Machine Learning

Bayesian Decision Theory, Maximum Likelihood, and Regularized Empirical Risk Minimization

Prof. Matthias Hein

Machine Learning Group
Department of Mathematics and Computer Science
Saarland University, Saarbrücken, Germany

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Bayesian interpretation of loss functions

Regression: $y_i = f(x_i) + \varepsilon_i$,

Bayesian: Model for distribution $p(y|X = x, f) \rightarrow$ model for distribution of ε.

Likelihood: $p(y|X = x, f)$ models: how *likely* is the output y given the point x and the function value $f(x)$?

Maximum likelihood estimation:
Use the function f which maximizes the likelihood.

$$f^*(x) := \operatorname*{arg\,max}_{f \in \mathcal{F}} \mathbb{E}_{Y|X=x}\Big[p(Y|X = x, f)\Big]$$

Bayesian interpretation of loss functions II

Correspondence to loss function:

$$L(y, f(x)) = -\log p(y|X = x, f(x)) + c,$$

$\Rightarrow$ Maximizing the likelihood $p(y|X = x, f(x))$ is **equivalent** to minimizing the loss $L(y, f(x))$.

Example:

$$p(y|X = x, f(x)) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\Big(-\frac{(y - f(x))^2}{2\sigma^2} \Big).$$

and so the corresponding loss function $L(y, f(x))$ is given as

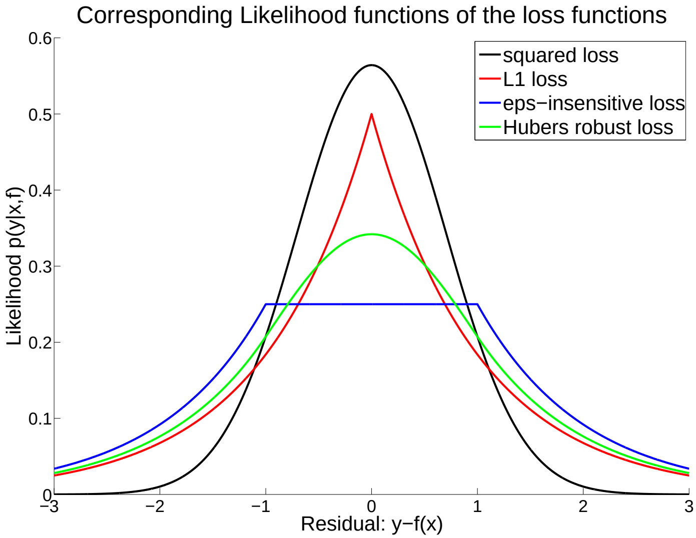
$$L(y, f(x)) = -\log p(y|X = x, f(x)) = \log(\sqrt{2\pi\sigma^2}) + \frac{\big(y - f(x)\big)^2}{2\sigma^2}.$$

Bayesian interpretation of loss functions III

With: $\varepsilon = y - f(x)$,

	$L(\lvert\varepsilon\rvert)$	$p(y\lvert x, f(x))$
squared loss	$\lvert\varepsilon\rvert^2$	$\frac{1}{\sqrt{\pi}} e^{-(y-f(x))^2}$,
L_1 - loss	$\lvert\varepsilon\rvert$	$\frac{1}{2} e^{-\lvert y-f(x)\rvert}$,
σ-insensitive	$(\lvert\varepsilon\rvert - \sigma)\mathbb{1}_{\lvert\varepsilon\rvert>\sigma}$	$\frac{1}{2+2\sigma} e^{-(\lvert y-f(x)\rvert-\varepsilon)\mathbb{1}_{\lvert y-f(x)\rvert>\sigma}}$,
Huber's robust loss	$\begin{cases} \frac{1}{2\sigma}\lvert\varepsilon\rvert^2 & \text{if } \lvert\varepsilon\rvert \leq \sigma \\ \lvert\varepsilon\rvert - \frac{\sigma}{2} & \text{if } \lvert\varepsilon\rvert > \sigma \end{cases}$	$\begin{cases} e^{-\frac{(y-f(x))^2}{2\sigma}} & \text{if } \lvert y-f(x)\rvert \leq \sigma \\ e^{-(\lvert y-f(x)\rvert - \frac{\sigma}{2})} & \text{if } \lvert y-f(x)\rvert > \sigma \end{cases}$

Bayesian interpretation of loss functions IV



Summary

- The optimal classifier for classification is the Bayes classifier. Extensions to cost-sensitive learning and the multi-class setting possible.
- Two schemes for solving multi-class problems: one-versus-all and one-versus-one.
- Discussion of the optimal function in regression (loss-dependent).
- Bayesian interpretation of loss functions $\Rightarrow$ Maximizing the likelihood is equivalent to minimizing the corresponding loss.

Empirical risk minimization

Problem: In order to compute the Bayes optimal learning rule we need to know the joint measure P on $\mathcal{X} \times \mathcal{Y}$,

but !

We do not know P but we have only the **training data** $(X_i, Y_i)_{i=1}^n$.

Idea: approximate the risk functional using the training data.

Empirical risk minimization II

Assumption: Training data $(X_i, Y_i)_{i=1}^n$ is an **i.i.d.** sample of the probability measure P on $\mathcal{X} \times \mathcal{Y}$.
i.i.d. = independently and identically distributed

- $(X_i, Y_i)_{i=1}^n$ are random variables,
- **independent**: joint density factorizes

$$p\big((x_1, y_1); (x_2, y_2); \ldots ; (x_n, y_n)\big) = \prod_{i=1}^{n} p_i(x_i, y_i).$$

- **identically distributed**:

$$p_i(x, y) = p_j(x, y), \qquad \forall i, j \in \{1, \ldots, n\}.$$

and $p(x, y)$ is the density of the data-generating measure P on $\mathcal{X} \times \mathcal{Y}$.

General Principle in Statistics

Statistics: Given an i.i.d. sample $(X_i)_{i=1}^n$, use the empirical measure

$$\mathrm{P}_n(x) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{x=X_i}$$

to approximate quantities of the data generating measure.

- **empirical mean**: $\mathbb{E}_{P_n}[X] = \frac{1}{n}\sum_{i=1}^n x\,\mathbb{1}_{x=X_i} = \frac{1}{n}\sum_{i=1}^n X_i$,
- **empirical variance**: $\mathrm{Var}[X] = \frac{1}{n}\sum_{i=1}^n \Big(X_i - \frac{1}{n}\sum_{j=1}^n X_j\Big)^2$,
- **empirical covariance**:
  $\mathrm{Cov}(X, Y) = \frac{1}{n}\sum_{i=1}^n X_i Y_i - \frac{1}{n}\sum_{i=1}^n X_i \,\frac{1}{n}\sum_{i=1}^n Y_i$,

$\boxed{\mathrm{P}_n \textbf{ approximates } \mathrm{P}}$

Empirical risk minimization III

Definition

Let $(X_i, Y_i)_{i=1}^n$ be an i.i.d. sample of P on $\mathcal{X} \times \mathcal{Y}$, which we call the **training sample**. The **empirical loss** is defined as

$$\mathbb{E}_{\mathrm{P}_n}[L(Y, f(X))] = \frac{1}{n}\sum_{i=1}^{n} L(Y_i, f(X_i)).$$

Given a class of functions $\mathcal{F}$, **empirical risk minimization** is defined as

$$f_n = \arg\min_{f \in \mathcal{F}} \mathbb{E}_{\mathrm{P}_n}[L(Y, f(X))] = \arg\min_{f \in \mathcal{F}} \frac{1}{n}\sum_{i=1}^{n} L(Y_i, f(X_i)),$$

where f_n is then learning rule based on the training sample.

Problems of Empirical risk minimization

- if the function class is too large it is likely that we overfit the training data,
- the mapping "data" to "learning rule" can be seen as an *inverse problem*.
  Definition of a **well-posed problem**:
  - a solution exists,
  - the solution is unique,
  - the solution depends continuously on the data.

  A problem which does not have one of these properties is called **ill-posed**. In particular the last two properties are most of the time not fulfilled in empirical risk minimization. In order to make problems well-posed one uses **regularization**.

Empirical risk minimization: Classification

Natural loss: 0-1-loss $L(y, f(x)) = \mathbb{1}_{y \neq f(x)}$.

Empirical risk minimization:
minimize the number of errors on the training set:

$$\frac{1}{n}\sum_{i=1}^{n} L(Y_i, f(X_i)) = \frac{1}{n}\sum_{i=1}^{n} \mathbb{1}_{Y_i \neq f(X_i)}.$$

Problem:

- for several classes of functions, empirical risk minimization leads to NP-hard problems
  $\Longrightarrow$ use of convex margin-based loss functions.

Empirical risk minimization: Regression

Standard loss: squared loss $L(y, f(x)) = (y - f(x))^2$.

$$f_n = \mathop{\arg\min}_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} (Y_i - f(X_i))^2$$

- $\mathcal{F} = \{f(x) = \langle w, x \rangle \mid w \in \mathbb{R}^d\}$, **linear least squares regression**.

Empirical risk minimization:

- function class $\mathcal{F}$ too large $\rightarrow$ overfitting,
- function class $\mathcal{F}$ too small $\rightarrow$ underfitting,

Idea: Use regularization together with a rather large function class $\mathcal{F}$.

Regularized empirical risk minimization

Definition

Let

- $(X_i, Y_i)_{i=1}^n$ be the training sample,
- $\mathcal{F}$ a fixed function class,
- $L(y, f(x))$ the loss function,
- $\Omega : \mathcal{F} \to \mathbb{R}_+$ the **regularization functional**.

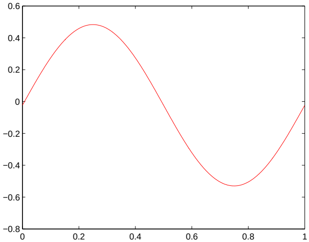
Then **regularized empirical risk minimization** is defined as

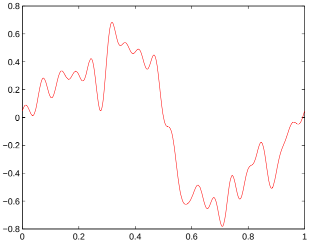
$$f_{n,\lambda} = \operatorname*{arg\,min}_{f \in \mathcal{F}} \frac{1}{n} \sum_{i=1}^{n} L(Y_i, f(X_i)) + \lambda\,\Omega(f),$$

where $\lambda \in \mathbb{R}_+$ is called the **regularization parameter**.

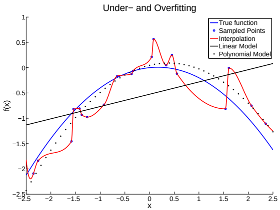
$\Longrightarrow$ This form of regularization is called **Tikhonov regularization**.

Trade-off between **fit of the data** and **complexity of the learning rule**.





Left: Relatively simple function, very smooth,
Right: Complex function, less smooth.



Regularized empirical risk minimization II

Equivalent formulation (Ivanov regularization):

Proposition

If the loss $L(y, f(x))$ and the regularization function $\Omega(f)$ are convex in f and the set $\{f \,|\, \Omega(f) < r\}$ is non-empty for every $r > 0$ and $\mathcal{F}$ is a convex set, then regularized empirical risk minimization is equivalent to the following problem:

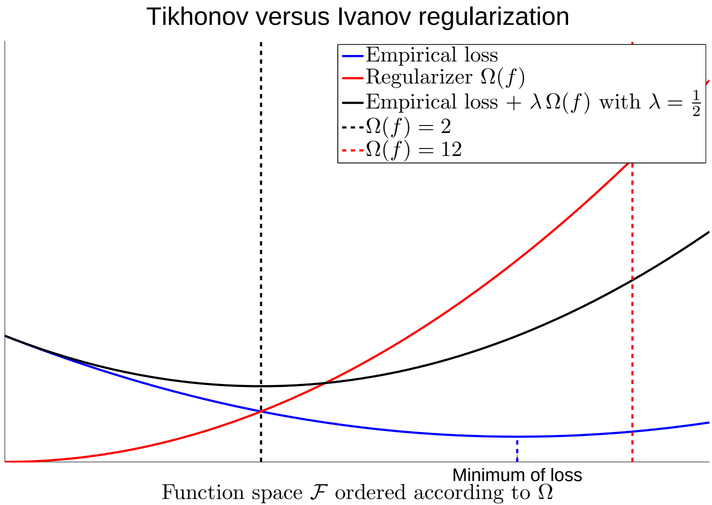
$$f_{n,r} = \underset{f \in \mathcal{F}, \quad \Omega(f) \leq r}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} L(Y_i, f(X_i)),$$

in the sense that there exists for each r a corresponding λ such that $f_{n,r} = f_{n,\lambda}$.

Proof:

- use of duality in convex optimization,
- in the lecture notes: proof for finite-dimensional function classes.

Tikhonov versus Ivanov regularization



Occam's razor

General Principle: prefer less complex function, as measured by Ω, if they have the same loss.

"Occam's razor":

Pluralitas non est ponenda sine necessitas.' (Plurality should not be posited without necessity.),

or similarly:

"Having two competing theories which make exactly the same predictions, the one that is simpler is the better."

Regularized empirical risk minimization IV

Regularization parameter λ: controls trade-off between fit and complexity.

Limits: $\lambda \to 0$ and $\lambda \to \infty$.

$$\lambda \to 0 \qquad \underset{\underset{f \in \mathcal{F}}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} L(Y_i, f(X_i))}{\arg\min} \Omega(f),$$

$$\lambda \to \infty \qquad \underset{\{f \in \mathcal{F} \,|\, \Omega(f)=0\}}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} L(Y_i, f(X_i))$$

Example: $f : \mathbb{R}^d \to \mathbb{R}$,

$$\Omega(f) = \int_{\mathbb{R}^d} \sum_{i=1}^{d} \left(\frac{\partial f}{\partial x^i}\right)^2 dx = \int_{\mathbb{R}^d} \|\nabla f\|^2 \, dx$$

$$\Omega(f) = 0 \quad \Longleftrightarrow \quad \exists\, c \in \mathbb{R}, \text{ such that } f(x) = c, \; \forall x \in \mathbb{R}^d.$$

Regularized empirical risk minimization IV

Related principle: **Structural risk minimization** proposed by Vapnik.

- empirical risk minimization over nested function classes $\mathcal{F}_n$, such that $\mathcal{F}_1 \subset \mathcal{F}_2 \subset \ldots$,
- as the size of the sample n increases one also allows more complex functions.

Example: start with the linear functions and then add polynomials of increasing order as n increases.

Relation I:

Empirical risk minimization
corresponds to
maximum likelihood estimation.

Relation II:

Regularized empirical risk minimization
corresponds to
maximum a posteriori estimation.

Maximum Likelihood Estimation

Problem: Given samples $x_1, \ldots, x_n$ identify the probability measure $p(x)$ which generated this sample.

General problem to difficult $\Longrightarrow$ parametric model of $p(x)$.

General Idea:

- parametric model of the data generating probability measure:

$$p(x \mid \theta) \qquad \text{(the likelihood)}.$$

- i.i.d. data $x_1, \ldots, x_n \implies p(x_1, \ldots, x_n \,|\theta) = \prod_{i=1}^n p(x_i \mid \theta)$.
- find parameter $\theta \in \Theta$ by maximizing the likelihood (resp. the log-likelihood)

$$\begin{aligned} \arg\max_{\theta \in \Theta} \prod_{i=1}^n p(x_i \mid \theta) &= \arg\max_{\theta \in \Theta} \log \Big(\prod_{i=1}^n p(x_i \mid \theta) \Big) \\ &= \arg\max_{\theta \in \Theta} \sum_{i=1}^n \log \big(p(x_i \mid \theta) \big) \end{aligned}$$

Maximum Likelihood Estimation - Example

Gaussian model:

$p(x|\mu) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$, the variance σ^2 is assumed to be known.

Maximum likelihood estimation of μ:

$$\begin{aligned} \underset{\mu \in \mathbb{R}}{\arg\max} \sum_{i=1}^{n} \log\big(p(x_i \,|\, \mu)\big) &= \underset{\mu \in \mathbb{R}}{\arg\max} \sum_{i=1}^{n} \Big(-\frac{\log\big(2\pi\sigma^2\big)}{2} - \frac{(x_i - \mu)^2}{2\sigma^2} \Big) \\ &= \underset{\mu \in \mathbb{R}}{\arg\min} \sum_{i=1}^{n} (x_i - \mu)^2 \end{aligned}$$

The objective is convex in $\mu \Longrightarrow$ Every local minimum is a global minimum.

The mean parameter μ^* maximizing the likelihood is:

$$\mu^* = \frac{1}{n} \sum_{i=1}^{n} x_i.$$

Empirical Risk Minimization and Maximum Likelihood

Maximum Likelihood:

- model for the conditional distribution = the **likelihood**: $p(y|x, f)$,
  f denotes the parameter of the model,
  $\mathcal{F}$ is the set of parameters.
- i.i.d. sample of the data $D = (X_i, Y_i)_{i=1}^n$.

Definition

The **maximum likelihood** solution f_{ML} is then defined as

$$f_{ML} = \arg\max_{f \in \mathcal{F}} \mathrm{P}(D|f) = \arg\max_{f \in \mathcal{F}} \prod_{i=1}^{n} \mathrm{P}(Y_i|X_i, f),$$

$$
\begin{array}{lcl}
\text{Model for } p(y|x, f(x)) & \longrightarrow & L(y, f(x)) = -\log p(y|x, f(x)), \\
\text{Loss function } L(y, f(x)) & \xrightarrow[\text{correspondence}]{\text{generally no}} & p(y|x, f(x)) = e^{-L(y,f(x))}.
\end{array}
$$

Proposition

Given an i.i.d. training sample $(X_i, Y_i)_{i=1}^n$, a class of functions $\mathcal{F}$ and a likelihood $p(y|x, f)$, then the **maximum likelihood solution** *f_{ML} agrees with the solution of* **empirical risk minimization** *f_n for the loss function $L(y, f(x)) = -\log p(y|x, f)$.*

- output space $\mathcal{Y}$ is discrete: likelihood is probability $\mathrm{P}(y|x, f)$,
- output space $\mathcal{Y}$ is continuous: likelihood is density $p(y|x, f)$.

Proof: By assumption we know $L(y, f(x)) = -\log \mathrm{P}(y|x, f)$, then

$$\begin{aligned}
f_{ML} &= \operatorname*{arg\,max}_{f \in \mathcal{F}} \mathrm{P}(D|f) = \operatorname*{arg\,max}_{f \in \mathcal{F}} \prod_{i=1}^{n} \mathrm{P}(Y_i|X_i, f) \\
&= \operatorname*{arg\,max}_{f \in \mathcal{F}} \quad \log \Big[\prod_{i=1}^{n} \mathrm{P}(Y_i|X_i, f) \Big] \\
&= \operatorname*{arg\,max}_{f \in \mathcal{F}} \quad \sum_{i=1}^{n} \log \mathrm{P}(Y_i|X_i, f) \\
&= \operatorname*{arg\,min}_{f \in \mathcal{F}} - \sum_{i=1}^{n} \log \mathrm{P}(Y_i|X_i, f) \\
&= \operatorname*{arg\,min}_{f \in \mathcal{F}} \sum_{i=1}^{n} L(Y_i, f(X_i)) = f_n,
\end{aligned}$$

Maximum A Posteriori Estimation

Idea: integrate **prior belief** on the model parameter θ

Realization: θ is random, we have a **prior distribution** $p(\theta)$.

MAP Estimation:

- prior distribution $p(\theta)$
- using Bayes rule

$$p(\theta \,|\, x_1, \ldots, x_n) = \frac{p(x_1, \ldots, x_n \,|\, \theta) p(\theta)}{p(x_1, \ldots, x_n)} = \frac{p(x_1, \ldots, x_n \,|\, \theta) p(\theta)}{\int_\Theta p(x_1, \ldots, x_n \,|\, \theta) p(\theta) d\theta}.$$

  The denominator is called the **partition function**.
- find parameter θ by maximizing the a posteriori distribution $p(\theta \,|\, x_1, \ldots, x_n)$

$$\arg\max_{\theta \in \Theta} \prod_{i=1}^{n} p(\theta \,|\, x_1, \ldots, x_n) = \arg\max_{\theta \in \Theta} \log \Big(p(x_1, \ldots, x_n \,|\, \theta) p(\theta) \Big)$$

$$= \arg\max_{\theta \in \Theta} \sum_{i=1}^{n} \log \big(p(x_i \,|\, \theta) \big) + \log \big(p(\theta) \big).$$

Maximum A Posteriori Estimation - Example

Gaussian model:

$p(x|\mu) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$, the variance σ^2 is assumed to be known.

$p(\mu) = \frac{1}{\sqrt{2\pi\sigma_\mu^2}} e^{-\frac{(\mu-\mu_0)^2}{2\sigma_\mu^2}}$, the variance σ_μ^2 is assumed to be known.

MAP estimation of μ:

$$\begin{aligned}\arg\max_{\mu\in\mathbb{R}} p(\mu \,|\, x_1, \ldots, x_n) &= \arg\max_{\mu\in\mathbb{R}} \sum_{i=1}^n \log\big(p(x_i \,|\, \mu)\big) + \log\big(p(\mu)\big) \\ &= \arg\min_{\mu\in\mathbb{R}} \frac{1}{2\sigma^2} \sum_{i=1}^n (x_i - \mu)^2 + \frac{1}{2\sigma_\mu^2}(\mu - \mu_0)^2\end{aligned}$$

The objective is convex in μ The MAP estimate of the mean parameter μ^* is:

$$\mu^* = \frac{1}{1 + \frac{\sigma^2}{n\sigma_\mu^2}} \frac{1}{n} \sum_{i=1}^n x_i \; + \; \frac{1}{1 + \frac{n\sigma_\mu^2}{\sigma^2}} \mu_0.$$

Ingredients:

- likelihood function $\mathrm{P}(y|x, f)$,
- set of parameters $\mathcal{F}$,
- **prior** $\mathrm{P}(f)$ over the function/parameter space $\mathcal{F}$.
  probability measure over the class of functions
  $\Longrightarrow$ which functions are more "likely" than others,
  $\Longrightarrow$ encodes **a priori** knowledge.

Maximum a posteriori estimation

Ingredients:

- likelihood function $\mathrm{P}(y|x, f)$,
- set of parameters $\mathcal{F}$,
- **prior** $\mathrm{P}(f)$ over the function/parameter space $\mathcal{F}$.
  probability measure over the class of functions
  $\Longrightarrow$ which functions are more "likely" than others,
  $\Longrightarrow$ encodes **a priori** knowledge.

Bayes theorem: Transform the prior and the likelihood into the **posterior probability** $\mathrm{P}(f|D)$,

$$\mathrm{P}(f|D) = \frac{\mathrm{P}(D|f)\mathrm{P}(f)}{\mathrm{P}(D)},$$

where $\mathrm{P}(D) = \int_{\mathcal{F}} \mathrm{P}(D|f)\mathrm{P}(f)df$.

MAP estimation II

Definition

The **maximum a posteriori** estimator for f is defined as

$$f_{MAP} = \arg\max_{f \in \mathcal{F}} \mathrm{P}(f|D) = \arg\max_{f \in \mathcal{F}} \prod_{i=1}^{n} \mathrm{P}(Y_i|X_i, f)\mathrm{P}(f),$$

where we have discarded $\mathrm{P}(D)$ since it is a constant.

Given a prior over functions $\mathrm{P}(f)$ we define the following regularization functional $\Omega(f)$,

$$\Omega(f) = -\log \mathrm{P}(f) \qquad \Longrightarrow \qquad \mathrm{P}(f) = e^{-\Omega(f)},$$

MAP estimation III

Proposition

The MAP estimator f_{MAP} agrees with the minimizer of $f_{\lambda=\frac{1}{n},n}$ of the regularized empirical risk minimization if

$$\begin{aligned} &\textbf{Loss function:} && L(y, f(x)) &&= -\log \mathrm{P}(y|x, f), \\ &\textbf{regularization functional:} && \Omega(f) &&= -\log \mathrm{P}(f). \end{aligned}$$

MAP estimation IV

Proof.

By assumption we know $L(y, f(x)) = -\log \mathrm{P}(y|x, f)$ and $\Omega(f) = -\log \mathrm{P}(f)$, then

$$\begin{aligned} f_{MAP} &= \arg\max_{f \in \mathcal{F}} \mathrm{P}(f|D) = \arg\max_{f \in \mathcal{F}} \prod_{i=1}^{n} \mathrm{P}(Y_i|X_i, f)\mathrm{P}(f) \\ &= \arg\max_{f \in \mathcal{F}} \sum_{i=1}^{n} \log \mathrm{P}(Y_i|X_i, f) + \log \mathrm{P}(f) \\ &= \arg\min_{f \in \mathcal{F}} \sum_{i=1}^{n} L(Y_i, f(X_i)) + \Omega(f) = f_{n,\lambda=\frac{1}{n}}. \end{aligned}$$

where we have used that the logarithm is a strictly increasing function. □

Full Bayesian treatment

Posterior predictive distribution:

$$p(x|D) = \int_\Theta p(x, \theta \,|\, D)\, d\theta = \int_\Theta p(x \,|\, \theta, D)\, p(\theta \,|\, D)\, d\theta$$

- $p(x|D)$ is **not** the true data-generating distribution !
- if the posterior $p(\theta \,|\, D)$ is very peaked, this is roughly the same as $p(x \,|\, \theta_{\mathrm{MAP}})$

Learning setting:

$$p(y \,|\, x, D) = \int_\Theta p(y \,|\, x, \theta)\, p(\theta \,|\, D)\, d\theta$$

Bayesians consider the full distribution $p(\theta \,|\, D)$ against the point estimate in the MAP estimation.