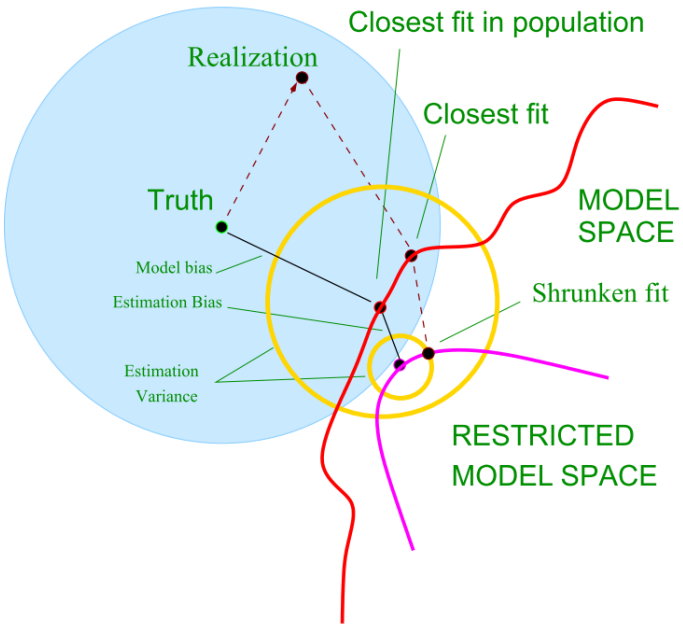
Introduction to Machine Learning

Introduction to Regularization



Learning goals

- XXX
- XXX

Motivation for Regularization

EXAMPLE: OVERFITTING

- Assume we want to predict the daily maximum **ozone level** in LA given a data set containing 50 observations.
- The data set contains 12 features describing time conditions (e.g., weekday, month), the weather (e.g., temperature at different weather stations, humidity, wind speed) or geographic variables (e.g., the pressure gradient).
- We fit a linear regression model using **all** of the features

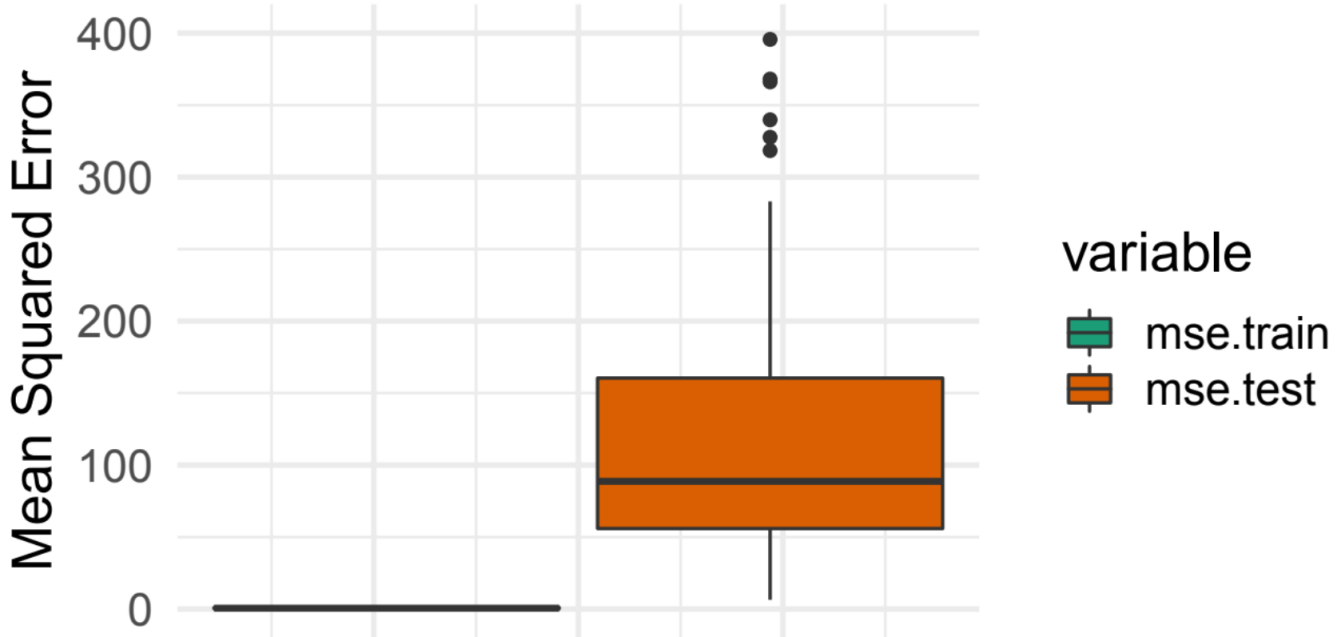
$$f(\mathbf{x} \mid \boldsymbol{\theta}) = \boldsymbol{\theta}^T \mathbf{x} = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_{12} x_{12}$$

  with the *L2* loss.
- We evaluate the performance with 10 times 10-fold CV.

We use (a subset of) the `Ozone` data set from the `mlbench` package. This way, we artificially create a "high-dimensional" dataset by reducing the number of observations drastically while keeping the number of features fixed.

EXAMPLE: OVERFITTING

While our model fits the training data almost perfectly (left), it generalizes poorly to new test data (right). We overfitted.



AVOID OVERFITTING

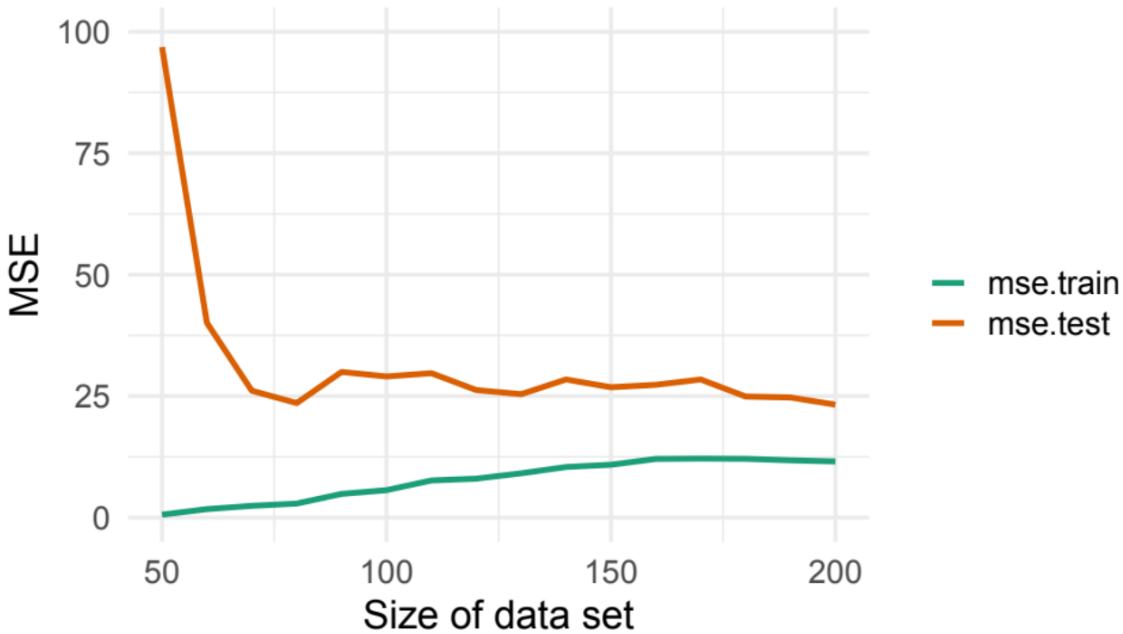
Why can **overfitting** happen? And how to avoid it?

1. Not enough data
   $\rightarrow$ collect **more data**
2. Data is noisy
   $\rightarrow$ collect **better data** (reduce noise)
3. Models are too complex
   $\rightarrow$ use **less complex models**
4. Aggressive loss optimization
   $\rightarrow$ **optimize less**

AVOID OVERFITTING

Approach 1: Collect more data

We explore our results for increased dataset size by 10 times 10-fold CV. The fit worsens slightly, but the test error decreases.



Good idea, but often not feasible in practice.

AVOID OVERFITTING

Approach 3: Reduce complexity

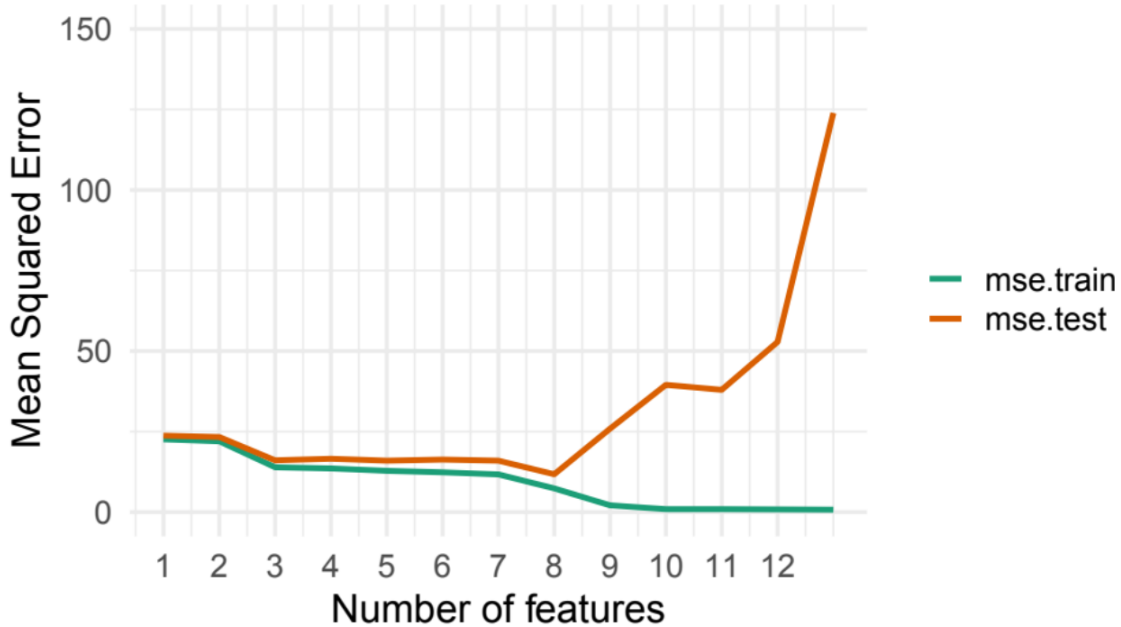
We try the simplest model we can think of: the constant model. For the *L2* loss, the optimal constant model is

$$f(\mathbf{x} \mid \boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} y^{(i)}$$

We then increase the complexity of the model step-by-step by adding one feature at a time.

AVOID OVERFITTING

We can control the complexity of the model by including/excluding features. We can try out all feature combinations and investigate the model fit.



Note: For simplicity, we added the features in one specific (clever) order, so we cheated a bit. Also note there are $2^{12} = 4096$ potential feature combinations.

AVOID OVERFITTING

Approach 4: Optimize less

Now we use polynomial regression with temperature as the only feature to predict the ozone level, i.e.,

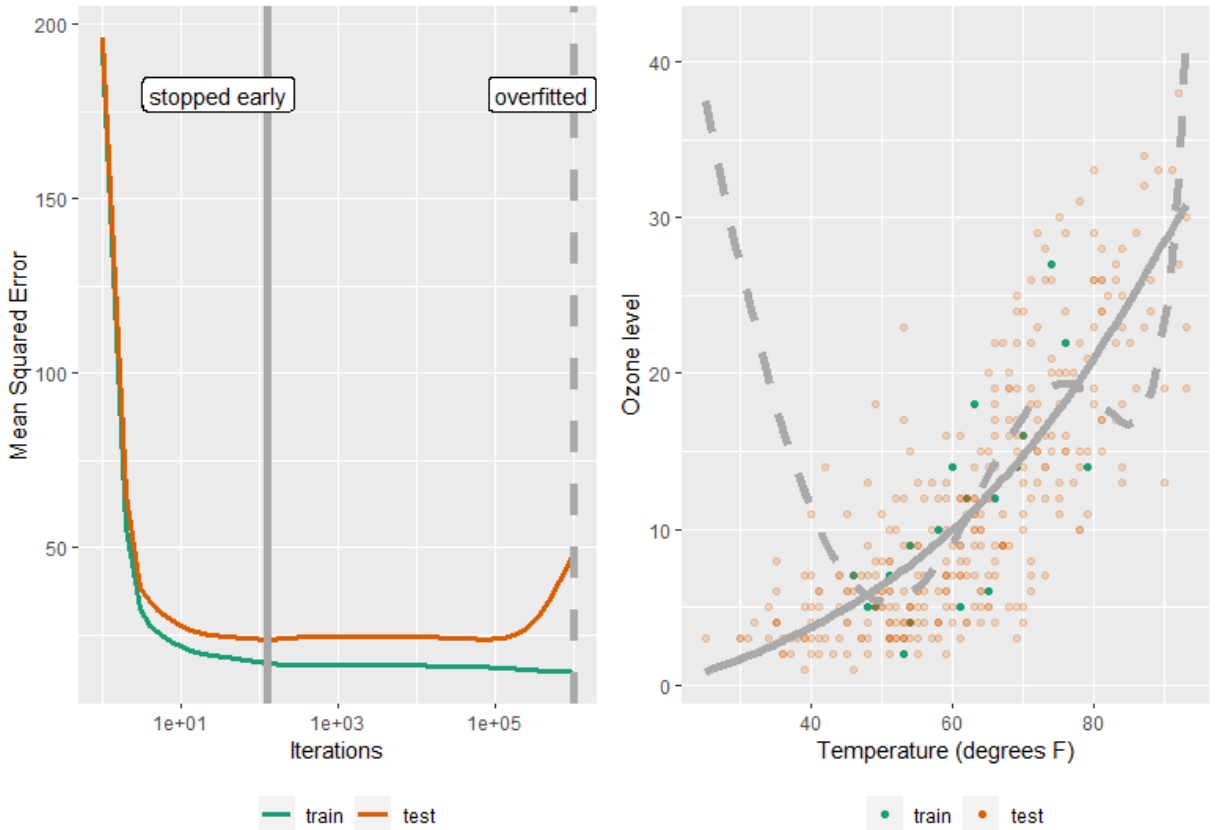
$$f(\mathbf{x} \mid \boldsymbol{\theta}) = \sum_{i=0}^{d} \theta_i (x_T)^i.$$

We choose $d = 15$, for which we get a very flexible model, which can be prone to overfitting for small data sets.

In this example, we don't solve for $\hat{\theta}$ directly, but instead, we use the gradient descent algorithm to find $\hat{\theta}$ stepwise.

AVOID OVERFITTING

We want to stop the optimization early when the generalization error starts to degrade.



Note: For polynomial regression, gradient descent usually needs many iterations before it starts to overfit. Hence a very small training set was chosen to accelerate this effect.

AVOID OVERFITTING

We have contradictory goals

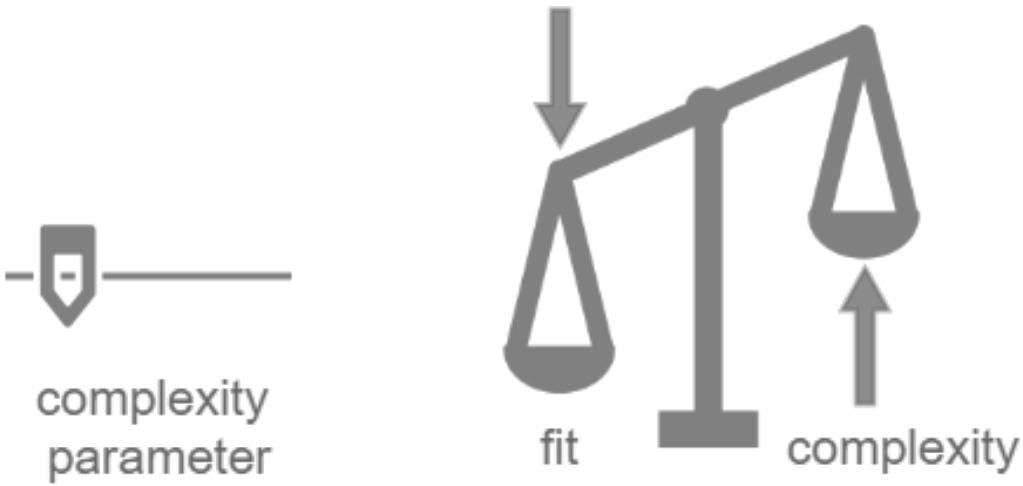
- **maximizing the fit** (minimizing the train loss)
- **minimizing the complexity** of the model.

We need to find the “sweet spot”.

AVOID OVERFITTING

Until now, we can either add a feature completely or not at all.

Instead of controlling the complexity in a discrete way by specifying the number of features, we might prefer to control the complexity **on a continuum** from simple to complex.



Regularized Empirical Risk Minimization

REGULARIZED EMPIRICAL RISK MINIMIZATION

Recall, empirical risk minimization with a complex hypothesis set tends to overfit. A major tool to handle overfitting is **regularization**.

In the broadest sense, regularization refers to any modification made to a learning algorithm that is intended to reduce its generalization error but not its training error.

Explicitly or implicitly, such modifications represent the preferences we have regarding the elements of the hypothesis set.

REGULARIZED EMPIRICAL RISK MINIMIZATION

Commonly, regularization takes the following form:

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

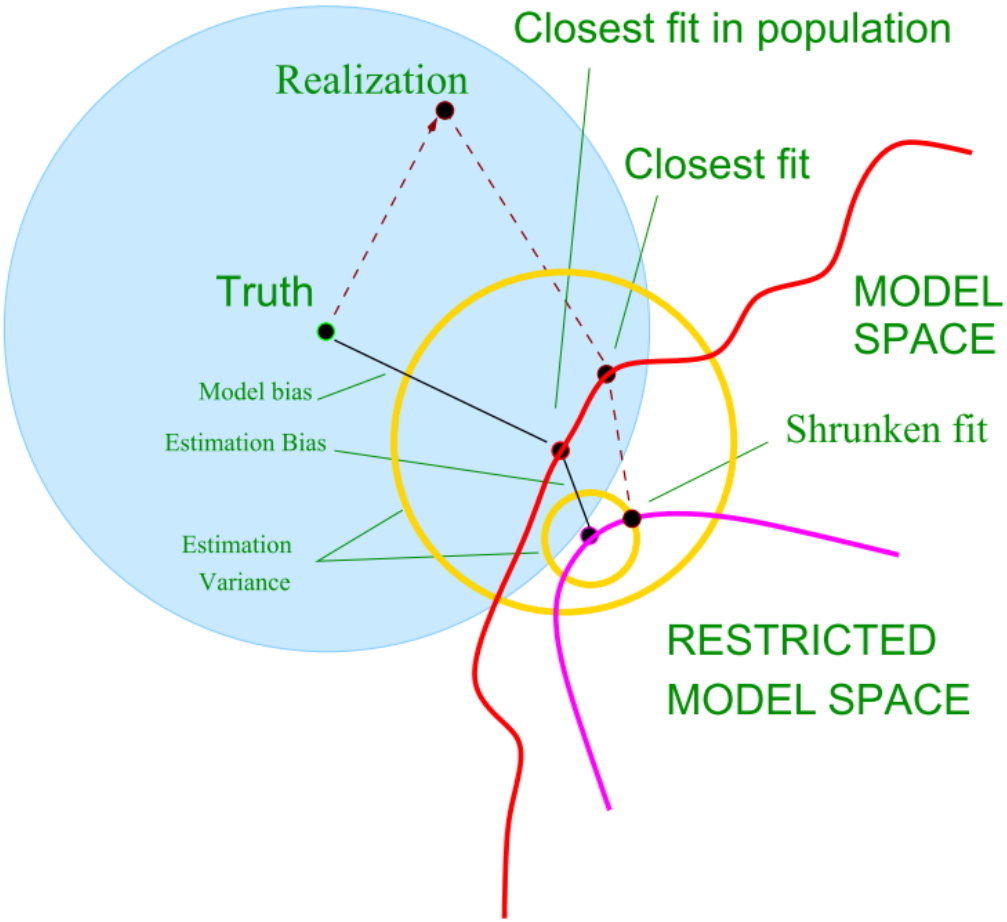
- $J(f)$ is called **complexity penalty**, **roughness penalty** or **regularizer**.
- $\lambda > 0$ is called **complexity control** parameter.
- It measures the "complexity" of a model and penalizes it in the fit.
- As for $\mathcal{R}_{\text{emp}}$, often $\mathcal{R}_{\text{reg}}$ and J are defined on $\boldsymbol{\theta}$ instead of f, so $\mathcal{R}_{\text{reg}}(\boldsymbol{\theta}) = \mathcal{R}_{\text{emp}}(\boldsymbol{\theta}) + \lambda \cdot J(\boldsymbol{\theta})$.

REGULARIZED EMPIRICAL RISK MINIMIZATION

Remarks:

- Note that we now face an optimization problem with two criteria:
  1. models should fit well (low empirical risk),
  2. but not be too complex (low $J(f)$).
- We decide to combine the two in a weighted sum and to control the trade-off via the complexity control parameter λ.
- λ is hard to set manually and is usually selected via cross-validation (see later).
- $\lambda = 0$: The regularized risk $\mathcal{R}_{\text{reg}}(f)$ reduces to the simple empirical $\mathcal{R}_{\text{emp}}(f)$.
- If λ goes to infinity, we stop caring about the loss/fit and models become as "simple" as possible.

REGULARIZED EMPIRICAL RISK MINIMIZATION



Hastie, The Elements of Statistical Learning, 2009 (p. 225)