# ECE-271A Statistical Learning I: Bayesian parameter estimation

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#### Bayesian estimation

last class we considered the Gaussian problem

$$P_{X|\mu}(X \mid \mu) = G(X, \mu, \sigma^2), \ \sigma^2 \text{ known}$$
  $P_{\mu}(\mu) = G(\mu, \mu_0, \sigma_0^2)$ 

and showed that

$$P_{\mu|T}(\mu \mid D) = G(x, \mu_n, \sigma_n^2)$$

$$P_{\mu|T}(\mu \mid D) = G(X, \mu_n, \sigma_n^2)$$

$$P_{X|T}(X \mid D) = G(X, \mu_n, \sigma^2 + \sigma_n^2)$$

$$\mu_n = \frac{n\sigma_0^2}{n\sigma_0^2 + \sigma^2} \hat{\mu}_{ML} + \frac{\sigma^2}{n\sigma_0^2 + \sigma^2} \mu_0$$

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

good example of various properties that are typical of Bayesian parameter estimates

#### **Properties**

- ► regularization:
  - if  $\sigma_0^2 = \sigma^2$  then  $\mu_n = \frac{n}{n+1} \hat{\mu}_{ML} + \frac{1}{n+1} \mu_0$   $= \frac{1}{n+1} \sum_{i=1}^{n+1} X_i, \quad \text{with } X_{i+1} = \mu_0$
- ▶ Bayes is equal to ML on a virtual sample with extra points
  - in this case, one additional point equal to the mean of the prior
  - for large n, extra point is irrelevant
  - for small n, it regularizes the Bayes estimate by
    - directing the posterior mean towards the prior mean
    - reducing the variance of the posterior  $\frac{1}{\sigma_n^2} = \frac{n}{\sigma^2} + \frac{1}{\sigma_0^2}$

## Conjugate priors

- note that
  - the prior  $P_{\mu}(\mu) = G(\mu, \mu_0, \sigma_0^2)$  is Gaussian
  - the posterior  $P_{\mu|T}(\mu \mid D) = G(x, \mu_n, \sigma_n^2)$  is Gaussian
- whenever this is the case (posterior in the same family as prior) we say that
  - $P_{\mu}(\mu)$  is a conjugate prior for the likelihood  $P_{X|\mu}(X \mid \mu)$
  - posterior  $P_{\mu|T}(\mu|D)$  is the reproducing density
- ► HW: a number of likelihoods have conjugate priors

Likelihood	Conjugate prior		
Bernoulli	Beta		
Poisson	Gamma		
Exponential	Gamma		
Normal (known $\sigma^2$ )	Gamma		

#### **Priors**

- potential problem of the Bayesian framework
  - "I don't really have a strong belief about what the most likely parameter configuration is"
- ▶ in these cases it is usual to adopt a non-informative prior
- the most obvious choice is the uniform distribution

$$P_{\Theta}(\theta) = \alpha$$

- ► there are, however, problems with this choice
  - if  $\theta$  is unbounded this is an improper distribution

$$\int_{0}^{\infty} P_{\Theta}(\theta) d\theta = \infty \neq 1$$

the prior is not invariant to all reparametrizations

#### Example

- ▶ consider  $\Theta$  and a new random variable  $\eta$  with  $\eta = e^{\Theta}$
- ▶ since this is a 1-to-1 transformation it should not affect the outcome of the inference process
- we check this by using the change of variables theorem
  - if y = f(x) then

$$P_{Y}(y) = \frac{1}{\left|\frac{\partial f}{\partial x}\right|_{x=f^{-1}(y)}} P_{X}(f^{-1}(y))$$

▶ in this case

$$P_{\eta}(\eta) = \frac{1}{\left|\frac{\partial e^{\theta}}{\partial \theta}\right|_{\theta = \log n}} P_{\Theta}(\log \eta) = \frac{1}{|\eta|} P_{\Theta}(\log \eta)$$

#### Invariant non-informative priors

- ▶ for uniform  $\eta$  this means that  $P_{\eta}(\eta)\alpha\frac{1}{|\eta|}$ , i.e. not constant ▶ this means that
  - there is no consistency between  $\Theta$  and h
  - a 1-to-1 transformation changes the non-informative prior into an informative one
- to avoid this problem the non-informative prior has to be invariant
- ▶ e.g. consider a location parameter:
  - a parameter that simply shifts the density
  - e.g. the mean of a Gaussian
- ▶ a non-informative prior for a location parameter has to be invariant to shifts, i.e. the transformation  $Y = \mu + c$

#### Location parameters

▶ in this case

$$P_{Y}(y) = \frac{1}{\left|\frac{\partial(\mu+c)}{\partial\mu}\right|_{\mu=y-c}} P_{\mu}(y-c) = P_{\mu}(y-c)$$

and, since this has to be valid for all c,

$$P_{Y}(y) = P_{\mu}(y)$$

hence

$$P_{\mu}(y-c)=P_{\mu}(y)$$

- which is valid for all c if and only if  $P_{\mu}(\mu)$  is uniform
- ▶ non-informative prior for location is  $P_{\mu}(\mu) \alpha 1$

#### Scale parameters

a scale parameter is one that controls the scale of the density

$$\sigma^{-1}f\left(\frac{X}{\sigma}\right)$$

e.g. the variance of a Gaussian distribution

▶ it can be shown that, in this case, the non-informative prior invariant to scale transformations is

$$P_{\sigma}(\sigma) = \frac{1}{\sigma}$$

▶ note that, as for location, this is an improper prior

- ▶ non-informative priors are the end of the spectrum where we don't know what parameter values to favor
- ▶ at the other end, i.e. when we are absolutely sure, the prior becomes a delta function

$$P_{\Theta}(\theta) = \delta(\theta - \theta_0)$$

▶ in this case

$$P_{\Theta|T}(\theta \mid D) \alpha P_{T|\Theta}(D \mid \theta) \delta(\theta - \theta_0)$$

and the predictive distribution is

$$P_{X|T}(X \mid D) \propto \int P_{X|\Theta}(X \mid \theta) P_{T|\Theta}(D \mid \theta) \delta(\theta - \theta_0) d\theta$$
$$= P_{X|\Theta}(X \mid \theta_0)$$

▶ this is identical to ML if  $\theta_0 = \theta_{ML}$ 

- ► hence,
  - ML is a special case of the Bayesian formulation,
  - where we are absolutely confident that the ML estimate is the correct value for the parameter
- but we could use other values for  $\theta_0$ . For example the value that maximizes the posterior

$$\theta_{MAP} = \underset{\theta}{\operatorname{arg\,max}} P_{\Theta|T}(\theta \mid D) = \underset{\theta}{\operatorname{arg\,max}} P_{T|\Theta}(D \mid \theta) P_{\Theta}(\theta)$$

this is called the MAP estimate and makes the predictive distribution equal to

$$P_{X|T}(X \mid D) = P_{X|\Theta}(X \mid \theta_{MAP})$$

▶ it can be useful when the true predictive distribution has no closed-form solution

- ▶ the natural question is then
  - "what if I don't get the prior right?"; "can I do terribly bad?"
  - "how robust is the Bayesian solution to the choice of prior?"
  - let's see how much the solution changes between the two extremes
- ▶ for the Gaussian problem
  - absolute certainty priors:  $P_{\mu}(\mu) = \delta(\mu \mu_p)$ 
    - MAP estimate: since  $P_{\mu|T}(\mu \mid D) = G(x, \mu_n, \sigma_n^2)$  we have

$$\mu_{p} = \mu_{n} = \frac{n\sigma_{0}^{2}}{n\sigma_{0}^{2} + \sigma^{2}} \mu_{ML} + \frac{\sigma^{2}}{n\sigma_{0}^{2} + \sigma^{2}} \mu_{0}$$

- ML estimate is  $\mu_p = \mu_{ML}$
- we have seen already that these are similar unless the sample is small (MAP = ML on sample with extra point)

- ▶ for the Gaussian problem
  - non-informative prior:
    - in this case it is  $P_{\mu}(\mu) \alpha 1$  or

$$P_{\mu}(\mu) = \lim_{\sigma_0^2 \to \infty} G(\mu, \mu_0, \sigma_0^2)$$

from which

$$\mu_{n} = \lim_{\sigma_{0}^{2} \to \infty} \left( \frac{n\sigma_{0}^{2}}{n\sigma_{0}^{2} + \sigma^{2}} \mu_{ML} + \frac{\sigma^{2}}{n\sigma_{0}^{2} + \sigma^{2}} \mu_{0} \right) = \mu_{ML}$$

$$\frac{1}{\sigma_n^2} = \lim_{\sigma_0^2 \to \infty} \left( \frac{n}{\sigma^2} + \frac{1}{\sigma_0^2} \right) = \frac{n}{\sigma^2} \iff \sigma_n^2 = \sigma_{ML}^2$$

and

$$P_{X|T}(X \mid D) = G(X, \mu_n, \sigma^2 + \sigma_n^2) = G\left(X, \mu_{ML}, \sigma^2\left(1 + \frac{1}{n}\right)\right)$$

- ▶ in summary, for the two prior extremes
  - delta prior centered on MAP:

$$P_{X|T}(X \mid D) = G(X, \mu_{MAP}, \sigma^2)$$

$$P_{X|T}(X \mid D) = G(X, \mu_{MAP}, \sigma^{2}) \qquad \mu_{MAP} = \frac{n\sigma_{0}^{2}}{n\sigma_{0}^{2} + \sigma^{2}} \mu_{ML} + \frac{\sigma^{2}}{n\sigma_{0}^{2} + \sigma^{2}} \mu_{0}$$

delta prior centered on ML:

$$P_{X|T}(X \mid D) = G(x, \mu_{ML}, \sigma^2)$$

non-informative prior

$$P_{X|T}(X \mid D) = G\left(X, \mu_{ML}, \sigma^2\left(1 + \frac{1}{n}\right)\right)$$

- ▶ all Gaussian, "qualitatively the same":
  - somewhat different parameters for small n; equal for large n
- this indicates robustness to "incorrect" priors!

- ▶ another example, problem 3.5.17 DHS (HW prob 3)
  - multivariate Bernoulli (d independent Bernoulli variables)
  - since Bernoulli is

$$P_{X|\Theta}(X \mid \theta) = \begin{cases} \theta, & X = 1 \\ 1 - \theta, & X = 0 \end{cases} = \theta^{X} (1 - \theta)^{1 - X}$$

multivariate likelihood is:

$$P_{X\mid\Theta}(X\mid\theta) = \prod_{i=1}^{d} \theta_{i}^{x_{i}} (1-\theta_{i})^{1-x_{i}}$$

• in (a) you show that if  $D = \{x^{(1)}, ..., x^{(n)}\}$  is a set of n iid samples, then

$$P_{T|\Theta}(D \mid \theta) = \prod_{i=1}^{d} \theta_i^{s_i} (1 - \theta_i)^{n - s_i}, \qquad s_i = \sum_{j=1}^{n} x_i^{(j)}$$

- ▶ another example, problem 3.5.17 DHS (HW prob 3)
  - in (b) you then show that if  $\Theta$  is uniform (non-informative) the predictive distribution is

$$P_{X|T}(X \mid D) = \prod_{i=1}^{d} \left( \frac{S_i + 1}{n+2} \right)^{X_i} \left( 1 - \frac{S_i + 1}{n+2} \right)^{1-X_i}$$

in (d) you show that comparing with

$$P_{X\mid\Theta}(X\mid\theta) = \prod_{i=1}^{d} \theta_{i}^{x_{i}} (1-\theta_{i})^{1-x_{i}}$$

- this can be interpreted as:
  - under Bayes, with a uniform prior, the predicted distribution is the same as the likelihood, with the parameter estimate

$$\hat{\theta}_i = \frac{s_i + 1}{n + 2}$$

- ▶ let's now consider the extreme of  $P_{\Theta}(\theta) = \delta(\theta \hat{\theta})$ 
  - ML: we know that

$$\hat{\theta}_i = \frac{S_i}{n}$$

and

$$P_{X|T}(X \mid D) = \prod_{i=1}^{d} \left(\frac{S_i}{n}\right)^{X_i} \left(1 - \frac{S_i}{n}\right)^{1 - X_i}$$

- this can be interpreted as:
  - the predicted distribution is the same as the likelihood, with the parameter estimate

$$\hat{\theta}_i = \frac{S_i}{n}$$

• MAP: given prior  $P_{\Theta} = \prod_{j} P_{\Theta_{j}}(\theta_{j})$  $\hat{\theta} = \arg\max_{\theta} \left\{ \log P_{T|\Theta}(D \mid \theta) + \log P_{\Theta}(\theta) \right\}$ 

and since

$$P_{T|\Theta}(D|\theta) = \prod_{i=1}^{d} \theta_i^{s_i} (1 - \theta_i)^{n - s_i}, \qquad s_i = \sum_{j=1}^{n} X_i^{(j)}$$

this is

$$\hat{\theta}_{i} = \arg\max_{\theta} \left\{ S_{i} \log \theta_{i} + (n - S_{i}) \log(1 - \theta_{i}) + \log P_{\Theta_{i}}(\theta_{i}) \right\}$$

i.e. the solution of

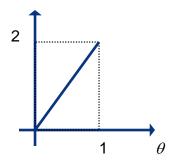
$$\frac{S_{i}}{\theta_{i}} - \frac{(n - S_{i})}{1 - \theta_{i}} + \frac{1}{P_{\Theta_{i}}(\theta_{i})} \frac{\partial}{\partial \theta_{i}} P_{\Theta_{i}}(\theta_{i}) = 0$$

let's consider some specific priors

• prior that favors "1"s

$$P_{\Theta_i}(\theta) = 2\theta$$

MAP solution:



$$\frac{S_i}{\theta_i} - \frac{(n - S_i)}{1 - \theta_i} + \frac{1}{\theta_i} = 0 \iff \hat{\theta}_i = \frac{S_i + 1}{n + 1}$$

and

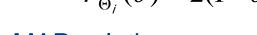
$$P_{X|T}(X \mid D) = \prod_{i=1}^{d} \left(\frac{S_i + 1}{n+1}\right)^{X_i} \left(1 - \frac{S_i + 1}{n+1}\right)^{1 - X_i}$$

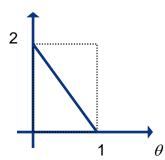
- this can be interpreted as:
  - the predicted distribution is the same as the likelihood, with the parameter estimate

$$\hat{\theta}_{i} = \frac{s_{i} + 1}{n + 1}$$

• prior that favors "0"s

$$P_{\Theta_i}(\theta) = 2(1-\theta)$$





MAP solution:

$$\frac{S_i}{\theta_i} - \frac{(n - S_i)}{1 - \theta_i} - \frac{1}{1 - \theta_i} = 0 \iff \hat{\theta}_i = \frac{S_i}{n + 1}$$

and

$$P_{X|T}(X \mid D) = \prod_{i=1}^{d} \left(\frac{S_i}{n+1}\right)^{X_i} \left(1 - \frac{S_i}{n+1}\right)^{1-X_i}$$

- this can be interpreted as:
  - the predicted distribution is the same as the likelihood, with the parameter estimate

$$\hat{\theta}_i = \frac{S_i}{n+1}$$

#### ▶ in summary

• all cases are of the form 
$$P_{X|T}(X \mid D) = \prod_{i=1}^{d} \hat{\theta}^{x_i} (1 - \hat{\theta})^{1 - x_i}$$

with

Estimator	$\hat{ heta}_{i}$	# tosses	# "1"s	interpretation
ML	$s_i/n$	n	S <sub>i</sub>	
MAP non-informative	$s_i/n$	n	S <sub>i</sub>	"the same"
MAP favor "1"s	$(s_i+1)/(n+1)$	n+1	s <sub>i</sub> +1	"add one 1"
MAP favor "0"s	$s_i/(n+1)$	n+1	S <sub>i</sub>	"add one 0"
Bayes non-informative	$(s_i+1)/(n+2)$	n+2	s <sub>i</sub> +1	"add one of each"

all cases qualitatively the same: "ML estimate on an extended sample with extra points that reflect the bias of the prior".

- these are all examples of regularization
- Q: what is the point of "adding one of each?" by Bayes non-informative?
  - the main problem of ML  $(s_i/n)$  is the "empty bin" problem
  - for small n,  $s_i$  is likely to be zero independently of the value of  $\theta_i$
  - this can lead to all sorts of problems, e.g. a likelihood ratio that goes to infinity
  - by adding "one of each" Bayes eliminates this problem
  - for richly populated bins it makes no difference, but it matters for empty bins
- note that this is consistent with the non-informative prior
  - empty bins are as likely as any other value
  - if we see a lot of them, we need to correct this

#### "empty bin" problem

- "why should I care?" this is unlikely if I have a large sample
- remember that "large" is always relative
- 10 bins in 1D transforms into 100 in 2D, 1000 in 3D, and 10<sup>d</sup> in a d-dimensional space
- when d is large, we are always in the "small sample" regime
- regularization usually makes a tremendous difference

#### example:

- histogram estimates in high-dimensional spaces
- e.g. histogram of English words for indexing web-pages
  - for each page, compute histogram  $C = (c_1, ..., c_w)$  where  $c_i$  is the # of times word i<sup>th</sup> word appeared in page
  - measure similarity between pages i,j with some function d(Ci,Ci)

- ▶ histogram similarity:
  - natural measure is the Kullback-Leibler divergence

$$d(C^{i},C^{j}) = \sum_{k=1}^{w} p_{k}^{i} \log \left(\frac{p_{k}^{i}}{p_{k}^{j}}\right)$$

where the probabilities are the counts after normalization

$$p_k^i = \sum_{k=0}^{c_k^i} c_k^i$$

- problem: log goes to infinity when  $p_k^j = 0!$
- for low-frequency words the noisy estimates are amplified by the ratio of probabilities
- the distance measure has a large variance

- ▶ Prob 3 on HW
  - the count vector C is distributed according to a multinomial distribution

$$P_{C}(C_{1},...,C_{W}) = \frac{n!}{\prod_{k=1}^{W} C_{k}!} \prod_{j=1}^{W} \pi_{j}^{c_{j}}$$

- where  $\pi_i$  is the probability of word j.
- since the  $\pi_i$  are probabilities, we can't use any prior here.
- distribution over vectors  $\pi = (\pi_1, ..., \pi_w)$  must satisfy the constraints of a probability mass function

$$\pi_j > 0$$

$$\sum_j \pi_j = 1$$

- ▶ Prob 3 on HW
  - one such distribution is the Dirichlet distribution

$$P_{\Pi}(\pi_1, \dots, \pi_W) = \frac{\Gamma\left(\sum_{j=1}^W u_j\right)}{\prod_{k=1}^W \Gamma\left(u_j\right)} \prod_{j=1}^W \pi_j^{u_j - 1}$$

- *u<sub>i</sub>* are hyper-parameters
- $\Gamma(.)$  is the gamma function

- ▶ Prob 3 on HW
  - on HW you will show that the posterior is

$$P_{\Pi|C}(\pi \mid C) = \frac{\Gamma\left(\sum_{j=1}^{W} C_j + U_j\right)}{\prod_{k=1}^{W} \Gamma\left(C_j + U_j\right)} \prod_{j=1}^{W} \pi_j^{c_j + U_j - 1}$$

- i.e. Dirichlet of hyper-parameters  $c_j + u_j$
- the prior parameters can be seen as additional counts that regularize the predictive distribution!

