# Probabilistic models - Bayesian Methods

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(Slides credit to David Rosenberg, He He, et al.)

NYU

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# 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)

$x \rightarrow$ one $y$

$x \rightarrow$ distribution of $y$

Categorial $\begin{cases} y=0 & 0.05 \\ y=1 & 0.95 \end{cases}$

Gaussian $N(\mu, \sigma^2)$

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  - **Generative**: $p(x, y)$ $= p(x)\, p(y|x) = p(y)\, p(x|y)$
- How to estimate the parameters of our model? Maximum likelihood estimation.

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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

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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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**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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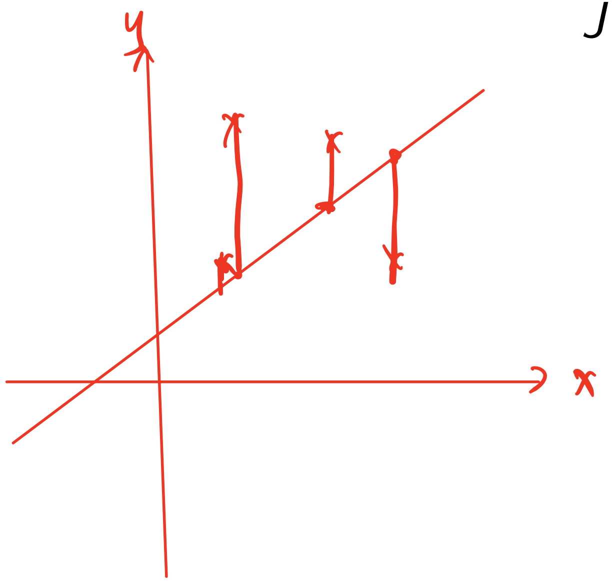
Note that

- 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.

## Parameter estimation

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

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



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$$\hat{\theta} = \arg\min_{\theta} (X\theta - \mathrm{y})^T (X\theta - \mathrm{y}). \tag{3}$$

$$= \theta^T X^T X \theta - 2X^T y \theta + y^T y$$

$$\frac{\partial}{\partial \theta} = 2X^T X\theta - 2X^T y = 0$$

$$X^T X \theta = X^T y \qquad \theta = (X^T X)^{-1} X^T y$$

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$(X^TX + \lambda I)^{-1}$

**Review questions**

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

Ridge Regression

pseudo-inverse of $X^TX$

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Next,

- Derive linear regression from a probabilistic modeling perspective.

# Assumptions in linear regression

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

where $\epsilon$ is the **residual error** capturing all unmodeled effects (e.g., noise).

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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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Next,

- Derive logistic regression for classification.

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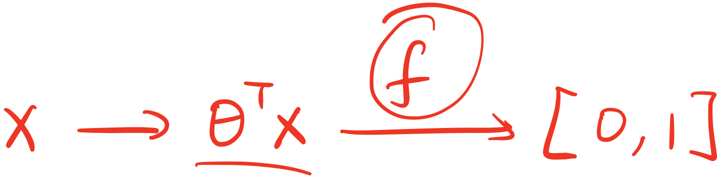

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- What is the mean of $Y \mid X = x$? $h(x)$. (Think how we parameterize the mean in linear regression)
- Need a function $f$ to map the linear predictor $\theta^T x$ in $\mathbb{R}$ to $(0,1)$:

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

# Logistic regression

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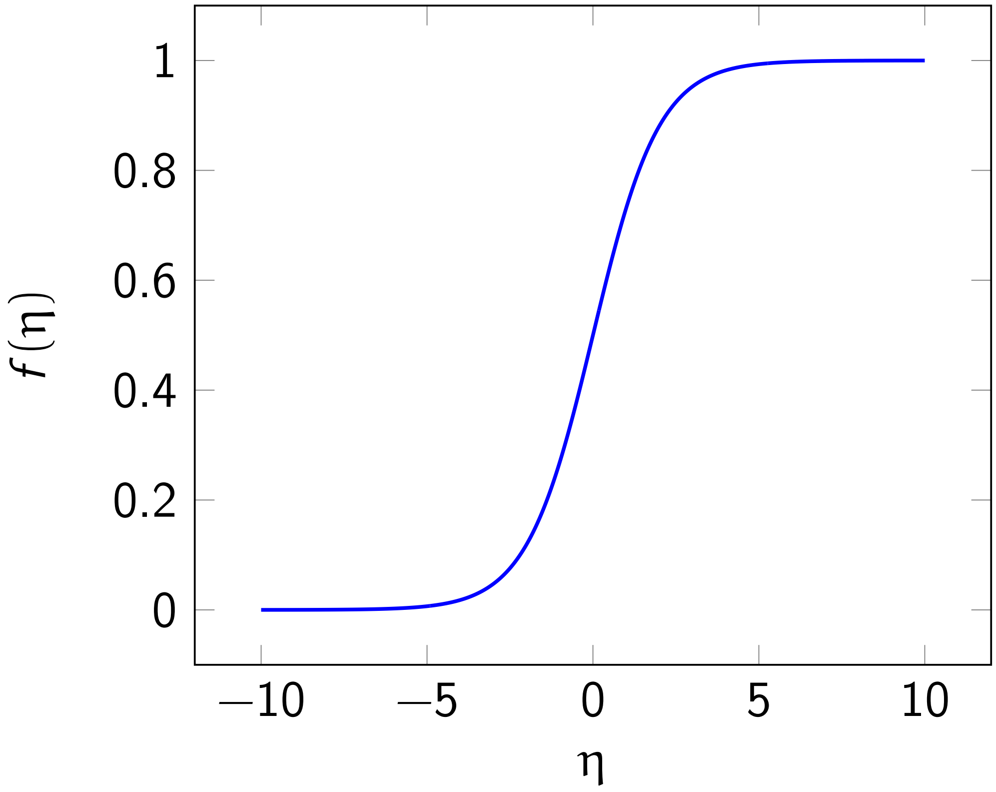


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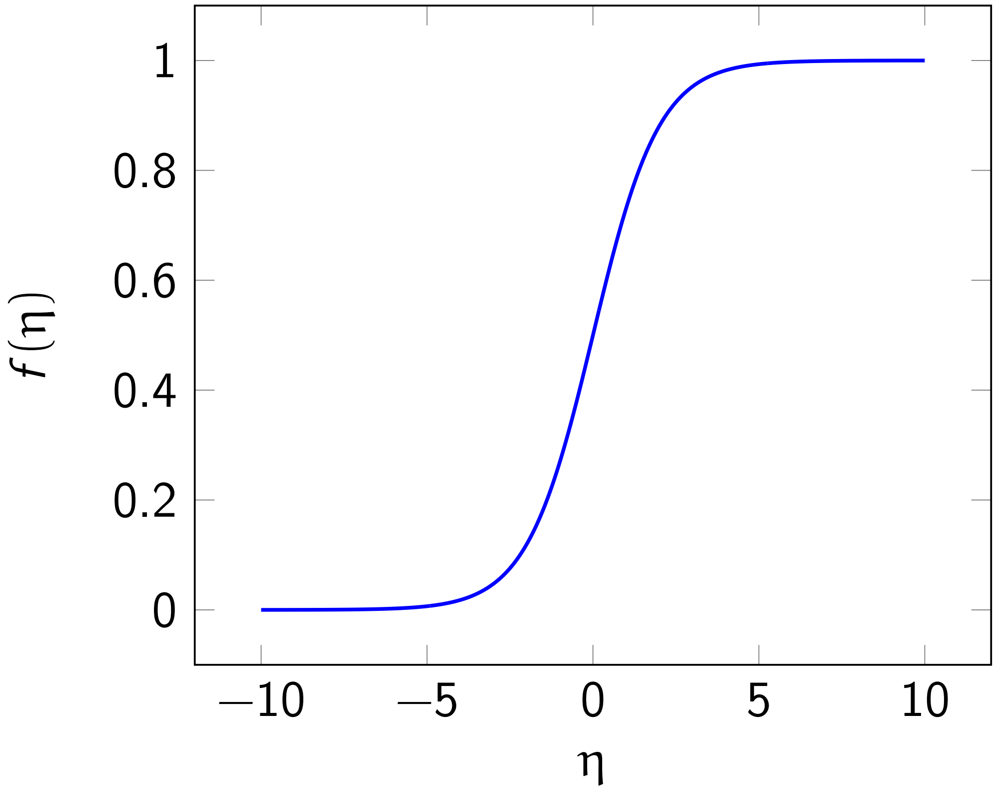


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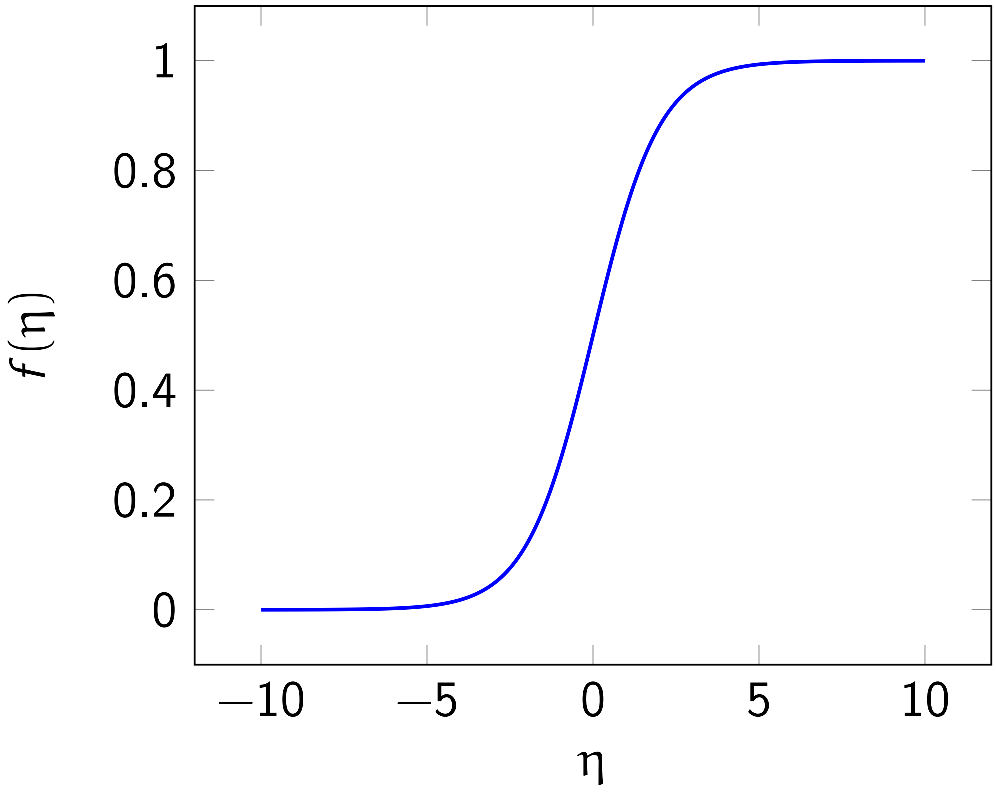


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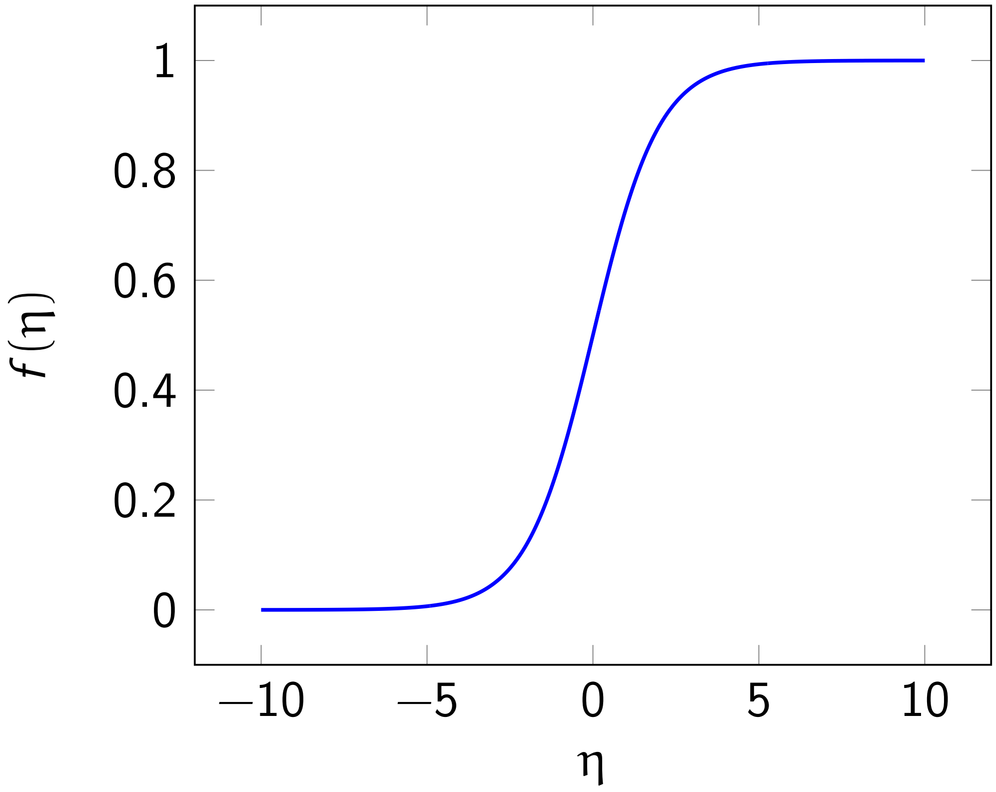


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- How do we extend it to multiclass classification? (more on this later)

# MLE for logistic regression

Similar to linear regression, let's estimate θ by maximizing the conditional log likelihood.

$$\max P(D) = \prod_{i=1}^{N} \left(1 - f(\theta^T x^{(n)})\right)^{1-y^{(n)}} \left(f(\theta^T x^{(n)})\right)^{y^{(n)}}$$

$$\Updownarrow$$

$$\max \underline{\log} P(D) = \sum_{i=1}^{N} \left(1 - y^{(n)}\right) \log\left(1 - f(\theta^T x^{(n)})\right) + y^{(n)} \log f(\theta^T x^{(n)}) \quad (21)$$

$$\frac{\partial}{\partial \theta} = 0 \implies \cdots$$

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

$$ \tag{26} $$

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$f'(z) = -(1+e^{-z})^{-2}(-e^{-z})$

$= f(z)\cdot(1-f(z))$

(26)

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

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

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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

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# A closer look at the gradient

LR: $$\frac{\partial l}{\partial \theta_i} = \sum_{n=1}^{N} \left(y^{(n)} - \theta^T x^{(n)}\right) x_i^{(n)}$$

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

- 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 |
|---|---|---|

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| | linear regression | logistic regression |
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| Combine the inputs | $\theta^T x$ (linear) | $\theta^T x$ (linear) |
| Output | real $Y \sim N(\theta^T x, \sigma^2)$ | categorical $Y \sim B(f(\theta^T x))$ |
| Conditional distribution | Gaussian | Bernoulli |
| Transfer function $f(\theta^T x)$ | identity | logistic |
| Mean $\mathbb{E}(Y \mid X = x; \theta)$ | $f(\theta^T x)$ | $f(\theta^T x)$ |

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Poisson

- $x$ 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 $\Theta$

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

**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)?

# Example: Construct Poisson regression

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

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- What's a good model for number of visitors (the output distribution)?

**Math review: Poisson distribution**

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

$$p(Y = k; \lambda) = \frac{\lambda^k e^{-\lambda}}{k!}, \qquad f: R \to R_{>0} \tag{29}$$

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

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

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

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

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

$\underset{w}{\text{argmax}}$

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

$\frac{\partial}{\partial w}$

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

# Multinomial Logistic Regression

handles > 2 classes

- 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:

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

$y = k$

$\vdots$

$$x \to \theta^T x \to \frac{f(\theta^T x)}{1 - f(\theta^T x)} \quad \begin{matrix} y = 1 \\ y = 0 \end{matrix}$$

# Multinomial Logistic Regression

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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 $\Theta$.
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:

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

(35)

# Generative modeling through the Bayes rule

Training:

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

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# Generative modeling through the Bayes rule

Training:

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

Testing:

$$p(y \mid x) \propto p(x \mid y)p(y)$$

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

$$(35)$$

# Generative modeling through the Bayes rule

Training:

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

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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$p(x, y)$

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What's the probability of a document $x$?

$P(x|y) = p(x_1, x_2, x_3, \cdots, x_d | y)$

$= p(y) p(x_1|y) \, p(x_2|x_1, y) \cdots p(x_d | x_1, x_2, \cdots, x_{d-1}, y)$

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

$p(x_d | x_1, x_2, \ldots x_{d-1}, y)$

$= p(x_d | y)$

# 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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2d+1

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Similarly,

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Similarly,

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

Thus,

$$p(x, y) = p(x \mid y)p(y) \tag{43}$$

$$= p(y) \prod_{i=1}^{d} p(x_i \mid y) \qquad \text{NB assumption} \tag{44}$$

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

$$P(D) = \prod_{n=1}^{N} p(x^{(n)}, y^{(n)})$$

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

$$\log P(D) = \sum_{n=1}^{N} \log p(y^{n}) + \sum_{i=1}^{d} \log(\theta \mathbb{I}(\cdot) + (1-\theta)\mathbb{I}(\cdot))$$

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).

$$ \tag{48} $$

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

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

$$\tag{48}$$

# MLE for our NB model

$\left(\sum \mathbb{I}(y=1)\right)\theta_{j,1} = \sum \mathbb{I}(y=1, x_j=1)$

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

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

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

$= 0 \quad \Rightarrow \left(1-\theta_{j,1}\right)\sum_{n=1}^{N}\mathbb{I}(y=1, x_j=1) = \theta_{j,1}\sum \mathbb{I}(y=1, x_j=0)$

$\left(\sum \mathbb{I}(y=1, x_j=1)+\mathbb{I}(y=1, x_j=0)\right)\theta_{j,1} = \sum \mathbb{I}(y=1, x_j=1)$

# 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:

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

# fake / # reviews

Exercise: show that

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

P(y=1)

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

# Review

tinyurl.com/ml-lec6

$p(x_d \mid x_1 \cdots x_k, y) = \frac{p(x_d \mid y)}{p(y)}$

NB assumption: conditionally independent features given the label

Recipe for learning a NB model: → Gaussian

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:

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

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# MLE for Gaussian NB

Show that

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

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

# Decision boundary of the Gaussian NB model

Is the Gaussian NB model a linear classifier?

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

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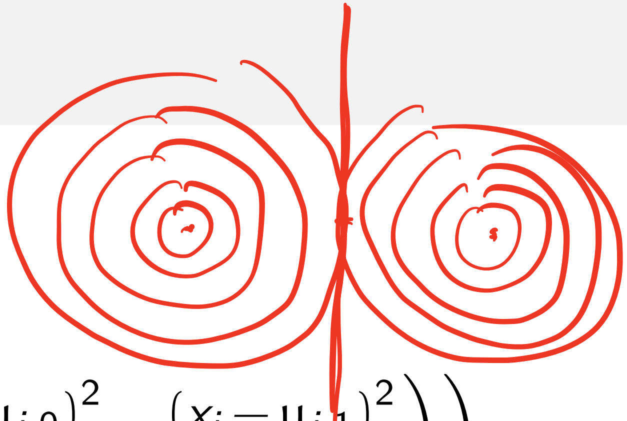

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$$\text{assume that } \sigma_{i,0} = \sigma_{i,1} = \sigma_i, \;\; (\theta_0 = 0.5) \tag{64}$$

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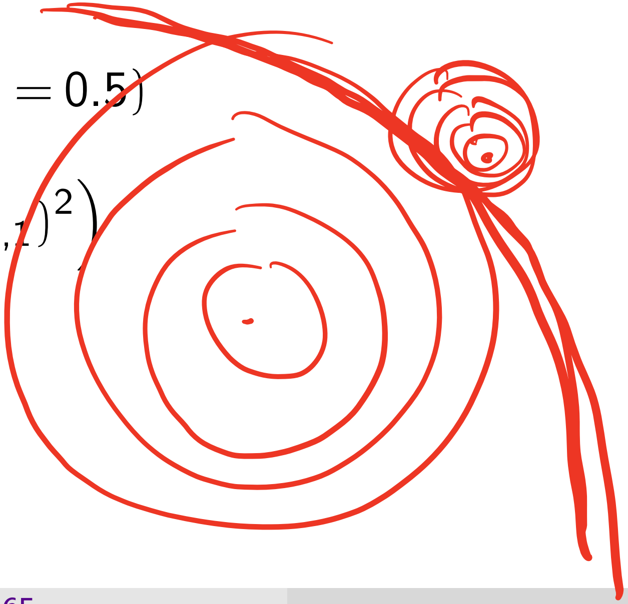

$$= \sum_{i=1}^{d} \frac{\mu_{i,1} - \mu_{i,0}}{\sigma_i^2} x_i + \frac{\mu_{i,0}^2 - \mu_{i,1}^2}{2\sigma_i^2} \quad \text{linear}$$

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# Decision boundary of the Gaussian NB model

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

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

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

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

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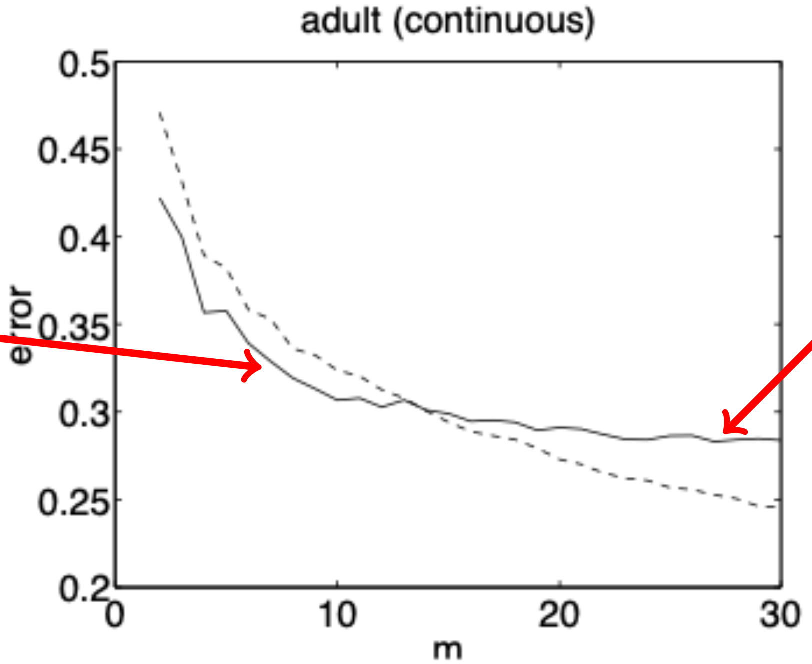
Given the same training data, is $\theta_{\text{LR}} = \theta_{\text{GNB}}$?

# 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.

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

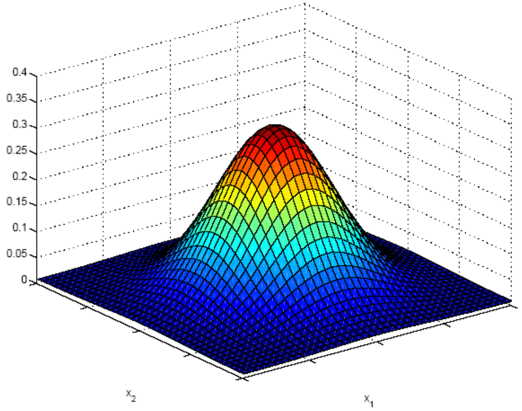
What if the GNB assumption is not true?

# Multivariate Gaussian Distribution

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

vector matrix

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



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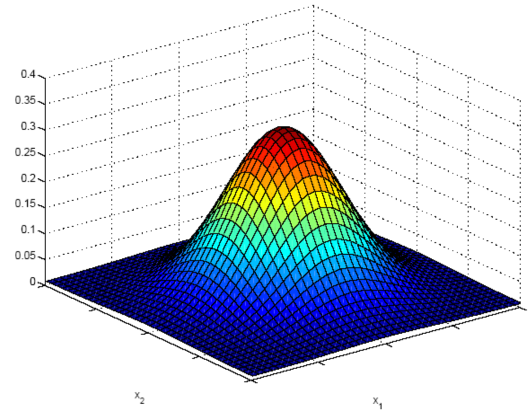


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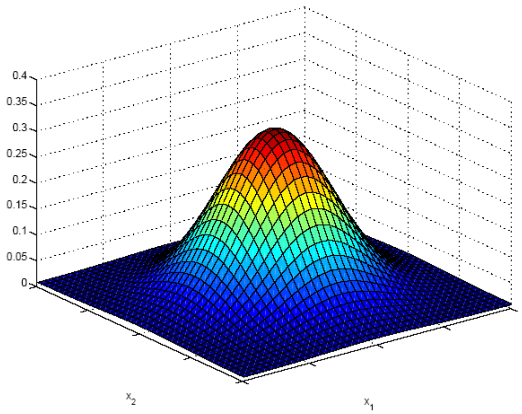
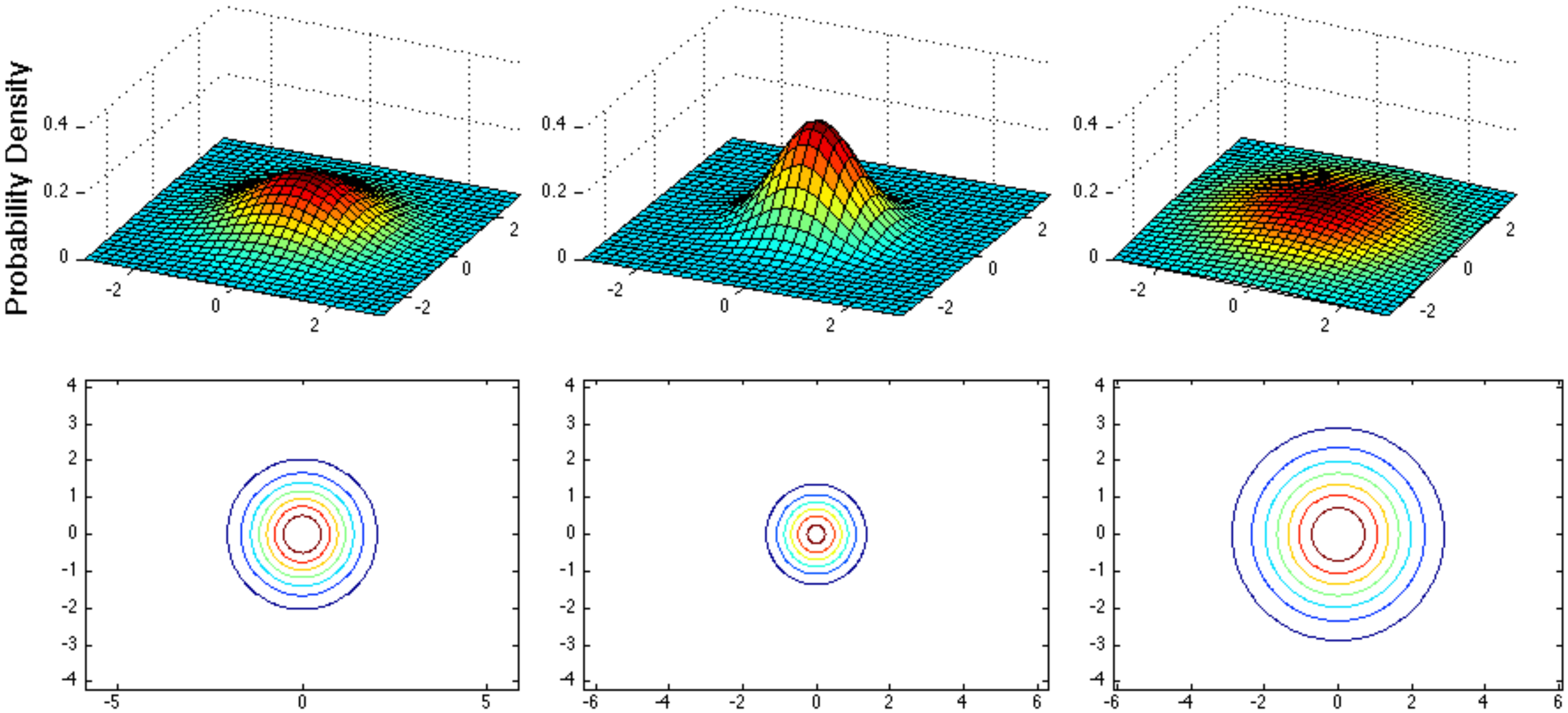



- Mahalanobis distance $(\mathbf{x}-\mu_k)^T\Sigma^{-1}(\mathbf{x}-\mu_k)$ measures the distance from $\mathbf{x}$ to $\mu$ in terms of $\Sigma$
- It normalizes for difference in variances and correlations

# Bivariate Normal

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



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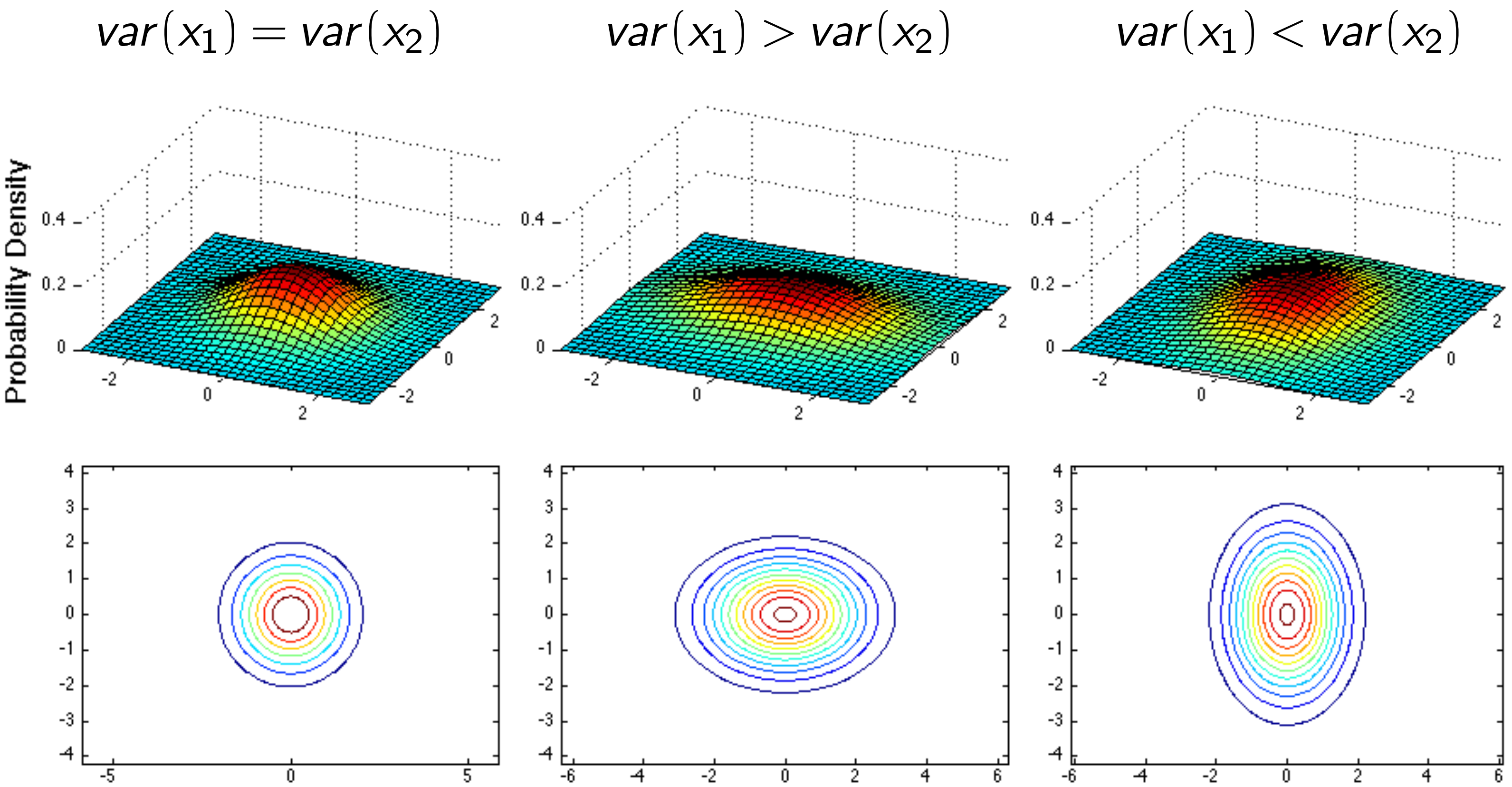

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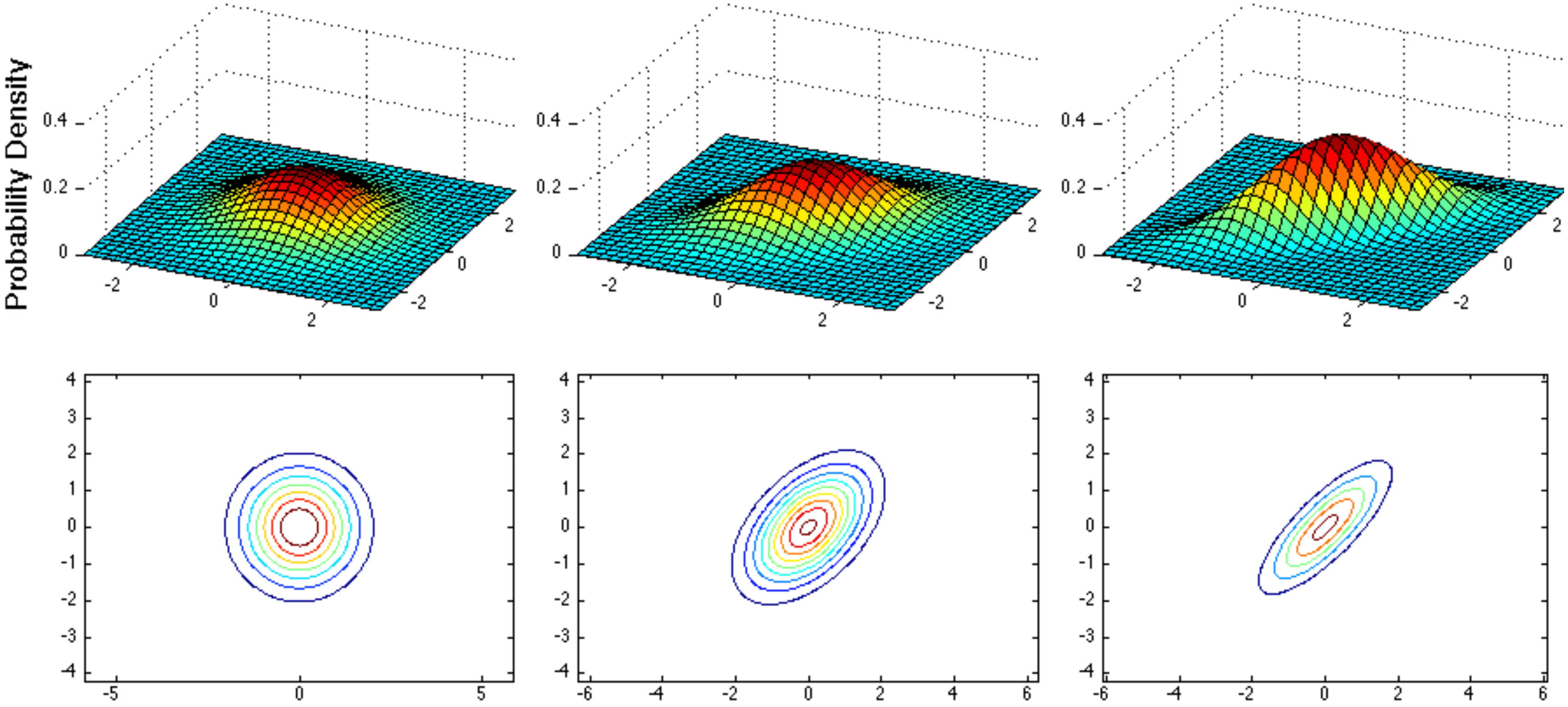
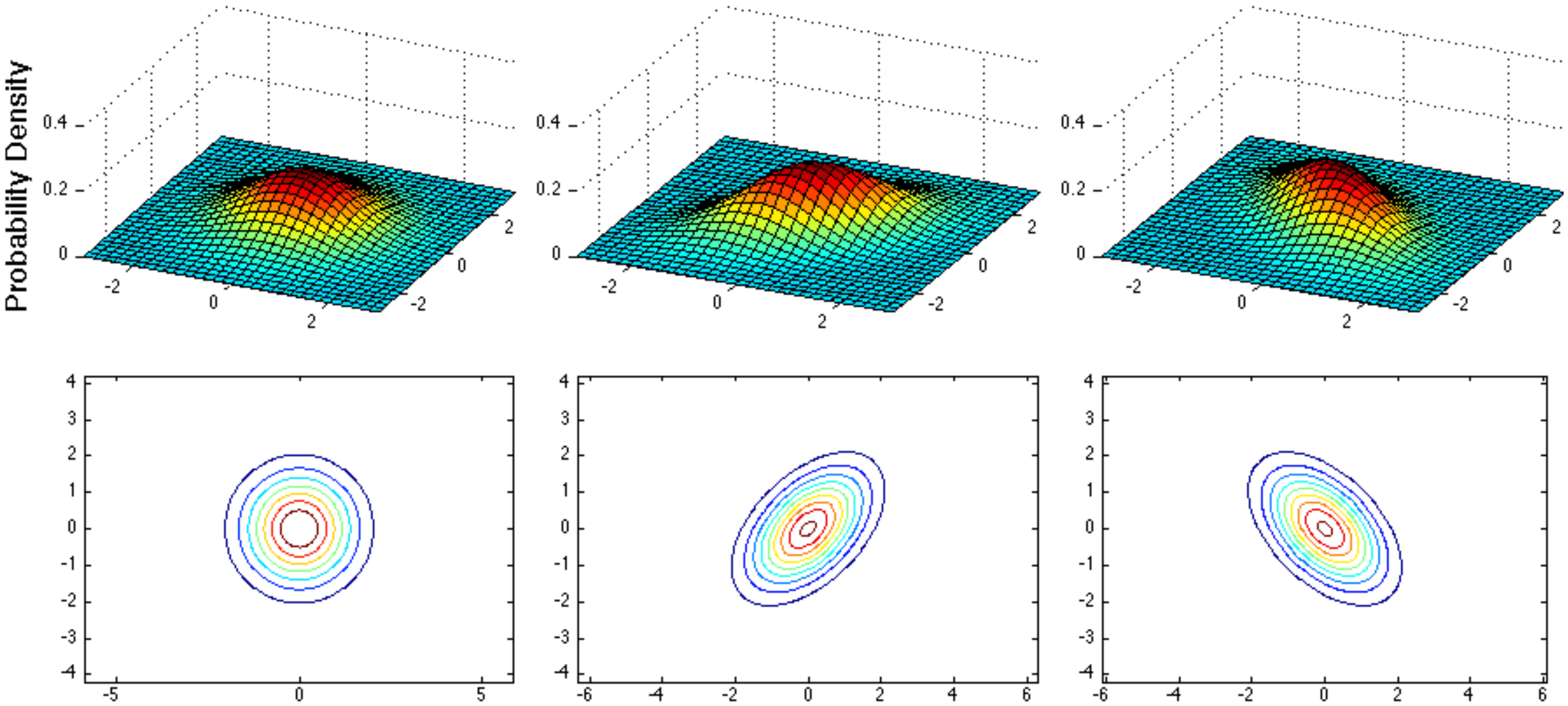
$$\Sigma = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} 1 & 0.5 \\ 0.5 & 1 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} 1 & 0.8 \\ 0.8 & 1 \end{pmatrix}$$



# Bivariate Normal

$Cov(x_1, x_2) = 0$ $\quad$ $Cov(x_1, x_2) > 0$ $\quad$ $Cov(x_1, x_2) < 0$



# Gaussian Bayes Classifier

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

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

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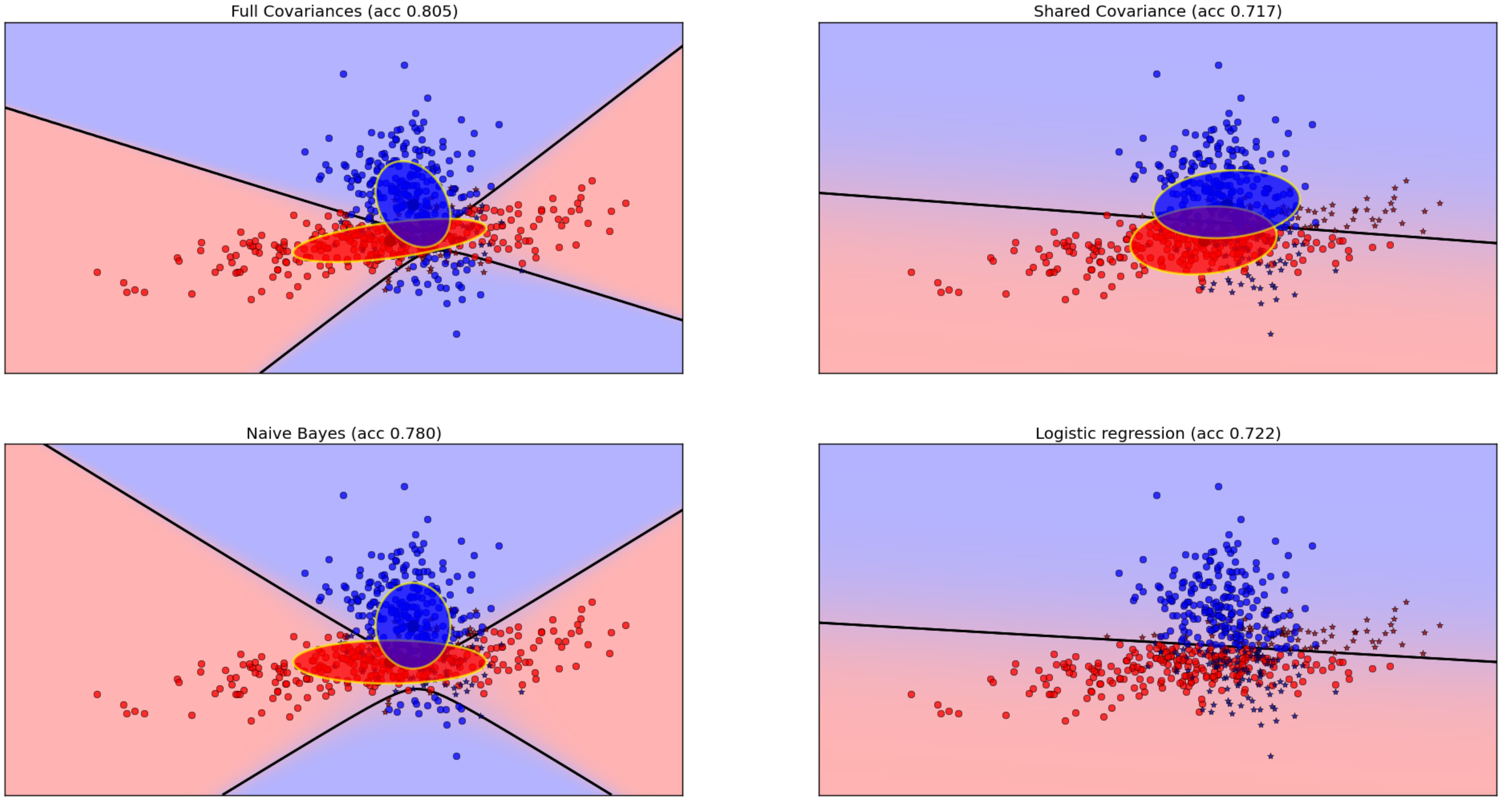
- $\Sigma_k$ has $\mathcal{O}(d^2)$ parameters - could be hard to estimate

# Example



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

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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

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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

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

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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 $\theta$, 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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- **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.
  - $n_h$: number of heads
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$$L_{\mathcal{D}}(\theta) = p(\mathcal{D} \mid \theta) = \theta^{n_h} (1-\theta)^{n_t}$$

- As usual, it is easier to maximize the log-likelihood function:

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

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- First order condition (equating the derivative to zero):

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

# Coin Flipping: MLE

- Data $\mathcal{D} = (H, H, T, T, T, T, T, H, \ldots, T)$, assumed i.i.d. flips.
  - $n_h$: number of heads
  - $n_t$: number of tails
- **Likelihood function** for data $\mathcal{D}$:

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

# Bayesian Statistics: Introduction

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  1. A parametric family of densities
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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 $\mathcal{D}$:

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

# The Posterior Distribution

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

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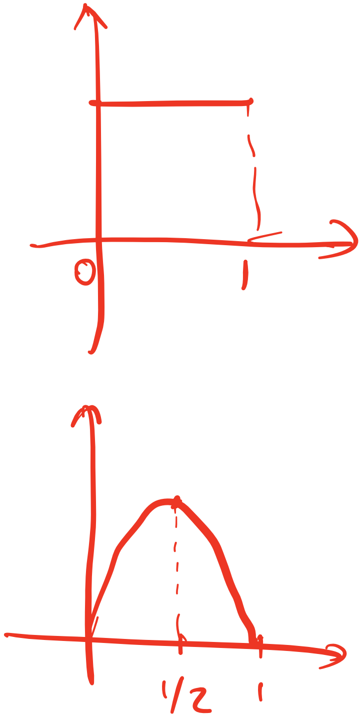

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  for $\theta \in \Theta = (0,1)$.
- We need a prior distribution $p(\theta)$ on $\Theta = (0,1)$.
- One convenient choice would be a distribution from the Beta family

# 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 http://commons.wikimedia.org/wiki/File:Beta_distribution_pdf.svg.

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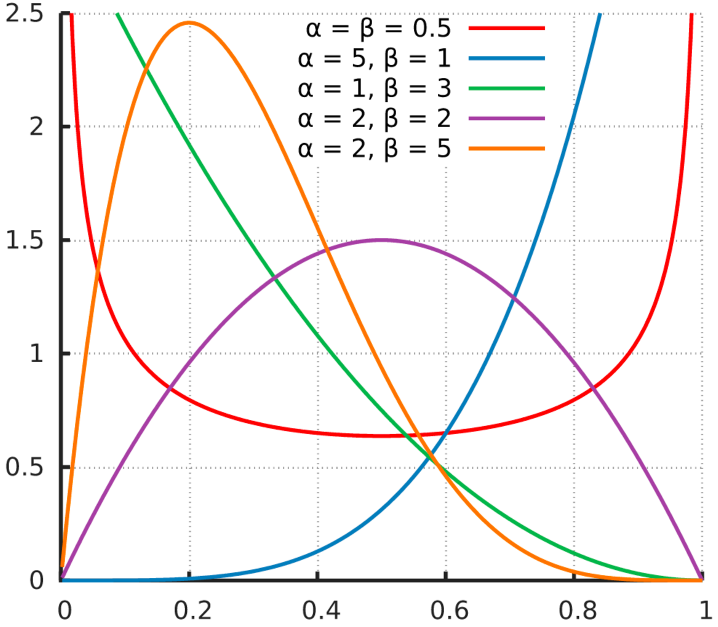


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- **Mode of Beta distribution:**

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

for $h, t > 1$.

# Coin Flipping: Posterior

- **Prior:**

$$\theta \sim \mathrm{Beta}(h, t)$$
$$p(\theta) \propto \theta^{h-1}(1-\theta)^{t-1}$$

D = (H, T, T, ...)

$n^h$ Heads
$n^t$ tails

# Coin Flipping: Posterior

- **Prior:**

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- **Likelihood function**

$$L(\theta) = p(\mathcal{D} \mid \theta) = \theta^{n_h}(1-\theta)^{n_t}$$

MLE: $\arg\max \theta^{n_h}(1-\theta)^{n_t}$

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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.

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

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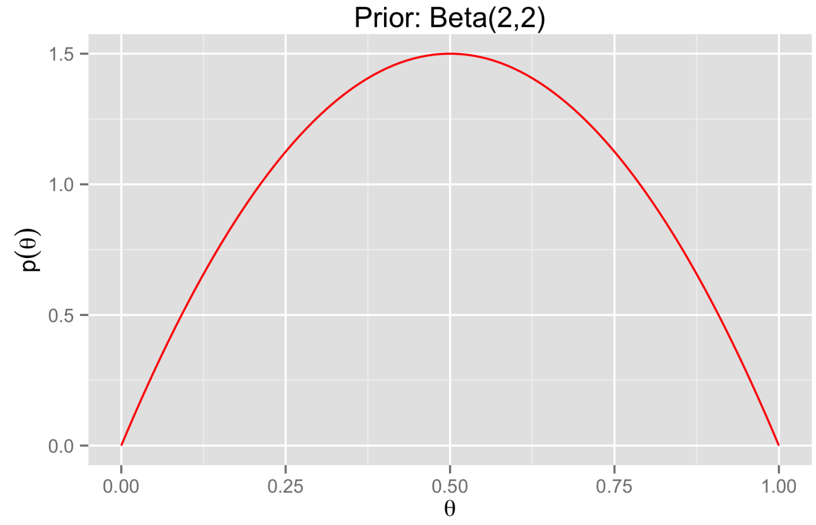

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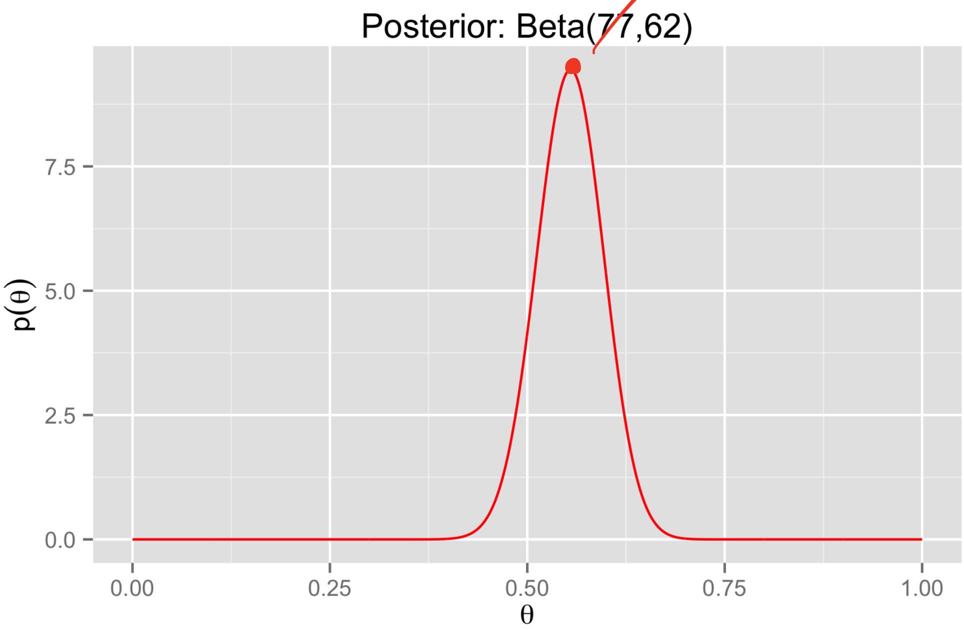
- **Posterior distribution:** $\theta \mid \mathcal{D} \sim \textbf{Beta}(77, 62)$:

mode / MAP $= \frac{77}{77+62}$



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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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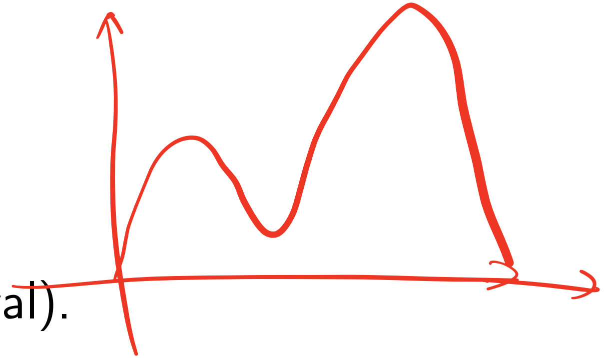

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- Select a point estimate using **Bayesian decision theory**:
  - Choose a loss function.
  - Find action **minimizing expected risk w.r.t. posterior**

0/1 loss → mode

loss: absolute loss → median

$|x - \hat{x}|$

square loss → mean