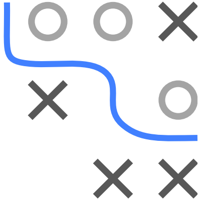
Introduction to Machine Learning



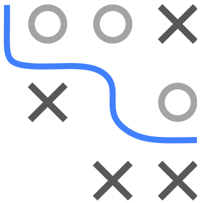
Regularization
Introduction

Learning goals

- Overfitting
- Motivation of regularization
- First overview of techniques
- Pattern of regularized ERM formula

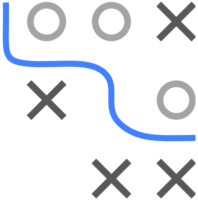
WHAT IS REGULARIZATION? I

Methods that add **inductive bias** to model, usually some “low complexity” priors (shrinkage and sparsity) to reduce overfitting and get better bias-variance tradeoff



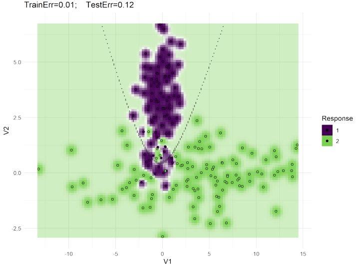
- **Explicit regularization**: penalize explicit measure of model complexity in ERM (e.g., $L1/L2$)
- **Implicit regularization**: early stopping, data augmentation, parameter sharing, dropout or ensembling
- **Structured regularization**: structural prior knowledge over groups of parameters or subnetworks (e.g., group lasso ▸ Yuan and Lin 2006)

RECAP: OVERFITTING I

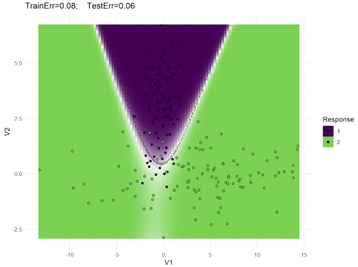


- Occurs when model reflects noise or artifacts in training data
- Model often then does not generalize well (small train error, high test error) – or at least works better on train than on test data

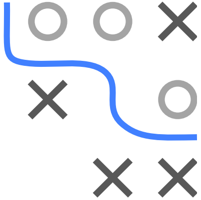
Overfitted model



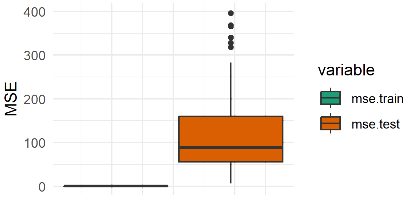
Appropriate model



EXAMPLE I: OVERFITTING I



- Data set: daily maximum **ozone level** in LA; $n = 50$
- 12 features: time (weekday, month); weather (temperature at stations, humidity, wind speed); pressure gradient
- Orig. data was subsetted, so it feels “high-dim.” now (low n in relation to p)
- LM with all features (L2 loss)
- MSE evaluation under 10×10 REP-CV



Model fits train data well, but generalizes poorly.

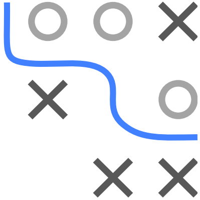
EXAMPLE II: OVERFITTING I

- We train an MLP and a CART on the mtcars data
- Both models are not regularized
- And configured to make overfitting more likely

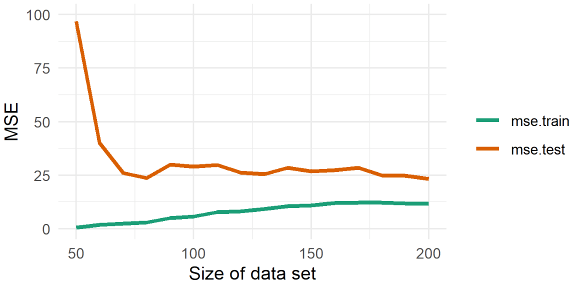
	Train MSE	Test MSE
Neural Network	1.47	345.84
CART	0.00	6.91

(And we now switch back to the Ozone example...)

AVOIDING OVERFITTING – COLLECT MORE DATA I



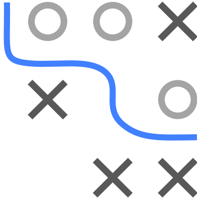
We explore our results for increased dataset size.



Fit slightly worsens, but test error decreases.

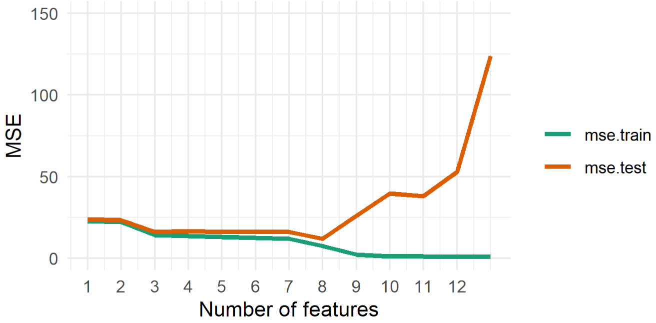
But: Often not feasible in practice.

AVOIDING OVERFITTING – REDUCE COMPLEXITY I



We try the simplest model: a constant. So for $L2$ loss the mean of $y^{(i)}$.

We then increase complexity by adding one feature at a time.



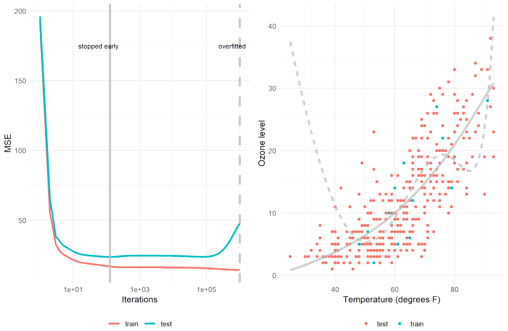
NB: We added features in a specific (clever) order, so we cheated a bit.

AVOIDING OVERFITTING – OPTIMIZE LESS I

Now: polynomial regression with temperature as single feature

$$f(\mathbf{x} \mid \boldsymbol{\theta}) = \sum_{k=0}^{d} \theta_k \cdot (x_T)^k$$

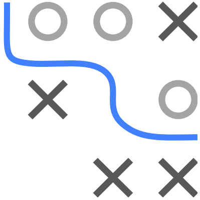
We set $d = 15$ to overfit to small data. To investigate early stopping, we don't analytically solve the OLS problem, but run GD stepwise.



We see: Early stopping GD can improve results.

NB: GD for poly-regr usually needs many iters before it starts to overfit, so we used a very small training set.

REGULARIZED EMPIRICAL RISK MINIMIZATION I

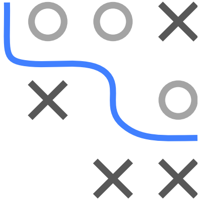


We have contradictory goals:

- **maximizing fit** (minimizing the train loss)
- **minimizing complexity** of the model

We saw how we can include features in a binary fashion.
But we would rather control complexity **on a continuum**.

REGULARIZED EMPIRICAL RISK MINIMIZATION I



Common pattern:

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

- $J(f)$: **complexity penalty**, **roughness penalty** or **regularizer**
- $\lambda \geq 0$: **complexity control** parameter
- The higher λ, the more we penalize complexity
- $\lambda = 0$: We just do simple ERM; $\lambda \to \infty$: we don't care about loss, models become as "simple" as possible
- λ is hard to set manually and is usually selected via CV
- As for $\mathcal{R}_{\text{emp}}$, $\mathcal{R}_{\text{reg}}$ and J are often defined in terms of $\boldsymbol{\theta}$:

$$\mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) + \lambda \cdot J(\boldsymbol{\theta})$$