

Learning Distributions (Parametric Approach)

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Machine Learning 10-701/15-781
Sept 12, 2012

The logo consists of the letters 'ML' in a bold, black, sans-serif font. A thick red horizontal line is positioned directly beneath the 'L'. The background behind the letters is a light gray with abstract, overlapping geometric shapes.

MACHINE LEARNING DEPARTMENT

The logo features a pattern of small, light gray dots arranged in a grid that tapers to the right. Below this pattern, the text 'Carnegie Mellon.' is written in a red, serif font, and 'School of Computer Science' is written in a smaller, black, sans-serif font below it.

Carnegie Mellon.
School of Computer Science

Announcement

- HW 1 is out – Due Sept 26

Your first consulting job

- A billionaire asks you a question:
 - He says: I have a coin, if I flip it, what's the probability it will fall with the head up?
 - You say: Please flip it a few times:



- You say: The probability is:
- **He says: Why???**
- You say: Because...

3/5

Bernoulli distribution

Data, $D =$



$$D = \{X_i\}_{i=1}^n, X_i \in \{H, T\}$$

- $P(\text{Heads}) = \theta$, $P(\text{Tails}) = 1 - \theta$
- Flips are **i.i.d.**:
 - **Independent** events
 - **Identically distributed** according to Bernoulli distribution

Choose θ that maximizes the probability of observed data

Maximum Likelihood Estimation

Choose θ that maximizes the probability of observed data

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

MLE of probability of head:

$$\hat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T} = 3/5 \text{ "Frequency of heads"}$$

Number of heads Number of tails

Maximum Likelihood Estimation

Choose θ that maximizes the probability of observed data

$$\begin{aligned}\hat{\theta}_{MLE} &= \arg \max_{\theta} P(D | \theta) \\ &= \arg \max_{\theta} \prod_{i=1}^n P(X_i | \theta) && \text{Independent draws} \\ &= \arg \max_{\theta} \prod_{i: X_i=H} \theta \prod_{i: X_i=T} (1 - \theta) && \text{Identically distributed} \\ &= \arg \max_{\theta} \underbrace{\theta^{\alpha_H} (1 - \theta)^{\alpha_T}}_{J(\theta)}\end{aligned}$$

Maximum Likelihood Estimation

Choose θ that maximizes the probability of observed data

$$\begin{aligned}\hat{\theta}_{MLE} &= \arg \max_{\theta} P(D | \theta) \\ &= \arg \max_{\theta} \underbrace{\theta^{\alpha_H} (1 - \theta)^{\alpha_T}}_{J(\theta)}\end{aligned}$$

$$\frac{\partial J(\theta)}{\partial \theta}$$

$$\Big|_{\theta=\hat{\theta}_{MLE}} = 0$$

$$\alpha_H(1 - \theta) - \alpha_T\theta \Big|_{\theta=\hat{\theta}_{MLE}} = 0$$

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

How many flips do I need?

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

- Billionaire says: I flipped 3 heads and 2 tails.
- You say: $\theta = 3/5$, I can prove it!
- He says: What if I flipped 30 heads and 20 tails?
- You say: Same answer, I can prove it!
- **He says: What's better?**
- You say: Hmm... The more the merrier???
- He says: Is this why I am paying you the big bucks???

Simple bound (Hoeffding's inequality)

- For $n = \alpha_H + \alpha_T$, and $\hat{\theta}_{MLE} = \frac{\alpha_H}{\alpha_H + \alpha_T}$
- Let θ^* be the true parameter, for any $\epsilon > 0$:

$$P(|\hat{\theta} - \theta^*| \geq \epsilon) \leq 2e^{-2n\epsilon^2}$$

PAC Learning

- PAC: Probably Approximate Correct
- Billionaire says: I want to know the coin parameter θ , within $\epsilon = 0.1$, with probability at least $1 - \delta = 0.95$.

How many flips?

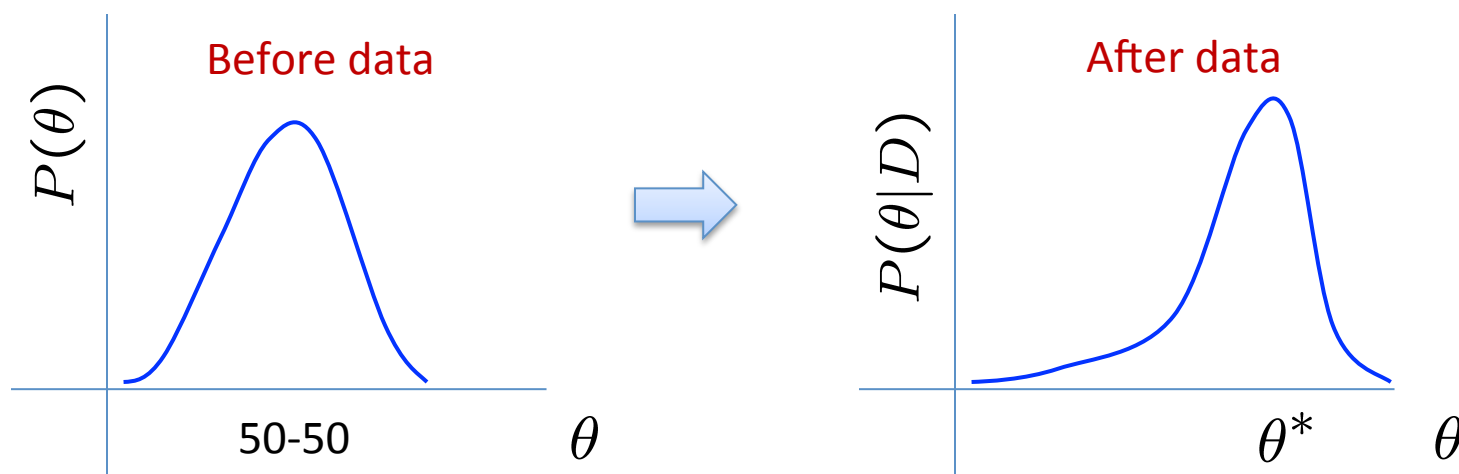
$$P(|\hat{\theta} - \theta^*| \geq \epsilon) \leq 2e^{-2n\epsilon^2}$$

Sample complexity

$$n \geq \frac{\ln(2/\delta)}{2\epsilon^2}$$

What about prior knowledge?

- Billionaire says: Wait, I know that the coin is “close” to 50-50. What can you do for me now?
- **You say: I can learn it the Bayesian way...**
- Rather than estimating a single θ , we obtain a distribution over possible values of θ



Bayesian Learning

- Use Bayes rule:

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

- Or equivalently:

$$P(\theta | \mathcal{D}) \propto P(\mathcal{D} | \theta)P(\theta)$$

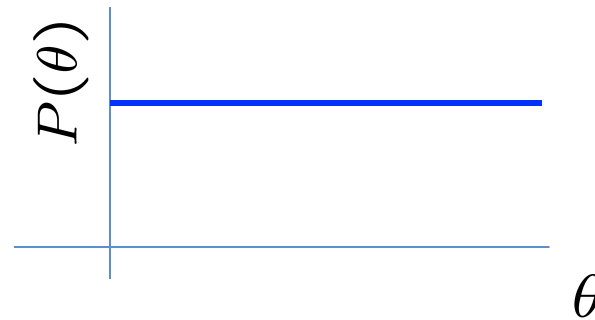
posterior likelihood prior



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

Prior distribution

- What about prior?
 - Represents expert knowledge (philosophical approach)
 - Simple posterior form (engineer's approach)
- Uninformative priors:
 - Uniform distribution
- Conjugate priors:
 - Closed-form representation of posterior
 - $P(\theta)$ and $P(\theta|D)$ have the same form



Conjugate Prior

- $P(\theta)$ and $P(\theta | D)$ have the same form

Eg. 1 Coin flip problem

Likelihood is \sim Binomial

$$P(\mathcal{D} | \theta) = \binom{n}{\alpha_H} \theta^{\alpha_H} (1 - \theta)^{\alpha_T}$$

If prior is Beta distribution,

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

Then posterior is Beta distribution

$$P(\theta | D) \sim \text{Beta}(\beta_H + \alpha_H, \beta_T + \alpha_T)$$

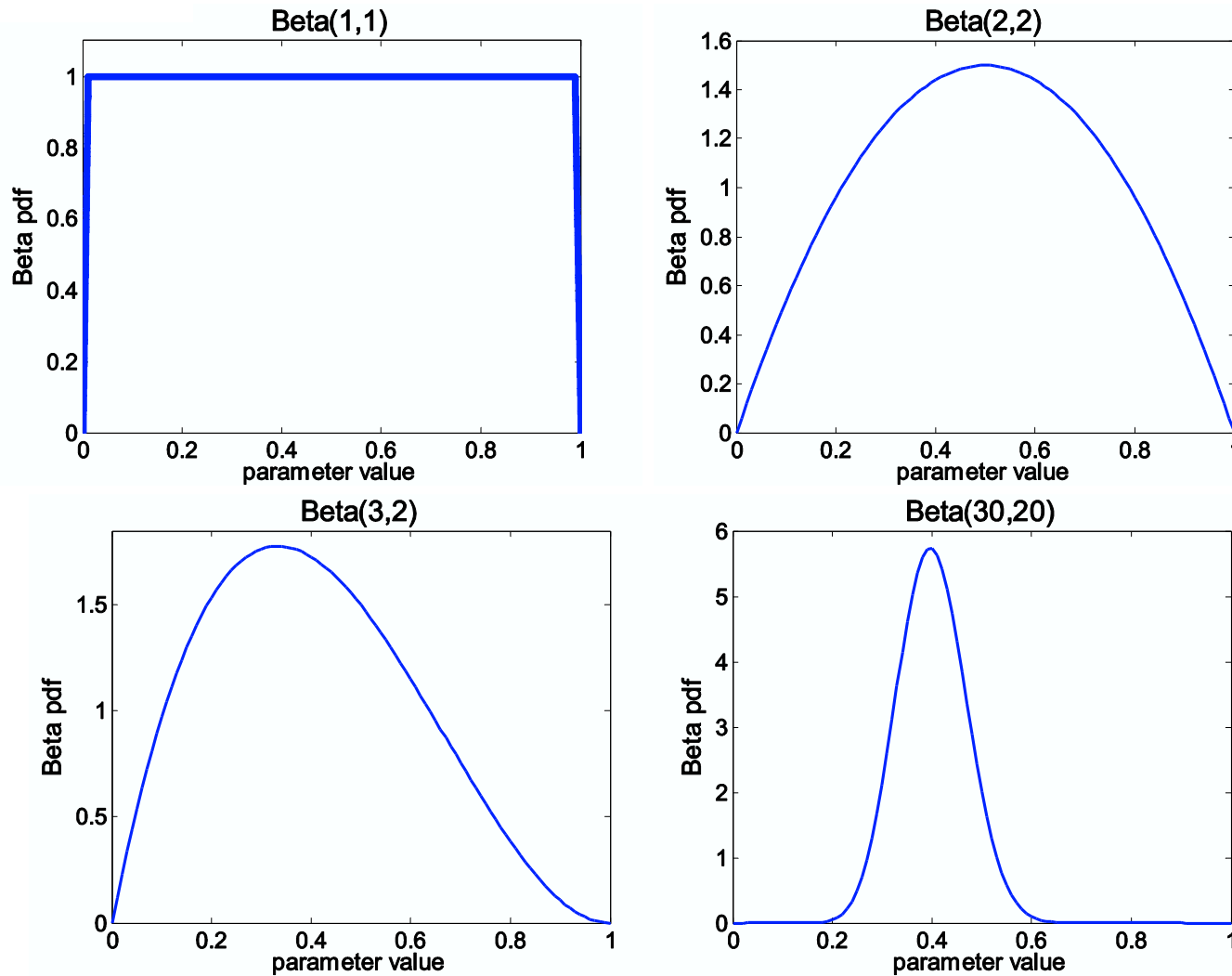
For Binomial, conjugate prior is Beta distribution.



Beta distribution

$$Beta(\beta_H, \beta_T)$$

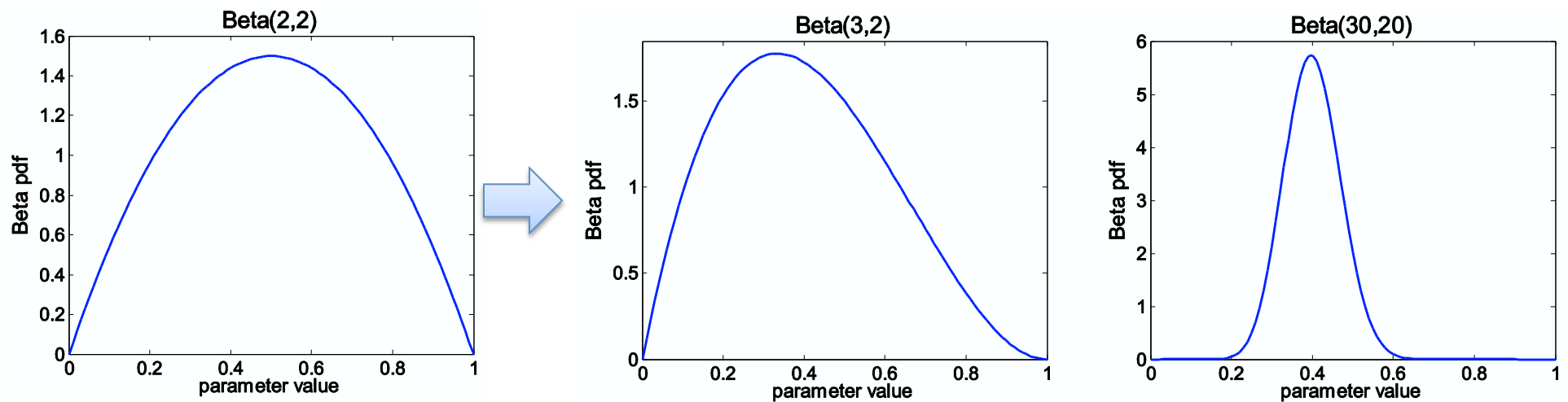
More concentrated as values of β_H, β_T increase



Beta conjugate prior

$$P(\theta) \sim \text{Beta}(\beta_H, \beta_T)$$

$$P(\theta|D) \sim \text{Beta}(\beta_H + \alpha_H, \beta_T + \alpha_T)$$



As $n = \alpha_H + \alpha_T$
increases

As we get more samples, effect of prior is “washed out”

Conjugate Prior

- $P(\theta)$ and $P(\theta|D)$ have the same form

Eg. 2 Dice roll problem (6 outcomes instead of 2)



Likelihood is \sim Multinomial($\theta = \{\theta_1, \theta_2, \dots, \theta_k\}$)

$$P(\mathcal{D} | \theta) = \frac{n!}{\alpha_1! \alpha_2! \dots \alpha_k!} \theta_1^{\alpha_1} \theta_2^{\alpha_2} \dots \theta_k^{\alpha_k} \quad \sum_{i=1}^k \alpha_i = n \quad \sum_{i=1}^k \theta_i = 1$$

If prior is Dirichlet distribution,

$$P(\theta) = \frac{\prod_{i=1}^k \theta_i^{\beta_i - 1}}{B(\beta_1, \dots, \beta_k)} \sim \text{Dirichlet}(\beta_1, \dots, \beta_k)$$

Then posterior is Dirichlet distribution

$$P(\theta|D) \sim \text{Dirichlet}(\beta_1 + \alpha_1, \dots, \beta_k + \alpha_k)$$

For Multinomial, conjugate prior is Dirichlet distribution.

Maximum A Posteriori Estimation

Choose θ that maximizes a posterior probability

$$\begin{aligned}\hat{\theta}_{MAP} &= \arg \max_{\theta} P(\theta | D) \\ &= \arg \max_{\theta} P(D | \theta)P(\theta)\end{aligned}$$

MAP estimate of probability of head:

$$P(\theta|D) \sim \text{Beta}(\beta_H + \alpha_H, \beta_T + \alpha_T)$$

$$\hat{\theta}_{MAP} = \frac{\alpha_H + \beta_H - 1}{\alpha_H + \beta_H + \alpha_T + \beta_T - 2} \quad \text{Mode of Beta distribution}$$

MLE vs. MAP

- Maximum Likelihood estimation (MLE)

Choose value that maximizes the probability of observed data

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

- Maximum *a posteriori* (MAP) estimation

Choose value that is most probable given observed data and prior belief

$$\begin{aligned}\hat{\theta}_{MAP} &= \arg \max_{\theta} P(\theta|D) \\ &= \arg \max_{\theta} P(D|\theta)P(\theta)\end{aligned}$$

When is MAP same as MLE?

MLE vs. MAP

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



What if we toss the coin too few times?

- You say: Probability next toss is a head = 0
- **Billionaire says: You're fired! ...with prob 1 😊**

$$\hat{\theta}_{MAP} = \frac{\alpha_H + \beta_H - 1}{\alpha_H + \beta_H + \alpha_T + \beta_T - 2}$$

- Beta prior equivalent to extra coin flips
- As $n \rightarrow 1$, prior is “forgotten”
- **But, for small sample size, prior is important!**

Bayesians vs. Frequentists

You are no good when sample is small

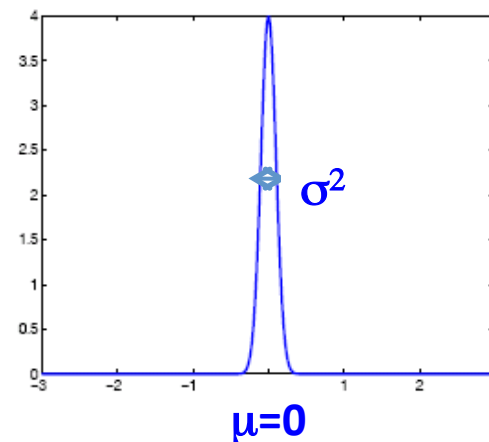
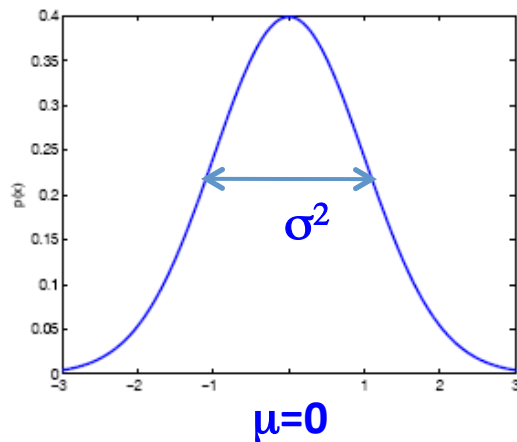


You give a different answer for different priors

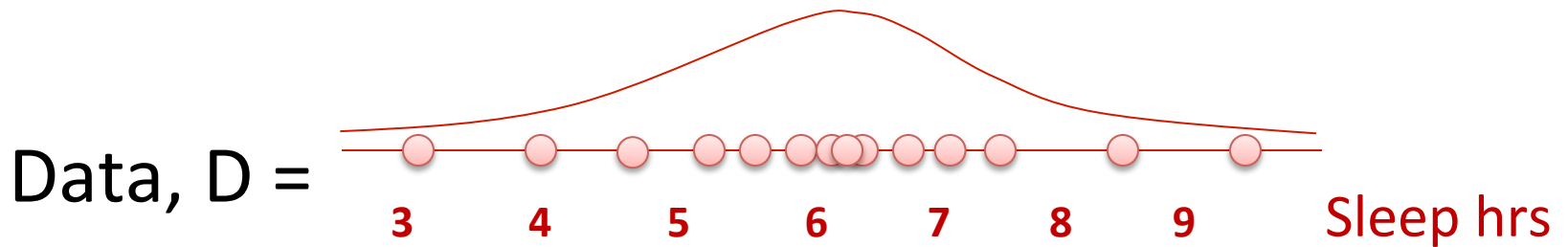
What about continuous variables?

- Billionaire says: If I am measuring a continuous variable, what can you do for me?
- **You say: Let me tell you about Gaussians...**

$$P(x \mid \mu, \sigma) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} = N(\mu, \sigma^2)$$



Gaussian distribution



- Parameters: μ – mean, σ^2 - variance
- Sleep hrs are **i.i.d.**:
 - **Independent** events
 - **Identically distributed** according to Gaussian distribution

Properties of Gaussians

- affine transformation (multiplying by scalar and adding a constant)
 - $X \sim N(\mu, \sigma^2)$
 - $Y = aX + b \text{ ! } Y \sim N(a\mu + b, a^2\sigma^2)$
- Sum of Gaussians
 - $X \sim N(\mu_X, \sigma_X^2)$
 - $Y \sim N(\mu_Y, \sigma_Y^2)$
 - $Z = X + Y \text{ ! } Z \sim N(\mu_X + \mu_Y, \sigma_X^2 + \sigma_Y^2)$

MLE for Gaussian mean and variance

Choose $\theta = (\mu, \sigma^2)$ that maximizes the probability of observed data

$$\begin{aligned}\hat{\theta}_{MLE} &= \arg \max_{\theta} P(D | \theta) \\ &= \arg \max_{\theta} \prod_{i=1}^n P(X_i | \theta) && \text{Independent draws} \\ &= \arg \max_{\theta} \prod_{i=1}^n \frac{1}{\sqrt{2\sigma^2}} e^{-(X_i - \mu)^2 / 2\sigma^2} && \text{Identically distributed} \\ &= \arg \max_{\theta = (\mu, \sigma^2)} \frac{1}{(2\sigma^2)^{n/2}} e^{-\sum_{i=1}^n (X_i - \mu)^2 / 2\sigma^2}\end{aligned}$$

MLE for Gaussian mean and variance

$$\hat{\mu}_{MLE} = \frac{1}{n} \sum_{i=1}^n x_i$$

$$\hat{\sigma}_{MLE}^2 = \frac{1}{n} \sum_{i=1}^n (x_i - \hat{\mu})^2$$

Note: MLE for the variance of a Gaussian is **biased**

- Expected result of estimation is **not** true parameter!
- Unbiased variance estimator:

$$\hat{\sigma}_{unbiased}^2 = \frac{1}{n-1} \sum_{i=1}^n (x_i - \hat{\mu})^2$$

MAP for Gaussian mean and variance

- Conjugate priors
 - Mean: Gaussian prior
 - Variance: Wishart Distribution

- Prior for mean:

$$P(\mu \mid \eta, \lambda) = \frac{1}{\lambda\sqrt{2\pi}} e^{-\frac{(\mu-\eta)^2}{2\lambda^2}} = N(\eta, \lambda^2)$$

MAP for Gaussian Mean

$$\hat{\mu}_{MLE} = \frac{1}{n} \sum_{i=1}^n x_i$$

$$\hat{\mu}_{MAP} = \frac{\frac{1}{\sigma^2} \sum_{i=1}^n x_i + \frac{\eta}{\lambda^2}}{\frac{n}{\sigma^2} + \frac{1}{\lambda^2}}$$

(Assuming known variance σ^2)

Independent of σ^2 if $\lambda^2 = \sigma^2/s$

MAP under Gauss-Wishart prior - Recitation

What you should know...

- Learning parametric distributions: form known, parameters unknown
 - Bernoulli (θ , probability of flip)
 - Gaussian (μ , mean and σ^2 , variance)
- MLE
- MAP