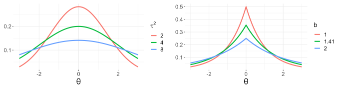
Introduction to Machine Learning

Regularization
Bayesian Priors



Learning goals

- RRM is same as MAP in Bayes
- Gaussian/Laplace prior corresponds to $L2/L1$ penalty

RRM VS. BAYES I

We already created a link between max. likelihood estimation and ERM.

Now we will generalize this for RRM.

Assume we have a parameterized distribution $p(y|\boldsymbol{\theta}, \mathbf{x})$ for our data and a prior $q(\boldsymbol{\theta})$ over our param space, all in Bayesian framework.

From Bayes theorem:

$$p(\boldsymbol{\theta}|\mathbf{x}, y) = \frac{p(y|\boldsymbol{\theta}, \mathbf{x})q(\boldsymbol{\theta})}{p(y|\mathbf{x})} \propto p(y|\boldsymbol{\theta}, \mathbf{x})q(\boldsymbol{\theta})$$

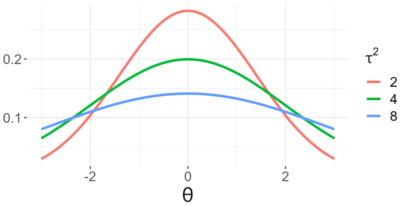
RRM VS. BAYES II

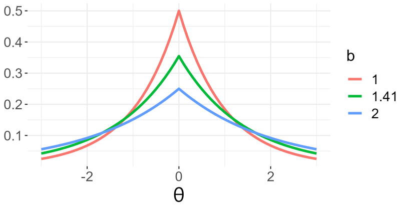
The maximum a posteriori (MAP) estimator of $\boldsymbol{\theta}$ is now the minimizer of

$$-\log p\left(y \mid \boldsymbol{\theta}, \mathbf{x}\right) - \log q(\boldsymbol{\theta}).$$

- Again, we identify the loss $L\left(y, f(\mathbf{x} \mid \boldsymbol{\theta})\right)$ with $-\log(p(y|\boldsymbol{\theta}, \mathbf{x}))$.
- If $q(\boldsymbol{\theta})$ is constant (i.e., we used a uniform, non-informative prior), the second term is irrelevant and we arrive at ERM.
- If not, we can identify $J(\boldsymbol{\theta}) \propto -\log(q(\boldsymbol{\theta}))$, i.e., the log-prior corresponds to the regularizer, and the additional λ, which controls the strength of our penalty, usually influences the peakedness / inverse variance / strength of our prior.

RRM VS. BAYES III





- $L2$ regularization corresponds to a zero-mean Gaussian prior with constant variance on our parameters: $\theta_j \sim \mathcal{N}(0, \tau^2)$
- $L1$ corresponds to a zero-mean Laplace prior: $\theta_j \sim \mathit{Laplace}(0, b)$. $\mathit{Laplace}(\mu, b)$ has density $\frac{1}{2b}\exp(-\frac{|\mu - x|}{b})$, with scale parameter b, mean μ and variance $2b^2$.
- In both cases, regularization strength increases as variance of prior decreases: more prior mass concentrated around 0 encourages shrinkage.
- Elastic-net regularization corresponds to a compromise between Gaussian and Laplacian priors ▸ Zou and Hastie 2005 ▸ Hans 2011

EXAMPLE: BAYESIAN L2 REGULARIZATION I

We can easily see the equivalence of *L*2 regularization and a Gaussian prior:

- Gaussian prior $\mathcal{N}_d(\mathbf{0}, diag(\tau^2))$ with uncorrelated components for $\boldsymbol{\theta}$:

$$q(\boldsymbol{\theta}) = \prod_{j=1}^{d} \phi_{0,\tau^2}(\theta_j) = (2\pi\tau^2)^{-\frac{d}{2}} \exp\left(-\frac{1}{2\tau^2}\sum_{j=1}^{d}\theta_j^2\right)$$

- MAP:

$$\begin{aligned}
\hat{\theta}^{\text{MAP}} &= \arg\min_{\boldsymbol{\theta}} \left(-\log p\left(y \mid \boldsymbol{\theta}, \mathbf{x}\right) - \log q(\boldsymbol{\theta})\right) \\
&= \arg\min_{\boldsymbol{\theta}} \left(-\log p\left(y \mid \boldsymbol{\theta}, \mathbf{x}\right) + \tfrac{d}{2}\log(2\pi\tau^2) + \frac{1}{2\tau^2}\sum_{j=1}^{d}\theta_j^2\right) \\
&= \arg\min_{\boldsymbol{\theta}} \left(-\log p\left(y \mid \boldsymbol{\theta}, \mathbf{x}\right) + \frac{1}{2\tau^2}\|\boldsymbol{\theta}\|_2^2\right)
\end{aligned}$$

- We see how the inverse variance (precision) $1/\tau^2$ controls shrinkage

EXAMPLE: BAYESIAN L2 REGULARIZATION II

- DGP $y = \theta + \varepsilon$ where $\varepsilon \sim \mathcal{N}(0, 1)$ and $\theta = 1$;
  with Gaussian prior on θ, so $\mathcal{N}(0, \tau^2)$ for $\tau \in \{0.25, 0.5, 2\}$
- For $n = 20$, posterior of θ and MAP can be calculated analytically
- Plotting the $L2$ regularized empirical risk $\mathcal{R}_{\text{reg}}(\theta) = \sum_{i=1}^{n}(y_i - \theta)^2 + \lambda\theta^2$ with $\lambda = 1/\tau^2$ shows that ridge solution is identical with MAP
- In our simulation, the empirical mean is $\bar{y} = 0.94$, with shrinkage toward 0 induced in the MAP