



# Robust and Trustworthy Deep Learning



THEMIS AI

January 11, 2023



# THEMIS AI

## Design, Advance, and Deploy Safe and Trustworthy AI



MIT



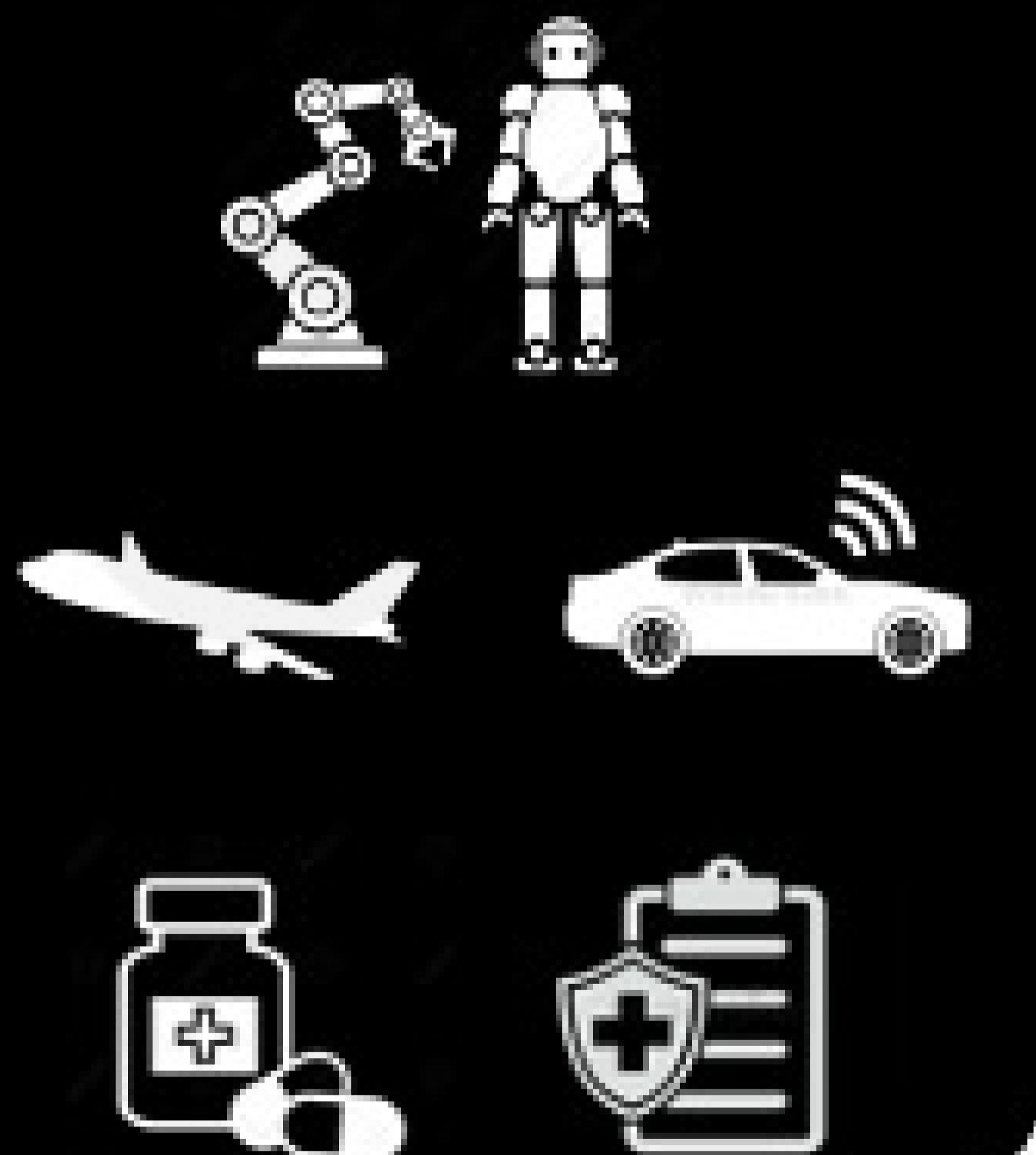
Scientific  
Innovation





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## Design, Advance, and Deploy Safe and Trustworthy AI



Scientific  
Innovation

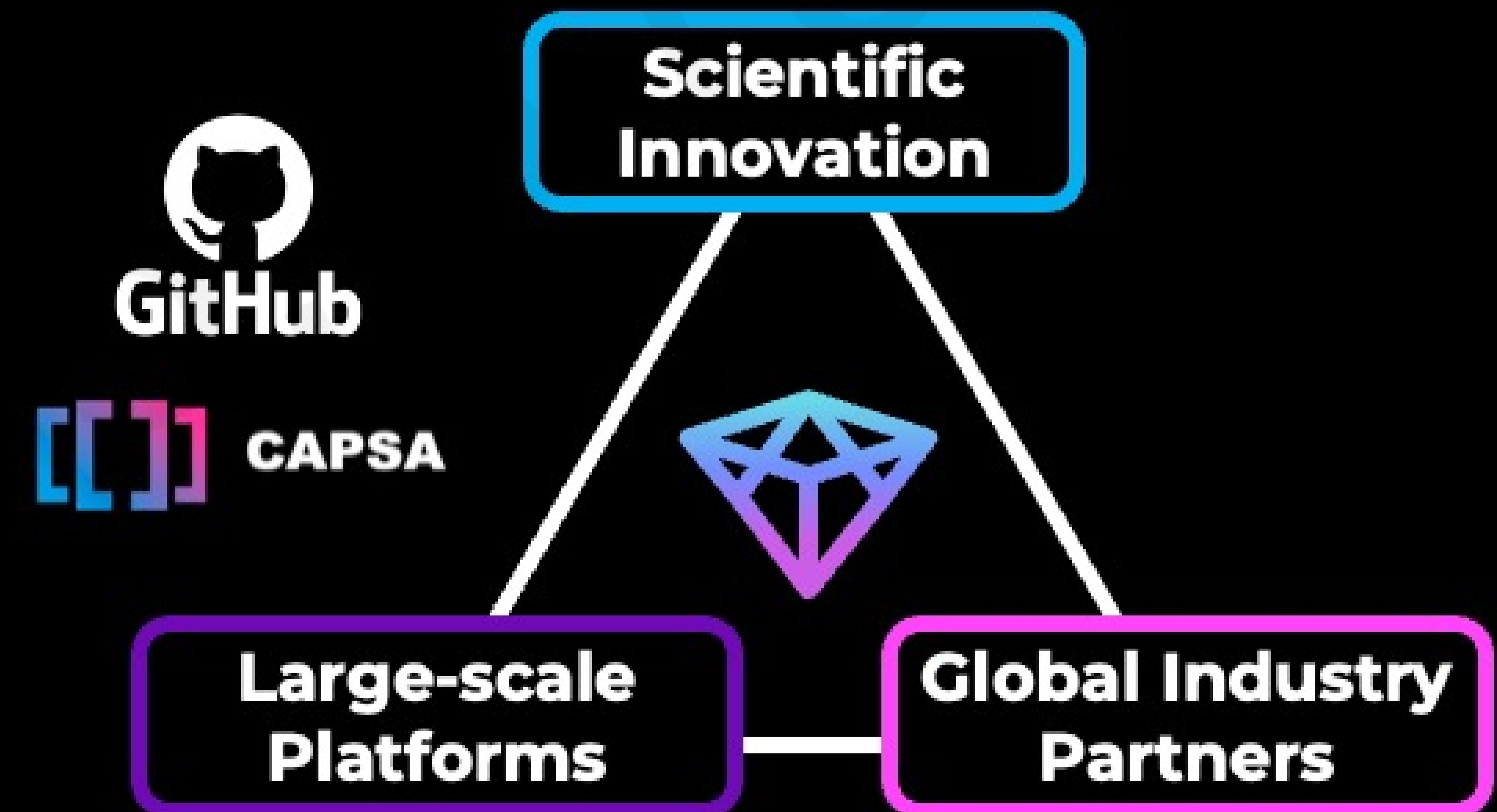


Global Industry  
Partners



# THEMIS AI

Design, Advance, and Deploy Safe and Trustworthy AI



# Robust and Trustworthy Deep Learning

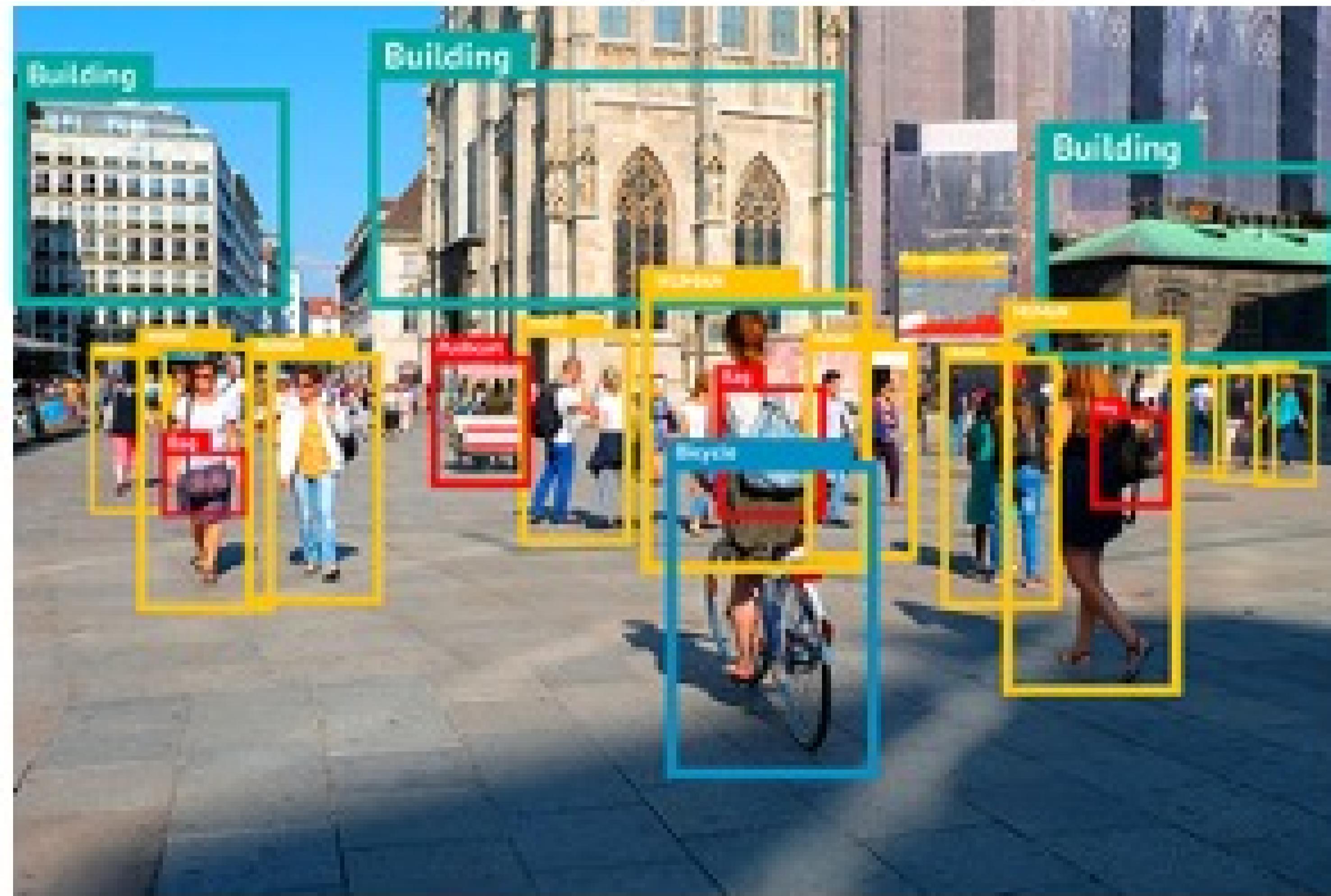
**Sadhana Lolla**

Machine Learning Scientist  
Themis AI



# AI in Safety-Critical Domains

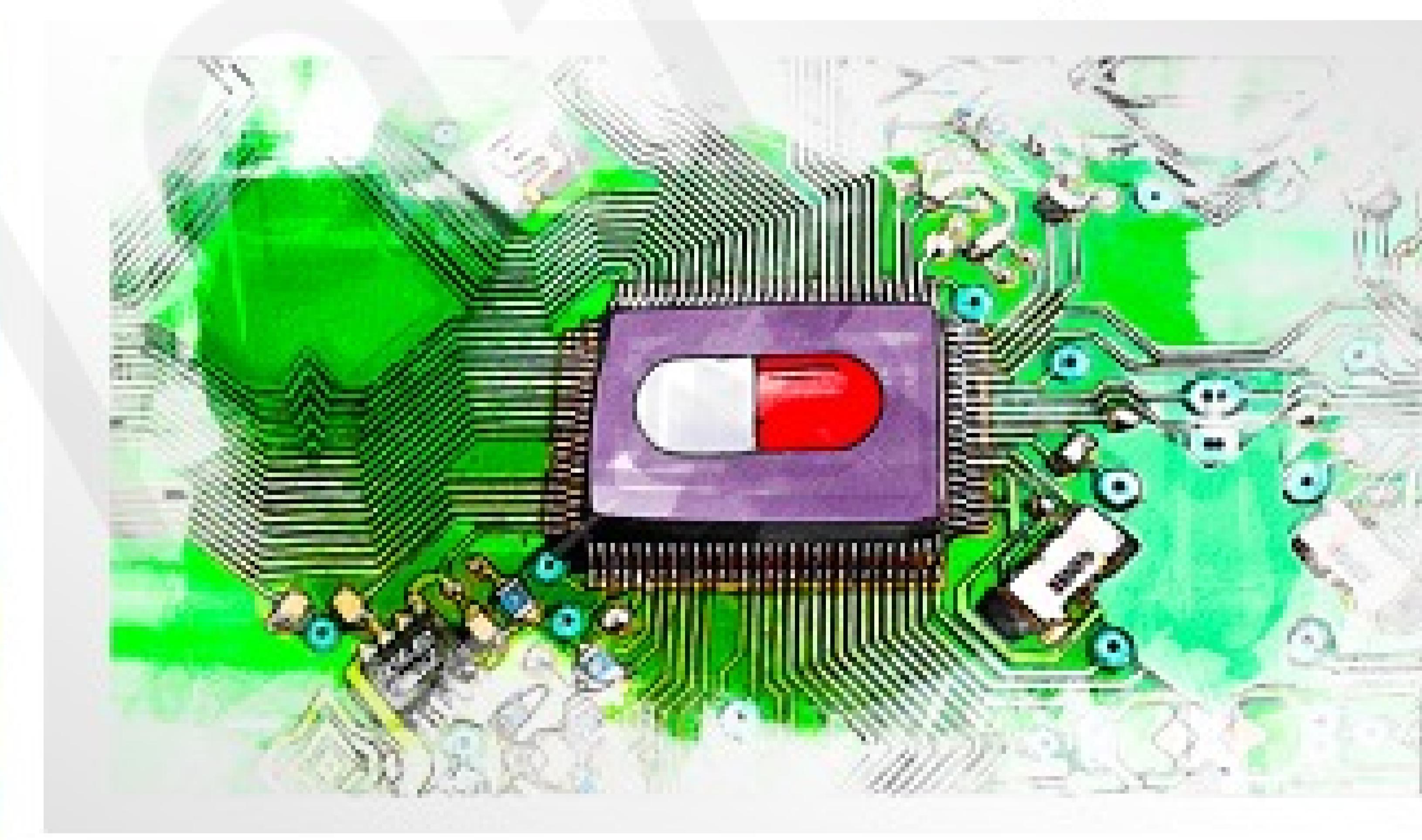
## Scene planning



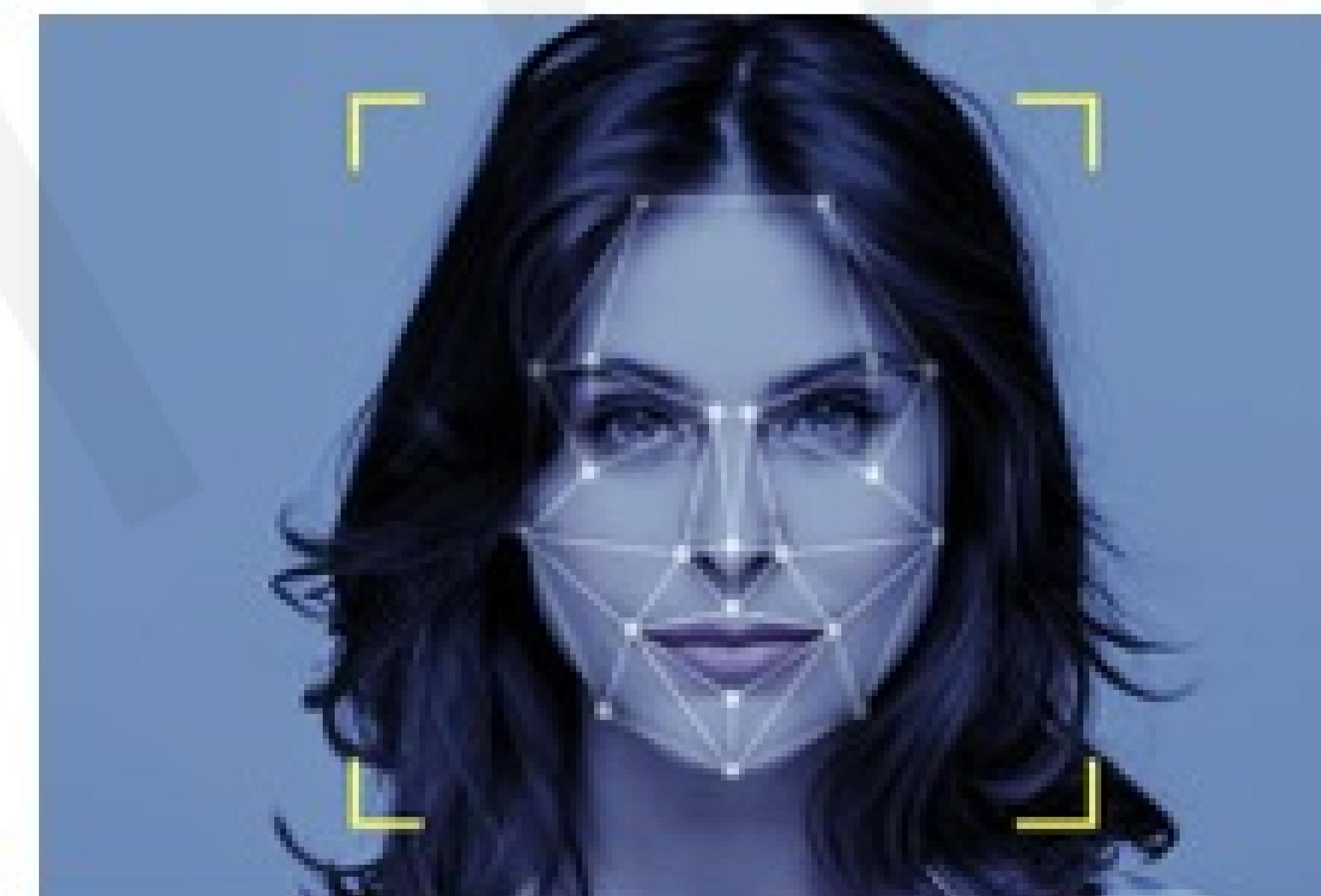
## Robot-assisted surgery



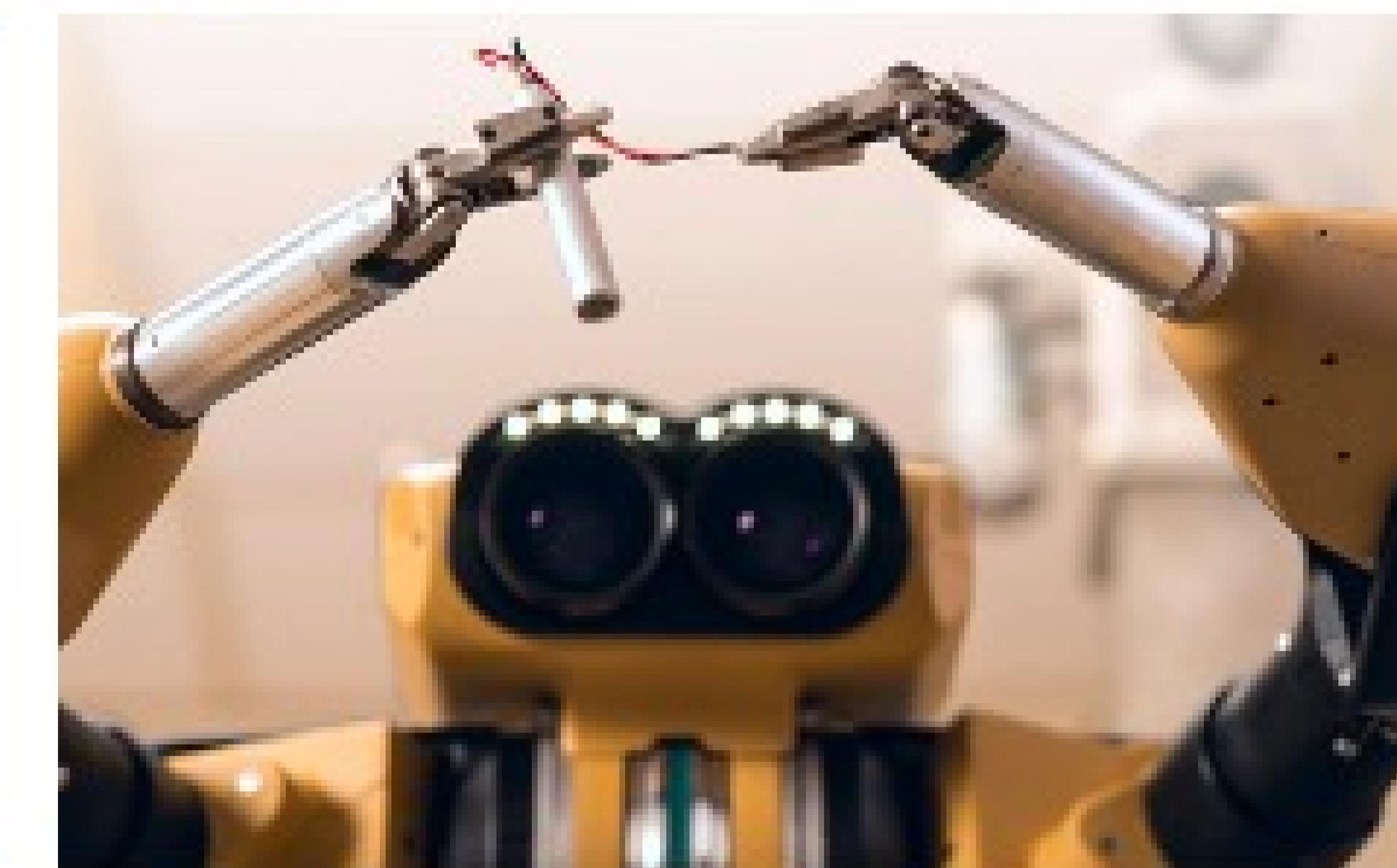
## Drug discovery



## Autonomous vehicles



## Facial recognition



## Robotics



## Diagnostics

# AI in the News

**Millions of black people affected by racial bias in health-care algorithms**

Artificial Intelligence has a gender bias problem – just ask Siri

GM's Cruise Recalls Self-Driving Software Involved in June Crash

*Microsoft Plans to Eliminate Face Analysis Tools in Push for 'Responsible A.I.'*

*The New Chatbots Could Change the World. Can You Trust Them?*

Tesla 'full self-driving' triggered an eight-car crash, a driver tells police

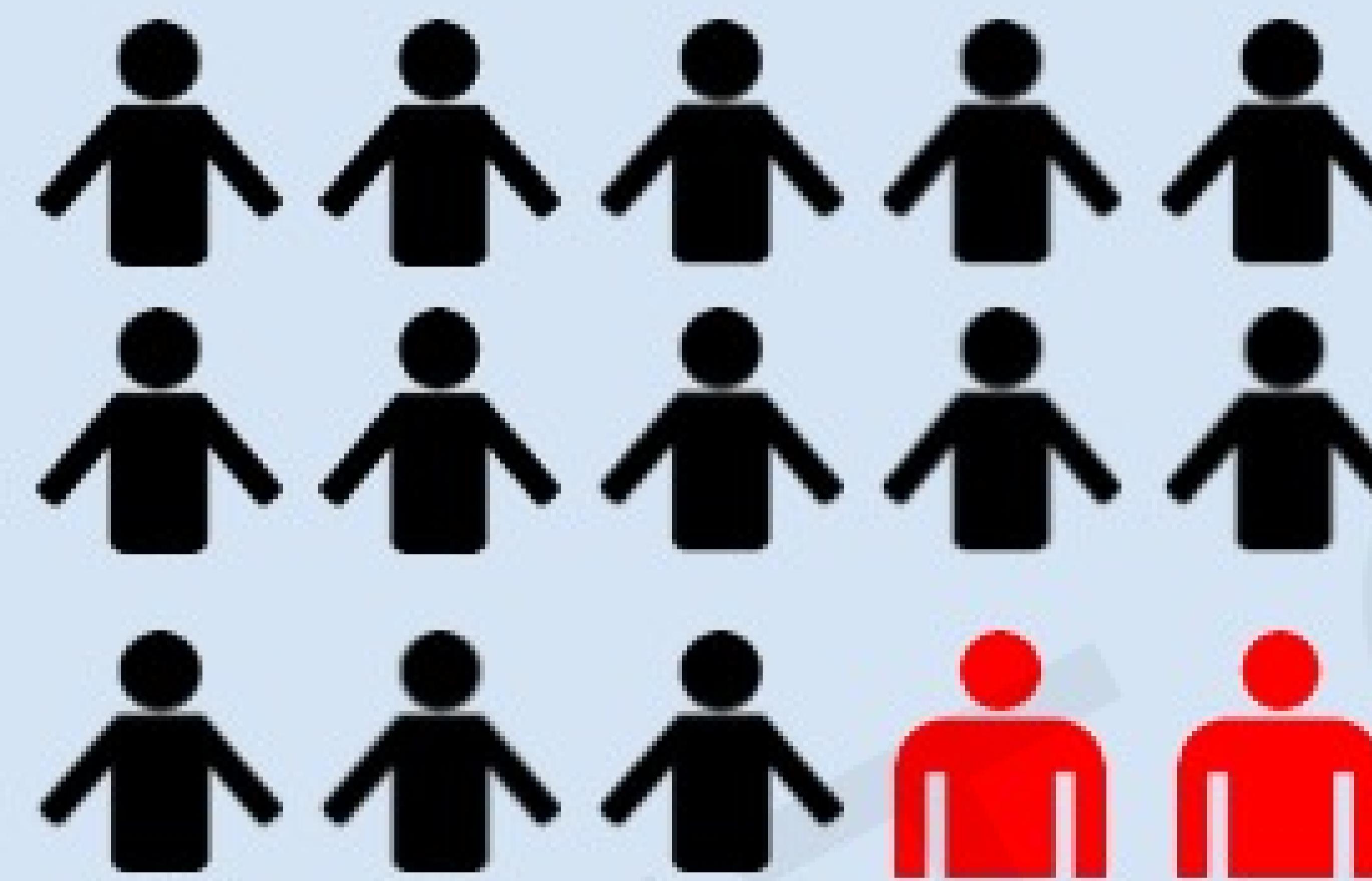
Minority Patients Often Left Behind By Health AI

*Many Facial-Recognition Systems Are Biased, Says U.S. Study*

**Risks Rise As Robotic Surgery Goes Mainstream**

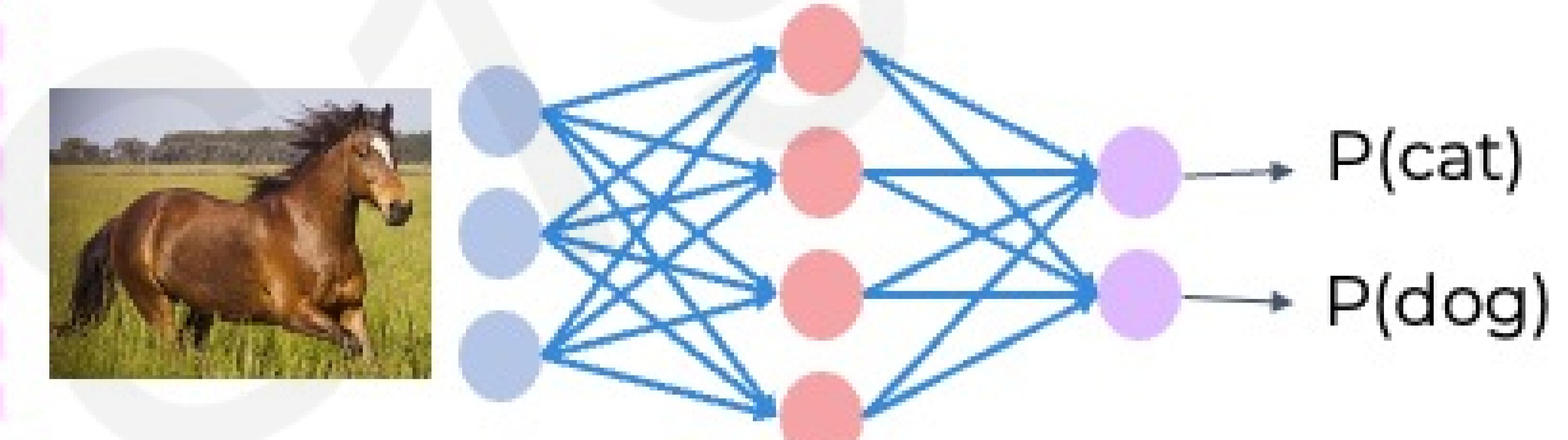
# Challenges for Robust Deep Learning

## Bias



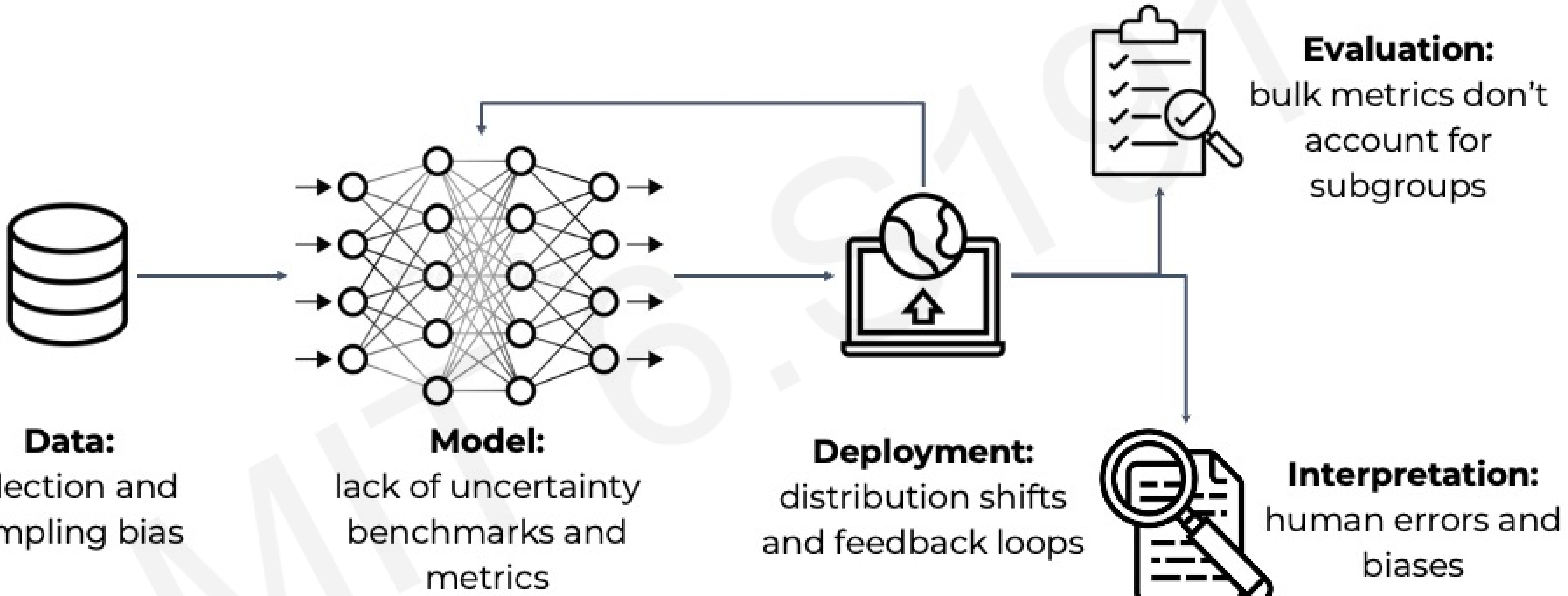
**What happens when  
models are skewed by  
sensitive feature inputs?**

## Uncertainty

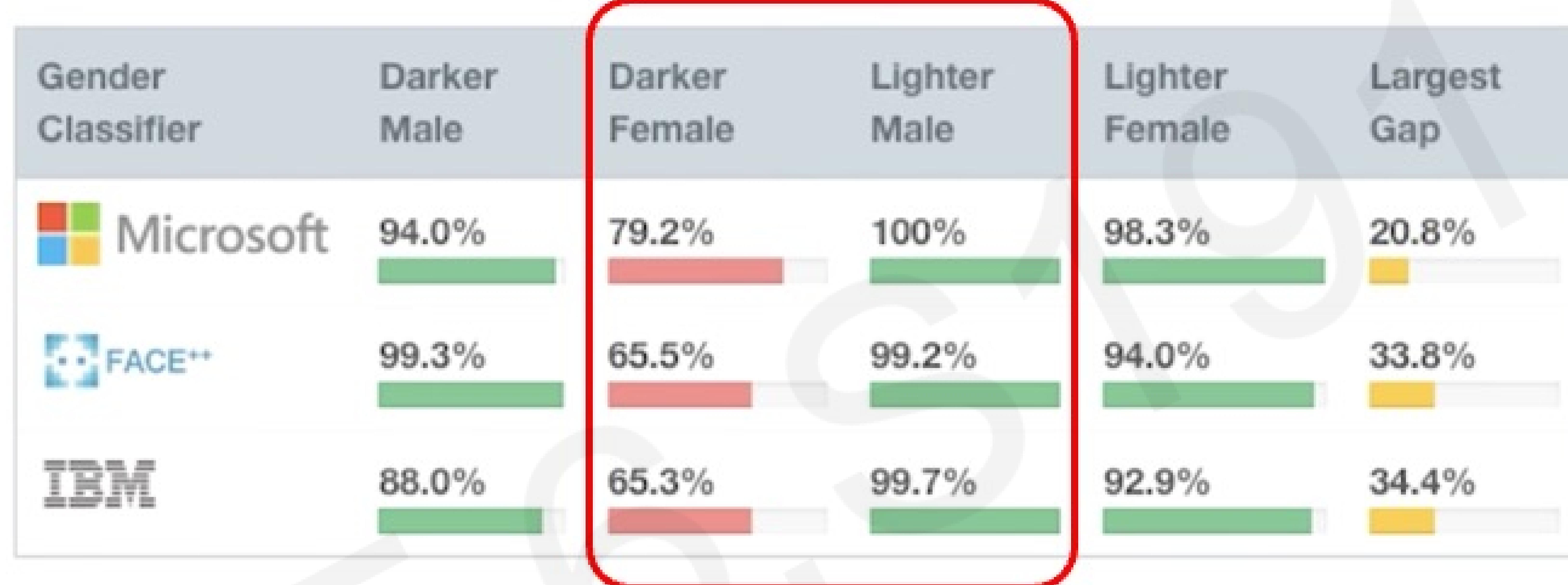


**Can we teach a model to  
recognize when it doesn't  
know the answer?**

# Bias in the AI Lifecycle



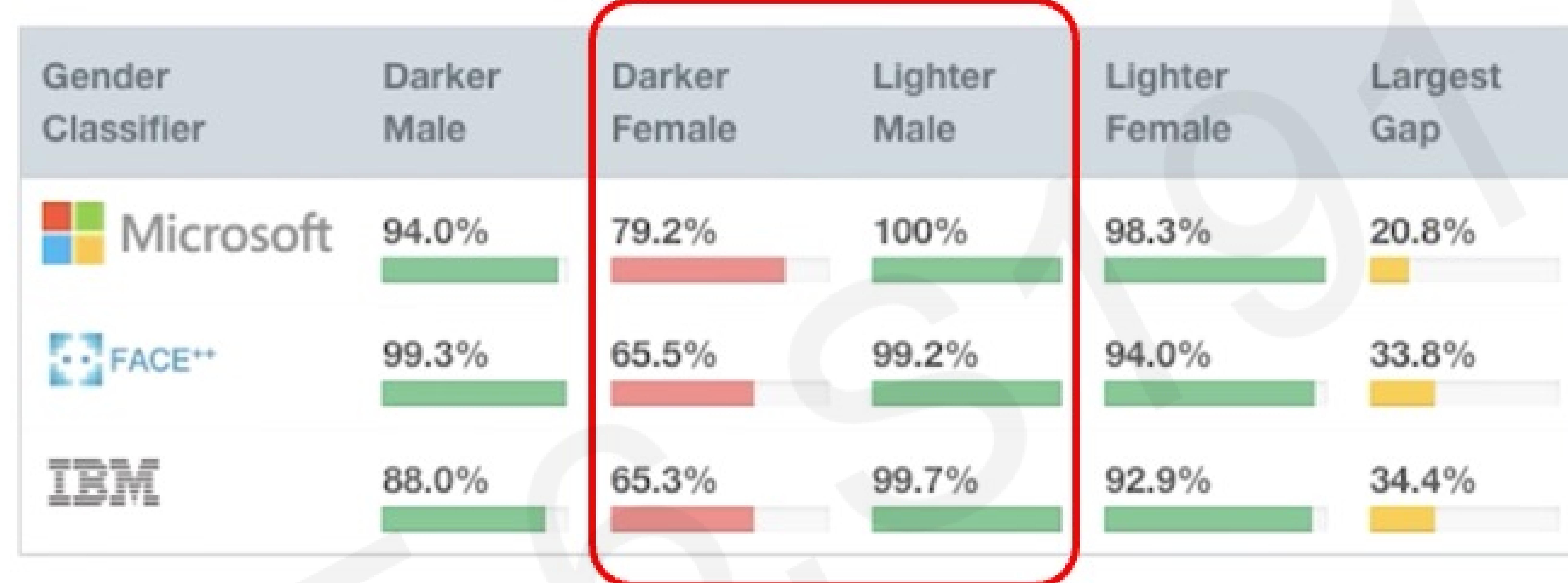
# Industry Example: Facial Detection



**What types of bias were present in these models?**

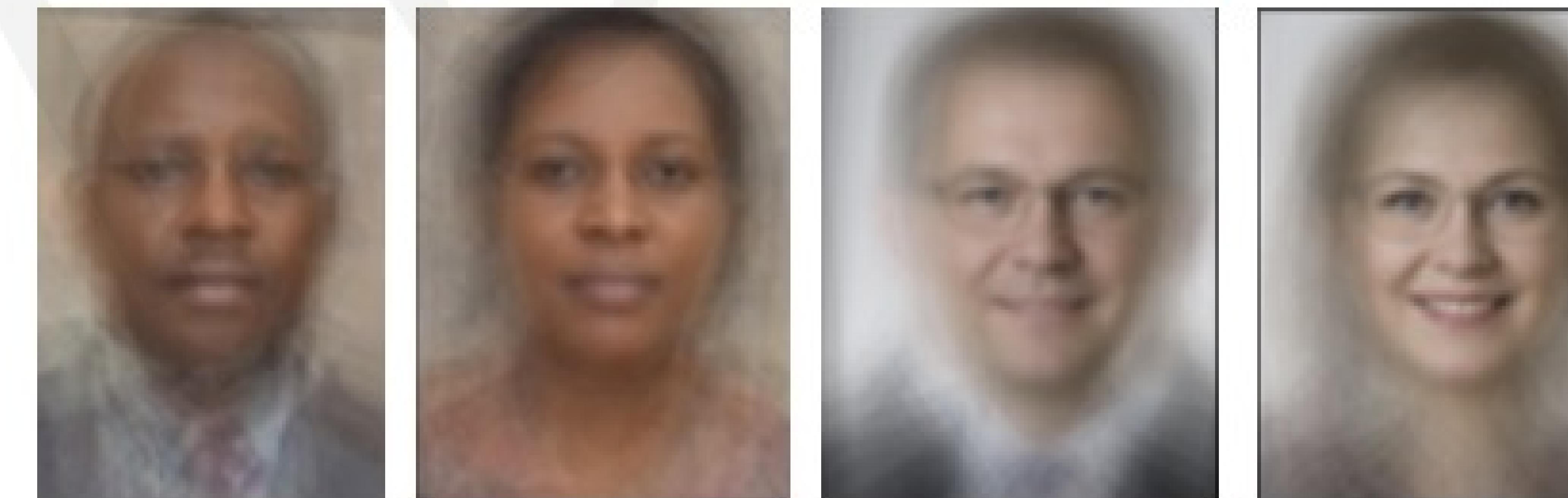
- Selection bias: proportion of data in dataset does not reflect the real world
- Evaluation bias: originally, these models were not evaluated on subgroups!

# Industry Example: Facial Detection



## Pilot Parliaments

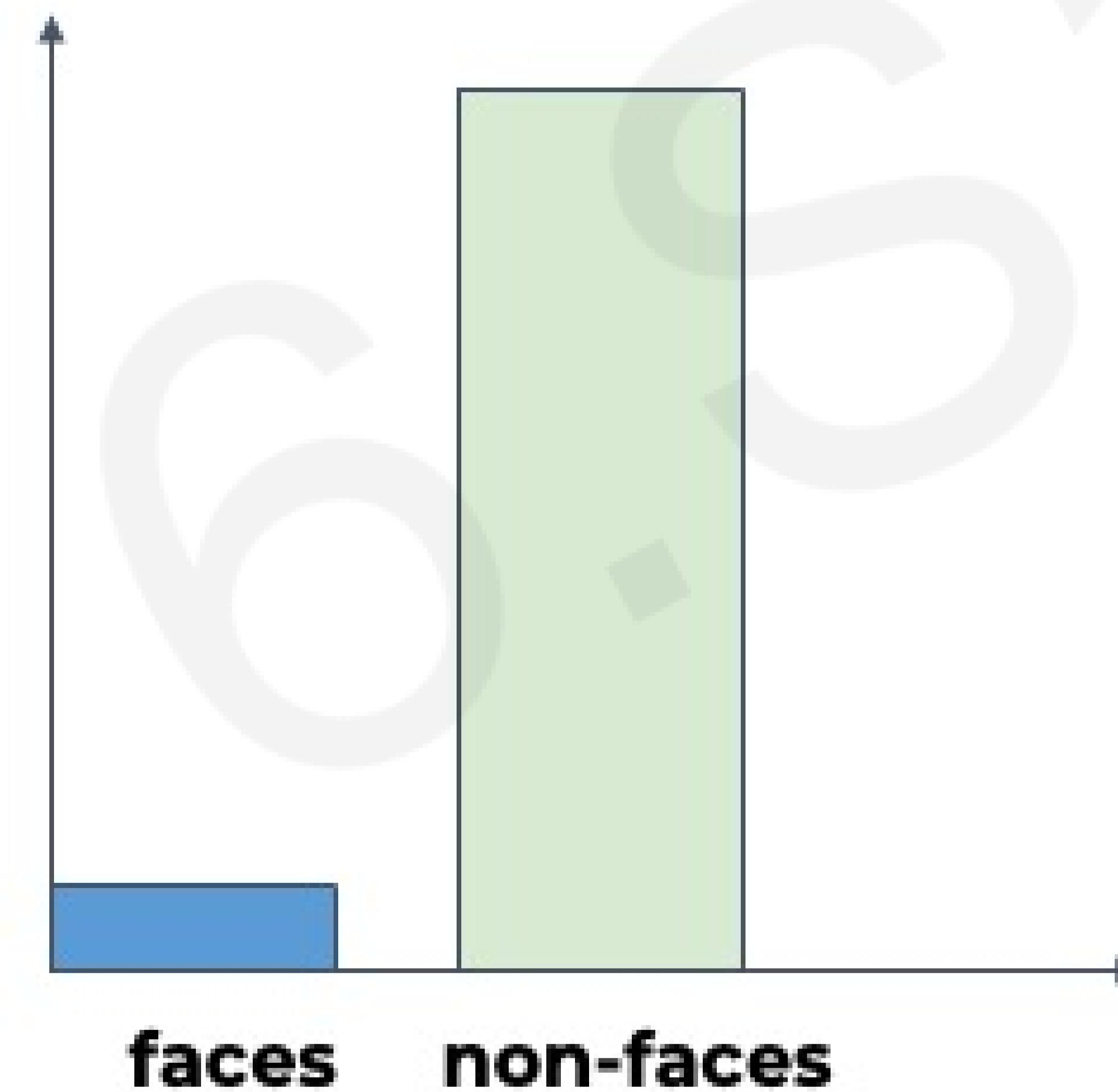
**Benchmark:** a dataset designed to uncover biases by balancing race and gender



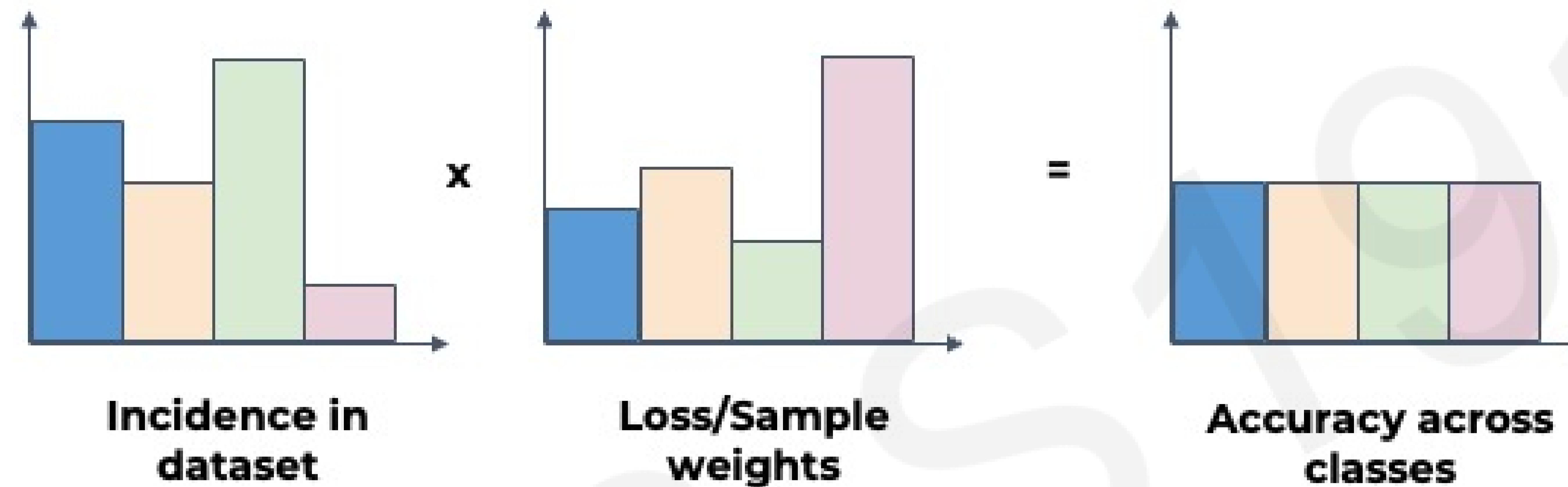
# Class Imbalance

What happens when some classes are more represented than others?

**Frequency of classes in dataset**



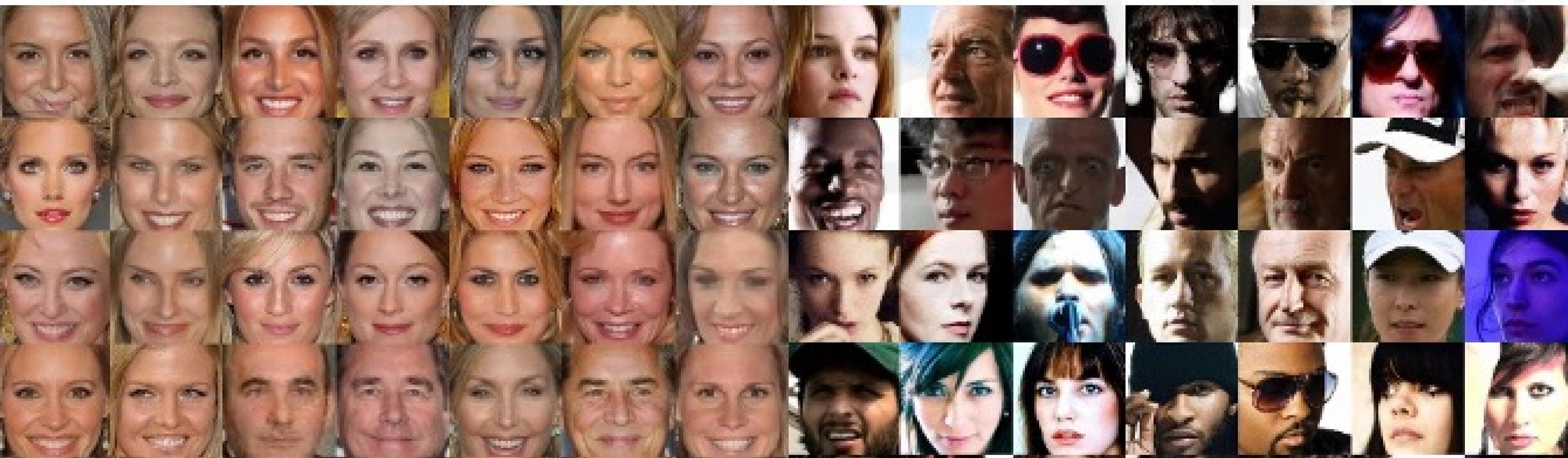
# Mitigating Class Imbalance



- **Sample Reweighting:** Sample more data points from underrepresented classes
- **Loss Reweighting:** Mistakes on underrepresented classes contribute more to loss
- **Batch Selection:** Choose randomly from classes so that every batch has an equal number of points per class

# What about *latent features*?

Variations **within the same class** are important to capture while debiasing; otherwise we may overgeneralize!

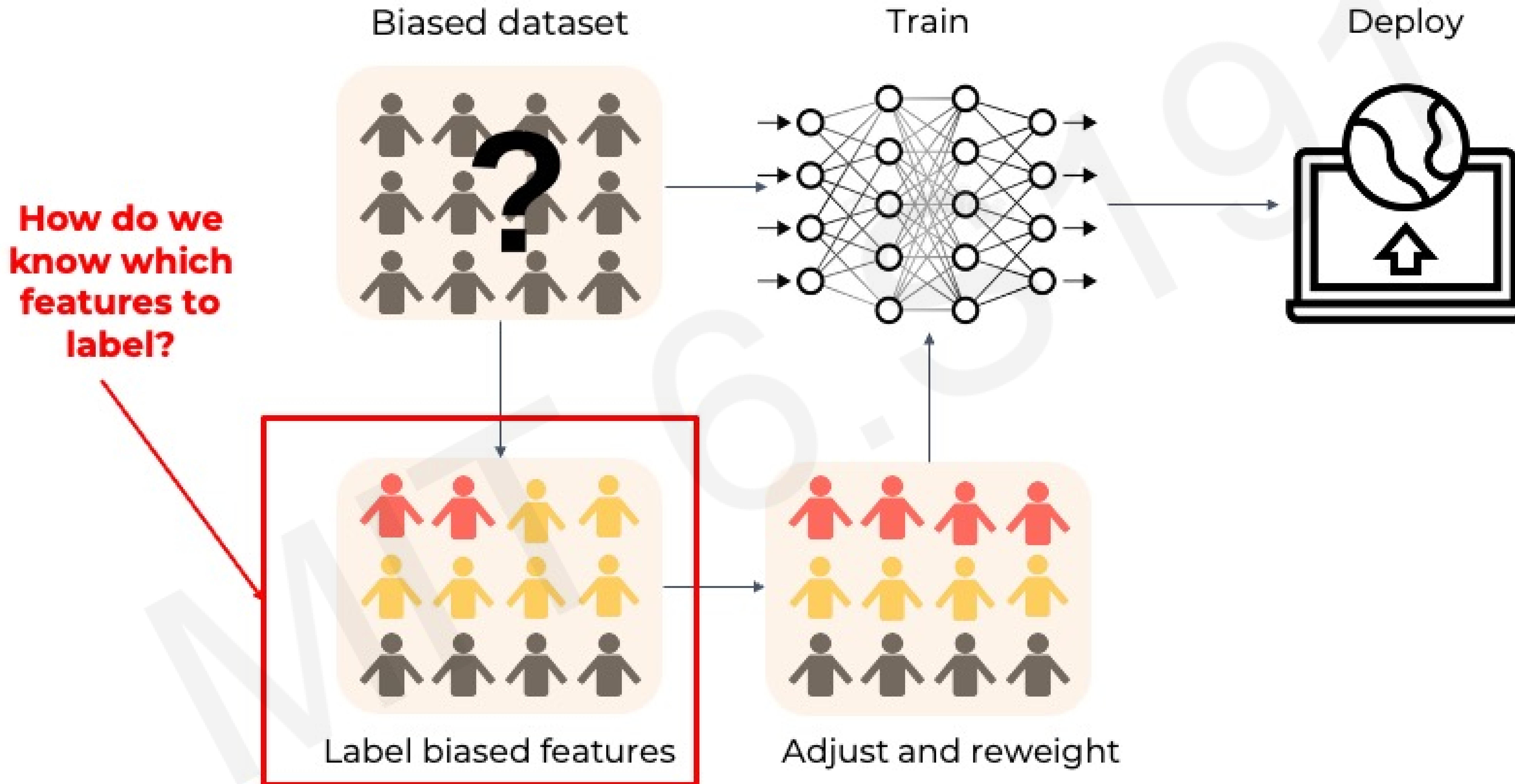


What are some latent features in the above dataset? Which ones may be underrepresented?

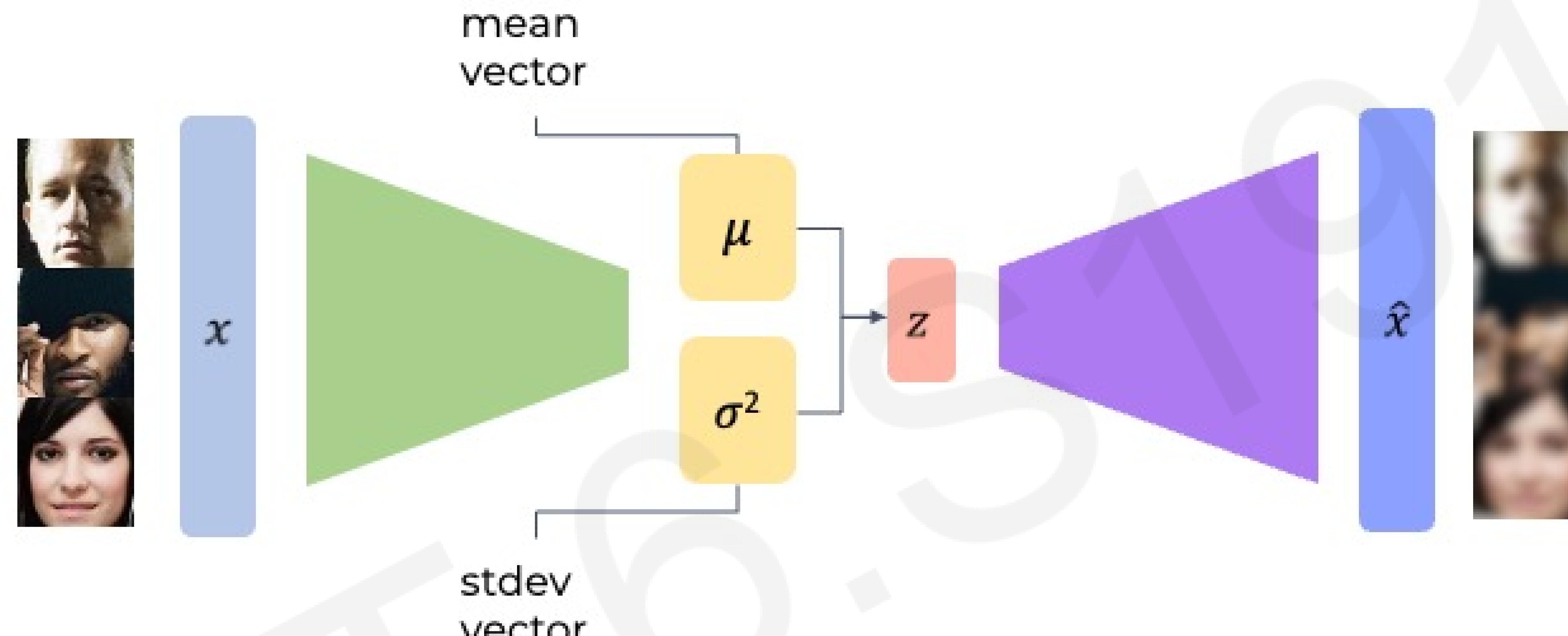


**Recall from lab 2 and lecture 4!**

# Why is debiasing latent features difficult?



# VAE Recap

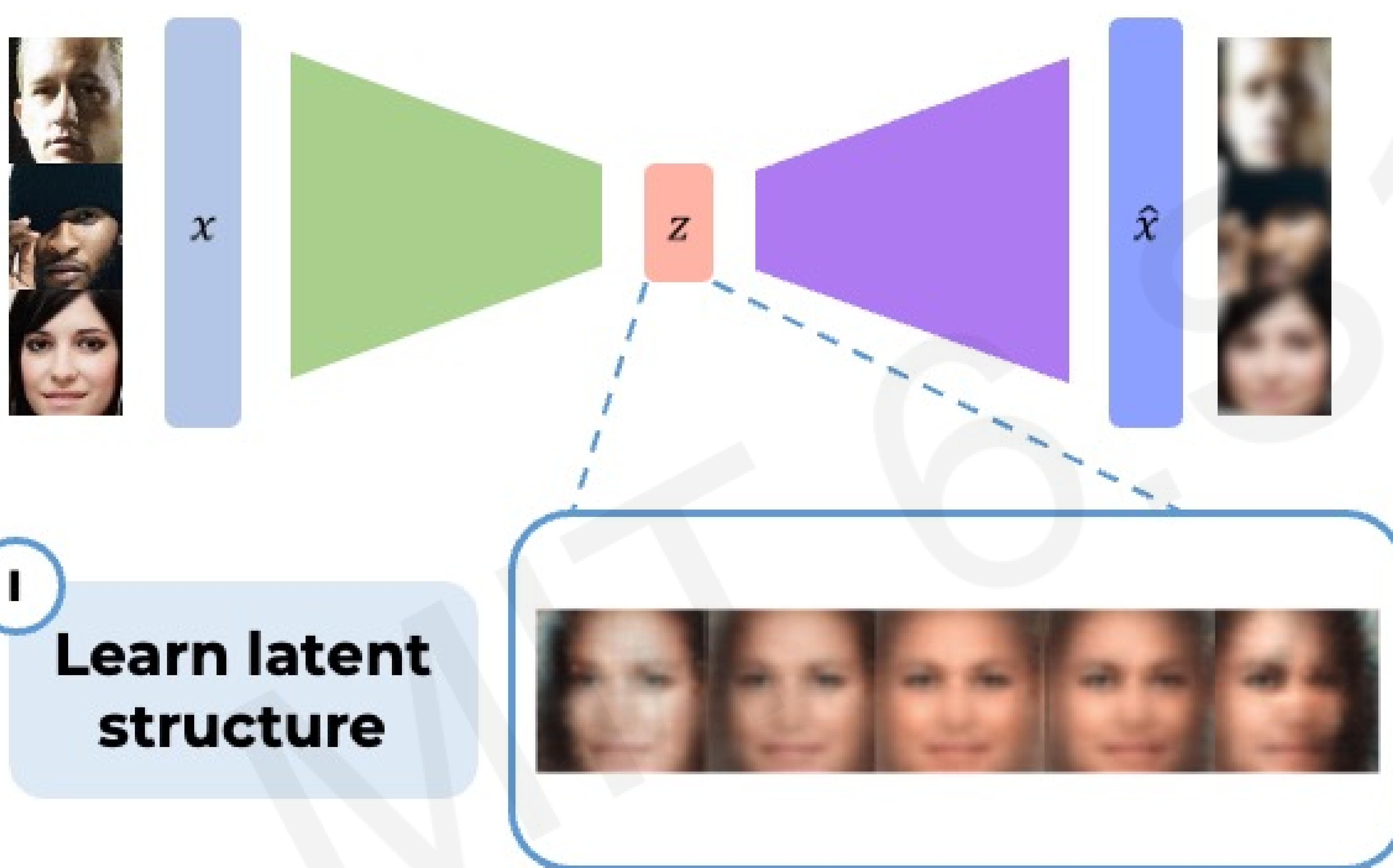


**Variational autoencoders (VAEs)** are a probabilistic twist on autoencoders!

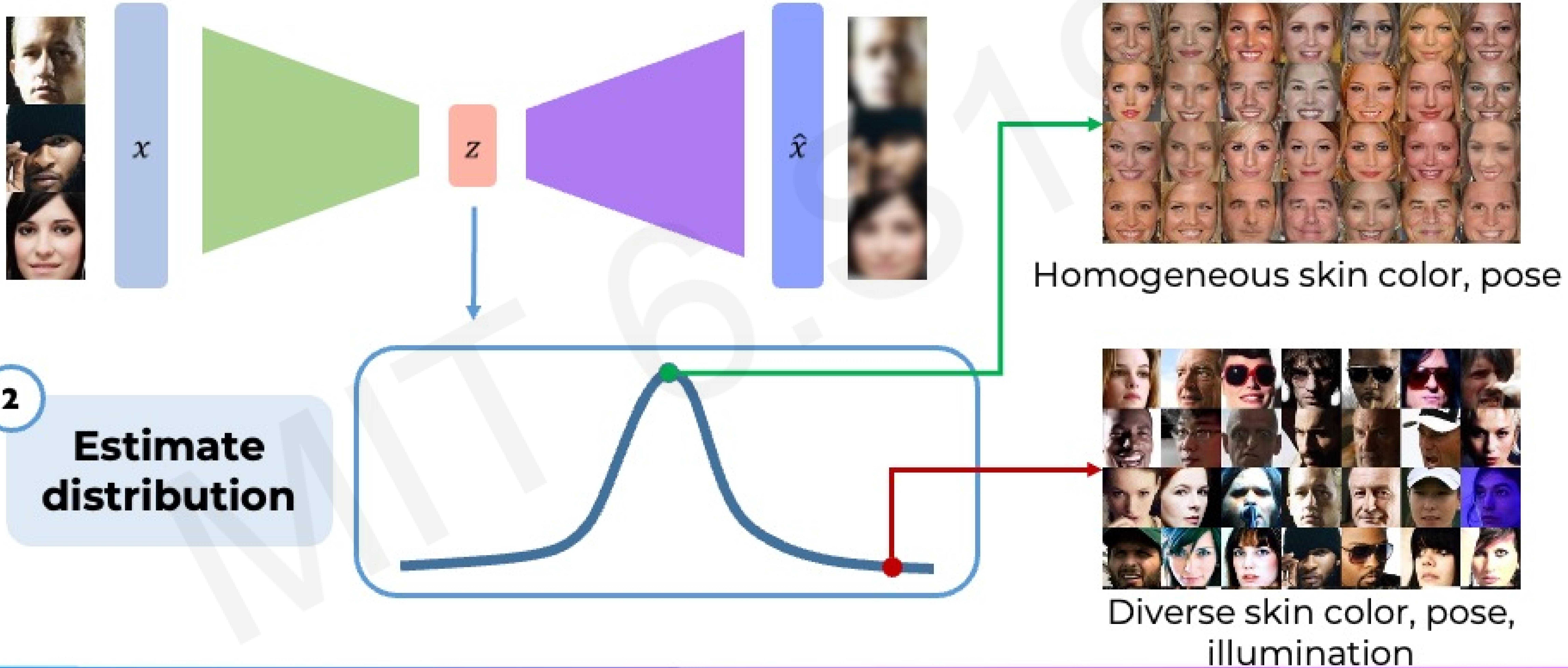


Recall from lab 2 and lecture 4!

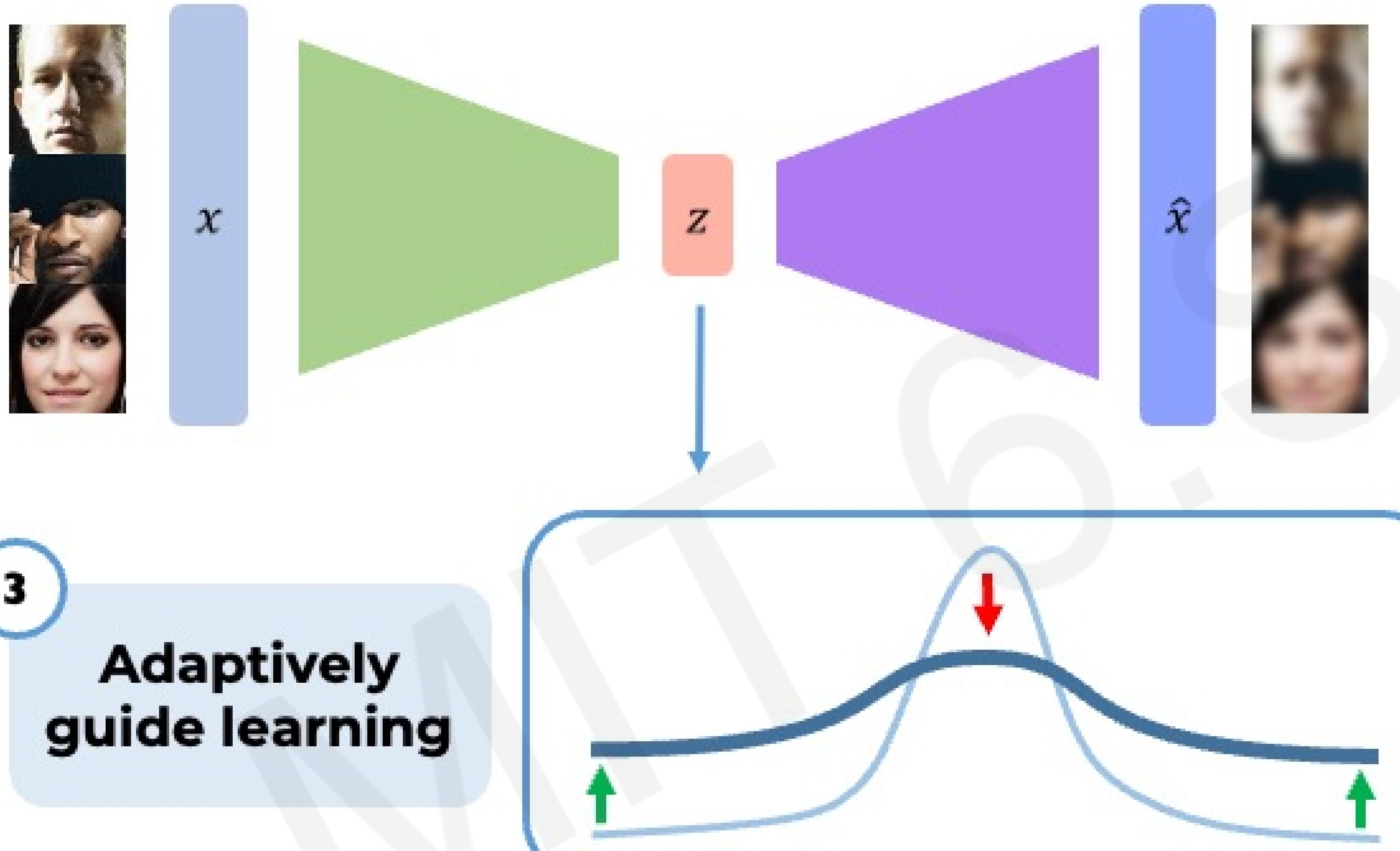
# Mitigating Bias Through Learned Latent Structure



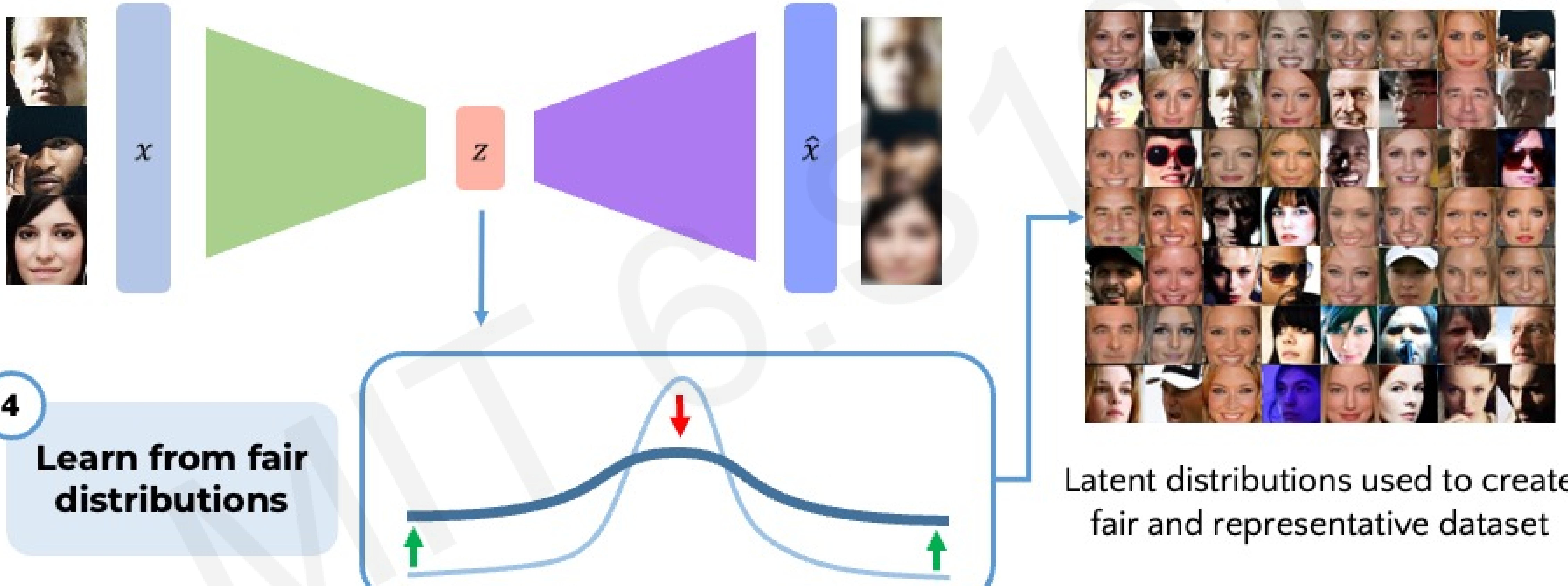
# Mitigating Bias Through Learned Latent Structure



# Mitigating Bias Through Learned Latent Structure



# Mitigating Bias Through Learned Latent Structure



# Using Latent Variables for Automated Debiasing

Approximate the distribution of the latent space with a joint histogram over the latent variables:

$$\hat{Q}(z|X) \propto \prod_i \hat{Q}_i(z_i|X)$$

**Estimated joint distribution**

*i* **Histogram for  
Independence every latent  
to approximate variable  $z_i$**

$$W(z(x)|X) \propto \prod_i \frac{1}{\hat{Q}_i(z_i(x)|X) + \alpha}$$

**Probability of  
selecting  
datapoint**

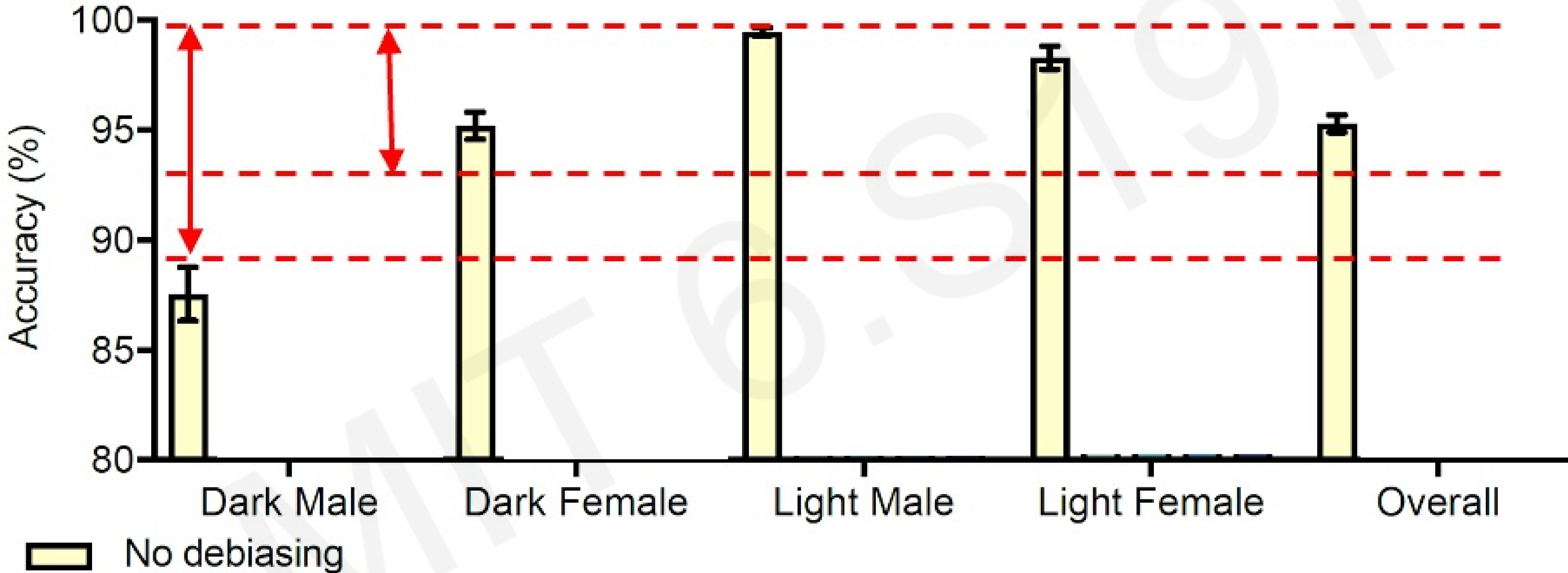
**Histogram for every  
latent variable  $z_i$**

**Debiasing  
parameter**



**Important for  
Lab 3!**

# Evaluation: Decreased Categorical Bias

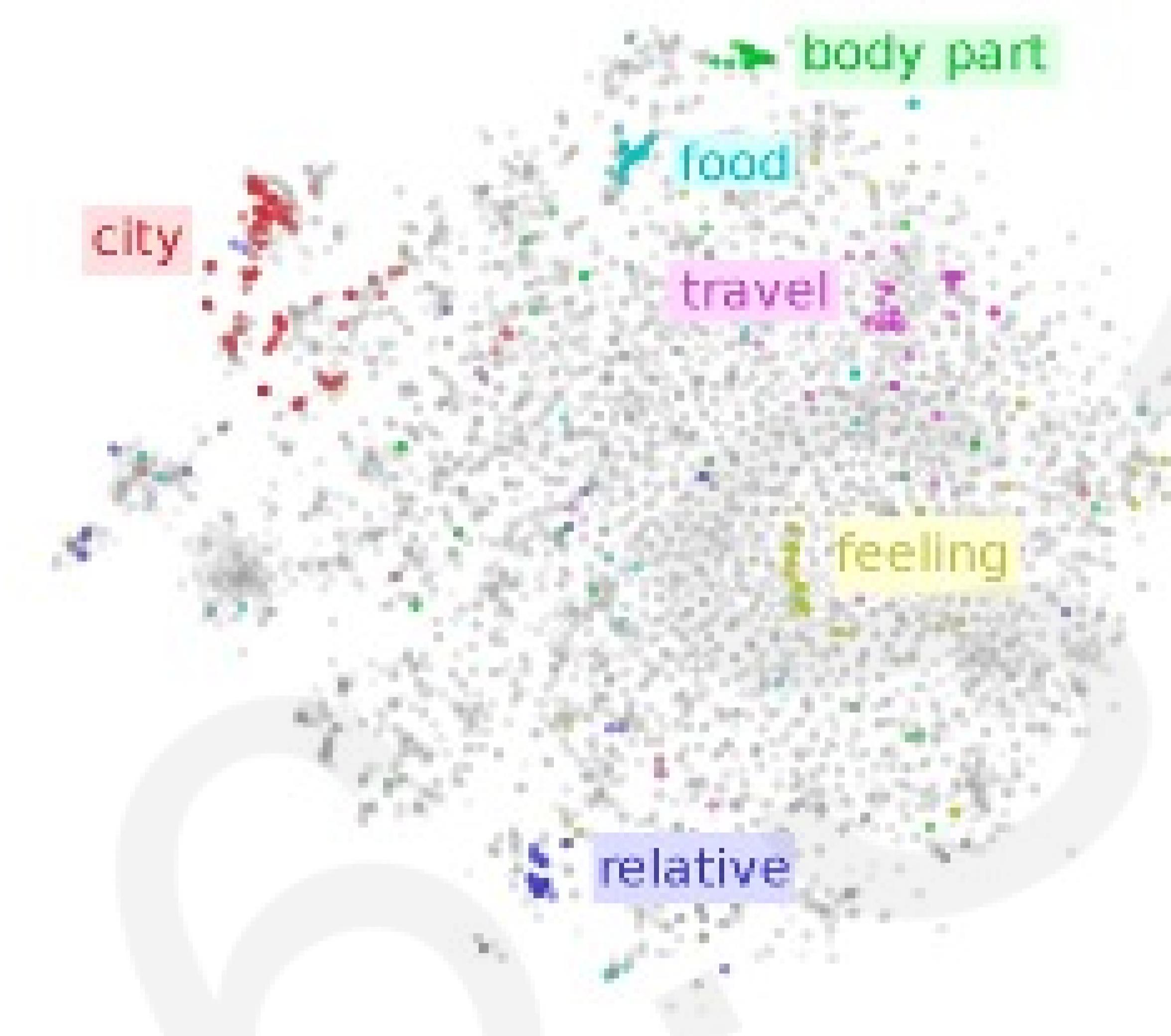


# Other examples of real-world bias



**Autonomous Driving**  
sunny, straight roads vs. adverse  
conditions

[Amini et al, IROS 2018]



**Language Modeling**  
Encodes gender biases

[Caliskan et al, Science 2017]

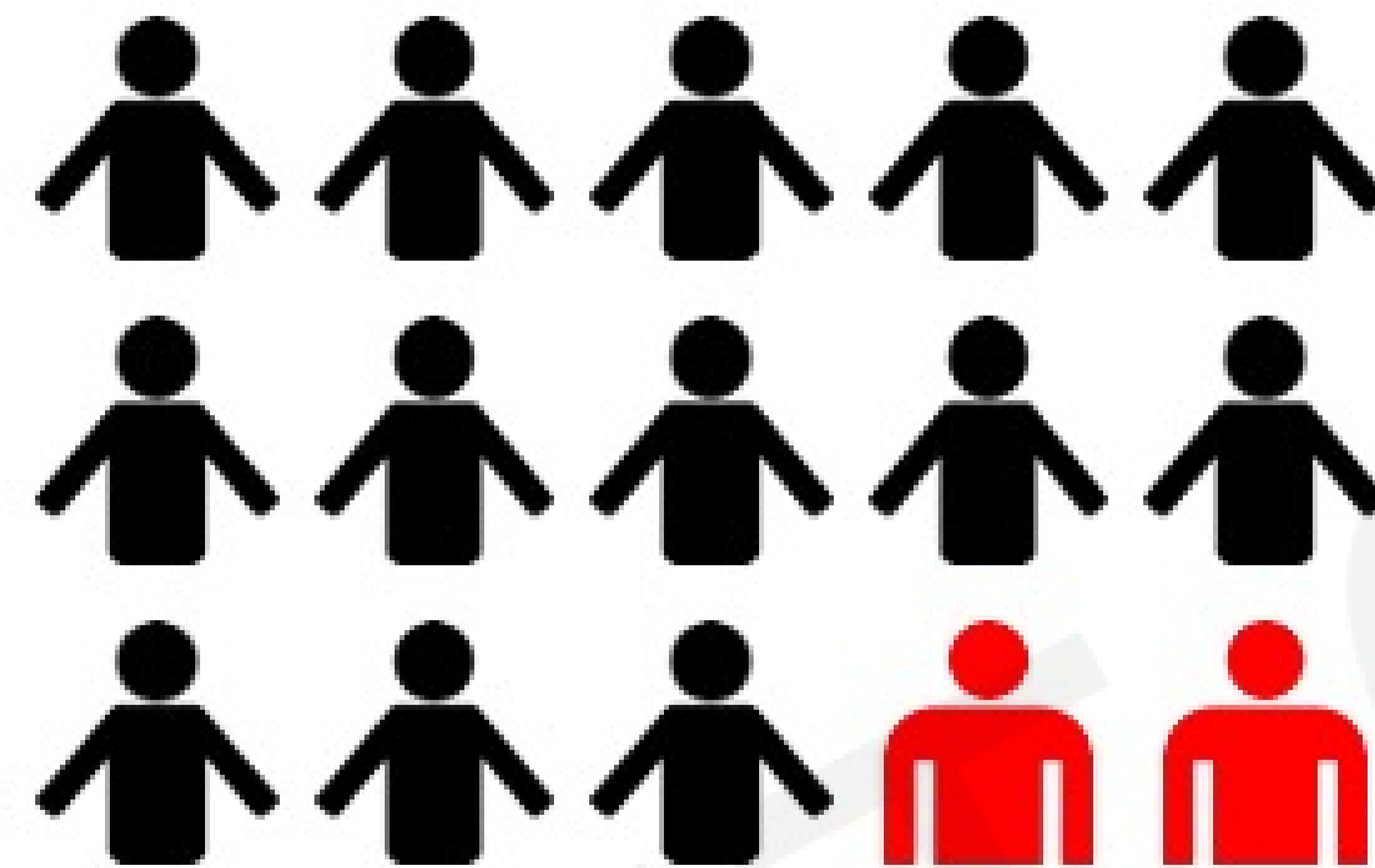


**Healthcare Recommendation  
Algorithms**  
Encodes racial biases

[Obermeyer et al, Science 2019]

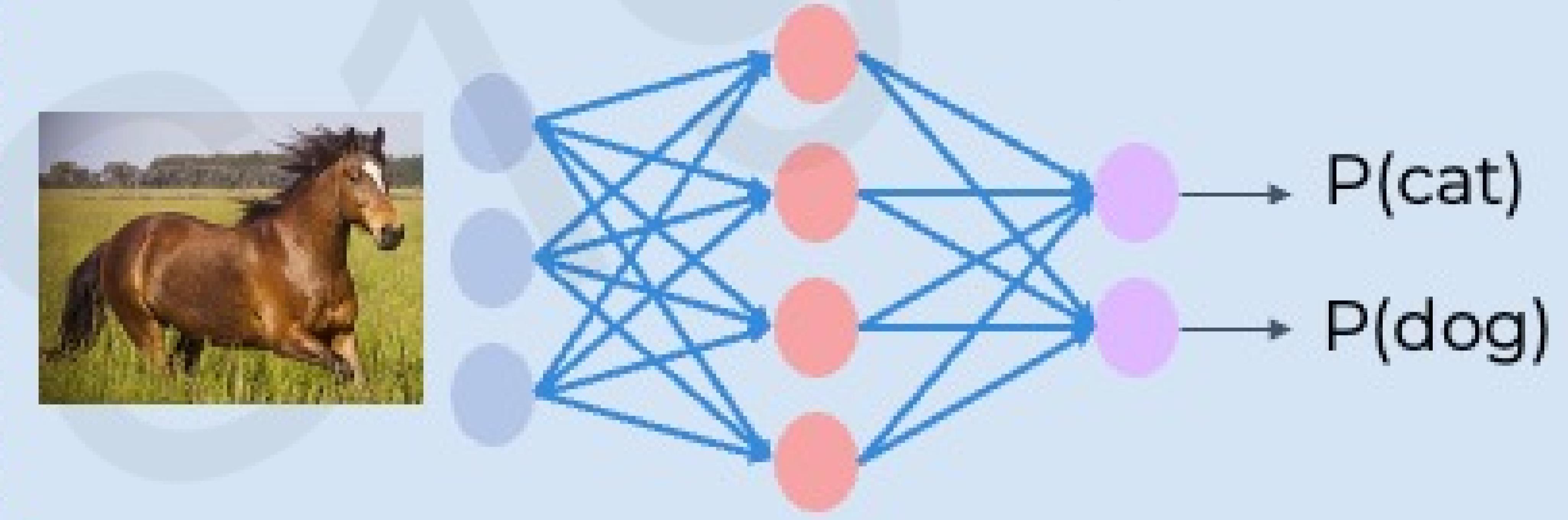
# Challenges for Robust Deep Learning

## Bias



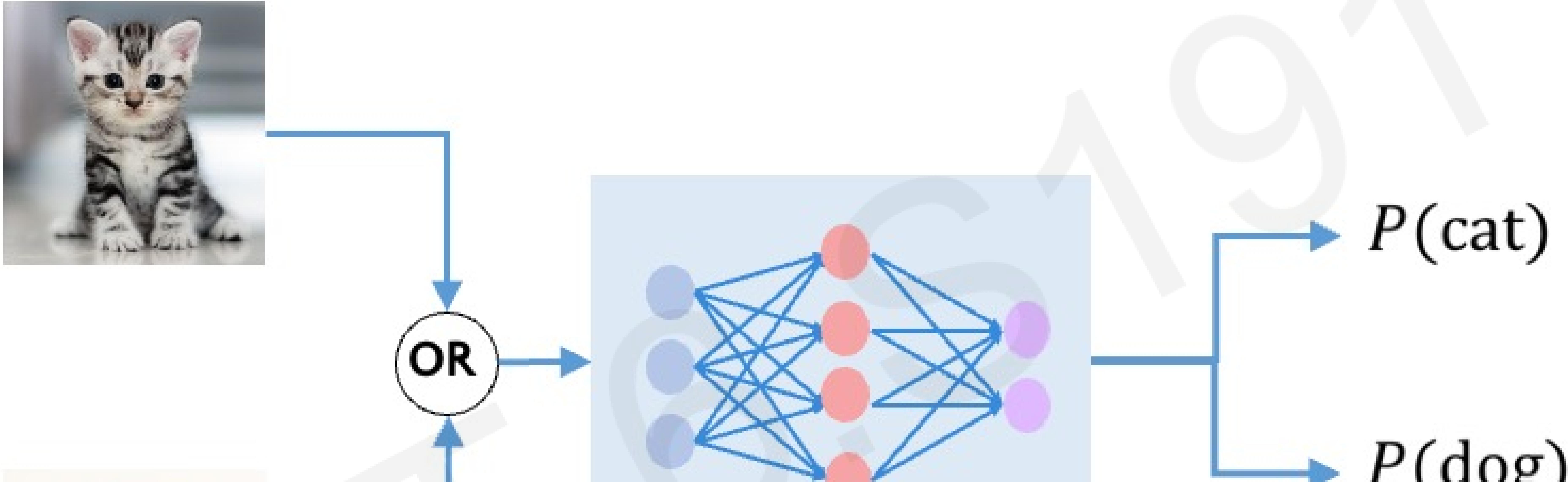
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## Uncertainty



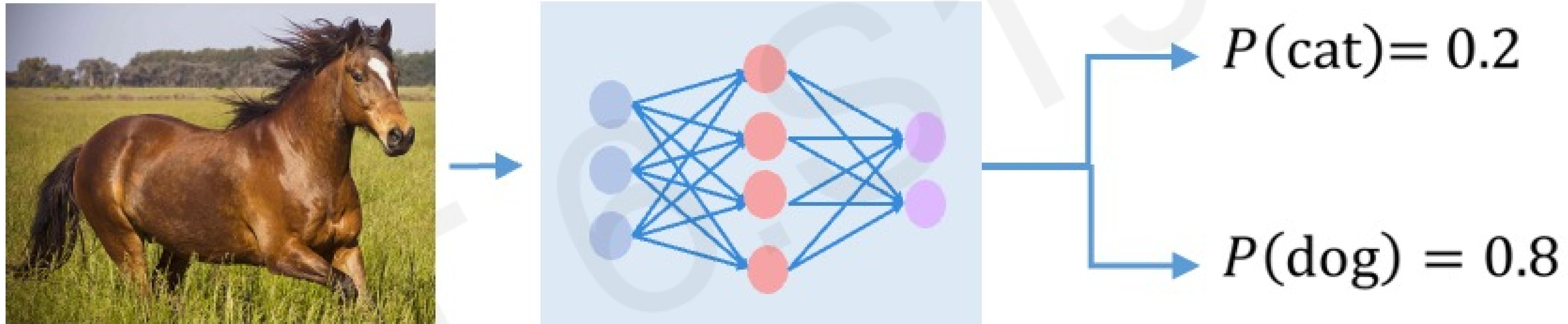
**Can we teach a model to  
recognize when it doesn't  
know the answer?**

# What is uncertainty?



# ...not to be confused with likelihood

Models output a **probability distribution** regardless of input; however, this is not a confidence score!



Uncertainty estimation gives us a measure of **confidence** in the prediction

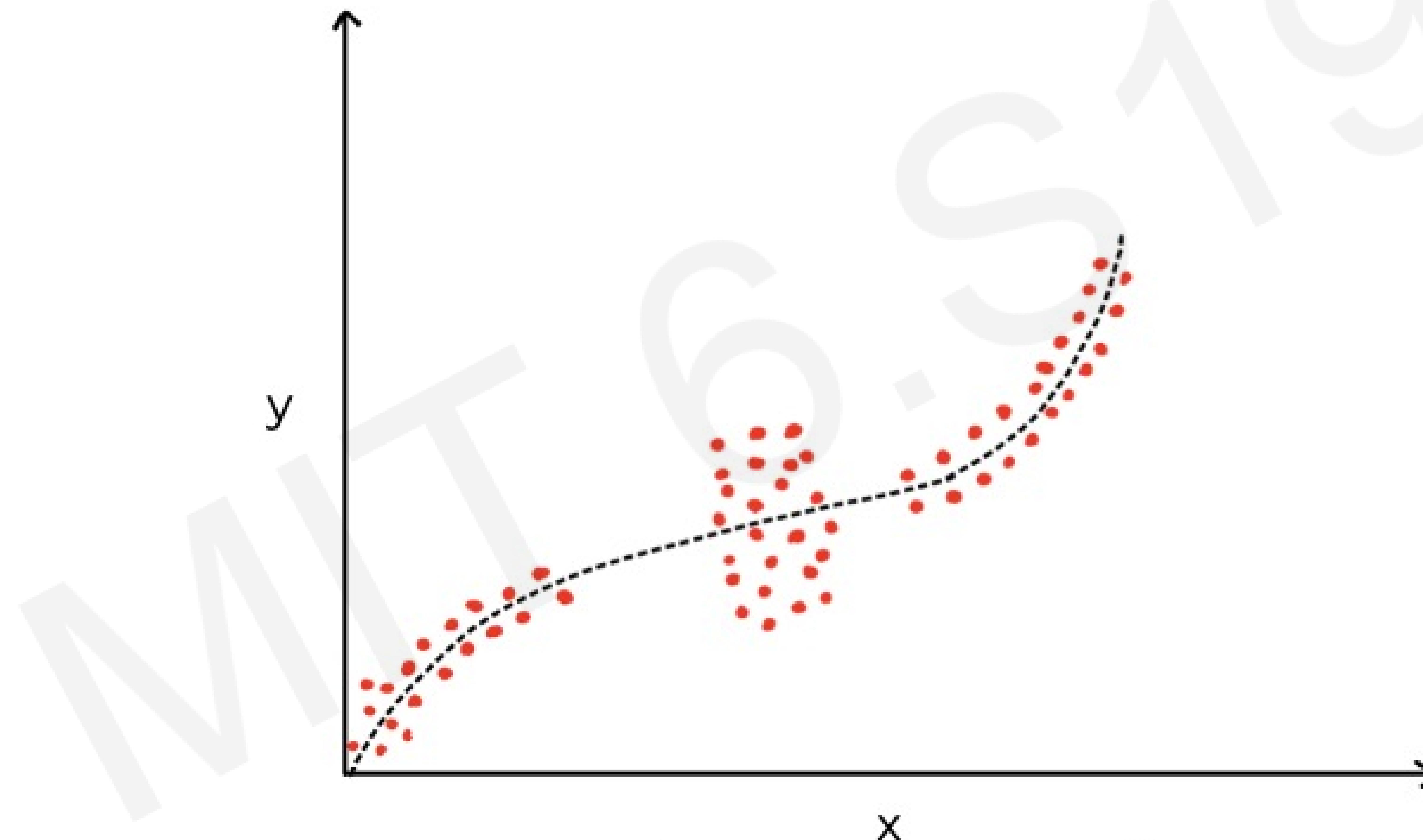
# To mitigate scenarios like this:



Teslas AI is confused

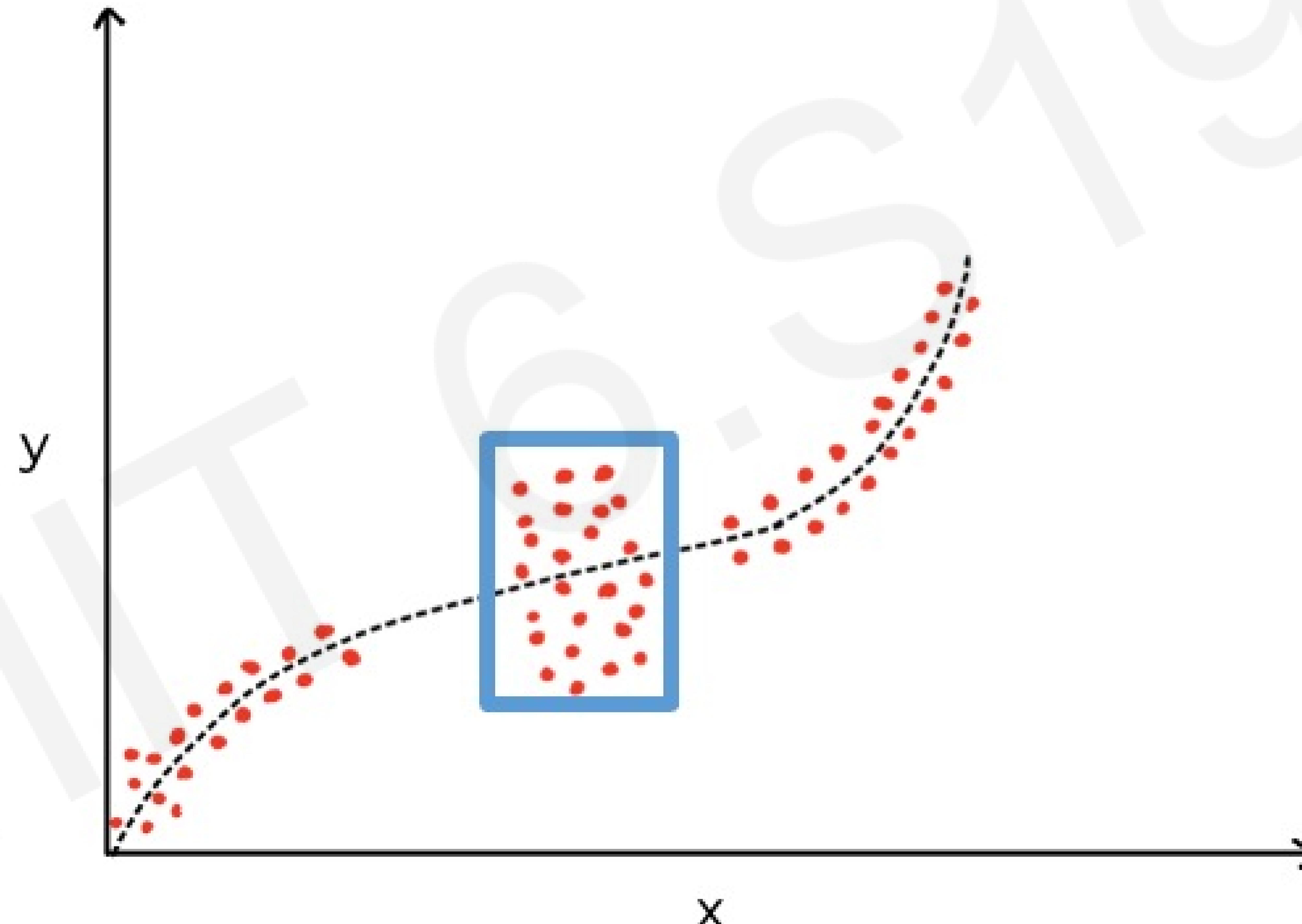
# Types of Uncertainty in Neural Networks

Let's say we're trying to estimate the curve  $y = x^3$ , and our dataset looks like the red points below:



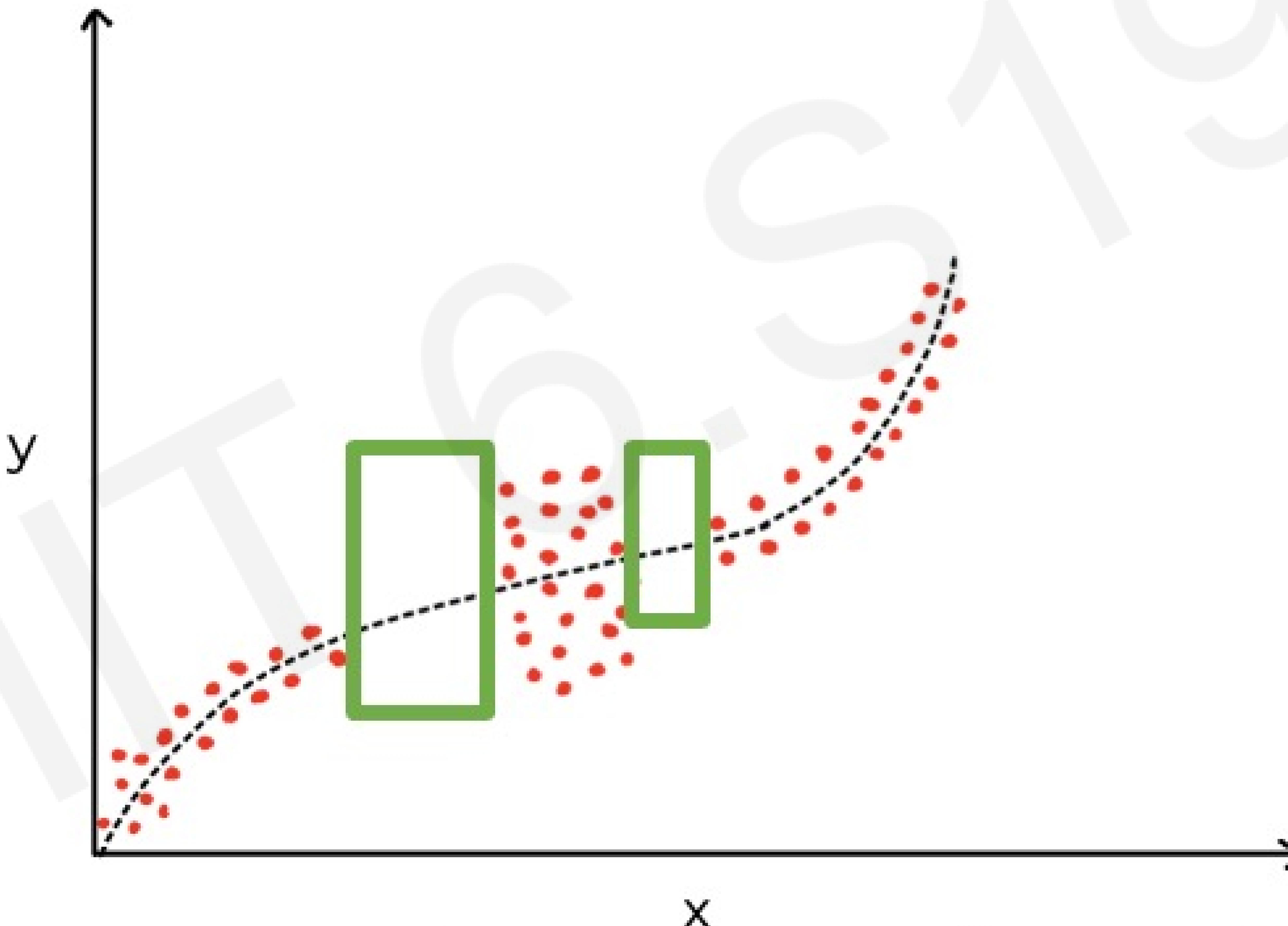
# Types of Uncertainty in Neural Networks

The boxed area shows a region of high **data uncertainty**: very similar inputs have drastically different outputs

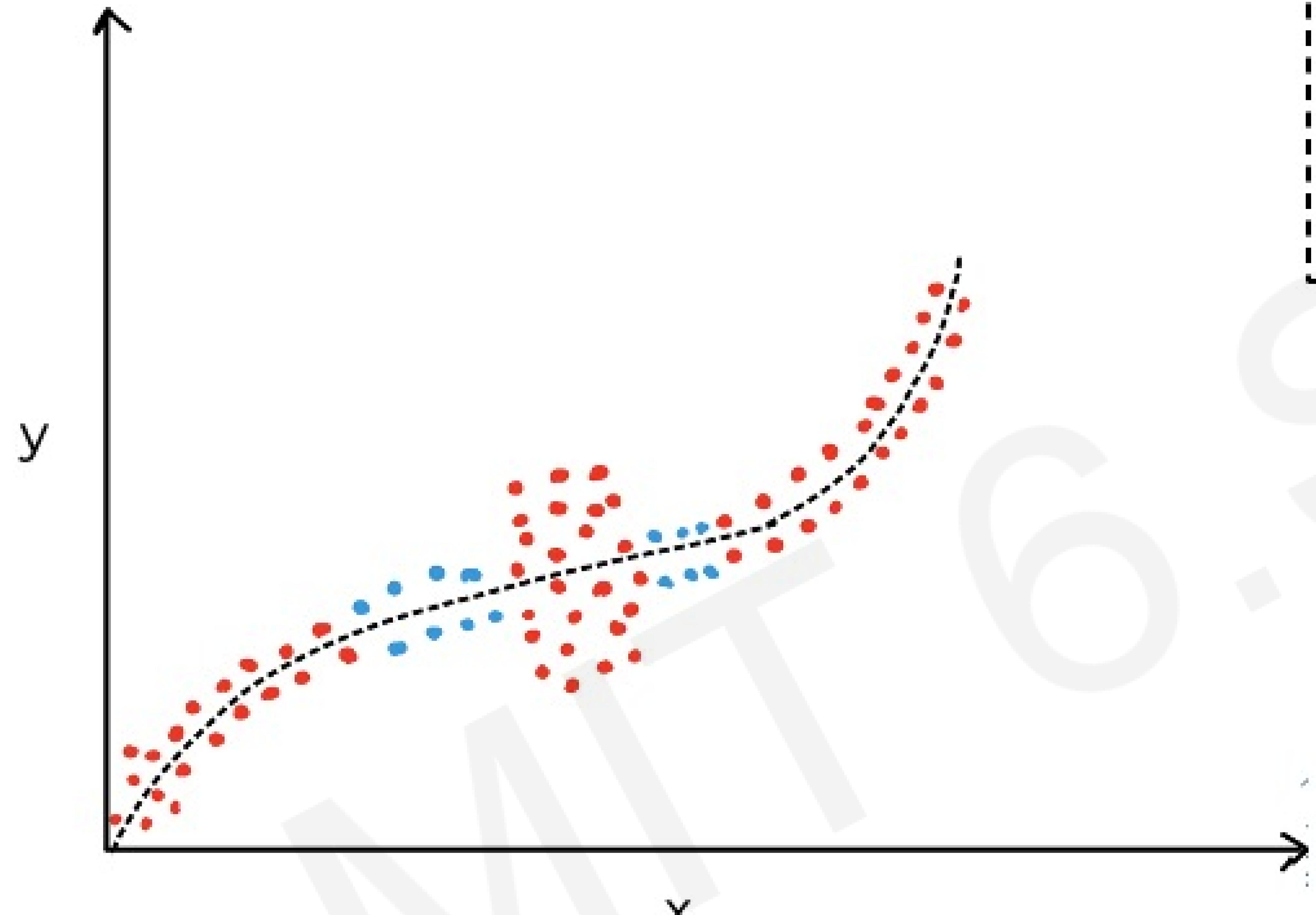


# Types of Uncertainty in Neural Networks

The boxed area shows a region of high **model uncertainty**:  
points here are out of distribution

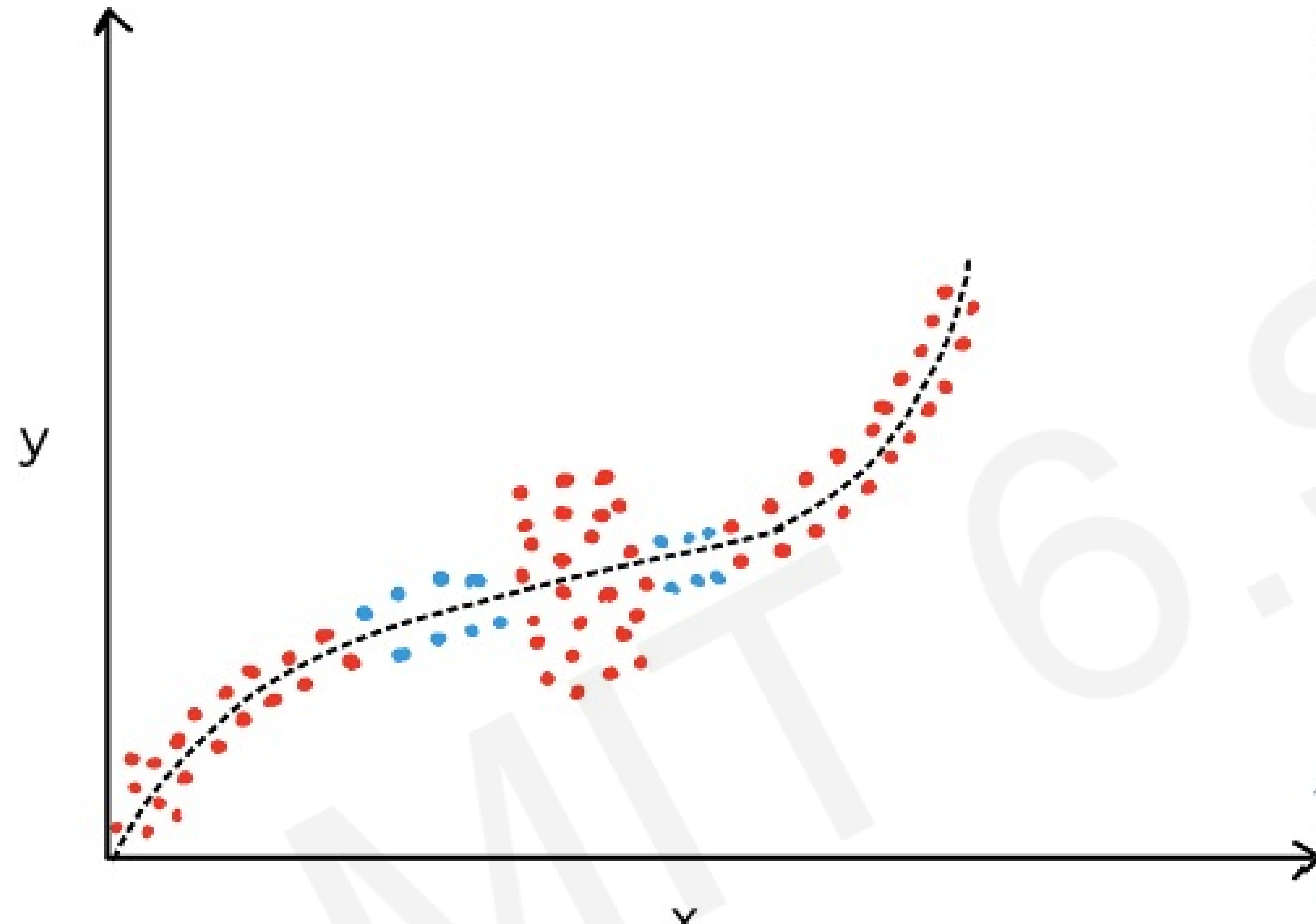


# Augmenting datasets to mitigate uncertainty



Would adding the **blue** training points to our dataset reduce uncertainty? If so, which type of uncertainty?

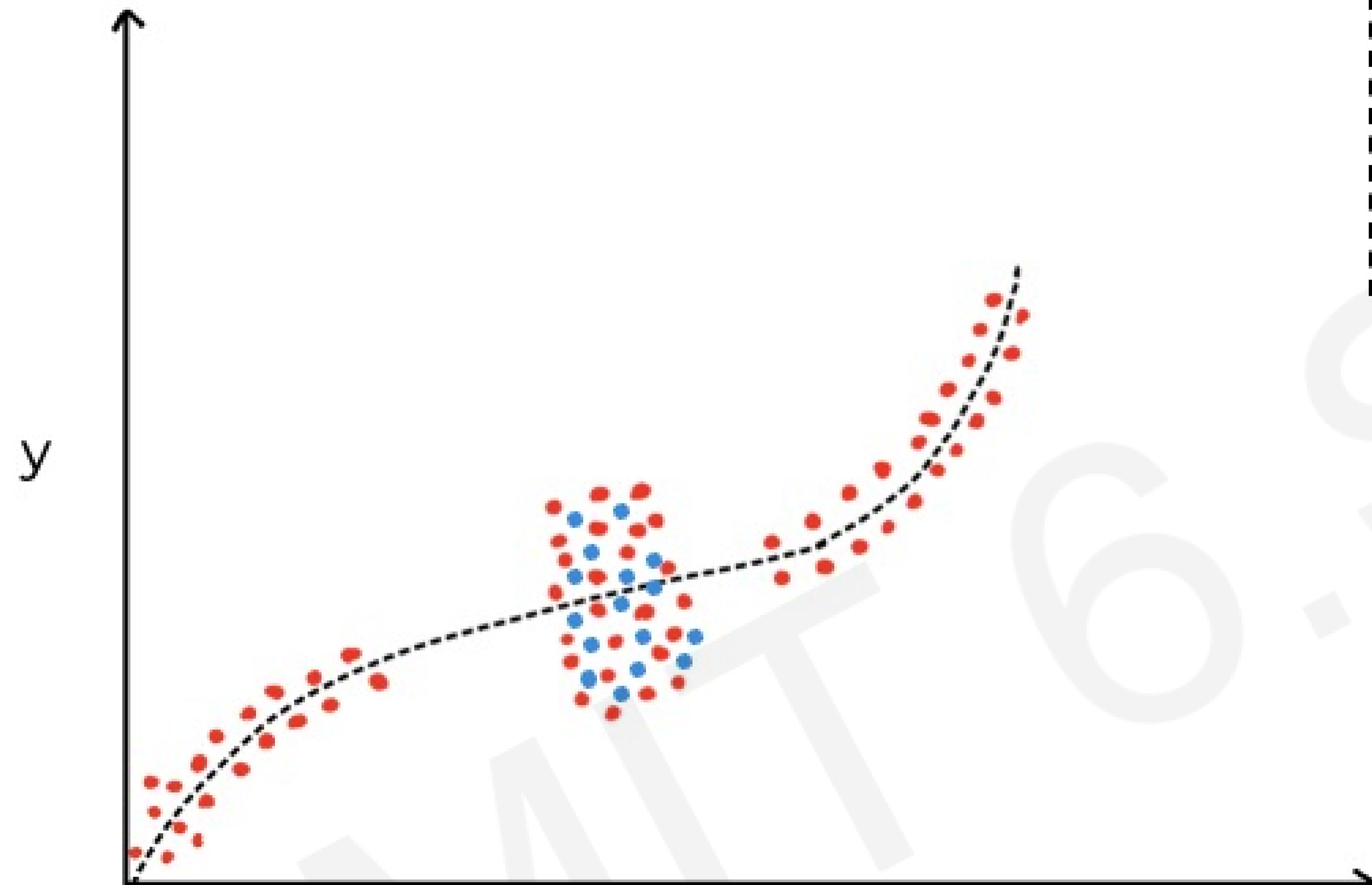
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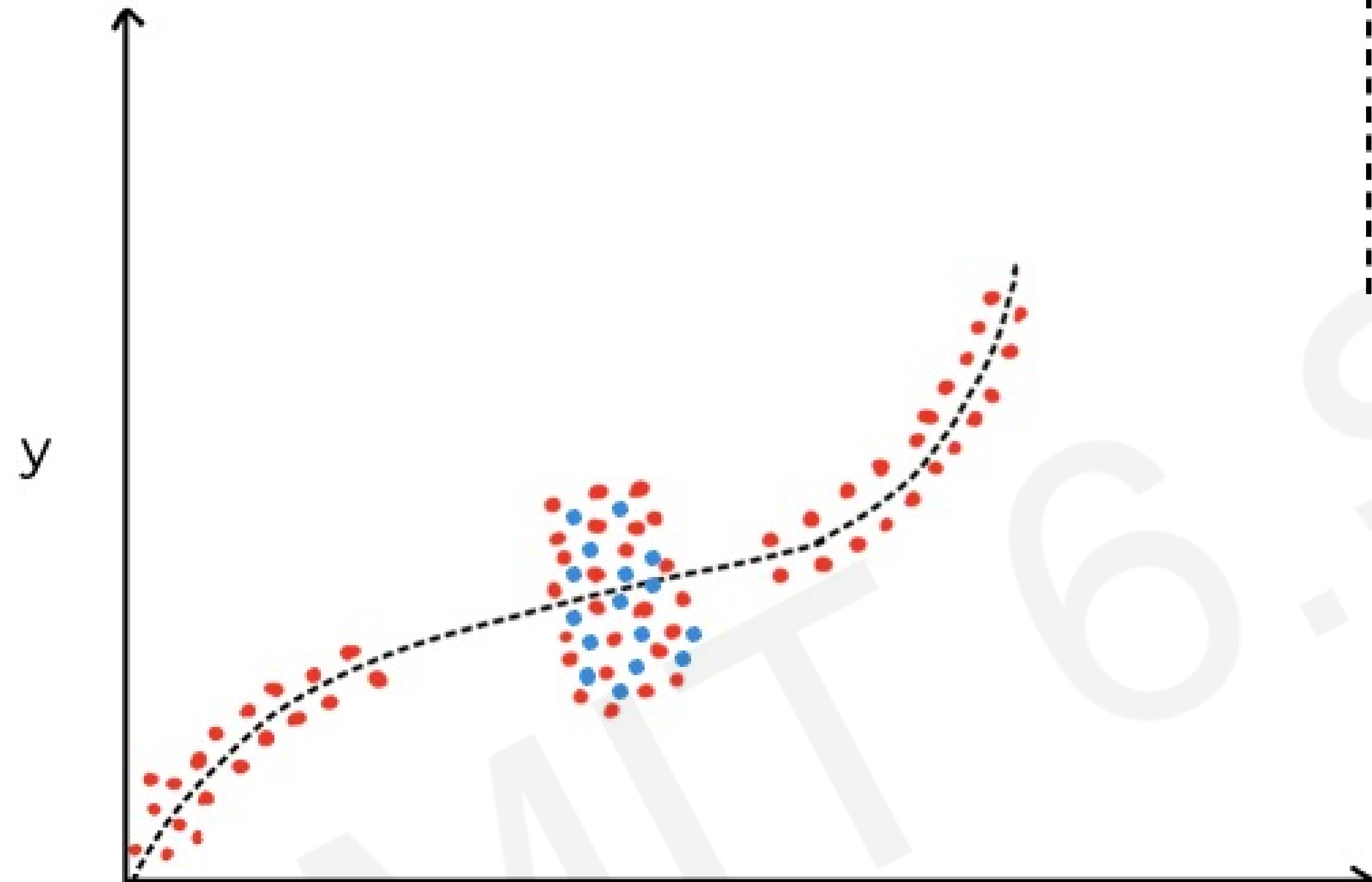
Model uncertainty is reduced by adding data!

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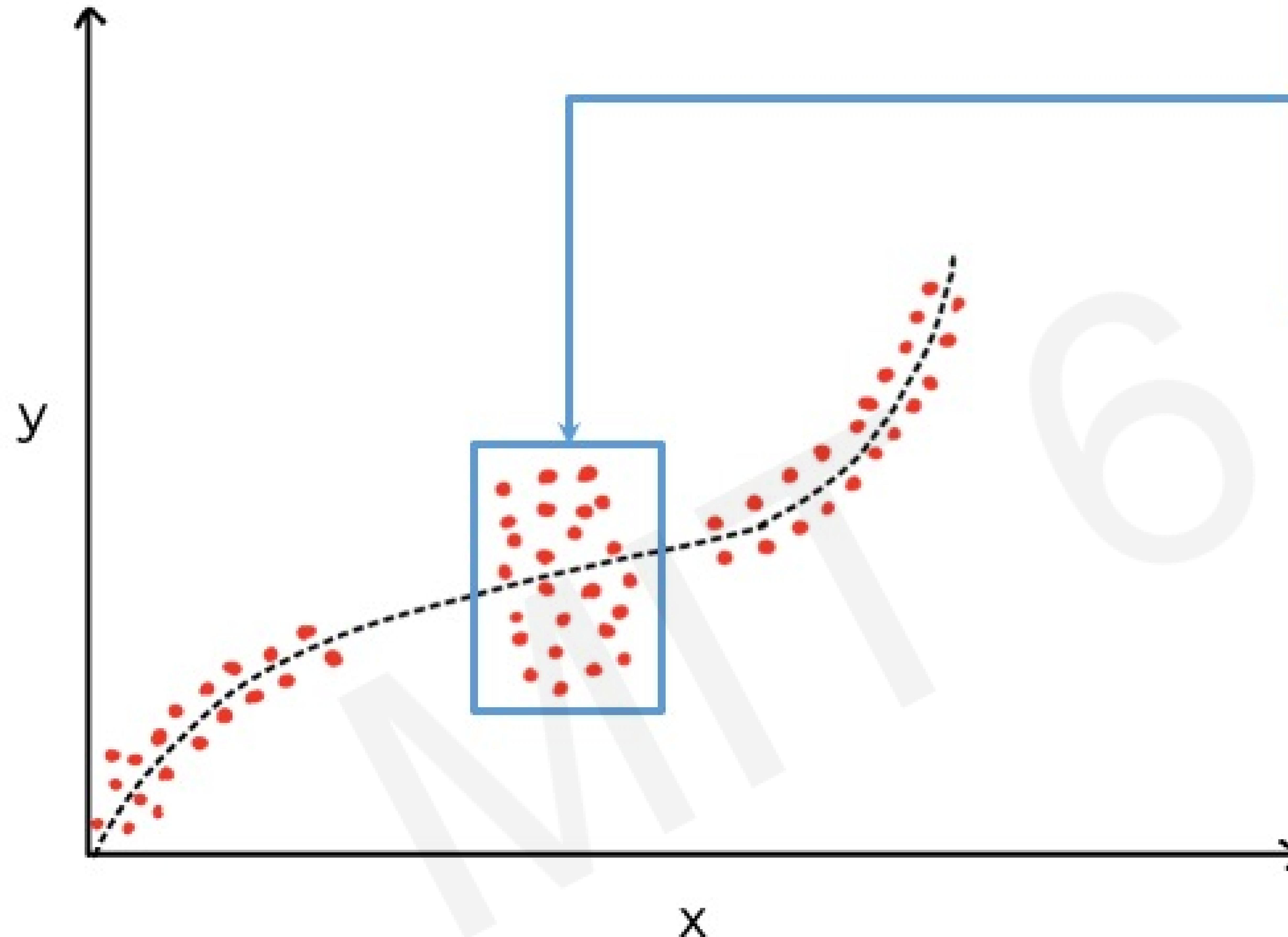
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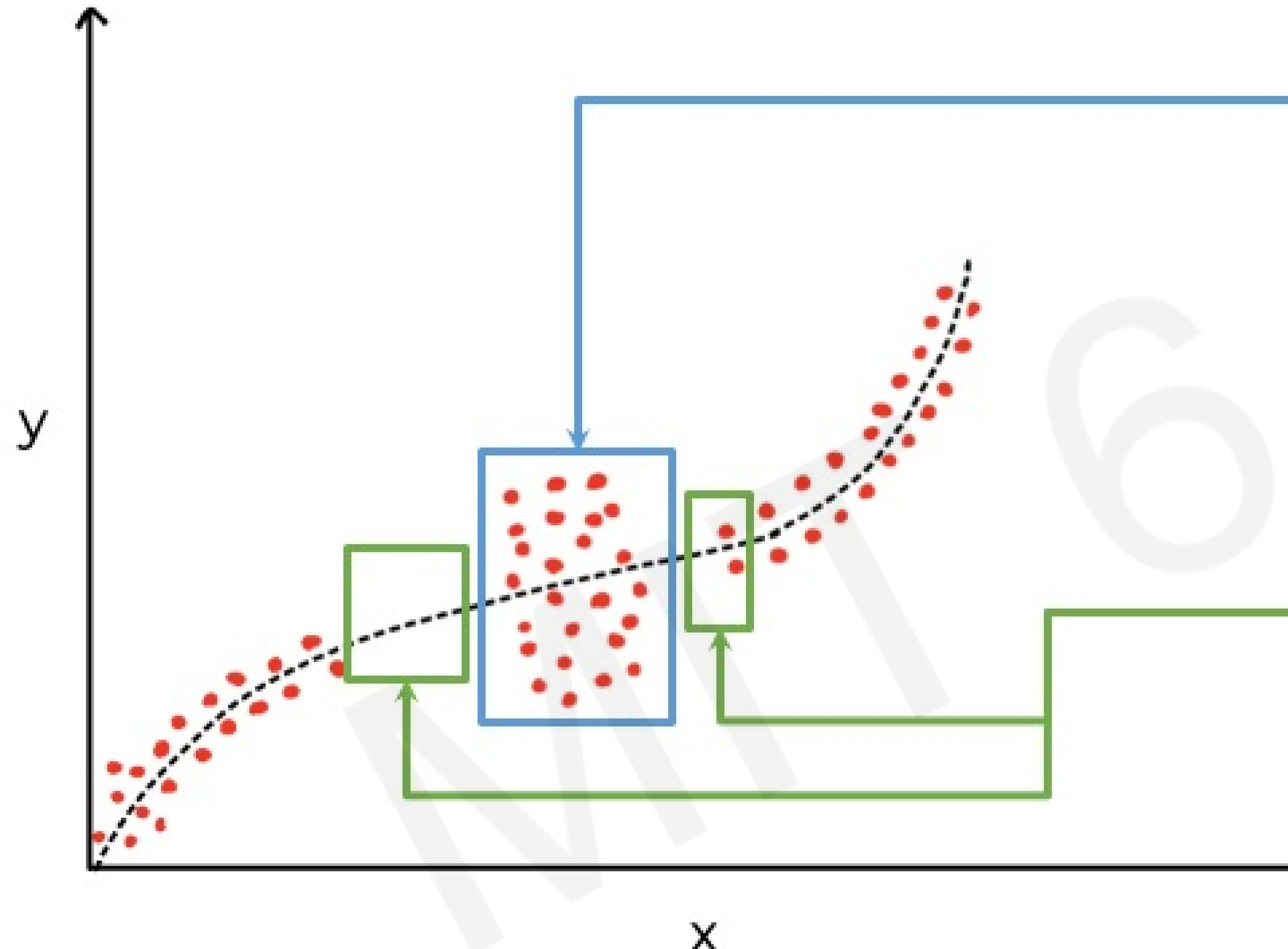
No-- data uncertainty is **irreducible!**

# Aleatoric vs. Epistemic Uncertainty



- **Aleatoric** uncertainty = data uncertainty
- Irreducible!
- Can be **directly learned from data**

# Aleatoric vs. Epistemic Uncertainty



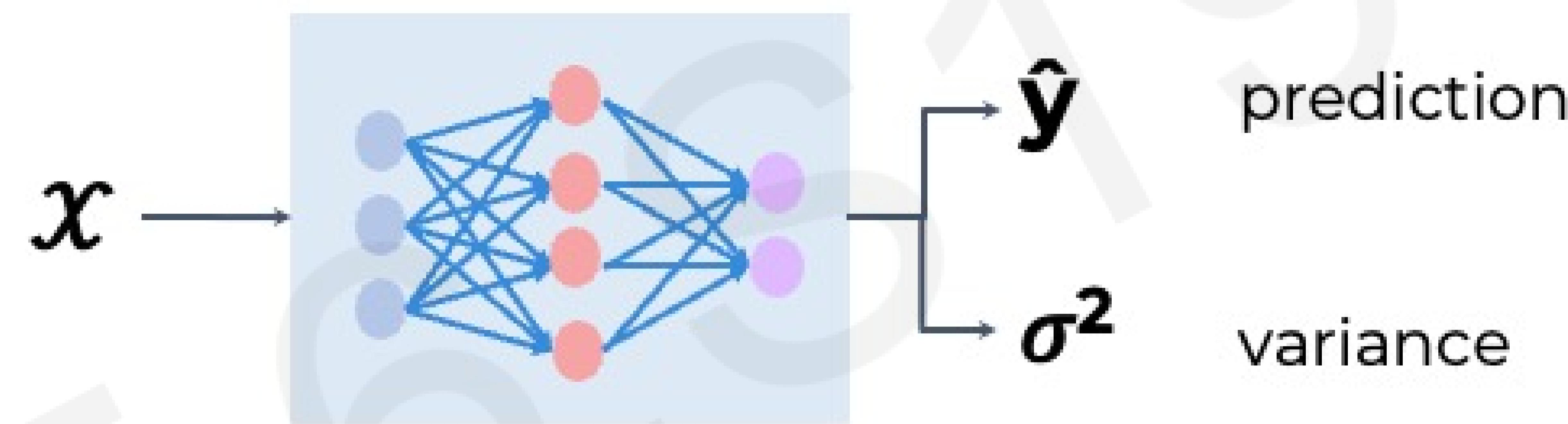
- **Aleatoric** uncertainty = data uncertainty
- Irreducible!
- Can be **directly learned from data**

- **Epistemic** uncertainty = model uncertainty
- Reducible by adding data!
- **Cannot** be directly learned from data

# Estimating Aleatoric Uncertainty: Regression

Goal: learn a set of **variances** corresponding to the input

Higher variance  $\rightarrow$  there is more uncertainty at this part of the dataset (more noise!)



$$f_{\theta}(x) \rightarrow \hat{y}, \sigma^2$$

This variance is **not constant**  
and depends on the value of  $x$ !

# Negative Log Likelihood Loss to Learn Variance

Our current loss function does not take into account variance:

$$\mathcal{L} = \frac{1}{N} \times \sum_{i=1}^N (\hat{y}_i - y_i)^2$$

By minimizing Mean Squared Error, we can learn the parameters of a multivariate **Gaussian** with mean  $y_i$  and **constant variance**.

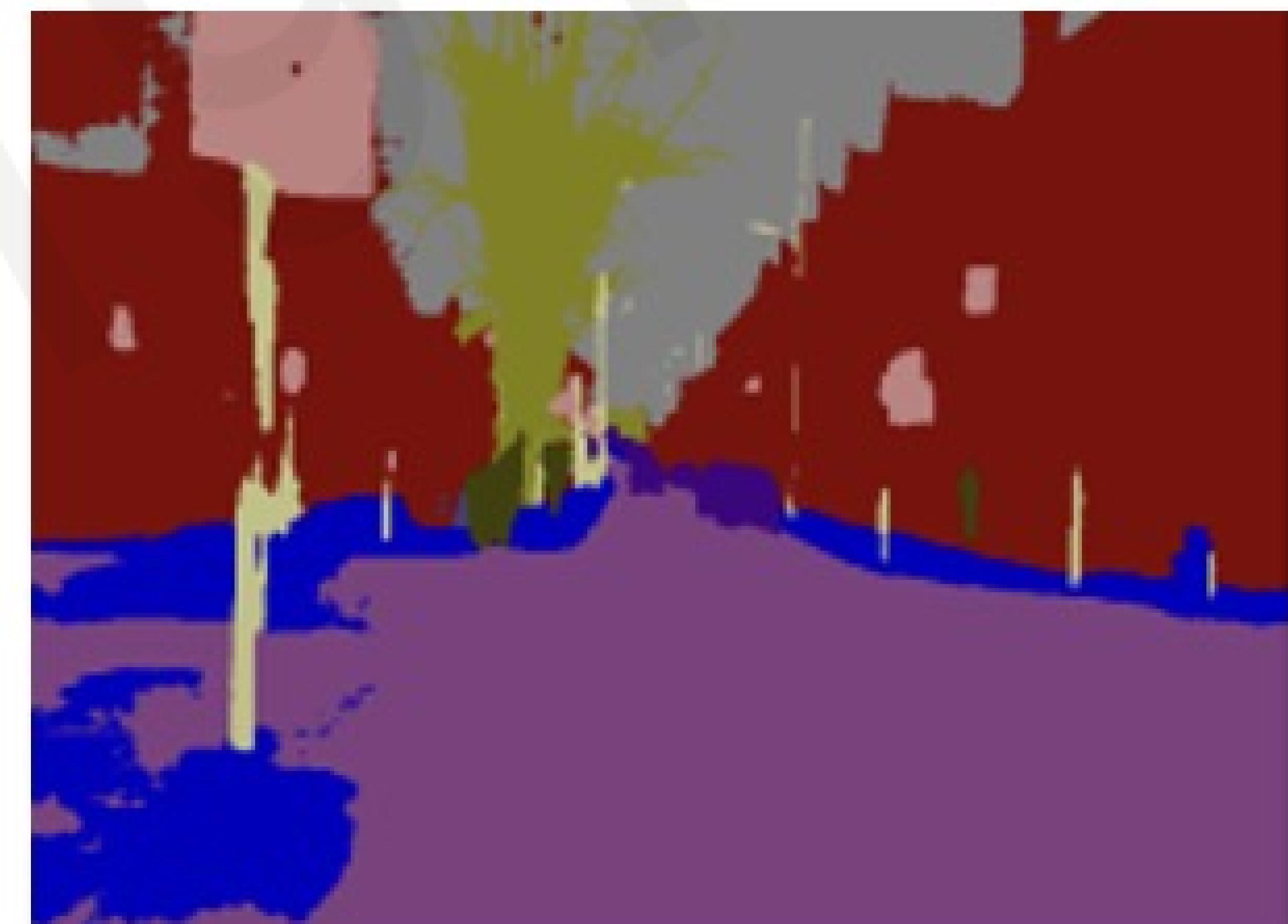
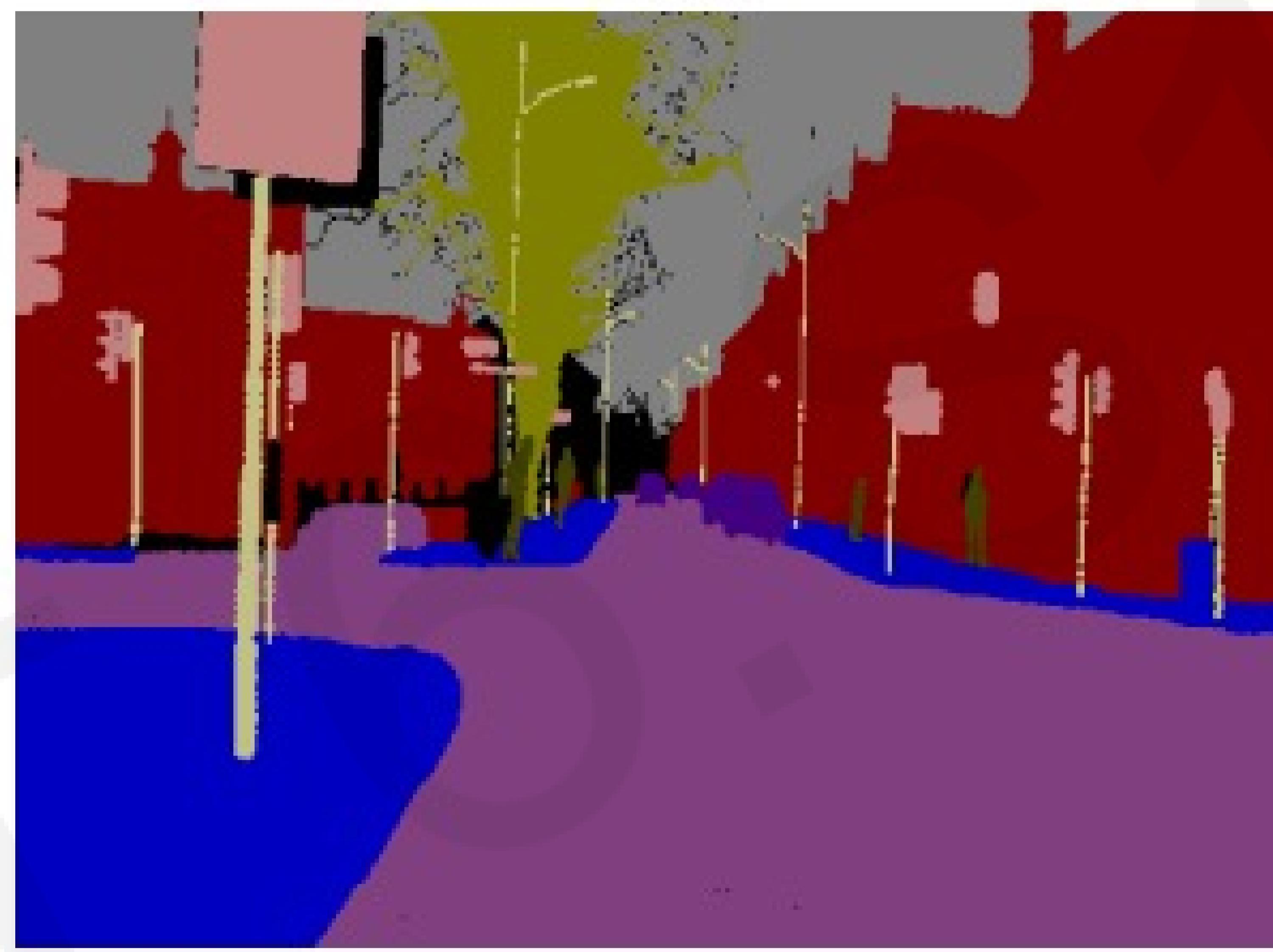
# Negative Log Likelihood Loss to Learn Variance

Negative Log Likelihood (NLL) is a **generalization** of MSE to **non-constant variances**:

$$\mathcal{L} = \frac{1}{N} \times \sum_{i=1}^N \frac{(\hat{y}_i - y_i)^2}{2\sigma_i^2} + \ln \sigma_i^2$$

# Aleatoric Uncertainty in the Real World: Semantic Segmentation

Semantic Segmentation: label every **pixel** of an image with its corresponding class



**Inputs:** RGB Images of scenes in cities

**Labels:** pixel-level masks of image

**Outputs:** predicted pixel-level masks of image

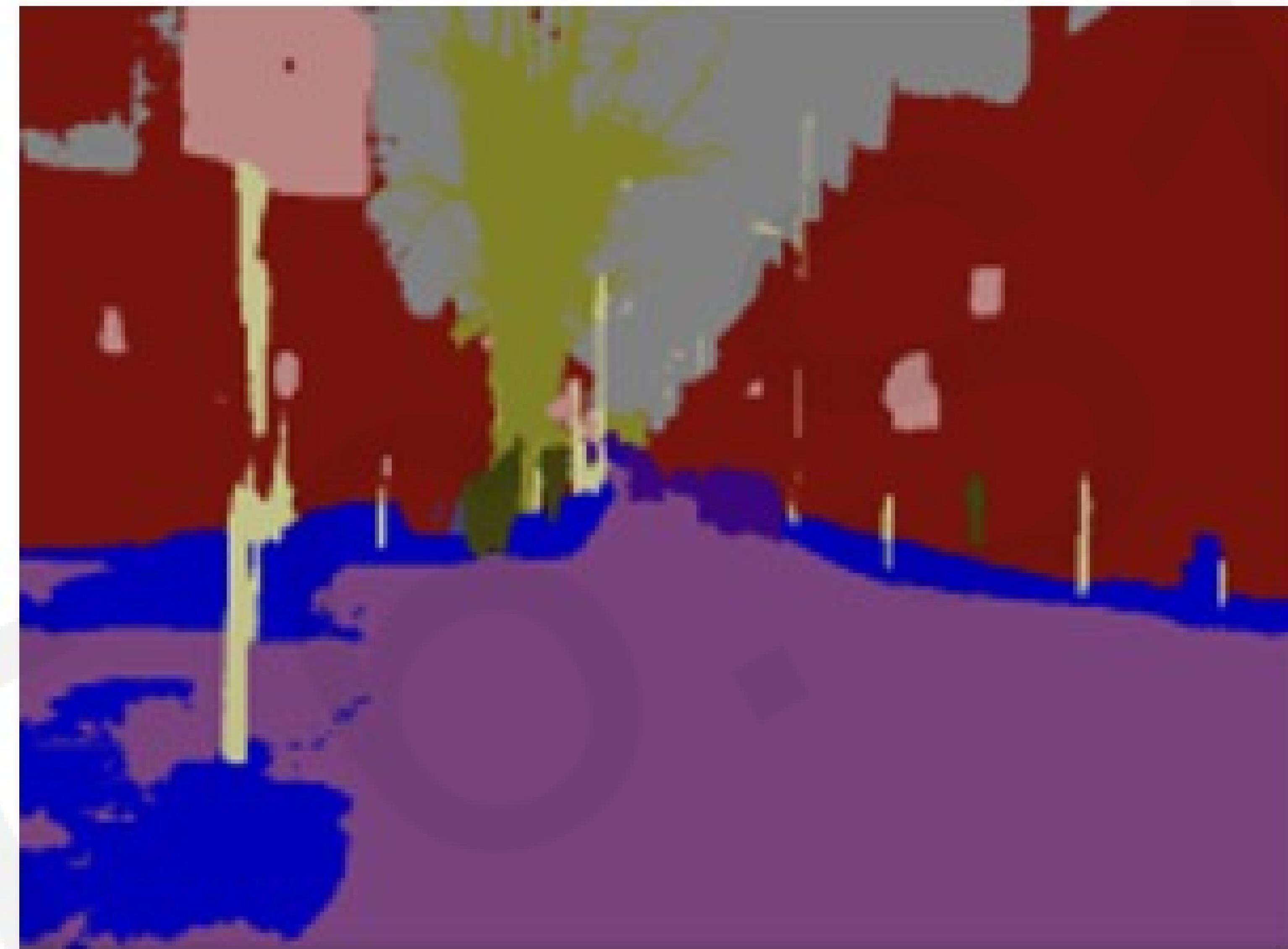
Which parts of this dataset have high **data** or aleatoric uncertainty?

# Aleatoric Uncertainty in the Real World: Semantic Segmentation

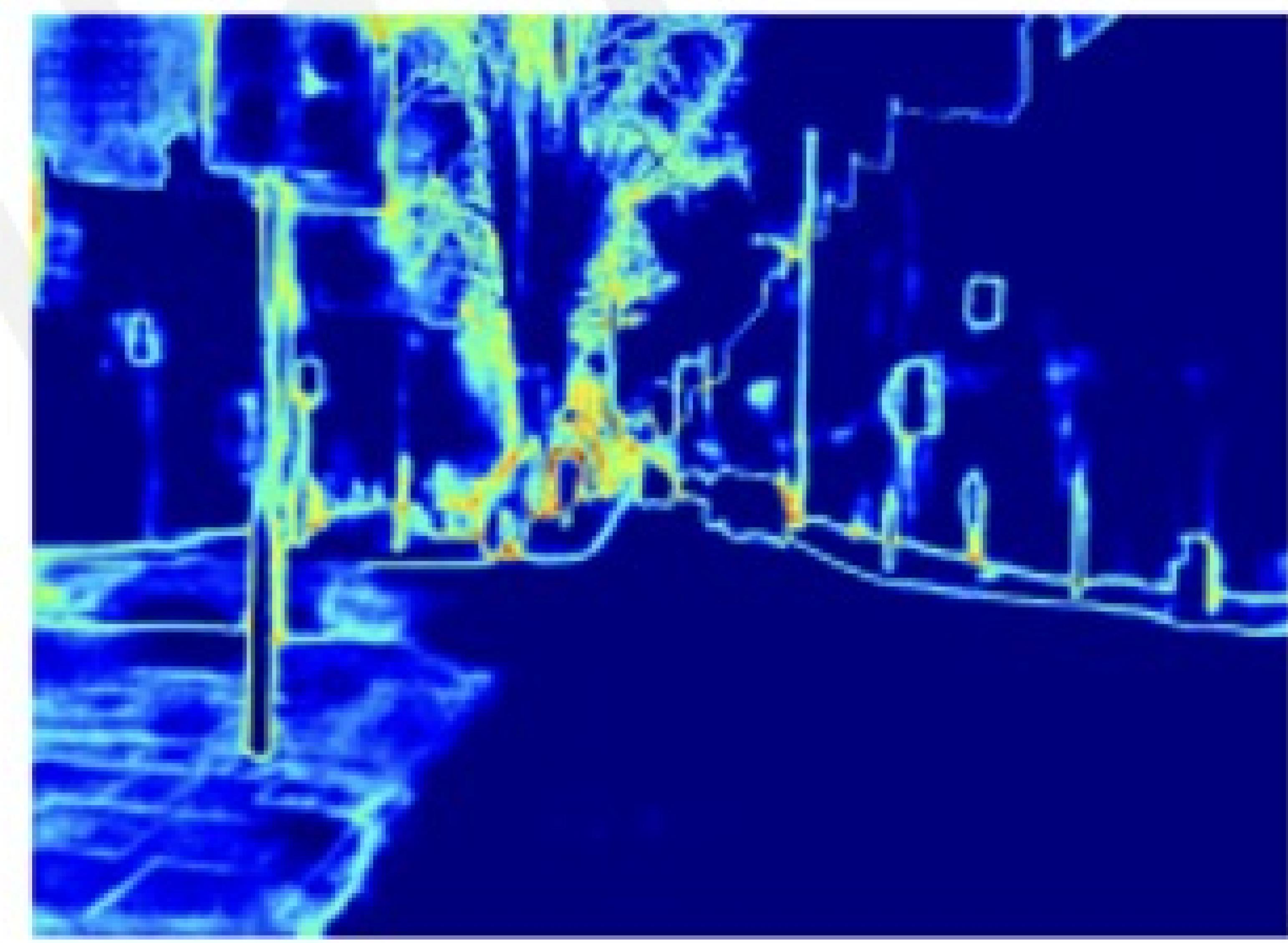
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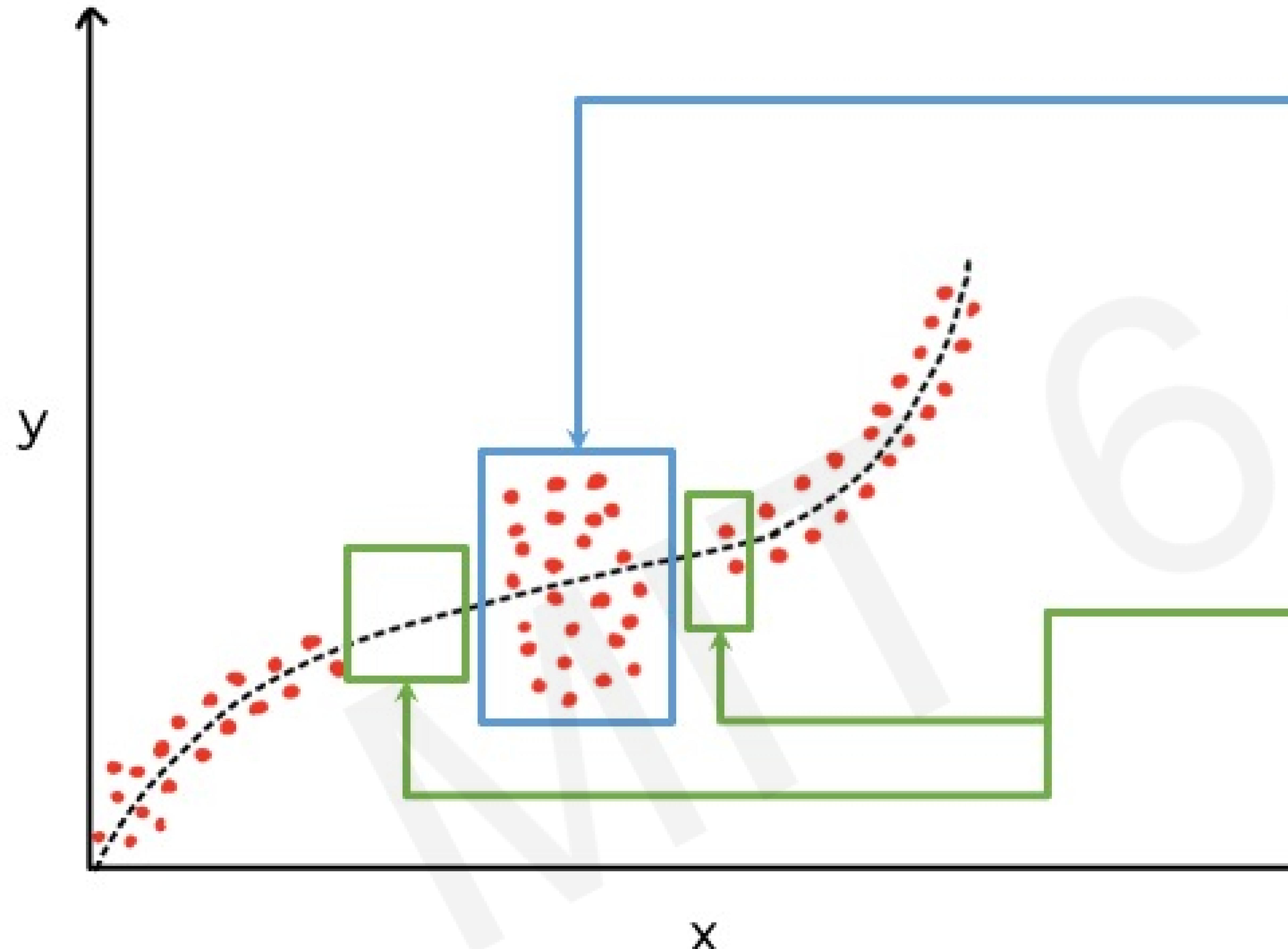


**Outputs:** pixel-level masks of labels



**Corners and boundaries** have high aleatoric uncertainty

# Aleatoric vs. Epistemic Uncertainty



- **Aleatoric** uncertainty = data uncertainty

- Irreducible!

- Can be **directly learned from data**

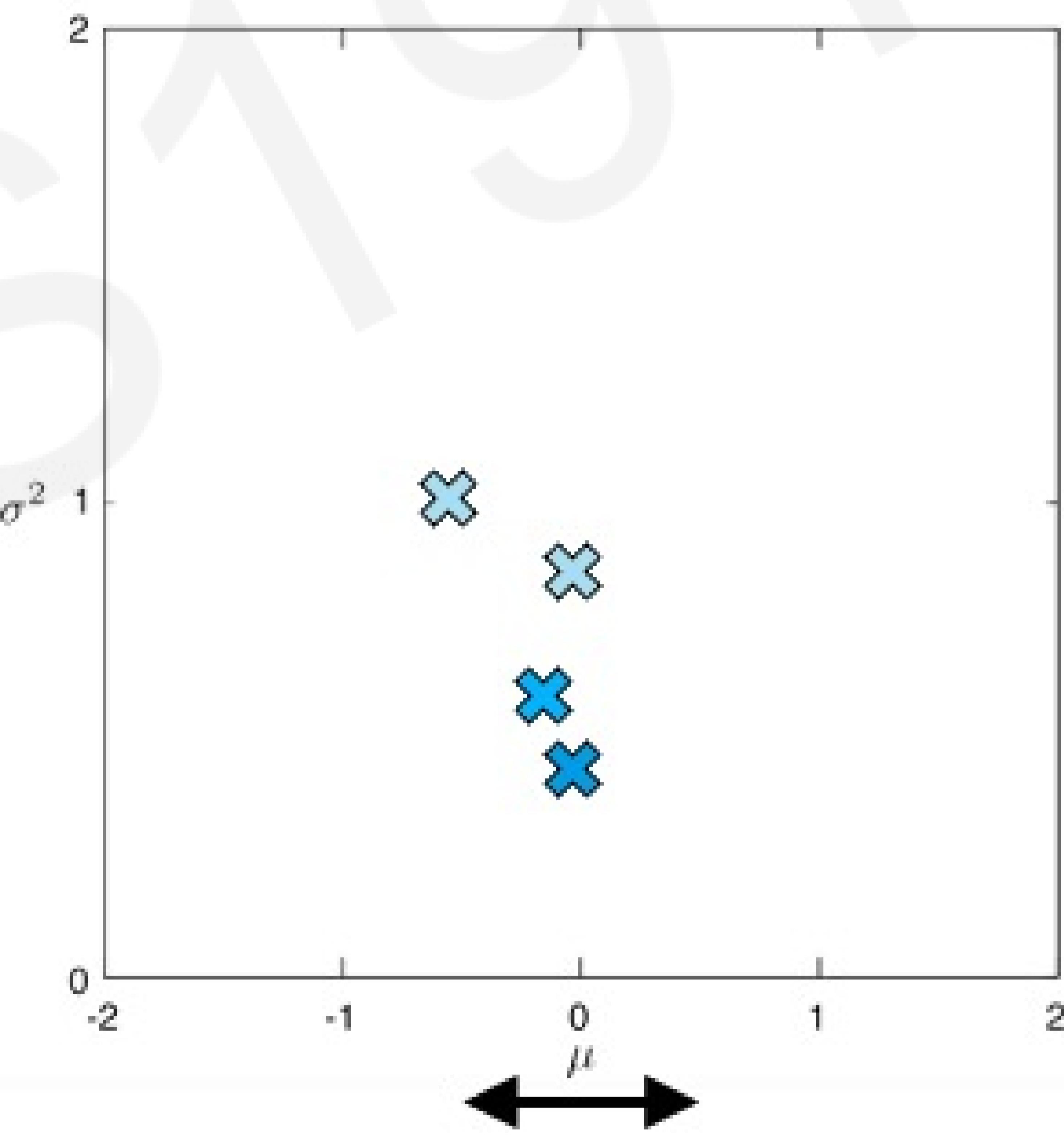
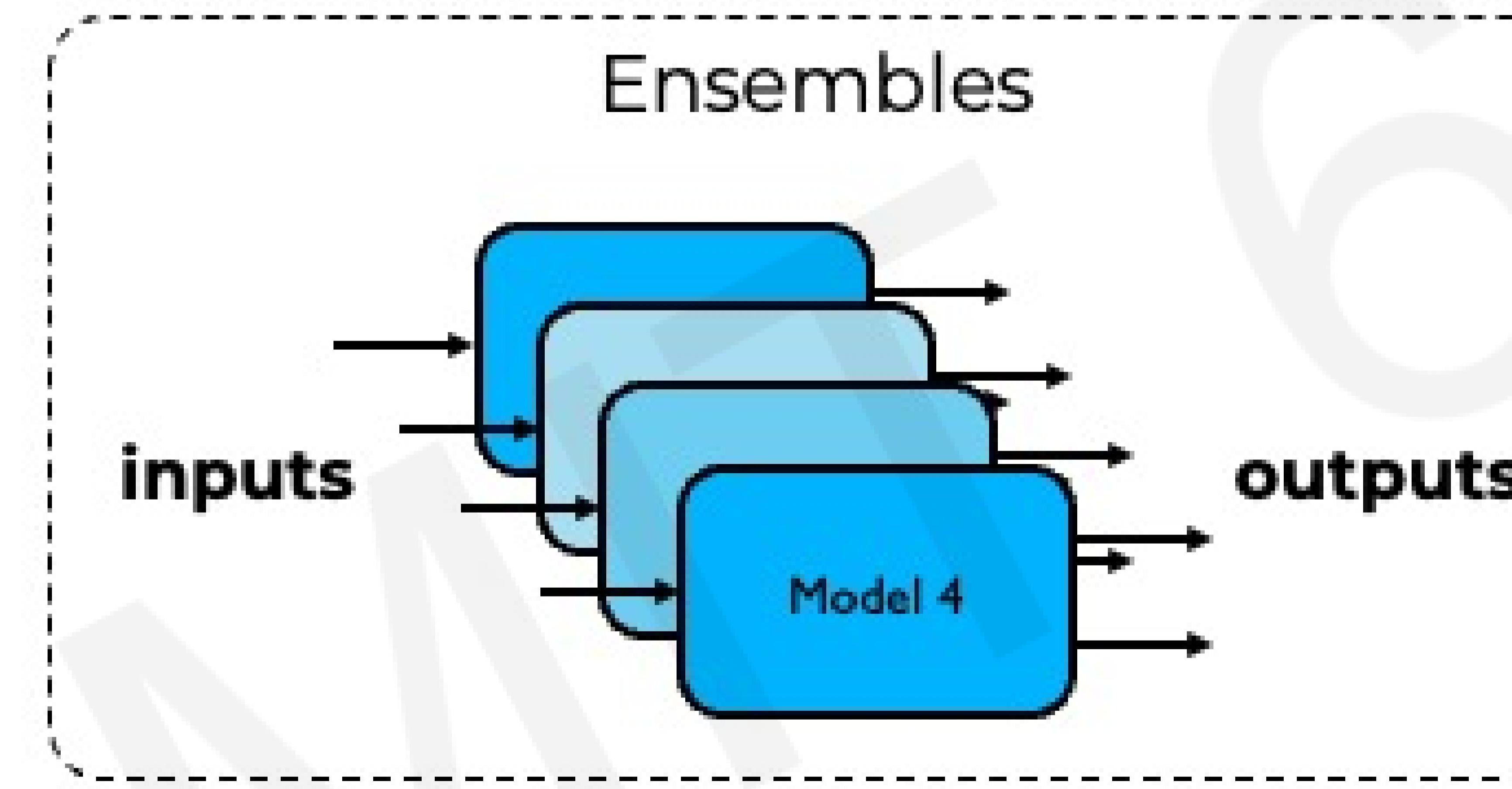
- **Epistemic** uncertainty = model uncertainty

- Reducible by adding data!

- **Cannot** be directly learned from data

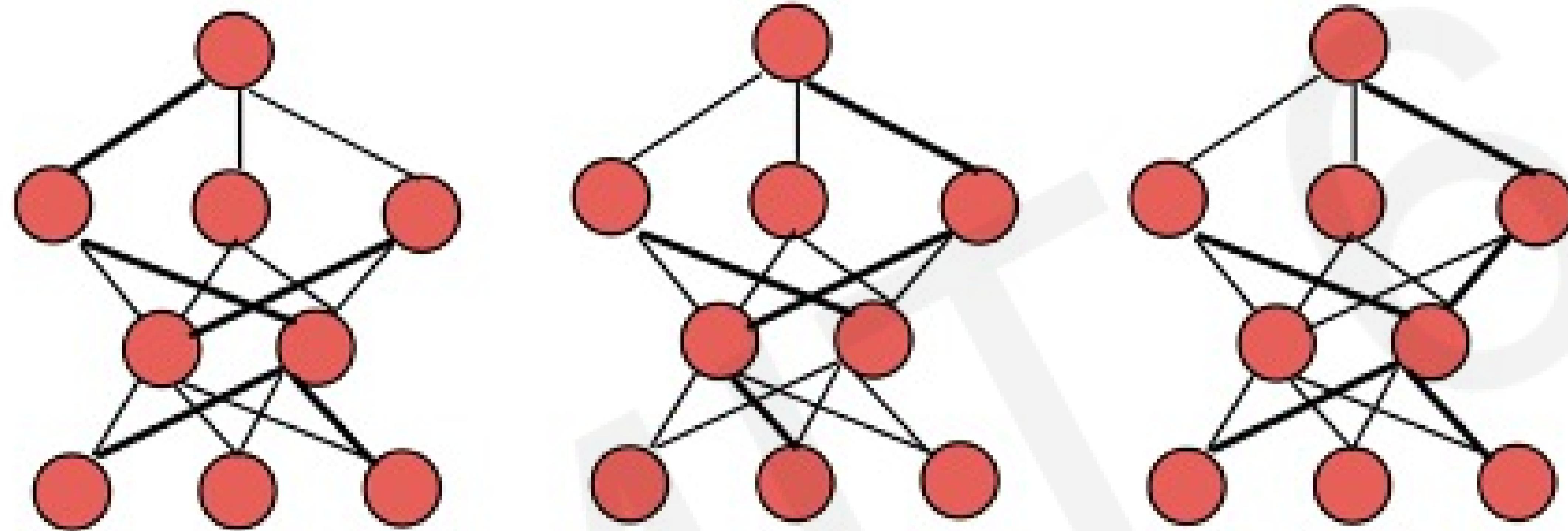
# Introduction to Estimating Epistemic Uncertainty

What if we train the same network multiple times (an **ensemble** of networks) and compare outputs?



# Estimating Epistemic Uncertainty through Sampling: Ensembling

- “Familiar” inputs → similar output for every network
- “Unfamiliar” inputs → different outputs for every network

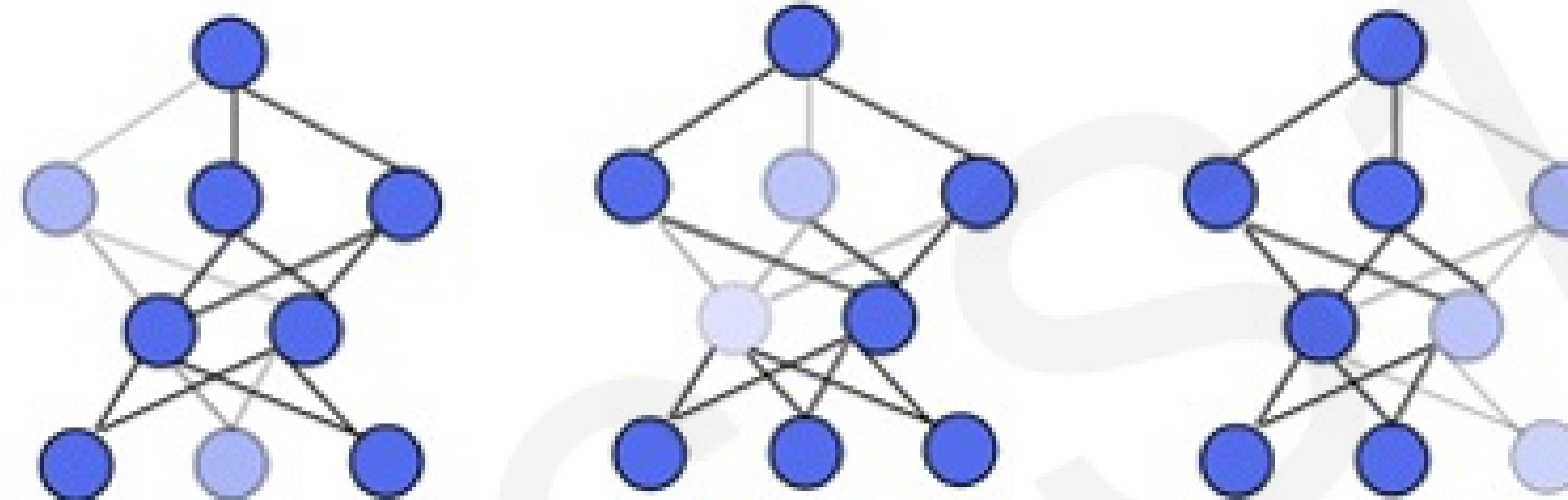


```
num_ensembles = 5
for i in range(num_ensembles):
    model = create_model(...)
    model.fit(...)
```

```
raw_predictions = [models[i].predict(x)
                    for i in range(num_ensembles)]
mu = np.mean(raw_predictions)
uncertainty = np.var(raw_predictions)
```

# Estimating Epistemic Uncertainty through Sampling: Dropout

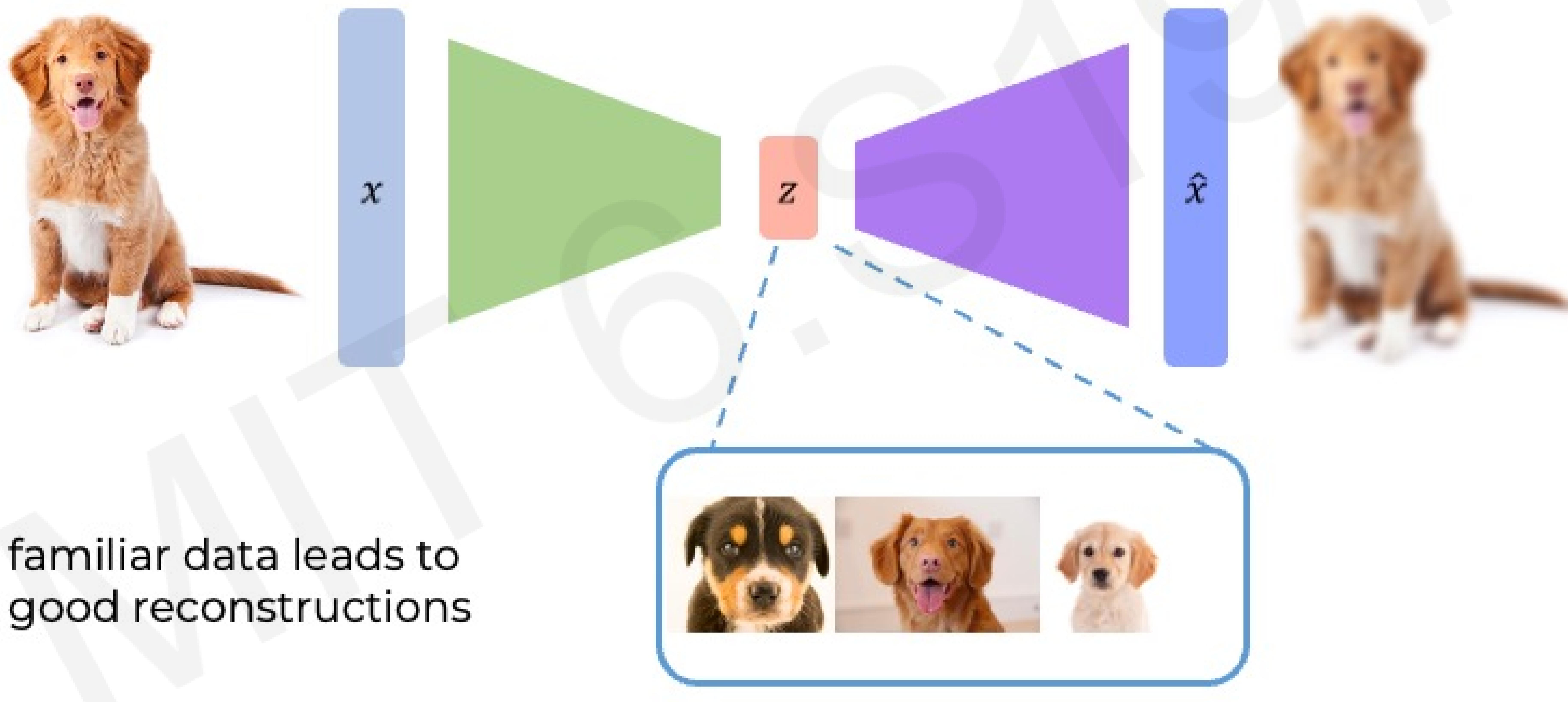
To introduce *stochasticity*, we can also add dropout layers and compute forward passes multiple times while saving memory and compute



```
for _ in range(T):
    forward_passes.append(model(x, dropout=True))
mu = np.mean(forward_passes)
uncertainty = np.var(forward_passes)
```

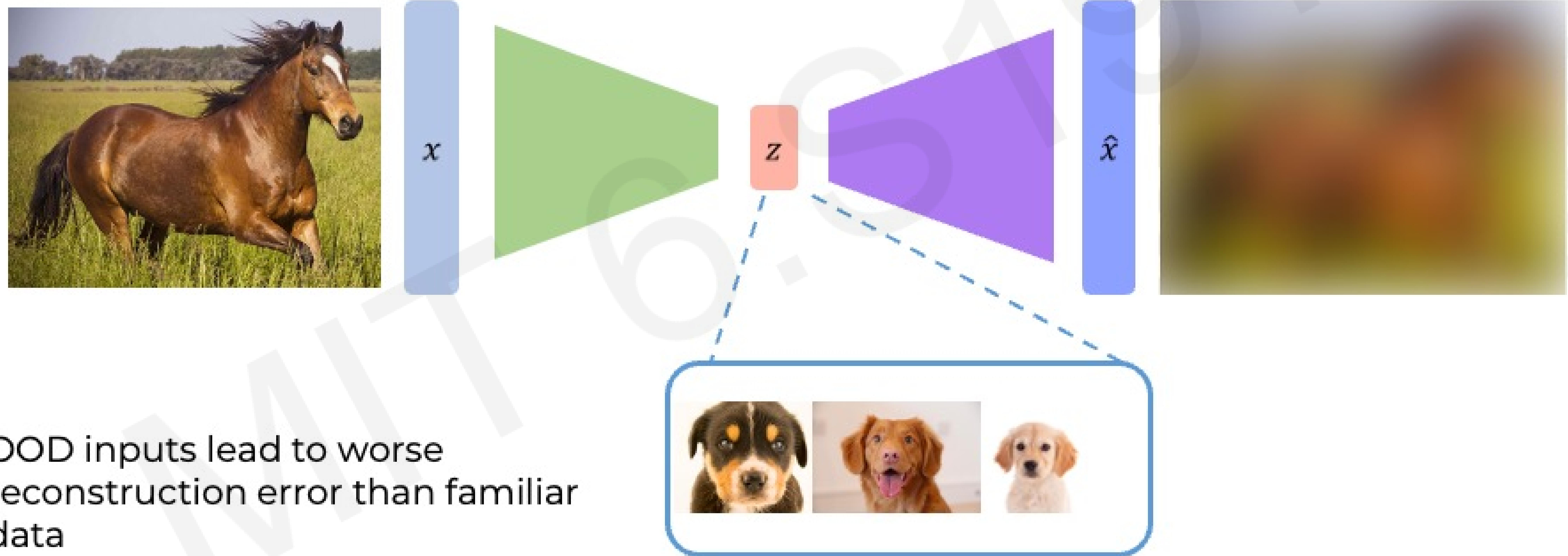
# Estimating Epistemic Uncertainty: Reconstruction Error

In addition to sampling, we can use reconstruction error to measure how confident the model is in a prediction



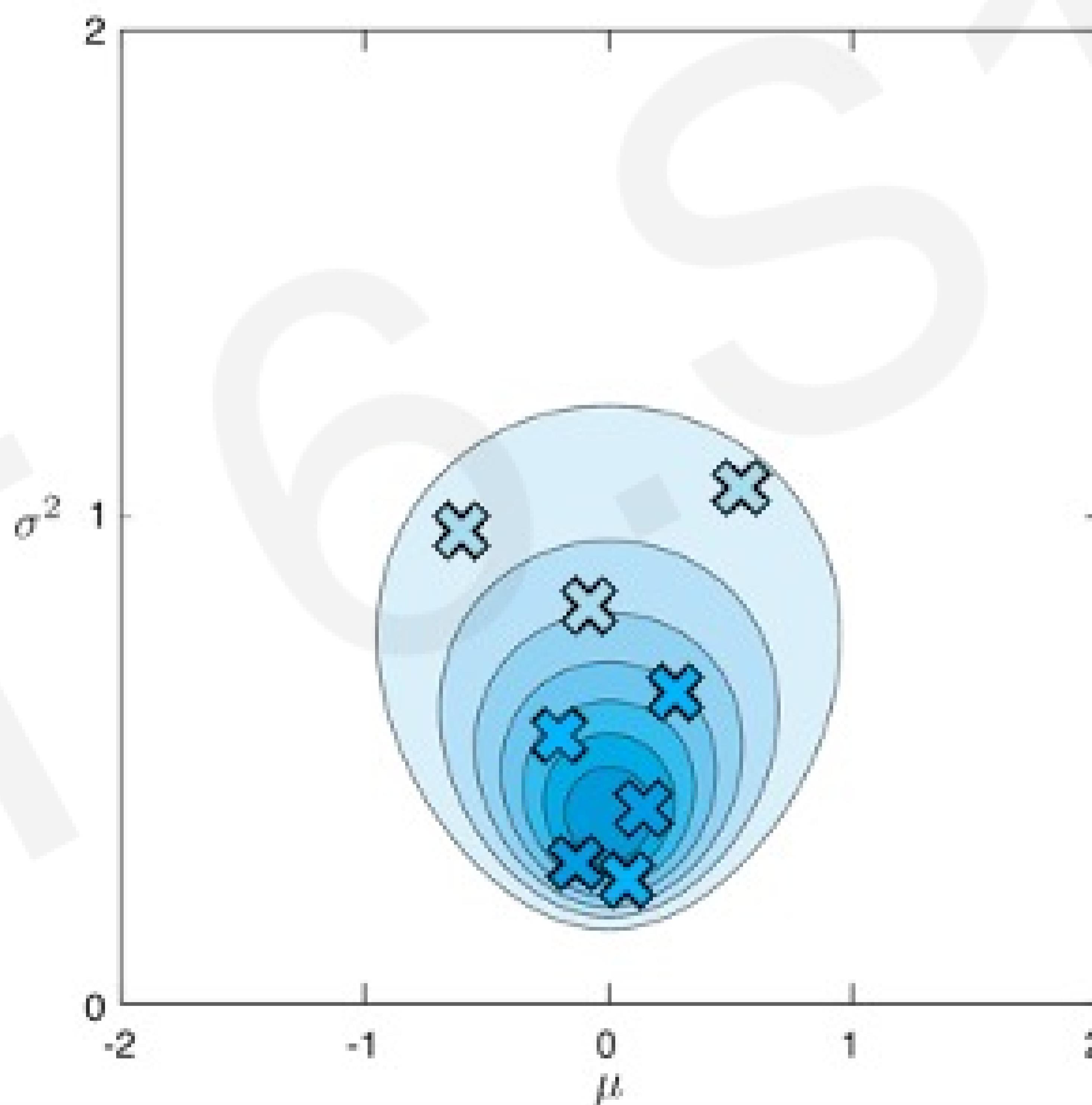
# Estimating Epistemic Uncertainty: Reconstruction Error

In addition to sampling, we can use reconstruction error to measure how confident the model is in a prediction



# Estimating Epistemic Uncertainty: Evidential Deep Learning

Learn the variance **directly**, without sampling by placing priors on the distribution that the evidence comes from.

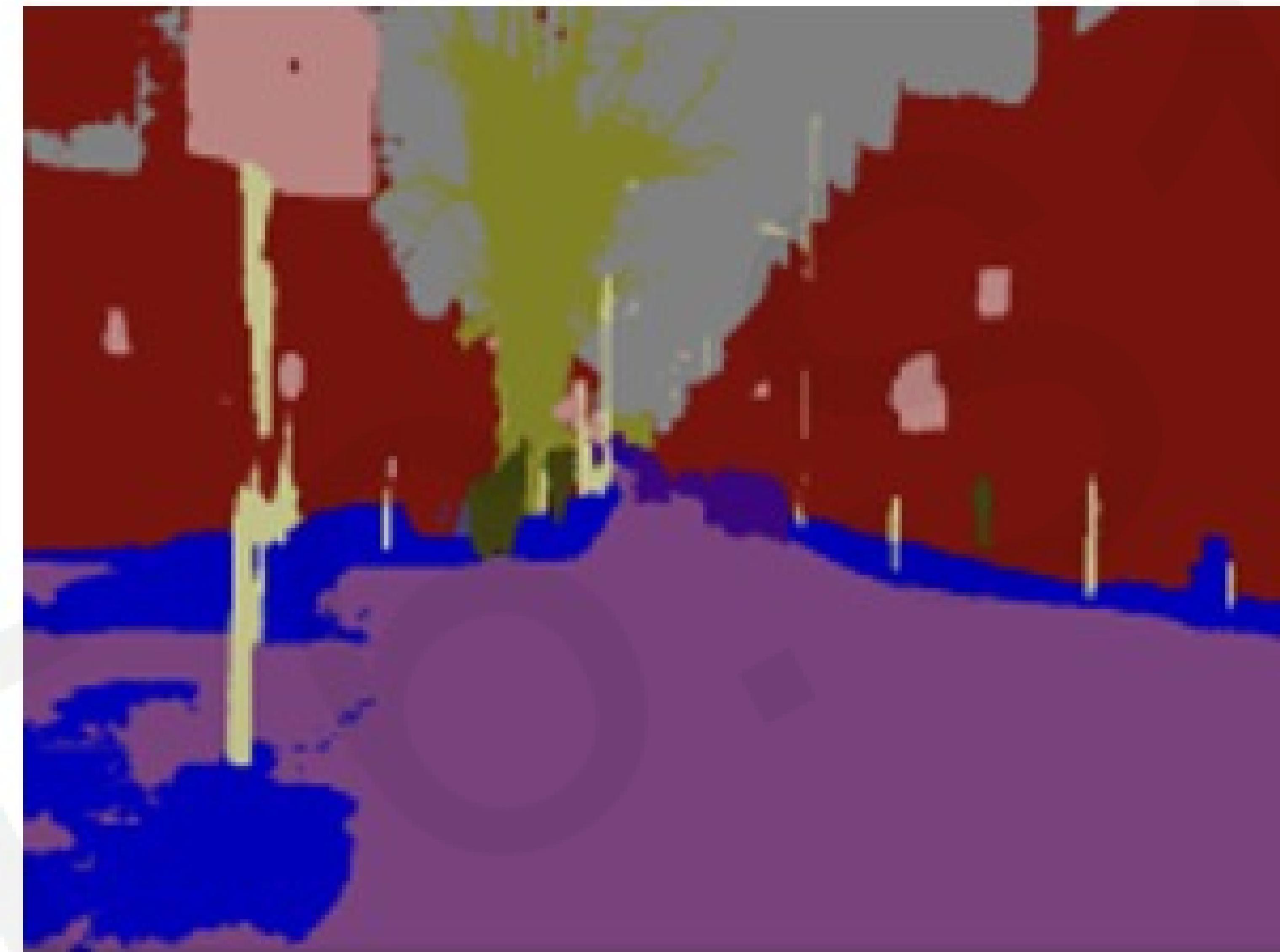


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Semantic Segmentation: label every **pixel** of an image with its corresponding class



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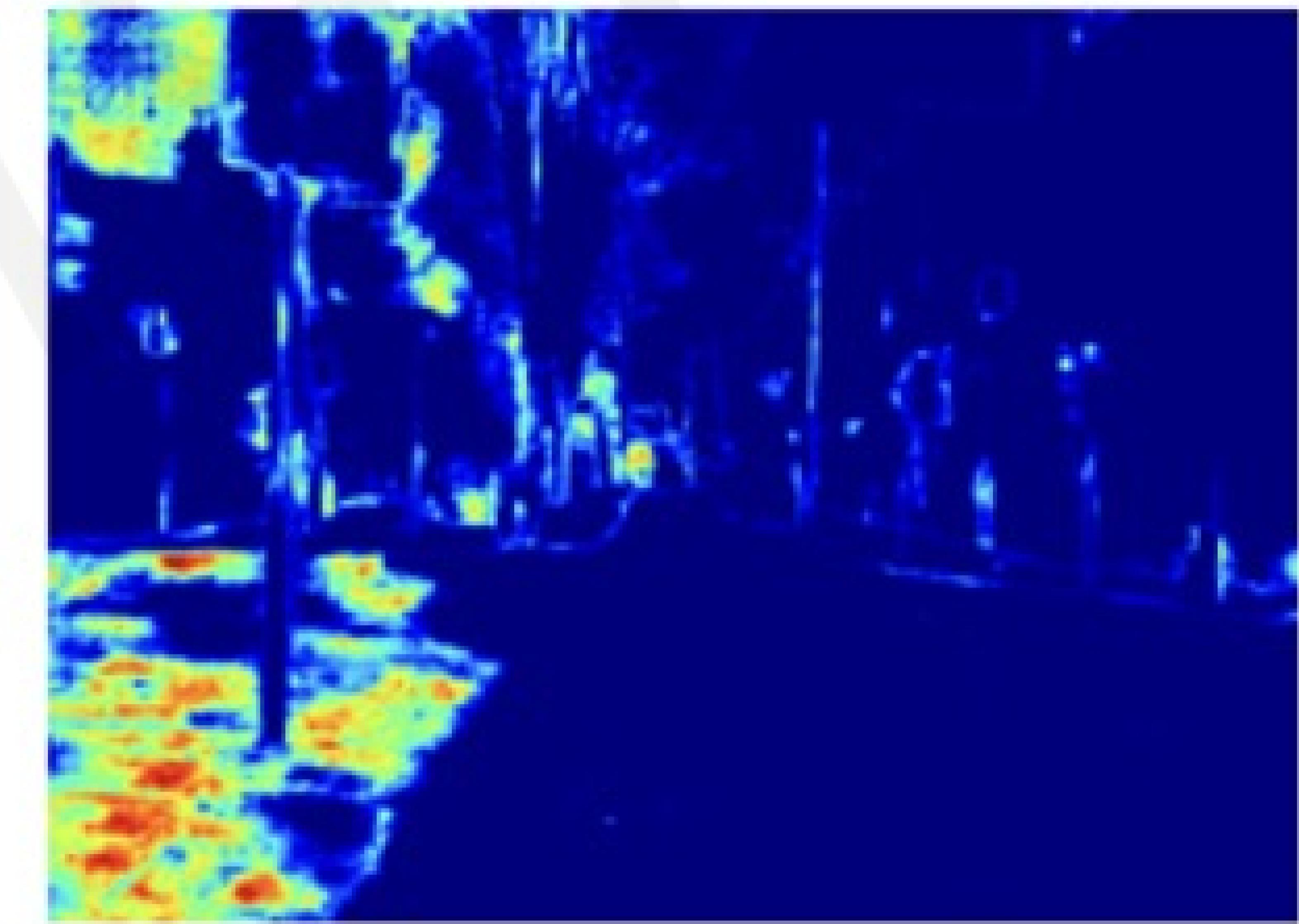
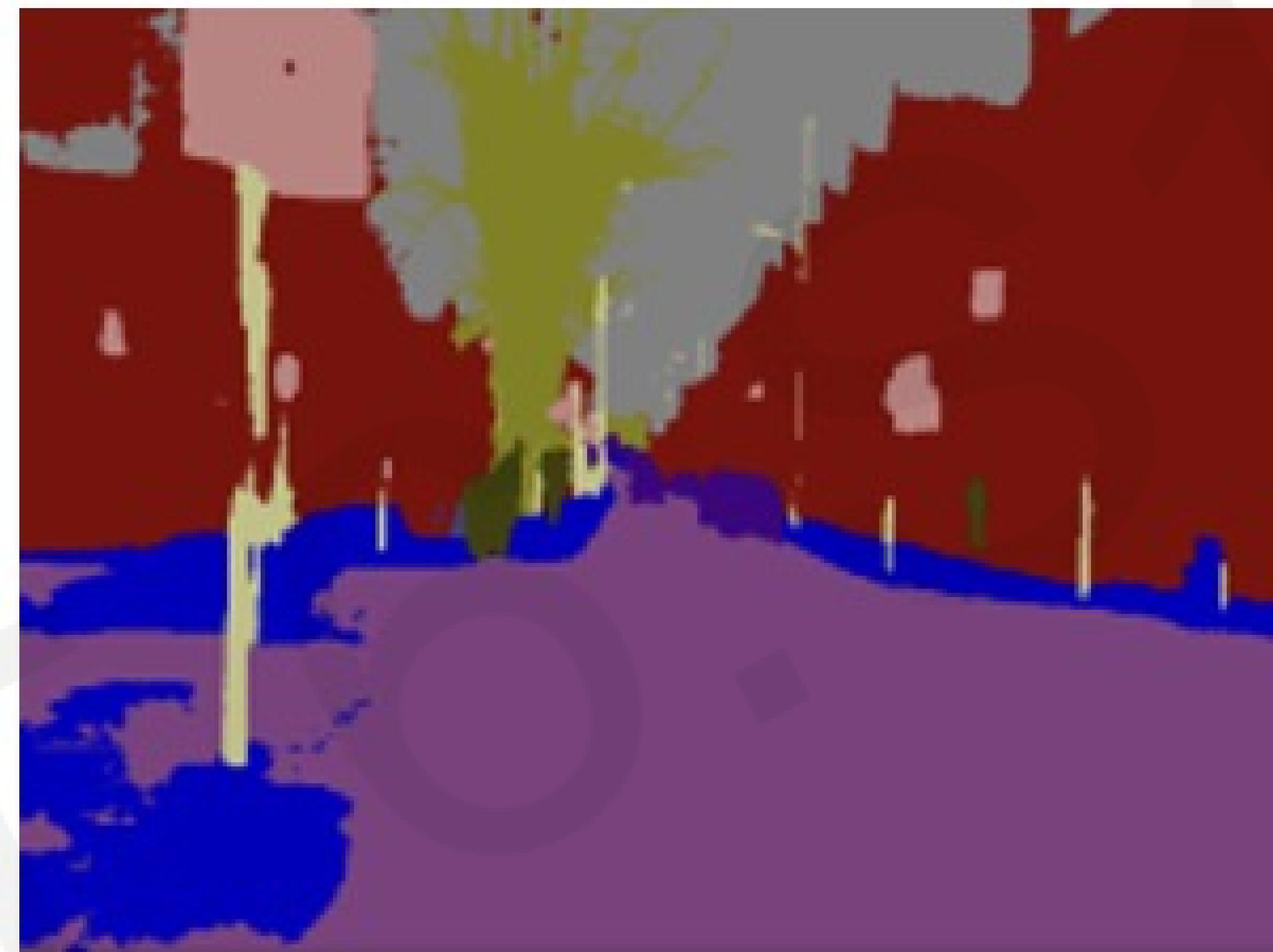


**Outputs:** pixel-level masks of labels

Which parts of this dataset have high **model** or epistemic uncertainty?

# Epistemic Uncertainty in the Real World: Semantic Segmentation

Semantic Segmentation: label every **pixel** of an image with its corresponding class



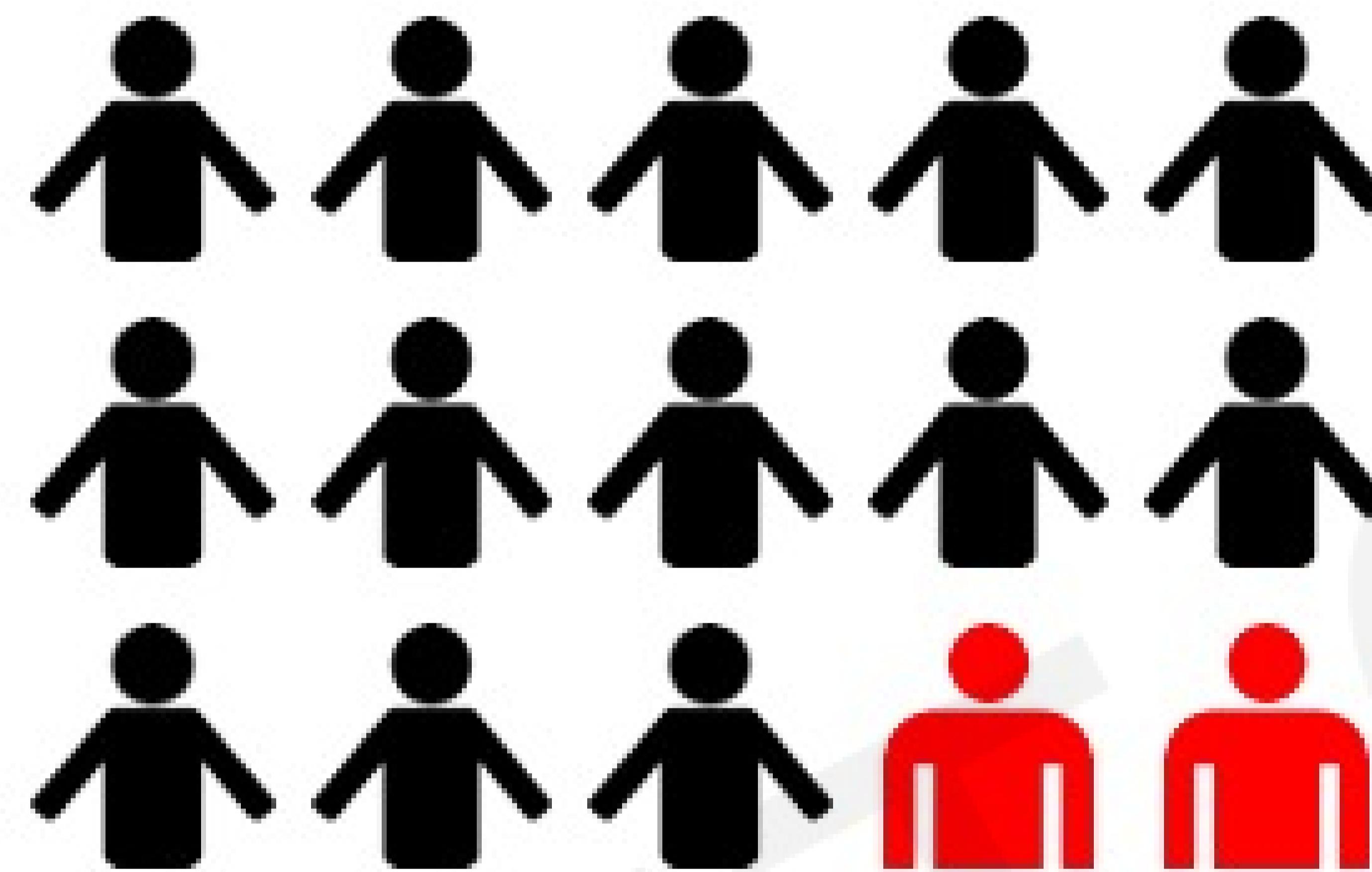
**Inputs:** RGB Images of scenes in cities

**Outputs:** pixel-level masks of labels

High epistemic uncertainty in areas of **discoloration**

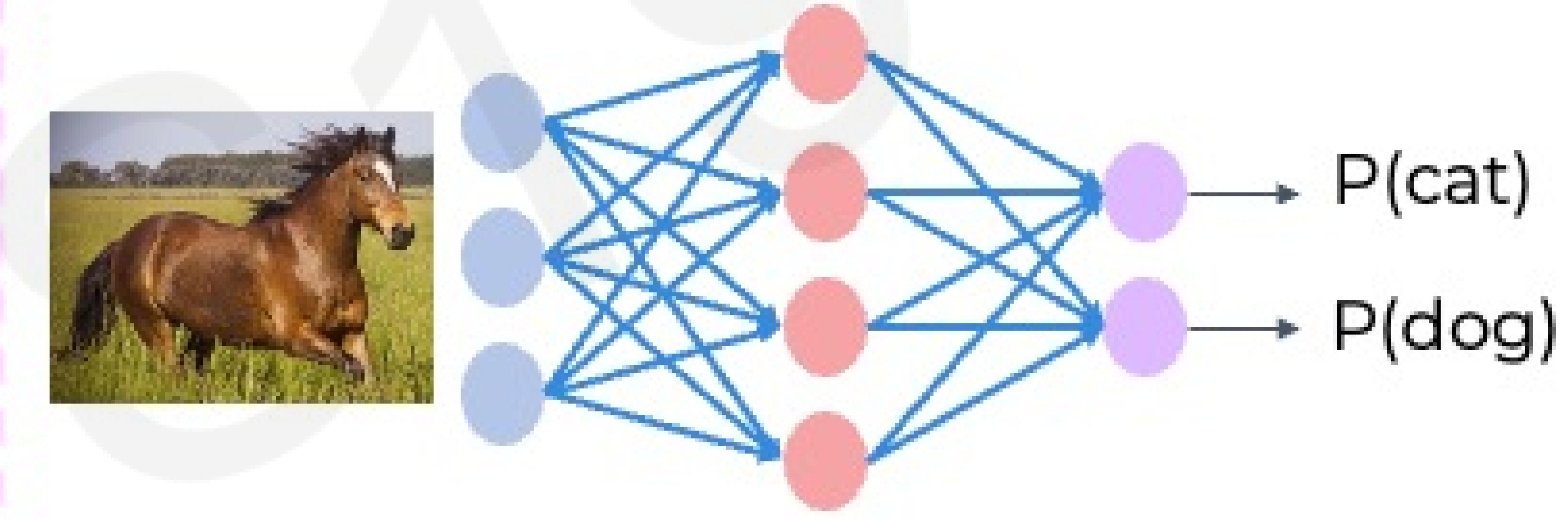
# Challenges for Robust Deep Learning

## Bias



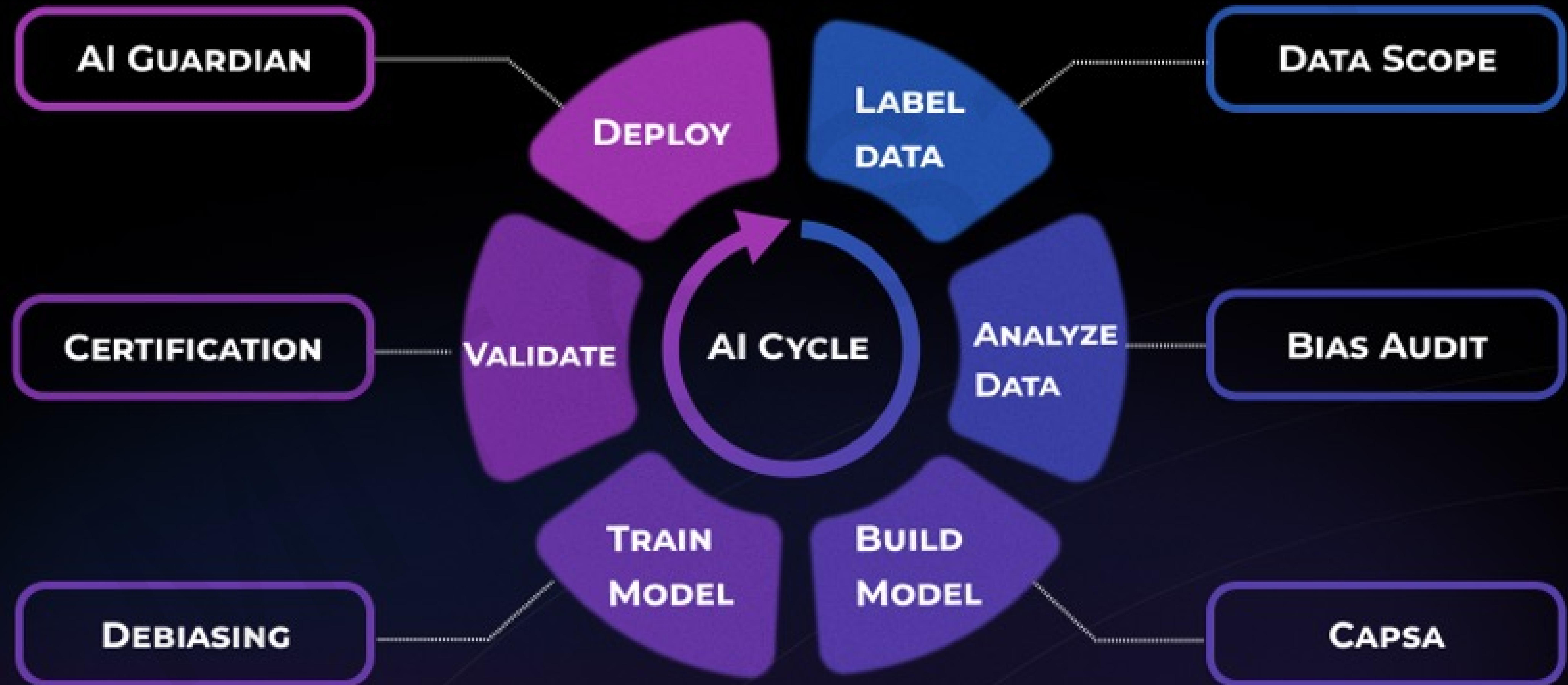
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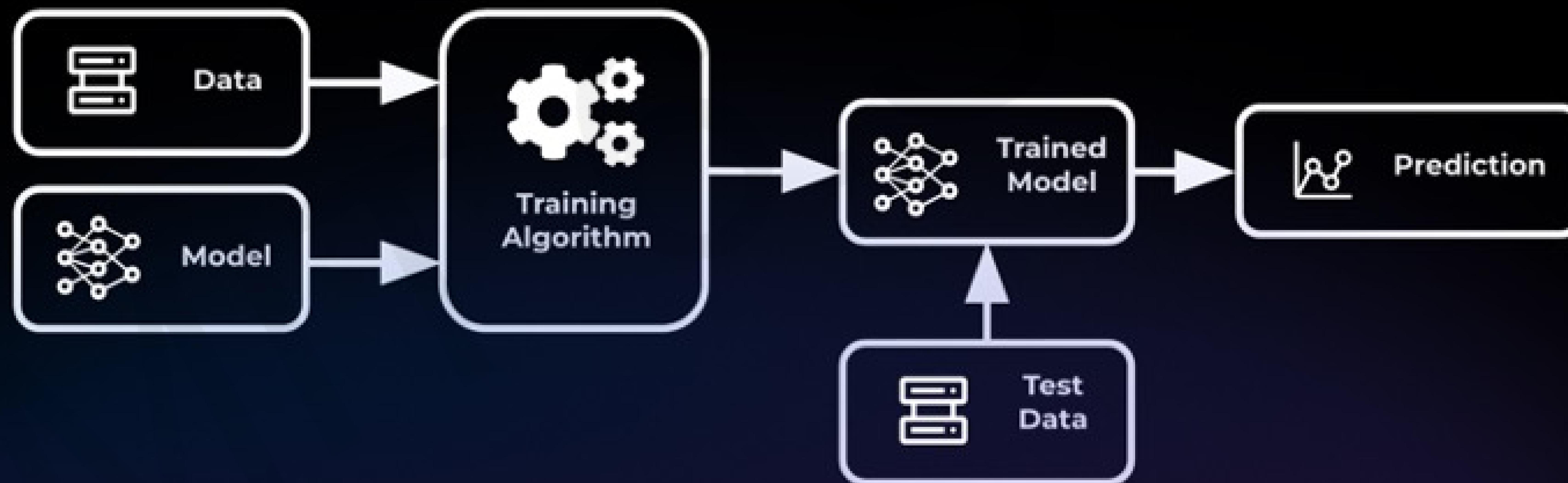


**Can we teach a model to  
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# Using Risk-Awareness to Transform AI Workflows

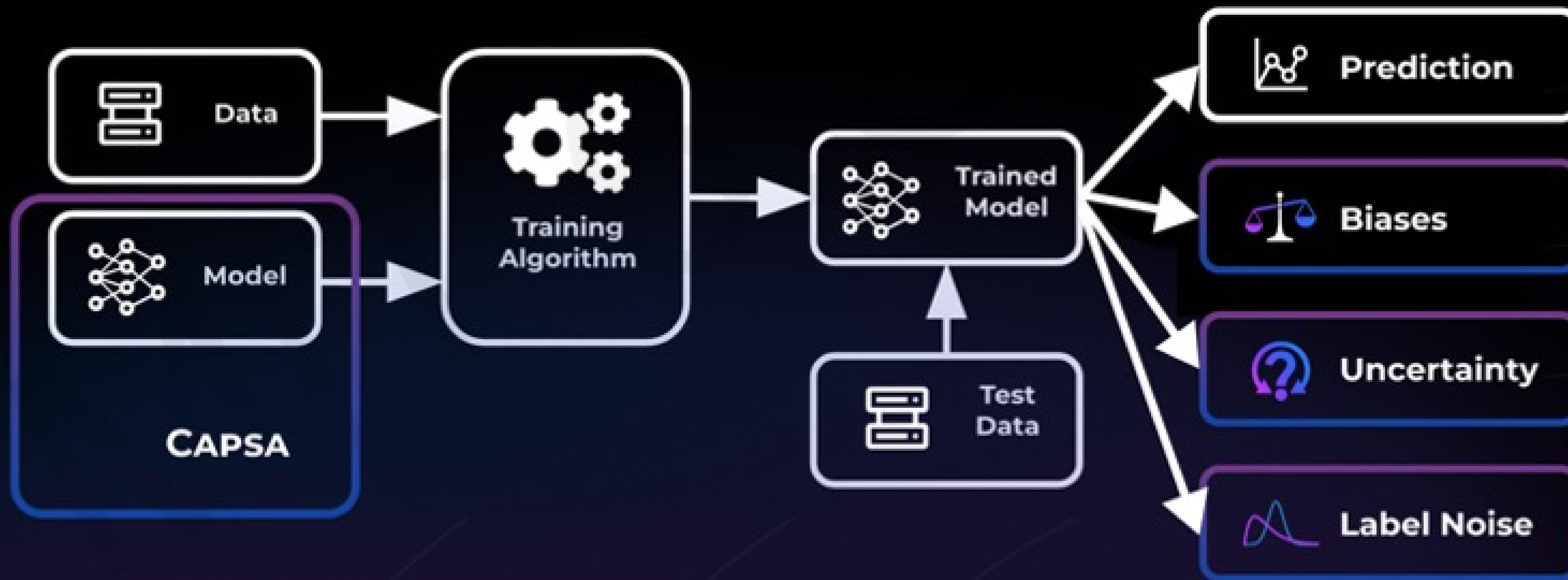


# CAPSA: A model-agnostic framework for risk estimation



# CAPSA: A model-agnostic framework for risk estimation

A Data- And Model-Agnostic Neural Network Wrapper  
For Risk-Aware Decision Making



\*Capsa: Latin Root For A Capsule Or Container

# Change the Future of Trustworthy AI With Us

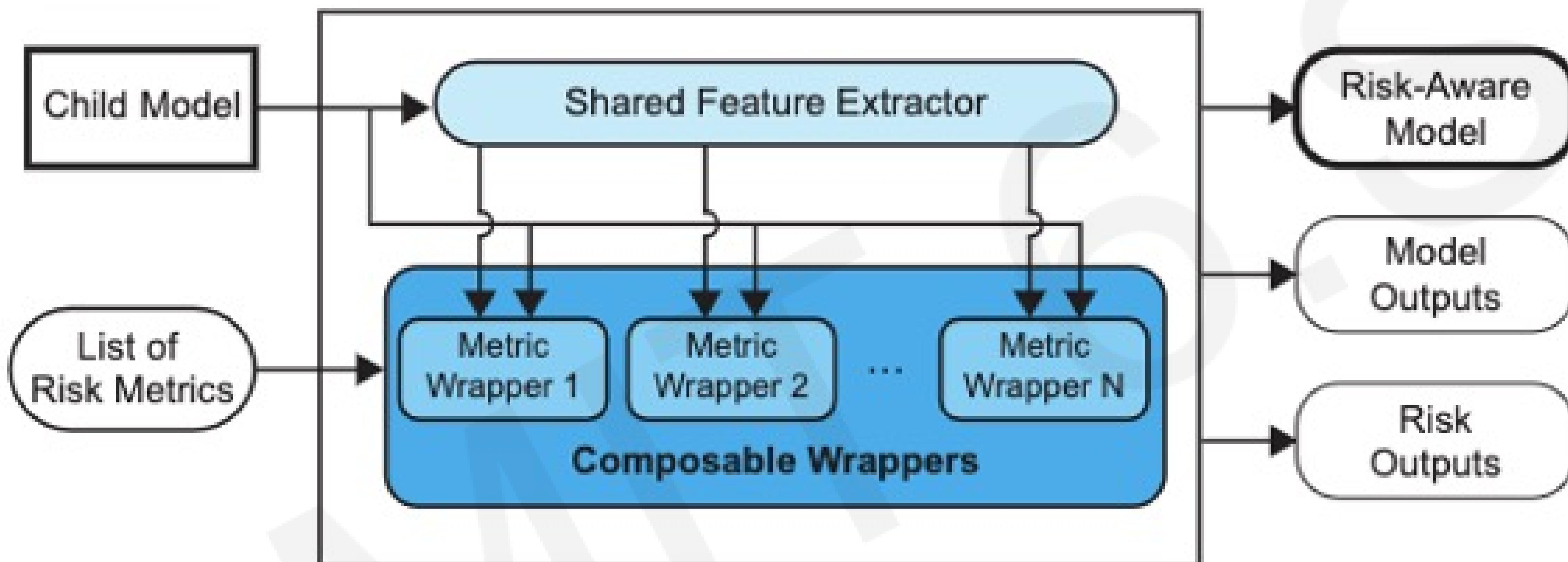
```
train_data, test_data = load_dataset()
model = build_model(n_layers, n_neurons, ...)
model.train(train_data)
preds = model.predict(test_data)
```

```
train_data, test_data = load_dataset()
model = build_model(n_layers, n_neurons, ...)
model = capsa.HistogramWrapper(model, ...)
model.train(train_data)
preds, bias = model.predict(test_data)
```

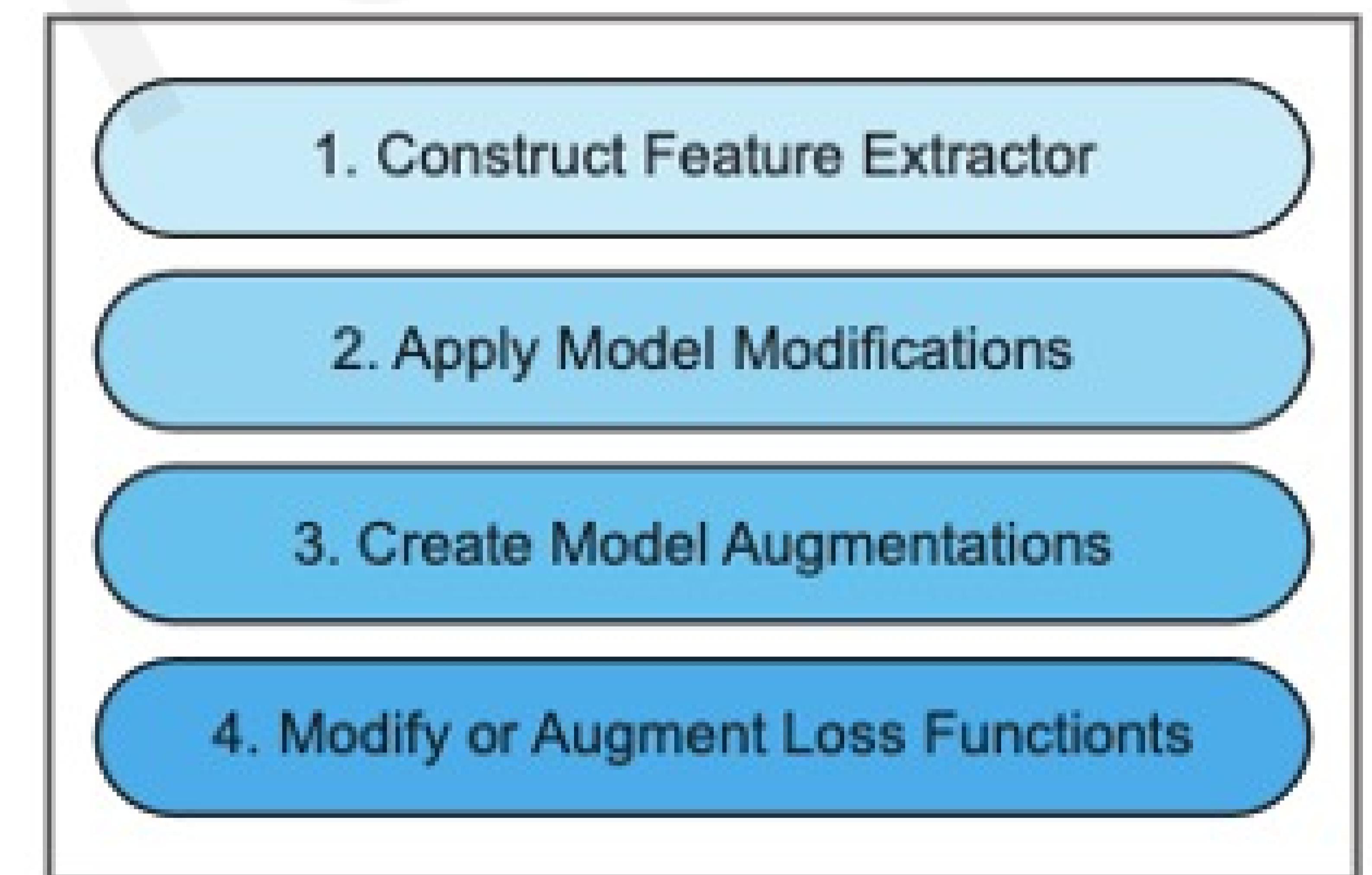
# CAPSA: A model-agnostic framework for risk estimation

CAPSA “wraps” models so that they are **risk-aware** by changing and adding necessary components for each metric wrapper.

## A. CAPSA: Converting Models to Risk-Aware Variants

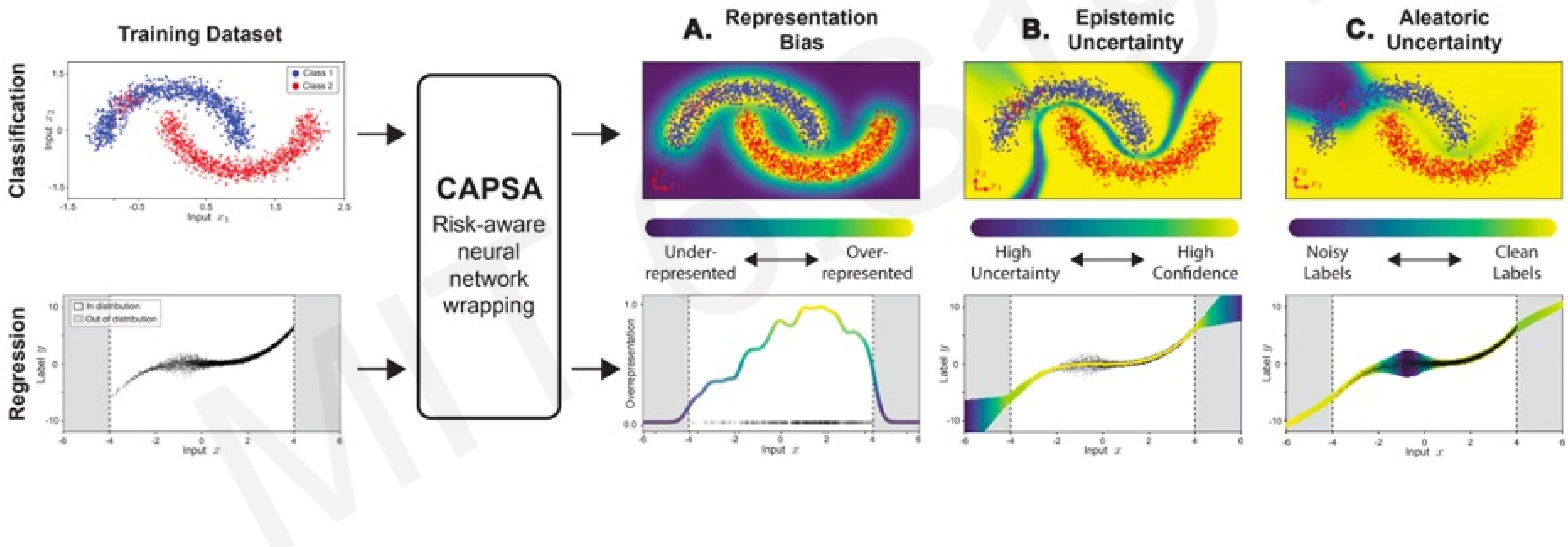


## B. Individual Metric Wrapper



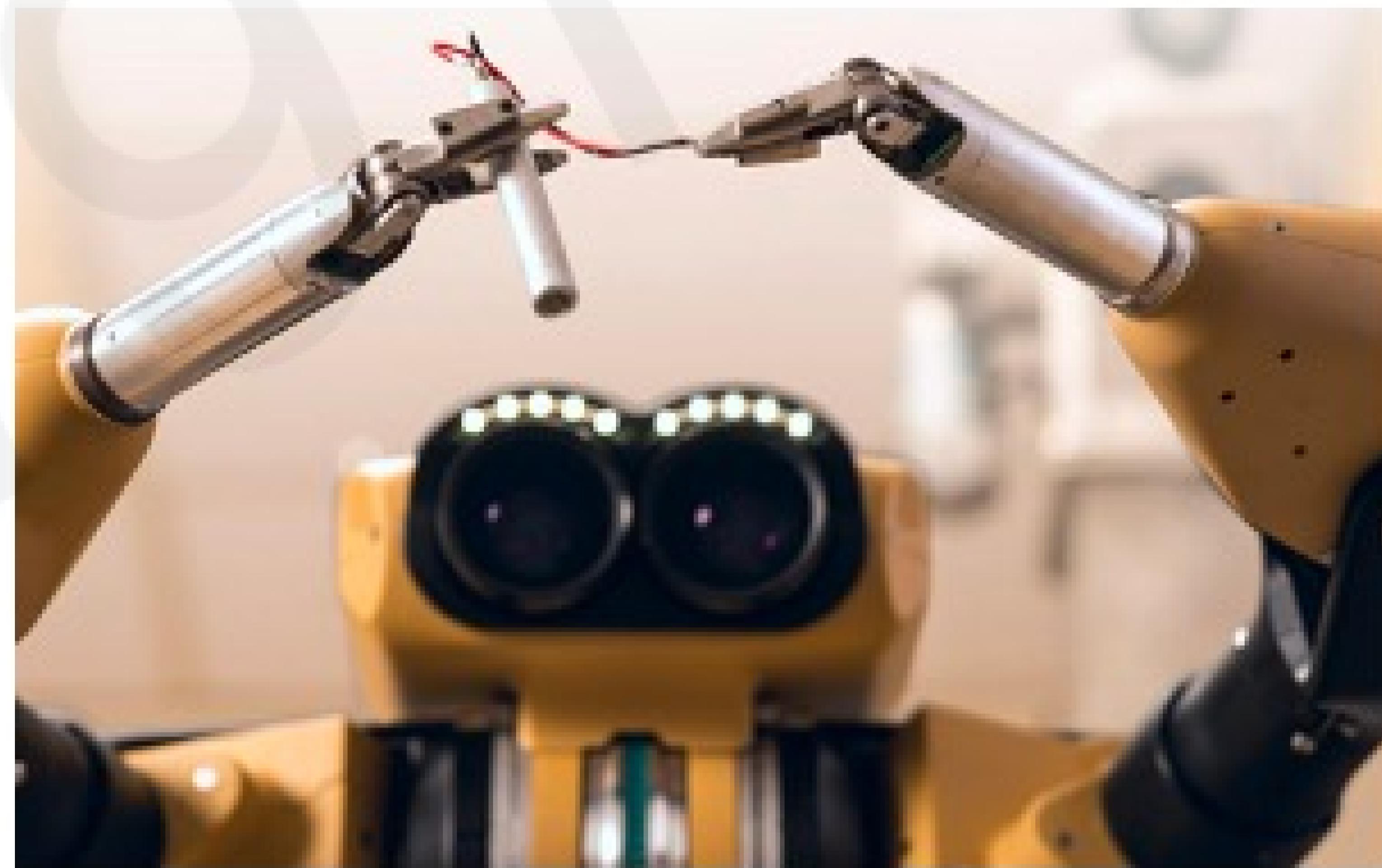
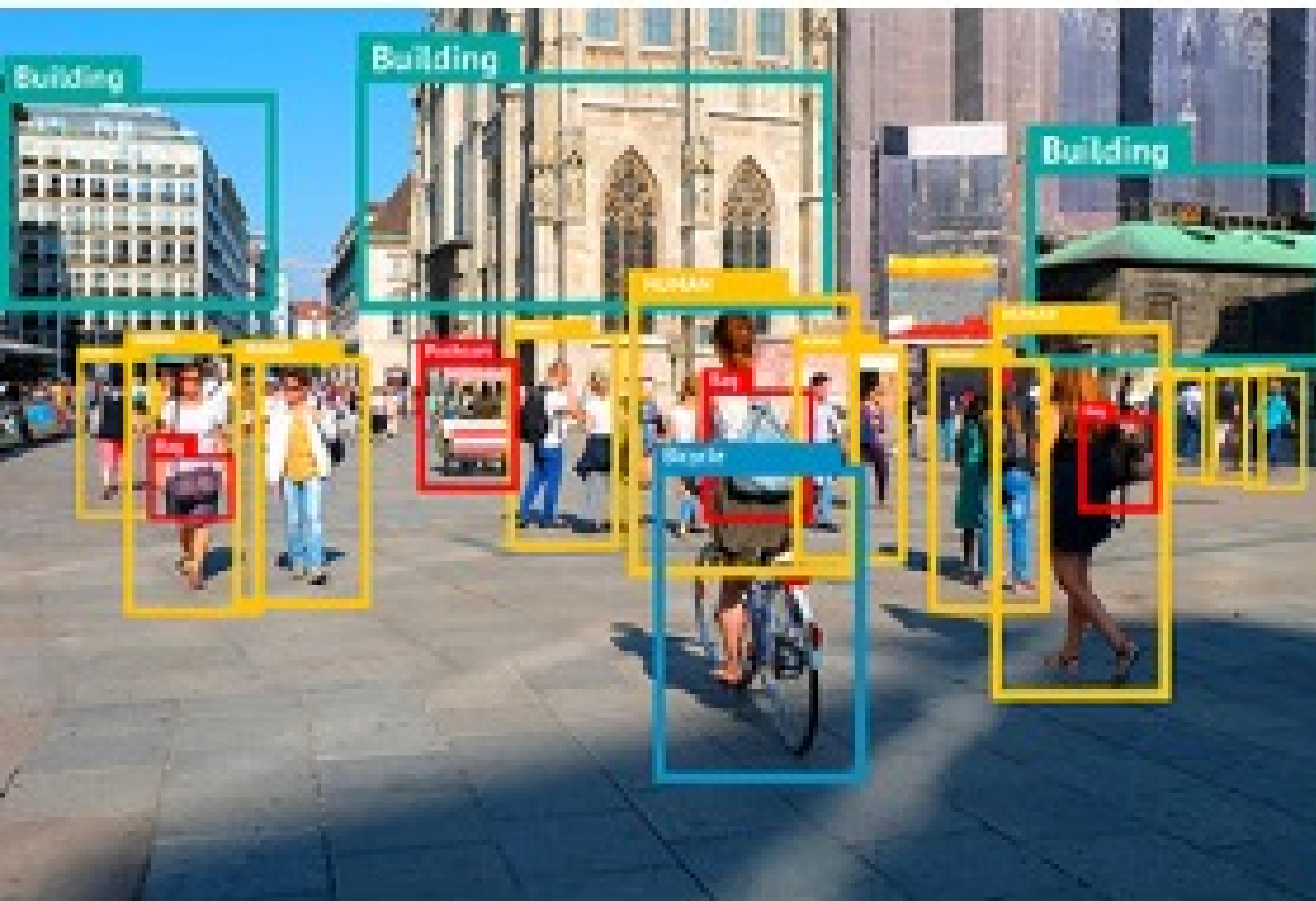
# CAPSA: A model-agnostic framework for risk estimation

Directly plugs into existing training pipelines, providing insight into **bias** (density and imbalance) as well as **aleatoric** (data), and **epistemic** (model) uncertainty



# Unlocking the Future of Trustworthy AI

Themis is unlocking the key to deploy deep learning safety across fields:

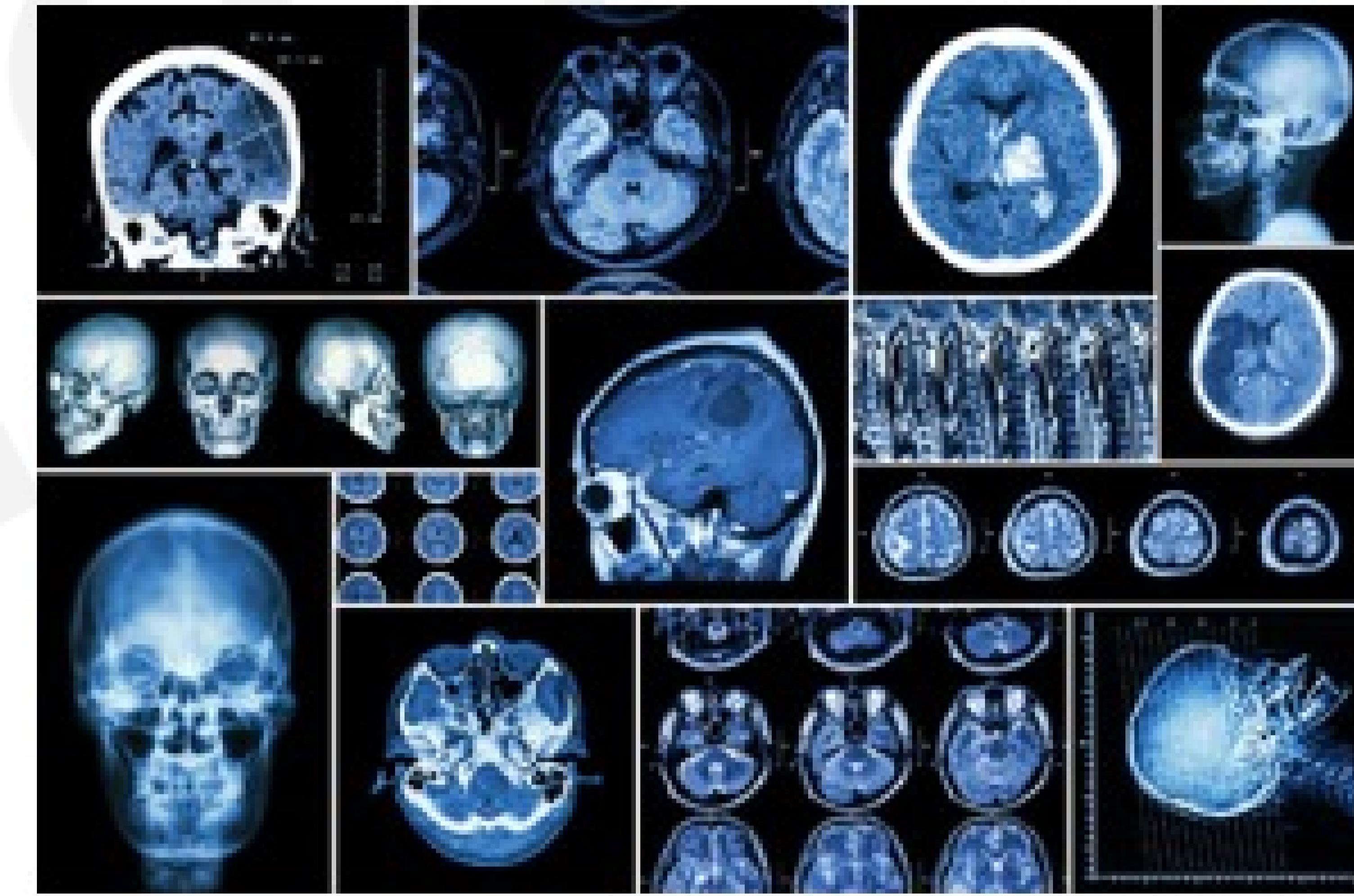
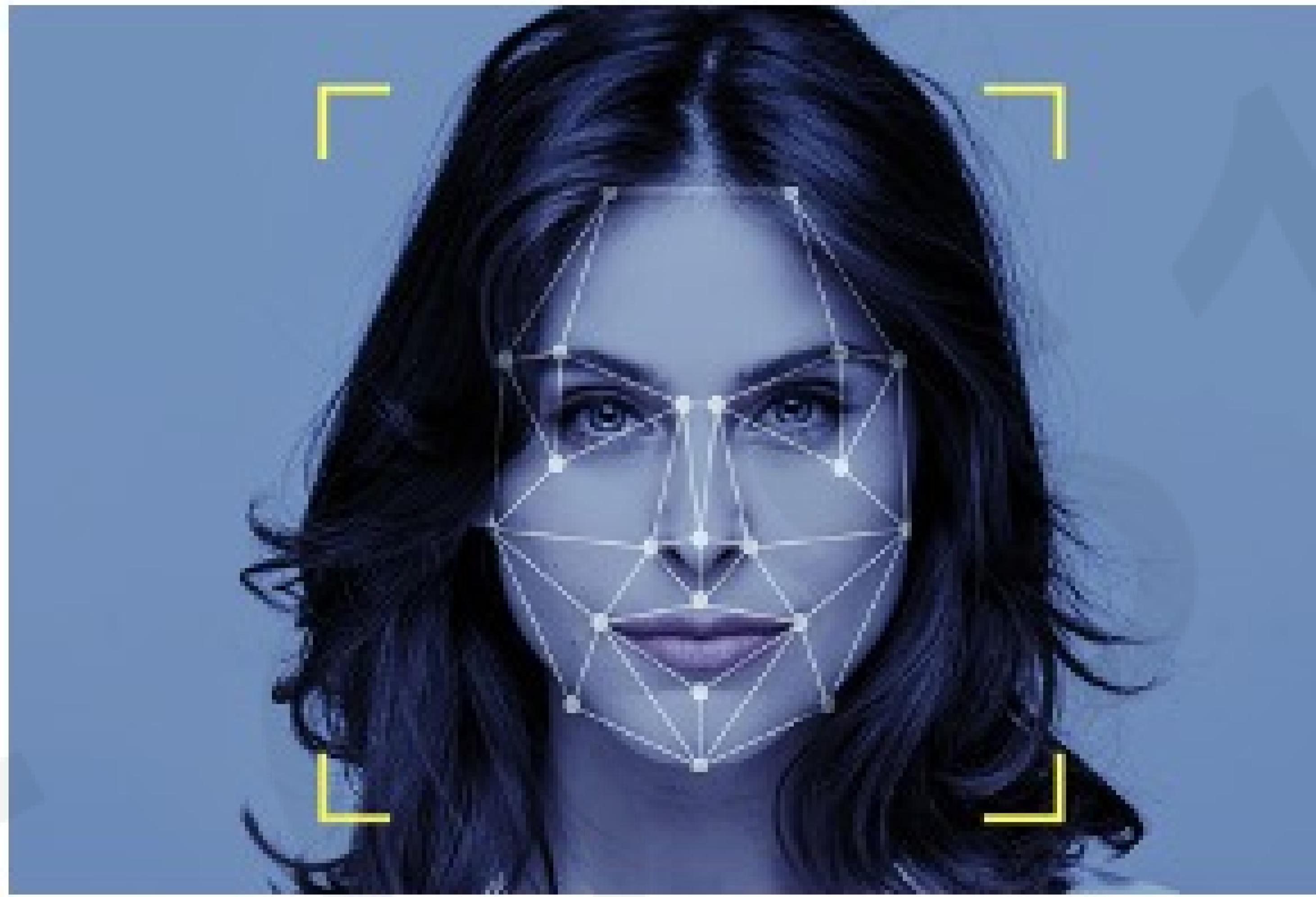


When should a human take control of an autonomous vehicle?

What types of data are underrepresented in commercial autonomous driving training pipelines?

# Unlocking the Future of Trustworthy AI

Themis technology can answer safety-critical questions across fields:



When is a model uncertain about a life-threatening diagnosis?

What types of patients might drug discovery algorithms be biased against?

**Today:** How can we improve commercial facial detection systems?

# Change the Future of Trustworthy AI Together With Us

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Workflows**



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