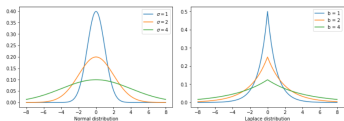


Introduction to Machine Learning

Regularization in Non-Linear Models and Bayesian Priors

Learning goals

- Understand that regularization and parameter shrinkage can be applied to non-linear models
- Know structural risk minimization
- Know how regularization risk minimization is the same as MAP in a Bayesian perspective, where the penalty corresponds to parameter prior.



SUMMARY: REGULARIZED RISK MINIMIZATION

If we should define ML in only one line, this might be it:

$$\mathcal{R}_{\text{reg}}(\theta) = \min_{\theta} \sum_{i=1}^n L\left(y^{(i)}, f\left(\mathbf{x}^{(i)} \mid \theta\right)\right) + \lambda \cdot J(\theta)$$

We can choose for a task at hand:

- the **hypothesis space** of f , which determines how features can influence the predicted y
- the **loss** function L , which measures how errors should be treated
- the **regularization** $J(\theta)$, which encodes our inductive bias and preference for certain simpler models

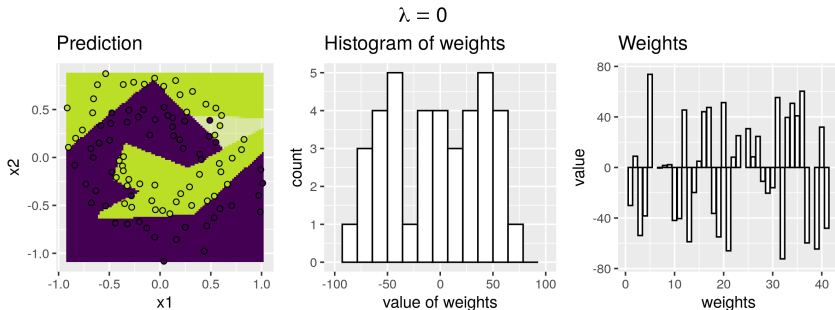
By varying these choices one can construct a huge number of different ML models. Many ML models follow this construction principle or can be interpreted through the lens of regularized risk minimization.

REGULARIZATION IN NONLINEAR MODELS

- So far we have mainly considered regularization in LMs.
- Can also be applied to non-linear models (with numeric parameters), where it is often important to prevent overfitting.
- Here, we typically use $L2$ regularization, which still results in parameter shrinkage and weight decay.
- By adding regularization, prediction surfaces in regression and classification become smoother.
- Note: In the chapter on non-linear SVMs we will study the effects of regularization on a non-linear model in detail.

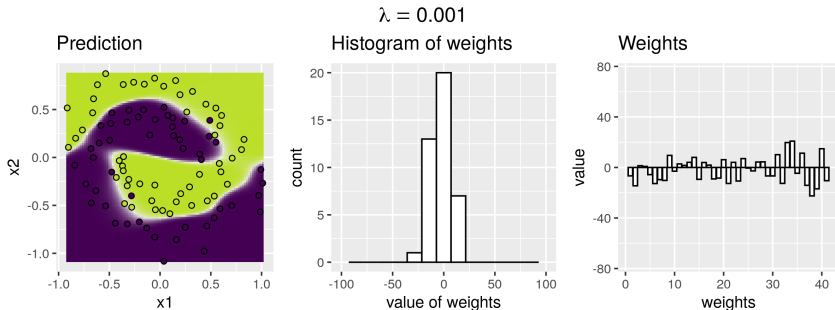
REGULARIZATION IN NONLINEAR MODELS

Setting: Classification for the spirals data. Neural network with single hidden layer containing 10 neurons and logistic output activation, regularized with L_2 penalty term for $\lambda > 0$. Varying λ affects smoothness of the decision boundary and magnitude of network weights:



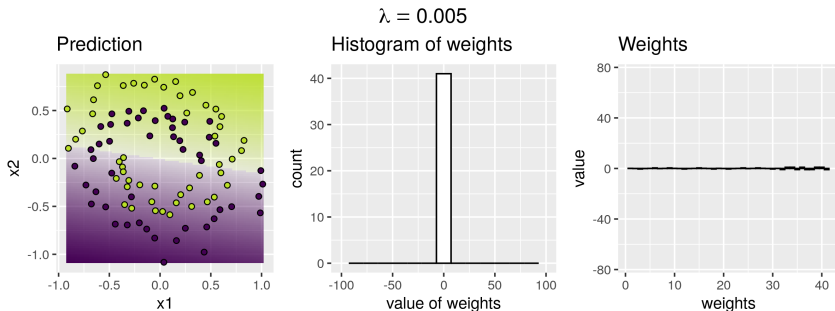
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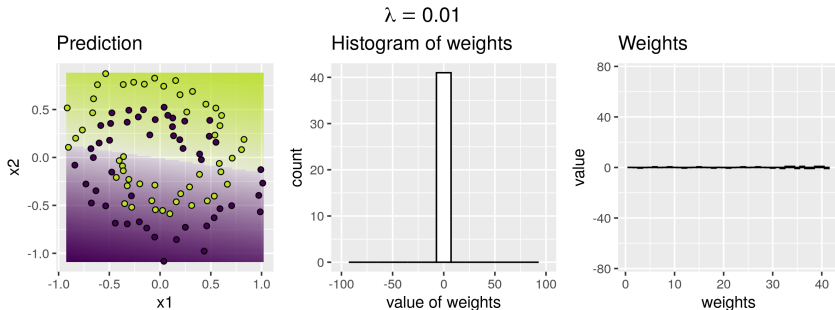
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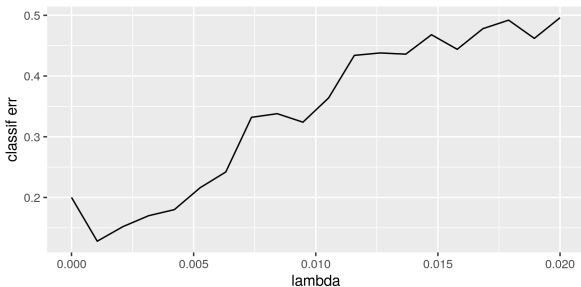
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REGULARIZATION IN NONLINEAR MODELS

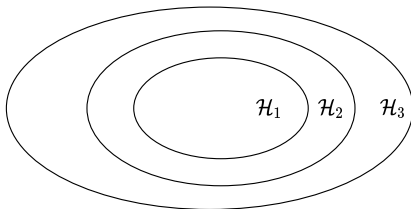
The prevention of overfitting can also be seen in CV. Same settings as before, but each λ is evaluated with repeated CV (10 folds, 5 reps).



We see the typical U-shape with the sweet spot between overfitting (LHS, low λ) and underfitting (RHS, high λ) in the middle.

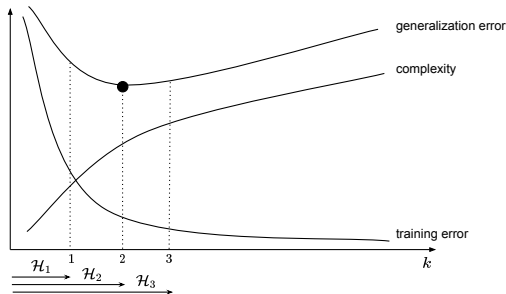
STRUCTURAL RISK MINIMIZATION

- Thus far, we only considered adding a complexity penalty to empirical risk minimization.
- Instead, structural risk minimization (SRM) assumes that the hypothesis space \mathcal{H} can be decomposed into increasingly complex hypotheses (size or capacity): $\mathcal{H} = \cup_{k \geq 1} \mathcal{H}_k$.
- Complexity parameters can be the, e.g. the degree of polynomials in linear models or the size of hidden layers in neural networks.



STRUCTURAL RISK MINIMIZATION

- SRM chooses the smallest k such that the optimal model from \mathcal{H}_k found by ERM or RRM cannot significantly be outperformed by a model from a \mathcal{H}_m with $m > k$.
- By this, the simplest model can be chosen, which minimizes the generalization bound.
- One challenge might be choosing an adequate complexity measure, as for some models, multiple complexity measures exist.

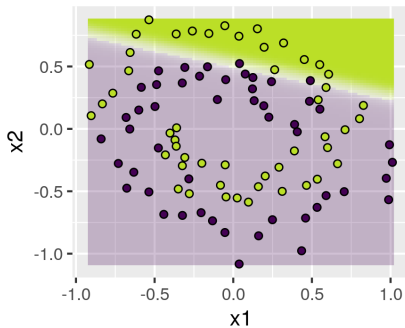


STRUCTURAL RISK MINIMIZATION

Setting: Classification for the spirals data. Neural network with single hidden layer containing k neurons and logistic output activation, L2 regularized with $\lambda = 0.001$. So here SRM and RRM are both used. Varying the size of the hidden layer affects smoothness of the decision boundary:

size of hidden layer = 1

Prediction

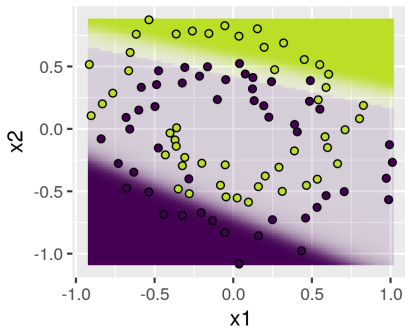


STRUCTURAL RISK MINIMIZATION

Setting: Classification for the spirals data. Neural network with single hidden layer containing k neurons and logistic output activation, L2 regularized with $\lambda = 0.001$. So here SRM and RRM are both used. Varying the size of the hidden layer affects smoothness of the decision boundary:

size of hidden layer = 2

Prediction

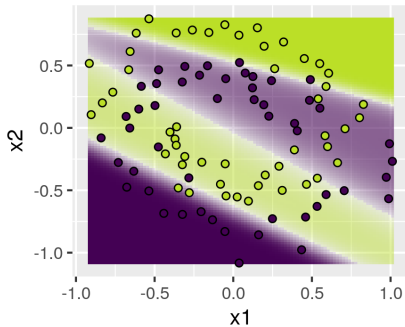


STRUCTURAL RISK MINIMIZATION

Setting: Classification for the spirals data. Neural network with single hidden layer containing k neurons and logistic output activation, L2 regularized with $\lambda = 0.001$. So here SRM and RRM are both used. Varying the size of the hidden layer affects smoothness of the decision boundary:

size of hidden layer = 3

Prediction

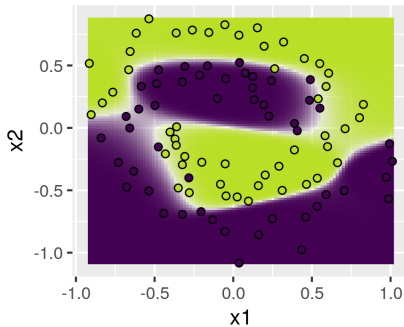


STRUCTURAL RISK MINIMIZATION

Setting: Classification for the spirals data. Neural network with single hidden layer containing k neurons and logistic output activation, L2 regularized with $\lambda = 0.001$. So here SRM and RRM are both used. Varying the size of the hidden layer affects smoothness of the decision boundary:

size of hidden layer = 5

Prediction

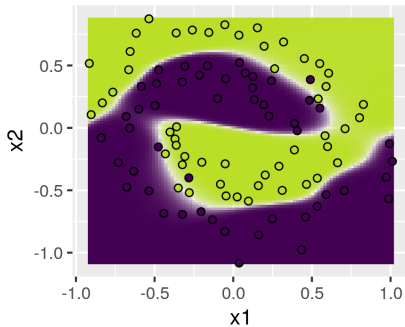


STRUCTURAL RISK MINIMIZATION

Setting: Classification for the spirals data. Neural network with single hidden layer containing k neurons and logistic output activation, L2 regularized with $\lambda = 0.001$. So here SRM and RRM are both used. Varying the size of the hidden layer affects smoothness of the decision boundary:

size of hidden layer = 10

Prediction

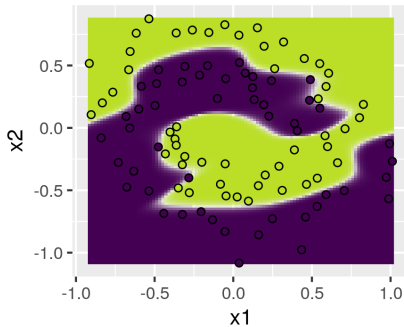


STRUCTURAL RISK MINIMIZATION

Setting: Classification for the spirals data. Neural network with single hidden layer containing k neurons and logistic output activation, L2 regularized with $\lambda = 0.001$. So here SRM and RRM are both used. Varying the size of the hidden layer affects smoothness of the decision boundary:

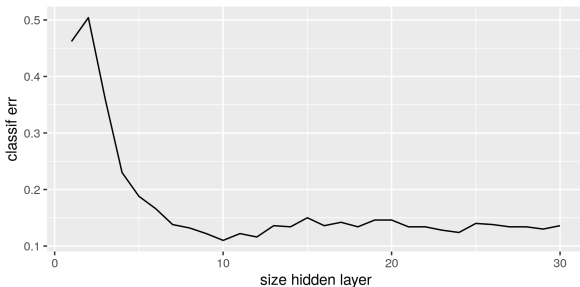
size of hidden layer = 100

Prediction



STRUCTURAL RISK MINIMIZATION

Again, complexity vs CV score.

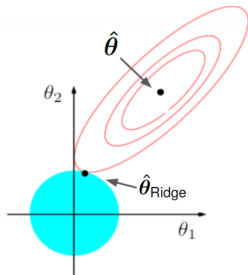


A minimal model with good generalization seems to have ca. 6-8 hidden neurons.

STRUCTURAL RISK MINIMIZATION AND RRM

Note that normal RRM can also be interpreted through SRM, if we rewrite the penalized ERM as constrained ERM.

$$\begin{aligned} \min_{\boldsymbol{\theta}} \quad & \sum_{i=1}^n L\left(y^{(i)}, f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right) \\ \text{s.t.} \quad & \|\boldsymbol{\theta}\|_2^2 \leq t \end{aligned}$$



We can interpret going through λ from large to small as through t from small to large. This constructs a series of ERM problems with hypothesis spaces \mathcal{H}_λ , where we constrain the norm of $\boldsymbol{\theta}$ to unit balls of growing size.

RRM VS. BAYES

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

Now we will generalize this for RRM.

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

From the Bayes theorem we know:

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

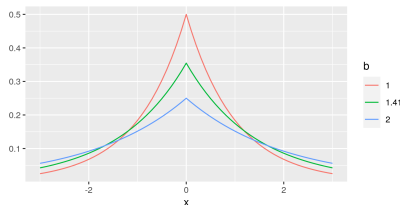
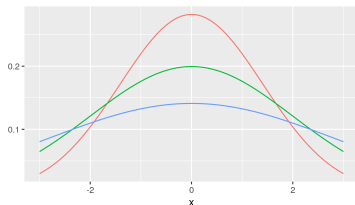
RRM VS. BAYES

The maximum a posteriori (MAP) estimator of θ is now the minimizer of

$$-\log p(y | \theta, \mathbf{x}) - \log q(\theta).$$

- Again, we identify the loss $L(y, f(\mathbf{x} | \theta))$ with $-\log(p(y|\theta, \mathbf{x}))$.
- If $q(\theta)$ 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 $J(\theta) \propto -\log(q(\theta))$, 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



- $L2$ 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: $\theta_j \sim \text{Laplace}(0, b)$. $\text{Laplace}(\mu, b)$ 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 the variance of the prior decreases: a prior probability mass more narrowly concentrated around 0 encourages shrinkage.

EXAMPLE: BAYESIAN L2 REGULARIZATION

We can easily see the equivalence of $L2$ regularization and a Gaussian prior:

- We define a Gaussian prior with uncorrelated components for θ :

$$q(\theta) = \mathcal{N}_d(\mathbf{0}, \text{diag}(\tau^2)) = \prod_{j=1}^d \mathcal{N}(0, \tau^2) = (2\pi\tau^2)^{-\frac{d}{2}} \exp\left(-\frac{1}{2\tau^2} \sum_{j=1}^d \theta_j^2\right).$$

- With this, the MAP estimator becomes

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

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