

**MACHINE LEARNING, SINGULARITY THEORY AND PHASE
TRANSITIONS
UNIVERSITY OF AMSTERDAM, 18-21 SEPTEMBER 2023**

Abstract

This is the program of an informal workshop organised at the University of Amsterdam around *Singular learning theory* and its burgeoning applications to the training dynamics of deep neural networks. This is a topic at the interface of machine learning, statistics and singularity theory in real-analytic geometry, so we expect a diverse audience, and the talks of the first day will provide some background from each discipline. Singular learning theory is an application of the tools of singularity theory to Bayesian statistics, and is a promising framework to understand some of the mysteries of modern deep learning. Our goal will be to understand the recent paper Quantifying degeneracy in singular models via the learning coefficient [4], both at a theoretical and practical level, and discuss work-in-progress on other deep learning systems.

PRACTICAL DETAILS

- The workshop will take place from Monday 18th to Thursday 21st, from 10:00 to 17:00.
- Everything will take place Room F1.15, in the building Science Park 107 of the Science Park campus of the University of Amsterdam.

OVERVIEW OF THE PROGRAM

- Monday 18st: Learning from data, singularity theory
 - Talk 1 (10:00-11:00): Machine learning, deep learning, mysteries (Zach Furman)
 - Talk 2 (11:00-12:00): Bayesian statistics and statistical learning theory (Alexander Gietelink Oldenziel)
 - Talk 3 (13:00-14:00): Regular and singular models (Simon Pepin Lehalleur)
 - Q& A, discussion, break (14:00-15:00)
 - Talk 4 (15:00-16:00) Analytic geometry and singularities (Louis Jaburi)
 - Talk 5 (16:00-17:00) Measuring degeneracy with the real log-canonical threshold (Simon Pepin Lehalleur)
- Tuesday 19st: Singular learning theory - overview and phase transitions
 - Q& A and discussion (10:00-11:00)
 - Talk 1 (11:00-12:00) Overview of singular learning theory and the free energy formula (Simon Pepin Lehalleur)
 - Talk 2 (13:00-14:00) Internal model selection and Bayesian phase transitions (Simon Pepin Lehalleur)
 - Discussion (14:15-16:00) On the larger picture of phase transitions in deep learning.
- Wednesday 20th : Singular learning practice - estimating learning coefficients and applications to phase transitions.
 - Talk 1 (10:00-11:00) “Quantifying degeneracy in singular models via the learning coefficient ” (Zach Furman)
 - Talk 2 (11:00-12:00) Computing $\hat{\lambda}$ in practice and applications (Stan van Wingerden)
 - Free afternoon!
- Thursday 21st: the fine print.
 - Discussion, work in small groups (10:00-12:00) DIY $\hat{\lambda}$: libraries, internals, APIs
 - Talk 2 (13:00-14:00) Computing RLCTs with algebraic geometry
 - Discussion, work in small groups (14:00-17:00) Looking more closely at the main results of SLT and their proofs.

MONDAY 18TH: LEARNING FROM DATA, SINGULARITY THEORY

Talk 1 (10:00-11:00) Machine learning, deep learning, mysteries.

- Discuss the basic framework of (supervised) machine learning ML: parametrized models, classifiers with loss functions, train and test datasets, etc.
- Introduce simple feed-forward neural networks, discuss tanh and ReLU activation functions.
- Briefly discuss how they are trained in practice: first-order optimization, stochastic gradient descent (SGD) - we will come back to this later on.
- Give an impressionistic overview of how successful deep learning has been in many domains.
- Explain some of the basic mysteries: why are such models trainable? Why do the trained models generalize so well and tend not to overfit? Can we understand the computational structure of trained models and how it forms during training?

Talk 2 (11:00-12:00) Bayesian statistics and statistical learning theory.

- Introduce the framework of Bayesian statistics as used by Watanabe. Explain how to work with a supervised learning ML model such as a DNN in this framework, with the mean square error. Discuss briefly the fact that this is very different from ML practice **Refs:** [1, §1.1-1.4]
- Introduce the basic quantities of statistical learning theory (which let us track how well the model is learning) and their relationships: generalization, training and cross-validation loss (and their averages), Kullback-Leibler divergence (empirical and averaged), marginal likelihood/partition function, free energy. Point out the difference between losses and errors. **Refs:**[1, §1.6-1.7], omitting WAIC.
- Show in particular that, in the setting of function approximation with mean square error and Gaussian noise, the function K is nothing but the L^2 -distance between the function predicted by the model and the true function (where L^2 is taken with respect to the distribution on inputs). This example is useful to keep in mind throughout the week, as functions are more concrete objects than probability distributions.
- Explain that one goal of statistical learning theory is to understand the behaviour of the various errors in the large n limit, and how the free energy is particularly important ([1, Rmk 10 in §1.7]. One could discuss [1, Example 1.9.4] of a simple Gaussian model where everything can be computed explicitly.

Talk 3 (13:00-14:00) Regular and singular models.

- Introduce the set of optimal parameters W_0 ; explain why we expect the posterior distribution to concentrate along W_0 and so why the “geometry” of W_0 , of K_n and K (in a so far imprecise sense) should be relevant to statistical learning theory.
- Discuss identifiable and non-identifiable models, noting in particular that W_0 is a point for identifiable models. Mention Doob’s theorem. Explain that DNNs are highly non-identifiable.
- Introduce the Fisher information matrix and its link with K . Define regular and singular models.
- State (semi-rigorously) the Bernstein-Von Mises theorem, which shows that for regular realizable models the posterior density converges in L^1 -norm to a Gaussian distribution centered at the optimal parameter. Mention that the starting point is the Laplace approximation for integral, and sketch the proof in 1d.
- Explain (maybe showing plots!) that this is very false for singular models.
- State the asymptotic free energy formula for regular models (perhaps only in the realizable case to keep things simple) [1, §4.2 Theorem 4]

Q& A, discussion, break (14:00-15:00). Possible discussion topics.

- What are standard approaches in statistical learning theory? Why do they fall short for deep learning?

- SGD vs Bayesian inference, what is known rigorously (e.g. in regular convex models)? empirically?

Talk 4 (15:00-16:00) Analytic geometry and singularities.

- Recall definition of smooth and real-analytic functions. Explain why real-analytic functions are better suited to “do geometry” (basically, their sets of solutions are reasonable geometric objects, “generically” manifolds, unlike sets of solutions of smooth functions). Explain why K is a real-analytic function for a tanh DNN.
- Discuss smooth and singular points of a real-analytic set (and the implicit function theorem), and critical points of a real-analytic function.
- Define Morse and Morse-Bott functions and state the Morse-Bott lemma. Connect this to regular/”minimally singular” statistical models.
- Define normal crossings functions and state embedded resolution of singularities for real-analytic functions, in the form used by Watanabe. Explain how this looks like in particular for a positive function like K .
- Briefly mention that, in practice, singularity theory for real-analytic functions can often be reduced to singularity theory for polynomials, and so to real algebraic geometry, which is convenient for some computations; note however that K itself is almost never a polynomial.
- If there is time (!), give example of ADE singularities and their resolutions.

Talk 5 (16:00-17:00) Measuring degeneracy with the real log-canonical threshold.

- Define the real log-canonical threshold (RLCT) or learning coefficient in terms of volume asymptotics, and closely related in terms of integrability.
- Introduce the “density of states” (DOS) function/distribution.
- Explain roughly, using the discussion of the regular case, why understanding the asymptotic behaviour of the DOS close to the optimal parameters is a key step to understanding the asymptotic behaviour of the partition function.
- Explain why the asymptotics of the DOS is closely related to the asymptotics of the volume function, and so the RLCT as defined above. Discuss also the log term and the multiplicity.
- Introduce the zeta function and give the characterization of the RLCT in terms of poles (mentioning the role of the Mellin transform)
- Explain that the zeta function can be computed on a resolution of singularities and give the resulting formula for the RLCT.
- Discuss basic properties of the RLCT (semi-continuity?), and give the formula in the minimally singular case (K Morse-Bott).
- If there is time (!), give example of ADE singularities as a case where we can compute the RLCT and they reflect the “complexity” of the singularity.

TUESDAY 18TH: SINGULAR LEARNING THEORY - THE CORE RESULTS

Q & A and discussion (10:00-11:00). Digesting the material from Monday, before going into the main results! Possible points that deserve clarification:

- Singularities are “measure-zero” objects, so why do we expect them to have any role in a probabilistic/statistical setting? Relatedly, machine learning systems are implemented on a computer, so with finite floating-point precision, so singularities should be “blurred out”; is this a reason to neglect them?

Talk 1 (11:00-12:00) Overview of the main results of SLT. This talk will discuss the main results of statistical learning theory from [2, 1], without proofs. The focus will be on the role of the RLCT as dominant term in the asymptotic expansion of the free energy of singular models.

Talk 2 (13:00-14:00): internal model selection and phase transitions in the Bayesian posterior. Besides Watanabe’s book, a useful reference for this is the talk of Dan Murfet .

- Introduce the general problem of model selection in Bayesian statistics [1, §8.1]
- Introduce local learning coefficients [4]
- Explain why the free energy formula implies phase transitions in the Bayesian posterior and discuss why this can be understood as a form of “internal model selection.” [2, §7.6] [1, §9.4]

Discussion (14:15-16:00): on the large picture of phase transitions in deep learning.

Phase transitions in the Bayesian framework of SLT are mathematically quantifiable phenomena, but we would like to use them to study the phase transitions which are observed empirically during SGD training in deep learning. To help translate between those two set-ups, ideas coming from the study of phase transitions in other contexts, and in particular statistical physics, should prove useful. Since this is very much an unfinished story, a discussion format seems appropriate.

WEDNESDAY 20TH: SINGULAR LEARNING PRACTICE - ESTIMATING LEARNING COEFFICIENTS AND APPLICATIONS TO PHASE TRANSITIONS

Talk 1 (10:00-11:00) “Quantifying degeneracy in singular models via the learning coefficient ”. Goal: present the paper [4] by Lau-Murfet-Wei.

Talk 2 (11:00-12:00) Computing $\hat{\lambda}$ in practice and applications.

Free afternoon!

THURSDAY 21ST: THE FINE PRINT

Discussion, work in small groups (10:00-12:00) DIY $\hat{\lambda}$: libraries, internals, APIs.

Talk 2 (13:00-14:00): Computing RLCTs with algebraic geometry.

- Explain why, in some cases, it is possible to reduce computations of RLCTs to the case of polynomials.
- Define blow-ups and explain that resolution of singularities can always be achieved by a sequence of blow-ups of smooth subvarieties.
- Choose a paper of Watanabe to illustrate the computation procedure.
- Could mention Newton polygons, toric methods, etc.

Discussion, work in small groups: (15:15-17:00) Looking at the details of the proofs and assumptions of SLT. Possible discussion topics:

- How realistic is the condition of relatively finite variance? There is at least one example in [1, §3.4 Example 19] which does not satisfy it and where the free energy formula does not hold; can we understand and generalize it?
- ReLU activations, which are popular in modern deep-learning architectures are only piecewise-analytic, so the theory above cannot be literally applied to it. What can be said nonetheless?
- Can we understand qualitatively the next order terms in the free energy formula? Do we expect large multiplicities to play a role? The prior only comes in the constant term, which is very complicated; can be say something about it, perhaps by analogy with the simple formula in the regular case?
- What does the singular fluctuation mean, really? And how should it manifest in practice?
- Can we interpret the description of the “renormalized posterior distribution” and its scaling law as in [2, §6.3] as a “singular Bernstein-Von Mises theorem”? Can we recover a form of the classical BVM theorem by applying this to regular models?
- Does SLT say something about generalization out-of-distribution?
- We haven’t discussed what Watanabe proves about maximum likelihood estimate in the singular context, but it is interesting and someone could try to summarize it.

- The function K (and hence the learning coefficient and other quantities relevant to statistical learning) depends in a complicated way of the interplay between the model and the true distribution. Can we quantify this interplay in some cases? For instance, if the true distribution has a certain symmetry property *and* the model contain a large subset of weights for which the model has this symmetry property, what does it imply about the structure of K ? Can we deduce something about (local) learning coefficients?
- Another interesting notion introduced in [3, §3] is the *parity* of the model, which has to do with the analytic continuation of $\sqrt{K(w)}$ and explains some sign issues in the core SLT theory. The result [3, Corollary 1] shows that WBIC for models with odd parity should be a better estimator than for models with even parity; do we observe this in practice?

REFERENCES

- [1] S. Watanabe, “Mathematical Theory of Bayesian Statistics”
- [2] S. Watanabe, “Algebraic Geometry and Statistical Learning Theory”
- [3] S. Watanabe, “A Widely applicable Bayesian Information Criterion”
- [4] E. Lau, D. Muref, S. Wei, “Quantifying degeneracy in singular models via the learning coefficient”, <https://arxiv.org/abs/2308.12108>