Bayesian Linear Regression

Vasilis Gkolemis

ATHENA RC — HUA

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Logistic Regression as a Probabilistic Model

- In binary classification, we model the probability of label $y \in \{0, 1\}$ given input $\mathbf{x} \in \mathbb{R}^d$:

$$p(y = 1 \mid \mathbf{x}, \mathbf{w}) = \sigma(\mathbf{w}^\top \mathbf{x})$$

- $\sigma(z) = \frac{1}{1+e^{-z}}$ is the logistic sigmoid function.
- In a Bayesian setting, we place a prior over $\mathbf{w}$ and infer the posterior:

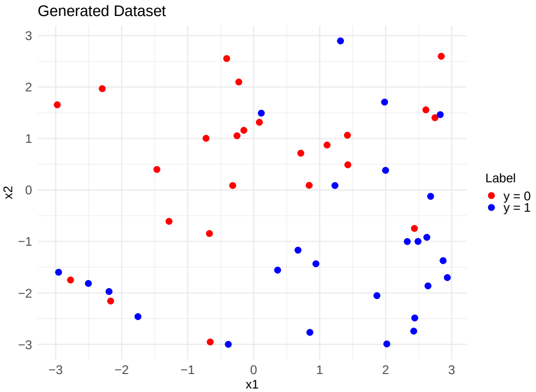
$$p(\mathbf{w} \mid \mathcal{D}) \propto p(\mathbf{w}) \prod_{n=1}^{N} p(y_n \mid \mathbf{x}_n, \mathbf{w})$$

Why Approximate Inference?

- The posterior is not analytically tractable due to the non-conjugate likelihood.
- The logistic sigmoid does not lead to a conjugate posterior with a Gaussian prior.
- Approximate inference methods are needed:
  - Laplace Approximation
  - Importance Sampling
  - Markov Chain Monte Carlo (MCMC)

2D Toy Example

- We create a small dataset with $N = 50$ samples:
  - $\mathbf{x}_n \in [-3, 3]^2$, $y_n \sim \mathrm{Bernoulli}(\sigma(\mathbf{w}^\top \mathbf{x}_n))$, where $\mathbf{w}^\star = (0.5, -0.6)$
- Classes are slightly overlapping to reflect realistic uncertainty.



Model Specification

- Prior over weights:

$$\mathbf{w} \sim \mathcal{N}(\mathbf{0}, \alpha^{-1}\mathbf{I})$$

- Likelihood:

$$p(\mathcal{D} \mid \mathbf{w}) = \prod_{n=1}^{N} \sigma(\mathbf{w}^\top \mathbf{x}_n)^{y_n}(1 - \sigma(\mathbf{w}^\top \mathbf{x}_n))^{1-y_n}$$

- Posterior:

$$p(\mathbf{w} \mid \mathcal{D}) \propto p(\mathbf{w})p(\mathcal{D} \mid \mathbf{w}) \quad \text{(approximated)}$$

Laplace Approximation: Idea

- Is it reasonable to approximate the posterior with a Gaussian?
- Yes:
  - It is an incremental improvement over MAP
  - Many ML methods rely on a single configuration; Laplace is a natural extension
  - When the posterior is dominated by a single mode
- No:
  - When the posterior is multimodal or highly skewed
  - Unfortunately, this is often the case in practice

$$p(\boldsymbol{\theta} \mid \mathcal{D}) \approx \mathcal{N}(\boldsymbol{\theta}; \boldsymbol{\mu}, \boldsymbol{\Sigma}), \quad \text{where:}$$

$\boldsymbol{\mu} =$ MAP estimate (mode of posterior), often denoted as $\hat{\boldsymbol{\theta}}$

$\boldsymbol{\Sigma} =$ inverse Hessian of the log posterior at the mode, denoted as $\mathbf{H}^{-1}$

Laplace Approximation: How it Works

$$p(\boldsymbol{\theta} \mid \mathcal{D}) \approx \mathcal{N}(\boldsymbol{\theta}; \boldsymbol{\mu} = \hat{\boldsymbol{\theta}}, \boldsymbol{\Sigma} = \mathbf{H}^{-1})$$

- Why setting $\boldsymbol{\mu}$ to $\hat{\boldsymbol{\theta}}$, i.e., the MAP estimate?
- $p(\boldsymbol{\theta} \mid \mathcal{D})$ is proportional to the product of the prior and likelihood: Search for the point that maximizes $L(\boldsymbol{\theta})p(\boldsymbol{\theta}) \Rightarrow$ MAP estimate

$$\hat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}} \log p(\boldsymbol{\theta} \mid \mathcal{D}) = \arg\max_{\boldsymbol{\theta}} \left(\log p(\boldsymbol{\theta}) + \sum_{i=1}^{N} \log p(y_i \mid \mathbf{x}_i, \boldsymbol{\theta}) \right)$$

- It is a simple optimization problem:
  - Use gradient-based methods (e.g., Newton-Raphson, L-BFGS)
  - Can easily solve high-dimensional problems, if autograd is available

Laplace Approximation: How it Works

$$p(\boldsymbol{\theta} \mid \mathcal{D}) \approx \mathcal{N}(\boldsymbol{\theta}; \boldsymbol{\mu} = \hat{\boldsymbol{\theta}}, \boldsymbol{\Sigma} = \mathbf{H}^{-1})$$

- Why setting $\boldsymbol{\Sigma}$ to $\mathbf{H}^{-1}$, i.e., the inverse Hessian?
- The MAP is a turning point. What happens there?
  - Imagine it as a mountain peak in the log-posterior landscape
  - The gradient vanishes: $\nabla \log p(\boldsymbol{\theta} \mid \mathcal{D})\big|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}} = 0$
  - The Hessian captures local curvature: $\mathbf{H} = -\nabla^2 \log p(\boldsymbol{\theta} \mid \mathcal{D})\big|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}}$
- $\mathbf{H} \in \mathbb{R}^{d \times d}$ (where d is the number of parameters), where:

$$\mathbf{H}_{ij} = -\frac{\partial^2 \log p(\boldsymbol{\theta} \mid \mathcal{D})}{\partial \theta_i \partial \theta_j}\bigg|_{\boldsymbol{\theta}=\hat{\boldsymbol{\theta}}}$$

- $\boldsymbol{\Sigma} = \mathbf{H}^{-1}$:
  - High curvature (large values in $\mathbf{H}$) means steep slope, low uncertainty
  - Low curvature (small values in $\mathbf{H}$) means flat slope, high uncertainty

Taylor Expansion and Laplace Approximation

- Taylor expansion approximates a function $f(\boldsymbol{\theta})$ around a point $\hat{\boldsymbol{\theta}}$ with a polynomial, i.e., a smooth curve:

$$f(\boldsymbol{\theta}) \approx f(\hat{\boldsymbol{\theta}}) + \nabla f(\hat{\boldsymbol{\theta}})^\top (\boldsymbol{\theta} - \hat{\boldsymbol{\theta}}) + \frac{1}{2}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})^\top \nabla^2 f(\hat{\boldsymbol{\theta}})(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})$$

- a second-order Taylor expansion around the MAP estimate is:

$$\log p(\boldsymbol{\theta} \mid \mathcal{D}) \approx \log p(\hat{\boldsymbol{\theta}} \mid \mathcal{D}) - \frac{1}{2}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})^\top \mathbf{H}(\boldsymbol{\theta} - \hat{\boldsymbol{\theta}})$$

  where $\mathbf{H} = -\nabla^2 \log p(\boldsymbol{\theta} \mid \mathcal{D})\big|_{\hat{\boldsymbol{\theta}}}$ is the (negative) Hessian at the mode.
- Exponentiating both sides gives the Laplace approximation of the posterior:

$$p(\boldsymbol{\theta} \mid \mathcal{D}) \approx \mathcal{N}(\boldsymbol{\theta}; \hat{\boldsymbol{\theta}}, \mathbf{H}^{-1})$$

Laplace Approximation: Summary

So the Laplace Approximation gives:

$$p(\boldsymbol{\theta} \mid \mathcal{D}) \approx \mathcal{N}(\boldsymbol{\theta}; \boldsymbol{\mu} = \hat{\boldsymbol{\theta}}, \boldsymbol{\Sigma} = \mathbf{H}^{-1})$$

- Computational considerations:
  - MAP estimate $\hat{\boldsymbol{\theta}}$ is a point estimate, not a distribution
  - If gradients are available, it is efficient to compute
  - Hessian $\mathbf{H}$ is computed at the MAP estimate
  - Up to $O(d^3)$ for inversion, where d is the number of parameters
  - Cannot work for very high-dimensional problems (e.g., $d > 1000$)
- Final conclusion:
  Laplace Approximation is easy to implement and compute but may be inaccurate if the posterior is multimodal or skewed.

Why Laplace Works in Logistic Regression

Consider Bayesian logistic regression:

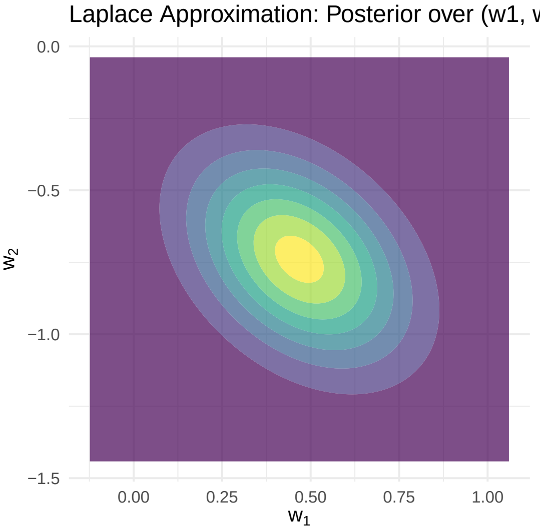
$$p(\boldsymbol{\theta} \mid \mathcal{D}) \propto p(\mathcal{D} \mid \boldsymbol{\theta}) \cdot p(\boldsymbol{\theta})$$

- **Likelihood:** $p(\mathcal{D} \mid \boldsymbol{\theta}) = \prod_n \sigma(\boldsymbol{\theta}^\top \mathbf{x}_n)^{y_n} (1 - \sigma(\boldsymbol{\theta}^\top \mathbf{x}_n))^{1-y_n}$
- **Prior:** $p(\boldsymbol{\theta}) = \mathcal{N}(\boldsymbol{\theta}; \mathbf{0}, \tau^2 \mathbf{I})$

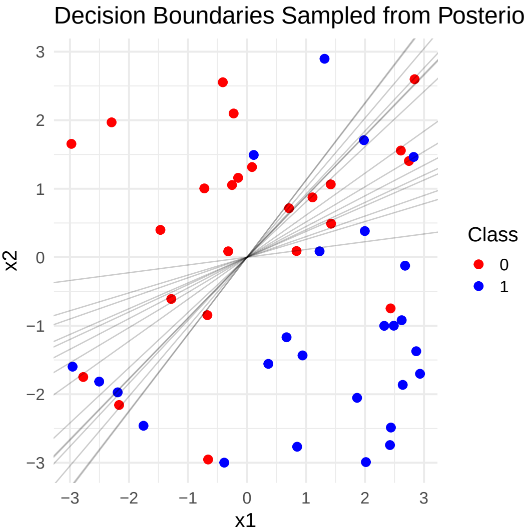
$$\Rightarrow p(\boldsymbol{\theta} \mid \mathcal{D}) = \text{Gaussian prior} \cdot \prod_n \text{sigmoid likelihood}$$

Conclusion: The posterior is a Gaussian (prior) where each sigmoid slices off a portion of the mass. The resulting distribution has a single mode, making Laplace a good approximation.

Laplace Approximation in our Toy Example



Laplace Approximation in our Toy Example



Importance Sampling: Motivation

- Goal: Compute expectations under a difficult distribution $p(\theta)$ (e.g., posterior).
- Direct sampling from $p(\theta)$ is hard or impossible.
- Instead, sample from a simpler proposal distribution $q(\theta)$.

$$\mathbb{E}_p[f(\theta)] = \int f(\theta)p(\theta)d\theta \quad \text{but} \quad p(\theta) \text{ is hard to sample from.}$$

Importance Sampling Estimator

$$\mathbb{E}_p[f(\theta)] = \int f(\theta)\frac{p(\theta)}{q(\theta)}q(\theta)d\theta = \mathbb{E}_q\left[f(\theta)w(\theta)\right]$$

where the importance weights are

$$w(\theta) = \frac{p(\theta)}{q(\theta)}.$$

Practical Importance Sampling

Given samples $\{\theta_i\}_{i=1}^N \sim q(\theta)$:

$$\hat{\mu} = \frac{\sum_{i=1}^N w_i f(\theta_i)}{\sum_{i=1}^N w_i}, \quad \text{where} \quad w_i = \frac{p(\theta_i)}{q(\theta_i)}.$$

- Weights are normalized to sum to 1.
- Effective when $q(\theta)$ covers $p(\theta)$ well.

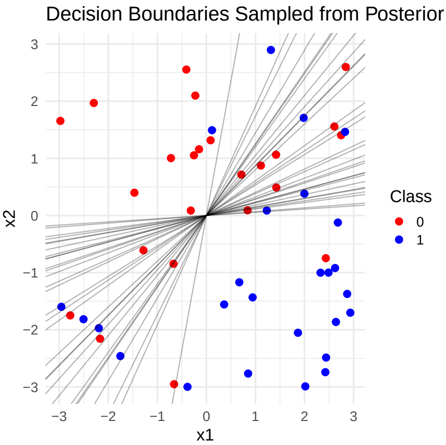
Importance Sampling in Bayesian Inference

- Target posterior: $p(\theta|X, y) \propto p(y|X, \theta)p(\theta)$.
- Proposal $q(\theta)$ can be prior or Laplace approximation.
- Importance weights:

$$w_i = \frac{p(y|X, \theta_i)p(\theta_i)}{q(\theta_i)}.$$

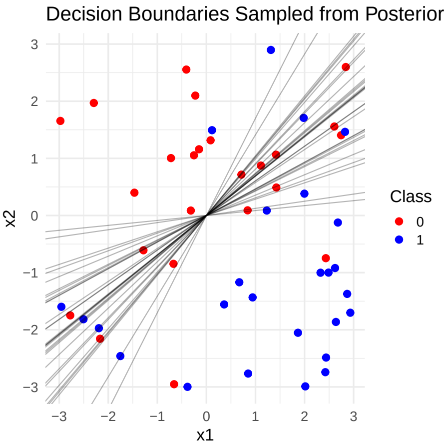
- Samples $\theta_i \sim q(\theta)$ weighted to approximate the posterior.

Importance Sampling with Prior Proposal



- Proposal distribution $q(\theta) = p(\theta)$ (prior).
- Samples drawn directly from prior.
- Importance weights correct for data likelihood.
- May have high variance if prior poorly matches posterior.

Importance Sampling with Laplace Approximation Proposal



- Proposal distribution $q(\theta) \approx \mathcal{N}(\hat{\theta}, H^{-1})$ (Laplace approx).
- Samples concentrated near MAP estimate.
- Importance weights reweight samples to correct approximation.
- Typically lower variance than prior proposal.

Markov Chain Monte Carlo (MCMC) for Bayesian Inference

- Goal: Sample from posterior distribution $p(\theta \mid X, y)$ when direct sampling is difficult.
- Construct a Markov chain whose stationary distribution is the posterior.
- Generates dependent samples that approximate the posterior as the chain runs.
- Widely applicable to complex models where exact inference is intractable.

Metropolis-Hastings Algorithm

- Start from an initial parameter $\theta^{(0)}$.
- At step t, propose θ^* from proposal distribution $q(\theta^* \mid \theta^{(t-1)})$.
- Calculate acceptance probability:

$$\alpha = \min\left(1, \frac{p(\theta^* \mid X, y)q(\theta^{(t-1)} \mid \theta^*)}{p(\theta^{(t-1)} \mid X, y)q(\theta^* \mid \theta^{(t-1)})}\right)$$

- Accept θ^* with probability α, else keep $\theta^{(t-1)}$.
- Ensures the chain converges to posterior distribution.

MCMC for Bayesian Logistic Regression

- Posterior $p(\theta \mid X, y) \propto p(y \mid X, \theta)p(\theta)$ is non-conjugate.
- MCMC provides a way to approximate the posterior without analytic form.
- Samples $\{\theta^{(t)}\}_{t=1}^{T}$ can be used for:
  - Estimating expectations (posterior means, variances).
  - Predictive distributions.
  - Visualizing uncertainty, e.g. decision boundary variation.

Practical Considerations

- **Burn-in**: Discard initial samples until chain stabilizes.
- **Thinning**: Keep every k-th sample to reduce autocorrelation.
- **Tuning**: Proposal distribution parameters (e.g., step size) affect acceptance rate and mixing.
- Diagnostics needed to check convergence (trace plots, effective sample size).

MCMC Samples: Decision Boundaries from Posterior