ECE-271A Statistical Learning I: Bayesian parameter estimation

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#### **Bayesian estimation**

Iast class we considered the Gaussian problem

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

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

and showed that

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

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

with

$$\mu_n = \frac{n\sigma_0^2}{n\sigma_0^2 + \sigma^2} \hat{\mu}_{ML} + \frac{\sigma^2}{n\sigma_0^2 + \sigma^2} \mu_0$$
$$\frac{1}{\sigma_n^2} = \frac{n}{\sigma^2} + \frac{1}{\sigma_0^2}$$

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

### **Properties**

#### regularization:

• if 
$$\sigma_0^2 = \sigma^2$$
 then  $\mu_n = \frac{n}{n+1}\hat{\mu}_{ML} + \frac{1}{n+1}\mu_0$   
=  $\frac{1}{n+1}\sum_{i=1}^{n+1}X_i$ , 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 ۲
- for large n, extra point is irrelevant
- for small n, it regularizes the Bayes estimate by  ${}^{\bullet}$ 
  - 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  $P_{\mu|T}(\mu | D) = G(x, \mu_n, \sigma_n^2)$  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 $\sigma^2$ )	al (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

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

• 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

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

### 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

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

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

$$\theta_{MAP} = \arg\max_{\theta} P_{\Theta|T}(\theta \mid D) = \arg\max_{\theta} P_{T|\Theta}(D \mid \theta) P_{\Theta}(\theta)$$

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

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

$$\mu_{MAP} = \frac{n\sigma_0^2}{n\sigma_0^2 + \sigma^2} \mu_{ML} + \frac{\sigma^2}{n\sigma_0^2 + \sigma^2} \mu_0$$

• 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

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

• multivariate likelihood is:

$$P_{X|\Theta}(X \mid \theta) = \prod_{i=1}^{d} \theta_i^{x_i} (1 - \theta_i)^{1 - x_i}$$

 in (a) you show that if D = {x<sup>(1)</sup>, ..., x<sup>(n)</sup>} 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 *Θ* 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

$$P_{X|\Theta}(X \mid \theta) = \prod_{i=1}^{d} \theta_i^{x_i} (1 - \theta_i)^{1 - x_i}$$

- 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 
$$P_{\Theta} = \prod_{i} P_{\Theta_i}(\theta_i)$$

$$\hat{\theta} = \arg \max_{\theta} \left\{ \log P_{T|\Theta}(D \mid \theta) + \log P_{\Theta}(\theta) \right\}$$

• and since

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

• 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:



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

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:



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

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 <sub>i</sub> /n	n	S <sub>i</sub>	
MAP non-informative	s <sub>i</sub> /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<sub>1</sub>, ..., c<sub>w</sub>) where c<sub>i</sub> is the # of times word i<sup>th</sup> word appeared in page
  - measure similarity between pages *i*,*j* with some function  $d(C^i, C^j)$

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

$$\mathcal{O}(\mathcal{C}^{i},\mathcal{C}^{j}) = \sum_{k=1}^{W} \mathcal{P}_{k}^{i} \log\left(\frac{\mathcal{P}_{k}^{i}}{\mathcal{P}_{k}^{j}}\right)$$

• where the probabilities are the counts after normalization

$$\boldsymbol{p}_{k}^{i} = \frac{\boldsymbol{C}_{k}^{i}}{\sum_{k} \boldsymbol{C}_{k}^{i}}$$

- 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

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

- 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

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

- *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

$$P_{\Pi|\mathcal{C}}(\pi \mid \mathcal{C}) = \frac{\Gamma\left(\sum_{j=1}^{W} \mathcal{C}_{j} + \mathcal{U}_{j}\right)}{\prod_{k=1}^{W} \Gamma\left(\mathcal{C}_{j} + \mathcal{U}_{j}\right)} \prod_{j=1}^{W} \pi_{j}^{\mathcal{C}_{j} + \mathcal{U}_{j} - 1}$$

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

