

# Week 3, Lecture 5 - Bayesian vs. frequentist approaches

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# Outline

- ▶ Administrative Issues
- ▶ Bayesian Statistics
- ▶ A Couple Examples

**Based on slides from Joyce Ho.**

# Frequentist vs Bayesian

## Frequentist

- ▶ Data are a repeatable random sample (there is a frequency)
- ▶ Underlying parameters remain constant during repeatable process
- ▶ Parameters are fixed
- ▶ Prediction via the estimated parameter value

## Bayesian

- ▶ Data are observed from the realized sample
- ▶ Parameters are unknown and described probabilistically (random variables)
- ▶ Data are fixed
- ▶ Prediction is expectation over unknown parameters

# Freq v. Bayes can hugely influence how we interpret the world



Figure: <https://xkcd.com/1132/>

# Bayesian statistics

## Bayesian - Derivation

Bayes' theorem may be derived from the definition of conditional probability:

$$P(A | B) = \frac{P(A \cap B)}{P(B)}, \text{ if } P(B) \neq 0$$

$$P(B | A) = \frac{P(B \cap A)}{P(A)}, \text{ if } P(A) \neq 0$$

because

$$P(B \cap A) = P(A \cap B)$$

$$\Rightarrow P(A \cap B) = P(A | B) P(B) = P(B | A) P(A)$$

$$\Rightarrow P(A | B) = \frac{P(B | A) P(A)}{P(B)}, \text{ if } P(B) \neq 0$$

# Classic Example: Binomial Experiment

- ▶ Given a sequence of coin tosses  $x_1, x_2, \dots, x_M$ , we want to estimate the (unknown) probability of heads:

$$P(H) = \theta$$

- ▶ The instances are independent and identically distributed samples
- ▶ Note that  $x$  can take on many possible values potentially if we decide to use a multinomial distribution instead

# Likelihood Function

- ▶ How good is a particular parameter?
  - ▶ Answer: Depends on how likely it is to generate the data

$$L(\theta; D) = P(D \mid \theta) = \sum_m P(x_m \mid \theta)$$

- ▶ Example: Likelihood for the sequence: H, T, T, H, H

$$L(\theta; D) = \theta(1 - \theta)(1 - \theta)\theta\theta = \theta^3(1 - \theta)^2$$



# Maximum Likelihood Estimate (MLE)

- ▶ Choose parameters that maximize the likelihood function
  - ▶ Commonly used estimator in statistics
  - ▶ Intuitively appealing
- ▶ In the binomial experiment, MLE for probability of heads

$$\hat{\theta} = \frac{N_H}{N_H + N_T}$$

- ▶ Optimization problem approach



# Is MLE the only option?

- ▶ Suppose that after 10 observations, MLE estimates the probability of a heads is 0.7, would you bet on heads for the next toss?
- ▶ How certain are you that the true parameter value is 0.7?
- ▶ Were there enough samples for you to be certain?

# Bayesian Approach

- ▶ Formulate knowledge about situation probabilistically
  - ▶ Define a model that expresses qualitative aspects of our knowledge (e.g., forms of distributions, independence assumptions)
  - ▶ Specify a **prior** probability distribution for unknown parameters in the model that expresses our beliefs about which values are more or less likely
- ▶ Compute the **posterior** probability distribution for the parameters, given observed data
- ▶ Posterior distribution can be used for:
  - ▶ Reaching conclusions while accounting for uncertainty
  - ▶ Make predictions by averaging over posterior distribution

# Posterior Distribution

- ▶ Posterior distribution for model parameters given the observed data combines the prior distribution with the likelihood function using Bayes' rule:

$$P(\theta \mid D) = \frac{P(\theta)P(D \mid \theta)}{P(D)}$$

- ▶ Denominator is just a normalizing constant so you can write it proportionally as:

$$\text{Posterior} \propto \text{Prior} \times \text{Likelihood}$$

- ▶ Predictions can be made by integrating with respect to posterior:

$$P(\text{newdata} \mid D) = \int_{\theta} P(\text{newdata} \mid \theta)P(\theta \mid D)$$

## Revisiting Binomial Experiment

- ▶ Prior distribution: uniform for  $\theta$  in  $[0, 1]$
- ▶ Posterior distribution:

$$P(\theta \mid x_1, \dots, x_M) \propto P(x_1, \dots, x_M \mid \theta) \times 1$$

- ▶ Example: 5 coin tosses with 4 heads, 1 tail
  - ▶ MLE estimate:

$$P(\theta) = \frac{4}{5} = 0.8$$

- ▶ Bayesian prediction:

$$P(x_{M+1} = H \mid D) = \int \theta P(\theta \mid D) d\theta = \frac{5}{7}$$



# Bayesian Inference and MLE

- ▶ MLE and Bayesian prediction differ
- ▶ However. . .
  - ▶ IF prior is well-behaved (i.e., does not assign 0 density to any “feasible” parameter value)
  - ▶ THEN both MLE and Bayesian prediction converge to the same value as the training data becomes infinitely large

# Features of the Bayesian Approach

- ▶ Probability is used to describe “physical” randomness and uncertainty regarding the true values of the parameters
  - ▶ Prior and posterior probabilities represent degrees of belief, before and after seeing the data
- ▶ Model and prior are chosen based on the knowledge of the problem and not, in theory, by the amount of data collected or the question we are interested in answering

# Priors

- ▶ Objective priors: noninformative priors that attempt to capture ignorance and have good frequentist properties
- ▶ Subjective priors: priors should capture our beliefs as well as possible. They are subjective but not arbitrary.
- ▶ Hierarchical priors: multiple levels of priors
- ▶ Empirical priors: learn some of the parameters of the prior from the data (“Empirical Bayes”)
  - ▶ Robust, able to overcome limitations of mis-specification of prior
  - ▶ Double counting of evidence / overfitting

# Conjugate Prior

- ▶ If the posterior distribution are in the same family as prior probability distribution, the prior and posterior are called conjugate distributions
- ▶ All members of the exponential family of distributions have conjugate priors

<b>Conjugate prior</b>		<b>Prior hyperparameter</b>	<b>Posterior hyperparameters</b>
<b>Likelihood distribution</b>			
Bernoulli	Beta	$\alpha, \beta$	$\alpha + \sum x_i, \beta + n - \sum x_i$
Multinomial	Dirichlet	$\alpha$	$\alpha + \sum x_i$
Poisson	Gamma	$\alpha, \beta$	$\alpha + \sum x_i, \beta + n$



# Linear Regression (Classic Approach)

$$y = w^\top x + \epsilon, \epsilon \sim N(0, \sigma^2)$$

$$P(y_i|w, x_i, \sigma^2) = N(w^\top x_i, \sigma^2)$$

$$P(y|w, X, \sigma^2) = \prod_i P(y_i|w, x_i, \sigma^2)$$

 maximize log likelihood

$$\max \ln(P(y|w, x, \sigma^2)) = \max \sum_i \ln(N(y_i|w, x_i, \sigma^2))$$

$$w_{\text{MLE}} = \operatorname{argmin}_w \frac{1}{2} \sum_i (y_i - x_i^\top w)^2$$

$$w = (X^\top X)^{-1} X^\top y$$

# Bayesian Linear Regression

- ▶ Prior is placed on either the weight,  $w$ , or the variance,  $\sigma$
- ▶ Conjugate prior for  $w$  is normal distribution

$$P(w) \sim N(\mu_0, S_0)$$

$$P(w | y) \sim N(\mu, S)$$

$$S^{-1} = S_0^{-1} + \frac{1}{\sigma^2} X^T X$$

$$\mu = S \left( S_0^{-1} \mu_0 + \frac{1}{\sigma^2} X^T y \right)$$

- ▶ Mean is weighted average of OLS estimate and prior mean, where weights reflect relative strengths of prior and data information

# Computing the Posterior Distribution

**Analytical integration** Works when “conjugate” prior distributions can be used, which combine nicely with the likelihood—usually not the case

**Gaussian approximation** Works well when there is sufficient data compared to model complexity—posterior distribution is close to Gaussian (Central Limit Theorem) and can be handled by finding its mode

**Markov Chain Monte Carlo** Simulate a Markov chain that eventually converges to the posterior distribution—currently the dominant approach

**Variational approximation** Cleverer way to approximate the posterior and maybe faster than MCMC but not as general and exact

# Approximate Bayesian Inference

- ▶ Stochastic approximate inference (MCMC)
  - ▶ Design an algorithm that draws sample from distribution
  - ▶ Inspect sample statistics
  - ▶ (Pros) Asymptotically exact
  - ▶ (Cons) Computationally expensive
  - ▶ (Cons) Tricky Engineering concerns
- ▶ Structural approximate inference (variational Bayes)
  - ▶ Use an analytical proxy that is similar to original distribution
  - ▶ Inspect distribution statistics of proxy
  - ▶ (Pros) Often insightful & fast
  - ▶ (Cons) Often hard work to derive
  - ▶ (Cons) Requires validation via sampling

# Markov Chain Monte Carlo

Markov Chain Monte Carlo

## A Simple Markov Chain



# Markov Chains

- ▶ A random process has Markov property iff:

$$p(X_t \mid x_{t-1}, X_{t-2}, \dots, X_1) = p(X_t \mid x_{t-1})$$

- ▶ Finite-state Discrete Time Markov Chains can be completely specified by the transition matrix  $P$

$$P = [p_{ij}]; p_{ij} = P[X_t = j \mid X_{t-1} = i]$$

- ▶ Stationarity: As  $t$  approaches infinity, the Markov chain converges in distribution to its stationary distribution (independent of starting position)

# Markov Chains

- ▶ Irreducible: any set of states can be reached from any other state in a finite number of moves
  - ▶ Assuming a stationary distribution exists, it is unique if the chain is irreducible
- ▶ Aperiodicity: greatest common divisor of return times to any particular state  $i$  is 1
- ▶ Ergodicity: if the Markov chain has a stationary distribution, aperiodic, irreducible then:

$$E_{\pi}[h(X)] = \frac{1}{N} \sum h(X^{(t)}) \text{ as } N \rightarrow \infty$$



# MCMC Algorithms

- ▶ Posterior distribution is too complex to sample from directly, simulate a Markov chain that converge (asymptotically) to the posterior distribution
  - ▶ Generating samples while exploring the state space using a Markov chain mechanism
  - ▶ Constructed so the chain spends more time in the important regions
  - ▶ Irreducible and aperiodic Markov chains with target distribution as the stationary distribution
- ▶ Can be very slow in some circumstances but is often the only viable approach to Bayesian inference using complex models

# The Monte Carlo Principle

- ▶ General Problem:

$$E_{\pi}[h(X)] = \int h(x)\pi(x)dx$$

- ▶ Instead, draw samples from the target density to estimate the function:
  - ▶  $X^{(1)}, X^{(2)}, \dots, X^{(N)} \sim \pi(x)$
  - ▶  $E_{\pi}[h(X)] \approx \frac{1}{N} \sum h(X^{(t)})$

# Metropolis-Hastings Algorithm

- ▶ Most popular MCMC (Metropolis, 1953; Hastings 1970)
- ▶ Main Idea:
  - ▶ Create a Markov chain whose transition matrix does not depend on the normalization term
  - ▶ Make sure the chain has a stationary distribution and is equal to the target distribution
  - ▶ After sufficient number of iterations, the chain converges to the stationary distribution

# Metropolis-Hasting Algorithm

At each iteration  $t$

- ▶ Step 1: Sample a candidate point from proposal distribution

$$y \sim q(y \mid x^{(t)})$$

- ▶ Step 2: Accept the next point with probability

$$\alpha(x^{(t)}, y) = \min \left[ 1, \frac{p(y)q(x^{(t)} \mid y)}{p(x^{(t)})q(y \mid x^{(t)})} \right]$$

# Illustration of Metropolis-Hasting Algorithm



# Variations of Proposal Distribution

- ▶ Random-walk is when proposal is dependent on previous state
  - ▶  $y \sim q(y \mid x^{(t)})$
- ▶ Symmetric proposal originally proposed by Metropolis (e.g., Gaussian distribution)
  - ▶  $q(x \mid y) \equiv q(y \mid x)$
- ▶ Independent sampler uses a proposal independent of  $x$ 
  - ▶  $q(y \mid x) \equiv q(y)$

# Metropolis-Hastings Notes

- ▶ Normalizing constant of the target distribution is not required
- ▶ Choice of proposal distribution is very important:
  - ▶ too narrow  $\rightarrow$  not enough mixing
  - ▶ too wide  $\rightarrow$  high correlations
- ▶ Usually  $q$  is chosen so the proposal distribution is easily to sample
- ▶ Easy to simulate several independent chains in parallel

# Acceptance Rates

- ▶ Important to monitor the acceptance rate (fraction of candidate draws that are accepted)
- ▶ Too high means the chain is not mixing well and not moving around the parameter space quickly enough
- ▶ Too low means algorithm is too inefficient (too many candidate draws)
- ▶ General rules of thumb:
  - ▶ Random walk: Somewhere between 0.25 and 0.50
  - ▶ Independent: Closer to 1 is preferred



# Gibbs Sampling (Geman & Geman, 1984)

- ▶ Popular in statistics and graphical models
- ▶ Special form of Metropolis-Hastings where we always accept a candidate point and we know the full conditional distributions
- ▶ Easy to understand, easy to implement
- ▶ Open-source, black-box implementations available

# Gibbs Sampling

Sample or update in turn:

$$X_1^{(t+1)} \sim \pi \left( x_1 \mid x_2^{(t)}, x_3^{(t)}, \dots, x_k^{(t)} \right)$$

$$X_2^{(t+1)} \sim \pi \left( x_2 \mid x_1^{(t+1)}, x_3^{(t)}, \dots, x_k^{(t)} \right)$$

$$X_3^{(t+1)} \sim \pi \left( x_3 \mid x_1^{(t+1)}, x_2^{(t+1)}, x_4^{(t)}, \dots, x_k^{(t)} \right)$$

...

$$X_k^{(t+1)} \sim \pi \left( x_k \mid x_1^{(t+1)}, x_2^{(t+1)}, \dots, x_{k-1}^{(t+1)} \right)$$

# Illustration of Gibbs Sampler



## Practicalities: Burn-In

- ▶ Convergence usually occurs regardless of our starting point, so can pick any feasible starting point
- ▶ Chain convergence varies depending on the starting point
- ▶ As a matter of practice, most people throw out a certain number of the first draws, known as the burn-in
- ▶ The remaining draws are closer to the stationary distribution and less dependent on the starting point
- ▶ Plot the time series for each quantity of interest and the auto-correlation functions to see if the chain has converged

# Practicalities: Number of Chains

- ▶ Suggestion: Experiment with different number of chains
- ▶ Several long runs (Gelman & Rubin, 1992)
  - ▶ Gives indication of convergence
  - ▶ Sense of statistical security
- ▶ One very long run (Geyer, 1992)
  - ▶ Reaches parts other schemes cannot reach

# Other Flavors of MC

- ▶ Auxiliary Variable Methods for MCMC
  - ▶ Hybrid Monte Carlo (HMC)
  - ▶ Slice Sampler
- ▶ Reversible jump MCMC
- ▶ Adaptive MCMC
- ▶ Sequential Monte Carlo (SMC) and Particle Filters

# Variational Approximation

Variational Approximation

# Bayesian Inference via Variational Approximation

- ▶ Related to “mean field” and other approximation methods from physics
- ▶ Idea: Find an approximate density that is maximally similar to the true posterior





# Kullback–Leibler divergence

$$D_{\text{KL}}(P\|Q) = - \sum_i P(i) \log \frac{Q(i)}{P(i)}$$

or

$$D_{\text{KL}}(P\|Q) = \int_{-\infty}^{\infty} p(x) \log \frac{p(x)}{q(x)} dx$$

# The Mean-Field Form

- ▶ A common way of restricting the class of approximate posterior is to consider those posteriors that factorize into independent partitions

$$q(\theta) = \prod_i q_i(\theta_i)$$

- ▶ Each  $q_i(\theta_i)$  is the approximate posterior for the  $i$ th subset of parameters
- ▶ This implies a straightforward algorithm for inference by cycling over each set of parameters given current sets of others

## Example: Variational Inference



Figure: Figure 10.4 from Bishop PRML

# Limitations and Criticisms of Bayesian Methods

- ▶ It is hard to come up with a prior (subjective) and the assumptions may be wrong
- ▶ Closed world assumption: need to consider all possible hypotheses for the data before observing the data
- ▶ Computationally demanding (compared to frequentist approach)
- ▶ Use of approximations weakens coherence argument

# Bayesian statistics

## Example problem - HIV test

- ▶ Rapid home tests will pick up an infection 97.7% of the time at 28 days after exposure (sensitivity).
- ▶ These same tests have a specificity of  $\sim 95\%$ .
- ▶ 0.34% of the US population is estimated to be infected.

Given a positive test, what is the chance of the average person in the US being infected?

How would this change if  $\sim 10\%$  of the population were infected?

# Implementation - PyMC3

```
import pymc3 as pm

n = 100
heads = 61

with pm.Model() as coin_context:
    p = pm.Beta('p', alpha=2, beta=2)
    y = pm.Binomial('y', n=n, p=p, observed=heads)
    trace = pm.sample()

pm.summary(t, varnames=['p'])
```

# Implementation - PyMC3

Output:

p:

Mean	SD	MC Error	95% HP
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0.615	0.050	0.002	[0.517
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Posterior quantiles:

2.5	25	50	75
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0.517	0.581	0.616	0.654
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# Implementation - emcee

```
import emcee

def lnprob(p):
    return lnprior(p) + lnobs(p, heads, n)

sampler = emcee.EnsembleSampler(nwalkers=3, ndim=1, lnprob=lnprob)

sampler.run_mcmc(pos, 500)

samples = sampler.chain
```



## Further Reading

- ▶ PyMC3 (python)
- ▶ emcee (python)
- ▶ Stan (C++, python, R)
- ▶ Bayesian Data Analysis
- ▶ Probabilistic Programming & Bayesian Methods for Hackers