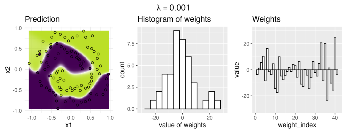
Introduction to Machine Learning

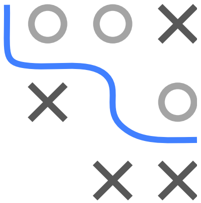
Regularization
Non-Linear Models and Structural Risk Minimization



Learning goals

- Regularization even more important in non-linear models
- Norm penalties applied similarly
- Structural risk minimization

SUMMARY: REGULARIZED RISK MINIMIZATION



If we define (supervised) ML in one line, this might be it:

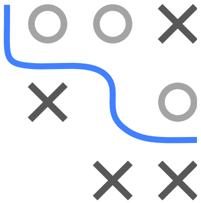
$$\min_{\boldsymbol{\theta}} \mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \min_{\boldsymbol{\theta}} \left(\sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right) + \lambda \cdot J(\boldsymbol{\theta}) \right)$$

Can choose for task at hand:

- **hypothesis space** of f, controls how features influence prediction
- **loss** function L, measures how errors are treated
- **regularizer** $J(\theta)$, encodes inductive bias

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 RRM.

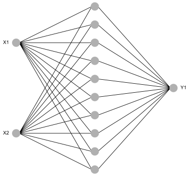
REGULARIZATION IN NONLINEAR MODELS

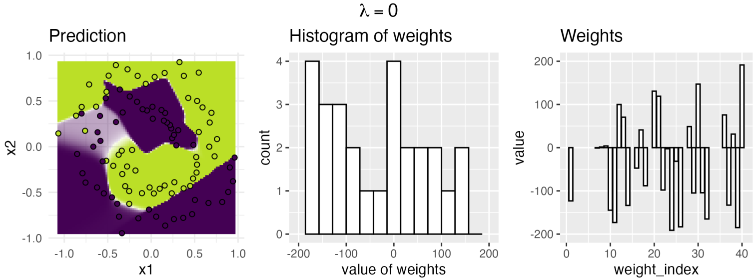


- So far we have mainly considered regularization in LMs
- Can in general also be applied to non-linear models; vector-norm penalties require numeric params
- Here, we typically use $L2$ regularization, which still results in parameter shrinkage and weight decay
- For non-linear models, regularization is even more important / basically required to prevent overfitting
- Commonplace in methods such as NNs, SVMs, or boosting
- Prediction surfaces / decision boundaries become smoother

REGULARIZATION IN NONLINEAR MODELS

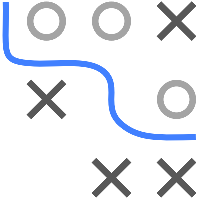
Classification for `spirals` data.
NN with single hidden layer, size 10, *L*2 penalty:





λ affects smoothness of decision boundary and magnitude of weights.
When λ is 0 (no regularization), absolute weights could be extremely large.

REGULARIZATION IN NONLINEAR MODELS



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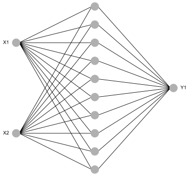

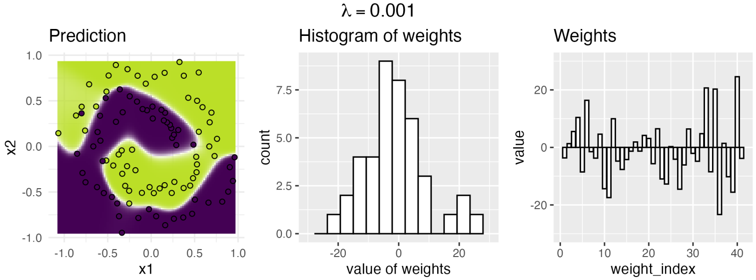

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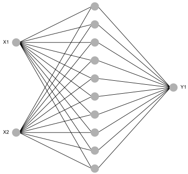

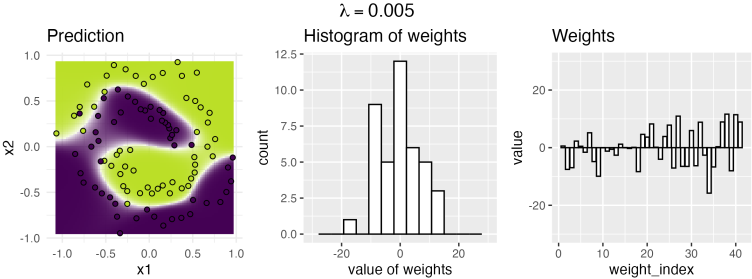

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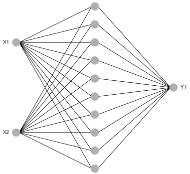

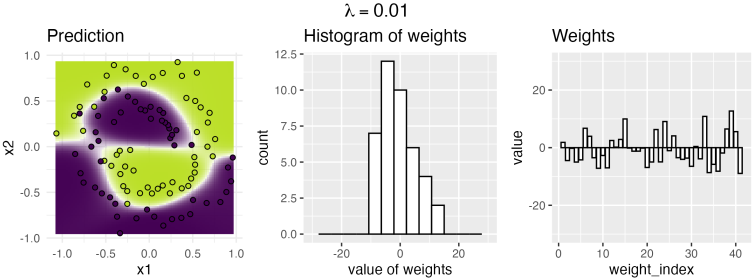

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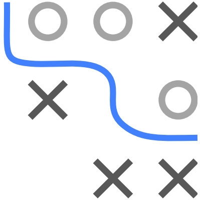
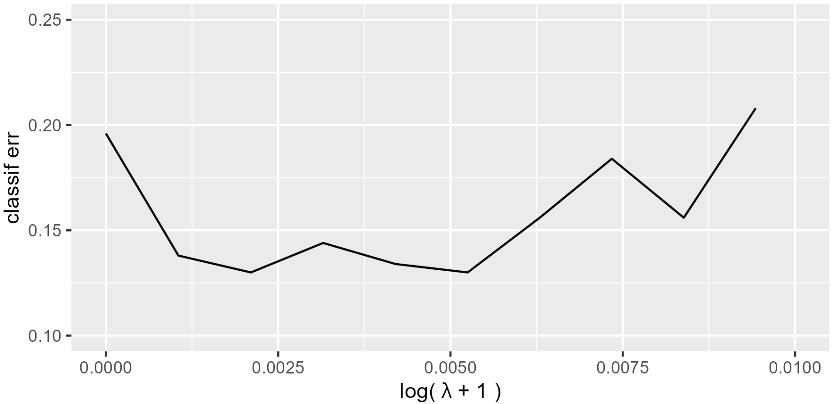


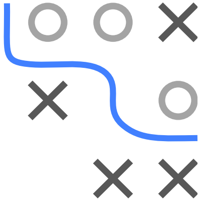
Prevention of overfitting can also be seen in CV.

Same settings as before, but each λ is evaluated with 5x10 REP-CV

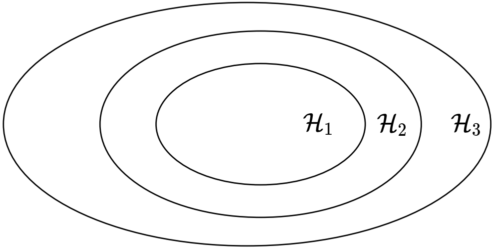


Typical U-shape with sweet spot between overfitting and underfitting

STRUCTURAL RISK MINIMIZATION



- Can also see this as an iterative process; more a “discrete” view on things
- SRM assumes that $\mathcal{H}$ can be decomposed into increasingly complex hypotheses: $\mathcal{H} = \cup_{k \geq 1} \mathcal{H}_k$
- Complexity parameters can be, e.g. the degree of polynomials in linear models or the size of hidden layers in neural networks



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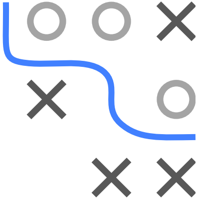
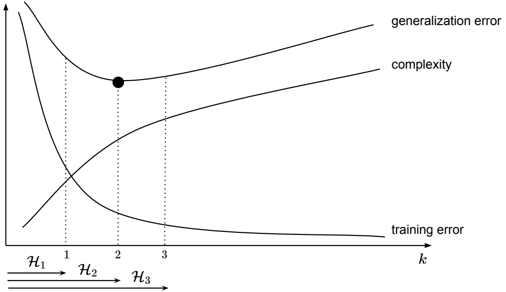


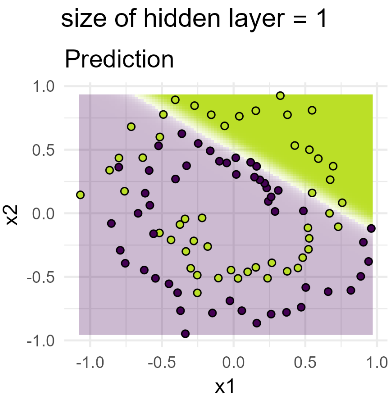
- SRM chooses the smallest k such that the optimal model from $\mathcal{H}_k$ found by ERM or RRM cannot significantly be outperformed by a model from a $\mathcal{H}_m$ with $m > k$
- Principle of Occam's razor
- One challenge might be choosing an adequate complexity measure, as for some models, multiple exist

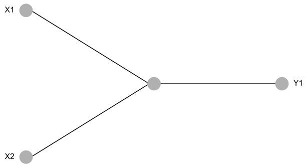


STRUCTURAL RISK MINIMIZATION

Again `spirals`.

NN with 1 hidden layer, and fixed (small) L2 penalty.





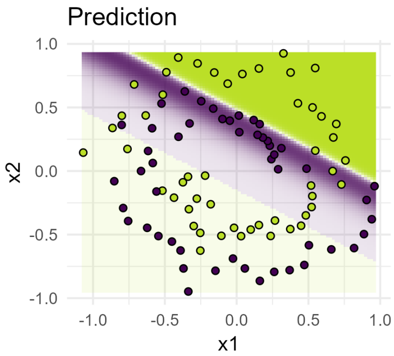
Size affects complexity and smoothness of decision boundary

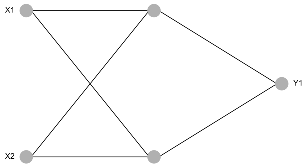
STRUCTURAL RISK MINIMIZATION

Again `spirals`.

NN with 1 hidden layer, and fixed (small) L2 penalty.

size of hidden layer = 2





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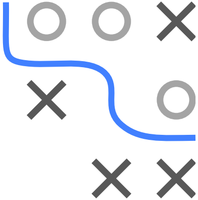
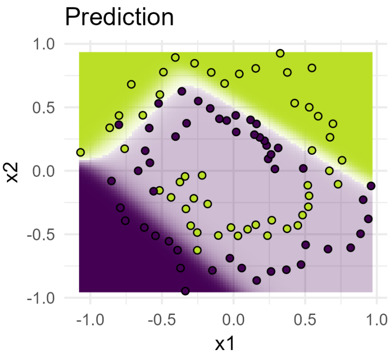
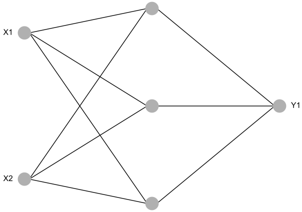


Again `spirals`.

NN with 1 hidden layer, and fixed (small) L2 penalty.

size of hidden layer = 3



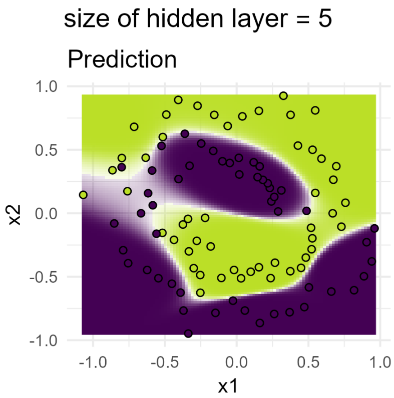


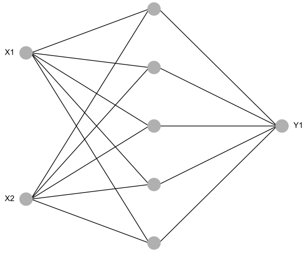
Size affects complexity and smoothness of decision boundary

STRUCTURAL RISK MINIMIZATION

Again `spirals`.

NN with 1 hidden layer, and fixed (small) L2 penalty.



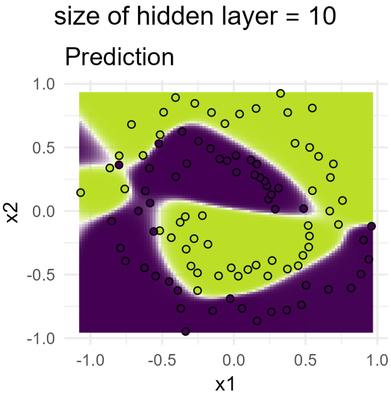


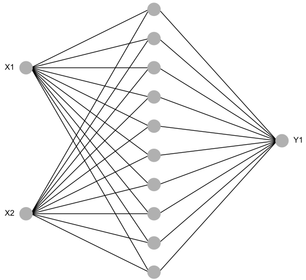
Size affects complexity and smoothness of decision boundary

STRUCTURAL RISK MINIMIZATION

Again `spirals`.

NN with 1 hidden layer, and fixed (small) L2 penalty.





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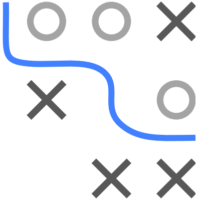
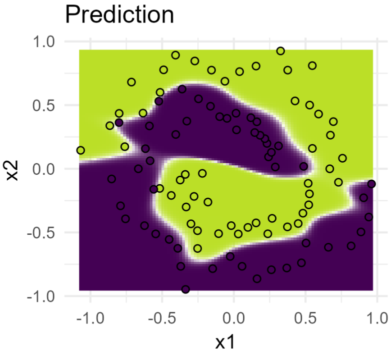
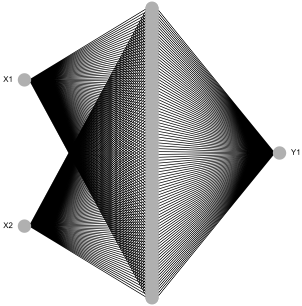


Again `spirals`.

NN with 1 hidden layer, and fixed (small) L2 penalty.

size of hidden layer = 100





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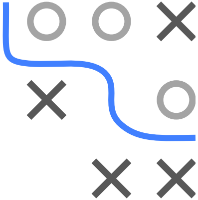
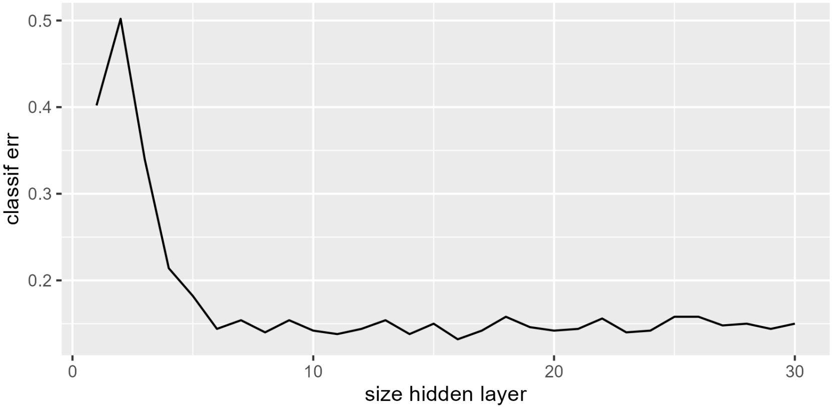
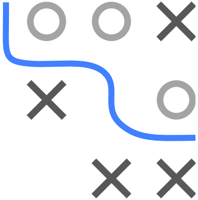


Again, complexity vs CV score.

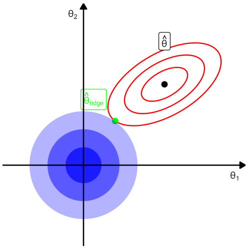


Minimal model with good generalization seems to size=10

STRUCTURAL RISK MINIMIZATION AND RRM



RRM can also be interpreted through SRM,
if we rewrite it in constrained form:



$$\min_{\boldsymbol{\theta}} \quad \sum_{i=1}^{n} L\left(y^{(i)}, f\left(\mathbf{x}^{(i)} \mid \boldsymbol{\theta}\right)\right)$$

$$\text{s.t.} \quad \|\boldsymbol{\theta}\|_2^2 \leq t$$

Can interpret going through λ from large to small as through t from small to large. Constructs series of ERM problems with hypothesis spaces $\mathcal{H}_\lambda$, where we constrain norm of $\boldsymbol{\theta}$ to unit balls of growing sizes.