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Active Learning

Data Mining Guestlecture

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Lecture Outline

- Lecture's Context
- Semi-Supervised Learning
- Active Learning
  - Motivation
  - Approaches
    - Uncertainty Sampling
    - Expected Error Reduction
    - Ensemble / Query by Committee
    - Probabilistic Active Learning
  - Evaluation
- Summary and Questions

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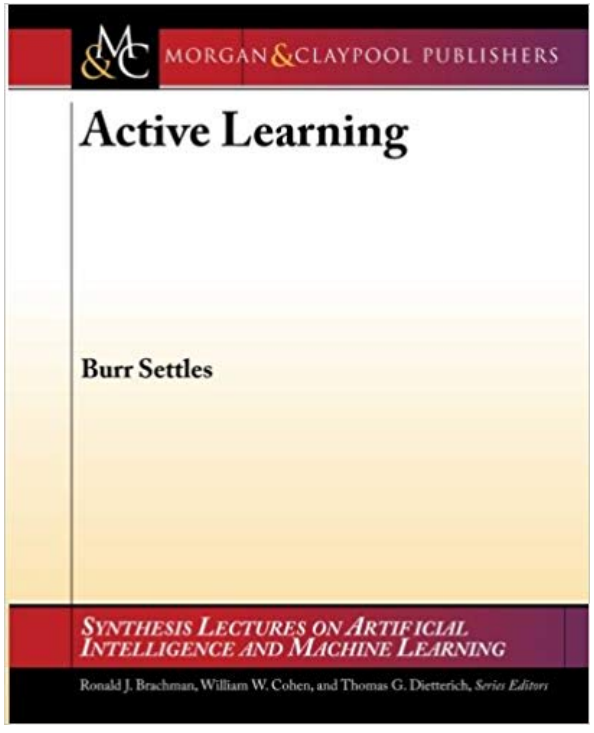
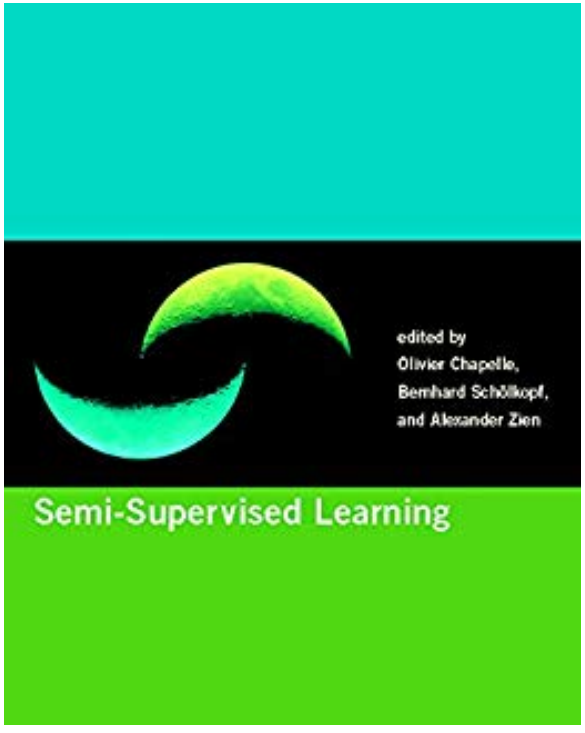
Recommended Literature on Active and Semi-Supervised Learning



(a) [Settles, 2012]



(b) [Chapelle et al., 2006]

Context of Active Learning within Data Mining / Machine Learning

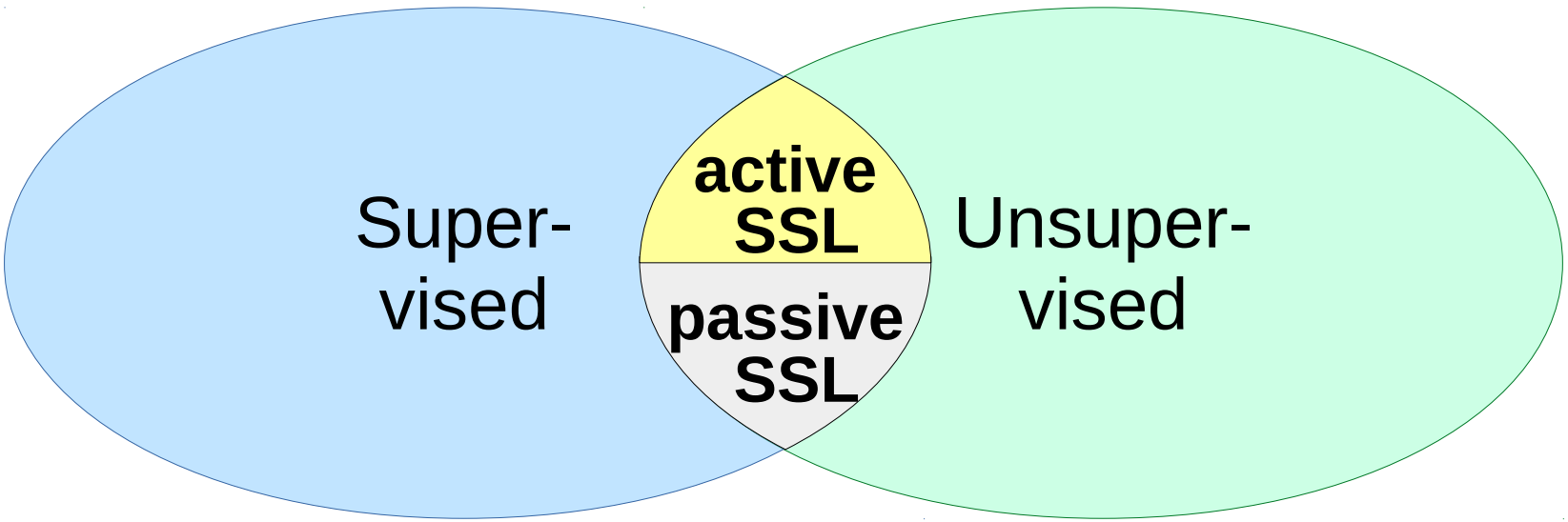
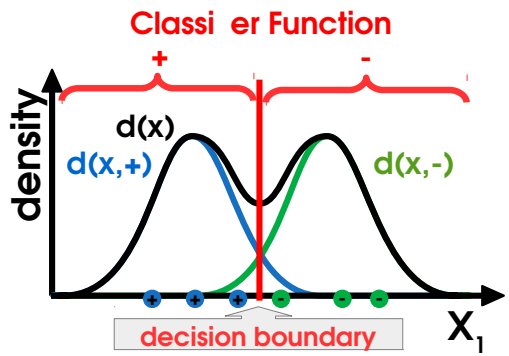


Figure: Context of Active Learning within Machine Learning

Supervised (Passive) Classification: Recapitulation

Credit Scoring: will a new order be paid?

amount X_1	...	default?
2.2	...	no
1.7	...	yes
1.3	...	yes
3.1	...	no
...	...	...



- **Historical Data**
  e.g. previous customer's records
- **Generate Training Sample** $\mathcal{L}$ with feature variables (e.g. order value X) and class label (e.g. default Y)
- **Aim: Classifier function** $f : X \to Y$
  E.g. using Bayes theorem

$$Pr(Y|X) = \frac{Pr(X|Y) \cdot Pr(Y)}{Pr(X)}$$

- **Estimate Distributions**
  joint distributions $d(X, Y)$ or posterior distributions
  $d(Y|X) = \frac{d(X,Y)}{d(X)}$
- **Derive Decision Boundary**
  at intersections of posterior distributions

Supervised Classification: Limitations

Common assumptions about the training data:

Data (features, labels) on each instance is

- *unbiased*
- *correct*
- *complete*
- and *available at once*
- available at *no cost* and *without the classifier controlling label selection*

What if these assumptions do not hold?

- Challenge for conventional supervised learning approaches[1]
  Requires techniques such as adaptive, active, semi-supervised, transfer learning

[1] See [Krempl et al., 2014b] in SIGKDD Explorations.

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Label Paucity:

- *Completeness* of information is not met:
  Only some labels are available
- **Semi-Supervised Classification**

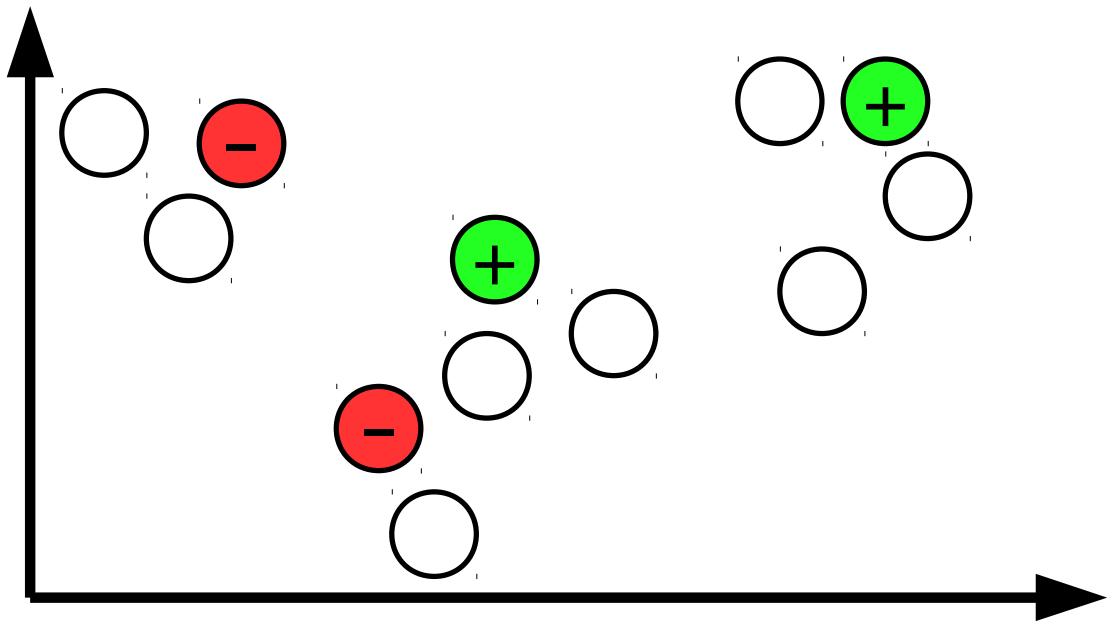

Figure: Classification with Partially Labelled Data

Semi-Supervised Learning[2]

Basic situation

- Not all data are labelled

Objective

- Use unlabelled data to improve classification model

Assumptions

Basic Assumption: There is some structure in the data

- Smoothness assumption
  - Neighbouring instances are similar w.r.t. class label, i.e.the closer, the more likely is a similar class label
  - We need to find low density regions
  - Decision boundary is placed in low-density regions
- Cluster assumption
  - Instances form clusters (subpopulations)
  - Within one cluster, similar label is more likely
  - In extreme case, label Y is conditionally independent of X given cluster Z
- Manifold assumption
  - Data are on a manifold of much lower dimension than the feature space
  - Learning the manifold eases classification (remedy against curse of dimensionality)

▸ Details of SSL Approaches

[2] See for example [Chapelle et al., 2006, Zhu, 2008].

Semi-Supervised Learning[3]

Basic situation

- Not all data are labelled

Objective

- Use unlabelled data to improve classification model

Assumptions

Basic Assumption: There is some structure in the data

- Smoothness assumption
- Cluster assumption
- Manifold assumption

Methods

- Self-Learning, Co-Learning
- Generative Models
- Low-density Separation
- Graph-Based Methods

▸ Details of SSL Approaches

[3] Literature survey by Zhu 2005 [Zhu, 2008].

SSL - Limitations

- Ex-post, passive viewpoint (we work with the data we have)
- What if we can influence which labels we obtain?

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Active Learning: Motivation[4]

Motivation

- some labels are expensive to obtain

Active Learning in Exemplary Applications

- Credit Scoring:
  E.g. costly to accept high risk clients for model building
- Brain Computer Interfaces:
  E.g. performing tasks for calibration can be tedious for user

Selection is important

- Even (or in particular!) in "Big Data" applications
- Efficient allocation of limited resources
- Sample where we **expect something interesting**

[4] See, e.g., [Settles, 2012, Fu et al., 2012, Zliobaitė et al., 2013].

Active Learning: Context & History

Context & Aim

- unlabelled data $\mathcal{U}$ is abundant,
- labelling is costly (small set of labelled data $\mathcal{L}$)
- control over the label selection process
- select the most valuable (informative) instances for labelling

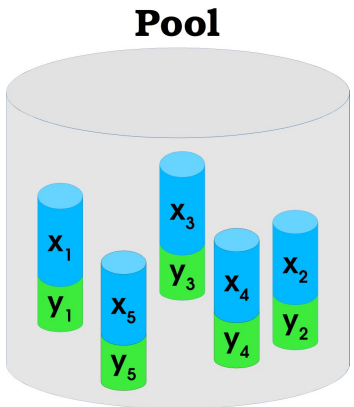
History

- Optimal experimental design [Fedorov, 1972]
- Learning with queries/query synthesis [Angluin, 1988]
- Selective sampling [Cohn et al., 1990]

Selective Data Acquisition Tasks[5]

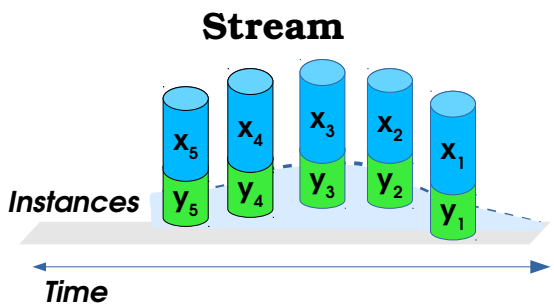
Active Learning Scenarios

- **Query synthesis**: example generated upon query
- **Pool** $\mathcal{U}$ of unlabelled data: static, repeated access
- **Stream**: sequential arrival, no repeated access



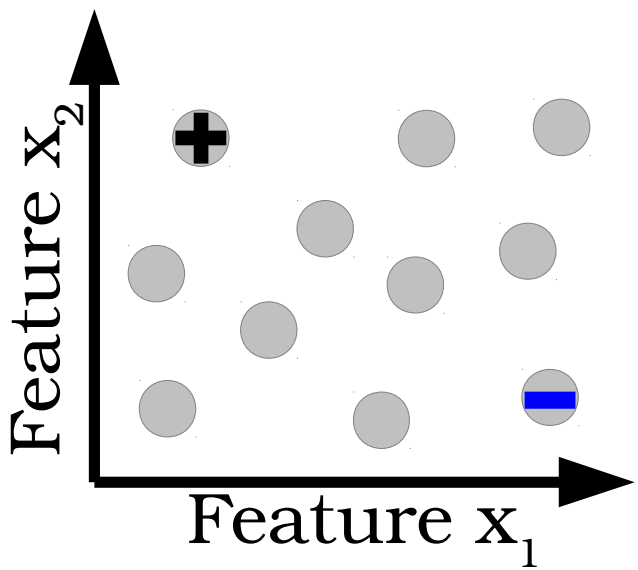
Type of Selected Information

- Active label acquisition
- Active feature (value) acquisition
- Active class selection, also denoted
  Active class-conditional example acquisition
- ...



[5] Own categorization, inspired by [Attenberg et al., 2011, Saar-Tsechansky et al., 2009, Settles, 2009].

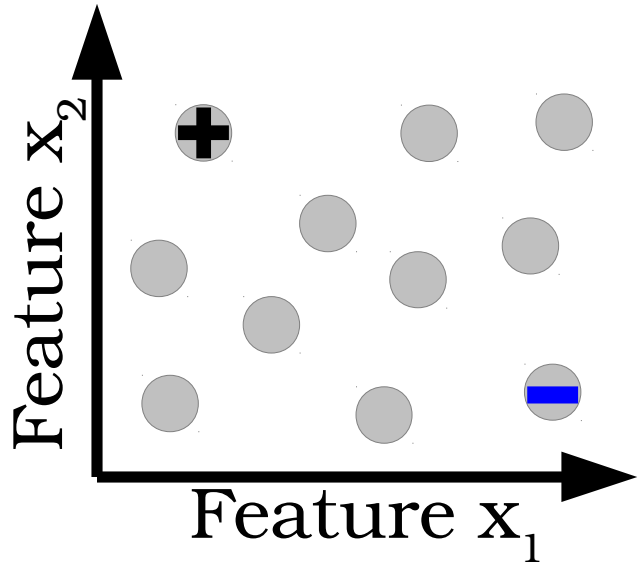
Active Learning Strategies: Motivating Example



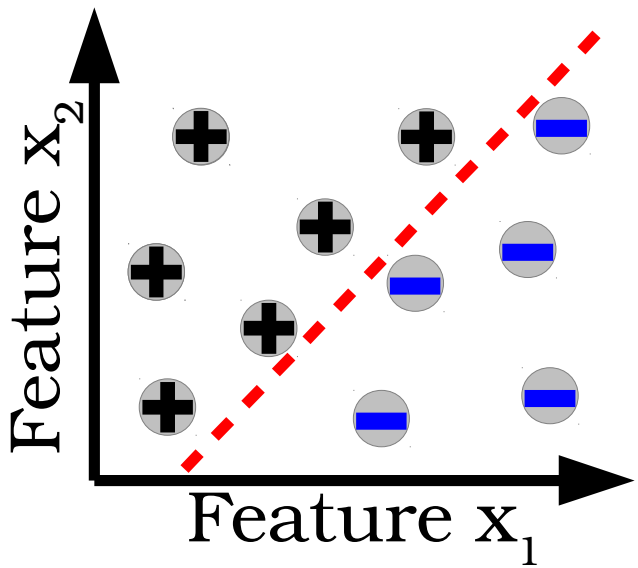
Example

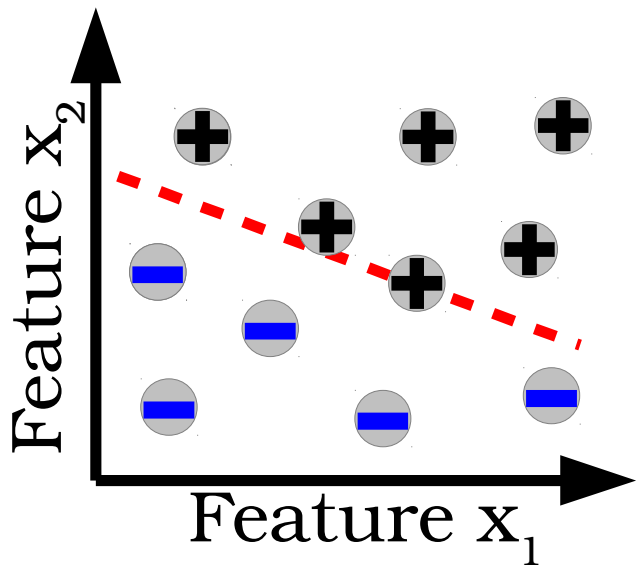
- Uniform distributed instances
- Which label to request?
- Idea: Try to *maximise diversity* of requested labels

Active Learning Strategies: Motivating Example



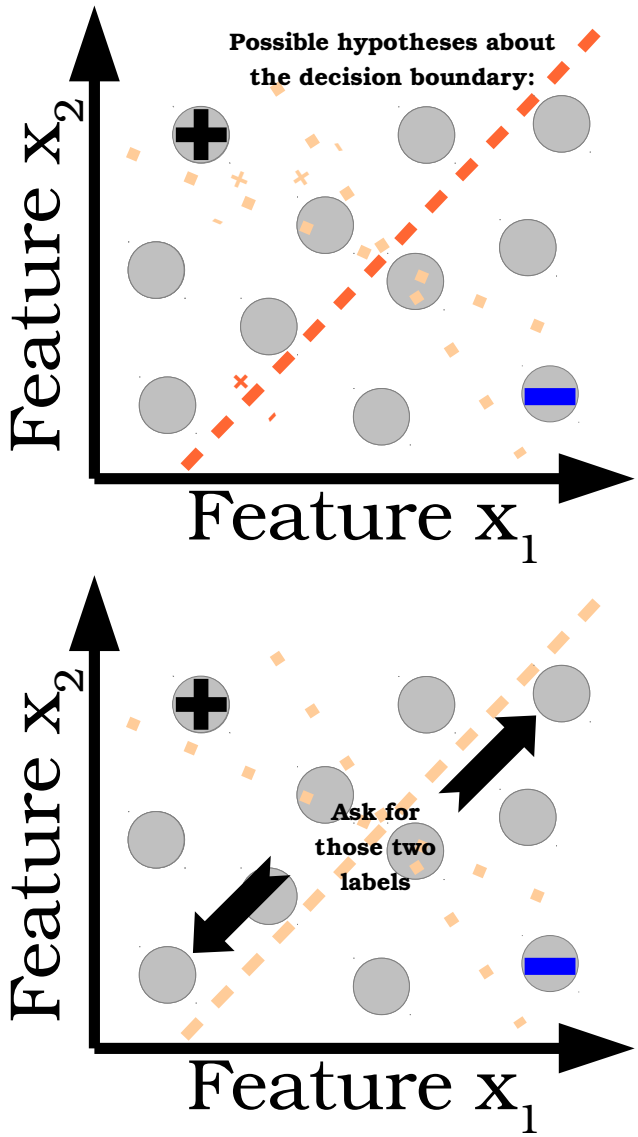
Based on these two labels, what are possible true label distributions?





and
many
others
. . .

Active Learning Strategies: Motivating Example



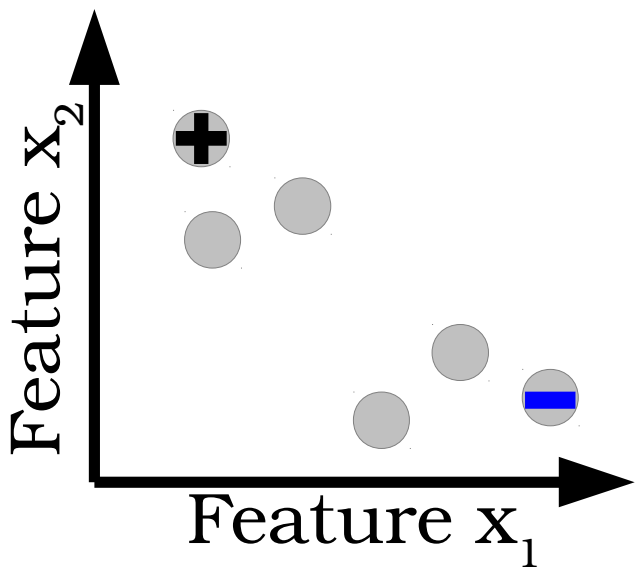
Problem

- Many distributions could have generated the data (see figure on the top left)
- How to know which one is the true one?

Core Ideas:

- *Maximise diversity* of requested labels
  - **Exploration** of feature space!
- *Reduce* the number of *remaining hypotheses* i.e. use the requested data to eliminate unlikely hypotheses
  - **Exploitation** of acquired knowledge!
  - Figure on the bottom left: Requesting labels at the top-right and bottom-left corners helps eliminating many possible hypotheses)
- But: Be aware of this **exploration vs. exploitation tradeoff**
- Furthermore, consider *density* for *sampling in high-density areas* rather than focusing on potentially irrelevant outliers

Active Learning Strategies: Motivating Example (2)



Example

- Multimodal distributed instances
- Which label to request?
- Idea: Try to *exploit structure* of data

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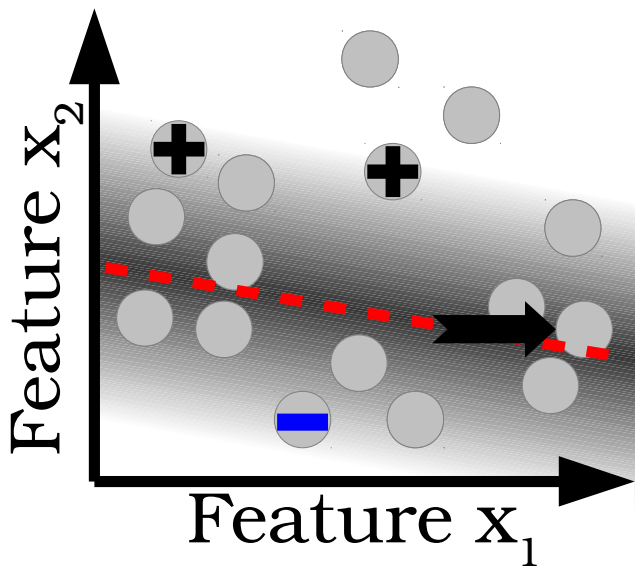
Active Learning Approaches

Selected Active Learning Approaches

- Uncertainty Sampling
- Expected Error Reduction
- Ensemble / Query by Committee
- Probabilistic Active Learning

Uncertainty-Based Strategy



Idea

Select those instances where we are least certain about the label

Approach:

- 3 labels preselected
- Linear classifier
- Use *distance to the decision boundary* as *uncertainty measure*

- **But: Is this a good uncertainty measure?**
- **Are there other ways of measuring uncertainty?**

Uncertainty Measures:

Three families of measures have been proposed[6]:

Margin

- Uncertainty is inverse proportional to the distance to the decision boundary
- *the closer* to the boundary, the *less certain*

Confidence (Posterior)

- Difference of the posteriors of different classes
- $abs\left(P(y=+|x) - P(y=-|x)\right)$
- *the higher* the difference, the *more certain*

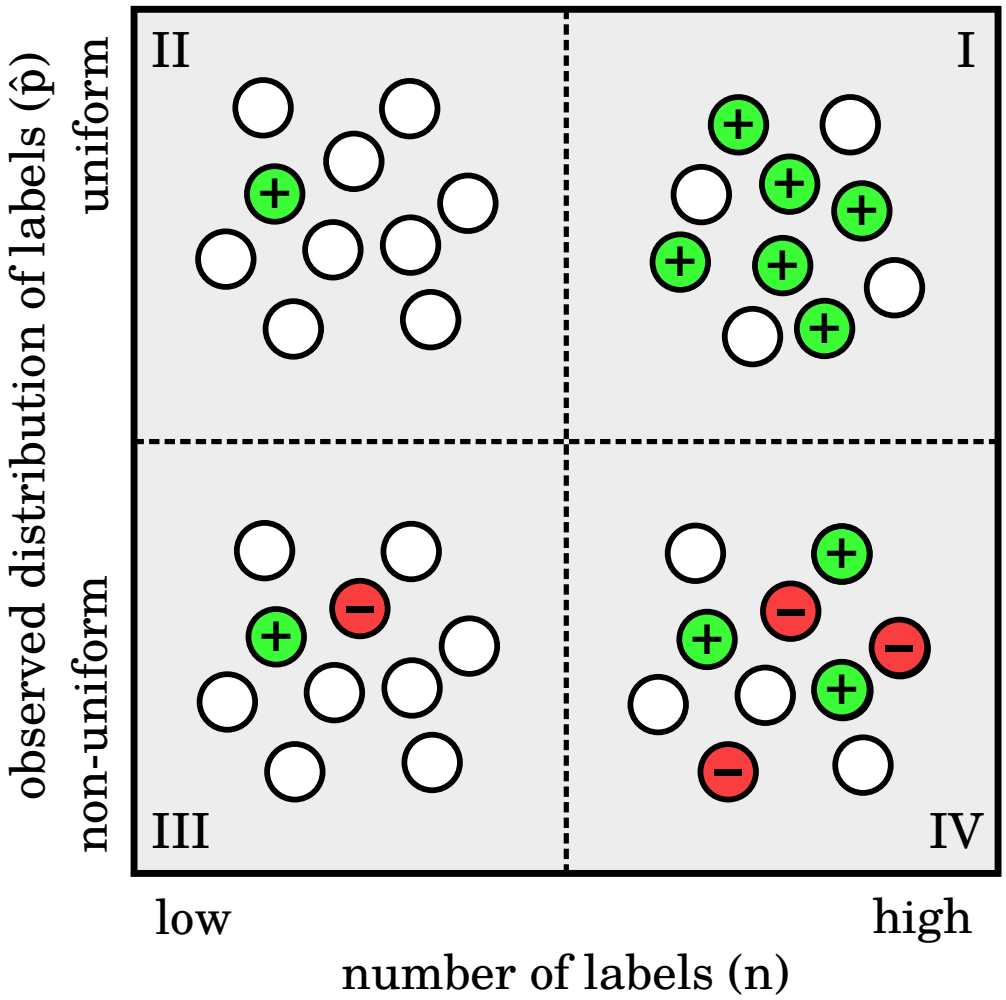
Entropy

- $-\sum_{y\in\{+,-\}} p(y|x)\log\left(p(y|x)\right)$
- *the higher* the entropy, the *less certain*

- **But how suitable are they?**

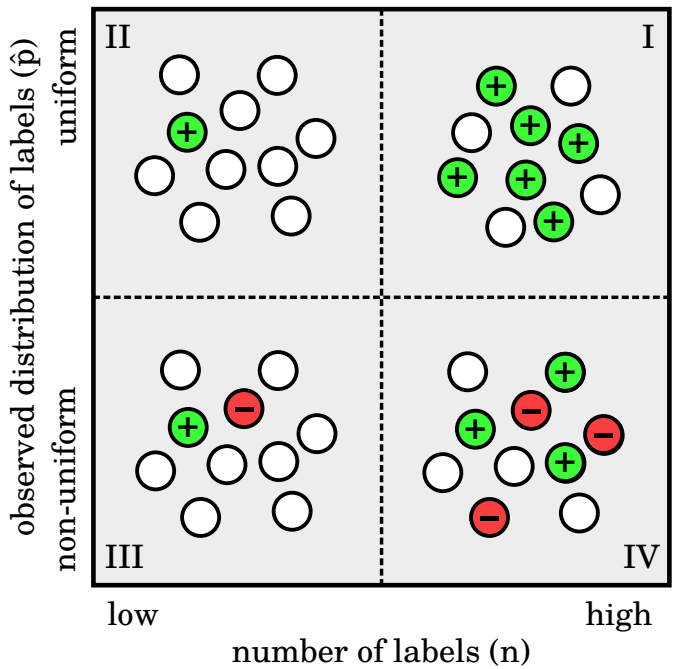
[6] See [Settles, 2012].

Exemplary AL Situations



- a label's value depends on the label information in its neighbourhood
- label information
  - number of labels
  - share of classes
- uncertainty sampling ignores **the number of similar labels**

Uncertainty Measures: Discussion



Margin

- Requests instances close to the decision boundary
- Avoids regions of low variance, ignores number of already requested labels

Confidence

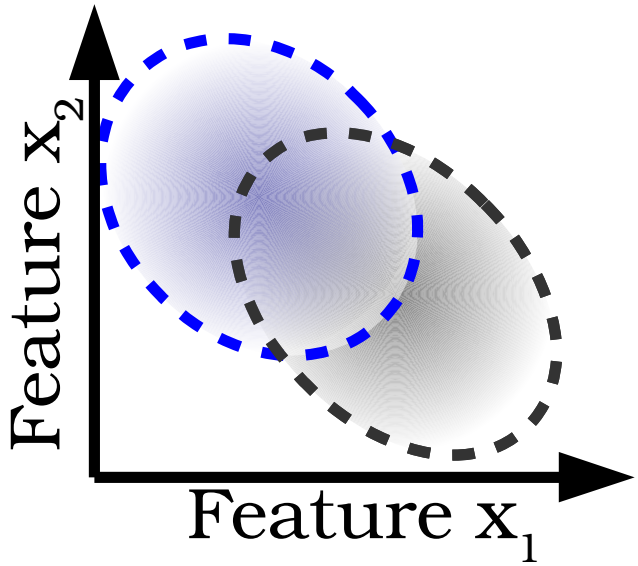
- Requests instances with low posterior difference
- Results in requests close to the decision boundary
- Again ignores the number of already requested labels

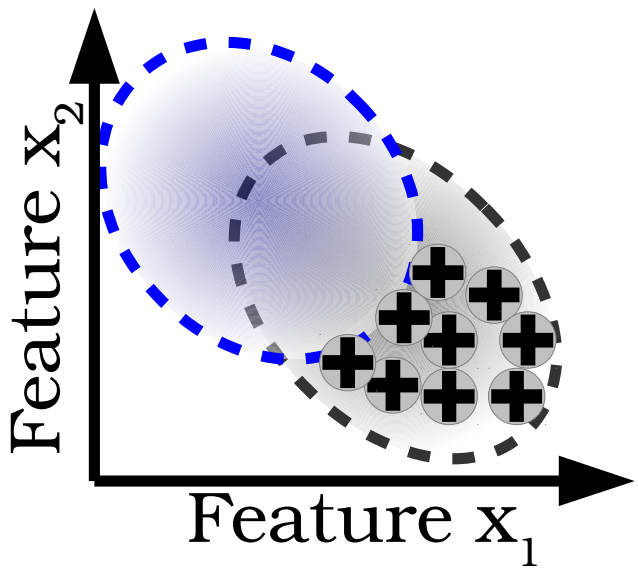
Entropy

- As above.

- **All those approaches ignore the number of previously requested labels!**

Error-Reduction Strategy





Observation

Valuable are instances that help us to improve.

Idea

Select instances that reduce the error the most

Observation

- Given the data on the left,
- generated by two Gaussian clusters,
- **where will we need many labels**?

- **Center: High variance**
  Some labels needed to learn that posteriors are equal, further labels will not improve classifier
- **Top-left, bottom-right: Low variance**
  Labels here are valuable, but a few may suffice
- **Top-right, bottom-left: Not frequent**
  The performance here is irrelevant

Error-Reduction Strategy

Formalisation: Compute *expected error reduction*

Approach

1. given current error rate e
2. for each possible outcome $\hat{y} \in \{+, -\}$ do
3. update classifier with $\hat{y}$
4. compute new error rate $e_{\hat{y}}$
5. compute error reduction $\delta_{\hat{y}} = e - e_{\hat{y}}$
6. compute weight $w_{\hat{y}}$ for this outcome $\hat{y}$
7. end
8. compute expected error reduction $E[\delta] = \sum_{\hat{y} \in \{+,-\}} w_{\hat{y}} \cdot \delta_{\hat{y}}$
9. request the label that maximises $E[\delta]$

Questions

1. How compute outcome-weights $w_{\hat{y}}$?
2. How compute new error rate $e_{\hat{y}}$?
   Specifically: On which data?

Error-Reduction Strategy

Outcome-Weights Computation

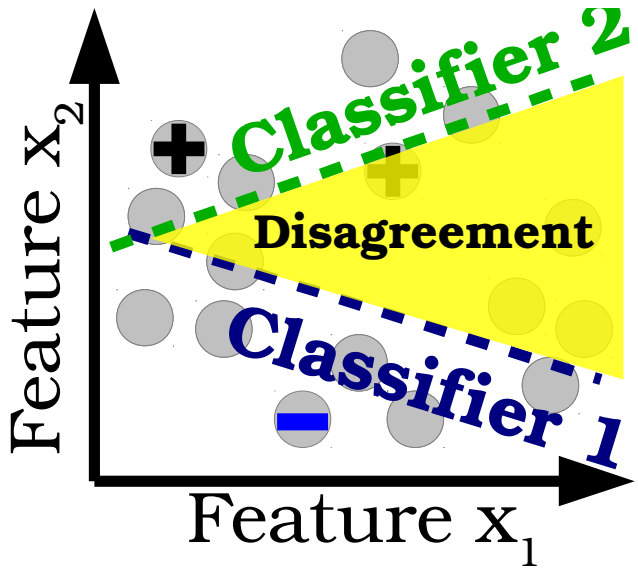
1. Average: Equal weights $w_{\hat{y}} = 0.5$ for all $\hat{y}$
2. Most likely: Weight the most likely outcome one
   (most likely based on the current classifiers prediction), the other outcome zero
3. Posterior-based: Use posterior estimates by current classifier as weights:
   $w_{\hat{y}} = \hat{p}(y = \hat{y}|x)$

- Variant 1: Favours exploration
  Only good for cases of high label variance
- Variant 2: Favours exploitation, similar to self-training
  Risk of getting stuck in the wrong hypothesis
- Variant 3: Inbetween one and two

Error-Rate Computation

- Use current classifier to label the unlabelled instances
  Similar to *self-training*
- Good estimate of the *generalisation capability*
- But: Might again lead to getting stuck in the wrong hypothesis

Ensemble-Based Strategy



Idea

Use disagreement between base classifiers

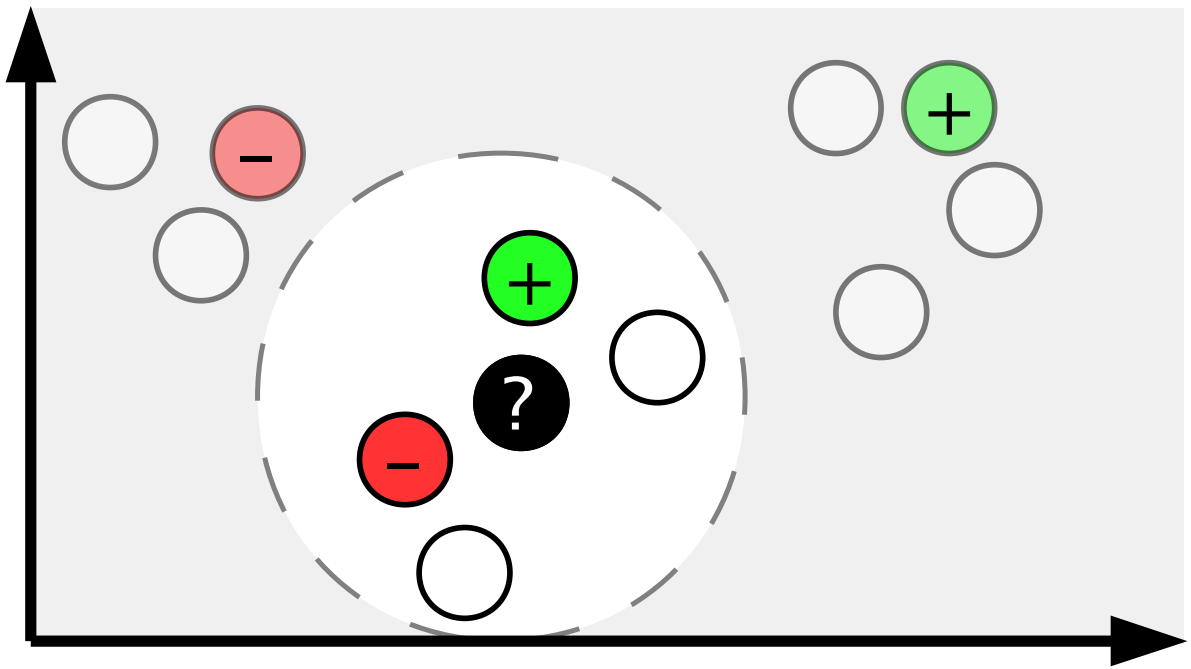
Approach

1. Get an initial set of labels
2. Split that set into (overlapping) subsets
3. On each subset, train a different base-classifier
4. Repeat
5. On each unlabelled instance do
6. Apply all base-classifiers
7. Request label, if base-classifiers disagree
8. Update all base-classifiers
9. Go to step 4
10. Until convergence

Probabilistic Active Learning: Illustrative Example

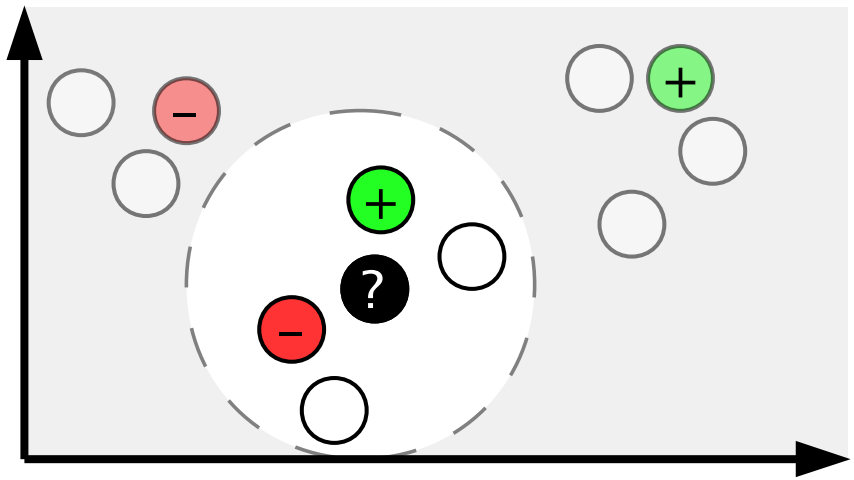
- Given: Dataset with labelled (⊖/⊕) and unlabelled (○) instances
- Objective: Select the most valuable candidate for labelling

How?



- **Decision Theoretic Approach:** Determine the gain in classification performance from labelling a candidate such as, e.g., $x_?$ (❓)

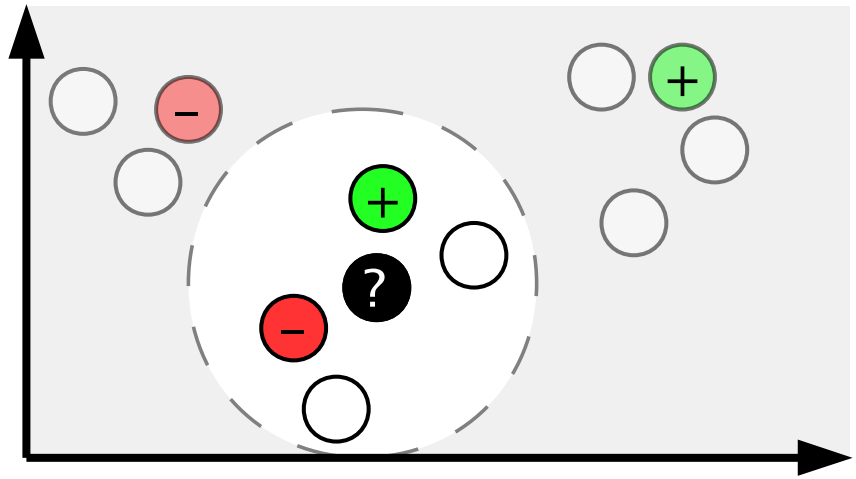
Principles of Probabilistic Active Learning [7]



- **How would we classify instances at the position of ?**
- Two neighbouring labels, half of them positive, half of them negative (**observed posterior** probability $\hat{p} = \hat{Pr}(Y = +|X = x_?) = 0.5$)
- Tie, e.g. let's classify instances here as negative

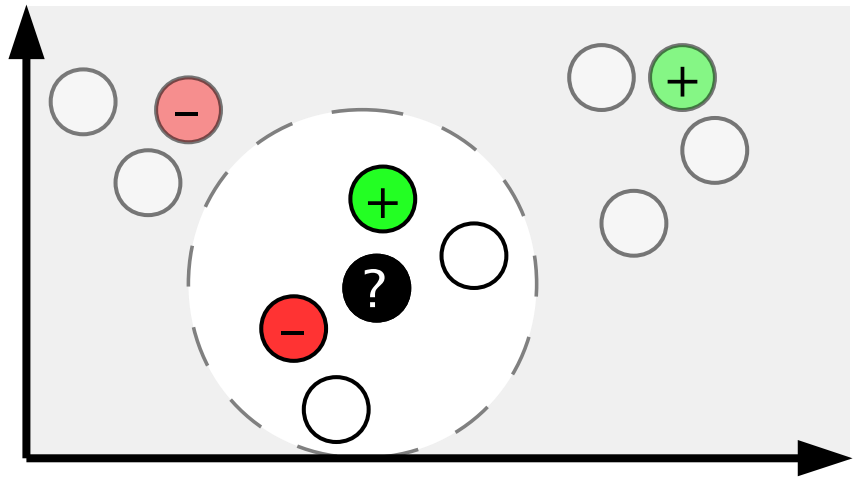
[7] See [Krempl et al., 2014a].

Principles of Probabilistic Active Learning



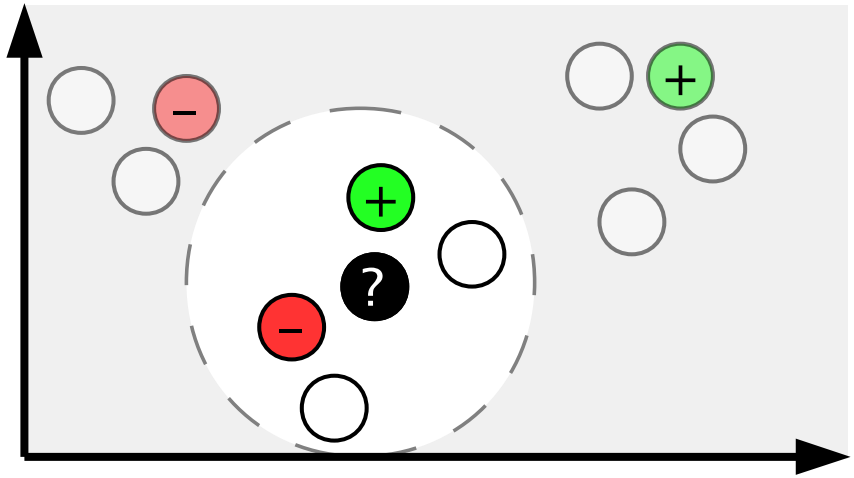
- **What is our current classification performance here, e.g. accuracy?**
- Depends on the **true posterior** probability $p = Pr(Y = +|X = x_?)$ here
- Unknown, but let's assume it to be, e.g., $p = 0.6$
- Then, our current accuracy is 40%

Principles of Probabilistic Active Learning



- **What happens if we get the label $y_?$ of $x_?$?**
- Depends on the **label's realisation**
- Unknown (yet), but let's assume it to be, e.g., positive: $y_? = +$
- Then, our classification rule changes to predicting positive labels
- Consequently, our current accuracy increases to 60%
- This results in a **gain in classification performance** by $+0.2$

Principles of Probabilistic Active Learning

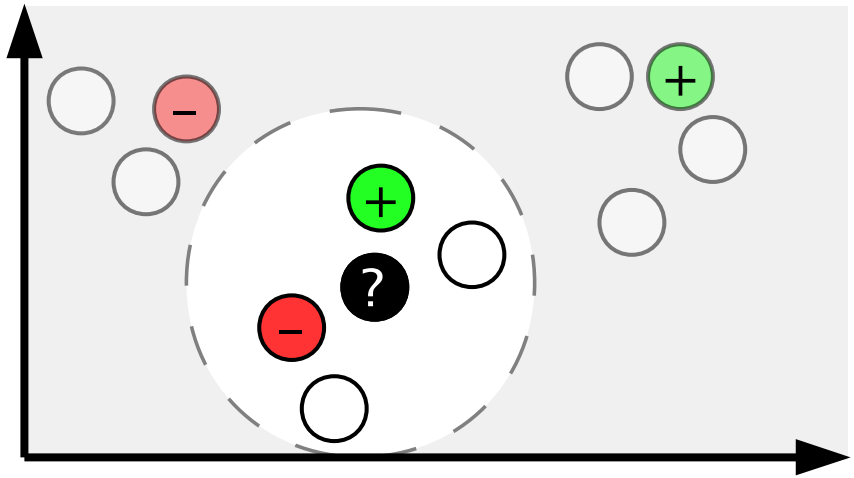


- **In reality we do not know the label realisation $y_?$ yet!**
- However, $y_?$ is the realisation of a **Bernoulli trial**:

$$\begin{array}{ccc} & y_? & \\ p \swarrow & & \searrow (1-p) \\ + & & - \end{array} \tag{1}$$

- Probability of success is the **true posterior** p
- E.g., in the case above, we get with $p = 0.6$ a positive label

Principles of Probabilistic Active Learning



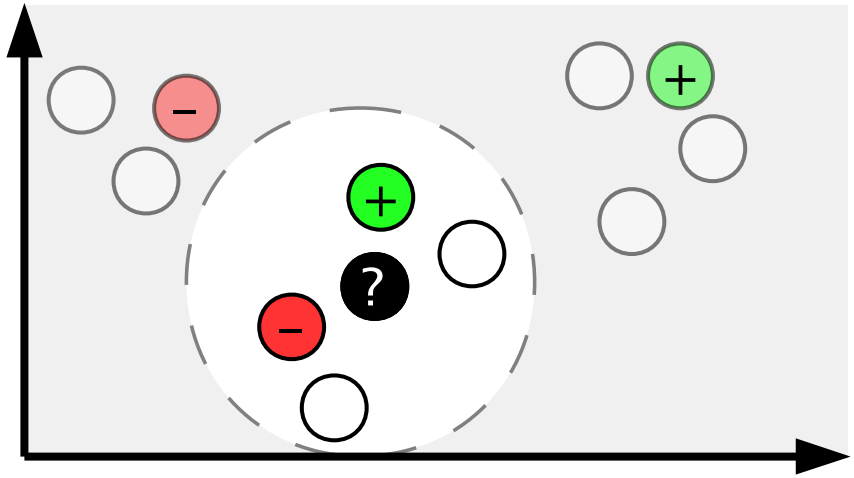
- **But how to determine p?**
- Unknown, but the already available labels provide some information:

  Let's summarise them by **label statistics** $\mathcal{ls} = (n_+, n_-)$, where
  - $n = n_+ + n_- = 2$ is the number of labels
  - $\hat{p} = \frac{n_+}{n_+ + n_-} = \frac{1}{2}$ is the share of positives therein (posterior estimate)

- These labels are the realisation of n Bernoulli trials with success probability p (*cmp. urn model*):

$$n_+ \sim \text{Binomial}_{n,p} = \text{Bin}_{n,p} \tag{2}$$

Principles of Probabilistic Active Learning



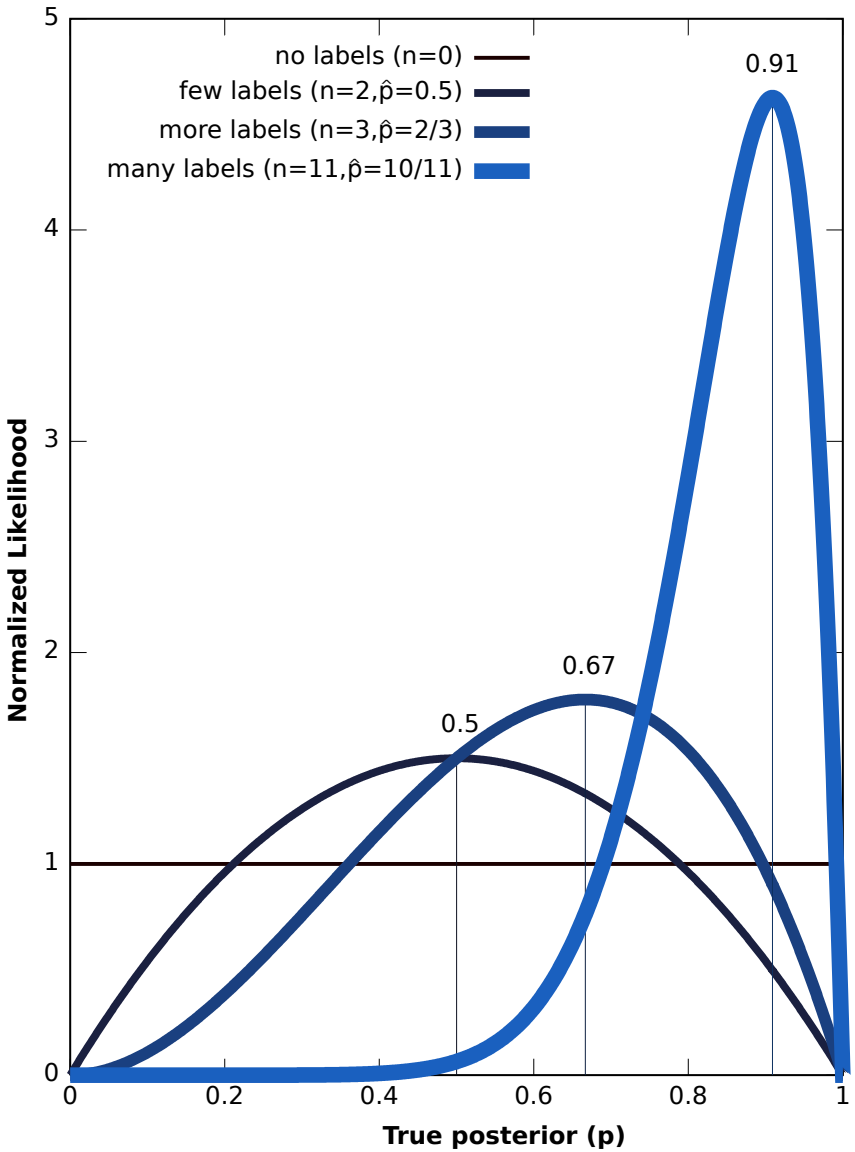
- The likelihood of p (as **parameter** of the above Binomial distribution), given the data $\mathcal{L} = (n_+, n_-)$ is

$$L(p|\mathcal{L}) = \mathrm{Bin}_{n_+ + n_-, p}(n_+) = \frac{\Gamma(n_+ + n_- + 1)}{\Gamma(n_+ + 1) \cdot \Gamma(n_- + 1)} \cdot p^{n_+} \cdot (1-p)^{n_-} \qquad (3)$$

- Normalising this likelihood yields the Beta distribution:

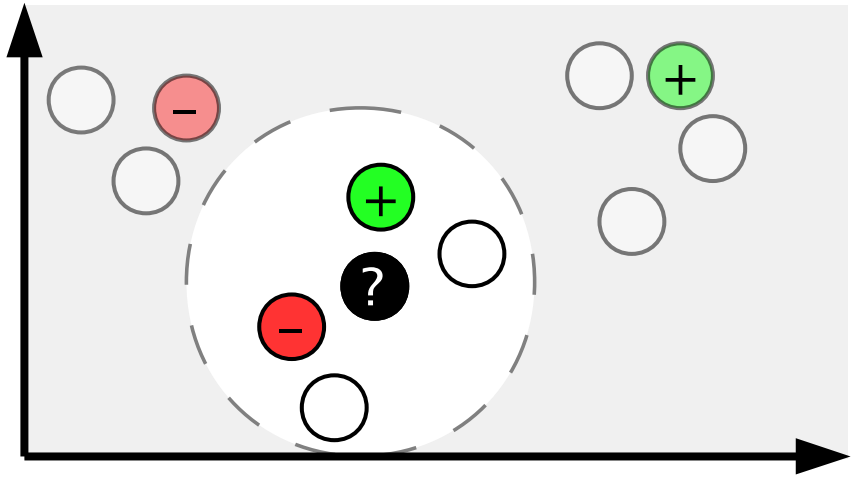
$$\omega_{\mathcal{L}}(p) = \frac{L(p|\mathcal{L})g(p)}{\int_0^1 L(\psi|\mathcal{L})g(\psi)\mathrm{d}\psi} = (n_+ + n_- + 1) \cdot L(p|\mathcal{L}) = \mathrm{Beta}_{\alpha,\beta}(p) \qquad (4)$$

Probabilistic Active Learning – Excursus: Beta Prior



- Uniform prior: Prior to the first label's arrival, all values of p are assumed equally plausible.
- A Bayesian approach yields for the normalised likelihood corresponds a beta distribution with parameters:
  - α Number of positive labels plus one
  - β Number of negative labels plus one
- Left: Plot of normalised likelihoods for different values of α, β
- The peak of this function becomes the more distinct, the more labels are obtained.

Principles of Probabilistic Active Learning



- Thus, given label statistics $\mathcal{ls} = (n_+, n_-)$ summarising labelled data,
- we have **two random variables**
  - the true posterior $P \sim \mathrm{Beta}_{n_+ +1, n_- +1}$
  - the label realisation $Y \sim \mathrm{Bernoulli}_p = \mathrm{Ber}_p$
- and calculate the **performance gain in expectation** over p, y

$$\mathrm{pgain}(\mathcal{ls}) = \mathrm{E}_p\left[\mathrm{E}_y\left[\mathrm{performancegain}_p(\mathcal{ls}, y)\right]\right] \tag{5}$$

$$= \int_0^1 \mathrm{Beta}_{\alpha,\beta}(p) \cdot \sum_{y \in \{0,1\}} \mathrm{Ber}_p(y) \cdot \mathrm{gain}_p(\mathcal{ls}, y)\,\mathrm{d}p \tag{6}$$

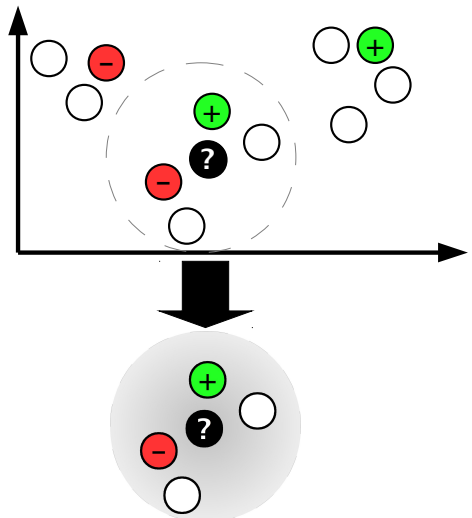
Probabilistic Gain

This **probabilistic gain** quantifies

- the *expected change* in classification performance
- at the *candidate's position* in feature space,
- in each and every *future classification* there,
- given that *one additional label* is acquired.

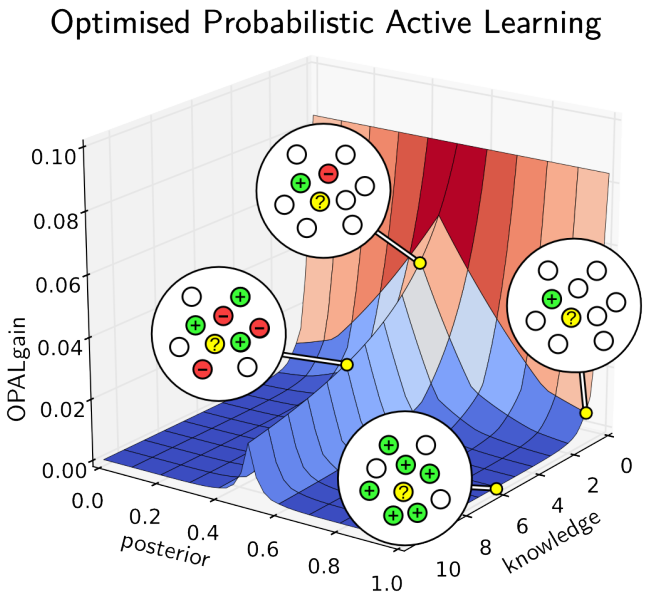
- Weight pgain with the density d_x *over labelled and unlabelled data* at the candidate's position.

- Select the candidate with highest density-weighted probabilistic gain.



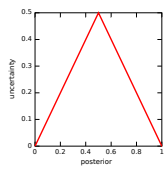
Probabilistic Gain – G_{OPAL}

Probabilistic Gain for Equal Misclassification Costs



- The probabilistic gain in accuracy as a function of $\mathcal{ls} = (n, \hat{p})$ is
- monotone with variable n,
- symmetric with respect to $\hat{p} = 0.5$,
- zero for irrelevant candidates.
- Compare to uncertainty:

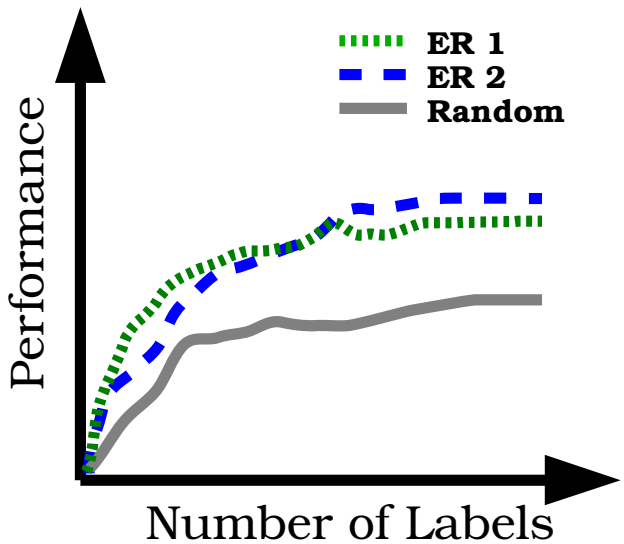
(in confidence) const. w.r.t. n:



Active Learning Strategies - Discussion

- Uncertainty-Based:
  fast and simple, *waste labels* in regions with high Bayesian error rate
- Error-Reduction:
  good quality, *high computational cost*
- Ensemble-Based:
  good quality, *convergence avoids unnecessary sampling* in regions with high Bayesian error rate, *conceptually easily understandable*, *multiple classifiers needed*
- Probabilistic Approach:
  good quality, *considering labelstatistics avoids unnecessary sampling* in regions with high Bayesian error rate

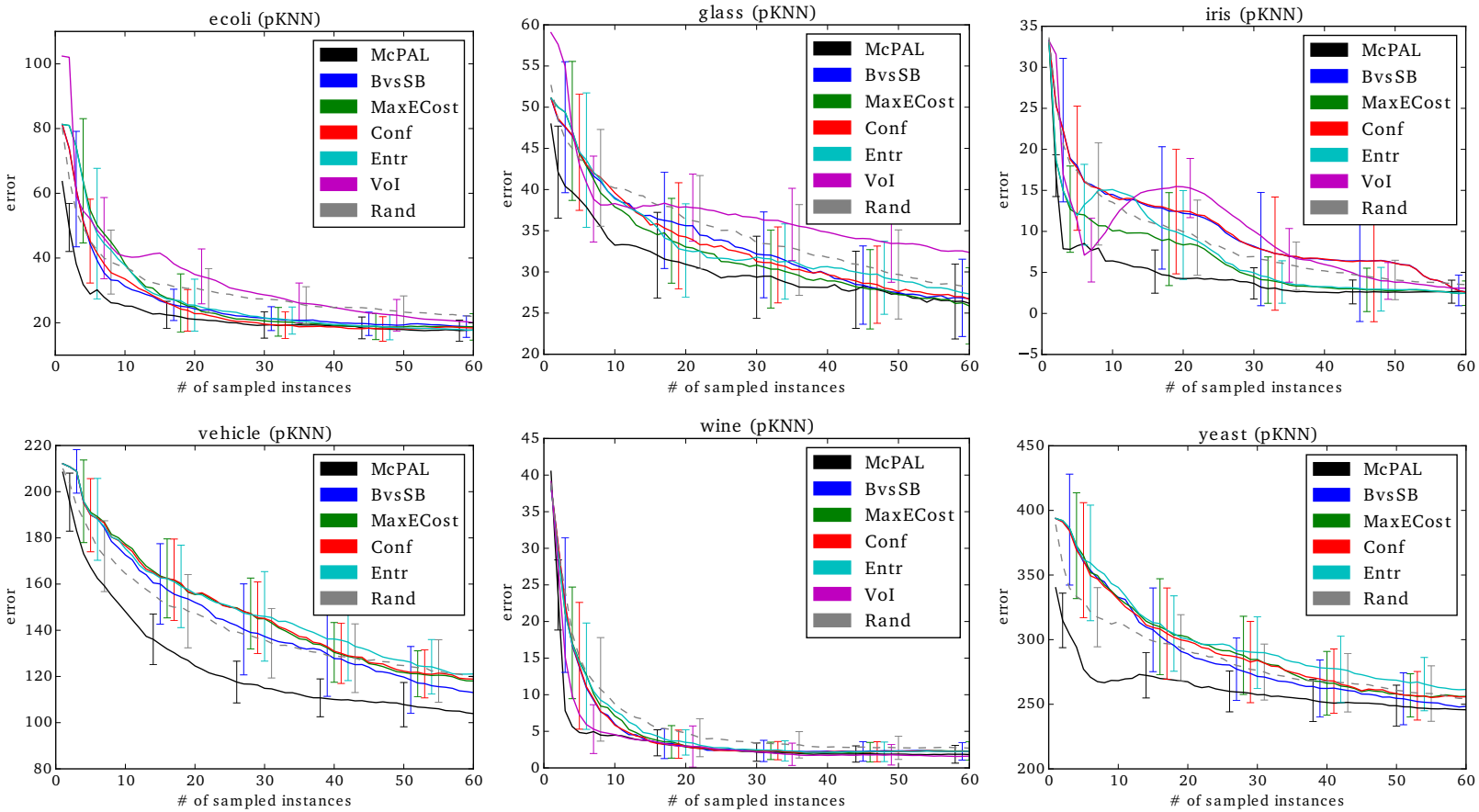
Evaluating Active Learning Approaches



Learning Curves

- Plot performance against the number of requested labels
- Expected Behaviour:
  - Performance increases with number of labels
  - Convergence: after ∞ label requests, all strategies should have the same performance
- Caveat: Allways compare using the same classifier!

Evaluation Example: Multi-Class Probabilistic AL (McPAL): (Selection[8])



Learning curves of mean misclassification cost (including standard deviation as error bars) of McPAL and its competitors on all six datasets using the pKNN classifier.

[8] For more results, please consult ECAI paper [Kottke et al., 2016].

Lecture Outline

- Lecture's Context
- Semi-Supervised Learning
- Active Learning
  - Motivation
  - Approaches
    - Uncertainty Sampling
    - Expected Error Reduction
    - Ensemble / Query by Committee
    - Probabilistic Active Learning
  - Evaluation
- Summary and Questions

Summary and Questions

Summary

- Motivation & Aim: Not all labels are available
- General Idea: Use structure of the data!
- Semi-Supervised Learning:
  - Assumptions: Smoothness, Clusters, or Manifold
  - Approaches: Self-Learning, Generative Models, Low-Density Separation, Graph-Based Models
- Active Learning:
  - Scenarios: Query Synthesis, Pool, Stream
  - Approaches: Uncertainty Sampling, Expected Error Reduction, Query by Committee, Probabilistic Active Learning
  - Evaluation: Learning Curves

Questions?

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SSL: Approaches

- Self-Learning, Co-Learning
- Generative Models
- Low-density Separation
- Graph-Based Methods

Generative Models

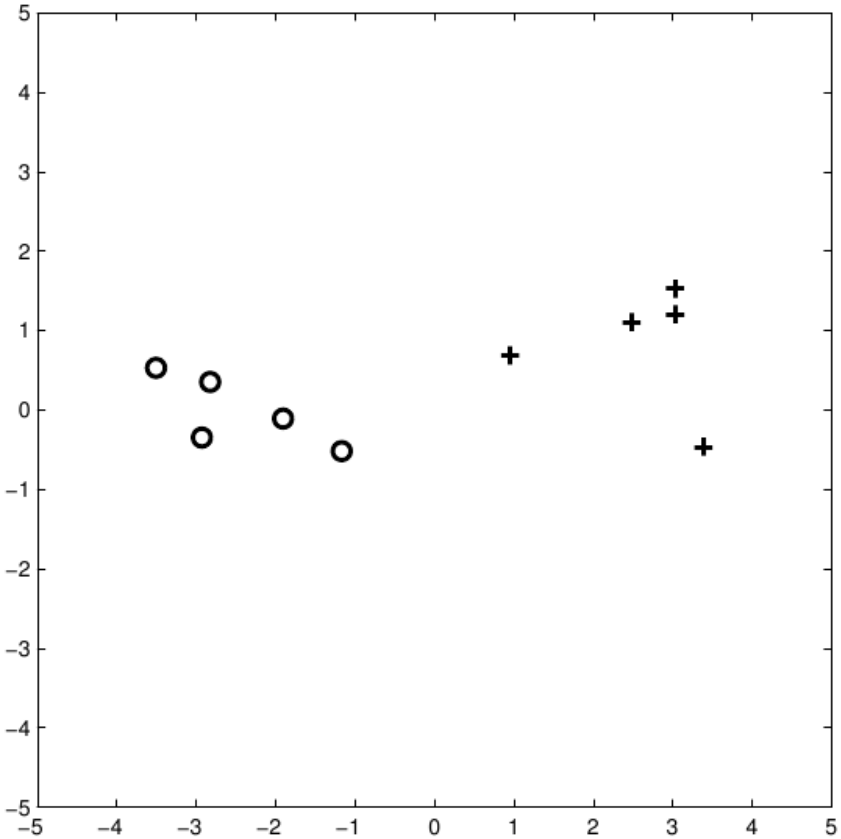
- **Assumption:**
  $P(X, Y) = P(Y)P(X|Y)$ with $P(X|Y)$ being an identifiably mixture distribution
- **Objective:**
  Identify generative model that produces the data
- **Basic Idea:**
  Learn distribution $P(X|Y)$ of each class $y \in Y$
  This requires some assumptions upon the generative model
- **Probabilistic approach:**
  Find likelihood–maximising parameter set Θ, e.g. using expectation–maximisation
- **Algorithmic approach:**
  Cluster – and – Label

Back to SSL Discussion

Generative Models - Example

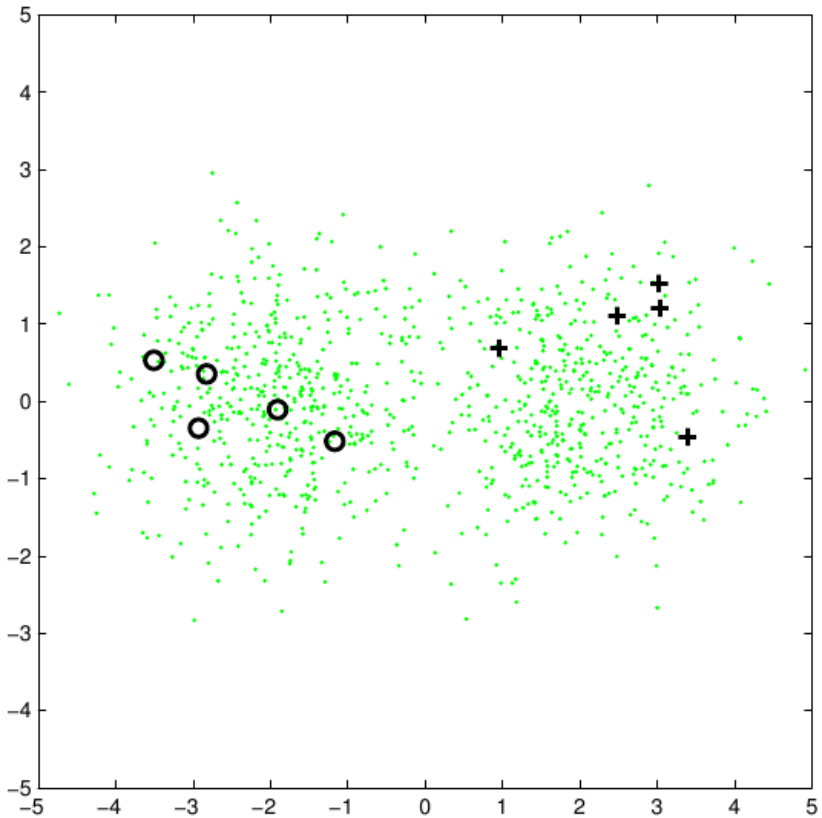
Gaussian Mixture Model Example[9]

Labelled data



Back to SSL Discussion

Labelled and unlabelled data

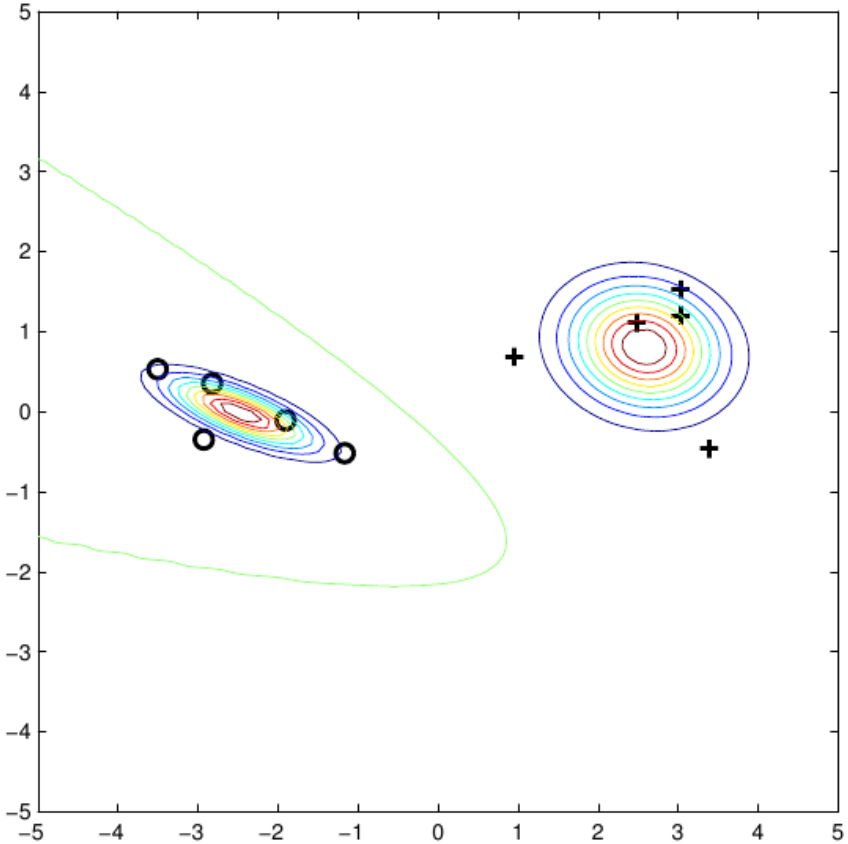


[9] Illustrations from Zhu 2005 [Zhu, 2008].

Generative Models - Example (2)

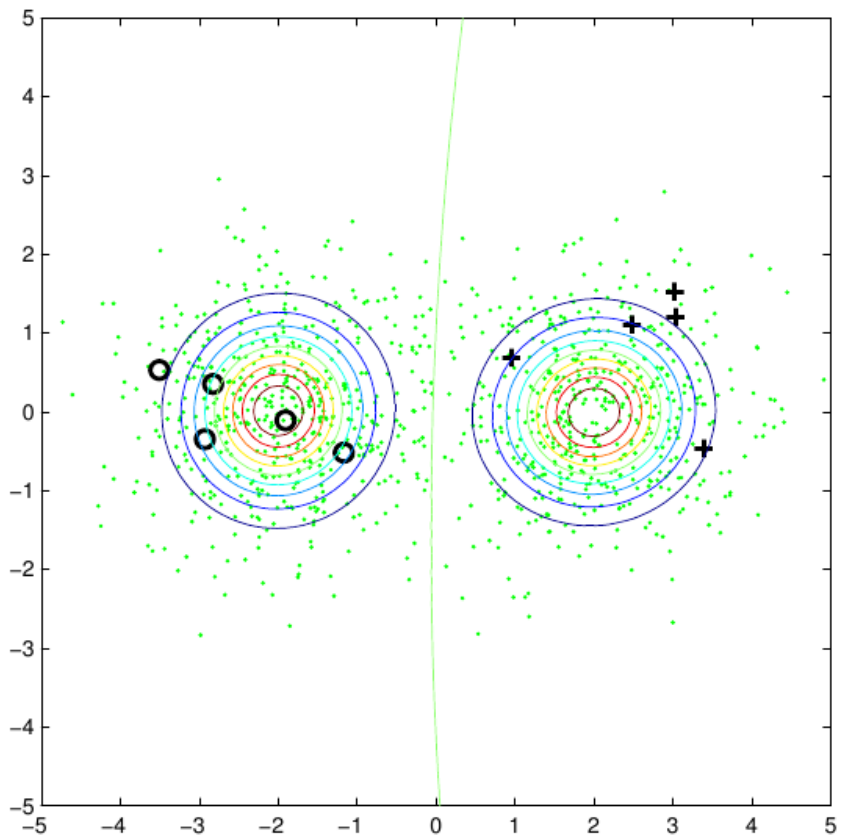
Gaussian Mixture Model Example[10]

Decision model learnt solely on labelled data



Back to SSL Discussion

Decision model learnt on all data



[10] Illustrations from Zhu 2005 [Zhu, 2008].

Generative Models - Challenges

- Identifiability
  It may happen, that solution is not unique, even if type of distributions involved is known

  Example from Zhu 2005:
  - Given $P(X) \sim U(0;1)$ and two labelled instances $(x_1 = 0.1; y_1 = +)$, $(x_2 = 0.9; y_2 = -)$
  - We know that $P(X|Y = +) \sim U(0;\tau)$ and $P(X|Y = -) \sim U(\tau;1)$, but we do not know value of τ
  - Different values of τ result in concurring models
    We can not identify the true model given the two instances
- Model correctness
  - If assumptions in the model are met, using unlabelled data increases quality of prediction model
  - But: Otherwise, model can be worse than a model based solely on labelled data
- Model fitting
  Parameter set might not be *global* optimum

Back to SSL Discussion

Low-Density Separation

- **Assumption:**
  Classes are separated by low density regions
- **Objective:**
  Placement of decision boundary in regions of low density
- **Approaches:**
  Transductive Support Vector Machines (TSVMs)
  Conventional SVM: aximize margin between labelled instances
  Transductive SVM: Maximize margin between all instances
  (i.e. labelled and unlabelled ones)

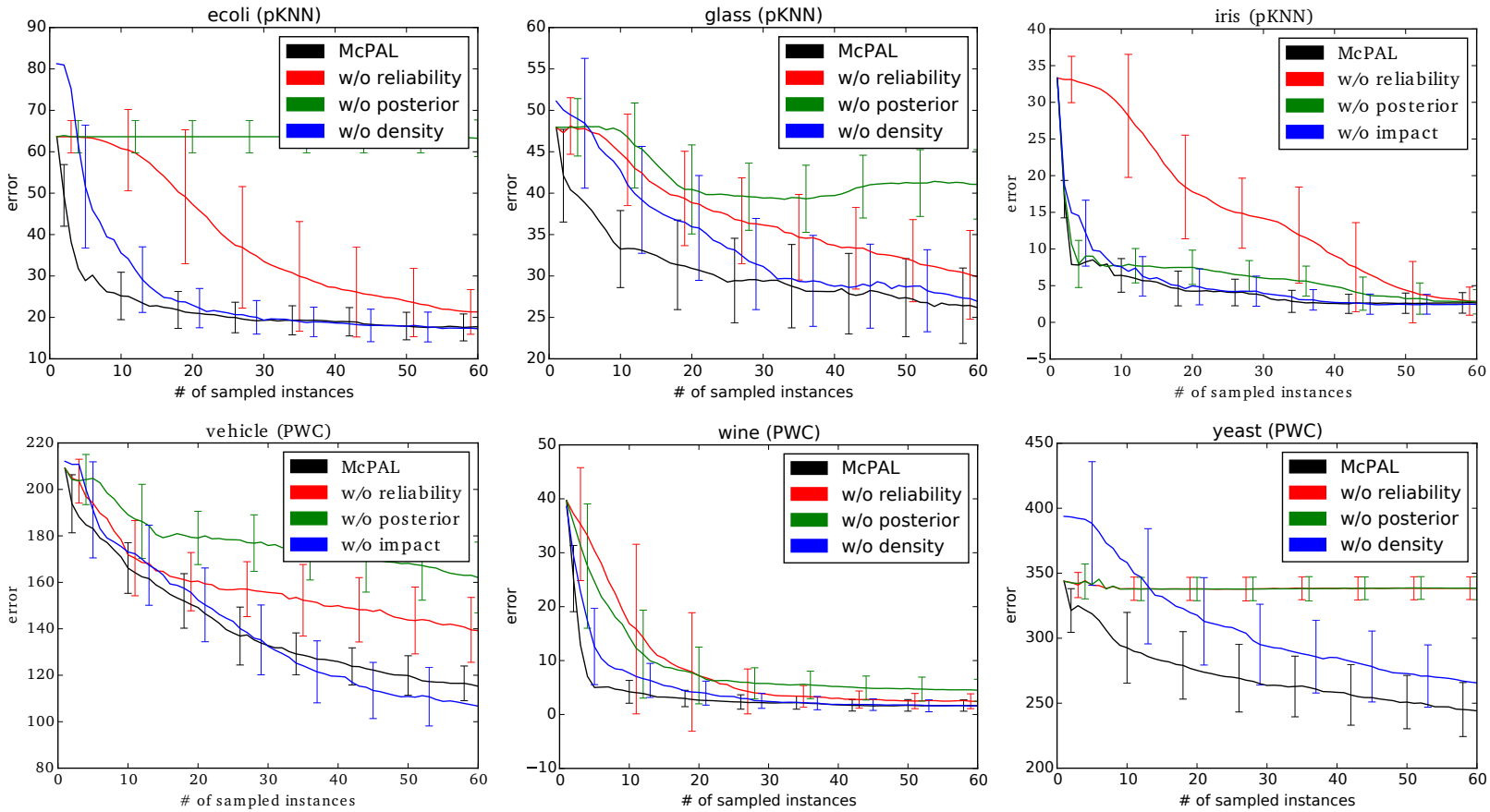
Graph-Based Methods

- **Assumption:**
  Manifold assumption, smoothness over graph
- **Approach:**
  - Represent data by a graph
  - Vertices/Nodes are labelled and unlabelled instances
    (e.g. connect an instance to its k nearest neighbours, or to all neighbours within some ϵ-neighbourhood)
  - Edges represent similarities
  - Estimate a function f on the graph,
    that is close to given labels and smooth to the whole graph
  - Use f to propagate label to neighbouring instances in graph

Back to SSL Discussion

Evaluation of Influence Factors

- Original McPAL compared to variants
- ignoring reliability: normalising the $\vec{k}$ vector to $\sum \vec{k} = n = 1$
- ignoring posterior: using uniform frequency estimate $k_i = n/C, 1 \leq i \leq C$
- ignoring density: setting it to a constant value



Learning curves in mean misclassification cost (including standard deviation as error bars).