

Bayesian Machine Learning

May 2024 - François HU https://curiousml.github.io/

Outline

Bayesian statistics

- Bayesian statistics and probabilistic model
- Analytical inference
- Conjugate priors

2 Latent Variable Models





5 Extensions and oral presentations

PREREQUISITE

THEORY

- 1. Notions of **probability & statistics**
- 2. Statistical Learning : supervised & unsupervised learning
- 3. Information theory : Entropy, KL-divergence, ...

APPLICATION

Python

ALGORITHM

Some « classical » supervised & unsupervised models









Gentle introduction to statistical learning

Simplified statistical learning process





Simplified statistical learning process





Simplified statistical learning process



















Aim during training phase : find θ such that $\forall (x, y) \in \mathcal{X} \times \mathcal{Y}, h_{\theta}(x) \approx y$

Usually in frequentist statistics we use the MLE : Maximum Likelihood Estimation $\hat{\theta}_{MLE} = \arg \max P(X | \theta)$ θ



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Example : Linear regression example (proof later in the course if needed)

θ



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- Cannot start with a « belief » hence not practical nor flexible
- Cannot express uncertainty of estimated model parameters and predictions _



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$$\mathcal{L} \times \mathcal{Y}, h_{\theta}(x) \approx y$$

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Aim during training phase : find θ such that $\forall (x, y) \in \mathcal{X} \times \mathcal{Y}, h_{\theta}(x) \approx y$

Problems :

- Only works well if we solve big data : $|X| \gg |\theta|$
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Usually in frequentist statistics we use the MLE : Maximum Likelihood Estimation $\hat{\theta}_{MLE} = \arg \max P(X | \theta)$

Why Bayesian methods ?

Examples of application of Bayesian Machine Learning



Supervised machine learning

Unsupervised machine learning

Others

Medical diagnosis

Patterns in customer dataset **Bayesian Non parametric Clustering (BNC)**

Reconstructing images from noisy images **Bayes theorem + MCMC**

Optimal character recognition (OCR)

Why Bayesian methods ?

Examples of application of Bayesian Machine Learning



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Why Bayesian methods ?

Examples of application of Bayesian Machine Learning



Supervised machine learning

Unsupervised machine learning

Others using more advanced techniques

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Probability

Relative **frequency** of an event in an infinite trials



Probability

Relative **frequency** of an event in an infinite trials



Random variable **Discrete** variable **Probability Mass Function** (PMF) 0.35 0.3 $P(X) = \begin{cases} 0.1 & \text{if } X = 1 \\ 0.3 & \text{if } X = 2 \\ 0.25 & \text{if } X = 3 \end{cases}$ 0.25 0.1 2 3 4 1 **Continuous** variable **Probability Density function** (PDF) $P(X \in [a, b]) = \int p(s)ds$ a b

Probability

Relative **frequency** of an event in an infinite trials







Probability

Relative **frequency** of an event in an infinite trials



Independence

Two random variables X and Y are **independent** if

$$P(X, Y) = P(X)P(Y)$$

joint probability

marginals

dependency : one dice

$$P([\bullet\bullet], \bullet\bullet]) = 0 \neq P([\bullet\bullet])P([\bullet\bullet]) = 1/6^2$$

independency : two dices

 $P([\bullet\bullet], [\bullet\bullet]) = P([\bullet\bullet])P([\bullet\bullet]) = 1/6^2$





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 $P([\bullet\bullet], [\bullet\bullet]) = P([\bullet\bullet])P([\bullet\bullet]) = 1/6^2$







 $P(X) = \cdots$



Conditional probability

probability of X given that Y happened

$$P(X \mid Y) = \frac{P(X, Y)}{P(Y)} \frac{\begin{array}{l} \text{Joint} \\ \text{probability} \end{array}}{\begin{array}{l} \text{Marginal} \end{array}}$$

Chain rule

 $P(X_1, X_2) = P(X_1 | X_2) \times P(X_2)$

$$P(X_1, X_2, X_3) = \cdots$$

 $P(X_1,\ldots,X_n)=\cdots$

Sum rule

discrete

 $P(X) = \cdots$

continuous

 $P(X) = \cdots$



Conditional probability

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$$P(X \mid Y) = \frac{P(X, Y)}{P(Y)} \frac{\text{Joint}}{\text{probability}}$$

Conditional Marginal

Chain rule

 $P(X_1, X_2) = P(X_1 | X_2) \times P(X_2)$ $P(X_1, X_2, X_3) = P(X_1 | X_2, X_3) \times P(X_2 | X_3) \times P(X_3)$ $P(X_1, \dots, X_n) = \cdots$

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Chain rule

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$$P(X_1, X_2, X_3) = P(X_1 | X_2, X_3) \times P(X_2 | X_3) \times P(X_3)$$

$$P(X_1, \dots, X_n) = \prod_{k=1,\dots,n} P(X_k | X_1, \dots, X_{k-1})$$

Sum rule

discrete

continuous

 $P(X) = \cdots$ $P(X) = \cdots$



Conditional probability

probability of X given that Y happened

$$P(X \mid Y) = \frac{P(X, Y)}{P(Y)} \frac{\text{Joint}}{\text{probability}}$$

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$$P(X_1, \dots, X_n) = \prod_{k=1,\dots,n} P(X_k | X_1, \dots, X_{k-1})$$

Sum rule

discrete continuous $P(X) = \sum_{Y \in \mathscr{Y}} P(X, Y) \qquad P(X) = \cdots$



Conditional probability

probability of X given that Y happened

$$P(X \mid Y) = \frac{P(X, Y)}{P(Y)} \frac{\text{Joint}}{\text{probability}}$$

Conditional Marginal

Chain rule

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Sum rule

discrete continuous

$$P(X) = \sum_{Y \in \mathscr{Y}} P(X, Y)$$
 $P(X) = \int_{Y \in \mathscr{Y}} P(X, Y) \cdot dY$



Conditional probability

probability of X given that Y happened

$$P(X \mid Y) = \frac{P(X, Y)}{P(Y)} \frac{\text{Joint}}{\text{probability}}$$

Conditional Marginal

Chain rule

$$P(X_1, X_2) = P(X_1 | X_2) \times P(X_2)$$

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Bayes theorem

Parameters

X Data



1. Introduction to bayesian statistics Frequentist VS Bayesian point of view



find θ such that $\forall (x, y) \in \mathcal{X} \times \mathcal{Y}, h_{\theta}(x) \approx y$


Frequentist VS Bayesian point of view



Frequentist VS Bayesian point of view



1. Introduction to bayesian statistics Frequentist VS Bayesian point of view







1. Introduction to bayesian statistics Frequentist VS Bayesian point of view



Problems in frequentist estimation :

- Only works well if we have big data : $|X| \gg |\theta|$
- Cannot start with a « belief » hence not practical nor flexible
- Cannot express uncertainty of estimated model parameters and predictions





1. Introduction to bayesian statistics Frequentist VS Bayesian point of view



Problems in frequentist estimation :

- Only works well if we have big data : $|X| \gg |\theta|$
- Cannot start with a « belief » hence not practical nor flexible
- **Cannot express uncertainty of estimated model parameters and predictions**

Bayes theorem

 $P(\theta | X) = \frac{P(X | \theta) \times P(\theta)}{P(X)}$



1. Introduction to bayesian statistics Bayesian point of view : classification





 $P(\theta | X_{train}, y_{train}) = \frac{P(y_{train} | X_{train}, \theta) \times P(\theta)}{P(y_{train} | X_{train})}$



1. Introduction to bayesian statistics Bayesian point of view : training





 $P(\theta | X_{train}, y_{train}) = \frac{P(y_{train} | X_{train}, \theta) \times P(\theta)}{P(y_{train} | X_{train})}$



Can regularize your model when training on your data



1. Introduction to bayesian statistics **Bayesian point of view : inference**





Can regularize your model when training on your data



1. Introduction to bayesian statistics Bayesian point of view : online learning





Can regularize your model when training on your data





Probabilistic graphical models : analysis using diagrammatic representations of probability distributions

Probabilistic graphical models : analysis using diagrammatic representations of probability distributions

Nodes : random variables
 Links : probabilistic relationships

Probabilistic graphical models : analysis using diagrammatic representations of probability distributions

Bayesian networks (Directed graphical models) Nodes : random variables
 Links : probabilistic relationships

Probabilistic graphical models : analysis using diagrammatic representations of probability distributions



Bayesian networks (Directed graphical models) Markov random fields (Undirected graphical models)



Probabilistic graphical models : analysis using diagrammatic representations of probability distributions

Bayesian networks (Directed graphical models)

The focus of our course !

Markov random fields (Undirected graphical models)



2. Probabilistic Graphical Model (PGM)

Probabilistic graphical models : analysis using diagrammatic representations of probability distributions

Bayesian networks (Directed graphical models)

Markov random fields (Undirected graphical models)

The focus of our course !

Model : joint probability over all variables



Nodes : random variables

Links : probabilistic relationships

Probabilistic graphical models : analysis using diagrammatic representations of probability distributions

Bayesian networks (Directed graphical models)

The focus of our course !

Model : joint probability over all variables



Markov random fields

(**Undirected** graphical models)

Example :



Nodes : random variables

Links : probabilistic relationships

 $P(X, Y) = \dots$

Probabilistic graphical models : analysis using diagrammatic representations of probability distributions

Bayesian networks (Directed graphical models)

The focus of our course !

Model : joint probability over all variables



Example :



Markov random fields

(**Undirected** graphical models)

Nodes : random variables

Links : probabilistic relationships

 $P(X, Y) = P(Y|X) \times P(X)$

Probabilistic graphical models : analysis using diagrammatic representations of probability distributions

Bayesian networks (Directed graphical models)

Markov random fields (Undirected graphical models)

The focus of our course !

Model : joint probability over all variables

 $P(X_1, \cdots, X_N) = \dots$

Example :



→ Nodes : random variables

Links : probabilistic relationships

$P(X, Y, Z) = \dots$

Features

 $X\,, Z\, {\rm conditionally}$ independent given Y

Probabilistic graphical models : analysis using diagrammatic representations of probability distributions

Bayesian networks (Directed graphical models)

Markov random fields (Undirected graphical models)

The focus of our course !

Model : joint probability over all variables

 $P(X_1, \cdots, X_N) = \dots$

Example :



→ Nodes : random variables

Links : probabilistic relationships

$P(X, Y, Z) = P(Y|X, Z) \times P(X, Z)$ $= P(Y|X, Z) \times P(X) \times P(Z)$

Features

 $X\,,Z\,{\rm conditionally}$ independent given Y

Probabilistic graphical models : analysis using diagrammatic representations of probability distributions

Bayesian networks (Directed graphical models)

Markov random fields (Undirected graphical models)

The focus of our course !

Model : joint probability over all variables

 $P(X_1, \cdots, X_N)$

Example :





$$= \prod_{i=1,\dots,N} P(X_i \mid parents(X_i))$$

$P(X, Y, Z) = P(Y|X, Z) \times P(X, Z)$ $= P(Y|X, Z) \times P(X) \times P(Z)$

Features

 $X\,,Z\,{\rm conditionally}$ independent given Y

Probabilistic graphical models : analysis using **diagrammatic representations** of probability distributions

Bayesian networks (**Directed** graphical models)

The focus of our course !

Model : joint probability over all variables

Markov random fields

Example :





 $P(X, Y) = P(Y|X) \times P(X)$ $P(X, Y, Z) = \dots$



 $P(Y, X_1, \cdots, X_N) =$

Probabilistic graphical models : analysis using **diagrammatic representations** of probability distributions

Markov random fields

Bayesian networks (**Directed** graphical models)

The focus of our course !

Model : joint probability over all variables



Example :





 $P(X, Y) = P(Y|X) \times P(X)$



2. Probabilistic model

Plates and examples of probabilistic model



2. Probabilistic model

Plates and examples of probabilistic model





2. Probabilistic model **Frequentist** linear regression

Reminder : Frequentist linear regression

 $x_i \in \mathbb{R}^d$

Scalar notation :

$$D = \{(x_1, y_1), \dots, (x_n, y_n)\}$$
$$y_i = x_i^T \theta + \epsilon_i$$

Matrix notation :

$$\mathbf{X} = (x_1, \dots, x_n) \text{ and } \mathbf{y} =$$
$$\mathbf{y} = \mathbf{X}^T \boldsymbol{\theta} + \boldsymbol{\epsilon}$$







$\min_{\theta} \|\theta^t X - y\|^2$



2. Probabilistic model **Frequentist** linear regression

Reminder : Frequentist linear regression

 $x_i \in \mathbb{R}^d$

Scalar notation :

Matrix notation :

$$D = \{(x_1, y_1), \dots, (x_n, y_n)\}$$

$$X = (x_1, \dots, x_n) \text{ and } y = y_i = x_i^T \theta + \epsilon_i$$

$$y = \mathbf{X}^T \theta + \epsilon_i$$

Proof : MLE for linear regression

$$\begin{aligned} x &= (x_{1_{1}\cdots_{1}}x_{n}), y = (y_{1_{1}}\cdots y_{n}), x_{i} \in IR^{d}, y_{i} \in R \\ & Y \wedge N(w^{T}x_{i}, e^{2}) \\ \Theta &= w \quad we \text{ suppose that } e^{2} \text{ is known} \\ & Y_{1_{1}\cdots_{i}}Y_{n} \text{ indep }, Y_{i} \sim N(w^{T}x_{i}, e^{2}) \quad OR \quad Y_{i} = w^{T}x_{i} + \varepsilon \\ & \text{likelihood} \qquad \qquad with \quad \varepsilon \wedge N(o_{i}e^{2}) \\ \Theta_{nLE} &= a_{1}g_{nax} \\ & \rho(y|x_{i}\Theta) \\ \Theta \in R^{d} \quad \rho(y_{1}|x_{i}\Theta) \\ & \rho(y_{1}|x_{i}\Theta) = \rho(y_{1_{1}\cdots_{i}}y_{n}|x_{1_{i}\cdots_{i}}x_{n_{i}}\Theta) = \prod_{i=1}^{n} \rho(y_{i}|x_{i_{i}}\Theta) \\ & = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}e^{2}} \exp\left(-\frac{1}{2e^{2}}(y_{i}-x_{i}^{T}w)^{2}\right) \\ & = \left(\frac{1}{\sqrt{2\pi}e^{1}}\right)^{n} \exp\left(-\frac{1}{2e^{2}}\sum_{i=1}^{n} (y_{i}-x_{i}^{T}w)^{2}\right) \end{aligned}$$







 $\min_{\theta} \|\theta^t X - y\|^2$

$$\frac{1}{|z\pi\tau\sigma^{2}|^{n/2}} e^{xp} \left(-\frac{1}{26^{2}}(y-x^{T}w)^{T}(y-x^{T}w)\right)$$

$$\frac{1}{|x\pi\sigma^{2}|^{n/2}} e^{xp} \left(-\frac{1}{26^{2}}(y-x^{T}w)^{T}(y-x^{T}w)\right)$$





2. Probabilistic model **Bayesian** linear regression

Bayesian Linear regression



 $P(\theta, y_i | x_i) = P(y_i | \theta, x_i) \times P(\theta)$



2. Probabilistic model **Bayesian** linear regression

Bayesian Linear regression



 $P(\theta, y_i | x_i) = P(y_i | \theta, x_i) \times P(\theta)$



2. Probabilistic model **Bayesian** linear regression

Bayesian Linear regression



$$P(\theta, y_i | x_i) = P(y_i | \theta, x_i) \times P(\theta)$$

$$P(y_i | \theta, x_i) = \mathcal{N}(y_i | \theta^T x_i, \sigma^2)$$

$$P(\theta) = \mathcal{N}(\theta | 0, \gamma^2)$$

Bayesian Linear regression



Frequentist linear regression

Objective: $\min_{\theta} \mathscr{L}(\theta) = \min_{\theta} ||\theta^{t}X - y||^{2}$ $\hat{\theta} = \arg\min_{\theta} \mathscr{L}(\theta)$ $\hat{\theta} = (X^{T}X)^{-1}X^{T}y$

Bayesian Linear regression



Frequentist linear regression

Objective: $\min_{\theta} \mathscr{L}(\theta) = \min_{\theta} \|\theta^t X - y\|^2$ $\hat{\theta} = \arg\min_{\alpha} \mathscr{L}(\theta)$ $\hat{\theta} = (X^T X)^{-1} X^T y$

Bayesian Linear regression



Theorem :

There exists $\lambda \in \mathbb{R}$ such that : $\underset{\theta}{\operatorname{arg max}} P(\theta | X, y) = \underset{\theta}{\operatorname{arg min}} \left\{ \|\theta^t X - y\|^2 + \lambda \|\theta\|^2 \right\}$

So by adding a normal prior on the weight we turned this problem into a L_2 regularised problem

Frequentist linear regression

Objective :
$$\min_{\theta} \mathscr{L}(\theta) = \min_{\theta} ||\theta^{t}X - y||^{2}$$

 $\hat{\theta} = \arg\min_{\theta} \mathscr{L}(\theta)$
 $\hat{\theta} = (X^{T}X)^{-1}X^{T}y$

Bayesian Linear regression



Theorem :

There exists $\lambda \in \mathbb{R}$ such that : $\underset{\theta}{\operatorname{arg max}} P(\theta | X, y) = \underset{\theta}{\operatorname{arg min}} \left\{ \|\theta^t X - y\|^2 + \lambda \|\theta\|^2 \right\}$

So by adding a normal prior on the weight we turned this problem into a L_2 regularised problem

Proof : left as an exercice

Frequentist linear regression

Objective :
$$\min_{\theta} \mathscr{L}(\theta) = \min_{\theta} ||\theta^{t}X - y||^{2}$$

 $\hat{\theta} = \arg\min_{\theta} \mathscr{L}(\theta)$
 $\hat{\theta} = (X^{T}X)^{-1}X^{T}y$



3. Analytical Inference Reminder of posterior distribution

Posterior distribution


3. Analytical Inference Reminder of posterior distribution

Posterior distribution



3. Analytical Inference Reminder of posterior distribution

Posterior distribution



3. Analytical Inference Maximum a posteriori (MAP) : definition & remarks

Posterior distribution



Remarks

- We have to avoid computing the evidence
- Naive approach : maximum a posteriori,

$$\hat{\theta}_{MAP} = \arg \max_{\theta} \left\{ \frac{P(\theta | X) \cdot P(\theta)}{P(X)} \right\}$$

 $= \arg \max P(X | \theta) \cdot P(\theta)$

This maximization can be done with numerical optimization problem

3. Analytical Inference Maximum a posteriori (MAP) : limitations

Posterior distribution



Limitations (among many others)

- 1. in general, not representative of bayesian methods : $\hat{\theta}_{MAP}$ is a point estimate like $\hat{\theta}_{MIF}$
 - can't compute credible intervals because it doesn't return a pdf/pmf (not a bayesian inference)
- 2. can't use online learning : the prior is not well updated

Remarks

- We have to avoid computing the evidence
- Naive approach : maximum a posteriori,

$$\hat{\theta}_{MAP} = \arg \max_{\theta} \left\{ \frac{P(\theta \mid X) \cdot P(\theta)}{P(X)} \right\}$$

- $= \arg \max P(X | \theta) \cdot P(\theta)$
- This maximization can be done with numerical optimization problem

3. Analytical Inference Maximum a posteriori (MAP) : book

For more theoretical details (and example on analytical inference) :







Posterior distribution



Posterior distribution



Remarks

- We have to avoid computing the evidence
- We can choose a convenient prior which enable us to compute the **posterior** :

Conjugate prior

Posterior distribution



Conjugate prior

 $P(\theta)$ is conjugate to $P(X | \theta)$ if the $P(\theta)$ and $P(\theta | X)$ lie in the same family of distributions (gaussian for example)

Remarks

- We have to avoid computing the evidence
- We can choose a convenient prior which enable us to compute the **posterior** :

Conjugate prior

Posterior distribution



Conjugate prior

 $P(\theta)$ is conjugate to $P(X | \theta)$ if the $P(\theta)$ and $P(\theta | X)$ lie in the same family of distributions (gaussian for example)

Example

 $P(\theta | X) = \frac{\mathcal{N}(X | \theta, \sigma^2) \times P(\theta)}{P(X)}$ $\mathcal{N}(\theta | \mu_{posterior}, \sigma_{posterior}^2)$

Remarks

- We have to avoid computing the evidence
- We can choose a convenient prior which enable us to compute the **posterior** :

Conjugate prior

 $\mathcal{N}(\theta \mid \mu_{prior}, \sigma_{prior}^2)$

In the context of a gaussian, the prior for the **mean** is a gaussian!

4. Conjugate distributions Limitations

Posterior distribution





- It computes the exact posterior
- Easy for online learning

Remarks

- We have to avoid computing the evidence
- We can choose a convenient prior which enable us to compute the **posterior** :

Conjugate prior



- For some (complex) models, the conjugate prior can be inadequate (improper prior)
- Can be unrealistic (non-informative prior)



Conjugate distributions : Exercices

5. Conjugate distributions **Exercices**

Exercice (left as an exercice, correction in the next lecture)

Show that $\mathcal{N}(\theta | x/2, 1/2) = \frac{\mathcal{N}(x | \theta, 1) \times \mathcal{N}(\theta | 0, 1)}{P(x)}$

Exercice (left as an exercice, correction in the next lecture) show the following equation

 $\Gamma(\gamma \mid \alpha_{posterior}, \beta_{posterior}) \qquad P(\gamma \mid x) = \frac{\mathcal{N}(x \mid \mu, \gamma^{-1}) \times P(\gamma)}{P(x)} \qquad \Gamma(\gamma \mid \alpha_{prior}, \beta_{prior})$ $\Gamma(\gamma \mid \alpha_{prior} + 1/2, \beta_{prior} + (x - \mu)^{2}/2)$

Exercice (left as an exercice, correction in the next lecture) show the following equation

 $B(\theta \mid \alpha_{posterior}, \beta_{posterior}) \qquad P(\theta \mid x) = \frac{Ber(x \mid \theta)}{P(\theta \mid x)}$

 $B(\theta | n_1 + \alpha_{prior}, n_0 + \beta_{prior})$



If you do these exercices before the next lecture, you'll have **bonus points**:

- 0.25 pts if only the reasoning is good
- **0.5 pts** if only some of them are correct
- **0.75 pts** if most of them are correct
- **1 pts** if all of them are correct





In the context of a gaussian, the prior for the **precision** is a gamma!

$$\frac{\theta^{n_1} \cdot (1 - \theta)^{n_0}}{B(\theta \mid \alpha_{prior}, \beta_{prior})}$$

$$\frac{\theta}{P(x)}$$

In the context of a Bernoulli distribution, the prior is a beta !











Oral presentations



Variational Inference



Causal Inference

