Supervised Learning
K Nearest Neighbors
Validation

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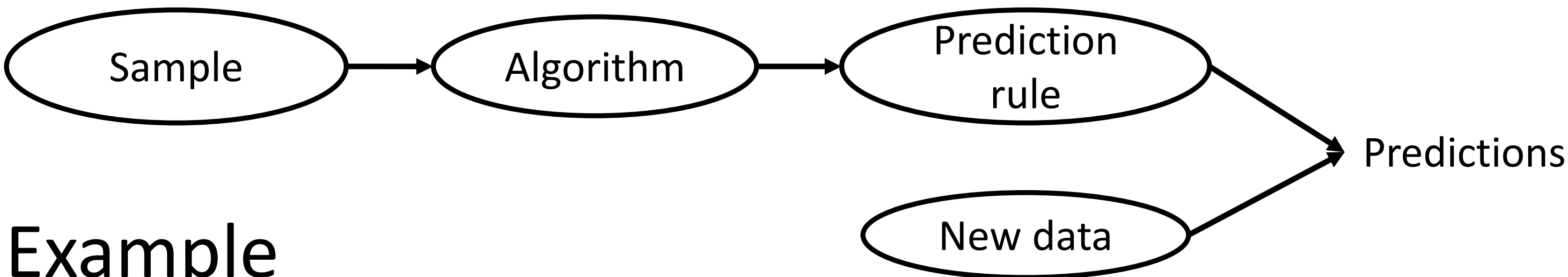
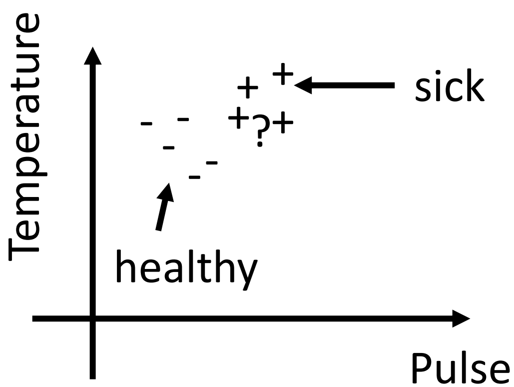
Supervised Learning

- Protocol



- Example



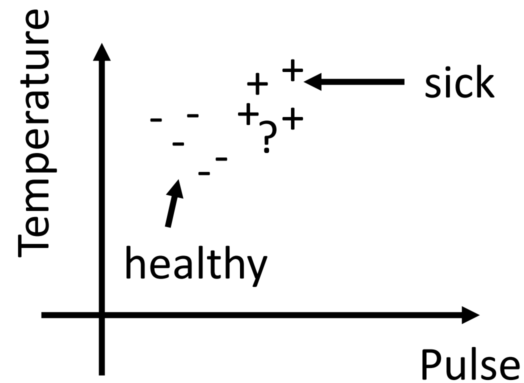
Supervised Learning

- More examples
  - (age, gender, weight) → height
  - (age, weight, height) → gender
  - (height(1), height(2), height(3)) → height(4)
- Notations
  - $\mathcal{X}$ – sample space (e.g., $\mathcal{X} = \mathbb{R}^d$)
  - $\mathcal{Y}$ – label space (e.g., Classification: $\mathcal{Y} = \{\pm 1\}$; Regression: $\mathcal{Y} = \mathbb{R}$)
  - $S = \{(X_1, Y_1), \ldots, (X_n, Y_n)\}$ – training sample (where $X_i \in \mathcal{X}$, $Y_i \in \mathcal{Y}$)
  - $h: \mathcal{X} \to \mathcal{Y}$ – a prediction rule / hypothesis
  - $\mathcal{H}$ - a set of prediction rules / a hypothesis set

K-Nearest Neighbors (K-NN)

- Algorithm: Predict X based on K nearest neighbors in S.

- Input: distance measure $d(x, x')$
- Examples:
  - Euclidian distance
  - Manhattan distance
  - Travel distance
  - Edit distance



- **The choice of d determines the success or failure of K-NN!**

Evaluation

- $\ell(y', y)$ – loss/error function
  Loss for predicting y' when the reality is y

- Examples:
  - Zero-one loss
    $$\ell(y', y) = \mathbb{I}(y' \neq y)$$
    $$= \begin{cases} 0, & if\ y' = y \\ 1, & if\ y' \neq y \end{cases}$$
  - Squared loss
    $$\ell(y', y) = (y' - y)^2$$
  - Absolute loss
    $$\ell(y', y) = |y' - y|$$

- **The loss function determines the cost of different mistakes!!!**

- Example: Fire alarm

Depends on the house

y' \ y	no fire	fire
no fire	0	5.000.000
fire	2.000	0

"constant"

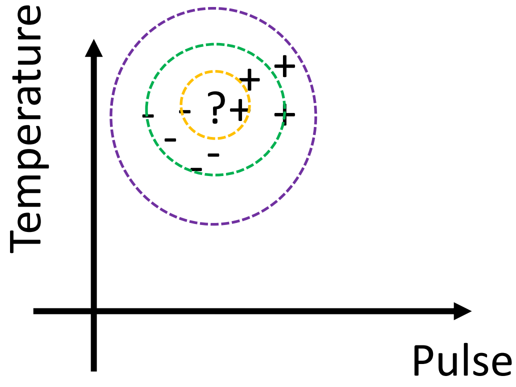
So far

- KNN – predict based on K nearest neighbors

- Input:
  - Distance measure $d(x, x')$ – domain knowledge

- Evaluation:
  - Loss function $\ell(y', y)$ – domain knowledge

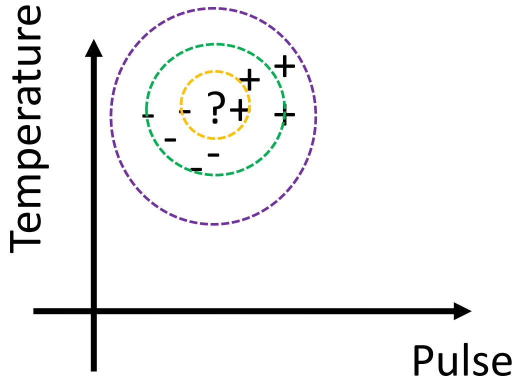
How to pick K?



- What is good/bad about small K?
  - Say, K=1?

- What is good/bad about large K?
  - Say, K=n?

How to pick K?



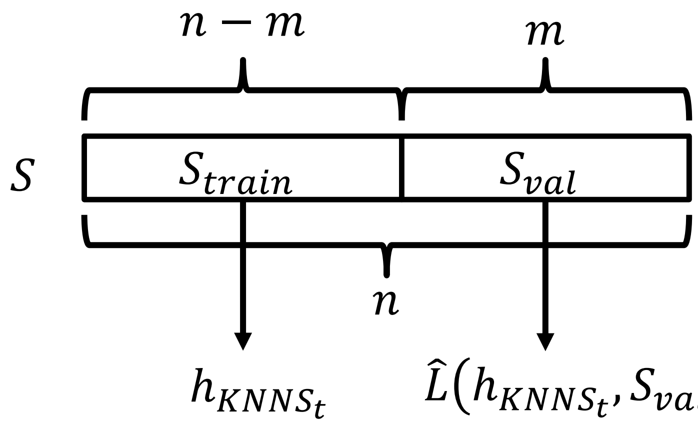
- Target: minimize the expected loss
  - $L(h_{KNN}) = \mathbb{E}[\ell(h_{KNN}(X), Y)]$

- Assumption
  - (X, Y) are sampled from a fixed (unknown) distribution $p(X, Y)$
  - The expectation is with respect to $p(X, Y)$

- Challenge: $p(X, Y)$ is unknown, and so is $L(h_{KNN})$

- How to estimate $L(h_{KNN})$?
  - Use the empirical loss $\hat{L}(h_{KNN}, S) = \frac{1}{n}\sum_{i=1}^{n} \ell(h_{KNN}(X_i), Y_i)$
  - What is $\hat{L}(h_{1NN}, S)$?
  - In general, $\hat{L}(h_{KNN}, S)$ is an underestimate of $L(h_{KNN})$.

Validation



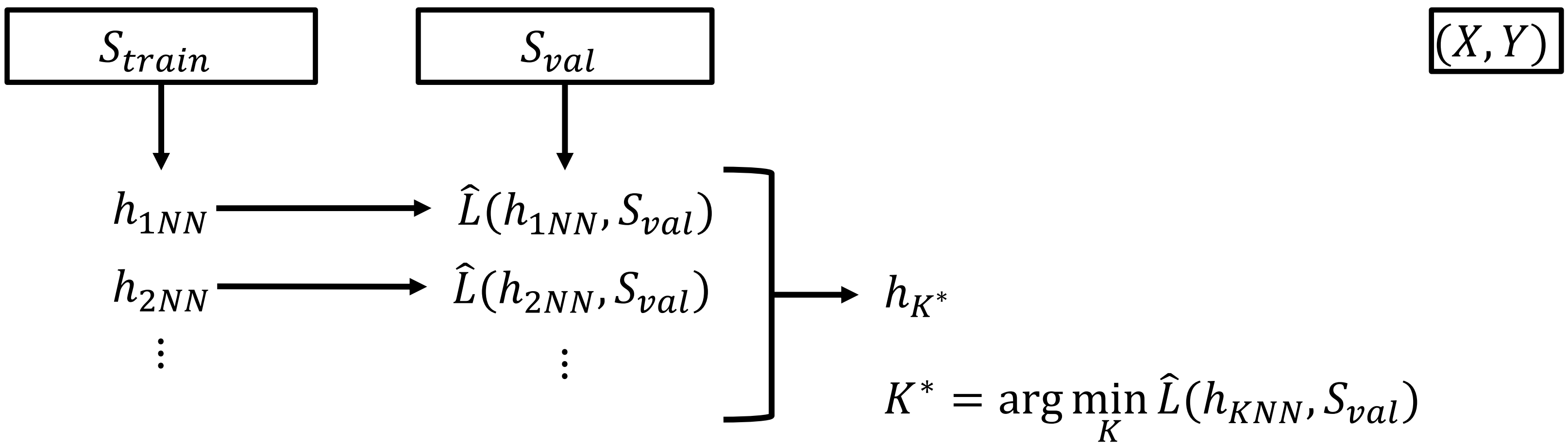
$\boxed{(X,Y)}$

$$\hat{L}(h_{KNNS_t}, S_{val}) = \frac{1}{m}\sum_{i=1}^{m} \ell(h_{KNNS_t}(X_i), Y_i)$$

- **Assumptions**
  - $\{(\boldsymbol{X_1}, \boldsymbol{Y_1}), \dots, (\boldsymbol{X_m}, \boldsymbol{Y_m})\}$ **are independent identically distributed (i.i.d.)**
  - **And come from the same distribution as new samples** $(\boldsymbol{X}, \boldsymbol{Y})$

- $\hat{L}(h_{KNNS_t}, S_{val})$ is an **unbiased** estimate of $L(h_{KNNS_t})$
  - $\mathbb{E}\left[\hat{L}(h_{KNNS_t}, S_{val})\right] = \mathbb{E}\left[\frac{1}{m}\sum_{i=1}^{m} \ell\left(h_{KNNS_t}(X_i), Y_i\right)\right] = \frac{1}{m}\sum_{i=1}^{m} \mathbb{E}[\,\ell\left(h_{KNNS_t}(X_i), Y_i\right)] = L\left(h_{KNNS_t}\right)$
  - From the perspective of h_{KNNS_t} the samples in S_{val} are indistinguishable from new samples (X, Y)

Selection of K

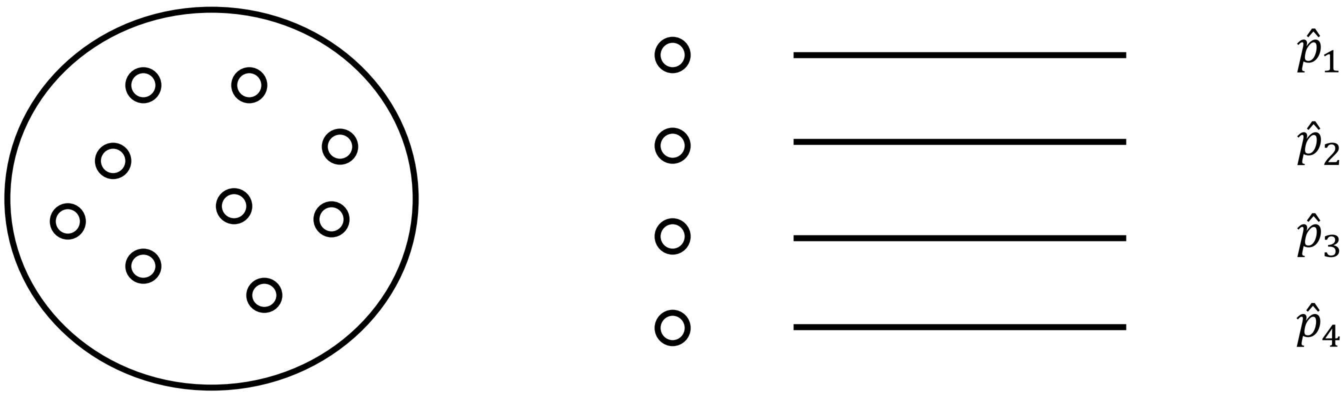


- **Selection introduces bias!**
  - Each $\hat{L}(h_{KNN}, S_{val})$ is an unbiased estimate of $L(h_{KNN})$
  - But $\hat{L}(h_{K^*NN}, S_{val})$ is a **biased** estimate of $L(h_{K^*NN})$!!!
    - From the perspective of h_{K^*NN} the samples in S_{val} are distinguishable from new samples (X,Y)
    - $\mathbb{E}[\ell(h_{K^*NN}(X_i), Y_i)] \neq \mathbb{E}[\ell(h_{K^*NN}(X), Y)]$

dependent!

in S_{val}

Illustration of Selection Bias



A bag of coins with bias p

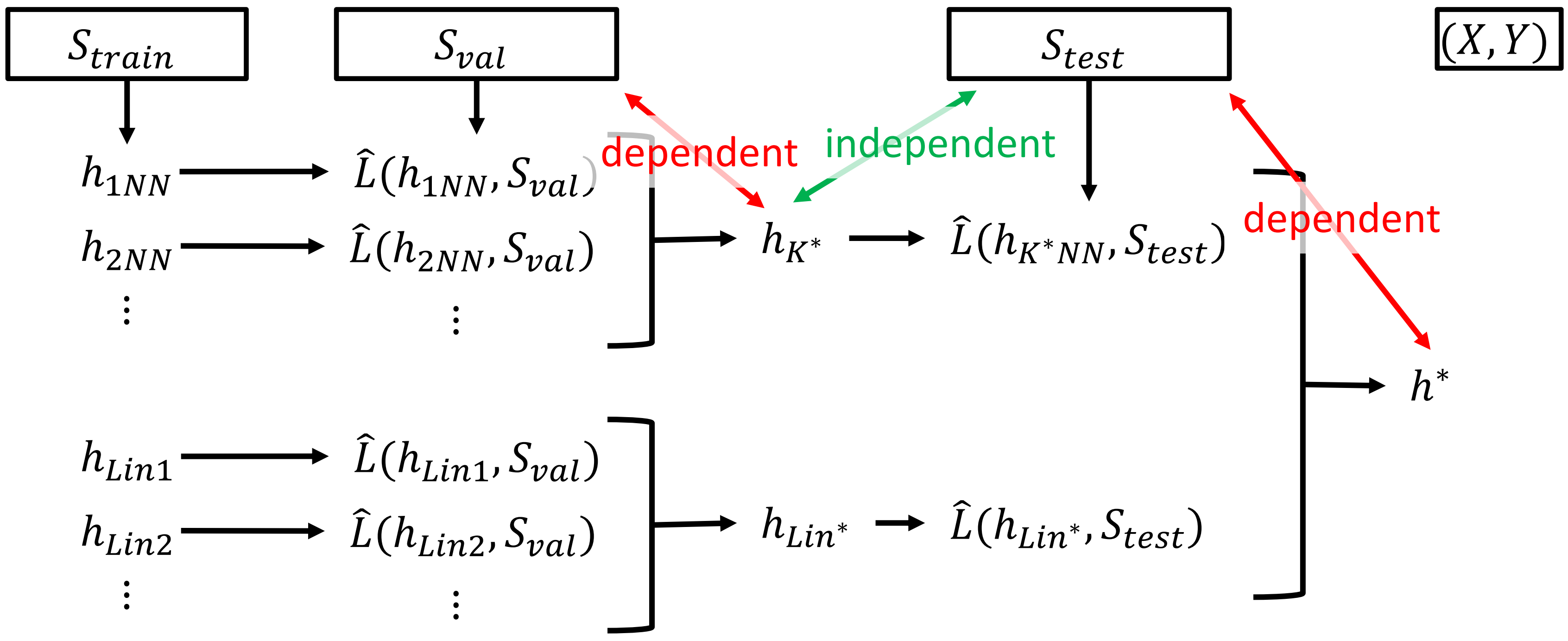
- $i^* = \arg\min_i \hat{p}_i$
- While each $\hat{p}_i$ is an unbiased estimate of p: $\mathbb{E}[\hat{p}_i] = p$
- $\hat{p}_{i^*}$ is a **biased** estimate of p: $\mathbb{E}[\hat{p}_{i^*}] \neq p$
- Outcome-based selection introduces bias!

So how can we estimate $L(h_{K^*NN})$?

$\boxed{S_{train}}$ $\quad$ $\boxed{S_{val}}$ $\quad$ $\boxed{(X,Y)}$

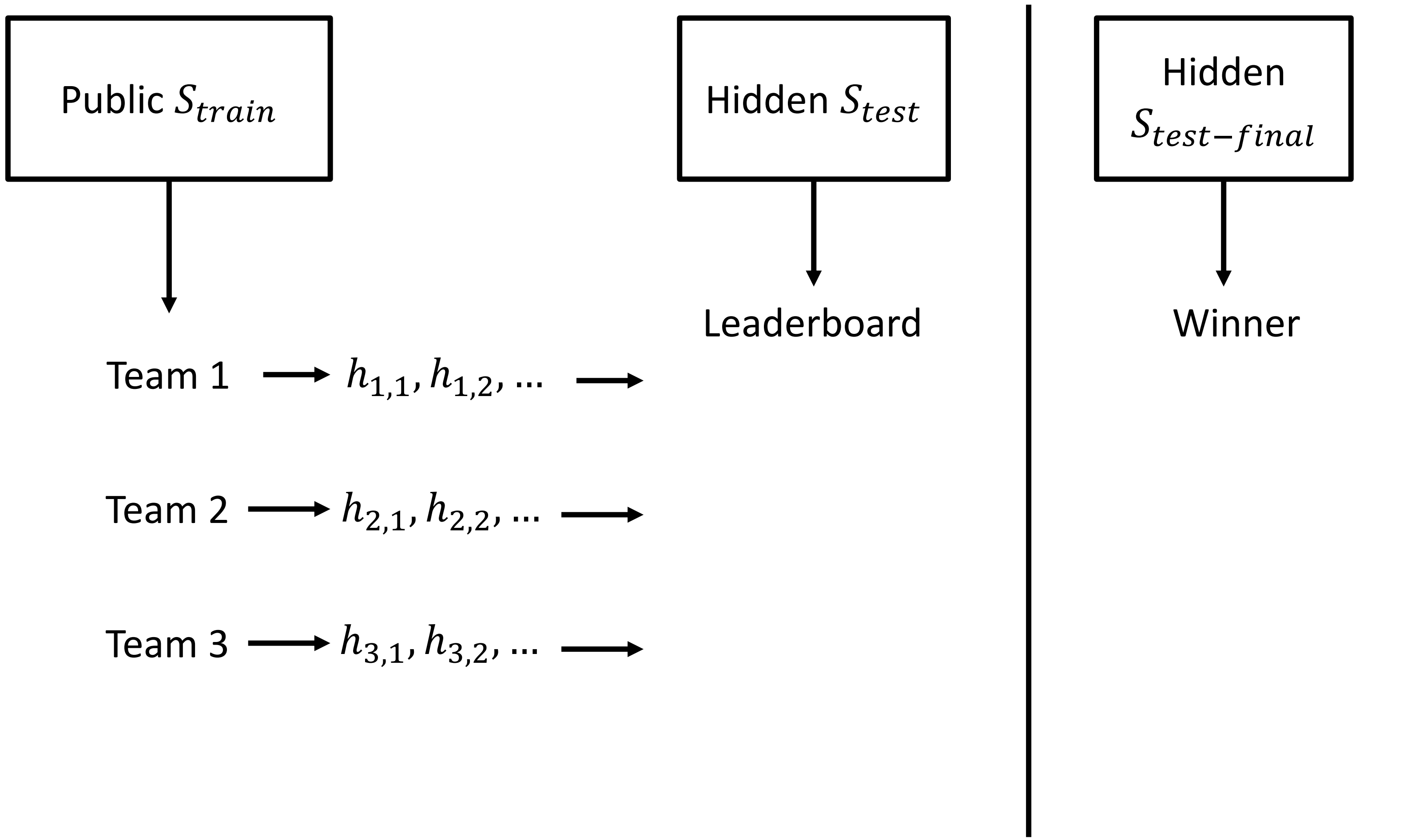
$$\left.\begin{array}{l} h_{1NN} \longrightarrow \hat{L}(h_{1NN}, S_{val}) \\ h_{2NN} \longrightarrow \hat{L}(h_{2NN}, S_{val}) \\ \quad\vdots \qquad\qquad\quad \vdots \end{array}\right] \longrightarrow h_{K^*}$$

Testing



- **It's not about how you call it; it's about how you use it!!!**
- $\hat{L}(h^*, S_{test})$ is a **biased** estimate of $L(h^*)$!

Respectable ML Competitions



Division of Responsibilities

- Evaluation/error measure $\ell(y', y)$ – domain knowledge

- Distance measure $d(x, x')$ – domain knowledge
  - But validation can be used to select a distance measure out of a set of candidates

- Selection of K and d – validation

- How to split the data (select m) – coming next

How to split the data into train/test/…?

- Consider the following extremes:

  - $m = 1$
    - $\hat{L}(h, S_{test}) \in \{0,1\}$, never approaches $L(h)$
  - $m = n - 1$
    - The training procedure only observes one label

- Do we need to reshuffle the data before splitting?
  - Theory: the data are assumed to be i.i.d., so it does not matter
  - Practice:
    - Yes, if the data are sorted by irrelevant parameter
    - No, if data order carries information relevant for testing, e.g., ordering by time

What can be said about $L(h)$ based on $\hat{L}(h, S_{val})$?

- $\hat{L}(h, S_{val})$ is an unbiased estimate of $L(h)$
- But consider the case $m = 1$:
  - $\hat{L}(h, S_{val}) \in \{0,1\}$ – never close to $L(h)$!

- Being unbiased is neither sufficient, nor necessary

- We need concentration!

Relation to “coin flips”

- $Z_i = \ell(h(X_i), Y_i) \in \{0,1\}$
  - Bernoulli random variable, “a coin flip”
- $\mathbb{E}[Z_i] = \mathbb{E}[\ell(h(X_i), Y_i)] = L(h) = p$
  - The bias of the coin
- $\hat{L}(h, S_{val}) = \frac{1}{m}\sum_i^m Z_i = \hat{p}_m$
  - An average of m “coin flips”
- How far can $\hat{p}_m$ be from p?