Bayesian Modeling: Foundations and Inference

ELG 5218 - Uncertainty Evaluation in Engineering Measurements and Machine Learning

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Learning goals

By the end of this lecture, you should be able to:

- Define **uncertainty quantification (UQ)**.
- Specify a Bayesian model using **prior**, **likelihood**, and **posterior**.
- Explain and compute **MLE** and **MAP**.
- Derive and interpret a simple conjugate update (Beta–Binomial).
- Compute and interpret **credible intervals** (central and HPD/HDI).
- Use the posterior to form the **posterior predictive distribution**.

Roadmap

- Introduction to UQ (what / why / how to represent uncertainty)
- Confidence intervals vs credible intervals (CI vs CrI)
- Bayesian inference framework (prior, likelihood, posterior, evidence)
- Conjugate priors and Beta–Binomial example
- Point estimation: MLE and MAP (and connection to regularization)
- Posterior summaries (mean/median/mode, intervals) and prediction (PPD)

What is Uncertainty Quantification?

Uncertainty Quantification (UQ) develops rigorous methods to characterize the impact of "limited knowledge" on quantities of interest.

Two fundamental sources of uncertainty

1. **Aleatoric Uncertainty**: inherent randomness in physical processes (irreducible)
2. **Epistemic Uncertainty**: lack of knowledge that can be reduced with more data/modeling

Key questions in UQ

- What is the expected value of our quantity of interest?
- How much does it vary (variance / standard deviation)?
- What range of values is plausible (intervals)?
- How do we update beliefs when new data arrive?

Example: Heart rate measurement reported as (60 ± 4) beats/minute.

Representing uncertainty

Common ways to express uncertainty:

1. **Standard error**: variability of an estimate
2. **Confidence intervals**: frequentist
3. **Credible intervals**: Bayesian
4. **Probability distributions**: full description of uncertainty
5. **Quantiles / moments**: extracted summaries

A point estimate without uncertainty quantification is incomplete.

A visual language for uncertainty

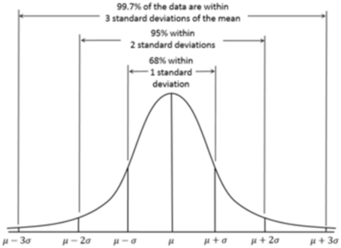


Figure: Normal distribution with interval bands

- Distributions communicate **shape** (skew, multimodality), not only spread.
- Intervals are summaries; distributions are the full story.

Confidence intervals: frequentist perspective

Definition: A 95% confidence interval (CI) is constructed so that:

95% of similarly constructed CIs contain the true parameter value.

Key properties

- The parameter θ is **fixed but unknown**
- The interval is **random** (depends on the sample)
- Interpretation is about **long-run frequency** across repeated sampling

What it does not mean:

$$\mathbb{P}\big(\theta \in [a, b]\big) = 0.95 \quad \textbf{WRONG}$$

Credible intervals: Bayesian perspective

Definition: A 95% credible interval (CrI) satisfies:

$$\mathbb{P}\big(\theta \in [a, b] \mid \text{data}\big) = 0.95$$

Key properties

- The parameter θ is treated as a **random variable**
- The interval is **fixed** (given the posterior)
- Interpretation is **posterior probability** (direct probability statement)

Two common credible intervals

1. **Central (equal-tailed)**: $\alpha/2$ mass in each tail
2. **HPD / HDI**: region(s) with highest posterior density

Credible intervals: central (equal-tailed)

Central interval: contains $\alpha/2$ probability in each tail.

$$\mathrm{CrI}_{1-\alpha} = \left[q_{\alpha/2},\ q_{1-\alpha/2}\right]$$

Example (95%):

$$\mathrm{CrI}_{0.95} = \left[q_{0.025},\ q_{0.975}\right]$$

Interpretation:

$$\mathbb{P}\big(\theta \in [q_{0.025}, q_{0.975}] \mid D\big) = 0.95$$

- simple and widely used
- may exclude the mode for skewed posteriors

Credible intervals: highest posterior density (HPD/HDI)

HPD/HDI: region with the highest posterior density containing $(1 - \alpha)$ mass.

Intuition

- all points inside are more credible than points outside
- typically shorter than equal-tailed intervals for skewed posteriors
- may be multi-interval for multimodal posteriors

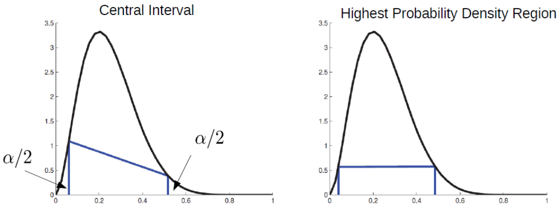


Figure: Central and HPD intervals

Comparison: CI vs CrI

Aspect	Confidence interval	Credible interval
Parameter	Fixed	Random variable
Interval	Random	Fixed (given posterior)
Uses prior?	No	Yes
Meaning	Long-run coverage	Posterior probability
Computation	Often analytic	Often via sampling / numeric

Modeling Data Probabilistically: A Simplistic View

- Assume a dataset $X = \{x_1, \ldots, x_N\}$ is generated from a probabilistic model with unknown parameters θ.
- For i.i.d. observations: $\quad x_1, \ldots, x_N \sim p(x \mid \theta)$.
- Plate notation: shaded nodes = observed; unshaded nodes = unknown / unobserved.
- Goal: estimate the unknowns (here, θ) given the observed data X.
- Use the learned model for prediction:

$$p(x^* \mid \theta) \quad \text{or} \quad p(x^* \mid X).$$

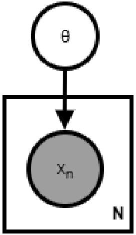
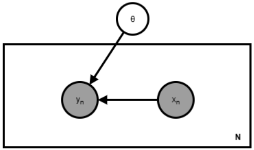


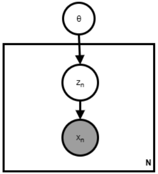
Figure: Simplified plate model for i.i.d. data

Modeling Data Probabilistically

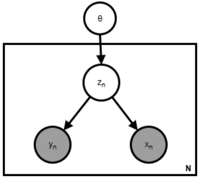
- This basic setup generalizes in many ways.
- Any node (even if observed) that we are uncertain about is modeled by a probability distribution.
- These nodes become the **random variables** of the model.
- The full model is specified via a **joint probability distribution** over all random variables.
- The goal is to **infer unknowns** of the model given the observed data.



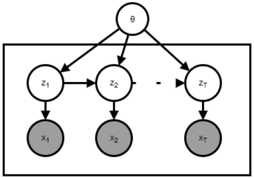
A Simple Supervised Learning Model



A Latent Variable Model for Unsupervised Learning



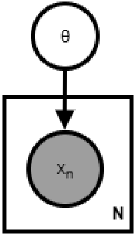
A Latent Variable Model for Supervised Learning



A Latent Variable Model for Sequential Data

Model Specification: Likelihood and Prior

- Probabilistic models require two key ingredients: **likelihood** and **prior**.
- **Likelihood** $p(x \mid \theta)$ ("observation model"): specifies how data is generated and measures data fit (loss) for a given θ.
- **Prior** $p(\theta)$: specifies how plausible parameter values are *a priori*; it often acts like a regularizer.
- Domain knowledge can guide both likelihood and prior choices.



$$p(\theta \mid X) \propto p(X \mid \theta)\, p(\theta)$$

Parameter Estimation vs. Bayesian Inference

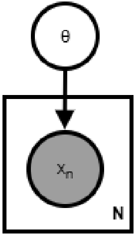
- A simplest approach is **point estimation**: find θ that makes the observed data most likely.

$$\hat{\theta} = \arg\max_{\theta} \log p(X \mid \theta).$$

- But a single point estimate does **not** quantify uncertainty in θ.
- **Bayesian inference** estimates the **full posterior**:

$$p(\theta \mid X) = \frac{p(X \mid \theta)\, p(\theta)}{p(X)} \propto \underbrace{p(X \mid \theta)}_{\text{Likelihood}} \times \underbrace{p(\theta)}_{\text{Prior}}.$$

- The posterior captures uncertainty in θ; we will study point estimation, Bayesian inference, and hybrids.



Posterior $=$ *Likelihood* $\times$ *Prior*
(normalized)

The Bayesian approach: overview

Core philosophy: Probability represents a *degree of belief*, updated with evidence.

Three key components

1. **Prior** $p(\theta)$: initial beliefs about parameters
2. **Likelihood** $p(D \mid \theta)$: probability of data given parameters
3. **Posterior** $p(\theta \mid D)$: updated beliefs after observing data

Goal

- compute posterior, summarize it, and make predictions for new observations $x^\star$

Bayes' theorem

$$\boxed{p(\theta \mid D) = \frac{p(D \mid \theta)\, p(\theta)}{p(D)}}$$

Components

- $p(\theta \mid D)$ posterior (what we want)
- $p(D \mid \theta)$ likelihood
- $p(\theta)$ prior
- $p(D)$ evidence / marginal likelihood (normalization)

$$p(\theta \mid D) \propto p(D \mid \theta)\, p(\theta)$$

$$p(D) = \int p(D \mid \theta)\, p(\theta)\, d\theta$$

Bayesian inference pipeline (big picture)

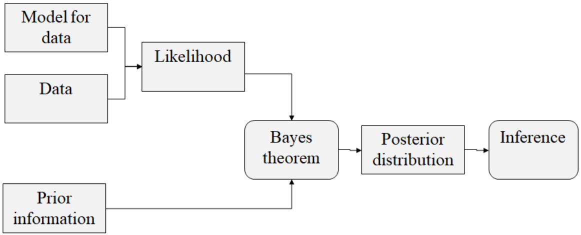


Figure: Bayesian inference

- Modeling: choose $p(D \mid \theta)$ and $p(\theta)$
- Inference: compute/approximate $p(\theta \mid D)$
- Decision/prediction: use posterior and posterior predictive

Prior distribution: encoding beliefs

Purpose: incorporate prior knowledge, stabilize inference, and regularize.

Types of priors

1. **Uninformative/flat**: minimal information (but still encodes assumptions)
2. **Weakly informative**: gentle regularization (prevents extreme values)
3. **Informative**: genuine prior knowledge (historical data, expert belief)
4. **Conjugate**: chosen for analytic convenience

Key principle: Posterior is a compromise between prior and likelihood; strong data can overwhelm weak priors.

How to choose a prior in practice

- **Domain knowledge:** expert judgment, historical datasets, physics constraints
- **Sensitivity analysis:** change priors and check how conclusions change
- **Prior predictive check:** sample from prior and see if it generates reasonable synthetic data
- **Weak vs strong:** with few observations, the prior matters more

Likelihood function: probability of data given parameters

$$p(D \mid \theta) = \prod_{i=1}^{N} p(x_i \mid \theta)$$

Likelihood is a model of the data-generating process

- The likelihood encodes sensor physics + imperfections.
- It is **not** "how likely x is"; it is "how likely y is, if x were true".
- Choosing the likelihood is often the most important modeling decision.

Typical likelihood choices

- **Binomial**: successes in n trials
- **Gaussian**: continuous measurements with additive noise
- **Poisson**: counts / event arrivals

Posterior distribution: updated beliefs

$$p(\theta \mid D) = \frac{p(D \mid \theta)\, p(\theta)}{p(D)}$$

Posterior interpretation

- **Mode** (MAP), **mean**, **median**
- **Spread**: uncertainty about θ
- **Quantiles**: credible intervals

Posterior predictive distribution (PPD)

Goal: predict a new observation $x^\star$.

$$p(x^\star \mid D) = \int p(x^\star \mid \theta)\, p(\theta \mid D)\, d\theta$$

Interpretation

- averages predictions over all plausible parameter values
- accounts for parameter uncertainty and observation noise

Plug-in approximation (often used, but weaker)

$$p(x^\star \mid D) \approx p(x^\star \mid \hat{\theta})$$

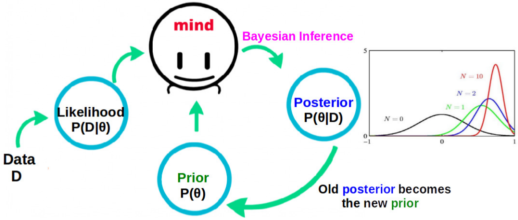


Figure: Bayesian Update

Conjugate priors: computational convenience

Definition: A prior is **conjugate** to a likelihood if the posterior has the same functional form as the prior.

Why it matters

- closed-form posterior (no sampling needed)
- easy to interpret updates
- sequential updating is straightforward

Likelihood	**Prior**	**Posterior**
Binomial / Bernoulli	Beta	Beta
Poisson	Gamma	Gamma
Gaussian (known σ)	Gaussian	Gaussian
Multinomial	Dirichlet	Dirichlet

When conjugacy breaks: optimization and approximation

- Many useful models do **not** have closed-form posteriors.
- Example: logistic regression likelihood (classification).
- Then we rely on:
  - **Optimization**: MAP via Newton / quasi-Newton.
  - **Approximation**: Laplace approximation, variational inference.
  - **Sampling**: MCMC (e.g., NUTS / HMC).

Lecture 2

Gaussian and linear models, Bayesian linear regression, and MAP logistic regression with Newton's method.

Beta–Binomial conjugacy: the canonical example

Model

- Prior: $\theta \sim \mathrm{Beta}(\alpha, \beta)$
- Likelihood: $k \sim \mathrm{Binom}(n, \theta)$
- Posterior: $\theta \mid k \sim \mathrm{Beta}(\alpha + k,\ \beta + n - k)$

Update rule

$$\alpha^\star = \alpha + k, \qquad \beta^\star = \beta + (n - k)$$

Pseudo-count interpretation

- prior contributes $\alpha - 1$ "successes" and $\beta - 1$ "failures"
- data contributes k successes and $n - k$ failures

Beta distribution: prior intuition

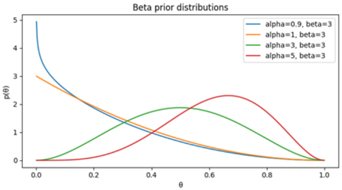


Figure: Beta prior shapes for different α with $\beta = 3$

- larger $\alpha + \beta \Rightarrow$ stronger prior (more concentrated)
- $\alpha > \beta$ biases belief toward larger θ; $\alpha < \beta$ toward smaller θ

Posterior derivation (up to proportionality)

Likelihood

$$p(k \mid \theta) \propto \theta^k (1-\theta)^{n-k}$$

Prior

$$p(\theta) \propto \theta^{\alpha-1}(1-\theta)^{\beta-1}$$

Posterior (unnormalized)

$$p(\theta \mid k) \propto \theta^{k+\alpha-1}(1-\theta)^{n-k+\beta-1}$$

Posterior in closed form

$$\theta \mid k, n \sim \mathrm{Beta}(\alpha + k,\ \beta + n - k)$$

Posterior moments

$$\mathbb{E}[\theta \mid k] = \frac{\alpha + k}{\alpha + \beta + n}$$

$$\mathrm{Var}[\theta \mid k] = \frac{(\alpha + k)(\beta + n - k)}{(\alpha + \beta + n)^2(\alpha + \beta + n + 1)}$$

Prior vs posterior (visual)

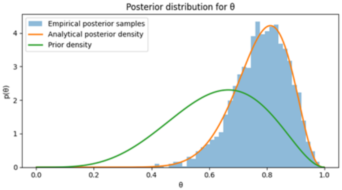


Figure: Prior and posterior density of θ

- Posterior shifts toward parameter values supported by data.
- Posterior becomes more concentrated as n increases.

How dataset size changes uncertainty

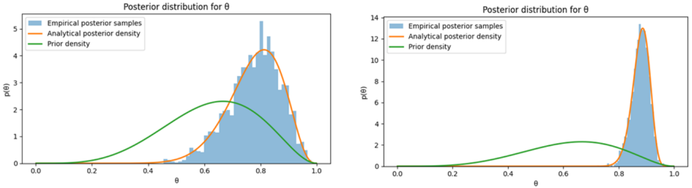


Figure: Posterior densities for $(k, n) = (9, 10)$ on the left and $(k, n) = (90, 100)$ on the right under the same prior.

- Same ratio k/n can imply very different uncertainty depending on n.

Why point estimates still matter

- Many applications require a single parameter value (for deployment simplicity).
- Point estimates are useful **summaries** of the posterior.
- MLE and MAP are the main point-estimation baselines.

Maximum Likelihood Estimation (MLE)

Definition: parameter value maximizing the likelihood.

$$\hat{\theta}_{\text{MLE}} = \arg\max_{\theta} \log p(D \mid \theta)$$

Binomial model

$$\log p(k \mid \theta, n) = k \log \theta + (n - k) \log(1 - \theta) + C$$

$$\frac{\partial}{\partial \theta} = \frac{k}{\theta} - \frac{n-k}{1-\theta} = 0 \quad \Rightarrow \quad \hat{\theta}_{\text{MLE}} = \frac{k}{n}$$

When to use: large sample sizes, purely data-driven estimation.

Maximum A Posteriori (MAP) estimation

Definition: parameter value maximizing the posterior.

$$\hat{\theta}_{\text{MAP}} = \arg\max_{\theta} \log \left[p(D \mid \theta) p(\theta) \right]$$

Beta–Binomial MAP

$$\hat{\theta}_{\text{MAP}} = \frac{k + \alpha - 1}{n + \alpha + \beta - 2}$$

- incorporates prior information
- acts like regularization (shrinkage toward the prior)
- still a point estimate (does not capture posterior uncertainty)

MLE vs MAP: practical example

Scenario: coin flip with $k = 7$ successes in $n = 10$ trials.
Prior: $\mathrm{Beta}(\alpha = 5, \beta = 3)$.

$$\hat{\theta}_{\text{MLE}} = \frac{7}{10} = 0.700 \qquad \hat{\theta}_{\text{MAP}} = \frac{7+5-1}{10+5+3-2} = \frac{11}{16} = 0.6875$$

Interpretation

- MLE uses only data.
- MAP balances data and prior (slight pull toward prior mean).
- With much more data, MLE and MAP converge.

MAP as regularization (ML viewpoint)

$$\hat{\theta}_{\text{MAP}} = \arg\min_{\theta} \Big(\underbrace{-\log p(D \mid \theta)}_{\text{data fit}} + \underbrace{-\log p(\theta)}_{\text{regularizer}} \Big)$$

- Gaussian prior on weights $\Rightarrow$ L2 regularization.
- Laplace prior $\Rightarrow$ L1 regularization.
- Prior encodes what parameter values are plausible *before* seeing data.

Summarizing the posterior from samples

If we have posterior samples $\{\theta^{(1)}, \ldots, \theta^{(S)}\}$, we can compute:

Central tendency

- mean: $\bar{\theta} = \frac{1}{S} \sum_{s=1}^{S} \theta^{(s)}$
- median: 50th percentile
- mode: most probable value (e.g., MAP)

Dispersion

- variance / standard deviation
- quantiles (IQR, 95% range)

Posterior predictive vs plug-in prediction

Posterior predictive

$$p(x^\star \mid D) = \int p(x^\star \mid \theta)\, p(\theta \mid D)\, d\theta$$

- accounts for parameter uncertainty
- often wider (more honest)

Plug-in

$$p(x^\star \mid D) \approx p(x^\star \mid \hat{\theta})$$

- simpler
- can be overconfident

Analytic vs Monte Carlo inference

- Conjugate models: compute posterior in closed form.
- General models: posterior may be intractable $\Rightarrow$ approximate inference.

Two views

- **Analytic:** derive posterior formula directly.
- **Sampling:** approximate posterior with samples (MC, MCMC).

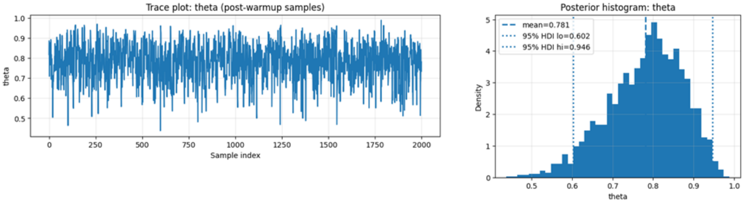


Figure: Posterior samples and their histogram

Evidence and Bayes factors

Marginal likelihood (evidence)

$$p(\boldsymbol{X}) = \int p(\boldsymbol{X} \mid \theta)\, p(\theta)\, d\theta$$

- Penalizes overly flexible models automatically ("Occam factor").
- Enables model comparison: $\mathrm{BF}_{10} = \dfrac{p(\boldsymbol{X} \mid M_1)}{p(\boldsymbol{X} \mid M_0)}$.

In conjugate models

You can compute evidence in closed form (e.g., Beta-Binomial). For complex models we approximate.

Key takeaways

- UQ asks: what is plausible, how variable, and how beliefs update with data.
- Bayesian inference: posterior $\propto$ likelihood $\times$ prior.
- MLE and MAP are point estimates; full Bayes keeps a distribution.
- Credible intervals (central/HPD) summarize posterior uncertainty.
- PPD averages over parameter uncertainty to avoid overconfidence.

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