Parametric Techniques

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Introduction

- When covering Bayesian Decision Theory, we assumed the full probabilistic structure of the problem was know.
- However, this is rarely the case in practice.
- Instead, we have some knowledge of the problem and some example data and we must estimate the probabilities.
- In the discriminants chapter, we learned how to estimate linear boundaries separating the data, assuming nothing about the specific structure of the data. Here, we resort to assuming some structure to the data and estimate the parameters of this structure.
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- **Parametric Models** – For a particular class ω_i, we consider a set of parameters $\boldsymbol{\theta}_i$ to fully define the likelihood model.
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  - For the Guassian, $\boldsymbol{\theta}_i = (\boldsymbol{\mu}_i, \boldsymbol{\Sigma}_i)$.
- **Supervised Learning** – we are working in a supervised situation where we have an set of training data:

$$\mathcal{D} = \{(\mathbf{x}, \omega)_1, (\mathbf{x}, \omega)_2, \ldots (\mathbf{x}, \omega)_N\} \quad (1)$$

Overview of the Methods

- **Intuitive Problem:** Given a set of training data, $\mathcal{D}$, containing labels for c classes, train the likelihood models $p(\mathbf{x}|\omega_i, \boldsymbol{\theta}_i)$ by estimating the parameters $\boldsymbol{\theta}_i$ for $i = 1, \ldots, c$.

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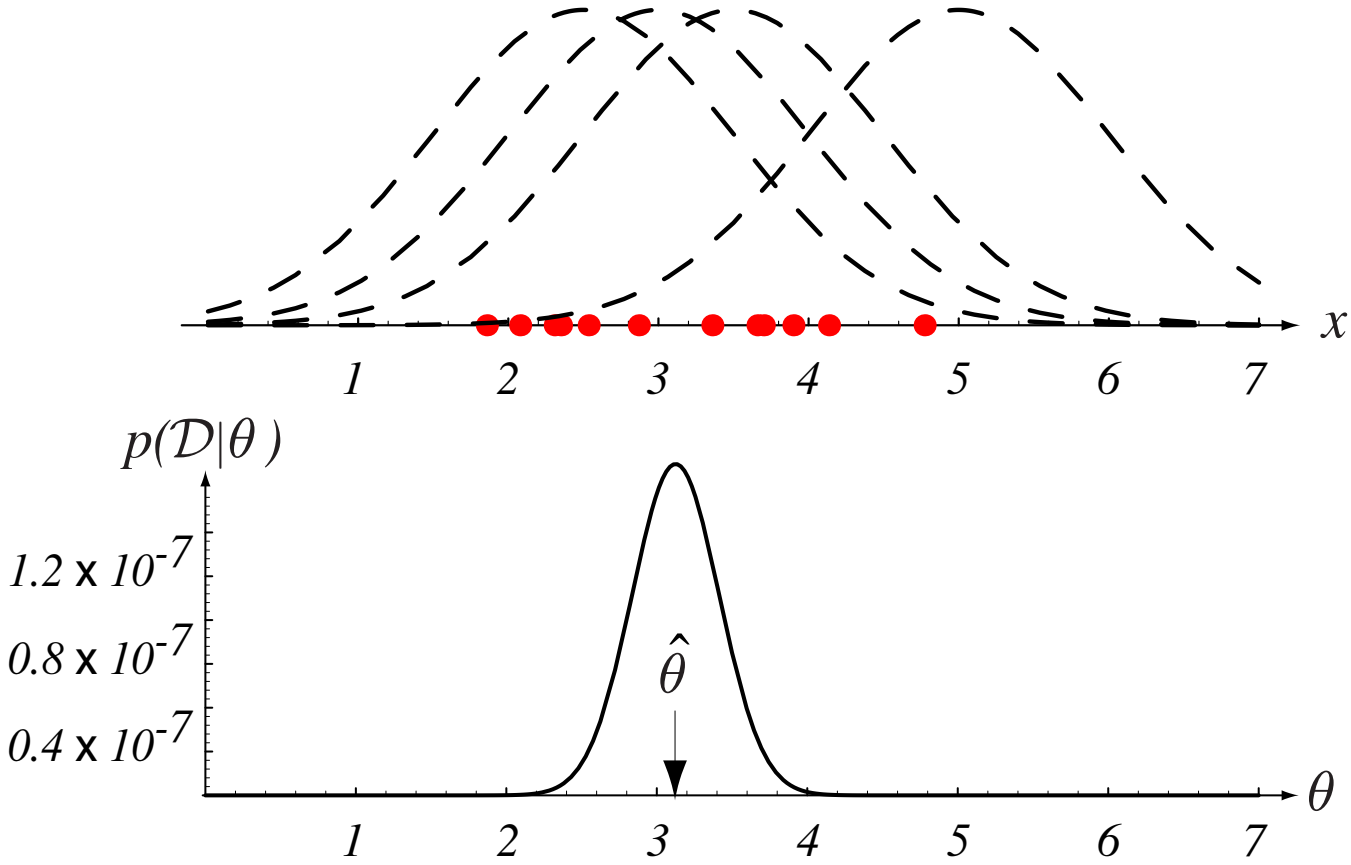
  - The best estimate of their value is the one that maximizes the probability of obtaining the samples in $\mathcal{D}$.
- **Bayesian Parameter Estimation**
  - Views the parameters as random variables having some known prior distribution.
  - The samples convert this prior into a posterior and revise our estimate of the distribution over the parameters.
  - We shall typically see that the posterior is increasingly peaked for larger $\mathcal{D}$ — *Bayesian Learning*.

Maximum Likelihood Intuition



- Underlying model is assumed to be a Gaussian of particular variance but unknown mean.

Preliminaries

- Separate our training data according to class; i.e., we have c data sets $\mathcal{D}_1, \ldots, \mathcal{D}_c$.
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- We thus have c separate problems of the form:

Definition

Use a set $\mathcal{D} = \{\mathbf{x}_1, \ldots, \mathbf{x}_n\}$ of training samples drawn independently from the density $p(\mathbf{x}|\boldsymbol{\theta})$ to estimate the unknown parameter vector $\boldsymbol{\theta}$.

(Log-)Likelihood

- Because we assume i.i.d. we have

$$p(\mathcal{D}|\boldsymbol{\theta}) = \prod_{k=1}^{n} p(\mathbf{x}_k|\boldsymbol{\theta}) \quad . \tag{2}$$

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- The log-likelihood is typically easier to work with both analytically and numerically.

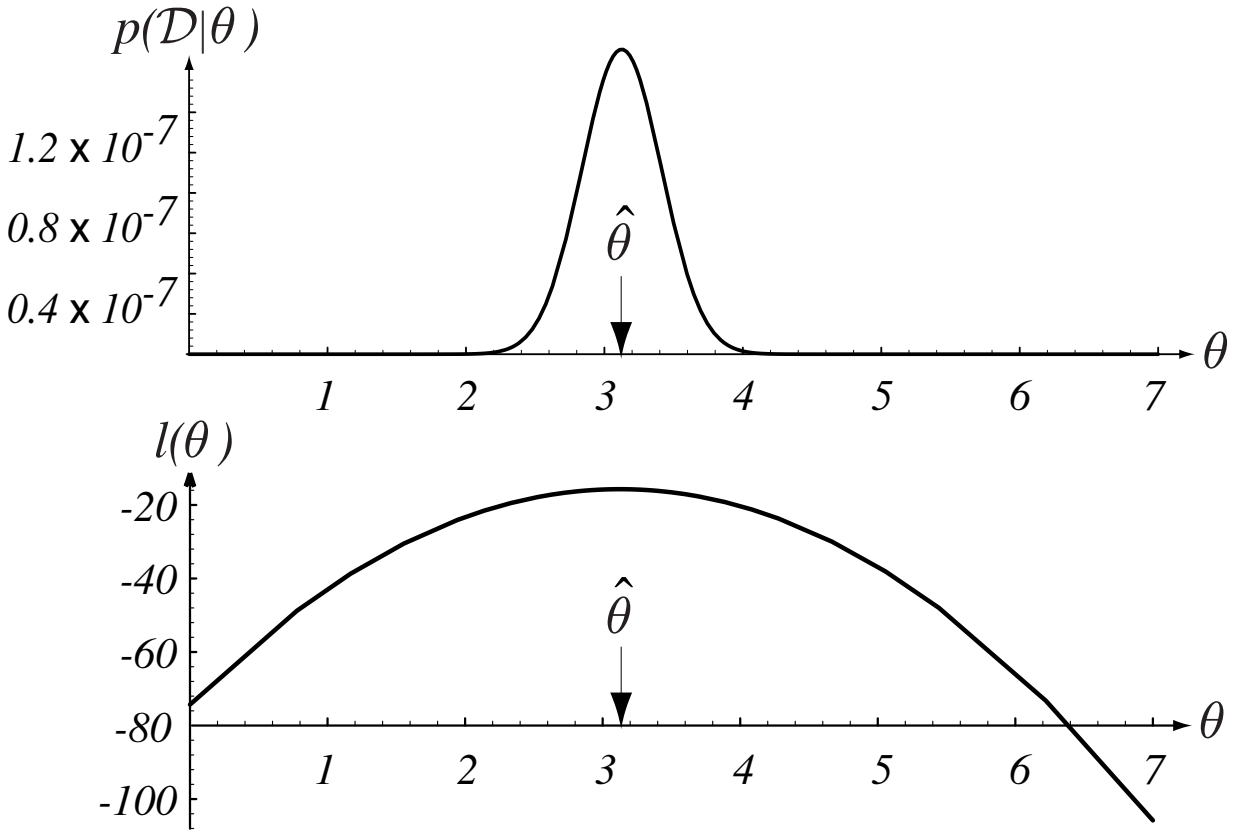
$$l_{\mathcal{D}}(\boldsymbol{\theta}) \equiv l(\boldsymbol{\theta}) \doteq \ln p(\mathcal{D}|\boldsymbol{\theta}) \tag{3}$$

$$= \sum_{k=1}^{n} \ln p(\mathbf{x}_k|\boldsymbol{\theta}) \tag{4}$$

Maximum (Log-)Likelihood

- The **maximum likelihood estimate** of $\boldsymbol{\theta}$ is the value $\hat{\boldsymbol{\theta}}$ that maximizes $p(\mathcal{D}|\boldsymbol{\theta})$ or equivalently maximizes $l_{\mathcal{D}}(\boldsymbol{\theta})$.

$$\hat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}} l_{\mathcal{D}}(\boldsymbol{\theta}) \tag{5}$$



Necessary Conditions for MLE

- For p parameters, $\boldsymbol{\theta} \doteq \begin{bmatrix} \theta_1 & \theta_2 & \dots & \theta_p \end{bmatrix}^{\mathsf{T}}$.
- Let $\boldsymbol{\nabla}_{\boldsymbol{\theta}}$ be the gradient operator, then $\boldsymbol{\nabla}_{\boldsymbol{\theta}} \doteq \begin{bmatrix} \frac{\partial}{\partial \theta_1} & \dots & \frac{\partial}{\partial \theta_p} \end{bmatrix}^{\mathsf{T}}$.
- The set of **necessary conditions** for the maximum likelihood estimate of $\boldsymbol{\theta}$ are obtained from the following system of p equations:

$$\boldsymbol{\nabla}_{\boldsymbol{\theta}} l = \sum_{k=1}^{n} \boldsymbol{\nabla}_{\boldsymbol{\theta}} \ln p(\mathbf{x}_k|\boldsymbol{\theta}) = 0 \tag{6}$$

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- A solution $\hat{\boldsymbol{\theta}}$ to (6) can be a true global maximum, a local maximum or minimum or an inflection point of $l(\boldsymbol{\theta})$.
- Keep in mind that $\hat{\boldsymbol{\theta}}$ is only an estimate. Only in the limit of an infinitely large number of training samples can we expect it to be the true parameters of the underlying density.

Gaussian Case with Known Σ and Unknown μ

- For a single sample point $\mathbf{x}_k$:

$$\ln p(\mathbf{x}_k|\boldsymbol{\mu}) = -\frac{1}{2}\ln\left[(2\pi)^d|\boldsymbol{\Sigma}|\right] - \frac{1}{2}(\mathbf{x}_k - \boldsymbol{\mu})^\mathsf{T}\boldsymbol{\Sigma}^{-1}(\mathbf{x}_k - \boldsymbol{\mu}) \quad (7)$$

$$\boldsymbol{\nabla}_{\boldsymbol{\mu}} \ln p(\mathbf{x}_k|\boldsymbol{\mu}) = \boldsymbol{\Sigma}^{-1}(\mathbf{x}_k - \boldsymbol{\mu}) \quad (8)$$

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$$\sum_{k=1}^{n} \boldsymbol{\Sigma}^{-1}(\mathbf{x}_k - \hat{\boldsymbol{\mu}}) = 0 \tag{9}$$

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- And we get the sample mean!

$$\hat{\boldsymbol{\mu}} = \frac{1}{n}\sum_{k=1}^{n} \mathbf{x}_k \tag{10}$$

Univariate Gaussian Case with Unknown μ and σ^2

The Log-Likelihood

- Let $\boldsymbol{\theta} = (\mu, \sigma^2)$. The log-likelihood of x_k is

$$\ln p(x_k|\boldsymbol{\theta}) = -\frac{1}{2}\ln\left[2\pi\sigma^2\right] - \frac{1}{2\sigma^2}(x_k - \mu)^2 \tag{11}$$

$$\boldsymbol{\nabla}_{\boldsymbol{\theta}} \ln p(x_k|\boldsymbol{\theta}) = \begin{bmatrix} \frac{1}{\sigma^2}(x_k - \mu) \\ -\frac{1}{2\sigma^2} + \frac{(x_k-\mu)^2}{2\sigma^2} \end{bmatrix} \tag{12}$$

Univariate Gaussian Case with Unknown μ and σ^2

Necessary Conditions

- The following conditions are defined:

$$\sum_{k=1}^{n} \frac{1}{\hat{\sigma}^2}(x_k - \hat{\mu}) = 0 \tag{13}$$

$$-\sum_{k=1}^{n} \frac{1}{\hat{\sigma}^2} + \sum_{k=1}^{n} \frac{(x_k - \hat{\mu})^2}{\hat{\sigma}^2} = 0 \tag{14}$$

Univariate Gaussian Case with Unknown μ and σ^2

ML-Estimates

- After some manipulation we have the following:

$$\hat{\mu} = \frac{1}{n}\sum_{k=1}^{n} x_k \tag{15}$$

$$\hat{\sigma}^2 = \frac{1}{n}\sum_{k=1}^{n}(x_k - \hat{\mu})^2 \tag{16}$$

- These are encouraging results – even in the case of unknown μ and σ^2 the ML-estimate of μ corresponds to the sample mean.

Bias

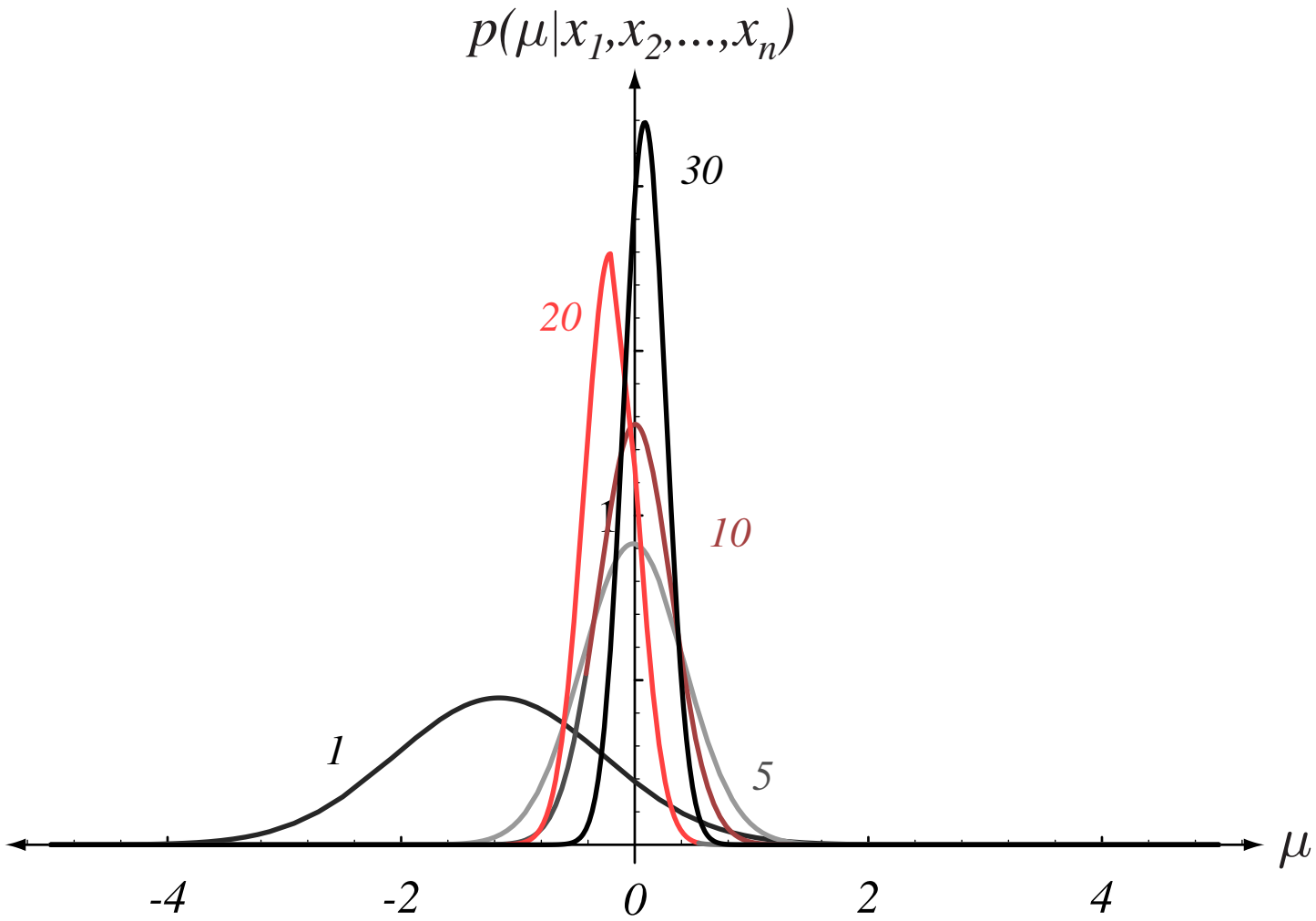
- The maximum likelihood estimate for the variance σ^2 is **biased**.
- The expected value over datasets of size n of the sample variance is not equal to the true variance

$$\mathcal{E}\left[\frac{1}{n}\sum_{i=1}^{n}(x_i - \hat{\mu})^2\right] = \frac{n-1}{n}\sigma^2 \neq \sigma^2 \tag{17}$$

- In other words, the ML-estimate of the variance systematically underestimates the variance of the distribution.
- As $n \to \infty$ the problem of bias is reduced or removed, but bias remains a problem of the ML-estimator.
- An unbiased ML-estimator of the variance is

$$\hat{\sigma}^2_{\text{unbiased}} = \frac{1}{n-1}\sum_{k=1}^{n}(x_k - \hat{\mu})^2 \tag{18}$$

Bayesian Parameter Estimation Intuition



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Bayesian Parameter Estimation

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Goal

Our ultimate goal is to estimate $p(\mathbf{x}|\mathcal{D})$, which is as close as we can come to estimating the unknown $p(\mathbf{x})$.

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- **Missing Data!** The samples will convert our prior $p(\boldsymbol{\theta})$ to a posterior $p(\boldsymbol{\theta}|\mathcal{D})$, by integrating the joint density over $\boldsymbol{\theta}$:

$$p(\mathbf{x}|\mathcal{D}) = \int p(\mathbf{x}, \boldsymbol{\theta}|\mathcal{D}) d\boldsymbol{\theta} \tag{19}$$

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- And, because the distribution of $\mathbf{x}$ is known given the parameters $\boldsymbol{\theta}$, we simplify to

$$p(\mathbf{x}|\mathcal{D}) = \int p(\mathbf{x}|\boldsymbol{\theta}) p(\boldsymbol{\theta}|\mathcal{D}) d\boldsymbol{\theta} \tag{21}$$

Linking Likelihood and the Parameter Distribution

$$p(\mathbf{x}|\mathcal{D}) = \int p(\mathbf{x}|\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathcal{D})d\boldsymbol{\theta}$$

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- If the posterior $p(\boldsymbol{\theta}|\mathcal{D})$ peaks very sharply for sample point $\hat{\boldsymbol{\theta}}$, then we obtain

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- What if the integral is not readily analytically computed?

The Posterior Density on the Parameters

- The primary task in Bayesian Parameter Estimation is the computation of the posterior density $p(\boldsymbol{\theta}|\mathcal{D})$.
- By Bayes formula

$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{1}{Z} p(\mathcal{D}|\boldsymbol{\theta}) p(\boldsymbol{\theta}) \tag{23}$$

- Z is a normalizing constant:

$$Z = \int p(\mathcal{D}|\boldsymbol{\theta}) p(\boldsymbol{\theta}) d\boldsymbol{\theta} \tag{24}$$

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- And, by the independence assumption on $\mathcal{D}$:

$$p(\mathcal{D}|\boldsymbol{\theta}) = \prod_{k=1}^{n} p(\mathbf{x}_k|\boldsymbol{\theta}) \tag{25}$$

- Let's see an example now.

Univariate Gaussian Case with Known σ^2

- Assume $p(x|\mu) \sim N(\mu, \sigma^2)$ with known σ^2.
- Whatever prior knowledge we know about μ is expressed in $p(\mu)$, which is known.

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- Indeed, we assume it too is a Gaussian

$$p(\mu) \sim N(\mu_0, \sigma_0^2) \ . \tag{26}$$

μ_0 represents our best guess of the value of the mean and σ_0^2 represents our uncertainty about this guess.

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  μ_0 represents our best guess of the value of the mean and σ_0^2 represents our uncertainty about this guess.
- Note: the choice of the prior as a Gaussian is not so crucial—it will simplify the mathematics. Rather, the more important assumption is that we know the prior.

Univariate Gaussian Case with Known σ^2

Training samples

- We assume that we are given samples $\mathcal{D} = \{x_1, \ldots, x_n\}$ from $p(x, \mu)$.
- Take some time to think through this point—unlike in MLE, we cannot assume that we have a single value of the parameter in the underlying distribution.

Univariate Gaussian Case with Known σ^2

Bayes Rule

- $$p(\mu|\mathcal{D}) = \frac{1}{Z} p(\mathcal{D}|\mu) p(\mu) \tag{27}$$
$$= \frac{1}{Z} \prod_k p(x_k|\mu) p(\mu) \tag{28}$$

- See how the training samples modulate our prior knowledge of the parameters in the posterior?

Univariate Gaussian Case with Known σ^2

Expanding...

- $$p(\mu|\mathcal{D}) = \frac{1}{Z}\prod_k \frac{1}{\sqrt{2\pi\sigma^2}}\exp\left[-\frac{1}{2}\left(\frac{x_k-\mu}{\sigma}\right)^2\right] \frac{1}{\sqrt{2\pi\sigma_0^2}}\exp\left[-\frac{1}{2}\left(\frac{\mu-\mu_0}{\sigma_0}\right)^2\right] \quad (29)$$

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- After some manipulation, we can see that $p(\mu|\mathcal{D})$ is an exponential function of a quadratic of μ, which is another way of saying a normal density.

$$p(\mu|\mathcal{D}) = \frac{1}{Z'}\exp\left[-\frac{1}{2}\left[\left(\frac{n}{\sigma^2}+\frac{1}{\sigma_0^2}\right)\mu^2 - 2\left(\frac{1}{\sigma^2}\sum_k x_k + \frac{\mu_0}{\sigma_0^2}\right)\mu\right]\right] \tag{30}$$

Univariate Gaussian Case with Known σ^2

Names of these convenient distributions...

- And, this will be true regardless of the number of training samples.
- In other words, $p(\mu|\mathcal{D})$ remains a normal as the number of samples increases.
- Hence, $p(\mu|\mathcal{D})$ is said to be a **reproducing density**.
- $p(\mu)$ is said to be a **conjugate prior**.

Univariate Gaussian Case with Known σ^2

Rewriting...

- We can write $p(\mu|\mathcal{D}) \sim N(\mu_n, \sigma_n^2)$. Then, we have

$$p(\mu|\mathcal{D}) = \frac{1}{\sqrt{2\pi\sigma_n^2}} \exp\left[-\frac{1}{2}\left(\frac{\mu-\mu_n}{\sigma_n}\right)^2\right] \tag{31}$$

- The new coefficients are

$$\frac{1}{\sigma_n^2} = \frac{n}{\sigma^2} + \frac{1}{\sigma_0^2} \tag{32}$$

$$\frac{\mu_n}{\sigma_n^2} = \frac{n}{\sigma^2}\overline{\mu}_n + \frac{\mu_0}{\sigma_0^2} \tag{33}$$

- $\overline{\mu}_n$ is the sample mean over the n samples.

Univariate Gaussian Case with Known σ^2

Rewriting...

- Solving explicitly for μ_n and σ_n^2

$$\mu_n = \left(\frac{n\sigma_0^2}{n\sigma_0^2 + \sigma^2} \right) \overline{\mu}_n + \frac{\sigma^2}{n\sigma_0^2 + \sigma^2} \mu_0 \tag{34}$$

$$\sigma_n^2 = \frac{\sigma_0^2 \sigma^2}{n\sigma_0^2 + \sigma^2} \tag{35}$$

shows explicitly how the prior information is combined with the training samples **to estimate the parameters of the posterior distribution**.

- After n samples, μ_n is our best guess for the mean of the posterior and σ_n^2 is our uncertainty about it.

Univariate Gaussian Case with Known σ^2

Uncertainty...

- What can we say about this uncertainty as n increases?

$$\sigma_n^2 = \frac{\sigma_0^2 \sigma^2}{n\sigma_0^2 + \sigma^2}$$

Univariate Gaussian Case with Known σ^2

Uncertainty...

- What can we say about this uncertainty as n increases?

$$\sigma_n^2 = \frac{\sigma_0^2 \sigma^2}{n\sigma_0^2 + \sigma^2}$$

- That each observation **monotonically decreases our uncertainty** about the distribution.

$$\lim_{n \to \infty} \sigma_n^2 = 0 \tag{36}$$

- In other terms, as n increases, $p(\mu|\mathcal{D})$ becomes more and more sharply peaked approaching a Dirac delta function.

Univariate Gaussian Case with Known σ^2

- What can we say about the parameter μ_n as n increases?

$$\mu_n = \left(\frac{n\sigma_0^2}{n\sigma_0^2 + \sigma^2} \right) \overline{\mu}_n + \frac{\sigma^2}{n\sigma_0^2 + \sigma^2} \mu_0$$

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- It is a convex combination between the sample mean $\overline{\mu}_n$ (from the observed data) and the prior μ_0.
- Thus, it always lives somewhere betweens $\overline{\mu}_n$ and μ_0.
- And, it approaches the sample mean as n approaches ∞:

$$\lim_{n \to \infty} \mu_n = \overline{\mu}_n \equiv \frac{1}{n} \sum_{k=1}^{n} x_k \tag{37}$$

Univariate Gaussian Case with Known σ^2

Putting it all together to obtain $p(x|\mathcal{D})$.

- Our goal has been to obtain an estimate of how likely a novel sample x is given the entire training set $\mathcal{D}$: $p(x|\mathcal{D})$.

$$p(x|\mathcal{D}) = \int p(x|\mu)p(\mu|\mathcal{D})d\mu \tag{38}$$

$$\begin{aligned} &= \int \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right] \\ &\quad \int \frac{1}{\sqrt{2\pi\sigma_n^2}} \exp\left[-\frac{1}{2}\left(\frac{\mu-\mu_n}{\sigma_n}\right)^2\right] \end{aligned} \tag{39}$$

$$= \frac{1}{2\pi\sigma\sigma_n} \exp\left[\frac{1}{2}\frac{(x-\mu_n)^2}{\sigma^2+\sigma_n^2}\right] f(\sigma,\sigma_n) \tag{40}$$

- Essentially, $p(x|\mathcal{D}) \sim N(\mu_n, \sigma^2+\sigma_n^2)$.

Some Comparisons

Maximum Likelihood

- Point Estimator

$$p(x|\mathcal{D}) = p(x|\hat{\boldsymbol{\theta}})$$

- Parameter Estimate

$$\hat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}} \ln p(\mathcal{D}|\boldsymbol{\theta})$$

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Bayesian

- Distribution Estimator

$$p(x|\mathcal{D}) = \int p(x|\boldsymbol{\theta})p(\boldsymbol{\theta}|\mathcal{D})d\boldsymbol{\theta}$$

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$$p(\boldsymbol{\theta}|\mathcal{D}) = \frac{1}{Z}p(\mathcal{D}|\boldsymbol{\theta})p(\boldsymbol{\theta})$$

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Comments on the two methods

- For reasonable priors, MLE and BPE are equivalent in the asymptotic limit of infinite training data.
- **Computationally** – MLE methods are preferred for computational reasons because they are comparatively simpler (differential calculus versus multidimensional integration).

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- **Confidence In Priors** – But, the Bayesian methods bring more information to the table. If the underlying distribution is of a different parametric form than originally assumed, Bayesian methods will do better.
- **Bias-Variance** – Bayesian methods make the bias-variance tradeoff more explicit by directly incorporating the uncertainty in the estimates.

Some Comparisons

Comments on the two methods

Take Home Message

There are strong theoretical and methodological arguments supporting Bayesian estimation, though in practice maximum-likelihood estimation is simpler, and when used for designing classifiers, can lead to classifiers that are nearly as accurate.

Recursive Bayesian Estimation

- Another reason to prefer Bayesian estimation is that it provides a natural way to incorporate additional training data as it becomes available.
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- Let a training set with n samples be denoted $\mathcal{D}^n$.
- Then, due to our independence assumption:

$$p(\mathcal{D}|\boldsymbol{\theta}) = \prod_{k=1}^{n} p(\mathbf{x}_k|\boldsymbol{\theta}) \tag{41}$$

we have

$$p(\mathcal{D}^n|\boldsymbol{\theta}) = p(\mathbf{x}_n|\boldsymbol{\theta})p(\mathcal{D}^{n-1}|\boldsymbol{\theta}) \tag{42}$$

Recursive Bayesian Estimation

- And, with Bayes Formula, we see that the posterior satisfies the recursion

$$p(\boldsymbol{\theta}|\mathcal{D}^n) = \frac{1}{Z} p(\mathbf{x}_n|\boldsymbol{\theta}) p(\boldsymbol{\theta}|\mathcal{D}^{n-1}) \quad . \tag{43}$$

- This is an instance of **on-line learning**.

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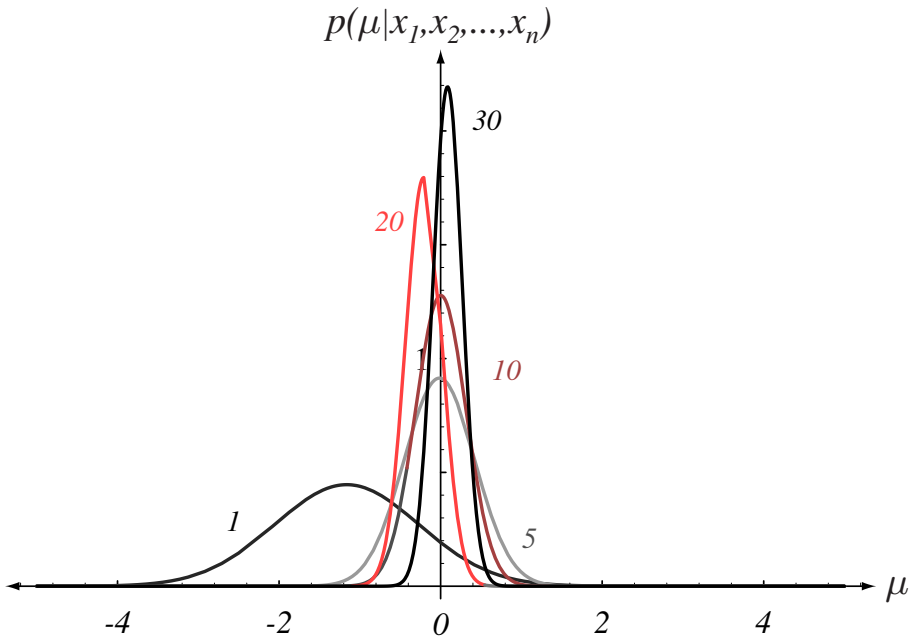
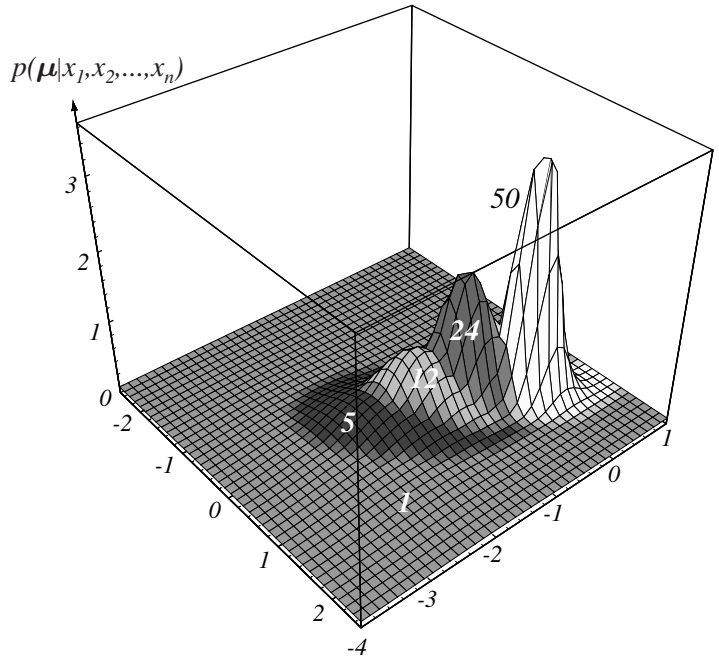
- This is an instance of **on-line learning**.
- In principle, this derivation requires that we retain the entire training set in $\mathcal{D}^{n-1}$ to calculate $p(\boldsymbol{\theta}|\mathcal{D}^n)$. But, for some distributions, we can simply retain the sufficient statistics, which contain all the information needed.

Recursive Bayesian Estimation





Example of Recursive Bayes

- Suppose we believe our samples come from a uniform distribution:

$$p(x|\theta) \sim U(0,\theta) = \begin{cases} 1/\theta & 0 \leq x \leq \theta \\ 0 & \text{otherwise} \end{cases} \tag{44}$$

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- We get a training data set $\mathcal{D} = \{4, 7, 2, 8\}$.

Example of Recursive Bayes

- When the first data point arrives, $x_1 = 4$, we get an improved estimate of θ:

$$p(\theta|\mathcal{D}^1) \propto p(x|\theta)p(\theta|\mathcal{D}^0) = \begin{cases} 1/\theta & 4 \leq \theta \leq 10 \\ 0 & \text{otherwise} \end{cases} \tag{46}$$

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- When the next data point arrives, $x_2 = 7$, we have

$$p(\theta|\mathcal{D}^2) \propto p(x|\theta)p(\theta|\mathcal{D}^1) = \begin{cases} 1/\theta^2 & 7 \leq \theta \leq 10 \\ 0 & \text{otherwise} \end{cases} \tag{47}$$

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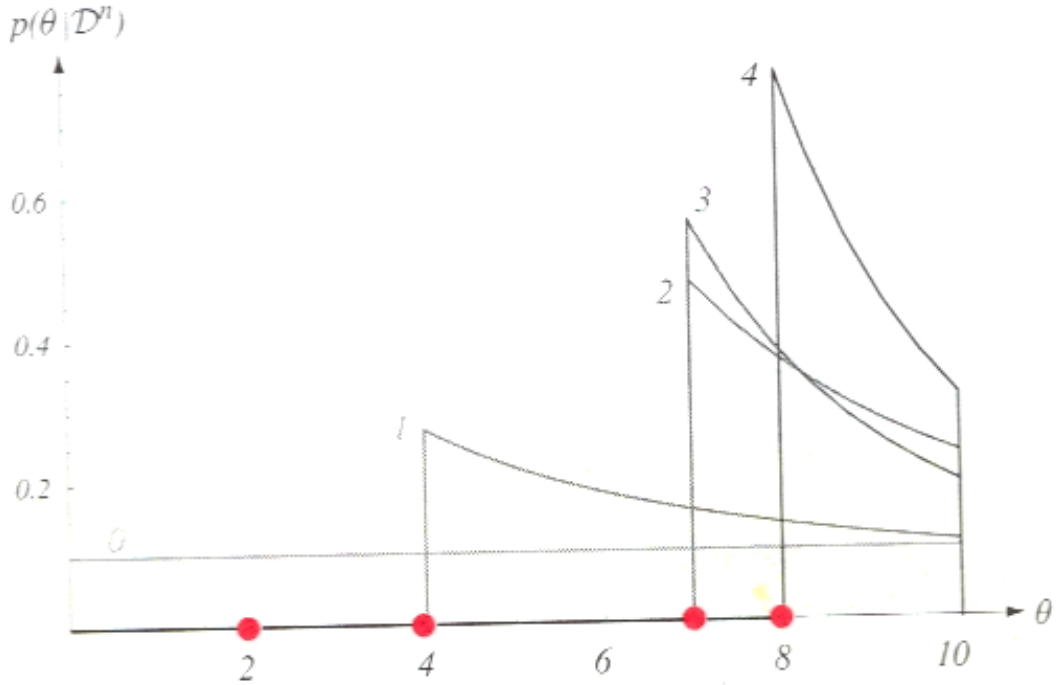
- And so on....

Example of Recursive Bayes

- Notice that each successive data sample introduces a factor of $1/\theta$ into $p(x|\theta)$.
- The distribution of samples is nonzero only for x values above the max, $p(\theta|\mathcal{D}^n) \propto 1/\theta^n$ for $\max_x[\mathcal{D}^n] \leq \theta \leq 10$.
- Our distribution is



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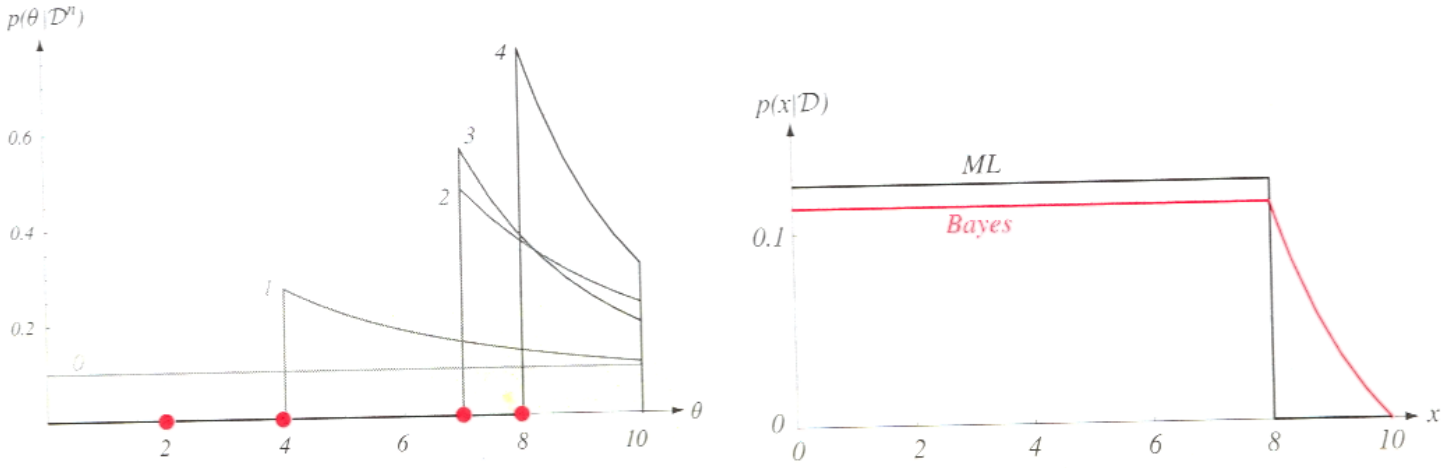

- The maximum likelihood solution is $\hat{\theta} = 8$, implying $p(x|\mathcal{D}) \sim U(0, 8)$.
- But, the Bayesian solution shows a different character:
  - Starts out flat.
  - As more points are added, it becomes increasingly peaked at the value of the highest data point.
  - And, the Bayesian estimate has a tail for points above 8 reflecting our prior distribution.