# STAT 991: Topics in Modern Statistical Learning Lecture 1

Edgar Dobriban

January 18, 2022

## Overview

Course information

Introduction to Topics

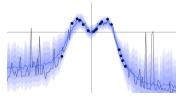
## Overview

#### Course information

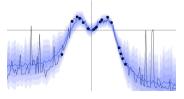
ntroduction to Topics

▶ This is an advanced graduate class of seminar type

- This is an advanced graduate class of seminar type
- The focus is on uncertainty quantification for machine learning methods: for instance conformal inference, prediction intervals/sets, calibration, OOD detection, etc.

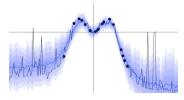


- ▶ This is an advanced graduate class of seminar type
- The focus is on uncertainty quantification for machine learning methods: for instance conformal inference, prediction intervals/sets, calibration, OOD detection, etc.



► All publicly available materials can be found on GitHub at https://github.com/dobriban/Topics-In-Modern-Statistical-Learning

- ▶ This is an advanced graduate class of seminar type
- ► The focus is on uncertainty quantification for machine learning methods: for instance conformal inference, prediction intervals/sets, calibration, OOD detection, etc.



- ► All publicly available materials can be found on GitHub at https://github.com/dobriban/Topics-In-Modern-Statistical-Learning
- ► Some materials will be available only on Canvas (at least temporarily)

▶ All lectures recorded. (At least) first two weeks online, rest currently planned in-person.

- ▶ All lectures recorded. (At least) first two weeks online, rest currently planned in-person.
- ► Zoom lecture expectations

- ▶ All lectures recorded. (At least) first two weeks online, rest currently planned in-person.
- Zoom lecture expectations
  - ► Mute yourself when not speaking

- ▶ All lectures recorded. (At least) first two weeks online, rest currently planned in-person.
- Zoom lecture expectations
  - ► Mute yourself when not speaking
  - Ask questions as we go along: Unmute yourself and ask question (aim for interactivity)

- ▶ All lectures recorded. (At least) first two weeks online, rest currently planned in-person.
- Zoom lecture expectations
  - ► Mute yourself when not speaking
  - Ask questions as we go along: Unmute yourself and ask question (aim for interactivity)
  - ► Camera on/off up to you

► Format:

- Format:
  - First several lectures by Edgar (and possible guests later)

- Format:
  - ► First several lectures by Edgar (and possible guests later)
  - ▶ Remaining lectures by students. We imagine a critical discussion of one or two papers per lecture; and several contiguous lectures on the same theme. The goal will be to develop a deep understanding of recent research (e.g., expect you to present proofs of results).

#### Format:

- ► First several lectures by Edgar (and possible guests later)
- ▶ Remaining lectures by students. We imagine a critical discussion of one or two papers per lecture; and several contiguous lectures on the same theme. The goal will be to develop a deep understanding of recent research (e.g., expect you to present proofs of results).
- ▶ The goal of the course will also be to identity new research directions.

#### Format:

- First several lectures by Edgar (and possible guests later)
- ▶ Remaining lectures by students. We imagine a critical discussion of one or two papers per lecture; and several contiguous lectures on the same theme. The goal will be to develop a deep understanding of recent research (e.g., expect you to present proofs of results).
- ▶ The goal of the course will also be to identity new research directions.
- Examples from past: three editions of Topics in Deep Learning: https://github.com/dobriban/Topics-in-deep-learning. Reseach topics came out: data augmentation, DeltaGrad.

- ► Format:
  - First several lectures by Edgar (and possible guests later)
  - ▶ Remaining lectures by students. We imagine a critical discussion of one or two papers per lecture; and several contiguous lectures on the same theme. The goal will be to develop a deep understanding of recent research (e.g., expect you to present proofs of results).
  - ▶ The goal of the course will also be to identity new research directions.
  - ► Examples from past: three editions of Topics in Deep Learning: https://github.com/dobriban/Topics-in-deep-learning. Reseach topics came out: data augmentation, DeltaGrad.
- As far I know, first course on this broad set of topics anywhere in the world. (sorry for the rough edges and omissions!)

- ► Format:
  - First several lectures by Edgar (and possible guests later)
  - ▶ Remaining lectures by students. We imagine a critical discussion of one or two papers per lecture; and several contiguous lectures on the same theme. The goal will be to develop a deep understanding of recent research (e.g., expect you to present proofs of results).
  - ▶ The goal of the course will also be to identity new research directions.
  - ► Examples from past: three editions of Topics in Deep Learning: https://github.com/dobriban/Topics-in-deep-learning. Reseach topics came out: data augmentation, DeltaGrad.
- As far I know, first course on this broad set of topics anywhere in the world. (sorry for the rough edges and omissions!)
- ► Goals:
  - 1. create an engaging, fun, but rigorous intellectual environment, where we will all learn and develop

- Format:
  - First several lectures by Edgar (and possible guests later)
  - Remaining lectures by students. We imagine a critical discussion of one or two papers per lecture; and several contiguous lectures on the same theme. The goal will be to develop a deep understanding of recent research (e.g., expect you to present proofs of results).
  - ▶ The goal of the course will also be to identity new research directions.
  - ► Examples from past: three editions of Topics in Deep Learning: https://github.com/dobriban/Topics-in-deep-learning. Reseach topics came out: data augmentation, DeltaGrad.
- As far I know, first course on this broad set of topics anywhere in the world. (sorry for the rough edges and omissions!)
- ► Goals:
  - 1. create an engaging, fun, but rigorous intellectual environment, where we will all learn and develop
  - 2. create broadly useful teaching materials

- ► Format:
  - First several lectures by Edgar (and possible guests later)
  - Remaining lectures by students. We imagine a critical discussion of one or two papers per lecture; and several contiguous lectures on the same theme. The goal will be to develop a deep understanding of recent research (e.g., expect you to present proofs of results).
  - ► The goal of the course will also be to identity new research directions.
  - ► Examples from past: three editions of Topics in Deep Learning: https://github.com/dobriban/Topics-in-deep-learning. Reseach topics came out: data augmentation, DeltaGrad.
- As far I know, first course on this broad set of topics anywhere in the world. (sorry for the rough edges and omissions!)
- ► Goals:
  - 1. create an engaging, fun, but rigorous intellectual environment, where we will all learn and develop
  - 2. create broadly useful teaching materials
- See syllabus for: Prerequsites, Feedback, Grading Policy

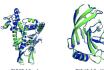


## Overview

Course information

Introduction to Topics

► Machine learning (ML): one of the most salient intellectual developments in today's world (part of broader "Data Sciences")



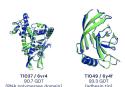
T1049 / 6y4f 93.3 GDT (adhesin tip)

Experimental result
 Computational prediction

(RNA polymerase domain)

Title: United Methodists Agree to Historic Split
Subtitle: Those who oppose gay marriage will form their own denomination
Article: After two days of intense debate, the United Methodist Church
has agreed to a historic split - one that is expected to end in the
creation of a new denomination, one that will be "theologically and
socially conservative," according to The Washington Post. The majority of
delegates attending the church's annual General Conference in May voted to
strengthen a ban on the ordination of LGBTQ clergy and to write new rules
that will "discipline" clergy who officiate at same-sex weddings. But
those who opposed these measures have a new plan: They say they will form a
separate denomination by 2020, calling their church the Christian Methodist
denomination.

► Machine learning (ML): one of the most salient intellectual developments in today's world (part of broader "Data Sciences")



Experimental result
 Computational prediction

Title: United Methodists Agree to Historic Split
Subtitle: Those who oppose gay marriage will form their own denomination
Article: After two days of intense debate, the United Methodist Church
has agreed to a historic split - one that is expected to end in the
creation of a new denomination, one that will be "theologically and
socially conservative," according to The Washington Post. The majority of
delegates attending the church's annual General Conference in May voted to
strengthen a ban on the ordination of LGBTQ clergy and to write new rules
that will "discipline" clergy who officiate at same-sex weddings. But
those who opposed these measures have a new plan: They say they will form a
separate denomination by 2020, calling their church the Christian Methodist
denomination.

Figure 3.14: The GPT-3 generated news article that humans had the greatest difficulty distinguishing from a written article (accuracy: 12%).

► AlphaFold (Science's 2021 "breakthrough of the year")

► Machine learning (ML): one of the most salient intellectual developments in today's world (part of broader "Data Sciences")

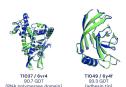


Experimental result
 Computational prediction

Title: United Methodists Agree to Historic Split
Subtitle: Those who oppose gay marriage will form their own denomination
Article: After two days of intense debate, the United Methodist Church
has agreed to a historic split - one that is expected to end in the
creation of a new denomination, one that will be "theologically and
socially conservative," according to The Washington Post. The majority of
delegates attending the church's annual General Conference in May voted to
strengthen a ban on the ordination of LGBTQ clergy and to write new rules
that will "discipline" clergy who officiate at same-sex weddings. But
those who opposed these measures have a new plan: They say they will form a
separate denomination by 2020, calling their church the Christian Methodist
denomination.

- AlphaFold (Science's 2021 "breakthrough of the year")
- ► GPT-3

► Machine learning (ML): one of the most salient intellectual developments in today's world (part of broader "Data Sciences")

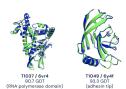


Experimental result
 Computational prediction

Title: United Methodists Agree to Historic Split
Subtitle: Those who oppose gay marriage will form their own denomination
Article: After two days of intense debate, the United Methodist Church
has agreed to a historic split - one that is expected to end in the
creation of a new denomination, one that will be "theologically and
socially conservative," according to The Washington Post. The majority of
delegates attending the church's annual General Conference in May voted to
strengthen a ban on the ordination of LGBTQ clergy and to write new rules
that will "discipline" clergy who officiate at same-sex weddings. But
those who opposed these measures have a new plan: They say they will form a
separate denomination by 2020, calling their church the Christian Methodist
denomination.

- AlphaFold (Science's 2021 "breakthrough of the year")
- ► GPT-3
- Pro-level skin cancer classification

► Machine learning (ML): one of the most salient intellectual developments in today's world (part of broader "Data Sciences")



Experimental result
 Computational prediction

Title: United Methodists Agree to Historic Split
Subtitle: Those who oppose gay marriage will form their own denomination
Article: After two days of intense debate, the United Methodist Church
has agreed to a historic split - one that is expected to end in the
creation of a new denomination, one that will be "theologically and
socially conservative," according to The Washington Post. The majority of
delegates attending the church's annual General Conference in May voted to
strengthen a ban on the ordination of LGBTQ clergy and to write new rules
that will "discipline" clergy who officiate at same-sex weddings. But
those who opposed these measures have a new plan: They say they will form a
separate denomination by 2020, calling their church the Christian Methodist
denomination.

- AlphaFold (Science's 2021 "breakthrough of the year")
- ► GPT-3
- Pro-level skin cancer classification
- Self-driving cars

▶ Machine learning (ML): one of the most salient intellectual developments in today's world (part of broader "Data Sciences")



Experimental result
 Computational prediction

Title: United Methodists Agree to Historic Split Subtitle: Those who oppose gay marriage will form their own denomination Article: After two days of intense debate, the United Methodist Church has agreed to a historic split - one that is expected to end in the creation of a new denomination, one that will be "theologically and socially conservative," according to The Washington Post. The majority of delegates attending the church's annual General Conference in May voted to strengthen a ban on the ordination of LGETQ clergy and to write new rules that will "discipline" clergy who officiate at same-sex weddings. But those who opposed these measures have a new plan: They say they will form a separate denomination by 2020, calling their church the Christian Methodist denomination.

- AlphaFold (Science's 2021 "breakthrough of the year")
- ► GPT-3
- Pro-level skin cancer classification
- Self-driving cars
- Deep learning for stock prediction

▶ Machine learning (ML): one of the most salient intellectual developments in today's world (part of broader "Data Sciences")



Experimental result
 Computational prediction

Title: United Methodists Agree to Historic Split
Subtitle: Those who oppose gay marriage will form their own denomination
Article: After two days of intense debate, the United Methodist Church
has agreed to a historic split - one that is expected to end in the
creation of a new denomination, one that will be "theologically and
socially conservative," according to The Washington Post. The majority of
delegates attending the church's annual General Conference in May voted to
strengthen a ban on the ordination of LGBTQ clergy and to write new rules
that will "discipline" clergy who officiate at same-sex weddings. But
those who opposed these measures have a new plan: They say they will form a
separate denomination by 2020, calling their church the Christian Methodist
denomination.

- AlphaFold (Science's 2021 "breakthrough of the year")
- ► GPT-3
- Pro-level skin cancer classification
- Self-driving cars
- Deep learning for stock prediction
- Causality and learning from natural experiments (a bit broader; Econ Nobel 2021)

► ML = Prediction

- ► ML = Prediction
  - ► Given *x* (inputs, features, covariates), predict *y* (outputs, outcomes)

- ► ML = Prediction
  - ► Given *x* (inputs, features, covariates), predict *y* (outputs, outcomes)

#### Examples

	X	У
AlphaFold	Protein sequence	3D structure
GPT-3	Text prompt	Answer
Skin cancer	Skin image	Cancer type
Self-driving car	3D environment, location,	Control signal

- ► ML = Prediction
  - ► Given *x* (inputs, features, covariates), predict *y* (outputs, outcomes)
- Examples

	X	У
AlphaFold	Protein sequence	3D structure
GPT-3	Text prompt	Answer
Skin cancer	Skin image	Cancer type
Self-driving car	3D environment, location,	Control signal

Less glitzy, but very important examples: predicting phenotype from genetic variables, Predicting response to medical treatment

# Uncertainty

► Given x, the answer y is often not uniquely determined

# Uncertainty

- ▶ Given x, the answer y is often not uniquely determined
  - even x may be measured with error

# Uncertainty

- Given x, the answer y is often not uniquely determined
  - even x may be measured with error
- Examples of uncertainty:

- ▶ Given x, the answer y is often not uniquely determined
  - even x may be measured with error
- Examples of uncertainty:
  - ► GPT-3: given text prompt, ...?

- ▶ Given x, the answer y is often not uniquely determined
  - even x may be measured with error
- Examples of uncertainty:
  - ► GPT-3: given text prompt, ...?
  - ► Self-driving cars: given 3D environment, location, ...?

- ▶ Given x, the answer y is often not uniquely determined
  - even x may be measured with error
- Examples of uncertainty:
  - ► GPT-3: given text prompt, ...?
  - ► Self-driving cars: given 3D environment, location, ...?
  - ► AlphaFold: given protein sequence, ...?

- ▶ Given x, the answer y is often not uniquely determined
  - even x may be measured with error
- Examples of uncertainty:
  - ► GPT-3: given text prompt, ...?
  - ► Self-driving cars: given 3D environment, location, ...?
  - ► AlphaFold: given protein sequence, ...?
  - Skin cancer classification: given skin image, ...?

- ▶ Given x, the answer y is often not uniquely determined
  - even x may be measured with error
- Examples of uncertainty:
  - ► GPT-3: given text prompt, ...?
  - Self-driving cars: given 3D environment, location, ...?
  - ► AlphaFold: given protein sequence, ...?
  - Skin cancer classification: given skin image, ...?
- ▶ Standard ML pipeline (see next) does not provide a solution

- ▶ Given x, the answer y is often not uniquely determined
  - even x may be measured with error
- Examples of uncertainty:
  - ► GPT-3: given text prompt, ...?
  - Self-driving cars: given 3D environment, location, ...?
  - ► AlphaFold: given protein sequence, ...?
  - Skin cancer classification: given skin image, ...?
- Standard ML pipeline (see next) does not provide a solution
  - Currently no "standard" method

For predicting  $x \in \mathcal{X} \mapsto y \in \mathcal{Y}$ ,

<sup>&</sup>lt;sup>1</sup>Ideally, uncertainty quantification methods should not depend on fitting methods

- For predicting  $x \in \mathcal{X} \mapsto y \in \mathcal{Y}$ ,
  - ▶ collect a sample of "training" data  $Z = \{(x_i, y_i), i = 1, ..., n\}$

<sup>&</sup>lt;sup>1</sup>Ideally, uncertainty quantification methods should not depend on fitting methods

- For predicting  $x \in \mathcal{X} \mapsto y \in \mathcal{Y}$ ,
  - ▶ collect a sample of "training" data  $Z = \{(x_i, y_i), i = 1, ..., n\}$
  - find a predictor (hypothesis)  $f: \mathcal{X} \mapsto \mathcal{Y}$  that "fits the data" well<sup>1</sup>

<sup>&</sup>lt;sup>1</sup>Ideally, uncertainty quantification methods should not depend on fitting methods

- ▶ For predicting  $x \in \mathcal{X} \mapsto y \in \mathcal{Y}$ ,
  - ightharpoonup collect a sample of "training" data  $Z = \{(x_i, y_i), i = 1, \dots, n\}$
  - find a predictor (hypothesis)  $f: \mathcal{X} \mapsto \mathcal{Y}$  that "fits the data" well<sup>1</sup>
- "Standard method": Empirical Risk Minimization (Wald, Vapnik, ...)

<sup>&</sup>lt;sup>1</sup>Ideally, uncertainty quantification methods should not depend on fitting methods one

- ▶ For predicting  $x \in \mathcal{X} \mapsto y \in \mathcal{Y}$ ,
  - ▶ collect a sample of "training" data  $Z = \{(x_i, y_i), i = 1, ..., n\}$
  - ▶ find a predictor (hypothesis)  $f: \mathcal{X} \mapsto \mathcal{Y}$  that "fits the data" well<sup>1</sup>
- ▶ "Standard method": Empirical Risk Minimization (Wald, Vapnik, ...)
  - lacktriangle Class of predictors  ${\cal H}$  (hypothesis class): linear models, deep nets, ...

<sup>&</sup>lt;sup>1</sup>Ideally, uncertainty quantification methods should not depend on fitting methods

- ▶ For predicting  $x \in \mathcal{X} \mapsto y \in \mathcal{Y}$ ,
  - ▶ collect a sample of "training" data  $Z = \{(x_i, y_i), i = 1, ..., n\}$
  - ▶ find a predictor (hypothesis)  $f: \mathcal{X} \mapsto \mathcal{Y}$  that "fits the data" well<sup>1</sup>
- "Standard method": Empirical Risk Minimization (Wald, Vapnik, ...)
  - ightharpoonup Class of predictors  ${\cal H}$  (hypothesis class): linear models, deep nets, ...
  - ▶ Loss function  $\ell: \mathcal{Y} \times \mathcal{Y} \mapsto [0, \infty)$

<sup>&</sup>lt;sup>1</sup>Ideally, uncertainty quantification methods should not depend on fitting methods

- ▶ For predicting  $x \in \mathcal{X} \mapsto y \in \mathcal{Y}$ ,
  - ▶ collect a sample of "training" data  $Z = \{(x_i, y_i), i = 1, ..., n\}$
  - ▶ find a predictor (hypothesis)  $f: \mathcal{X} \mapsto \mathcal{Y}$  that "fits the data" well<sup>1</sup>
- "Standard method": Empirical Risk Minimization (Wald, Vapnik, ...)
  - lacktriangle Class of predictors  ${\cal H}$  (hypothesis class): linear models, deep nets, ...
  - ▶ Loss function  $\ell: \mathcal{Y} \times \mathcal{Y} \mapsto [0, \infty)$
  - lacktriangle Run some algorithm to approximately minimize empirical risk, finding  $\hat{f}$

$$\min_{f\in H} R_n(f,Z) = \frac{1}{n} \sum_{i=1}^n \ell(f(x_i), y_i)$$

<sup>&</sup>lt;sup>1</sup>Ideally, uncertainty quantification methods should not depend on fitting methods

- ▶ For predicting  $x \in \mathcal{X} \mapsto y \in \mathcal{Y}$ ,
  - ▶ collect a sample of "training" data  $Z = \{(x_i, y_i), i = 1, ..., n\}$
  - ▶ find a predictor (hypothesis)  $f: \mathcal{X} \mapsto \mathcal{Y}$  that "fits the data" well<sup>1</sup>
- "Standard method": Empirical Risk Minimization (Wald, Vapnik, ...)
  - lacktriangle Class of predictors  ${\cal H}$  (hypothesis class): linear models, deep nets, ...
  - ▶ Loss function  $\ell: \mathcal{Y} \times \mathcal{Y} \mapsto [0, \infty)$
  - lacktriangle Run some algorithm to approximately minimize empirical risk, finding  $\hat{f}$

$$\min_{f \in H} R_n(f, Z) = \frac{1}{n} \sum_{i=1}^n \ell(f(x_i), y_i)$$

Empirically evaluate: obtain new "test" dataset  $Z' = \{(x_i', y_i'), i = 1, \dots, n'\}$ , find test loss  $R_{n'}(\hat{f}, Z')$ 

<sup>&</sup>lt;sup>1</sup>Ideally, uncertainty quantification methods should not depend on fitting methods

- ▶ For predicting  $x \in \mathcal{X} \mapsto y \in \mathcal{Y}$ ,
  - ▶ collect a sample of "training" data  $Z = \{(x_i, y_i), i = 1, ..., n\}$
  - ▶ find a predictor (hypothesis)  $f: \mathcal{X} \mapsto \mathcal{Y}$  that "fits the data" well<sup>1</sup>
- "Standard method": Empirical Risk Minimization (Wald, Vapnik, ...)
  - lacktriangle Class of predictors  ${\cal H}$  (hypothesis class): linear models, deep nets, ...
  - ▶ Loss function  $\ell: \mathcal{Y} \times \mathcal{Y} \mapsto [0, \infty)$
  - lacktriangle Run some algorithm to approximately minimize empirical risk, finding  $\hat{f}$

$$\min_{f \in H} R_n(f, Z) = \frac{1}{n} \sum_{i=1}^n \ell(f(x_i), y_i)$$

- Empirically evaluate: obtain new "test" dataset  $Z' = \{(x'_i, y'_i), i = 1, ..., n'\}$ , find test loss  $R_{n'}(\hat{f}, Z')$
- ► Works... (perhaps surprisingly)

<sup>&</sup>lt;sup>1</sup>Ideally, uncertainty quantification methods should not depend on fitting methods

► Uncertainty = probability<sup>2</sup>

<sup>&</sup>lt;sup>2</sup>what is the meaning of "probability", or the source of randomness? discuss later

- ► Uncertainty = probability<sup>2</sup>
- ► Goal: Make probabilistic statements about predictions

<sup>&</sup>lt;sup>2</sup>what is the meaning of "probability", or the source of randomness? discuss later

- ► Uncertainty = probability<sup>2</sup>
- ► Goal: Make probabilistic statements about predictions
- Examples:

<sup>&</sup>lt;sup>2</sup>what is the meaning of "probability", or the source of randomness? discuss later

- ► Uncertainty = probability<sup>2</sup>
- Goal: Make probabilistic statements about predictions
- Examples:
  - ▶ Upper Confidence Prediction:  $P(y \le f(x)) \ge 1 \alpha$ , for some  $\alpha \in (0,1)$

<sup>&</sup>lt;sup>2</sup>what is the meaning of "probability", or the source of randomness? discuss later

- ► Uncertainty = probability<sup>2</sup>
- Goal: Make probabilistic statements about predictions
- Examples:
  - ▶ Upper Confidence Prediction:  $P(y \le f(x)) \ge 1 \alpha$ , for some  $\alpha \in (0,1)$
  - ▶ Prediction Interval:  $P(f_l(x) \le y \le f_u(x)) \ge 1 \alpha$ , for some  $\alpha \in (0,1)$

<sup>&</sup>lt;sup>2</sup>what is the meaning of "probability", or the source of randomness? discuss later

- Uncertainty = probability<sup>2</sup>
- ► Goal: Make probabilistic statements about predictions
- Examples:
  - ▶ Upper Confidence Prediction:  $P(y \le f(x)) \ge 1 \alpha$ , for some  $\alpha \in (0,1)$
  - ▶ Prediction Interval:  $P(f_l(x) \le y \le f_u(x)) \ge 1 \alpha$ , for some  $\alpha \in (0,1)$
  - ▶ Prediction Set: for some mapping C of inputs to subsets of  $\mathcal{Y}$ :  $P(y \in C(x)) \geqslant 1 \alpha$ , for some  $\alpha \in (0,1)$ . Or, conditional guarantee

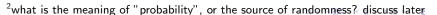
$$P_Z(P_{(x,y)}(y \in C(x; Z)) \geqslant 1 - \alpha) \geqslant 1 - \delta$$

- Uncertainty = probability<sup>2</sup>
- ► Goal: Make probabilistic statements about predictions
- Examples:
  - ▶ Upper Confidence Prediction:  $P(y \le f(x)) \ge 1 \alpha$ , for some  $\alpha \in (0,1)$
  - ▶ Prediction Interval:  $P(f_l(x) \le y \le f_u(x)) \ge 1 \alpha$ , for some  $\alpha \in (0,1)$
  - ▶ Prediction Set: for some mapping C of inputs to subsets of  $\mathcal{Y}$ :  $P(y \in C(x)) \geqslant 1 \alpha$ , for some  $\alpha \in (0,1)$ . Or, conditional guarantee

$$P_Z(P_{(x,y)}(y \in C(x;Z)) \geqslant 1-\alpha) \geqslant 1-\delta$$

Calibration: for all appopriate t,

$$P(f(x) = y | p(x) = t) \approx t$$





- ► Uncertainty = probability<sup>2</sup>
- ► Goal: Make probabilistic statements about predictions
- Examples:
  - ▶ Upper Confidence Prediction:  $P(y \le f(x)) \ge 1 \alpha$ , for some  $\alpha \in (0,1)$
  - ▶ Prediction Interval:  $P(f_l(x) \le y \le f_u(x)) \ge 1 \alpha$ , for some  $\alpha \in (0,1)$
  - ▶ Prediction Set: for some mapping C of inputs to subsets of  $\mathcal{Y}$ :  $P(y \in C(x)) \geqslant 1 \alpha$ , for some  $\alpha \in (0,1)$ . Or, conditional guarantee

$$P_Z(P_{(x,y)}(y \in C(x;Z)) \geqslant 1-\alpha) \geqslant 1-\delta$$

Calibration: for all appopriate t,

$$P(f(x) = y | p(x) = t) \approx t$$

- ▶ Or... you name it: conditional on x, or on y, or only partial, or under dependence, or structured settings, or...
- ► Is uncertainty ever good?

<sup>&</sup>lt;sup>2</sup>what is the meaning of "probability", or the source of randomness? discuss later

Probability: what does it mean? where does it come from?

- Probability: what does it mean? where does it come from?
- ▶ this is a deeper question than one might think. There is an entire area of the philosophy of probability and statistics.

- Probability: what does it mean? where does it come from?
- ▶ this is a deeper question than one might think. There is an entire area of the philosophy of probability and statistics.
- For us the most common way of thinking is the frequency interpretation:

- Probability: what does it mean? where does it come from?
- ▶ this is a deeper question than one might think. There is an entire area of the philosophy of probability and statistics.
- ► For us the most common way of thinking is the frequency interpretation:
  - ▶  $P(x \in A)$  is the long-term average over repeated experiments of the same type of the event that the observed quantity x belongs to the set A

- Probability: what does it mean? where does it come from?
- ▶ this is a deeper question than one might think. There is an entire area of the philosophy of probability and statistics.
- For us the most common way of thinking is the frequency interpretation:
  - ▶  $P(x \in A)$  is the long-term average over repeated experiments of the same type of the event that the observed quantity x belongs to the set A
  - problems with this in ML?

- Probability: what does it mean? where does it come from?
- ▶ this is a deeper question than one might think. There is an entire area of the philosophy of probability and statistics.
- ► For us the most common way of thinking is the frequency interpretation:
  - ▶  $P(x \in A)$  is the long-term average over repeated experiments of the same type of the event that the observed quantity x belongs to the set A
  - problems with this in ML?
- Other interpretations: subjective beliefs (Dempster-Shafer), betting (Kelly), ...

- Probability: what does it mean? where does it come from?
- ▶ this is a deeper question than one might think. There is an entire area of the philosophy of probability and statistics.
- ► For us the most common way of thinking is the frequency interpretation:
  - ▶  $P(x \in A)$  is the long-term average over repeated experiments of the same type of the event that the observed quantity x belongs to the set A
  - problems with this in ML?
- Other interpretations: subjective beliefs (Dempster-Shafer), betting (Kelly), ...
- The language of probability is already at the core of theoretical ML: generalization bounds, probabilistic ML (graphical models), Bayesian methods, etc. so it is already widely accepted

▶ Q1. Why/when do we need uncertainty quantification?

- ▶ Q1. Why/when do we need uncertainty quantification?
- ▶ There are problems where uncertainty quantification is almost moot:

- Q1. Why/when do we need uncertainty quantification?
- There are problems where uncertainty quantification is almost moot:
  - 1. non-prediction/subjective problems, e.g., what is the best tasting food?

- ▶ Q1. Why/when do we need uncertainty quantification?
- There are problems where uncertainty quantification is almost moot:
  - 1. non-prediction/subjective problems, e.g., what is the best tasting food?
  - 2. deterministic problems, e.g., compute 3+4

- ▶ Q1. Why/when do we need uncertainty quantification?
- There are problems where uncertainty quantification is almost moot:
  - 1. non-prediction/subjective problems, e.g., what is the best tasting food?
  - 2. deterministic problems, e.g., compute 3 + 4
  - 3. low-stake problems where very quick decisions need to be taken, e.g., show ads on website

- ▶ Q1. Why/when do we need uncertainty quantification?
- There are problems where uncertainty quantification is almost moot:
  - 1. non-prediction/subjective problems, e.g., what is the best tasting food?
  - 2. deterministic problems, e.g., compute 3 + 4
  - 3. low-stake problems where very quick decisions need to be taken, e.g., show ads on website
  - 4. problems with a lack of data or adequate computational resources, e.g., can I predict tomorrow's weather?

- ▶ Q1. Why/when do we need uncertainty quantification?
- There are problems where uncertainty quantification is almost moot:
  - 1. non-prediction/subjective problems, e.g., what is the best tasting food?
  - 2. deterministic problems, e.g., compute 3 + 4
  - 3. low-stake problems where very quick decisions need to be taken, e.g., show ads on website
  - 4. problems with a lack of data or adequate computational resources, e.g., can I predict tomorrow's weather?
  - 5. very complex problems that depend on multiple domains, where prediction is inherently near-impossible, e.g., can NWS predict the weather 100 years in advance?

- ▶ Q1. Why/when do we need uncertainty quantification?
- ► There are problems where uncertainty quantification is almost moot:
  - 1. non-prediction/subjective problems, e.g., what is the best tasting food?
  - 2. deterministic problems, e.g., compute 3 + 4
  - 3. low-stake problems where very quick decisions need to be taken, e.g., show ads on website
  - 4. problems with a lack of data or adequate computational resources, e.g., can I predict tomorrow's weather?
  - 5. very complex problems that depend on multiple domains, where prediction is inherently near-impossible, e.g., can NWS predict the weather 100 years in advance?
- ▶ A1: So it makes most sense in some of the following settings

- ▶ Q1. Why/when do we need uncertainty quantification?
- ► There are problems where uncertainty quantification is almost moot:
  - 1. non-prediction/subjective problems, e.g., what is the best tasting food?
  - 2. deterministic problems, e.g., compute 3 + 4
  - 3. low-stake problems where very quick decisions need to be taken, e.g., show ads on website
  - 4. problems with a lack of data or adequate computational resources, e.g., can I predict tomorrow's weather?
  - 5. very complex problems that depend on multiple domains, where prediction is inherently near-impossible, e.g., can NWS predict the weather 100 years in advance?
- ▶ A1: So it makes most sense in some of the following settings
  - 1. objective prediction problems

- ▶ Q1. Why/when do we need uncertainty quantification?
- ► There are problems where uncertainty quantification is almost moot:
  - 1. non-prediction/subjective problems, e.g., what is the best tasting food?
  - 2. deterministic problems, e.g., compute 3 + 4
  - 3. low-stake problems where very quick decisions need to be taken, e.g., show ads on website
  - 4. problems with a lack of data or adequate computational resources, e.g., can I predict tomorrow's weather?
  - 5. very complex problems that depend on multiple domains, where prediction is inherently near-impossible, e.g., can NWS predict the weather 100 years in advance?
- ▶ A1: So it makes most sense in some of the following settings
  - 1. objective prediction problems
  - 2. there is no easily computed clear single answer

- ▶ Q1. Why/when do we need uncertainty quantification?
- ► There are problems where uncertainty quantification is almost moot:
  - 1. non-prediction/subjective problems, e.g., what is the best tasting food?
  - 2. deterministic problems, e.g., compute 3 + 4
  - 3. low-stake problems where very quick decisions need to be taken, e.g., show ads on website
  - 4. problems with a lack of data or adequate computational resources, e.g., can I predict tomorrow's weather?
  - 5. very complex problems that depend on multiple domains, where prediction is inherently near-impossible, e.g., can NWS predict the weather 100 years in advance?
- ▶ A1: So it makes most sense in some of the following settings
  - 1. objective prediction problems
  - 2. there is no easily computed clear single answer
  - 3. the stakes are somewhat high, and/or there is time to take into account the uncertainty we care about this

- ▶ Q1. Why/when do we need uncertainty quantification?
- ► There are problems where uncertainty quantification is almost moot:
  - 1. non-prediction/subjective problems, e.g., what is the best tasting food?
  - 2. deterministic problems, e.g., compute 3 + 4
  - 3. low-stake problems where very quick decisions need to be taken, e.g., show ads on website
  - 4. problems with a lack of data or adequate computational resources, e.g., can I predict tomorrow's weather?
  - 5. very complex problems that depend on multiple domains, where prediction is inherently near-impossible, e.g., can NWS predict the weather 100 years in advance?
- ▶ A1: So it makes most sense in some of the following settings
  - 1. objective prediction problems
  - 2. there is no easily computed clear single answer
  - 3. the stakes are somewhat high, and/or there is time to take into account the uncertainty we care about this
  - 4. there is data and computational resources

- ▶ Q1. Why/when do we need uncertainty quantification?
- There are problems where uncertainty quantification is almost moot:
  - 1. non-prediction/subjective problems, e.g., what is the best tasting food?
  - 2. deterministic problems, e.g., compute 3 + 4
  - 3. low-stake problems where very quick decisions need to be taken, e.g., show ads on website
  - 4. problems with a lack of data or adequate computational resources, e.g., can I predict tomorrow's weather?
  - 5. very complex problems that depend on multiple domains, where prediction is inherently near-impossible, e.g., can NWS predict the weather 100 years in advance?
- ▶ A1: So it makes most sense in some of the following settings
  - 1. objective prediction problems
  - 2. there is no easily computed clear single answer
  - 3. the stakes are somewhat high, and/or there is time to take into account the uncertainty we care about this
  - 4. there is data and computational resources
  - 5. relatively simple, isolated problem



Q2. why via probability?

- Q2. why via probability?
- Sometimes one can/has to perform uncertainty quantification via other means

- ▶ Q2. why via probability?
- Sometimes one can/has to perform uncertainty quantification via other means
  - 1. Sometimes one can just provide a range, e.g., the high and low predicted precipitation for tomorrow, without any probabilistic interpretation

- Q2. why via probability?
- Sometimes one can/has to perform uncertainty quantification via other means
  - 1. Sometimes one can just provide a range, e.g., the high and low predicted precipitation for tomorrow, without any probabilistic interpretation
  - 2. Sometimes the data collection process is entirely out of the user's control, or it is not possible to formulate a probabilistic model, e.g., scraping web data

- ▶ Q2. why via probability?
- Sometimes one can/has to perform uncertainty quantification via other means
  - 1. Sometimes one can just provide a range, e.g., the high and low predicted precipitation for tomorrow, without any probabilistic interpretation
  - 2. Sometimes the data collection process is entirely out of the user's control, or it is not possible to formulate a probabilistic model, e.g., scraping web data
- ► A2: So some of the reasons/settings are

- Q2. why via probability?
- Sometimes one can/has to perform uncertainty quantification via other means
  - 1. Sometimes one can just provide a range, e.g., the high and low predicted precipitation for tomorrow, without any probabilistic interpretation
  - Sometimes the data collection process is entirely out of the user's control, or it is not possible to formulate a probabilistic model, e.g., scraping web data
- ► A2: So some of the reasons/settings are
  - 1. If we want to be precise, and be able to use the answers for downstream calculations (e.g., to calculate an expected risk to a shipping company, we need probabilistic interpretation of the range of precipitation)

- Q2. why via probability?
- Sometimes one can/has to perform uncertainty quantification via other means
  - 1. Sometimes one can just provide a range, e.g., the high and low predicted precipitation for tomorrow, without any probabilistic interpretation
  - Sometimes the data collection process is entirely out of the user's control, or it is not possible to formulate a probabilistic model, e.g., scraping web data
- ► A2: So some of the reasons/settings are
  - 1. If we want to be precise, and be able to use the answers for downstream calculations (e.g., to calculate an expected risk to a shipping company, we need probabilistic interpretation of the range of precipitation)
  - 2. In the sciences, a dominating paradigm is to collect a small amount of data in a controlled way, and make inferences based on that

Q3. how via probability?

- Q3. how via probability?
- ► A3: Can start by following the most well established frameworks There is well-developed scholarship, methods and results

- Q3. how via probability?
- ► A3: Can start by following the most well established frameworks There is well-developed scholarship, methods and results
  - Statistical inference and prediction

- Q3. how via probability?
- ► A3: Can start by following the most well established frameworks There is well-developed scholarship, methods and results
  - ► Statistical inference and prediction
    - Confidence intervals (Neyman '37)

- Q3. how via probability?
- ► A3: Can start by following the most well established frameworks There is well-developed scholarship, methods and results
  - ► Statistical inference and prediction
    - ► Confidence intervals (Neyman '37)
    - Prediction/tolerance regions (Wilks '41, Wald, Tukey 40's)

- Q3. how via probability?
- ► A3: Can start by following the most well established frameworks There is well-developed scholarship, methods and results
  - ► Statistical inference and prediction
    - ► Confidence intervals (Neyman '37)
    - Prediction/tolerance regions (Wilks '41, Wald, Tukey 40's)
    - decision theoretic prediction (Takeuchi '75-'80)

- Q3. how via probability?
- ► A3: Can start by following the most well established frameworks There is well-developed scholarship, methods and results
  - ► Statistical inference and prediction
    - Confidence intervals (Neyman '37)
    - Prediction/tolerance regions (Wilks '41, Wald, Tukey 40's)
    - decision theoretic prediction (Takeuchi '75-'80)
  - Computer Science

- Q3. how via probability?
- ► A3: Can start by following the most well established frameworks There is well-developed scholarship, methods and results
  - ► Statistical inference and prediction
    - Confidence intervals (Neyman '37)
    - Prediction/tolerance regions (Wilks '41, Wald, Tukey 40's)
    - decision theoretic prediction (Takeuchi '75-'80)
  - Computer Science
    - Conformal prediction (Vovk et al., '98-)

- Q3. how via probability?
- ► A3: Can start by following the most well established frameworks There is well-developed scholarship, methods and results
  - ► Statistical inference and prediction
    - Confidence intervals (Neyman '37)
    - Prediction/tolerance regions (Wilks '41, Wald, Tukey 40's)
    - decision theoretic prediction (Takeuchi '75-'80)
  - Computer Science
    - Conformal prediction (Vovk et al., '98-)
    - ► The most popular current methods (Ensembles, Test-time model pertubation & augmentation, etc; Gal, Balasubramanian, ... )

- Q3. how via probability?
- ► A3: Can start by following the most well established frameworks There is well-developed scholarship, methods and results
  - Statistical inference and prediction
    - Confidence intervals (Neyman '37)
    - Prediction/tolerance regions (Wilks '41, Wald, Tukey 40's)
    - decision theoretic prediction (Takeuchi '75-'80)
  - Computer Science
    - Conformal prediction (Vovk et al., '98-)
    - ► The most popular current methods (Ensembles, Test-time model pertubation & augmentation, etc; Gal, Balasubramanian, ... )
  - Applied areas

- Q3. how via probability?
- ► A3: Can start by following the most well established frameworks There is well-developed scholarship, methods and results
  - Statistical inference and prediction
    - Confidence intervals (Neyman '37)
    - Prediction/tolerance regions (Wilks '41, Wald, Tukey 40's)
    - decision theoretic prediction (Takeuchi '75-'80)
  - Computer Science
    - Conformal prediction (Vovk et al., '98-)
    - ► The most popular current methods (Ensembles, Test-time model pertubation & augmentation, etc; Gal, Balasubramanian, ...)
  - Applied areas
    - Meteorology: calibration (aka validity, Miller, '63)

- Q3. how via probability?
- ► A3: Can start by following the most well established frameworks There is well-developed scholarship, methods and results
  - Statistical inference and prediction
    - Confidence intervals (Neyman '37)
    - Prediction/tolerance regions (Wilks '41, Wald, Tukey 40's)
    - decision theoretic prediction (Takeuchi '75-'80)
  - Computer Science
    - Conformal prediction (Vovk et al., '98-)
    - ► The most popular current methods (Ensembles, Test-time model pertubation & augmentation, etc; Gal, Balasubramanian, ... )
  - Applied areas
    - Meteorology: calibration (aka validity, Miller, '63)
- ► There is no universally accepted approach. Some are mainly theoretically justified, some mainly empirically. Big open problem: can we have both?

► Q4: why now?

- ▶ Q4: why now?
- ► A4: Several reasons

- ▶ Q4: why now?
- A4: Several reasons
  - ▶ ML already successful in some cases, but still growing in popularity

- ▶ Q4: why now?
- A4: Several reasons
  - ▶ ML already successful in some cases, but still growing in popularity
  - there are some approaches to uncertainty quantification, but none fully satisfying.

- ▶ Q4: why now?
- ► A4: Several reasons
  - ML already successful in some cases, but still growing in popularity
  - there are some approaches to uncertainty quantification, but none fully satisfying.
  - ▶ One of the most exciting areas at the interface of statistics and ML. A lot of great work being done right now, by great research groups. You can be part of it!

Go into any or all of the above in deep detail

- Go into any or all of the above in deep detail
- Overview by Edgar (mainly theory/methods), following lecture notes

- Go into any or all of the above in deep detail
- Overview by Edgar (mainly theory/methods), following lecture notes
- Followed by student lectures on topics of interest (can be theory/methods/algorithms/computation/applications...).

- Go into any or all of the above in deep detail
- Overview by Edgar (mainly theory/methods), following lecture notes
- Followed by student lectures on topics of interest (can be theory/methods/algorithms/computation/applications...).
  - ▶ Roughly one lecture per student. Can work in teams of up to two, and then present two lectures together. Treat it as a course project.

- Go into any or all of the above in deep detail
- Overview by Edgar (mainly theory/methods), following lecture notes
- Followed by student lectures on topics of interest (can be theory/methods/algorithms/computation/applications...).
  - ▶ Roughly one lecture per student. Can work in teams of up to two, and then present two lectures together. Treat it as a course project.
  - ▶ Topics are suggested on the website (Mostly based on important or recent papers). Hopefully we can have some coherent structure (but do not aim for perfect).

- Go into any or all of the above in deep detail
- Overview by Edgar (mainly theory/methods), following lecture notes
- Followed by student lectures on topics of interest (can be theory/methods/algorithms/computation/applications...).
  - ▶ Roughly one lecture per student. Can work in teams of up to two, and then present two lectures together. Treat it as a course project.
  - ▶ Topics are suggested on the website (Mostly based on important or recent papers). Hopefully we can have some coherent structure (but do not aim for perfect).
  - ► There will be a Google sheet where you can sign up.

- Go into any or all of the above in deep detail
- Overview by Edgar (mainly theory/methods), following lecture notes
- Followed by student lectures on topics of interest (can be theory/methods/algorithms/computation/applications...).
  - Roughly one lecture per student. Can work in teams of up to two, and then present two lectures together. Treat it as a course project.
  - ▶ Topics are suggested on the website (Mostly based on important or recent papers). Hopefully we can have some coherent structure (but do not aim for perfect).
  - ► There will be a Google sheet where you can sign up.
  - Meet with Edgar one week in advance of your lecture to get feedback on your plan. Back and forth as you work on your presentation. Prepare cca 60-75 mins, to allow for discussion. Practice your presentation. Provide final presentation 24 hours in advance.

- Go into any or all of the above in deep detail
- Overview by Edgar (mainly theory/methods), following lecture notes
- Followed by student lectures on topics of interest (can be theory/methods/algorithms/computation/applications...).
  - Roughly one lecture per student. Can work in teams of up to two, and then present two lectures together. Treat it as a course project.
  - Topics are suggested on the website (Mostly based on important or recent papers). Hopefully we can have some coherent structure (but do not aim for perfect).
  - ► There will be a Google sheet where you can sign up.
  - Meet with Edgar one week in advance of your lecture to get feedback on your plan. Back and forth as you work on your presentation. Prepare cca 60-75 mins, to allow for discussion. Practice your presentation. Provide final presentation 24 hours in advance.
  - ► Can talk about your own work, But need to provide thorough introduction of the broader context, the technical tools, proofs etc. More of a lecture than a research talk.

- Go into any or all of the above in deep detail
- Overview by Edgar (mainly theory/methods), following lecture notes
- Followed by student lectures on topics of interest (can be theory/methods/algorithms/computation/applications...).
  - Roughly one lecture per student. Can work in teams of up to two, and then present two lectures together. Treat it as a course project.
  - Topics are suggested on the website (Mostly based on important or recent papers). Hopefully we can have some coherent structure (but do not aim for perfect).
  - ► There will be a Google sheet where you can sign up.
  - Meet with Edgar one week in advance of your lecture to get feedback on your plan. Back and forth as you work on your presentation. Prepare cca 60-75 mins, to allow for discussion. Practice your presentation. Provide final presentation 24 hours in advance.
  - Can talk about your own work, But need to provide thorough introduction of the broader context, the technical tools, proofs etc. More of a lecture than a research talk.
  - Aim to identify, discuss, and even answer, research questions.



#### This course: to do now

Website for topics: https://github.com/dobriban/ Topics-In-Modern-Statistical-Learning

#### This course: to do now

- Website for topics: https://github.com/dobriban/ Topics-In-Modern-Statistical-Learning
- ▶ Google sheet to sign up for presentations: https://docs.google.com/spreadsheets/d/ 11YcUl1Z4pFdfQdJWzGQFmSkPqECblSnLuhBaugEJB10/edit?usp= sharing
  - Sign up for one or multiple topics

#### This course: to do now

- Website for topics: https://github.com/dobriban/ Topics-In-Modern-Statistical-Learning
- Google sheet to sign up for presentations: https://docs.google.com/spreadsheets/d/ 11YcUl1Z4pFdfQdJWzGQFmSkPqECblSnLuhBaugEJB10/edit?usp= sharing
  - Sign up for one or multiple topics
- Student introductions