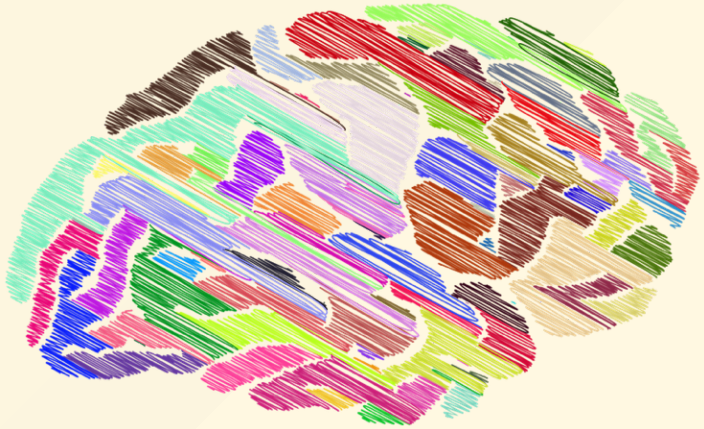
PAC-Bayesian Theory



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Agenda for today

1. Recap on VC theory
2. Bayesian data modelling
3. PAC-Bayes theorem
4. PAC-Bayes for NNs
5. PAC-Bayesian model comparison

VC theory

We proved that:

$$\mathbb{P}\left[\text{for any } f \in F \;\middle|\; \text{train error} - \text{test error}\right| \geq \varepsilon\Big] \leq \frac{2\,\mathbb{E}_X[N(F,X)]}{\exp\left(m\frac{\varepsilon^2}{2}\right)}$$

In words: the chance that any classifier gets substantially different error on randomly drawn train and test sets (each containing m datapoints) depends on a tradeoff between m and the average number of distinct labellings the function class F can apply to $2m$ datapoints X drawn from the data distribution.

Basic mechanism of VC theory

① If a classifier $f \in F$ gets very different train and test error, then from the point of view of that classifier something very imbalanced and unlikely happened in the data sampling.

② But if there are lots and lots of classifiers, then it can become quite likely that something unlikely happens to one of them.

③ VC theory's advice is thus to limit the number of classifiers, as measured by realisable dichotomies on a finite sample.

Pitfalls of VC theory

- neural nets still generalise even when they are capable of realising all 2^m dichotomies of m points.

- asking for no classifier $f \in F$ to overfit is overkill. We only care about the classifier found by the optimiser.

- the VC bound we derived is blind to the complexity of the training labels —— the complexity measure (RHS) only depends on the inputs.

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Bayes' theorem

A Bayesian will tell you that all a data scientist needs is:

$$P(\text{model} \mid \text{data}) = \frac{P(\text{data} \mid \text{model})\, P(\text{model})}{P(\text{data})}$$

(likelihood) (prior)

(posterior)

(evidence)

... but there's a jarring contrast to deep learning — we train a single model, we don't find a posterior distribution over models. Let's ignore this for a moment.

What is the Bayesian evidence?

The denominator of Bayes' thm will be very important to us.

$$\underbrace{P(\text{model}\,|\,\text{data})}_{\text{(posterior)}} = \frac{\overbrace{P(\text{data}\,|\,\text{model})}^{\text{(likelihood)}}\ \overbrace{P(\text{model})}^{\text{(prior)}}}{\underbrace{P(\text{data})}_{\text{(evidence)}}}$$

"evidence" for the model class:

$$P(\text{data}) = \sum_{\text{all models}} P(\text{data}\,|\,\text{model})\ P(\text{model}).$$

It's the probability of randomly sampling a model from the prior and finding that it fits the data.

Evidence for a NN

For a classification problem, a natural likelihood function is

$$P(\text{data} \mid \text{model}) = \begin{cases} 1 & \text{if model fits all training labels} \\ 0 & \text{otherwise.} \end{cases}$$

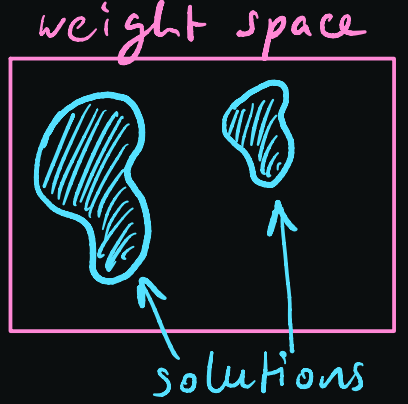
The evidence then simplifies to

$$P(\text{data}) = \sum_{\substack{\text{models that fit} \\ \text{all labels}}} P(\text{model}).$$

total prior probability of models that get 100% training acc.

Think of this as:

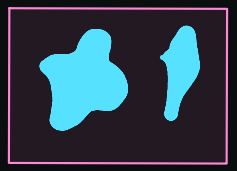
$$\text{evidence} = \frac{\text{volume of solutions}}{\text{volume of weight space}}.$$



Properties of the evidence

The evidence has some nice properties:

① For a fixed NN architecture, we might expect it to to reflect the "hardness" of the dataset.



easy data
⇒ more solutions

hard data
⇒ fewer solutions

② For a fixed dataset, we might expect it to reflect the suitability of an NN architecture.

good architecture
⇒ more solutions

bad architecture
⇒ fewer solutions

Connection to generalisation?

③ The evidence has an information theoretic interpretation:

draws from the prior to find a solution $\approx \frac{1}{\text{evidence}}$

$\Rightarrow$ a <u>random</u> solution can be described by the random seed and $\approx \log \frac{1}{\text{evidence}}$ additional bits.

So it seems like a good candidate for a fairly general purpose complexity measure.

David MacKay wrote in 1995:

"Empirically, the correlation between the evidence and generalization error is often good ... but a theoretical connection between the two is not yet established."

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Basic mechanism of PAC-Bayes

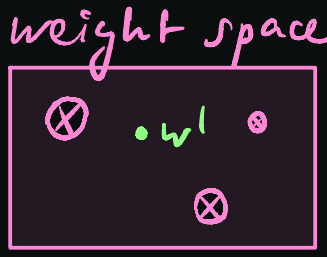
Draw a fresh iid train and test set.

Next, draw a random weight vector w from the weight space.

Q1: would you expect w to have similar train and test error?

A1: Yes!

Next, I look at the training data, and decide to exclude 5% of weight vectors:



You draw a random weight vector w' from the 95% that remain.

Q2: would you expect w' to have similar train and test error?

A2: Yes! Excluding 5% of weight vectors can't change much.

a simplified version.

Statement of the result

PAC-Bayes: the fewer the weight vectors that are excluded by the training data, the better a random solution will generalise.

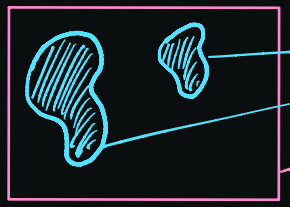
More formally, for a proportion $1-\delta$ of iid training sets,

$$\underset{\text{solutions}}{\text{averaged over}}\left[\text{population error}\right] \leq \frac{\log\left(\frac{1}{\text{evidence}}\right) + \log\left(\frac{2m}{\delta}\right)}{m-1}.$$

where: m = # training points

a solution is a weight vector that gets 100% train acc

$$\text{evidence} = \frac{\text{volume of solutions}}{\text{volume of weight space}}$$



Deriving the result (sketch)

On HW4 we show: $$\mathbb{E}_{w\sim Q}\, h(w) \leq \frac{KL(Q\|P) + \ln \mathbb{E}_{w\sim P} e^{\beta h(w)}}{\beta}.$$

- set $\beta = m-1$ (# train points -1)
- set P to the prior on weight space
- set Q to the prior restricted to the solutions

$$\Rightarrow KL(Q\|P) = \log \frac{1}{P(\text{all solutions})} = \log \frac{1}{\text{evidence}}$$

- set $h(w)$ to the generalisation error of weight vector w
  ↪ for $w \sim Q$, w gets 0% train error $\Rightarrow$ $h(w)$ measures population error.

<u>Critical step</u>: since P does not depend on the train set, then we would expect $\ln \mathbb{E}_{w\sim P} e^{\beta h(w)}$ to be small. In fact, we can show that for a fraction $(1-\delta)$ of iid train sets, $\ln \mathbb{E}_{w\sim P} e^{\beta h(w)} \leq \ln \frac{2m}{\delta}$.

Proving this requires doing some statistics. See references on website.

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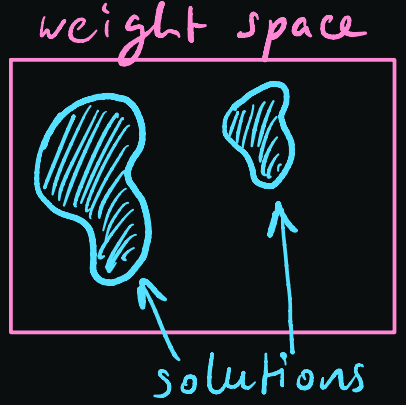
Evidence for a neural net

PAC – Bayes: for a fraction $(1-\delta)$ of iid train sets,

$$\underset{\text{over solutions}}{\text{averaged}}\left[\text{population error}\right] \leq \frac{\log\left(\frac{1}{\text{evidence}}\right) + \log\left(\frac{2m}{\delta}\right)}{m-1}.$$

Recall:

$$\text{evidence} = \frac{\text{volume of solutions}}{\text{volume of weight space}}.$$



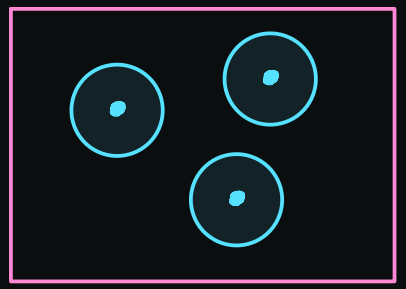
How can we compute the evidence for a neural net?

Attempt #1: sharpness/flatness

IDEA: if a solution is "flatter" then the evidence will be larger.

Think of "flatness" as the amount we can perturb a solution w before we induce a misclassification.

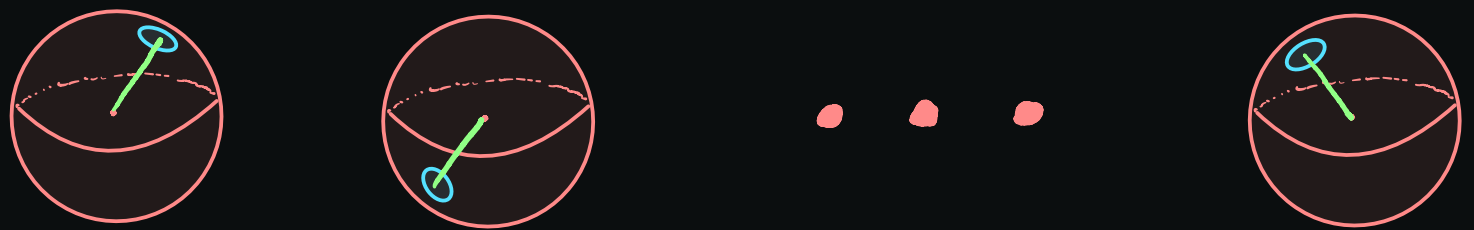
Let's model the solution space as being comprised of K such non-intersecting solutions:



Attempt #1: sharpness/flatness

To work this idea through, let's consider a neural net composed of n neurons with fan-in d, each with a weight vector w satisfying $\sum_{i=1}^{d} w_i = 0$, $\sum_{i=1}^{d} w_i^2 = 1$.

Geometrically, a solution weight vector is a point on the Cartesian product of n $(d-2)$-spheres:



Define "flatness" to be the max angle α we can arbitrarily rotate every neuron through without causing a misclassification.

Attempt #1: sharpness/flatness

Letting the prior be uniform over the n hyperspheres, we get:

$$\text{evidence} = \frac{\text{volume of solutions}}{\text{volume of weight space}} = K \times \left[\frac{\text{area of } \bigcirc}{\text{area of } \bigcirc}\right]^n$$

Geometry result: the proportion of a $(d-2)$ sphere's surface area taken up by a cap of angle α satisfies:

$$\frac{\text{area of } \bigcirc}{\text{area of } \bigcirc} \geq \frac{1}{2} \sin^{(d-2)} \frac{\alpha}{2}.$$

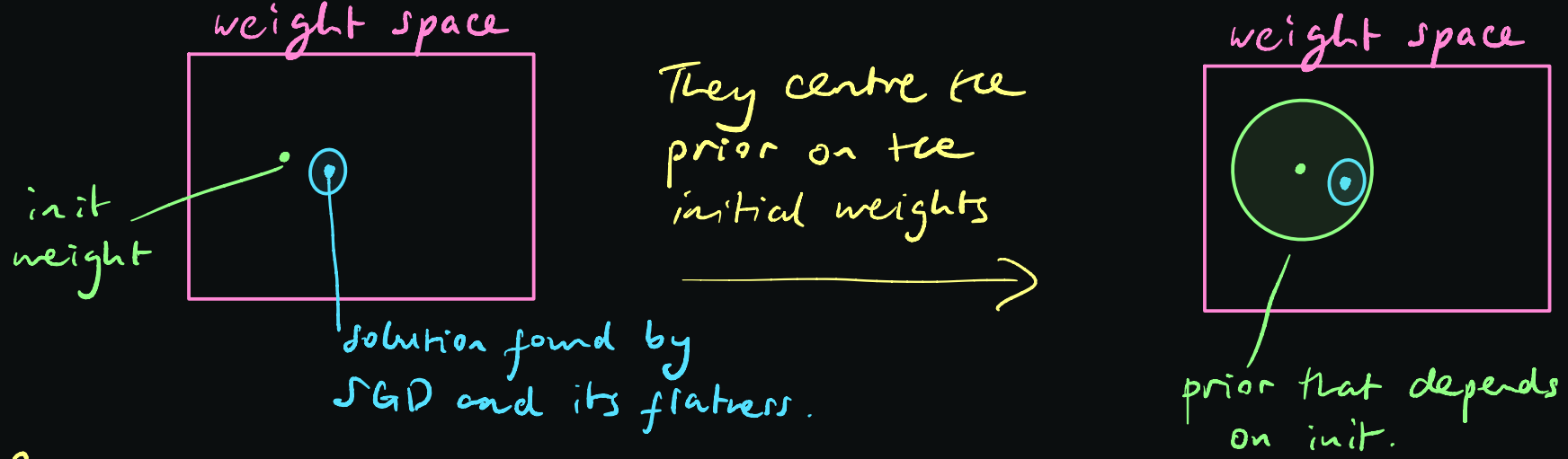
$$\Rightarrow \boxed{\text{evidence} \geq \frac{K}{2^n} \sin^{n(d-2)} \frac{\alpha}{2}}$$

This depends on # degrees of freedom $n(d-2)$, but also on the number of solutions K.

Attempt #2: breaking symmetries

Problem with the previous approach: we don't know K.

Dziugaite & Roy overcome this by using a different prior:



Problem: they don't know how large the prior should be.

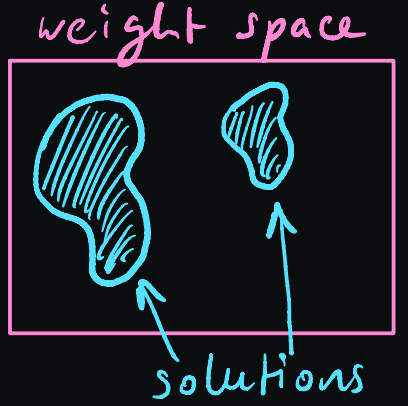
Solution: they derive PAC-Bayes bounds for many priors of varying size, and choose the best one in hindsight.

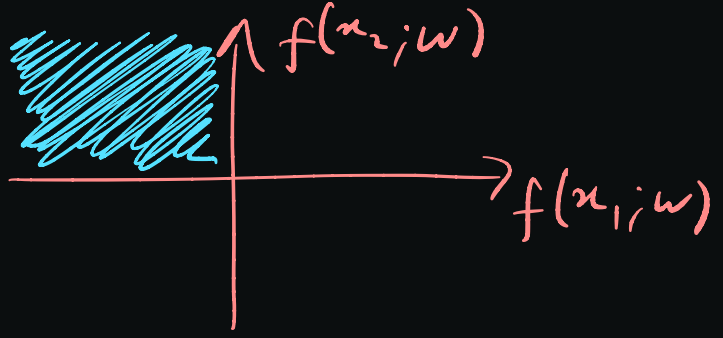
This leads to non-vacuous generalisation bounds for neural nets, although choosing over many priors pays a cost in terms of failure probability.

Attempt #3: infinite width

The structure of the solution manifold in weight space is complicated.

But in function space, it is simple!





For binary classification, it is an orthant.

So for ∞-ly wide NN binary classifiers, by the NNGP correspondence,

$$\text{evidence} = \mathbb{P}_{z \sim \mathcal{N}(0,\Sigma)}\left[\text{sign}(z) = y\right]$$

Σ: NNGP covariance.

y: vector of training labels

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Comparing two architectures

What is any of this good for?

Suppose we want to know which of two NN architectures is better on a certain task, a Bayesian would tell us to compare the evidence for each architecture.

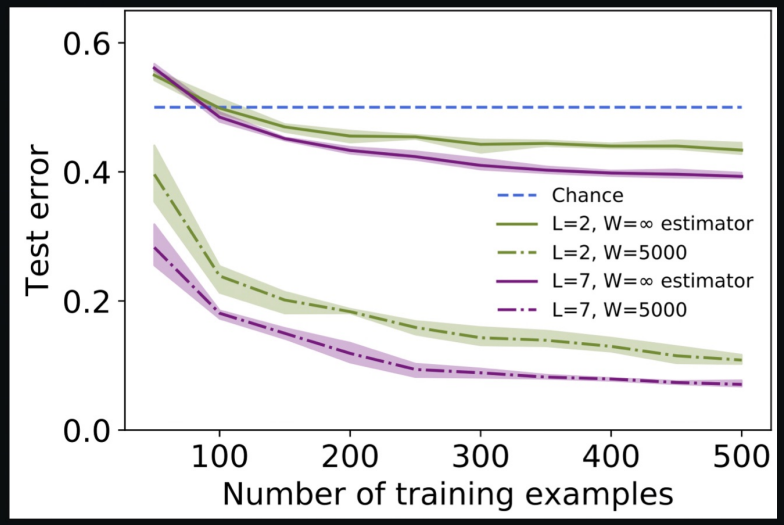
good architecture
⇒ more solutions
⇒ more evidence

bad architecture
⇒ fewer solutions
⇒ less evidence

PAC-Bayes goes further — it says we'd expect random solutions from the architecture with more evidence to generalise better.

An example

Want to choose between a 7-layer MLP and a 2-layer MLP for classifying MNIST digits as even or odd.



comparing the PAC-Bayes upper bound estimated for infinitely wide networks versus the empirical test error at finite width as a fn. of training set size.

Seems to be a viable tool for model comparison!

Summary

- PAC-Bayes relates the expected generalisation error of a random solution to the volume of weight space excluded by the training data.
- The complexity measure is $\log \frac{1}{\text{Bayesian evidence}}$.
- Yields generalisation bounds that are non-vacuous, and can be used to perform model comparison or compare the hardness of different datasets.

Next lecture

Project ideas.