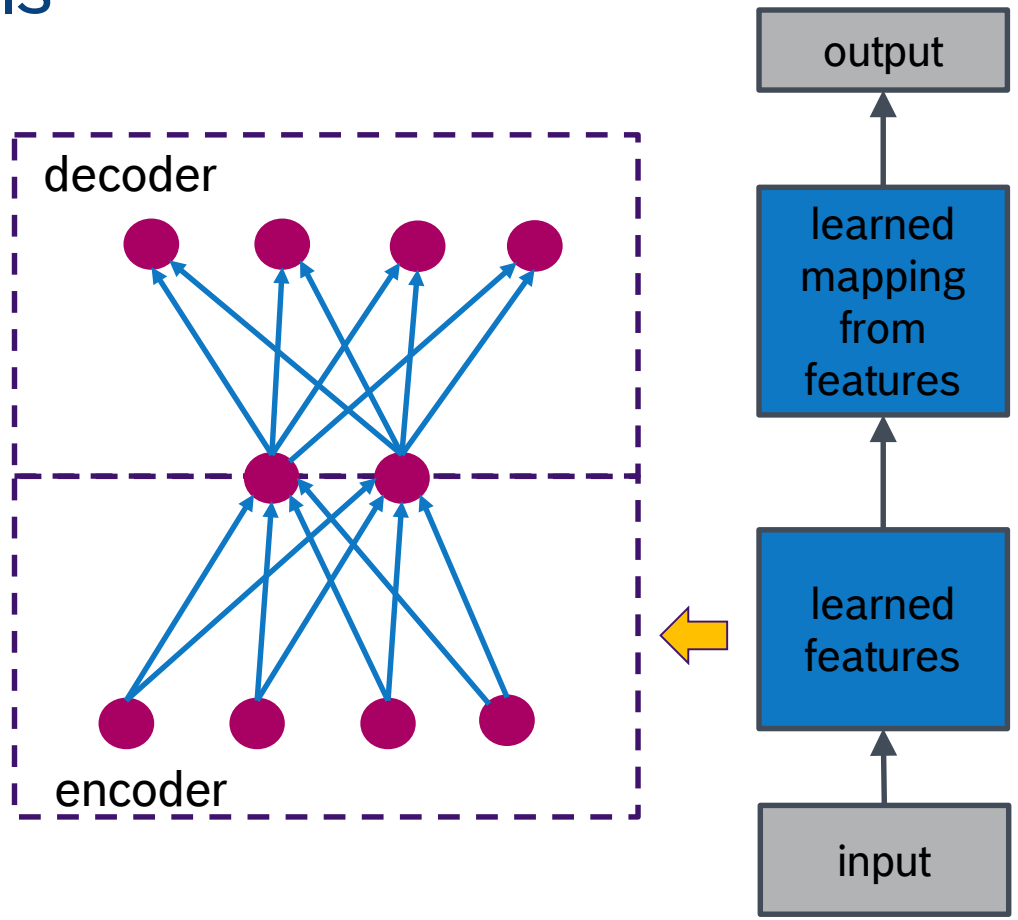






The Path to Deep Learning
Second Generation: Shallow Models

- Learn the representation too!
  - Separately: *e.g.* **auto-encoders**
  - Jointly with the mapping: **end-to-end learning**
- Better, but we still need to cover a large **abstraction gap**



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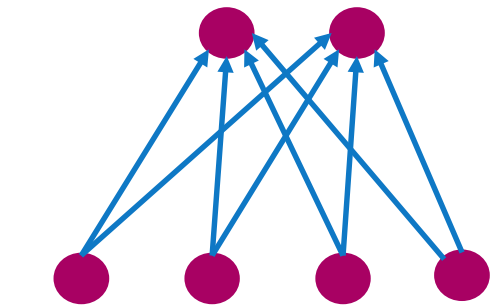
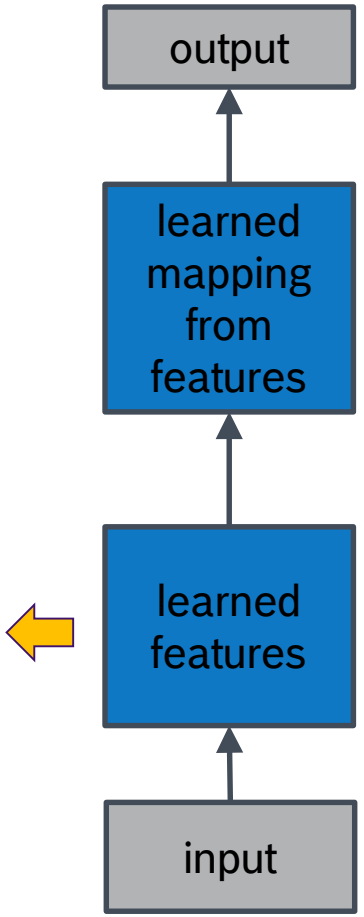


encoder



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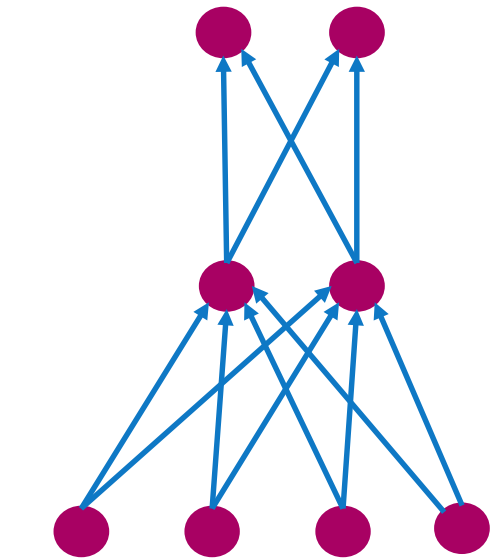
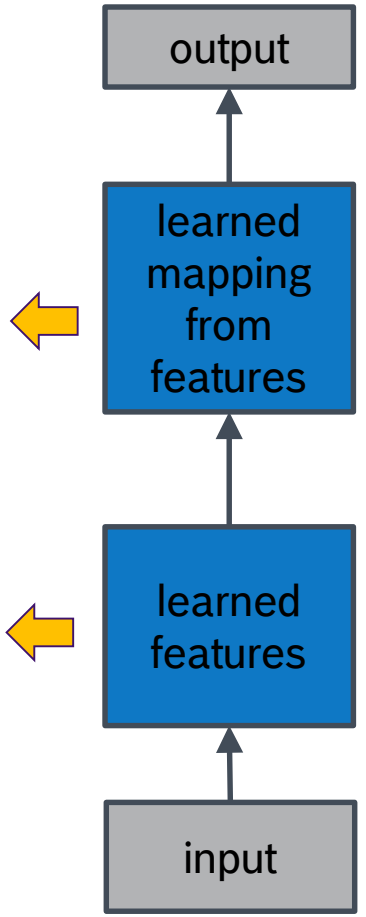
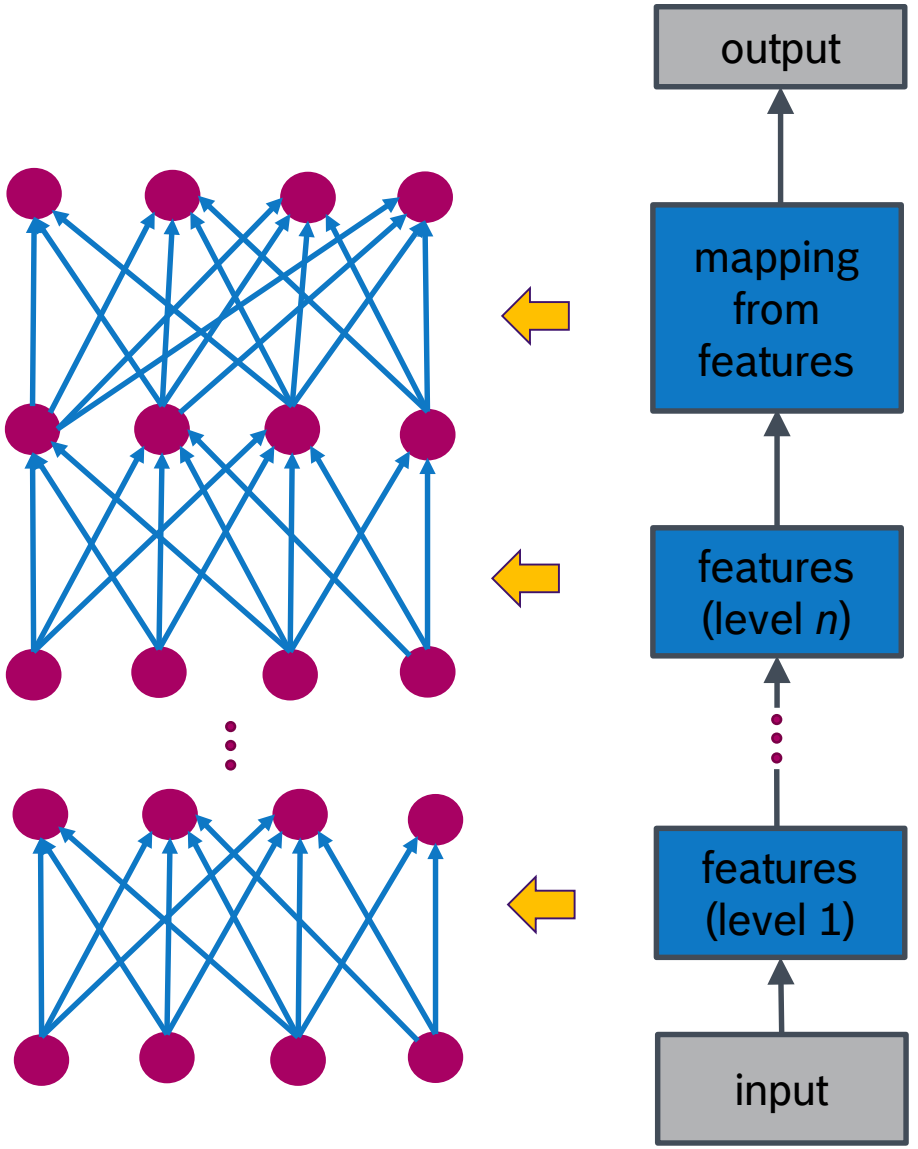




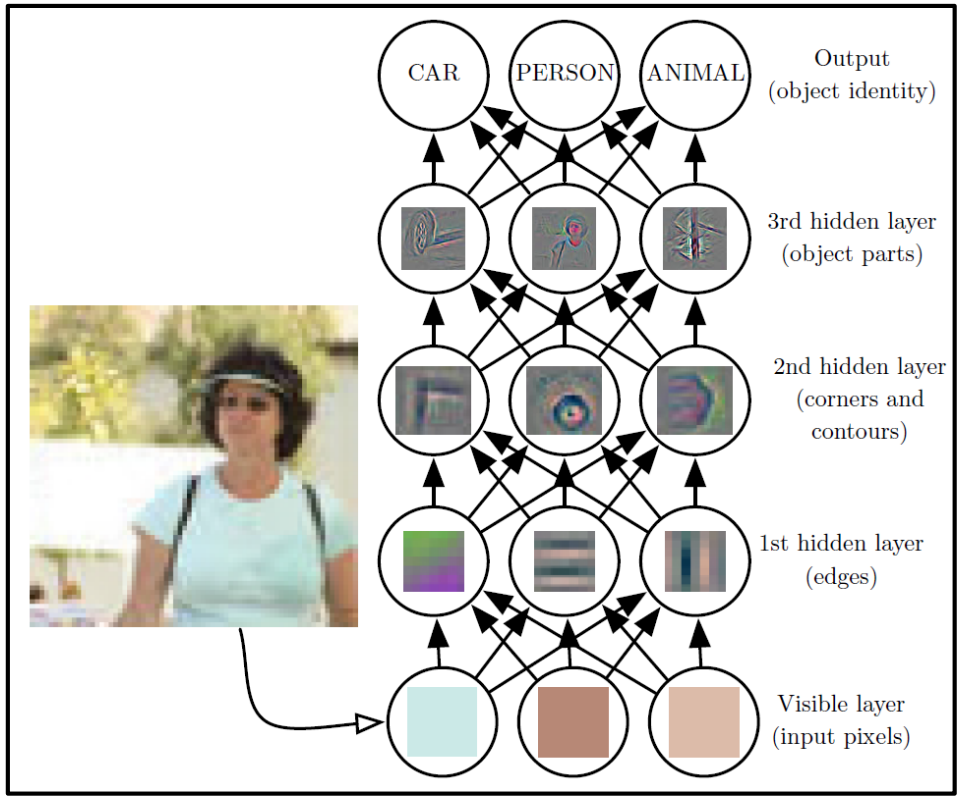
The Path to Deep Learning
Third Generation: Deep Learning

- Why not learn a hierarchy of features?
- This is **deep learning**
- Examples:
  - **deep auto-encoders**
  - **multi-layer-perceptron (MLP)**
  - **convolutional neural networks (CNNs)**



The Path to Deep Learning
Third Generation: Deep Learning

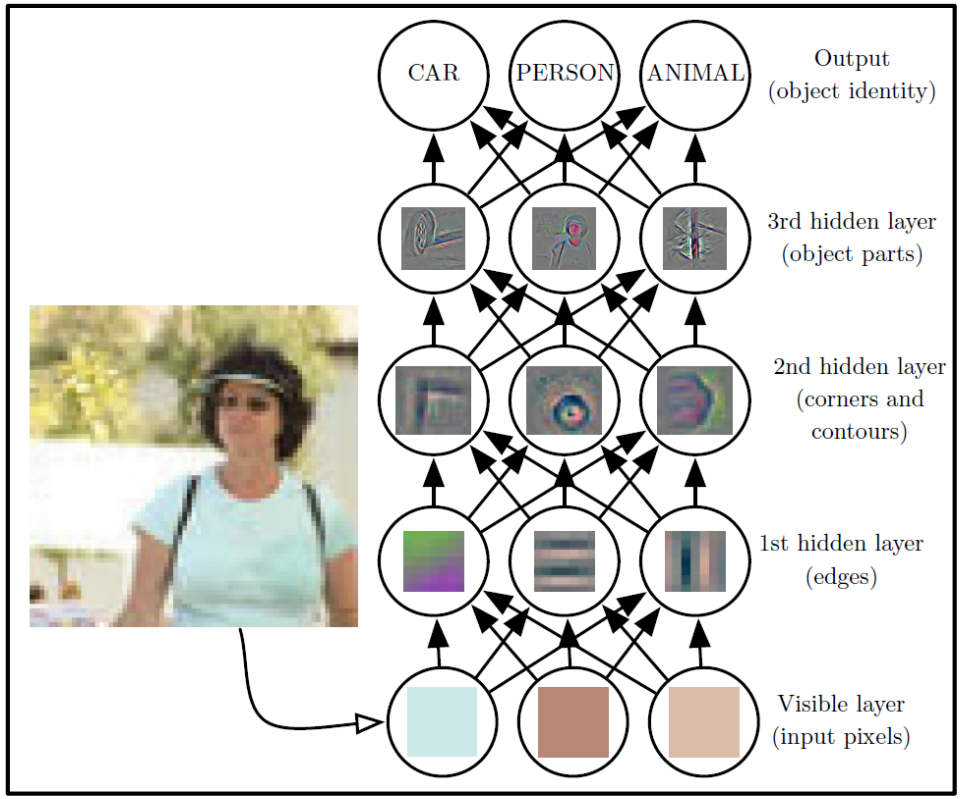
- Pros:
  - Near human performance on many hard problems
  - Fully scalable to any problem domain
- Cons:
  - Need large amounts of data
  - Expensive to train and run



The Path To Deep Learning

A Dual View of Deep Learning

- **Representational:** function composition
  - layer: a simple function (multi-dimensional)
  - layer output: a new representation of the input
- **Computational:** computer program
  - layer: set of parallel instructions
  - layer output: state of computer memory (may not be entirely input-related!)

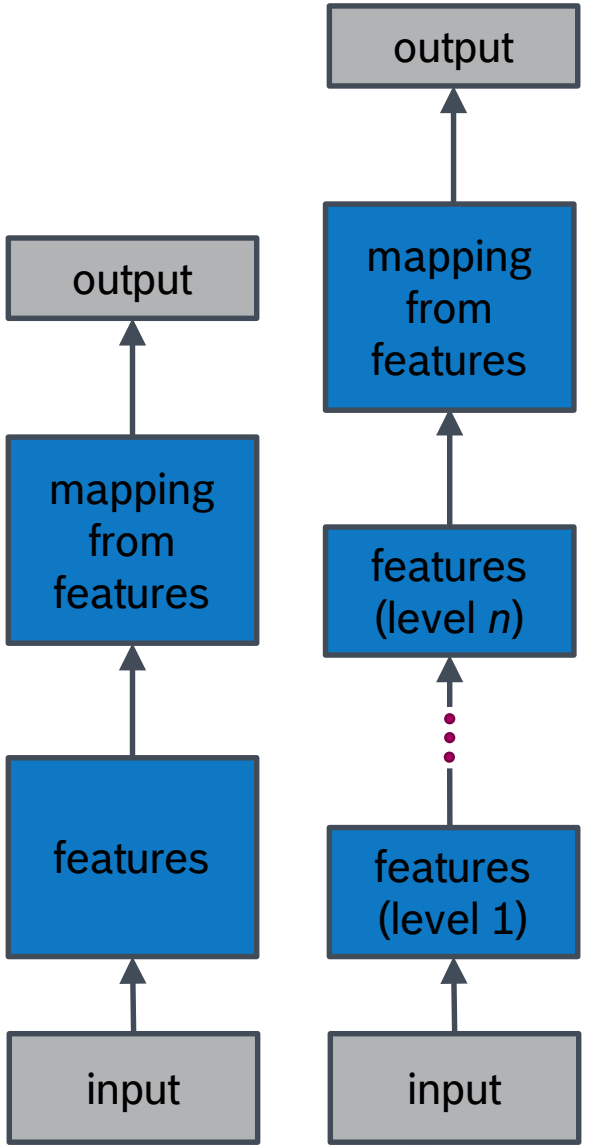


The Path To Deep Learning

Deep or not deep?

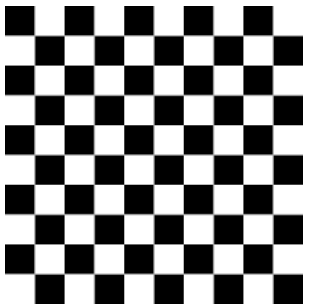
- No single definition of depth:
  - Maximum number of instructions to evaluate the entire output?
  - Maximum number of concepts to arrive at the output representation?
- No clear definition of deep:
  - Having at least 4 layers? (some authors)
  - In any case:

    *A **deep model** is a model with more learned instructions/concepts than a traditional machine learning model.*

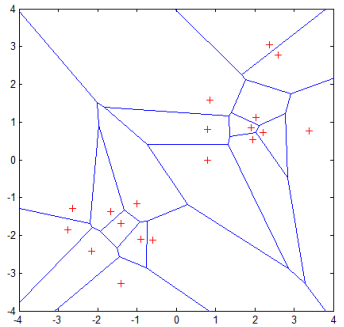


The Path to Deep Learning
Distributed Representations

- We need to **dis-entangle** factors of variation
- Example: recognize cars/trucks/birds of three colors (red, green, blue)
- Encodings:
  - Option 1: all combinations => 9 features
  - Option 2: **distributed representation** => 6 features (3 for object type, 3 for color)
- Deep models can learn distributed representations!



Entangled features



kNN in image space needs one example in each cell!

The Path To Deep Learning

Recap

- We need to address the **abstraction gap**
- Extremely Difficult:
  - Representations are not conspicuous!
  - Hard to dis-entangle factors of variation
- Hand designed features
  - Time consuming to design
  - Do not generalize across problems
  - Brittle to variations (illuminations, pose changes)
- Learned feature hierarchies (**end-to-end learning**)
  - Trade training data for design time
  - Generalize across problems
  - Increased variance
  - Distributed representations of the world
- **Deep learning** is just end-to-end learning with a lot of feature levels

REFERENCES

Deep Learning for Computer Vision
References

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- [5] Zhang, A. and Lipton, Z.C. and Li, M. and Smola, J.A., "*Dive into Deep Learning*", *2017*, https://d2l.ai/