7.1 Overfitting

Machine Learning 1: Foundations

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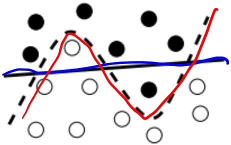
Overfitting Dilemna

Given too few data we do not know which classifier works better: a simple or complex one.

Overfitting Dilemna

Given too few data we do not know which classifier works better: a simple or complex one.

training: small data



Overfitting Dilemna

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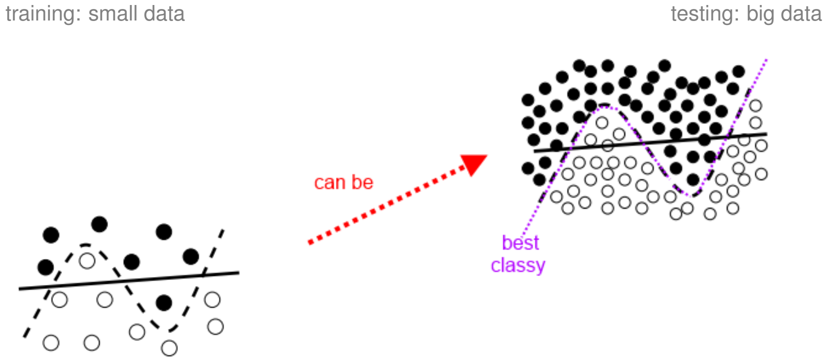

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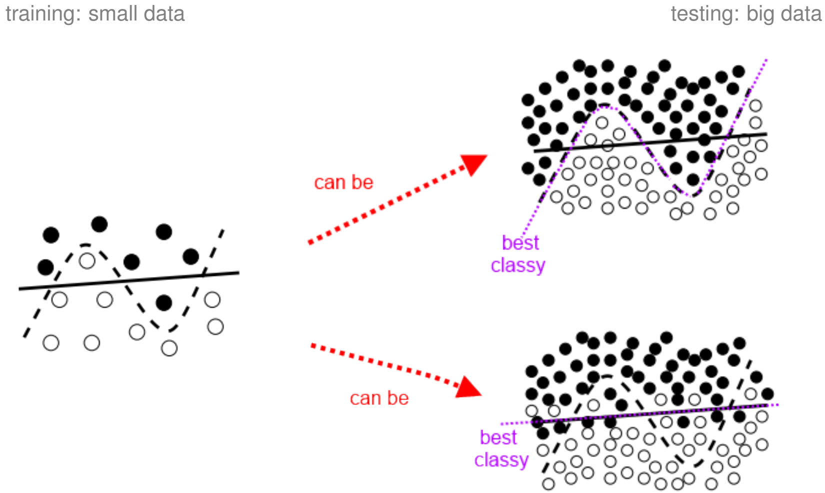
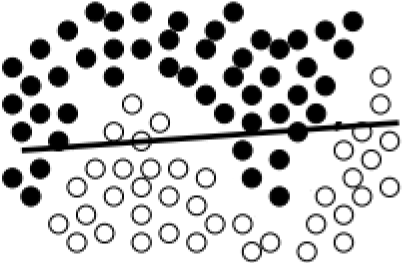


Two things can go wrong...



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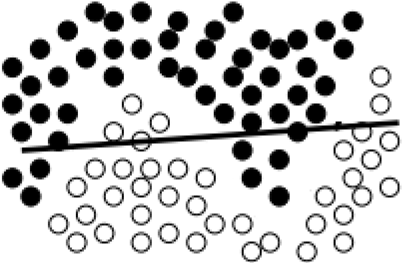

Underfitting

Learning a too simple classifier that is not complex enough to describe the training data well.

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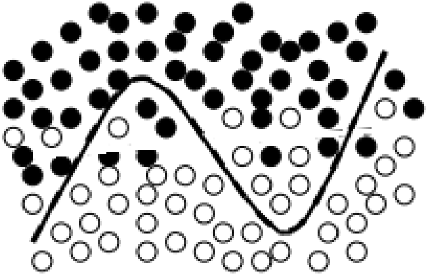

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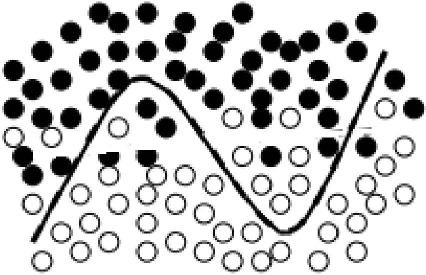

Overfitting

Learning a too complex classifier that fits the training data “too well”

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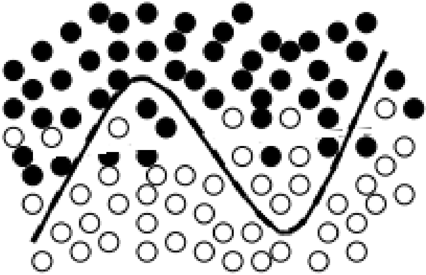

Overfitting

Learning a too complex classifier that fits the training data “too well” (does not “generalize” to new data)

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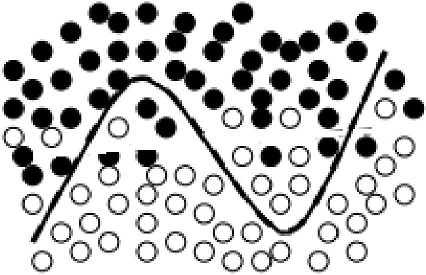

Overfitting

Learning a too complex classifier that fits the training data “too well” (does not “generalize” to new data)

Generalization

Predict accurately for new (previously unseen) examples.

Example: SVM with **polynomial** kernel

Polynomial kernel of degree $m \in \mathbb{N}$

Defined as:

$$k(\mathbf{x}, \tilde{\mathbf{x}}) := (\langle \mathbf{x}, \tilde{\mathbf{x}} \rangle + b)^m, \quad b \in \mathbb{R}_+$$

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Prediction functions are degree-m polynomials:

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

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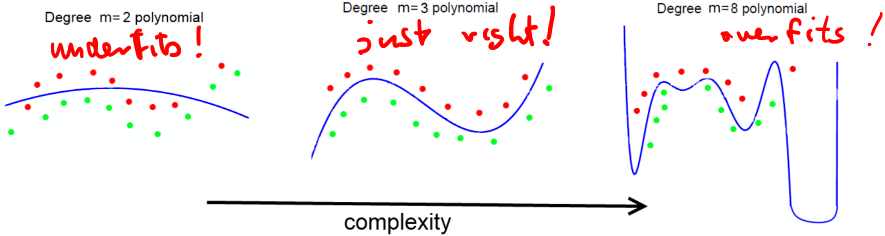
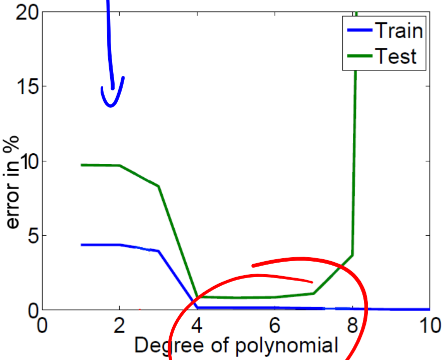


Typical result

under-fitting

overfitting



just right

Example: SVM with **Gaussian** kernel

Gaussian kernel with bandwidth $\sigma > 0$

$$k(\mathbf{x}, \tilde{\mathbf{x}}) := \exp\left(-\frac{1}{2\sigma^2}\|\mathbf{x} - \tilde{\mathbf{x}}\|^2\right)$$

Demo:

`https://cs.stanford.edu/~karpathy/svmjs/demo/`

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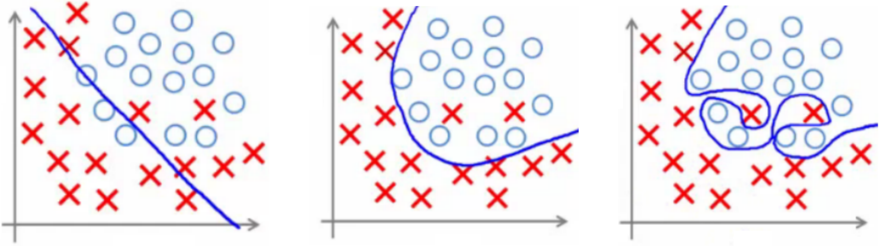


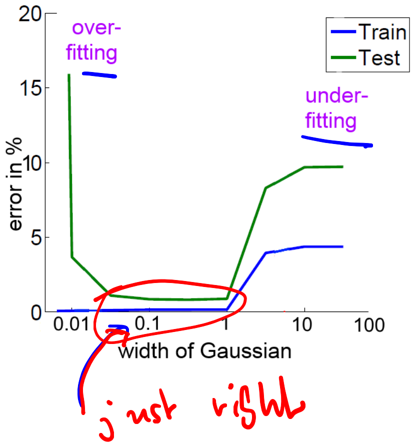
large width — under-fitting

moderate width — just right

small width — over-fitting

complexity

Typical result



Similar Behavior of Various Other Learning Machines

k-nearest neighbor algorithm:

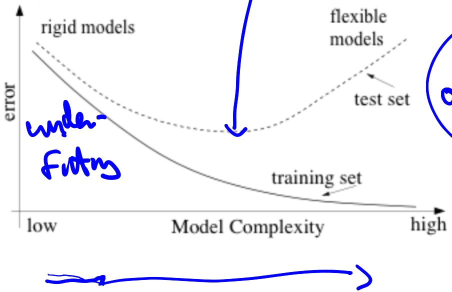
- too small *k*: overfits
- too large *k*: underfits

Deep learning

- Architecture that is too deep
  & has too many neurons and connections: overfits
- Architecture that is too shallow
  & has too few neurons and connections: underfits

Big Picture

just right



overfitting

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Even the simplest classifiers can overfit, e.g.:

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How to avoid under- and overfitting?

Solution

Choose an (overly) complex model (thus avoiding **under**fitting), but use a technique called **regularization** to avoid **over**fitting