# Machine Intelligence:: Deep Learning
# Week 7

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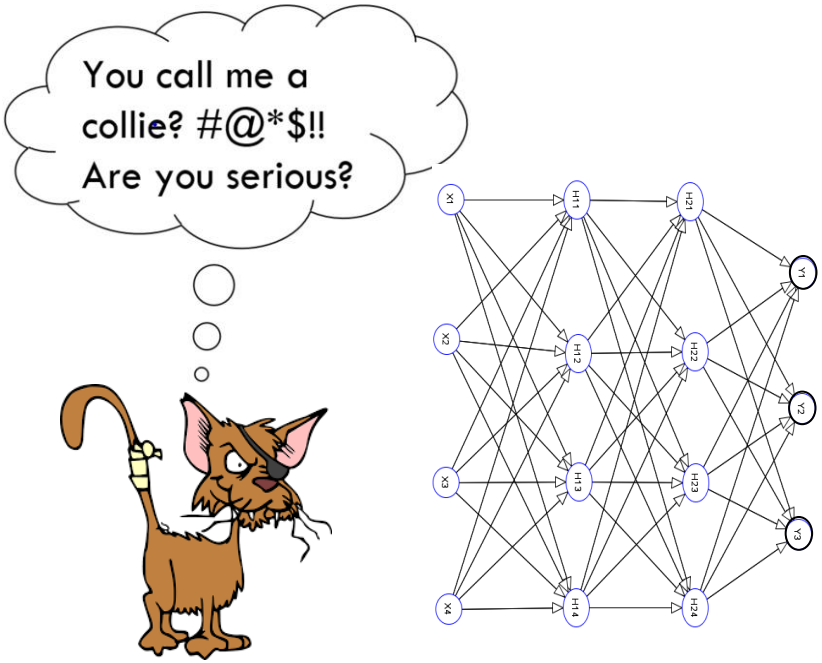
Ensembling approaches for improving the performance and uncertainty estimates of NN models by taking into account the algorithmic epistemic uncertainty.

# Outline:

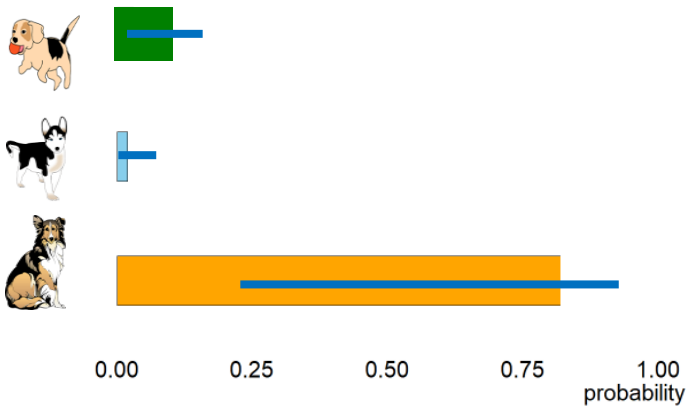
- Bayes
  - Motivation of Bayesian Models
  - Bayes the Hackers way
  - Approximative Bayes via Variational Inference
  - Pseudo approximative Bayes via MC Dropout

# A non-Bayesian NN cannot ring the alarm

**What happens if we present a novel class to the CNN?**




**Plain wrong !**




**We need some error bars!**

# Recall some points on uncertainty from last lecture

- We have different uncertainty components when working with NN
  - Model choice uncertainty
    - which model/architecture should we use?
  - Aleatoric uncertainty = data inherent variablilty
    - We capture aleatoric uncertainty by the spread of the predicted conditional probability distribution, e.g. Variance/Entropy for numeric/categorial data
  - Algorithmic uncertainty
    - Training twice the same NN-architecture with the same data does not yield the same trained model
    - Random intialization, random mini-batch splits, random augmentation
  - Epistemic uncertainty
    - The lack of knowledge due to a lack of information, such as too few data or a lack of understanding leading to the wrong model choice

- Deep Ensembling is always good to get a better model
    - Better prediction performance: The NLL of an ensemble is better or equal than the mean NLL of the members
    - We can quantify the algorithmic uncertainty of the model

# Bayesian Neural Networks

# Bayesian modeling does also kind of ensembling

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

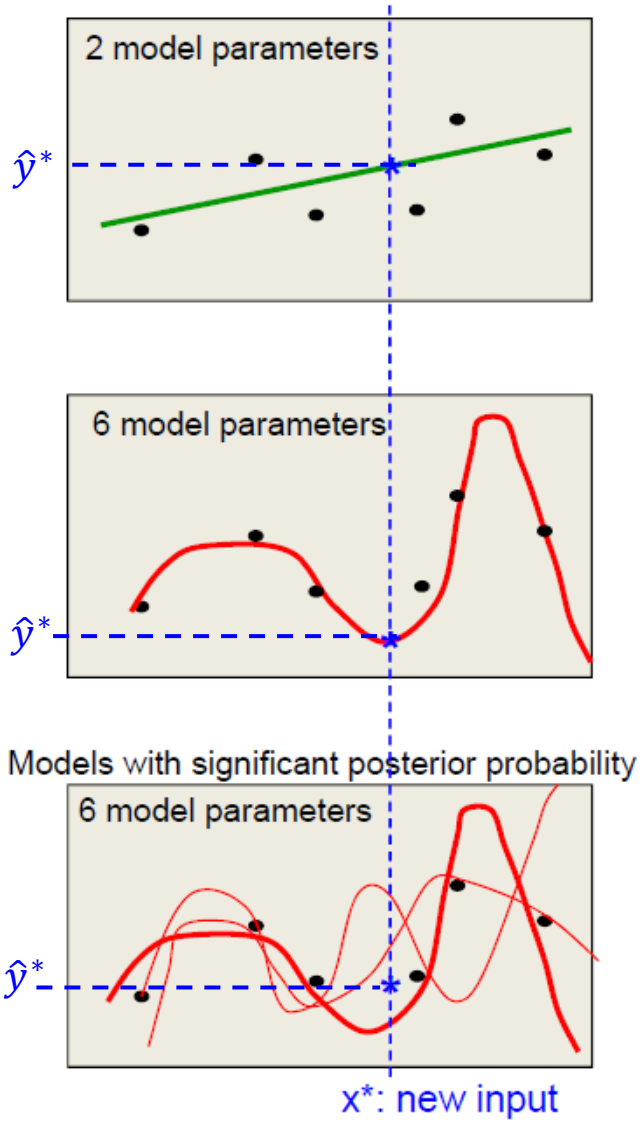
**Bayesian's strategy:**
Use the model complexity you believe in.

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.

$$p(Y|x^*, D) = \int p(y|x^*, \theta) \cdot w(\theta)\ d\theta$$

$\hat{y}^*$=E(Y|x*,D)




Weighted average of different predictions
the weights are the «posteriors of the the parameters» tuned w.r.t. the train data

# Bayesian statistics

- The Bayesian Theorem

$$P(A|B) = \frac{P(B|A)P(A)}{P(B)}$$

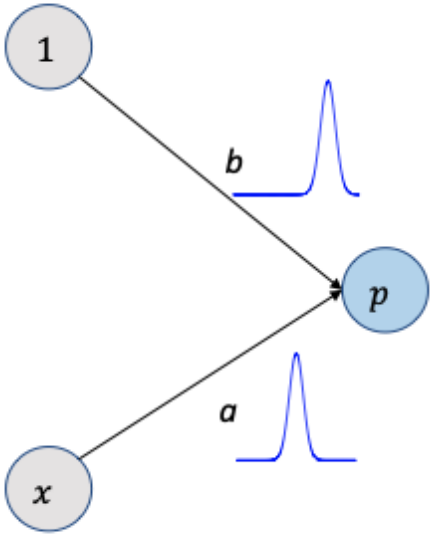
- Applied to $A = \theta$ and $B = D$
  - Parameters $\theta$ of a model e.g. weights *w* of NN
  - Training data *D*

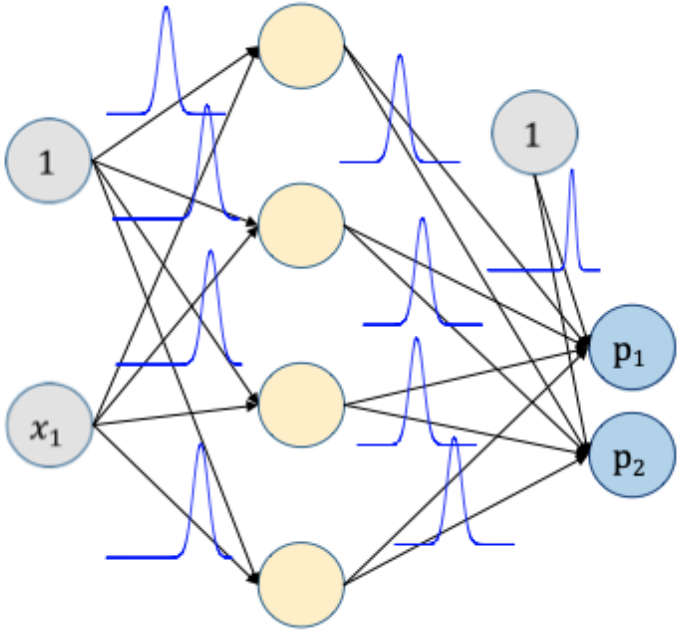
$$p(\theta|D) = \frac{p(D|\theta)p(\theta)}{p(D)}$$

  - $p(\theta|D)$ posterior or the model parameters $\theta$ after seeing the train data D
  - $p(D|\theta)$ likelihood of the train data D
  - $p(\theta)$ prior or the model parameters $\theta$ before seeing any data
  - $p(D)$ evidence (just a normalization constant)

# Bayesian Neural* Networks (BNN)

- In a fitted Bayesian Model, such as a Bayesian NN, the parameters (weights) are not fixed numbers but come from a (posterior) distribution

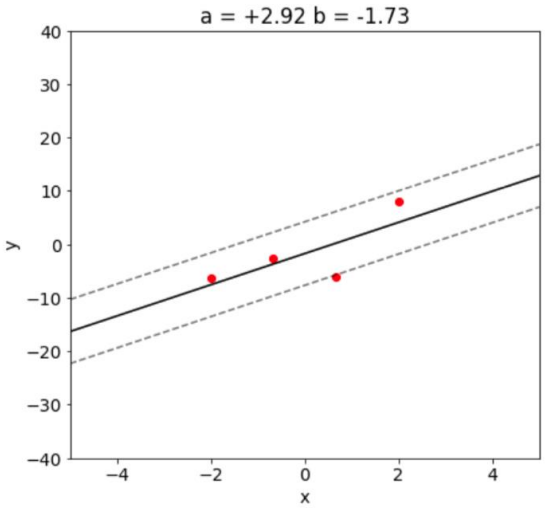


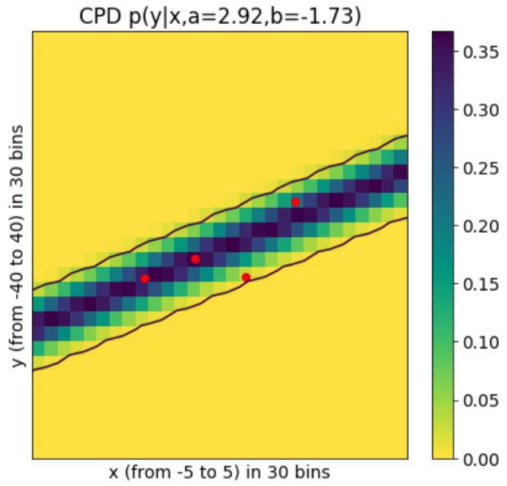




*Don't confuse Bayesian Networks (DAGs) with Bayesian Neural Networks

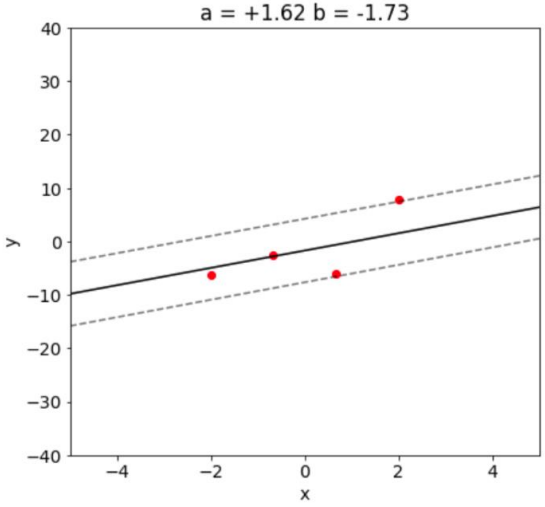
# Bayes the hackers' way

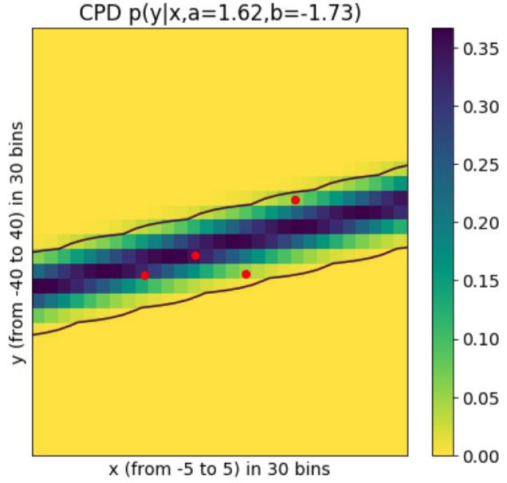
Let's look at good old linear regression to understand the gist of the Bayes idea. Assume $\sigma = 3$ to be known.




With parameter values $(a_{ML}, b_{ML})$ yielding the maximial likelihood for train data (usual way)

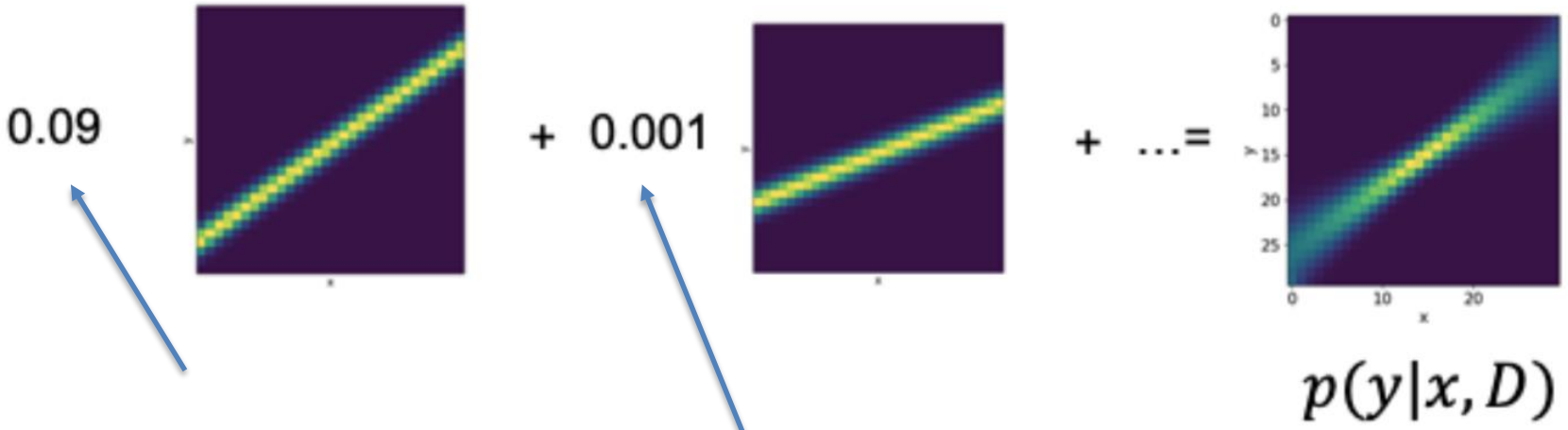



With parameter values $(a, b)$ yielding a slightly smaller likelihood for train data

# Combining different fits to get the conditional predictive distribution for $(Y|\mathbf{x})$ given the model was trained on $\mathbf{D}$

Also take the other fits with different parameters into account and weight them




Hightest weight for MaxLike

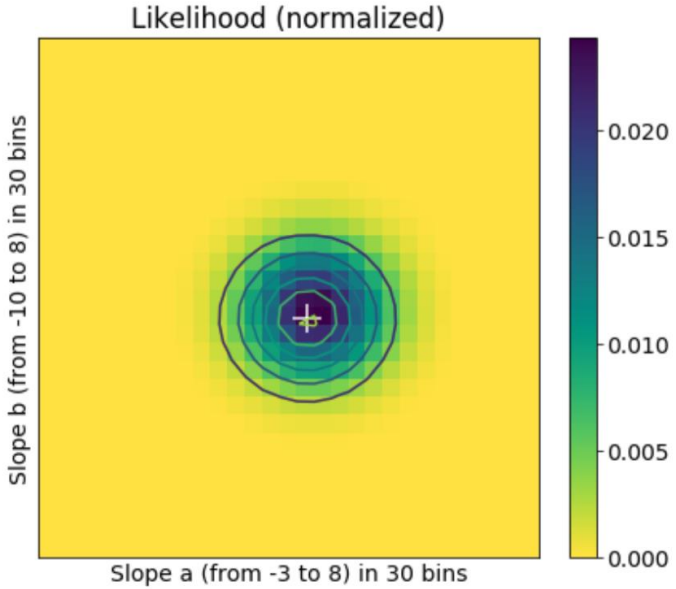
Less likely solutions get a smaller weight

Question: How to get the weight?

Idea: use the (normalized) likelihood $p_{\mathrm{norm}}(D|(a,b))$ as weights !

# Don't put all egg's in one Basket

- Also take other solutions for parameters $a$, $b$ into account




$$p_{\text{norm}}(D|(a,b)) = \frac{p(D|(a,b))}{\sum_w p(D|(a,b))}$$

Normalized likelihood $p_{\text{norm}}(D|(a,b))$ serve as weights

$$\mathrm{p}(y|x,D) = \sum_a \sum_b p(y|x,(a,b)) \cdot p_{\text{norm}}(D|(a,b))$$

Likelihood at 30x30 different positions of a and b. Normalized to be one.

https://github.com/tensorchiefs/ dl_book/blob/master/chapter_07 /nb_ch07_02.ipynb

# Resulting condtional posterior predictive distribution

$$\mathrm{p}(y|x, D) = \sum_a \sum_b p(y|x, (a, b)) \cdot p_{\mathrm{norm}}(D|(a, b))$$

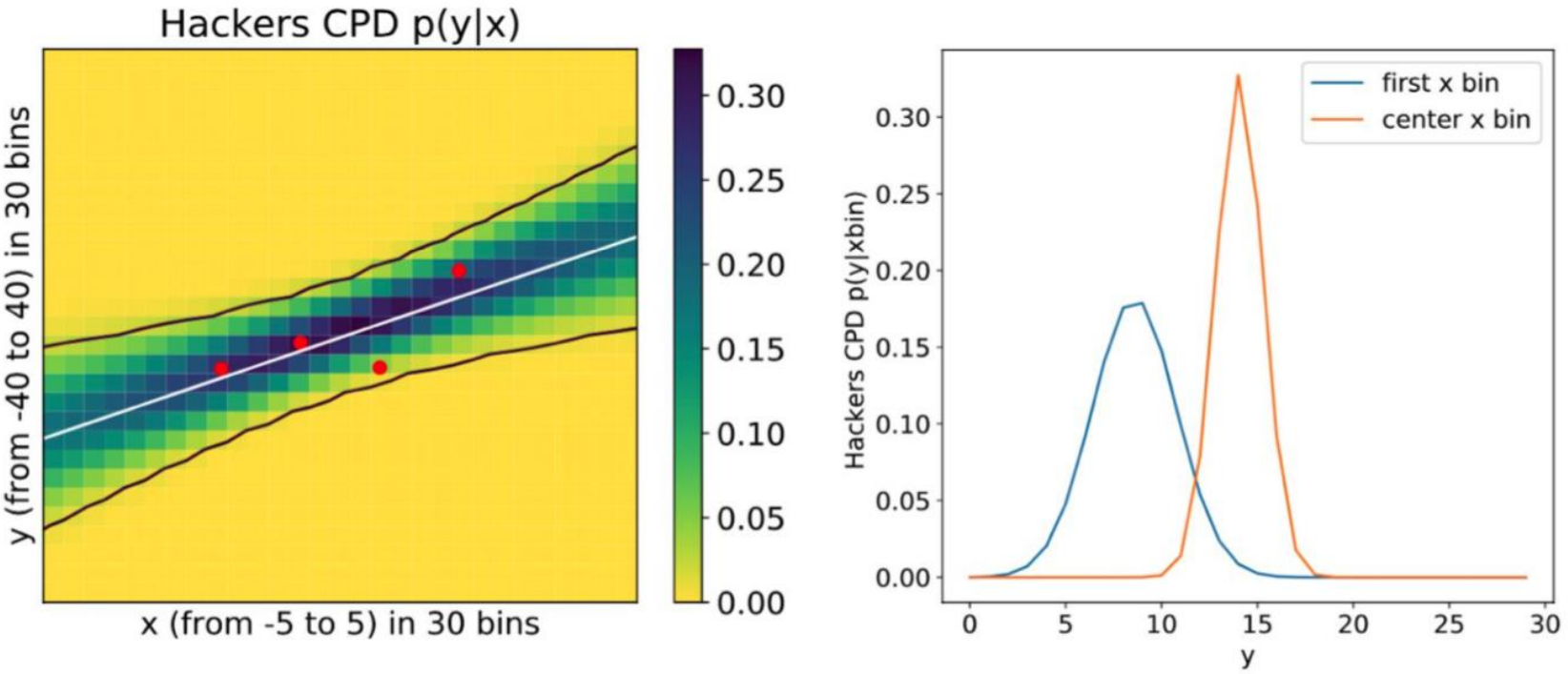
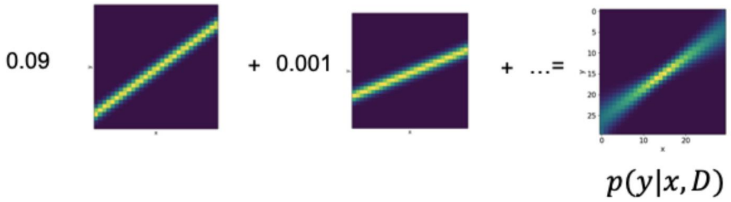



**Figure 7.6 The predictive distribution for the Bayesian linear regression model, trained with the four data points shown on the left side by the color-code and on the right as conditional distribution at two different *x* positions. You can clearly see that the uncertainty gets larger when leaving the *x*-regions where there's data.**

# Revisiting the Hackers' example: Get Bayesian predictive posterior as ensemble by weighted averaging different models




$p(y|x, D)$

- Hacker's way

weight

$$\mathrm{p}(y|x, D) = \sum p(y|x, w) \cdot p_{\mathrm{norm}}(D|w) = \sum p(y|x, w) \cdot \frac{p(D|(a,b))}{\sum_w p(D|(a,b))}$$

- Bayes

weight

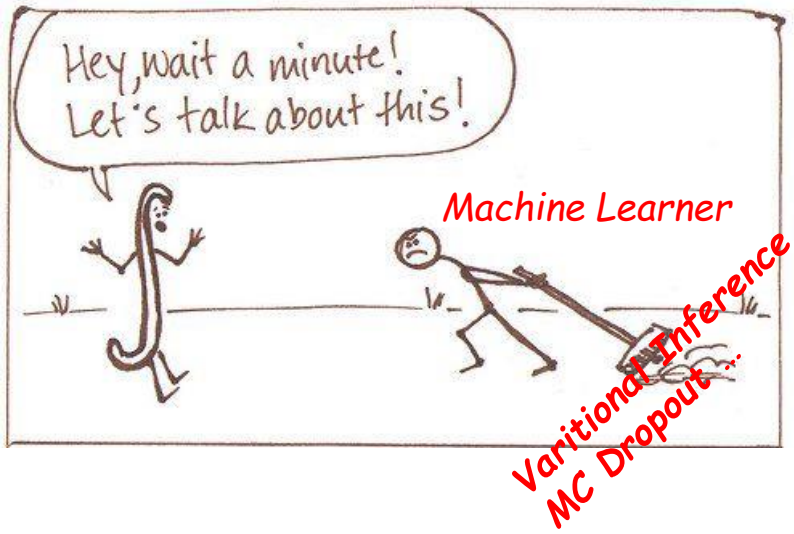
$$\mathrm{p}(y|x, D) = \sum_w p(y|x, w) \cdot p(w|D) = \sum_w p(y|x, w) \cdot \frac{p(D|w)p(w)}{\sum_w p(D|w)p(w)}$$

→ The Hacker's way is Bayes, if we assume a uniform prior $p(w) = \mathrm{const}$

# Computing the posterior can get difficult due to $\int_\theta$

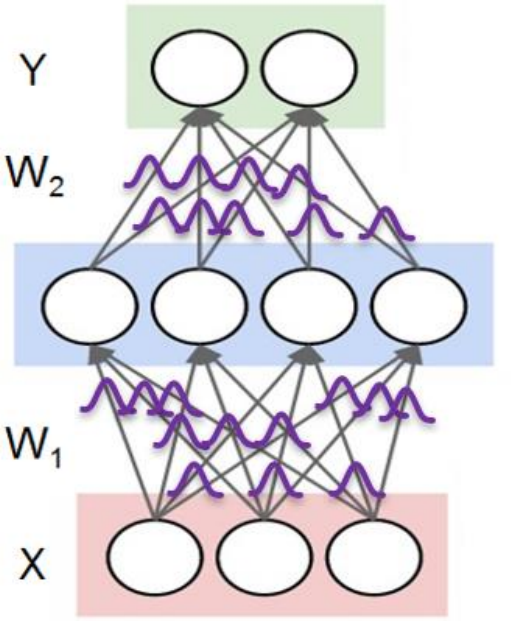
Posterior : $p(\theta|D) = \frac{p(D|\theta)p(\theta)}{p(D)} = \frac{p(D|\theta)p(\theta)}{\int_\theta p(D|\theta)p(\theta)d\theta} \sim p(D|\theta)p(\theta)$

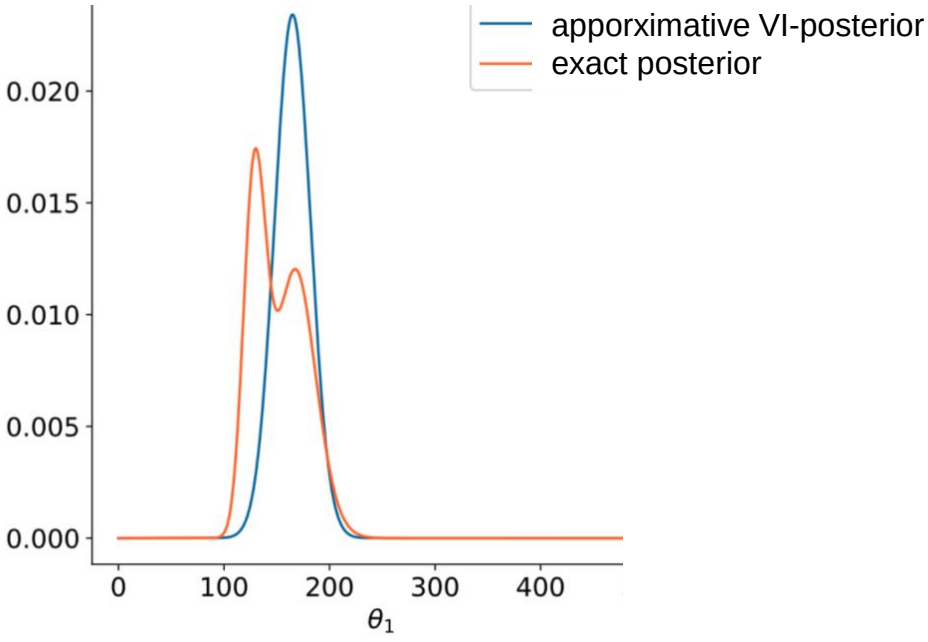
- $p(D|\theta)$ likelihood - easy ☺
- $p(\theta)$ prior – easy ☺
- $\int_\theta p(D|\theta)p(\theta)d\theta$ - hard ☹




- Bayesian Mantra:
  The posterior is proportional to the likelihood times the prior

# Variational Inference to get an approximate posterior



# Approximative Bayes via Variational Inference

- Layers for Variational Inferene :
  - Use VI Flipout layer instead normal Conv layer

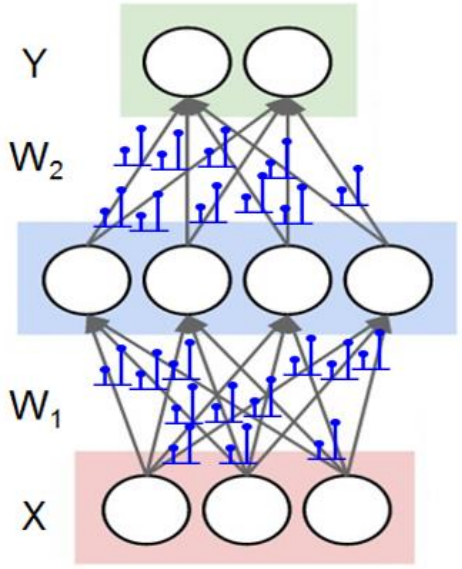
```
model_vi.add(tfp.layers.Convolution2DFlipout(16,kernel_size=(3,3),
                padding="same", activation = 'relu',
                kernel_divergence_fn=kernel_divergence_fn))
```

Instead of

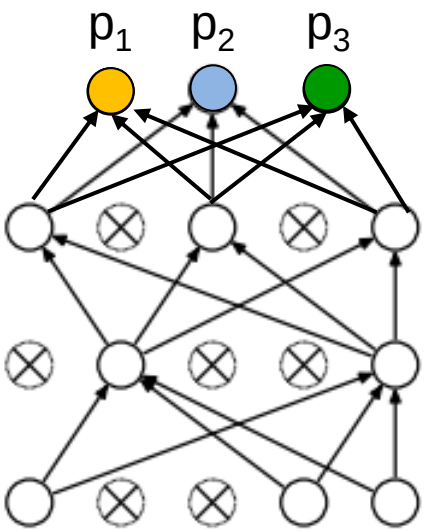
```
model.add(Convolution2D(16,kernel_size=(3,3),padding="same", activation = 'relu'))
```

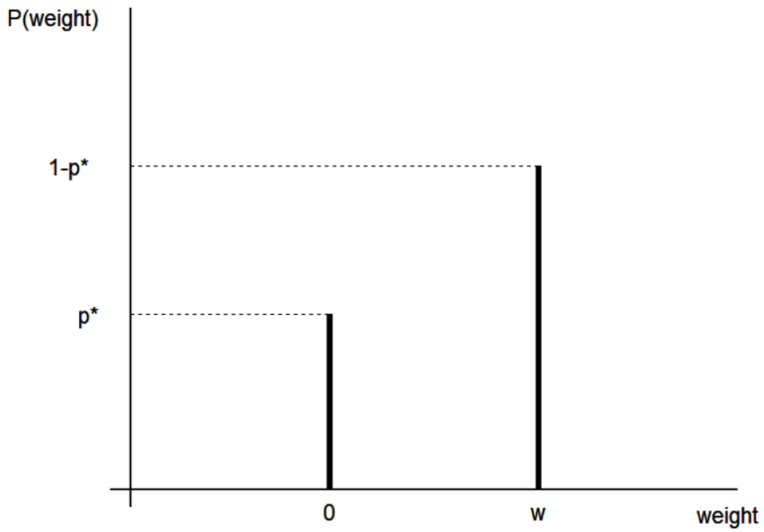
Remark: we skip the theory of Variational Inference

# MC Dropout as approximate Bayes



# Recall: Classical Dropout only during training

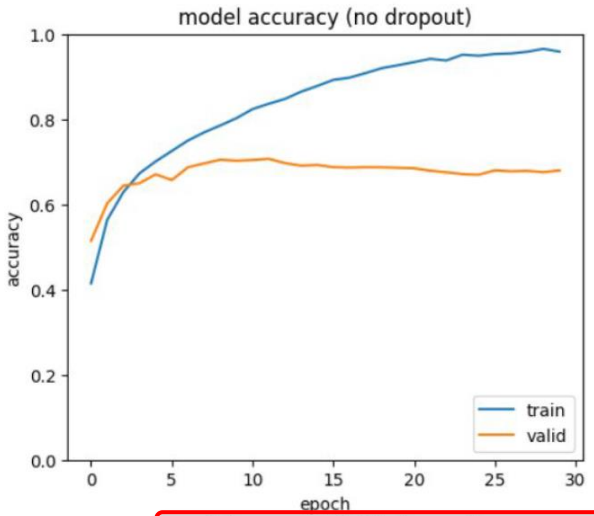


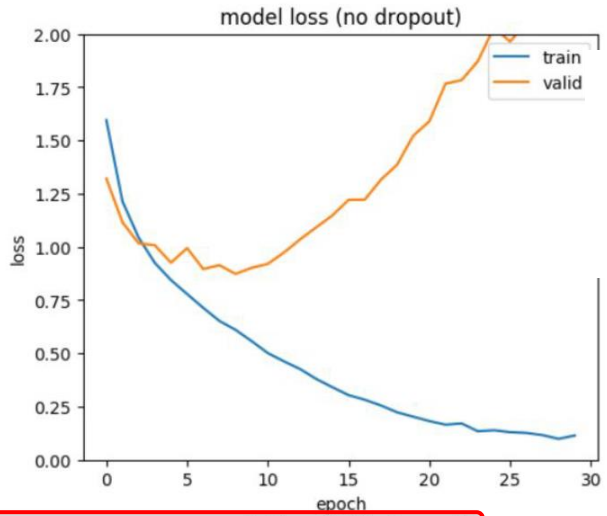



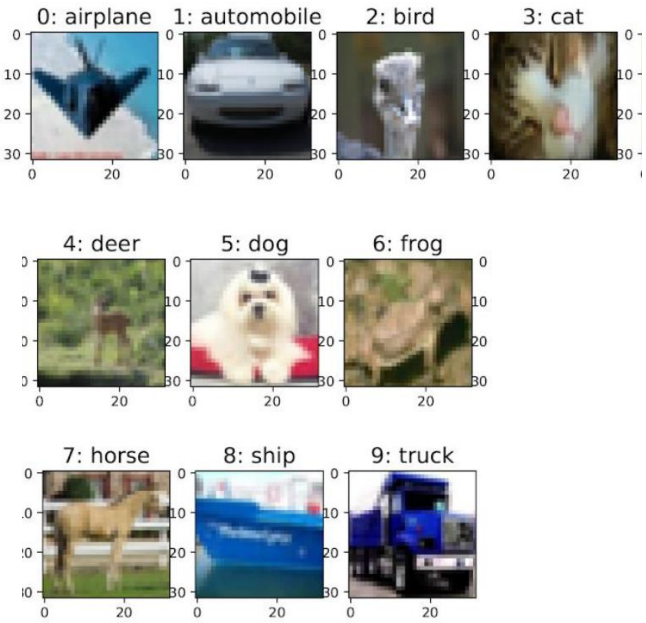

Using dropout during training implies:

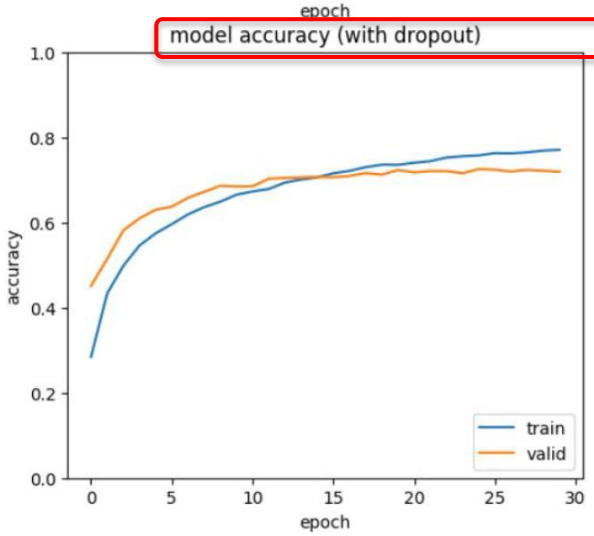
- In each training step only weights to not-dropped units are updated → we train a sparse sub-model NN
- For non-Bayesian NN we freeze the weights after training to a value $w \cdot p^*$

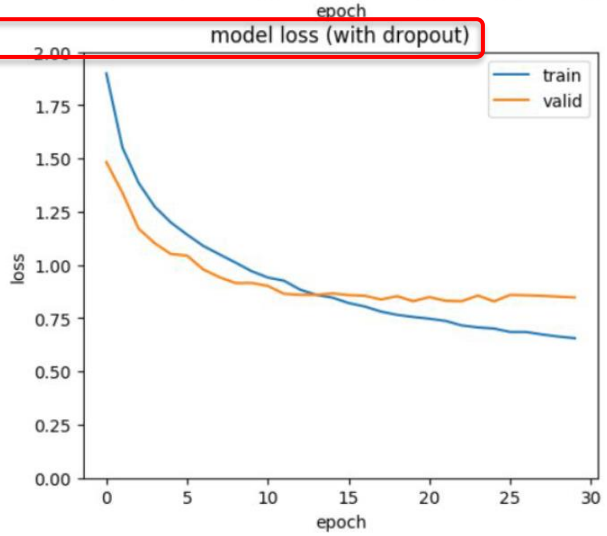
# Recall: Dropout fights overfitting in a CIFAR10 CNN



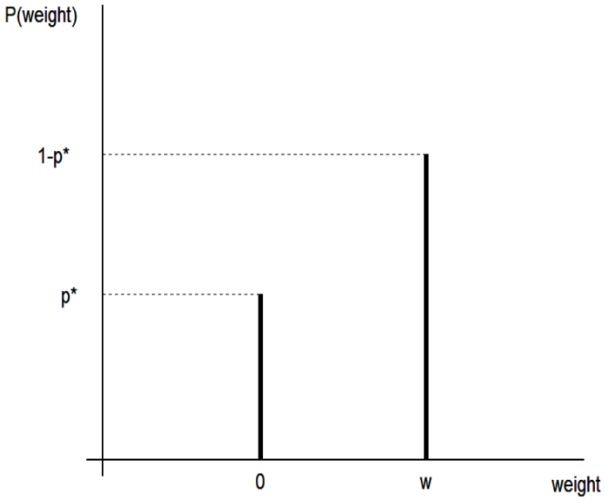



# From Dropout during training to MC Dropout during test time

# Bayesian NN via MC Dropout

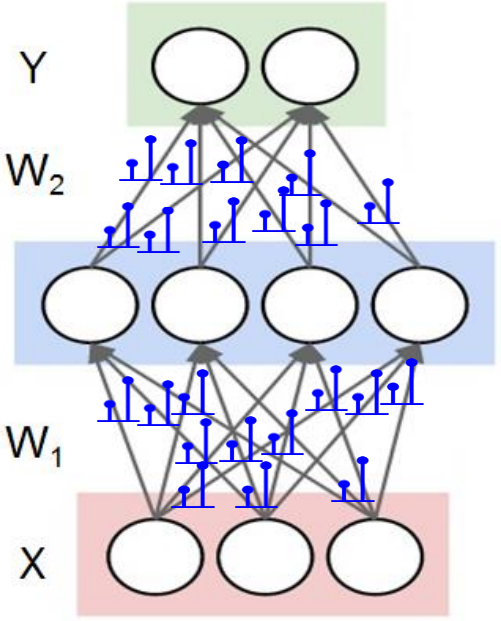
Yarin Gal et al. (2015):
Via Dropout training we learned a whole weight distribution for each connection.
We can sample from this Bernoulli-kind weight distribution by performing dropout during test time and use the dropout-trained NN as Bayesian NN.
Gal showed that doing dropout approximates VI with a Bernoulli-kind variational distribution $q_\theta$ (instead of a Gaussian).

Learned
Bernoulli-kind distribution




Dropout in
test time

MC dropout NN




Weights have
Bernoulli-kind distribution

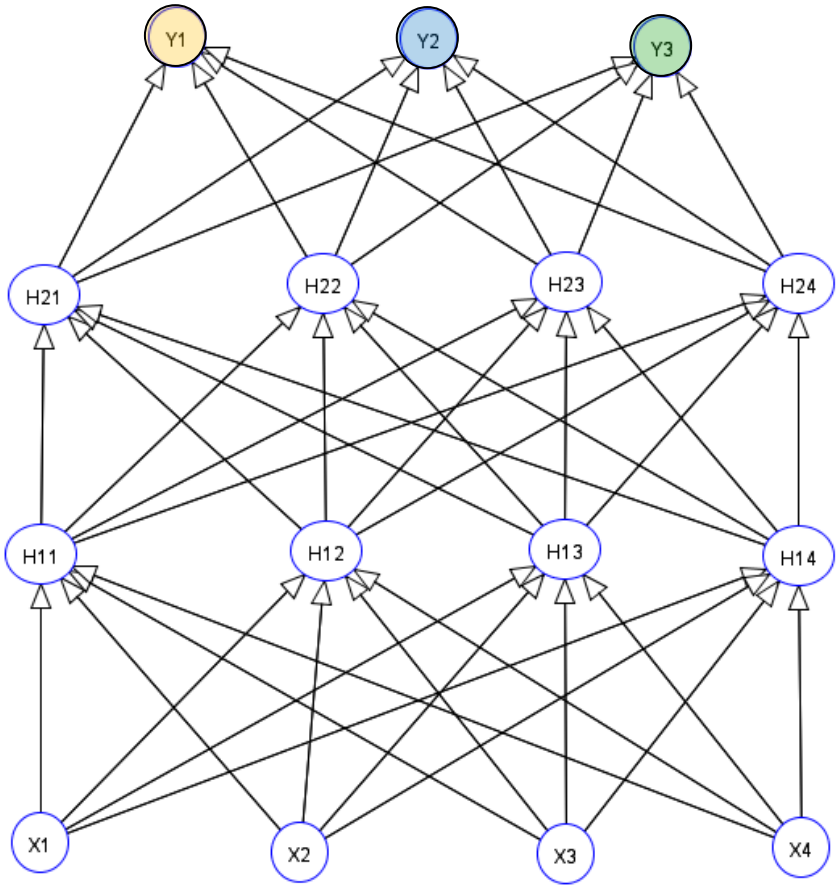
Which parameter has this $q_\theta$?

The value $w$.

# When using Dropout only during training

For non-Bayesian NN we freeze the weights after training to a value $w \cdot p^*$ and use then the trained NN for prediction:

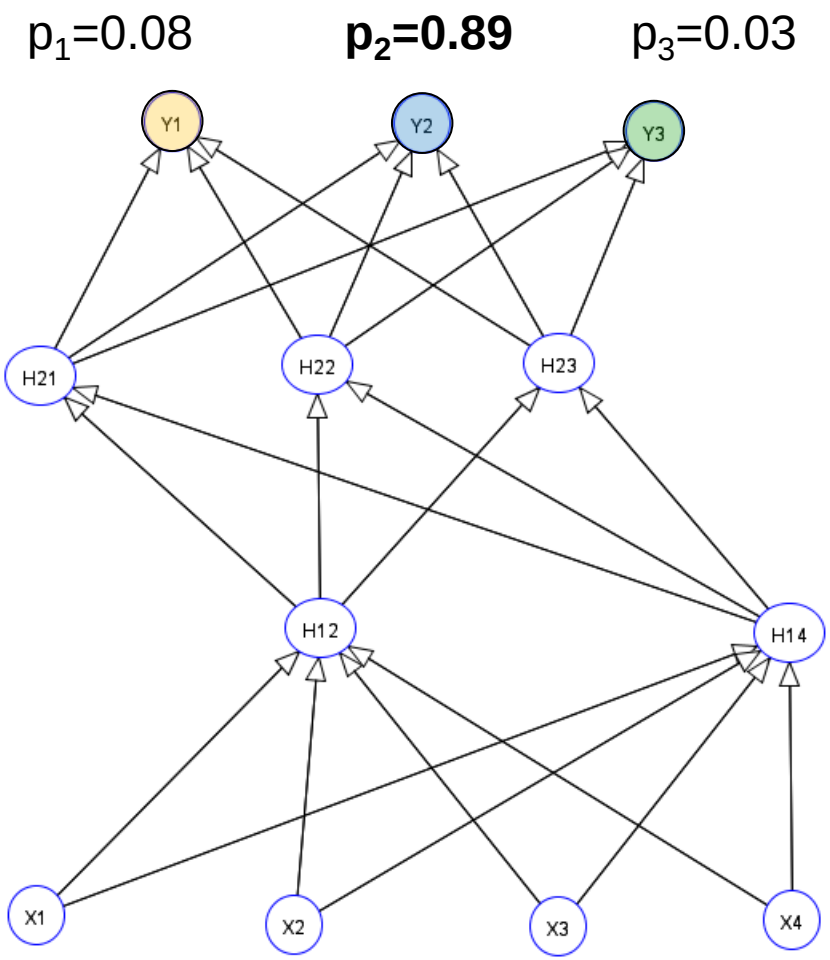
$p_1$=0.07 **$p_2$=0.91** $p_3$=0.02

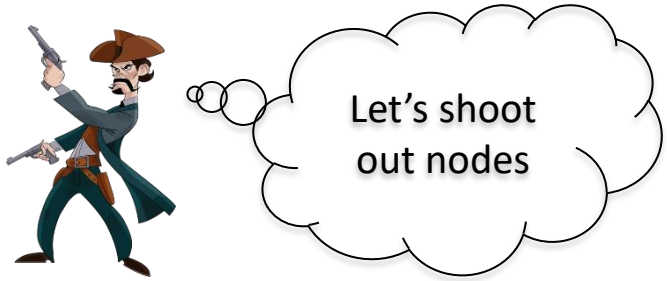



Probability of predicted class: **$p_{max}$**

Input: image pixel values

# MC Dropout during test time: Run 1



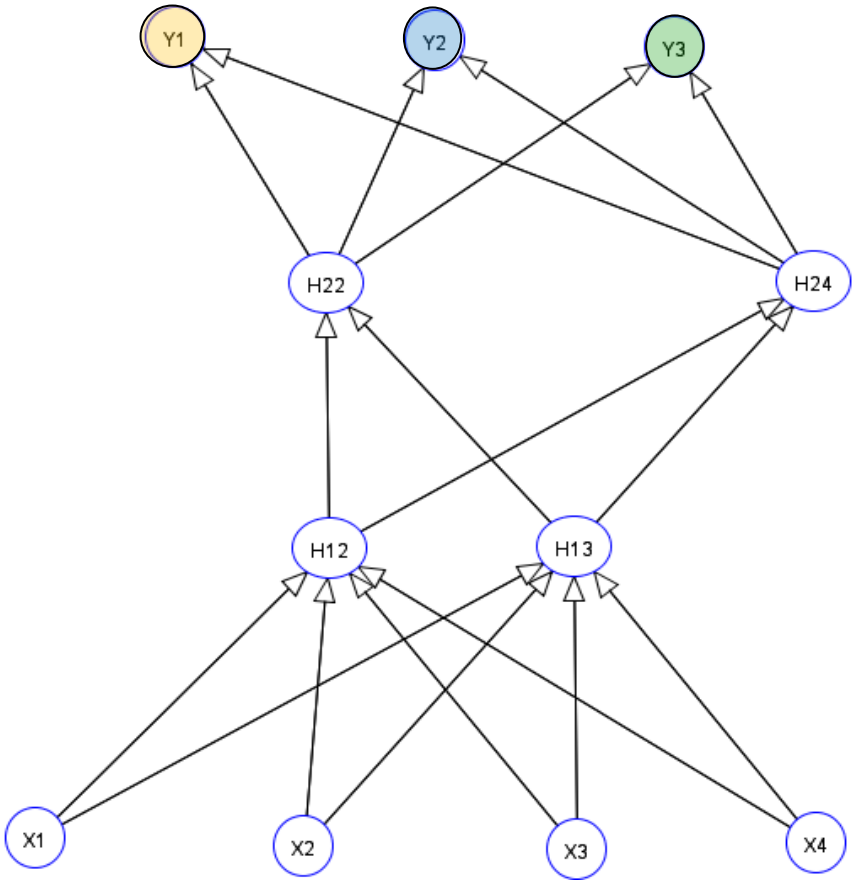



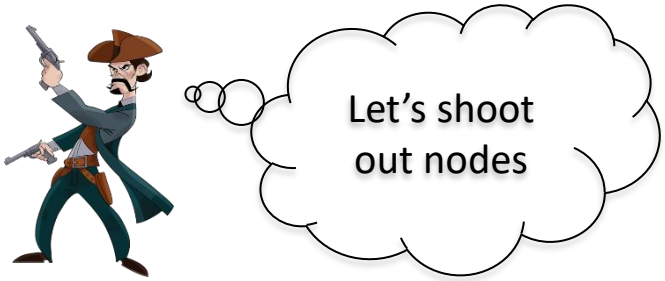

Stochastic dropout of units

**Same input image**

# MC Dropout during test time: Run 2

$p_1$=0.11 **$p_2$=0.81** $p_3$=0.08

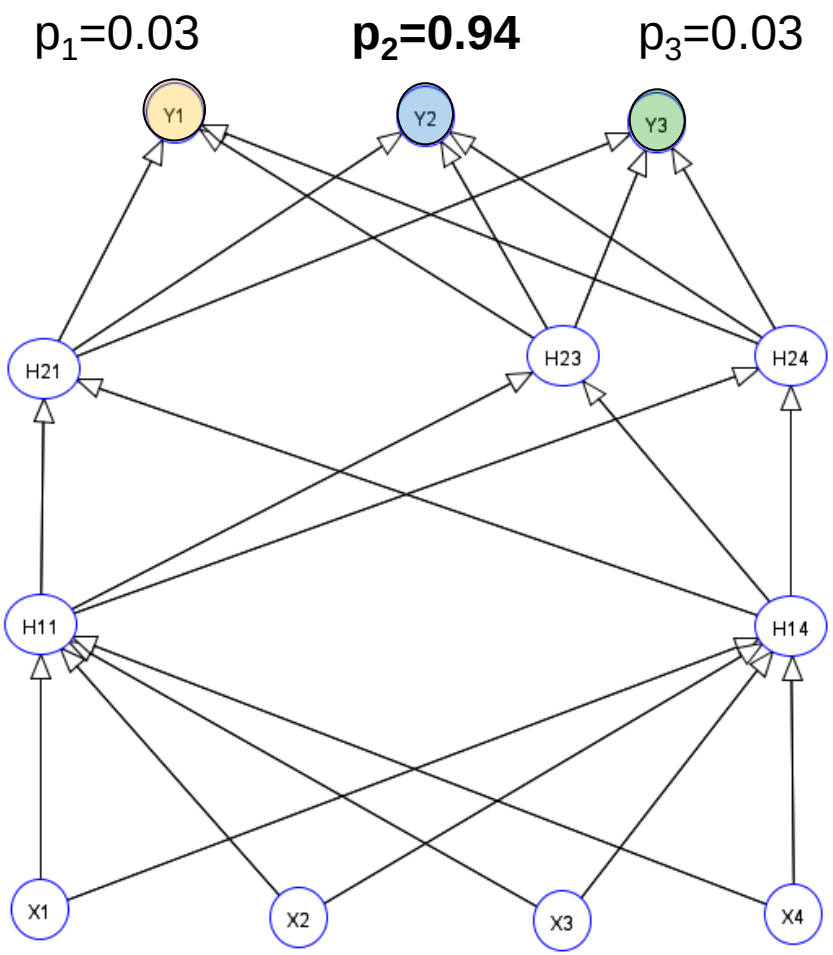


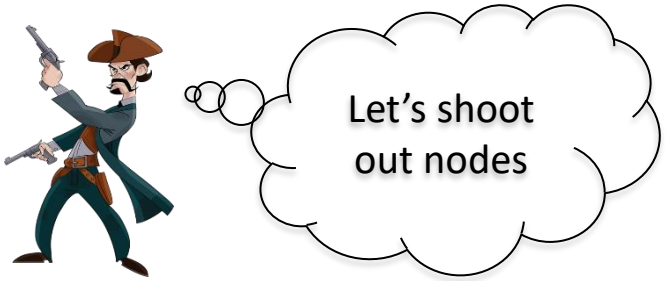




Stochastic dropout of units

**Same input image**

# MC Dropout during test time: Run 3



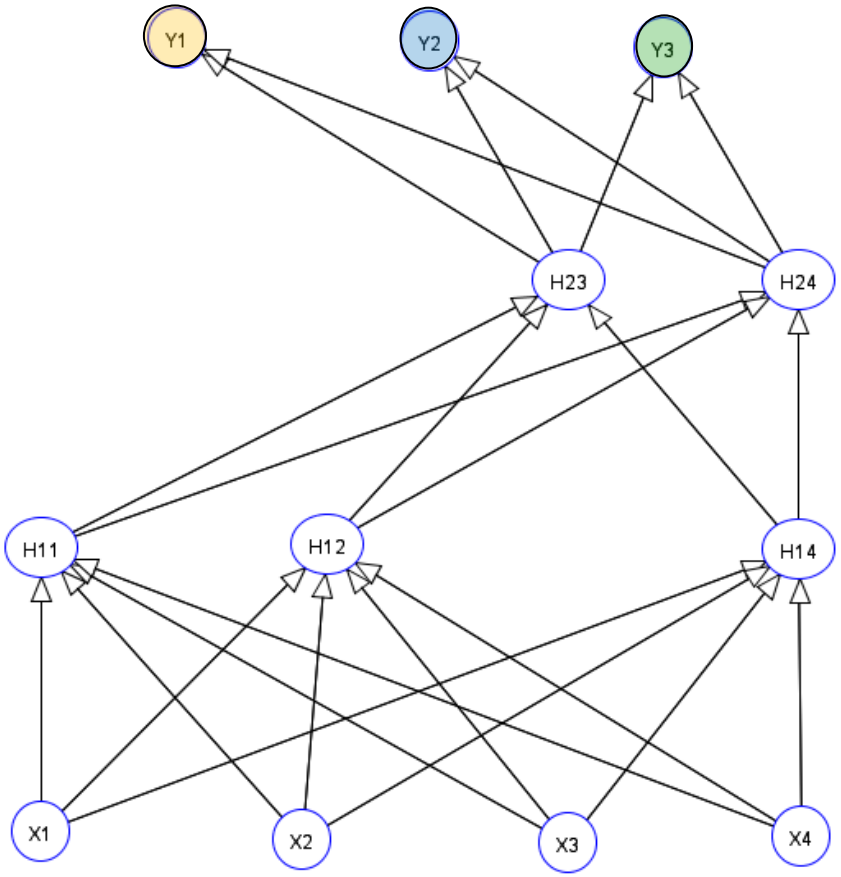



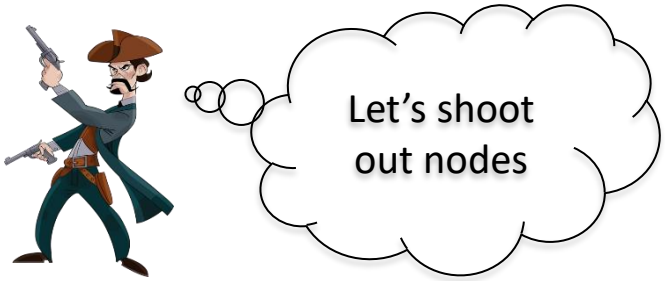

Stochastic dropout of units

**Same input image**

# MC Dropout during test time: Run 4

$p_1$=0.16 **$p_2$=0.78** $p_3$=0.06



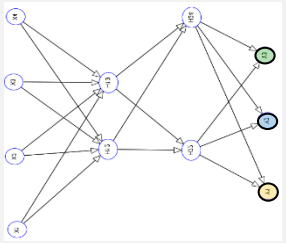



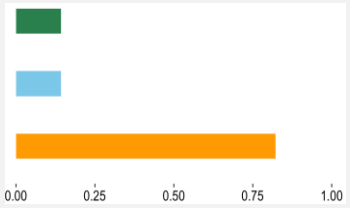

Stochastic dropout of units

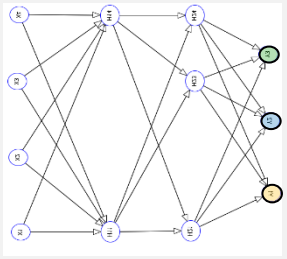
**Same input image**

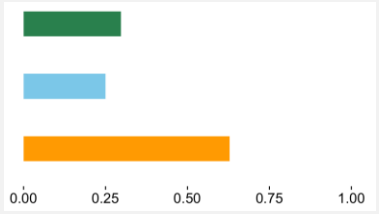
# MC Dropout during test time yields a multivariate predictive distribution for the parameters

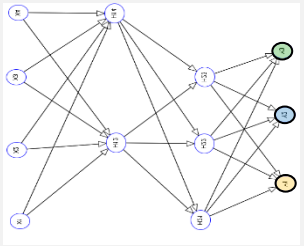
Many Dropout Runs in forward pass

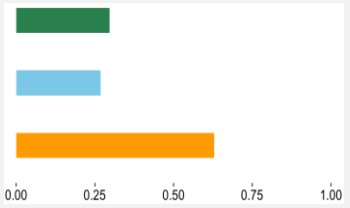




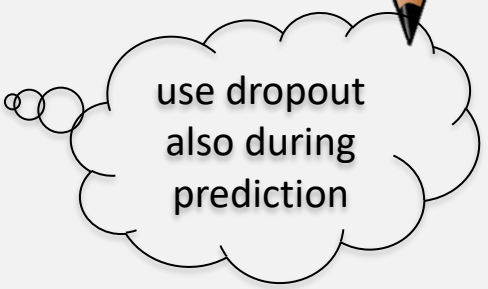



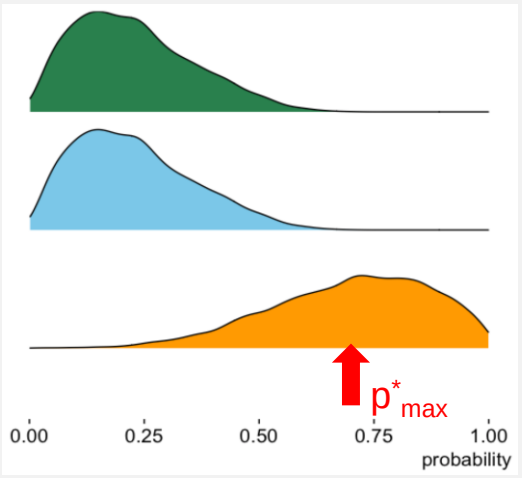





...

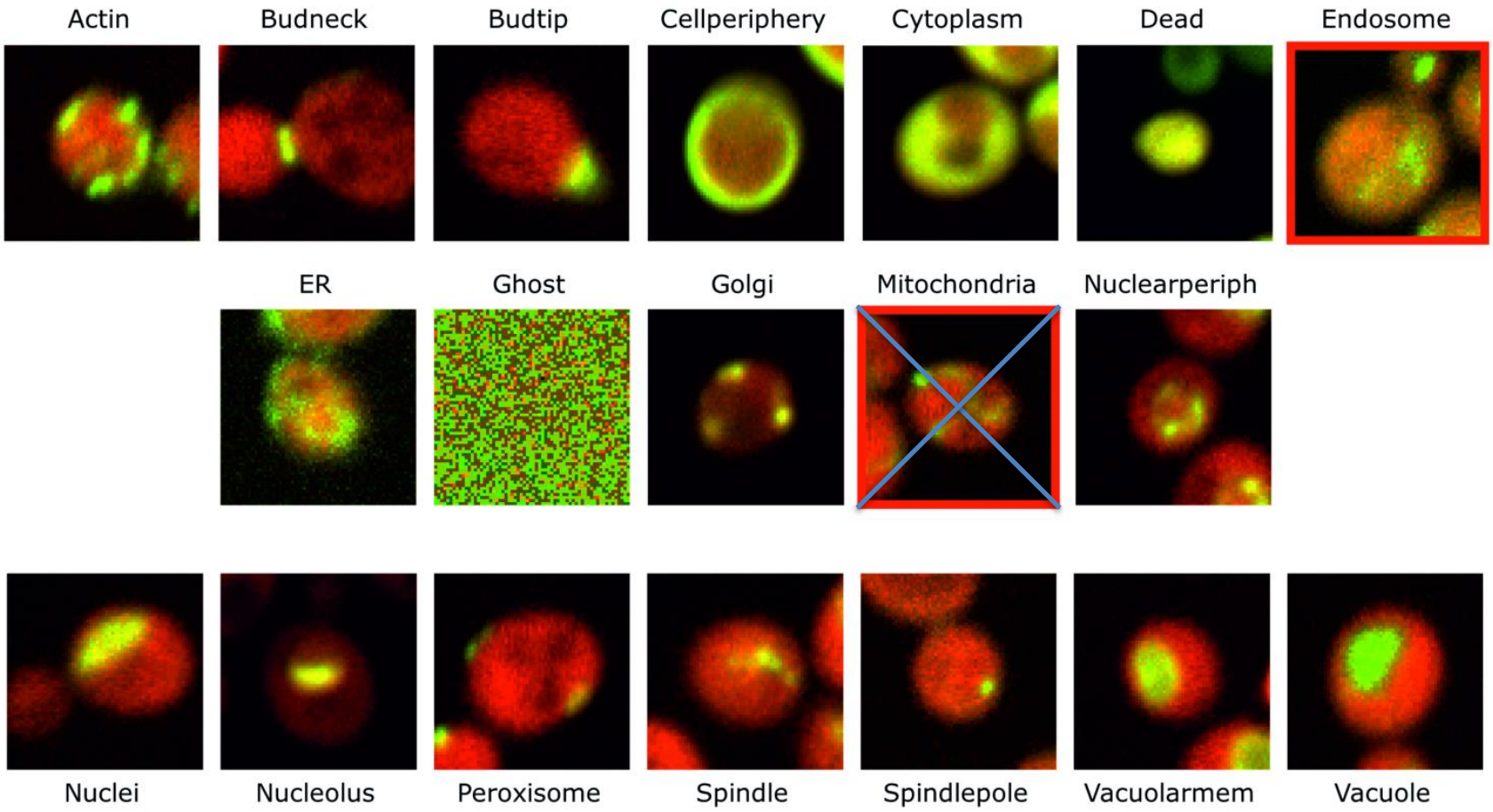



CNN predicts class “collie”
but with high uncertainty

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

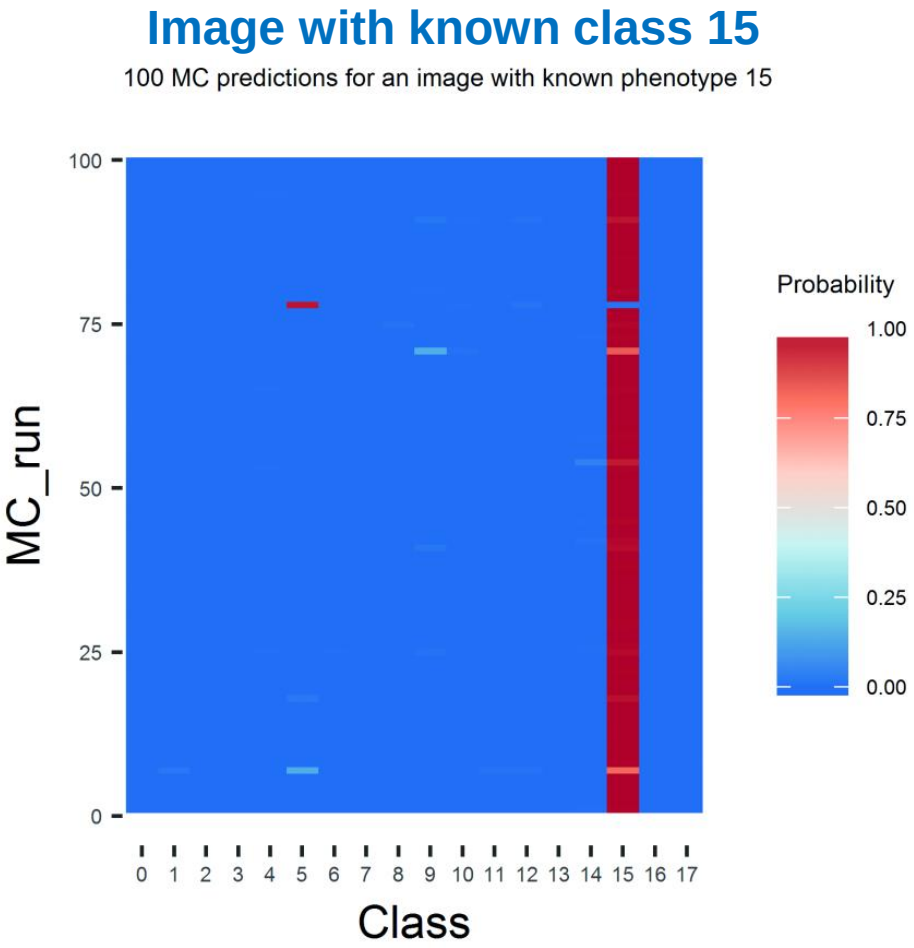
# Experiment with unknown phenotype




Dürr O, Murina E, Siegismund D, Tolkachev V, Steigele S, Sick B. Know when you don't know, Assay Drug Dev Technol. 2018

# Probability distribution from MC dropout runs

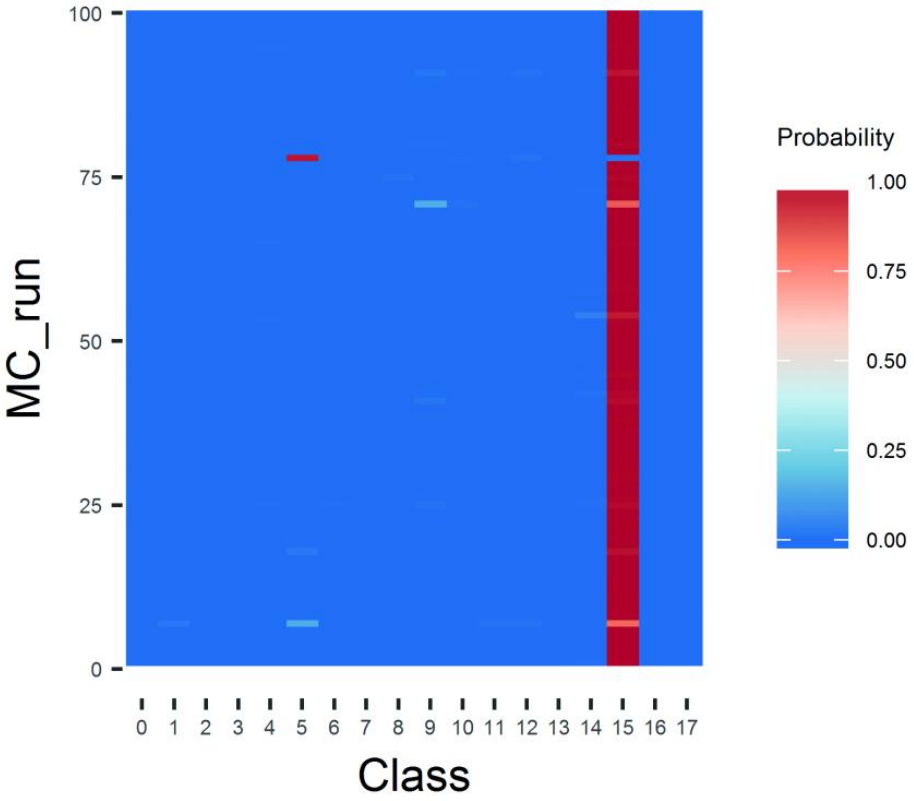
## Image with known class 15



# Probability distribution from MC dropout runs

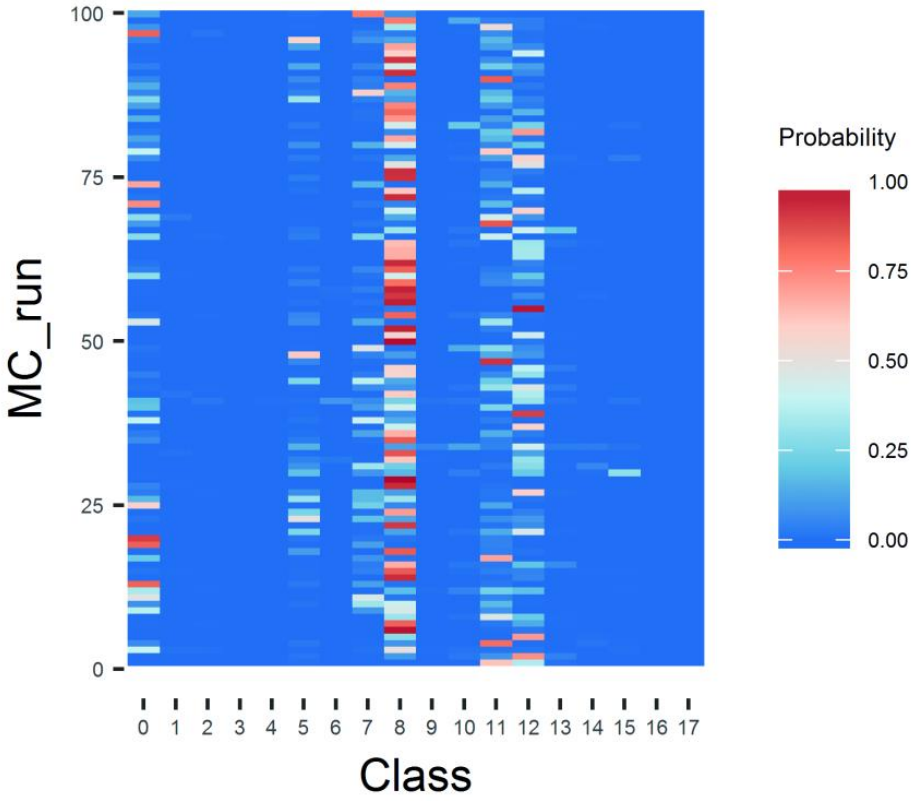
## Image with known class 15

100 MC predictions for an image with known phenotype 15



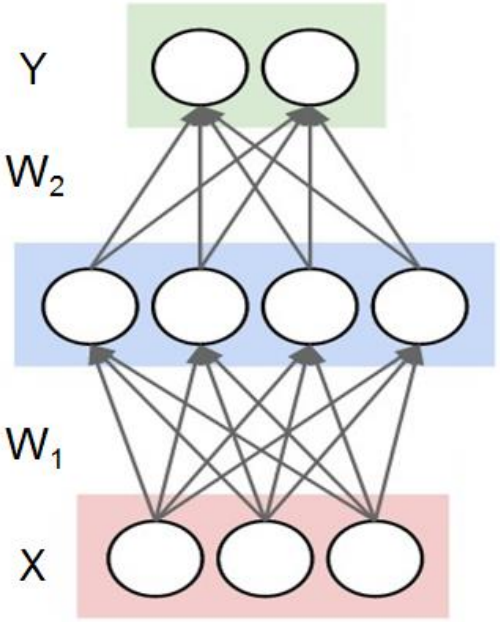

## Image with unknown class

100 MC predictions for an image with an unknown phenotype



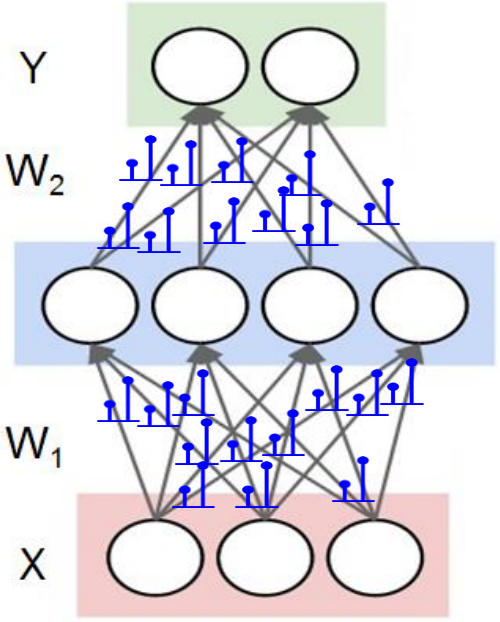
# Non-Bayesian and Bayesian NNs

Non-Bayesian NN



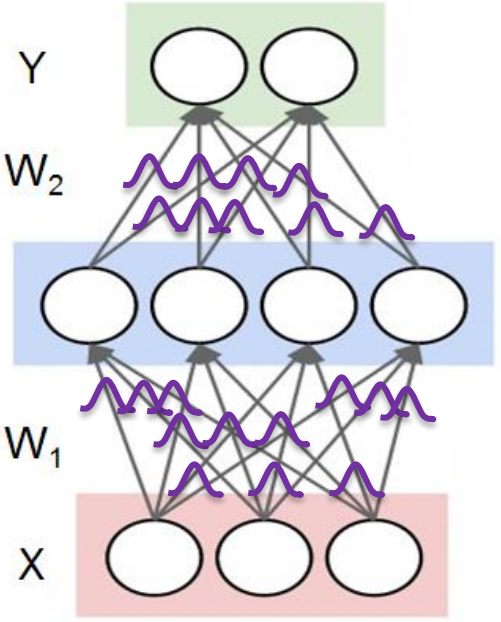

**Weights are fixed**

MC dropout Bayesian NN




**Weights have Bernoulli-kind distribution**

VI Bayesian NN

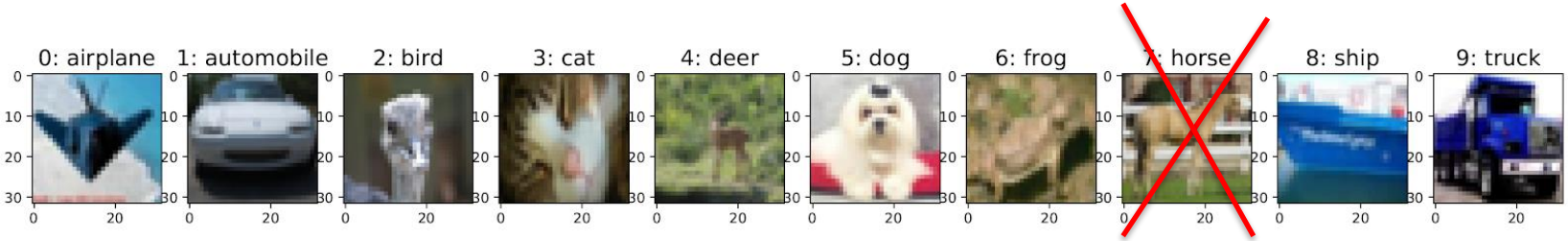



**Weights have Gaussian distribution**

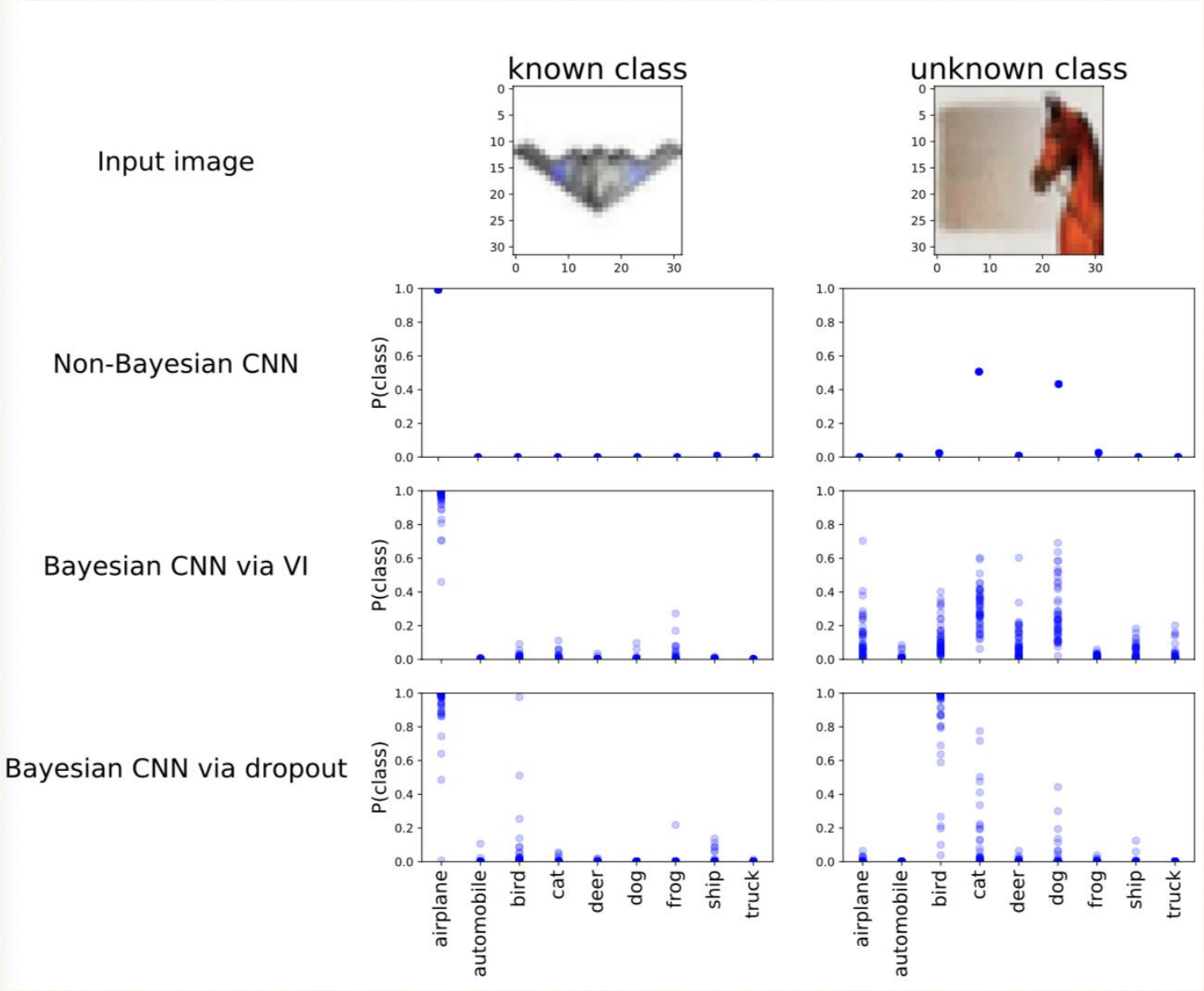
# Hands-on Time

[Notebook 17]

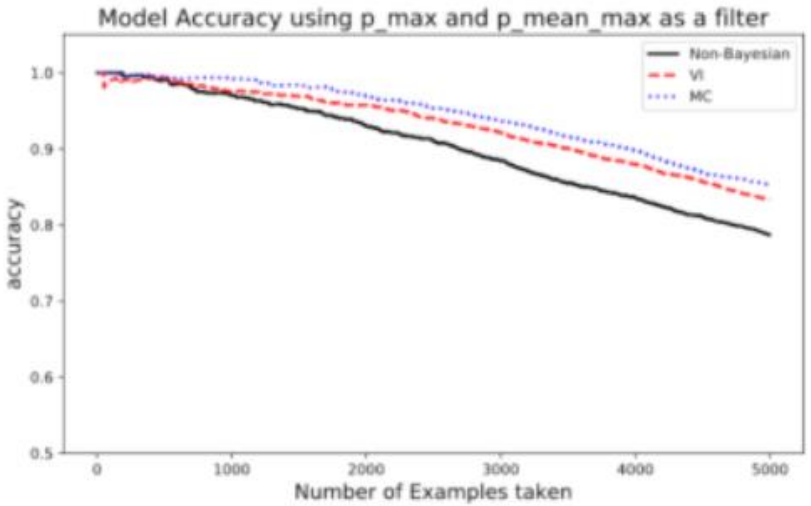
Train a CNN with only 9 of the 10 classes and investigate if the uncertainties are different when predicting images from known or unknown classes.

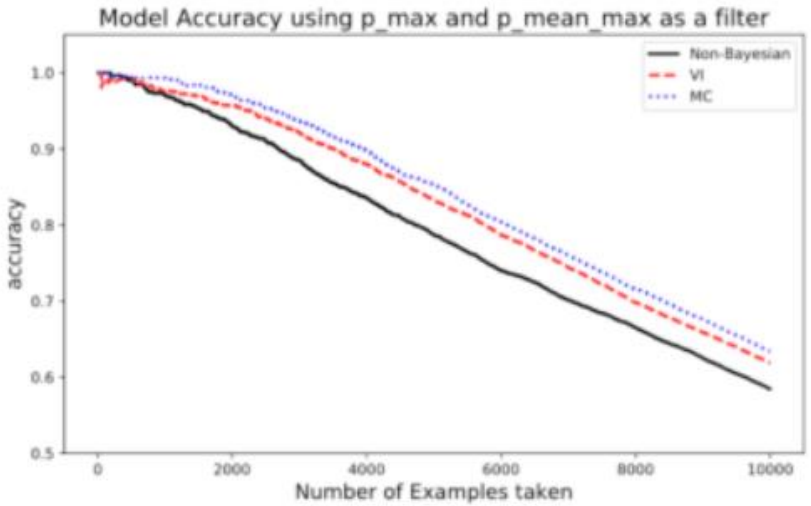


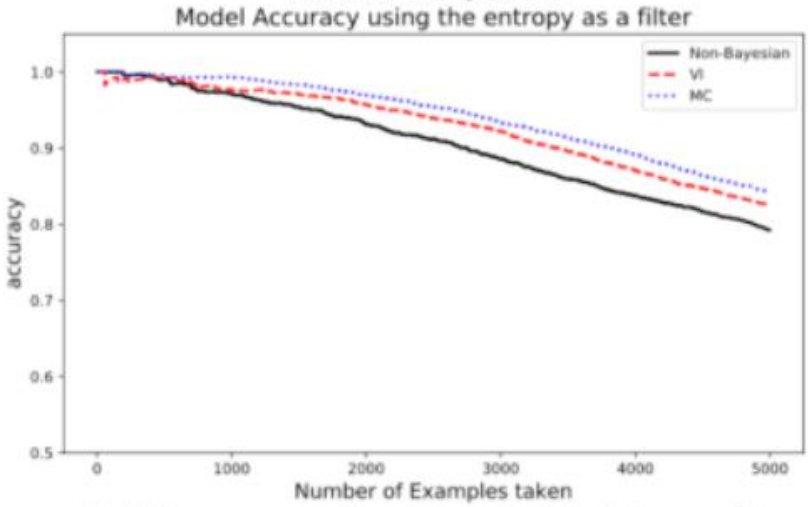
# Looking at the predictive distribution!

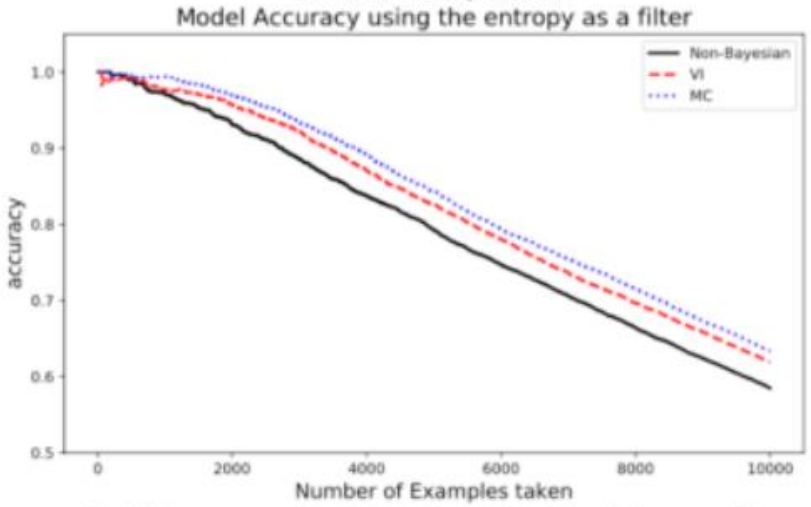


# Filtering experiment to compare uncertainty measures




Uncertainty from non-Bayesian NN is less good in filtering out wrong classifications than uncertainty measures from Bayesian variants of the NN.

# Take home message

- Using some kind of ensembling or Bayes improve almost all models

- To get a better prediction performance and uncertainty measuers we need to take into account different uncertainty contributions in the model fitting process
  - Work with probabilistic models and fit conditional outcome distributions (capture aleatoric uncertainty)
  - Ensembling of probabilistic models (add algorithmic uncertainty contribution)
  - Bayes (add epistemic uncertainty contribution)
    - Approximative Bayesian NN via Variational Inference (VI)
    - Pseudo apprixmative Bayesian NN via MC Dropout

- For MC dropout we need to fit a NN with dropout which has as many parameters as a classical NN. We also turn on dropout during prediction and then average different MC dropout predictions.

- For deep ensembles we need to train several NNs (typical 3 to 5) with different random initialization. We then average the predictions of these NNs. Deep ensembles are computationally more costly but provide typically better prediction performance (and also better uncertainty measures) than MC dropout.