Quantification

Predicting Class Frequencies via Supervised Learning

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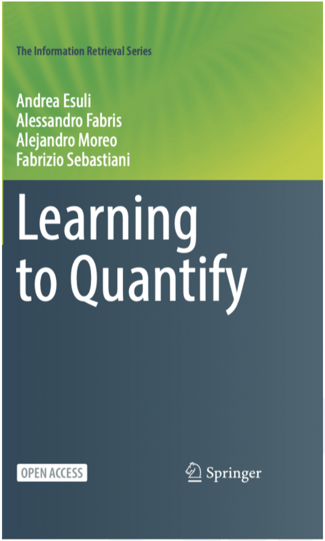
What this course is about

- A course about a special type of application contexts for supervised learning technologies, i.e., the contexts in which our interest is not at the individual level but at the aggregate level
- Many fields of human activity focus not on the "micro" level but on the "macro" level (e.g., the social sciences, political science, epidemiology, ecological modelling, market research)
- In these fields we don't care about individuals, we care about populations; we don't care about the needle, but we care about the haystack



The Information Retrieval Series

Andrea Esuli
Alessandro Fabris
Alejandro Moreo
Fabrizio Sebastiani

Learning to Quantify

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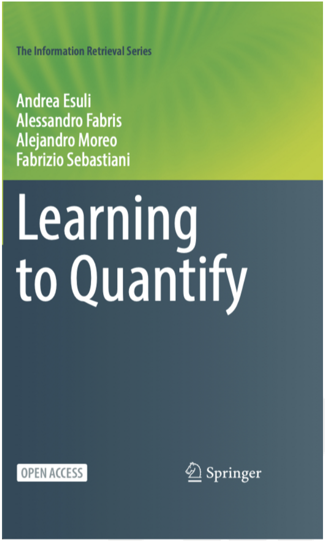
Springer

Andrea Esuli, Alessandro Fabris, Alejandro Moreo, Fabrizio Sebastiani. Learning to Quantify. Springer Nature, 2023. Download for free at https://bit.ly/3JgEMJ0

What this course is about

- Learning to Quantify (aka quantification) stands to classification as aggregate data stand to individual data
- This course is an introduction to this field, to its applications, to the methods for performing quantification, and to the methods for evaluating quantification systems



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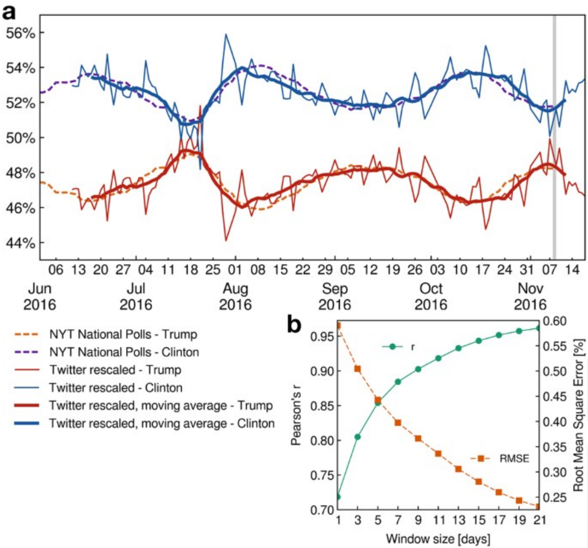
What is “Learning to Quantify” (a.k.a. quantification)?



What is "Learning to Quantify" (a.k.a. quantification)?

- In many applications of classification, the real goal is determining the relative frequency of each class in the unlabelled data. This task has come to be called quantification.
- E.g.
  - Among this week's tweets concerning the next presidential elections, what is the fraction of ProDemocrat ones?
  - Among this week's posts about the Apple Watch Ultra posted on forums, what is the fraction of VeryNegative ones?
  - How are these fractions evolving over time?
- Otherwise called "learning to quantify", "supervised prevalence estimation", "class prior estimation", "prior estimation", "class distribution estimation", ...
- Relative frequencies otherwise called "prevalence values", "class priors", "priors", "class fractions", "class percentages", ...

P. González, A. Castaño, N. Chawla, and J. del Coz. A review on quantification learning. *ACM Computing Surveys*, 50(5): 74:1–74:40, 2017.

What is “Learning to Quantify” (a.k.a. quantification)?

- A fully supervised task (unless otherwise noted)
- A task “simpler” (i.e., less general) than classification
    - Vapnik’s principle : *If you possess a restricted amount of information for solving some problem, try to solve the problem directly and never solve a more general problem as an intermediate step. It is possible that the available information is sufficient for a direct solution but is insufficient for solving a more general intermediate problem.*

What is “Learning to Quantify” (a.k.a. quantification)?

- An “asymmetric” learning task, since training examples are individual labelled items and test examples are samples of individual unlabelled items

(Binary) Task	Model	Training		Test		Type
		Examples	Labels	Examples	Labels	
Classification	$h : \mathcal{X} \rightarrow \{+1, -1\}$	Individual items	Classes	Individual items	Classes	Symmetric
Regression	$h : \mathcal{X} \rightarrow \mathbb{R}$	Individual items	Real values	Individual items	Real values	Symmetric
Learning from Label Proportions	$h : 2^{\mathcal{X}} \rightarrow [0, 1]$	Samples of individual items	Real values in [0,1]	Samples of individual items	Real values in [0,1]	Symmetric
Quantification	$h : 2^{\mathcal{X}} \rightarrow [0, 1]$	Individual items	Classes	Samples of individual items	Real values in [0,1]	Asymmetric

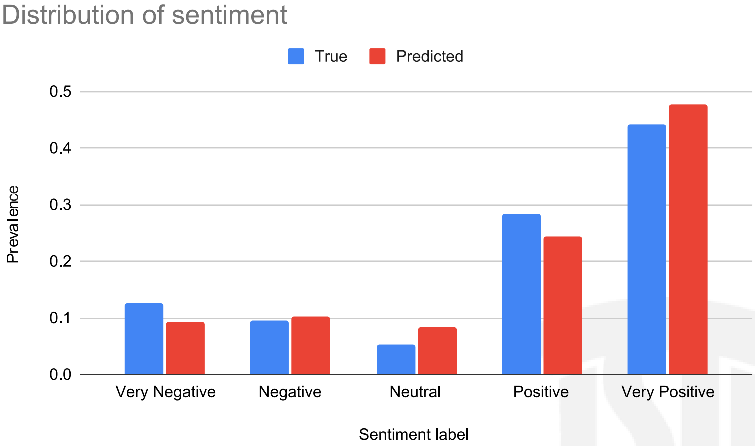
- Studied within ML, DM, NLP, and has given rise to learning methods and evaluation measures specific to it, and independent of those for classification
- The task is of independent interest in statistics and data mining, while it is often only ancillary (i.e., functional to generating better classifiers, or to performring other downstream ML tasks) in machine learning
- Still a fairly unknown task among potential users

Structure of this course

1. Introduction
2. Applications of quantification in ML, DM, NLP
3. Evaluation measures and evaluation protocols for quantification
4. Supervised learning methods for quantification (+ hands-on session)
5. Advanced topics
6. Conclusions

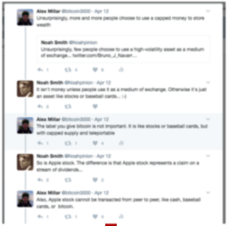
What is quantification?

- Quantification may also be defined as the task of approximating a true distribution by a predicted distribution



- As a result, evaluation measures for quantification evaluate how well a predicted distribution approximates the true distribution

Example applications of quantification



Alex Millar @bitcoin3000 · Apr 12
Unsurprisingly, more and more people choose to use a capped money to store wealth

> **Noah Smith** @Noahpinion
> Unsurprisingly, few people choose to use a high-volatility asset as a medium of exchange... twitter.com/Bruno_J_Navarr...

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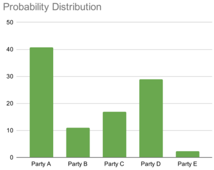
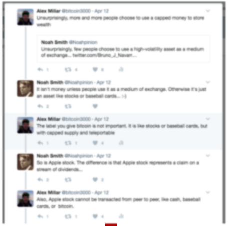


Example applications of quantification



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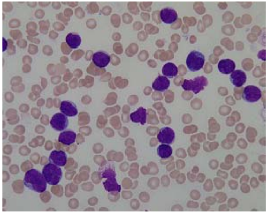
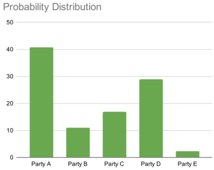
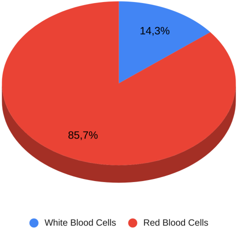
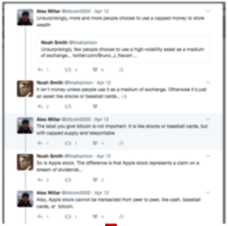






Example applications of quantification



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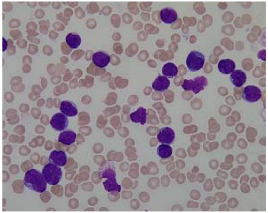
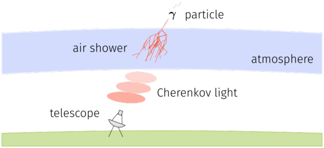
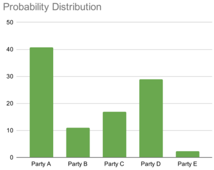
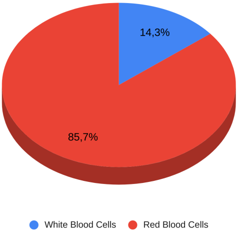
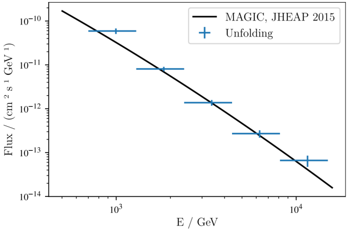










The suboptimality of “Classify and Count”

- Quantification can trivially be solved via the Classify and Count (CC) method:
  1. Train a classifier
  2. Classify all the unlabelled data items in the sample
  3. For each class, count how many unlabelled data items have been attributed to the class
  4. Divide each count by the total number of unlabelled data items
- However, CC proves a suboptimal quantification method, for two main independent reasons:
  1. Classifier bias
  2. Presence of dataset shift

1. CC delivers suboptimal results under classifier bias

- Even if it relies on a good classifier, CC is not necessarily a good quantifier, even in the absence of dataset shift:

	$y = 1$	$y = 0$
$\hat{y} = 1$	TP	FP
$\hat{y} = 0$	FN	TN

h_1	$y = 1$	$y = 0$
$\hat{y} = 1$	95	20
$\hat{y} = 0$	5	480

h_2	$y = 1$	$y = 0$
$\hat{y} = 1$	70	30
$\hat{y} = 0$	30	470

#ActualPositives = 100 (16.7%)
#ActualNegatives = 500 (83.3%)
#Instances = 600

#Errors=25, Accuracy=96%
#PredictedPositives=115 (19.1%)
#ActualPositives=100 (16.7%)

#Errors=60, Accuracy=90%
#PredictedPositives=100 (16.7%)
#ActualPositives=100 (16.7%)

- Paradoxically, for quantification purposes, we should base CC on h_2 rather than on h_1
- Situations such as the above are realistic, since classifiers are usually trained to minimize the number of errors, and not to optimize error balancing
- This implies that quantification is a task in its own right, since the goals of classification and those of quantification do not coincide

2. CC delivers suboptimal results under dataset shift

- Even if it relies on a classifier trained to optimize error balancing, CC may deliver suboptimal results in the presence of dataset shift (DS – aka dataset "drift")
- DS defined as the case in which $P_L(X, Y) \neq P_U(X, Y)$, i.e., as the case in which the IID assumption does not hold
  - L: the data distribution from which the training data are sampled
  - U: the data distribution from which the unlabelled (test) data are sampled
- When dataset shift is present, U are also called out-of-distribution (OOD) data

2. CC delivers suboptimal results under dataset shift

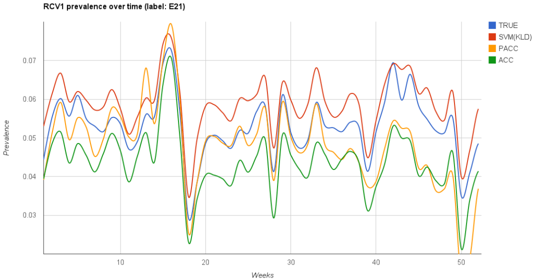
- DS may derive
  - from variations in the environment that the data represent (real shift); i.e. the environment is not stationary, and the operating ("test") conditions were not the same at training time;
    - E.g., prevalence of terrorism-related news before or after 9/11;
  - from the fact that the (training) data misrepresent the environment (virtual shift): i.e., the process of labelling training data may have introduced "sample selection bias":
    - intentionally (e.g., when oversampling the minority class)
    - unintentionally (e.g., if active learning is used)
- CC is suboptimal under DS because CC is usually based on classifiers trained under the IID assumption, which is not verified under DS
- Unlike (say) in "continual learning", in quantification we assume that we cannot acquire any labelled data from U

2. CC delivers suboptimal results under dataset shift

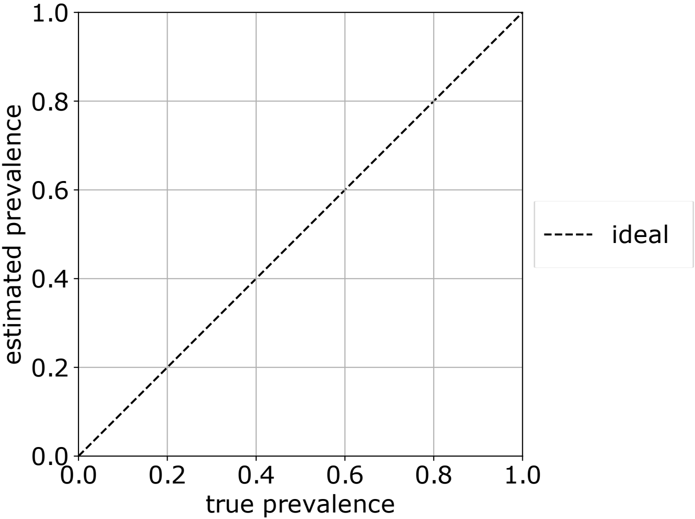
- The DS literature identifies three main DS types, depending on whether we are in the presence of "$X \rightarrow Y$ problems" (causal learning) or "$Y \rightarrow X$ problems" (anti-causal learning)
- In $X \rightarrow Y$ problems we may write $P(X, Y) = P(Y|X)P(X)$
  - E.g., weather forecasting, avalanche prediction from causes
  - In this case we may have covariate shift, defined as the case in which $P_L(X) \neq P_U(X)$ but $P_L(Y|X) = P_U(Y|X)$
  - E.g., avalanche prediction in different geographical areas
- In $Y \rightarrow X$ problems we may write $P(X, Y) = P(X|Y)P(Y)$
  - E.g., handwritten digit recognition, authorship attribution, predicting illnesses from symptoms
  - In this case we may have prior probability shift (aka "label shift"), defined as the case in which $P_L(Y) \neq P_U(Y)$ but $P_L(X|Y) = P_U(X|Y)$
  - E.g., applying to binary digits a handwritten digit recognizer trained on decimal digits
- We have concept shift if either $P_L(Y|X) \neq P_U(Y|X)$
  or $P_L(X|Y) \neq P_U(X|Y)$

2. CC delivers suboptimal results under dataset shift

- Quantification has been mostly studied in the prior probability shift scenario; research in the covariate shift scenario is scarce, while research in the concept shift scenario is nonexistent
- The reason why quantification research has concentrated on prior probability shift is that
  - The dominant experimental protocol in quantification research (the "artificial prevalence protocol" – APP) simulates prior probability shift
  - Performing quantification means assuming that class prevalence values may vary, and covariate shift does not imply that these values vary (e.g., the "faulty sensor" scenario)



CC delivers biased results



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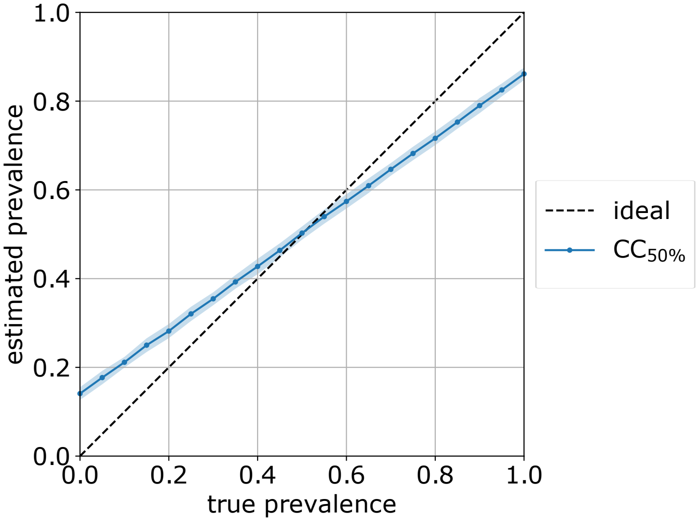

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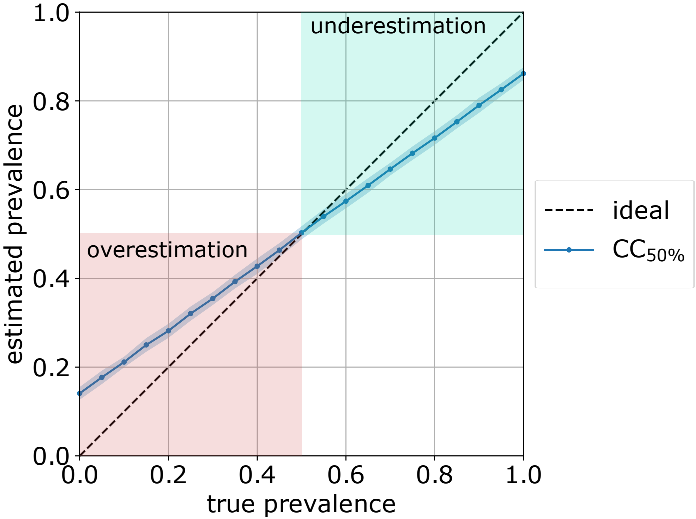

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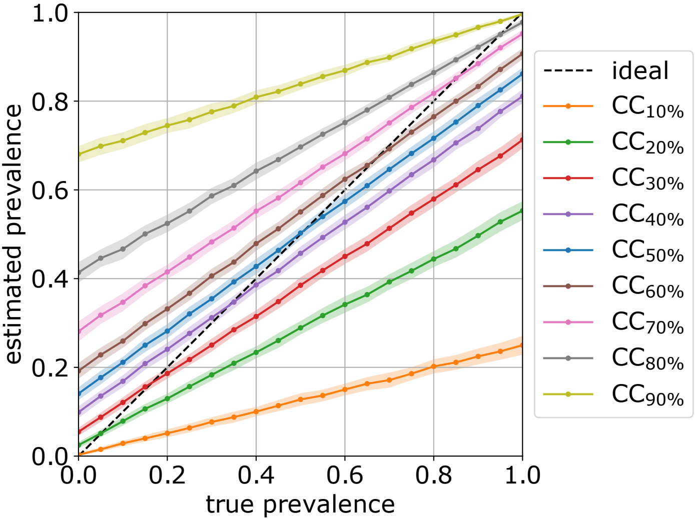

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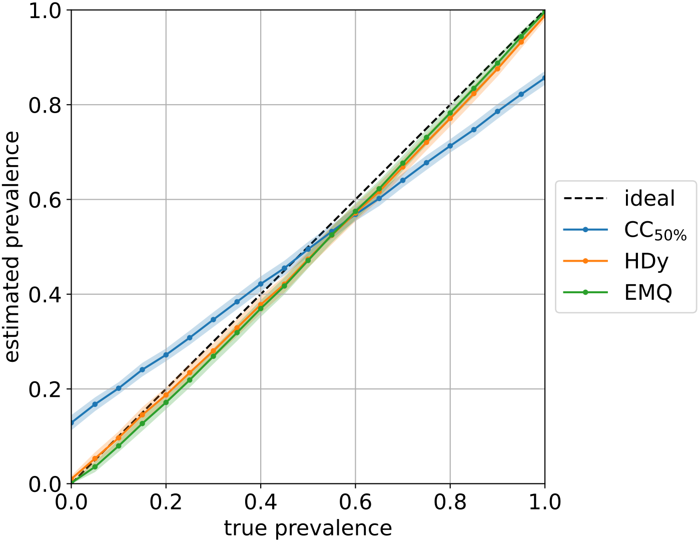

Why does CC deliver biased results?

- Example: the Optimal Bayes Classifier
- For all $\mathbf{x} \in U$ we have

$$p(y|\mathbf{x}) = \frac{p_U(\mathbf{x}|y)p_U(y)}{p_U(\mathbf{x})} \tag{1}$$

- Since $p_U(\mathbf{x}|y)$ and $p_U(y)$ are unknown, they need to be estimated on the training set L, i.e.,

$$\hat{p}(y|\mathbf{x}) = \frac{p_L(\mathbf{x}|y)p_L(y)}{p_U(\mathbf{x})} \tag{2}$$

$$\hat{p}_U(y) = \sum_{\mathbf{x}\in U} \hat{p}(y|\mathbf{x}) \tag{3}$$

- However, in the presence of PPS, $p_U(y)$ is (very) different from $p_L(y)$, so estimating $p_U(y)$ via $p_L(y)$ leads to inaccurate (classification AND quantification) results

Historical development

- The history of quantification research is highly non-linear (task discovered and re-discovered from within different disciplines)
- 1st stage : interest in the "estimation of class priors" in machine learning
  - Goal : making classifiers robust to the presence of prior probability shift and better attuned to the characteristics of the data to which they need to be applied
  - Earliest recorded method is (Vucetic & Obradovic, 2001), most influential one is (Saerens et al., 2002)
- 2nd stage : interest in "quantification" from data mining / text mining
  - Goal : estimating quantities and trends from unlabelled data
  - Earliest recorded work is (Forman, 2005), where the term "quantification" was coined
  - It is the applications from these fields that have provided the impetus behind the most recent wave of research in quantification

G. Forman. Counting positives accurately despite inaccurate classification. ECML 2005.

Slobodan Vucetic, Zoran Obradovic: Classification on Data with Biased Class Distribution. ECML 2001.

Marco Saerens, Patrice Latinne, Christine Decaestecker: Adjusting the Outputs of a Classifier to New a Priori Probabilities: A Simple Procedure. Neural Computation, 2002

Related but different: Screening tests in epidemiology

- Quantification is reminiscent of “prevalence estimation from screening tests” in epidemiology
- Screening test : a test that a patient undergoes in order to check if she has a given pathology; can be used for epidemiological purposes when administered to a certain population
- Screening tests are often imperfect, i.e., they may generate
  - false positives (patient incorrectly diagnosed with the pathology)
  - false negatives (patient incorrectly diagnosed to be free from the pathology)
- Testing a patient is thus akin to classifying an item
- Main differences:
  - no supervised learning is involved
  - a screening test typically has known and fairly constant “sensitivity” (recall) and “specificity” (1−fallout), while the same usually does not hold for a classifier
- Some currently used quantification methods indeed derive from methods used for prevalence estimation from screening tests

Related but different: Density estimation

- Quantification is similar to density estimation (e.g., estimating the prevalence of yellow balls in a large urn containing coloured balls).
- However, in traditional density estimation
  1. We can deterministically assess whether each item belongs to the class (variable y_j can be observed); in quantification this does not hold
  2. It is impossible / economically not viable to assess class membership for each single item (e.g., we do not want to inspect every single ball in the urn); in quantification this does not hold

Related but different: Density estimation

- Quantification is thus closely related to classification, where 1 and 2 also do not hold. However,
  - in classification the goal is correctly estimating the true class of each single individual (quantification is concerned “not with the needle, but with the haystack”);
  - classification is applied to individual items, and not to batches of such examples

Related but different: Collective classification

- A task seemingly related to quantification is collective classification (CoC), as in e.g., the classification of networked items. Similarly to quantification, in CoC the classification of an instance is not viewed in isolation of the other instances.
- However, the focus of CoC is on improving the accuracy of classification by exploiting relationships between the items to classify (e.g., hypertextual documents). CoC
  - assumes the existence of explicit relationships between the objects to classify (which quantification does not)
  - is evaluated at the individual level, rather than at the aggregate level as quantification.

Structure of this lecture

1. Introduction
2. Applications of quantification in ML, DM, NLP
3. Evaluation measures and evaluation protocols for quantification
4. Supervised learning methods for quantification (+ hands-on session)
5. Advanced topics
6. Resources and shared tasks
7. Conclusions

1. Characterizing the haystack

- Many fields of human activity are not concerned with individual data but with aggregate data only, often broken down according to variables of interest (e.g., age group, gender, religion, job type, geographical region). Examples are
  - Social sciences and political sciences
  - Epidemiology
  - Market research
  - Ecological modelling
  - ...
- In these fields, whenever the variable of study (Y) is not explicit, quantification (instead of classification) is what is needed

1. Characterizing the haystack: The social sciences

- "Computational social science": the big new paradigm spurred by the availability of big data from social networks
- Within the social sciences, the individuals on which we perform quantification are persons
- Example quantification endeavours are
    - Quantification by topic, e.g., as in establishing the prevalence of a certain topical class within respondents of a survey
    - Sentiment quantification, e.g., the goal of most works that do "sentiment classification of Twitter data" is estimating class prevalences
    - Stance quantification, i.e., detecting the prevalence of individuals that have a certain stance towards a given issue or topic ("target")
- Political science : e.g., predicting election results / monitoring support for a political party by estimating the prevalence of blog posts / tweets that have a certain stance towards the party
- Most works in these fields still use "classify and count", mostly due to lack of awareness of the existence of alternative quantification methods

1. Characterizing the haystack: The social sciences

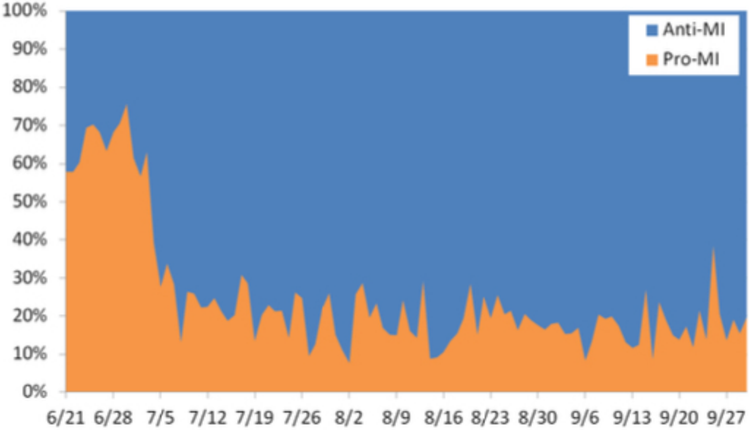

Figure: Temporal trend in the proportions of tweets supporting or opposing military intervention in Egypt during the “Arab spring” in summer 2013.

Borge-Holthoefer, J., Magdy, W., Darwish, K., and Weber, I. (2015). Content and network dynamics behind Egyptian political polarization on Twitter. In Proceedings of CSCW 2015.

1. Characterizing the haystack: Ecological modelling

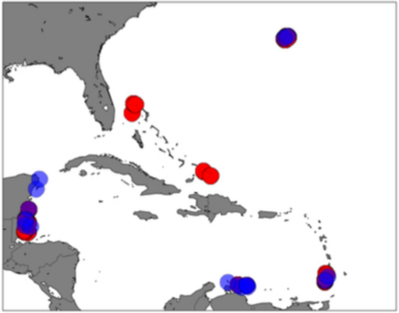

Figure: Using quantification for estimating the prevalence of different species of living beings on the seabed; red circles indicate the locations where the training data were collected while blue circles indicate the locations where the unlabelled data to which the trained model was applied were collected.

Beijbom, O., Hoffman, J., Yao, E., Darrell, T., Rodriguez-Ramirez, A., Gonzalez-Rivero, M., and Hoegh-Guldberg, O. (2015). Quantification in-the-wild: Datasets and baselines. NIPS 2015 Workshop on Transfer and Multi-Task Learning.

1. Characterizing the haystack: Ecological modelling

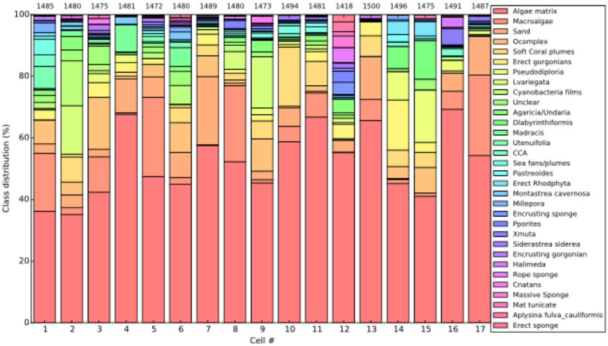

Figure: Class prevalence of each of 32 living species in seabed cover as estimated via quantification technology; the different columns represent different samples on which quantification has been performed.

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1. Characterizing the haystack

- Market Research : estimating the distribution of consumers' attitudes towards products, product features, or marketing strategies; e.g.,
    - quantifying customers' attitudes from verbal responses to open-ended questions (Esuli and Sebastiani, 2010)
- Epidemiology : tracking the incidence and the spread of diseases; e.g.,
    - estimate pathology prevalence from clinical reports where pathologies are diagnosed
    - estimate the prevalence of different causes of death from "verbal autopsies", i.e., from verbal accounts of symptoms
- Other :
    - estimating the proportions of different types of cells in blood samples
    - estimating the proportion of no-shows within a set of bookings

A. Esuli and F. Sebastiani. Machines that learn how to code open-ended survey data. *International Journal of Market Research* 52(6):775–800, 2010.

2. Applications to downstream tasks

- Improving classification accuracy : improving the performance of classifiers when deployed on data characterized by prior probability shift
  - An instance of domain adaptation
- Improving word sense disambiguation accuracy : e.g., tuning a word sense disambiguator to a domain characterized by sense priors different from those of the training set
- Estimating the fairness of a classifier with respect to a sensitive attribute
- Estimating the fairness of a ranker with respect to a sensitive attribute
- Estimating the accuracy of a classifier on out-of-distribution data

Marco Saerens, Patrice Latinne, Christine Decaestecker: Adjusting the Outputs of a Classifier to New a Priori Probabilities: A Simple Procedure. Neural Computation, 2002

YS Chan and HT Ng. Estimating class priors in domain adaptation for word sense disambiguation. *Proceedings of ACL 2006*.

A Fabris, A Esuli, A Moreo, and F Sebastiani. Measuring Fairness under Unawareness of Sensitive Attributes: A Quantification-Based Approach. *Journal of Artificial Intelligence Research* 2023.

Structure of this lecture

1. Introduction
2. Applications of quantification in ML, DM, NLP
3. Evaluation measures and evaluation protocols for quantification
4. Supervised learning methods for quantification (+ hands-on session)
5. Advanced topics
6. Resources and shared tasks
7. Conclusions

Notation and terminology

- Domain $\mathcal{X}$ of items (documents), set $\mathcal{Y}$ of classes
- Different brands of classification :
  - Binary classification: each item has exactly one of $\mathcal{Y} = \{y_1, y_2\}$ (which we often write $\mathcal{Y} = \{\oplus, \ominus\}$)
  - Single-label multi-class classification (SLMC): each item has exactly one of $\mathcal{Y} = \{y_1, ..., y_n\}$, with $n > 2$
  - Multi-label multi-class classification (MLMC): each item may have zero, one, or several among $\mathcal{Y} = \{y_1, ..., y_n\}$, with $n > 1$
    - MLMC is often reduced to binary by solving n independent binary classification problems
  - Ordinal classification (aka "ordinal regression"): each item has exactly one of $\mathcal{Y} = (y_1 \preceq ... \preceq y_n)$, where $\preceq$ is a total order and $n > 2$
  - Metric regression: each item has a real-valued score from the range $[\alpha, \beta]$
- For each such brand of classification we will be interested in its "quantification equivalent"
- Most of our discussion will be framed in terms of SLMC quantification

How do we evaluate quantification methods?

- Evaluating quantification means measuring how well a predicted probabilistic distribution $\hat{p}(y)$ fits a true distribution $p(y)$
- The goodness of fit (or lack thereof) between two categorical distributions can be computed via divergence functions, defined as the functions $D(p, \hat{p})$ which enjoy
  1. $D(p, \hat{p}) = 0$ only if $p = \hat{p}$ (identity of indiscernibles)
  2. $D(p, \hat{p}) \geq 0$ (non-negativity)
- If a divergence also enjoys
  - $D(p, q)$ implies $D(q, p)$ (symmetry)
  - $D(p, q) + D(q, r) \geq D(p, r)$ (triangle inequality)

  then it is a distance; but symmetry and the triangle inequality are not essential for the purposes of quantification

F. Sebastiani. Evaluation measures for quantification: An axiomatic approach, *Information Retrieval Journal*, 2019.

How do we evaluate quantification methods?

- Divergences may also enjoy (as exemplified in the binary case)

  3. If $\hat{p}'(y_1) = p(y_1) - a$ and $\hat{p}''(y_1) = p(y_1) + a$, then $D(p, \hat{p}') = D(p, \hat{p}'')$ (impartiality)
     - Enforces the notion that underestimation and overestimation are equally serious
     - E.g., if D enjoys impartiality, it considers estimating $p(y) = .20$ as $\hat{p}(y) = .10$ or as $\hat{p}(y) = .30$ equally serious mistakes

  4. If $\hat{p}'(y_1) = p'(y_1) \pm a$ and $\hat{p}''(y_1) = p''(y_1) \pm a$, with $p'(y_1) < p''(y_1) \leq 0.5$, then $D(p, \hat{p}') > D(p, \hat{p}'')$ (relativity)
     - Enforces the notion that estimation errors of the same absolute magnitude are more serious for rare classes;
     - E.g., if D enjoys relativity, it considers predicting $\hat{p}(y) = 0.01$ when $p(y) = 0.02$ more serious than predicting $\hat{p}(y) = 0.49$ when $p(y) = 0.50$

How do we evaluate quantification methods?

- Q: Which evaluation function is more desirable?

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- A: It depends on the application; arguably, for some applications relativity is desired, while for some others it is not; e.g.
- Application 1: estimating the prevalence of illnesses in a given region / age group. Here, relativity is desired (since, e.g., a .01 estimation error may be tolerable if $p(y) = .40$ but not if $p(y) = .0001$).

How do we evaluate quantification methods?

- Q: Which evaluation function is more desirable?
- A: It depends on the application; arguably, for some applications relativity is desired, while for some others it is not; e.g.
- Application 1: estimating the prevalence of illnesses in a given region / age group. Here, relativity is desired (since, e.g., a .01 estimation error may be tolerable if $p(y) = .40$ but not if $p(y) = .0001$).
- Application 2: predicting the prevalence of no-shows on a flight-by-flight basis. Here, relativity is undesired (since, e.g., a .02 estimation error has the same impact if $p(y) = .05$ and if $p(y) = .20$).
- Identity of indiscernibles, non-negativity, and impartiality, are arguably always desirable

How do we evaluate quantification methods?

- Divergences frequently used for evaluating (binary, SLMC, and MLMC) quantification are
  - $\mathrm{AE}(p, \hat{p}) = \frac{1}{|\mathcal{Y}|}\sum_{y\in\mathcal{Y}} |\hat{p}(y) - p(y)|$ (Absolute Error)
  - $\mathrm{RAE}(p, \hat{p}) = \frac{1}{|\mathcal{Y}|}\sum_{y\in\mathcal{Y}} \frac{|\hat{p}(y) - p(y)|}{p(y)}$ (Relative Absolute Error)
  - $\mathrm{KLD}(p, \hat{p}) = \sum_{y\in\mathcal{Y}} p(y)\log\frac{p(y)}{\hat{p}(y)}$ (Kullback-Leibler Divergence)

	Impartiality	Relativity
Absolute Error	Yes	No
Relative Absolute Error	Yes	Yes
Kullback-Leibler Divergence	No	Yes

- AE and RAE are indeed the most satisfactory measures of quantification error
- For MLMC quantification, "macroaveraged" versions of these measures, obtained by averaging them across the classes, are used

Fabrizio Sebastiani. Evaluation Measures for Quantification: An Axiomatic Approach. Information Retrieval Journal 23(3):255-288, 2020

How do we evaluate quantification methods?

- RAE and KLD may sometimes be undefined due to the presence of zero denominators.
- To solve this we can smooth $p(y)$ and $\hat{p}(y)$ via additive smoothing and use the smoothed versions in place of the original ones; the smoothed version of $p(y)$ is

$$p_s(y) = \frac{\epsilon + p(y)}{\epsilon|\mathcal{Y}| + \sum_{y \in \mathcal{Y}} p(y)} \tag{4}$$

- $\epsilon = \dfrac{1}{2|S|}$ is often used as a smoothing factor

Multi-objective loss functions

- The “paradox of quantification”:

h_1		actual	
		y	$\overline{y}$
pred	y	0	1000
	$\overline{y}$	1000	0

h_2		actual	
		y	$\overline{y}$
pred	y	990	0
	$\overline{y}$	10	1000

- h_1 yields better AE / RAE / KLD than h_2, but we intuitively prefer h_2 to h_1
- It is difficult to trust an aggregative quantifier if it is not based on a good enough classifier ...

Multi-objective loss functions

- The MOLF multi-objective loss function (Milli et al., 2013) strives to keep both classification and quantification error low

$$\begin{aligned}\mathrm{MOLF}(p,\hat{p}) &= \sum_{y_j\in\mathcal{Y}} |\,\mathrm{FP}_j^2 - \mathrm{FN}_j^2\,| \\ &= \sum_{y_j\in\mathcal{Y}} (\mathrm{FN}_j + \mathrm{FP}_j)\cdot|\,\mathrm{FN}_j - \mathrm{FP}_j\,|\end{aligned}$$

  since
  - $|\,\mathrm{FN}_j - \mathrm{FP}_j\,|$ is a measure of quantification error
  - $(\mathrm{FN}_j + \mathrm{FP}_j)$ is a measure of classification error
- It makes sense to use MOLF as a loss function to minimize, but not as a measure for evaluating quantification accuracy
- It applies to "aggregative" quantifiers only

L. Milli, A. Monreale, G. Rossetti, F. Giannotti, D. Pedreschi, F. Sebastiani. Quantification trees. ICDM 2013, pp. 528–536.

J. Barranquero, J. Díez, and J. del Coz. Quantification-oriented learning based on reliable classifiers. *Pattern Recognition* 48(2):591–604, 2015.

Measures for evaluating ordinal quantification

- Ordinal classification $\equiv$ SLMC classification when there is a total order on the n classes
- Important in the social sciences, where ordinal scales are often used to elicit human evaluations (e.g., product reviews)
- Important also in astrophysics, where ordinal scales are used to "bin" energy levels of astroparticles
- The most frequently used measure for ordinal quantification is the (normalized) Earth Mover's Distance (aka "Wasserstein metric")

$$\mathrm{EMD}(p,\hat{p}) = \frac{1}{|\mathcal{Y}|-1} \sum_{j=1}^{|\mathcal{Y}|-1} |\sum_{i=1}^{j} \hat{p}(y_i) - \sum_{i=1}^{j} p(y_i)| \tag{5}$$

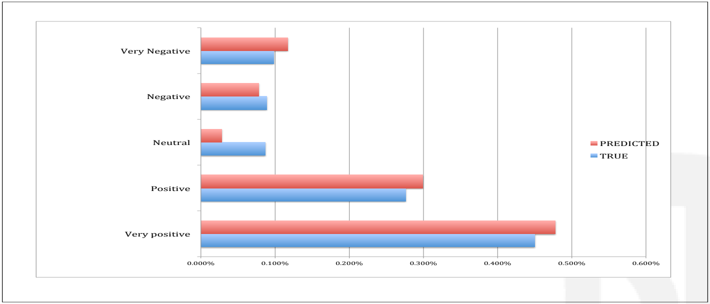
- The EMD is the "ordinal analogue" of absolute error

A. Esuli and F. Sebastiani. Sentiment quantification. *IEEE Intelligent Systems* 25(4):72–75, 2010.

Mirko Bunse, Alejandro Moreo, Fabrizio Sebastiani, and Martin Senz. Ordinal quantification through regularization. ECML/PKDD 2022.

Measures for evaluating ordinal quantification

- The EMD may be seen as measuring the “minimum effort” to turn the predicted distribution into the true distribution, where the effort is measured by
  - the probability masses that need to be moved between one class and another;
  - the “distance” travelled by these probability masses



Experimental protocols for evaluating quantification

- Any test set used for testing the accuracy of classification can obviously be used as a sample σ also for evaluating quantification
- However, while for classification a set of k unlabelled datapoints provides k test datapoints, for quantification a set of k unlabelled datapoints provides only 1 test datapoint
- An experimental protocol for quantification is an algorithm for extracting, from a test set of labelled datapoints, a set $U = \{\sigma_1, \sigma_2, ...\}$ of samples on which quantifiers should be tested
- Different protocols must be chosen for different quantification tasks (binary, multiclass, multilabel, ordinal)

G. Forman. Counting positives accurately despite inaccurate classification. ECML 2005.

Andrea Esuli, Alejandro Moreo, and Fabrizio Sebastiani. LeQua@CLEF2022: Learning to Quantify. ECIR 2022.

Alejandro Moreo, Manuel Francisco, and Fabrizio Sebastiani. Multi-Label Quantification. arXiv:2211.08063 [cs.LG].

Mirko Bunse, Alejandro Moreo, Fabrizio Sebastiani, and Martin Senz. Ordinal quantification through regularization. ECML/PKDD 2022.

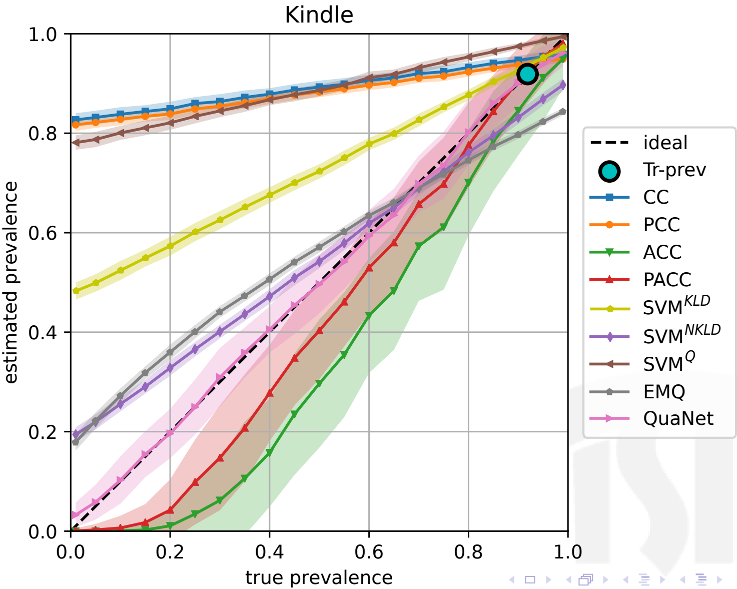
Experimental protocols for evaluating quantification

- Two main protocols are used in the literature:
  - The artificial-prevalence protocol (APP): take a standard dataset split into L and U, and extract a set of samples that exhibits the highest possible diversity in terms of class distribution
    - **Pros**: challenging, since some samples exhibit high amounts of PPS
    - **Cons**: samples with unrealistically high amounts of PPS may influence the results too much + only deals with PPS
  - The natural-prevalence protocol (NPP): pick one or more standard datasets that represent a wide array of class prevalence values
    - **Pros**: experimental setting is realistic
    - **Cons**: class prevalence values and shift values may not be varied at will
- The NPP has almost been abandoned now, due to the difficulty of finding datasets that are challenging enough, i.e., displaying substantial amounts of PPS, and sizeable enough
- Research is ongoing for defining protocols that simulate types of dataset shift other than PPS

G. Forman. Counting positives accurately despite inaccurate classification. ECML 2005.

A. Esuli and F. Sebastiani. Optimizing text quantifiers for multivariate loss functions. *ACM Transactions on Knowledge Discovery and Data*, 9(4):Article 27, 2015.

The APP for the binary case: An example



The artificial-prevalence protocol in the multiclass case

- The APP in the binary case consists of
  1. establishing a grid of values in the [0,1] interval, e.g., $G = \{0.00, 0.05, ..., 0.95, 1.00\}$
  2. for each value $\alpha \in G$ extract, by random sampling with replacement, m samples of k datapoints each such that the prevalence $p_{\sigma}(y_1)$ of the positive class in the sample is α;
  3. use the set of $|G| \times m$ extracted samples as the test set for evaluating quantifiers.
- Using the APP in the multiclass case can be problematic since, given a grid G, the number of samples that can be extracted via the above method is $O(g^n)$
- We can then resort to extracting samples whose distribution is extracted uniformly at random from the unit $(n-1)$-simplex
- However, in order to guarantee randomness we need to avoid naive extraction algorithms ...

Sampling uniformly at random from the unit simplex

- The naive algorithm (NA):
  1. Given a set of classes $\mathcal{Y}$, generate a vector $A = \langle a_1, \ldots, a_{(|\mathcal{Y}|-1)} \rangle$ of datapoints sampled uniformly at random from [0,1]
  2. Obtain a vector $P = \langle p_1, \ldots, p_{|\mathcal{Y}|} \rangle$ by defining

$$p_i = \begin{cases} a_i \prod_{j=1}^{i-1}(1-a_j) & \text{if } i < |\mathcal{Y}| \\ (1 - \sum_{j=1}^{|\mathcal{Y}|-1} p_j) & \text{if } i = |\mathcal{Y}| \end{cases}$$

  3. Use P as the distribution of class prevalence values for generating sample σ

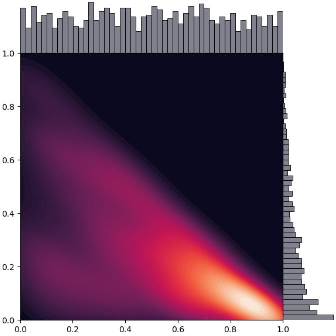


Figure: Distribution of datapoints $\langle p_1, p_2, p_3 \rangle$ sampled via the NA on the unit 2-simplex.

Sampling uniformly at random from the unit simplex

- The IID algorithm (IIDA):
  1. Given a set of classes $\mathcal{Y}$, generate a vector $A = \langle a_1, ..., a_{|\mathcal{Y}|} \rangle$ of datapoints sampled uniformly at random from [0,1]
  2. Obtain a vector $P = \langle p_1, ..., p_{|\mathcal{Y}|} \rangle$ by normalizing A to unit length
  3. Use P as the distribution of class prevalence values for generating sample σ

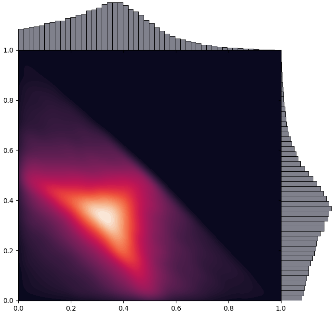


Figure: Distribution of datapoints $\langle p_1, p_2, p_3 \rangle$ sampled via the IIDA on the unit 2-simplex.

Sampling uniformly at random from the unit simplex

- The Kraemer algorithm (KA):
    1. Given a set of classes $\mathcal{Y}$, generate a vector $A = \langle a_1, ..., a_{(|\mathcal{Y}|-1)} \rangle$ of datapoints sampled uniformly at random from [0,1]
    2. Sort the a_i's to obtain $B = \langle b_1 \leq ... \leq b_{(|\mathcal{Y}|-1)} \rangle$, and define $b_0 = 0$ and $b_{|\mathcal{Y}|} = 1$
    3. Obtain a vector $P = \langle p_1, ..., p_{|\mathcal{Y}|} \rangle$ by defining $p_i = b_i - b_{(i-1)}$ for all $i \in \{1, ..., |\mathcal{Y}|\}$
    4. Use P as the distribution of class prevalence values for generating sample σ

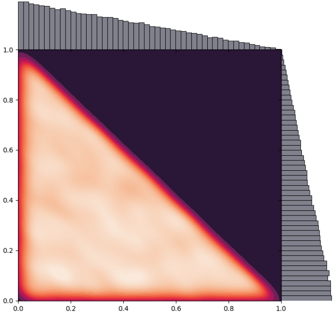
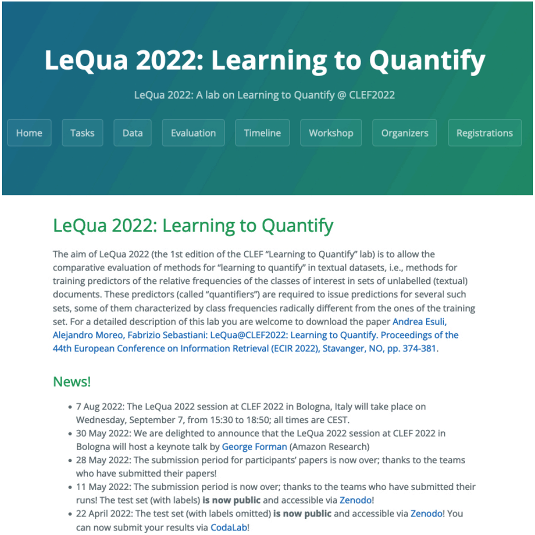


Figure: Distribution of datapoints $\langle p_1, p_2, p_3 \rangle$ sampled via the KA on the unit 2-simplex.

Smith, Noah A. and Tromble, Roy W., Sampling uniformly from the unit simplex, Technical report, Johns Hopkins University, 2004. https://www.cs.cmu.edu/~nasmith/papers/smith+tromble.tr04.pdf

LeQua @ CLEF 2022

- LeQua @ CLEF 2022: a "lab" (i.e., data challenge) explicitly devoted to learning to quantify
- Goal: supporting LtQ research by providing a tightly controlled environment for the comparative evaluation of LtQ systems



LeQua 2022: Learning to Quantify

LeQua 2022: A lab on Learning to Quantify @ CLEF2022

LeQua 2022: Learning to Quantify

The aim of LeQua 2022 (the 1st edition of the CLEF "Learning to Quantify" lab) is to allow the comparative evaluation of methods for "learning to quantify" in textual datasets, i.e., methods for training predictors of the relative frequencies of the classes of interest in sets of unlabelled (textual) documents. These predictors (called "quantifiers") are required to issue predictions for several such sets, some of them characterized by class frequencies radically different from the ones of the training set. For a detailed description of this lab you are welcome to download the paper Andrea Esuli, Alejandro Moreo, Fabrizio Sebastiani: LeQua@CLEF2022: Learning to Quantify. Proceedings of the 44th European Conference on Information Retrieval (ECIR 2022), Stavanger, NO, pp. 374-381.

News!

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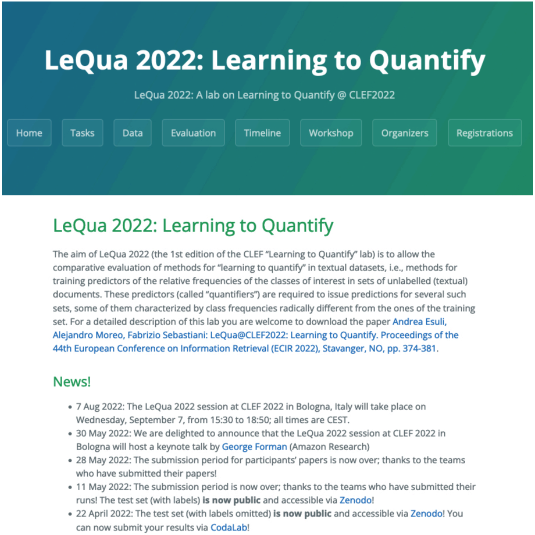
- 30 May 2022: We are delighted to announce that the LeQua 2022 session at CLEF 2022 in Bologna will host a keynote talk by George Forman (Amazon Research)
- 28 May 2022: The submission period for participants' papers is now over; thanks to the teams who have submitted their papers!
- 11 May 2022: The submission period is now over; thanks to the teams who have submitted their runs! The test set (with labels) **is now public** and accessible via Zenodo!
- 22 April 2022: The test set (with labels omitted) **is now public** and accessible via Zenodo! You can now submit your results via CodaLab!

https://lequa2022.github.io/

LeQua @ CLEF 2022

- Used Amazon product reviews as the data
- Provided 4 subtasks, for every choice of “binary vs. multiclass” × “raw documents vs. vectors”
- Binary quantification addressed sentiment (Positive vs. Negative) while multiclass quantification addressed topic (28 classes denoting types of merchandise)



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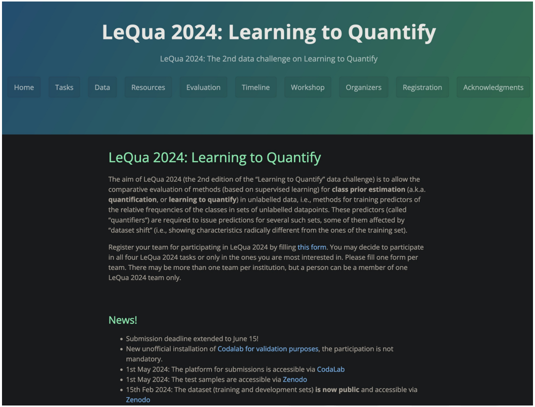
https://lequa2022.github.io/

LeQua @ ECML/PKDD 2024

- Provided 4 subtasks
  1. Binary quantification under PPS
  2. Multiclass quantification under PPS
  3. Ordinal quantification under PPS
  4. Binary quantification under covariate shift
- Data are (again) Amazon product reviews
- Data already provided in vector form



LeQua 2024: Learning to Quantify
LeQua 2024: The 2nd data challenge on Learning to Quantify
Home
Tasks
Data
Resources
Evaluation
Timeline
Workshop
Organizers
Registration
Acknowledgments

LeQua 2024: Learning to Quantify

The aim of LeQua 2024 (the 2nd edition of the "Learning to Quantify" data challenge) is to allow the comparative evaluation of methods (based on supervised learning) for **class prior estimation** (a.k.a. **quantification**, or **learning to quantify**) in unlabelled data, i.e., methods for training predictors of the relative frequencies of the classes in sets of unlabelled datapoints. These predictors (called "quantifiers") are required to issue predictions for several such sets, some of them affected by "dataset shift" (i.e., showing characteristics radically different from the ones of the training set).

Register your team for participating in LeQua 2024 by filling this form. You may decide to participate in all four LeQua 2024 tasks or only in the ones you are most interested in. Please fill one form per team. There may be more than one team per institution, but a person can be a member of one LeQua 2024 team only.

News!

- Submission deadline extended to June 15!
- New unofficial installation of Codalab for validation purposes, the participation is not mandatory.
- 1st May 2024: The platform for submissions is accessible via CodaLab
- 1st May 2024: The test samples are accessible via Zenodo
- 15th Feb 2024: The dataset (training and development sets) **is now public** and accessible via Zenodo

https://lequa2024.github.io/

Structure of this course

1. Introduction
2. Applications of quantification in ML, DM, NLP
3. Evaluation measures and evaluation protocols for quantification
4. Supervised learning methods for quantification (+ hands-on session)
5. Advanced topics
6. Conclusions

Advanced topics (hints)

- Multi-label quantification
- Ordinal quantification
- Regression quantification
- Cross-lingual text quantification
- Quantification for data streams
- Quantification for networked data
- Cost-sensitive quantification
- ...

Advanced topics (hints)

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Multi-label quantification

- Multi-label multi-class (MLMC) quantification: each item may have zero, one, or several among $\mathcal{Y} = \{y_1, ..., y_n\}$, with $n > 1$
- MLMC quantification is often reduced to binary quantification by solving n independent binary quantification problems; this is the baseline that all "truly" MLMC quantification methods are supposed to beat
- The reduction to binary does not allow to leverage possible stochastic correlations between classes; e.g., we may notice from training data that many datapoints in class "Republican" are also in class "LovesGolf"
- Work in MLMC classification has shown that leveraging these correlations brings about higher accuracy

Multi-label quantification

- For simplicity, we will deal with aggregative quantification methods only
- The most trivial class of solutions to MLMC quantification is BC+BA, which consists of using n binary classifiers and, on top of them, n instances of a binary aggregative quantification method
- A slightly less trivial class of solutions is MLC+BA, which consists of using a truly multi-label classifier and, on top of it, n instances of a binary aggregative quantification method
- Another less trivial class of solutions is BC+MLA, which consists of using n independent binary classifiers and, on top of them, a truly multi-label quantification method
- The most interesting class of solutions is MLC+MLA, which consists of using a truly multi-label classifier and, on top of it, a truly multi-label quantification method

Alejandro Moreo, Manuel Francisco, Fabrizio Sebastiani. Multi-label quantification. arXiv:2211.08063 [cs.LG], 2022.

Multi-label quantification

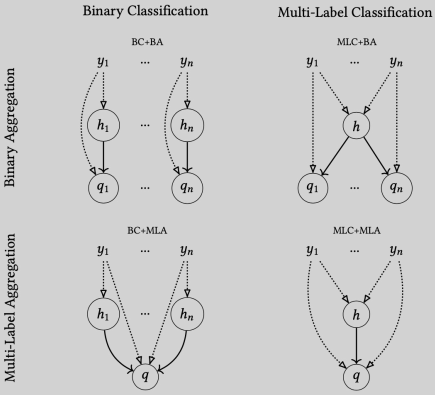

Fig. 2. The four groups of multi-label quantification methods. Dotted lines connecting class labels with a model (classifier or quantifier) indicate that the model learns from (or has access to) the class labels of the training datapoints. Solid lines connecting classifiers with quantifiers indicate a transfer of outputs from the classifier to the quantifier. With a slight deviation from our notation, here *h* denotes any classifier, hard or soft.

Alejandro Moreo, Manuel Francisco, Fabrizio Sebastiani. Multi-label quantification. arXiv:2211.08063 [cs.LG], 2022.

Multi-label quantification

- Best-performing system so far: the regression-based MLC+MLA quantification method (Moreo et al. 2022):
  1. Take a multi-label quantifier q trained via a MLC+BA quantification method
  2. Put a regressor $r : \mathbb{R}^n \rightarrow \mathbb{R}^n$ on top of it that takes as input a vector of n "uncorrected" prevalence values and returns a vector of n "corrected" prevalence values
  3. Train the regressor with a set of pairs $(\hat{\mathbf{p}}^q_{\sigma_i}, \mathbf{p}_{\sigma_i})$, where
     - $\hat{\mathbf{p}}^q_{\sigma_i}$ is the vector of the n prevalence values estimated by q
     - $\mathbf{p}_{\sigma_i}$ is the vector of the n true prevalence values
- The regressor is thus trained to leverage the stochastic dependencies among the classes
- This method can be used also if the MLC+BA underlying method is non-aggregative
- (Moreo et al. 2022) provide an experimental protocol specific to multi-label quantification, that can be used for evaluation and also for generating the σ_i's to be used in Step 3 above

Alejandro Moreo, Manuel Francisco, Fabrizio Sebastiani. Multi-label quantification. arXiv:2211.08063 [cs.LG], 2022.

Ordinal quantification

- Ordinal quantification is SLMC quantification when there is a total order $\mathcal{Y} = (y_1 \preceq \ldots \preceq y_n)$ on the classes
- Mis-assigning probability mass to a neighbouring class is less serious than mis-assigning it to a faraway class; EMD is thus a good evaluation measure;
- Few research works conducted on this task
  - Early OQ algorithms are (da San Martino et al., 2016) and (Esuli, 2016)
  - "Unfolding" algorithms in the astrophysics literature (Bunse, 2018)
  - More recent algorithms are (Bunse et al., 2022) and (Castaño et al, 2022)

Ordinal quantification

- Class of OQ methods based on regularization (Bunse et al., 2022)
- Basic idea: take an algorithm for SLMC quantification, and introduce a "regularization" that penalizes "unlikely" assignments of probability mass
- "Likely $\approx$ Smooth", i.e., sharp differences between $p_\sigma(y_i)$ and $p_\sigma(y_{i+1})$ are considered unlikely
- Several algorithms proposed along these lines, including o-ACC, o-PACC, o-SLD

Ordinal quantification

- E.g., o-ACC, an ordinal version of ACC:
- ACC amounts to solving for $\mathbf{p}$ the system of linear equations $\mathbf{q} = \mathbf{M}\mathbf{p}$, where $\mathbf{q} \in \mathbb{R}^n$ are the prevalence estimates obtained via CC and $\mathbf{M}$ is the misclassification matrix.
- Least-squares solutions to this system are found by computing

$$\mathrm{argmin}_{\mathbf{p}} \|\mathbf{q} - \mathbf{M}\mathbf{p}\|_2^2$$

- We introduce a regularization term that penalizes non-smooth solutions

$$\mathrm{argmin}_{\mathbf{p}} \|\mathbf{q} - \mathbf{M}\mathbf{p}\|_2^2 + \frac{\tau}{2} \left(\mathbf{C}\mathbf{p}\ \right)^2 \tag{6}$$

where the Tikhonov matrix $\mathbf{C}$ is such that

$$\frac{1}{2} \left(\mathbf{C}\mathbf{p}\ \right)^2 = \frac{1}{2} \sum_{i=2}^{n-1} \left(-[\mathbf{p}]_{i-1} + 2[\mathbf{p}]_i - [\mathbf{p}]_{i+1}\right)^2 \tag{7}$$

Mirko Bunse, Alejandro Moreo, Fabrizio Sebastiani, Martin Senz: Ordinal Quantification Through Regularization. ECML/PKDD (5) 2022: 36-52

Open challenges for quantification

- Quantification has not received the same attention as classification; therefore, many open problems still remain; there is a need, e.g., to

  1. Investigate non-aggregative quantification methods more extensively, since they are the true realization of "Vapnik's principle"
  2. Investigate transductive quantification methods, to take advantage of the fact that transductive contexts are "easier"
  3. Devise methods for exploiting the full potential of deep learning for quantification
  4. Investigate explainable quantification methods
  5. Investigate the relationships between quantification and types of dataset shift other than PPS

Structure of this course

1. Introduction
2. Applications of quantification in ML, DM, NLP
3. Evaluation measures and evaluation protocols for quantification
4. Supervised learning methods for quantification (+ hands-on session)
5. Advanced topics
6. Conclusions

Conclusion

- Growing awareness that quantification is going to be more and more important; given the advent of big data, application contexts will spring up in which we will simply be happy with analysing data at the aggregate (rather than at the individual) level
- Takeaway message to users of supervised learning: when
  - You are using classification
  - Your only goal is to obtain aggregate results, i.e., class prevalence estimates

  your work would probably benefit from using quantification technology instead of classification technology

Questions?

Thank you!

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