# Probabilistic models - Bayesian Methods

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## Logistics

- 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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  - Conditional:  $p(y \mid x)$
  - Generative: p(x,y)
- How to estimate the parameters of our model? Maximum likelihood estimation.
- Compare and contrast conditional and generative models.

## Conditional models

## Linear regression

Linear regression is one of the most important methods in machine learning and statistics. **Goal**: Predict a real-valued **target** y (also called response) from a vector of **features** x (also called covariates).

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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  $\theta$ ) to predict y from x:

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

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.

Loss function We estimate  $\theta$  by minimizing the squared loss (the least square method):

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

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### Review questions

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

### Review

#### We've seen

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### Next,

• Derive linear regression from a probabilistic modeling perspective.

• x and y are related through a linear function:

$$y = \theta^T x + \epsilon, \tag{4}$$

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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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#### Gradient of the likelihood

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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#### Review

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#### However,

- Sometimes Gaussian distribution is not a reasonable assumption, e.g., classification
- Can we use the same modeling approach for other prediction tasks?

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#### However,

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- Can we use the same modeling approach for other prediction tasks?

#### Next,

• Derive logistic regression for classification.

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Consider binary classification where  $Y \in \{0,1\}$ . What should be the distribution  $Y \mid X = x$ ?

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- What is the mean of  $Y \mid X = x$ ?

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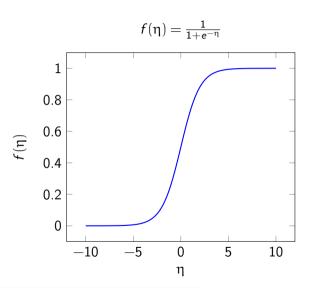
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- What is the mean of  $Y \mid X = x$ ? h(x). (Think how we parameterize the mean in linear regression)
- Need a function f to map the linear predictor  $\theta^T x$  in  $\mathbb{R}$  to (0,1):

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

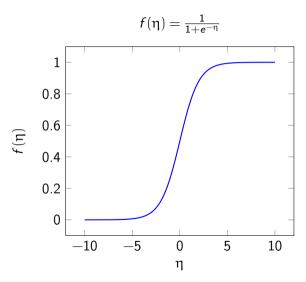
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•  $p(y \mid x) = Bernoulli(f(\theta^T x)).$ 

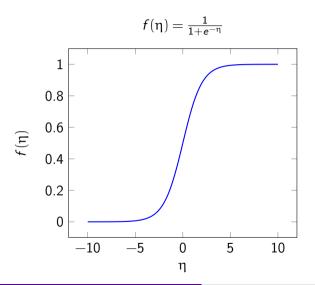
17 / 73

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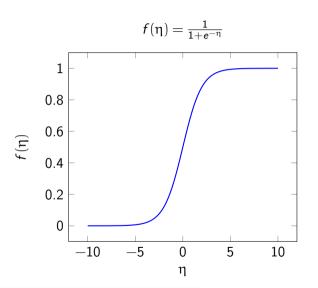


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- Exercise: show that the log odds is

$$\log \frac{p(y=1 \mid x)}{p(y=0 \mid x)} = \theta^{T} x.$$
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 $\implies$  linear decision boundary (19)

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

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(21)

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

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

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#### Math review: Chain rule

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

(26)

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$$= \left( \frac{y^{(n)}}{f^n} - \frac{1 - y^{(n)}}{1 - f^n} \right) \frac{\partial f^n}{\partial \theta_i}$$

$$\frac{d}{dx} \ln x = \frac{1}{x}$$
(24)

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 $\partial \ell^n \quad \partial \ell^n \partial f^n$ 

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

$$\frac{\partial}{\partial \theta_{i}} = \frac{\partial}{\partial f^{n}} \frac{\partial}{\partial \theta_{i}} \qquad (23)$$

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

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

$$= \left(y^{(n)} - f^{n}\right)x_{i}^{(n)} \qquad \text{simplify by algebra} \qquad (26)$$

(23)

19 / 73 Mengve Ren (NYU) CSCI-GA 2565 Oct 17, 2023

#### Math review: Chain rule

 $\partial \ell^n \quad \partial \ell^n \partial f^n$ 

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

$$\frac{\partial v}{\partial \theta_{i}} = \frac{\partial v}{\partial f^{n}} \frac{\partial v}{\partial \theta_{i}} \qquad (23)$$

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

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$$= \left(v^{(n)} - f^{n}\right)x_{i}^{(n)} \qquad \text{simplify by algebra} \qquad (26)$$

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

Mengye Ren (NYU)

CSCI-GA 2565

Oct 17, 2023

$$\frac{\partial \ell}{\partial \theta_i} = \sum_{n=1}^{N} (y^{(n)} - f(\theta^T x^{(n)})) x_i^{(n)}$$
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#### A closer look at the gradient

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#### A closer look at the gradient

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(27)

- 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

# 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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# 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

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

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

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

- 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  $\theta \in \Theta$
- ullet Choose a transfer function that maps a linear predictor in  ${\mathbb R}$  to  $\Theta$

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

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

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#### Math review: Poisson distribution

Given a random variable  $Y \in 0, 1, 2, ...$  following Poisson( $\lambda$ ), we have

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

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

Standard approach is to take

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

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

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

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

$$= \sum_{i=1}^{n} \left[ y_{i} w^{T} x_{i} - \exp \left( w^{T} x_{i} \right) - \log \left( y_{i} ! \right) \right]$$
 (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  $y \in \{1, ..., k\}$  as

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

Recipe for contructing a conditional distribution for prediction:

- Oefine 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  $\Theta$ .
- (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  $p(y \mid x; \theta)$  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  $\arg \max_{y \in \mathcal{Y}} p(x, y; \theta)$ .

Training:

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

(35)

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$$p(y \mid x)$$

(35)

Training:

$$p(x,y) = p(x \mid y)p(y)$$
(33)

Testing:

$$p(y \mid x) = \frac{p(x \mid y)p(y)}{p(x)}$$

Bayes rule

(35)

(34)

Training:

$$p(x,y) = p(x \mid y)p(y)$$
(33)

Testing:

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

$$\underset{y}{\operatorname{arg\,max}} p(y \mid x) = \underset{y}{\operatorname{arg\,max}} p(x \mid y) p(y)$$
(35)

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

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

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

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What's the probability of a document x?

$$p(x \mid y) = p(x_1, ..., x_d \mid y)$$

$$= p(x_1 \mid y)p(x_2 \mid y, x_1)p(x_3 \mid y, x_2, x_1) ... p(x_d \mid y, x_{d-1}, ..., x_1)$$
 chain rule (38)

$$= \prod_{i=1}^{d} p(x_i \mid y, x_{< i})$$
 (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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**Challenge**:  $p(x_i | y, x_{< i})$  is hard to model (and estimate), especially for large *i*. Solution:

#### Naive Bayes assumption

Features are conditionally independent given the label:

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

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

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Similarly,

$$p(y=1) = \theta_0. \tag{42}$$

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Similarly,

$$\rho(y=1) = \theta_0. \tag{42}$$

Thus.

$$p(x,y) = p(x \mid y)p(y)$$

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

$$= p(y) \prod_{i=1}^{d} \theta_{i,y} \mathbb{I}\{x_i = 1\} + (1 - \theta_{i,y}) \mathbb{I}\{x_i = 0\}$$
(43)
$$(44)$$

Indicator function I{condition} evaluates to 1 if "condition" is true and 0 otherwise.

(41)

#### 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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(46)

$$= \frac{\partial}{\partial \theta_{i,1}} \sum_{n=1}^{N} \log \left( \theta_{j,y^{(n)}} \mathbb{I} \left\{ x_j^{(n)} = 1 \right\} + \left( 1 - \theta_{j,y^{(n)}} \right) \mathbb{I} \left\{ x_j^{(n)} = 0 \right\} \right) \quad \text{ignore } i \neq j \quad (47)$$

(48)

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).

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

$$&= \frac{\partial}{\partial \theta_{j,1}} \sum_{n=1}^{N} \log \left( \theta_{j,y^{(n)}} \mathbb{I} \left\{ x_{j}^{(n)} = 1 \right\} + \left( 1 - \theta_{j,y^{(n)}} \right) \mathbb{I} \left\{ x_{j}^{(n)} = 0 \right\} \right) \qquad \text{ignore } i \neq j \quad (47)$$

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

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

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

#### MLE solution for our NB model

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

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

In practice, count words:

number of fake reviews containing "absolutely" number of fake reviews

Exercise: show that

$$\theta_{j,0} = \frac{\sum_{n=1}^{N} \mathbb{I}\left\{y^{(n)} = 0 \land x_{j}^{(n)} = 1\right\}}{\sum_{n=1}^{N} \mathbb{I}\left\{y^{(n)} = 0\right\}}$$

$$(50)$$

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

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.
- Stimate 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.

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

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

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

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 (52)

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

Likelihood of the data:

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

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

#### MLE for Gaussian NB

Log likelihood:

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

(58)

(59)

#### MLF for Gaussian NB

Log likelihood:

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

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

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

(58)

(59)

Log likelihood:

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

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

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

(59)

Log likelihood:

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

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

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

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

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

#### MLE for Gaussian NB

Log likelihood:

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

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

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

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

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

#### MLE for Gaussian NB

Show that

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

$$\theta_{k} = \frac{\sum_{n:y^{(n)}=k} 1}{M} \qquad \text{(class prior)}$$

$$(60)$$

Is the Gaussian NB model a linear classifier?

(66)

Is the Gaussian NB model a linear classifier?

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

(66)

Is the Gaussian NB model a linear classifier?

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

$$= \log \frac{\theta_0}{1-\theta_0} + \sum_{i=1}^{d} \left(\log \sqrt{\frac{\sigma_{i,0}^2}{\sigma_{i,1}^2}} + \left(\frac{(x_i - \mu_{i,0})^2}{2\sigma_{i,0}^2} - \frac{(x_i - \mu_{i,1})^2}{2\sigma_{i,1}^2}\right)\right)$$
(62)

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(63)

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

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

$$=\sum_{i=1}^{d}\frac{\mu_{i,1}-\mu_{i,0}}{\sigma_{i}^{2}}x_{i}+\frac{\mu_{i,0}^{2}-\mu_{i,1}^{2}}{2\sigma_{i}^{2}}$$

linear

(66)

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

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

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(68)

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(69)

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(68)where else have we seen it?

(69)

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

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

# Naive Bayes vs logistic regression

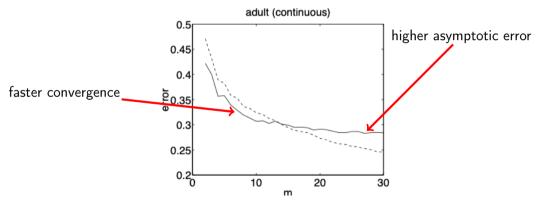
	logistic regression	Gaussian naive Bayes
model type	conditional/discriminative	generative
parametrization	$p(y \mid x)$	p(x   y), p(y)
assumptions on $Y$	Bernoulli	Bernoulli
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Given the same training data, is  $\theta_{LR}=\theta_{GNB}?$ 

#### 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.

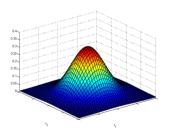
- Data points are generated from Gaussian distributions for each class
- Each dimension is independently generated
- Shared variance

What if the GNB assumption is not true?

#### Multivariate Gaussian Distribution

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

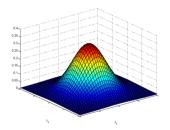
$$p(\mathbf{x}) = \frac{1}{(2\pi)^{d/2} |\Sigma|^{1/2}} \exp\left[ -\frac{1}{2} (\mathbf{x} - \mathbf{\mu})^T \Sigma^{-1} (\mathbf{x} - \mathbf{\mu}) \right]$$



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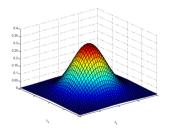


• Mahalanobis distance  $(x - \mu_k)^T \Sigma^{-1} (x - \mu_k)$  measures the distance from x to  $\mu$  in terms of  $\Sigma$ 

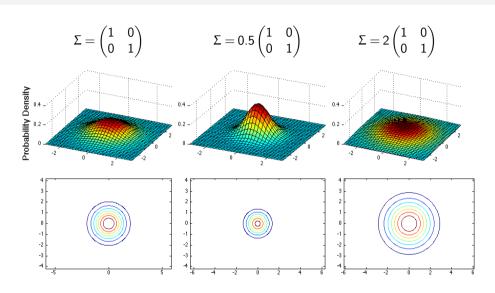
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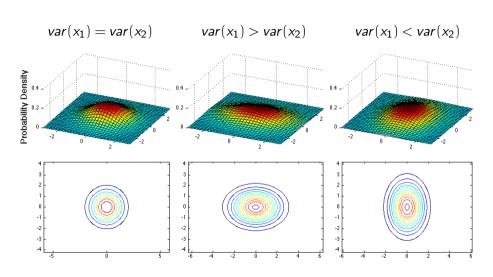
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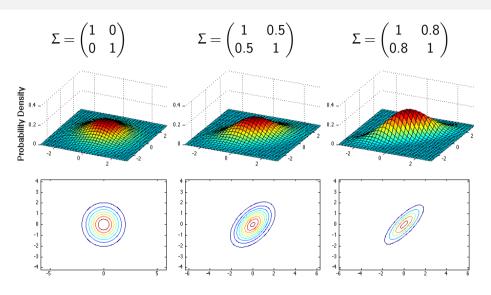
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- It normalizes for difference in variances and correlations



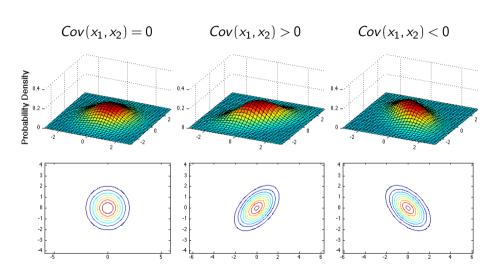


Mengye Ren (NYU) CSCI-GA 2565 Oct 17, 2023

46 / 73



47 / 73



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

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

where  $|\Sigma_k|$  denotes the determinant of the matrix, and d is dimension of x

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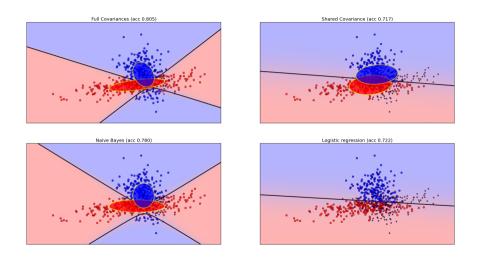
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- $\Sigma_k$  has  $O(d^2)$  parameters could be hard to estimate

# Example



### Gaussian Bayes Binary Classifier Cases

Different cases on the covariance matrix:

- Full covariance: Quadratic decision boundary
- Shared covariance: Linear 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.

### Summary

- 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.

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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
- $\theta$  is a parameter in a [finite dimensional] parameter space  $\Theta$ .

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- where  $p(y \mid \theta)$  is a density on a sample space  $\mathcal{Y}$ , and
- $\theta$  is a parameter in a [finite dimensional] parameter space  $\Theta$ .
- 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).

• We're still working with a parametric family of densities:

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55 / 73 Mengve Ren (NYU) CSCI-GA 2565 Oct 17, 2023

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- But instead of  $\theta$ , 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  $\theta$ .

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  - **Efficiency:** (Roughly speaking)  $\hat{\theta}_n$  is as accurate as we can get from a sample of size n.
- Maximum likelihood estimators are consistent and efficient under reasonable conditions.

Mengye Ren (NYU) CSCI-GA 2565 Oct 17, 2023 56/73

# Example of Point Estimation: Coin Flipping

• Parametric family of mass functions:

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

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

- Data  $\mathfrak{D} = (H, H, T, T, T, T, T, H, ..., T)$ , assumed i.i.d. flips.
  - n<sub>h</sub>: number of heads
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• As usual, it is easier to maximize the log-likelihood function:

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

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$$\frac{n_h}{\theta} - \frac{n_t}{1 - \theta} = 0 \iff \theta = \frac{n_h}{n_h + n_t}$$

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Bayesian Statistics: Introduction

### Bayesian Statistics

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- The prior reflects our belief about  $\theta$ , before seeing any data.

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- **2** A **prior distribution**  $p(\theta)$  on parameter space  $\Theta$ .
- Putting the pieces together, we get a joint density on  $\theta$  and  $\mathfrak{D}$ :

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

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Mengye Ren (NYU) CSCI-GA 2565 Oct 17, 2023 63/73

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

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## Coin Flipping: Bayesian Model

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

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- One convenient choice would be a distribution from the Beta family

CSCI-GA 2565 Oct 17, 2023 64 / 73

Prior:

$$\theta \sim \operatorname{Beta}(\alpha, \beta)$$
 $p(\theta) \propto \theta^{\alpha-1} (1-\theta)^{\beta-1}$ 

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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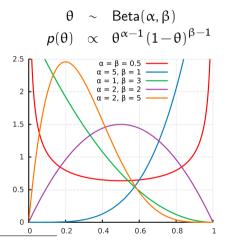


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• Prior:

$$\theta \sim \operatorname{Beta}(h,t)$$
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Mengye Ren (NYU) CSCI-GA 2565 Oct 17, 2023 67/73

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

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#### Definition

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

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

Mengye Ren (NYU) CSCI-GA 2565 Oct 17, 2023 69/73

#### Coin Flipping: Concrete Example

• Suppose we have a coin, possibly biased (parametric probability model):

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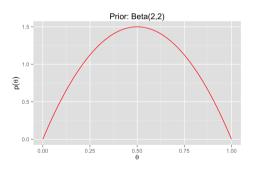
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Mengye Ren (NYU) CSCI-GA 2565 Oct 17, 2023 70/73

• Next, we gather some data  $\mathfrak{D} = \{H, H, T, T, T, T, T, T, H, \dots, T\}$ :

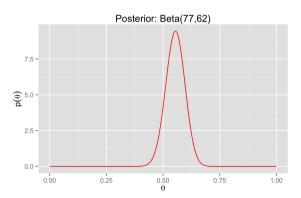
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• Posterior distribution:  $\theta \mid \mathcal{D} \sim \text{Beta}(77, 62)$ :



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- Common options:
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  - maximum a posteriori (MAP) estimate  $\hat{\theta} = \arg \max_{\theta} p(\theta \mid D)$ 
    - 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