Google DeepMind

Evaluation and calibration of AI models with *uncertain* ground truth

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a collaboration between Google DeepMind and Health

Outline

Contents:

- ❏ Uncertainty from annotator disagreement
- ❏ Statistical framework
- ❏ Measuring uncertainty
- ❏ Evaluating AI models
- ❏ Case study in dermatology:
  - ❏ Results
  - ❏ Bonus: calibration
- ❏ Conclusion and outlook

Promise: you will start to question any "ground truth" labels you come across!

``Bird", "cat", or "frog"?

"Hemangioma" or "Melanoma"?
Benign or cancer?

Standard evaluation of supervised models

Observation

Correct/good prediction?

AI prediction

“bird”

Standard evaluation of supervised models

Unknown true label

?

Observation

Correct/good prediction?

AI prediction

"bird"

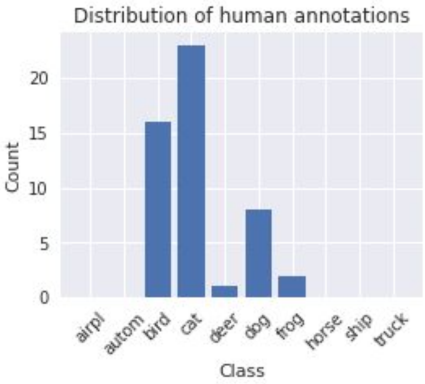
Standard evaluation of supervised models

Unknown true label

?

Observation

Annotations



Annotators disagree!

?

AI prediction

"bird"

Joshua C. Peterson*, Ruairidh M. Battleday*, Thomas L. Griffiths, & Olga Russakovsky. Human uncertainty makes classification more robust. ICCV'19.

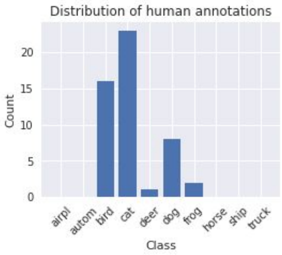
Standard evaluation of supervised models

Unknown true label

?

Observation

Annotations



Majority vote

“cat”

Ignores disagreement!

Incorrect!

AI prediction

“bird”

Standard evaluation of supervised models

Unknown true label

?

Observation

Annotations

b^1: {*Pyogenic granuloma* (Low)} {*Hemangioma* (Med)} {*Melanoma* (High)}
b^2 {*Angiokeratoma of skin* (Low)} {*Atypical Nevus* (Med)}
b^3: {*Hemangioma* (Med)} {*Melanocytic Nevus* (Low), *Melanoma* (High), *O/E – ecchymoses present* (Low)}
b^4: {*Hemangioma* (Med), *Melanoma* (High), *Skin Tag* (Low)}
b^5: {*Melanoma* (High)}
b^6: {*Hemangioma* (Med)} {*Melanoma* (High)} {*Melanocytic Nevus* (Low)}

Conditions, Low/Med/High risk conditions

Y. Liu et al. A deep learning system for differential diagnosis of skin diseases. Nature Medicine, 2020.

Standard evaluation of supervised models

Unknown true label

?

Observation

Annotations

b¹: {*Pyogenic granuloma* (Low)} {***Hemangioma*** (Med)} {*Melanoma* (High)}
b² {*Angiokeratoma of skin* (Low)} {*Atypical Nevus* (Med)}
b³: {***Hemangioma*** (Med)} {*Melanocytic Nevus* (Low), *Melanoma* (High), *O/E - ecchymoses present* (Low)}
b⁴: {***Hemangioma*** (Med), *Melanoma* (High), *Skin Tag* (Low)}
b⁵: {*Melanoma* (High)}
b⁶: {***Hemangioma*** (Med)} {*Melanoma* (High)} {*Melanocytic Nevus* (Low)}

Majority voting is non-trivial

?

AI prediction

"Hemangioma"

Standard evaluation of supervised models

Unknown true label

?

Observation

Annotations

b[1]: {*Pyogenic granuloma* (Low)} {*Hemangioma* (Med)} {*Melanoma* (High)}
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b[3]: {*Hemangioma* (Med)} {*Melanocytic Nevus* (Low), *Melanoma* (High), *O/E – ecchymoses present* (Low)}
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b[5]: {*Melanoma* (High)}
b[6]: {*Hemangioma* (Med)} {*Melanoma* (High)} {*Melanocytic Nevus* (Low)}

?

AI prediction *set*

"Hemangioma"

"Atypical Nevus"

"Melanocytic Nevus"

Standard evaluation of supervised models

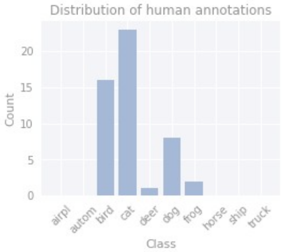
Unknown true label	Observation	Annotations	Majority vote		AI model
y^* →	x →	b^1 ⋮ b^R →	y	↔ Standard metric	

Unknown true label

?

Observation

Annotations



Majority vote

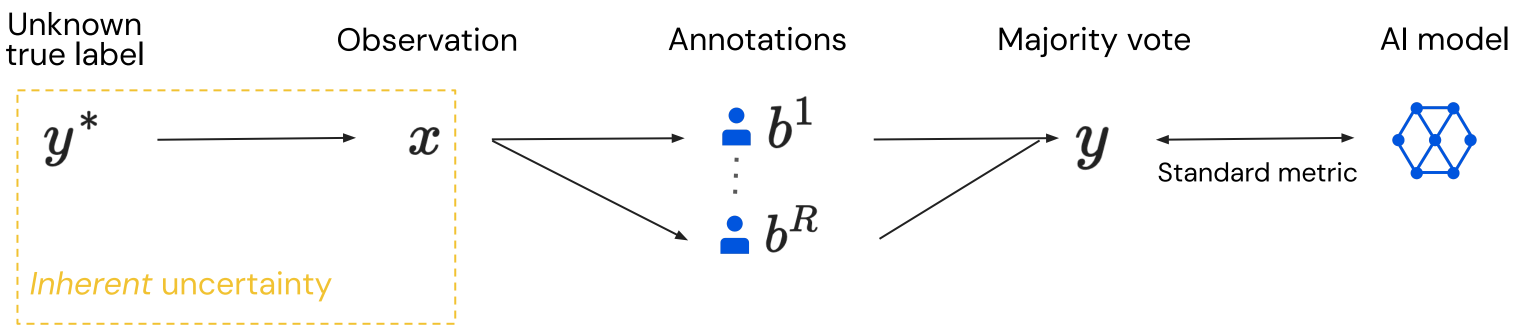
"cat"

Incorrect!

AI prediction

"bird"

Inherent uncertainty

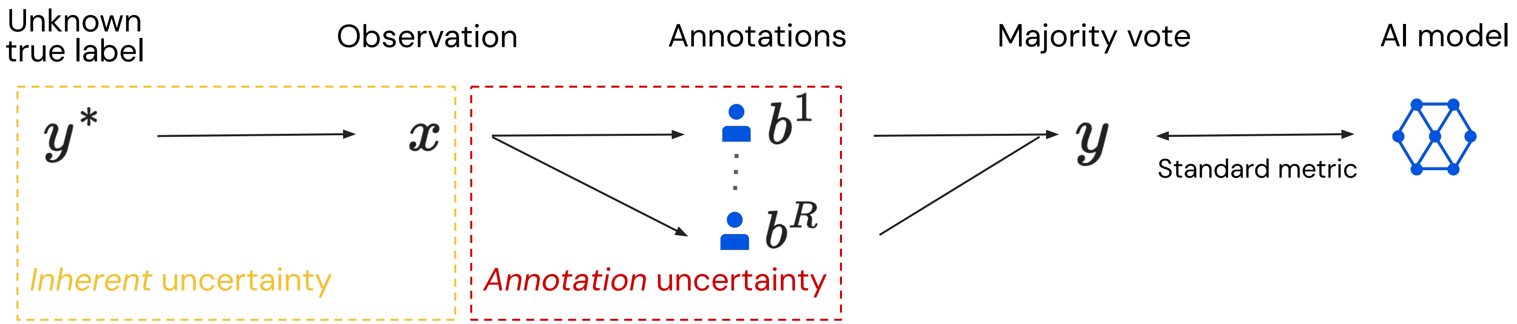


Inherent uncertainty = limited observational information:
(typically called data uncertainty)

- Low-resolution images in image recognition (e.g., CIFAR10)
- Single 2D view in 3D reconstruction
- Missing meta information or no option to question the patient in health
- ...

TL;DR: $p(y^*|x)$ is not one-hot and has high entropy!

Annotation uncertainty

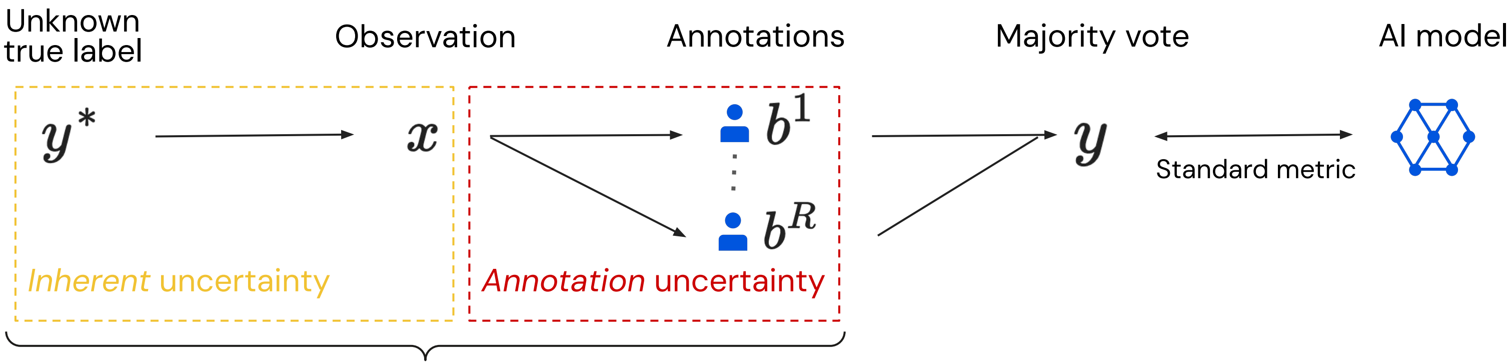


Annotation uncertainty = uncertainty induced through human annotators:

- Subjective tasks
- Inexperience of annotators
- Insufficient training of annotators
- Inappropriate annotation tool
- Different biases or background from annotators

TL;DR: annotation is difficult and we have to trust experts.

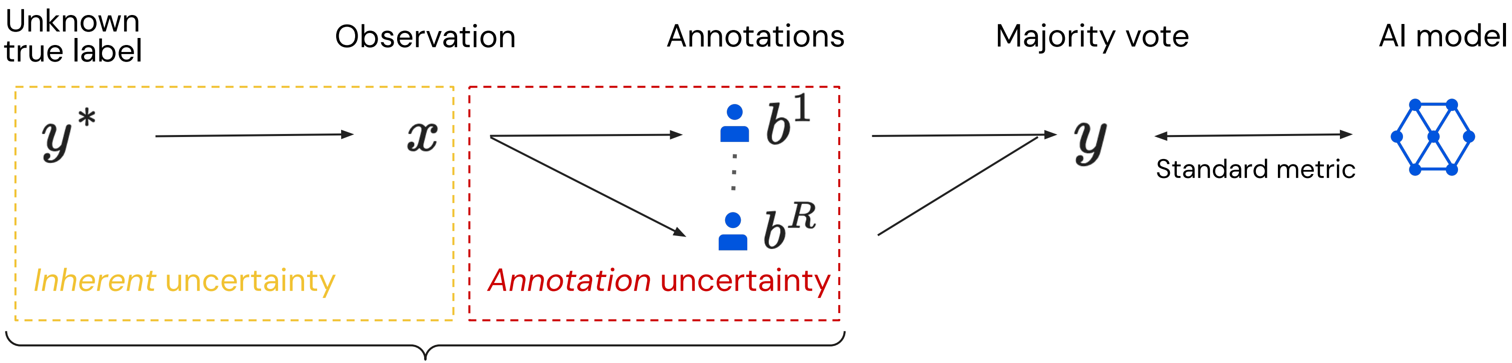
Ground truth uncertainty



Ground truth uncertainty = inherent + annotation uncertainty

- We observe both through annotator **disagreement**
- Often impossible to disentangle inherent and annotation uncertainty

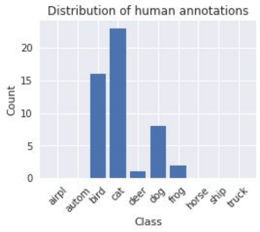
Ground truth uncertainty



Ground truth uncertainty = inherent + annotation uncertainty

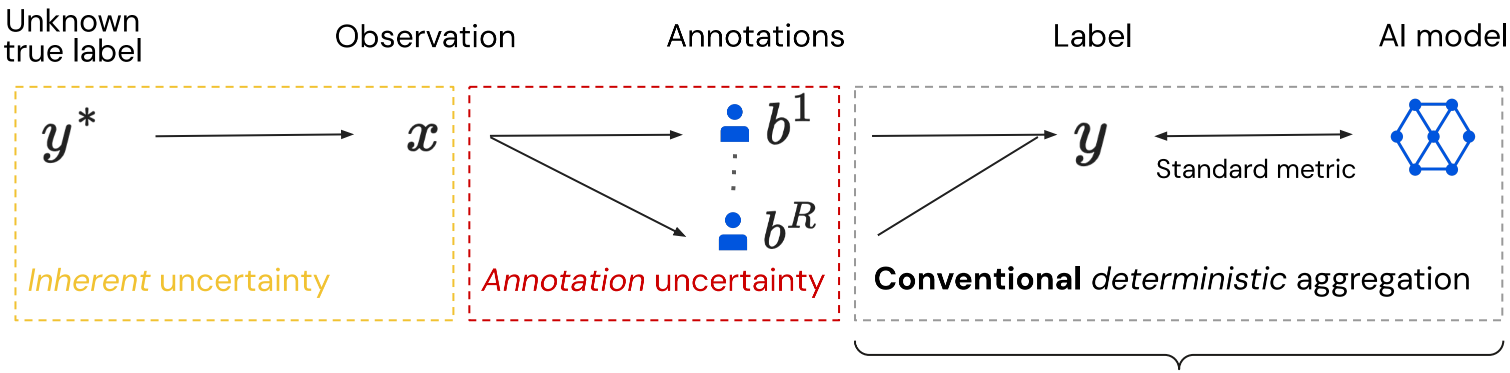
- We observe both through annotation disagreement
- Usually we cannot disentangle between inherent and annotation uncertainty

Inherent uncertainty



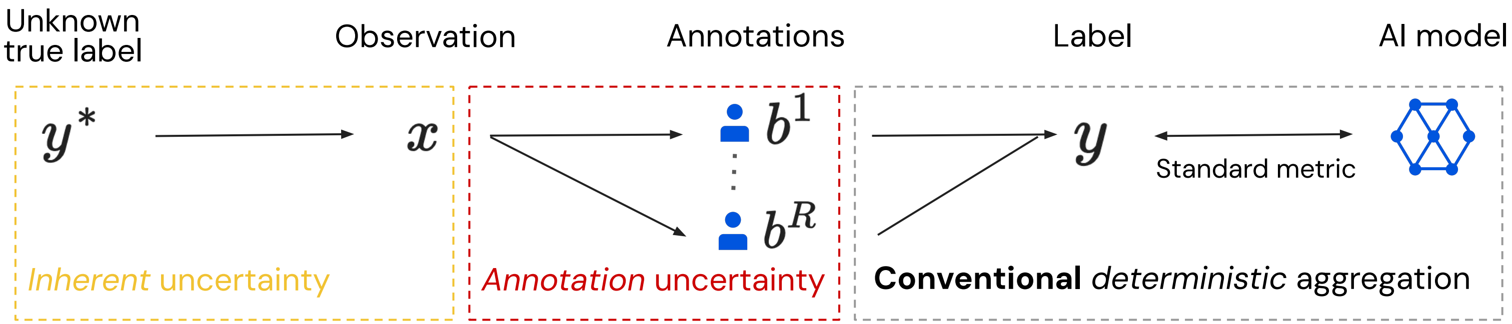
Annotation uncertainty

Deterministic aggregation ignores uncertainty



Simple majority voting or deterministic aggregation ignores this uncertainty

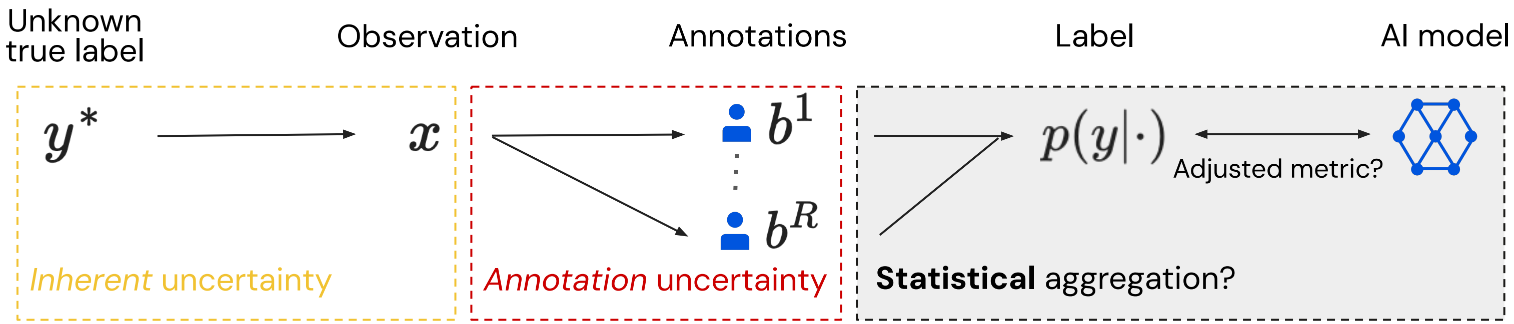
Deterministic aggregation ignores uncertainty



Deterministic aggregation ignores ground truth uncertainty:

- Ignores large parts of the annotators
- Might evaluate against the wrong labels
- Does not quantify uncertainty on top of metrics

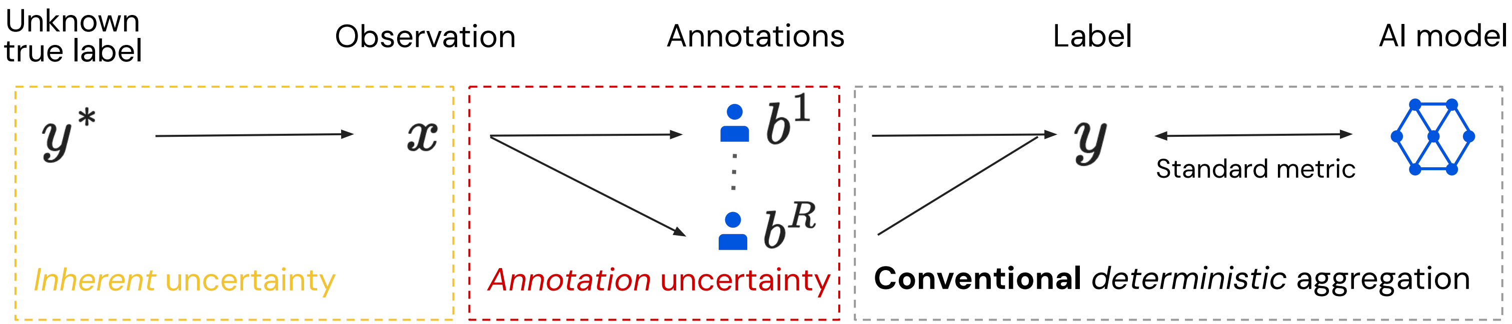
Deterministic aggregation ignores uncertainty



Can we use a statistical aggregation model to account for uncertainty?

- Statistical aggregation of annotations
- Adjust evaluation metrics by uncertainty

Deterministic aggregation ignores uncertainty



Deterministic aggregation:

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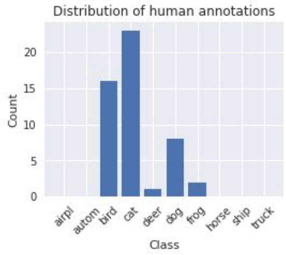
- ➔ Does not quantify uncertainty on top of metrics



Introducing *plausibilities*

Confidential — Google DeepMind

Observation

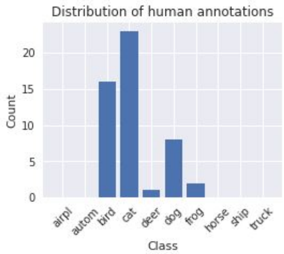
Annotations

b^1

⋮

b^R

Plausibilities $\hat{\lambda}$



?

AI prediction

“bird”

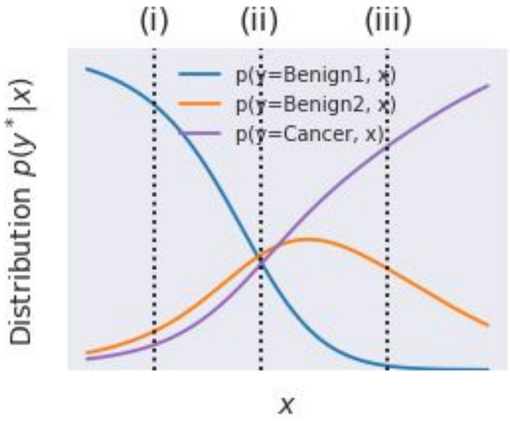
$$\underbrace{\text{Annotations} \rightarrow \text{Plausibilities } \hat{\lambda}}$$

Deterministic aggregation approximates posterior $p(y^*|x)$
using a point estimate $\hat{\lambda}$

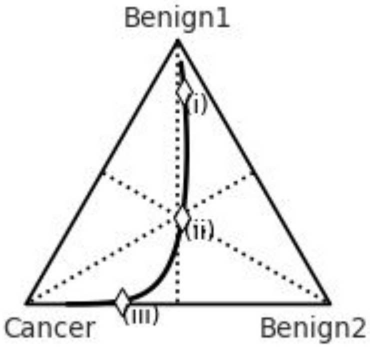
- “Plausibilities” = how *plausible* is a label given the annotations
- In this talk: categorical distributions over classes

Plausibilities on one-dimensional toy example

Example cases

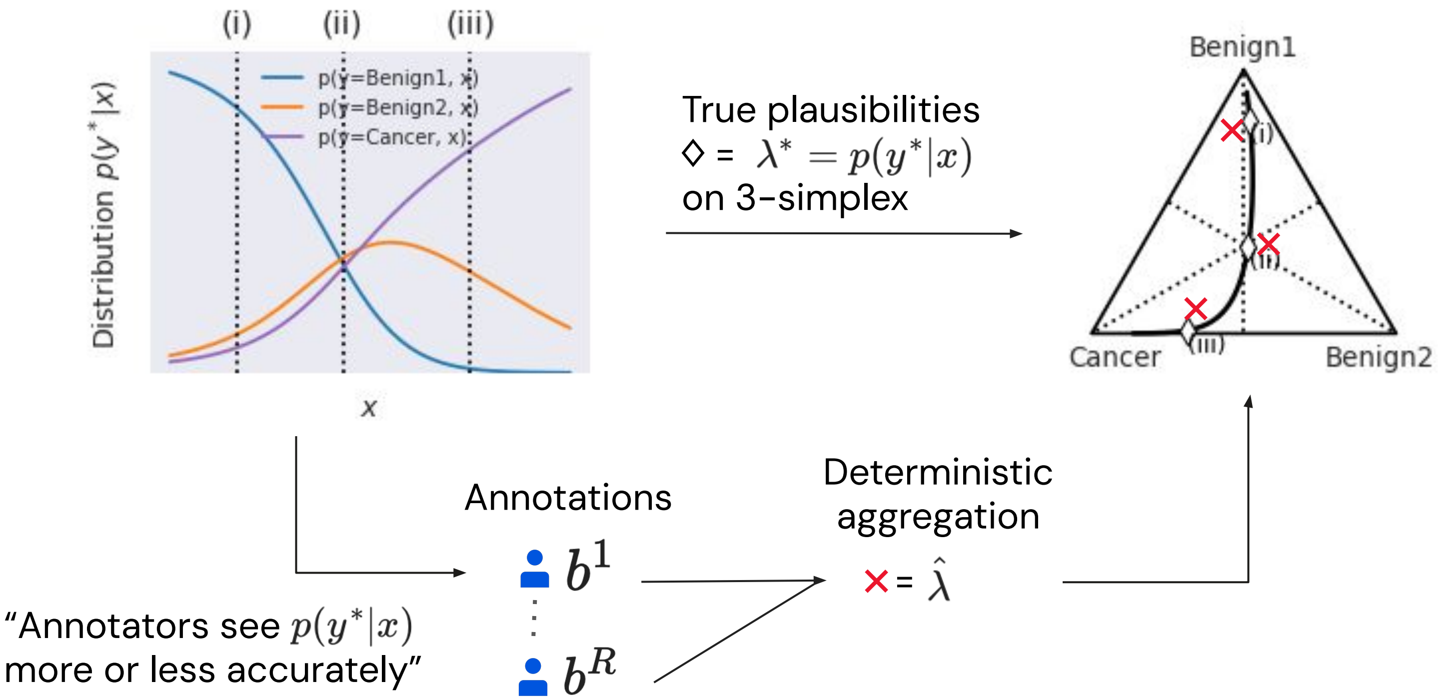


True plausibilities
◊ = $\lambda^* = p(y^*|x)$
on 3-simplex

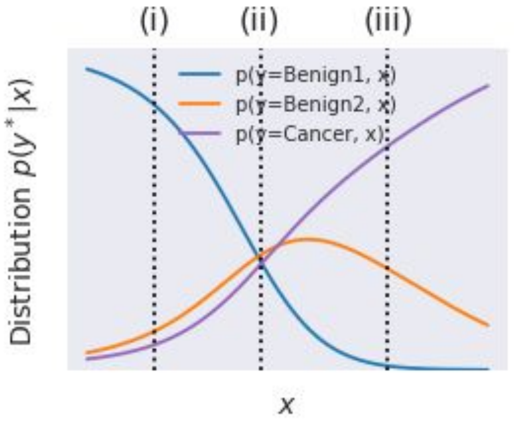


Inherent uncertainty =
location on simplex

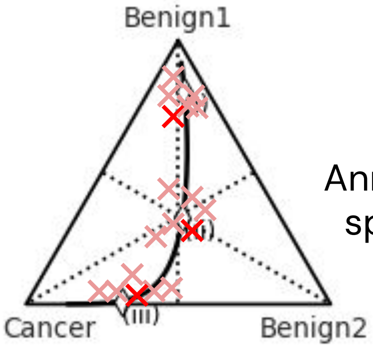
Point estimates from deterministic aggregation



Variation in plausibilities through re-annotating



True posterior
◇ = $\lambda^* = p(y^*|x)$
on 3-simplex



Annotation uncertainty =
spread of plausibilities

Annotations

b^1

⋮

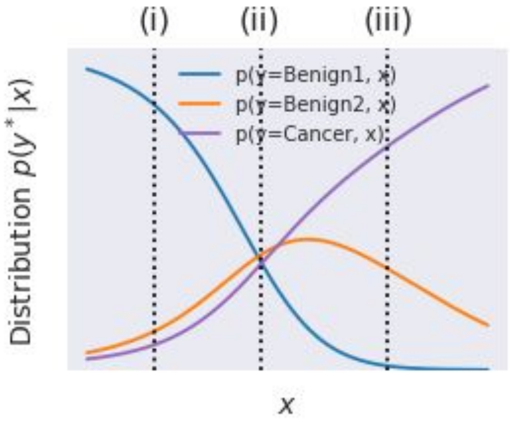
b^R

Deterministic
aggregation

× = $\hat{\lambda}$

Different annotators yield
different plausibilities $\hat{\lambda}$

Statistical aggregation



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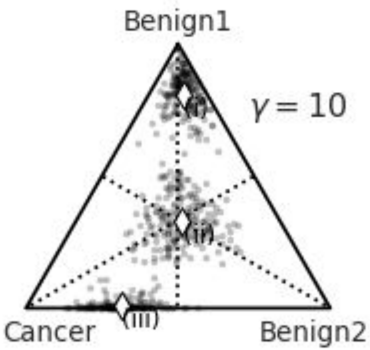


$b^r \sim p(b|\lambda^*)$

Annotation model

b^1

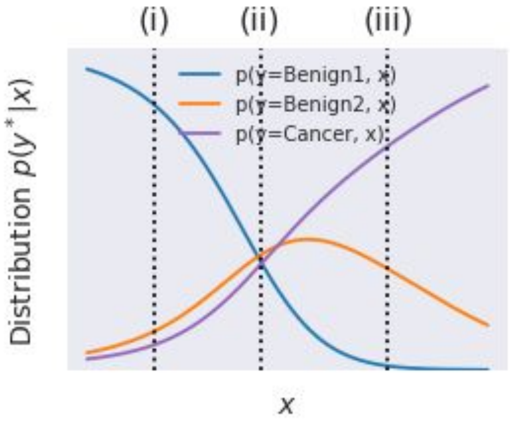
$\vdots$

b^R

$\lambda^m \sim p_\gamma(\lambda|b, x)$

Statistical aggregation model

Annotator *reliability* in statistical aggregation



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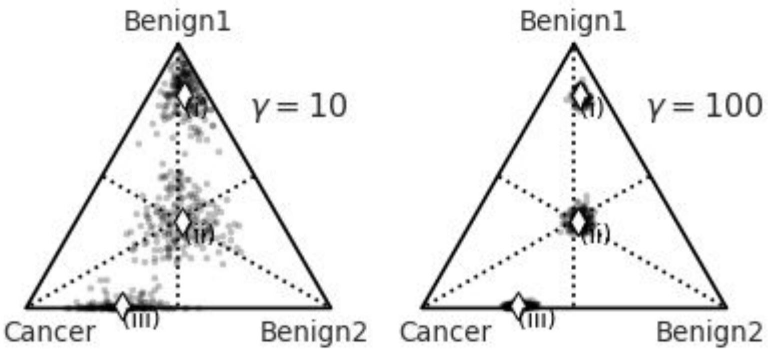


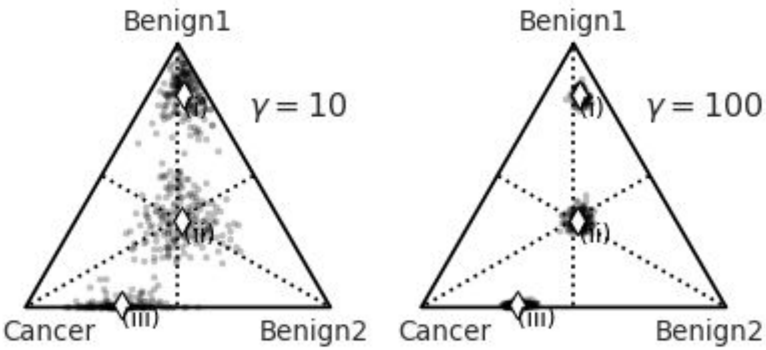
$b^r \sim p(b|\lambda^*)$

b^1
⋮
b^R

$\lambda^m \sim p_\gamma(\lambda|b, x)$

Reliability γ = lower or higher prior trust in annotators

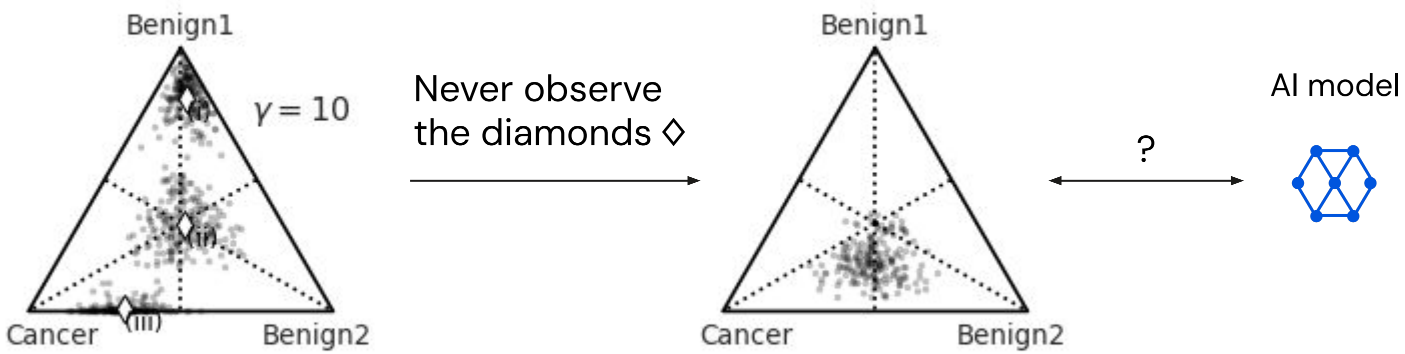
Conclusion: plausibilities on toy example



Ground truth uncertainty on the simplex:

- Location of plausibilities on simplex = inherent uncertainty
- Spread of plausibilities = annotation uncertainty

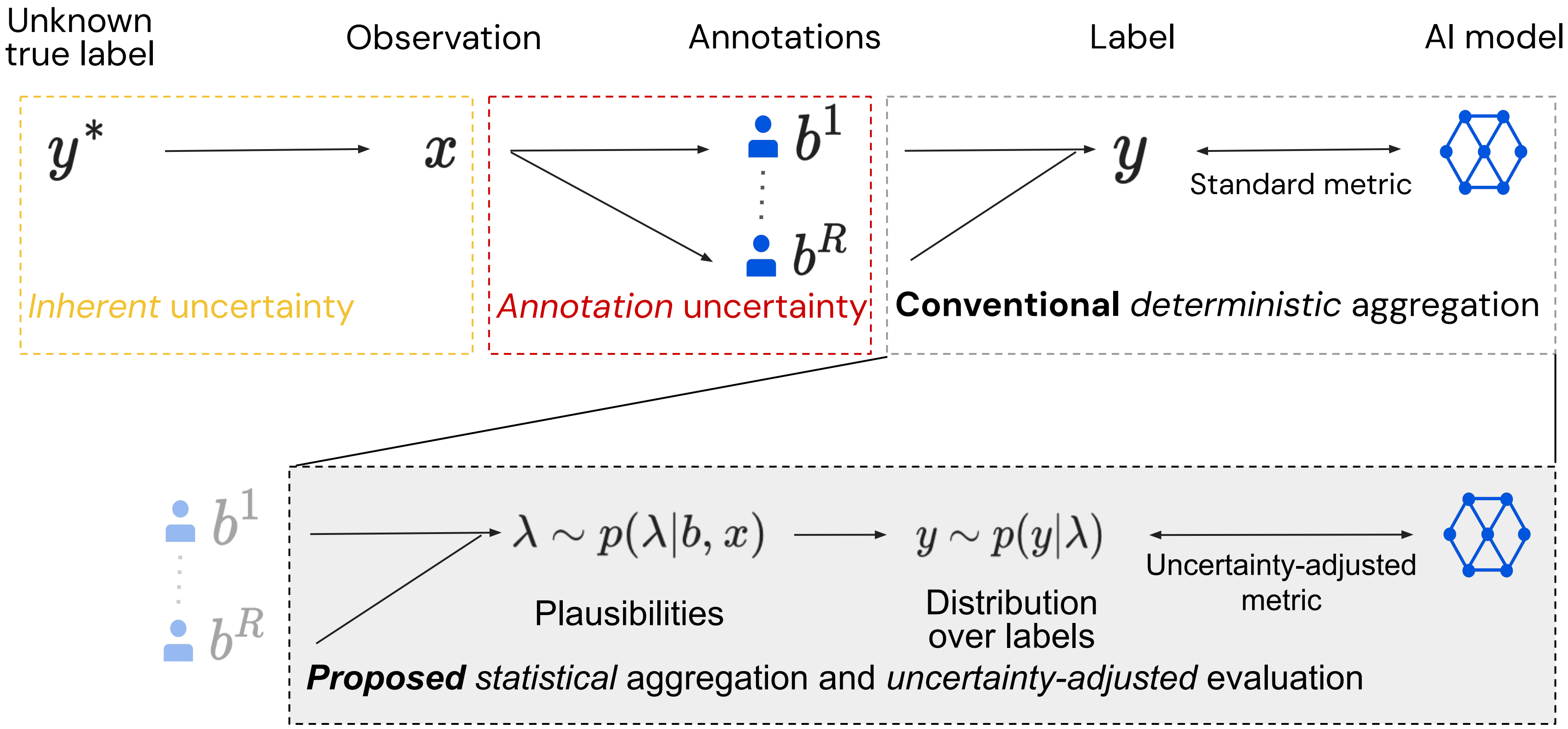
Conclusion: plausibilities on toy example



Statistically modeling aggregation:

- Allows to disentangle inherent and annotation uncertainty to some extent (subject to modeling assumptions, depending on reliability)
- Avoids expensive re-annotation to get uncertainty estimates

Summary: proposed statistical framework

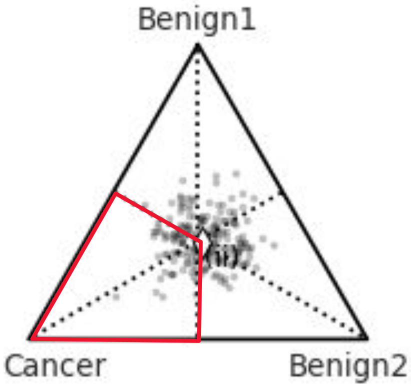


Measuring annotation uncertainty

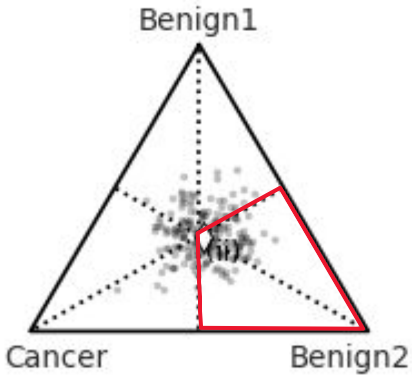
- How *certain* is it that y is the top-1 label?

$$\mathrm{Certainty}(y; b, x) = \mathbb{E}_{p(\lambda|b,x)}\left[\delta[y = \arg\max_j \lambda_j]\right]$$

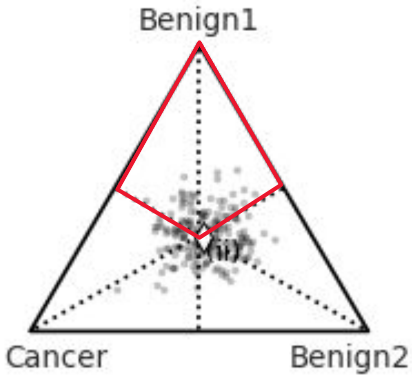
Certainty(Cancer)



Certainty(Benign2)



Certainty(Benign1)



Measuring annotation uncertainty

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$$\mathrm{Certainty}(y; b, x) = \mathbb{E}_{p(\lambda|b,x)}\left[\delta[y = \arg\max_j \lambda_j]\right]$$

- What is the highest certainty across labels?

$$\mathrm{AnnotationCertainty}(b, x) = \max_y \mathrm{Certainty}(y; b, x)$$

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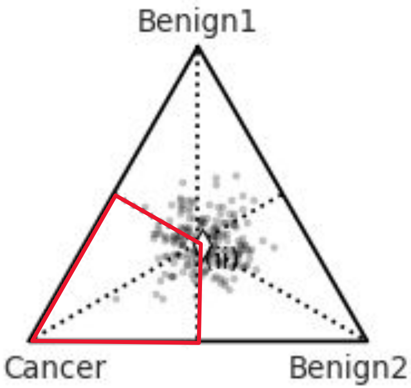
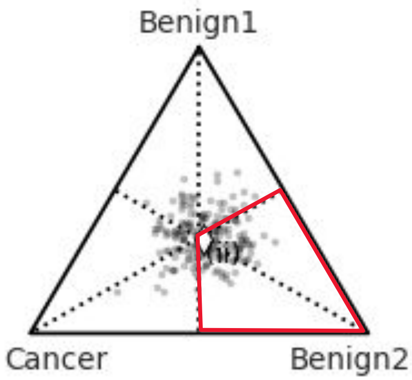
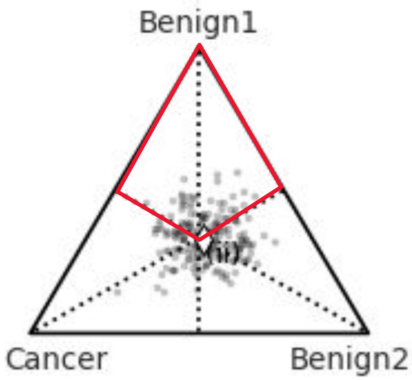


Certainty(Benign2)



Certainty(Benign1)

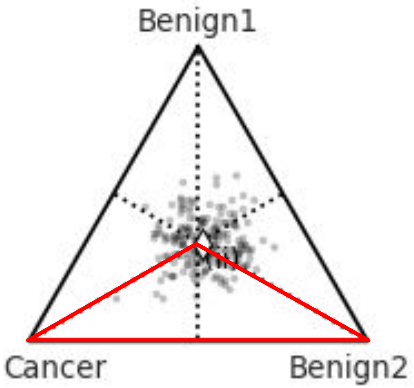


Measuring annotation uncertainty

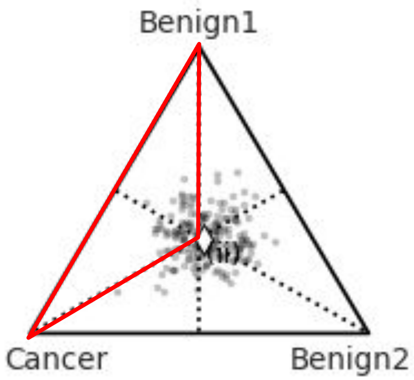
- Can also quantify certainty of label sets Y :

$$\text{Certainty}(Y; b, x) = \mathbb{E}_{p(\lambda|b,x)} \left[\delta[Y = \text{top\_k}(\lambda)]\right]$$

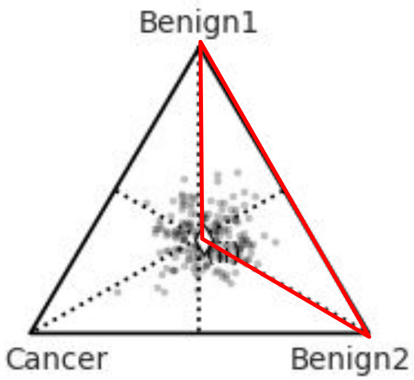
Certainty({Cancer, Benign2})



Certainty({Cancer, Benign2})



Certainty({Benign1, Benign2})



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- What is the highest certainty across labels?

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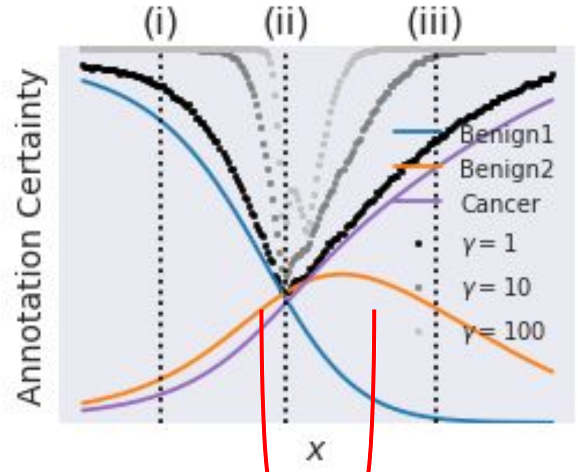
Measuring annotation uncertainty

- Annotation certainty on toy example for different reliabilities γ :

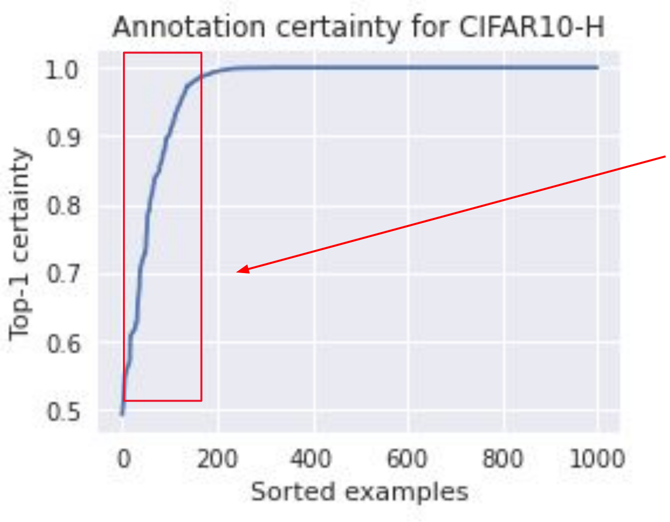


Different reliabilities

Top-1 label uncertain irrespective of
how much we trust our annotators

Measuring annotation uncertainty

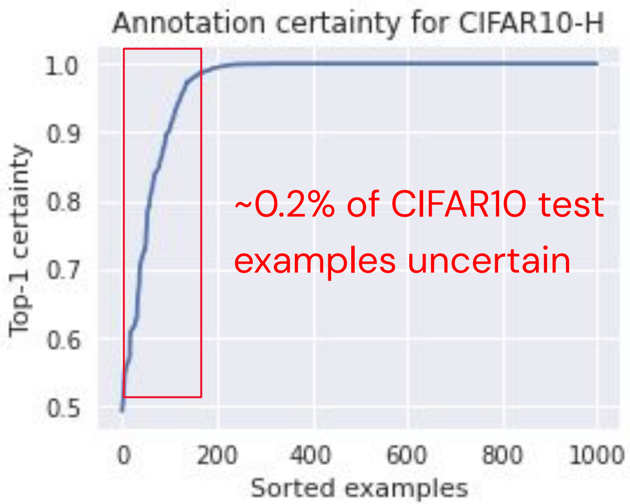
- Annotation certainty on CIFAR10 using annotations from CIFAR10-H:



- 178 examples with annotation certainty < 99%
- This is ~0.2% of all CIFAR10 test examples

Measuring annotation uncertainty

- Annotation certainty on CIFAR10 using annotations from CIFAR10-H:



[Papers with Code leaderboard](#):

μ2Net	99.49	2022
ViT-L/16	99.42	2020
CaiT-M-36 U 224	99.4	2021
CvT-W24	99.39	2021
BiT-L	99.37	2019
ViT-B	99.3	2022

Improvements within 0.2%

Uncertainty-adjusted (top-k) accuracy

Given a model that yields a top-k prediction set $C_{\text{top-}k}(x)$:

$$\text{UA-Accuracy}_{\text{top-}k} = \mathbb{E}_{p(x)}\mathbb{E}_{p(\lambda|b,x)}\left[\delta[\arg\max_j \lambda_j \in C_{\text{top-}k}(x)]\right]$$

Uncertainty-adjusted (top-k) accuracy

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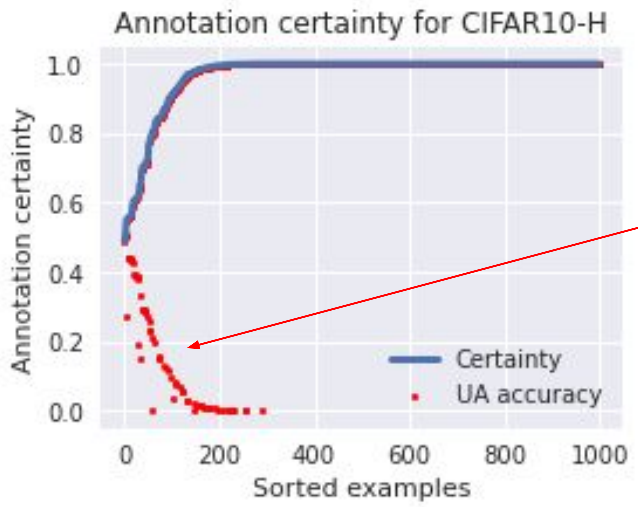

- $C_{\text{top-}k}(x)$ = <u>original CIFAR10 labels</u> (k = 1)

➔ Even CIFAR10 labels perform poorly on uncertain examples!

Case study: dermatology

Observation

Annotations

b^1: {*Pyogenic granuloma* (Low)} {*Hemangioma* (Med)} {*Melanoma* (High)}
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b^5: {*Melanoma* (High)}
b^6: {*Hemangioma* (Med)} {*Melanoma* (High)} {*Melanocytic Nevus* (Low)}

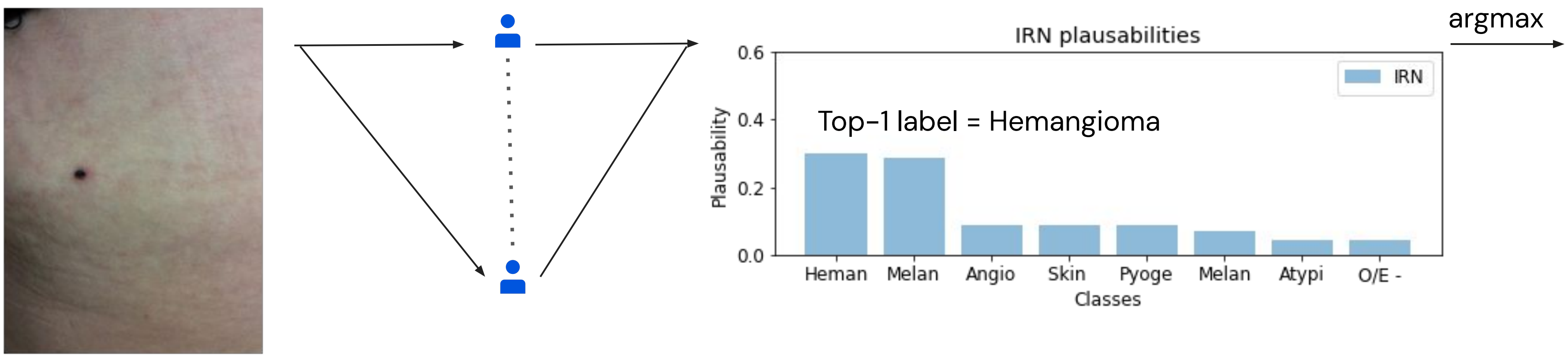
Partial rankings to model differential diagnoses

Case study: deterministic aggregation using IRN

Task: predict dermatological conditions from images.

- Inverse rank normalization (IRN) to aggregate annotators' differential diagnoses.

Observation | Annotations | Plausibilities $\hat{\lambda}$



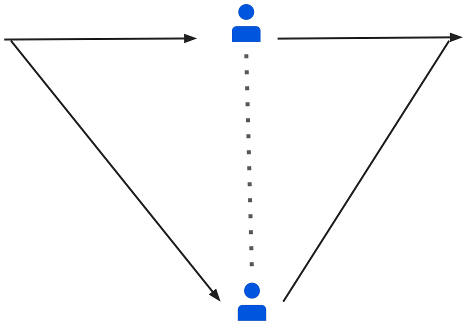
Case study: statistical aggregation using PrIRN

Task: predict dermatological conditions from images.

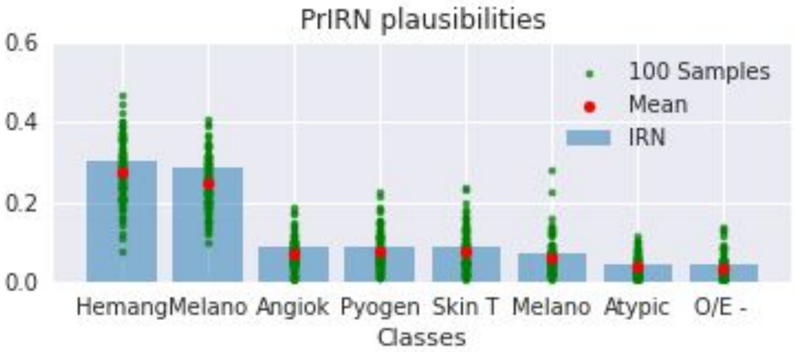
- Plackett-Luce or probabilistic IRN (PrIRN) to model $p(\lambda|b)$

Observation

Annotations



Plausibilities $\lambda^m \sim p_\gamma(\lambda|b)$



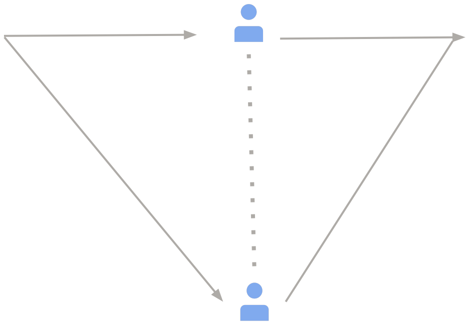
Case study: statistical aggregation using PrIRN

Task: predict dermatological conditions from images.

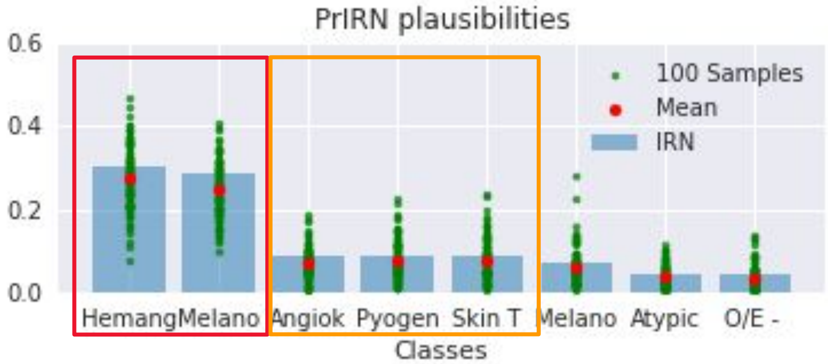
- Plackett-Luce or probabilistic IRN to model $p(\lambda|b)$

Observation

Annotations



Plausibilities $\lambda^m \sim p_\gamma(\lambda|b)$

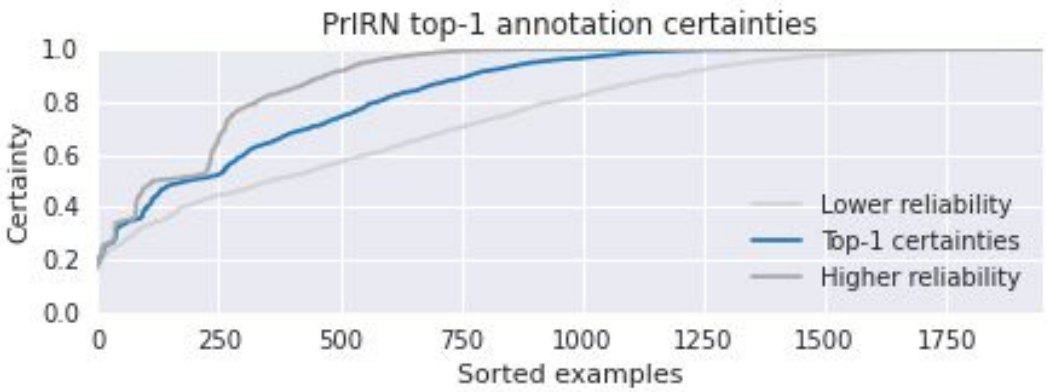


Top-1 condition changes easily
= low annotation certainty

3rd, 4th, 5h conditions also
change easily

High annotation uncertainty

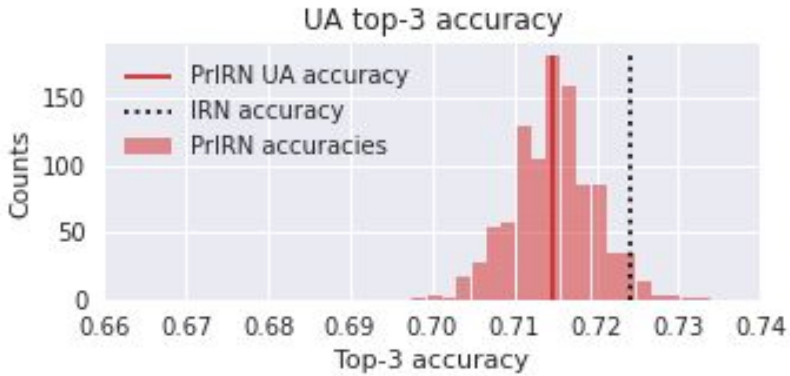
- Significant portions of cases with high annotation uncertainty:



➔ In discussions with dermatologists often attributed to inherent uncertainty

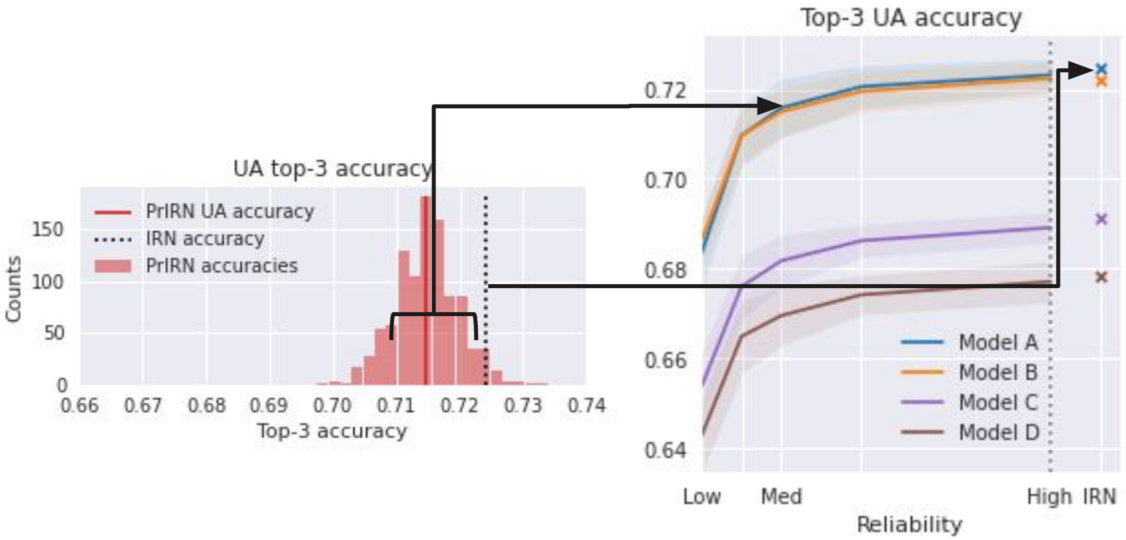
Uncertainty-adjusted top-3 accuracy

- Across cases / per plausibility:



➔ Significant variation in top-3 accuracy

Evaluation across annotator reliabilities

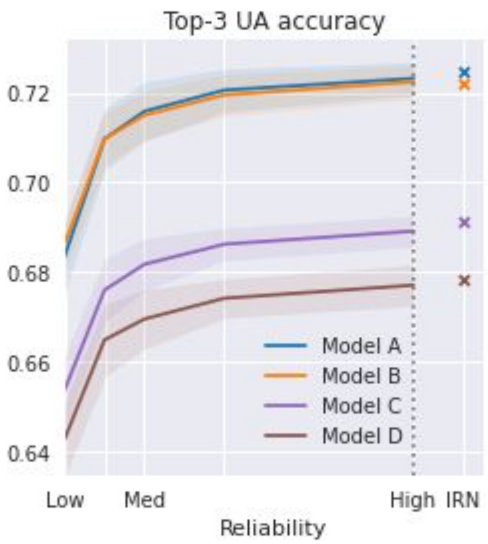


- UA accuracy varies significantly by reliability
- IRN implicitly evaluates infinite annotator reliability
- Large spread/uncertainty in accuracies (shaded)

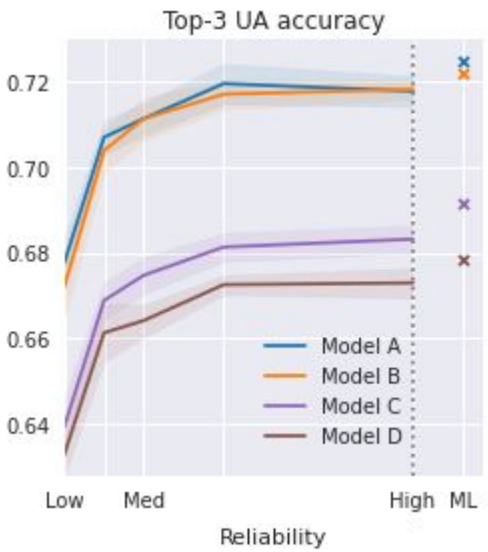
Alternative statistical aggregation methods

- Alternative statistical aggregation models exhibit different results:

PrIRN



Plackett-Luce



➔ Aggregation is a mode choice usually not made explicit!

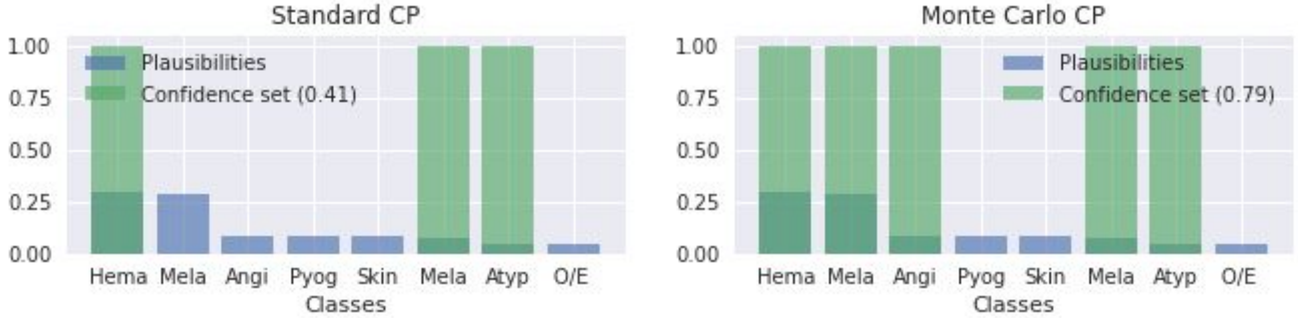
Bonus: calibration with uncertain ground truth

Calibration usually based on ground truth labels on a calibration/validation set:

- Conformal prediction uses ground truth labels to calibrate a softmax threshold τ
- Threshold used to predict confidence sets of classes at test time instead of the top-k:

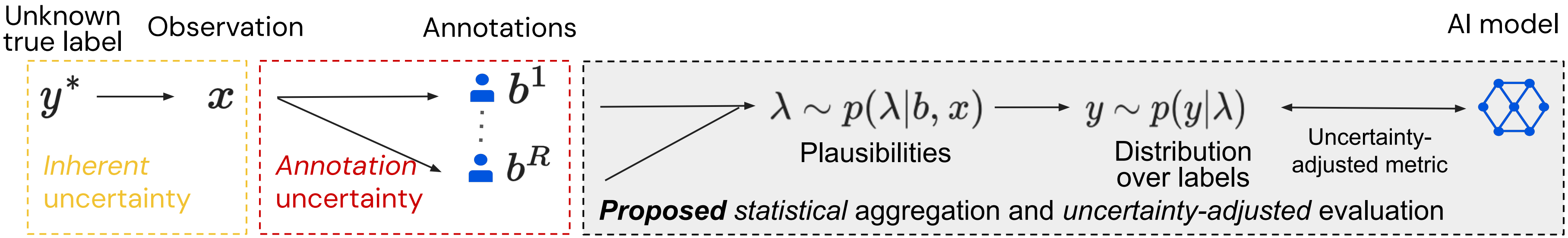
$$C_{\text{top-}k}(x) \longrightarrow C_{\text{CP}}(x) := \{k \in [K] : k - \text{th softmax} \geq \tau\}$$

- We propose *Monte Carlo* conformal prediction to calibrate directly against the annotations

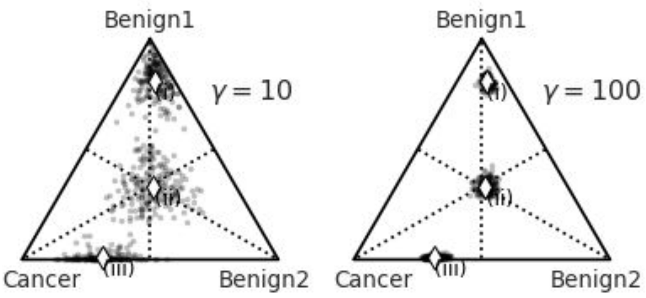


Conclusion

Proposed a statistical framework for dealing with ground truth uncertainty:



- ➔ Ground truth uncertainty = inherent + annotation uncertainty (location + spread of plausibilities)
- ➔ *Annotation certainty* explicitly measures annotation uncertainty
- ➔ Uncertainty-adjusted metrics to evaluate and evaluate models



More: arxiv.org/abs/2307.02191 | arxiv.org/abs/2307.09302 | davidstutz.de | dstutz@google.com