Ensembles in machine learning

(simple) theory and (simple) practice

Pierre-Alexandre Mattei

Not many new things in this talk, but I will also talk about some joint ongoing work with ***Damien Garreau, Raphaël Razafindralambo, Rémy Sun, Frédéric Precioso***

see ***Mattei & Garreau, Are Ensembles Getting Better all the Time?****, 2024 arXiv:2311.17885*

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Institut interdisciplinaire d'intelligence artificielle

Menu of the day

1. Historical intro
2. Some basic examples of ensembles used in practice
   - MC dropout
   - Deep ensembles
3. When and why ensembling works? Some empirics
4. When and why ensembling works? The case of convex losses
5. Nonconvex subtleties

1

Ensembles in stats and machine learning, a brief history

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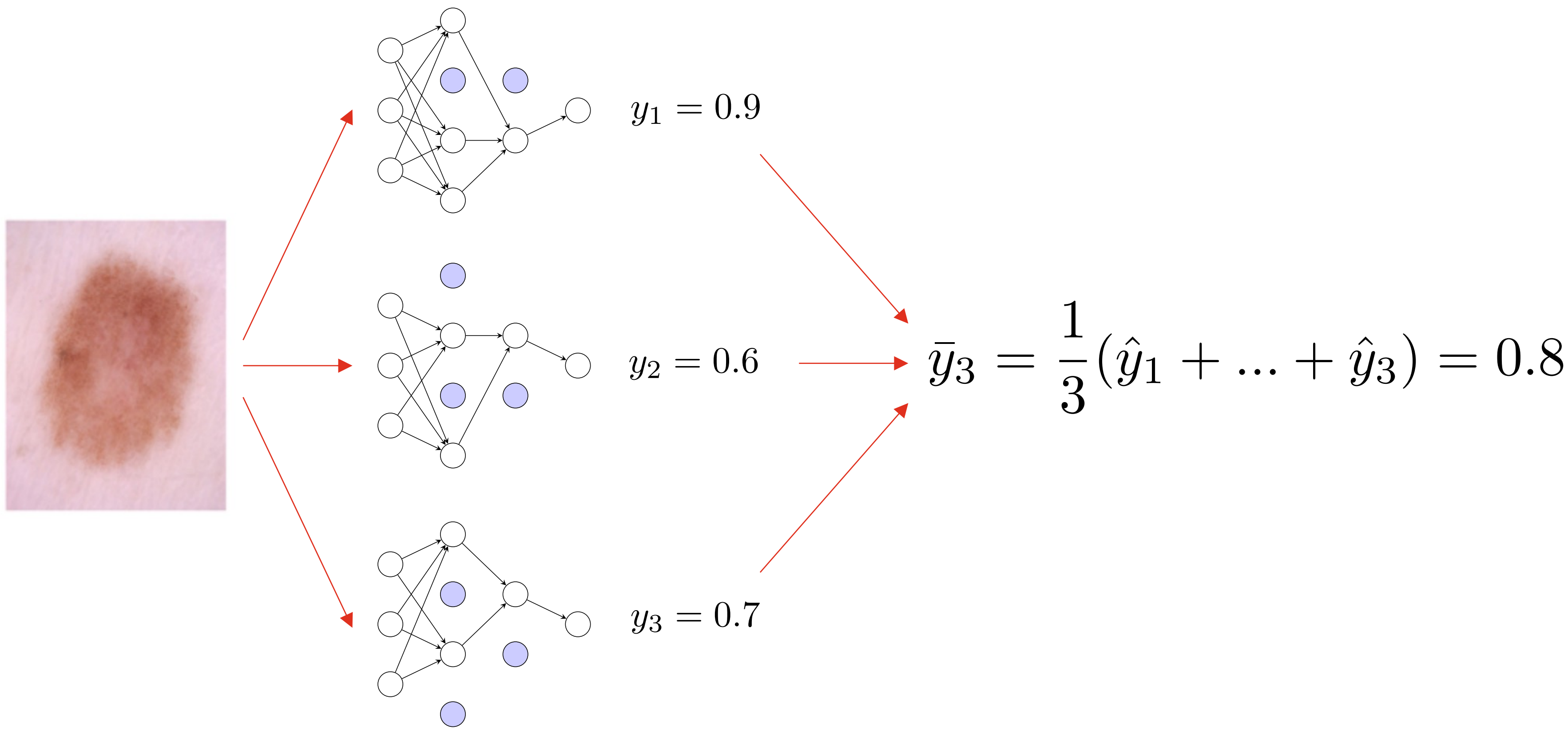

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- Breiman, *Random forests*, Machine Learning, 2000
  - A variant of bagging where base models are **randomised decision trees**

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❖ Krogh and Vedeslby, *Neural Network Ensembles, Cross Validation, and Active Learning*, NeurIPS, 1995

What are ensembles? Trends of the 2020s

- For **tabular data**, ensembles of decision trees (random forest, boosting) still perform better than deep learning.
    - Grinsztajn, Oyallon, and Varoquaux, *Why do tree-based models still outperform deep learning on typical tabular data?*, NeurIPS 2022

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- Ensembling also works well together with deep learning.
    - In **Monte Carlo dropout (MC dropout)**, base models are **versions of a single network with several dropout masks**
        - Gal and Ghahramani, *Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning*, ICML 2016

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        - Lakshminarayanan, Pritzel, Blundell, *Simple and Scalable Predictive Uncertainty Estimation using Deep Ensembles*, NeurIPS 2017

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Both MC dropout and deep ensembles work extremely well especially with respect to “uncertainty aware” metrics like the cross-entropy, but are a bit less impressive in terms of accuracy.

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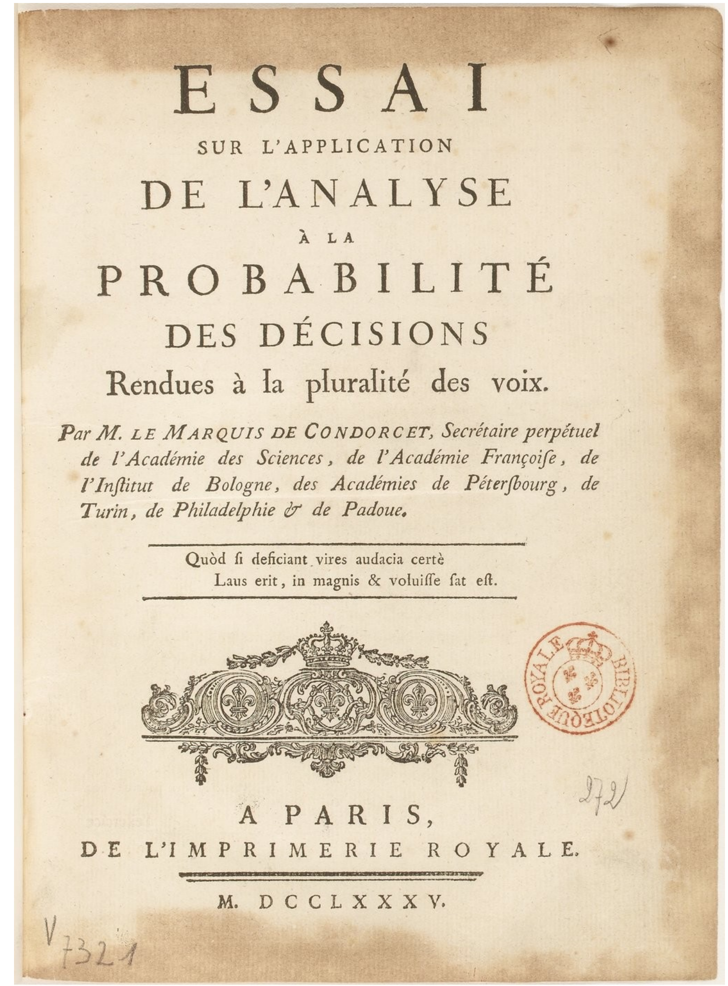
- At the end of the 1700s, **Condorcet** proposed a mathematical formalisation of this argument that is somewhat close to what we'll see today. His main applications were politics and jurys.


ESSAI

SUR L'APPLICATION

DE L'ANALYSE

À LA

PROBABILITÉ

DES DÉCISIONS

Rendues à la pluralité des voix.

Par M. LE MARQUIS DE CONDORCET, Secrétaire perpétuel de l'Académie des Sciences, de l'Académie Françoiſe, de l'Inſtitut de Bologne, des Académies de Péterſbourg, de Turin, de Philadelphie & de Padoue.

Quòd ſi deficiant vires audacia certè
Laus erit, in magnis & voluiſſe ſat eſt.

A PARIS,

DE L'IMPRIMERIE ROYALE.

M. DCCLXXXV.

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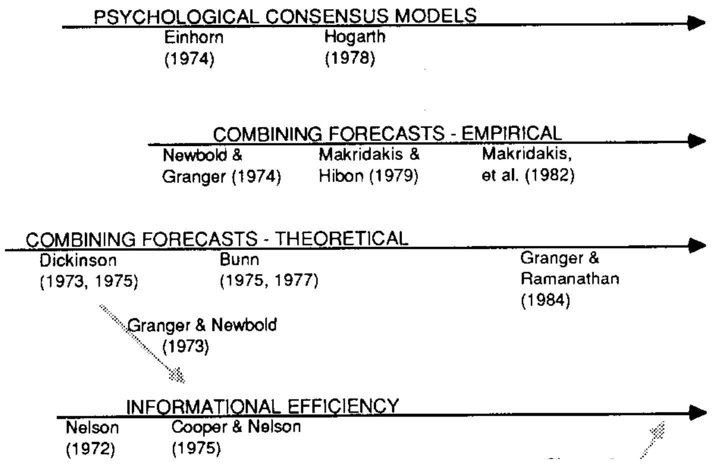
- **Economists, econometricians and forecasters** have used ensembles from the 60s.
  - Clemen, *Combining forecasts: A review and annotated bibliography*, International Journal of Forecasting, 1989



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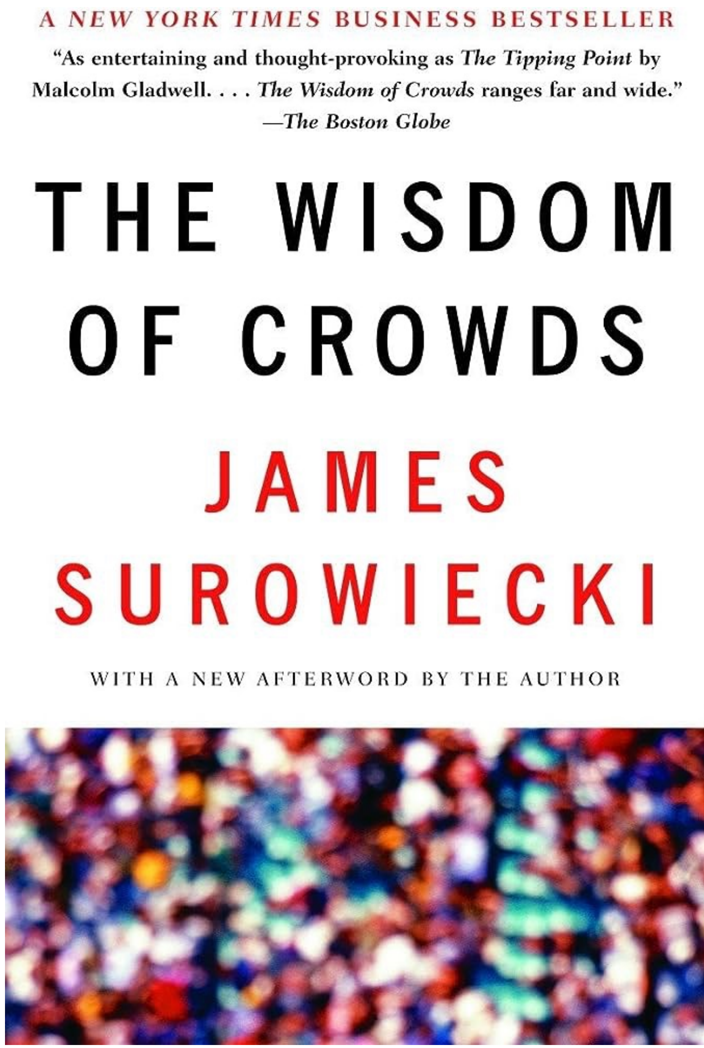
- The key idea behing ensembles is that **groups are collectively better at decision-making than individals**. This is an old idea, that goes way beyond ML.

- The phrase « wisdom of crowds », popularised by Surowiecki's bestselling book, is often used to summarise this idea



What ensembles will we be looking at today

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- While this is very general, other ensembles that do not satisfy this property exist, but we will not be looking at them today: **boosting**, **Bayesian model averaging**, ensembles of different physical models for weather forecasting…
    - Kuncheva, *Combining Pattern Classifiers: Methods and Algorithms (2nd edition)*, Wiley, 2014

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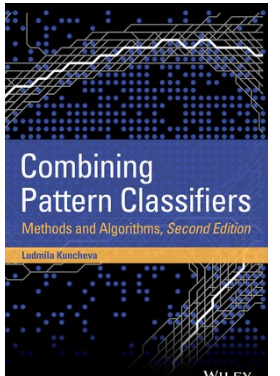

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Basic but popular ensembles of neural nets

Deep ensembles

- **Train n neural nets on the same dataset, with the same training algorithm but different random seeds.**

- Weirdly enough, it generally outperforms bagging of deep nets.

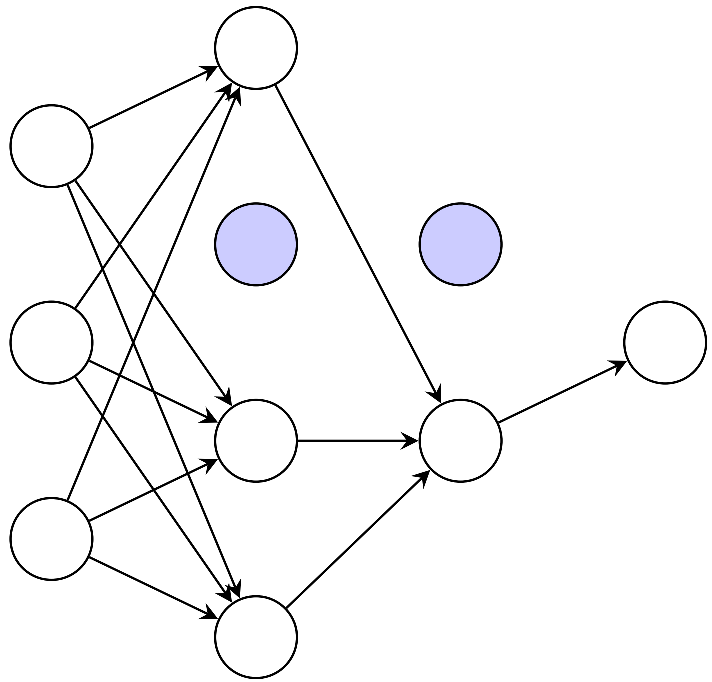
- Again, we can average the networks as we see fit, for instance just average the outputs.

- This can be used for **any deep learning task**, not only classification, but segmentation, generative modelling (R. Razafindralambo's talk on Monday), regression…

- Related to Bayesian deep learning:
    - Wild et al., **A Rigorous Link between Deep Ensembles and (Variational) Bayesian Methods**, NeurIPS 2023

MC dropout

- Train a neural net once, but with dropout activated.
- **Then, average the networks obtained using different (random) dropout masks.**



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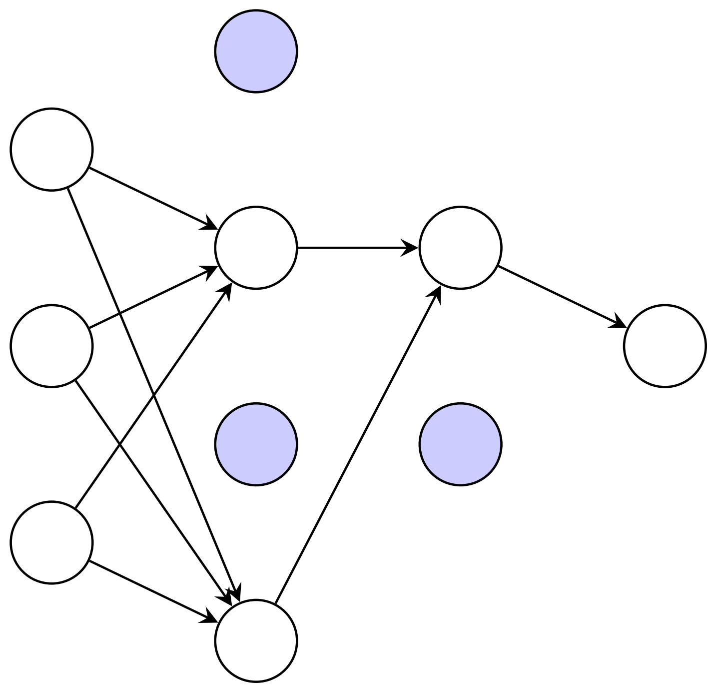

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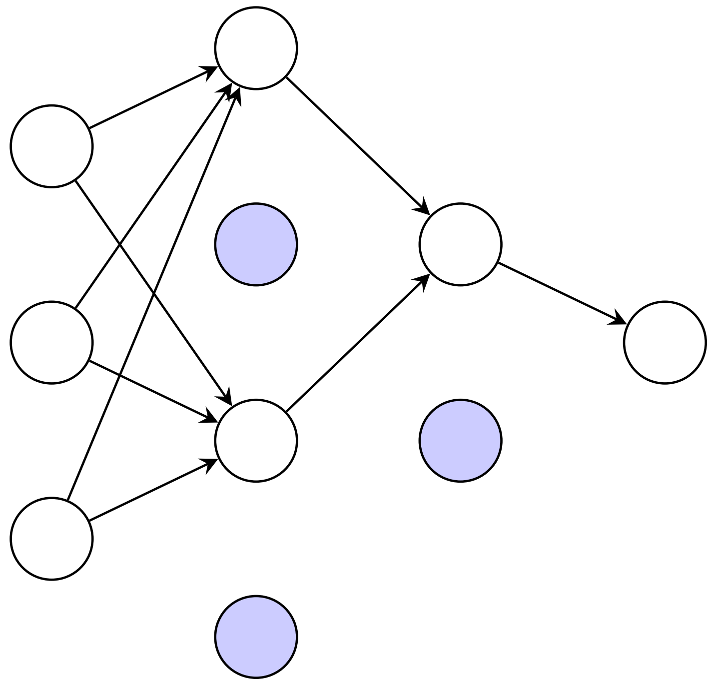

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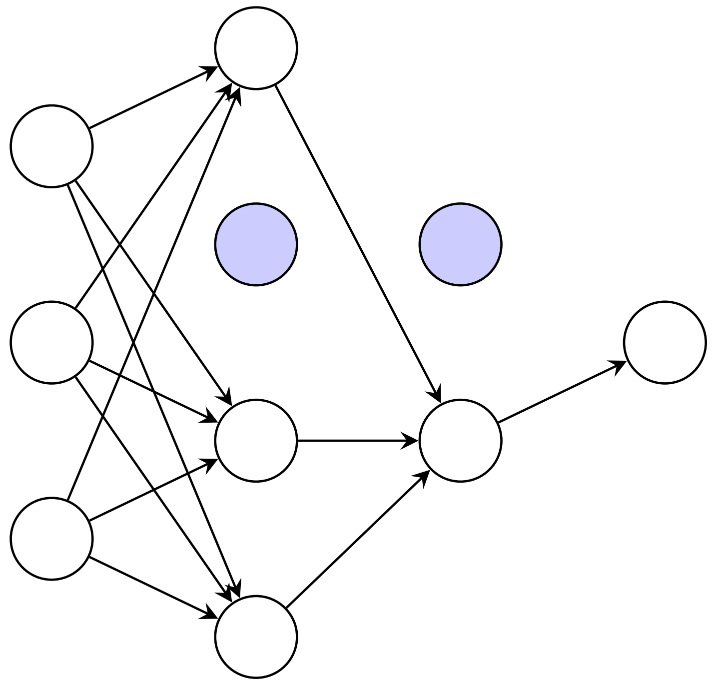

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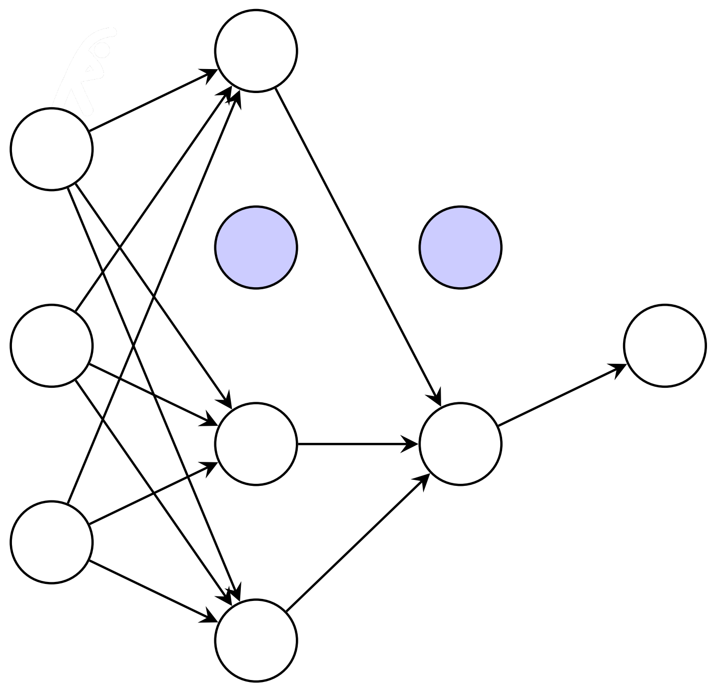


Loose relationship with Bayesian inference:

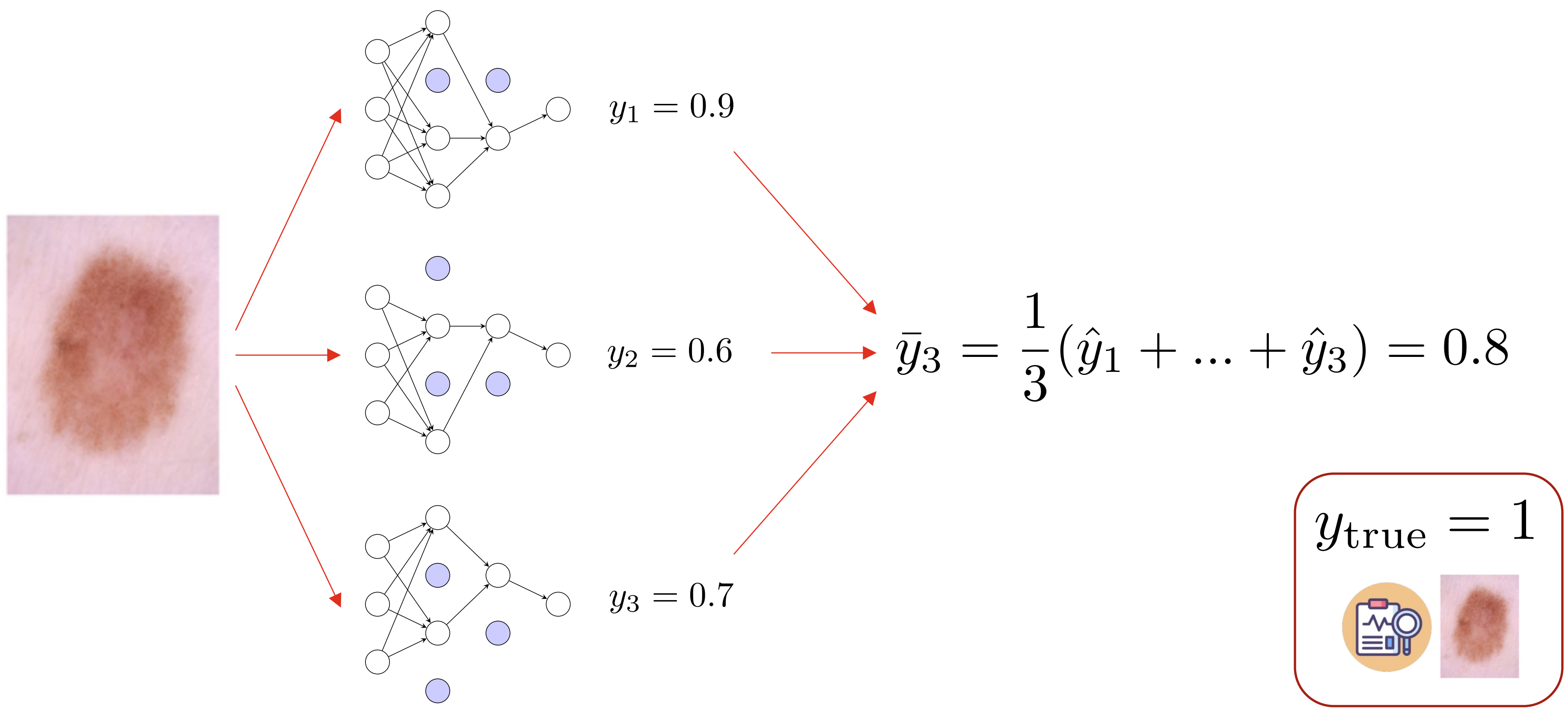
➢ Hron et al., Variational Bayesian dropout: pitfalls and fixes, ICML 2023

3

When and why ensembles work?

some empirics

MC dropout for medical image classification



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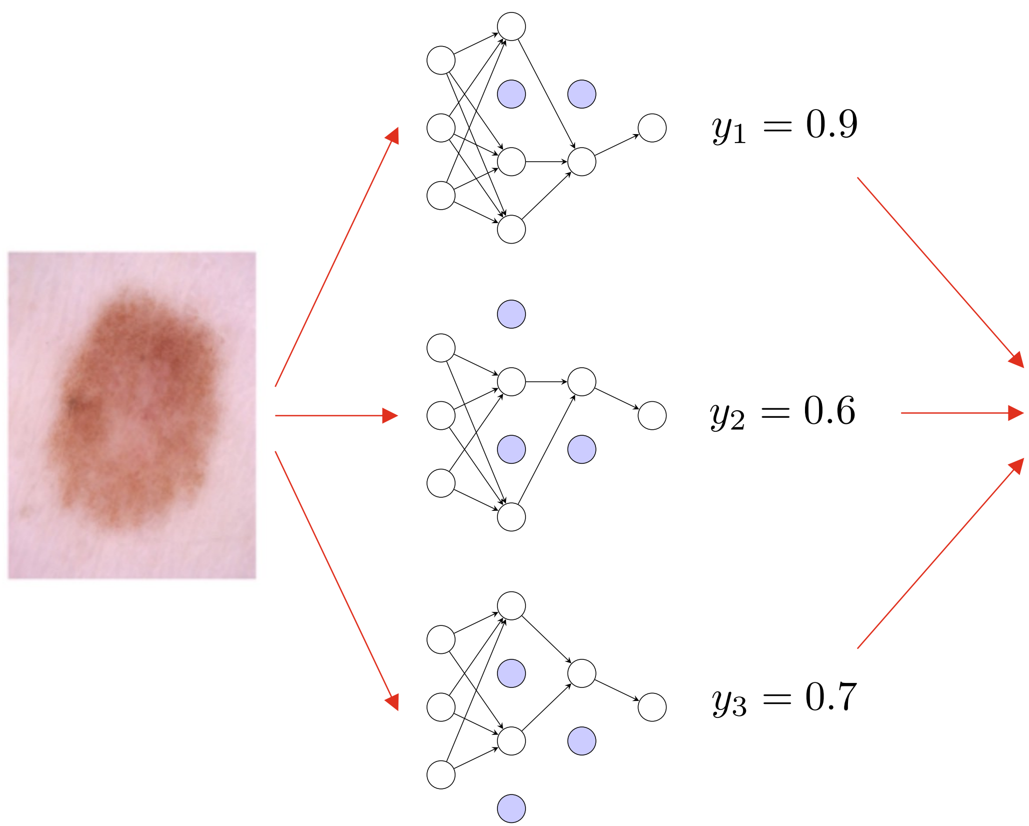
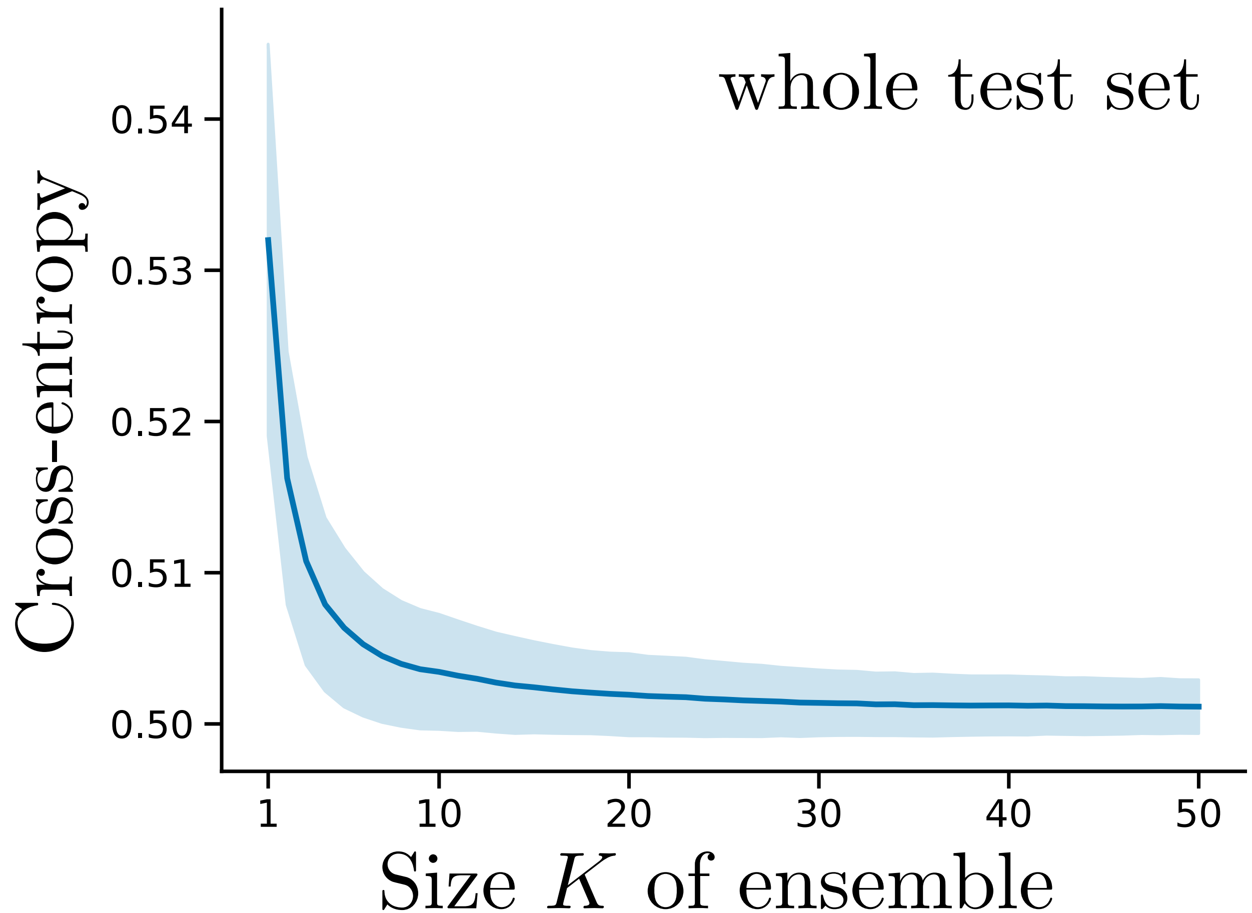


$$\bar{y}_3 = \frac{1}{3}(\hat{y}_1 + \ldots + \hat{y}_3) = 0.8$$

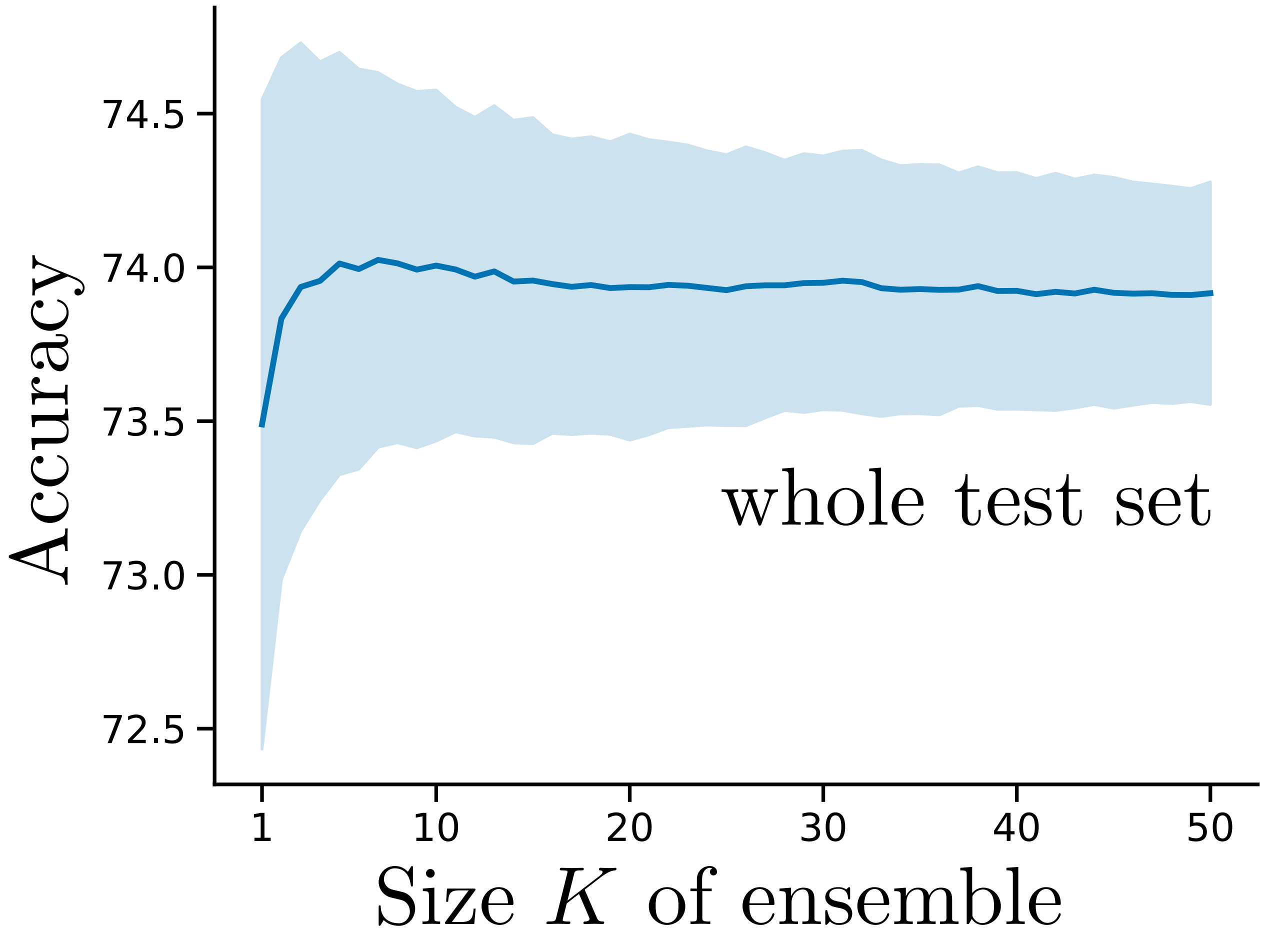
$y_{\text{true}} = 1$

“Infinite ensemble” $\bar{y}_\infty = \mathbb{E}[y_k] = \lim \bar{y}_K$

Ensembles seem to be getting better and better 😀



Ensembles seem to be getting better and better? Really? 🤔



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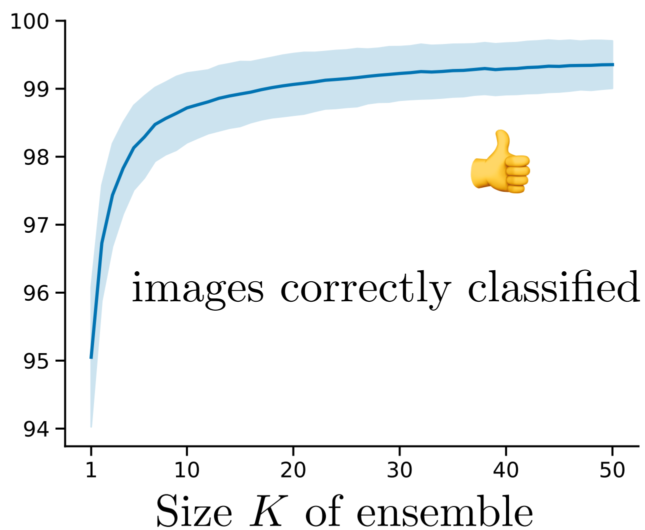

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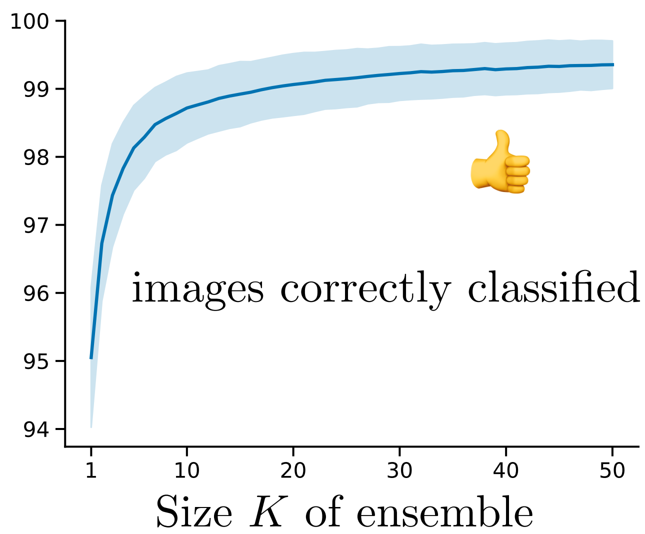

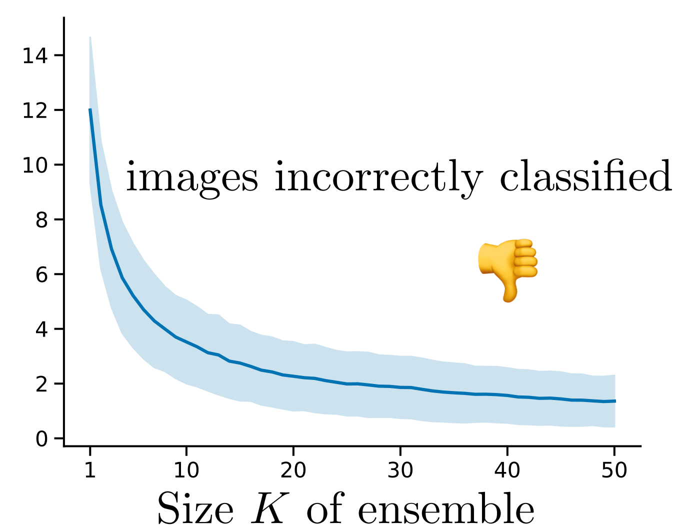

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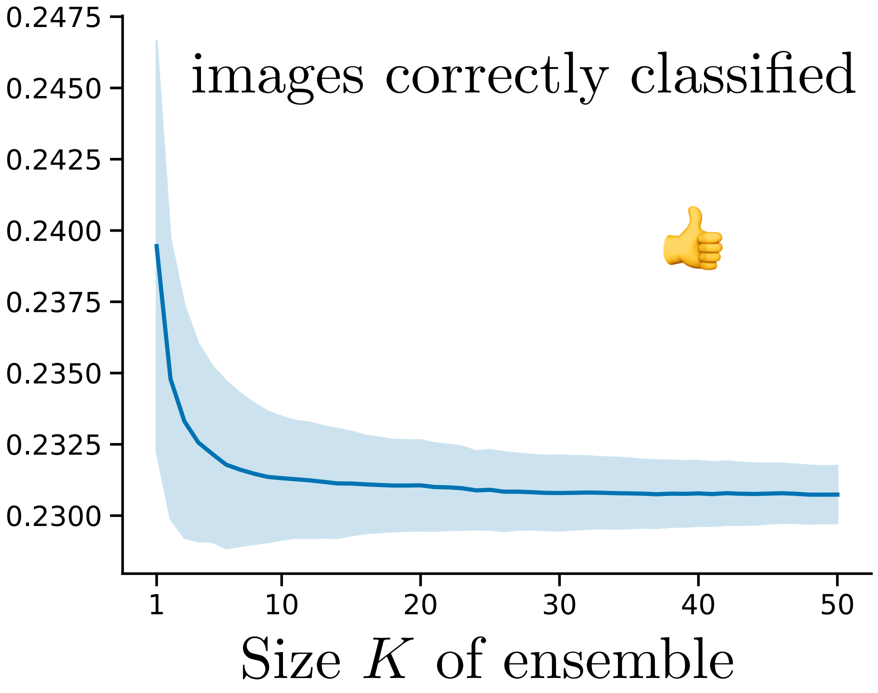
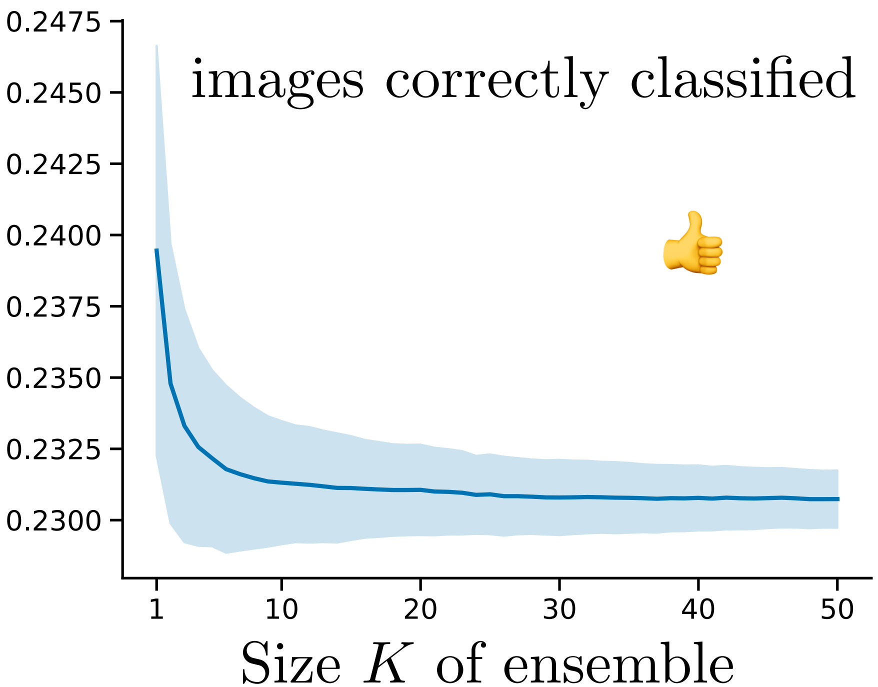
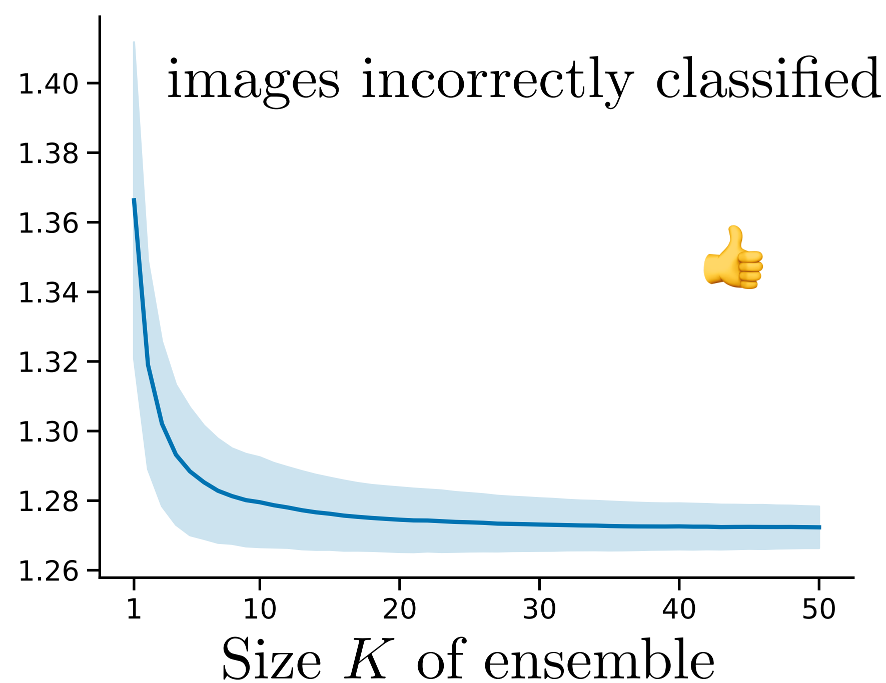


What about the cross entropy?

- Dividing the dataset into the same parts is harmless for the monotonicity of the cross-entropy. It seems that **the cross-entropy is always getting better and better!**





The behaviour we just saw is typical

- These observations are incredibly universal, and were previously highlighted for random forests by Probst and Boulesteix (2018) who looked at **308 data sets!**

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Our goal is to provide a theoretical explaination for these behaviours.

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  - **Cross-entropy and Brier score are convex**, which is not the case of classification error/AUC.

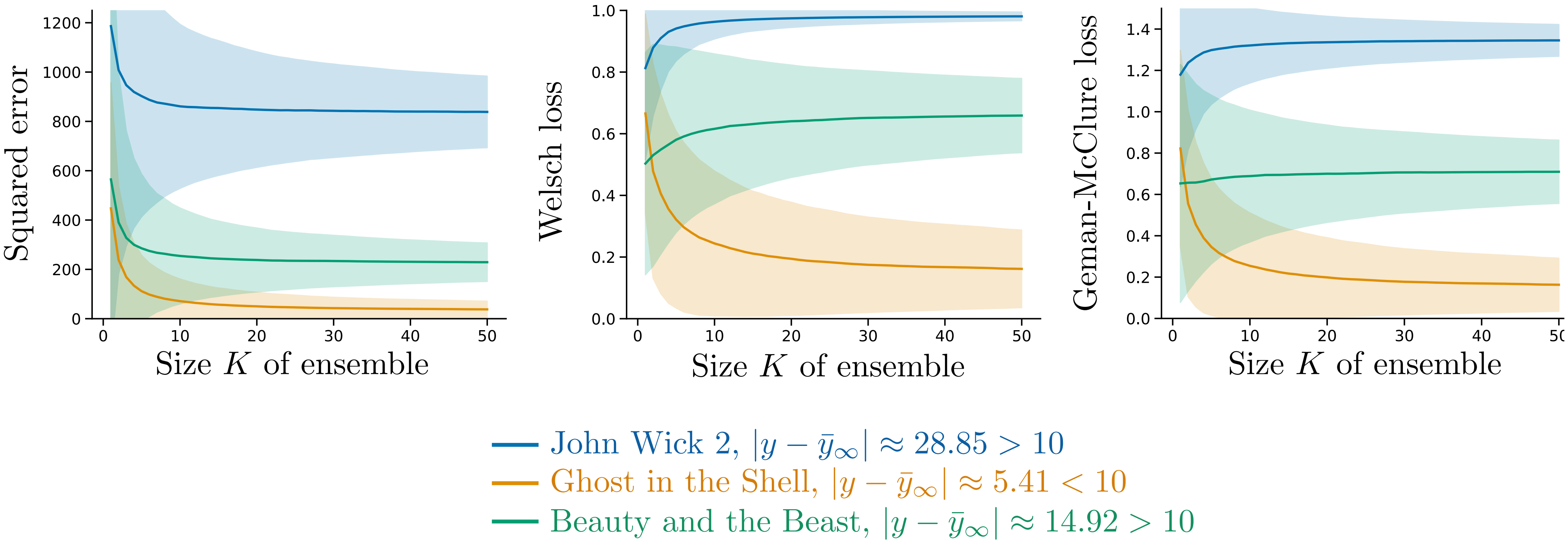
- Our main contribution is to show that this convexity divide is responsible for the results we just saw. We will essentially show that

  - **For convex losses, ensembles are getting better all the time**

  - **For convex losses, ensembles are improving over "good" data points and getting worse over "bad" data points.**

This goes beyond classification!

- While we only talked about classification so far, **these insights are true as long as there is an ensemble and a loss function**, for instance in regression, parameter estimation, or collective intelligence.
- Here a crowd was asked to **predict the ratings of upcoming movies**



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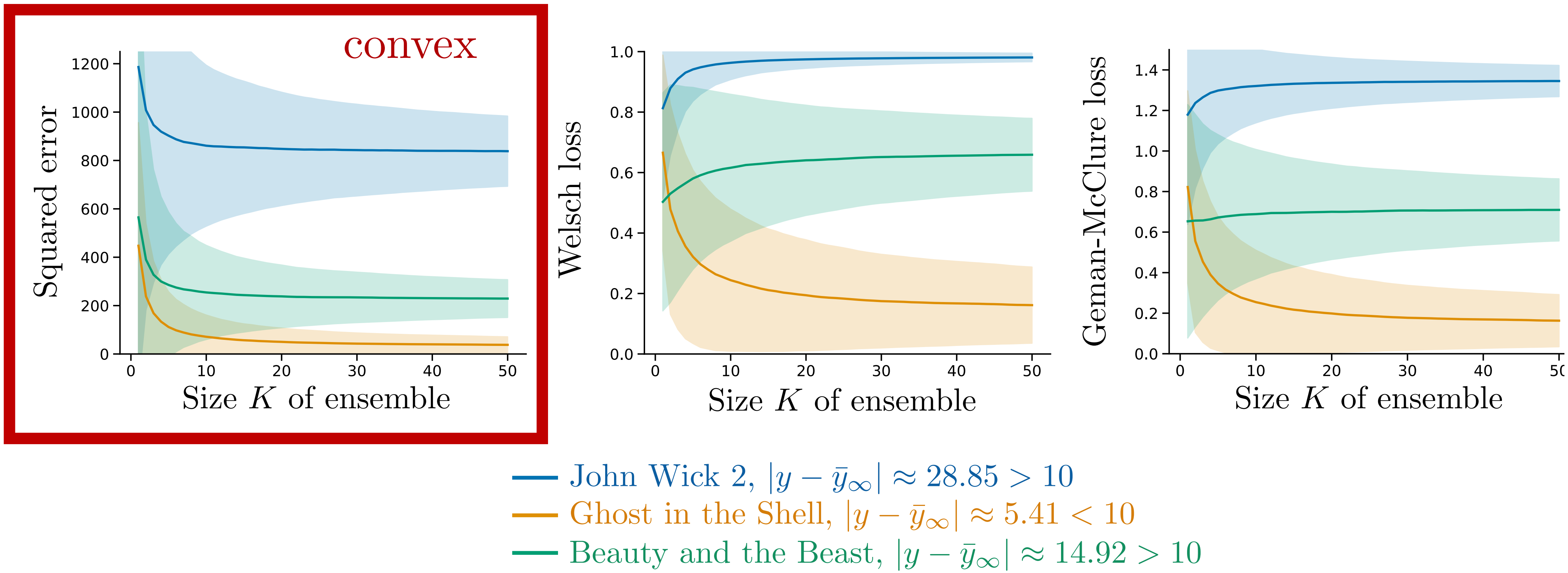

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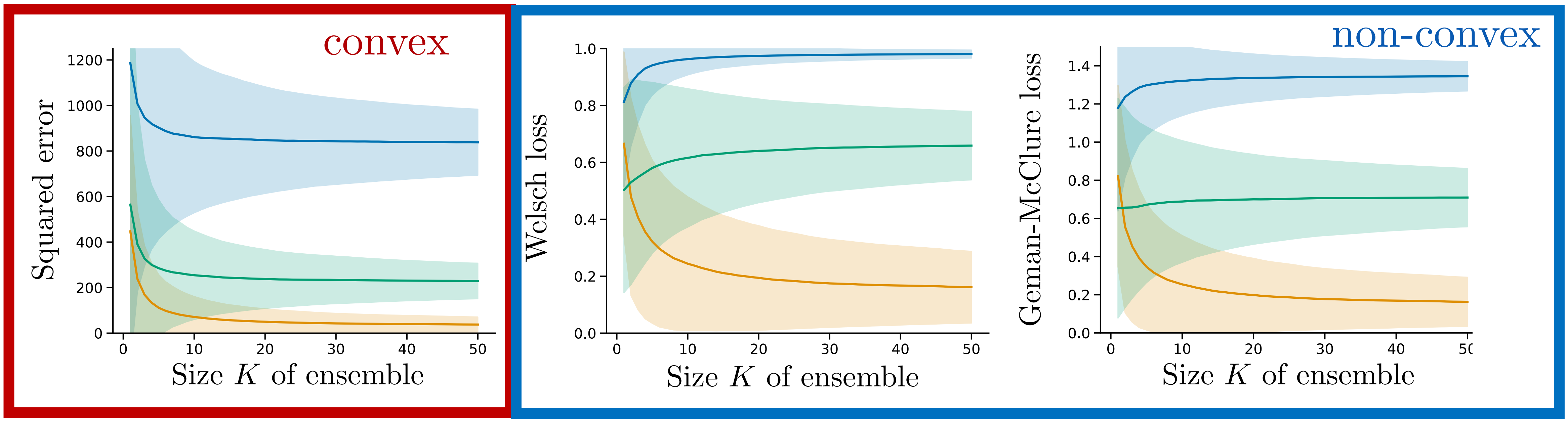

John Wick 2, $|y - \bar{y}_\infty| \approx 28.85 > 10$
Ghost in the Shell, $|y - \bar{y}_\infty| \approx 5.41 < 10$
Beauty and the Beast, $|y - \bar{y}_\infty| \approx 14.92 > 10$

4

For convex losses, ensembles are getting better all the time

Formalising the problem

- We have predictions $\hat{y}_1, \ldots, \hat{y}_K \in C$ (e.g. the predictive probabilities of K neural nets for a single given image), and we want to look at the **average prediction**

$$\bar{y}_K = \frac{1}{K} \sum_{k=1}^{K} \hat{y}_k$$

- We also assume that we have a **loss function** $L : C \to \mathbb{R}$

- Since we want to have results on the influence of the predictions at the **data point level**, we assume that everything is fixed except the $\hat{y}s$.

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$$\overline{y}_\infty = \mathbb{E}\left[\hat{y}_1\right] = \cdots = \mathbb{E}\left[\hat{y}_K\right]$$

Form

All these assumptions are true for random forests, deep ensembles, bagging,…

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Refresher: Jensen's inequality

- If we assume that the loss is convex, we have **convexity and averages**, so using Jensen's seems like a good idea.
- Reminder: in its general form, Jensen's states that $f(\mathbb{E}[x]) \leq \mathbb{E}[f(x)]$ when f is convex and these expectations exist.
- A useful version is its **finite form**

$$f\left(\frac{1}{K}\sum_{k=1}^{K} x_k\right) \leq \frac{1}{K}\sum_{k=1}^{K} f(x_k)$$

Jensen's and ensembles, old school classics

- Using the finite form of Jensen's gives

$$L(\overline{y}_K) \leq \frac{1}{K} \sum_{k=1}^{K} L(\hat{y}_k)$$

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Average loss of the individual models

Loss of the worst model

For this, we don't even need to assume that the predictions are random variables!

Jensen's and ensembles, old school classics

- Using the finite form of Jensen's gives

$$L(\overline{y}_K) \leq \frac{1}{K}\sum_{k=1}^{K} L(\hat{y}_k) \leq \max_{k\in\{1,\ldots,K\}} L(\hat{y}_k)$$

- If $\hat{y}_1, \ldots, \hat{y}_K$ are exchangeable with mean $\overline{y}_\infty = \mathbb{E}\left[\hat{y}_1\right] = \cdots = \mathbb{E}\left[\hat{y}_K\right]$, Jensen's further gives

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Loss of the "infinite" ensemble

Average loss of a finite ensemble

Jensen's and ensembles, old and new

- The arguments of the previous slides were already used in the ensemble papers from the 90s (Michael Perrone's 1993 PhD thesis, Krogh and Vedelsby, 1995, Breiman, 1996).
- When L is the squared error, this is just another way to say that **ensembling reduces the variance**
- The summary was that **an ensemble with a single model is worse than one with a finite number of models $K \geq 2$, which is in turn worse than one with an infinite number of models.**

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- The summary was that **an ensemble with a single model is worse than one with a finite number of models $K \geq 2$, which is in turn worse than one with an infinite number of models.**
- But this says nothing about the question that really interests us : **Is it always true that an ensemble of K models performs better than an ensemble of $K-1$ models?**
- Actually, playing around with Jensen's inequality allows to have a simple answer to that question.

Playing around with Jensen's

- Our goal is to use Jensen's to show that ensembles are getting better, i.e. that

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- Using Jensen's then gives us

$$L\left(\frac{1}{K}\sum_{k=1}^{K}\hat{y}_k\right) \leq \frac{1}{K}\sum_{j=1}^{K}L\left(\frac{1}{K-1}\sum_{k\neq j}\hat{y}_k\right)$$

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- Averaging this expression gives

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Equals $\mathbb{E}\left[L\left(\overline{y}_{K-1}\right)\right]$ because of exchangeability

Ensembles get better for convex losses

- We have just shown that, when the predictions are exchangeable and the loss is convex, **ensembles are monotonically getting better**

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  - Also related to **the monotonicity of IWAE bounds**, as first noticed by this paper
    - Noh et al., *Regularizing deep neural networks by noise: Its interpretation and optimization*, NeurIPS 2017

5

What happens for nonconvex losses?

Can we reuse what we did for non-convex losses?

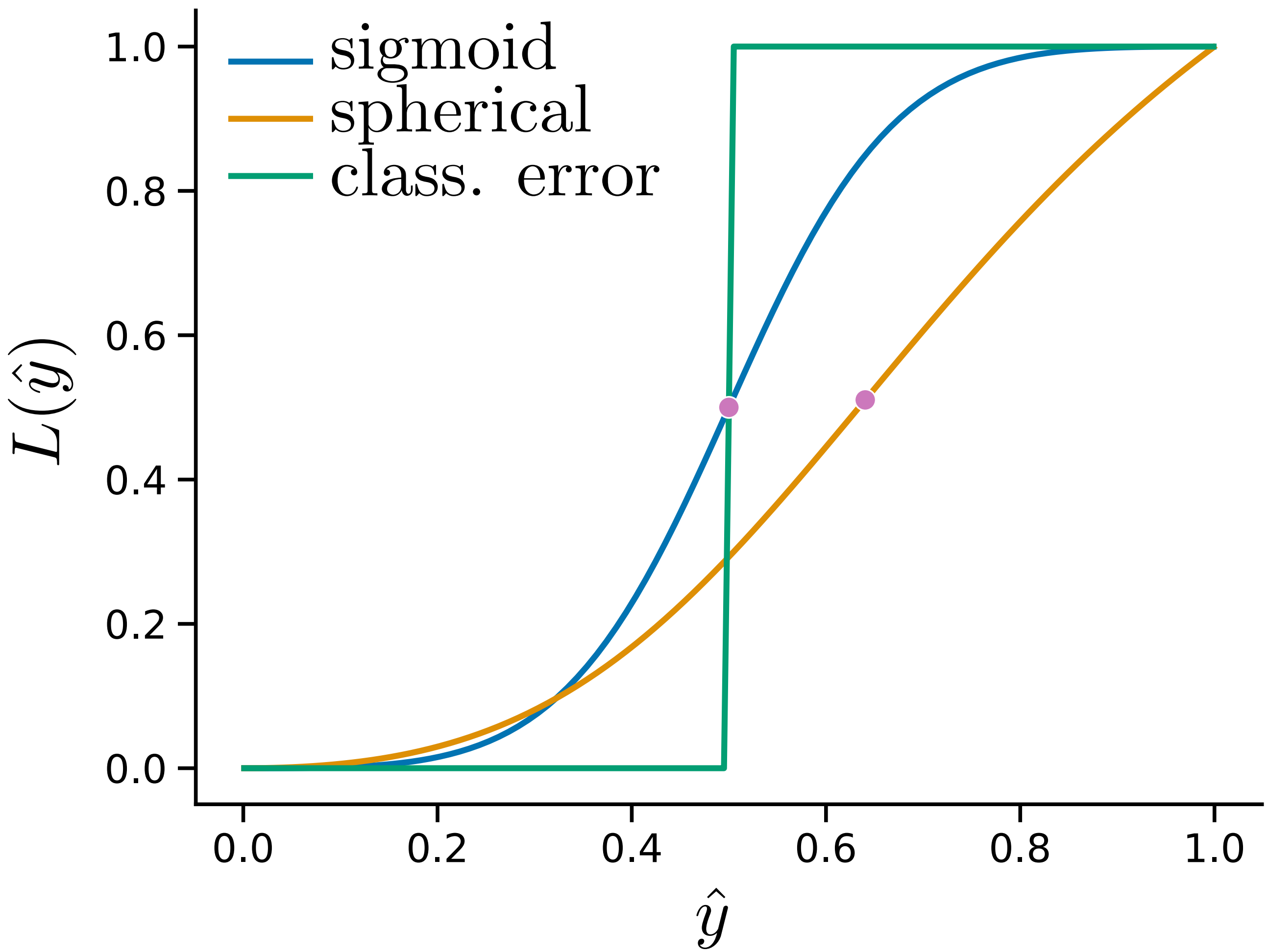
- There is an instance of nonconvex loss that can be tackled by the convex theory! Is we have a **concave loss then ensembles are always getting worse:**

$$\mathbb{E}\left[L\left(\overline{y}_K\right)\right] \geq \mathbb{E}\left[L\left(\overline{y}_{K-1}\right)\right]$$

- Of course concave loss do not exist in real life, but this still gives us some insights about what’s going on.

- Indeed, some losses are convex in some part of the prediction space, and convex in another part. **If our predictions mostly end up in the concave part, we can expect our ensembles to get worse!**

Some nonconvex losses for binary classification



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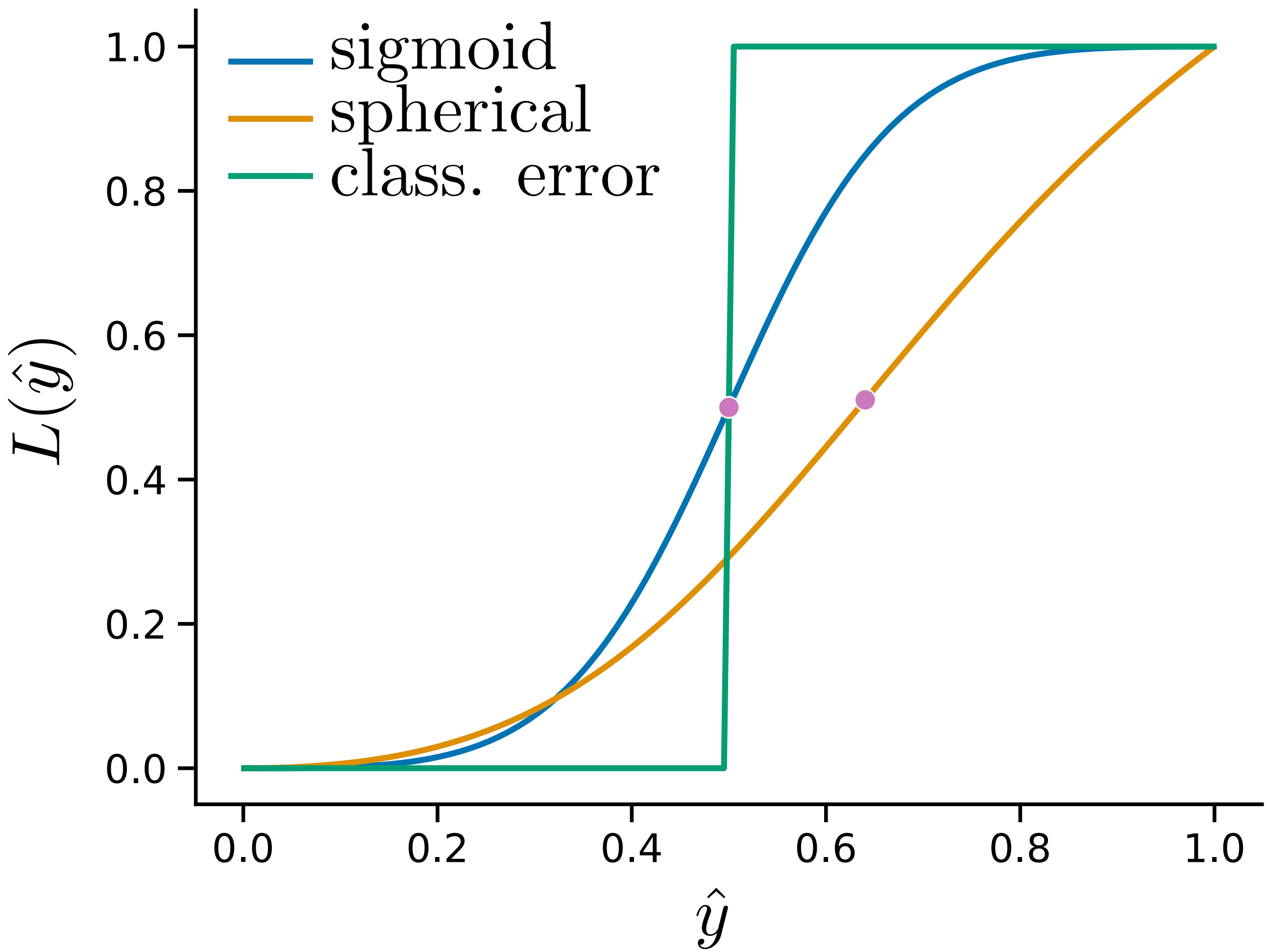

- The smooth losses are **convex when predictions are « right »** (above the purple inflexion point) and **concave when they are « wrong »**.

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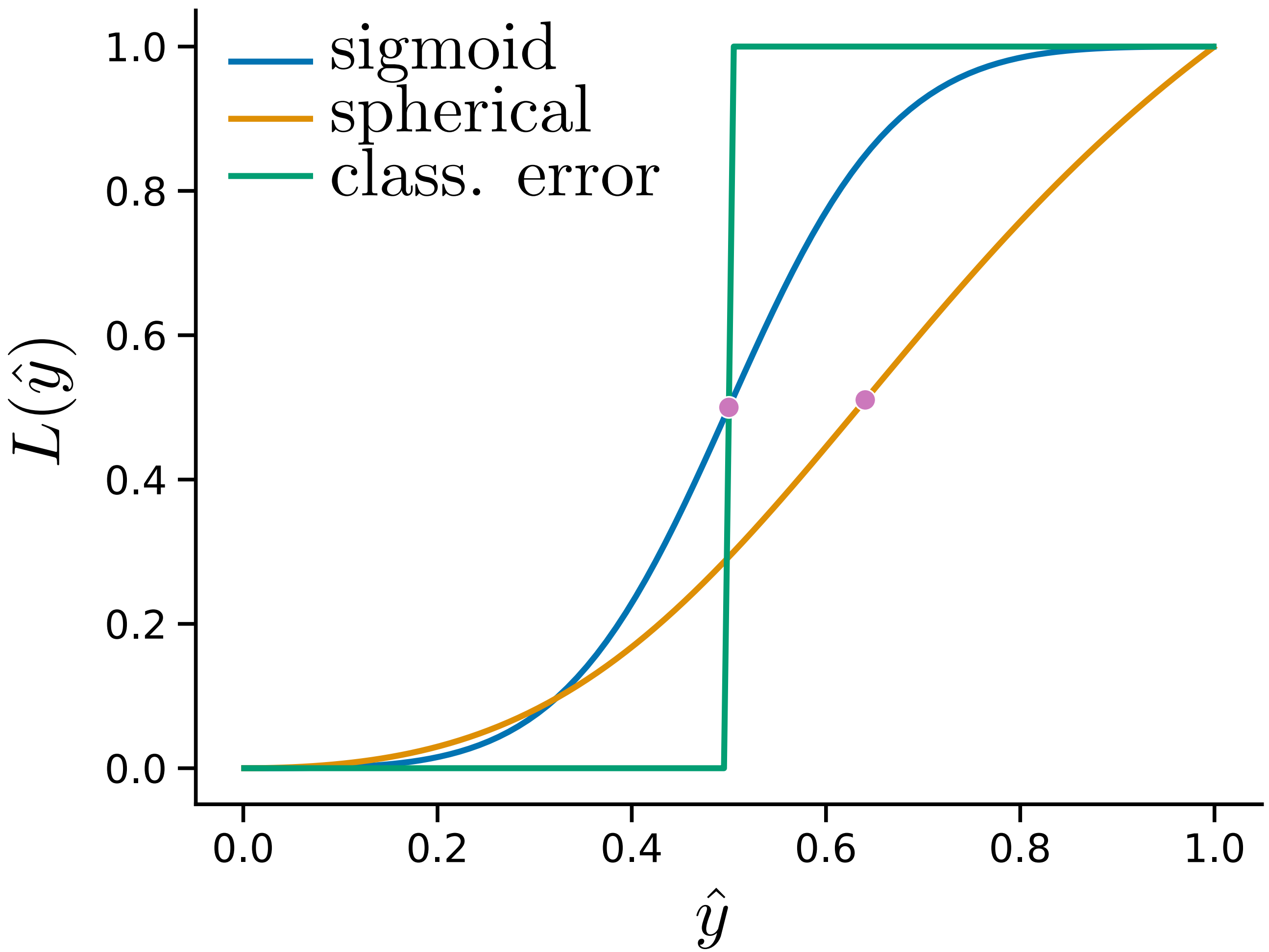

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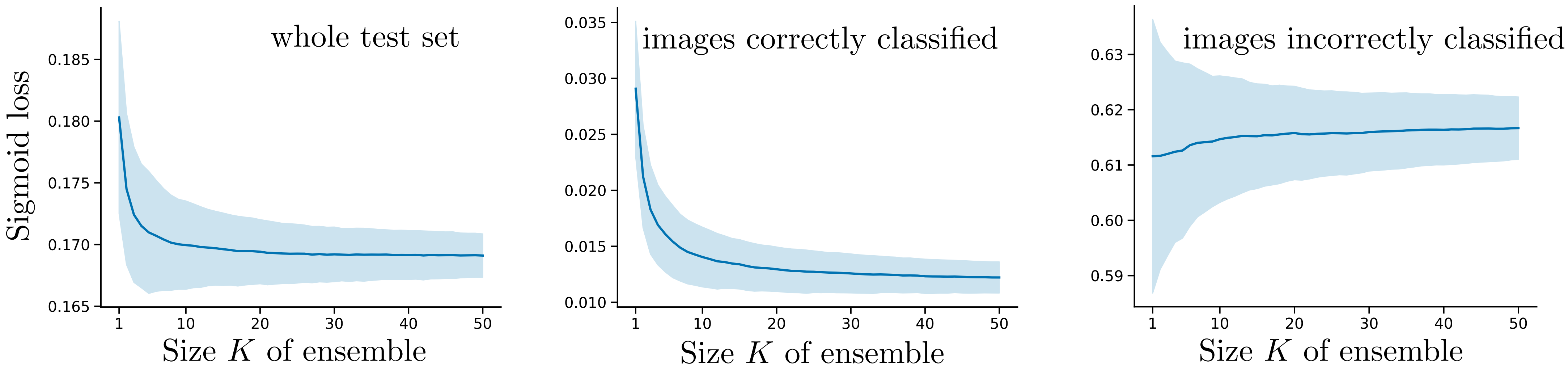
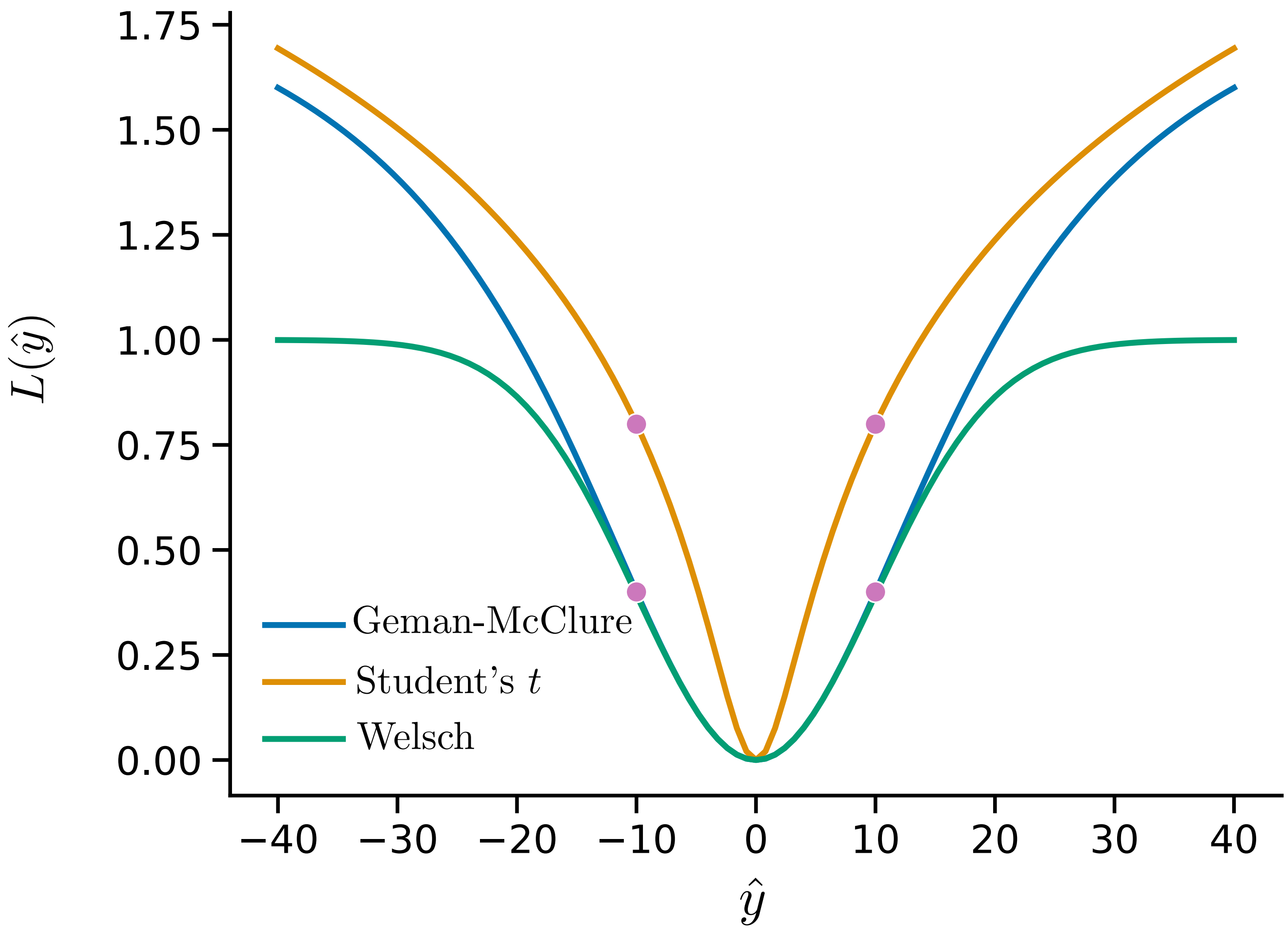
- The classification error can be approximated by the sigmoid loss

The sigmoid loss behaves roughly like the classification error

Good ensembles get better, bad ones get worse

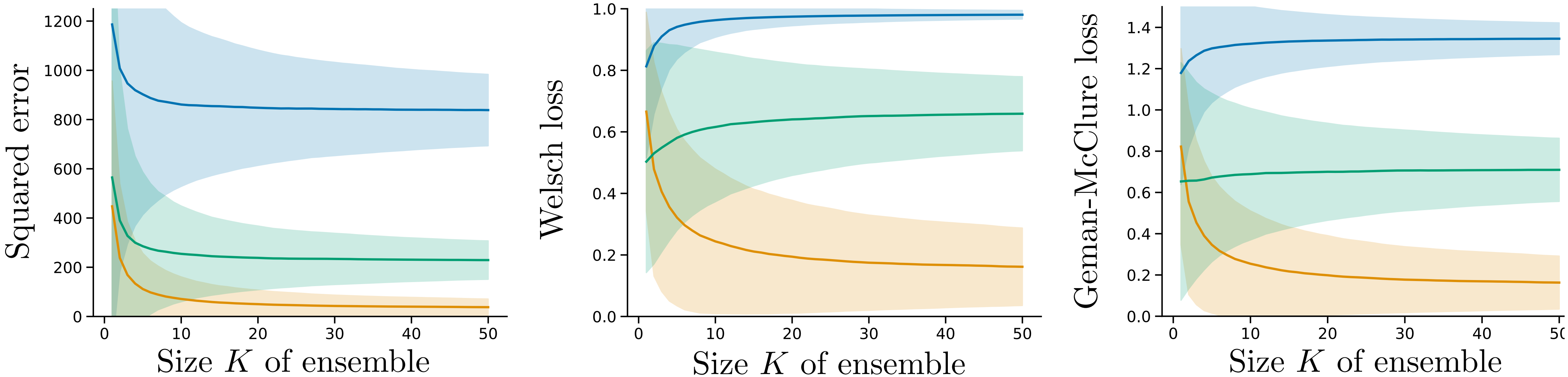


Some nonconvex losses for regression



- The smooth losses are **convex when predictions are « right »** (above the purple inflexion point) and **concave when they are « wrong »**.
- The classification error can be approximated by the sigmoid loss
- Same insights for regressions losses.

Again, good ensembles get better, bad ones get worse for nonconvex losses



John Wick 2, $|y - \bar{y}_\infty| \approx 28.85 > 10$

Ghost in the Shell, $|y - \bar{y}_\infty| \approx 5.41 < 10$

Beauty and the Beast, $|y - \bar{y}_\infty| \approx 14.92 > 10$

We can formalise this!

Theorem. Let $\hat{y}_1, \ldots, \hat{y}_K \in C$ be nondegenerate i.i.d. random variables whose first 5 moments are finite, and L be a function with continuous and bounded partial derivatives of order up to 5, with Hessian matrix H. Then

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The proof essentially relies on a fourth order Taylor expansion of the loss.

What about the classification error?

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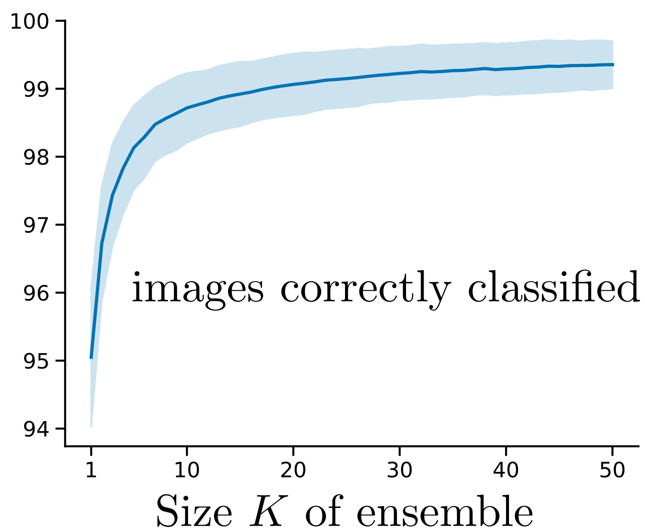
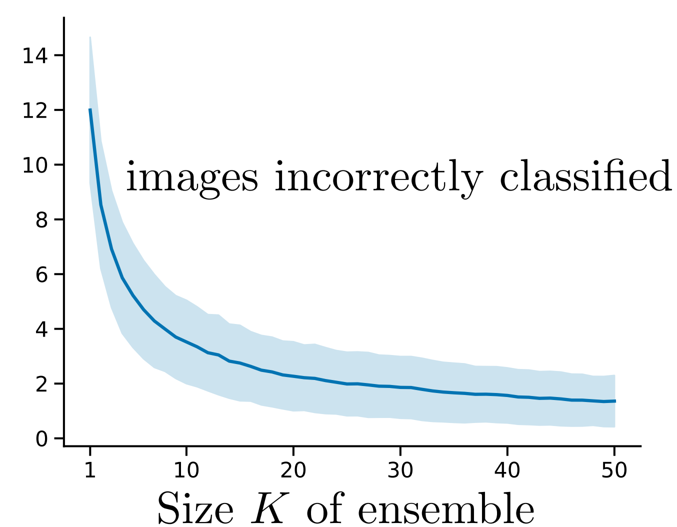
- Since the accuracy is well-approximated by the sigmoid loss, the previous result seems to indicate that **the accuracy will be increasing for points well classified**, and **decreasing for points misclassified**. In practice, we saw in the beginning that this was indeed the case





Can we show the previous conjecture?

- Surprisingly, things get very weird for the classification error.

- **We were looking for a quick and natural proof**
  - using the fact that the sigmoid approximates the classification error
  - using the fact that the result is true if the $\hat{y}s$ are Gaussian and then use the central limit theorem (or Berry-Esseen, or large deviations?)

- **Nothing worked.** And for good reason. Indeed, we found that there is a very simple counter–example that dates back to Condorcet (1785) !

Condorcet's counter-example for binary classification

- For binary classification when the true label is 0, the average error is just
$$\mathbb{E}[L(\overline{y}_k)] = \mathbb{P}(\overline{y}_K \geq 0.5)$$
- Now, let $\hat{y}_1, \cdots, \hat{y}_K \sim \mathcal{B}(\overline{y}_\infty)$
- We would very like $\mathbb{E}[L(\overline{y}_k)]$ to be decreasing if $\overline{y}_\infty < 0.5$ and increasing if $\overline{y}_\infty > 0.5$

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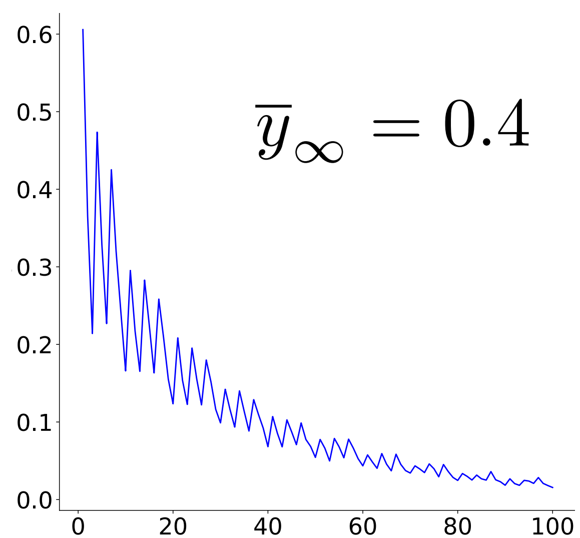
but…

Non-monotonicity seems to be there because of the potential ties, ie when $\overline{y}_K = 0.5$



We did manage to do something!

Let $\hat{y}_1, \ldots, \hat{y}_K \in \mathbb{R}^{n_{\text{Cl}}}$ be i.i.d. random variables. Then

1. If the prediction is asymptotically correct (Weird assumption 1), then the ensemble is eventually getting better: for K large enough,

$$\mathbb{E}\left[L\left(\overline{y}_K\right)\right] < \mathbb{E}\left[L\left(\overline{y}_{K-1}\right)\right], \tag{1}$$

2. If the prediction is asymptotically completely incorrect (Weird assumption 2), then the ensemble is eventually getting better: for K large enough,

$$\mathbb{E}\left[L\left(\overline{y}_K\right)\right] > \mathbb{E}\left[L\left(\overline{y}_{K-1}\right)\right]. \tag{2}$$

Proof idea: use strong large deviation theorems: Bahadur-Ranga Rao-Petrov for binary classification and Joutard for multiclass.

Our basic (kinda new) tool

Theorem 1 (monotonicity of tail probabilities, univariate) *Let* $X_1, \ldots, X_n$ *be i.i.d. random variables with finite expectation* μ*, and let* $\varepsilon > 0$*. Assume furthermore that*

1. $\mathbb{E}\left[\mathrm{e}^{tX_1}\right] < +\infty$ *for all* $t \in \mathbb{R}$*;*
2. $\mathbb{P}\left(X_1 > \mu + \epsilon\right) > 0$*;*
3. X_1 *is absolutely continuous with respect to the Lebesgue measure;*

or, alternatively to (3),

(3bis) X_1 *is a lattice random variable and* $\mathbb{P}\left(X_1 = \mu + \epsilon\right) > 0$*.*

Then, $\mathbb{P}\left(\overline{X}_n \geq \mu + \varepsilon\right)$ *and* $\mathbb{P}\left(\overline{X}_n > \mu + \varepsilon\right)$ *are both strictly decreasing for all* n *large enough.*

Similar result in the multivariate case but much more complicated...

Conclusion

- From a practical perspective, our results strengthen and confirm the message of Probst and Boulesteix: **ensemble size should not be tuned, and ensembles should be as large as possible.**

- **This work was solely about the « pure variance reduction effect » of generic ensembles**. Of course, this is a **very small part of the story**

- Theoretical work on specific kinds of ensembles is also very important
  - Scornet and Hooker, **Theory of Random Forests: A Review**, HAL-05006431, 2025
  - Wild et al., **A Rigorous Link between Deep Ensembles and (Variational) Bayesian Methods**, NeurIPS 2023
  - Hron et al., **Variational BayesiaVariational Bayesian dropout: pitfalls and fixes**, ICML 2023