Uncertainty in Recurrent Decision Tree Classifiers

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Explainable Machine Learning

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What?

Setting

- Image classification: many powerful architectures exist
- Prominent example: ResNet
- Popular models only yield classification
- No reasoning behind classification

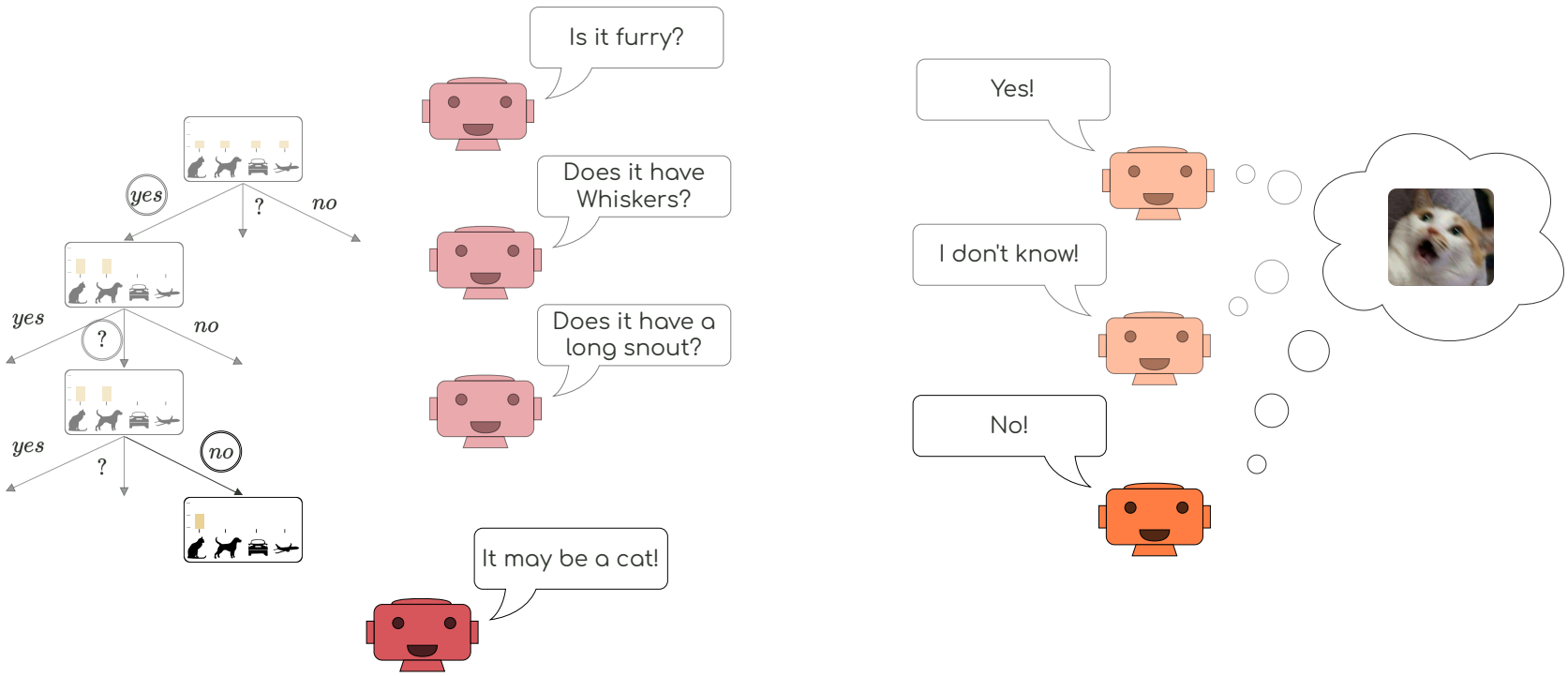
What?

What is a Recurrent Decision Tree Classifier?

- Alaniz et al. [1] propose RDTC
- Two communicating agents
- Left: ask questions — right: look at data and answer them
- Unfolding tree reveals reasoning behind classification

What?

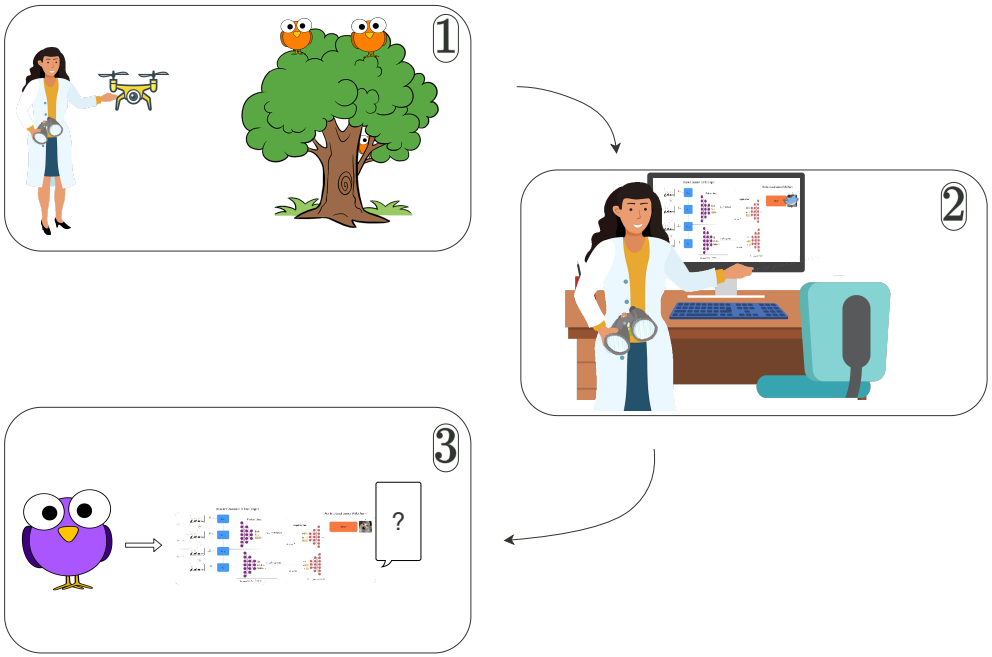
Introducing Uncertainty to a RDTC



- Right agent is aware of uncertainties
- Communicates this to left agent

Why do we need uncertainty?

A Practical Example...



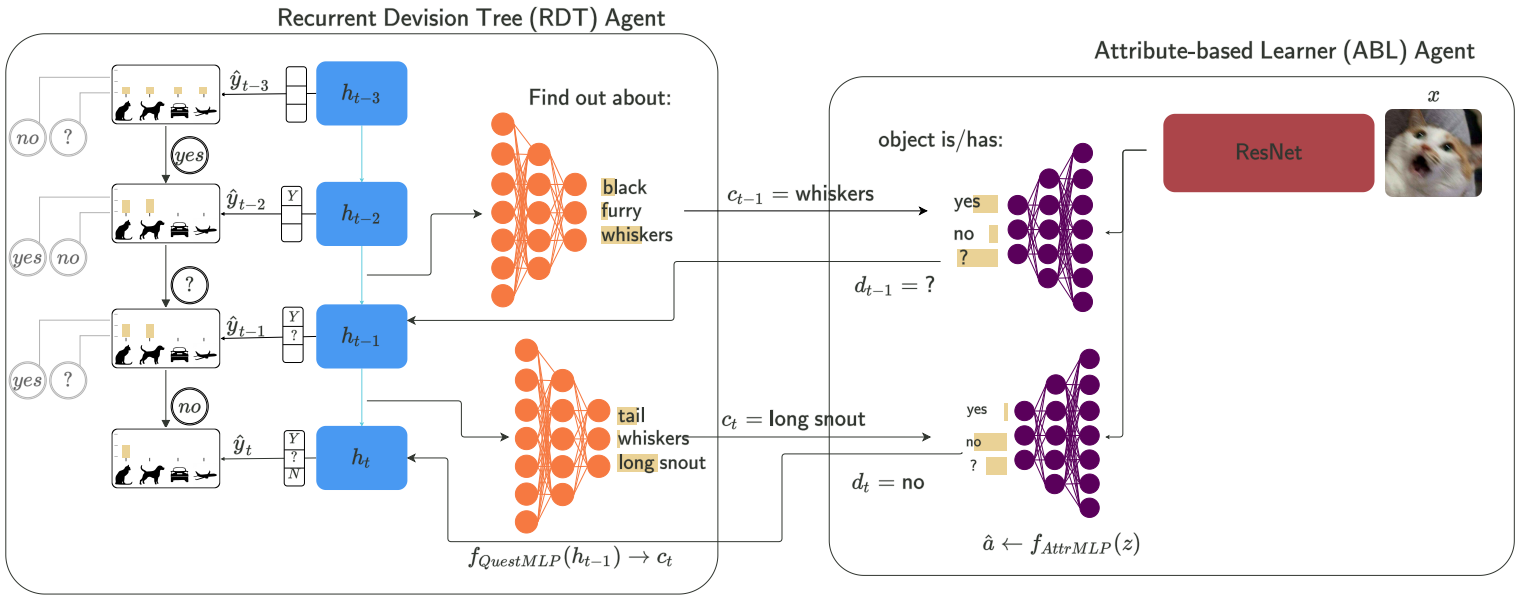
- Ornithologist surveys area using drone and CV software
- Classification is automated with our model
- Bird species unknown to model yield high uncertainty
- Those can be classified manually

Introduction

- RDTC by Alaniz et al. [1] yields decision tree
- Decision tree is build through communication of agents
- Our aim is to introduce uncertainty to RDTC
- Uncertainty allows model to i.e. detect OOD examples

How?

Architecture

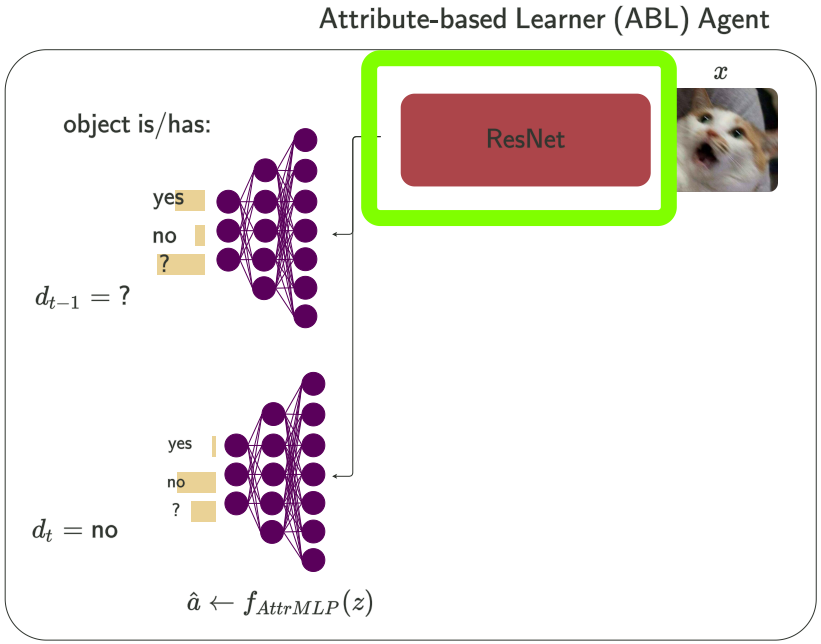


- RDT can not see the images and only ask if attribute is present
- The AbL can see the image and answer RDT's questions

Attribute-based Learner

Extracting features: ResNet

- Extract features using ResNet
- Then pass to $f_{AttrMLP}$



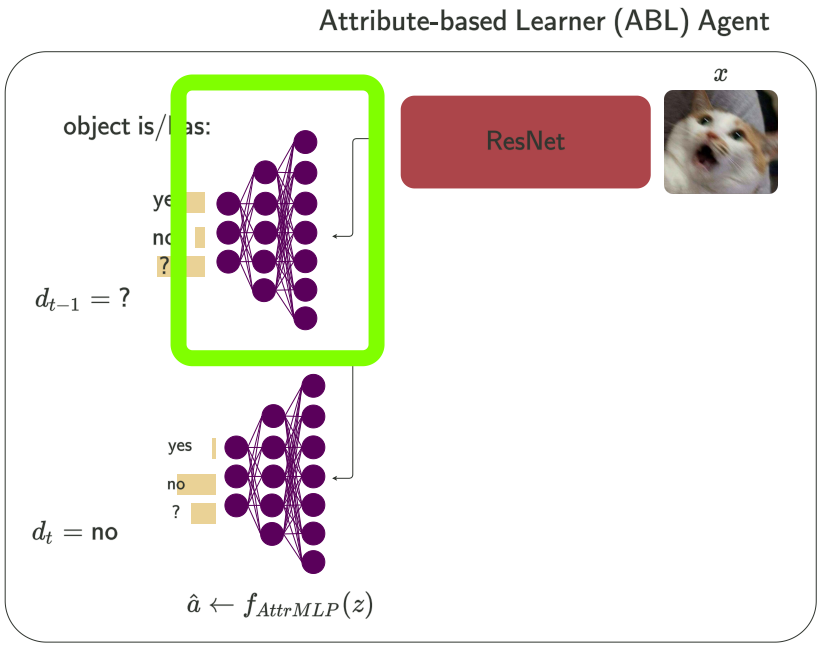
Attribute-based Learner

Mapping features to attributes: Attribute MLP

- Map features to answers
- Yes, No, ? for each attribute
- Discrete answers with TempSoftmax

$$\frac{exp((log\ \pi_i)/\tau)}{\sum_{j=1}^{K} exp((log\ \pi_j)/\tau)}$$

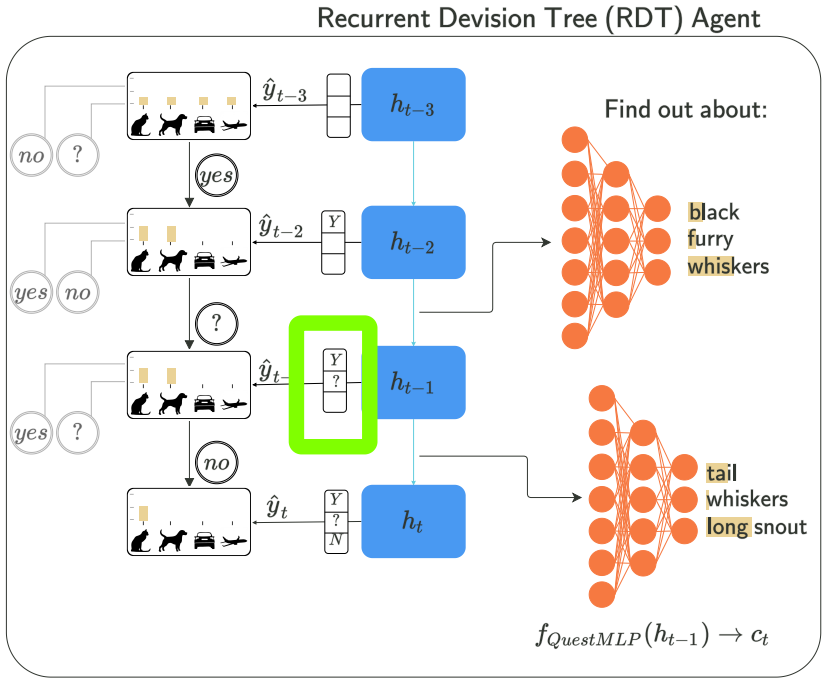
$$= \hat{a}$$



Recurrent Decision Tree

Storing decisions: Explicit memory

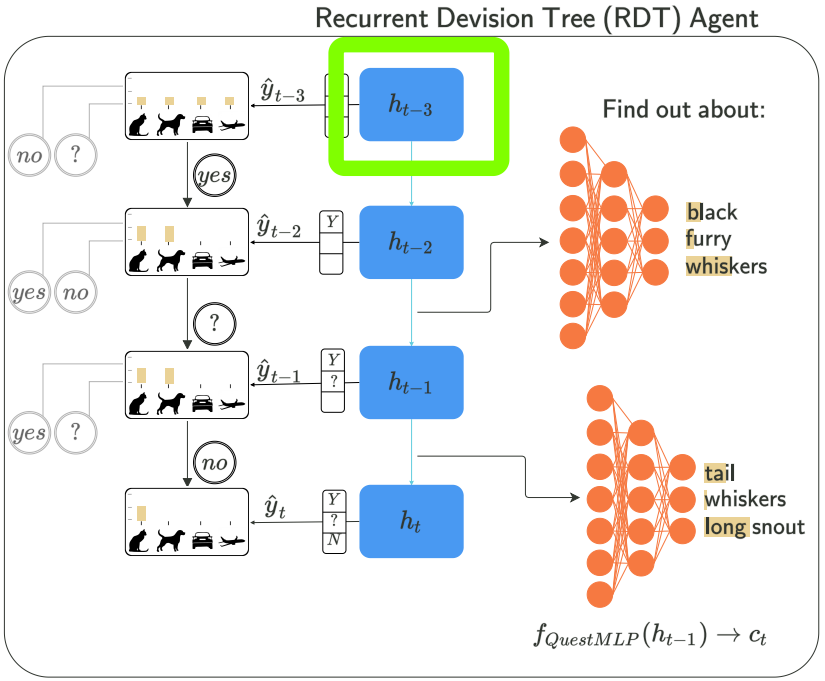
- store questions (indices)
- and answers
- iteratively increases



Recurrent Decision Tree

Keeping track: LSTM

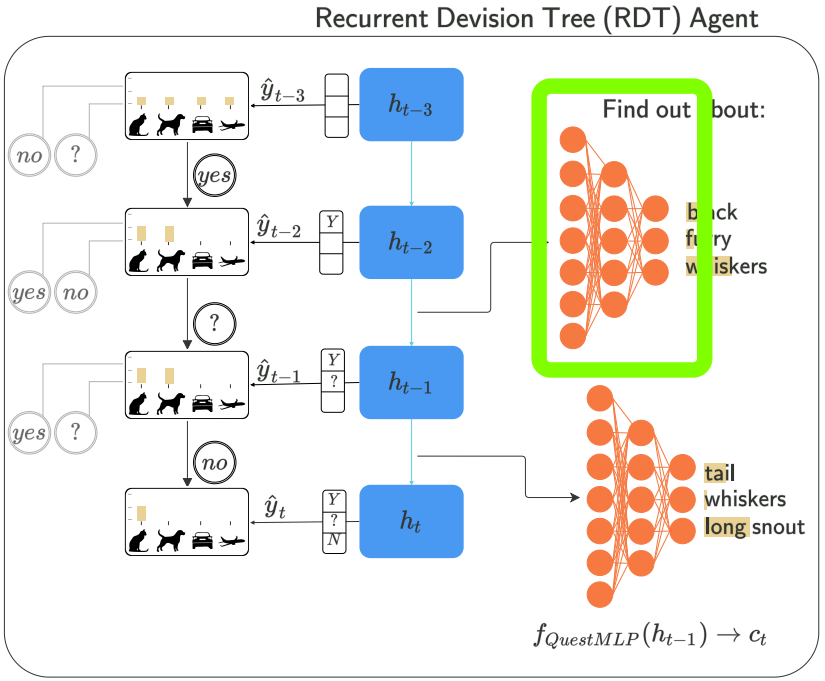
- Hidden state based on memory
- Basis for next question
- Basis for classification



Recurrent Decision Tree

Choosing questions: Question MLP

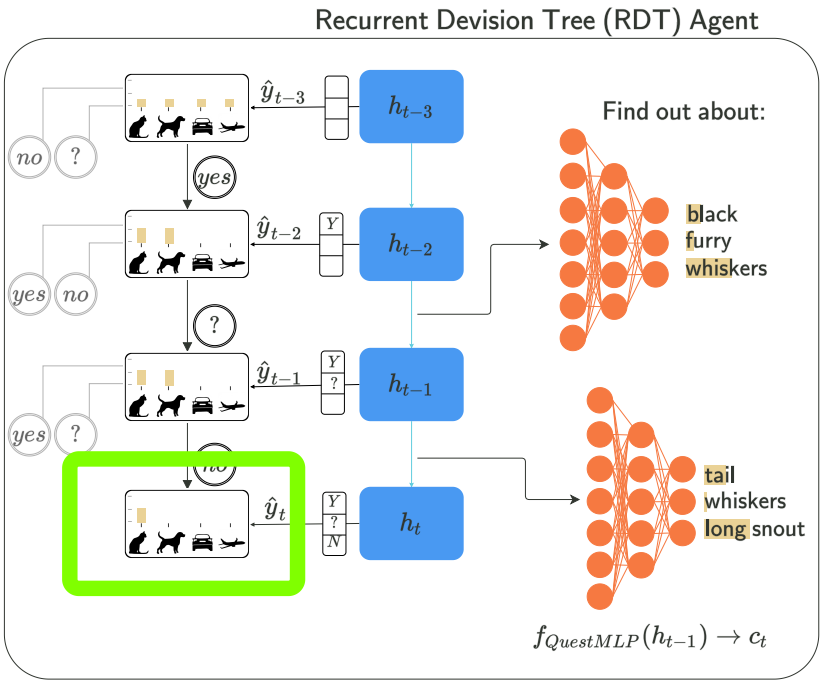
- Pose new question c_t
- $c_t \sim p(c_t)$
- Sample from categorical distribution
- With GumbelSoftmax
- $d_t = \hat{a}\,[c_t]$



Recurrent Decision Tree

Making a classification: Class MLP

- Classification in each communication step
- For classification loss



- Optimize for class (and attribute accuracy)

$$\mathcal{L} = \frac{1}{T}\sum_{t=1}^{T}\left[(1-\lambda)\underbrace{\mathcal{L}_{CE}(y,\hat{y}_t)}_{Class} + \lambda\underbrace{\mathcal{L}_{CE}(\alpha_{y,c_t},\hat{\alpha}_{c_t})}_{Attr}\right]$$

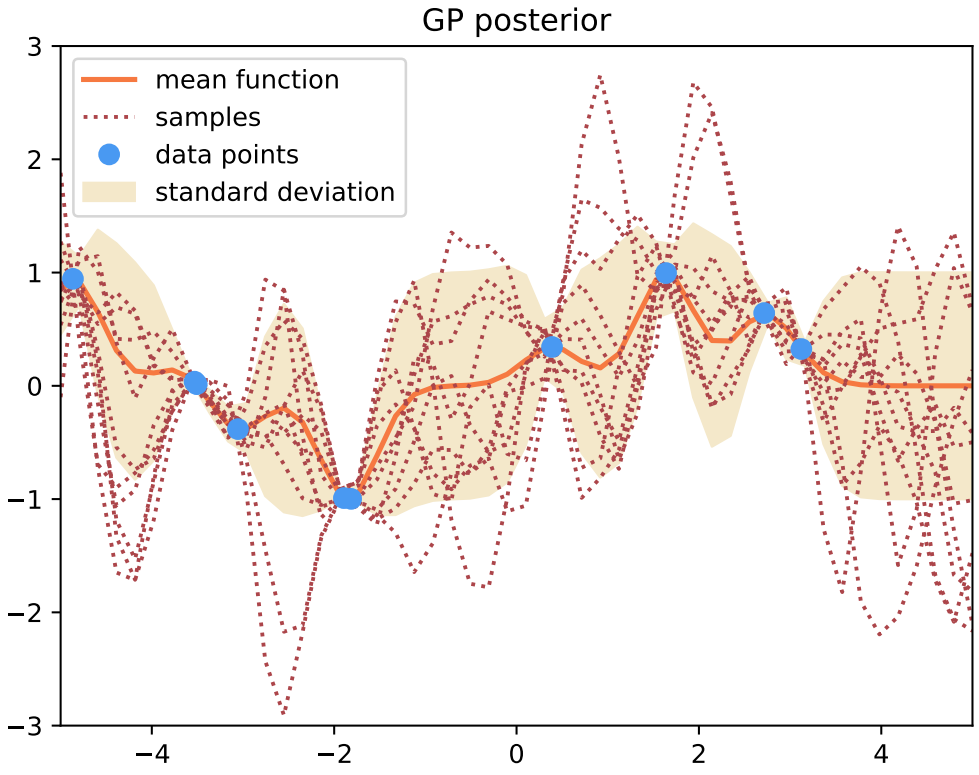
- λ can be used to balance the two loss terms
- For all of our experiments, we use $\lambda = 0.2$
- Discourage deep trees

The RDTC Model [1]

- AbL can see data, and answer all questions in advance
- RDT can choose attributes to question
- Get answer through indexing
- Joint objective of maximizing class and attribute accuracy

Background

A small excursion to Gaussian Processes (GP)



- Data can be described by (infinitely) many functions
- GP is PDF over these functions
- Intuition: → GP yields probability for function values
- Parameterized by mean function and covariance function
- Variance corresponds to model uncertainty

- Why care about GP's?
- Neural net is set of weighted linear functions, activated by non-linearity
- PDF over each weight $\rightarrow$ finite GP
- Neural net $\approx$ GP
- $\rightarrow$ Extract model uncertainty from a neural net
- Proof by Gal and Ghahramani [2]
- $\rightarrow$ Theoretical foundation for estimating uncertainty in RDTC

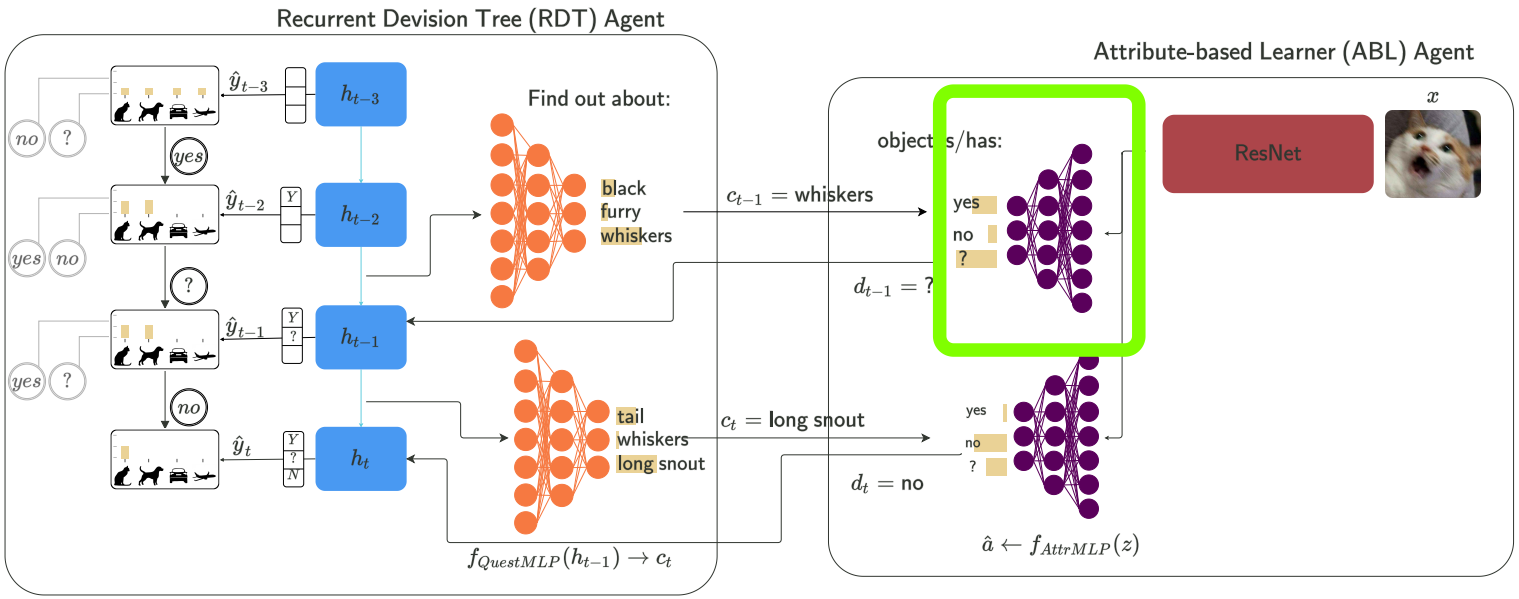
- Posterior over functions requires computing integrals
- Intractable integrals require methods of variational inference
  - GP objective $\rightarrow$ minimization objective
- For covariance function $\rightarrow$ Monte-Carlo integration
- Approximated GP's objective can be rewritten as dropout net
- Variance arising from dropout $\rightarrow$ model uncertainty

Dropout Uncertainty Estimation [2]

- Dropout net as special case of GP
- GP uses approximation techniques
- Rewrite GP objective as dropout net objective
- Proofed by Gal and Ghahramani [2]
- We use this for uncertainty estimation

How?

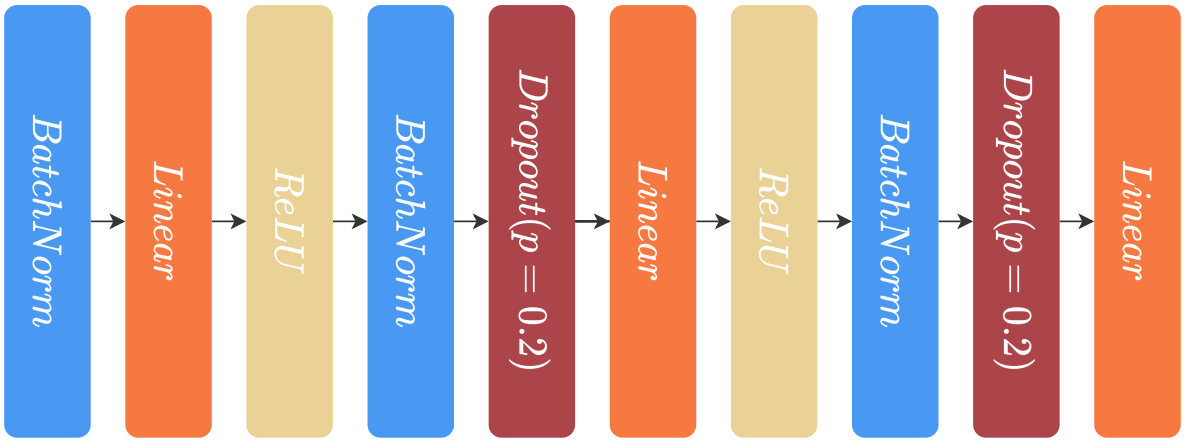
How do we get uncertainty information?



- Use Gal and Ghahramani's [2] proof to estimate uncertainty
- We want AbL to say '?' in the case of high uncertainty
- Make $f_{AttrMLP}$ a dropout MLP
- After extracting features $\rightarrow$ compute $Var(n\ forward\ passes)$

Getting Uncertainty Information

Estimating Uncertainty in the AbL

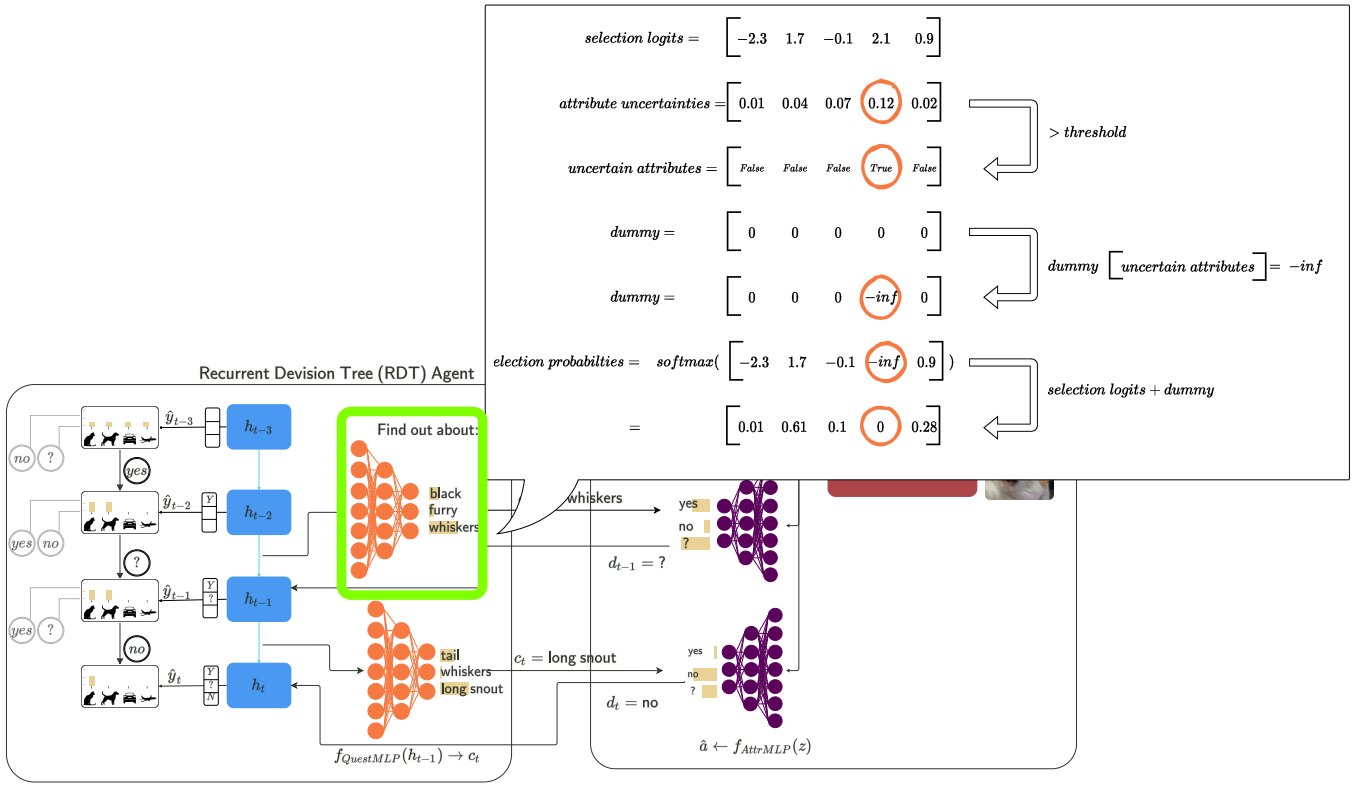


- We include dropout layers in $f_{AttrMLP}$
- We tested different configurations
- Combination of batchnorm and dropout worked best

- We use uncertainty in two different strategies
  - Prevent model from asking about uncertain attributes
    $\rightarrow$ remRDTC
  - We give the model the ability to answer with 'I don't know'
    $\rightarrow$ extRDTC
- Attribute uncertain if above threshold hyperparameter
- Don't allow the model to use gradients from uncertain attributes
- Uncertainty information remains inductive bias

Using Uncertainty Information

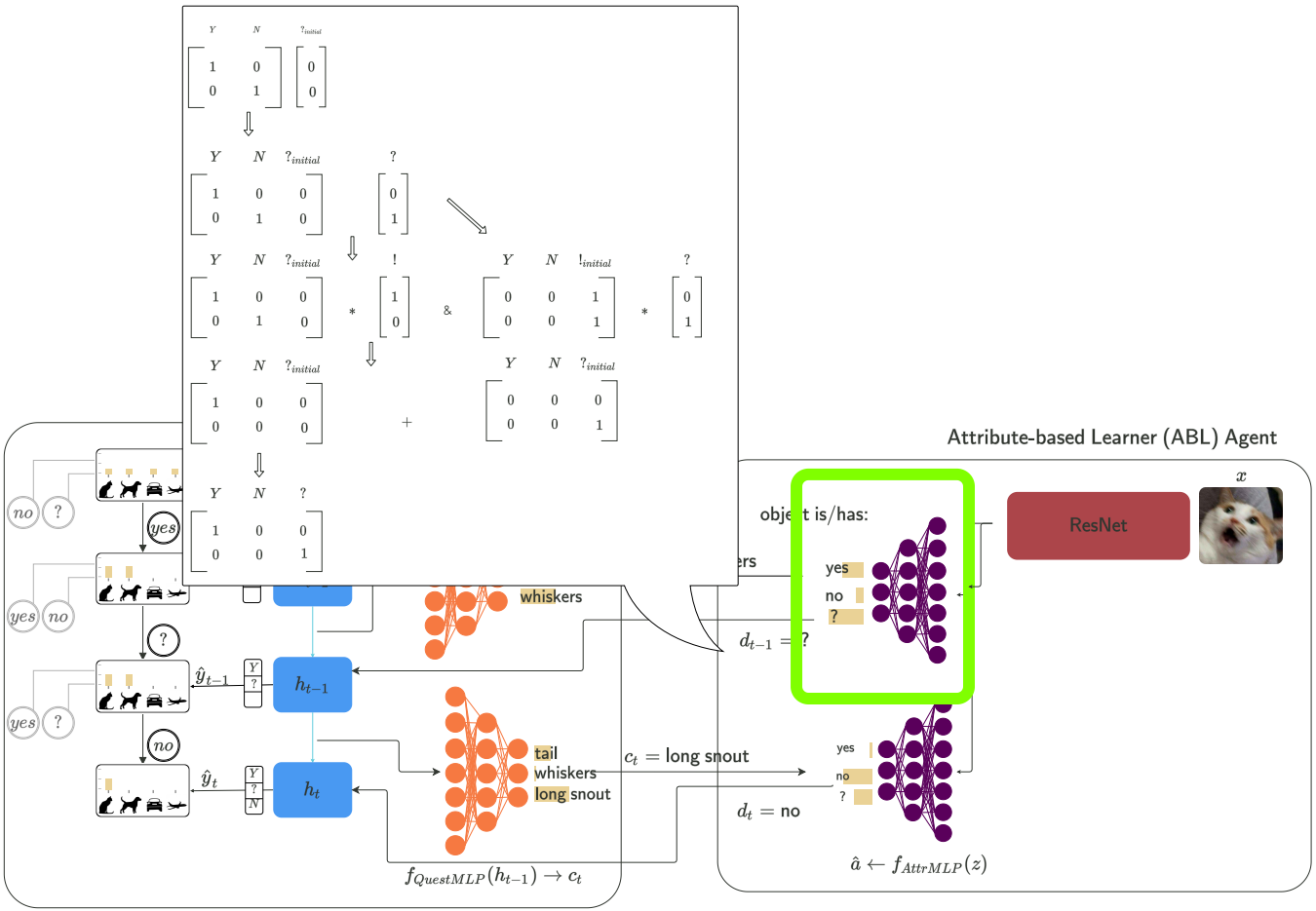
remRDTC - Removing uncertain attributes



- Idea: Skip uncertain questions
- Reminder: output from $f_{QuestMLP}$ is attribute index
- If attribute deemed uncertain, replace logit with $-\infty$
  $\rightarrow$ Gumbel softmax cannot pick these attributes

Using Uncertainty Information

extRDTC - Extending the vocabulary



- Idea: AbL can say 'I don't know'
- Binary vector with 1s where uncertainty is above threshold
- Append to initial answer
- Prevent conflicting answers

Introducing Uncertainty

- Use proof of Gal and Ghahramani [2] to estimate uncertainty in RDTC [1]
- Estimate uncertainty in $f_{AttrMLP}$
- Uncertainty information is used in two strategies
  - remRDTC
  - extRDTC

Experiments

- RDTC is now aware of, and can express its uncertainties
- In experiments, we:
  - Investigate uncertainty and its relationship to other variables
  - Test our model on OOD data
  - Test the model's performance on benchmark datasets

Experiments

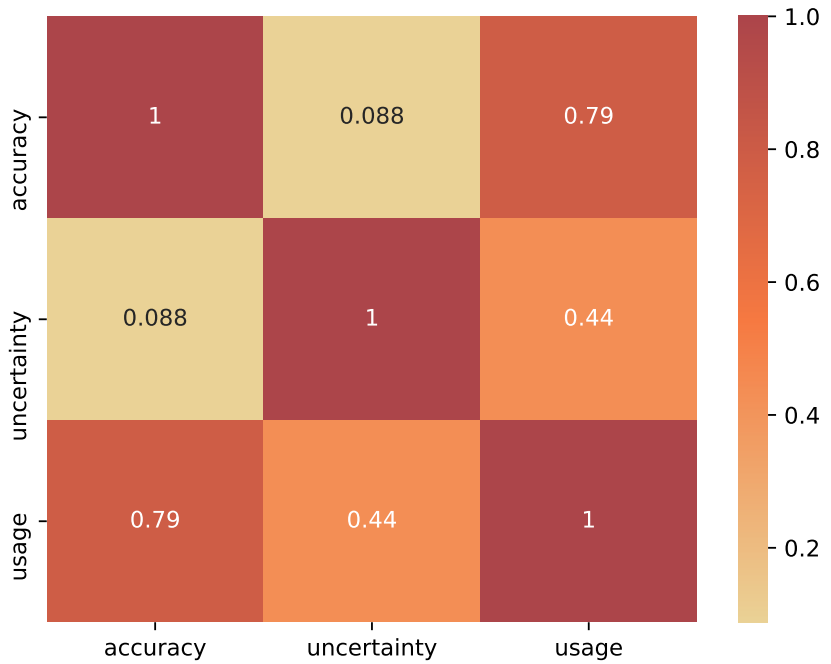
Datasets with attributes

- Animals with Attributes 2 (AWA2)
  - medium size, coarse grained
- aPY
  - small size, coarse grained
- CUB
  - large size, fine grained

Experiments

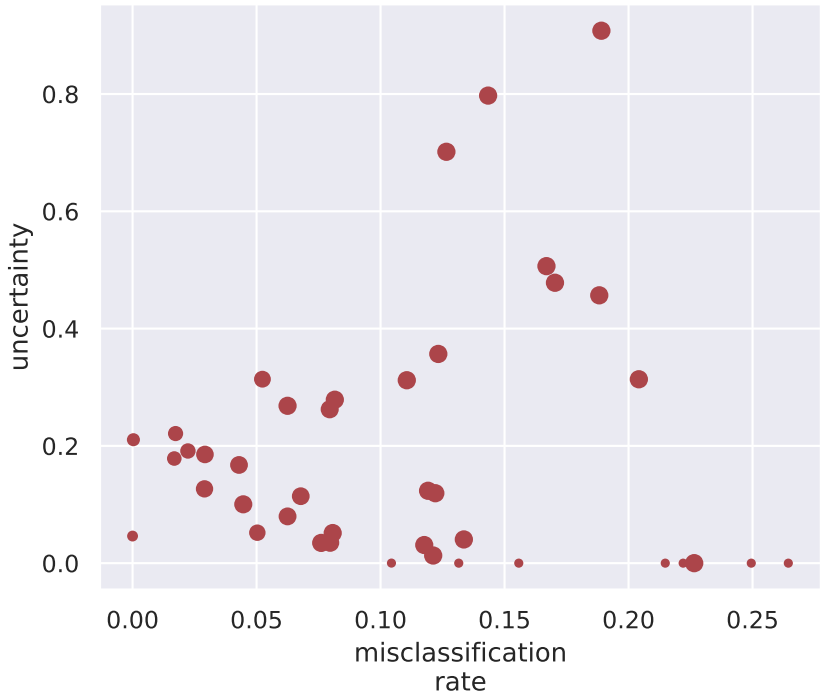
Investigating Uncertainties in CUB

- Misclassification rate, uncertainty, and usage of attributes



- Positive correlation between usage and accuracy
- Almost no correlation between uncertainty and accuracy

- Uncertainty, misclassification rate, usage (size $\propto$ usage)

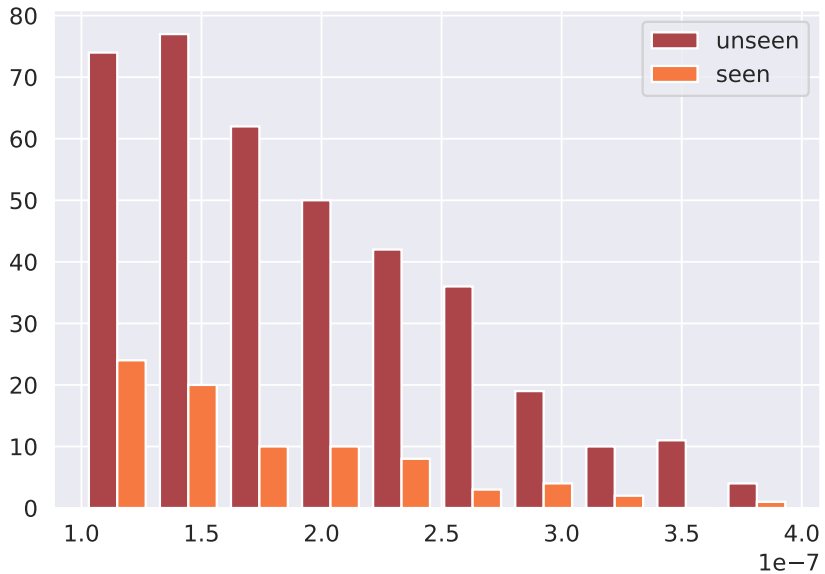


- Uncertain attribute seem to be misclassified more often

Experiments

OOD Detection

- We test extRDTC in zero shot setting (using CUB)
- $\frac{1}{4}$ of classes not seen in training
- Histogram of uncertainty values of seen and unseen classes



- Unseen classes have higher uncertainty values

Experiments

Comparison to other models

- Decision Tree (DT)
  - Use extracted ResNet features
  - Try to split until every leaf node corresponds to one class
- Explainable Decision Tree (XDT)
  - Use learned attribute representations instead of features
  - Attribute representations from $f_{AttrMLP}$
- dNDF [4]
  - Every node is parameterized differentiable function
  - Leaf nodes represent class distributions
  - Learn the optimal route through the tree for each example

- aRDTC
  - RDTC with $\lambda > 0$
- randRDTC
  - Random baseline
  - Like remRDTC, but uncertainty vector is generated randomly
- ResNet
  - Not explainable
  - Trained on ImageNet, fine-tuned for specific datasets

Experiments

Results on Benchmark Datasets

	AWA2	aPY	CUB
ResNet [3]	98.2± 0.0	85.1± 0.6	**79.0**± 0.2
DT	78.0± 0.4	64.3± 0.6	19.3± 0.3
dNDF[4]	97.6± 0.2	85.0± 0.6	73.8± 0.3
RDTC[1]	98.0± 0.1	85.7± 0.7	78.1± 0.2
XDT	73.9± 0.9	59.9± 1.5	4.9± 1.3
aRDTC[1]	98.6	86.1	77.9± 0.6
remRDTC(ours)	**98.7**	86.4	77.7
extRDTC(ours)	**98.7**	85.4	77.8
randtRDTC	98.5	**86.5**	76.8

Experiments

Results on Benchmark Datasets

CUB	aRDTC [1]	randRDTC	remRDTC(Ours)	extRDTC(Ours)
Class	**77.9**	76.8	77.7	77.8
Attribute	84.9	83.9	**87.0**	86.9

Experiments

- RDTC prefers attributes that it rarely misclassifies
- Uncertain attributes seem to be misclassified more often
- Unseen classes yield higher uncertainty
- Both remRDTC and extRDTC perform well on benchmark tasks

Discussion

Looking back...

- The right kind of uncertainty?
  - Uncertainty arising from noise or occlusions is not considered
  - Dropout Uncertainty Estimation lacks empirical proof
- Other methods of uncertainty estimation
  - Often computationally expensive
  - Open area of research
- Beyond attribute uncertainty
  - Estimate uncertainty in other parts of the model (i.e. $f_{ClassMLP}$)

Conclusions

A qualitative Example

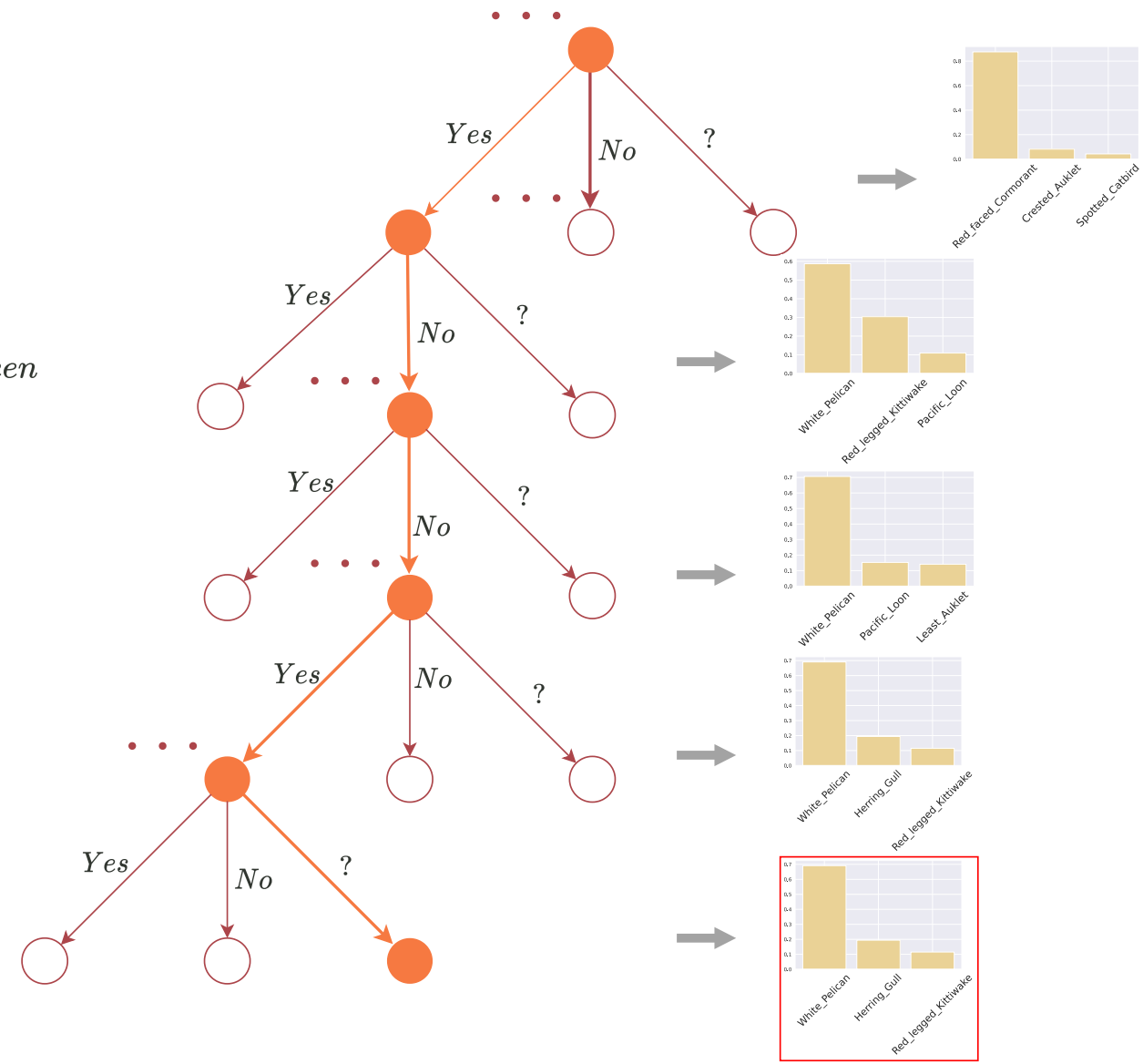
has_size :: small

has_wing_color :: olive

has_under_tail_color :: green

has_nape_color :: black

has_belly_pattern :: solid



Conclusions

- Estimate uncertainty based on Gal and Ghahramani [2]
- Used in RDTC by Alaniz et al. [1]
- Two strategies: remRDTC and extRDTC
- We investigate uncertainty and relationship to other variables
- OOD examples yield high uncertainty
- Uncertain RDTC's achieve SOTA accuracy

References

[1] S. Alaniz, D. Marcos, and Z. Akata. Learning decision trees recurrently through communication. ICML XXAI Workshop, 2020.

[2] Y. Gal and Z. Ghahramani. Dropout as a bayesian approximation: Representing model uncertainty in deep learning. In international conference on machine learning, pages 1050–1059, 2016.

[3] K. He, X. Zhang, S. Ren, and J. Sun. Deep residual learning for image recognition. In Proceedings of the IEEE conference on computer vision and pattern recognition, pages 770–778, 2016.

[4] P. Kontschieder, M. Fiterau, A. Criminisi, and S. Rota Bulo. Deep neural decision forests. In Proceedings of the IEEE international conference on computer vision, pages 1467–1475, 2015.