Probabilistic view

Machine Learning and Data Mining, 2021

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Why probability?

- Machine learning often deals with random quantities
- Sources of uncertainty:
  - Inherent stochasticity of the system being modelled
  - Lack of information
  - Incomplete modelling (discarding information for the sake of simplicity, computability, etc.)

Probability recap

Probability

- Frequentist:
  - **relative frequency** of occurrence of an experiment's outcome, when repeating the experiment

Example: coin toss

Toss a coin N times (H – number of ‘heads’, T – number of ‘tails’)
Probability:

$$P('\text{heads}') = \lim_{N \to +\infty} \frac{H}{N}$$

$$P('\text{tails}') = \lim_{N \to +\infty} \frac{T}{N} = 1 - P('\text{heads}')$$

Probability

- Frequentist:
  - **relative frequency** of occurrence of an experiment's outcome, when repeating the experiment
- Bayesian:
  - **degree of belief**

Example: doctor analyzes a patient and says that the patient has 40% probability of having the flu (we can’t “repeat” this patient)

Random variable

- A variable that can take values randomly
- Can think of it as variable enumerating possible outcomes of a random event
  - E.g., for the coin toss:

$$x = \begin{cases} 0, & 'heads' \\ 1, & 'tails' \end{cases}$$

take

Random variable

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  - E.g., for the coin toss:

$$\mathrm{x} = \begin{cases} 0, & '\mathrm{heads}' \\ 1, & '\mathrm{tails}' \end{cases}$$

  - A bit more complex example – number of coin tosses with ‘heads’ out of N tosses total:

$$\mathrm{n} = n \in \{0, \ldots, N\}$$

random variable

possible value it may take

Probability mass function (PMF)

- Defined for discrete variables
- Equals to probability for the variable x to take a given value x:

$$P(\mathrm{x} = x)$$

- or just $P(x)$ – omitting the name of the variable
- Joint probability distribution – probability for several random variables to take some particular values simultaneously:

$$P\left(\mathrm{x} = x, \mathrm{y} = y\right) \equiv P(x,\ y)$$

- PMF must:
  - be defined on all possible states of the variable
  - take values in the $[0, 1]$ interval
  - sum to 1 over all possible outcomes (probability for anything to happen)

Probability density function (PDF)

- Defined for continuous variables
- Equals to:

$$p(x) = \lim_{\delta x \to 0} P\big(\mathrm{x} \in (x, x + \delta x)\big)/\delta x$$

- PDF must:
  - be defined on all possible states of the variable
  - be ≥ 0 (can be higher than 1 though)
  - integrate to 1 over all possible outcomes (probability for anything to happen):

$$\int_{\mathrm{X}} p(x)dx = 1$$

Expectation and variance

- Expectation:

For a discrete variable

$$\mathbb{E}[\mathrm{x}] = \sum_{\mathrm{X}} xP(x)$$

For a continuous variable

$$\mathbb{E}[\mathrm{x}] = \int_{X} xp(x)dx$$

  – Meaning: **average outcome**

- Variance:

$$\mathrm{Var}[x] = \mathbb{E}\left[(\mathrm{x} - \mathbb{E}[x])^2\right] = \mathbb{E}\left[x^2\right] - (\mathbb{E}[x])^2$$

  – Meaning: **spread of the outcomes**

Some distributions

- Uniform[a, b]:

$$p(x) = \frac{1}{b-a} = const$$

- Binomial:

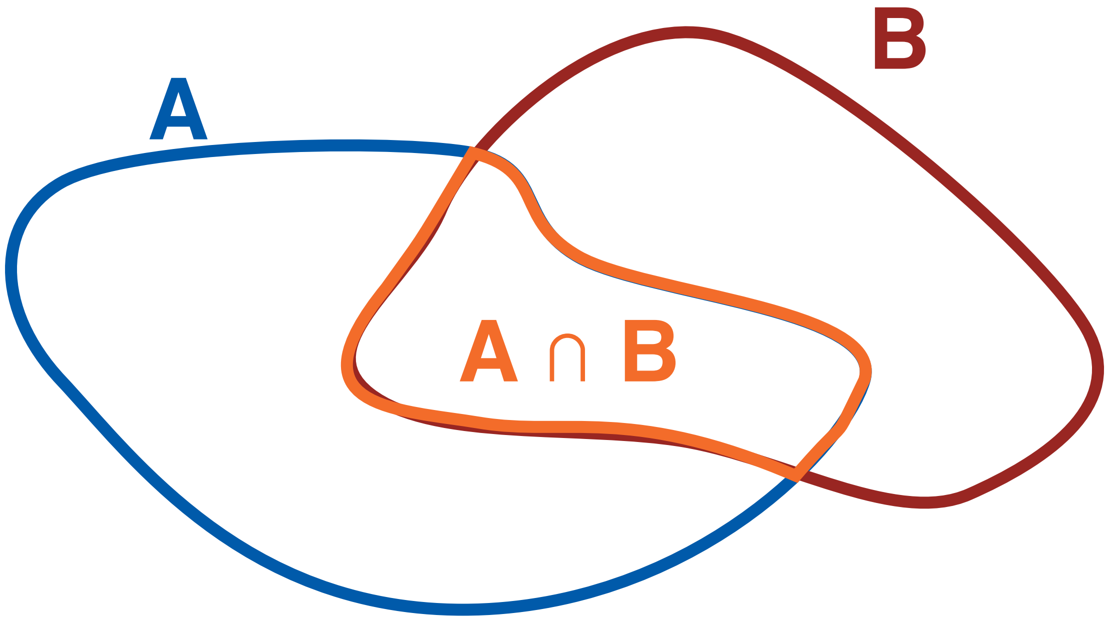
$$P(k) = \frac{n!}{k!(n-k)!} p^k (1-p)^{n-k}$$

- Normal distribution:

$$p(x) \equiv \mathcal{N}\left(x \,\middle|\, \mu, \sigma^2\right) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

Conditional probability

$$P(A \mid B) = \frac{P(A \cap B)}{P(B)}$$



For PDF: $$p\left(x \mid y\right) = \frac{p\left(x, y\right)}{p\left(y\right)}$$

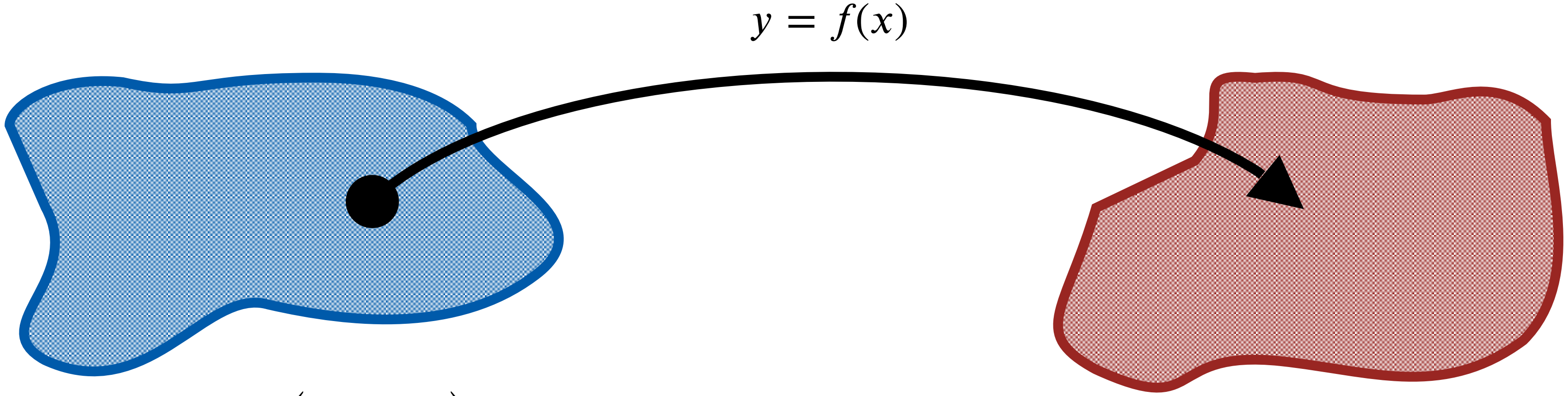
– i.e. we're renormalizing $p(x, y)$ as a distribution of only x for some fixed y

Probabilistic view on supervised learning

Problem setup

$\mathscr{X}$ – a set of objects

$\mathscr{Y}$ – a set of targets



A dataset: $D = \{ \left(x_i, \ y_i \right) : i = 1, \ 2, \dots, \ N \}$

$$x_i \in \mathscr{X}, \ \ y_i = f(x_i) \in \mathscr{Y}$$

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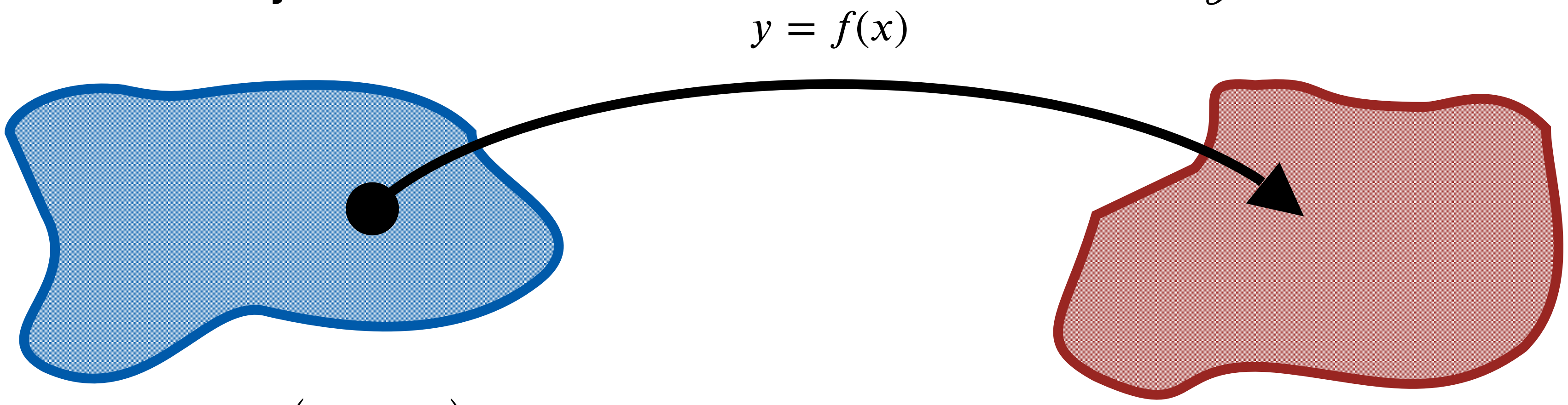

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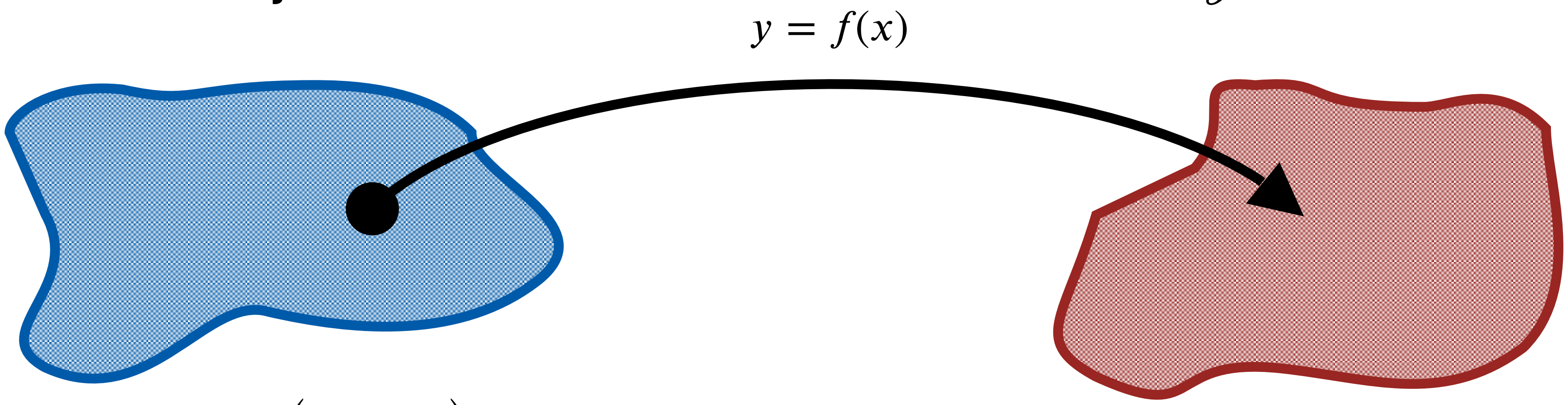

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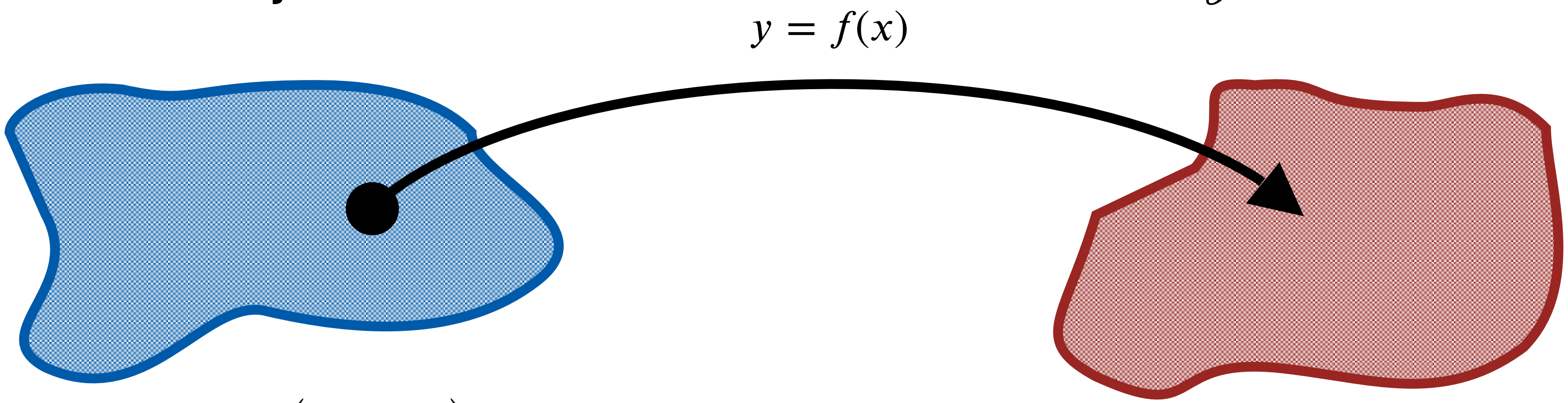

A dataset: $D = \{(x_i,\ y_i) : i = 1,\ 2, \ldots,\ N\}$

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– There's some **underlying probability distribution** $p(x,\ y)$

– $(x_i,\ y_i)$ are drawn from $p(x,\ y)$, **independently** for each i

– Can also say that for a given x_i, the target y_i is drawn from $p(y \quad x)$

Deterministic and stochastic components

- With this view, we can separate deterministic and stochastic parts of the true mapping:

$$y \;\; x = f(x) + \varepsilon(x)$$

Deterministic part (expectation)

$$f(x) = \mathbb{E}\left[y \;\; x\right] \equiv \int y \cdot p\left(y \middle| x\right) dy$$

Random part (noise)

$$\varepsilon(x) = y \;\; x - \mathbb{E}\left[y \;\; x\right]$$

Probabilistic model

Let's make an assumption about data:

$$y \quad x = f(x) + \varepsilon$$

Assume that **label noise** is **normally distributed:**

$$\varepsilon \sim \mathcal{N}\left(0, \sigma_\varepsilon^2\right)$$

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We want our model $\hat{f}_\theta(x)$ to fit the true dependence $f(x)$, i.e. we **define a probabilistic model**:

$$y \quad x \sim \mathcal{N}\left(\hat{f}_\theta(x),\ \sigma_\varepsilon^2\right)$$

Probabilistic model

Our model can be fitted with the **maximum likelihood** approach:

$$L = \prod_{i=1\ldots N} \mathcal{N}\left(y_i \,\middle|\, \hat{f}_\theta(x_i),\ \sigma_\varepsilon^2\right) \to \max_\theta$$

"The observed data is most probable"

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Max. likelihood = min. negative log likelihood

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$$= C \cdot \sum_{i=1\dots N} \left(y_i - \hat{f}_\theta(x_i)\right)^2 + const \to \min_\theta$$

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MSE loss $\iff$ Prob. model with normal label noise!

Summary

- Machine Learning often deals with **randomness** (intrinsic, lack of information, incomplete modelling)
- Supervised learning problems can be posed in the probabilistic context
- The mapping between features and labels can be decomposed into **deterministic** and **stochastic** parts
- There's a **probabilistic model** behind the loss function

- Food for thought: what probabilistic model would correspond to minimizing MAE loss: $\frac{1}{N}\sum_i \left| y_i - \hat{f}(x_i) \right|$?