Estimating Probabilities from Data

MLE and MAP

Maria-Florina Balcan

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What does this has to do with function approximation?

Instead of learning $\mathrm{F}: \mathrm{X} \rightarrow \mathrm{Y}$, learn P(Y|X).

Can design algorithms that learn functions with uncertain outcomes (e.g., predicting tomorrow's stock price) **and that incorporate prior knowledge to guide learning** (e.g., a bias that tomorrow's stock price is likely to be similar to today's price).

The Joint Distribution

Example: Boolean variables A,B,C

A	B	C	Prob
0	0	0	0.30
0	0	1	0.05
0	1	0	0.10
0	1	1	0.05
1	0	0	0.05
1	0	1	0.10
1	1	0	0.25
1	1	1	0.10

- The key to building probabilistic models is to define a set of random variables, and to consider the joint probability distribution over them.

The Joint Distribution

Recipe for making a joint distribution of M variables:

1. Make a truth table listing all combinations of values (M Boolean variables $\rightarrow 2^M$ rows).

2. For each combination of values, say how probable it is.

3. By the axioms of probability, these probabilities must sum to 1.

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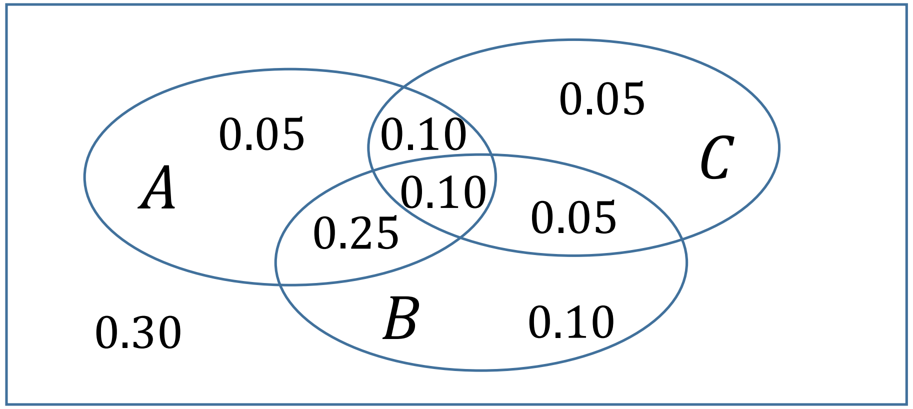

Using the Joint Distribution

Once we have the Joint Distribution, can ask for the probability of **any** logical expression involving these variables

College Degree	Hours worked	Wealth	prob
No	40.5-	Medium	0.253122
No	40.5-	Rich	0.0245895
No	40.5+	Medium	0.0421768
No	40.5+	Rich	0.0116293
Yes	40.5-	Medium	0.331313
Yes	40.5-	Rich	0.0971295
Yes	40.5+	Medium	0.134106
Yes	40.5+	Rich	0.105933

$$\mathrm{P(E)} = \sum_{\text{rows matching E}} \mathrm{P(row)}$$

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$$\mathrm{P}(\text{College} \,\&\, \text{Medium}) = 0.4654$$

$$\mathrm{P}(E) = \sum_{\text{rows matching } E} \mathrm{P}(\text{row})$$

Using the Joint Distribution

Once we have the Joint Distribution, can ask for the probability of **any** logical expression involving these variables

$$\mathrm{P(Medium)} = 0.7604$$

College Degree	Hours worked	Wealth	prob
No	40.5-	Medium	0.253122
No	40.5-	Rich	0.0245895
No	40.5+	Medium	0.0421768
No	40.5+	Rich	0.0116293
Yes	40.5-	Medium	0.331313
Yes	40.5-	Rich	0.0971295
Yes	40.5+	Medium	0.134106
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$$\mathrm{P(E)} = \sum_{\text{rows matching E}} \mathrm{P(row)}$$

Inference with the Joint Distribution

Once we have the Joint Distribution, can ask for the probability of **any** logical expression involving these variables

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$$\mathrm{P(College\ |Medium)} = \frac{0.4654}{0.7604} = 0.612$$

$$\mathrm{P(E_1 \mid E_2)} = \frac{\mathrm{P(E_1 \wedge E_2)}}{\mathrm{P(E_2)}} = \frac{\sum_{\text{rows matching } \mathrm{E_1} \text{ and } \mathrm{E_2}} \mathrm{P(row)}}{\sum_{\text{rows matching } \mathrm{E_2}} \mathrm{P(row)}}$$

Learning and the Joint Distribution

Suppose we want to learn the function f: $\langle C, H \rangle \rightarrow W$

Equivalently, $P(W \mid C, H)$

One solution: learn joint distribution from data, calculate $P(W \mid C, H)$

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No	40.5-	Medium	0.253122
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$$\text{e.g., } P(W = \text{rich} | C = \text{no}, H = 40.5\,-) = \frac{0.0245895}{0.0245895 + 0.253122}$$

Idea: learn classifiers by learning $P(Y \mid X)$

Consider $Y = \text{Wealth}$

$X = \langle \text{CollegeDegree}, \text{HoursWorked} \rangle$

College Degree	Hours worked	Wealth	prob
No	40.5-	Medium	0.253122
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College Degree	Hours worked	P(rich|C,HW)	P(medium|C,HW)
No	< 40.5	.09	.91
No	> 40.5	.21	.79
Yes	< 40.5	.23	.77
Yes	> 40.5	.38	.62

Estimating Probabilities from Data

MLE and MAP

Estimating the Bias of a Coin

Problem: Assume we can flip a coin with bias θ several times. Estimate the probability that it turns out heads when we flip it?

X=1 X=0

Each flip yields a Boolean value for X, X~ Bernoulli(θ)

Bernoulli Random Variable $P(X = 1) = \theta$; $P(X = 0) = 1 - \theta$

We flip it repeatedly, observing the outcome:

- It turns Heads (i.e. X=1) α_H times
- It turns Tails (i.e. X=0) α_T times

How can we estimate the probability of heads $\theta = P(X = 1)$?

Estimating the Bias of a Coin

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How can we estimate the probability of heads $\theta = P(X = 1)$?

Two Cases:

- Case 1: 100 flips. E.g., 51 Heads (X=1) and 49 tails (X=0)
- Case 2: 3 flips. E.g., 2 Heads (X=1) and 1 tails (X=0)

Principles of Estimating Probabilities

Principle 1: Maximum Likelihood Estimation E.g., 51 Heads (X=1) and 49 tails (X=0)

Choose parameter $\hat{\theta}$ that maximizes likelihood of observed data $P(\mathrm{data}|\hat{\theta})$

$$\hat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_T + \alpha_H}$$

Principle 2: Maximum Aposteriori Probability E.g., 2 Heads (X=1) and 1 tails (X=0)

Choose parameter $\hat{\theta}$ that maximizes likelihood the posterior prob $P(\hat{\theta}|\mathrm{data})$

$$\hat{\theta}_{MAP} = \frac{\alpha_H + \#\mathrm{halucinated\_Hs}}{(\alpha_T + \#\mathrm{halucinated\_Ts}) + (\alpha_H + \#\mathrm{halucinated\_Hs})}$$

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Maximum Likelihood Estimation for Bernoulli Variables

$P(X = 1) = \theta \qquad P(X = 0) = 1 - \theta$

Data D: {1, 0, 0, 1, … }

Flips produce data D with α_H heads (X=1) and α_T tails (X=0)

Flips are i.i.d.:

- independent events
- identically distributed according to the Bernoulli distribution

MLE estimate: choose the value of θ that makes D most probable.

Intuition: we are more likely to observe data D if we are in a world where the appearance of this data is highly probable. Therefore, we should estimate θ by assigning it whatever value maximizes the probability of having observed D.

Maximum Likelihood Estimation for Bernoulli Variables

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Data D: {1, 0, 0, 1, … }

Flips produce data D with α_H heads (X=1) and α_T tails (X=0)

Flips are i.i.d.:

- independent events
- identically distributed according to the Bernoulli distribution

Therefore $P(D|\theta) = \theta(1-\theta)(1-\theta)\theta \ldots = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$

$$\hat{\theta}_{MLE} = \mathrm{argmax}_\theta\, P(D|\theta)$$

$$\hat{\theta}_{MLE} = \mathrm{argmax}_\theta\, \ln P(D|\theta)$$

Maximum Likelihood Estimation for Bernoulli Variables

$P(X=1)=\theta \qquad P(X=0)=1-\theta$

Data D: {1, 0, 0, 1, … } $\qquad \alpha_H$ heads and α_T tails

$$\hat{\theta}_{MLE} = \arg\max_{\theta} \ln P(D|\theta)$$
$$= \arg\max_{\theta} \ln[\theta^{\alpha_H}(1-\theta)^{\alpha_T}]$$

Set derivative to 0. $\qquad \dfrac{d}{d\,\theta} \ln P(D|\theta) = 0$

$$\frac{d}{d\,\theta} \ln P(D|\theta) = \frac{d}{d\,\theta}[\alpha_H \ln\theta + \alpha_T \ln(1-\theta)] = \frac{\alpha_H}{\theta} - \frac{\alpha_T}{1-\theta}$$

$$\frac{d}{d\,\theta} \ln\theta = \frac{1}{\theta}$$

Therefore $\qquad \hat{\theta}_{MLE} = \dfrac{\alpha_H}{\alpha_T + \alpha_H}$

Summary: MLE for Bernoulli Variables

Problem: Assume we can flip a coin with bias θ several times. Estimate the probability that it turns out heads when we flip it?

Each flip yields a Boolean value for X, X~ Bernoulli(θ)

Bernoulli Random Variable $P(X = 1) = \theta$; $P(X = 0) = 1 - \theta$

$$P(X) = \theta^{X}(1-\theta)^{1-X}$$

Data D of independently, identically distributed (i.i.d) flips produces α_H heads (X=1) and α_T tails (X=0)

Therefore $P(D|\theta) = (\alpha_1, \alpha_0|\theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$

$$\hat{\theta}_{MLE} = \operatorname{argmax}_{\theta} P(D|\theta) = \frac{\alpha_H}{\alpha_T + \alpha_H}$$

High Probability Bound, Sample Complexity

Problem: Assume we can flip a coin with bias θ several times. Estimate the probability that it turns out heads when we flip it?

X=1 X=0

$P(X = 1) = \theta$

Data D: {1, 0, 0, 1, … }

α_H heads and α_T tails; $n = \alpha_0 + \alpha_1$

$$\hat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_T + \alpha_H}$$

Hoeffding Inequality:

For any $\epsilon > 0$, $P(|\hat{\theta}_{MLE} - \theta| \geq \epsilon) \leq 2\, e^{-2n\epsilon^2}$

High Probability Bound: Want to know the coin parameter θ within $\epsilon > 0$ with probability at least $1 - \delta$. How many flips?

Set $P(|\hat{\theta}_{MLE} - \theta| \geq \epsilon) \leq 2\, e^{-2n\epsilon^2} \leq \delta$ Solve for n: $n \geq \frac{\ln\frac{2}{\delta}}{2\,\epsilon^2}$

Principles of Estimating Probabilities

Principle 1: Maximum Likelihood Estimation

Choose parameter $\hat{\theta}$ that maximizes likelihood of observed data $P(\text{data}|\hat{\theta})$

$$\hat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_T + \alpha_H}$$

Principle 2: Maximum Aposteriori Probability

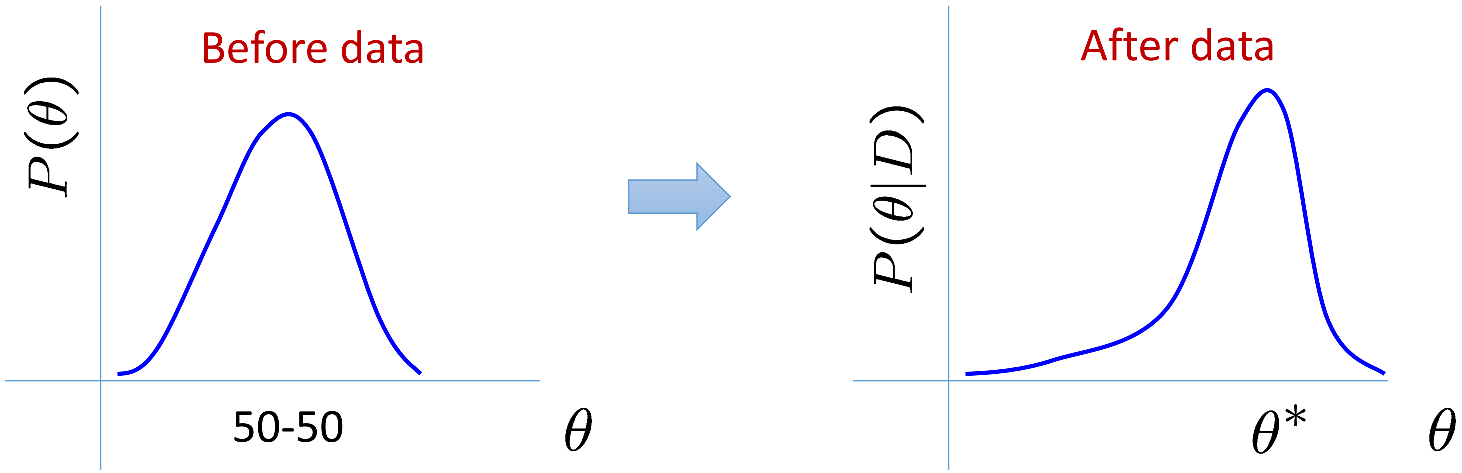
Choose parameter $\hat{\theta}$ that maximizes likelihood the posterior prob $P(\hat{\theta}|\text{data})$

$$\hat{\theta}_{MAP} = \frac{\alpha_H + \#\text{halucinated\_Hs}}{(\alpha_T + \#\text{halucinated\_Ts}) + (\alpha_H + \#\text{halucinated\_Hs})}$$

What if we have prior knowledge?

Prior Knowledge: E.g., I know that the coin is “close” to 50-50.

MAP estimate: we should choose the value of Theta that is most probable, given the observed data D and our prior assumptions summarized by $\mathbf{P(\theta)}$.



Bayesian Learning

Use Bayes Rule:

$$P(\theta|D) = \frac{P(D|\theta)P(\theta)}{P(D)}$$

Equivalently:

$$P(\theta|D) \propto P(D|\theta) \cdot P(\theta)$$

posterior likelihood prior

Bayes, Thomas (1763) An essay towards solving a problem in the doctrine of chances. *Philosophical Transactions of the Royal Society of London*, 53:370-418

MAP estimate: choose parameter $\hat{\theta}$ that maximizes the posterior prob $P(\hat{\theta}|\text{data})$, i.e. it chooses the value that is most probable given observed data and prior belief

Principles of Estimating Probabilities

Principle 1: Maximum Likelihood Estimation (MLE)

Choose parameter $\hat{\theta}$ that maximizes likelihood of observed data $P(D|\hat{\theta})$

$$\hat{\theta}_{MLE} = \mathrm{argmax}_{\theta} P(D|\theta)$$

Principle 2: Maximum Aposteriori Probability (MAP)

Choose parameter $\hat{\theta}$ that maximizes likelihood the posterior prob $P(\hat{\theta}|D)$, i.e. it chooses the value that is most probable given observed data and prior belief

$$\hat{\theta}_{MAP} = \mathrm{argmax}_{\theta} P(\theta|D) \quad = \mathrm{argmax}_{\theta}\, P(D|\theta)P(\theta)$$

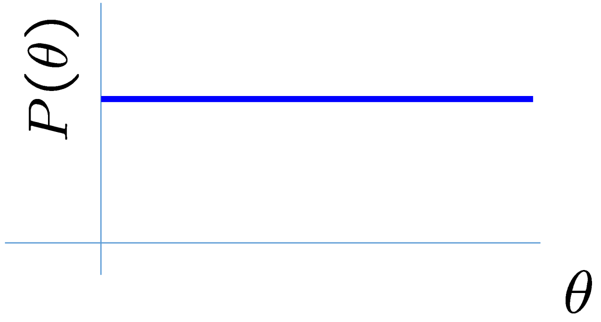
As $n \to \infty$, prior is forgotten

For small sample sizes, prior is important

Which Prior Distribution?

- Prior represents the experts knowledge.
- Simple posterior form (engineer's approach).

Uninformative Prior

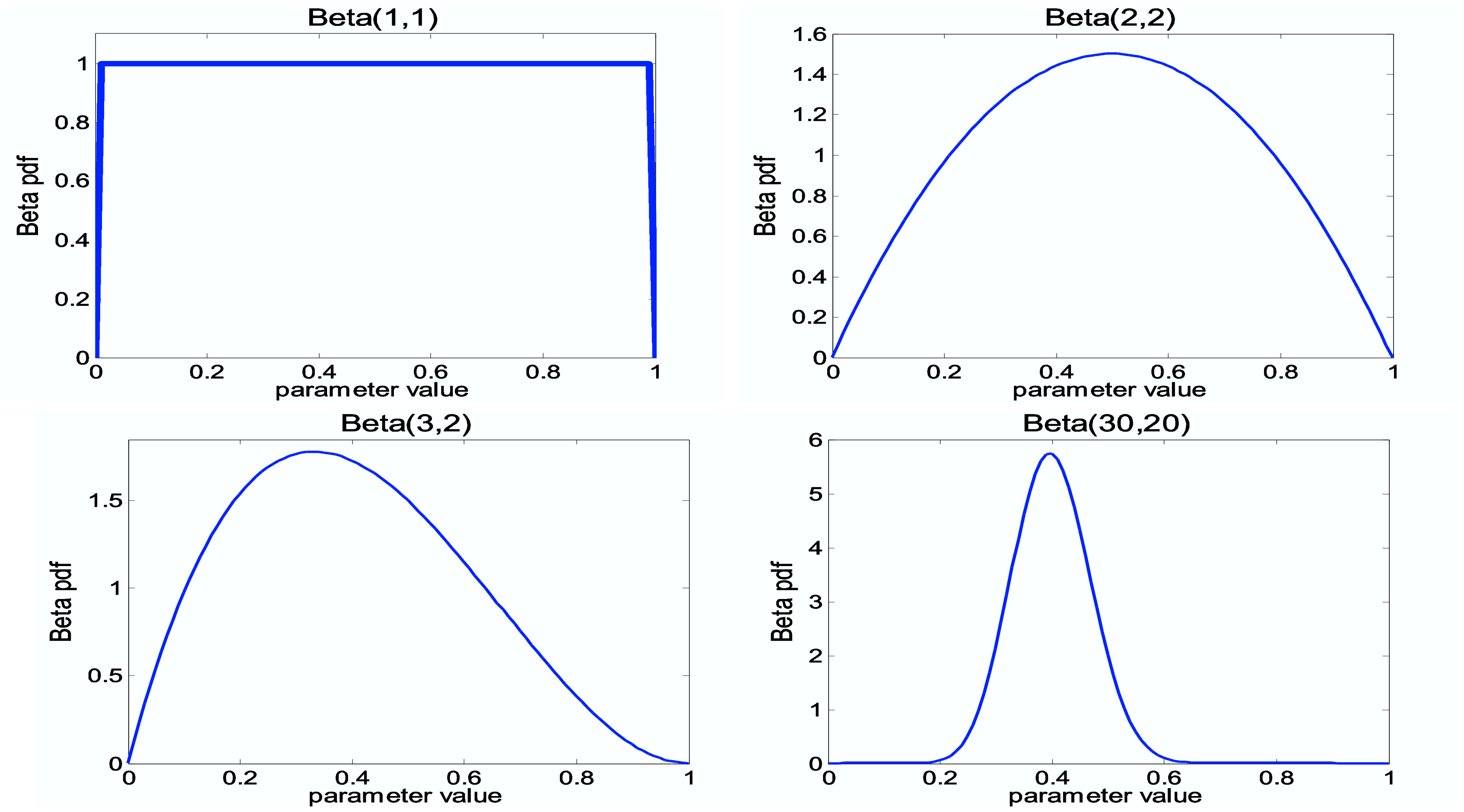


Conjugate Prior

- Closed-form expression of posterior.
- $P(\theta)$ and $P(\theta|D)$ have **same** form.

Beta Prior Distribution

Assume $\theta \sim \mathrm{Beta}(\beta_H, \beta_T)$ I.e., $P(\theta) = \frac{\theta^{\beta_H - 1}(1-\theta)^{\beta_T - 1}}{B(\beta_H, \beta_T)}$



More concentrated as values of β_H, β_T increase

MAP Estimate for Bernoulli Variables with Beta Prior Distribution

Assume $\theta \sim \mathrm{Beta}(\beta_H, \beta_T)$ I.e., $P(\theta) = \frac{\theta^{\beta_H - 1}(1-\theta)^{\beta_T - 1}}{B(\beta_H, \beta_T)}$

Likelihood function $P(D|\theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$

Posterior: $P(\theta|D) \propto P(D|\theta)P(\theta)$

$$P(\theta|D) \propto \theta^{\alpha_H + \beta_H - 1}(1-\theta)^{\alpha_T + \beta_T - 1}$$

Interpretation: like MLE, but *hallucinating* $\beta_H - 1$ additional heads & $\beta_T - 1$ additional tails

$$\hat{\theta}_{MAP} = \frac{\alpha_H + \beta_H - 1}{(\alpha_T + \beta_T - 1) + (\alpha_H + \beta_H - 1)}$$

Note: as we get more sample effect of prior washed out.

Conjugate Priors

Likelihood function: $P(D|\theta)$

Prior: $P(\theta)$

Posterior: $P(\theta|D) \propto P(D|\theta)P(\theta)$

Conjugate Prior: $P(\theta)$ is the conjugate prior for the likelihood function $P(D|\theta)$ if the forms of $P(\theta)$ and $P(\theta|D)$ are the same.

MAP Estimate for Bernoulli Variables with Beta Prior Distribution

Likelihood function $P(D|\theta) = \theta^{\alpha_H}(1-\theta)^{\alpha_T}$ (Binomial)

If prior is beta distribution, $\theta \sim \text{Beta}(\beta_H, \beta_T)$ I.e., $P(\theta) = \frac{\theta^{\beta_H - 1}(1-\theta)^{\beta_T - 1}}{B(\beta_H, \beta_T)}$

then posterior : $P(\theta|D) \propto P(D|\theta)P(\theta) \propto \theta^{\alpha_H + \beta_H - 1}(1-\theta)^{\alpha_T + \beta_T - 1} \sim \text{Beta}(\alpha_H + \beta_H, \alpha_T + \beta_T)$

Therefore

$$\hat{\theta}_{MAP} = \frac{\alpha_H + \beta_H}{(\alpha_T + \beta_T - 1) + (\alpha_H + \beta_H - 1)}$$

Mode of Beta distribution

MAP Estimate for Dice Rolling with Dirichlet Prior Distribution

Dice Roll Problem: 6 outcomes instead of 2.

Likelihood function is $\sim \mathrm{Multinomial}(\theta_1, \ldots, \theta_k)$ $P(D|\theta) = \theta_1^{\alpha_1}\theta_2^{\alpha_2} \cdots \theta_k^{\alpha_k}$

If prior is Dirichlet distribution, $\theta \sim \mathrm{Dirichlet}(\beta_1, \beta_2, \ldots, \beta_k)$ $P(\theta) = \frac{\prod_{i=1}^{k} \theta_i^{\beta_i - 1}}{B(\beta_1, \beta_2, \ldots, \beta_k)}$

then posterior:

$$P(\theta|D) \propto P(D|\theta)P(\theta) \propto \mathrm{Dirichlet}(\alpha_1 + \beta_1, \ldots, \alpha_k + \beta_k)$$

For Multinomial, conjugate prior is Dirichlet.

Principles of Estimating Probabilities

Principle 1: Maximum Likelihood Estimation (MLE)

Choose parameter $\hat{\theta}$ that maximizes likelihood of observed data $P(D|\hat{\theta})$

$$\hat{\theta}_{MLE} = \text{argmax}_{\theta} P(D|\theta)$$

Principle 2: Maximum Aposteriori Probability (MAP)

Choose parameter $\hat{\theta}$ that maximizes likelihood the posterior prob $P(\hat{\theta}|D)$, i.e. it chooses the value that is most probable given observed data and prior belief

$$\hat{\theta}_{MAP} = \text{argmax}_{\theta} P(\theta|D) \quad = \text{argmax}_{\theta}\, P(D|\theta)P(\theta)$$

As $n \to \infty$, prior is forgotten

For small sample sizes, prior is important

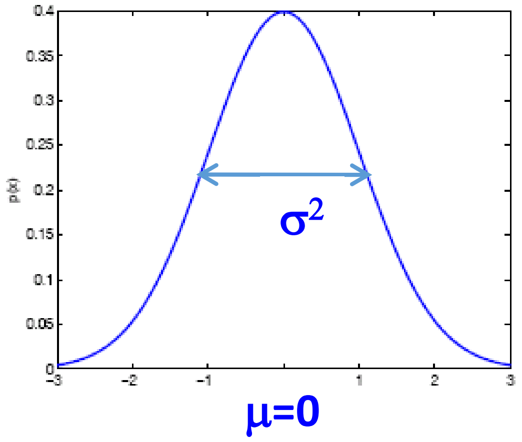
Bayesians vs. Frequentists

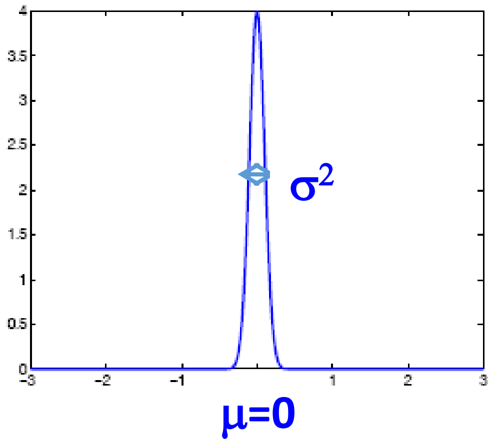
What About Continuous Random Variables?

Gaussian Random Variable

$X \sim N(\mu, \sigma)$, then

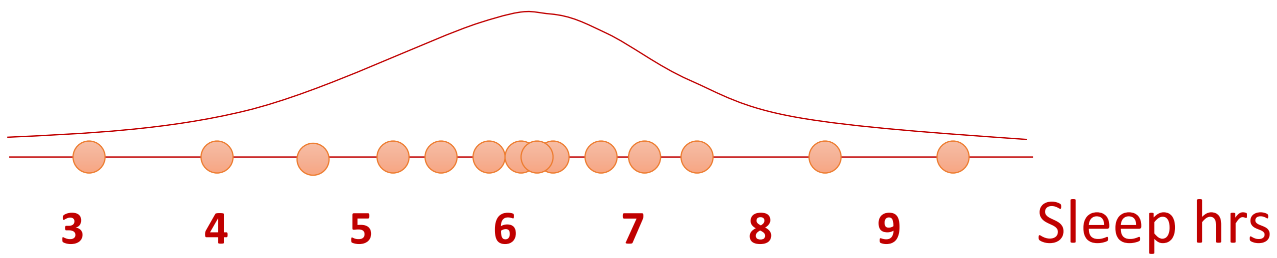
$$p(x|\mu,\sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{\sigma^2}}$$





What About Continuous Random Variables?

Observed data D:



Parameters: μ- mean, σ^2 variance

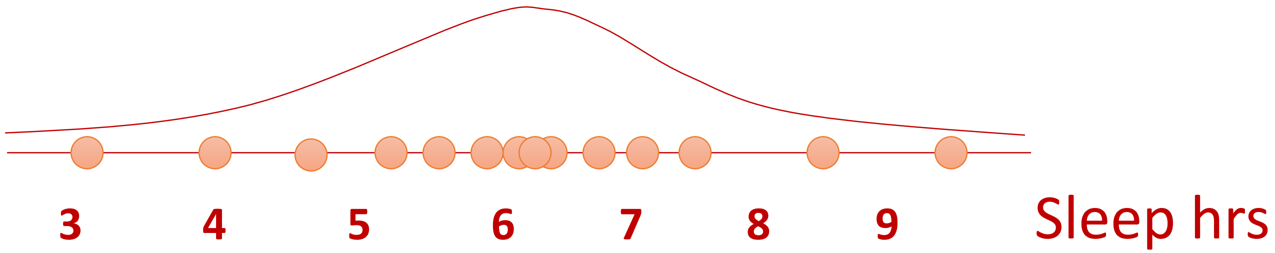
Sleep hours are i.i.d.:

- independent events
- identically distributed according to Gaussian distribution

Goal: estimate μ, σ

MLE for Mean of Gaussian

Observed data D:



Probability of i.i.d. samples $D = \{x_1, \ldots, x_N\}$ $\quad P(D|\mu,\sigma) = \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^{N} \prod_{\{i=1\ldots N\}} e^{-\frac{(x_i-\mu)^2}{\sigma^2}}$

Log-likelihood of data $\quad \ln P(D|\mu,\sigma) = \ln\left(\frac{1}{\sigma\sqrt{2\pi}}\right)^{N} \prod_{\{i=1\ldots N\}} e^{-\frac{(x_i-\mu)^2}{\sigma^2}}$

$$\ln P(D|\mu,\sigma) = -N\ln\left(\sigma\sqrt{2\pi}\right) - \sum_{\{i=1,\ldots,N\}} \frac{(x_i-\mu)^2}{\sigma^2}$$

MLE for Mean of Gaussian

Probability of i.i.d. samples $D = \{x_1, \ldots, x_N\}$ $\quad P(D|\mu,\sigma) = \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^{N} \prod_{\{i=1,\ldots,N\}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$

$$\ln P(D|\mu,\sigma) = -N\ln\left(\sigma\sqrt{2\pi}\right) - \sum_{\{i=1,\ldots,N\}} \frac{(x_i-\mu)^2}{2\sigma^2}$$

$$\frac{d}{d\,\mu}\ln P(D|\mu,\sigma) = -\sum_{\{i=1,\ldots,N\}} \frac{d}{d\,\mu}\frac{(x_i-\mu)^2}{2\sigma^2} = 2\sum_{\{i=1,\ldots,N\}} \frac{(x_i-\mu)}{2\sigma^2}$$

Set $\frac{d}{d\,\mu}\ln P(D|\mu,\sigma) = 0$ $\quad$ Therefore $\sum_{\{i=1,\ldots,N\}}(x_i-\mu) = 0$ $\quad \hat{\mu}_{MLE} = \frac{\sum_i x_i}{N}$

MLE for Variance of Gaussian

Probability of i.i.d. samples $D = \{x_1, \ldots, x_N\}$ $\quad P(D|\mu,\sigma) = \left(\frac{1}{\sigma\sqrt{2\pi}}\right)^N \prod_{\{i=1\ldots N\}} e^{-\frac{(x_i-\mu)^2}{2\sigma^2}}$

$$\ln P(D|\mu,\sigma) = -N\ln\left(\sigma\sqrt{2\pi}\right) - \sum_{\{i=1,\ldots,N\}} \frac{(x_i-\mu)^2}{2\sigma^2}$$

$$\frac{d}{d\,\sigma}\ln P(D|\mu,\sigma) = -N\frac{d}{d\,\sigma}\ln\left(\sigma\sqrt{2\pi}\right) - \sum_{\{i=1,\ldots,N\}} \frac{d}{d\,\sigma}\frac{(x_i-\mu)^2}{2\sigma^2} = -\frac{N}{\sigma} + 2\sum_{\{i=1,\ldots,N\}} \frac{(x_i-\mu)^2}{2\sigma^3}$$

Set $\frac{d}{d\,\mu}\ln P(D|\mu,\sigma) = 0$ $\qquad$ Therefore $\quad \hat{\sigma}_{MLE} = \frac{\sum_i (x_i-\hat{\mu})^2}{N}$

Learning Gaussian Parameters

MLE:

$$\hat{\sigma}_{MLE} = \frac{\sum_i (x_i - \mu)^2}{N}$$

$$\hat{\mu}_{MLE} = \frac{\sum_i x_i}{N}$$

Bayesian learning/estimation is also possible.

Conjugate priors:

Mean: Gaussian prior

Variance: Wishart distribution

What You Should Know

- MLE, MAP
- Coins, Dice, Gaussian