Guarantees for Machine Learning, Fall 2023

Lecture 1: Introduction and concentration bounds

Class intro

Objective. Develop graduate students into researchers who can

- understand and criticize papers in ML theory
- conjecture and prove new theorems that with high impact

Prerequisites

- Familiar with core machine learning concepts
- Should be comfortable writing rigorous mathematical proofs (for D-MATH courses)

Course structure

- First part: classical techniques for non-asymptotic risk bounds
  - Core reference: Martin Wainwright: High-dimensional statistics (available for free online via ETH)
- Second part: projects that review and extend current papers

Logistics

- Class website sml.inf.ethz.ch/gml23/syllabus.html
- Lecture slides will be uploaded after lectures at the latest
- TAs: Konstantin Donhauser, Julia Kostin (Office hours on request)
- Internet platforms to sign up for: moodle (announcements, questions, teammate search), Gradescope (assignments)
- Important date announcements: in class and per email

Evaluation & enrollment

Evaluation

- 2 homeworks (10%), midterm (50%), project (40%)
- HWs:
  - randomly select questions graded by TAs
  - check HW release schedule on the website
- Project (in groups of two):
  - Pick a paper from list according to your interests & background on (**October 13**)
  - Discussion & extension of one theoretical paper
  - 15-20 min Presentation in last four weeks
  - $\geq$ 10 page written report (due **January 12**)

Enrollment

- Current waitlist: ~75. Admitted: 30. Limit for admissions: 30
- By experience, everybody who wants to take it, can
- Final deadline to de-register: **October 11th** else no-show
- Others welcome to audit as long as there is space

Who is here?

Which department?

1. Computer Science
2. Mathematics/Statistics
3. Data Science
4. EE & Robotics
5. Others

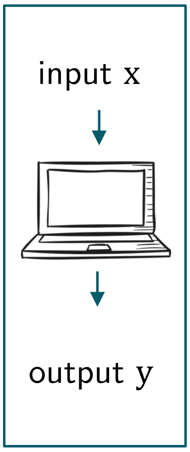
What stage of your studies are you?

1. Masters
2. PhD student
3. Bachelors

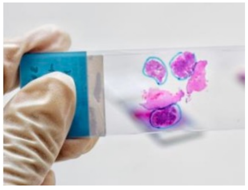
Plan for today

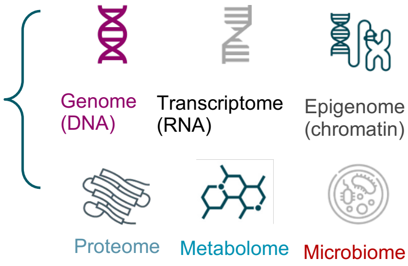
- Statistical perspective on the supervised learning pipeline
- Evaluation of an estimator using the excess risk
- Concentration bounds of empirical means

Recap: (Supervised) Machine Learning - Classification



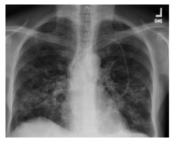
x: multiomics





y: cancer survival

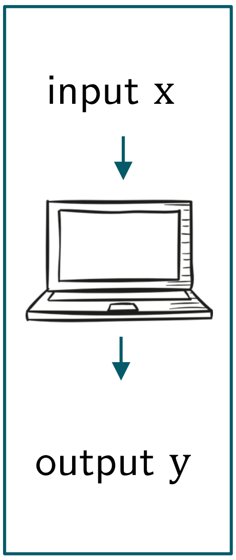
x: -Ray images



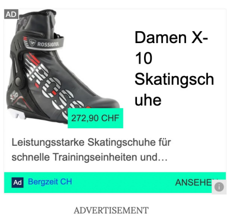
y: pneumonia or healthy

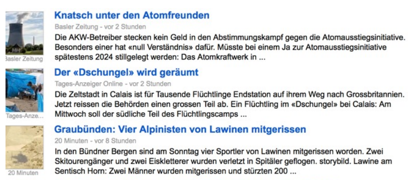
Figure 1: Classification examples

Recap: (Supervised) Machine Learning - Regression

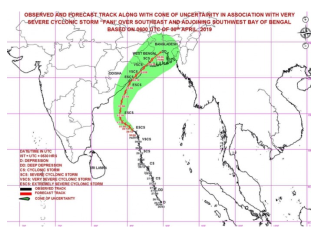


x: User data & article/advertisement





x: storm track



y: Probability of click / purchase

y: storm speed

Figure 2: Regression examples

Statistical Perspective on (supervised) Machine Learning

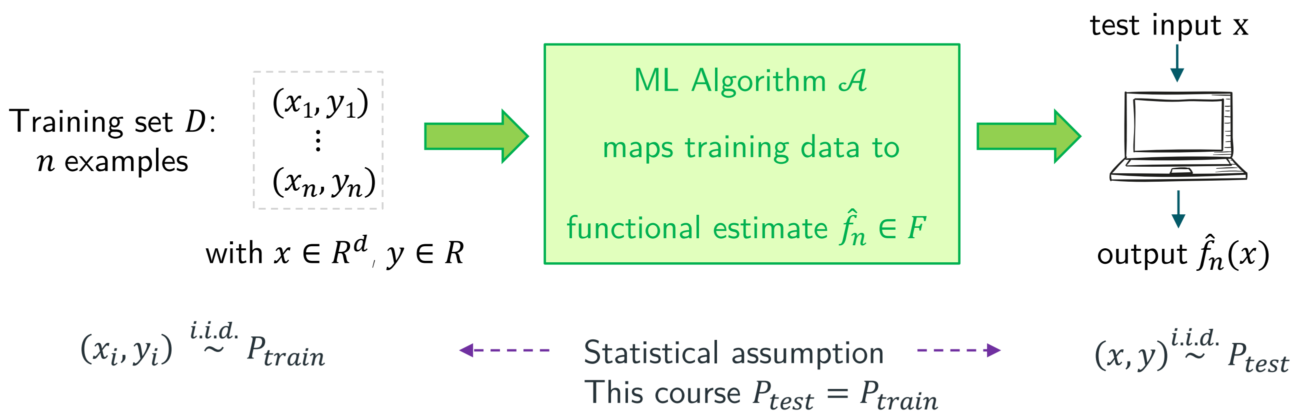


Figure 3: Supervised learning pipeline from statistical point of view

- some examples for $\mathbb{P} = \mathbb{P}_{train} = \mathbb{P}_{test}$ include
  - regression: marginal dist. over x and $y = f^\star(x) + \epsilon$ for random ϵ
  - classification: generative such as Gaussian mixture model or discriminative: marginal dist. over x and $y = \text{sign}(f^\star(x))$
- The estimate $\hat{f}_n \in \mathcal{F}$ depends on $(x_i, y_i)_{i=1}^n$ (i.e. is random) and is in some function class (e.g. linear, neural network etc.)

Evaluation of an estimator $\widehat{f}_n$

Whether $\widehat{f}_n$ is "good" is decided during test time: On average over test points (x, y), we'd like the predictions $\widehat{f}_n(x)$ to be close to y

- We measure "close" via a pointwise loss ℓ,
  e.g. $\ell((x, y), f) = (f(x) - y)^2$ for regression
  or $\ell(x, y; f) = \mathbb{1}_{f(x)=y}$ for classification
- We call the average loss of any function f the *population risk*
  $R(f) := R(f; \mathbb{P}) = \mathbb{E}\ell((x, y); f)$
- We further call the training loss of any f the *empirical risk*
  $R_n(f) := R(f; \mathcal{D}) = \frac{1}{n} \sum_{i=1}^n \ell((x_i, y_i); f)$ estimate is
- In the next lectures we'll consider the empirical risk minimization paradigm where

$$\widehat{f}_n := \arg\min_{f \in \mathcal{F}} R_n(f)$$

Evaluation of an estimator $\widehat{f}_n$

Q: For classification, is $R(\widehat{f}_n) = 20\%$ bad or good?

A: Depends on how hard the task is! Perhaps it's not possible to achieve perfect accuracy!

We should compare population risk of $\widehat{f}_n$ with that of the best possible function *if we knew the full distribution*, i.e. evaluate the excess risk:

$$\mathcal{E}_R(n) := R(\widehat{f}_n) - \inf_f R(f) \leq UB(...)$$

Grab a neighbor: Designate a presenter. Discuss for 5 minutes.

1. How is the population risk of an estimator related to its test error?
2. Which parameters of the problem and algorithm does the excess risk depend on? What happens to the excess risk of an estimator $\widehat{f}_n$ when we vary these parameters? Categorize the phenomena
3. What are tradeoffs when we consider the *empirical risk minimizer* $\widehat{f}_n := \arg\min_{f \in \mathcal{F}} R_n(f)$

Questions on the excess risk

1. Population risk vs. test error

- Test error on n' new samples follows $R_{n'}(\widehat{f}_n) \to R_n(\widehat{f}_n)$ by law of large numbers (LLN)

2. Excess risk depends on model class $\mathcal{F}$, dimensionality of the data d, sample size n and consists of the following factors and trends

- approximation error (if $f^\star = \arg\min_f R(f)$ is complicated): larger $\mathcal{F}$, smaller d better
- optimization error (due to optimization algorithm): Lipschitz, (strong) convex loss ℓ better
- statistical error (due to finite sample and noise): larger n (usually) better (depends on $\mathcal{F}, d$ as well) of course $\leftarrow$ this course

3. Tradeoffs: Larger $\mathcal{F}$, bigger effect of noise (statistical error) but smaller approx error (variance vs. bias)

This course: Non-asymptotic take on statistical "Guarantees for Machine Learning"

We introduce general frameworks to analyze excess risk and compute concrete upper (and lower) bounds s.t. with prob. at least $1-\delta$

$$R(\widehat{f}_n) - R(f^\star) \leq UB(n, d, \mathcal{F}, f^\star)$$

where we assume $f^\star = \arg min_f R(f)$ exists.

Questions we'd like to answer:

1. Does UB converge to 0 as n increases? (consistency)

1. If I collect double as much data, how much do I decrease my excess risk? $\rightarrow$ boils down to the exponent of n (statistical rate)

This course focuses on 2. We'll now discuss some probabilistic basics that give a sense for what to expect from course later.

Excess risk decomposition

- Recall the population risk $R(f) = \mathbb{E}\ell((X, Y); f)$
- Recall the empirical risk $R_n(f) = \frac{1}{n}\sum_{i=1}^n \ell((X_i, Y_i); f)$
- Remember we want to bound the excess risk

$$R(\widehat{f}_n) - R(f^\star) = R(\widehat{f}_n) - R_n(\widehat{f}_n) + \overbrace{R_n(\widehat{f}_n) - R_n(f^\star)}^{T_3 \leq 0} + R_n(f^\star) - R(f^\star)$$
$$\leq \underbrace{R(\widehat{f}_n) - R_n(\widehat{f}_n)}_{T_1} + \underbrace{R_n(f^\star) - R(f^\star)}_{T_2}$$

Question: Are T_1 and T_2 qualitatively similarly hard to bound? Is $T_3 \leq 0$ always true? Briefly discuss with your neighbor.

- $T_3 \leq 0$ is only true when $f^\star \in \mathcal{F}$!
- T_1 is harder than T_2 since it's a sum of dependent variables whereas T_2 is difference between an emprical mean and its expectation.

Concentration bounds for single random variables (R.V.)

- *Markov* inequality: $\mathbb{P}(X \geq t) \leq \frac{\mathbb{E}X}{t}$ for $X \geq 0$;
- Markov used on $e^{\lambda(X-\mathbb{E}X)}$ for $\lambda \geq 0$ yields the *Chernoff* bound

$$\mathbb{P}(X - \mathbb{E}X \geq t) \leq \inf_{\lambda \geq 0} \frac{\mathbb{E}[e^{\lambda(X-\mathbb{E}X)}]}{e^{\lambda t}}$$

  where the inf is effectively over all $\lambda \geq 0$ where the moment generating function (MGF) $\mathbb{E}e^{\lambda X}$ exists

We can use Chernoff to get tighter bounds for R.V. X with short tails

Definition (Sub-Gaussian random variables)

A random variable X with mean μ is sub-Gaussian w/ parameter σ if

$$\mathbb{E}e^{\lambda(X-\mu)} \leq e^{\lambda^2\sigma^2/2} \quad \text{for all } \lambda \in \mathbb{R}$$

- For σ sub-Gaussians using Chernoff we obtain the tail bound

$$\mathbb{P}(X - \mathbb{E}X \geq t) \leq \inf_{\lambda \geq 0} e^{\frac{\lambda^2\sigma^2}{2} - \lambda t} = e^{-\frac{t^2}{2\sigma^2}}$$

Examples for sub-Gaussian random variables

- Gaussians $\mathcal{N}(0, \sigma^2)$ are sub-Gaussian with parameter σ
- *Rademacher variables* $\epsilon = -1, +1$ with equal probability $1/2$ are sub-Gaussian with parameter $\sigma = 1$
  - We can directly compute and bound their MGF

$$\mathbb{E}e^{\lambda\epsilon} = \frac{1}{2}(e^{-\lambda} + e^{\lambda}) \leq e^{\lambda^2/2}$$

- Almost surely bounded in $[a, b]$ (exercise)

Empirical means of independent subgaussians

Lemma (Hoeffding's inequality)

For i.i.d sub-Gaussian R.V. X_i, it holds that

$$\mathbb{P}(\frac{1}{n}\sum_{i=1}^{n} X_i - \mathbb{E}X \geq t) \leq e^{-\frac{nt^2}{2\sigma^2}}$$

Neighbor-Q: Prove Hoeffding's inequality

- Recall sub-Gaussian: $\mathbb{E}e^{\lambda(X-\mu)} \leq e^{\lambda^2\sigma^2/2}$ for all $\lambda \in \mathbb{R}$
- Recall Chernoff for sub-Gaussians: $\mathbb{P}(X - \mathbb{E}X \geq t) \leq e^{-\frac{t^2}{2\sigma^2}}$

Proof of Hoeffding's inequality

1. We can apply Chernoff on the mean of n independent random variables with moment generating function

$$\mathbb{E}e^{\lambda(\frac{1}{n}\sum_{i=1}^{n}(X_i - \mathbb{E}X_i))} = \prod_{i=1}^{n} \mathbb{E}e^{\frac{\lambda}{n}(X_i-\mu)} = [\mathbb{E}e^{\frac{\lambda}{n}(X_i-\mu)}]^n$$

1. Hence, the mean of n i.i.d. sub-Gaussian variables is sub-Gaussian with parameter $\frac{\sigma}{\sqrt{n}}$ since $\mathbb{E}e^{\lambda(\frac{1}{n}\sum_{i=1}^{n}(X_i - \mathbb{E}X_i))} \leq e^{\frac{\lambda^2\sigma^2}{2n^2}n}$
1. yielding Hoeffding's inequality for the mean of iid sub-Gaussians

$$\mathbb{P}(\frac{1}{n}\sum_{i=1}^{n} X_i - \mathbb{E}X \geq t) \leq e^{-\frac{nt^2}{2\sigma^2}}$$

Q: How can we now use Hoeffding's inequality to bound the term T_2?

Syllabus of course

The courses focuses on bounding T_2 using so-called uniform convergence.

We'll cover

- uniform convergence using Rademacher and Gaussian complexity
- metric entropy and chaining to bound the complexity
- application to non-parametric regression (kernel methods)
- minimax lower bounds
- theory for overparameterized models

References

Concentration bounds:

- MW Chapters 2

Excess risk:

- MW Chapter 4