Mathematics for Machine Learning

— When Models Meet Data

Probabilistic Modeling & Inference

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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.
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- **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.
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  - 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 $\boldsymbol{\theta}$:
  - Maximum likelihood estimation (MLE)
  - Maximum a posteriori estimation (MAP)
- We can then obtain a *single-best* value of $\boldsymbol{\theta}$ (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 $p(\boldsymbol{\theta})$, and a likelihood function, the posterior

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

then by applying Bayes' theorem,

$$p(\mathcal{X}) = \int p(\mathcal{X} \mid \boldsymbol{\theta})p(\boldsymbol{\theta})\mathrm{d}\boldsymbol{\theta}.$$

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    - It has been marginalized/integrated out.

Bayesian Inference (3/3)

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- 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 $\boldsymbol{\theta}^*$ of the parameters.
  - Key computational problem: optimization.
  - Prediction: straightforward.
- Bayesian inference yields a distribution.
  - Key computational problem: integration.
  - Prediction: solving another integration problem.

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Latent Variables

- Sometimes it is useful to have additional variable (besides $\boldsymbol{\theta}$) as part of the model.
    - We call them latent variables.
    - They do not parametrize the model explicitly.
    - E.g., mixture of K Gaussians (further reading link).
- 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:

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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 $\boldsymbol{\theta}$:

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    - Resort to approximation.

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

Discussions