Probability and Statistics

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COMP 64101 – Reasoning and Learning under Uncertainty
Lecture 1





Topics: Probability

"I know it's Tuesday. It's a good day for math!"

Max Mintz

- Discrete vs Continuous Distributions (Murphy, 2023, § 2.1.2 2.1.3)
- Bayes' Rule (Murphy, 2023, § 2.1.5 2.1.6)
- Some Common Probability Distributions (Murphy, 2023, § 2.2 2.3)
 - Mixture of Gaussians (Murphy, 2023, § 28.2.1)
- Markov Chains (Murphy, 2023, § 2.6)

Topics: Statistics

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- (Some Concepts of) Bayesian Statistics (Murphy, 2023, § 3.2)
- (Some Concepts of) Frequentist Statistics (Murphy, 2023, § 3.3)
- Maximum Likelihood Estimator and the EM Algorithm (Murphy, 2023, § 6.5.3)

Probability Space

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- ullet Ω is the sample space (possible outcomes from an experiment)
- \mathcal{F} is the event space (σ -algebra), a collection of subsets of Ω
- ullet $\mathbb{P}:\mathcal{F} \rightarrow [0,1]$ is the probability measure

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- $\Omega = \{\omega_1 = (H, H), \omega_2 = (H, T), \omega_3 = (T, H), \omega_4 = (T, T)\}$
- $\mathcal{F} = 2^{\Omega}$, so $|\mathcal{F}| = 2^4 = 16$
- $\mathbb{P}(\{\omega_i\}) = 1/4$, $i \in \{1, ..., 4\}$, and the probability of the other sets in \mathcal{F} follows by additivity (next slide)

• $\mathbb{P}(E) \geq 0$, for all $E \in \mathcal{F}$

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 - Only Finite Additivity: Subjectivist Approach to Probability de Finetti (1974, 1975)
 - Super/Subadditivity: Imprecise Approach to Probability Walley (1991);
 Augustin et al. (2014)

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- Can we assign a number to each element of Ω (i.e. to each outcome of our experiment of interest)?
- Yes, via a Random Variable (rv)

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- Example cont'd: Number of Heads via rv

$$X(\omega_1) = 2$$
, $X(\omega_2) = X(\omega_3) = 1$, $X(\omega_4) = 0$

- Random Variable need not assign only numbers to the outcomes of the experiment
- In general, we call state space \mathcal{X} the range¹ of rv X, i.e. $\mathcal{X} = X(\Omega)$

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$$p_X(a) = \mathbb{P}[X^{-1}(a)], \quad X^{-1}(a) := \{\omega \in \Omega : X(\omega) = a\}$$

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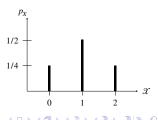
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Example cont'd: pmf is

•
$$p_X(0) = \mathbb{P}(\{(T, T)\}) = 1/4$$

•
$$p_X(1) = \mathbb{P}(\{(H, T), (T, H)\}) = 1/2$$

•
$$p_X(2) = \mathbb{P}(\{(H, H)\}) = 1/4$$



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Continuous Random Variables

- Experiments with continuous outcome
- ullet $\Omega\subseteq\mathbb{R}$, and $X(\omega)=\omega$, so that $\mathcal{X}=\Omega$
- **Example:** The duration of some event (in seconds), so $\Omega = \{t \in \mathbb{R}_+ : t \leq T_{\text{max}}\}$

Conditional Probability

• Consider events E_1 and E_2 , and suppose $\mathbb{P}(E_2) > 0$. Then, conditional probability of E_1 given E_2 is

$$\mathbb{P}(E_1 \mid E_2) := \frac{\mathbb{P}(E_1 \cap E_2)}{\mathbb{P}(E_2)}$$

• In turn, $\mathbb{P}(E_1 \cap E_2) = \mathbb{P}(E_1 \mid E_2)\mathbb{P}(E_2) = \mathbb{P}(E_2 \mid E_1)\mathbb{P}(E_1)$

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- Conditional probability measures how likely an event E_1 is, given that event E_2 has happened

A Note on Independent Events

• E_1 and E_2 are independent events if

$$\mathbb{P}(E_1 \cap E_2) = \mathbb{P}(E_1)\mathbb{P}(E_2)$$

• If both $\mathbb{P}(E_1) > 0$ and $\mathbb{P}(E_2) > 0$, this is equivalent to

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• E_1 and E_2 are conditionally independent given E_3 if

$$\mathbb{P}(E_1 \cap E_2 \mid E_3) = \mathbb{P}(E_1 \mid E_3)\mathbb{P}(E_2 \mid E_3)$$

Bayes' Theorem

• Consider events E_1 and E_2 , and suppose $\mathbb{P}(E_1), \mathbb{P}(E_2) > 0$. Then, Bayes' rule is

$$\mathbb{P}(\textit{E}_1 \mid \textit{E}_2) = \frac{\mathbb{P}(\textit{E}_2 \mid \textit{E}_1)\mathbb{P}(\textit{E}_1)}{\mathbb{P}(\textit{E}_2)}$$

• Discrete case with $|\mathcal{X}| = K$,

$$p(X = k \mid E) = \frac{p(E \mid X = k)p(X = k)}{\sum_{k'=1}^{K} p(E \mid X = k')p(X = k')}$$

ullet Continuous case, e.g. with $\mathcal{X}=\mathbb{R}$,

$$p(x \mid E) = \frac{p(E \mid x)p(x)}{\int_{\mathcal{X}} p(E \mid x)p(x)dx}$$

Common Discrete Distributions

- Let $\mathcal{X} = \{1, ..., K\}$
- Binomial: $X \sim \text{Bin}(N, \mu)$, $p(x) = \binom{N}{x} \mu^x (1 \mu)^{N-x}$
 - $\binom{N}{x} := \frac{N!}{(N-x)!x!}$ and $\mu \in [0,1]$
 - Number x of successes in a sequence of N independent experiments, each asking a yes—no question, and having success probability μ
 - Implement it in Python: here

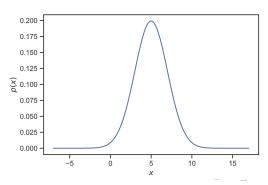
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 - Implement it in Python: here
- Categorical: $X \sim \text{Cat}(\theta)$, $p_X(k) = \theta_k$
 - $m{ heta}$ is a probability vector, and hence belongs to unit simplex $\Delta^{K-1}\subset\mathbb{R}^K$
 - $p_X(k) = \theta_k \to \text{probability that } X \text{ is equal to } k$; such probability is the k^{th} entry of parameter θ
 - Fundamental for Classification Problems
 - Implement it in Python: here



Univariate Gaussian Distribution

- \bullet $\mathcal{X} = \mathbb{R}$
- Gaussian: $X \sim \mathcal{N}(\mu, \sigma^2)$, $p(x) = \frac{1}{\sigma \sqrt{2\pi}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$
 - $\mu \in \mathbb{R}$, $\sigma^2 \in \mathbb{R}_+$
 - Ubiquitous in science; parly because of the Central Limit Theorem
 - Standard Normal: $\mu = 0$, $\sigma = 1$
 - Sensitive to outliers
 - Implement it in Python: here, § 5

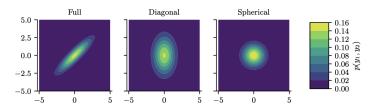


The Holy Grail

• Multivariate Normal: $X \sim \mathcal{N}(\mu, \Sigma)$, $p(x) = \frac{1}{(2\pi)^{D/2} |\Sigma|^{1/2}} \exp\left[-\frac{1}{2}(x-\mu)^{\top} \Sigma^{-1}(x-\mu)\right]$ • $\mu \in \mathbb{R}^D$, $\Sigma \in \mathbb{R}^{D \times D}$

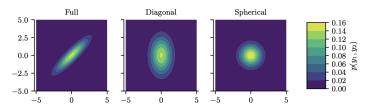
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 - $\mu \in \mathbb{R}^D$, $\Sigma \in \mathbb{R}^{D \times D}$
 - Full Covariance Matrix: D(D+1)/2 parameters; we divide by 2 since Σ is symmetric
 - Diagonal covariance matrix: D parameters, and 0s in the off-diagonal terms
 - Spherical covariance matrix: $\Sigma = \sigma^2 I_D$, so only one free parameter σ



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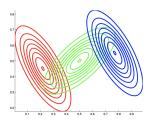
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Implement it in Python: here

Mixture of Gaussians

- Gaussian mixture model (GMM): $p(x) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mu_k, \Sigma_k)$
 - The π_k 's are non-negative and sum up to 1
 - If we let the number of mixture components grow sufficiently large, a GMM can approximate any smooth distribution over \mathbb{R}^D
 - GMMs are often used for unsupervised clustering of real-valued data samples $x_n \in \mathbb{R}^D$





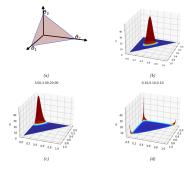
• Implement it in Python: here

Dirichlet Distribution (Unit Simplex Δ^{K-1})

•
$$X \sim \text{Dir}(\alpha)$$
, $p(x) \propto \prod_{k=1}^K x_k^{\alpha_k - 1}$,

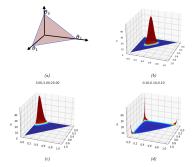
Dirichlet Distribution (Unit Simplex Δ^{K-1})

- $X \sim \text{Dir}(\alpha)$, $p(x) \propto \prod_{k=1}^K x_k^{\alpha_k 1}$, $\alpha \in \Delta^{K-1}$ and $\alpha_0 = \sum_{k=1}^K \alpha_k$
- α_0 controls how peaked the distribution is, and the α_k 's control where the peak occurs
- Mean: $\mathbb{E}(x_k) = \alpha_k/\alpha_0$



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- Useful to quantify epistemic and aleatoric uncertainties in classification problems
- Implement it in Python: here

Markov Chains

- Let $(x_t)_{t\in\mathbb{N}}$ be a sequence of elements of \mathbb{R}^D
- Markov property: $p(x_{t+\tau} \mid x_1, \dots, x_t) = p(x_{t+\tau} \mid x_t)$

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- Markov property: $p(x_{t+\tau} \mid x_1, \dots, x_t) = p(x_{t+\tau} \mid x_t)$
- In turn, we have that $p(x_1, ..., x_T) = p(x_1) \prod_{t=2}^{T} \underbrace{p(x_t \mid x_{t-1})}_{\text{transition function}}$
 - This is a Markov model (MM)
- If $p(x_t \mid x_{t-1})$ is indep. of time, the MM is called stationary
- Implement it in Python: here

Markov Chains

- Stationary distribution π : intuitively, it is the long term distribution over states
- Finding π: (Murphy, 2023, § 2.6.4)
- Stationary distributions need not always exist (Murphy, 2023, § 2.6.4.3 - 2.6.4.4)

Statistics

- Probability theory: modeling the distribution over observed data outcomes D given known parameters θ by computing $p(D \mid \theta)$
- Statistics: inverse problem. Infer the unknown parameters θ given observations, i.e. compute $p(\theta \mid D)$

- Parameter θ as unknown (rv), and data D as fixed and known
- Represent uncertainty about θ , after seeing data D, by computing the posterior distribution via Bayes' rule

$$p(\theta \mid D) = \frac{p(\theta)p(D \mid \theta)}{\int_{\Theta} p(\theta)p(D \mid \theta)d\theta} \propto p(\theta)p(D \mid \theta)$$

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- Marginal likelihood: $p(D) = \int_{\Theta} p(\theta)p(D \mid \theta)d\theta$, normalization constant, crucial in Bayesian Model Selection (BMS)

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- Example: see (Murphy, 2023, § 3.2.1)
 - If we assume iid data, then $p(D \mid \theta) = \prod_{y \in D} p(y \mid \theta)$
 - $p(y \mid \theta)$: distributions we introduced before, e.g. a Binomial

Bayesian Statistics: MAP

Maximum A Posteriori estimate (MAP):

$$\hat{\theta}_{\mathsf{map}} = \argmax_{\theta \in \Theta} p(\theta \mid D) = \argmax_{\theta \in \Theta} [\log p(\theta) + \log p(D \mid \theta)]$$

- It is the posterior mode (most probable value)
- Confront it with the MLE

$$\mathop{\arg\max}_{\theta\in\Theta}p(D\mid\theta)=\mathop{\arg\max}_{\theta\in\Theta}\log p(D\mid\theta)$$

- An extra component coming from the prior $p(\theta)$
- If we use uniform prior $p(\theta) \propto 1$, MAP = MLE

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- If we use uniform prior $p(\theta) \propto 1$, MAP = MLE
- Implement it in Python: here and (Murphy, 2023, § 6.5.3)

Bayesian Statistics: Posterior Predictive

Posterior Predictive Distribution:

$$p(y \mid D) = \int_{\Theta} p(y \mid \theta) p(\theta \mid D) d\theta$$

$$= \mathbb{E}_{\theta \sim p(\theta \mid D)} [p(y \mid \theta)]$$
(1)

- Given the data D we observed, it tells us what is the probability that the next observation is some value y
- Implement it in Python: here

Bayesian Statistics: Posterior Predictive

- In ML: interested in predicting outcomes y given input features x
- Use conditional probability of the form $p(y \mid x, \theta)$ (e.g. coming from a neural network)
- (Conditional) likelihood is $p(D \mid \theta) = \prod_{(x,y) \in D} p(y \mid x, \theta)$

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- (Conditional) likelihood is $p(D \mid \theta) = \prod_{(x,y) \in D} p(y \mid x, \theta)$
- Eq. (1) then becomes

$$p(y \mid x, D) = \int_{\Theta} p(y \mid x, \theta) p(\theta \mid D) d\theta$$
$$= \mathbb{E}_{\theta \sim p(\theta \mid D)} [p(y \mid x, \theta)]$$

- By integrating out the unknown parameters, we reduce the chance of overfitting
 - We are computing the weighted average of predictions from an infinite number of models

Frequentist Statistics: Basic Concepts

- Frequentist statistics: uncertainty by calculating how a quantity estimated from data (e.g. a parameter) would change if the data were changed
 - Captured by the sampling distribution of an estimator
- This notion of variation across repeated trials: uncertainty modeling by the frequentist approach

Frequentist Statistics: Sampling Distribution

- Estimator: decision procedure that specifies what action to take given some observed data *D*
 - Parameter estimation: the action space is to return a parameter vector via function δ , so $\hat{\theta} = \delta(D)$, e.g. the MLE
- Sampling distribution of an estimator: distribution of results we would see if we applied the estimator multiple times to different datasets sampled from some distribution
 - Parameter estimation: it is the distribution of $\hat{\theta}$, viewed as a random variable that depends on the random sample D
- Implement it in Python: here

Frequentist Statistics: Drawbacks

- Frequentist Statistics has some counterintuitive properties (Murphy, 2023, § 3.3.5 - 3.3.6)
- Popular because easy, taught at UG level, sometimes faster to implement than Bayesian
- "Inside every Non-Bayesian, there is a Bayesian struggling to get out", D. Lindley, cf. Jaynes (2002)
- CAREFUL: Bayesian approach is only as correct as its modeling assumptions
 - Check sensitivity of the conclusions to the choice of prior (and likelihood): BMS

Selecting the Prior: Conjugate Priors

- A prior $p(\theta) \in \mathcal{P}$ is a conjugate prior for a likelihood function $p(D \mid \theta)$ if the posterior is in the same parameterized family as the prior, i.e. $p(\theta \mid D) \in \mathcal{P}$
- ullet That is, ${\cal P}$ is closed under Bayesian updating
- Conjugate priors simplify the computation of the posterior (Murphy, 2023, § 3.4)
- Implement it in Python: here

Selecting the Prior: Noninformative Priors

- When we have little or no domain specific knowledge, desirable to use a noninformative prior, to "let the data speak for itself"
- No unique way to define such priors, and they all encode some kind of knowledge
 - Better to use the term minimally informative prior (Murphy, 2023, § 3.5)
- Implement it in Python: here

Other Statistical Concepts

Model selection: we have a set of different models \mathcal{M} , each of which may fit the data to different degrees, and each of which may make different assumptions

- How to pick the best model from this set, or to average over all of them
- Assumed that the "true" model is in M (Murphy, 2023, § 3.8)
- Model checking: Bayesian inference is "optimal", but only if the modeling assumptions are correct. How to assess if a model is reasonable?
 - We assume that we do not have a specific alternative model in mind
 - We see if the data we observe is "typical" of what we might expect if our model were correct (Murphy, 2023, § 3.9)



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