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Uncertainty in DL models

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Remark: Much of the material has been developed together with Elvis Murina and Oliver Dürr

Topics

- **Capturing uncertainty in statistics**
  - Functional uncertainty – model family
  - Epistemic uncertainty - model parameter values
  - Aleatoric uncertainty - data variation
  - Frequentist's vs Bayesian's approach to capture epistemic uncertainty
- **Capturing uncertainty in DL?**
  - Bayesian DL
  - Using dropout during test-time to do Bayesian DL
  - Using `TF probability` to do probabilistic modeling → Oliver takes over
- **Your projects**
  - Spotlight talks
  - Poster session

Uncertainties

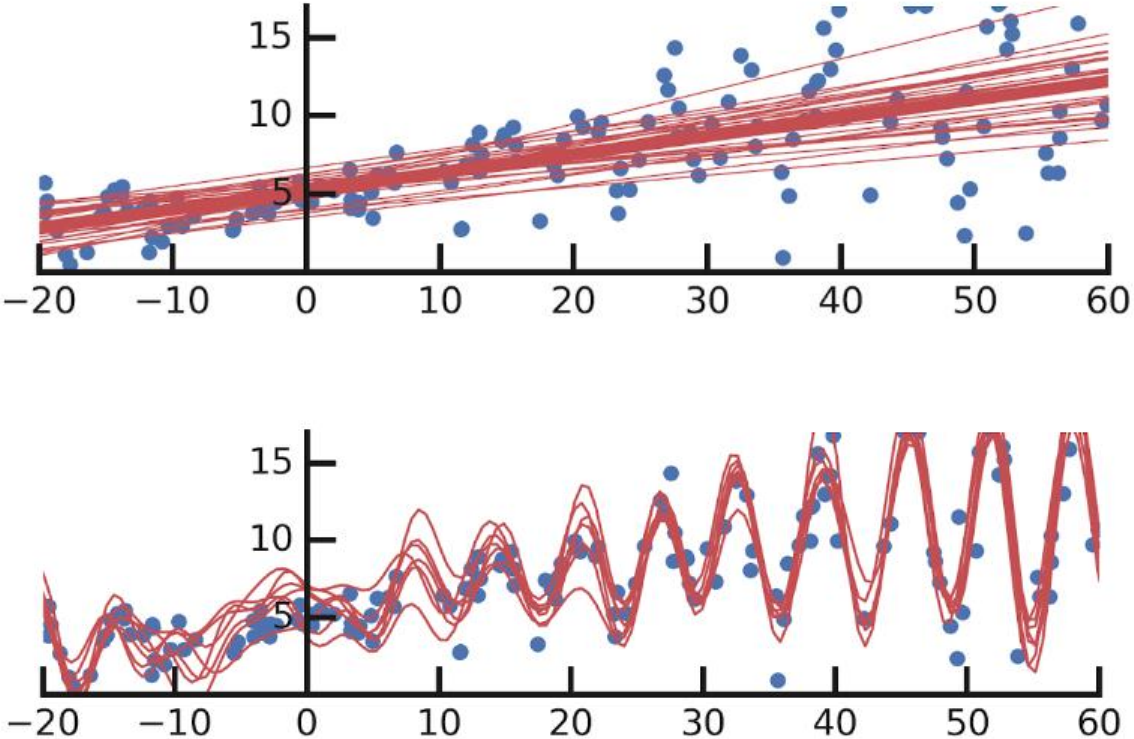


Image credits: [TFp]

Functional uncertainty: Linear model or sinus with increasing amplitude?

Epistemic uncertainty: What values do we need to pick for the model parameters?

Aleatoric uncertainty: How much do the individual data vary?

Which kind of uncertainties do talk about?

- **Functional uncertainty**
  - How sure can we be to have fitted the correct model?
    → this uncertainty depends on our field knowledge but gets usually also smaller if we collect more data which allows to detect a potential bias more easily

- **Aleatoric uncertainty**
  - data variability inherent to the data generating process
    → this uncertainty does not get small when we collect more data

- **Epistemic uncertainty**
  - Uncertainty of the model parameter estimates
    → this uncertainty goes down when we collect more data

Recap: Linear regression in statistics

Model for the <u>c</u>onditional <u>p</u>robability <u>d</u>istribution

CPD: $Y_{X_i} = (Y|X_i) \sim N(\mu_{x_i}, \sigma^2)$

$Y_x \in \mathbb{R}$

$\mu_x \in \mathbb{R}$

μ_x is modeled

σ^2 is independent of the predictor values

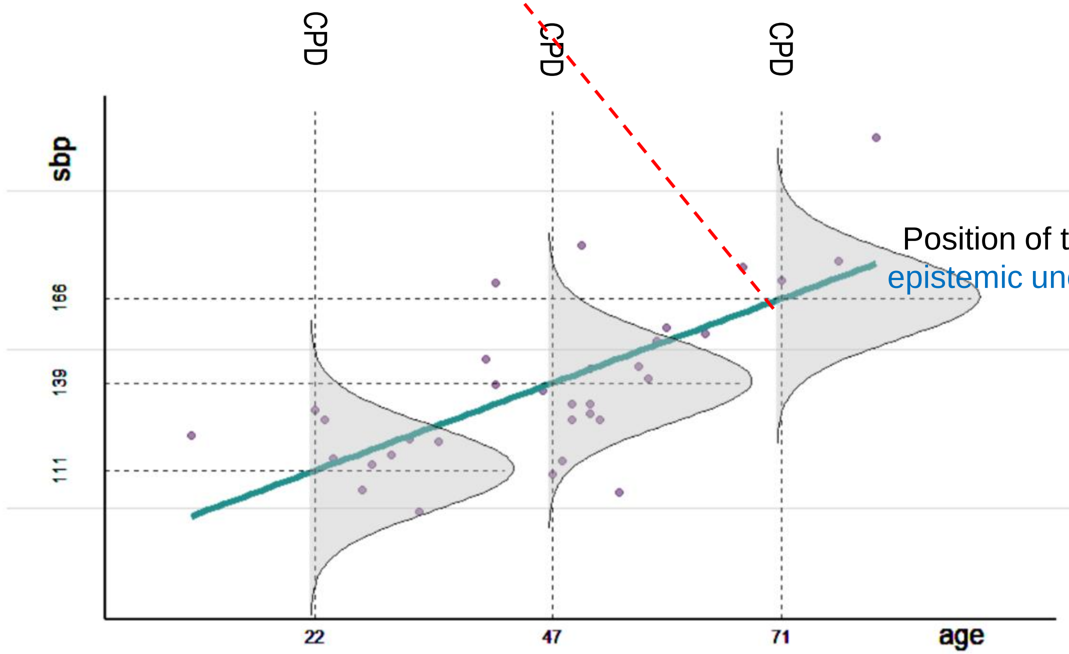
$$y_i = \beta_0 + \beta_1 \cdot x_{i1} + \varepsilon_i$$

$$E\left(Y_{X_i}\right) = \mu_{x_i} = (\mu|X=x_i) = \beta_0 + \beta_1 \cdot x_{i1}$$

$$\mathrm{Var}(Y_{X_i}) = \mathrm{Var}(Y|X_i) = \mathrm{Var}(\varepsilon_i) = \sigma^2$$

$$\varepsilon_i \text{ i.i.d.} \sim N(0, \sigma^2)$$

Variability of data: aleatoric uncertainty



Position of the line: epistemic uncertainty

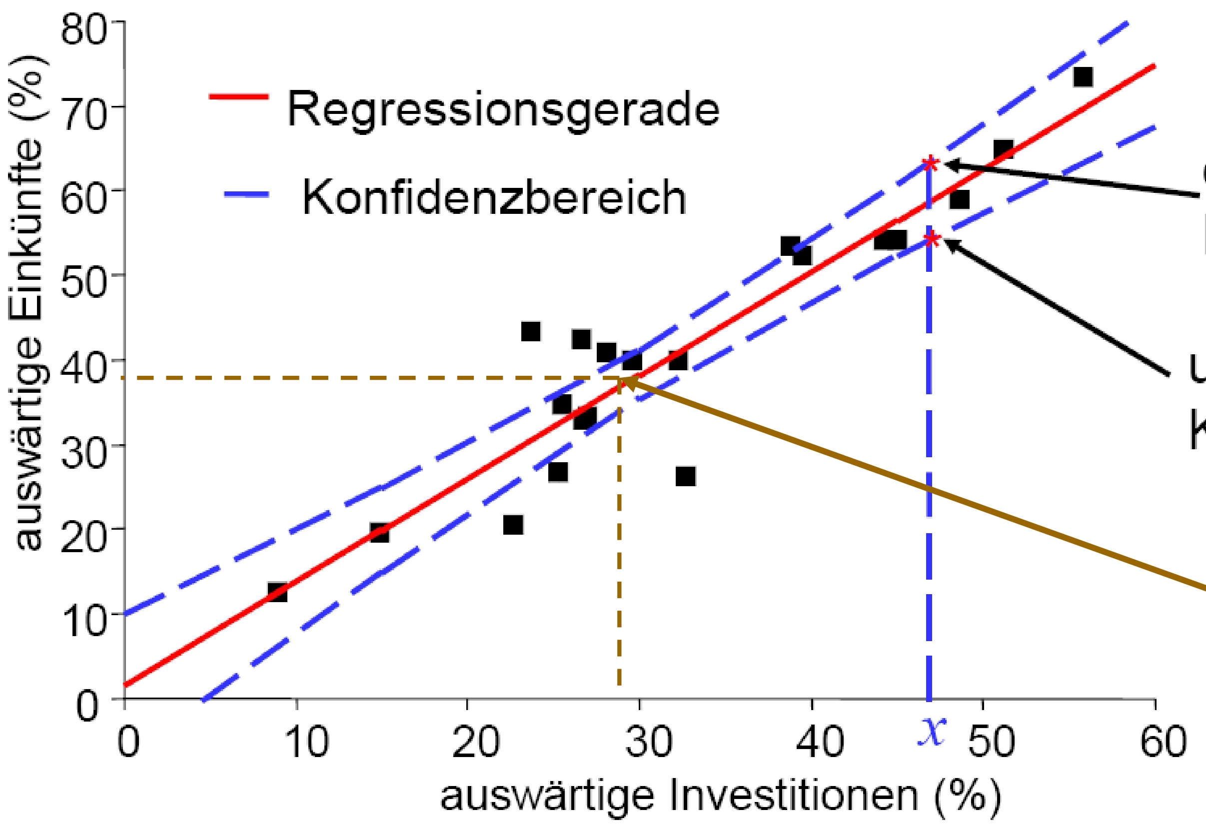
Confidence Interval quantifies epistemic uncertainty

Model for the conditional probability distribution

CPD: $Y_{X_i} = (Y|X_i) \sim N(\mu_{x_i}, \sigma^2)$

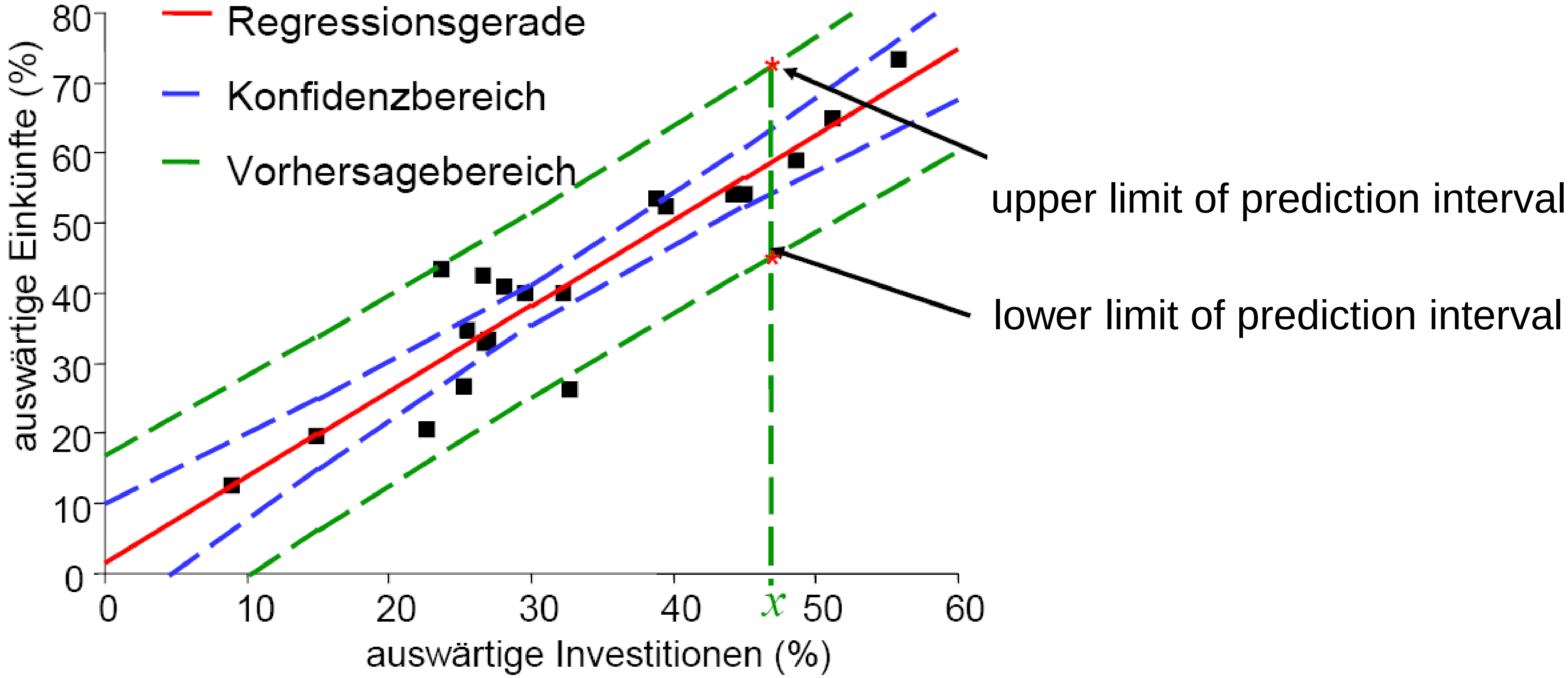
We can determine at each position x_i the confidence interval for μ_{x_i}

$$\hat{\mu}_{x_i} \pm q^{t_{n-2}}_{\alpha/2} \cdot se(\hat{\mu}_{x_i})$$



The fitted regression line runs always through the center of the data

Prediction Interval quantifies also aleatoric uncertainties



The confidence interval quantifies the uncertainty of the parameter μ
(“epistemic uncertainty“)

The prediction interval quantifies the variation of the data
(“ aleatoric uncertainty plus epistemic uncertainty“)

Confidence and Prediction Interval: Formula

$$Y_i = a + bX_i + \varepsilon_i$$

CI for μ

$$\hat{\mu}_x \pm q^{t_{n-2}}{}_{\alpha/2} \cdot se(\hat{\mu}_x)$$

$$se(\hat{\mu}_x) = \sqrt{\hat{\sigma}^2 \cdot \left(\frac{1}{n} + \frac{(x - \overline{x})^2}{\sum (x_i - \overline{x})^2}\right)}$$

epistemic uncertainty

CI for σ

$$\hat{\sigma} = \sqrt{\frac{1}{n-2} \sum_{i=1}^{n} r^2{}_i}$$

$$\hat{\sigma} \pm q^{t_{n-2}}{}_{\alpha/2} \cdot se(\hat{\sigma})$$

$$se(\hat{\sigma}) = \sqrt{\hat{\sigma}^2 \cdot \left(1 + \frac{1}{n} + \frac{(x - \overline{x})^2}{\sum (x_i - \overline{x})^2}\right)}$$

epistemic uncertainty

PI for y

$$\hat{\mu}_x \pm q^{t_{n-2}}{}_{\alpha/2} \cdot se(y_x)$$

$$se(y_x)^2 = se(\hat{\mu}_x)^2 + \hat{\sigma}^2$$

aleatoric uncertainty

Recap: Binary classification in statistics

CPD: $Y_{X_i} = (Y|X_i) \sim \mathrm{Ber}(p_{x_i})$

$Y_x \in \{0,1\}$, $p_x \in [0,1]$

$$\log\left(\frac{p_{x_i}}{1-p_{x_i}}\right) = \beta_0 + \beta_1 x_{i1}$$

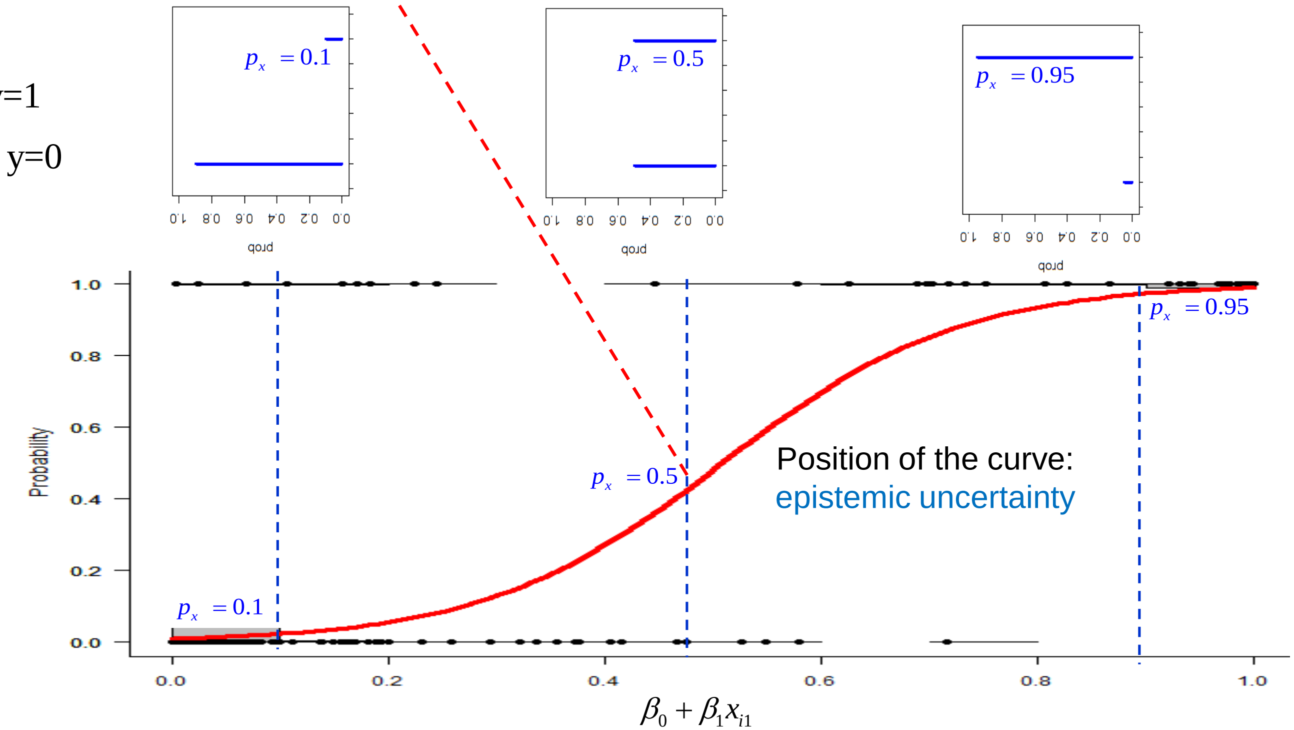
$$E(Y_{x_i}) = E(Y=1 \mid X = x_i) = p_{x_i} = \frac{e^{\beta_0+\beta_1 x_{i1}}}{1+e^{\beta_0+\beta_1 x_{i1}}}$$

$$\mathrm{Var}(Y_{x_i}) = p_{x_i} \cdot (1-p_{x_i})$$

Variability of data: aleatoric uncertainty

p_x is modeled

$$P(Y \mid X = x) = \begin{cases} p_x & , y=1 \\ 1-p_x & , y=0 \end{cases}$$



Bayes inference: linear regression

Model for the conditional probability distribution

CPD: $Y_{X_i} = (Y|X_i) \sim N(\omega_0 + \omega_1 X_i\ , \sigma^2)$

$\omega_0 \sim N(0, s^2_{\omega_0}),\ \omega_1 \sim N(0, s^2_{\omega_1}),\ \sigma^2 \sim N(0, s^2_{\sigma^2})$

before seeing data we set

$p(\omega)$ prior distribution

ω are the model parameter

In Bayes we assume that parameter come from a (prior) distribution.
We can sample parameter values and check possible realizations of models:

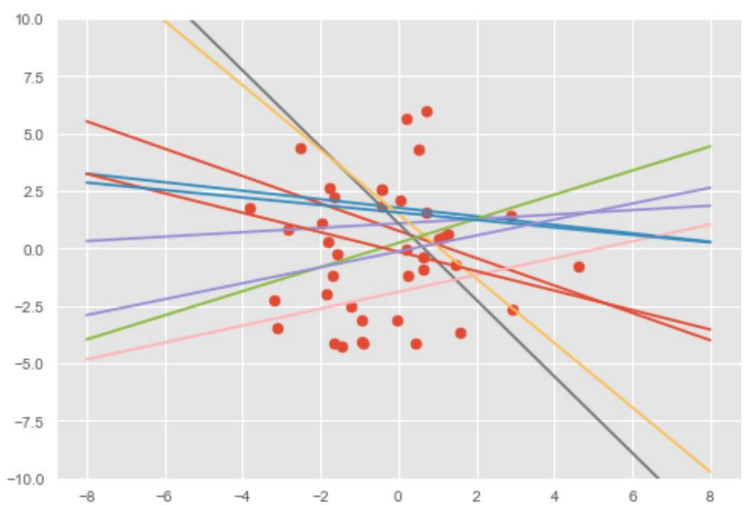


Image credits: to be added

Learning in the Bayesian framework

After we have seen some data

we can update the distribution of

the parameter

→ posterior distribution

likelihood prior

$$p(\omega\,|X,Y) = \frac{p(Y|\omega,X)\cdot p(\omega)}{p(Y|X)}$$

normalizer=marginal likelihood

$$p(Y|X) = \int p(Y|X,\omega)\cdot p(\omega)\,d\omega$$

We can capture the epistemic uncertainty by the interval in which 95% of all possible models are located.

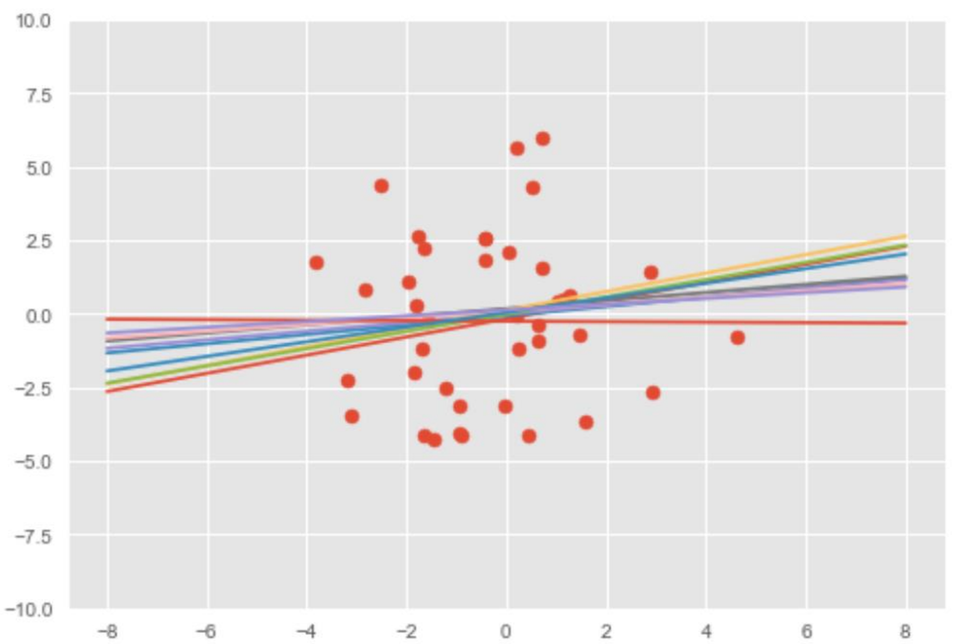


Image credits: to be added

Prediction with flexible Frequentist's vs Bayesian's models

Frequentist's strategy:
You can only use a complex model if you have enough data!

Bayesian's strategy:

Use the model complexity you believe in.

Do not just use the best fitting model.

Do use the full posterior distribution over parameter settings leading to vague predictions since many different parameter settings have significant posterior probability.

$$p\left(y^*|x^*,X,Y\right) = \int p(y^*|x^*,\omega)\cdot p\left(\omega\,|X,Y\right)d\omega$$

prediction via marginalization over ω:

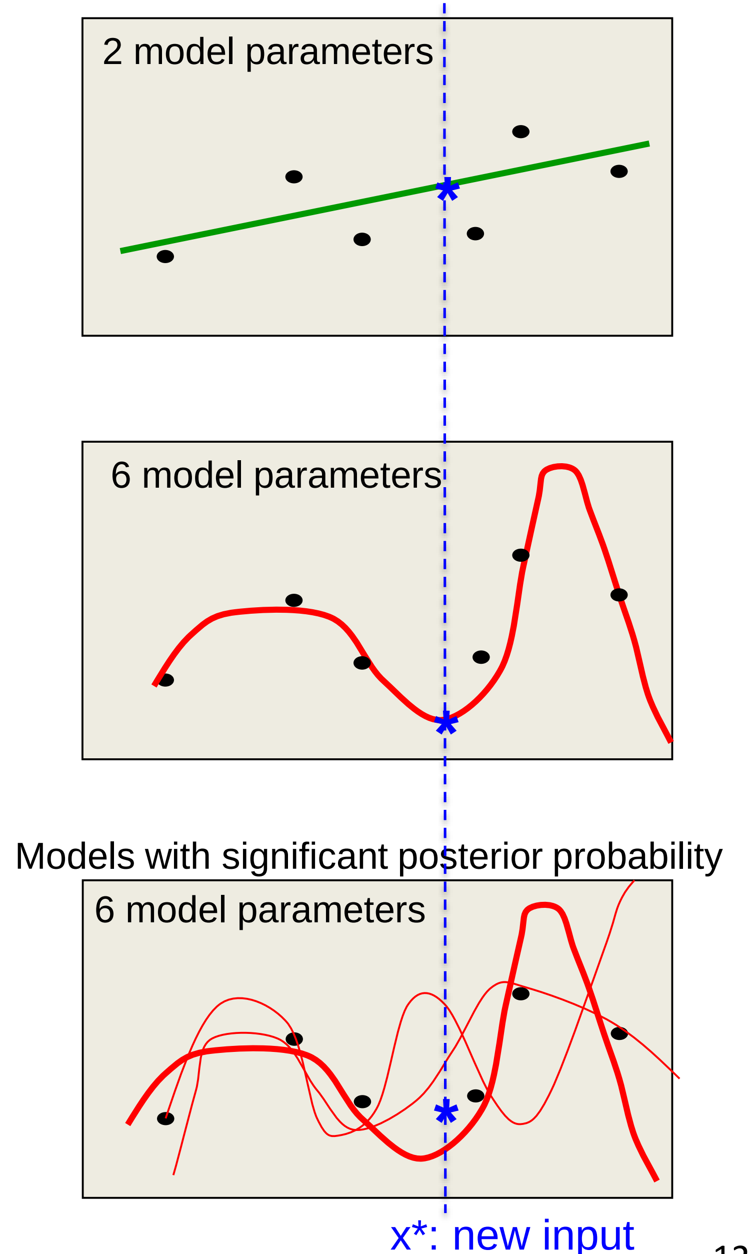


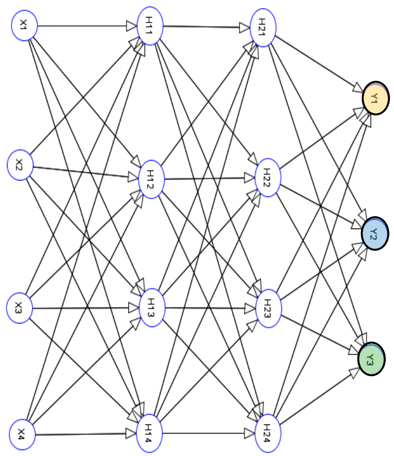
Image credits: Hinton coursera course

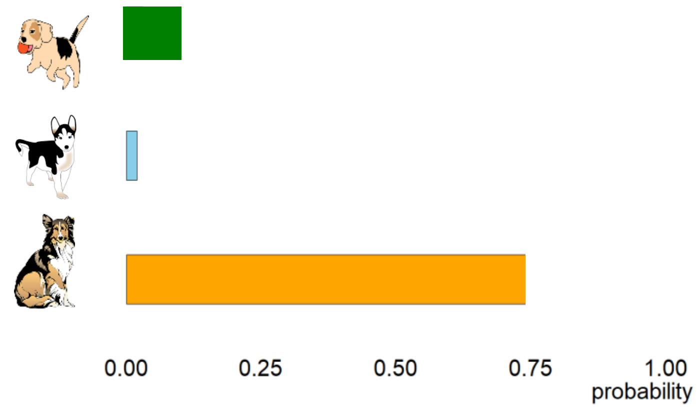
DL can also be used for regression and classification, but…

Can DL quantify uncertainty?

What do we get from a DL classification model?

Suppose you train a classifier to discriminate between 3 dog breeds





The prediction is “collie” because it gets the highest probability: p_{max}=0.75

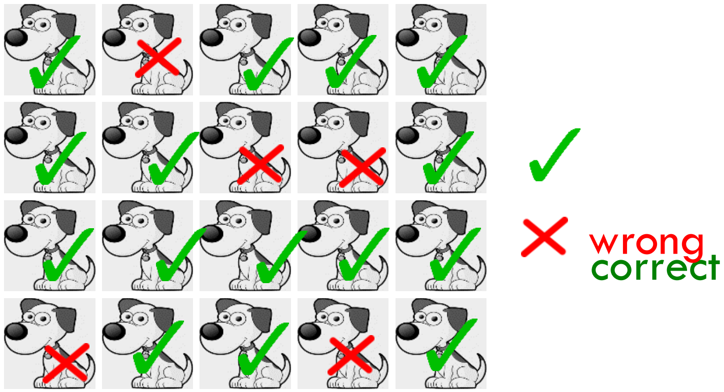
What is the probability telling?

p_{max}=0.75

Among many predications that had p_{max}=0.75, we expect that on average 75% of these predictions are correct and only 25% predictions are wrong

→ Then the classifier produces *calibrated probabilities*

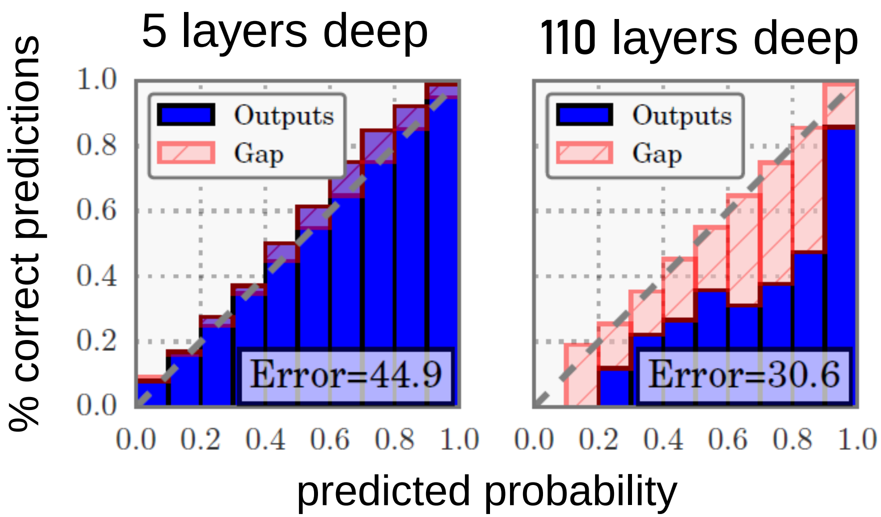
Sample of images where the predicted class got p=0.75:



Do CNNs produce calibrated probabilities?

Guo et al. (2017)
[On Calibration of Modern NN]

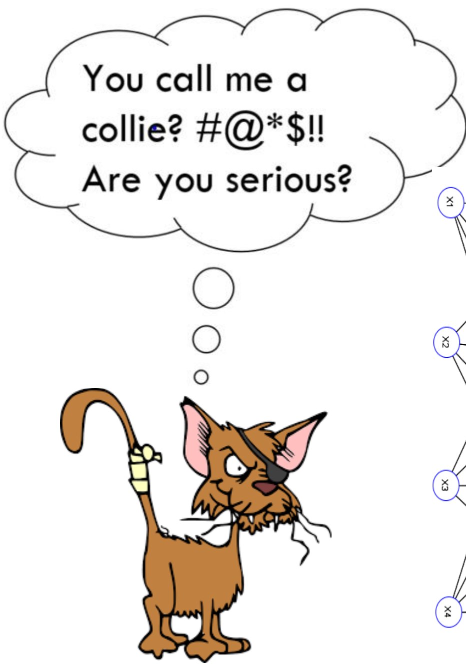
The deeper CNNs get
- the fewer miss-classifications
- the less well calibrated they get

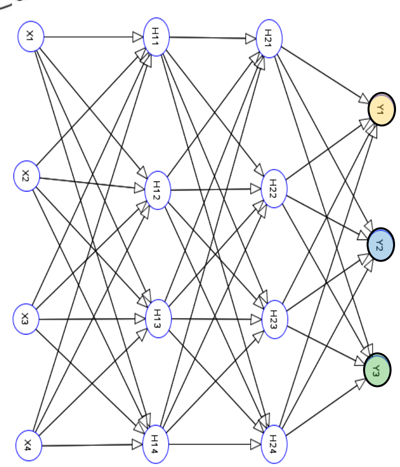


Good news:
deep NN can be "recalibrated" and then we get calibrated probabilities.

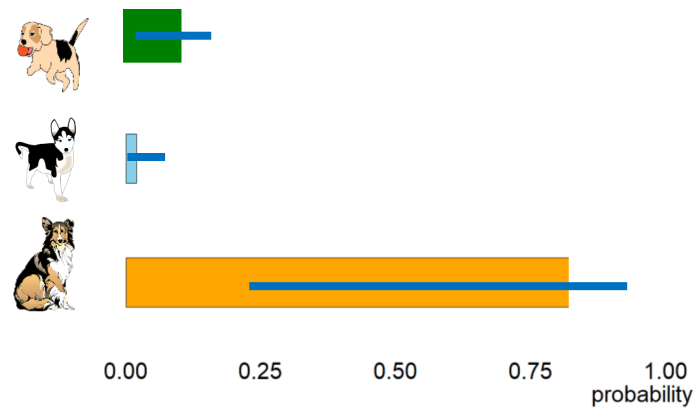
CNNs yield high accuracy
and calibrated probabilities, but...

What happens if a novel class is presented to the CNN?



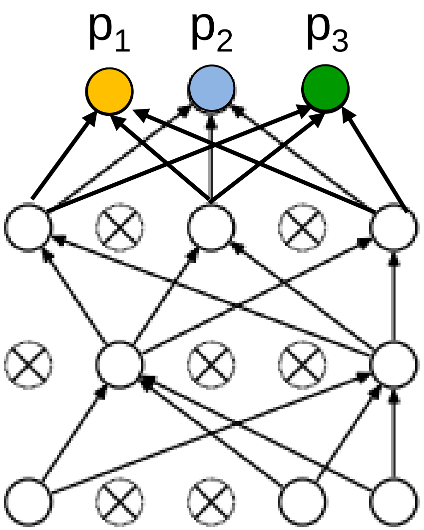


Plain wrong !



We need some error bars!

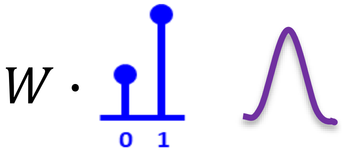
MC Dropout and Bayesian Neural Networks

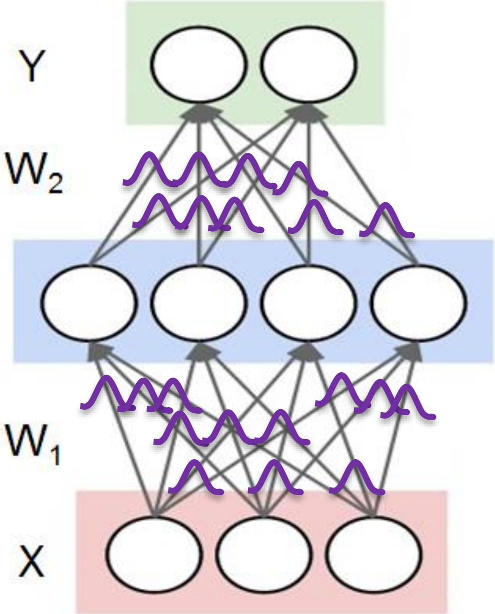


MC Dropout
Randomly drop nodes in each run
→ Ususally done during training

Dropout in test time

Yarin Gal* (2015): we learn a whole weight distribution



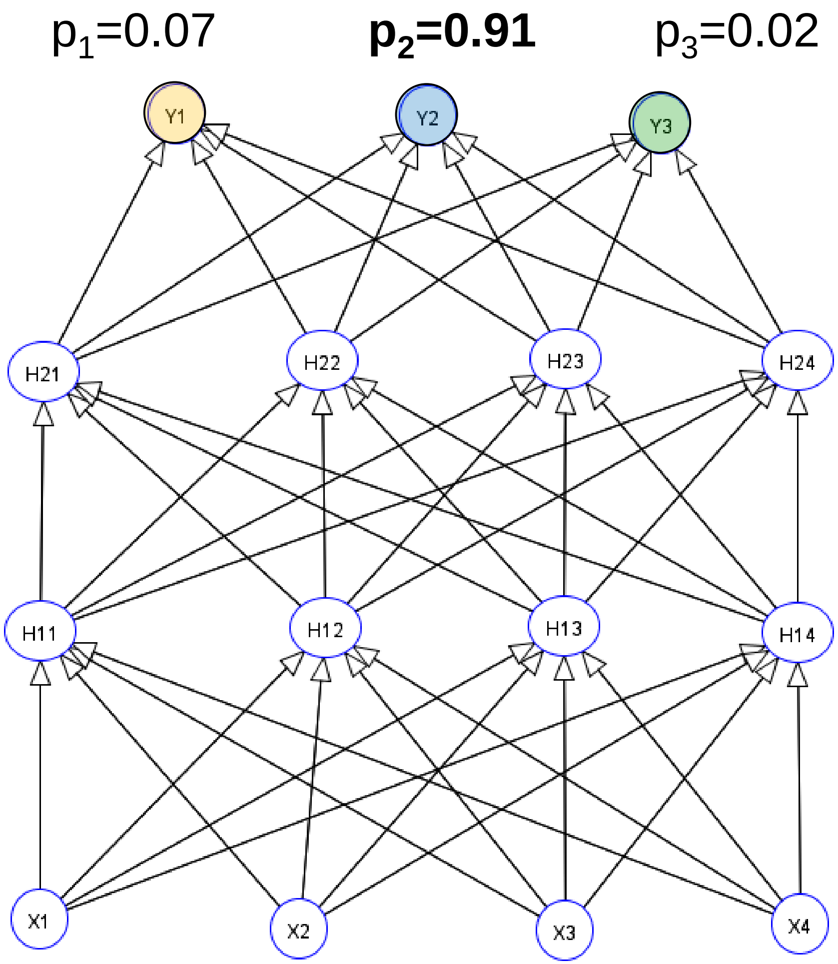


Bayesian NN

→ We should sample from weight distribution during test time

*Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning https://arxiv.org/abs/1506.02142

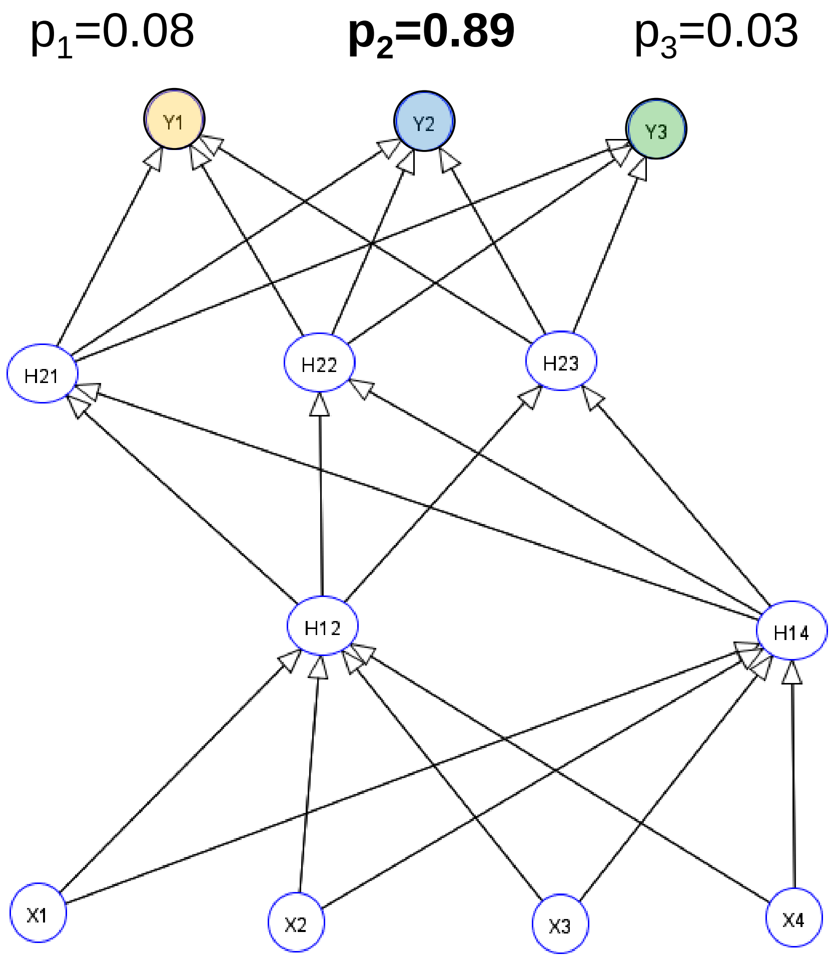
No MC Dropout

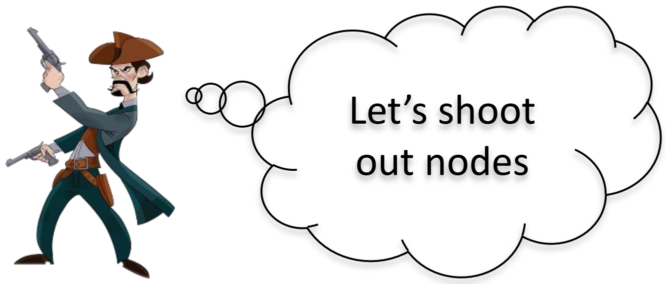


Probability of predicted class: $\mathbf{p_{max}}$

Input: image pixel values

Use dropout at test time: Run 1

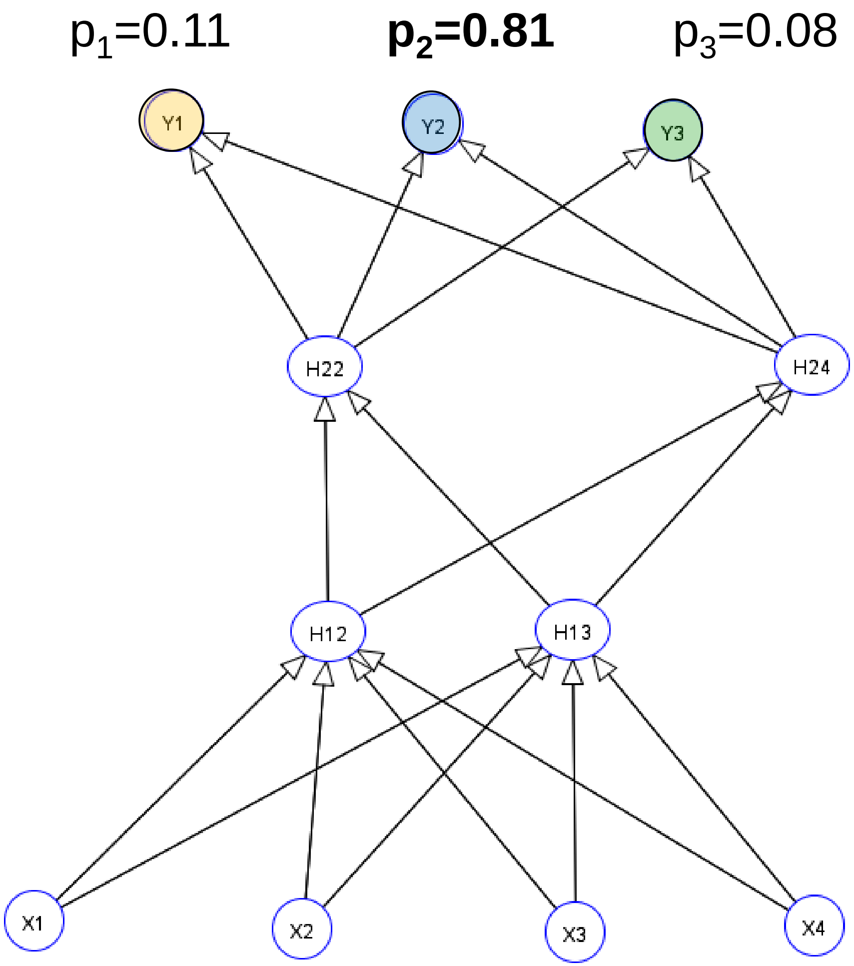


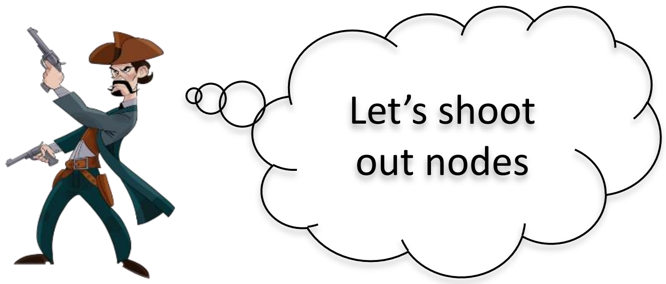


Stochastic dropout of units

Same input image

Use dropout at test time: Run 2

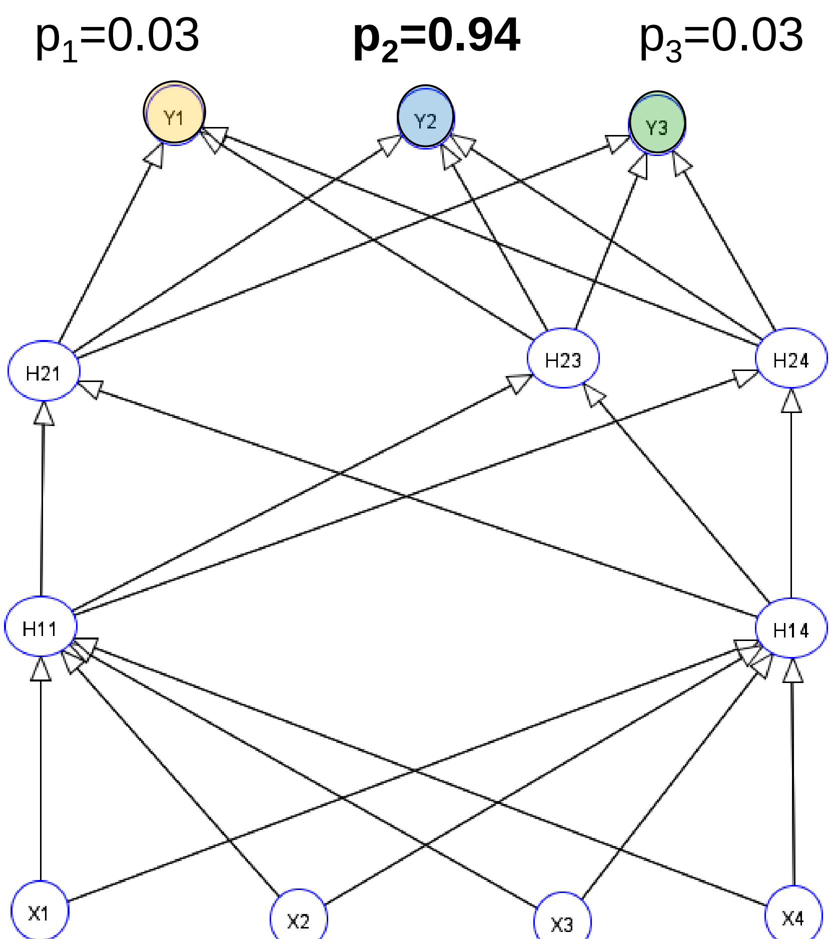


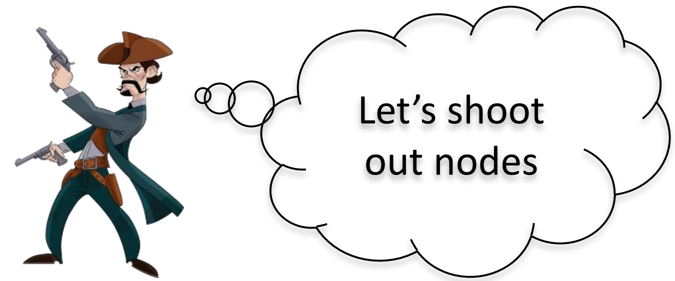


Stochastic dropout of units

Same input image

Use dropout at test time: Run 3

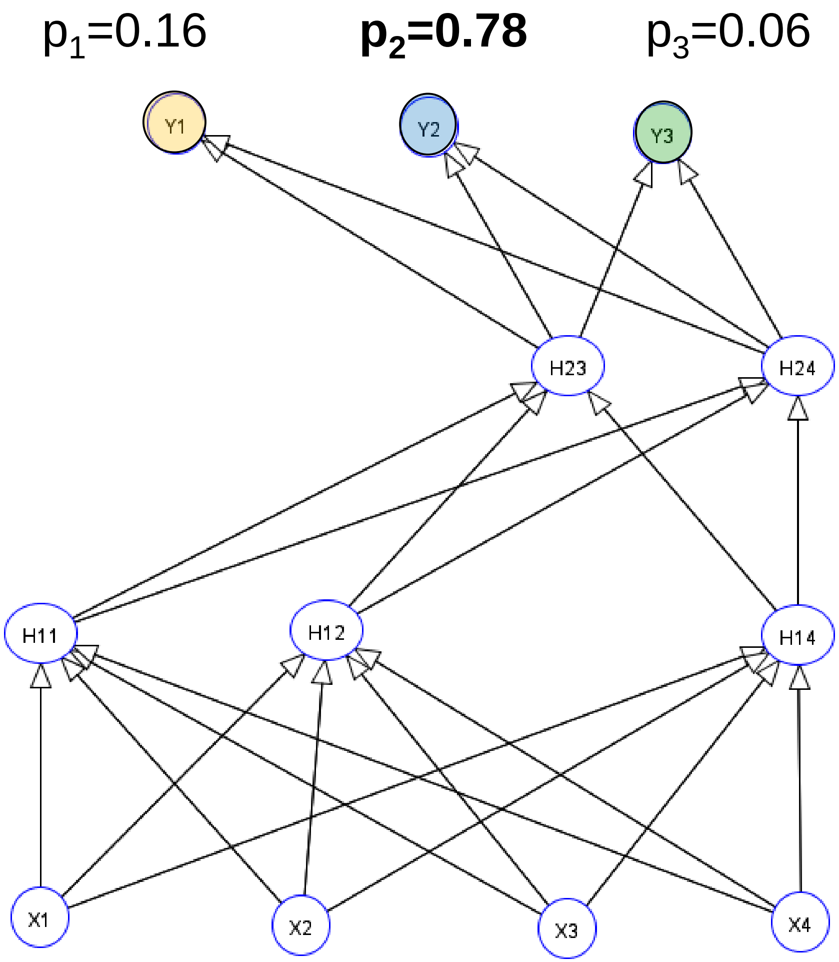


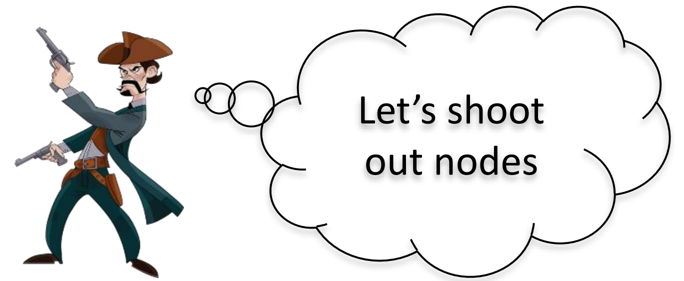


Stochastic dropout of units

Same input image

Use dropout at test time: Run 4



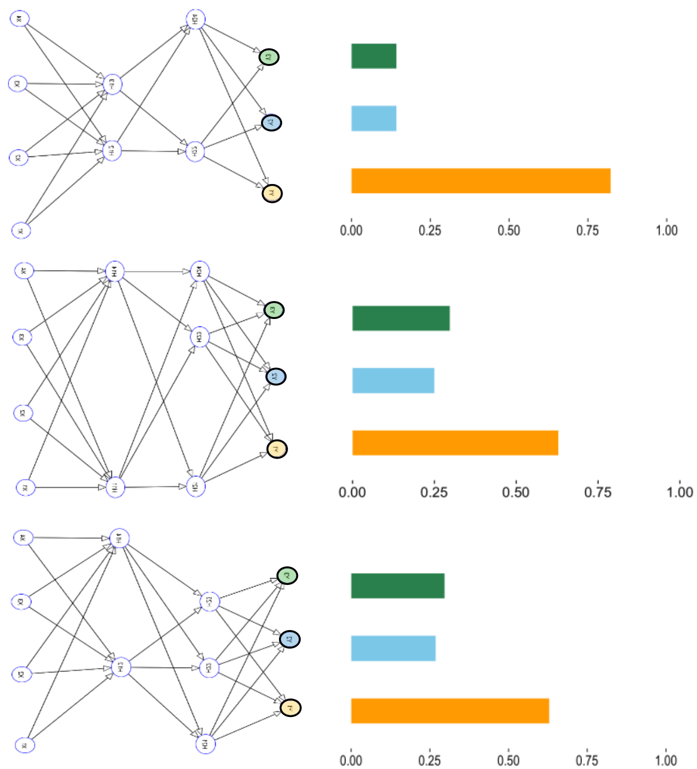


Stochastic dropout of units

Same input image

MC probability prediction

Many Dropout Runs in forward pass



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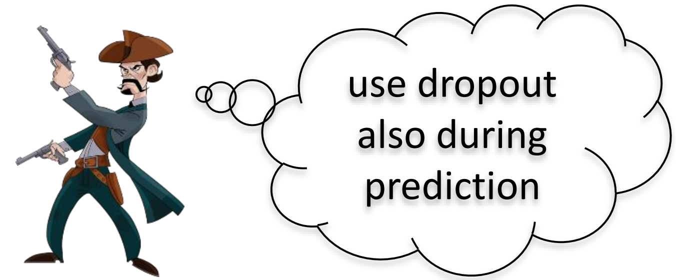
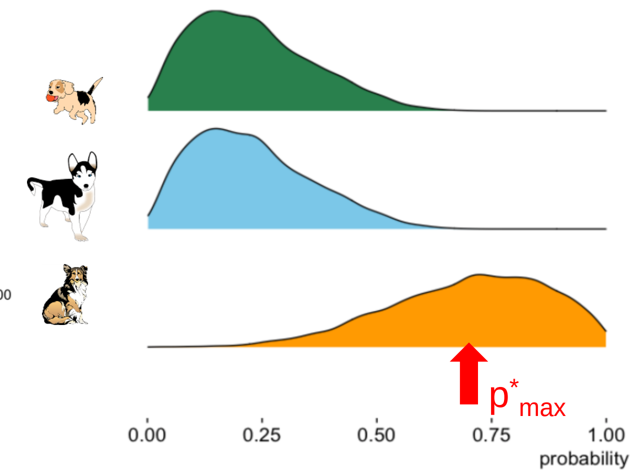




CNN predicts class
“collie”
but with high uncertainty

Remark: Mean of marginal give components of mean in multivariate distribution.

What to get from the MC* probability distribution

The center of mass quatifies the predicted probablilty

p^*_{max}

The spread quantifies in addition the uncertainty of the predicted probability

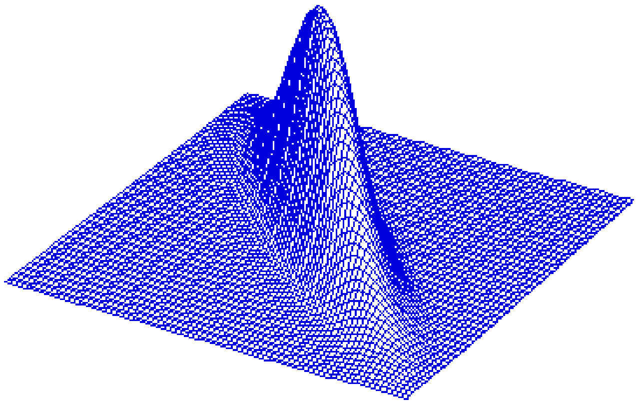
σ^* total standard deviation

PE^* entropy,

MI^* mutual information

VR* variation ratio

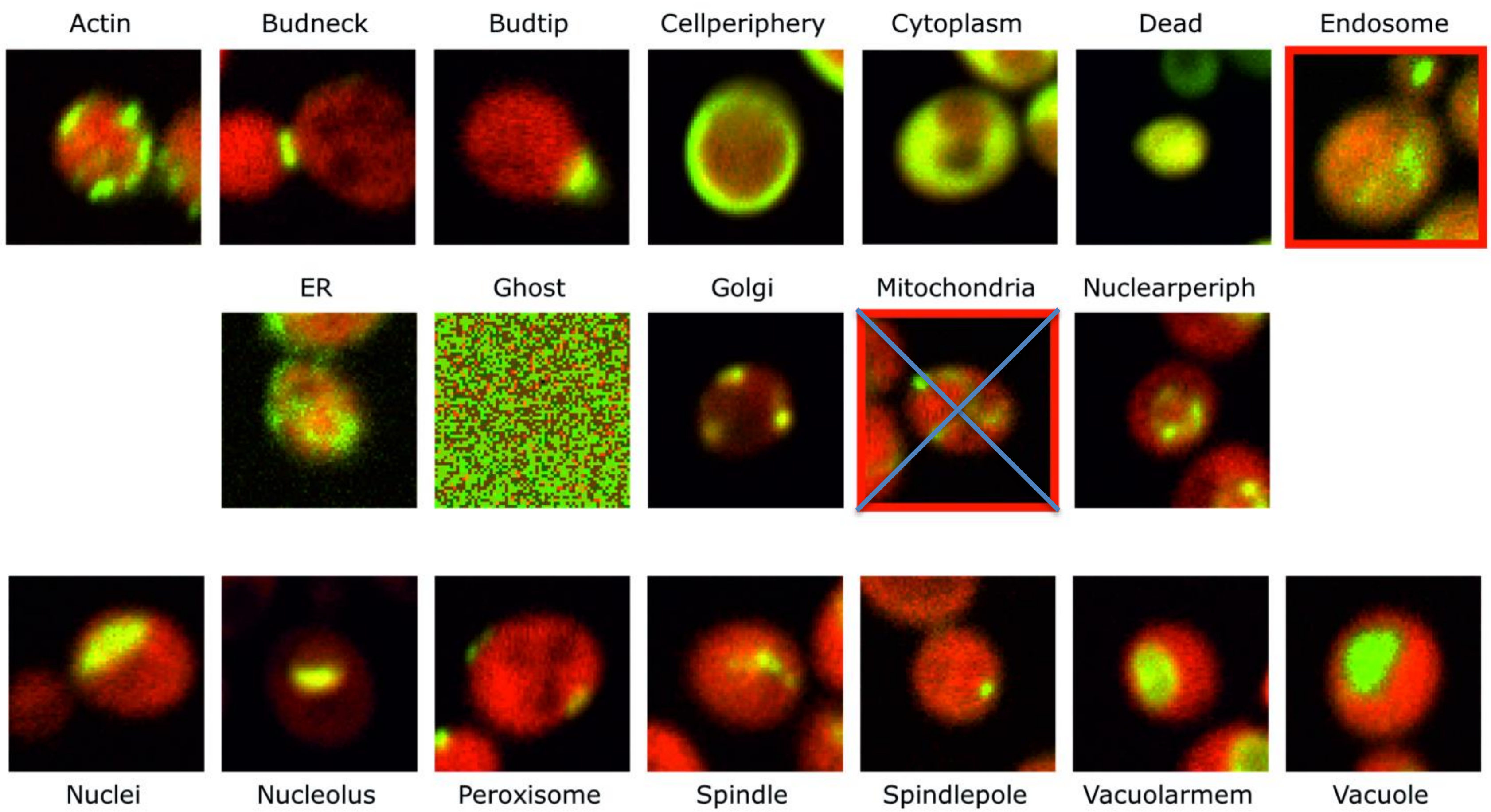
f* vote ratio



Remark: to go from image to patient level we use the average of all measures as baseline

Evaluate method on some real data

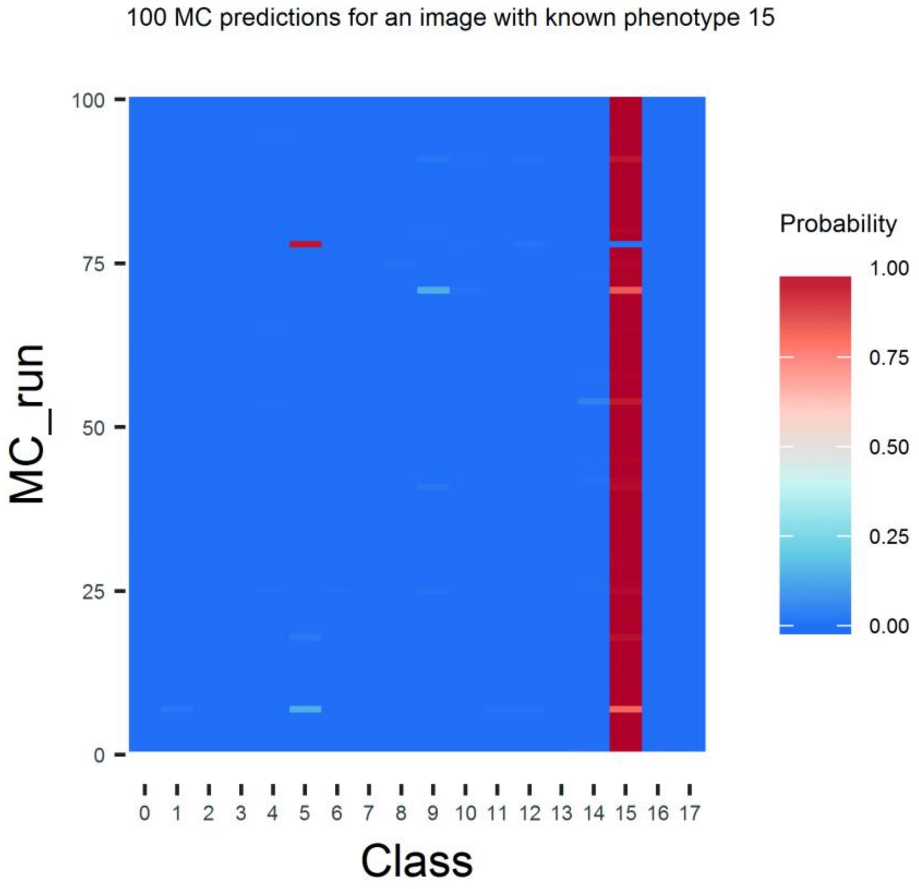
Experiment with unknown phenotype



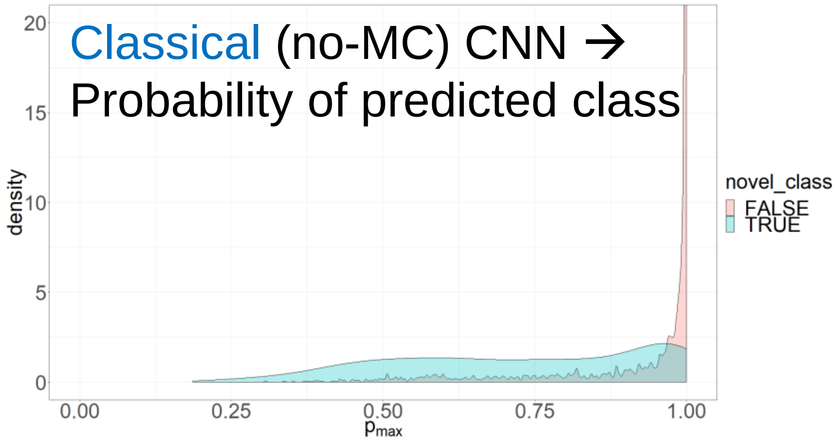
Dürr O, Murina E, Siegismund D, Tolkachev V, Steigele S, Sick B. Know when you don’t know, Assay Drug Dev Technol.

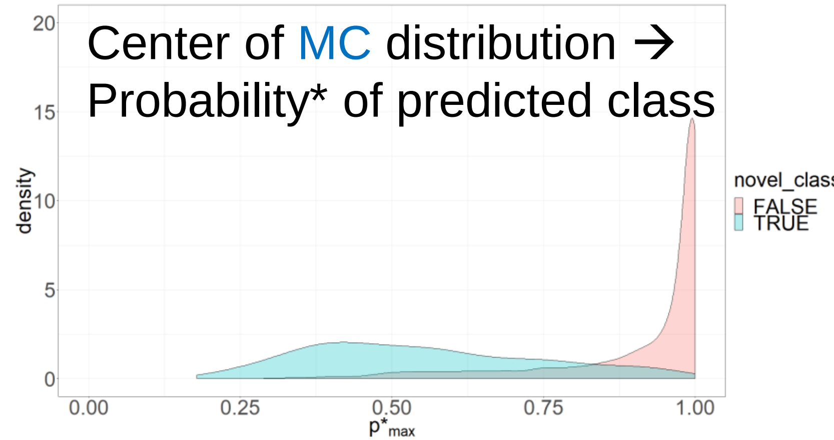
Probability distribution from MC dropout runs

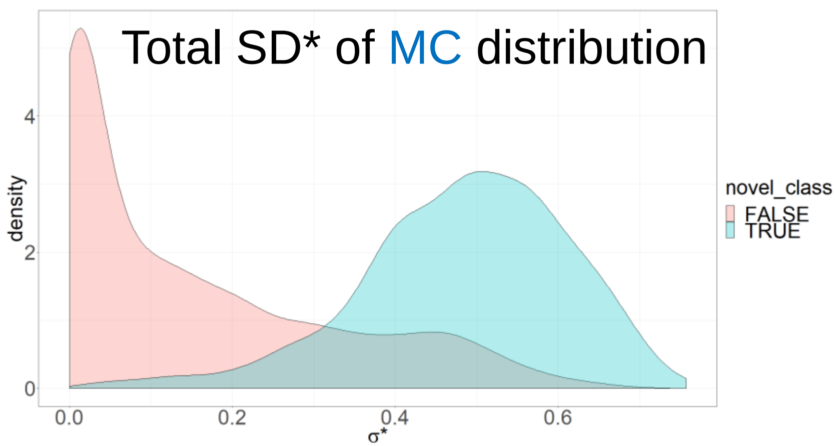
Image with known class 15

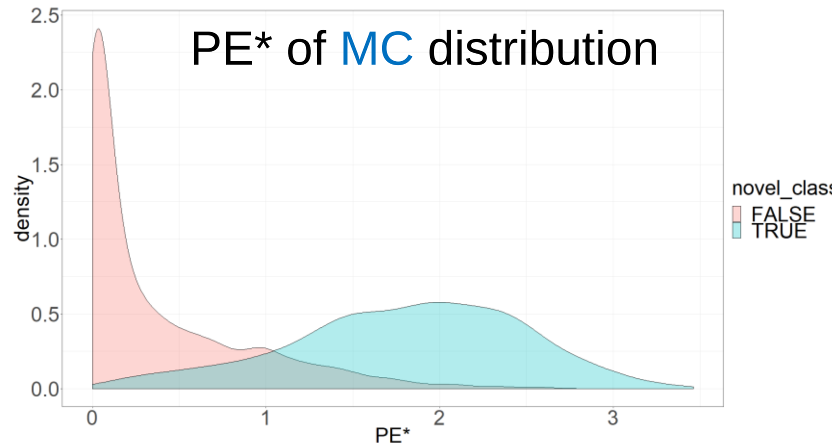


Do known/novel classes yield different values for probability and uncertainty measures?

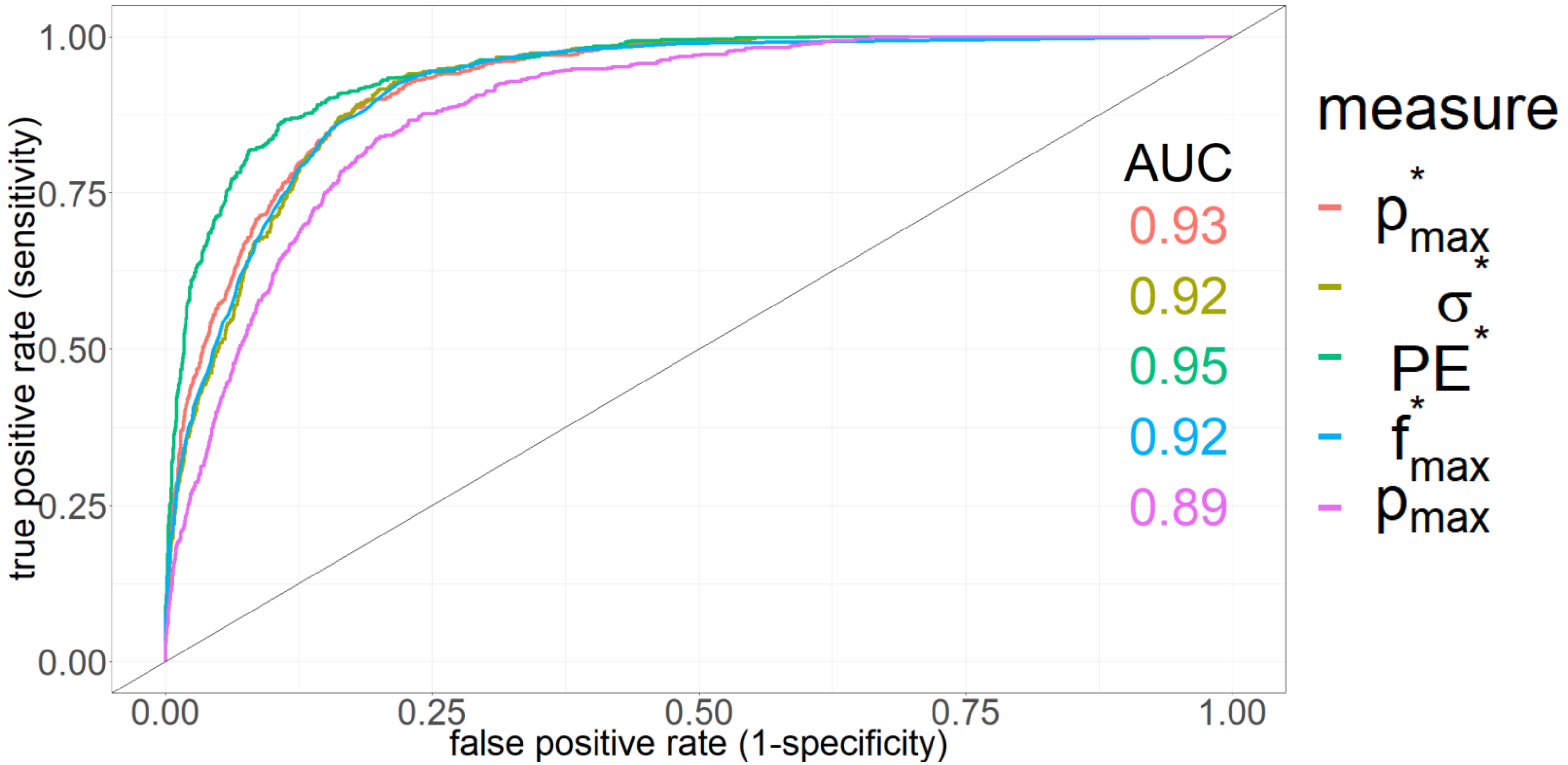








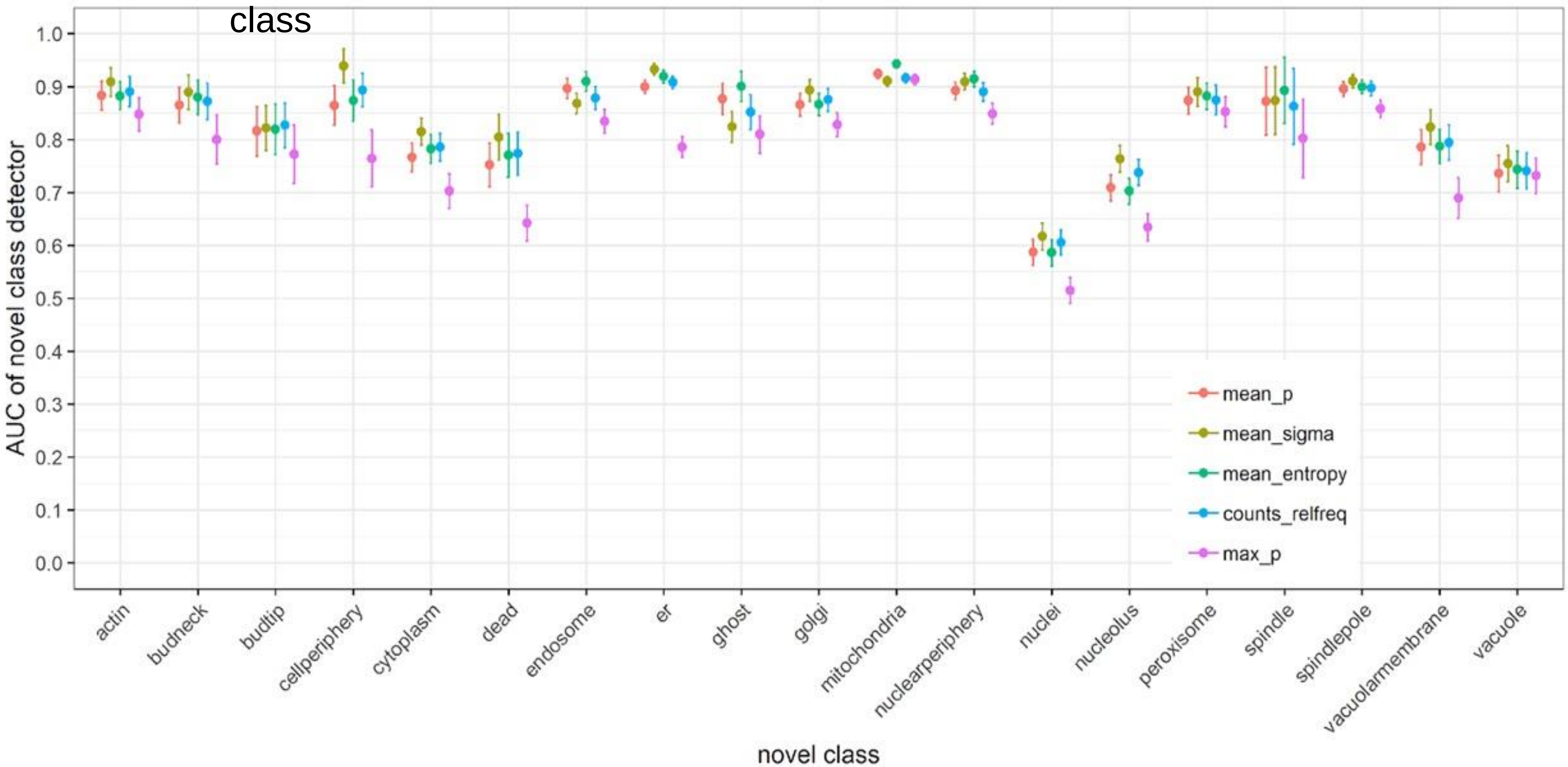
How good are novel/unusual classes identifiable?



All **MC Dropout based appoaches are superior compared** to the non-MC approach.

Dropout uncertainty measures outperform traditional CNN probability

CV experiment where each phenotyp is once in the role of the novel class



Creating custom layers in keras

```
keras.layers.Dropout(0.5)(x, training=True)
```

Or define a lambda layer which does the trick:

```
from keras.layers.core import Lambda # needed to build the custom layer
from keras import backend as K #Now we have access to the backend (could be tensorflow,
```

Define your custom function

```
def mcdropout(x):
  #return tf.nn.dropout(x=x, keep_prob=0.33333) #using TensorFlow
  return K.dropout(x, level=0.5) # beeing agnostic of the backend
```

Here you could do anything possible in TF
`tf.add(x, 10)`
…

Include your custom function as a layer

```
model = Sequential()
model.add(Lambda(mcdropout, input_shape=(5,)))
#model.add(Dense(10))
#... Usually you would have many more layers
model.compile(loss='categorical_crossentropy',optimizer='adam')
```

https://github.com/oduerr/dl_tutorial/blob/master/tensorflow/keras/using_tf_in_keras.ipynb

Conclusion

MC Dropout during test time

→ yields uncertainty measures for each individual classification

→ helps to identify uncertain cases

→ allows to indicate novel classes

→ yields new probability estimates leading to higher accuracy