Bayesian Logistic Regression

ELG 5218 - Uncertainty Evaluation in Engineering Measurements and Machine Learning

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February 1, 2026

Outline: Bayesian Logistic Regression

- **Motivation and Model**
  - Logistic regression as a discriminative model
  - Likelihood function and Bayesian prior
- **Intractability and Approximation**
  - Non-conjugacy of logistic likelihood and Gaussian prior
  - Posterior not analytically tractable
  - Laplace approximation: MAP estimation + Hessian
- **Inference and Prediction**
  - Approximate predictive distribution
  - Application to failure prediction in engineering
- **Implementation using MCMC**
- **Laplace Deep Dive (Backup)**

Notepad: Laplace_Approximation_Logistic_Regression.ipynb

The Logistic Regression Model

Discriminative Classification:

- We model $p(y|x, \boldsymbol{w})$ directly using the logistic sigmoid function $\sigma(\cdot)$.
- Prediction: $\mu = \sigma(\boldsymbol{w}^\top \boldsymbol{x}) = \frac{1}{1+\exp(-\boldsymbol{w}^\top \boldsymbol{x})}$.
- Likelihood (Bernoulli):

$$p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{w}) = \prod_{n=1}^{N} \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n)^{y_n}(1 - \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n))^{1-y_n}$$

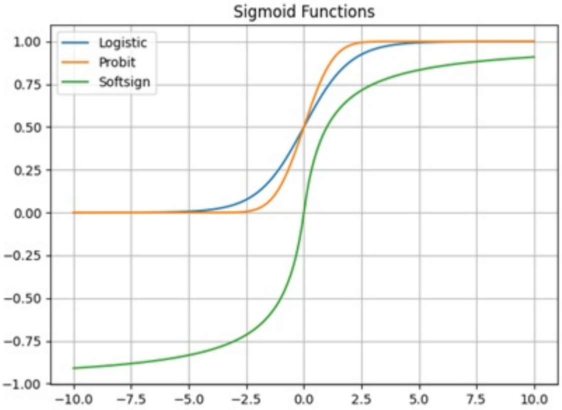
The Bayesian Goal:

- Introduce a prior on weights: $p(\boldsymbol{w}) = \mathcal{N}(\boldsymbol{w}|\boldsymbol{0}, \alpha^{-1}\boldsymbol{I})$.
- Compute the **Posterior**: $p(\boldsymbol{w}|\boldsymbol{y}, \boldsymbol{X}) \propto p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{w})p(\boldsymbol{w})$.
- Compute the **Predictive Distribution**: $p(y_*|\boldsymbol{x}_*, \boldsymbol{y}, \boldsymbol{X})$.

Sigmoid Functions

Sigmoid Options:

- **Logistic:** Simple closed form, standard choice. Heavy tails; posterior not conjugate with a Gaussian prior.
- **Probit:** Gaussian CDF; lighter tails, links to latent-Gaussian models. More expensive; posterior still intractable.
- **Softsign:** Cheap and smooth, but not a probability model and poorly calibrated.



The Intractability Problem

Why is this harder than Linear Regression?

Posterior Distribution

$$p(\boldsymbol{w}|\boldsymbol{y}, \boldsymbol{X}) \propto \underbrace{\prod_{n=1}^{N} \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n)^{y_n}(1-\sigma(\boldsymbol{w}^\top \boldsymbol{x}_n))^{1-y_n}}_{\text{Likelihood (Sigmoids)}} \times \underbrace{\exp\left(-\frac{\alpha}{2}\boldsymbol{w}^\top \boldsymbol{w}\right)}_{\text{Prior (Gaussian)}}$$

- The likelihood is a product of sigmoids; the prior is Gaussian.
- They are **not conjugate**.
- The product is **not** a Gaussian (and not a standard distribution).
- The normalization constant $Z = \int p(\boldsymbol{y}|\boldsymbol{X}, \boldsymbol{w})p(\boldsymbol{w})d\boldsymbol{w}$ is analytically intractable.

Solution: We must use approximations. Today: **The Laplace Approximation**.

Why We Use Laplace Approximation

Why Not Use Standard Loss?

- Classification usually optimized via *cross-entropy* (negative log-likelihood).
- Works for point estimation (MLE/MAP), but **does not give the posterior**.
- Logistic likelihood and Gaussian prior are **not conjugate** $\rightarrow$ posterior integral is intractable.

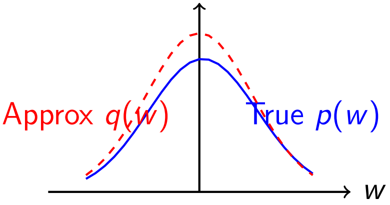
Why Laplace Approximation?

- Approximates the posterior by a Gaussian around the MAP.
- Makes Bayesian logistic regression computationally feasible.

The Laplace Approximation

Idea: Approximate the intractable posterior $p(\boldsymbol{w}|\mathcal{D})$ with a Gaussian $q(\boldsymbol{w})$.

1. Find the mode of the posterior, $\boldsymbol{w}_{MAP}$ (Maximum A Posteriori).
2. Compute the curvature (Hessian) of the log-posterior at the mode.
3. Construct a Gaussian centered at $\boldsymbol{w}_{MAP}$ with covariance determined by the curvature.



$$\ln p(\boldsymbol{w}|\mathcal{D}) \approx \ln p(\boldsymbol{w}_{MAP}|\mathcal{D}) - \frac{1}{2}(\boldsymbol{w} - \boldsymbol{w}_{MAP})^\top \boldsymbol{A}(\boldsymbol{w} - \boldsymbol{w}_{MAP})$$

$$q(\boldsymbol{w}) = \mathcal{N}(\boldsymbol{w}|\boldsymbol{w}_{MAP}, \boldsymbol{A}^{-1})$$

Where $\boldsymbol{A} = -\nabla\nabla \ln p(\boldsymbol{w}|\mathcal{D})|_{\boldsymbol{w}_{MAP}}$ (Negative Hessian).

Step 1: Finding w_{MAP}

We maximize the log-posterior:

$$\ln p(\boldsymbol{w}|\mathcal{D}) = -\frac{\alpha}{2}\boldsymbol{w}^\top \boldsymbol{w} + \sum_{n=1}^{N}\{y_n \ln \mu_n + (1 - y_n)\ln(1 - \mu_n)\} + \text{const}$$

where $\mu_n = \sigma(\boldsymbol{w}^\top \boldsymbol{x}_n)$.

Gradient (∇E):

$$\nabla \ln p(\boldsymbol{w}|\mathcal{D}) = -\alpha\boldsymbol{w} + \sum_{n=1}^{N}(y_n - \mu_n)\boldsymbol{x}_n = -\alpha\boldsymbol{w} + \boldsymbol{X}^\top(\boldsymbol{y} - \boldsymbol{\mu})$$

Algorithm: Since this is convex, we use **gradient descent** .

$$\boldsymbol{w}_{new} = \boldsymbol{w}_{old} - \boldsymbol{\eta}\nabla E(\boldsymbol{w}_{old})$$

Step 2: The Hessian Matrix

To apply Newton-Raphson and find the Laplace covariance, we need the second derivatives.

$$\boldsymbol{H} = \nabla\nabla \ln p(\boldsymbol{w}|\mathcal{D}) = -\alpha \boldsymbol{I} - \sum_{n=1}^{N} \mu_n(1-\mu_n)\boldsymbol{x}_n\boldsymbol{x}_n^\top$$

In matrix notation:

$$\boldsymbol{H} = -(\alpha \boldsymbol{I} + \boldsymbol{X}^\top \boldsymbol{S}\boldsymbol{X})$$

where $\boldsymbol{S}$ is a diagonal weighting matrix with elements $S_{nn} = \mu_n(1-\mu_n)$.

The Laplace Approximation Result

The posterior is approximated as Gaussian $q(\boldsymbol{w}) = \mathcal{N}(\boldsymbol{w}|\boldsymbol{w}_{MAP}, \Sigma_N)$ with:

$$\Sigma_N^{-1} = \alpha \boldsymbol{I} + \boldsymbol{X}^\top \boldsymbol{S}\boldsymbol{X}$$

Predictive Distribution: The Challenge

We have the posterior $q(\boldsymbol{w})$. Now we want to predict class y_* for a new input $\boldsymbol{x}_*$.

$$p(y_* = 1|\boldsymbol{x}_*, \mathcal{D}) = \int p(y_* = 1|\boldsymbol{x}_*, \boldsymbol{w})q(\boldsymbol{w})d\boldsymbol{w}$$

$$= \int \sigma(\boldsymbol{w}^\top \boldsymbol{x}_*)\mathcal{N}(\boldsymbol{w}|\boldsymbol{w}_{MAP}, \Sigma_N)d\boldsymbol{w}$$

Problem: This is the convolution of a Sigmoid and a Gaussian.

- Still analytically intractable!
- However, it's a 1D integral of a projected Gaussian.

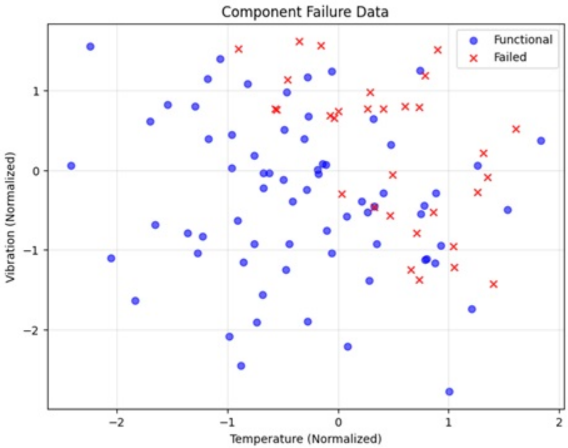
Engineering Example: Component Failure Prediction

Scenario: We want to predict mechanical component failure based on sensor data.

- x_1: Operating Temperature (Normalized)
- x_2: Vibration Frequency (Normalized)
- $y \in \{0, 1\}$: Functional vs. Failed

Why Bayesian?

- We have limited failure data (rare events).
- We need to know **when** the model is uncertain to trigger manual inspection.



Synthetic Failure Data

Implementation in NumPyro

Defining a Bayesian Logistic Regression model in probabilistic code:

Python/NumPyro Code

```
def logistic_model(X, y=None):
    # 1. Priors (Gaussian regularization)
    w = numpyro.sample("w", dist.Normal(0, 1).expand([2]))
    b = numpyro.sample("b", dist.Normal(0, 1))

    # 2. Logits
    logits = jnp.dot(X, w) + b

    # 3. Likelihood (Bernoulli)
    with numpyro.plate("data", len(X)):
        numpyro.sample("obs", dist.Bernoulli(logits=logits), obs=y)
```

Numpyro: What are `plate`, `jnp.dot`, and `numpyro.sample`?

1) `numpyro.plate("data", N)`
Declares an i.i.d. dimension of size N and vectorizes the computation. For a Bernoulli likelihood,
$\log p(\mathbf{y} \mid X, \theta) = \sum_{n=1}^{N} \log \text{Bernoulli}\big(y_n\,;\,\sigma(\mathbf{w}^\top \mathbf{x}_n + b)\big).$

2) `jnp.dot(X, w)`
Matrix–vector product. With $X \in \mathbb{R}^{N \times D}$ and $w \in \mathbb{R}^D$, it returns logits $\in \mathbb{R}^N$ where $\text{logits}_n = \sum_{j=1}^{D} X_{nj} w_j$.

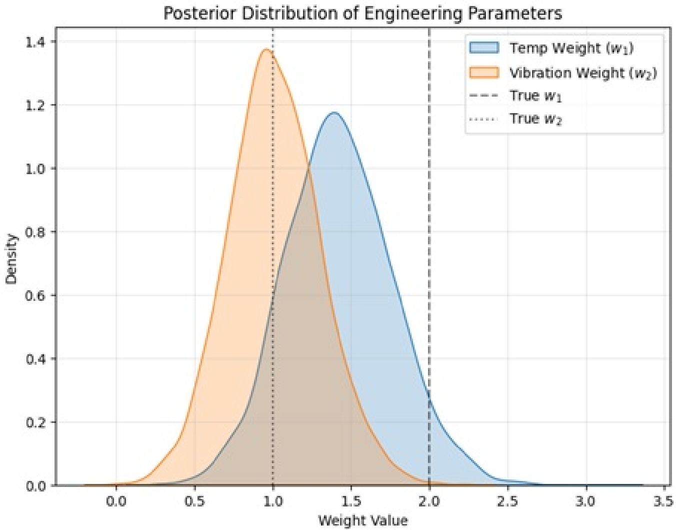
3) `numpyro.sample(name, dist, obs=None)`
Creates a random variable site from a distribution. Used for priors and likelihood. When `obs` is provided, the node is *observed* and contributes its log-probability; when omitted, NumPyro will draw from the distribution during prior/predictive simulation.

Posterior Uncertainty in Parameters

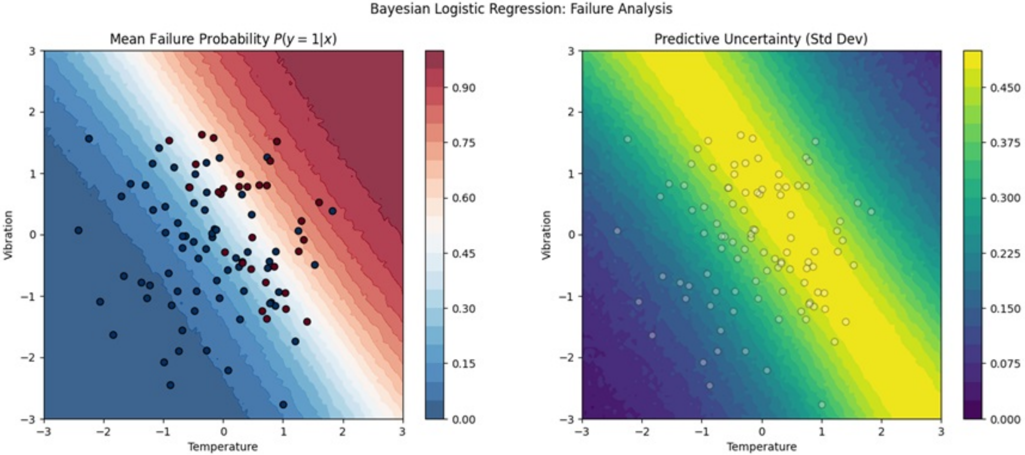
Instead of a single "best fit" weight vector $\hat{\mathbf{w}}_{MLE}$, we get a distribution over possible weights.

- **Blue:** Temperature Sensitivity (w_1)
- **Orange:** Vibration Sensitivity (w_2)

We are more confident about w_1 (narrower peak) than w_2.



Visualizing Predictive Uncertainty



- **Left:** Mean probability of failure (The Decision Boundary).
- **Right:** Predictive Standard Deviation (Where is the model confused?).

Reading the Posterior Predictive Maps

Left: Mean Failure Probability

- Color $= \mathbb{E}_w[\sigma(w^\top x + b)]$.
- Black contour at 0.5 is the decision boundary.
- High Temp + High Vibration $\Rightarrow$ red (high failure risk).

Right: Predictive Uncertainty (Std of y)

- Peaks near the boundary (mean ≈ 0.5) and in sparse regions.
- Decomposes into aleatoric $E[p(1-p)]$ and epistemic $\mathrm{Var}(p)$.
- Use high-uncertainty flags for additional inspection.

Summary

1. **Theory:** Logistic Regression likelihood $\times$ Gaussian Prior $\neq$ Gaussian Posterior.
2. **Approximation:** We used Laplace Approx (Taylor Series) to estimate $p(\boldsymbol{w}|\mathcal{D}) \approx \mathcal{N}(\boldsymbol{w}_{MAP}, \boldsymbol{H}^{-1})$.
3. **Implementation:** Modern tools like NumPyro allow full MCMC inference for critical engineering applications where uncertainty quantification is key.

Summary:

1. Bayesian Logistic Regression is non-conjugate.
2. **Laplace Approximation**:
   - Fit MAP via IRLS.
   - Use Hessian for Covariance Σ_N.
3. **Predictive Distribution**:
   - Convolve Sigmoid with Gaussian.
   - Result: "Moderated" Sigmoid (less confident predictions when uncertain).

Other Approaches (Higher accuracy/cost):

- **Variational Inference (VI):** Optimizes a lower bound on marginal likelihood. (Jaakkola & Jordan, 2000).
- **MCMC:** Metropolis-Hastings or Hamiltonian Monte Carlo (Gold standard, slow).
- **EP (Expectation Propagation):** Often more accurate than Laplace for logistic regression.

Backup slides about Laplace approximation

Learning goals

- Understand the **Hessian** as *curvature* (1D) and *curvature + coupling* (multi-D).
- Understand the **Laplace approximation** as a local Gaussian approximation around the MAP.
- See when Laplace works well (unimodal, near-Gaussian) and when it fails (multimodal, skewed).
- Apply Laplace to **Bayesian logistic regression**: approximate posterior + credible intervals + predictive bands.

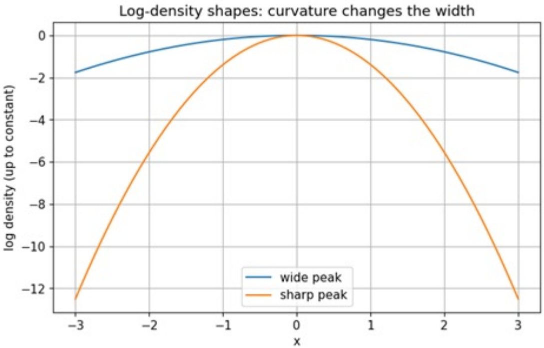
Hessian in 1D: second derivative = curvature

For a 1D function $f(x)$:

- $f'(x)$ is the **slope**.
- $f''(x)$ is how the slope changes: the **curvature**.

For a *log-density* peak:

- **More curvature** (more negative f'' at the peak) $\Rightarrow$ **narrower** uncertainty.
- **Less curvature** $\Rightarrow$ **wider** uncertainty.

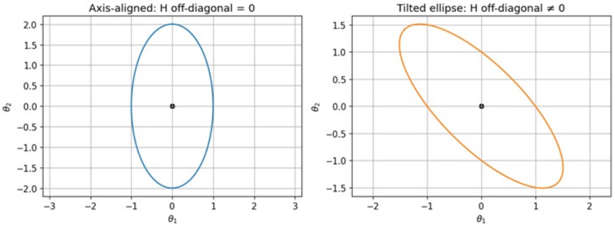


Hessian in 2D: curvature + coupling

In many dimensions, the Hessian is a matrix: $H_{ij}(\theta) = \frac{\partial^2 f}{\partial\theta_i \partial\theta_j}$.

Intuition:

- Diagonal entries: curvature in each coordinate direction.
- Off-diagonal entries: **coupling** (how directions interact) $\Rightarrow$ tilted ellipses.



Near a mode, if the negative log posterior looks like $U(\theta) \approx U(\hat{\theta}) + \frac{1}{2}(\theta - \hat{\theta})^\top H(\theta - \hat{\theta})$, then the covariance is approximately $\Sigma \approx H^{-1}$.

Laplace approximation: the one-line story

Goal: approximate a difficult posterior $p(\theta \mid y)$ by a Gaussian.
Define the negative log posterior:

$$U(\theta) = -\log p(\theta \mid y).$$

Step 1 (MAP): find the mode / MAP

$$\hat{\theta} = \arg\min_{\theta} U(\theta).$$

Step 2 (curvature): compute the Hessian at the MAP

$$H = \nabla^2 U(\hat{\theta}).$$

Step 3 (Gaussian): approximate

$$p(\theta \mid y) \approx \mathcal{N}\big(\hat{\theta},\ H^{-1}\big).$$

Translation: *mode becomes mean; curvature becomes covariance.*

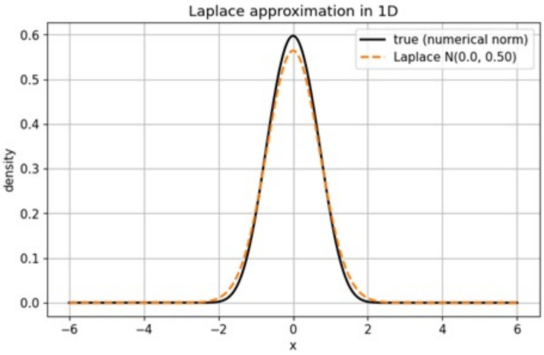
Example: a slightly non-Gaussian target

Consider

$$p(x) \propto \exp(-x^2 - 0.1x^4).$$

It is not exactly Gaussian (tails differ), but it is *approximately* Gaussian near its peak.
At the mode $\hat{x} = 0$:

$$U(x) = x^2 + 0.1x^4, \quad U''(0) = 2 \Rightarrow \sigma^2 \approx 1/2.$$



Why it becomes Gaussian: quadratic log-density

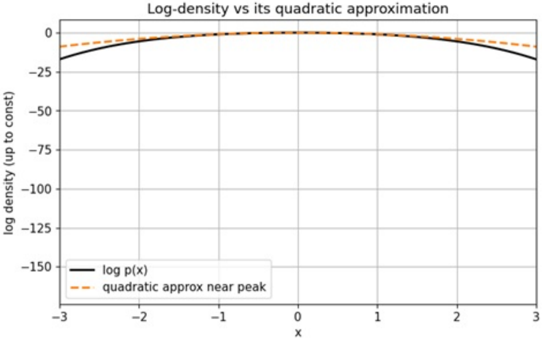
A Gaussian has a **quadratic** in the exponent:

$$\mathcal{N}(\mu, \sigma^2) \propto \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right).$$

Laplace approximates the log-density by a quadratic around the peak:

$$\log p(x) \approx \log p(\hat{x}) - \tfrac{1}{2} H (x - \hat{x})^2.$$

Exponentiating this quadratic gives a Gaussian.

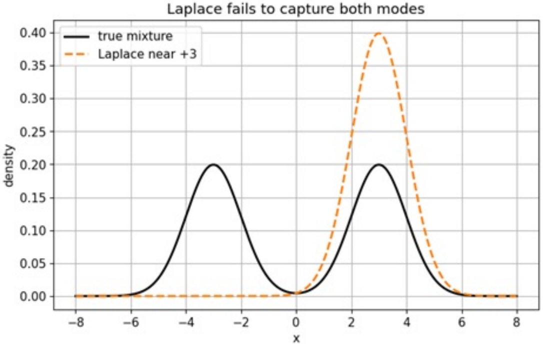


Failure case: multimodal posterior

If the target has **multiple peaks**, a single Gaussian around one peak cannot capture the whole distribution.
Example mixture:

$$p(x) = \tfrac{1}{2}\mathcal{N}(-3, 1) + \tfrac{1}{2}\mathcal{N}(3, 1).$$

Laplace around the right peak captures only that mode and ignores the other.
Takeaway: Laplace works best for *unimodal, near-Gaussian* posteriors.



Key takeaways

- **Hessian** = curvature (2nd derivatives); off-diagonals mean coupling/correlation.
- **Laplace**: approximate $p(\theta \mid y)$ by $\mathcal{N}(\hat{\theta}, H^{-1})$.
- Works best when posterior is **unimodal** and **locally Gaussian**.
- Can be misleading for **multimodal**, **skewed**, or **heavy-tailed** posteriors.
- For more accurate uncertainty, use **HMC/NUTS** (NumPyro/Stan) — Laplace is fast and interpretable.

Acknowledgements/ Document preparation

This document was developed and converted into LaTeX slides and formatted with assistance from ChatGPT (OpenAI) and CoPilot (Microsoft). The instructor modified the source text and verified the final structure and wording.