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7.3 Regularization

Machine Learning 1: Foundations

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What is Regularization?

SVM, LR, and ANN employ regularization:

$$\min_{[W,]\ b,\mathbf{w}} \underbrace{\frac{1}{2}\|\mathbf{w}\|^2 \left[+\frac{1}{2}\sum_{l=1}^{L}\|W_l\|^2\right]}_{\text{regularizer } R(\theta)} + \underbrace{C}_{\substack{\text{regularization}\\ \text{constant}}} \underbrace{\sum_{i=1}^{n}\ell\left(y_i\left(\langle\mathbf{w},\phi(\mathbf{x}_i)\rangle + b\right)\right)}_{\text{loss } L(\theta)},$$

denoting $\theta := (b, \mathbf{w}, [, W])$, with the gray terms only for ANNs.

Influence of the regularization constant C

- high C
  $\Rightarrow$ focus on getting the loss small, not the regularizer
  $\Rightarrow$ low regularization & high overfitting
- low $C \Rightarrow$ high regularization & low overfitting

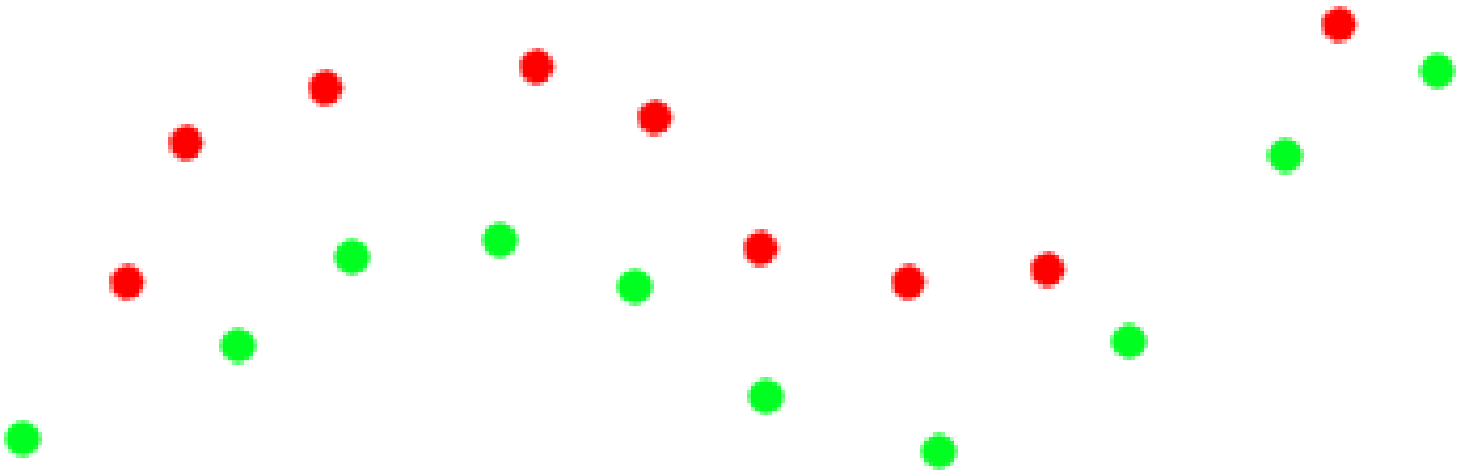
Why does it work?

Why It Works: Example of Polynomial Kernel

Recall: prediction functions are degree-m polynomials:

$$f(\mathbf{x}) = \langle \mathbf{w}, \phi(\mathbf{x}) \rangle = \sum_{i=(i_1,\ldots,i_d) \in \mathbb{N}_0^d : \sum_{j=1}^d i_j \leq m} w_i c_i x_1^{i_1} \cdots x_d^{i_d}$$

Consider classifying this data with a degree-8 polynomial:



The more regularization, the smaller the coefficients

- leads to smoother functions

Why Regularization Works: Regularizer in Constraint

Using a Lagrangian argument, one can show that

$$\min_{\theta} \quad \underbrace{R(\theta)}_{\text{regularizer}} + \underbrace{C}_{\substack{\text{regularization} \\ \text{constant}}} \underbrace{L(\theta)}_{\text{loss}}$$

is equivalent to

$$\begin{aligned} \min_{\theta} \quad & L(\theta) \\ \text{s.t.} \quad & R(\theta) \leq \tilde{C} \end{aligned}$$

for some adequate choice of $\tilde{C}$.

Proof (Non-mandatory Material)

By the Lagrangian duality theorem (L),

$$
\begin{aligned}
& & \min_{\theta} \quad & L(\theta) \quad \text{s.t.} \quad R(\theta) \leq \tilde{C} \\
&\overset{(L)}{=} \max_{\lambda \geq 0} \min_{\theta} \quad & L(\theta) + \lambda(R(\theta) - \tilde{C}) \\
&\overset{(L)}{=} \min_{\theta} \max_{\lambda \geq 0} \quad & L(\theta) + \lambda(R(\theta) - \tilde{C}) \\
&= \min_{\theta} \quad & L(\theta) + \lambda^*(R(\theta) - \tilde{C}) \\
&= \min_{\theta} \quad & L(\theta) + \underbrace{\lambda^*}_{=:C} R(\theta),
\end{aligned}
$$

where (θ^*, λ^*) is the optimal value the above min-max problem.

□

Why Regularization Works: Regularizer in Constraint

Interpretation of SVM/LR/ANN with regularizer in constraint:

- By changing $\tilde{C}$ we can control the size of the set

$$\left\{\theta : R(\theta) \leq \tilde{C}\right\},$$

  from which we pick the parameters $\theta := (b, \mathbf{w}, [, W])$ of the classifier

Bottom line: The **larger** the set, the more likely the algorithm will pick a function

- that describes the training data well
- but does not generalize well