COMP90051 **Statistical Machine Learning**

Semester 2, 2017

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2. Statistical Schools

THE UNIVERSITY OF MELBOURNE

Adapted from slides by Ben Rubinstein

Statistical Schools of Thought

Remainder of deck is to provide *intuition* into how algorithms in this subject come about and inter-relate

Based on Berkeley CS 294-34 tutorial slides by Ariel Kleiner

Frequentist Statistics

- Abstract problem
  - Given: $X_1, X_2, \ldots, X_n$ drawn i.i.d. from some distribution
  - Want to: identify unknown distribution
- Parametric approach ("**parameter estimation**")
  - Class of models $\{p_\theta(x): \theta \in \Theta\}$ indexed by parameters Θ (could be a real number, or vector, or ….)
  - Select $\hat{\theta}\ (x_1, \ldots, x_n)$ some function (or statistic) of data

Hat means estimate or estimator

- Examples
  - Given n coin flips, determine probability of landing heads
  - Building a classifier is a very related problem

How do Frequentists Evaluate Estimators?

- Bias: $B_\theta(\hat{\theta}) = E_\theta[\hat{\theta}(X_1, \dots, X_n)] - \theta$
- Variance: $Var_\theta(\hat{\theta}) = E_\theta[(\hat{\theta} - E_\theta[\hat{\theta}])^2]$
  - Efficiency: estimate has minimal variance
- Square loss vs bias-variance

$$E_\theta\left[\left(\theta - \hat{\theta}\right)^2\right] = [B(\theta)]^2 + Var_\theta(\hat{\theta})$$

- Consistency: $\hat{\theta}(X_1, \dots, X_n)$ converges to θ as *n* gets big

… more on this later in the subject …

Subscript θ means data *really* comes from p_θ

$\hat{\theta}$ still function of data

Is this "*Just Theoretical*"™ ?

- Recall Lecture 1 →

COMP90051 Machine Learning (S2 2017) L1

Evaluation (Supervised Learners)

- How you measure quality depends on your problem!
- Typical process
  - Pick an evaluation metric comparing label vs prediction
  - Procure an independent, labelled test set
  - "Average" the evaluation metric over the test set
- Example evaluation metrics
  - Accuracy, Contingency table, Precision-Recall, ROC curves
- When data poor, cross-validate

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- Those evaluation metrics? They're just estimators of a performance parameter
- Example: error
- Bias, Variance, etc. indicate quality of approximation

Maximum-Likelihood Estimation

- A general principle for designing estimators
- Involves optimisation
- $\hat{\theta}(x_1, \ldots, x_n) = \underset{\theta \in \Theta}{\operatorname{argmax}} \prod_{i=1}^{n} p_\theta(x_i)$
  - Question: Why a *product*?

Fischer

Example I: Normal

- Know data comes from Normal distribution with variance 1 but unknown mean; find mean
- MLE for mean
  * $p_\theta(x) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}(x-\theta)^2\right)$
  * Maximising likelihood yields $\hat{\theta} = \frac{1}{n}\sum_{i=1}^{n} x_i$
- Exercise: derive MLE for *variance* σ^2 based on $p_\theta(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2\sigma^2}(x-\mu)^2\right)$ with $\theta = (\mu, \sigma^2)$

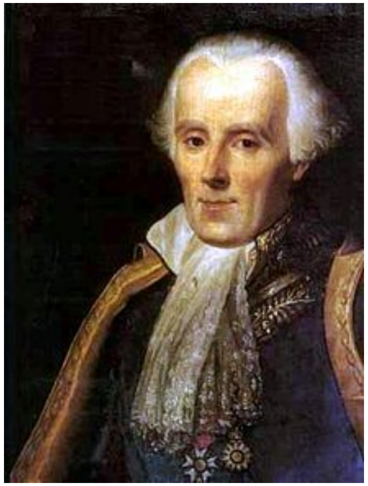
Example II: Bernoulli

- Know data comes from Bernoulli distribution with unknown parameter (e.g., biased coin); find mean
- MLE for mean
  - $p_\theta(x) = \begin{cases} \theta, & \text{if } x = 1 \\ 1-\theta, & \text{otherwise} \end{cases} = \theta^x(1-\theta^{1-x})$
  - Maximising likelihood yields $\hat{\theta} = \frac{1}{n}\sum_{i=1}^{n} x_i$

MLE 'algorithm'

1. given data $x_1, \ldots, x_n$ define probability distribution, p_θ, assumed to have generated the data
2. express likelihood of data, $\prod_{i=1}^{n} p_\theta(x_i)$ (usually its *logarithm*... why*?)*
3. optimise to find *best* (most likely) parameters $\hat{\theta}$
    1. take partial derivatives of log likelihood wrt θ
    2. set to 0 and solve
       (failing that, use iterative gradient method)

Bayesian Statistics



Laplace

- Probabilities correspond to beliefs
- Parameters
  - Modeled as r.v.'s having distributions
  - Prior belief in θ encoded by prior distribution $\mathrm{P}(\theta)$
  - Write likelihood of data P(X) as conditional $\mathrm{P}(\mathrm{X}|\theta)$
  - Rather than point estimate $\hat{\theta}$, Bayesians update belief $\mathrm{P}(\theta)$ with observed data to $\mathrm{P}(\theta|X)$ the posterior distribution

More Detail (Probabilistic Inference)

Bayes

- Bayesian machine learning
  - Start with prior $\mathrm{P}(\theta)$ and likelihood $\mathrm{P}(X|\theta)$
  - Observe data $X = x$
  - Update prior to posterior $\mathrm{P}(\theta|X = x)$
- We'll later cover tools to get the posterior
  - Bayes Theorem: reverses order of conditioning

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

  - Marginalisation: eliminates unwanted variables

$$\mathrm{P}(X = x) = \sum_t P(X = x, \theta = t)$$

Example

- We model $X|\theta$ as $N(\theta, 1)$ with prior $N(0,1)$
- Suppose we observe X=1, then update posterior

$$P(\theta|X = 1) = \frac{P(X = 1|\theta)P(\theta)}{P(X=1)}$$

$$\propto P(X = 1|\theta)P(\theta)$$

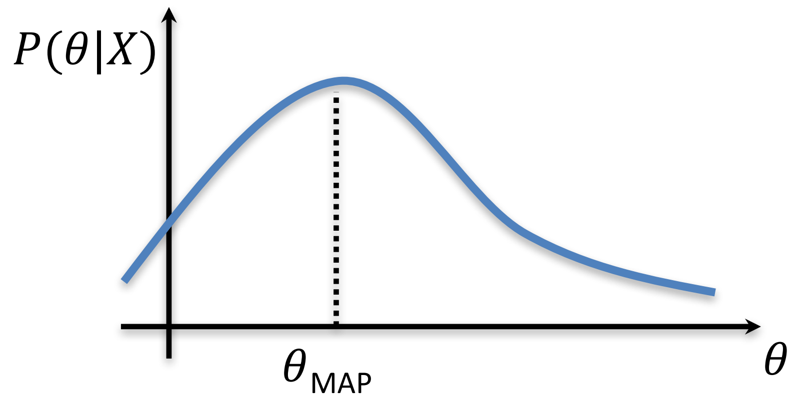
$$= \left[\frac{1}{\sqrt{2\pi}} exp\left(-\frac{(1-\theta)^2}{2}\right)\right]\left[\frac{1}{\sqrt{2\pi}} exp\left(-\frac{\theta^2}{2}\right)\right]$$

$$\propto N(0.5,0.5)$$

NB: allowed to push constants out front and "ignore" as these get taken care of by normalisation

How Bayesians Make Point Estimates

- They don't, unless forced at gunpoint!
  - The posterior carries full information, why discard it?
- But, there are common approaches
  - Posterior mean $E_{\theta|X}[\theta] = \int \theta P(\theta|X) d\theta$
  - Posterior mode $\underset{\theta}{\operatorname{argmax}} P(\theta|X)$ (max a posteriori or MAP)



MLE in Bayesian context

- MLE formulation: find parameters that best fit data
$$\hat{\theta} = \operatorname{argmax}_\theta P(X = x|\theta)$$
- Consider the MAP under a Bayesian formulation
$$\begin{aligned}\hat{\theta} &= P(\theta|X = x) \\ &= \operatorname{argmax}_\theta \frac{P(X = x|\theta)P(\theta)}{P(X = x)} \\ &= \operatorname{argmax}_\theta P(X = x|\theta)P(\theta)\end{aligned}$$
- Difference is **prior** $P(\theta)$; assumed *uniform* for MLE

Parametric vs Non-Parametric Models

Parametric	Non-Parametric
Determined by fixed, finite number of parameters	Number of parameters grows with data, potentially infinite
Limited flexibility	More flexible
Efficient statistically and computationally	Less efficient

Examples to come! There are non/parametric models in both the frequentist and Bayesian schools.

Generative vs. Discriminative Models

- X's are instances, Y's are labels (supervised setting!)
  - Given: i.i.d. data $(X_1, Y_1),\ldots,(X_n, Y_n)$
  - Find model that can predict Y of new X
- Generative approach
  - Model full joint $P(X, Y)$
- Discriminative approach
  - Model conditional $P(Y|X)$ only
- Both have pro's and con's

Examples to come! There are generative/discriminative models in both the frequentist and Bayesian schools.

Summary

- Philosophies: frequentist vs. Bayesian
- Principles behind many learners:
  * MLE
  * Probabilistic inference, MAP
- Discriminative vs. Generative models