

Probabilistic models - Bayesian Methods

Mengye Ren

NYU

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- Midterm next week Oct 24 4:55 - 6:55 PM (same as lecture).
- Send me your course project group by Oct 20 (NetID + NYU ID, Email title contains **CSCI-GA 2565**).
- Course project 2 page proposal due Oct 27.

Overview

Why probabilistic modeling?

- A unified framework that covers many models, e.g., linear regression, logistic regression
- Learning as **statistical inference**
- Principled ways to incorporate your belief on the data generating distribution (inductive biases)

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- How to estimate the parameters of our model? Maximum likelihood estimation.
- Compare and contrast conditional and generative models.

Conditional models

Linear regression

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Examples:

- Predicting house price given location, condition, build year etc.
- Predicting medical cost of a person given age, sex, region, BMI etc.
- Predicting age of a person based on their photos.

Problem setup

Data Training examples $\mathcal{D} = \{(x^{(n)}, y^{(n)})\}_{n=1}^N$, where $x \in \mathbb{R}^d$ and $y \in \mathbb{R}$.

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Model A *linear* function h (parametrized by θ) to predict y from x :

$$h(x) = \sum_{i=0}^d \theta_i x_i = \theta^T x, \quad (1)$$

where $\theta \in \mathbb{R}^d$ are the **parameters** (also called weights).

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Note that

- We incorporate the **bias term** (also called the intercept term) into x (i.e. $x_0 = 1$).
- We use superscript to denote the example id and subscript to denote the dimension id.

Parameter estimation

Loss function We estimate θ by minimizing the **squared loss** (the least square method):

$$J(\theta) = \frac{1}{N} \sum_{n=1}^N \left(y^{(n)} - \theta^T x^{(n)} \right)^2. \quad (\text{empirical risk}) \quad (2)$$

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- Let $X \in \mathbb{R}^{N \times d}$ be the **design matrix** whose rows are input features.
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Review questions

- Derive the solution for linear regression.
- What if $X^T X$ is not invertible?

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Next,

- Derive linear regression from a probabilistic modeling perspective.

Assumptions in linear regression

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$$y = \theta^T x + \epsilon, \quad (4)$$

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In practice, we maximize the **log likelihood** $\ell(\theta)$, or equivalently, minimize the negative log likelihood (NLL).

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Recall that we obtained the normal equation by setting the derivative of the squared loss to zero. Now let's compute the derivative of the likelihood w.r.t. the parameters.

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- Derive **logistic regression** for classification.

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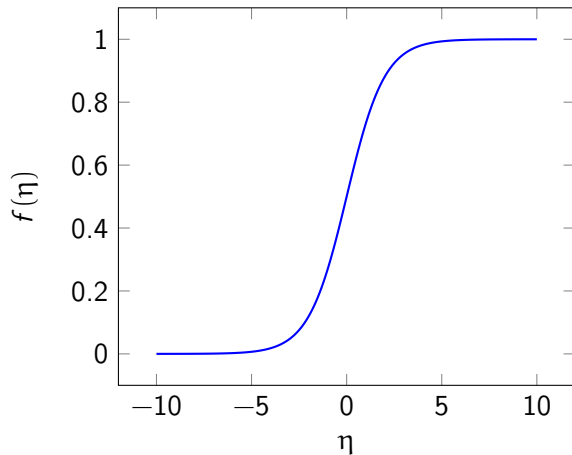
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- What is the mean of $Y | X = x$? $h(x)$. (Think how we parameterize the mean in linear regression)
- Need a function f to map the linear predictor $\theta^T x$ in \mathbb{R} to $(0, 1)$:

$$f(\eta) = \frac{1}{1 + e^{-\eta}} \quad \text{logistic function} \quad (17)$$

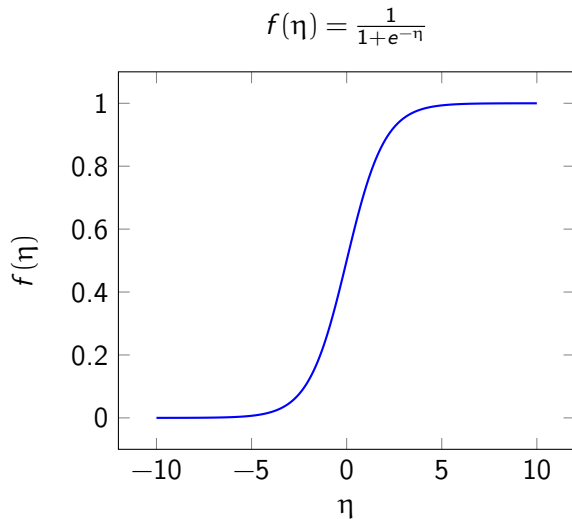
Logistic regression

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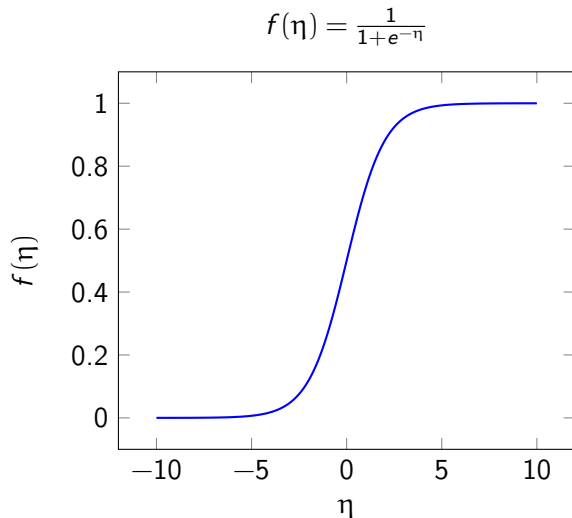
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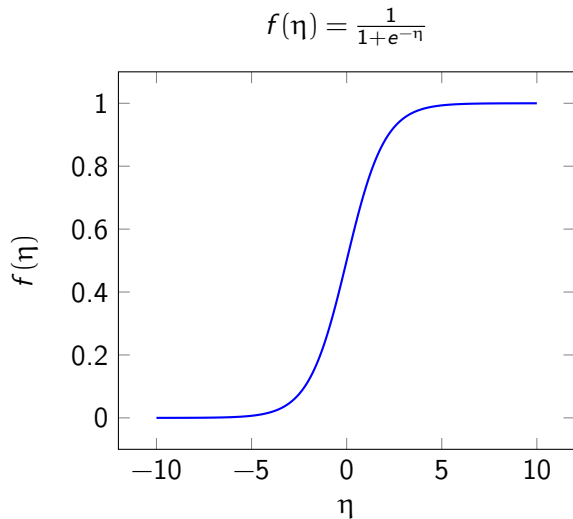


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- **Exercise:** show that the **log odds** is

$$\log \frac{p(y = 1 | x)}{p(y = 0 | x)} = \theta^T x. \quad (18)$$

$$\implies \text{linear decision boundary} \quad (19)$$

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- How do we extend it to multiclass classification? (more on this later)

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- Closed-form solutions are not available.
- But, the likelihood is concave—[gradient ascent](#) gives us the unique optimal solution.

$$\theta := \theta + \alpha \nabla_{\theta} \ell(\theta). \quad (22)$$

Gradient descent for logistic regression

Math review: Chain rule

If z depends on y which itself depends on x , e.g., $z = (y(x))^2$, then $\frac{dz}{dx} = \frac{dz}{dy} \frac{dy}{dx}$.

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$$= \left(\frac{y^{(n)}}{f^n} - \frac{1 - y^{(n)}}{1 - f^n} \right) \left(f^n (1 - f^n) x_i^{(n)} \right) \quad \text{Exercise: apply chain rule to } \frac{\partial f^n}{\partial \theta_i} \quad (25)$$

$$= (y^{(n)} - f^n) x_i^{(n)} \quad \text{simplify by algebra} \quad (26)$$

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If z depends on y which itself depends on x , e.g., $z = (y(x))^2$, then $\frac{dz}{dx} = \frac{dz}{dy} \frac{dy}{dx}$.

Likelihood for a single example: $\ell^n = y^{(n)} \log f(\theta^T x^{(n)}) + (1 - y^{(n)}) \log(1 - f(\theta^T x^{(n)}))$.

$$\frac{\partial \ell^n}{\partial \theta_i} = \frac{\partial \ell^n}{\partial f^n} \frac{\partial f^n}{\partial \theta_i} \quad (23)$$

$$= \left(\frac{y^{(n)}}{f^n} - \frac{1 - y^{(n)}}{1 - f^n} \right) \frac{\partial f^n}{\partial \theta_i} \quad \frac{d}{dx} \ln x = \frac{1}{x} \quad (24)$$

$$= \left(\frac{y^{(n)}}{f^n} - \frac{1 - y^{(n)}}{1 - f^n} \right) \left(f^n (1 - f^n) x_i^{(n)} \right) \quad \text{Exercise: apply chain rule to } \frac{\partial f^n}{\partial \theta_i} \quad (25)$$

$$= (y^{(n)} - f^n) x_i^{(n)} \quad \text{simplify by algebra} \quad (26)$$

The full gradient is thus $\frac{\partial \ell}{\partial \theta_i} = \sum_{n=1}^N (y^{(n)} - f(\theta^T x^{(n)})) x_i^{(n)}$.

A closer look at the gradient

$$\frac{\partial \ell}{\partial \theta_i} = \sum_{n=1}^N (y^{(n)} - f(\theta^T x^{(n)})) x_i^{(n)} \quad (27)$$

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- Does this look familiar?
- Our derivation for linear regression and logistic regression are quite similar...
- Next, a more general family of models.

Compare linear regression and logistic regression

linear regression	logistic regression
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	linear regression	logistic regression
Combine the inputs	$\theta^T x$ (linear)	$\theta^T x$ (linear)

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Transfer function $f(\theta^T x)$	identity	logistic

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	linear regression	logistic regression
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Conditional distribution	Gaussian	Bernoulli
Transfer function $f(\theta^T x)$	identity	logistic
Mean $\mathbb{E}(Y X = x; \theta)$	$f(\theta^T x)$	$f(\theta^T x)$

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Transfer function $f(\theta^T x)$	identity	logistic
Mean $\mathbb{E}(Y X = x; \theta)$	$f(\theta^T x)$	$f(\theta^T x)$

- x enters through a linear function.
- The main difference between the formulations is due to different conditional distributions.
- Can we generalize the idea to handle other output types, e.g., positive integers?

Construct a generalized regression model

Task: Given x , predict $p(y | x)$

Modeling:

- Choose a parametric family of distributions $p(y; \theta)$ with parameters $\theta \in \Theta$
- Choose a transfer function that maps a linear predictor in \mathbb{R} to Θ

$$\underbrace{x}_{\in \mathbb{R}^d} \mapsto \underbrace{w^T x}_{\in \mathbb{R}} \mapsto \underbrace{f(w^T x)}_{\in \Theta} = \theta, \quad (28)$$

Learning: MLE: $\hat{\theta} \in \arg \max_{\theta} \log p(\mathcal{D}; \theta)$

Inference: For prediction, use $x \rightarrow f(w^T x)$

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Example: Construct Poisson regression

Say we want to predict the number of people entering a restaurant in New York during lunch time.

- What features would be useful?
- What's a good model for number of visitors (the **output distribution**)?

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Math review: Poisson distribution

Given a random variable $Y \in 0, 1, 2, \dots$ following $\text{Poisson}(\lambda)$, we have

$$p(Y = k; \lambda) = \frac{\lambda^k e^{-\lambda}}{k!}, \quad (29)$$

where $\lambda > 0$ and $\mathbb{E}[Y] = \lambda$.

The Poisson distribution is usually used to model the number of events occurring during a fixed period of time.

Example: Construct Poisson regression

We've decided that $Y | X = x \sim \text{Poisson}(\eta)$, what should be the transfer function f ? x enters linearly:

$$x \mapsto \underbrace{w^T x}_{\mathbb{R}} \mapsto \lambda = \underbrace{f(w^T x)}_{(0, \infty)}$$

Standard approach is to take

$$f(w^T x) = \exp(w^T x).$$

Likelihood of the full dataset $\mathcal{D} = \{(x_1, y_1), \dots, (x_n, y_n)\}$:

$$\log p(y_i; \lambda_i) = [y_i \log \lambda_i - \lambda_i - \log(y_i!)] \quad (30)$$

$$\log p(\mathcal{D}; w) = \sum_{i=1}^n [y_i \log [\exp(w^T x_i)] - \exp(w^T x_i) - \log(y_i!)] \quad (31)$$

$$= \sum_{i=1}^n [y_i w^T x_i - \exp(w^T x_i) - \log(y_i!)] \quad (32)$$

Multinomial Logistic Regression

- Say we want to get the predicted categorical distribution for a given $x \in \mathbb{R}^d$.
- First compute the scores ($\in \mathbb{R}^k$) and then their softmax:

$$x \mapsto (\langle w_1, x \rangle, \dots, \langle w_k, x \rangle) \mapsto \theta = \left(\frac{\exp(w_1^T x)}{\sum_{i=1}^k \exp(w_i^T x)}, \dots, \frac{\exp(w_k^T x)}{\sum_{i=1}^k \exp(w_i^T x)} \right)$$

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- We can write the conditional probability for any $y \in \{1, \dots, k\}$ as

$$p(y | x; w) = \frac{\exp(w_y^T x)}{\sum_{i=1}^k \exp(w_i^T x)}.$$

Recipe for constructing a conditional distribution for prediction:

- ① Define input and output space (as for any other model).
- ② Choose the output distribution $p(y | x; \theta)$ based on the task
- ③ Choose the transfer function that maps $w^T x$ to a Θ .
- ④ (The formal family is called “generalized linear models”.)

Learning:

- Fit the model by maximum likelihood estimation.
- Closed solutions do not exist in general, so we use gradient ascent.

Generative models

We've seen

- Model the conditional distribution $p(y | x; \theta)$ using generalized linear models.
- (Previously) Directly map x to y , e.g., perceptron.

Next,

- Model the **joint distribution** $p(x, y; \theta)$.
- Predict the label for x as $\arg \max_{y \in \mathcal{Y}} p(x, y; \theta)$.

Generative modeling through the Bayes rule

Training:

$$p(x, y) \tag{33}$$

(35)

Generative modeling through the Bayes rule

Training:

$$p(x, y) = p(x | y)p(y) \quad (33)$$

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$$p(y | x) = \frac{p(x | y)p(y)}{p(x)} \quad \text{Bayes rule} \quad (34)$$

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$$p(x, y) = p(x | y)p(y) \quad (33)$$

Testing:

$$p(y | x) = \frac{p(x | y)p(y)}{p(x)} \quad \text{Bayes rule} \quad (34)$$

$$\arg \max_y p(y | x) = \arg \max_y p(x | y)p(y) \quad (35)$$

Naive Bayes (NB) models

Let's consider binary text classification (e.g., fake vs genuine review) as a motivating example.

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Bag-of-words representation of a document

- ["machine", "learning", "is", "fun", "."]
- $x_i \in \{0, 1\}$: whether the i -th word in our vocabulary exists in the input

$$\mathbf{x} = [x_1, x_2, \dots, x_d] \quad \text{where } d = \text{vocabulary size} \quad (36)$$

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$$x = [x_1, x_2, \dots, x_d] \quad \text{where } d = \text{vocabulary size} \quad (36)$$

What's the probability of a document x ?

$$p(x | y) = p(x_1, \dots, x_d | y) \quad (37)$$

$$= p(x_1 | y) p(x_2 | y, x_1) p(x_3 | y, x_2, x_1) \dots p(x_d | y, x_{d-1}, \dots, x_1) \quad \text{chain rule} \quad (38)$$

$$= \prod_{i=1}^d p(x_i | y, x_{<i}) \quad (39)$$

Naive Bayes assumption

Challenge: $p(x_i | y, x_{<i})$ is hard to model (and estimate), especially for large i .

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Solution:

Naive Bayes assumption

Features are **conditionally independent** given the label:

$$p(x | y) = \prod_{i=1}^d p(x_i | y). \quad (40)$$

A strong assumption in general, but works well in practice.

Parametrize $p(x_i | y)$ and $p(y)$

For binary x_i , assume $p(x_i | y)$ follows Bernoulli distributions.

$$p(x_i = 1 | y = 1) = \theta_{i,1}, \quad p(x_i = 1 | y = 0) = \theta_{i,0}. \quad (41)$$

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Similarly,

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Thus,

$$p(x, y) = p(x | y)p(y) \quad (43)$$

$$= p(y) \prod_{i=1}^d p(x_i | y) \quad \text{NB assumption} \quad (44)$$

$$= p(y) \prod_{i=1}^d \theta_{i,y} \mathbb{I}\{x_i = 1\} + (1 - \theta_{i,y}) \mathbb{I}\{x_i = 0\} \quad (45)$$

Indicator function $\mathbb{I}\{\text{condition}\}$ evaluates to 1 if “condition” is true and 0 otherwise.

MLE for our NB model

We maximize the likelihood of the data $\prod_{n=1}^N p_{\theta}(x^{(n)}, y^{(n)})$ (as opposed to the *conditional* likelihood we've seen before).

(48)

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$$\frac{\partial}{\partial \theta_{j,1}} \ell = \frac{\partial}{\partial \theta_{j,1}} \sum_{n=1}^N \sum_{i=1}^d \log \left(\theta_{i,y^{(n)}} \mathbb{I} \{x_i^{(n)} = 1\} + (1 - \theta_{i,y^{(n)}}) \mathbb{I} \{x_i^{(n)} = 0\} \right) + \log p_{\theta_0}(y^{(n)})$$

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$$= \sum_{n=1}^N \mathbb{I} \{y^{(n)} = 1 \wedge x_j^{(n)} = 1\} \frac{1}{\theta_{j,1}} + \mathbb{I} \{y^{(n)} = 1 \wedge x_j^{(n)} = 0\} \frac{1}{1 - \theta_{j,1}} \quad \text{ignore } y^{(n)} = 0 \quad (48)$$

MLE solution for our NB model

Set $\frac{\partial}{\partial \theta_{j,1}} \ell$ to zero:

$$\theta_{j,1} = \frac{\sum_{n=1}^N \mathbb{I} \left\{ y^{(n)} = 1 \wedge x_j^{(n)} = 1 \right\}}{\sum_{n=1}^N \mathbb{I} \left\{ y^{(n)} = 1 \right\}} \quad (49)$$

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In practice, count words:

$$\frac{\text{number of fake reviews containing "absolutely"}}{\text{number of fake reviews}}$$

Exercise: show that

$$\theta_{j,0} = \frac{\sum_{n=1}^N \mathbb{I}\{y^{(n)} = 0 \wedge x_j^{(n)} = 1\}}{\sum_{n=1}^N \mathbb{I}\{y^{(n)} = 0\}} \quad (50)$$

$$\theta_0 = \frac{\sum_{n=1}^N \mathbb{I}\{y^{(n)} = 1\}}{N} \quad (51)$$

NB assumption: **conditionally independent** features given the label

Recipe for learning a NB model:

- 1 Choose $p(x_i | y)$, e.g., Bernoulli distribution for binary x_i .
- 2 Choose $p(y)$, often a categorical distribution.
- 3 Estimate parameters by MLE (same as the strategy for conditional models) .

Next, NB with continuous features.

NB with continuous inputs

Let's consider a multiclass classification task with continuous inputs.

$$p(x_i | y) \sim \mathcal{N}(\mu_{i,y}, \sigma_{i,y}^2) \quad (52)$$

$$p(y = k) = \theta_k \quad (53)$$

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Likelihood of the data:

$$p(\mathcal{D}) = \prod_{n=1}^N p(y^{(n)}) \prod_{i=1}^d p(x_i^{(n)} | y^{(n)}) \quad (54)$$

$$= \prod_{n=1}^N \theta_{y^{(n)}} \prod_{i=1}^d \frac{1}{\sqrt{2\pi}\sigma_{i,y^{(n)}}} \exp\left(-\frac{1}{2\sigma_{i,y^{(n)}}^2} \left(x_i^{(n)} - \mu_{i,y^{(n)}}\right)^2\right) \quad (55)$$

MLE for Gaussian NB

Log likelihood:

$$\ell = \sum_{n=1}^N \log \theta_{y^{(n)}} + \sum_{n=1}^N \sum_{i=1}^d \log \frac{1}{\sqrt{2\pi}\sigma_{i,y^{(n)}}} - \frac{1}{2\sigma_{i,y^{(n)}}^2} \left(x_i^{(n)} - \mu_{i,y^{(n)}} \right)^2 \quad (56)$$

(58)

(59)

MLE for Gaussian NB

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$$\frac{\partial}{\partial \mu_{j,k}} \ell = \frac{\partial}{\partial \mu_{j,k}} \sum_{n: y^{(n)}=k} -\frac{1}{2\sigma_{j,k}^2} \left(x_j^{(n)} - \mu_{j,k} \right)^2 \quad \text{ignore irrelevant terms} \quad (57)$$

$$(58)$$

$$(59)$$

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Set $\frac{\partial}{\partial \mu_{j,k}} \ell$ to zero:

$$\mu_{j,k} = \frac{\sum_{n:y^{(n)}=k} x_j^{(n)}}{\sum_{n:y^{(n)}=k} 1} \quad (59)$$

MLE for Gaussian NB

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Set $\frac{\partial}{\partial \mu_{j,k}} \ell$ to zero:

$$\mu_{j,k} = \frac{\sum_{n:y^{(n)}=k} x_j^{(n)}}{\sum_{n:y^{(n)}=k} 1} = \text{sample mean of } x_j \text{ in class } k \quad (59)$$

Show that

$$\sigma_{j,k}^2 = \frac{\sum_{n:y^{(n)}=k} \left(x_j^{(n)} - \mu_{j,k}\right)^2}{\sum_{n:y^{(n)}=k} 1} = \text{sample variance of } x_j \text{ in class } k \quad (60)$$

$$\theta_k = \frac{\sum_{n:y^{(n)}=k} 1}{N} \quad (\text{class prior}) \quad (61)$$

Decision boundary of the Gaussian NB model

Is the Gaussian NB model a linear classifier?

(66)

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$$\log \frac{p(y = 1 | x)}{p(y = 0 | x)} = \log \frac{p(x | y = 1)p(y = 1)}{p(x | y = 0)p(y = 0)} \quad (62)$$

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$$= \log \frac{\theta_0}{1-\theta_0} + \sum_{i=1}^d \left(\log \sqrt{\frac{\sigma_{i,0}^2}{\sigma_{i,1}^2}} + \left(\frac{(x_i - \mu_{i,0})^2}{2\sigma_{i,0}^2} - \frac{(x_i - \mu_{i,1})^2}{2\sigma_{i,1}^2} \right) \right) \quad \text{quadratic} \quad (63)$$

$$\text{assume that } \sigma_{i,0} = \sigma_{i,1} = \sigma_i, \quad (\theta_0 = 0.5) \quad (64)$$

$$= \sum_{i=1}^d \frac{1}{2\sigma_i^2} \left((x_i - \mu_{i,0})^2 - (x_i - \mu_{i,1})^2 \right) \quad (65)$$

$$= \sum_{i=1}^d \frac{\mu_{i,1} - \mu_{i,0}}{\sigma_i^2} x_i + \frac{\mu_{i,0}^2 - \mu_{i,1}^2}{2\sigma_i^2} \quad \text{linear} \quad (66)$$

Decision boundary of the Gaussian NB model

Assuming the variance of each feature is the same for both classes, we have

$$\log \frac{p(y=1|x)}{p(y=0|x)} = \sum_{i=1}^d \frac{\mu_{i,1} - \mu_{i,0}}{\sigma_i^2} x_i + \frac{\mu_{i,0}^2 - \mu_{i,1}^2}{2\sigma_i^2} \quad (67)$$

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$$(69)$$

$$\theta_i = \frac{\mu_{i,1} - \mu_{i,0}}{\sigma_i^2} \quad \text{for } i \in [1, d] \quad (70)$$

$$\theta_0 = \sum_{i=1}^d \frac{\mu_{i,0}^2 - \mu_{i,1}^2}{2\sigma_i^2} \quad \text{bias term} \quad (71)$$

Naive Bayes vs logistic regression

	logistic regression	Gaussian naive Bayes
model type	conditional/discriminative	generative
parametrization	$p(y x)$	$p(x y), p(y)$
assumptions on Y	Bernoulli	Bernoulli
assumptions on X	—	Gaussian
decision boundary	$\theta_{\text{LR}}^T x$	$\theta_{\text{GNB}}^T x$

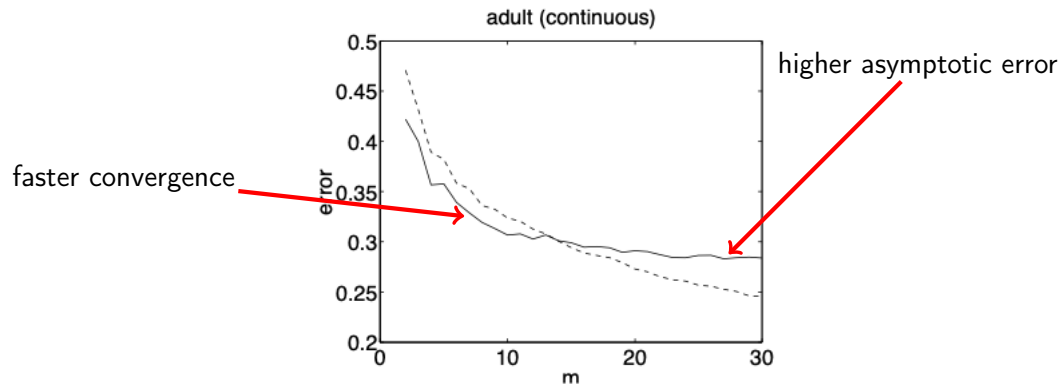
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Given the same training data, is $\theta_{\text{LR}} = \theta_{\text{GNB}}$?

Generative vs discriminative classifiers

Ng, A. and Jordan, M. (2002). [On discriminative versus generative classifiers: A comparison of logistic regression and naive Bayes](#). In Advances in Neural Information Processing Systems 14.



Solid line: naive Bayes; dashed line: logistic regression.

Naive Bayes vs logistic regression

Logistic regression and Gaussian naive Bayes converge to the same classifier asymptotically, assuming the GNB assumption holds.

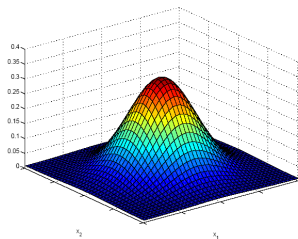
- Data points are generated from Gaussian distributions for each class
- Each dimension is independently generated
- Shared variance

What if the GNB assumption is not true?

Multivariate Gaussian Distribution

- $\mathbf{x} \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$, a Gaussian (or normal) distribution defined as

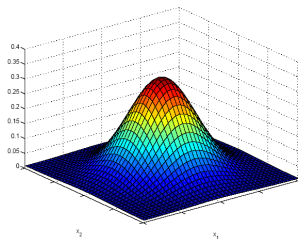
$$p(\mathbf{x}) = \frac{1}{(2\pi)^{d/2} |\boldsymbol{\Sigma}|^{1/2}} \exp \left[-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right]$$



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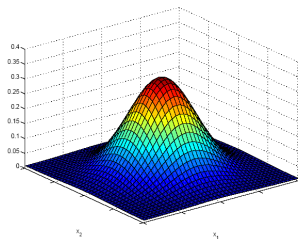


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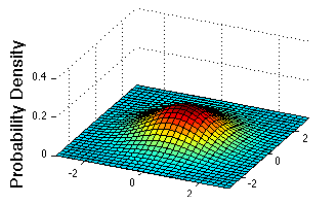
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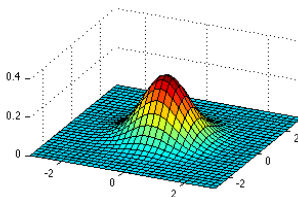
- Mahalanobis distance $(x - \mu_k)^T \Sigma^{-1} (x - \mu_k)$ measures the distance from x to μ in terms of Σ
- It normalizes for difference in variances and correlations

Bivariate Normal

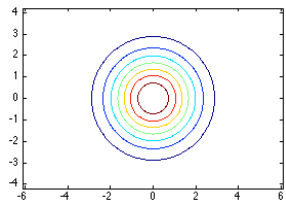
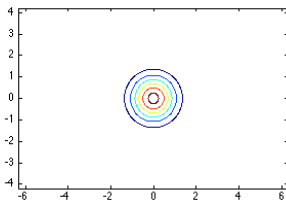
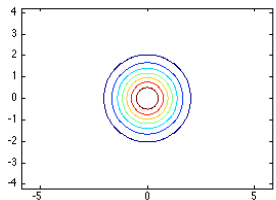
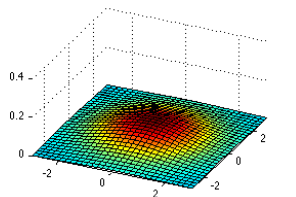
$$\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$



$$\Sigma = 0.5 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

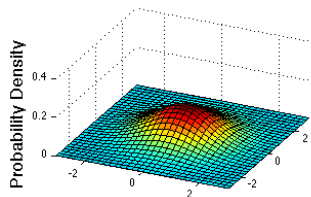


$$\Sigma = 2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

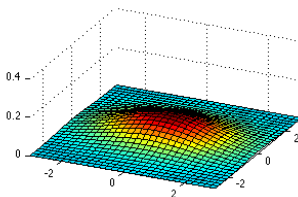


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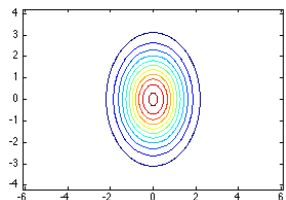
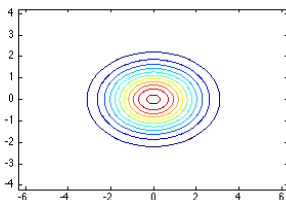
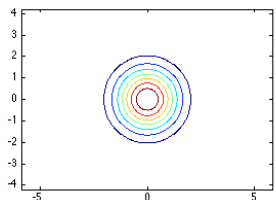
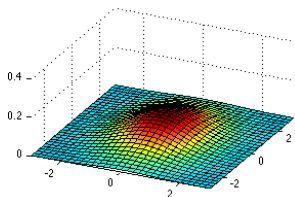
$$\text{var}(x_1) = \text{var}(x_2)$$



$$\text{var}(x_1) > \text{var}(x_2)$$

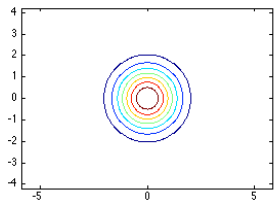
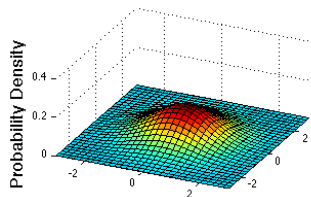


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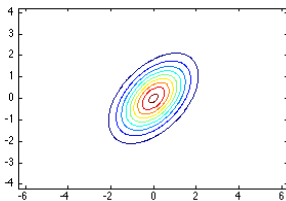
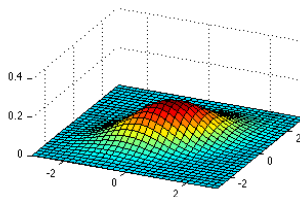


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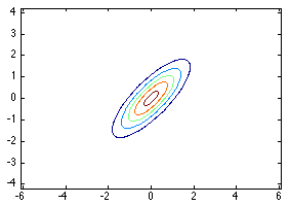
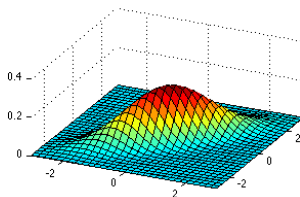
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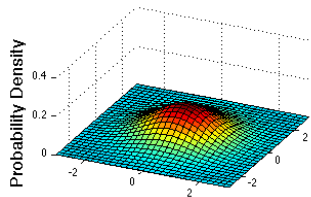


$$\Sigma = \begin{pmatrix} 1 & 0.8 \\ 0.8 & 1 \end{pmatrix}$$

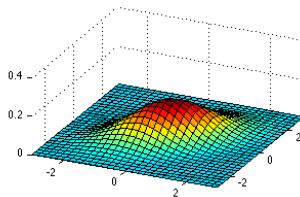


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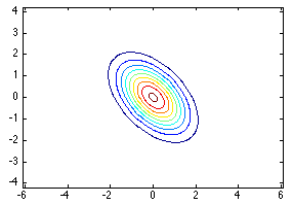
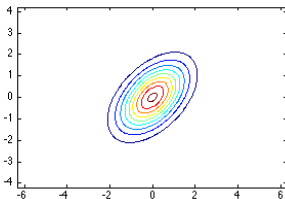
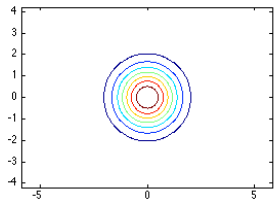
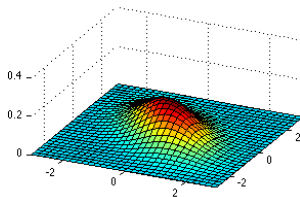
$$\text{Cov}(x_1, x_2) = 0$$



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Gaussian Bayes Classifier

- Gaussian Bayes Classifier in its general form assumes that $p(\mathbf{x}|y)$ is distributed according to a multivariate normal (Gaussian) distribution
- Multivariate Gaussian distribution:

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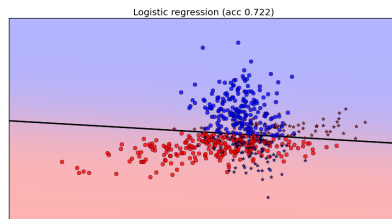
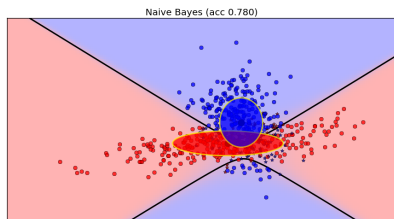
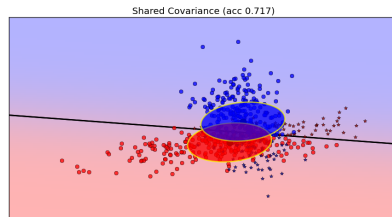
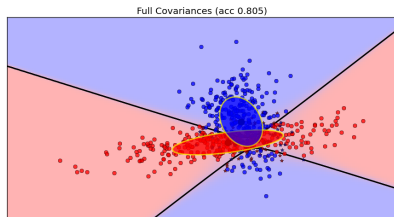
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- Σ_k has $\mathcal{O}(d^2)$ parameters - could be hard to estimate

Example



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Different cases on the covariance matrix:

- Full covariance: Quadratic decision boundary
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GBC vs. Logistic Regression:

- If data is truly Gaussian distributed, then shared covariance = logistic regression.
- But logistic regression can learn other distributions.

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- Probabilistic framework of using maximum likelihood as a more principled way to derive loss functions.
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- Conditional vs. generative
- Generative models the joint distribution, and may lead to more assumption on the data.
- When there is very few data point, it may be hard to model the distribution.
- Is there an equivalent “regularization” in a probabilistic framework?

Bayesian ML: Classical Statistics

Parametric Family of Densities

- A **parametric family of densities** is a set

$$\{p(y \mid \theta) : \theta \in \Theta\},$$

- where $p(y \mid \theta)$ is a density on a **sample space** \mathcal{Y} , and
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- where $p(y | \theta)$ is a density on a **sample space** \mathcal{Y} , and
- θ is a **parameter** in a [finite dimensional] **parameter space** Θ .
- This is the common starting point for a treatment of classical or Bayesian statistics.
- In this lecture, whenever we say “density”, we could replace it with “mass function.” (and replace integrals with sums).

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- But instead of θ , we have data \mathcal{D} : y_1, \dots, y_n sampled i.i.d. from $p(y | \theta)$.
- Statistics is about how to get by with \mathcal{D} in place of θ .

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- **Maximum likelihood estimators** are consistent and efficient under reasonable conditions.

Example of Point Estimation: Coin Flipping

- Parametric family of mass functions:

$$p(\text{Heads} \mid \theta) = \theta,$$

for $\theta \in \Theta = (0, 1)$.

Coin Flipping: MLE

- Data $\mathcal{D} = (H, H, T, T, T, T, T, H, \dots, T)$, assumed i.i.d. flips.
 - n_h : number of heads
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- As usual, it is easier to maximize the log-likelihood function:

$$\begin{aligned}\hat{\theta}_{\text{MLE}} &= \arg \max_{\theta \in \Theta} \log L_{\mathcal{D}}(\theta) \\ &= \arg \max_{\theta \in \Theta} [n_h \log \theta + n_t \log(1 - \theta)]\end{aligned}$$

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Bayesian Statistics: Introduction

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- The prior reflects our belief about θ , **before seeing any data**.

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- ① A parametric family of densities

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- Putting the pieces together, we get a joint density on θ and \mathcal{D} :

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

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- The posterior represents the **rationally updated belief** about θ , after seeing \mathcal{D} .

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- Maximum a posteriori: Find $\hat{\theta}_{MAP}$ Maximize the posterior distribution.

Coin Flipping: Bayesian Model

- Recall that we have a parametric family of mass functions:

$$p(\text{Heads} \mid \theta) = \theta,$$

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- We need a prior distribution $p(\theta)$ on $\Theta = (0, 1)$.
- One convenient choice would be a distribution from the Beta family

Coin Flipping: Beta Prior

- Prior:

$$\begin{aligned}\theta &\sim \text{Beta}(\alpha, \beta) \\ p(\theta) &\propto \theta^{\alpha-1} (1-\theta)^{\beta-1}\end{aligned}$$

Figure by Horas based on the work of Krishnavedala (Own work) [Public domain], via Wikimedia Commons
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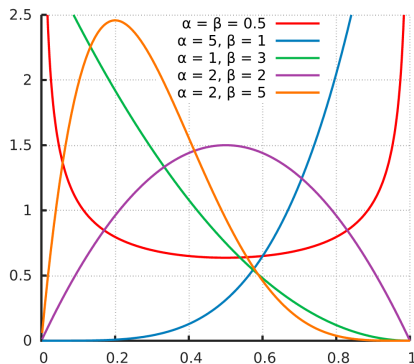


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- Mode of Beta distribution:

$$\arg \max_{\theta} p(\theta) = \frac{h-1}{h+t-2}$$

for $h, t > 1$.

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- Interpretation:

- Prior initializes our counts with h heads and t tails.
- Posterior increments counts by observed n_h and n_t .

Sidebar: Conjugate Priors

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A family of distributions π is **conjugate to** parametric model P if for any prior in π , the posterior is always in π .

- The beta family is conjugate to the coin-flipping (i.e. Bernoulli) model.

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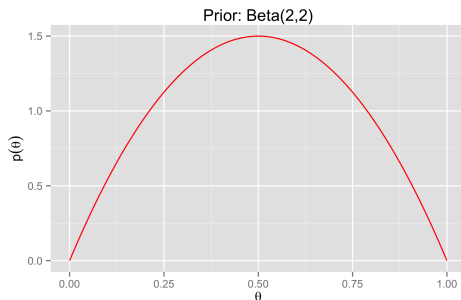
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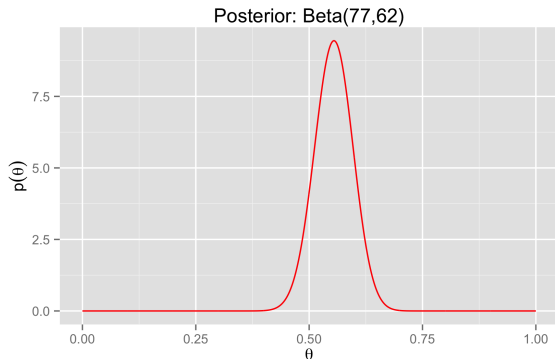
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- Next, we gather some data $\mathcal{D} = \{H, H, T, T, T, T, T, H, \dots, T\}$:
- Heads: 75 Tails: 60
 - $\hat{\theta}_{\text{MLE}} = \frac{75}{75+60} \approx 0.556$
- **Posterior distribution:** $\theta \mid \mathcal{D} \sim \text{Beta}(77, 62)$:



Bayesian Point Estimates

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- Common options:
 - **posterior mean** $\hat{\theta} = \mathbb{E}[\theta \mid \mathcal{D}]$
 - **maximum a posteriori (MAP) estimate** $\hat{\theta} = \arg \max_{\theta} p(\theta \mid \mathcal{D})$
 - Note: this is the **mode** of the posterior distribution

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- Select a point estimate using **Bayesian decision theory**:
 - Choose a loss function.
 - Find action **minimizing expected risk w.r.t. posterior**

Bayesian Decision Theory

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- Ingredients:
 - **Parameter space** Θ .
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- A **Bayes action** a^* is an action that minimizes posterior risk:

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Important Cases

- Squared Loss : $\ell(\hat{\theta}, \theta) = (\theta - \hat{\theta})^2 \Rightarrow$ posterior mean
- Zero-one Loss: $\ell(\theta, \hat{\theta}) = \mathbb{1}[\theta \neq \hat{\theta}] \Rightarrow$ posterior mode
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- Optimal decision depends on the loss function and the posterior distribution.
- We will derive the square loss case next.

Bayesian Point Estimation: Square Loss

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- The **Bayes action** for **square loss** is the posterior mean.

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 - Exercise: Show this.

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- **Bayes action is**

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$$\begin{aligned}r(\hat{\theta}) &= \mathbb{E} \left[\mathbb{1}[\theta \neq \hat{\theta}] \mid \mathcal{D} \right] \\&= \mathbb{P}(\theta \neq \hat{\theta} \mid \mathcal{D}) \\&= 1 - \mathbb{P}(\theta = \hat{\theta} \mid \mathcal{D}) \\&= 1 - p(\hat{\theta} \mid \mathcal{D})\end{aligned}$$

- **Bayes action** is

$$\hat{\theta} = \arg \max_{\theta \in \Theta} p(\theta \mid \mathcal{D})$$

- This $\hat{\theta}$ is called the **maximum a posteriori (MAP)** estimate.
- The MAP estimate is the **mode** of the posterior distribution.

Interim summary

Recap and Interpretation

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 - **prior distribution** on Θ
 - For decision making, we need a **loss function**.

Recap: Conditional Probability Models

Conditional Probability Modeling

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- Outcome space \mathcal{Y}
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- where $p(y \mid x, \theta)$ is a density on **outcome space** \mathcal{Y} for each x in **input space** \mathcal{X} , and
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- This is the common starting point for either classical or Bayesian regression.

Classical treatment: Likelihood Function

- **Data:** $\mathcal{D} = (y_1, \dots, y_n)$
- The probability density for our data \mathcal{D} is

$$p(\mathcal{D} \mid x_1, \dots, x_n, \theta) = \prod_{i=1}^n p(y_i \mid x_i, \theta).$$

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- For fixed \mathcal{D} , the function $\theta \mapsto p(\mathcal{D} \mid x, \theta)$ is the **likelihood function**:

$$L_{\mathcal{D}}(\theta) = p(\mathcal{D} \mid x, \theta),$$

where $x = (x_1, \dots, x_n)$.

- The **maximum likelihood estimator (MLE)** for θ in the family $\{p(y | x, \theta) | \theta \in \Theta\}$ is

$$\hat{\theta}_{\text{MLE}} = \arg \max_{\theta \in \Theta} L_{\mathcal{D}}(\theta).$$

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- The corresponding prediction function is

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Bayesian Conditional Probability Models

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- Posterior represents the **rationally updated beliefs** after seeing \mathcal{D} .
- Each θ corresponds to a prediction function,
 - i.e. the conditional distribution function $p(y \mid x, \theta)$.

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- We may want to use
 - $\hat{\theta} = \mathbb{E}[\theta \mid \mathcal{D}, x]$ (the posterior mean estimate)
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 - $\hat{\theta} = \arg \max_{\theta \in \Theta} p(\theta \mid \mathcal{D}, x)$ (the MAP estimate)
- depending on our loss function.

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- and a prior distribution $p(\theta)$ on this set.
- Having set our Bayesian model, how do we predict a distribution on y for input x ?
- We don't need to make a discrete selection from the hypothesis space: we **maintain uncertainty**.

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Comparison to Frequentist Approach

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- In the Bayesian approach, we integrate out over Θ w.r.t. $p(\theta | \mathcal{D})$ and predict with

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- Each of these can be derived from $p(y \mid x, \mathcal{D})$.

Gaussian Regression Example

Example in 1-Dimension: Setup

- Input space $\mathcal{X} = [-1, 1]$ Output space $\mathcal{Y} = \mathbb{R}$
- Given x , the world generates y as

$$y = w_0 + w_1 x + \varepsilon,$$

where $\varepsilon \sim \mathcal{N}(0, 0.2^2)$.

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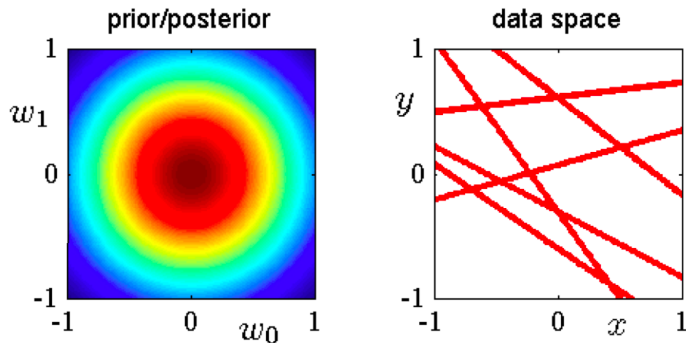
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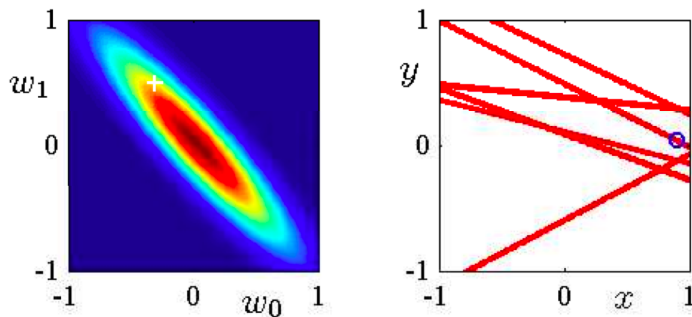
Example in 1-Dimension: Prior Situation

- **Prior distribution:** $w = (w_0, w_1) \sim \mathcal{N}(0, \frac{1}{2}I)$ (Illustrated on left)



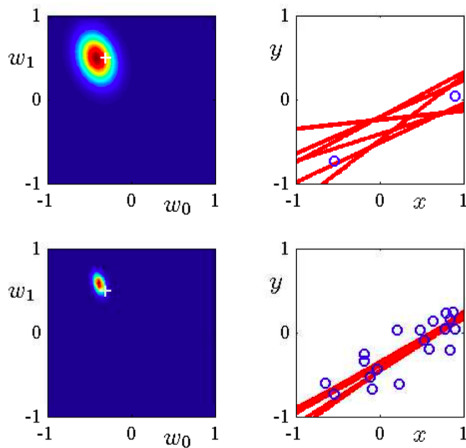
- On right, $y(x) = \mathbb{E}[y \mid x, w] = w_0 + w_1 x$, for randomly chosen $w \sim p(w) = \mathcal{N}(0, \frac{1}{2}I)$.

Example in 1-Dimension: 1 Observation



- On left: posterior distribution; white cross indicates true parameters
- On right:
 - blue circle indicates the training observation
 - red lines, $y(x) = \mathbb{E}[y | x, w] = w_0 + w_1 x$, for randomly chosen $w \sim p(w|\mathcal{D})$ (posterior)

Example in 1-Dimension: 2 and 20 Observations



Bishop's PRML Fig 3.7

Gaussian Regression: Closed form

Closed Form for Posterior

- Model:

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- **Posterior Variance Σ_P gives us a natural uncertainty measure.**

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which is of course the ridge regression solution.