Introduction to Data Science - 1MS041

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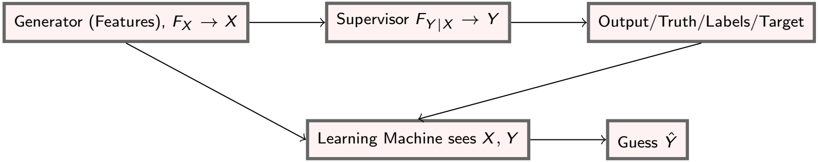
HT 2023

Supervised learning

Setup

1. The generator of the data G
2. The supervisor S
3. The learning machine LM.



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The pattern recognition problem

Minimize

$$R(\lambda) = \int L(y, g_\lambda(x)) dF(x, y) = \mathbb{E}[L(Y, g_\lambda(X))]$$

where $(X, Y) \sim F(x, y)$, where $g_\lambda \in \mathcal{M}$.

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Assume that $Z = ((X_1, Y_1), (X_2, Y_2), \ldots, (X_n, Y_n)) \overset{\text{IID}}{\sim} F(x, y)$ is a sequence of $\mathbb{R}^{m+1}$ valued random variables taking values in the data space $\mathbb{X} \times \mathbb{Y}$. We define the empirical risk for a function $g : \mathbb{X} \to \mathbb{Y}$ as

$$\hat{R}_n(g) = \hat{R}_n(Z; g) = \frac{1}{n} \sum_{i=1}^{n} L(Y_i, g(X_i)).$$

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Given a model space $\mathcal{M}$ we consider

$$\hat{g}_n^* := \hat{g}_n^*(Z) := \arg\min_{g \in \mathcal{M}} \hat{R}_n(g).$$

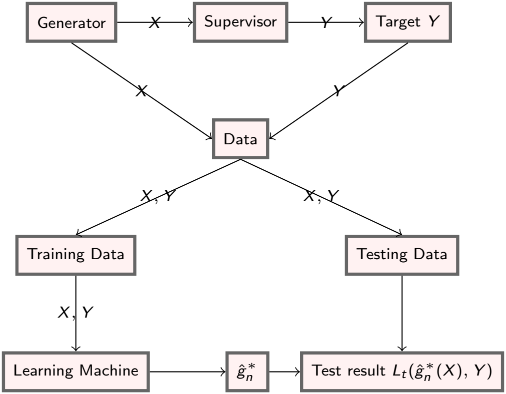
Trained model

The decision function

$$\hat{g}_n^* := \hat{g}_n^*(Z) := \arg\min_{g \in \mathcal{M}} \hat{R}_n(g)$$

is what we call the trained model.

Supervised learning



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$$\hat{g} = \arg\min_{\phi \in \mathcal{M}} \hat{R}_n(g)$$

- The empirical testing error is

$$\hat{R}_m(\hat{g}) = \frac{1}{m} \sum_{i=n+1}^{m} L(\hat{g}(X_i), Y_i)$$

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Our true testing error is

$$\mathbb{E}[L(\hat{g}(X), Y) \mid T_{rain}]$$

that is, given the training data T_{rain} we want the empirical test error to be an estimate of the true test error.

Point of view

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- Make a lot of assumptions about the data, and make guarantees before we fit our model. Think linear regression assuming everything is Gaussian.
- We make very little assumptions on data, fit our model and then test it. We want to design a test measurement that is well behaved no matter what (think bounded).

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- We think of the actual fitting procedure on the training data as a black box.
- This black box gives out a decision function, we say, OK lets test it.
- We perform a test on data that never went into the black box and want to give guarantees for the empirical test error!
- Thus we can just choose a different measurement than the loss.

Metrics

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- We are free to choose the underlying loss function L when testing.
- We can also consider conditional Risk.

Metrics

1. Consider the conditional risk

$$R_1(\lambda) = \mathbb{P}(Y = 1 \mid g_\lambda(X) = 1) = \mathbb{E}[\mathbb{1}_{Y=1} \mid g_\lambda(X) = 1]$$

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Guarantees

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Consider now the $0-1$ loss L, and let us be given a decision function g. Let us also assume that we have some i.i.d. testing data $T_{est} = \{(X_1, Y_1), \ldots, (X_m, Y_m)\}$.

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- $L(g(X_i), Y_i) \in \{0, 1\}$ is certainly a bounded random variable.
- Since $\{(X_1, Y_1), \dots, (X_m, Y_m)\}$ is an i.i.d. seqence, so is $L(g(X_1), Y_1), \dots, L(g(X_m), Y_m)$.

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- Denote $Z_i = L(g(X_i), Y_i)$, by using Hoeffdings inequality we thus get

$$\mathbb{P}(|\overline{Z}_m - \mathbb{E}[Z_1]| \geq \epsilon) \leq 2e^{-2m\epsilon^2}.$$

Confidence intervals

Then for $\alpha \in (0, 1)$ we have for $\delta = \frac{1}{\sqrt{m}}\sqrt{\frac{1}{2}\ln\left(\frac{2}{\alpha}\right)}$

$$\mathbb{P}(\overline{Z}_m - \delta \leq \mathbb{E}[Z_1] \leq \overline{Z}_m + \delta) \geq 1 - \alpha.$$

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- $\overline{Z}_n$ is thus our empirical risk.

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Define the conditional random variable $Z = Y \mid (g_\lambda(X) = 1)$, then we will get $Z_1, \ldots, Z_k$ coming from $(X_1, Y_1), \ldots, (X_m, Y_m)$ where k is the number of observations for which $g_\lambda(X_i) = 1$.

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- $Z_i \in \{0, 1\}$ so we can again use Hoeffding, but note, for $\alpha \in (0, 1)$ we have for $\delta = \frac{1}{\sqrt{k}}\sqrt{\frac{1}{2}\ln\left(\frac{2}{\alpha}\right)}$

$$\mathbb{P}(\overline{Z}_k - \delta \leq \mathbb{E}[Z_1] \leq \overline{Z}_k + \delta) \geq 1 - \alpha.$$