CHAPTER 16:

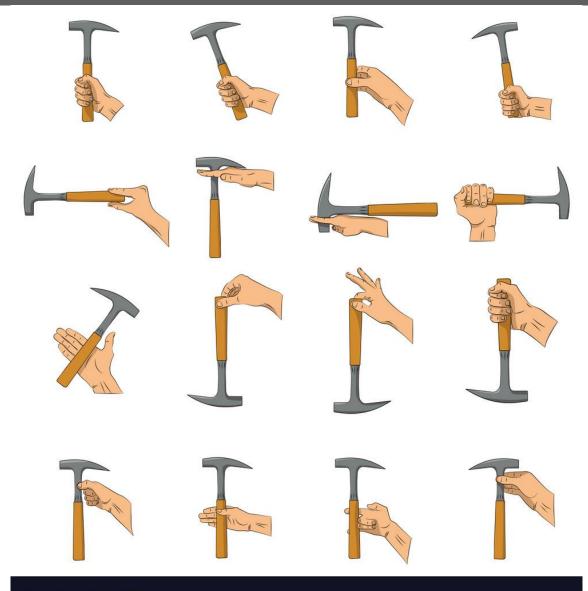
BAYESIAN ESTIMATION

Stella Grasshof

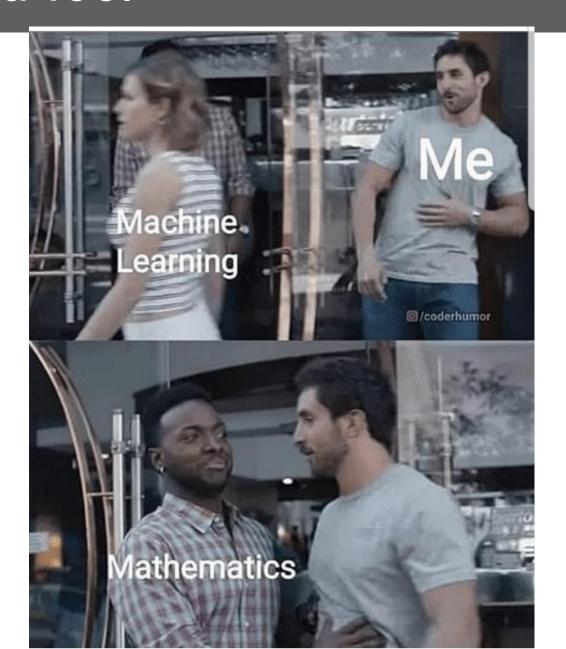
Overview

- Repeat
- □ Bayesian estimation
- Bayesian estimation of unknown mean
- Bayesian regression
- ☐ Howto Prior
- □ Model Quality

Math is a tool



Math is a tool

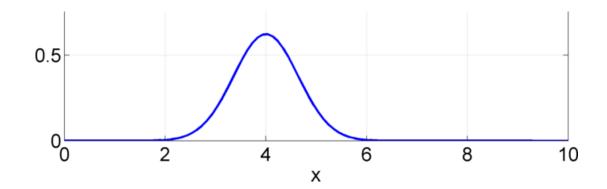


1D Normal

$$X \sim \mathcal{N}(\mu, \sigma^2)$$
$$E[X] = \mu, Var[X] = \sigma^2$$

p.d.f.
$$f(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma^2}\right)^2\right]$$

c.d.f.
$$\Phi(x) = P(X \le x)$$

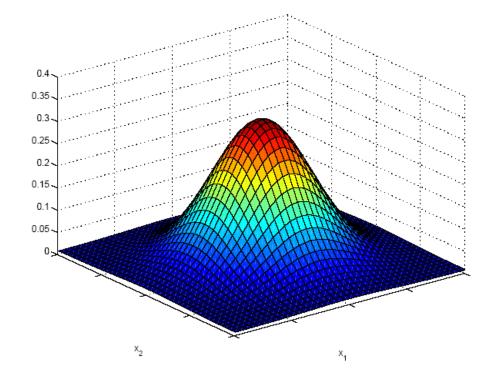


multidimsional Normal

D-dimensional: $x \in \mathbb{R}^D$

$$oldsymbol{x} \sim \mathcal{N}(oldsymbol{\mu}, oldsymbol{\Sigma})$$

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



Discrete Binomial

$$X \sim B(n,k)$$

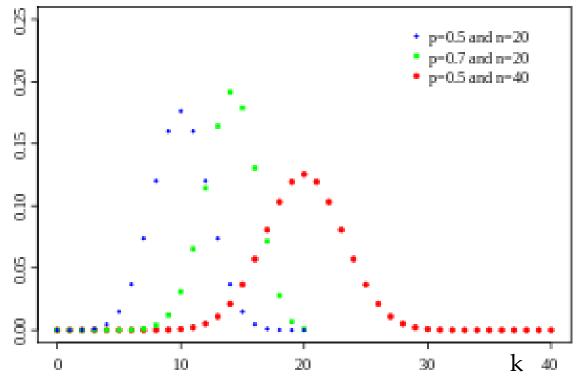
$$E[X] = np, Var[X] = np(1-p)$$

p.d.f.

$$f(k) = \binom{n}{k} p^k (1-p)^{n-k} \ \exists$$

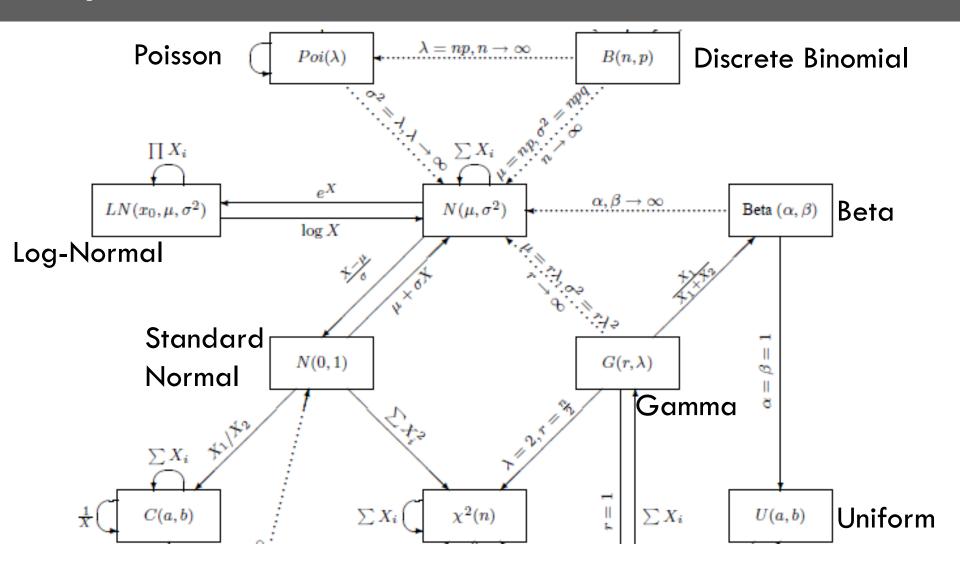
c.d.f.

$$F(x) = P(X \le x)$$



https://en.wikipedia.org/wiki/Binomial_distribution

Table 3.1: Common Exponential Distributions and their Sufficient Statistics.						
Name	Distribution	Domain		s		
Normal	$p(x \boldsymbol{\theta}) = \sqrt{\frac{\theta_2}{2\pi}} e^{-(1/2)\theta_2(x-\theta_1)^2}$	$\theta_2 > 0$	V(200)	$\frac{\frac{1}{n}\sum_{k=1}^{n}x_{k}}{\frac{1}{n}\sum_{k=1}^{n}x_{k}^{2}}$ $\frac{1}{n}\sum_{k=1}^{n}\mathbf{x}_{k}$		
Multi- variate Normal	$p(\mathbf{x} \boldsymbol{\theta}) = \frac{p(\mathbf{x} \boldsymbol{\theta})}{(2\pi)^{d/2}} e^{-(1/2)(\mathbf{x}-\boldsymbol{\theta}_1)^t \boldsymbol{\Theta}_2(\mathbf{x}-\boldsymbol{\theta}_1)}$	Θ_2 positive definite		$\begin{bmatrix} \frac{1}{n} \sum\limits_{k=1}^{n} \mathbf{x}_{k} \\ \frac{1}{n} \sum\limits_{k=1}^{n} \mathbf{x}_{k} \mathbf{x}_{k}^{t} \end{bmatrix}$		
Exponential	$ \begin{aligned} p(x \theta) &= \\ \theta e^{-\theta x} & x \ge 0 \\ 0 & \text{otherwise} \end{aligned} $	$\theta > 0$	10 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	$\frac{1}{n}\sum_{k=1}^{n}x_{k}$		
Rayleigh	$p(x \theta) = \begin{cases} 2\theta x e^{-\theta x^2} & x \ge 0\\ 0 & \text{otherwise} \end{cases}$	$\theta > 0$		$\frac{1}{n}\sum_{k=1}^{n}x_{k}^{2}$		
Maxwell	$p(x \theta) = \begin{cases} \frac{4}{\sqrt{\pi}} \theta^{3/2} x^2 e^{-\theta x^2} & x \ge 0\\ 0 & \text{otherwise} \end{cases}$	$\theta > 0$	15 12 2 1 1 1 1 1 1	$\frac{1}{n}\sum_{k=1}^{n}x_{k}^{2}$		
Gamma	$p(x \boldsymbol{\theta}) = \begin{cases} \frac{\theta_2^{\theta_1+1}}{\Gamma(\theta_1+1)} x^{\theta_1} e^{-\theta_2 x} & x \ge 0\\ 0 & \text{otherwise} \end{cases}$	$\theta_1 > -1$ $\theta_2 > 0$	01 = -2 03 = -2	$ \left[\left(\prod_{k=1}^{n} x_k \right)^{1/n} \right] \\ \frac{1}{n} \sum_{k=1}^{n} x_k $		
Beta	$\begin{cases} p(x \boldsymbol{\theta}) = \\ \frac{\Gamma(\theta_1 + \theta_2 + 2)}{\Gamma(\theta_1 + 1)\Gamma(\theta_2 + 1)} x^{\theta_1} (1 - x)^{\theta_2} \\ 0 \le x \le 1 \\ 0 \text{otherwise} \end{cases}$	$\theta_1 > -1$ $\theta_2 > -1$	9-13	$\begin{bmatrix} \frac{1}{n} \sum_{k=1}^{n} x_k \\ \left(\prod_{k=1}^{n} x_k \right)^{1/n} \\ \left(\prod_{k=1}^{n} (1 - x_k) \right)^{1/n} \end{bmatrix}$		
Poisson	$P(x \theta) = \frac{\theta^x}{x!}e^{-\theta}$ $x = 0, 1, 2,$	$\theta > 0$	1 1 1 1 1 1 1 1	$\frac{1}{n}\sum_{k=1}^{n}x_{k}$		
Bernoulli	(1)	$0 < \theta < 1$	1 1 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	$\frac{1}{n}\sum_{k=1}^{n}x_{k}$		
Binomial	$P(x \theta) = \frac{m!}{x!(m-x)!} \theta^x (1-\theta)^{m-x} \\ x = 0, 1,, m$	$0 < \theta < 1$	n = 10	$\frac{1}{n}\sum_{k=1}^n x_k$		
Multinomial	$P(\mathbf{x} \boldsymbol{\theta}) = \\ \frac{m! \prod_{i=1}^{d} \theta_i^{x_i}}{\prod_{i=1}^{d} x_i!} \qquad x_i = 0, 1,, m \\ \sum_{i=1}^{d} x_i = m$	$0 < \theta_i < 1$ $\sum_{i=1}^d \theta_i = 1$	$R(x \theta)$ $M = 12$ M	$\frac{1}{n}\sum_{k=1}^{n}\mathbf{x}_{k}$		



Source: script "Biometrie", 2009, Prof. Ziegler, Lübeck

Repeat: ML vs. MAP

Task: Given data \mathcal{X} , estimate parameter θ

□ Maximum Likelihood (ML)

$$\theta_{\mathrm{ML}} = \underset{\theta}{\mathrm{arg\,max}} \ p(\mathcal{X}|\theta)$$

Likelihood

□ Maximum A Posteriori (MAP)

$$egin{aligned} heta_{\mathrm{MAP}} &= rg \max_{ heta} & p(heta|\mathcal{X}) & \mathbf{p}(\mathcal{X}| heta)p(heta) & \mathbf{p}(\mathcal{X}| heta)p(heta) & \mathbf{p}(\mathcal{X}) & \mathbf{p}(\mathcal{X}) & \mathbf{p}(\mathcal{X}) & \mathbf{p}(\mathcal{X}) & \mathbf{p}(\mathcal{X}) & \mathbf{p}(\mathcal{X}| heta)p(heta) & \mathbf{p}(\mathcal{X}| heta)p(heta)p(heta) & \mathbf{p}(\mathcal{X}| heta)p(heta)p($$

Posterior

Bayes' Rule

give point estimates: one fixed parameter θ

Bayesian Approach

- 1. Prior is pdf $p(\theta)$
 - lacktriangle high weight in regions where heta is likely
 - **low** weight in regions where θ is **unlikely**
- 2. Assume parameter θ is not fixed generate several estimates θ and average, weighted by probabilities

	1.	2.
$\theta_{\mathrm{ML}} = \operatorname*{argmax}_{\theta} p(\mathcal{X} \theta)$	×	×
$\theta_{\text{MAP}} = \underset{\theta}{\operatorname{argmax}} \ p(\mathcal{X} \theta)p(\theta)$	√	×

Repeat: ML vs. MAP

Maximum Likelihood (ML)

$$heta_{ ext{ML}} = rgmax_{ heta} p(\mathcal{X}| heta)$$
 $ext{$\square$ Maximum A Posteriori (MAP)}$

$$\theta_{\text{MAP}} = \underset{\theta}{\operatorname{arg\,max}} p(\mathcal{X}|\theta)p(\theta)$$

├ one fixed parameter

Bayes

Parameter θ is random variable with prior $p(\theta)$

$$\theta_{\text{Bayes}} = E[\theta|\mathcal{X}] = \int \theta p(\theta|\mathcal{X}) d\theta$$

Frequentist vs. Bayesian

Frequentist Approach

- \square Assumes unknown, fixed parameter θ
- \square Estimates θ with some confidence
- Prediction by estimated parameter value

Bayesian Approach

- Unknown parameters as random variables
- Probability quantifies uncertainty
- □ Prediction by expectation over unknown parameters

Consider coin toss example

probability of heads
$$\widehat{p} = \frac{\#\{\text{Heads}\}}{\#\{\text{Tosses}\}}$$

$$\mathcal{X} = \{1, 1, 1, 0, 0, 1, 1, 0, 1\} \implies \widehat{p} = \frac{6}{9}$$

$$\mathcal{X} = \{1, 1, 1\} \implies \widehat{p} = \frac{3}{3} = 1$$

Consider a Casino

- □ Machine A: 3 wins out of 4 plays
- □ Machine B: 81 wins out of 121 plays

Which Machine would you choose?

- by intuition: Bbecause more samples = reliable
- □ ML estimate

$$\hat{\theta}_{ML,A} = \frac{3}{4} \approx 0.75$$
 $\hat{\theta}_{ML,B} = \frac{81}{121} \approx 0.67$

Consider a Casino

- □ Machine A: 3 wins out of 4 plays
- □ Machine B: 81 wins out of 121 plays

Binomial distribution pdf:

$$p(k|n,\theta) = P(X=k) = \binom{n}{k} \theta^k (1-\theta)^{n-k}$$

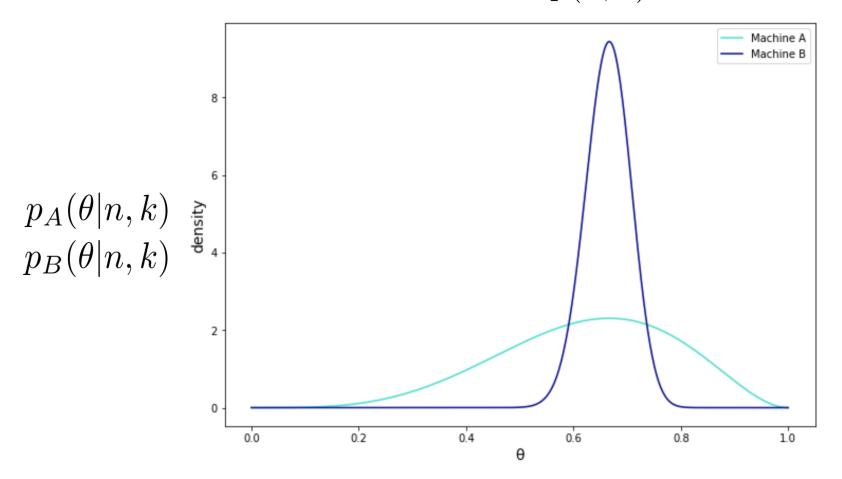
□ MAP estimate

$$\widehat{\theta}_{\text{MAP}} = \underset{\theta}{\operatorname{arg\,max}} \ p(n, k | \theta) p(\theta)$$

Detailed steps on learnit

$$\widehat{\theta}_{\mathrm{MAP},A} = \widehat{\theta}_{\mathrm{MAP},B} \approx 0.667$$

Bayes
$$p(\theta|\mathrm{Data}) = p(\theta|n,k) = \frac{p(n,k|\theta)p(\theta)}{p(n,k)}$$



 $p_A(\theta|n,k)$



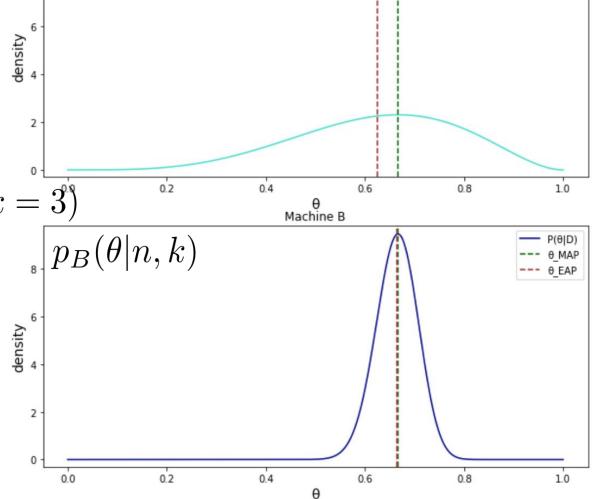
Expected A Posteriori (EAP)

$$\theta_{\text{Bayes,A}} = \mathrm{E}(\theta|\mathcal{X}_A)$$

$$= \mathrm{E}(\theta|n=4, k=3)$$

 $\theta_{\mathrm{Bayes,A}} \approx 0.625$

$$\theta_{\rm Bayes,B} \approx 0.664$$



Machine A

 $P(\theta|D)$

θ_MAP θ EAP

https://towardsdatascience.com/mle-map-and-bayesian-inference-3407b2d6d4d9

Consider a Casino

- □ Machine A: 3 wins out of 4 plays
- □ Machine B: 81 wins out of 121 plays

Estimated winning probability:

$$\square$$
 ML estimate $\widehat{ heta}_{\mathrm{ML},A} = 0.75,$

 $\theta_{\mathrm{ML},B} \approx 0.67$

$$\square$$
 MAP estimate $\widehat{ heta}_{\mathrm{MAP},A}pprox 0.667,$

- $\theta_{\text{MAP},B} \approx 0.667$
- \square Bayes estimate $\theta_{\mathrm{Bayes,A}} pprox 0.625$
- $\theta_{\rm Bayes,B} \approx 0.664$

Likelihood or Bayes?

- Bayes uses more information than ML solutions:
 - additional training data changes the estimate
 - Uncertainty of estimate is well reflected
- But Bayes is often complex to compute therefore sampling of the posterior

=> Choice of Likelihood or Bayes depends on problem

Bayesian Approach

$$p(x'|\mathcal{X}) = \int p(x'|\theta)p(\theta|\mathcal{X})d\theta$$

- In certain cases, it is easy to integrate
- Conjugate priorPosterior has the same density as prior
- Sampling (Markov Chain Monte Carlo)
 Sample from the posterior and average
- Approximate the posteriorwith a model easier to integrate

 \square Assume data is Gaussian $f(x) = \mathcal{N}(\mu, \sigma^2)$

$$p(\mathcal{X}|\mu,\sigma^2) = \prod f(x_n|\mu,\sigma^2)$$

□ Gaussian Prior

$$p(\mu) = \mathcal{N}(\mu_0, \sigma_0^2)$$

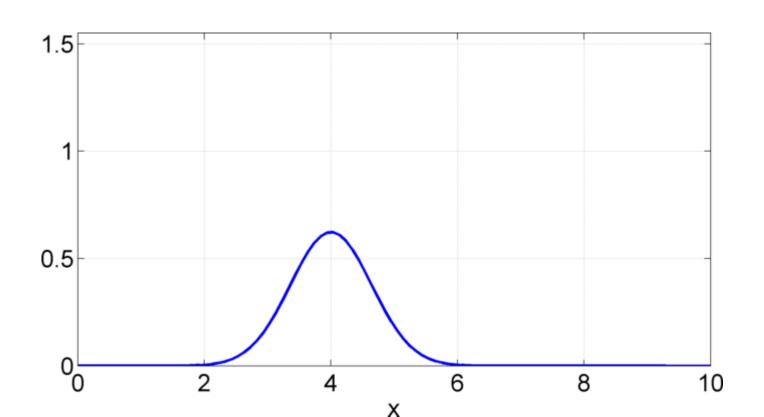
Posterior is Gaussian

$$p(\mu|\mathcal{X}) \propto p(\mu)p(\mathcal{X}|\mu) = \mathcal{N}(\mu_N, \sigma_N^2)$$

$$\mu_N = \frac{\sigma^2}{N\sigma_0^2 + \sigma^2}\mu_0 + \frac{N\sigma_0^2}{N\sigma_0^2 + \sigma^2}m \qquad m = \frac{1}{N}\sum_{n=1}^N x_n$$

$$\frac{1}{\sigma_N^2} = \frac{1}{\sigma_0^2} + \frac{N}{\sigma^2}$$

 \Box Gaussian Prior $p(\mu) = \mathcal{N}(\mu_0 = 4, \sigma_0^2 = 0.8^2)$ assumption of prior knowledge!

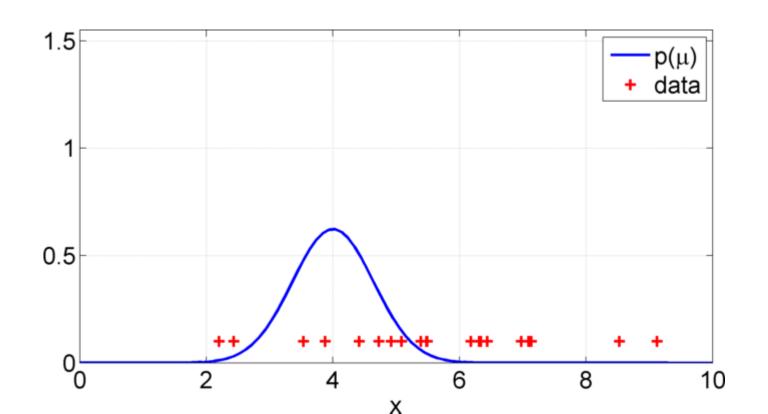


□ Gaussian Prior

$$p(\mu) = \mathcal{N}(\mu_0 = 4, \sigma_0^2 = 0.8^2)$$

Data

$$p(\mathcal{X}|\mu) = \mathcal{N}(m = 6, \sigma^2 = 1.5^2)$$

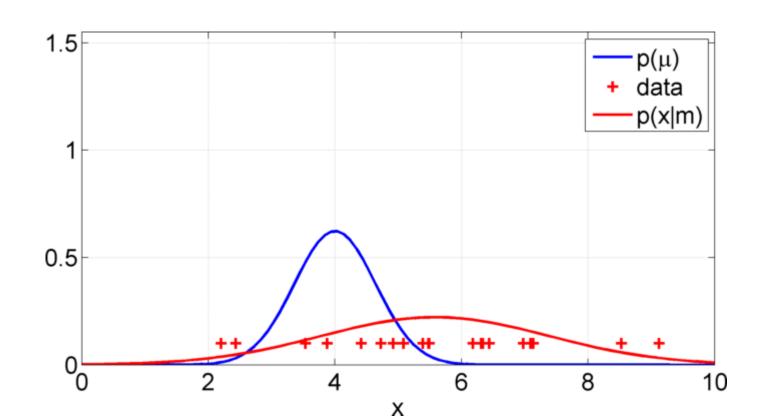


□ Gaussian Prior

$$p(\mu) = \mathcal{N}(\mu_0 = 4, \sigma_0^2 = 0.8^2)$$

Data

$$p(\mathcal{X}|\mu) = \mathcal{N}(m = 6, \sigma^2 = 1.5^2)$$



□ Gaussian Prior

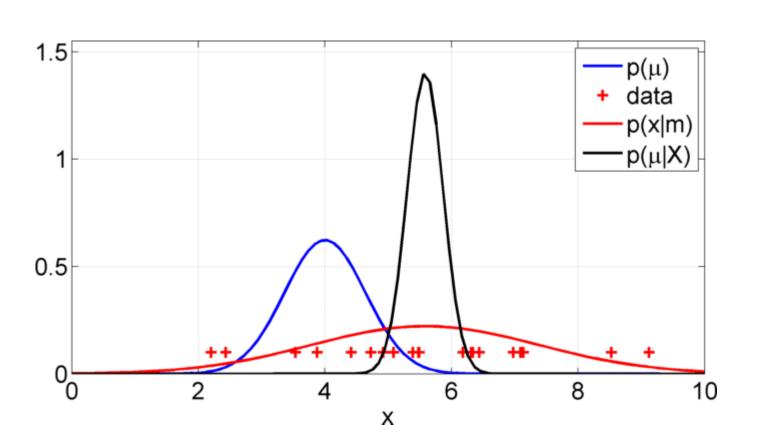
$$p(\mu) = \mathcal{N}(\mu_0 = 4, \sigma_0^2 = 0.8^2)$$

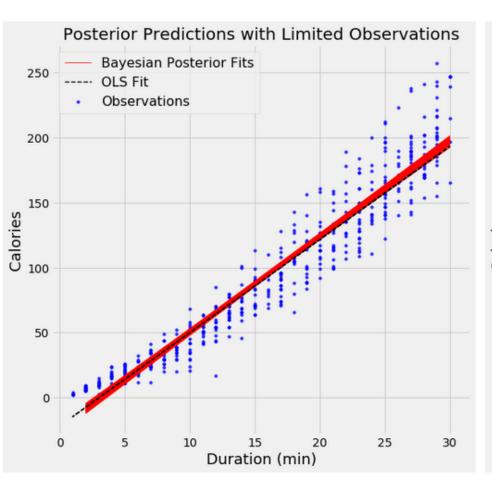
Data

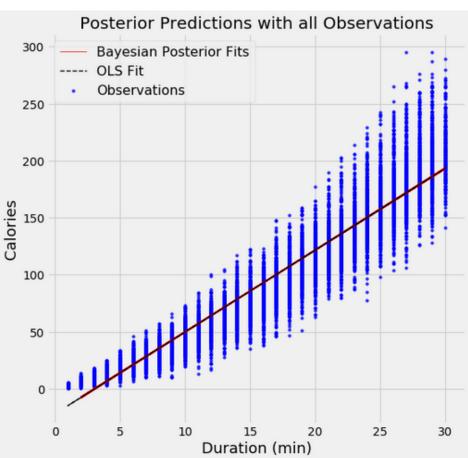
$$p(\mathcal{X}|\mu) = \mathcal{N}(m = 6, \sigma^2 = 1.5^2)$$

Posterior

$$p(\mu|\mathcal{X}) = \mathcal{N}(\mu_N = 5.7, \sigma_N^2 = 0.3^2)$$







https://towardsdatascience.com/introduction-to-bayesian-linear-regression-e66e60791ea7

Line with Gaussian error

$$r_n = f(\boldsymbol{x}_n) = w_0 + w_1 \boldsymbol{x}_n + \epsilon, \quad \epsilon \sim \mathcal{N}(0, 1/\beta)$$

 $r_n = f(\boldsymbol{x}_n) = \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n + \epsilon, \quad \epsilon \sim \mathcal{N}(0, 1/\beta), \ \boldsymbol{w} = (w_0, w_1)^{\mathrm{T}}$

 \square Assume samples $oldsymbol{x}_n, r_n, \ n=1,\ldots,N$

$$p(r_n|\boldsymbol{x}_n, \boldsymbol{w}, \beta) \sim \mathcal{N}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n, 1/\beta)$$

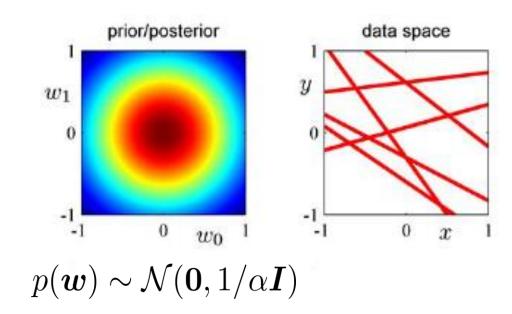
□ ML estimate

$$\boldsymbol{w}_{\mathrm{ML}} = (\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X})^{-1}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{r}$$

 \square Assume prior $p(\boldsymbol{w}) \sim \mathcal{N}(\boldsymbol{0}, 1/\alpha \boldsymbol{I})$

likelihood

No data N=0



Line with Gaussian error

$$r_n = f(\boldsymbol{x}_n) = \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n + \epsilon, \quad \epsilon \sim \mathcal{N}(0, 1/\beta), \ \boldsymbol{w} = (w_0, w_1)^{\mathrm{T}}$$

 \square Assume samples $\boldsymbol{x}_n, r_n, \ n=1,\ldots,N$

$$p(r_n|\boldsymbol{x}_n, \boldsymbol{w}, \beta) \sim \mathcal{N}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n, 1/\beta)$$

□ ML and MAP estimate

$$\boldsymbol{w}_{\mathrm{ML}} = (\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X})^{-1}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{r} \quad \boldsymbol{w}_{\mathrm{MAP}} = \beta((\alpha \boldsymbol{I} + \beta \boldsymbol{X}^{\mathrm{T}}\boldsymbol{X})^{-1})\boldsymbol{X}^{\mathrm{T}}\boldsymbol{r}$$

- \square Assume prior $p(\boldsymbol{w}) \sim \mathcal{N}(\boldsymbol{0}, 1/\alpha \boldsymbol{I})$
- $_{\square}$ posterior $p(oldsymbol{w}|oldsymbol{X},oldsymbol{r})\propto p(oldsymbol{X},oldsymbol{r}|oldsymbol{w})p(oldsymbol{w})$

Line with Gaussian error

$$r_n = f(\boldsymbol{x}_n) = \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n + \epsilon, \quad \epsilon \sim \mathcal{N}(0, 1/\beta), \ \boldsymbol{w} = (w_0, w_1)^{\mathrm{T}}$$

 \square Assume samples $oldsymbol{x}_n, r_n, \ n=1,\ldots,N$

$$p(r_n|\boldsymbol{x}_n, \boldsymbol{w}, \beta) \sim \mathcal{N}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n, 1/\beta)$$

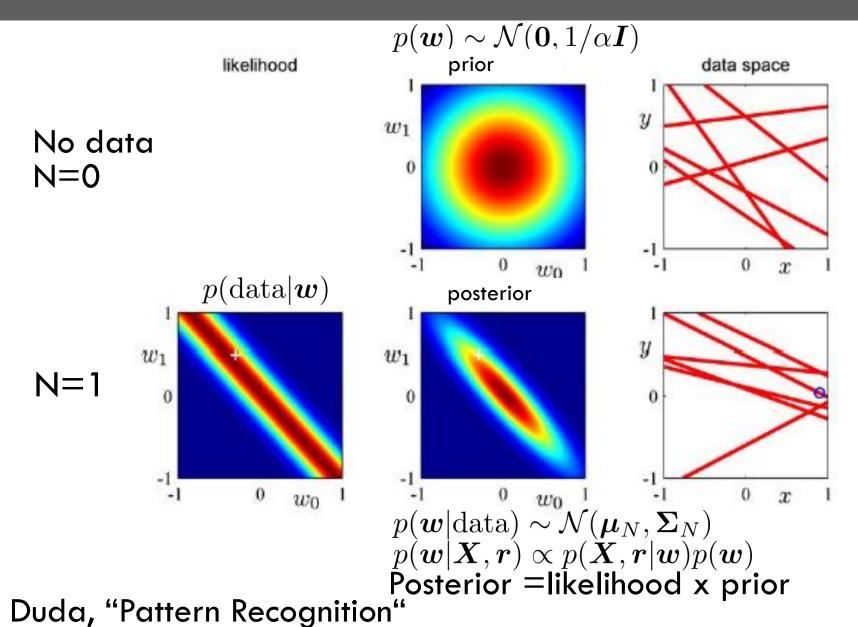
□ ML and MAP estimate

$$\boldsymbol{w}_{\mathrm{ML}} = (\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X})^{-1}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{r} \quad \boldsymbol{w}_{\mathrm{MAP}} = \beta((\alpha \boldsymbol{I} + \beta \boldsymbol{X}^{\mathrm{T}}\boldsymbol{X})^{-1})\boldsymbol{X}^{\mathrm{T}}\boldsymbol{r}$$

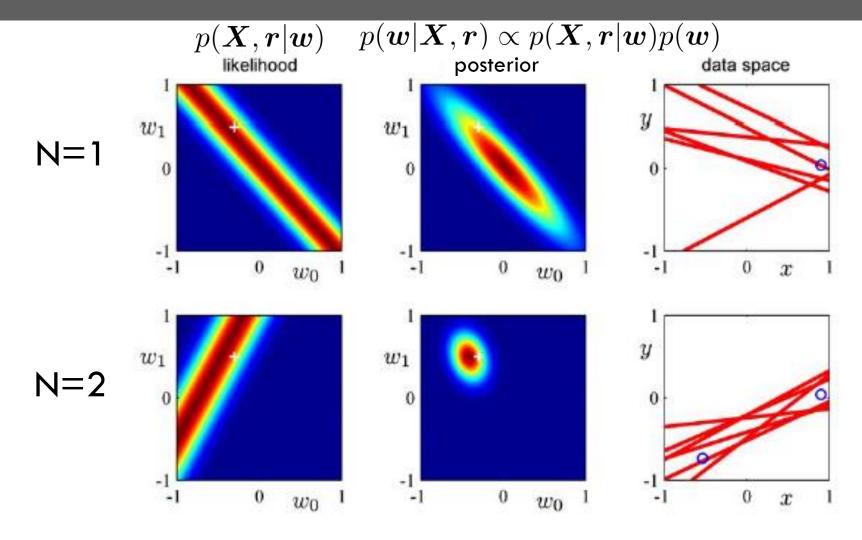
- \square Assume prior $p(\boldsymbol{w}) \sim \mathcal{N}(\boldsymbol{0}, 1/\alpha \boldsymbol{I})$
- $_{\square}$ posterior $p(m{w}|m{X},m{r}) \sim \mathcal{N}(m{\mu}_N,m{\Sigma}_N)$

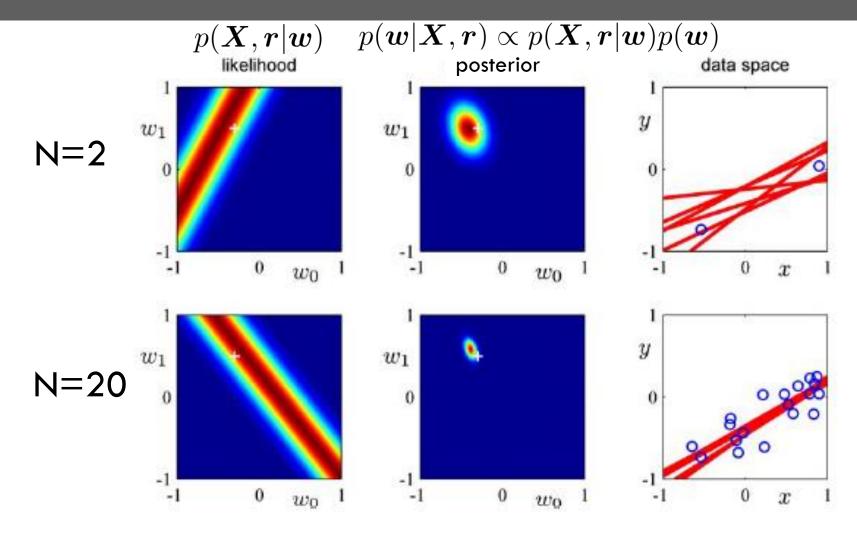
$$oldsymbol{\mu}_N = eta oldsymbol{\Sigma}_{oldsymbol{N}} oldsymbol{X}^{\mathrm{T}} oldsymbol{r}$$

$$\Sigma_N = (\alpha \boldsymbol{I} + \beta \boldsymbol{X}^{\mathrm{T}} \boldsymbol{X})^{-1}$$



32





Line with Gaussian error

$$r_n = f(\boldsymbol{x}_n) = \boldsymbol{w}^{\mathrm{T}} \boldsymbol{x}_n + \epsilon, \quad \epsilon \sim \mathcal{N}(0, 1/\beta), \ \boldsymbol{w} = (w_0, w_1)^{\mathrm{T}}$$

 \square Assume samples $\boldsymbol{x}_n, r_n, \ n=1,\ldots,N$

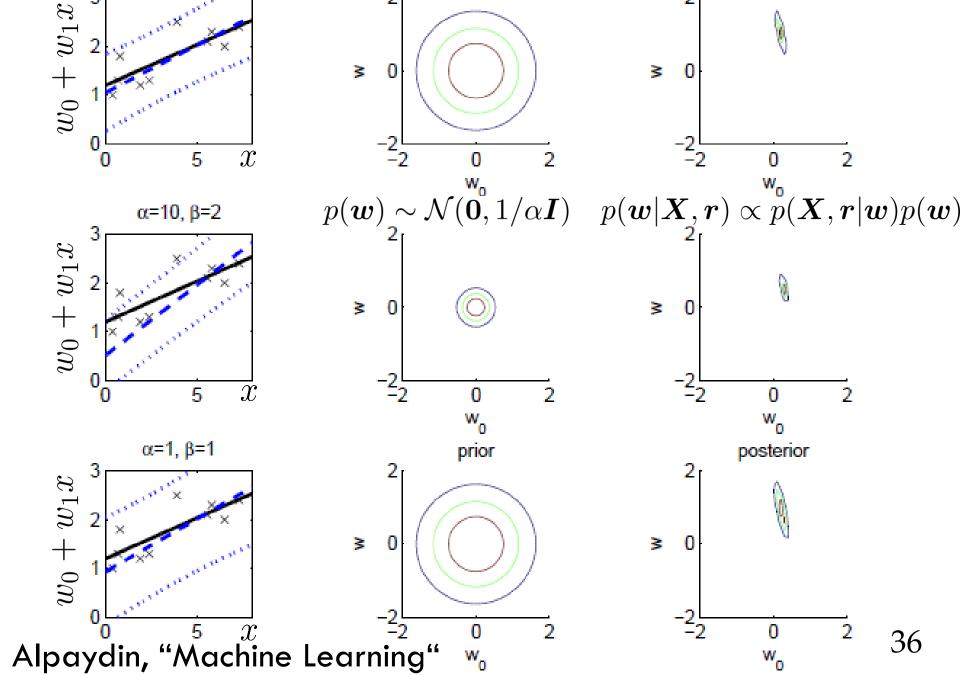
$$p(r_n|\boldsymbol{x}_n, \boldsymbol{w}, \beta) \sim \mathcal{N}(\boldsymbol{w}^{\mathrm{T}}\boldsymbol{x}_n, 1/\beta)$$

□ ML and MAP estimate

$$\boldsymbol{w}_{\mathrm{ML}} = (\boldsymbol{X}^{\mathrm{T}}\boldsymbol{X})^{-1}\boldsymbol{X}^{\mathrm{T}}\boldsymbol{r} \quad \boldsymbol{w}_{\mathrm{MAP}} = \beta((\alpha \boldsymbol{I} + \beta \boldsymbol{X}^{\mathrm{T}}\boldsymbol{X})^{-1})\boldsymbol{X}^{\mathrm{T}}\boldsymbol{r}$$

- \square Assume prior $p(\boldsymbol{w}) \sim \mathcal{N}(\boldsymbol{0}, 1/\alpha \boldsymbol{I})$

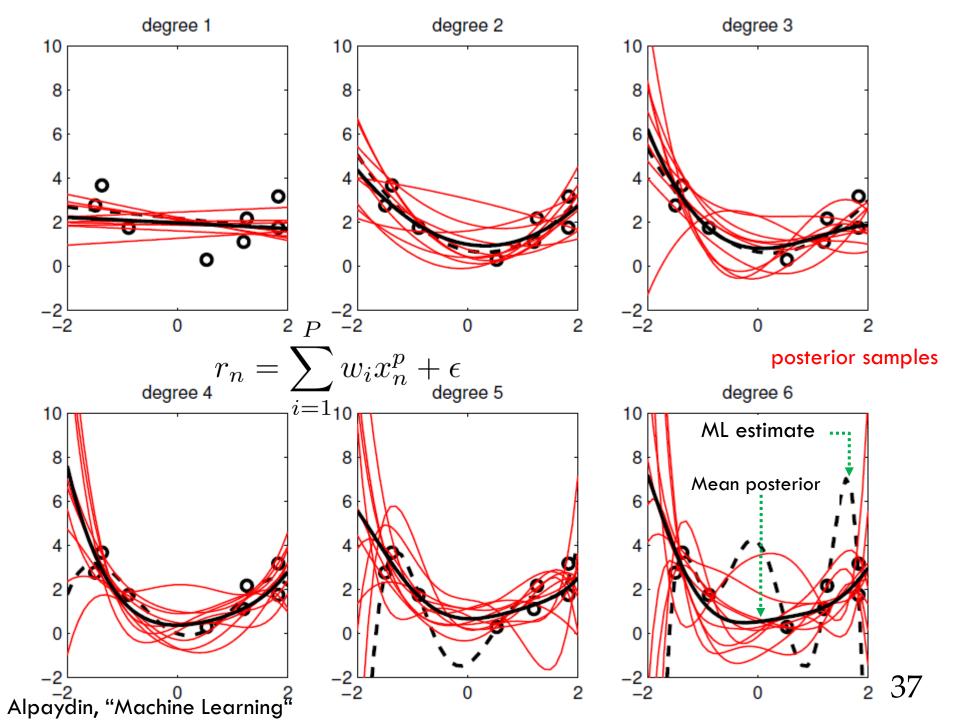
$$egin{aligned} egin{aligned} posterior & p(m{w}|m{X},m{r}) \sim \mathcal{N}(m{\mu}_N,m{\Sigma}_N) \ & m{\mu}_N = eta m{\Sigma}_N m{X}^{\mathrm{T}}m{r} \ & m{\Sigma}_N = (lpha m{I} + eta m{X}^{\mathrm{T}}m{X})^{-1} \end{aligned}$$



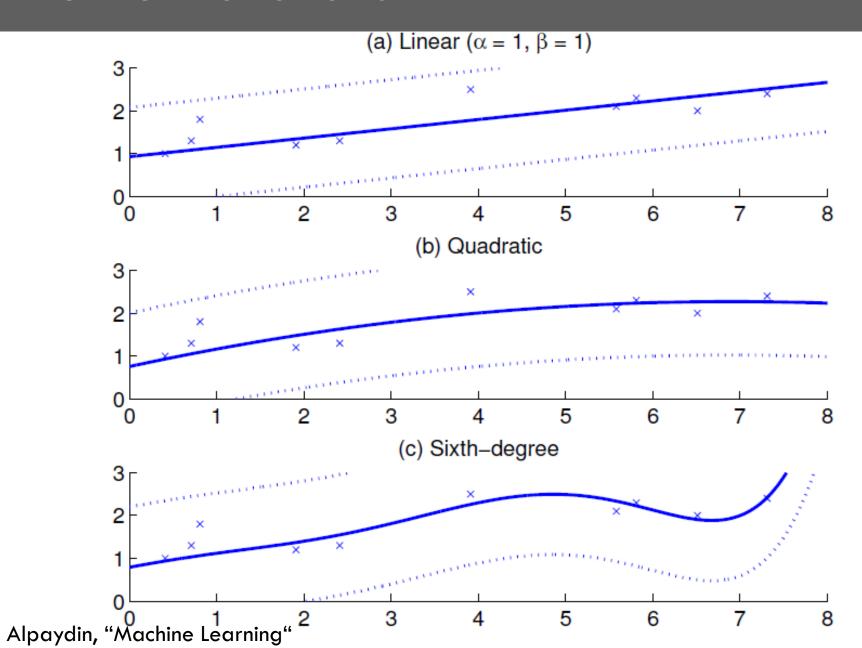
prior

posterior

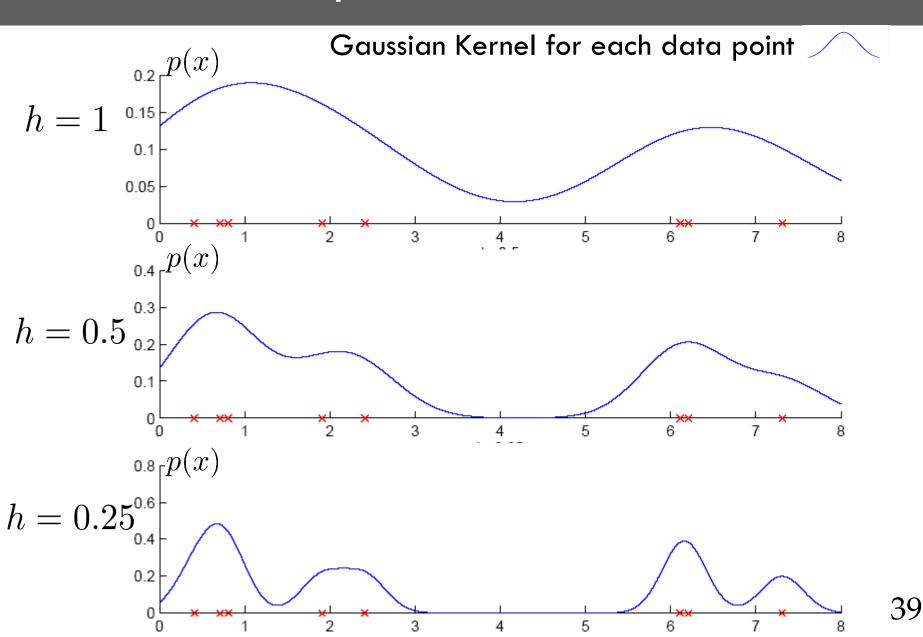
α=1, β=2



Kernel Functions

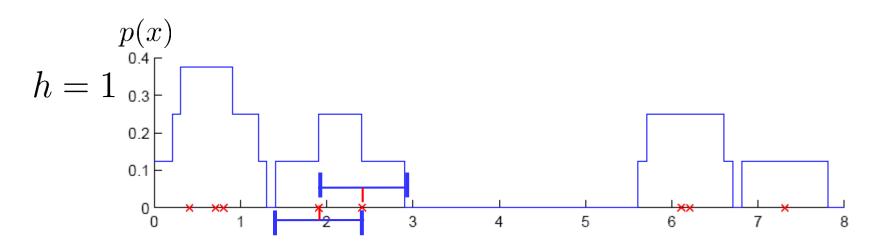


Reminder: Nonparametric Kernel Estimator



Nonparametric Bayes

- Similar to k-NN and Parzen windows:training set = parameters
- Model complexity can increases more data
 (in practice up to N, potentially to infinity)

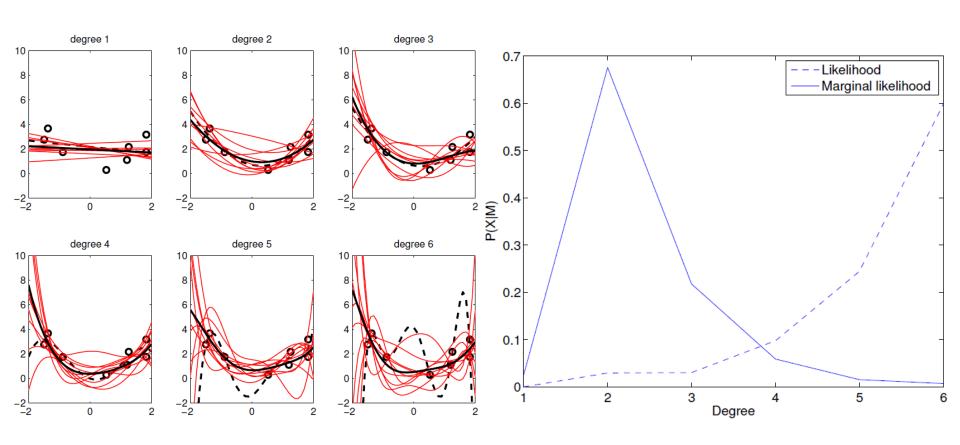


Howto Prior

- Defining a prior is subjective
- Uninformative prior if no prior preference
- - □ Level II $p(x|\mathcal{X}) = \int p(x|\theta)p(\theta|\mathcal{X},\alpha)p(\alpha) \ d\alpha$
 - lacktriangle Level II ML/Empirical Bayes: Use one good $lpha^*$

$$p(x|\mathcal{X}) = \int p(x|\theta)p(\theta|\mathcal{X}, \alpha^*) \ d\theta$$

Bayesian Model Comparison



Bayesian Model Comparison

o Marginal likelihood of a model ${\mathcal M}$

$$p(X|\mathcal{M}) = \int p(X|\theta, \mathcal{M}) p(\theta|\mathcal{M}) d\theta$$

Posterior probability of model given data

$$p(\mathcal{M}|\mathcal{X}) = \frac{p(\mathcal{X}|\mathcal{M})p(\mathcal{M})}{p(\mathcal{X})}$$

□ Bayes' factor

$$\frac{P(\mathcal{M}_1|\mathcal{X})}{P(\mathcal{M}_0|\mathcal{X})} = \frac{P(\mathcal{X}|\mathcal{M}_1)}{P(\mathcal{X}|\mathcal{M}_0)} \frac{P(\mathcal{M}_1)}{P(\mathcal{M}_0)}$$

Approximations

$$\square \qquad \mathsf{BIC} \qquad \log p(\mathcal{X}|\mathcal{M}) \approx \mathsf{BIC} \equiv \log p(\mathcal{X}|\theta_{ML}, \mathcal{M}) - \frac{|\mathcal{M}|}{2} \log N$$

$$\triangle$$
 AIC $\equiv \log p(\mathcal{X}|\theta_{ML}, \mathcal{M}) - |\mathcal{M}|$

Summary

- □ ML and MAP give fixed parameter estimates
- □ Bayes
 - assumes parameter is random variable
 - gives more information
 - is more complex
 - we can sample more data