# Supervised Learning

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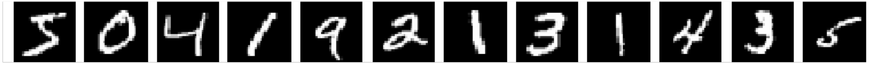
Introduction to Machine Learning

# Table of Contents

# Handwritten Digit Classification (MNIST)



our goal: assign the correct digit class to images

**5 0 4 1 9 2 1 3 1 4 3 5**

input $X$: 28x28 = 784 pixels with values between 0 (black) and 1 (white)

output $Y$: digit class 0, 1, . . ., 9

# Spam Detection with the Enron Dataset

**spam**

Subject: follow up
here ’ s a question i ’ ve been wanting to ask you , are you feeling down but too embarrassed to go to the doc to get your m / ed ’ s ?
here ’ s the answer , forget about your local p harm . acy and the long waits , visits and embarassments . . do it all in the privacy of your own home , right now . http : / / chopin . manilamana . com / p / test / duet it ’ s simply the best and most private way to obtain the stuff you need without all the red tape .

**ham**

Subject: darrin presto
amy :
please follow up as soon as possible with darrin presto regarding a real time interview . i forwarded his resume to you last week . he can be reached at 509 - 946 - 7879
thanks
greg

Our goal: classify new emails as spam or “ham“ (not spam).

input $X$: sequences of characters (emails), output $Y$: label spam or ham

# Wind Speed Prediction

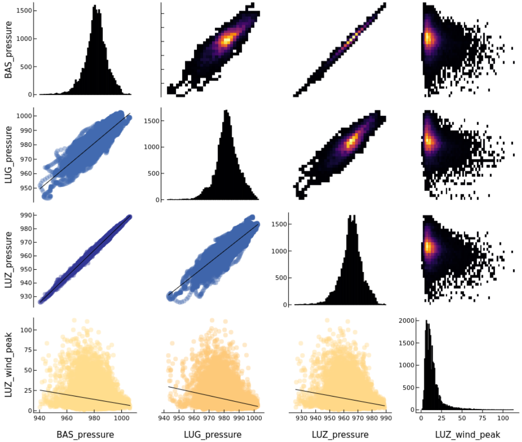
- SwissMeteo data: hourly measurements for 5 years from different stations (Bern, Basel, Luzern, Lugano, etc.).
- Our goal: given measurements at different stations, predict wind speed in Luzern 5 hours later.

# Wind Speed Prediction

| time | BAS_pressure | LUG_pressure | ... | LUZ_pressure | LUZ_wind_peak |
|---|---|---|---|---|---|
| $x_{11} = 2015010100$ | $x_{12} = 997.1$ | $x_{13} = 998.6$ | $\dots$ | $x_{1p} = 980.0$ | $y_1 = 13.0$ |
| $x_{21} = 2015010101$ | $x_{22} = 997.3$ | $x_{23} = 998.8$ | $\dots$ | $x_{2p} = 979.9$ | $y_2 = 6.8$ |
| $\vdots$ | $\vdots$ | $\vdots$ | $\ddots$ | $\vdots$ | |
| $x_{n1} = 2017123123$ | $x_{n2} = 972.7$ | $x_{n3} = 981.5$ | $\dots$ | $x_{np} = 957.5$ | $y_n = 11.9$ |

- $p$ **input** variables $X = (X_1, X_2, \dots, X_p)$
  e.g. $X_1$ `time`, $X_2$ `BAS_pressure`, $X_3$ `LUG_pressure`
  also called: **predictors, independent variables, features**
- **output** variable $Y$ e.g. `LUZ_wind_peak`
  also called: **response, dependent variable**
- $n$ **measurements** or **data points**

# Always Look at Raw Data!

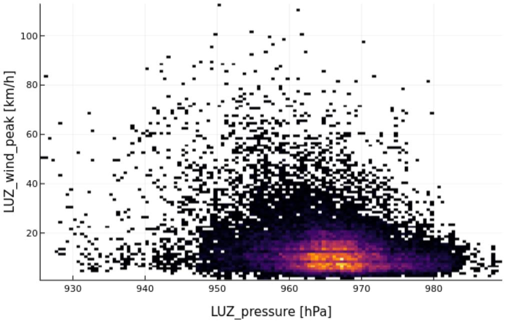



- **on diagonal**: 1D histogram
- **lower triangle**: scatter plot & trend line
- **upper triangle**: 2D histogram

## Observations

1. LUZ_wind_peak has a long tail.
2. For low pressures there are outliers of strong wind.
3. Pressure in Basel and Luzern is highly correlated.
4. ...

# Wind Speed Prediction




- The higher the pressure in Luzern, the less probable it is to have strong winds.
- There is no function `LUZ_wind_peak` = $f$(`LUZ_pressure`) that can describe this data; instead we use conditional probability densities $p$(`LUZ_wind_peak` | `LUZ_pressure`).

# Table of Contents

# Data Generating Processes

It is useful to think of our datasets as samples from **data generating processes** for the input X and the conditional output Y|X.

- **MNIST** X: people write digits $\rightarrow$ people take standardized photos thereof.
  Y|X: different people label the same photo X.
- **Spam** X: people write emails.
  Y|X: different people classify the same email X as spam or not.
- **Weather** X: the weather acts on sensors in weather stations.
  Y|X: the weather evolves from X and is measured again 5 hours later.

Using samples from these data generating processes, supervised learning aims at learning something about the conditional processes, i.e how Y depends on X.

# Where Does Noise Come From?

For most data generating processes we **cannot measure all factors** that determine the outcome.

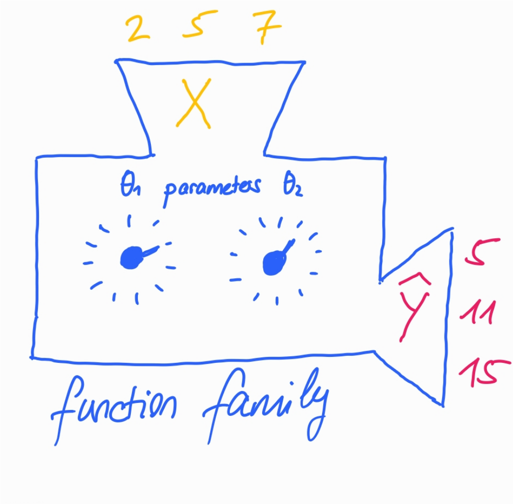
$\Rightarrow$ **same values of the measured factors can cause different outcomes.**

- **MNIST** Different persons may label the same handwritten digit differently.
- **Spam** What is spam for somebody, may not be spam for someone else.
- **Weather** Even when all considered weather stations measure exactly the same values at time $t_1$ and $t_2$, the full state of the weather at $t_1$ differs most likely from the one at $t_2$.

In machine learning we treat the effect of unmeasured factors as noise with certain probability distributions.

# Table of Contents

# How Does Supervised Learning Work?




**Function Family**

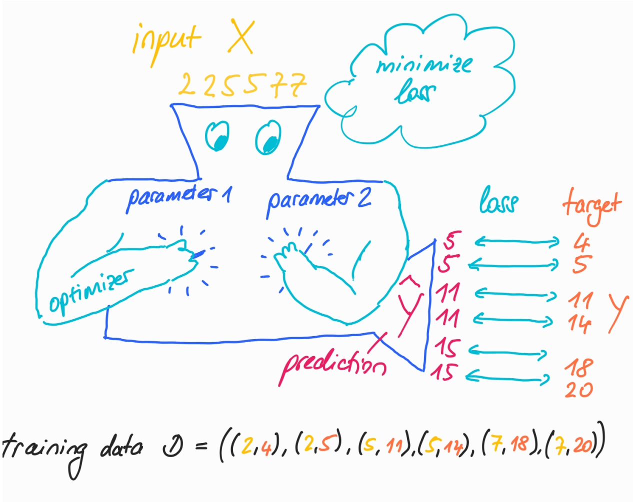
- We change the parameters.
- The machine computes $\hat{y}$ given parameters $\theta$ and $x$.

For example

$$\hat{y} = f_\theta(x) = \theta_0 + \theta_1 x$$

When we change the parameters $\theta_0$ and $\theta_1$, we change the way $\hat{y}$ depends on $x$.

# How Does Supervised Learning Work?




**Loss Minimizing Machine**

- We specify
  1. the training data
  2. the function family (model)
  3. the loss function $L(y, \hat{y})$
  4. the optimizer
- The machine changes the parameters with the help of the optimizer until the loss is minimal.

For example: linear regression

# Training Loss and Test Loss

- **Training Set** $\mathcal{D}$: Data used by the machine to tune the parameters.
- **Training Loss of Function** $f$: $\mathcal{L}(f, \mathcal{D}) = \frac{1}{n} \sum_{i=1}^{n} L(y_i, f(x_i))$
- **Test Loss of Function** $f$ **at** $x$ **for a Conditional Data Generating Process**: $\mathrm{E}_{Y|x}\left[L(Y, f(x))\right]$ = expected loss under the conditional generating process.
- **Test Loss of Function** $f$ **for a Joint Data Generating Process**: $\mathrm{E}_{X,Y}\left[L(Y, f(X))\right]$ = expected loss under the joint generating process.
- **Test Set** $\mathcal{D}_{\text{test}}$: Data from the same generating process as the training set, not used for parameter tuning.
- **Test Loss of Function** $f$ **for a Test Set** $\mathcal{D}_{\text{test}}$: $\mathcal{L}(f, \mathcal{D}_{\text{test}})$ = same computation as for the training loss but for a test set.

# Blackboard: Linear Regression as a Loss Minimizing Machine

**Data Generating Process**

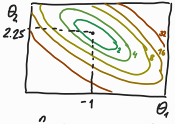
$$y = 2x - 1 + \varepsilon \,, \quad E[\varepsilon] = 0 \quad Var[\varepsilon] = \sigma^2$$

**Training Data**

$$\big((x_1 = 0, y_1 = -1), (x_2 = 2, y_2 = 4), (x_3 = 2, y_3 = 3)\big)$$

**Function Family**

$$\hat{y} = \theta_0 + \theta_1 \cdot x$$




**Loss Function**

$$L(\theta) = L(\theta_1, \theta_2) = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \frac{1}{n} \sum_{i=1}^{n} (y_i - \theta_0 - \theta_1 x_i)^2$$

$$= \frac{1}{3} \Big( (-1 - \theta_0)^2 + (4 - \theta_0 - 2\theta_1)^2 + (3 - \theta_0 - 2\theta_1)^2 \Big)$$

**Optimizer**: Default

**Solution**: $\hat{\theta}_0 = -1 \,, \hat{\theta}_1 = 2.25 \,, \quad L(\hat{\theta}) = \frac{2}{3} \cdot 0.5^2$

**Test Loss at $x_0$**:

$$E\Big[\big(\underbrace{2x_0 - \cancel{1} + \varepsilon}_{y} \underbrace{+ \cancel{1} - 2.25x_0}_{-\hat{y}}\big)^2\Big] = (0.25x_0)^2 + \sigma^2$$

**Test Data**:

$$\big((x_1 = 1, y_1 = 0), (x_2 = 2, y_2 = 3), (x_3 = 3, y_3 = 5), (x_4 = 0, y_4 = -1)\big)$$

$$\Rightarrow \text{(Empirical) Test Loss} = \frac{1}{4}\left(0.25^2 + 0.5^2 + 0.75^2 + 0^2\right)$$

# Quiz

Suppose we have training data $\mathcal{D} = ((0,1),(2,9))$ and test data $\mathcal{D}_{\text{test}} = ((0,0),(3,20))$, define a function family $f(x) = \theta_0 + \theta_1 x^2$ and loss function $L(y,\hat{y}) = |y - \hat{y}|$.

Correct or wrong?

1. The training loss is minimal for $\hat{\theta}_0 = 1$ and $\hat{\theta}_1 = 2$.
2. The test loss of $f(x) = 1 + 2x^2$ at $x = 0$ for the conditional data generating process is 1.
3. The test loss of $f(x) = 1 + 2x^2$ for the test set is 1.

# Supervised Learning with MLJ: Linear Regression

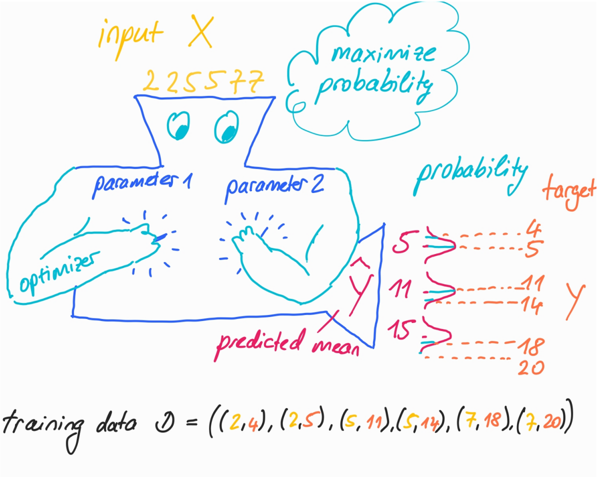
```
model = LinearRegressor()     # function family, loss function and optimizer
mach = machine(model, X, y)  # training data with input X and output y
fit!(mach)                    # fit the machine
fitted_params(mach)           # inspect the fitted parameters
ŷ = predict(mach)             # make predictions on the training data
ŷtest = predict(mach, Xtest) # make predictions on the test data
```

# Which Loss Functions Should We Use?

- Is the mean squared error always a good loss?
- What kind of loss would be good in a classification setting (e.g. MNIST)?
- How should we choose the loss when we know something about the noise distribution?

All these questions have a straight-forward answer, if we use a **family of probability distributions** (instead of a family of functions) and estimate the parameters with a **maximum likelihood approach** (instead of minimizing a hand-picked loss).

# How Does Supervised Learning Work?




**Likelihood Maximizing Machine**

- We specify
  1. the training data
  2. the family of probability distributions (model)
  3. the optimizer
- The machine changes the parameters with the help of the optimizer until the likelihood of the parameters is maximal.

For example: linear regression

# The Likelihood Function

For a family of conditional probability distributions $P(y|x,\theta)$ and training data $\mathcal{D} = ((x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n))$ the **likelihood function** is defined as

$$\ell(\theta) = \prod_{i=1}^{n} P(y_i|x_i,\theta)\,.$$

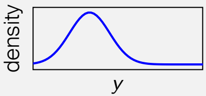
This is the probability of all the responses $y_i$ given all the inputs $x_i$ for a given value of the parameters $\theta$.

In practice it is usually more convenient to work with the **log-likelihood function**

$$\log \ell(\theta) = \sum_{i=1}^{n} \log P(y_i|x_i,\theta)$$

# The Normal, Bernoulli and Categorical Distribution

## Normal




$$p(y|x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(y-f(x))^2}{2\sigma^2}}$$

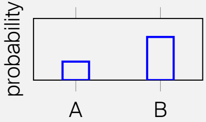
$f(x)$: a number

mean: $f(x)$

variance: $\sigma^2$

mode: $f(x)$

## Bernoulli




$$p(\mathrm{A}|x) = p_\mathrm{A} = \sigma(f(x))$$

$f(x)$: a number

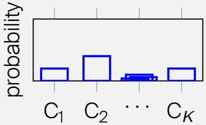
sigmoid/logistic function

$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

$$p(\mathrm{B}|x) = 1 - p_\mathrm{A} = \sigma(-f(x))$$

mode: A if $p_\mathrm{A} > p_\mathrm{B}$

## Categorical




$$p(\mathrm{C}_i|x) = p_{\mathrm{C}_i} = s(f(x))_i$$

$f(x)$: a vector of $K$ numbers

softmax function

$$s(x)_i = \frac{e^{x_i}}{\sum_{j=1}^{K} e^{x_j}}$$

mode: X with largest $p_\mathrm{X}$.

# Blackboard: The Normal, Bernoulli and Categorical Distribution

## Normal

$f(x) = 1 \,,\; \sigma = 2$

$$Pr(y \in [-0.05, 0.05]) \approx 0.1 \cdot \frac{1}{\sqrt{2\pi} \cdot 2} e^{-\frac{(0-1)^2}{2 \cdot 2^2}} \approx 0.017$$

## Bernoulli

$f(x) = 3$

$$Pr(y = A) = \frac{1}{1+e^{-3}} \approx 0.95$$

$$Pr(y = B) \approx \frac{1}{1+e^{3}} \approx 0.05$$

## Categorical

$$f(x) = \begin{pmatrix} 3 \\ -2 \\ 1 \\ 0 \end{pmatrix}$$

$$Pr(y = A) = \frac{e^3}{e^3 + e^{-2} + e^1 + e^0} \approx 0.84$$

$$Pr(y = D) = \frac{e^0}{e^3 + e^{-2} + e^1 + e^0} \approx 0.04$$

# Blackboard: Maximum Likelihood Estimation

Data Generating Process

$P(y = A \mid x) = \text{Bernoulli}(2x - 1)$

$y = A$ if $\sigma(2x - 1) > \varepsilon$, $\varepsilon \sim \text{Uniform}([0,1])$

Training Data

$((x_1 = 0, y_1 = B), (x_2 = 2, y_2 = A), (x_3 = 3, y_3 = B))$

Family of Distributions

$P(y = A \mid x, \theta) = \sigma(\theta_0 + \theta_1 x)$

Log-Likelihood Function

$$\log \ell(\theta) = \log \ell(\theta_0, \theta_1) = \sum_{i=1}^{n} \log P(y_i \mid x_i, \theta)$$

$$= \log \sigma(-\theta_0) + \log \sigma(\theta_0 + 2\theta_1) + \log \sigma(-\theta_0 - 3\theta_1)$$

Optimizer : Default

Solution : $\hat{\theta}_0 \approx -1.3$ $\hat{\theta}_1 \approx 0.3$ $\log \ell(\hat{\theta}) \approx -1.9$

Test Log-Likelihood at $x_0$ : $E[\log P(Y \mid x_0)]$

$$\underbrace{\sigma(2x_0 - 1)}_{P(Y=A \mid x_0)} \cdot \log \underbrace{\sigma(0.3x_0 - 1.3)}_{P(Y=A \mid x_0, \hat{\theta})} + \underbrace{\sigma(-2x_0 + 1)}_{P(Y=B \mid x_0)} \log \underbrace{\sigma(-0.3x_0 + 1.3)}_{P(Y=B \mid x_0, \hat{\theta})}$$

# Supervised Learning with MLJ: Linear Classification

```
model = LogisticClassifier() # distribution family and optimizer
mach = machine(model, X, y)  # training data with input X and output y
fit!(mach)                   # fit the machine
fitted_params(mach)          # inspect the fitted parameters
p̂  = predict(mach)            # predicted probabilities on the training data
p̂ ₐ = pdf.(p̂ , "A")           # predicted probabilities of class "A"
ŷ = predict_mode(mach)       # class with highest predicted probability
```

# Nomenclature

For some models (families of probability distributions) with linear function $f(x)$ we see occasionally specific names for the likelihood maximizing machine.

- Gaussian (normal distribution): Linear Regression
- Bernoulli: Logistic Regression or Linear Binary Classification
- Categorical: Multinomial Logistic Regression or Multiclass Linear Regression (or Classification)
- Poisson: Poisson Regression

Later we will see that there are natural generalizations for all these models with non-linear $f(x)$, where $f(x)$ is for example given by a neural network.

# Summary

We use a training set to find a conditional distribution that captures some regularities of the conditional data generation process. The goal is to find a conditional distribution that minimizes the test loss of the joint data generation process. With a test set we can assess how close we are at reaching this goal.

| Supervised Learning as Loss Minimization | Supervised Learning as Likelihood Maximization |
|---|---|
| We provide<br>1. training data<br>2. function family<br>3. loss function<br>4. optimizer | We provide<br>1. training data<br>2. probability distribution family<br>3. optimizer<br>The negative log-likelihood function of the parameters implicitly defines a loss function. |
| It is not (always) obvious what kind of loss function to take for classification problems or regression problems with a specific noise distributions | We take the binomial for binary classification problems and the categorical for other classification problems. Regression with other noise distribution is also possible. |

# Suggested Reading

The following chapters from "An Introduction to Statistical Learning" (second edition, `https://www.statlearning.com`) are complementary to the material presented in this lecture. It is not mandatory to read them, but maybe it helps to better understand the material of this lecture.

- 3.1 Simple Linear Regression
- 4.1 An Overview of Classification
- 4.2 Why Not Linear Regression?
- 4.3 Logistic Regression