Generative Approach to Classification: Naïve Bayes

Estimating Probabilities from Data: MLE and MAP

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Admin

HWK 1: due today.

Recitation: Tue, 5:00 – 6:30 (see Piazza post)

Estimating Probabilities from Data: MLE and MAP

Useful Readings:

Mitchell, http://www.cs.cmu.edu/%7Etom/mlbook/Joint MLE MAP.pdf

Murphy, chapters 3,4

The Joint Distribution

Example: Boolean variables A,B,C

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

A	В	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

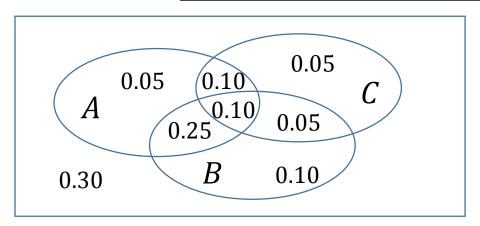
The Joint Distribution

Example: Boolean variables A,B,C

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.

A	В	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



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

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

Using the Joint Distribution

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

P(College & Medium) = 0.4654

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

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

Using the Joint Distribution

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

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
C	Yes	40.5-	Medium	0.331313
	Yes	40.5-	Rich	0.0971295
${\sf C}$	Yes	40.5+	Medium	0.134106
	Yes	40.5+	Rich	0.105933

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

Inference with 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
2_	Yes	40.5-	Rich	0.0971295
	Yes	40.5+	Medium	0.134106
	Yes	40.5+	Rich	0.105933

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

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

Learning and the Joint Distribution

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

Equivalently, P(W | C, H)

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

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

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

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

Consider Y = Wealth

 $X = \langle CollegeDegree, HoursWorked \rangle$

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

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

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

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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- It turns Tails (i.e. X=0) α_T times

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 $P(\text{data}|\hat{\theta})$

$$\hat{\theta}_{\text{MLE}} = \frac{\alpha_{\text{H}}}{\alpha_{\text{T}} + \alpha_{\text{H}}}$$

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 $P(\hat{\theta}|data)$

$$\hat{\theta}_{MAP} = \frac{\alpha_{H} + \#halucinated_Hs}{(\alpha_{T} + \#halucinated_Ts) + (\alpha_{H} + \#halucinated_Hs)}$$

Principles of Estimating Probabilities



Principle 1: Maximum Likelihood Estimation

E.g., 51 Heads (X=1) and 49 tails (X=0)

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Maximum Likelihood Estimation for Bernoulli Variables

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

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

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

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

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

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

$$\hat{\theta}_{MLE} = argmax_{\theta} \ ln \ P(D|\theta)$$

Maximum Likelihood Estimation for Bernoulli Variables

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

Data D: $\{1, 0, 0, 1, ...\}$ α_H heads and α_T tails

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

$$= \operatorname{argmax}_{\theta} \ln [\theta^{\alpha_{\text{H}}} (1 - \theta)^{\alpha_{\text{T}}}]$$

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

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



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

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

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?



X=1X=0

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

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

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

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

$$\hat{\theta}_{\text{MLE}} = \operatorname{argmax}_{\theta} P(D|\theta) = \frac{\alpha_{\text{H}}}{\alpha_{\text{T}} + \alpha_{\text{H}}}$$

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?



$$P(X = 1) = \theta$$

X=1

Data D: {1, 0, 0, 1, ... }
$$\alpha_H \text{ heads and } \alpha_T \text{ tails; } n = \alpha_0 + \alpha_1$$

$$\hat{\theta}_{\text{MLE}} = \frac{\alpha_{\text{H}}}{\alpha_{\text{T}} + \alpha_{\text{H}}}$$

Hoeffding Inequality:

For any
$$\epsilon > 0$$
, $P(|\widehat{\theta}_{MLE} - \theta| \ge \epsilon) \le 2 e^{-2n\epsilon^2}$

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

Set
$$P(|\widehat{\theta}_{MLE} - \theta| \ge \epsilon) \le 2 e^{-2n\epsilon^2} \le \delta$$
 Solve for n: $n \ge \frac{\ln^2_{\delta}}{2 \epsilon^2}$

Principles of Estimating Probabilities



Principle 1: Maximum Likelihood Estimation

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

$$\hat{\theta}_{\text{MLE}} = \frac{\alpha_{\text{H}}}{\alpha_{\text{T}} + \alpha_{\text{H}}}$$

Principle 2: Maximum Aposteriori Probability

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

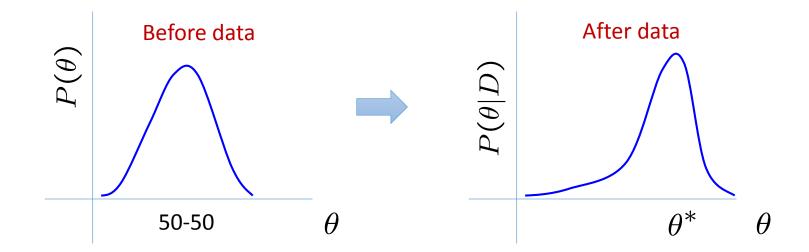
$$\hat{\theta}_{MAP} = \frac{\alpha_{H} + \#halucinated_Hs}{(\alpha_{T} + \#halucinated_Ts) + (\alpha_{H} + \#halucinated_Hs)}$$

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 $P(\theta)$.



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 $P(\hat{\theta}|data)$, 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 $P(D|\hat{\theta})$

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

Principle 2: Maximum Aposteriori Probability (MAP)

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

$$\hat{\theta}_{MAP} = \operatorname{argmax}_{\theta} P(\theta|D) = \operatorname{argmax}_{\theta} P(D|\theta) P(\theta)$$

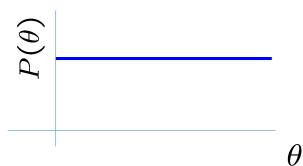
As $n \to \infty$, prior is forgotten

For small sample sizes, prior is important

Which Prior Distribution?

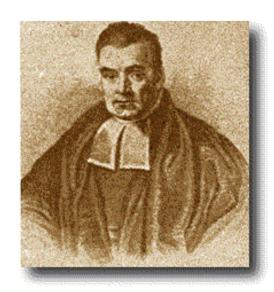
- Prior represents the experts knowledge.
- Simple posterior form (engineer's approach).

Uninformative Prior



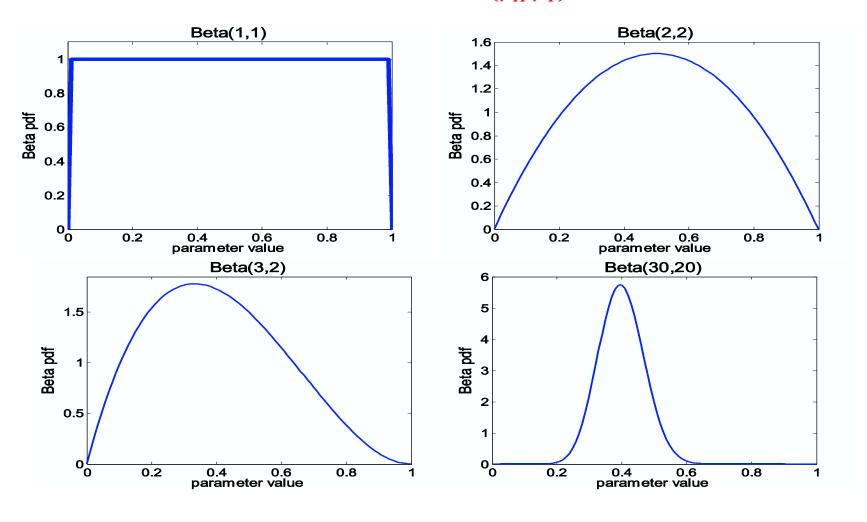
Conjugate Prior

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



Beta Prior Distribution

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



More concentrated as values of β_H , β_T increase

MAP Estimate for Bernoulli Variables with Beta Prior Distribution



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

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 eta_H-1 additional heads & eta_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 : $P(\theta|D) \propto P(D|\theta)P(\theta) \propto \theta^{\alpha_H + \beta_H - 1}(1-\theta)^{\alpha_T + \beta_T - 1} \sim Beta(\alpha_H + \beta_H, \alpha_T + \beta_T)$

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
$$\sim$$
 Multinomial $(\theta_1, ..., \theta_k)$ $P(D|\theta) = \theta_1^{\alpha_1} \theta_2^{\alpha_2} \cdots \theta_k^{\alpha_k}$
If prior is Dirichlet distribution, $\theta \sim \text{Dirichlet}(\beta_1, \beta_2, ..., \beta_k)$
$$P(\theta) = \frac{\prod_{i=1}^k \theta_i^{\beta_i - 1}}{B(\beta_1, \beta_2, ..., \beta_k)}$$

then posterior:

$$P(\theta|D) \propto P(D|\theta)P(\theta) \propto Dirichlet(\alpha_1 + \beta_1, ..., \alpha_k + \beta_k)$$

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 $P(D|\hat{\theta})$

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

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

$$\hat{\theta}_{MAP} = \operatorname{argmax}_{\theta} P(\theta|D) = \operatorname{argmax}_{\theta} P(D|\theta) P(\theta)$$

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

For small sample sizes, prior is important

Bayesians vs. Frequentists

You are no good when sample is small

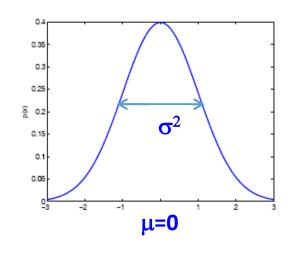


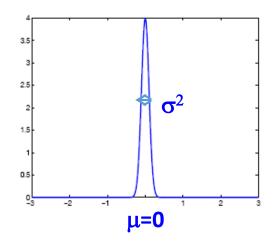
You give a different answer for different priors

What About Continuous Random Variables?

Gaussian Random Variable

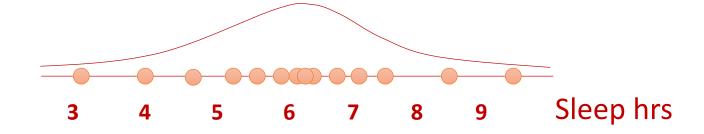
$$X \sim N(\mu, \sigma)$$
, then
$$p(x|\mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{\sigma^2}}$$





What About Continuous Random Variables?

Observed data D:



Parameters: μ - mean, σ^2 variance

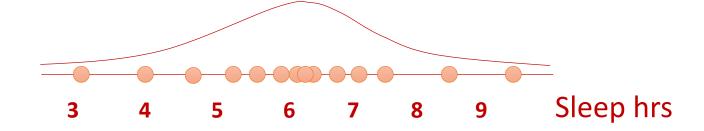
Sleep hours are i.i.d.:

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

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

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

MLE for Mean of Gaussian

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

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

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

Set
$$\frac{d}{du} \ln P(D|\mu, \sigma) = 0$$

Therefore
$$\sum_{\{i=1,...,N\}} (x_i - \mu) = 0$$

$$\hat{\mu}_{MLE} = \frac{\sum_{i} x_{i}}{N}$$

MLE for Variance of Gaussian

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

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

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

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

Learning Gaussian Parameters

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

$$\widehat{\mu}_{MLE} = \frac{\sum_{i} x_{i}}{N}$$

Bayesian learning/estimation is also possible.

Conjugate priors:

Mean: Gaussian prior

Variance: Wishart distribution

What you should know

- MLE, MAP
- Coins, Dice, Gaussian