Active Learning & Experimental Design

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Heavily modified, of course, by **Lyle Ungar**

Strategies for choosing which points to label

Active learning: sequential, *ad hoc*

Experimental design: simultaneous, principled

Motivation

- **Labeling data is often expensive**
  - Unlabeled data is often cheap
- **Not all labels are equally useful**
- **We want to collect the "best" data at minimal cost**

What observations should one label?

Toy examples

Assume you are learning $y = ax+b$ **for** x **on** $[-1,1]$.

You can pick two x**'s to get** y**'s for.**

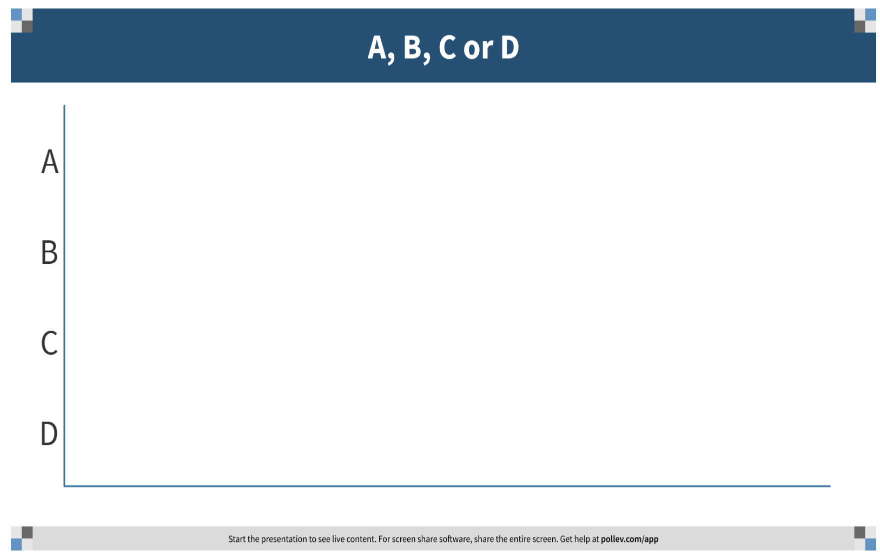
What two values would you pick?

A) -1/3, 1/3

B) -1, 1

C) 0, 1

D) Something else



Toy examples

Assume you are learning *y* = *f*(*x*) for *x* a scalar

You are learning an SVM classifier on [-1.1].

You can pick 4 *x*'s to get *y*'s for.

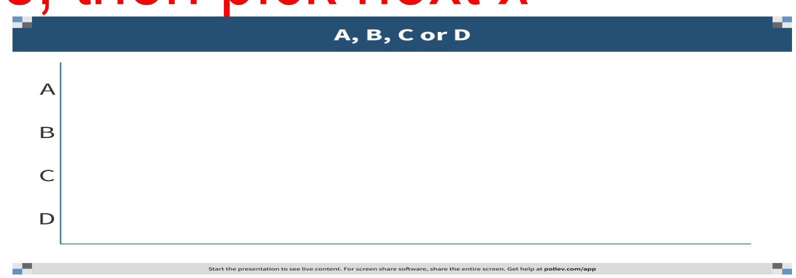
What strategy would you use to pick *x*'s?

A) Pick -1, -1/3, 1/3, 1

B) Pick -1, 1, see what the answer is, then pick next *x*

C) Pick -1/3, 1/3, see what the answer is, then pick next *x*

D) Something else



Toy Example: 1D classifier

Unlabeled data: labels are all 0 then all 1 (left to right)

Classifier (threshold function): $h_w(x) = 1$ if $x > w$ (0 otherwise)

Goal: find transition between 0 and 1 labels in minimum steps

Naïve method: choose points to label at random on line

- Requires O(n) training data to find underlying classifier

Better method: binary search for transition between *0* and *1*

- Requires O(log n) training data to find underlying classifier
- Exponential reduction in training data size!

Example: collaborative filtering

- **Users usually rate only a few movies**
  - ratings are“expensive”
- **Which movies do you show users to best extrapolate movie preferences?**

[Yu et al. 2006]

Example: collaborative filtering

- **Baseline algorithms:**
  - Random: *m* movies randomly
  - Most Popular Movies: *m* most frequently rated movies
- **Most popular movies is not better than random!**
- **Popular movies rated highly by all users; do not discriminate tastes**

[Yu et al. 2006]

Active Learning

- **Active learning**
  - Uncertainty sampling
  - Information-based loss functions
- **Optimal experimental design**
- **Response surface modeling**

Active Learning

- **Given existing data (*X*,*y*), choose where to collect more labels**
  - Assume access to cheap unlabeled points
  - Make a query to obtain expensive label
  - Want to find labels that are "informative"
  - **Output:** Classifier / predictor
- **Similar to "active learning" in classrooms**
  - Students ask questions, receive a response, and ask more questions
  - Contrast: passive learning: student just listens to lecturer

Active Learning Setup

- Active learner picks which data point *x* to query
- Receive label ("response") *y* from an oracle
- Update parameters *w* of the model
- Repeat

- Query selected to minimize some loss function ("risk")

Active Learning

- **Heuristic methods for reducing risk:**
  - Select "*most uncertain*" data point
  - Select "*most informative*" data point

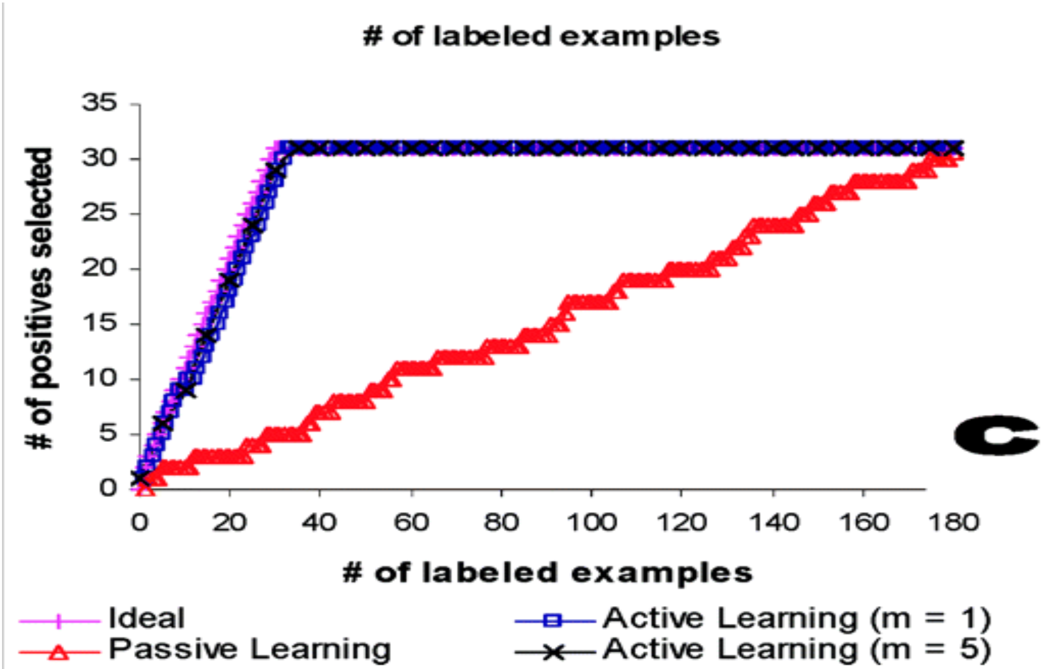
Uncertainty Sampling

- **Query the item (x) that the current classifier is *most uncertain* about**
- **Needs measure of uncertainty**
- **Examples:**
  - Entropy
  - Least confident predicted label
  - Euclidean distance (e.g. point closest to margin in SVM)

When might this fail?

Example: Gene expression and Cancer classification

- Active learning takes 31 points to achieve same accuracy as passive learning with 174



Liu 2004

Information-based Loss Function

- **Above methods looked at uncertainty at a single point**
  - Does not look at expected effect of adding the point on the model
- **Better: quantify the information gained**
  - Maximize **KL divergence** between posterior and prior

$$KL(P\|\pi) = \#\text{ of bits gained about model}$$

  - Maximize reduction in **model entropy** between posterior and prior (reduce number of bits required to describe distribution)
- **Where have we seen something similar?**

[MacKay, 1992]

KL divergence as info gain

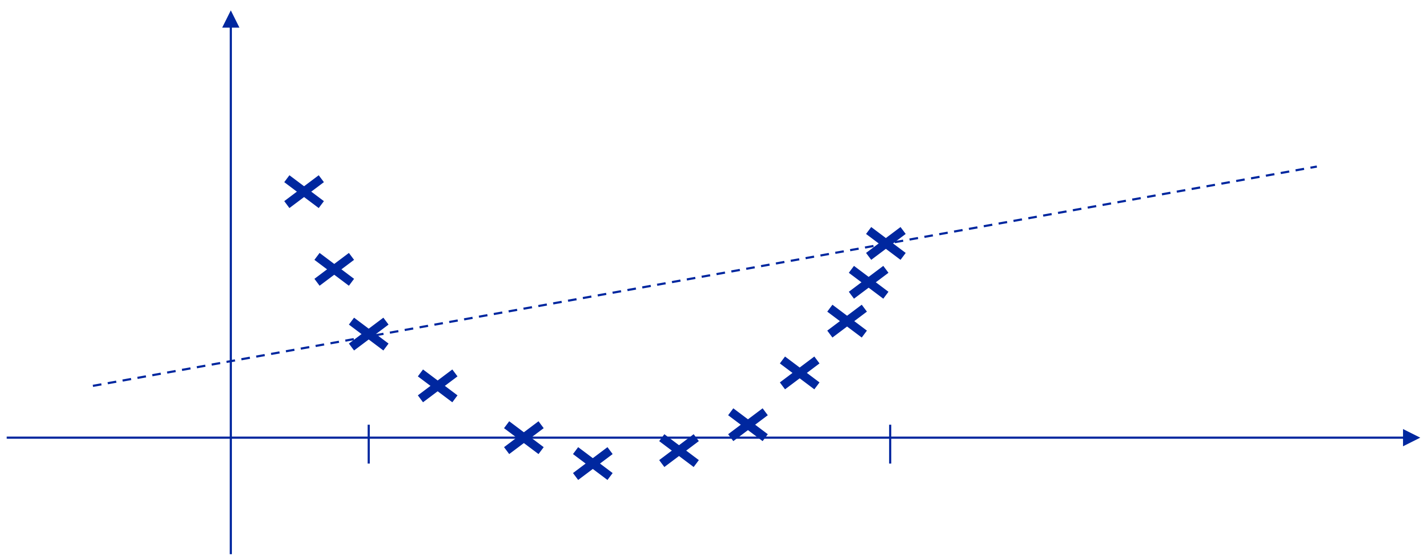
- **The KL divergence measures the information gain expected from query** (x'):

$$KL(\, p(\theta \mid x, x') \,||\, p(\theta \mid x))$$

- **Goal:** choose a query that *maximizes* the KL divergence between the updated posterior probability and the current posterior probability
  - This represents the largest expected information gain

Active learning warning

- Choice of data is only as good as the model itself
- Assume a linear model, then two data points are sufficient
- What happens when data are not linear?



Active Learning = Sequential Experimental Design

- Active learning
  - Uncertainty sampling
  - Information-based loss functions
- **Optimal experimental design**
- Response surface modeling

Optimal Experimental Design

- **Active learning heuristics mostly perform well**
  - but sometimes fail
- **Optimal experimental design gives**
  - theoretical criteria for choosing which points to label
  - given specific assumptions and objectives

It fails, too, if the assumptions aren't met.

Optimal Experimental Design

- **Given a model with parameters *w*,**
  - What queries are maximally informative
- **“Best” minimizes variance of estimate of *w***
- **Linear models**
  - Optimal design does not depend on ***w*** !
- **Non-linear models**
  - Depends on ***w****;* often use Taylor expansion to linear model

Goal: Minimize variance of *w*

If $y = \boldsymbol{x}^T\beta + \varepsilon$ then $\boldsymbol{w} = (\boldsymbol{X}^T\boldsymbol{X})^{-1}\boldsymbol{X}^T\boldsymbol{y}$

$\boldsymbol{w} \sim N(\beta, \sigma^2(\boldsymbol{X}^T\boldsymbol{X})^{-1})$ $\varepsilon \sim N(0, \sigma^2)$

We want to minimize the variance of our parameter estimate **w**, so pick training data **X** to minimize $(\mathbf{X}^T\mathbf{X})^{-1}$

But that is a matrix, so we need to reduce it to a scalar

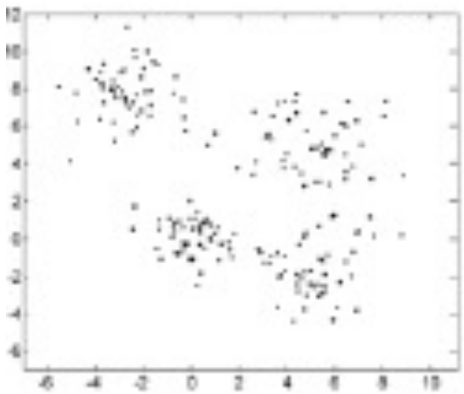
- ***A-optimal*** **(average) design minimizes** *trace*$(\boldsymbol{X}^T\boldsymbol{X})^{-1}$
- ***D-optimal*** **(determinant) design minimizes** *log det*$(\boldsymbol{X}^T\boldsymbol{X})^{-1}$
- ***E-optimal*** **(extreme) design minimizes** *max eigenvalue of* $(\boldsymbol{X}^T\boldsymbol{X})^{-1}$

Alphabet soup of other criteria (C-, G-, L-, V-, etc.)

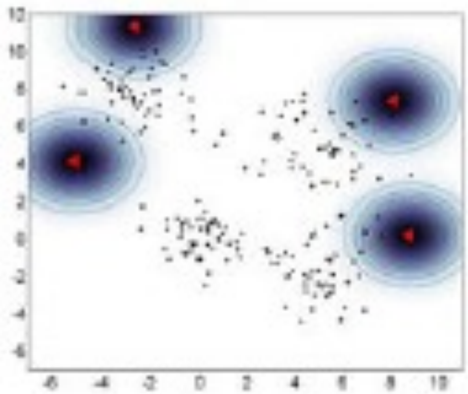
A-Optimal Design

- ***A-optimal* design minimizes the trace of $(X^TX)^{-1}$**
  - Equivalent to minimizing the Frobeneous norm
  - Chooses points near the border of the dataset
  - Trace of a matrix is the sum of its eigenvalues

Example: mixture of four Gaussians



(a) Data set



(b) A-optimal design

[Yu et al., 2006]

Practicalities

- **Sometimes you can generate an *x* arbitrarily**
- **More often you need to select from a set of given *x*'s**
  - This can be an expensive search!

Experimental Design

- Active learning
  - Uncertainty sampling
  - Information-based loss functions
- Optimal experimental design
- **Response surface modeling**
  - Fit curve only near optimum

Response Surface Methods

- **Goal: find an x to minimize** y **(for an unknown function** $y = f(\mathbf{x})$)
  - Using gradient descent
  - E.g., find optimal conditions for growing cell cultures
- **Procedure**
  - **Initialize:** Given a set of datapoints, $(\mathbf{X},\mathbf{y})$, fit $y = f(\mathbf{x};\mathbf{w})$
    - This is the "response surface"
  - **Repeat**
    - Pick the next $\mathbf{x}_i$ by doing gradient descent on $f(\mathbf{x})$
    - Measure the corresponding y_i (e.g. by taking action $\mathbf{x}_i$)
    - Use $(\mathbf{x}_i, y_i)$ to update the response surface $f(\mathbf{x})$
- **We only care about fitting close to the optimum**

Response Surface Modeling

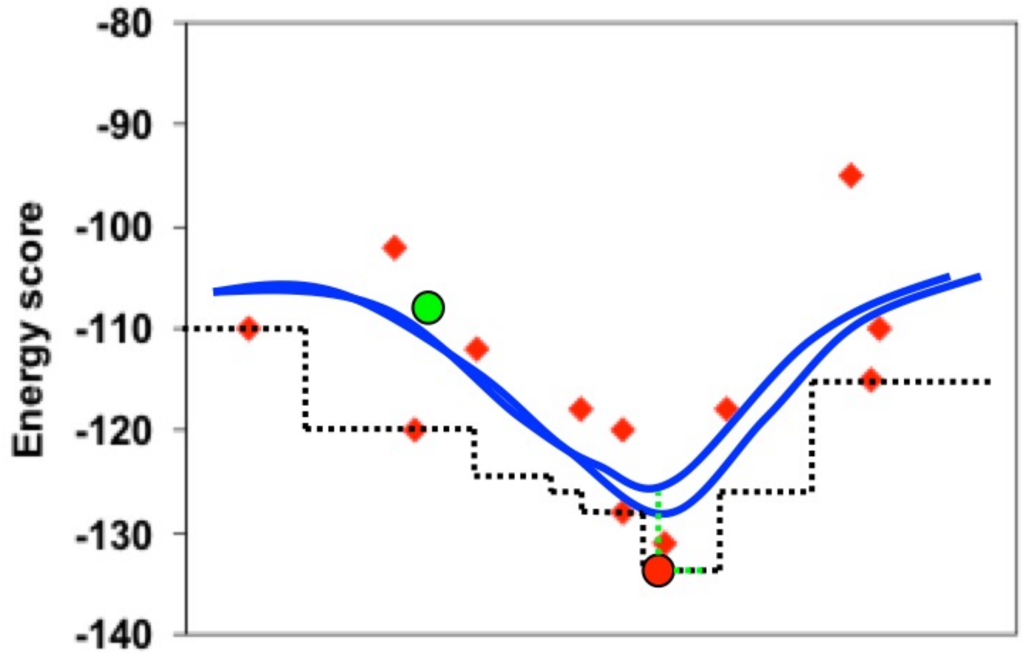
Goal: find the minimum of unknown function y = f(x)

Initialize: Given a set of datapoints, ***(X,y)***, fit $y = \boldsymbol{f(x;w)}$

Repeat

- Pick the next $\boldsymbol{x_i}$ using gradient descent on $f(\boldsymbol{x})$
- Measure the corresponding y_i
- Use $(\boldsymbol{x_i}, y_i)$ to update the response surface $f(\boldsymbol{x;w})$

Taking action ***x*** lets you observe the corresponding reward y. This new point (**x**,y) is added to the training data to better estimate **w**



[Blum, unpublished]

What you should know

- **Active learning**
  - Uncertainty sampling
  - Query by committee
  - Information-based loss functions
- **Optimal experimental design**
  - A-optimal design
  - D-optimal design
  - E-optimal design
  - *All minimize the variance in estimate of **w***
- **Response surface methods**

Sample where models is uncertain

Sample where model disagree

Maximize information gain

Minimize trace= $\Sigma \lambda_i$ of $(X^TX)^{-1}$

Minimize det= $\Pi \lambda_i$ of $(X^TX)^{-1}$

Minimize largest eigenvalue $max\ \lambda_i$ of $(X^TX)^{-1}$

Sequential experiments for optimization