Probabilistic models - Bayesian Methods

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Oct 17, 2023

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

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

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):

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

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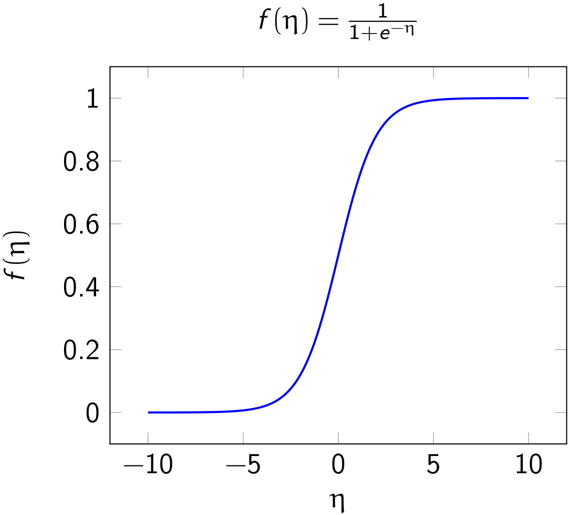
- What is the mean of $Y \mid X = x$? $h(x)$. (Think how we parameterize the mean in linear regression)
- Need a function f to map the linear predictor $\theta^T x$ in $\mathbb{R}$ to $(0,1)$:

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

Logistic regression



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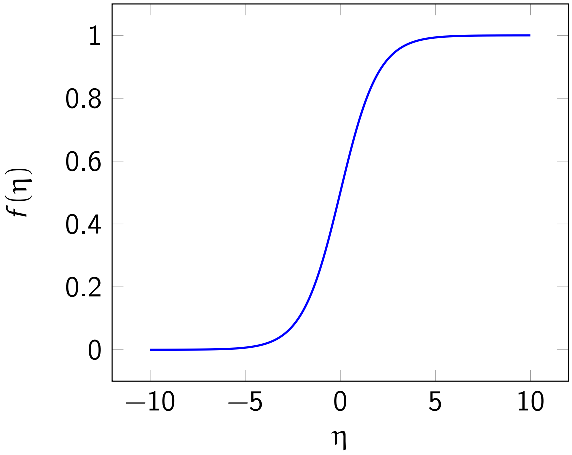

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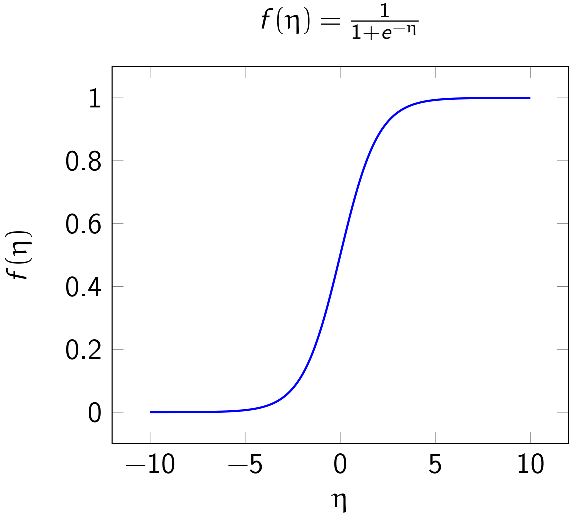

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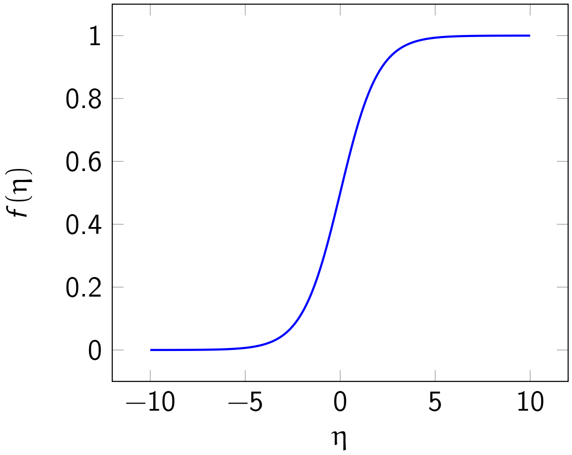

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- How do we extend it to multiclass classification? (more on this later)

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

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

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

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

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 $\frac{dz}{dx} = \frac{dz}{dy}\frac{dy}{dx}$.

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

$$\frac{\partial \ell^n}{\partial \theta_i} = \frac{\partial \ell^n}{\partial f^n}\frac{\partial f^n}{\partial \theta_i} \tag{23}$$

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

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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

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

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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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	linear regression	logistic regression
Combine the inputs	$\theta^T x$ (linear)	$\theta^T x$ (linear)
Output	real	categorical
Conditional distribution	Gaussian	Bernoulli
Transfer function $f(\theta^T x)$	identity	logistic

Compare linear regression and logistic regression

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

Compare linear regression and logistic regression

	linear regression	logistic regression
Combine the inputs	$\theta^T x$ (linear)	$\theta^T x$ (linear)
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Conditional distribution	Gaussian	Bernoulli
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Mean $\mathbb{E}(Y \mid X = x; \theta)$	$f(\theta^T x)$	$f(\theta^T x)$

- 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 $p(y \mid x)$
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

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

Learning: MLE: $\hat{\theta} \in \arg\max_{\theta} \log p(\mathcal{D}; \hat{\theta})$
Inference: For prediction, use $x \to f(w^T x)$

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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 $Y \in 0, 1, 2, \ldots$ following Poisson(λ), we have

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

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 $Y \mid X = x \sim \text{Poisson}(\eta)$, what should be the transfer function f?

x enters linearly:

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

Standard approach is to take

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

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

$$\log p(y_i; \lambda_i) = [y_i \log \lambda_i - \lambda_i - \log(y_i!)] \tag{30}$$

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

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

Multinomial Logistic Regression

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

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

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

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

Review

Recipe for contructing a conditional distribution for prediction:

1. Define input and output space (as for any other model).
2. Choose the output distribution $p(y \mid x; \theta)$ 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

Review

We've seen

- Model the conditional distribution $p(y \mid x; \theta)$ 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:

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

$$\tag{35}$$

Generative modeling through the Bayes rule

Training:

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

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Generative modeling through the Bayes rule

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$$p(y \mid x) = \frac{p(x \mid y)p(y)}{p(x)} \qquad \text{Bayes rule} \tag{34}$$

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Generative modeling through the Bayes rule

Training:

$$p(x, y) = {\color{blue}p(x \mid y)}{\color{red}p(y)} \tag{33}$$

Testing:

$$p(y \mid x) = \frac{p(x \mid y)p(y)}{p(x)} \qquad \text{Bayes rule} \tag{34}$$

$$\arg\max_y p(y \mid x) = \arg\max_y p(x \mid y)p(y) \tag{35}$$

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

$$x = [x_1, x_2, \ldots, x_d] \quad \text{where } d = \text{vocabulary size} \tag{36}$$

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What's the probability of a document x?

$$\begin{aligned}
p(x \mid y) &= p(x_1, \ldots, x_d \mid y) && (37)\\
&= p(x_1 \mid y)p(x_2 \mid y, x_1)p(x_3 \mid y, x_2, x_1) \ldots p(x_d \mid y, x_{d-1}, \ldots, x_1) \qquad \text{chain rule} && (38)\\
&= \prod_{i=1}^{d} p(x_i \mid y, x_{<i}) && (39)
\end{aligned}$$

Naive Bayes assumption

Challenge: $p(x_i \mid y, x_{<i})$ 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:

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

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

Parametrize $p(x_i \mid y)$ and $p(y)$

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

$$p(x_i = 1 \mid y = 1) = \theta_{i,1}, \;\; p(x_i = 1 \mid y = 0) = \theta_{i,0}. \tag{41}$$

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Similarly,

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Thus,

$$\begin{aligned}
p(x, y) &= p(x \mid y) p(y) && (43) \\
&= p(y) \prod_{i=1}^{d} p(x_i \mid y) && \text{NB assumption} \quad (44) \\
&= p(y) \prod_{i=1}^{d} \theta_{i,y} \mathbb{I}\{x_i = 1\} + (1 - \theta_{i,y}) \mathbb{I}\{x_i = 0\} && (45)
\end{aligned}$$

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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$$\frac{\partial}{\partial \theta_{j,1}} \ell = \frac{\partial}{\partial \theta_{j,1}} \sum_{n=1}^{N} \sum_{i=1}^{d} \log\left(\theta_{i,y^{(n)}} \mathbb{I}\left\{x_i^{(n)} = 1\right\} + \left(1 - \theta_{i,y^{(n)}}\right) \mathbb{I}\left\{x_i^{(n)} = 0\right\}\right) + \log p_{\theta_0}(y^{(n)}) \tag{46}$$

(48)

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

MLE solution for our NB model

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

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

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In practice, count words:

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

Exercise: show that

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

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

Review

NB assumption: conditionally independent features given the label

Recipe for learning a NB model:

1. Choose $p(x_i \mid y)$, 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.

$$p(x_i \mid y) \sim \mathcal{N}(\mu_{i,y}, \sigma^2_{i,y}) \tag{52}$$

$$p(y = k) = \theta_k \tag{53}$$

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$$p(y = k) = \theta_k \tag{53}$$

Likelihood of the data:

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

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

MLE for Gaussian NB

Log likelihood:

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

(58)

(59)

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

(58)

(59)

MLE for Gaussian NB

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$$= \sum_{n:y^{(n)}=k} \frac{1}{\sigma_{j,k}^2} \left(x_j^{(n)} - \mu_{j,k} \right) \tag{58}$$

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

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

MLE for Gaussian NB

Log likelihood:

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

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

MLE for Gaussian NB

Show that

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

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

Decision boundary of the Gaussian NB model

Is the Gaussian NB model a linear classifier?

(66)

Decision boundary of the Gaussian NB model

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$$\log \frac{p(y=1 \mid x)}{p(y=0 \mid x)} = \log \frac{p(x \mid y=1)p(y=1)}{p(x \mid y=0)p(y=0)} \tag{62}$$

(66)

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

(66)

Decision boundary of the Gaussian NB model

Is the Gaussian NB model a linear classifier?

$$\log \frac{p(y=1 \mid x)}{p(y=0 \mid x)} = \log \frac{p(x \mid y=1)p(y=1)}{p(x \mid y=0)p(y=0)} \tag{62}$$

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

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

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

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

Decision boundary of the Gaussian NB model

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

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

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

Naive Bayes vs logistic regression

	logistic regression	Gaussian naive Bayes
model type	conditional/discriminative	generative
parametrization	$p(y \mid x)$	$p(x \mid y)$, $p(y)$
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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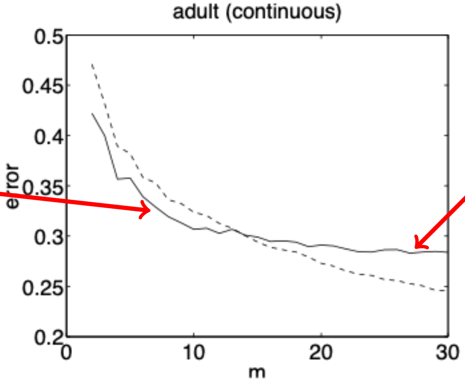
Given the same training data, is $\theta_{\mathrm{LR}} = \theta_{\mathrm{GNB}}$?

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.

faster convergence

higher asymptotic error



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.

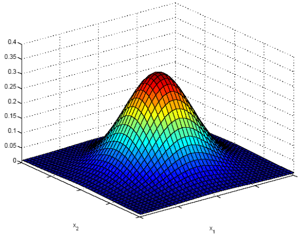
- Data points are generated from Gaussian distributions for each class
- Each dimension is independently generated
- Shared variance

What if the GNB assumption is not true?

Multivariate Gaussian Distribution

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

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



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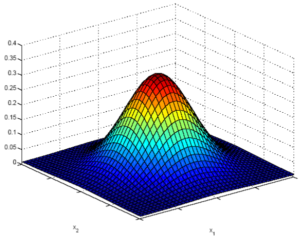

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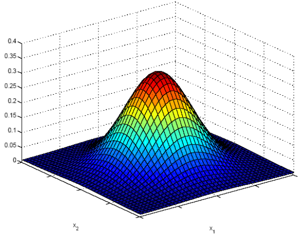
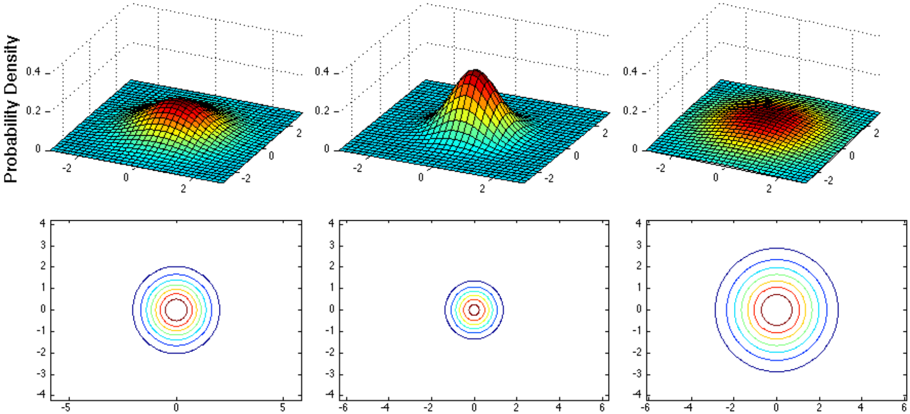


- Mahalanobis distance $(x-\mu_k)^T\Sigma^{-1}(x-\mu_k)$ measures the distance from x to μ in terms of Σ
- It normalizes for difference in variances and correlations

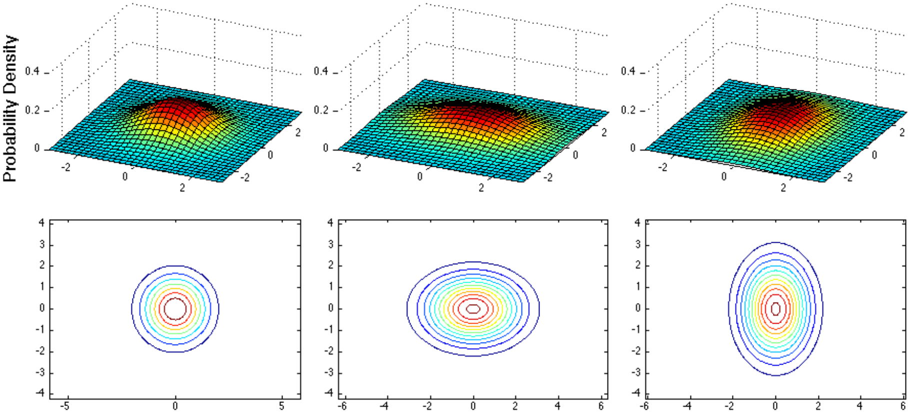
Bivariate Normal

$$\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \Sigma = 0.5 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \Sigma = 2 \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$



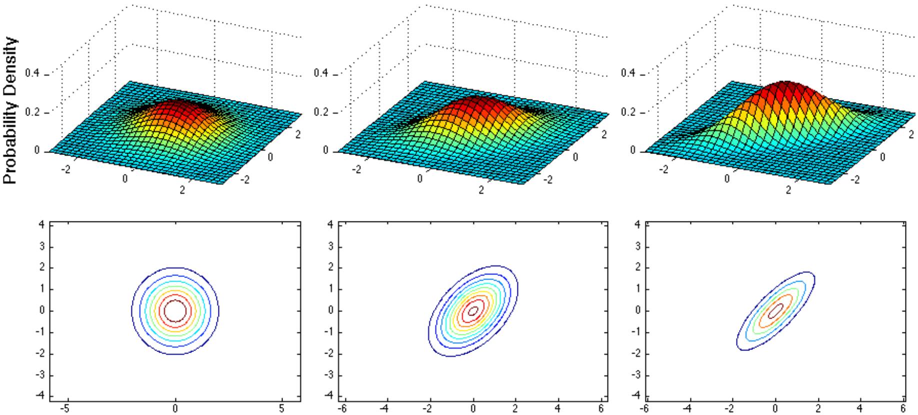
Bivariate Normal

$var(x_1) = var(x_2)$ $\quad$ $var(x_1) > var(x_2)$ $\quad$ $var(x_1) < var(x_2)$



Bivariate Normal

$$\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} 1 & 0.5 \\ 0.5 & 1 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} 1 & 0.8 \\ 0.8 & 1 \end{pmatrix}$$



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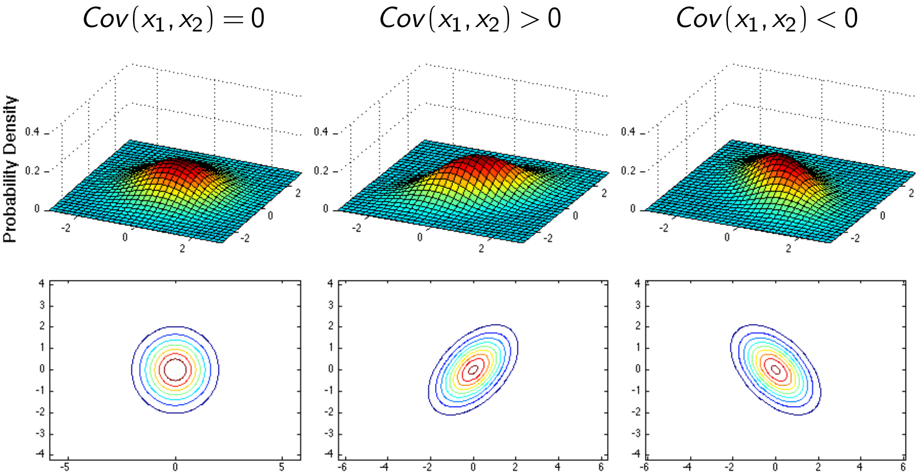

Gaussian Bayes Classifier

- Gaussian Bayes Classifier in its general form assumes that $p(\mathbf{x}|y)$ is distributed according to a multivariate normal (Gaussian) distribution
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$$p(\mathbf{x}|t=k) = \frac{1}{(2\pi)^{d/2}|\Sigma_k|^{1/2}} \exp\left[-\frac{1}{2}(\mathbf{x}-\boldsymbol{\mu}_k)^T \Sigma_k^{-1}(\mathbf{x}-\boldsymbol{\mu}_k)\right]$$

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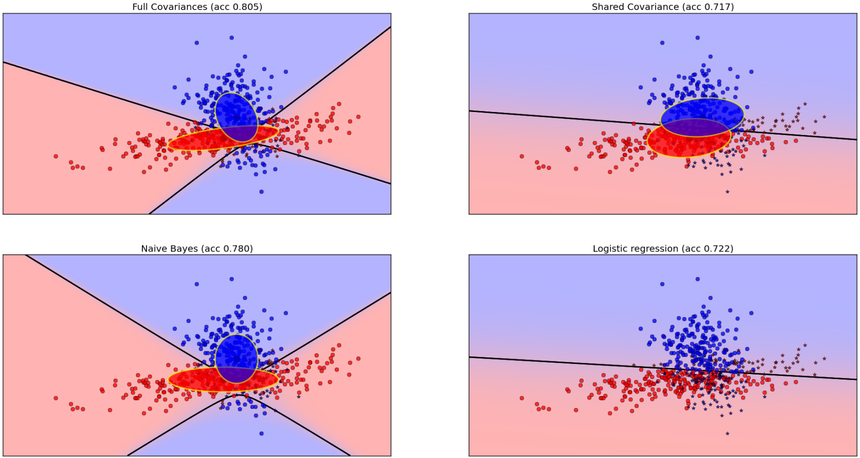
- Σ_k has $\mathcal{O}(d^2)$ parameters - could be hard to estimate

Example



Full Covariances (acc 0.805)
Shared Covariance (acc 0.717)
Naive Bayes (acc 0.780)
Logistic regression (acc 0.722)

Gaussian Bayes Binary Classifier Cases

Different cases on the covariance matrix:

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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.

Summary

- Probabilistic framework of using maximum likelihood as a more principled way to derive loss functions.
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- Probabilistic framework of using maximum likelihood as a more principled way to derive loss functions.
- 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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- 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 $\mathcal{D}$: $y_1, \ldots, y_n$ sampled i.i.d. from $p(y \mid \theta)$.
- 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 $\mathcal{D} = (H, H, T, T, T, T, T, H, \ldots, T)$, assumed i.i.d. flips.
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$$\begin{aligned} \hat{\theta}_{\text{MLE}} &= \underset{\theta \in \Theta}{\arg\max} \log L_{\mathcal{D}}(\theta) \\ &= \underset{\theta \in \Theta}{\arg\max} \left[n_h \log \theta + n_t \log(1-\theta) \right] \end{aligned}$$

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$\hat{\theta}_{\mathrm{MLE}}$ is the empirical fraction of heads.

Bayesian Statistics: Introduction

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- A **prior distribution** $p(\theta)$ is a distribution on the parameter space Θ.
- The prior reflects our belief about θ, **before seeing any data**.

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  2. A **prior distribution** $p(\theta)$ on parameter space Θ.
- 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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- Where $\propto$ means we've dropped factors that are independent of θ.

Coin Flipping: Bayesian Model

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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}
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Figure by Horas based on the work of Krishnavedala (Own work) [Public domain], via Wikimedia Commons http://commons.wikimedia.org/wiki/File:Beta_distribution_pdf.svg.

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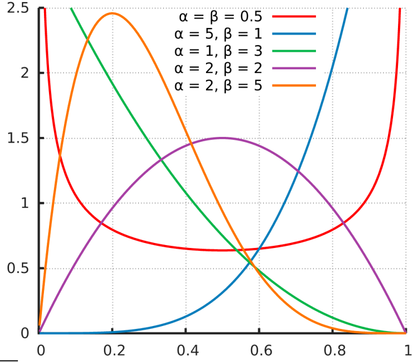

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- **Mean of Beta distribution:**

$$\mathbb{E}\theta = \frac{h}{h+t}$$

Coin Flipping: Beta Prior

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

- **Mean of Beta distribution:**

$$\mathbb{E}\theta = \frac{h}{h+t}$$

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

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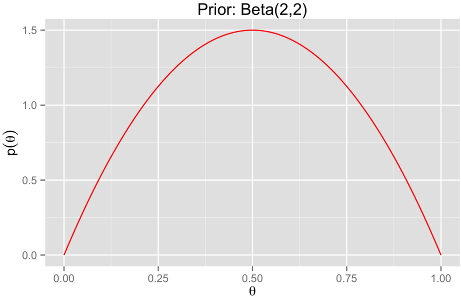

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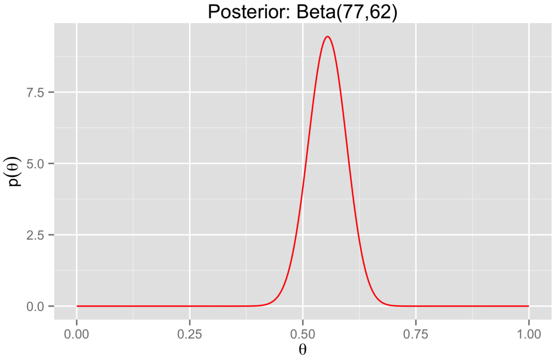

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    - **posterior mean** $\hat{\theta} = \mathbb{E}[\theta \mid \mathcal{D}]$
    - **maximum a posteriori (MAP) estimate** $\hat{\theta} = \arg\max_\theta p(\theta \mid \mathcal{D})$
        - Note: this is the **mode** of the posterior distribution

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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**

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

$$
r(a^*) = \min_{a \in \mathcal{A}} r(a)
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Important Cases

- Squared Loss : $\ell(\hat{\theta}, \theta) = \left(\theta - \hat{\theta}\right)^2 \quad \Rightarrow$ posterior mean
- Zero-one Loss: $\ell(\theta, \hat{\theta}) = \mathbb{1}[\theta \neq \hat{\theta}] \quad \Rightarrow$ posterior mode
- Absolute Loss : $\ell(\hat{\theta}, \theta) = \left|\theta - \hat{\theta}\right| \quad \Rightarrow$ posterior median

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

Interim summary

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  - 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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- This is the common starting point for either classical or Bayesian regression.

Classical treatment: Likelihood Function

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

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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 $x = (x_1, \ldots, x_n)$.

Maximum Likelihood Estimator

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

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

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- The corresponding prediction function is

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Bayesian Conditional Probability Models

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$$\begin{aligned} p(\theta \mid \mathcal{D}, x) &\propto p(\mathcal{D} \mid \theta, x) p(\theta) \\ &= \underbrace{L_{\mathcal{D}}(\theta)}_{\text{likelihood}} \underbrace{p(\theta)}_{\text{prior}} \end{aligned}$$

- 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)
  - $\hat{\theta} = \text{median}[\theta \mid \mathcal{D}, x]$
  - $\hat{\theta} = \arg\max_{\theta \in \Theta} p(\theta \mid \mathcal{D}, x)$ (the MAP estimate)
- depending on our loss function.

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

$$p(y \mid x, \mathcal{D}) = \int p(y \mid x; \theta) p(\theta \mid \mathcal{D}) \, d\theta$$

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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 $\mathcal{Y} = \mathbf{R}$
- Given x, the world generates y as

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

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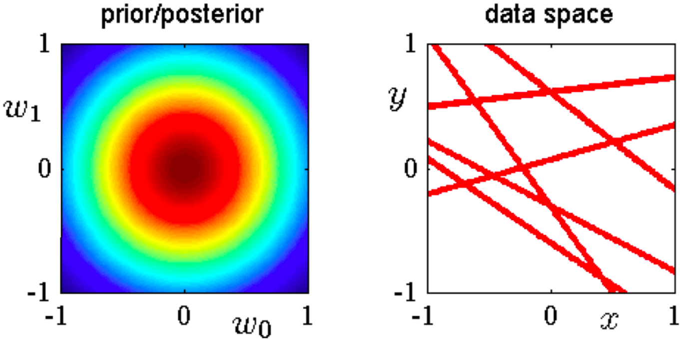
Example in 1-Dimension: Prior Situation

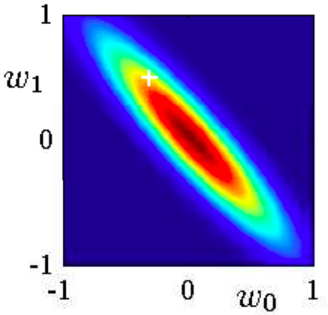
- **Prior distribution:** $w = (w_0, w_1) \sim \mathcal{N}\left(0, \frac{1}{2}I\right)$ (Illustrated on left)

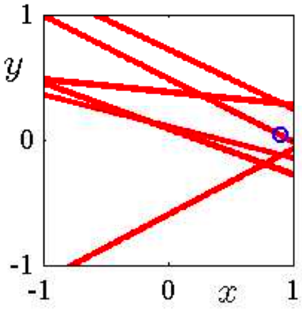


- On right, $y(x) = \mathbb{E}[y \mid x, w] = w_0 + w_1 x$, for randomly chosen $w \sim p(w) = \mathcal{N}\left(0, \frac{1}{2}I\right)$.

Bishop's PRML Fig 3.7

Example in 1-Dimension: 1 Observation

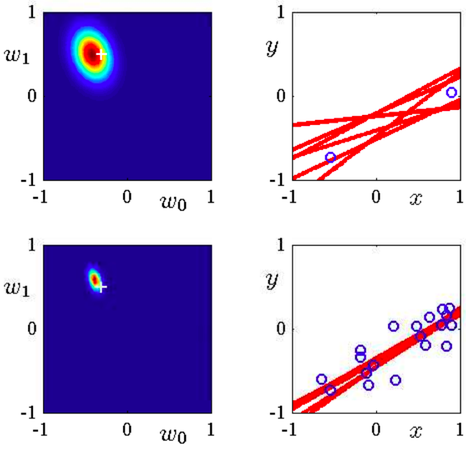




- On left: posterior distribution; white cross indicates true parameters
- On right:
  - blue circle indicates the training observation
  - red lines, $y(x) = \mathbb{E}[y \mid x, w] = w_0 + w_1 x$, for randomly chosen $w \sim p(w|\mathcal{D})$ (posterior)

Bishop's PRML Fig 3.7

Example in 1-Dimension: 2 and 20 Observations



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Gaussian Regression: Closed form

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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.