Machine Learning (Week 8 Lecture) Naive **Bayes** Classifier and **Bayes**ian Classification

Debasis Ganguly
Debasis.Ganguly@glasgow.ac.uk

School of Computing Science
University of Glasgow

November 20, 2025

Introduction

D. Ganguly

Refresher on Bayes Theorem

Naive Bayes

NB for Categorical data

NB for Non-categorical data

Bayesian Logistic Regression

Laplace approximation

MCMC sampling

Classification under Uncertainties

- Last 2 weeks of Classification:
  - Binary and multi-class parametric approaches - Logistic Regression and Softmax Regression
  - Non-parametric approach: K-NN (Doesn't learn any parameters).
- **Today about application of Bayesian**:
  - As a **Classifier**: Naive Bayes (NB) - Learns an abstraction from the data but does not learn parameters by gradient descent.
  - As a **Model calibrator**: Address uncertainties in data/model by **calibrating model confidences**.

Problem: Which bin did the ball come from?

- Two identical looking bins: A (●, ●, ●, ●, ●), and B (●, ●, ●, ●, ●)
- You are blind-folded and asked to select a ball from a bin (you don't know which bin that is).

Menti-Quiz (Code: 2131-2255)

You observe a ● ball. Which likely bin did the ball come from?

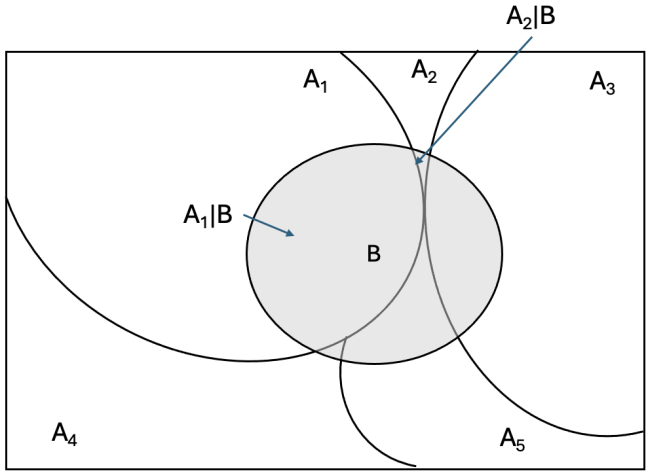
Problem: Which bin did the ball come from?

- Two identical looking bins: A (●, ●, ●, ●, ●), and B (●, ●, ●, ●, ●)
- You are blind-folded and asked to select a ball from a bin (you don't know which bin that is).

Menti-Quiz (Code: 2131-2255)

You observe a ● ball. Which likely bin did the ball come from?

Bayes Theorem



- A_i - Hypotheses/Causes (forms a partition over the set of all possibilities)
- B - Evidence/Effect, i.e., one that is observed.

Most likely hypothesis that has led to **an observation**

$$P(A_i|B) = \frac{\underbrace{P(B|A_i)}_{\text{reverse causation}} \underbrace{P(A_i)}_{\text{prior}}}{P(B)}$$

$$P(A_i|B) = \frac{P(B|A_i)P(A_i)}{\sum_j P(B|A_j)P(A_j)}$$

Solution: Which bin did the ball come from?

Compute the **priors**

- $P(\bullet|A) = 3/5$, $P(\bullet|A) = 2/5$, $P(\bullet|B) = 1/5$, $P(\bullet|B) = 4/5$
- P(A) = P(B) = 1/2 (No other information is given)

Apply Bayes Theorem to compute **posteriors**

- $P(B|\bullet) = P(\bullet|B)P(B)/\mathrm{P}(\bullet)$
- $= P(\bullet|B)P(B)/\ (P(\bullet|A)P(A) + P(\bullet|B)P(B))$
- $= \frac{1/5 \times 1/2}{3/5 \times 1/2 + 1/5 \times 1/2} = \frac{1/10}{3/10 + 1/10} = 1/4.$

From drawing balls to building a classification model

For classification

- Bins (A_i): Hypothesis $\equiv$ **Class**
- Ball (B): An observed Value of a **Categorical Feature**

Menti-Quiz (Code: 2131-2255)

Revisit the ball sampling problem: You now draw two balls blindfolded, and you observe both are red (●, ●). Will your estimate change? Why?

Refresher on Bayes Theorem

Naive Bayes

NB for Categorical data

NB for Non-categorical data

Bayesian Logistic Regression

Laplace approximation

MCMC sampling

From drawing balls to building a classification model

For classification

- Bins (A_i): Hypothesis $\equiv$ **Class**
- Ball (B): An observed Value of a **Categorical Feature**

Menti-Quiz (Code: 2131-2255)

Revisit the ball sampling problem: You now draw two balls blindfolded, and you observe both are red (●, ●). Will your estimate change? Why?

- Balls $\equiv$ Observed features (e.g., terms in an email that you received).
- You then have to find the likely class $\equiv$ Predict a class of an instance (e.g., predict if the email is spam or not).

Refresher on Bayes Theorem

Naive Bayes

NB for Categorical data

NB for Non-categorical data

Bayesian Logistic Regression

Laplace approximation

MCMC sampling

Independence Assumption

- Labelled training data $\equiv$ knowing the content of the two bins.
- Each bin $\equiv$ a class (spam or not spam).

Independence Assumption

- Labelled training data $\equiv$ knowing the content of the two bins.
- Each bin $\equiv$ a class (spam or not spam).
- Estimate probabilities of the form: $P(x = \text{cheap}|y = \text{SPAM})$.
- You need to **aggregate** these probabilities $\equiv$ assuming that drawing a ball is independent of drawing another.

Independence Assumption

- Labelled training data $\equiv$ knowing the content of the two bins.
- Each bin $\equiv$ a class (spam or not spam).
- Estimate probabilities of the form: $P(x = \text{cheap}|y = \text{SPAM})$.
- You need to **aggregate** these probabilities $\equiv$ assuming that drawing a ball is independent of drawing another.
- Here it means:
  - **A term** in an observed document **is independent of another**.
- Naive: Indicates this simplistic assumption.

Bayes Theorem to Invert Priors to Posteriors

- At inference time, you don't know the y value. You're given an instance $\mathbf{x}$.
- You need to compute $P(y = k|\mathbf{x})$ for each k and then take the maximum.
- In our example, choose the max between $P(y = 1|\mathbf{x})$ and $P(y = 2|\mathbf{x})$.

Bayes Theorem - Invert class priors to class posteriors

- $P(y = k|\mathbf{x}) = \frac{P(\mathbf{x}|y=k).P(y=k)}{Z}$
- $Z = \sum_{k'=1}^{M} P(\mathbf{x}|y = k').P(y = k')$.
- $P(\mathbf{x}|y = k) = \prod_{x \in \mathbf{x}} P(x|y = k)$ (**features are independent**, i.e., sampling a blue ball is independent of sampling an yellow ball).

Refresher on Bayes Theorem

Naive Bayes

NB for Categorical data

NB for Non-categorical data

Bayesian Logistic Regression

Laplace approximation

MCMC sampling

Naive Bayes

- Naive Bayes: Classifier that's somewhere in the middle of a parametric (logistic regression) and non-parametric classification (K-NN).
- Unlike a non-parametric classifier it learns a representation from the training set.
- Unlike a parametric classifier, it doesn't learn via back-propagation of error (i.e., doesn't learn from mistakes).

Naive Bayes works on Categorical Data

- Works for discrete-valued data instances, i.e., where the values of each component of a data instance are categorical.
- Examples of classifiers working with discrete-valued data:
  - A combination of age-range and income-bracket $\mapsto$ sanction loan (0/1).
  - Documents (comprised of terms) $\mapsto$ Spam (0/1).

Categorical Data Example: Loan Sanction Classifier

- Age-range $\in$ { Young (20-35), Middle_aged (36-55), Seniors (>55) }, i.e., one of {Y, M, S} (category names). You can think of these as integers, i.e., Y=1 and so on.

Categorical Data Example: Loan Sanction Classifier

- Age-range $\in$ { Young (20-35), Middle_aged (36-55), Seniors (>55) }, i.e., one of {Y, M, S} (category names). You can think of these as integers, i.e., Y=1 and so on.
- Income-bracket $\in$ {Low_income (1), Average_income (2), Above_average_income (3), High_income (4) }.

Categorical Data Example: Loan Sanction Classifier

- Age-range $\in$ { Young (20-35), Middle_aged (36-55), Seniors (>55) }, i.e., one of {Y, M, S} (category names). You can think of these as integers, i.e., Y=1 and so on.
- Income-bracket $\in$ {Low_income (1), Average_income (2), Above_average_income (3), High_income (4) }.
- Given training data of the following form:

Age-range	Income-bracket	Loan sanctioned
1	1	0
2	2	1
	...	
3	4	0

Categorical Data Example: Loan Sanction Classifier

- Age-range $\in$ { Young (20-35), Middle_aged (36-55), Seniors (>55) }, i.e., one of {Y, M, S} (category names). You can think of these as integers, i.e., Y=1 and so on.
- Income-bracket $\in$ {Low_income (1), Average_income (2), Above_average_income (3), High_income (4) }.
- Given training data of the following form:

Age-range	Income-bracket	Loan sanctioned
1	1	0
2	2	1
	...	
3	4	0

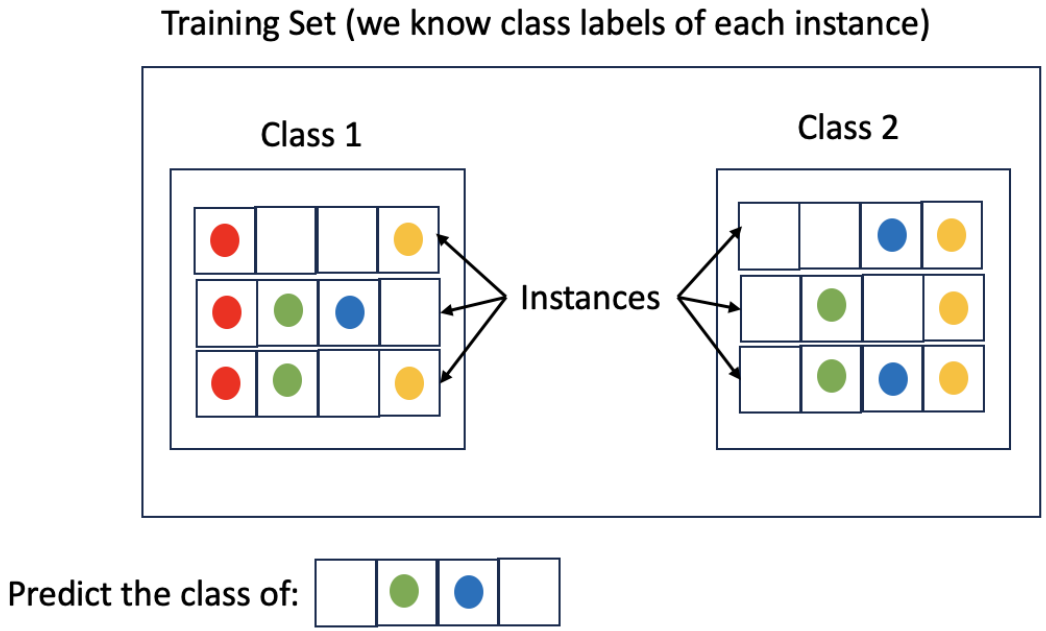
- Prediction Task:

Age-range	Income-bracket	Loan sanctioned
3	2	?

Categorical Data Example: Document Classification

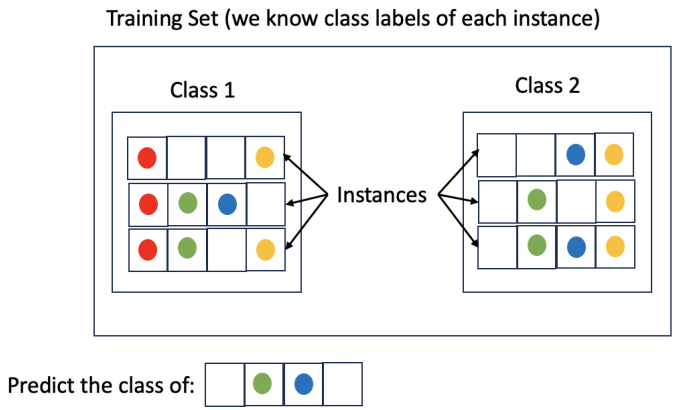
- $V = \{\text{Set of all unique terms}\}$ (called **vocabulary**).
- Each document is a $|V|$-sized vector, each index corresponds to a term.
- Value 1 if term present, else 0.
- Example: consider the following four term world.
  - $V = \{buy, product, cheap, review\}$.
  - $D_1 = \{buy, cheap, product\}, \mathbf{d}_1 = (1, 1, 1, 0), SPAM(D_1) = 1$.
  - $D_2 = \{product, review\}, \mathbf{d}_2 = (0, 0, 1, 1), SPAM(D_2) = 0$.
  - Example task: Predict if a document is spam or not.

Sampling with replacement



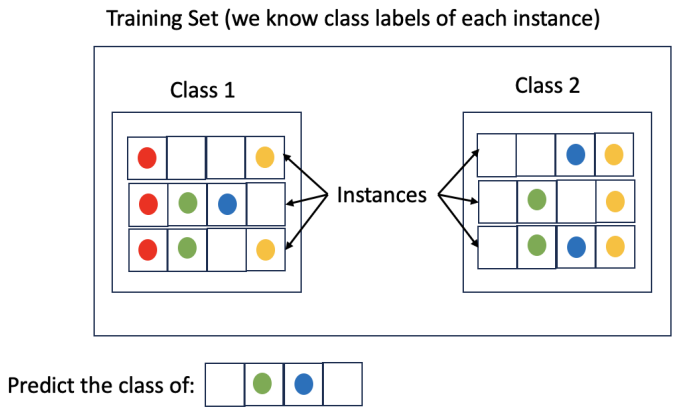
- Intuitions:
  1. Yellow/Green absence or presence doesn't really matter?
  2. Red not present $\approx$ Class 2.
  3. Blue present $\approx$ Class 2 (sort of puts more confidence that this is indeed class 2).
- We now need to **formalise the intuitions**.

Modeling the class priors



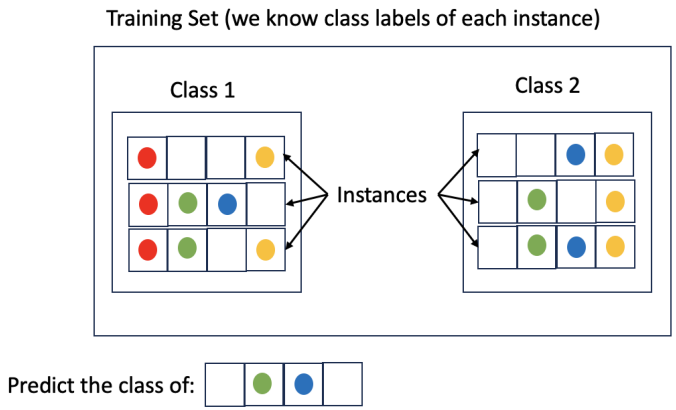
- Compute the **class priors** for each feature (balls).
- $P(x = Red|y = 1) = 3/3$
  - 3 red balls out of 3 total instances in class 1.
  - You can also estimate this to be $3/8$ (3 red balls out of a total of 8 balls)
- $P(x = Red|y = 2) = 0$.

Modeling the class priors



- Compute the **class priors** for each feature (balls).
- $P(x = Red|y = 1) = 3/3$
  - 3 red balls out of 3 total instances in class 1.
  - You can also estimate this to be $3/8$ (3 red balls out of a total of 8 balls)
- $P(x = Red|y = 2) = 0$.
- Repeat for all colors.

Modeling the class priors



- Compute the **class priors** for each feature (balls).
- $P(x = Red|y = 1) = 3/3$
  - 3 red balls out of 3 total instances in class 1.
  - You can also estimate this to be $3/8$ (3 red balls out of a total of 8 balls)
- $P(x = Red|y = 2) = 0$.
- Repeat for all colors.
- You now have a table of the following form:

Class	Color (Feature value)	Probability
Red	1	$3/3 = 1$
	...	
Green	2	$2/3$

Numerical Example of posterior computation

- $\mathbf{x}_{test}$ (we simply write as $\mathbf{x}$) $= \{\text{G, B}\}$.

Feature $\rightarrow$ Class Priors

$$P(\mathbf{x} = \{G, B\}|y = 1)$$

$$= P(G|y = 1)\,P(B|y = 1)$$

$$= \frac{2}{3} \times \frac{1}{3} = \frac{2}{9}$$

$$P(\mathbf{x} = \{G, B\}|y = 2)$$

$$= P(G|y = 2)P(B|y = 2)$$

$$= \frac{2}{3} \times \frac{2}{3} = \frac{4}{9}$$

Class Priors

$$P(y = 1) = \frac{3}{6} = \frac{1}{2}$$

$$P(y = 1) = \frac{3}{6} = \frac{1}{2}$$

Numerical Example of posterior computation

- Compute the normalisation constant (denominator in Bayes):
- $Z = \frac{2}{9}\frac{1}{2} + \frac{4}{9}\frac{1}{2} = \frac{1}{3}$.

$$P(y = 1|\mathbf{x} = \{G, B\})$$

$$= P(\mathbf{x}|y = 1)\ P(y = 1)\ /\ Z$$

$$= \frac{2}{9}\ \frac{1}{2} \times 3 = \frac{1}{3}$$

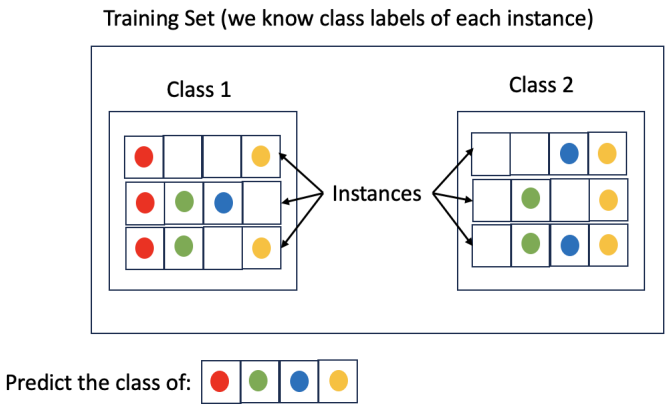
$$P(y = 2|\mathbf{x} = \{G, B\})$$

$$= P(\mathbf{x}|y = 1)P(y = 1)/Z$$

$$= \frac{4}{9}\frac{1}{2} \times 3 = \frac{2}{3}$$

- So, we predict $\mathbf{x} = \{G, B\}$ to class 2 (and that conforms to our intuitions).

Smoothing of Probabilities

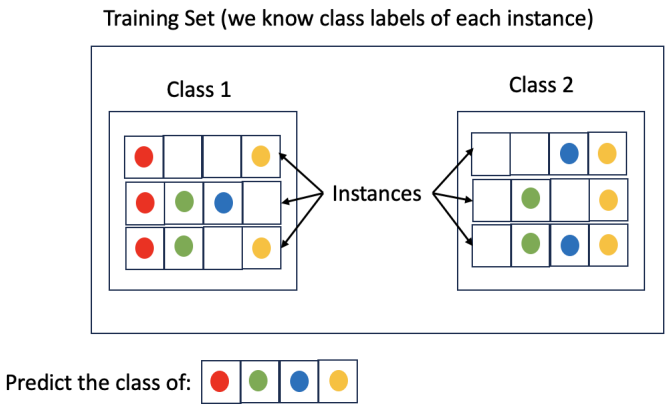


- What do we predict for $\mathbf{x}_{test} = \{R, G, B, Y\}$?

Menti-Quiz (Code: 2131-2255)

$P(x = Red|y = 2) = 0$. Is that good?

Smoothing of Probabilities



- What do we predict for $\mathbf{x}_{test} = \{R, G, B, Y\}$?

Menti-Quiz (Code: 2131-2255)

$P(x = Red|y = 2) = 0$. Is that good?

Laplace Smoothing

- Add 1 to the numerator and K (#categories) to the denominator.
- In our example, number of categories is 4 (Size of the set {R, G, B, Y}).
- $P(x = Red|y = 2) = \frac{1+\text{Count}(x=Red|y=2)}{\#categories+Count(class2)} = \frac{1+0}{4+7}$.
- And all other probabilities need to be adjusted in the same way.
- **Homework**:
  - Work out the posterior probability estimates with this modified notion of defining the smoothed probabilities.
  - Predict the class of $\mathbf{x}_{test} = \{R, G, B, Y\}$.

Some practical considerations

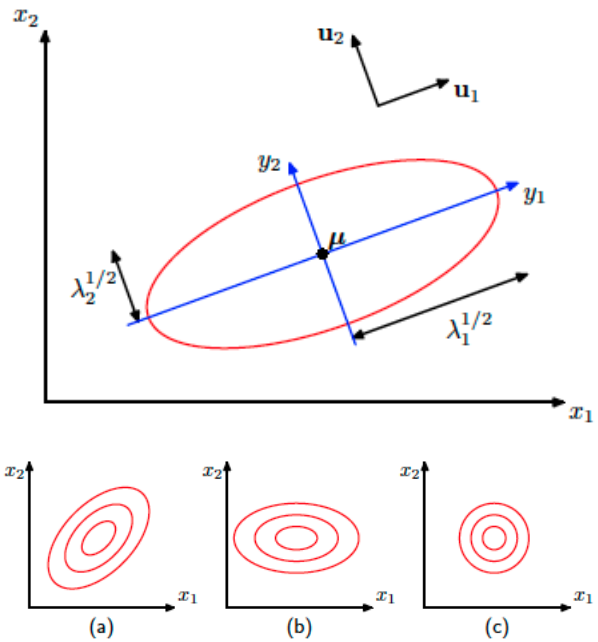
- Independence assumption requires computing:
  - $P(\mathbf{x}|y = k) = \prod_{x \in \mathbf{x}} P(x|y = k)$.
- Leads to floating point arithmetic underflows with large dimensions. Why?
- Because we're multiplying numbers that are all < 1.
- An elegant engineering solution is to work with the $\log(1 + P)$s, and predict the log-likelihoods.

A refresher on Gaussians

m-dimensional Gaussian

$$P(\mathbf{x}|\mathcal{N}(\boldsymbol{\mu}, \Sigma)) \propto \exp(-(\mathbf{x}-\boldsymbol{\mu})^T \Sigma^{-1}(\mathbf{x}-\boldsymbol{\mu}))$$

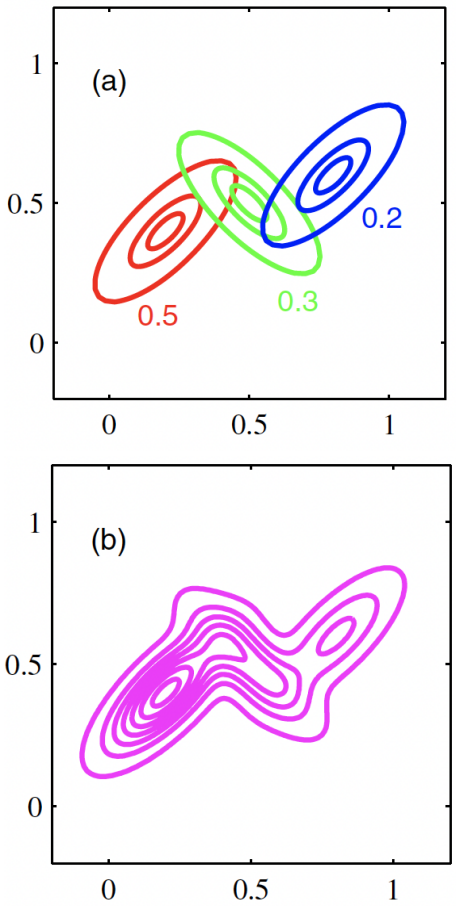
- $\boldsymbol{\mu} \in \mathbb{R}^m$ - the centroid is a vector of m dimensions
- $\Sigma \in \mathbb{R}^m \times \mathbb{R}^m$ - the spread matrix is of size $m \times m$



- Figure on the left shows a 2D example.
- Effect of the spread matrix:
  - a) $((1, 1), (1, 1))$ – Anisotropic w/ cross correlation
  - b) $((5, 0), (0, 1))$ – Anisotropic w/o cross correlation
  - c) $((1, 0), (0, 1))$ – Isotropic

Colab notebook:

Mixture of Gaussians (MoG)



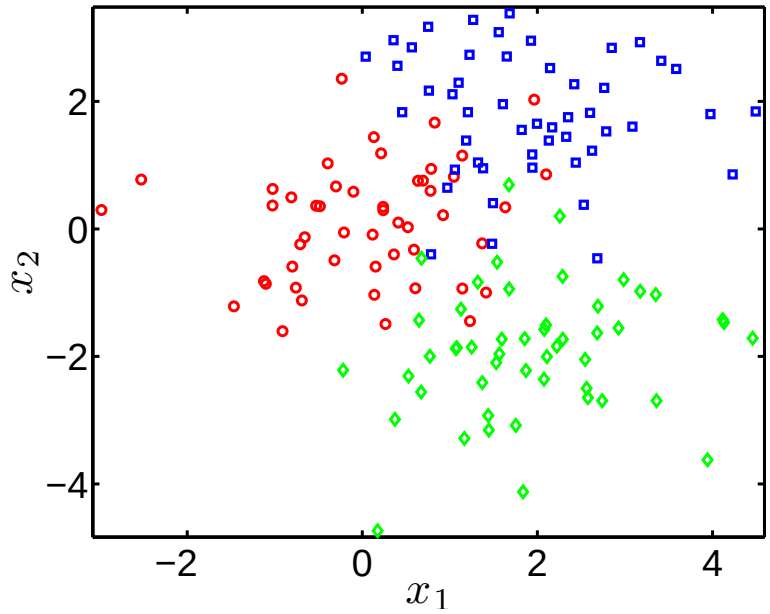
Gaussian Mixture distribution

$$\sum_{i=1}^{k} p_i \mathcal{N}(\boldsymbol{\mu}_i, \Sigma_i)$$

- p_i: Prior belief that an observed point $\mathbf{x}$ is generated by the i^{th} component.
- Posterior: Given $\mathbf{x}$, the likelihood that it is generated from the i^{th} component -
  - $P(Y = i|\mathbf{x}) = (\mathbf{x} - \boldsymbol{\mu}_i)^T \Sigma_i^{-1} (\mathbf{x} - \boldsymbol{\mu}_i)$

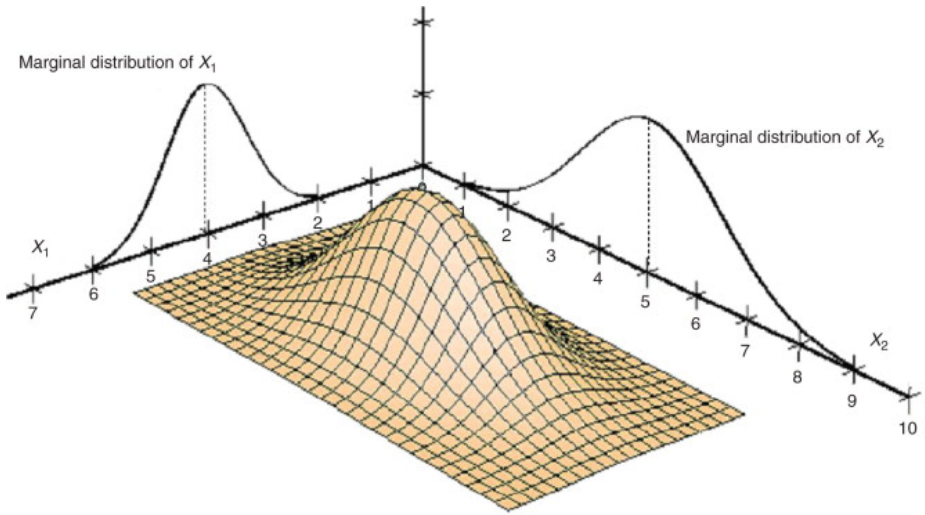
NB for non-categorical data, e.g., images?

- Assume that data follows an MoG (Mixture of Gaussians).
- Example:



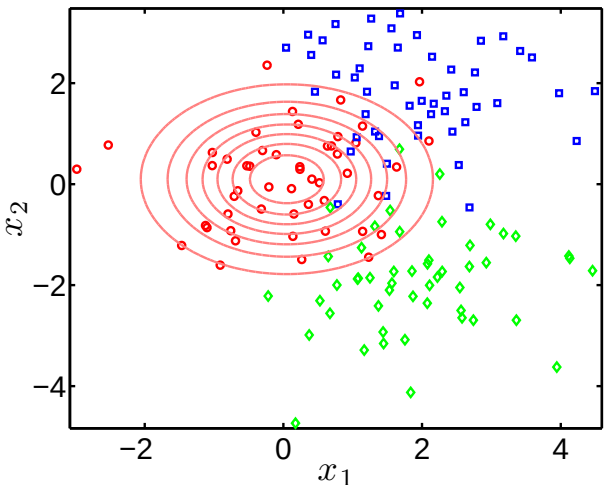
- 2D data: $\mathbf{x} = (x_1, x_2)$.
- $K = 3$ classes.
- $P(y = k) = 1/\#classes$ – uniform class priors.

Marginals of Gaussians



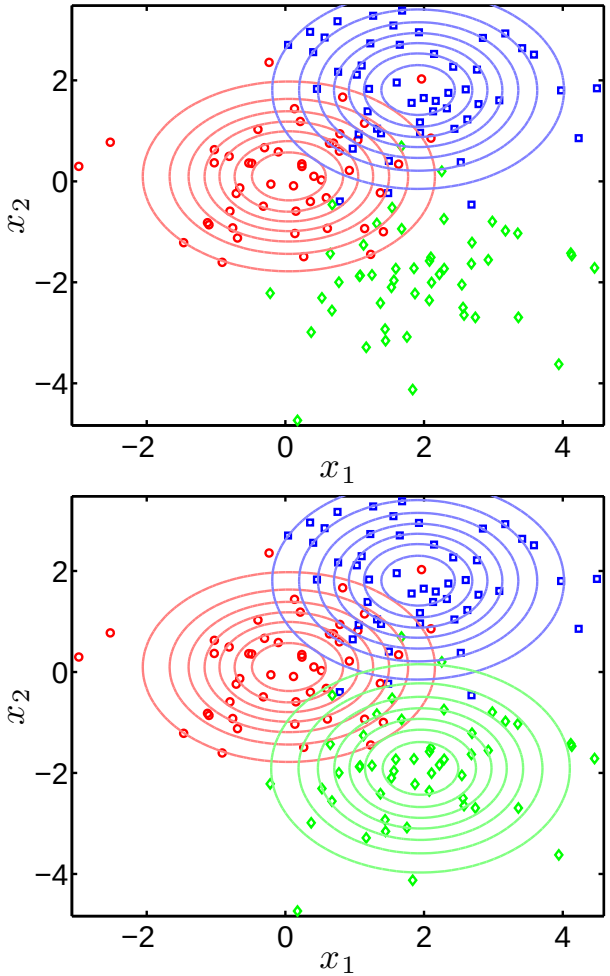
- A marginal of a Gaussian is a projection on to a lower dimension (analogous to a shadow) .
  - The projections themselves are Gaussians.
  - The two projections combined is **not equivalent** to the mixture distribution (except when cross-correlation components are 0s)
  - In NB, we work with the projections.

NB Algorithm (Training)



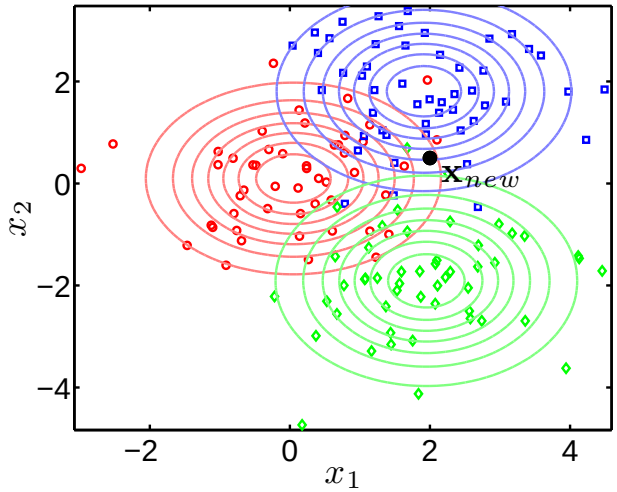
- Each component a Gaussian with parameters $\boldsymbol{\mu}$ and Σ.
- For NB, Σ is w/o cross-correlation (independence of features).
- Hence, for dimension d we work with d number of **univariate (1-d) Gaussians**, each with parameters μ_i and σ_i $(i = 1, \ldots, d)$.
- In the example, for the given red points, calculate μ^R and σ^R.
  - $\mu^R = \frac{1}{|R|} \sum_{\mathbf{x}:y(x)=R} \mathbf{x}$
  - $\sigma_i^R = \frac{1}{|R|} \sum_{\mathbf{x}:y(x)=R} \sqrt{(\mathbf{x}_i - \mu_i^R)^2}$

NB Algorithm (Training)



- Repeat the same steps for the green and the blue components.
  - $\mu^G = \frac{1}{|G|} \sum_{\mathbf{x}:y(x)=G} \mathbf{x}$
  - $\sigma_i^G = \frac{1}{|G|} \sum_{\mathbf{x}:y(x)=G} \sqrt{(\mathbf{x}_i - \mu_i^G)^2}$

NB Algorithm (Inference)



- For each given point $\mathbf{x}_{new}$:
- Compute the posterior likelihoods for each component, e.g., for red:
- $P(\mathbf{x_{new}} = R) = (\mathbf{x} - \mu^{\mathbf{R}})^T((\sigma_1^R, 0)(0, \sigma_2^R))^{-1}(\mathbf{x} - \mu^{\mathbf{R}})$
- Similarly, $P(\mathbf{x_{new}} = G) = (\mathbf{x} - \mu^{\mathbf{G}})^T((\sigma_1^G, 0)(0, \sigma_2^G)^{-1}(\mathbf{x} - \mu^{\mathbf{G}})$, and so on.
- Multiply all these posteriors with the class priors, i.e., $P(\mathbf{x_{new}} = R) \leftarrow P(\mathbf{x_{new}} = R) \times P(R)$, and so on.
- Classify the point to be in the class with the highest probability.

Calibration of Model Confidence

Menti-Quiz (Code: 2131-2255)

Let's see how confident humans are!

Refresher on Bayes Theorem

Naive Bayes

NB for Categorical data

NB for Non-categorical data

Bayesian Logistic Regression

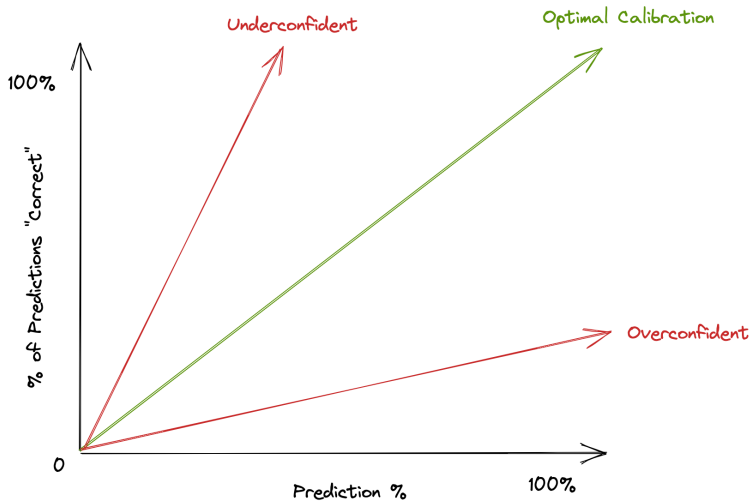
Laplace approximation

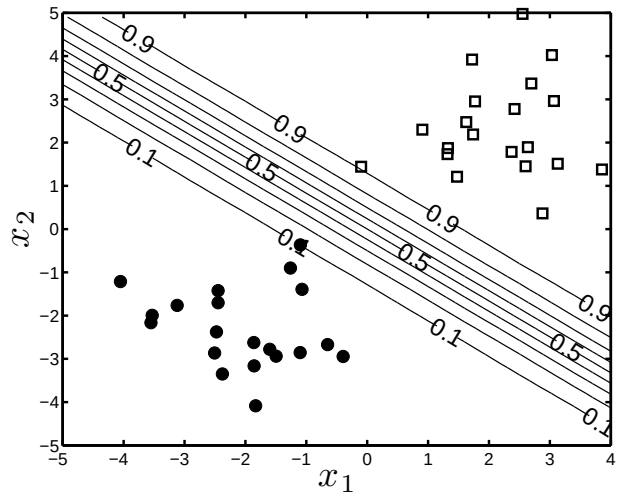
MCMC sampling

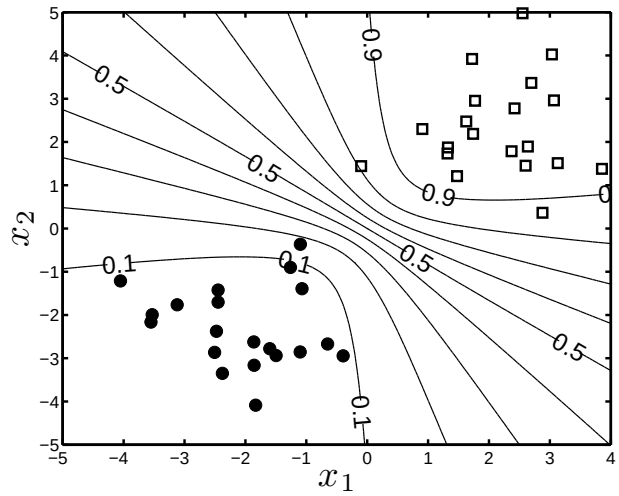
Calibration of Model Confidence

Menti-Quiz (Code: 2131-2255)

Let's see how confident humans are!







Introduction

D. Ganguly

Refresher on Bayes Theorem

Naive Bayes

NB for Categorical data

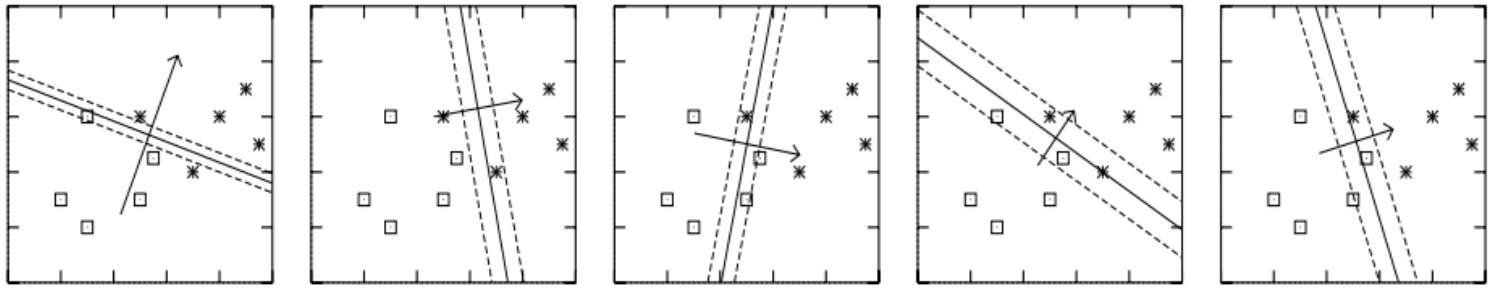
NB for Non-categorical data

Bayesian Logistic Regression

Laplace approximation

MCMC sampling

Model the parameter (weight) priors



- Which decision boundary is better?
- Can estimations change if we see more data samples?

The Core Equation

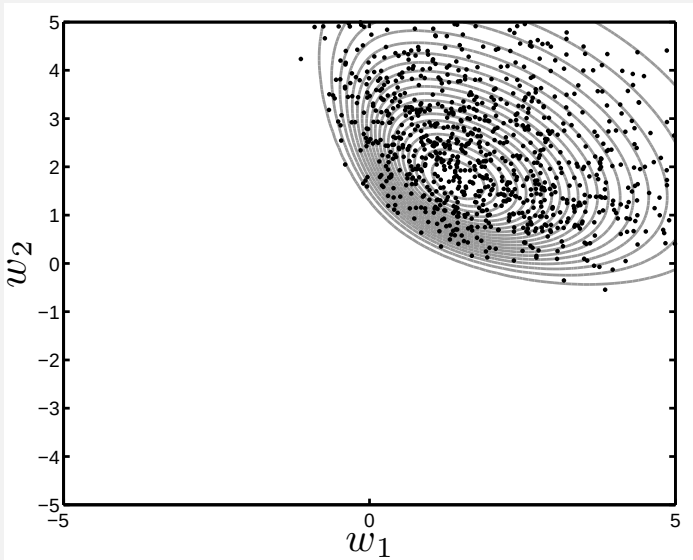
$$\underbrace{P(Y|X,\mathcal{D})}_{\text{Overall belief}} = \int \underbrace{P(Y|X,\theta)}_{\text{Belief with one model}} \underbrace{P(\theta|\mathcal{D})d\theta}_{\text{Model likelihood}}$$

- Aggregate the different beliefs of explaining your data samples by various models $P(Y|X,\theta)$ weighted by their priors $P(\theta|\mathcal{D})$.

Bayesian: Addresses Model Uncertainty

A Bayesian approach

- Doesn't estimate a single point, but rather a distribution.
- In the **data space**: Observed data is sampled from an underlying distribution (e.g., an MoG).
- Analogously, points in the parameter space are also sampled from a distribution $\implies$ **not a single solution** but **a distribution that yields potential solutions**.



Variational Approximation

- **Approximate** $p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$ with another distribution.
  - $p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$: Model parameter uncertainty, i.e., the **distribution of model parameters** given the training data.

Refresher on Bayes Theorem

Naive Bayes

NB for Categorical data

NB for Non-categorical data

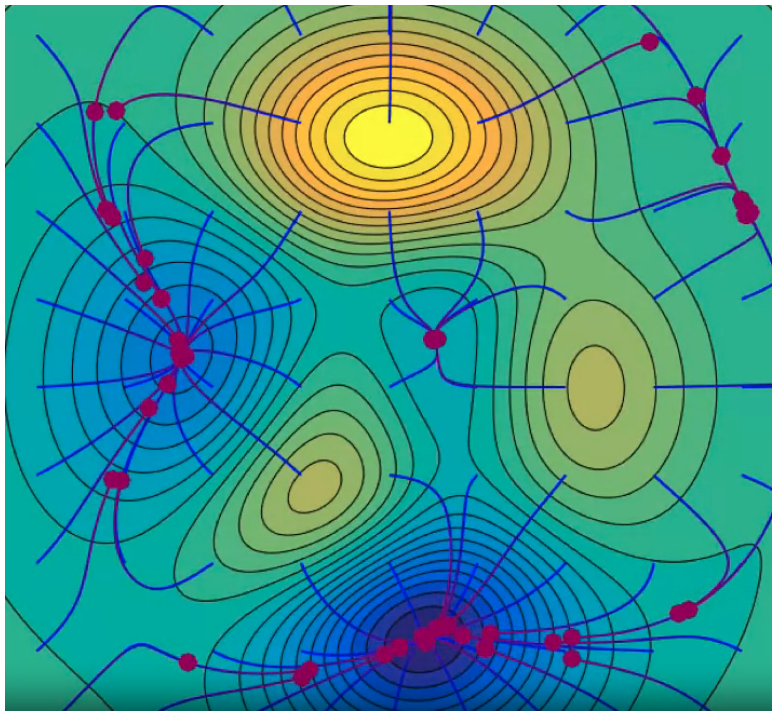
Bayesian Logistic Regression

Laplace approximation

MCMC sampling

Variational Approximation

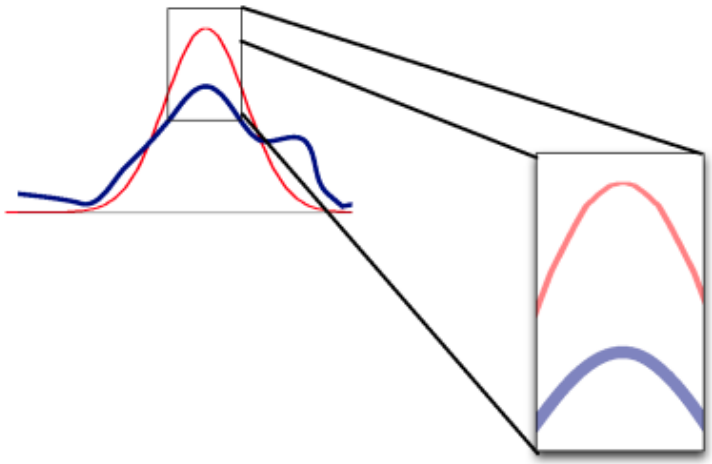
- **Approximate** $p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$ with another distribution.
  - $p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$: Model parameter uncertainty, i.e., the **distribution of model parameters** given the training data.
  - Realise that: with data perturbation or a different starting point of MAP (gradient descent), we may converge on different decision boundaries.



Variational Approximation by Laplace Algorithm

Variational distribution $q(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$

- Should be **similar in behaviour** to the distribution that we want to approximate.
- We then need an algorithm to estimate the parameters of this variational distribution q.



- Fit the variational distribution at the **mode (most likely region)** of the original distribution.
  - This is the region where we want a close fit.
  - Rest doesn't matter that much.

Laplace approximation

- Approximate $p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$ with a Gaussian:
  $q(\mathbf{w}|\mathbf{X}, \mathbf{t}) = \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$
- We now need to estimate the values of $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$.

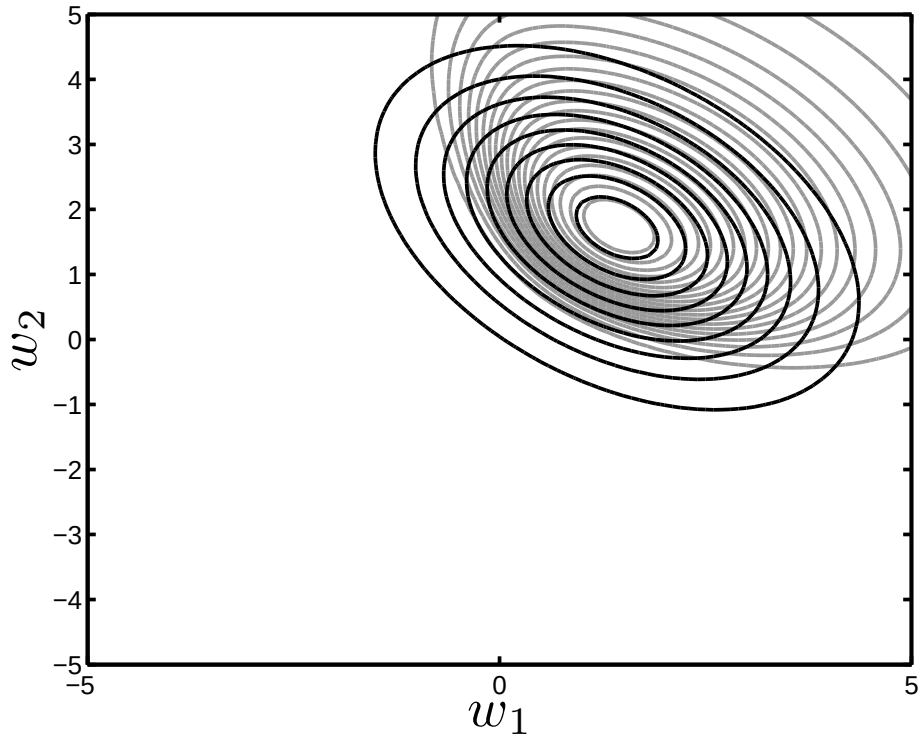
Posterior likelihood

$g = p(\mathbf{t}|\mathbf{X}, \mathbf{w})p(\mathbf{w}|\sigma^2)$ - distribution of model predictions
$\widehat{\mathbf{w}} = \underset{\mathbf{w}}{\text{argmax}} \ \log g(\mathbf{w}; \mathbf{X}, \mathbf{t}, \sigma^2)$ – the mode of this distribution

Consider the point estimate as the mode

$$\boldsymbol{\mu} = \widehat{\mathbf{w}}, \ \boldsymbol{\Sigma}^{-1} = \underbrace{- \left. \frac{\partial \log g(\mathbf{w}; \mathbf{X}, \mathbf{t}, \sigma^2)}{\partial \mathbf{w} \partial \mathbf{w}^{\mathsf{T}}} \right|_{\widehat{\mathbf{w}}}}_{\text{spread of the variational}}$$

Laplace approximation for logistic regression



- Dark lines – approximation.
- Light lines – $\propto$ $p(\mathbf{w}|\mathbf{X}, \mathbf{t}, \sigma^2)$.
- Approximation is OK.
- As expected, it gets worse as we travel away from the mode.

Predictions with the Laplace approximation

- We have $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ as an approximation to $p(\mathbf{w}|\mathbf{X}, \mathbf{t})$.
- Can we use it to make predictions?
- Need to evaluate:

$$\begin{aligned} P(T_{\text{new}} = 1|\mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t}) &= \mathbf{E}_{\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})} \{P(T_{\text{new}} = 1|\mathbf{x}_{\text{new}}, \mathbf{w})\} \\ &= \int \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma}) \frac{1}{1 + \exp(-\mathbf{w}^{\mathsf{T}}\mathbf{x}_{\text{new}})} \, d\mathbf{w} \end{aligned}$$

- We can't quantitatively evaluate the integral. So, what was the point?

Sampling from $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$ is easy

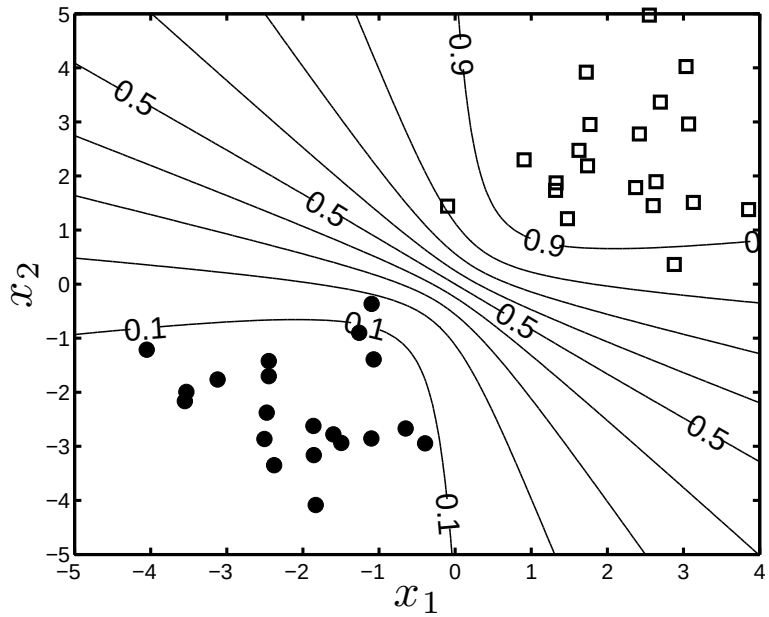
And we can approximate an expectation with samples!

Predictions with the Laplace approximation

Expectation over samples

Draw S samples $\mathbf{w}_1, \ldots, \mathbf{w}_S$ from $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$

$$\mathbf{E}_{\mathcal{N}(\boldsymbol{\mu},\boldsymbol{\Sigma})}\left\{P(T_{\text{new}} = 1|\mathbf{x}_{\text{new}}, \mathbf{w})\right\} \approx \frac{1}{S}\sum_{s=1}^{S}\frac{1}{1+\exp(-\mathbf{w}_s^{\mathsf{T}}\mathbf{x}_{\text{new}})}$$

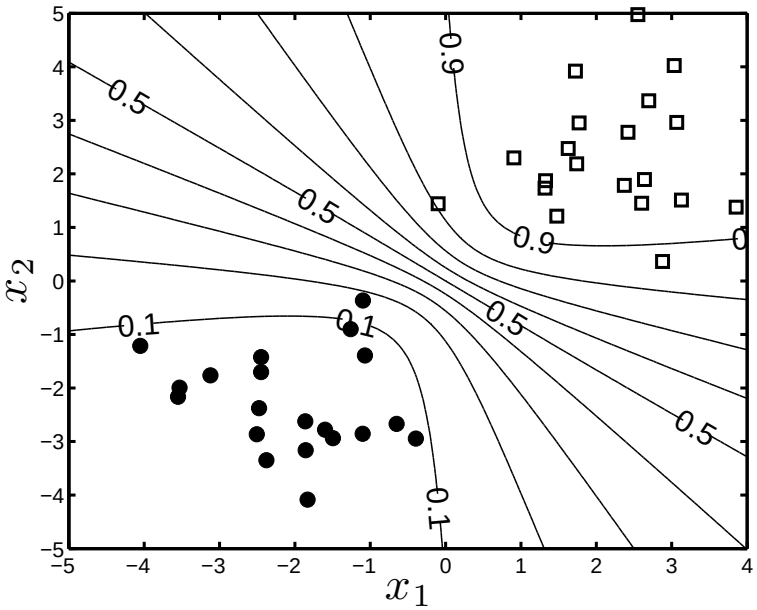


- Contours of $P(T_{\text{new}} = 1|\mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t})$.
- Better than those from the point prediction?

Predictions with the Laplace approximation

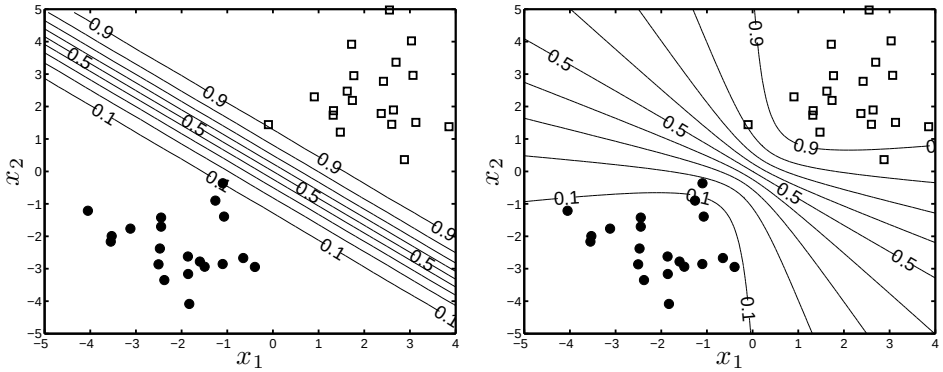
Predictions averaged over many classifiers

$$\mathbf{E}_{\mathcal{N}(\boldsymbol{\mu},\boldsymbol{\Sigma})}\{P(T_{\text{new}}=1|\mathbf{x}_{\text{new}},\mathbf{w})\} \approx \frac{1}{S}\sum_{s=1}^{S}\frac{1}{1+\exp(-\mathbf{w}_s^{\mathsf{T}}\mathbf{x}_{\text{new}})}$$



- This classifier is **less certain** in its predictions.
- Only if a point is **close to a centroid of a class**, the classifier's posterior probability is high.

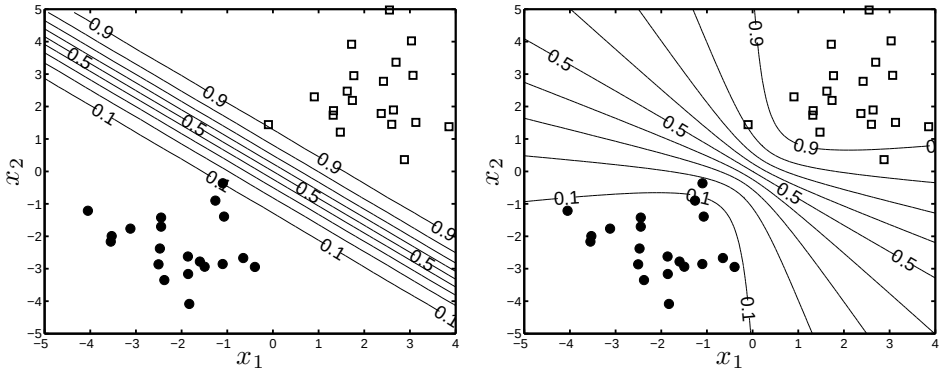
Point prediction v Laplace approximation



Menti-Quiz (Code: 2131-2255)

Why the difference? Explain

Point prediction v Laplace approximation



Menti-Quiz (Code: 2131-2255)

Why the difference? Explain

MCMC Sampling

Laplace Algorithm

- Computationally expensive!
- Suffers from curse of dimensionality.
- We relying on sampling for the eventual predictions.
  - Do we then need to estimate a parametric distribution to be able to sample from it?
  - No - let's motivate the idea of **Rejection Sampling**.

Refresher on Bayes Theorem

Naive Bayes

NB for Categorical data

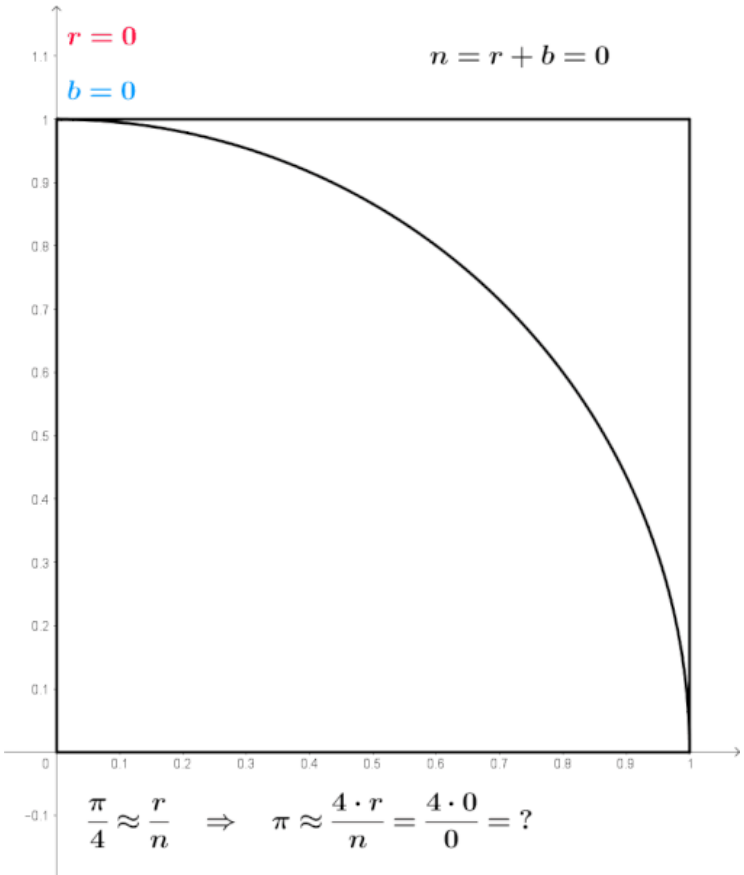
NB for Non-categorical data

Bayesian Logistic Regression

Laplace approximation

MCMC sampling

The idea of Rejection Sampling



Analogy

- Curve that defines a quadrant of a circle $\equiv$ True distribution of $\mathbf{w}$.
- Both are unknown.

- Use a criterion to decide whether a sample is to be considered or rejected.
- Compute stats on the acceptance vs. rejection to estimate the desired distribution.

Metropolis-Hastings

MH Sampling

Similar to the idea of accepting or rejecting if a point lies within a unit radius or not for computing π.

Proposal and acceptance

- Produces a sequence of samples – $\mathbf{w}_1, \mathbf{w}_2, \ldots, \mathbf{w}_s, \ldots$
- Consider the last sample accepted: $\mathbf{w}_{s-1}$
- First *propose* a **candidate** $\mathbf{w}_s$ ($\widetilde{\mathbf{w}_s}$) based on $\mathbf{w}_{s-1}$.
- Then decide whether or not to *accept* $\widetilde{\mathbf{w}_s}$
  - If accepted, $\mathbf{w}_s = \widetilde{\mathbf{w}_s} \implies$ we moved in the parameter space!
  - If not, $\mathbf{w}_s = \mathbf{w}_{s-1} \implies$ try again!

Refresher on Bayes Theorem

Naive Bayes

NB for Categorical data

NB for Non-categorical data

Bayesian Logistic Regression

Laplace approximation

MCMC sampling

MH – proposal

- Treat $\widetilde{\mathbf{w}_s}$ as a random variable **conditioned on** $\mathbf{w}_{s-1}$
- Define $p(\widetilde{\mathbf{w}_s}|\mathbf{w}_{s-1})$
  - Note that this does not necessarily have to be similar to posterior we're trying to sample from.
- Can be **any distribution**! So, choose a parametric distribution that is easy to work with.

Introduction

D. Ganguly

Refresher on Bayes Theorem

Naive Bayes

NB for Categorical data

NB for Non-categorical data

Bayesian Logistic Regression

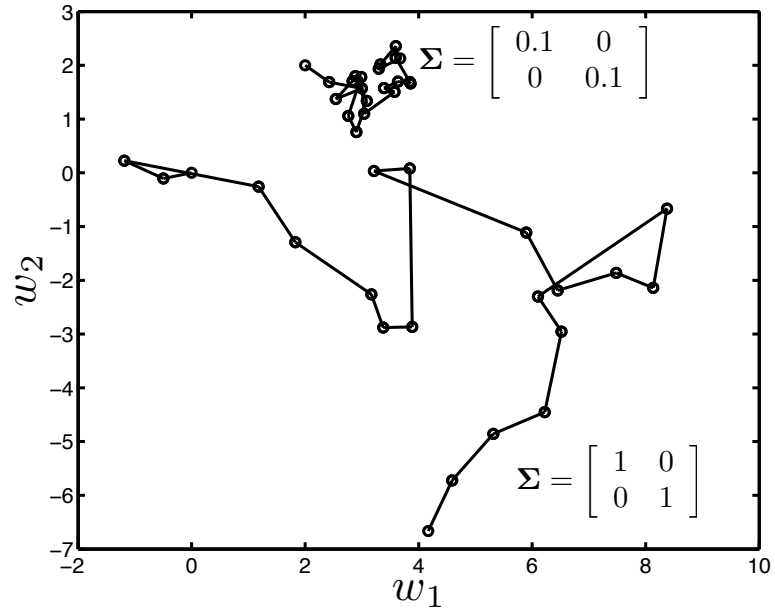
Laplace approximation

MCMC sampling

MH – proposal

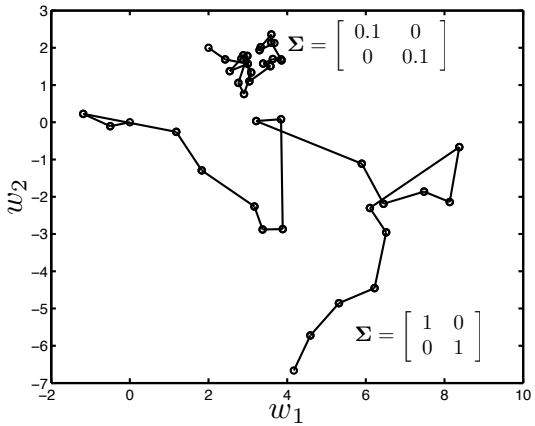
- Treat $\widetilde{\mathbf{w}_s}$ as a random variable **conditioned on** $\mathbf{w}_{s-1}$
- Define $p(\widetilde{\mathbf{w}_s}|\mathbf{w}_{s-1})$
  - Note that this does not necessarily have to be similar to posterior we're trying to sample from.
- Can be **any distribution**! So, choose a parametric distribution that is easy to work with.
- Use a Gaussian centred on $\mathbf{w}_{s-1}$ with some covariance:

$$p(\widetilde{\mathbf{w}_s}|\mathbf{w}_{s-1}, \mathbf{\Sigma}_p) = \mathcal{N}(\mathbf{w}_{s-1}, \mathbf{\Sigma}_p)$$



Random Walk in MH

- Start from a random point on the parameter space.
- Estimations get better with a higher number of iterations.



- What is the role of σ in MH sampling?
- High σ:
  - **Aggressive** exploration.
  - Effective if point estimate $\widehat{\mathbf{w}}$ is bad.
- Low σ:
  - **Conservative** exploration.
  - More exploitation: works well if point estimate $\widehat{\mathbf{w}}$ is good.

MH Acceptance for Symmetric Variational

- p: Distribution that we want to approximate.
- Acceptance probability r.

Acceptance probability r

$$r = \min(1, \frac{p(\widetilde{\mathbf{w}_s}|\mathbf{X}, \mathbf{t}, \sigma^2)}{p(\mathbf{w}_{s-1}|\mathbf{X}, \mathbf{t}, \sigma^2)}.$$

- If more probable (better) sample drawn ($p(\widetilde{\mathbf{w}_s})$) then **always accept it**.
- Else accept it with some probability r.
- Small r means that:
  - $p(\widetilde{\mathbf{w}_s})$ is small – this model is not likely to be effective. Hence accept only with a small probability.
  - $p(\mathbf{w}_{s-1}|\mathbf{X}, \mathbf{t}, \sigma^2)$ is high – we already have got good solutions; risky to explore more.

MH Acceptance for Asymmetric Variational

Acceptance probability r

$$r = \min(1, \frac{p(\widetilde{\mathbf{w}_s}|\mathbf{X}, \mathbf{t}, \sigma^2)}{p(\mathbf{w}_{s-1}|\mathbf{X}, \mathbf{t}, \sigma^2)} \frac{p(\mathbf{w}_{s-1}|\widetilde{\mathbf{w}_s}, \mathbf{\Sigma}_p)}{p(\widetilde{\mathbf{w}_s}|\mathbf{w}_{s-1}, \mathbf{\Sigma}_p)}).$$

- The ratio of $p(\mathbf{w}_{s-1}|\widetilde{\mathbf{w}_s}, \mathbf{\Sigma}_p)$ and $p(\widetilde{\mathbf{w}_s}|\mathbf{w}_{s-1}, \mathbf{\Sigma}_p)$ is called the Hastings correction.
- High $p(\mathbf{w}_{s-1}|\widetilde{\mathbf{w}_s}, \mathbf{\Sigma}_p)$: We can explain our existing model with the new model (**Good Exploitation**).
- Low $p(\widetilde{\mathbf{w}_s}|\mathbf{w}_{s-1}, \mathbf{\Sigma}_p)$: The new model is different from what we have seen so far (**Good Exploration**).

MH for Logistic Regression

Generic Formula

$$r = \min(1, \frac{p(\widetilde{\mathbf{w}_s}|\mathbf{X}, \mathbf{t}, \sigma^2)}{p(\mathbf{w}_{s-1}|\mathbf{X}, \mathbf{t}, \sigma^2)} \frac{p(\mathbf{w}_{s-1}|\widetilde{\mathbf{w}_s}, \mathbf{\Sigma}_p)}{p(\widetilde{\mathbf{w}_s}|\mathbf{w}_{s-1}, \mathbf{\Sigma}_p)}).$$

In Logistic Regression

$$r = \min(1, \frac{g(\widetilde{\mathbf{w}_s}; \mathbf{X}, \mathbf{t}, \sigma^2)}{g(\mathbf{w}_{s-1}; \mathbf{X}, \mathbf{t}, \sigma^2)} \frac{p(\mathbf{w}_{s-1}|\widetilde{\mathbf{w}_s}, \mathbf{\Sigma}_p)}{p(\widetilde{\mathbf{w}_s}|\mathbf{w}_{s-1}, \mathbf{\Sigma}_p)}).$$

- Replace $p(\mathbf{w}|\mathbf{X})$ with the cross-entropy posterior g (as we did for Laplace Approximation).

Refresher on Bayes Theorem

Naive Bayes

NB for Categorical data

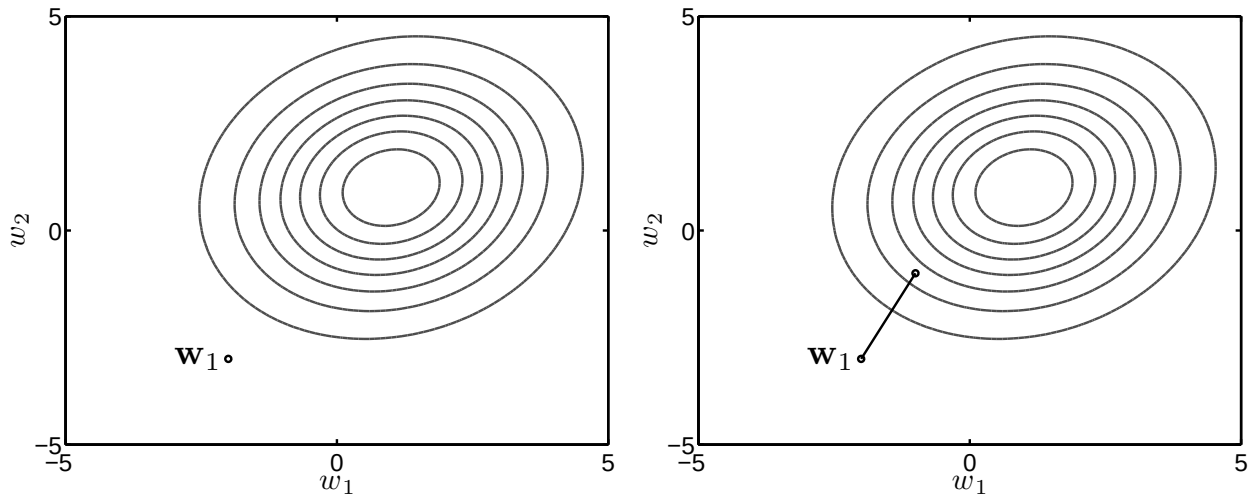
NB for Non-categorical data

Bayesian Logistic Regression

Laplace approximation

MCMC sampling

MH – walkthrough



Menti-Quiz (Code: 2131-2255)

Why do we accept the first sample?

Introduction

D. Ganguly

Refresher on Bayes Theorem

Naive Bayes

NB for Categorical data

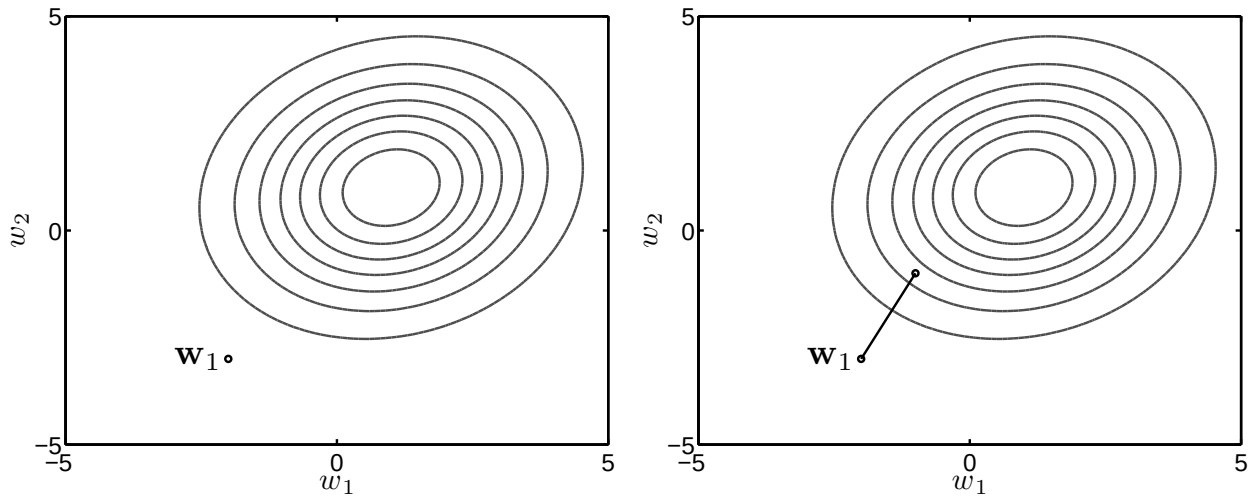
NB for Non-categorical data

Bayesian Logistic Regression

Laplace approximation

MCMC sampling

MH – walkthrough



Menti-Quiz (Code: 2131-2255)

Why do we accept the first sample?

Introduction

D. Ganguly

Refresher on Bayes Theorem

Naive Bayes

NB for Categorical data

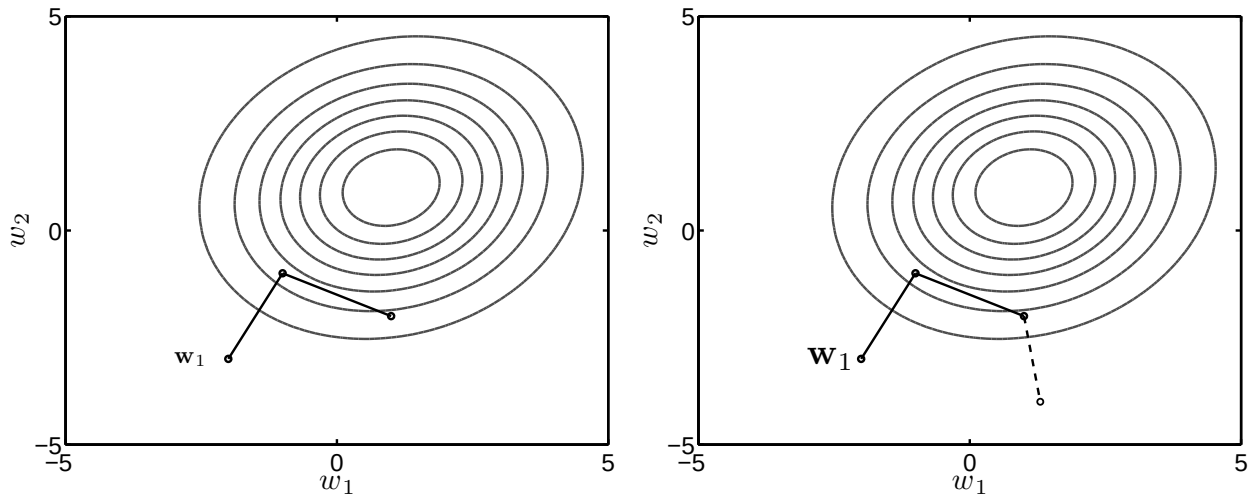
NB for Non-categorical data

Bayesian Logistic Regression

Laplace approximation

MCMC sampling

MH – walkthrough



Menti-Quiz (Code: 2131-2255)

Why do we reject the third sample?

Introduction

D. Ganguly

Refresher on Bayes Theorem

Naive Bayes

NB for Categorical data

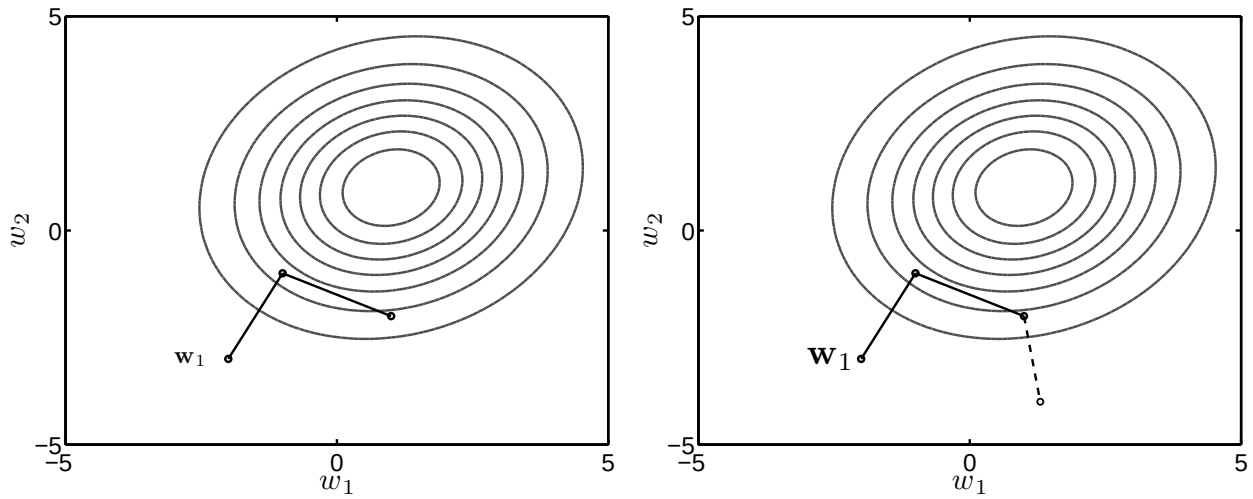
NB for Non-categorical data

Bayesian Logistic Regression

Laplace approximation

MCMC sampling

MH – walkthrough



Menti-Quiz (Code: 2131-2255)

Why do we reject the third sample?

Introduction

D. Ganguly

Refresher on Bayes Theorem

Naive Bayes

NB for Categorical data

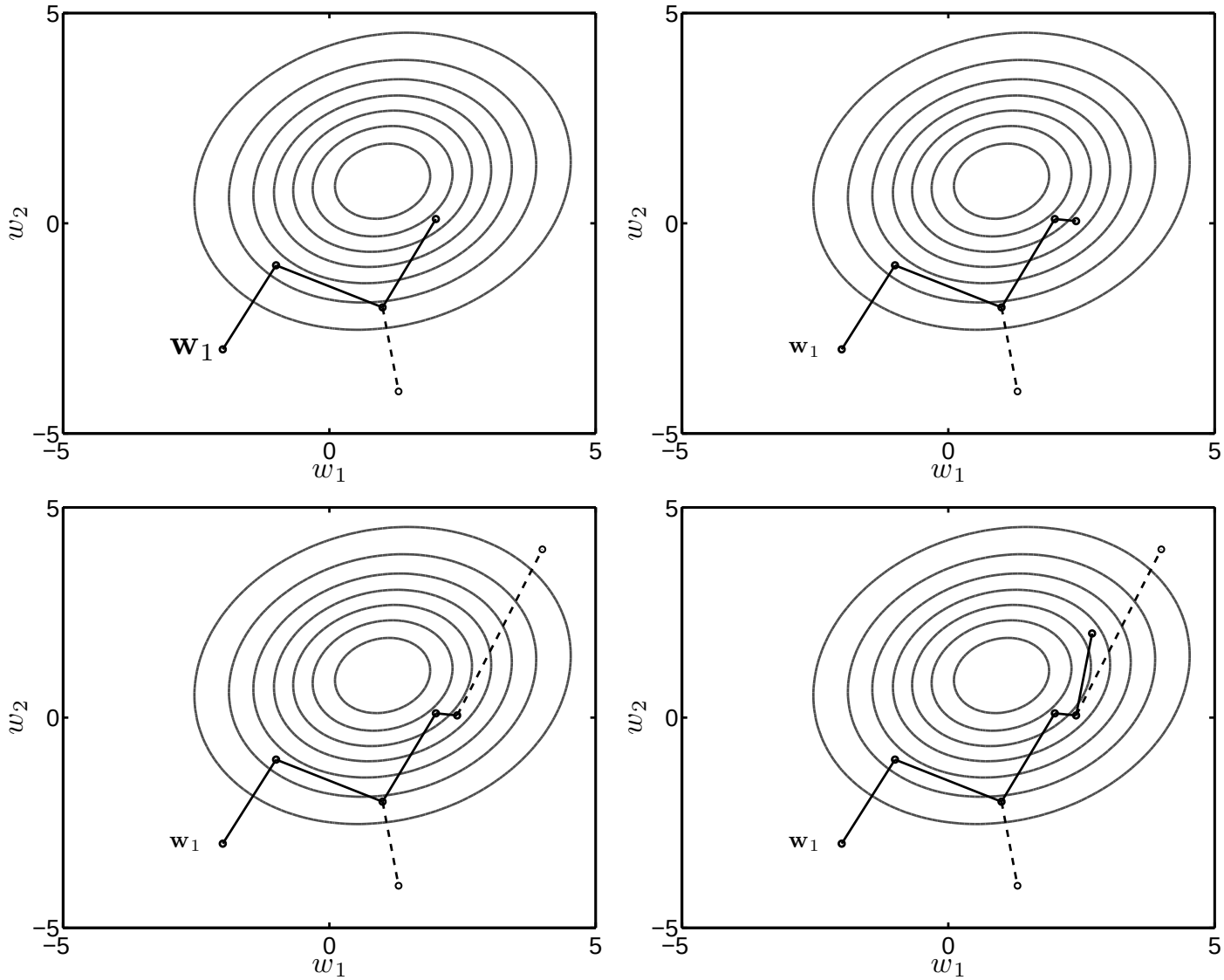
NB for Non-categorical data

Bayesian Logistic Regression

Laplace approximation

MCMC sampling

MH – walkthrough



Refresher on Bayes Theorem

Naive Bayes

NB for Categorical data

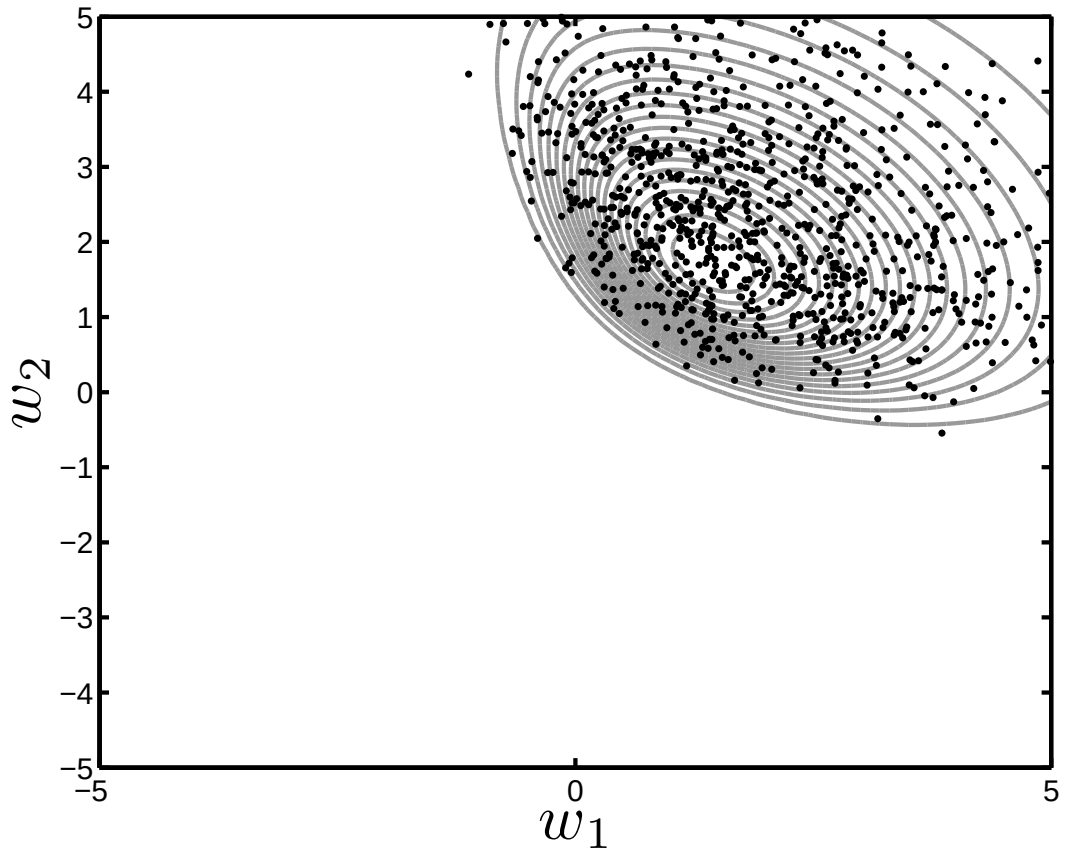
NB for Non-categorical data

Bayesian Logistic Regression

Laplace approximation

MCMC sampling

What do the samples look like?

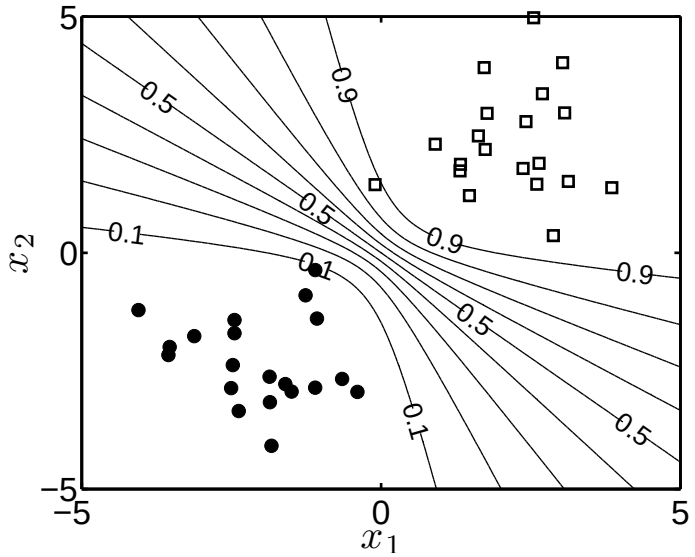


- 1000 samples from the posterior using MH.

Predictions with MH

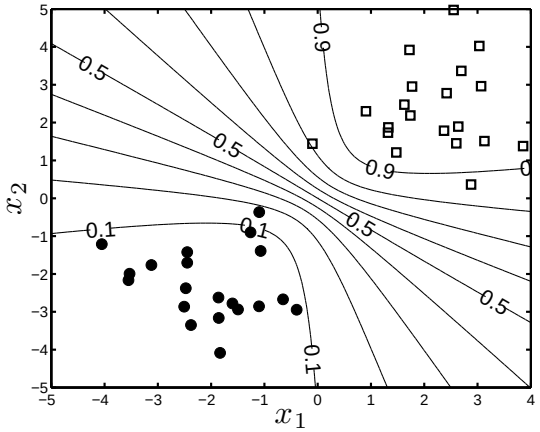
- MH provides us with a set of samples – $\mathbf{w}_1, \ldots, \mathbf{w}_S$.
- These can be used like the samples from the Laplace approximation:

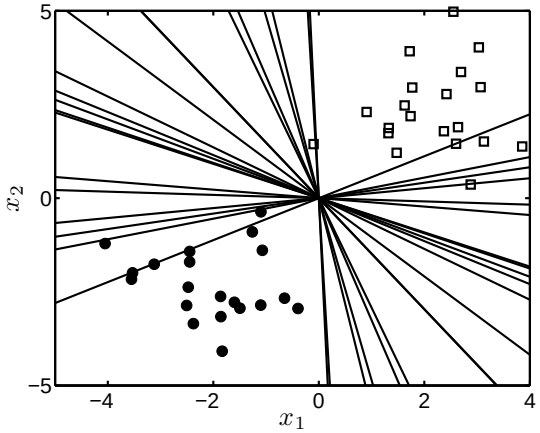
$$P(t_{\text{new}} = 1 | \mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t}, \sigma^2) = \mathbf{E}_{p(\mathbf{w}|\mathbf{X},\mathbf{t},\sigma^2)} \{P(t_{\text{new}} | \mathbf{x}_{\text{new}}, \mathbf{w})\}$$
$$\approx \frac{1}{S} \sum_{s=1}^{S} \frac{1}{1 + \exp(-\mathbf{w}_s^T \mathbf{x}_{\text{new}})}$$



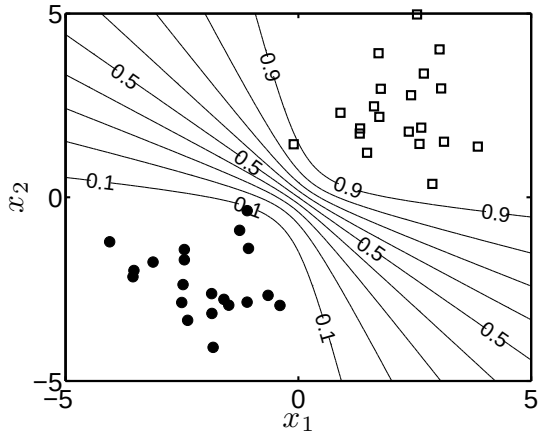
- Contours of $P(t_{\text{new}} = 1 | \mathbf{x}_{\text{new}}, \mathbf{X}, \mathbf{t}, \sigma^2)$

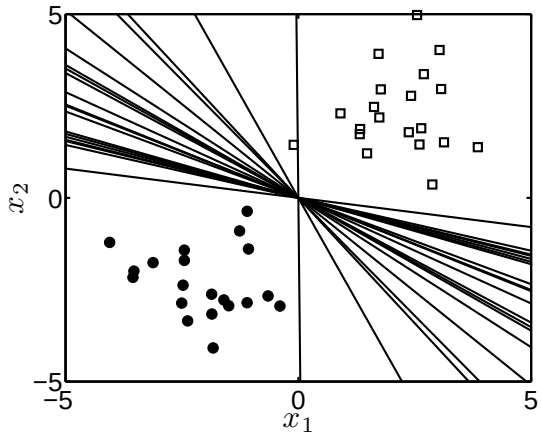
Laplace v MH





- Laplace approximation allows some *bad* boundaries.
- Hence over-compensates for uncertainty modeling.
- See how close the 0.9 contours are to the centroids.





- MH is more selective.
- Achieves the right amount of calibration for uncertainty.
- See that the 0.9 contours aren't too close to the centroids.

Summary

- Two applications of Bayes Theorem in Machine Learning.
- First: To build a classifier based on the independence assumption of features.
- Second: Calibrate model confidences for uncertainties.
- Two specific algorithms for extending the MAP estimate.
  - Laplace Approximation - Involves **estimating parameters of a distribution** and samples.
  - Metropolis Hastings - **No need to estimate parameters**. Find the distribution by rejection sampling.
- **Next week**:
  - Bayesian is a calibration approach - no direct modeling of uncertainty in the objective function.
  - Will discuss a **more direct approach** of modeling uncertainty - **Support Vector Machines**.
  - **Change in the objective function** itself.

Refresher on Bayes Theorem

Naive Bayes

NB for Categorical data

NB for Non-categorical data

Bayesian Logistic Regression

Laplace approximation

MCMC sampling