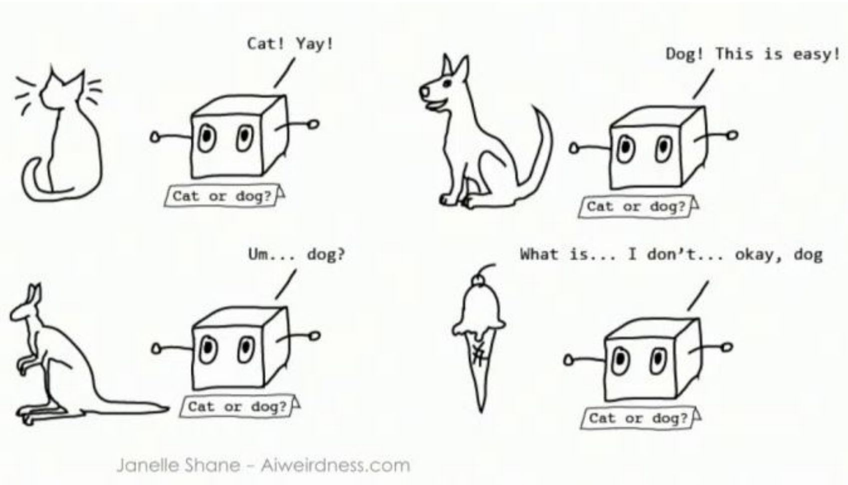
Cat! Yay!
Cat or dog?
Dog! This is easy!
Cat or dog?
Um... dog?
Cat or dog?
What is... I don't... okay, dog
Cat or dog?
Janelle Shane - Aiweirdness.com

Uncertainty reasoning and machine learning

Uncertainty, Decision and Evaluation in Machine Learning

Vu-Linh Nguyen

Chaire de Professeur Junior, Laboratoire Heudiasyc
Université de technologie de Compiègne

AOS4 master courses

Who is more reliable?

An example: Assume we travel to a small village

- There are **two doctors** who can give suggestion on whether a patient suffers from at least one type of serious cancers.
- Either "yes (y)" or "don't know (y/n)" ⟶ go to the closest hospital for further diagnosis
- People ask you "who is more reliable?" given historical record on 1000 patients.

True situations	50 y	50 y	400 n	500 n
Dr. A's predictions	50 y	**50 n**	400 n	400 n + 100 y
Dr. B's predictions	50 y	**40 y/n + 10 n**	400 n	400 n + 100 y

Which model is more reliable?

Another example: Assume we travel to another village

- There are **3 pre-trained models** which can give suggestion on whether a patient suffers from at least one type of serious cancers.
- Either "yes (y)" or "don't know (y/n)" ⟶ go to the closest hospital for further diagnosis
- People ask you "which model is more reliable?" given historical record on 1000 patients.

True situations	50 y	50 y	400 n	500 n
C's predictions	50 y	**50 n**	400 n	**400 n + 100 y**
D's predictions	50 y	**40 y/n + 10 n**	400 n	**400 n + 100 y**
E's predictions	50 y	**40 y/n + 10 n**	400 n	**450 n + 50 y/n**

Go beyond the predictive performance?

It might be safer to defer our answer until we know more about

- how the **models** were learned and make their predictions
- how robust their predictions are (under the presence of noise)
- the decision-making process (cost, consequence, etc.)
- ...

Objectives

After this lecture students should be able to

- conceptually describe the Imprecise Dirichlet model (IDM) [1]
- use IDM in K-nn classifiers with fixed windows [8]
- evaluate classifiers based on IDM and related models [4, 10]

Outline

- Inference from Multinomial Data
- Imprecise Dirichlet Model (IDM)
- (Parzen) Window Classifiers
- Evaluate Classifiers

Basic setup:

- Univariate discrete variable V
- A finite set of possible outcomes $v \in \mathcal{V}$
- Each possible outcome is assigned a **probability value** $\theta_v := P(V = v) = P(\{v\})$

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Questions

- How to model and estimate θ_v?
- How to do inference?
- How to handle small data?
- How to handle missing/partial data?

Frequentist, Bayesian and Imprecise approaches

Axioms

1. Positive: $\theta_v \geq 0$ for all outcomes $v \in \mathcal{V}$
2. Additive: $P(S) = \sum_{v \in S} \theta_v$ for all events $S \subseteq \mathcal{V}$
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Three approaches (discussed in this lecture):

4F. **Frequentist**: $\boldsymbol{\theta} = \{\theta_v | v \in \mathcal{V}\}$ is **not** a random variable (VR).

4B. **Bayesian**: $\boldsymbol{\theta} = \{\theta_v | v \in \mathcal{V}\}$ is a RV $\longleftarrow$ **prior uncertainty** (PU) is described by **a distribution**.

4I. **Imprecise**: $\boldsymbol{\theta} = \{\theta_v | v \in \mathcal{V}\}$ is a RV $\longleftarrow$ PU is described by **a set of distribution** $\boldsymbol{\theta} \in \Theta$.

Some Inference Problems

Multinomial data:

- Given the observed data $\boldsymbol{D}$ where v appear n_v times, $v \in \mathcal{V}$:
- Let $n = \sum_v n_v$ and $\boldsymbol{n} = \{n_v | v \in \mathcal{V}\}$

Multinomial likelihood:

- $\propto$: is proportional to.
- $L(\boldsymbol{\theta}|\boldsymbol{D}) \propto \prod_{v \in \mathcal{V}} (\theta_v)^{n_v}$.

Make inferences about

- the **unknown** $\boldsymbol{\theta}$
- some derived parameter of interest $g(\boldsymbol{\theta})$
- future observations $\boldsymbol{D}'$

(Few) Potential Applications

Multinomial data:

- Given the observed data $\boldsymbol{D}$ where v appear n_v times, $v \in \mathcal{V}$:
- Let $n = \sum_v n_v$ and $\boldsymbol{n} = \{n_v | v \in \mathcal{V}\}$
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Make inferences about

- the **unknown** $\boldsymbol{\theta}$, e.g., its best estimate $\boldsymbol{\theta}^*$
- some derived parameter of interest $g(\boldsymbol{\theta})$

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Make inferences about

- the **unknown** $\boldsymbol{\theta}$, e.g., its best estimate $\boldsymbol{\theta}^*$
- some derived parameter of interest $g(\boldsymbol{\theta})$

You would find such a problem in

- **Parzen window classifiers**
- (Credal) Decision trees, Naive Bayesian/credal Classifier (Lecture 4)
- Ensembles (Trees, Neural Nets, etc.)
- Bayesian Neural Nets

Outline

- Inference from Multinomial Data
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  - Frequentist and Bayesian Approaches
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Frequentist (Recap)

Axioms

1. Positive: $\theta_v \geq 0$ for all outcomes $v \in \mathcal{V}$
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4F. **Frequentist**: $\boldsymbol{\theta} = \{\theta_v | v \in \mathcal{V}\}$ is **not** a random variable (VR).

Estimate $\boldsymbol{\theta}$:

- **Frequencies**: Maximum likelihood estimation (MLE) gives $\theta_v^* = {n_v}/{n}$

Frequentist: Comments

- Does not take into account the **importance of sample size** $\longleftarrow$ **Sources of uncertainty**!

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Coin	Small	Large
Flips	2	$2 \cdot 10^6$
Heads	50%	50%
Tails	50%	50%

- For both coins, a frequentist says

$$\theta^*_{\text{Head}} = \theta^*_{\text{Tail}} = {}^1\!/_2$$

Frequentist: Comments

- Does not take into account the **importance of sample size** ⟵ **Sources of uncertainty**!

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Frequentist: Comments (Cont.)

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Coin	Small	Large
Flips	2	$2 \cdot 10^6$
Heads	$[0,1]$	$[5,10]$
Tails	$[1,2]$	$[5, 2 \cdot 10^6]$

- Can we use frequencies to estimate θ^*_{Head} and θ^*_{Tail}?
- What can you say about the reliability of the estimate for each coin?

Bayesian (Recap)

Axioms

1. Positive: $\theta_v \geq 0$ for all outcomes $v \in \mathcal{V}$
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4B. **Bayesian**: $\boldsymbol{\theta} = \{\theta_v | v \in \mathcal{V}\}$ is a RV $\longleftarrow$ **prior uncertainty** (PU) is described by **a distribution**.

Bayesian estimates:

- **posterior mean** θ_v^* of θ_v: $E(\theta_v)$
- **posterior mean** $\theta_v^* | \boldsymbol{D}$ of $\theta_v | \boldsymbol{D}$: $E(\theta_v | \boldsymbol{D})$

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- **posterior mean** $\theta_v^* | \boldsymbol{D}$ of $\theta_v | \boldsymbol{D}$: $E(\theta_v | \boldsymbol{D})$
- We can also use **posterior mode**

Dirichlet Model

Prior uncertainty: $\boldsymbol{\theta} \sim \text{Diri}(\boldsymbol{\alpha}) = \text{Diri}(s\boldsymbol{f})$

- Prior strengths (hyperparameter): α_v, $v \in \mathcal{V}$
- Total strength (hyperparameter): $s := \sum_{v \in \mathcal{V}} \alpha_v$
- Prior frequencies: $\boldsymbol{f} := \{f_v | v \in \mathcal{V}\}$ with $f_v := \alpha_v / s$, $v \in \mathcal{V}$
- $\theta_v \sim \text{Beta}(sf_v, s\sum_{v' \neq v} f_{v'})$
- $\boldsymbol{\theta}|\boldsymbol{D} \sim \text{Diri}(\boldsymbol{n} + \boldsymbol{\alpha}) = \text{Diri}(\boldsymbol{n} + s\boldsymbol{f})$
- $\theta_x|\boldsymbol{D} \sim \text{Beta}(n_v + sf_v, \sum_{v' \neq v} n_{v'} + s\sum_{v' \neq v} f_{v'})$

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Bayesian estimates:

- **posterior mean** θ_v^* of θ_v: $E(\theta_v) = f_v$
- **posterior mean** $\theta_v^* | \boldsymbol{D}$ of $\theta_v | \boldsymbol{D}$:

$$E(\theta_k | \boldsymbol{D}) = (n_v + \alpha_v)/(n+s) = (n_v + sf_v)/(n+s)$$

Dirichlet Model: Hyperparameters

Solutions for fixed *n* are usually **symmetric Dirichlet priors**

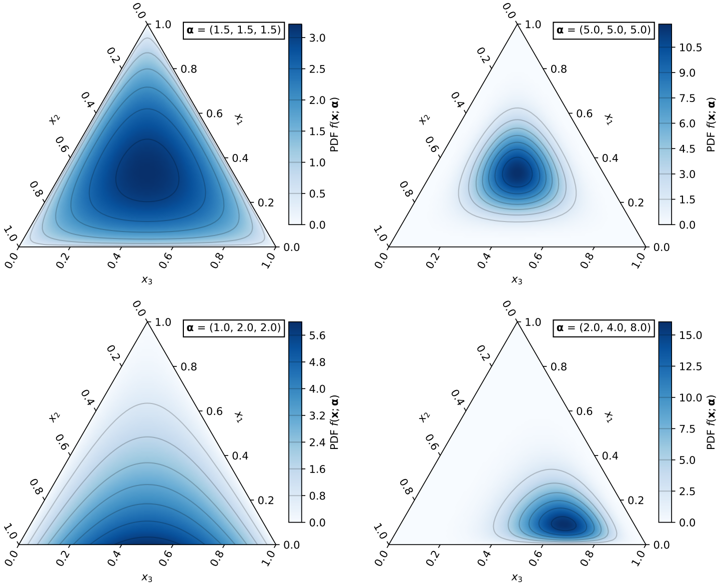
- Prior frequencies: $f_v = {}^{1}\!/\!_{|\mathcal{V}|}$, $v \in \mathcal{V}$
- Total strength: $s = g'(|\mathcal{V}|)$

Dirichlet Model: Hyperparameters

Solutions for fixed n are usually **symmetric Dirichlet priors**

- Prior frequencies: $f_v = {}^1\!/_{|\mathcal{V}|}$, $v \in \mathcal{V}$
- Total strength: $s = g'(|\mathcal{V}|)$

Advocators	α_v	s
Haldane (1948)	0	0
Perks (1947)	${}^1\!/_{|\mathcal{V}|}$	1
Jeffreys (1946, 1961)	${}^1\!/_2$	${}^{|\mathcal{V}|}\!/_2$
Bayes-Laplace	1	$|\mathcal{V}|$


α = (1.5, 1.5, 1.5)
α = (5.0, 5.0, 5.0)
α = (1.0, 2.0, 2.0)
α = (2.0, 4.0, 8.0)
PDF f(x; α)
x1
x2
x3

The Importance of Sample Size (Exercise 1)

Coin	Small	Large
Flips	2	$2 \cdot 10^6$
Heads	50%	50%
Tails	50%	50%

- For both coins, a frequentist says

$$p_{\text{Heads}} = p_{\text{Tails}} = 1/2$$

- Do Bayesians say the same thing?

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Coin	Small	Large
Flips	4	$4 \cdot 10^6$
Heads	25%	25%
Tails	75%	75%

- For both coins, a frequentist says

$$p_{\text{Heads}} = 0.25, p_{\text{Tails}} = 0.75$$

- Do Bayesians say the same thing?

The Importance of Sample Size (Exercise 1)

Coin	Small	Large
Flips	2	$2 \cdot 10^6$
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Advocators	α_x	s	p^S_H	p^S_T	p^L_H	p^L_T
Haldane (1948)	0	0	???	???	???	???
Perks (1947)	$1/\lvert\mathcal{V}\rvert$	1	???	???	???	???
Jeffreys (1946, 1961)	$1/2$	$\lvert\mathcal{V}\rvert/2$	???	???	???	???
Bayes-Laplace	1	$\lvert\mathcal{V}\rvert$	???	???	???	???

The Importance of Sample Size (Solution 1)

Coin	Small	Large
Flips	2	$2 \cdot 10^6$
Heads	50%	50%
Tails	50%	50%

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$$p_{\text{Heads}} = p_{\text{Tails}} = {}^1\!/_2$$

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  Yes!

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Advocators	α_V	s	p^S_{H}	p^S_{T}	p^L_{H}	p^L_{T}
Haldane (1948)	0	0	0.25	0.75	0.25	0.75
Perks (1947)	$1/\lvert\mathcal{V}\rvert$	1	0.3	0.7	0.25	0.75
Jeffreys (1946, 1961)	$1/2$	$\lvert\mathcal{V}\rvert/2$	0.3	0.7	0.25	0.75
Bayes-Laplace	1	$\lvert\mathcal{V}\rvert$	0.33	0.67	0.25	0.75

The Importance of Sample Size (Exercise 2)

Coin	Small	Large
Flips	2	$2 \cdot 10^6$
Heads	0%	0%
Tails	100%	100%

- For both coins, a frequentist says

$$p_{\text{Heads}} = 0, p_{\text{Tails}} = 1$$

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The Importance of Sample Size (Exercise 2)

Coin	Small	Large
Flips	2	$2 \cdot 10^6$
Heads	0%	0%
Tails	100%	100%

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Advocators	α_x	s	p_H^S	p_T^S	p_H^L	p_T^L
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Perks (1947)	$1/\lvert\mathcal{V}\rvert$	1	???	???	???	???
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Bayes-Laplace	1	$\lvert\mathcal{V}\rvert$	???	???	???	???

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Advocators	α_x	s	p^S_{H}	p^S_{T}	p^L_{H}	p^L_{T}
Haldane (1948)	0	0	0	1	0	1
Perks (1947)	$1/\lvert\mathcal{V}\rvert$	1	0.17	0.83	$3 \cdot 10^{-7}$	$1 - 3 \cdot 10^{-7}$
Jeffreys	$1/\lvert\mathcal{V}\rvert$	1	0.17	0.83	$3 \cdot 10^{-7}$	$1 - 3 \cdot 10^{-7}$
Bayes-Laplace	1	$\lvert\mathcal{V}\rvert$	0.25	0.75	$5 \cdot 10^{-7}$	$1 - 5 \cdot 10^{-7}$

Dirichlet Model (DM): Comments

- Does not (naturally) take into account missing/partial data

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Coin	Small	Large
Flips	2	$2\cdot 10^6$
Heads	$[0,1]$	$[5,10]$
Tails	$[1,2]$	$[5,2\cdot 10^6]$

- Can we use DM to estimate θ^*_{Head} and θ^*_{Tail}?
- What can you say about the reliability of the estimate for each coin?

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- Inference from Multinomial Data
- Imprecise Dirichlet Model (IDM)
  - Frequentist and Bayesian Approaches
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Imprecise (Recap)

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Interval estimates:

- **posterior mean** θ_v^* of θ_v:

$$E(\theta_v) \in [\underline{E}(\theta_v), \overline{E}(\theta_v)]$$

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$$E(\theta_v | \boldsymbol{D}) \in [\underline{E}(\theta_v | \boldsymbol{D}), \overline{E}(\theta_v | \boldsymbol{D})]$$

Imprecise Dirichlet Model

Prior uncertainty: $\mathbf{\Theta} = \{\boldsymbol{\theta} \sim \text{Diri}(\boldsymbol{\alpha}) = \text{Diri}(s\boldsymbol{f}) | \sum_{v \in \mathcal{V}} \alpha_v = s\}$

- Hyperparameter: s = **degree of imprecision** in the inferences
- Prior frequencies: $\boldsymbol{f} := \{f_v | v \in \mathcal{V}\}$ with $f_v := \alpha_v / s$, $v \in \mathcal{V}$
- $\theta_v \sim \text{Beta}(sf_v, s\sum_{v' \neq v} f_{v'})$
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- $\theta_x|\boldsymbol{D} \sim \text{Beta}(n_v + sf_v, \sum_{v' \neq v} n_{v'} + s\sum_{v' \neq v} f_{v'})$

Posterior mean $\theta_v^*|\boldsymbol{D}$ of $\theta_v|\boldsymbol{D}$:

$$E(\theta_v|\boldsymbol{D}) \in [\underline{E}(\theta_v|\boldsymbol{D}), \overline{E}(\theta_v|\boldsymbol{D})], \tag{1}$$

$$\underline{E}(\theta_v|\boldsymbol{D}) = {}^{n_v}/_{(n+s)}, \tag{2}$$

$$\overline{E}(\theta_v|\boldsymbol{D}) = {}^{(n_v+s)}/_{(n+s)}. \tag{3}$$

The Importance of Sample Size (Exercise 3)

Coin	Small	Large
Flips	2	$2 \cdot 10^6$
Heads	50%	50%
Tails	50%	50%

- For both coins, a frequentist says
$$\theta_{\text{Heads}} = \theta_{\text{Tails}} = 1/2$$
- Bayesians would say the same thing
- Would IDM say the same thing?

The Importance of Sample Size (Exercise 3)

Coin	Small	Large
Flips	2	$2 \cdot 10^6$
Heads	50%	50%
Tails	50%	50%

- For both coins, a frequentist says

$$\theta_{\text{Heads}} = \theta_{\text{Tails}} = 1/2$$

- Bayesians would say the same thing
- Would IDM say the same thing?

	$\underline{P}^S_{\text{H}}$	$\overline{P}^S_{\text{H}}$	$\underline{P}^L_{\text{H}}$	$\overline{P}^L_{\text{H}}$
$s = 1$	???	???	???	???
$s = 2$	???	???	???	???

The Importance of Sample Size (Solution 3)

Coin	Small	Large
Flips	2	$2 \cdot 10^6$
Heads	50%	50%
Tails	50%	50%

- For both coins, a frequentist says

$$\theta_{\text{Heads}} = \theta_{\text{Tails}} = 1/2$$

- Bayesians would say the same thing
- Would IDM say the same thing?

	$\underline{P}_{\text{H}}^{S}$	$\overline{P}_{\text{H}}^{S}$	$\underline{P}_{\text{H}}^{L}$	$\overline{P}_{\text{H}}^{L}$
$s = 1$	0.33	0.67	$0.5 - 3 \cdot 10^{-7}$	$0.5 + 3 \cdot 10^{-7}$
$s = 2$	0.25	0.75	$0.5 - 5 \cdot 10^{-7}$	$0.5 + 5 \cdot 10^{-7}$

The Importance of Sample Size (Exercise 4)

Coin	Small	Large
Flips	2	$2 \cdot 10^6$
Heads	0%	0%
Tails	100%	100%

- For both coins, a frequentist says

$$\theta_{\text{Heads}} = 0, \theta_{\text{Tails}} = 1$$

- Bayesians would say different things
- What would IDM say?

The Importance of Sample Size (Exercise 4)

Coin	Small	Large
Flips	2	$2 \cdot 10^6$
Heads	0%	0%
Tails	100%	100%

- For both coins, a frequentist says

$$\theta_{\text{Heads}} = 0, \theta_{\text{Tails}} = 1$$

- Bayesians would say different things
- What would IDM say?

Advocators	α_x	s	p^S_{H}	p^S_{T}	p^L_{H}	p^L_{T}
Haldane (1948)	0	0	0	1	0	1
Perks (1947)	$1/\lvert\mathcal{V}\rvert$	1	0.17	0.83	$3 \cdot 10^{-7}$	$1 - 3 \cdot 10^{-7}$
Jeffreys	$1/\lvert\mathcal{V}\rvert$	1	0.17	0.83	$3 \cdot 10^{-7}$	$1 - 3 \cdot 10^{-7}$
Bayes-Laplace	1	$\lvert\mathcal{V}\rvert$	0.25	0.75	$5 \cdot 10^{-7}$	$1 - 5 \cdot 10^{-7}$

The Importance of Sample Size (Exercise 4)

Coin	Small	Large
Flips	2	$2 \cdot 10^6$
Heads	0%	0%
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$$\theta_{\text{Heads}} = 0, \theta_{\text{Tails}} = 1$$

- Bayesians would say different things
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Advocators	α_x	s	p_{H}^S	p_{T}^S	p_{H}^L	p_{T}^L
Haldane (1948)	0	0	0	1	0	1
Perks (1947)	$1/\lvert\mathcal{V}\rvert$	1	0.17	0.83	$3 \cdot 10^{-7}$	$1 - 3 \cdot 10^{-7}$
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IDM	$\underline{P}_{\text{H}}^S$	$\overline{P}_{\text{H}}^S$	$\underline{P}_{\text{H}}^L$	$\overline{P}_{\text{H}}^L$
$s = 1$	???	???	???	???
$s = 2$	???	???	???	???

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IDM	$\underline{P}^S_{\text{H}}$	$\overline{P}^S_{\text{H}}$	$\underline{P}^L_{\text{H}}$	$\overline{P}^L_{\text{H}}$
$s = 1$	0	0.33	0	$5 \cdot 10^{-7}$
$s = 2$	0	0.50	0	10^{-6}

The case of Partial/Missing Data

What if we only know $n_v \in \boldsymbol{n}_v \subset \{0, 1, \ldots, n\}$?

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- Imprecise approaches provide nice tools to handle such data sets [8]
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Interval posterior mean $\theta_v^* | \mathscr{D}$ of $\theta_v | \mathscr{D}$:

$$E(\theta_v|\mathscr{D}) \in [\underline{E}(\theta_v|\mathscr{D}), \overline{E}(\theta_v|\mathscr{D})], \quad (4)$$

$$\underline{E}(\theta_v|\mathscr{D}) = \min_{\boldsymbol{D} \in \mathscr{D}} \underline{E}(\theta_v|\boldsymbol{D}) = \min_{\boldsymbol{D} \in \mathscr{D}} {}^{n_v}/_{(n+s)}, \quad (5)$$

$$\overline{E}(\theta_v|\mathscr{D}) = \max_{\boldsymbol{D} \in \mathscr{D}} \overline{E}(\theta_v|\boldsymbol{D}) = \max_{\boldsymbol{D} \in \mathscr{D}} {}^{(n_v+s)}/_{(n+s)}. \quad (6)$$

Determine $\mathscr{D}$ (Exercise 5)

Coin	Small	Large
Flips	2	$2 \cdot 10^6$
Heads	$[0,1]$	$[5,10]$
Tails	$[1,2]$	$[5, 2 \cdot 10^6]$

- Recap: $\mathscr{D} = \{\boldsymbol{D} | n_v \in \boldsymbol{n}_v, \sum_{v \in \mathcal{V}} n_v = n\}$
- What is $\mathscr{D}^S$ for the first coin?
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- What is $\mathscr{D}^L$ for the second coin?

Coin	Small	$\boldsymbol{D}_1$	$\boldsymbol{D}_2$
Flips	2	2	2
Heads	$[0,1]$	0	1
Tails	$[1,2]$	2	1

Determine $\mathscr{D}$ (Exercise 5)

Coin	Small	Large
Flips	2	$2 \cdot 10^6$
Heads	$[0,1]$	$[5,10]$
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Coin	Small	$\boldsymbol{D}_1$	$\boldsymbol{D}_2$
Flips	2	2	2
Heads	$[0,1]$	0	1
Tails	$[1,2]$	2	1

Coin	Large	$\boldsymbol{D}_1$	$\boldsymbol{D}_2$	$\boldsymbol{D}_3$	$\boldsymbol{D}_4$	$\boldsymbol{D}_5$	$\boldsymbol{D}_6$
Flips	$n = 2 \cdot 10^6$	n	n	n	n	n	n
Heads	$[5,10]$	???	???	???	???	???	???
Tails	$[5,n]$	???	???	???	???	???	???

Determine $\mathscr{D}$ (Solution 5)

Coin	Small	Large
Flips	2	$2 \cdot 10^6$
Heads	$[0,1]$	$[5,10]$
Tails	$[1,2]$	$[5, 2\cdot 10^6]$

- Recap: $\mathscr{D} = \{\boldsymbol{D} | n_v \in \boldsymbol{n}_v, \sum_{v \in \mathcal{V}} n_v = n\}$
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Coin	Small	$\boldsymbol{D}_1$	$\boldsymbol{D}_2$
Flips	2	2	2
Heads	$[0,1]$	0	1
Tails	$[1,2]$	2	1

Coin	Large	$\boldsymbol{D}_1$	$\boldsymbol{D}_2$	$\boldsymbol{D}_3$	$\boldsymbol{D}_4$	$\boldsymbol{D}_5$	$\boldsymbol{D}_6$
Flips	$n = 2 \cdot 10^6$	n	n	n	n	n	n
Heads	$[5,10]$	5	6	7	8	9	10
Tails	$[5,n]$	$n-5$	$n-6$	$n-7$	$n-8$	$n-9$	$n-10$

Compute Lower and Upper Expectations (Exercise 6)

Interval posterior mean $\theta_v^*|\mathscr{D}$ of $\theta_v|\mathscr{D}$:

$$\underline{E}(\theta_v|\mathscr{D}) = \min_{\boldsymbol{D}\in\mathscr{D}} \underline{E}(\theta_v|\boldsymbol{D}) = \min_{\boldsymbol{D}\in\mathscr{D}} {}^{n_v}/_{(n+s)}, \quad (7)$$

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Coin	Small	$\boldsymbol{D}_1$	$\boldsymbol{D}_2$	$\underline{E}(\theta_v\|\mathscr{D})$	$\overline{E}(\theta_v\|\boldsymbol{D})$
Flips	2	2	2		
Heads	[0,1]	0	1	???	???
Tails	[1,2]	2	1	???	???

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Coin	Small	$\boldsymbol{D}_1$	$\boldsymbol{D}_2$	$\underline{E}(\theta_v\|\mathscr{D})$	$\overline{E}(\theta_v\|\boldsymbol{D})$
Flips	2	2	2		
Heads	$[0,1]$	0	1	???	???
Tails	$[1,2]$	2	1	???	???

Coin	Large	$\boldsymbol{D}_1$	...	$\boldsymbol{D}_6$	$\underline{E}(\theta_v\|\mathscr{D})$	$\overline{E}(\theta_v\|\boldsymbol{D})$
Flips	$n = 2\cdot 10^6$	n	...	n		
Heads	$[5,10]$	5	...	10	???	???
Tails	$[5,n]$	$n-5$	...	$n-10$	???	???

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Coin	Small	$\boldsymbol{D}_1$	$\boldsymbol{D}_2$	$\underline{E}(\theta_v\|\mathscr{D})$	$\overline{E}(\theta_v\|\boldsymbol{D})$
Flips	2	2	2		
Heads	$[0,1]$	0	1	$^{s}/_{(2+s)}$	$^{(1+s)}/_{(2+s)}$
Tails	$[1,2]$	2	1	$^{(1+s}/_{(2+s)}$	$^{(2+s)}/_{(2+s)}$

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Coin	Large	$\boldsymbol{D}_1$	…	$\boldsymbol{D}_6$	$\underline{E}(\theta_v\|\mathscr{D})$	$\overline{E}(\theta_v\|\boldsymbol{D})$
Flips	$n = 2\cdot 10^6$	n	…	n		
Heads	$[5,10]$	5	…	10	${}^{(5+s)}/_{(n+s)}$	${}^{(10+s)}/_{(n+s)}$
Tails	$[5,n]$	$n-5$	…	$n-10$	${}^{(n-10+s)}/_{(n+s)}$	${}^{(n-5+s)}/_{(n+s)}$

Outline

- Inference from Multinomial Data
- Imprecise Dirichlet Model (IDM)
- (Parzen) Window Classifiers
- Evaluate Classifiers

Pazen Window Classifiers [5]

Basic setup and assumption

- Given training data $\boldsymbol{D} \subset \mathscr{X} \times \mathscr{Y}$, a distance $d(\boldsymbol{x}, \boldsymbol{x}')$, and a threshold ϵ
- For each instance $\boldsymbol{x}$, determine $\boldsymbol{D}_\epsilon(\boldsymbol{x}) = \{\boldsymbol{x}' \in \boldsymbol{D} | d(\boldsymbol{x}, \boldsymbol{x}') \leq \epsilon\}$
- $\boldsymbol{D}_\epsilon(\boldsymbol{x})$ can be used to estimate $\boldsymbol{\theta}|\boldsymbol{x} := \boldsymbol{\theta}|\boldsymbol{D}_\epsilon(\boldsymbol{x})$

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Optimal decision rules

- Let $\ell : \mathscr{Y} \times \mathscr{Y} \longmapsto \mathbb{R}_+$ be any loss function.
- The Bayes-optimal prediction of ℓ on $\boldsymbol{x}$ is

$$y_\ell^{\boldsymbol{\theta}} = \operatorname*{argmin}_{\overline{y} \in \mathscr{Y}} \sum_{y \in \mathscr{Y}} \ell(\overline{y}, y) \theta_y | \boldsymbol{x}$$

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$$y_\ell^{\boldsymbol{\theta}} = \operatorname*{argmin}_{\overline{y} \in \mathscr{Y}} \sum_{y \in \mathscr{Y}} \ell(\overline{y}, y) \theta_y | \boldsymbol{x}$$
- If ℓ is subset 0/1 loss, i.e. $\ell(\overline{y}, y) = \mathbb{1}(\overline{y} \neq y)$, then (Check!)
$$y_\ell^{\boldsymbol{\theta}} = \operatorname*{argmax}_{\overline{y} \in \mathscr{Y}} \theta_{\overline{y}} | \boldsymbol{x}$$

Learning Problem

Given $\boldsymbol{D}_\epsilon(\boldsymbol{x})$, we can

- Count $n = |\boldsymbol{D}_\epsilon(\boldsymbol{x})|$ and n_y, for any $y \in \mathscr{Y} \longleftarrow \sum_{y \in \mathscr{Y}} n_y = n$
- Estimate $\boldsymbol{\theta}|\boldsymbol{x}$ using MLE, DM, etc.

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What would we do if $\boldsymbol{D}$ contains

- a small number of instances
- and/or missing/partial data?

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$\boldsymbol{x}' \in \boldsymbol{D}_\epsilon(\boldsymbol{x})$	$Y' \subset \mathscr{Y} = \{\text{Apple}, \text{Banana}, \text{Tomato}\}$
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$\boldsymbol{x}'_5$	Tomato
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Learning Problem (Cont.)

Given $\boldsymbol{D}_{\epsilon}(\boldsymbol{x})$, we can

- Count $n = |\boldsymbol{D}_{\epsilon}(\boldsymbol{x})|$ and $\boldsymbol{n}_y$ for $y \in \mathscr{Y}$
- Determine $\mathscr{D} = \{\boldsymbol{D} | n_y \in \boldsymbol{n}_y, \sum_{y \in \mathscr{Y}} n_y = n\}$

Learning Problem (Cont.)

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- Count $n = |\boldsymbol{D}_\epsilon(\boldsymbol{x})|$ and $\boldsymbol{n}_y$ for $y \in \mathscr{Y}$
- Determine $\mathscr{D} = \{\boldsymbol{D} | n_y \in \boldsymbol{n}_y, \sum_{y \in \mathscr{Y}} n_y = n\}$

Using IDM to estimate **interval posterior mean** $\theta_y^*|\mathscr{D}$ of $\theta_y|\mathscr{D}$:

$$\underline{E}(\theta_y|\boldsymbol{x}) = \min_{\boldsymbol{D}\in\mathscr{D}} \underline{E}(\theta_y|\boldsymbol{x}) = \min_{\boldsymbol{D}\in\mathscr{D}} {n_y}/{(n+s)}, \tag{11}$$

$$\overline{E}(\theta_y|\boldsymbol{x}) = \max_{\boldsymbol{D}\in\mathscr{D}} \overline{E}(\theta_y|\boldsymbol{D}) = \max_{\boldsymbol{D}\in\mathscr{D}} {(n_y+s)}/{(n+s)}. \tag{12}$$

Determine Possible Precise Data Set (Exercise 7)

$\boldsymbol{x}' \in \boldsymbol{D}_\epsilon(\boldsymbol{x})$	$Y \subset \mathcal{Y} = \{\text{Apple}, \text{Banana}, \text{Tomato}\}$
$\boldsymbol{x}'_1$	Apple or Banana, but not Tomato
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$$n = 7, \boldsymbol{n}_A = ???, \boldsymbol{n}_B = ???, \boldsymbol{n}_T = ??? \qquad (13)$$

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	$\boldsymbol{D}_1$	$\boldsymbol{D}_2$	$\boldsymbol{D}_3$	$\boldsymbol{D}_4$	$\boldsymbol{D}_5$	$\boldsymbol{D}_6$	$\boldsymbol{D}_7$	$\boldsymbol{D}_8$
n_A	???	???	???	???	???	???	???	???
n_B	???	???	???	???	???	???	???	???
n_T	???	???	???	???	???	???	???	???

Determine Possible Precise Data Set (Solution 7)

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$$n = 7\,, \boldsymbol{n}_A = \{0, 1, 2\}\,, \boldsymbol{n}_B = \{2, 3, 4\}\,, \boldsymbol{n}_T = \{2, 3, 4\} \quad (14)$$

Determine Possible Precise Data Set (Solution 7)

$\boldsymbol{x}' \in \boldsymbol{D}_\epsilon(\boldsymbol{x})$	$Y \subset \mathscr{Y} = \{\text{Apple}, \text{Banana}, \text{Tomato}\}$
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$$n = 7\,, \boldsymbol{n}_A = \{0, 1, 2\}\,, \boldsymbol{n}_B = \{2, 3, 4\}\,, \boldsymbol{n}_T = \{2, 3, 4\} \tag{14}$$

	$\boldsymbol{D}_1$	$\boldsymbol{D}_2$	$\boldsymbol{D}_3$	$\boldsymbol{D}_4$	$\boldsymbol{D}_5$	$\boldsymbol{D}_6$	$\boldsymbol{D}_7$	$\boldsymbol{D}_8$
n_A	0	0	1	1	1	2	2	2
n_B	3	4	2	3	4	2	3	4
n_T	4	3	4	3	2	4	3	3

Compute Lower and Upper Expectations (Exercise 8)

	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8
n_A	0	0	1	1	1	2	2	2
n_B	3	4	2	3	4	2	3	4
n_T	4	3	4	3	2	4	3	3

Using IDM to estimate **interval posterior mean** $\theta^*_y|\mathscr{D}$ of $\theta_y|\mathscr{D}$:

$$\underline{E}(\theta_y|\boldsymbol{x}) = \min_{\boldsymbol{D}\in\mathscr{D}} \underline{E}(\theta_y|\boldsymbol{x}) = \min_{\boldsymbol{D}\in\mathscr{D}} n_y/(n+s), \qquad (15)$$

$$\overline{E}(\theta_y|\boldsymbol{x}) = \max_{\boldsymbol{D}\in\mathscr{D}} \overline{E}(\theta_y|\boldsymbol{D}) = \max_{\boldsymbol{D}\in\mathscr{D}} (n_y+s)/(n+s). \qquad (16)$$

Compute Lower and Upper Expectations (Exercise 8)

	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8
n_A	0	0	1	1	1	2	2	2
n_B	3	4	2	3	4	2	3	4
n_T	4	3	4	3	2	4	3	3

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	$\underline{E}(\theta_y\|\boldsymbol{x})$	$\overline{E}(\theta_y\|\boldsymbol{x})$
A	???	???
B	???	???
T	???	???

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	$\underline{E}(\theta_y\|\boldsymbol{x})$	$\overline{E}(\theta_y\|\boldsymbol{x})$
A	$^{0}/_{(7+s)}$	$^{(2+s)}/_{(7+s)}$
B	$^{2}/_{(7+s)}$	$^{(4+s)}/_{(7+s)}$
T	$^{2}/_{(7+s)}$	$^{(4+s)}/_{(7+s)}$

Compute Lower and Upper Expectations

- For any $y \in \mathscr{Y}$, let

$$\underline{n}_y = \sum_{\boldsymbol{x}' \in \boldsymbol{D}} \mathbb{1}(y = Y'), \quad (19)$$

$$\overline{n}_y = \sum_{\boldsymbol{x}' \in \boldsymbol{D}} \mathbb{1}(y \in Y'). \quad (20)$$

- Compute **interval posterior mean** $\theta_y^*|\mathscr{D}$ of $\theta_y|\mathscr{D}$:

$$\underline{E}(\theta_y|\boldsymbol{x}) \underline{n}_y/(n+s), \quad (21)$$

$$\overline{E}(\theta_y|\boldsymbol{x}) = (\overline{n}_y+s)/(n+s). \quad (22)$$

Compute Lower and Upper Bound Expectation (Again)

$\boldsymbol{x}' \in \boldsymbol{D}_\epsilon(\boldsymbol{x})$	$Y \subset \mathscr{Y} = \{\text{Apple}, \text{Banana}, \text{Tomato}\}$
$\boldsymbol{x}'_1$	Apple or Banana, but not Tomato
$\boldsymbol{x}'_2$	Banana or Tomato, but not Apple
$\boldsymbol{x}'_3$	Apple or Tomato, but not Banana
$\boldsymbol{x}'_4$	Tomato
$\boldsymbol{x}'_5$	Tomato
$\boldsymbol{x}'_6$	Banana
$\boldsymbol{x}'_7$	Banana

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	$\underline{n}_y$	$\overline{n}_y$	$\underline{E}(\theta_y \vert \boldsymbol{x})$	$\overline{E}(\theta_y \vert \boldsymbol{x})$
A	0	2	$0/(7+s)$	$(2+s)/(7+s)$
B	2	4	$2/(7+s)$	$(4+s)/(7+s)$
T	2	4	$2/(7+s)$	$(4+s)/(7+s)$

Set-Valued Predictions [6, 7] (Recap)

E-admissibility Rule:

- An optimal prediction is

$$Y^{E}_{\ell,\mathbf{\Theta}|\boldsymbol{x}} = \{y \in \mathscr{Y} \,|\, \exists \boldsymbol{\theta}|\boldsymbol{x} \in \mathbf{\Theta}|\boldsymbol{x} \text{ s.t. } y = y_{\ell}^{\boldsymbol{\theta}|\boldsymbol{x}}\}.$$

- Computation: Solving linear programs, etc.

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Package: github.com/Haifei-ZHANG/Probability-Sets-Model

Outline

- Inference from Multinomial Data
- Imprecise Dirichlet Model (IDM)
- (Parzen) Window Classifiers
- Evaluate Classifiers
  - The cases of Singleton Prediction
  - The cases of Set-Valued Predictions

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(Few) Commonly Used Criteria

Predictive ability (on a test set):

- Let $\ell : \mathscr{Y} \times \mathscr{Y} \longmapsto \mathbb{R}_+$ be any loss function.
- Compute (average) loss on the test set

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(Few) Other criteria:

- Model complexity (Storage memory)
- Training and/or Inference time
- Robustness: Under the presence of noise
- Trustworthiness: Explainability, interpretability, etc.

Calibration Error (See Lecture 6)

Confidence calibration [2]:

$$P(y = \arg\max_{y \in \mathcal{Y}} \theta_y | \boldsymbol{x} \text{ such that } \max_{y \in \mathcal{Y}} \theta_y | \boldsymbol{x} = \beta) = \beta, \forall \beta \in [0, 1]. \tag{23}$$

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Classwise calibration [9]:

$$P(y \text{ such that } \theta_y | \boldsymbol{x} = \beta_y) = \beta_y, y \in \mathcal{Y}, \beta \in [0,1]. \tag{24}$$

- May be harder to ensure, compared to **confidence calibration**

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Distribution calibration [3]:

$$P(y \text{ such that } \boldsymbol{\theta} | \boldsymbol{x} = \boldsymbol{q}) = \boldsymbol{q}, \forall \boldsymbol{q} \in \triangle^{|\mathcal{Y}|}, \quad (25)$$

where $\triangle^{|\mathcal{Y}|}$ is the $|\mathcal{Y}|$-dimensional simplex

- May be harder to ensure, compared to the **above notions**.

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Predictive ability (on a test set):

- We can use any loss function $\ell : 2^{\mathscr{Y}} \times \mathscr{Y} \longmapsto \mathbb{R}_+$.
- If we use utility metric $u = 1 - \ell$, replacing $\min$ by $\max$.
- Set-based utility functions [10]: $u(Y, y) = \mathbb{1}(y \in Y)g(|Y|)$
- Few commonly used utility function [4]:

$$g_\alpha(|Y|) = \frac{\alpha}{|Y|} + \frac{\alpha - 1}{|Y|^2},.$$

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Set-Based Utility Functions

Few commonly used **utility functions**:

$$g_\alpha(|Y|) = \frac{\alpha}{|Y|} - \frac{\alpha - 1}{|Y|^2}.$$

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Reward to cautiousness:

- u_{50}: $\alpha = 1 \longleftarrow$ no reward.
- u_{65}: $\alpha = 1.6$, moderate reward.
- u_{80}: $\alpha = 2.2$, big reward.
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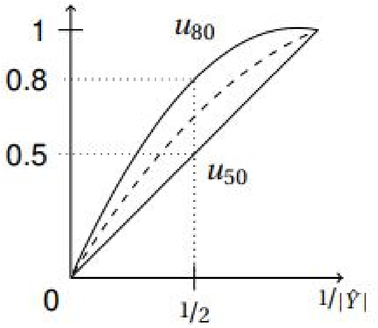

Set-Based Utility Functions (Exercise 9)

Question: Prove that $g_\alpha(|Y|) \leq 1$ if $\alpha \leq 3$.

Coverage Error (See Lecture 6)

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