

Mathematics for Machine Learning

— When Models Meet Data

Probabilistic Modeling & Inference

Joseph Chuang-Chieh Lin

Department of Computer Science & Engineering,
National Taiwan Ocean University

Fall 2025

Credits for the resource

- The slides are based on the textbooks:
 - *Marc Peter Deisenroth, A. Aldo Faisal, and Cheng Soon Ong: Mathematics for Machine Learning. Cambridge University Press. 2020.*
 - *Arnold J. Insel, Lawrence E. Spence, Stephen H. Friedberg: Linear Algebra, 4th Edition. Prentice Hall. 2013.*
 - *Howard Anton, Chris Rorres, Anton Kaul: Elementary Linear Algebra, 12th Edition. Wiley. 2019.*
- We could partially refer to the monograph:
Francesco Orabona: A Modern Introduction to Online Learning.
<https://arxiv.org/abs/1912.13213>

Outline

- 1 Probabilistic Models & Bayesian Inference
- 2 Latent-Variable Models

Motivation

- We are concerned with prediction of future events and decision making.
- We build models that describe the **generative process** that generates the observed data.
- For example, consider the outcome of a coin-flip experiment ("heads" or "tails").

Motivation

- We are concerned with prediction of future events and decision making.
- We build models that describe the **generative process** that generates the observed data.
- For example, consider the outcome of a coin-flip experiment ("heads" or "tails").
 - Define a parameter μ which describes the probability of "heads" (the parameter of a Bernoulli distribution).

Motivation

- We are concerned with prediction of future events and decision making.
- We build models that describe the **generative process** that generates the observed data.
- For example, consider the outcome of a coin-flip experiment ("heads" or "tails").
 - Define a parameter μ which describes the probability of "heads" (the parameter of a Bernoulli distribution).
 - Then, we can sample an outcome $x \in \{\text{head, tail}\}$ from the Bernoulli distribution $p(x | \mu) = \text{Ber}(\mu)$.

Motivation

- We are concerned with prediction of future events and decision making.
- We build models that describe the **generative process** that generates the observed data.
- For example, consider the outcome of a coin-flip experiment ("heads" or "tails").
 - Define a parameter μ which describes the probability of "heads" (the parameter of a Bernoulli distribution).
 - Then, we can sample an outcome $x \in \{\text{head, tail}\}$ from the Bernoulli distribution $p(x | \mu) = \text{Ber}(\mu)$.
- **Note:** μ is **unknown** in advance and can **never be observed directly**.

Motivation

- We are concerned with prediction of future events and decision making.
- We build models that describe the **generative process** that generates the observed data.
- For example, consider the outcome of a coin-flip experiment ("heads" or "tails").
 - Define a parameter μ which describes the probability of "heads" (the parameter of a Bernoulli distribution).
 - Then, we can sample an outcome $x \in \{\text{head, tail}\}$ from the Bernoulli distribution $p(x | \mu) = \text{Ber}(\mu)$.
- **Note:** μ is **unknown** in advance and can **never be observed directly**.
- We need mechanisms to learn something about μ given observed outcomes of coin-flip.

Probabilistic Models

- The benefit of using probabilistic models:
 - A unified and consistent set of tools from probability theory for modeling, inference, prediction, and model selection.
- $p(\mathbf{x}, \boldsymbol{\theta})$: the joint distribution of the observed variables \mathbf{x} and the hidden parameters $\boldsymbol{\theta}$.

Probabilistic Models

- The benefit of using probabilistic models:
 - A unified and consistent set of tools from probability theory for modeling, inference, prediction, and model selection.
- $p(\mathbf{x}, \boldsymbol{\theta})$: the joint distribution of the observed variables \mathbf{x} and the hidden parameters $\boldsymbol{\theta}$. It encapsulates the information:
 - The prior and the likelihood.
 - The marginal likelihood $p(\mathbf{x})$ (though integrating out the parameters is required.)
 - The posterior (obtained by dividing the joint by the marginal likelihood).

Probabilistic Models

- The benefit of using probabilistic models:
 - A unified and consistent set of tools from probability theory for modeling, inference, prediction, and model selection.
- $p(\mathbf{x}, \boldsymbol{\theta})$: the joint distribution of the observed variables \mathbf{x} and the hidden parameters $\boldsymbol{\theta}$. It encapsulates the information:
 - The prior and the likelihood.
 - The marginal likelihood $p(\mathbf{x})$ (though integrating out the parameters is required.)
 - The posterior (obtained by dividing the joint by the marginal likelihood).
- Therefore, a probabilistic model is specified by the joint distribution of **all** its random variables.

Bayesian Inference (1/3)

- We have already learnt two ways of estimating model parameters θ :
 - Maximum likelihood estimation (MLE)
 - Maximum a posteriori estimation (MAP)
- We can then obtain a *single-best* value of θ (solving an optimization problem), then we can use them to make predictions.
- Having the full posterior distribution around can be useful and leads to more robust decisions.

Bayesian Inference (2/3)

- Bayesian inference: finding such a posterior distribution.
- For a dataset \mathcal{X} , a parameter prior $p(\theta)$, and a likelihood function, the posterior

$$p(\theta | \mathcal{X}) = \frac{p(\mathcal{X} | \theta)p(\theta)}{p(\mathcal{X})},$$

then by applying Bayes' theorem,

$$p(\mathcal{X}) = \int p(\mathcal{X} | \theta)p(\theta)d\theta.$$

Bayesian Inference (2/3)

- Bayesian inference: finding such a posterior distribution.
- For a dataset \mathcal{X} , a parameter prior $p(\theta)$, and a likelihood function, the posterior

$$p(\theta | \mathcal{X}) = \frac{p(\mathcal{X} | \theta)p(\theta)}{p(\mathcal{X})},$$

then by applying Bayes' theorem,

$$p(\mathcal{X}) = \int p(\mathcal{X} | \theta)p(\theta)d\theta.$$

- Propagate uncertainty from the parameters to the data. Specifically, with a distribution $p(\theta)$, our predictions will be

$$p(\mathbf{x}) = \int p(\mathbf{x} | \theta)p(\theta)d\theta$$

Bayesian Inference (2/3)

- Bayesian inference: finding such a posterior distribution.
- For a dataset \mathcal{X} , a parameter prior $p(\theta)$, and a likelihood function, the posterior

$$p(\theta | \mathcal{X}) = \frac{p(\mathcal{X} | \theta)p(\theta)}{p(\mathcal{X})},$$

then by applying Bayes' theorem,

$$p(\mathcal{X}) = \int p(\mathcal{X} | \theta)p(\theta)d\theta.$$

- Propagate uncertainty from the parameters to the data. Specifically, with a distribution $p(\theta)$, our predictions will be

$$p(\mathbf{x}) = \int p(\mathbf{x} | \theta)p(\theta)d\theta = \mathbb{E}_{\theta}[p(\mathbf{x} | \theta)],$$

which no longer depend on the model parameters θ .

Bayesian Inference (2/3)

- Bayesian inference: finding such a posterior distribution.
- For a dataset \mathcal{X} , a parameter prior $p(\theta)$, and a likelihood function, the posterior

$$p(\theta | \mathcal{X}) = \frac{p(\mathcal{X} | \theta)p(\theta)}{p(\mathcal{X})},$$

then by applying Bayes' theorem,

$$p(\mathcal{X}) = \int p(\mathcal{X} | \theta)p(\theta)d\theta.$$

- Propagate uncertainty from the parameters to the data. Specifically, with a distribution $p(\theta)$, our predictions will be

$$p(\mathbf{x}) = \int p(\mathbf{x} | \theta)p(\theta)d\theta = \mathbb{E}_{\theta}[p(\mathbf{x} | \theta)],$$

which no longer depend on the model parameters θ .

- It has been marginalized/integrated out.

Bayesian Inference (3/3)

$$p(\mathbf{x}) = \int p(\mathbf{x} | \boldsymbol{\theta}) p(\boldsymbol{\theta}) d\boldsymbol{\theta} = \mathbb{E}_{\boldsymbol{\theta}}[p(\mathbf{x} | \boldsymbol{\theta})],$$

- The prediction becomes an average over all plausible values of $\boldsymbol{\theta}$.
 - The plausibility is encapsulated by the distribution $p(\boldsymbol{\theta})$.

Computational Issues

- MLE or MAP yields a consistent point estimate θ^* of the parameters.
 - Key computational problem: optimization.
 - Prediction: straightforward.
- Bayesian inference yields a **distribution**.
 - Key computational problem: integration.
 - Prediction: solving another integration problem.

Outline

1 Probabilistic Models & Bayesian Inference

2 Latent-Variable Models

Latent Variables

- Sometimes it is useful to have additional variable (besides θ) as part of the model.
 - We call them **latent variables**.
 - They do not parametrize the model explicitly.
 - E.g., mixture of K Gaussians.
- Latent variables can
 - Describe the data-generation process.
 - Increase the interpretability of the model.
 - Simplify the structure of the model.

In the Data Generation Process

Denote data by \mathbf{x} , the model parameter by $\boldsymbol{\theta}$ and the latent variables by \mathbf{z} , we obtain the conditional distribution:

$$p(\mathbf{x} \mid \mathbf{z}, \boldsymbol{\theta}).$$

In the Data Generation Process

Denote data by x , the model parameter by θ and the latent variables by z , we obtain the conditional distribution:

$$p(x | z, \theta).$$

⇒ Generate data for any model parameter and latent variables.

In the Data Generation Process

Denote data by \mathbf{x} , the model parameter by $\boldsymbol{\theta}$ and the latent variables by \mathbf{z} , we obtain the conditional distribution:

$$p(\mathbf{x} \mid \mathbf{z}, \boldsymbol{\theta}).$$

- ⇒ Generate data for any model parameter and latent variables.
- We place a prior $p(\mathbf{z})$ on the given latent variables \mathbf{z} .

In the Data Generation Process

Denote data by \mathbf{x} , the model parameter by $\boldsymbol{\theta}$ and the latent variables by \mathbf{z} , we obtain the conditional distribution:

$$p(\mathbf{x} \mid \mathbf{z}, \boldsymbol{\theta}).$$

- ⇒ Generate data for any model parameter and latent variables.
- We place a prior $p(\mathbf{z})$ on the given latent variables \mathbf{z} .

A Two-Step Procedure for Parameter Learning & Inference

- ① Compute the likelihood $p(\mathbf{x} \mid \boldsymbol{\theta})$ (not depending on \mathbf{z}).
- ② Use the likelihood for parameter estimation or Bayesian inference.

Likelihood in Terms of Marginal Distribution

What we already have: a conditional distribution

$$p(\mathbf{x} \mid \mathbf{z}, \boldsymbol{\theta}).$$

We need to marginalize out the latent variables to have the predictive distribution of the data given the model parameters $\boldsymbol{\theta}$:

$$p(\mathbf{x} \mid \boldsymbol{\theta}) = \int p(\mathbf{x} \mid \mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z}) d\mathbf{z},$$

Likelihood in Terms of Marginal Distribution

What we already have: a conditional distribution

$$p(\mathbf{x} \mid \mathbf{z}, \boldsymbol{\theta}).$$

We need to marginalize out the latent variables to have the predictive distribution of the data given the model parameters $\boldsymbol{\theta}$:

$$p(\mathbf{x} \mid \boldsymbol{\theta}) = \int p(\mathbf{x} \mid \mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z}) d\mathbf{z},$$

Note that $p(\mathbf{z})$ is a prior,

Likelihood in Terms of Marginal Distribution

What we already have: a conditional distribution

$$p(\mathbf{x} \mid \mathbf{z}, \boldsymbol{\theta}).$$

We need to marginalize out the latent variables to have the predictive distribution of the data given the model parameters $\boldsymbol{\theta}$:

$$p(\mathbf{x} \mid \boldsymbol{\theta}) = \int p(\mathbf{x} \mid \mathbf{z}, \boldsymbol{\theta}) p(\mathbf{z}) d\mathbf{z},$$

Note that $p(\mathbf{z})$ is a prior, and $p(\mathbf{x} \mid \boldsymbol{\theta})$ does not depend on \mathbf{z} .

Bayesian Inference in a Latent Variable Model

- MAP estimation is also straightforward:

Bayesian Inference in a Latent Variable Model

- MAP estimation is also straightforward:
 - Place a prior $p(\theta)$ and use Bayes' theorem to obtain

Bayesian Inference in a Latent Variable Model

- MAP estimation is also straightforward:
 - Place a prior $p(\theta)$ and use Bayes' theorem to obtain

$$p(\theta | \mathcal{X}) = \frac{p(\mathcal{X} | \theta)p(\theta)}{p(\mathcal{X})}$$

Bayesian Inference in a Latent Variable Model

- MAP estimation is also straightforward:
 - Place a prior $p(\theta)$ and use Bayes' theorem to obtain

$$p(\theta | \mathcal{X}) = \frac{p(\mathcal{X} | \theta)p(\theta)}{p(\mathcal{X})}$$

⇒ a posterior distribution over the model parameters given a dataset \mathcal{X} .

Bayesian Inference in a Latent Variable Model

- MAP estimation is also straightforward:
 - Place a prior $p(\theta)$ and use Bayes' theorem to obtain

$$p(\theta | \mathcal{X}) = \frac{p(\mathcal{X} | \theta)p(\theta)}{p(\mathcal{X})}$$

- ⇒ a posterior distribution over the model parameters given a dataset \mathcal{X} .
- $p(\mathcal{X} | \theta)$ requires the marginalization of latent variables \mathbf{z} .

Bayesian Inference in a Latent Variable Model

- MAP estimation is also straightforward:
 - Place a prior $p(\theta)$ and use Bayes' theorem to obtain

$$p(\theta | \mathcal{X}) = \frac{p(\mathcal{X} | \theta)p(\theta)}{p(\mathcal{X})}$$

- ⇒ a posterior distribution over the model parameters given a dataset \mathcal{X} .
- $p(\mathcal{X} | \theta)$ requires the marginalization of latent variables \mathbf{z} .

$$p(\mathbf{x} | \theta) = \int p(\mathbf{x} | \mathbf{z}, \theta)p(\mathbf{z})d\mathbf{z},$$

- Resort to approximation.

A Posterior on the Latent Variables

Similarly we can have

$$p(\mathbf{z} | \mathcal{X}) = \frac{p(\mathcal{X} | \mathbf{z})p(\mathbf{z})}{p(\mathcal{X})}, \quad p(\mathcal{X} | \mathbf{z}) = \int p(\mathcal{X} | \mathbf{z}, \boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta},$$

A Posterior on the Latent Variables

Similarly we can have

$$p(\mathbf{z} | \mathcal{X}) = \frac{p(\mathcal{X} | \mathbf{z})p(\mathbf{z})}{p(\mathcal{X})}, \quad p(\mathcal{X} | \mathbf{z}) = \int p(\mathcal{X} | \mathbf{z}, \boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta},$$

$p(\mathbf{z})$: the prior on \mathbf{z} ; $p(\mathcal{X} | \mathbf{z})$ requires us to integrate out $\boldsymbol{\theta}$.

A Posterior on the Latent Variables

Similarly we can have

$$p(\mathbf{z} | \mathcal{X}) = \frac{p(\mathcal{X} | \mathbf{z})p(\mathbf{z})}{p(\mathcal{X})}, \quad p(\mathcal{X} | \mathbf{z}) = \int p(\mathcal{X} | \mathbf{z}, \boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta},$$

$p(\mathbf{z})$: the prior on \mathbf{z} ; $p(\mathcal{X} | \mathbf{z})$ requires us to integrate out $\boldsymbol{\theta}$.

- It may be difficult to solve the integrals analytically.
- Marginalizing out both the latent variables and the model parameters at the same time is not possible in general.

A Posterior on the Latent Variables

Similarly we can have

$$p(\mathbf{z} | \mathcal{X}) = \frac{p(\mathcal{X} | \mathbf{z})p(\mathbf{z})}{p(\mathcal{X})}, \quad p(\mathcal{X} | \mathbf{z}) = \int p(\mathcal{X} | \mathbf{z}, \boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta},$$

$p(\mathbf{z})$: the prior on \mathbf{z} ; $p(\mathcal{X} | \mathbf{z})$ requires us to integrate out $\boldsymbol{\theta}$.

- It may be difficult to solve the integrals analytically.
- Marginalizing out both the latent variables and the model parameters at the same time is not possible in general.
- An easier quantity to compute:

A Posterior on the Latent Variables

Similarly we can have

$$p(\mathbf{z} | \mathcal{X}) = \frac{p(\mathcal{X} | \mathbf{z})p(\mathbf{z})}{p(\mathcal{X})}, \quad p(\mathcal{X} | \mathbf{z}) = \int p(\mathcal{X} | \mathbf{z}, \boldsymbol{\theta})p(\boldsymbol{\theta})d\boldsymbol{\theta},$$

$p(\mathbf{z})$: the prior on \mathbf{z} ; $p(\mathcal{X} | \mathbf{z})$ requires us to integrate out $\boldsymbol{\theta}$.

- It may be difficult to solve the integrals analytically.
- Marginalizing out both the latent variables and the model parameters at the same time is not possible in general.
- An easier quantity to compute:

$$p(\mathbf{z} | \mathcal{X}, \boldsymbol{\theta}) = \frac{p(\mathcal{X} | \mathbf{z}, \boldsymbol{\theta})p(\mathbf{z})}{p(\mathcal{X} | \boldsymbol{\theta})}.$$

- $p(\mathbf{z})$: the prior on \mathbf{z} ; $p(\mathcal{X} | \mathbf{z}, \boldsymbol{\theta})$: given.

Discussions