Vapnik-Chervonenkis learning theory

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Courtesy: M.I. Schlesinger.

Outline of the talk:

- Classifier design.
- Mathematical formulation of the risk describing process of learning.
- Upper bound = guaranteed risk.
- VC-dimension calculation.
- Structural risk minimization.
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Classifier design (1)

The object of interest is characterized by observable properties $x \in X$ and its class membership (unobservable, hidden state) $y \in Y$, where X is the space of observations and Y the set of hidden states.

The objective of a classifier design is to find the optimal decision function $q^*\colon X \to Y$.

Bayesian decision theory solves the problem of minimization of the Bayesian risk

$$R(q) = \sum_{x,y} p_{XY}(x,y)\, W(y, q(x))$$

given the following quantities:

- $p_{XY}(x,y)$, $\forall x \in X$, $y \in Y$ – the statistical model of the dependence of the observable properties (measurements) on class membership.
- $W(y, q(x))$ the loss of decision $q(x)$ if the true class is y.

Classifier design (2)

Constraints or penalties for different errors depend on the application problem formulation.

However, in applications typically:

- None of the probabilities are known, e.g., $p(x|y)$, $p(y)$, $\forall x \in X$, $y \in Y$.
- The designer is only given a training multi-set $T = \{(x_1, y_1) \dots (x_L, y_L)\}$, where L is the length (size) of the training multi-set.
- The desired properties of the classifier $q(x)$ are assumed.

Note: Non-Bayesian decision theory offers the solution to the problem if $p(x|y)$, $\forall x \in X$, $y \in Y$ are known, but $p(y)$ are unknown (or do not exist).

Classifier design via parameter estimation

- Assume $p(x, y)$ have a particular form, e.g., a mixture of Gaussians, piece-wise constant, etc., with a finite (i.e., small) number of parameters Θ_y.
- Estimate the parameters Θ_y from the training multi-set T.
- Solve the classifier design problem (i.e., minimize the risk) by substituting the estimated $\hat{p}(x, y)$ for the true (and unknown) probabilities $p(x, y)$.

– : There is no direct relationship between known properties of estimated $\hat{p}(x, y)$ and the properties (typically the risk) of the obtained classifier $q'(x)$.

– : If the true $p(x, y)$ is not of the assumed form then $q'(x)$ may be arbitrarily bad, even if the size of training set L approaches infinity!

\+ : Implementation is often straightforward, especially if parameters Θ_y for each class are assumed independent.

\+ : Performance on real data can be predicted empirically from performance on training set (divided to training set and validation set, e.g., crossvalidation).

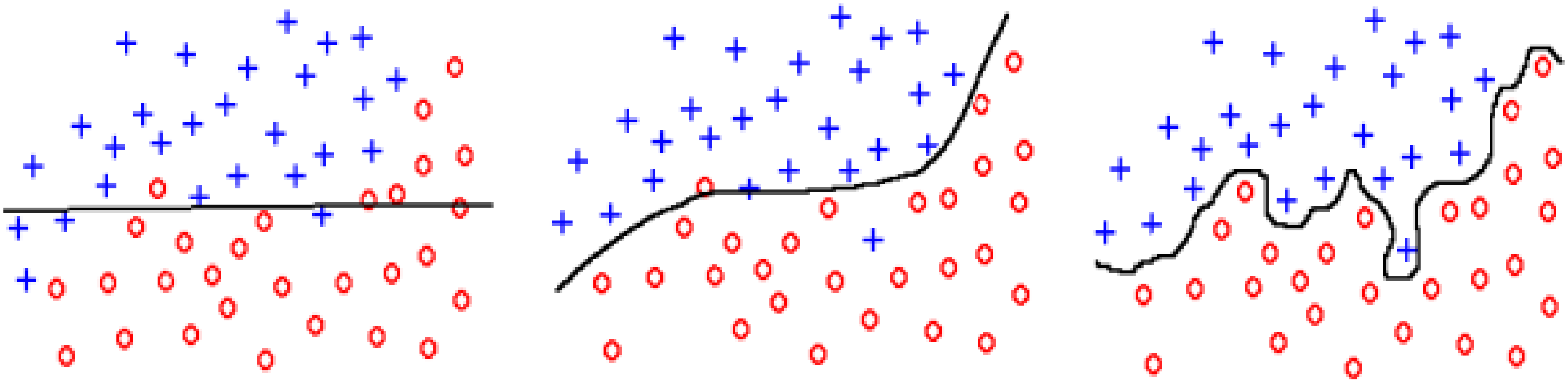
Learning in statistical pattern recognition

- Choose a class Q of decision functions (classifiers) $q\colon X \to Y$.
- Find $q^* \in Q$ by minimizing some criterion function on the training set that approximates the risk $R(q)$ (which cannot be computed).
- Learning paradigm is defined by the approximating criterion function:

1. Maximizing likelihood.
   Example: Estimating the probability density.
2. Using a non-random training set.
   Example: Image analysis.
3. Empirical risk minimization in which the true risk is approximated by the error rate on the training set.
   Examples: Perceptron, Neural nets (Back-propagation), etc.
4. Structural risk minimization.
   Example: SVM (Support Vector Machines).

Overfitting and underfitting

- How rich class Q of classifiers $q(x, \Theta)$ should be used?
- The problem of generalization is a key problem of pattern recognition: a small empirical risk R_{emp} need not imply a small true expected risk R!



underfit fit overfit

Asymptotic behavior

- For infinite training data, the law of large number assures

$$\lim_{L \to \infty} R_{\mathrm{emp}}(\Theta) = R(\Theta)\ .$$

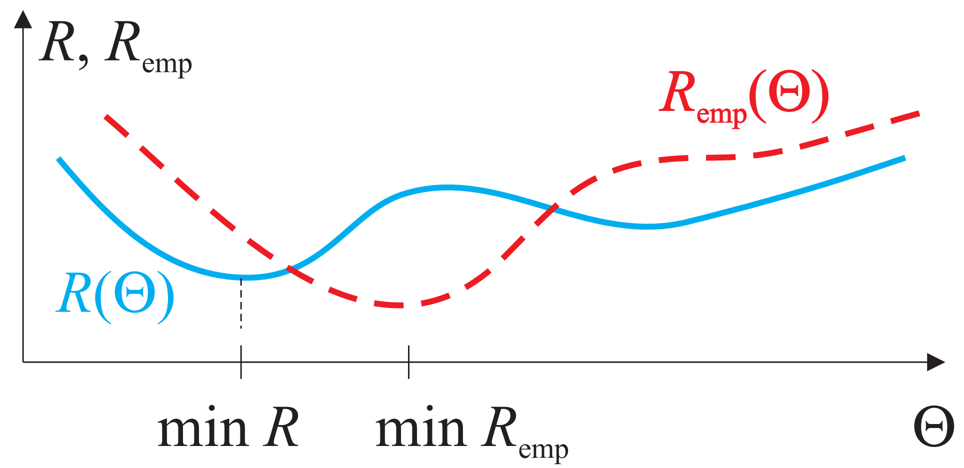
- In general, unfortunately, there is no guarantee for a solution based on the expected risk minimization because

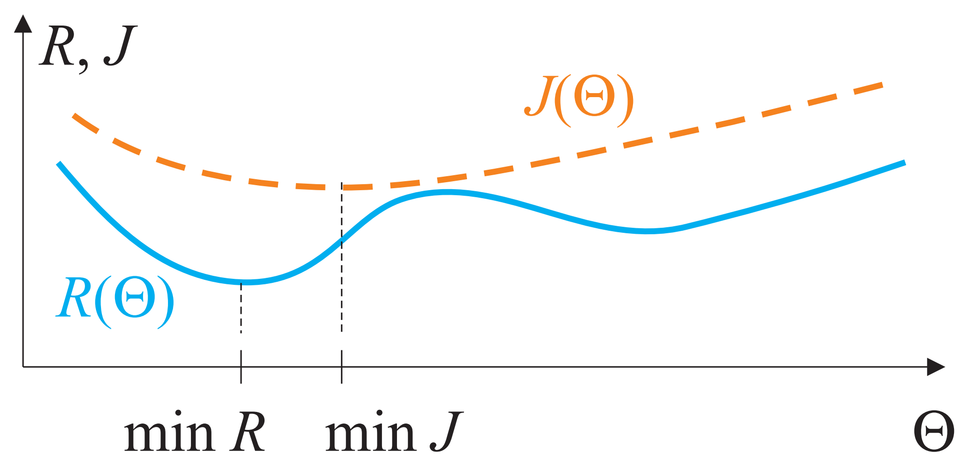
$$\operatorname*{argmin}_{\Theta} R_{\mathrm{emp}}(\Theta) \neq \operatorname*{argmin}_{\Theta} R(\Theta)\ .$$

Performance on training data is often better than on test data (or real performance).

The idea of the guaranteed risk

- Idea: add a prior (called also regularizer).
- This regularizer favors a simpler strategy, cf., Occam razor.
- Vapnik-Chervonenkis learning theory introduces a guaranteed risk $J(\Theta)$, $R(\Theta) \leq J(\Theta)$, with the probabilistic confidence η.
- The upper bound $J(\Theta)$ may be so large (meaning pessimistic) that it can be useless.





The upper bound of a true risk

- The upper bound was derived by Chervonenkis and Vapnik in the 1970s.
- With the confidence η, $0 \leq \eta \leq 1$,

$$R(\Theta) \leq J(\Theta) = R_{\mathrm{emp}}(\Theta) + \sqrt{\frac{h\left(\log\left(\frac{2L}{h}\right) + 1\right) - \log\left(\frac{\eta}{4}\right)}{L}} \, .$$

where L is the length of the training multi-set, h is the VC-dimension of the class of strategies $q(x, \Theta)$.

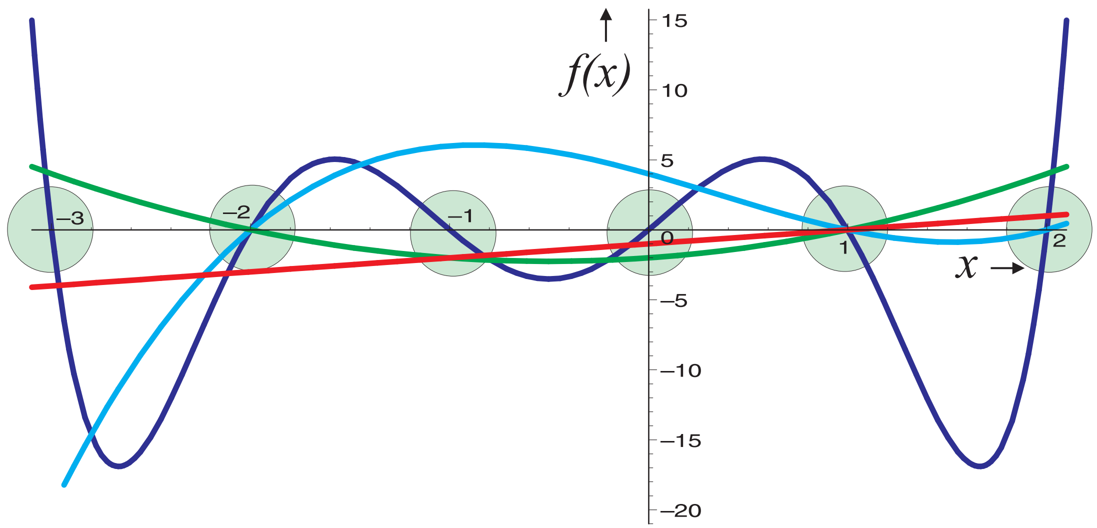
- Note that the above upper bound is independent of the true $p(x, y)$!!
- It is the worst case upper bound valid for all possible $p(x, y)$.
- Structural risk minimization means minimizing the upper bound $J(\Theta)$.
(We will return to structural risk minimization after we explain how to compute VC-dimension.)

Vapnik-chervonenkis dimension

- It is a number characterizing the decision strategy.
- Abbreviated VC-dimension.
- Named after Vladimir Vapnik and Alexey Chervonenkis

  (Appeared in their book in Russian. V. Vapnik, A. Chervonenkis: Pattern Recognition Theory, Statistical Learning Problems, Nauka, Moskva, 1974).
- It is one of the core concepts in Vapnik-Chervonenkis theory of learning.
- In the original 1974 publication, it was called capacity of a class of strategies.
- The VC dimension is a measure of the capacity of a statistical classification algorithm.

VC-dimension, the idea informally



$$
\begin{aligned}
f_1(x) &= (x-1)\\
f_2(x) &= (x-1)(x+2)\\
f_3(x) &= (x-2)(x-1)(x+2)\\
f_6(x) &= (x-2)(x-1)\,x\,(x+1)\\
&\qquad (x+2)(x+3)
\end{aligned}
$$

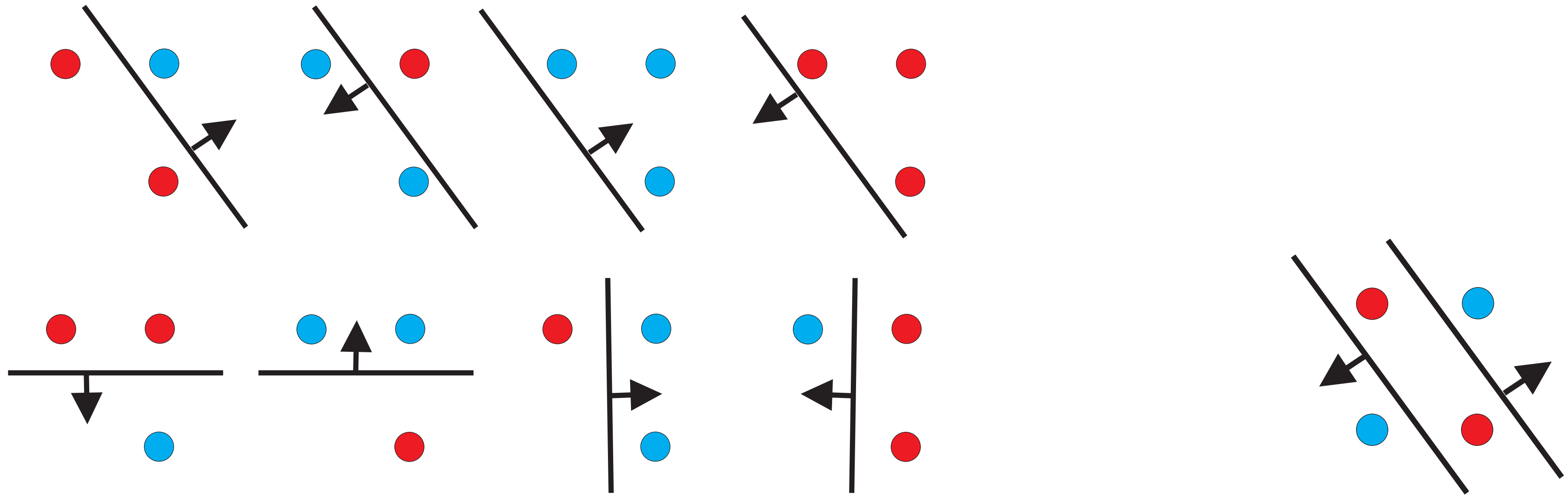
Light green circles symbolize data points.

- The VC-dimension (capacity) of a classification strategy tells how complicated it can be.
- An example: the thresholding a high-degree polynomial. If a very high-degree polynomial is used, it can be very wiggly, and can fit a training set exactly (overfit). Such a polynomial has a high capacity and problems with generalization.
- A linear function, e.g., has a low VC-dimension.

Shattering

- Consider a classification strategy q with some parameter vector Θ.
- The strategy q can shatter a set of data points $x_1, x_2, \ldots, x_n$ if, for all possible assignments of labels $y \in Y$ to data points, there exists a parameter Θ such that the model q makes no errors when evaluating that set of data points.

Shattering example: q is a line in a 2D feature space.



3 points, shattered

4 points, undivisible

VC-dimension h, definition

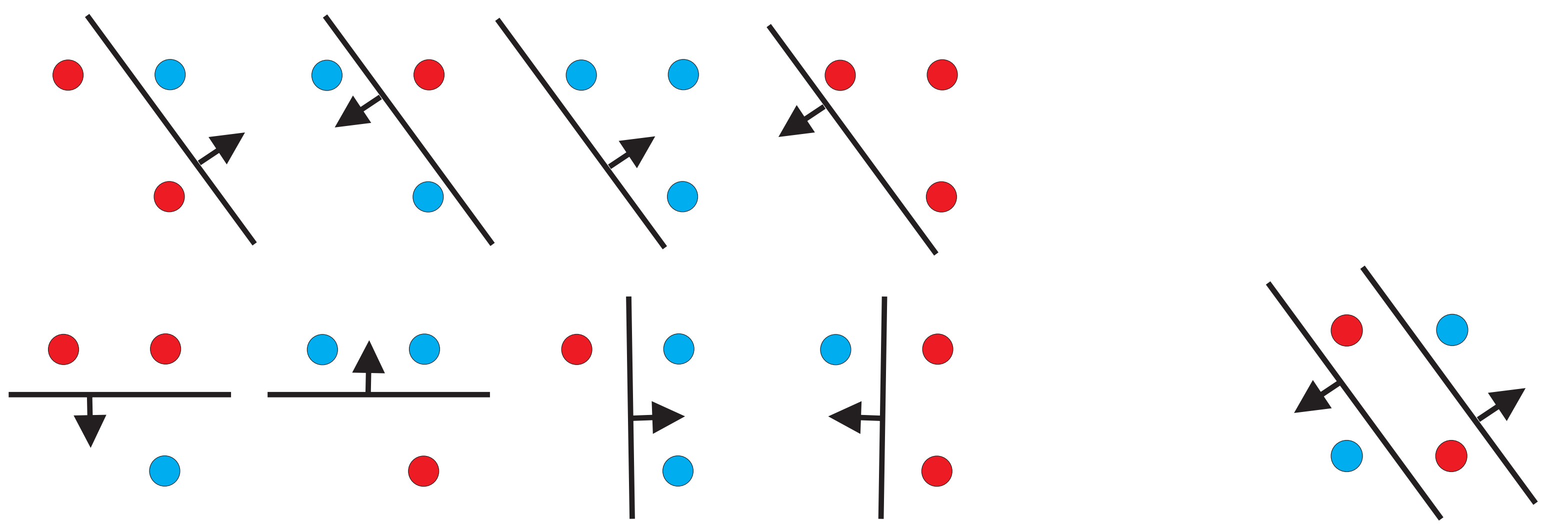
- Consider a set of dichotomic strategies $q(x, \Theta) \in Q$.
- The set consisting of h data points (observations) can be labelled in 2^h possible ways.
- A strategy $q \in Q$ exists which assigns labels correctly to all possible configurations.

  (Process of finding all possible configurations with correctly assigned labels is called shattering.)
- VC-dimension (definition) is the maximal number h of data points (observations) that can be shattered.

VC-dimension of a linear strategy in a 2D feature space

- A set of parameters $\Theta = \{\Theta_0, \Theta_1, \Theta_2\}$.
  A linear strategy $q(x, \Theta) = \Theta_1\, x_1 + \Theta_2\, x_2 + \Theta_0$.

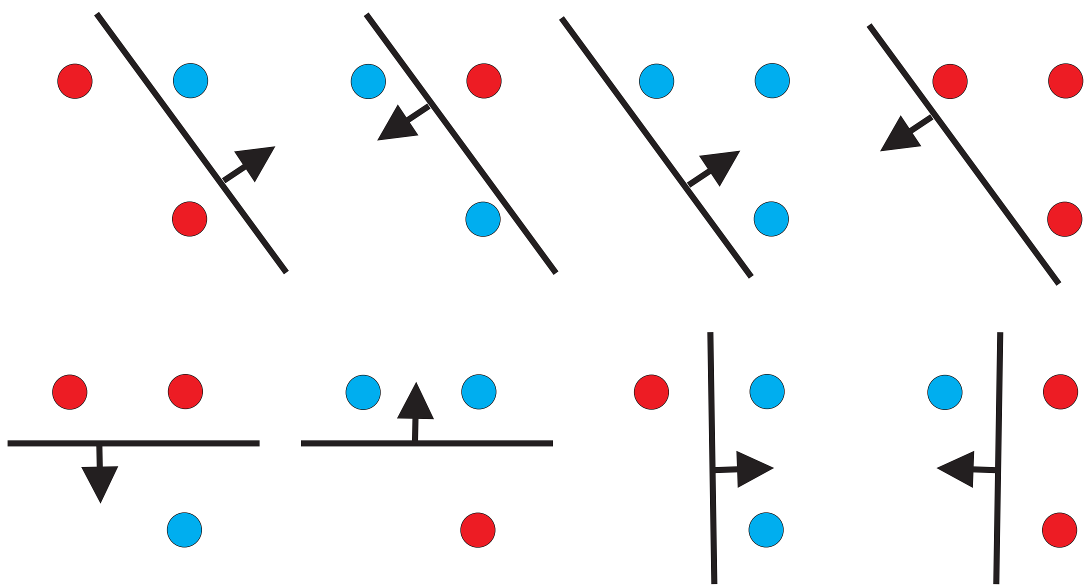
- Shattering example (revisited):



3 points, shattered *4 points, undivisible*

- 3 points in 2D space $(n = 2)$ can be shattered.
  There was counter example given that 4 points cannot be shattered.
  $\Rightarrow$ VC-dimension $h = 3$.

VC-dimension for a linear strategy in a n-dimensional space



A special case, n=2.

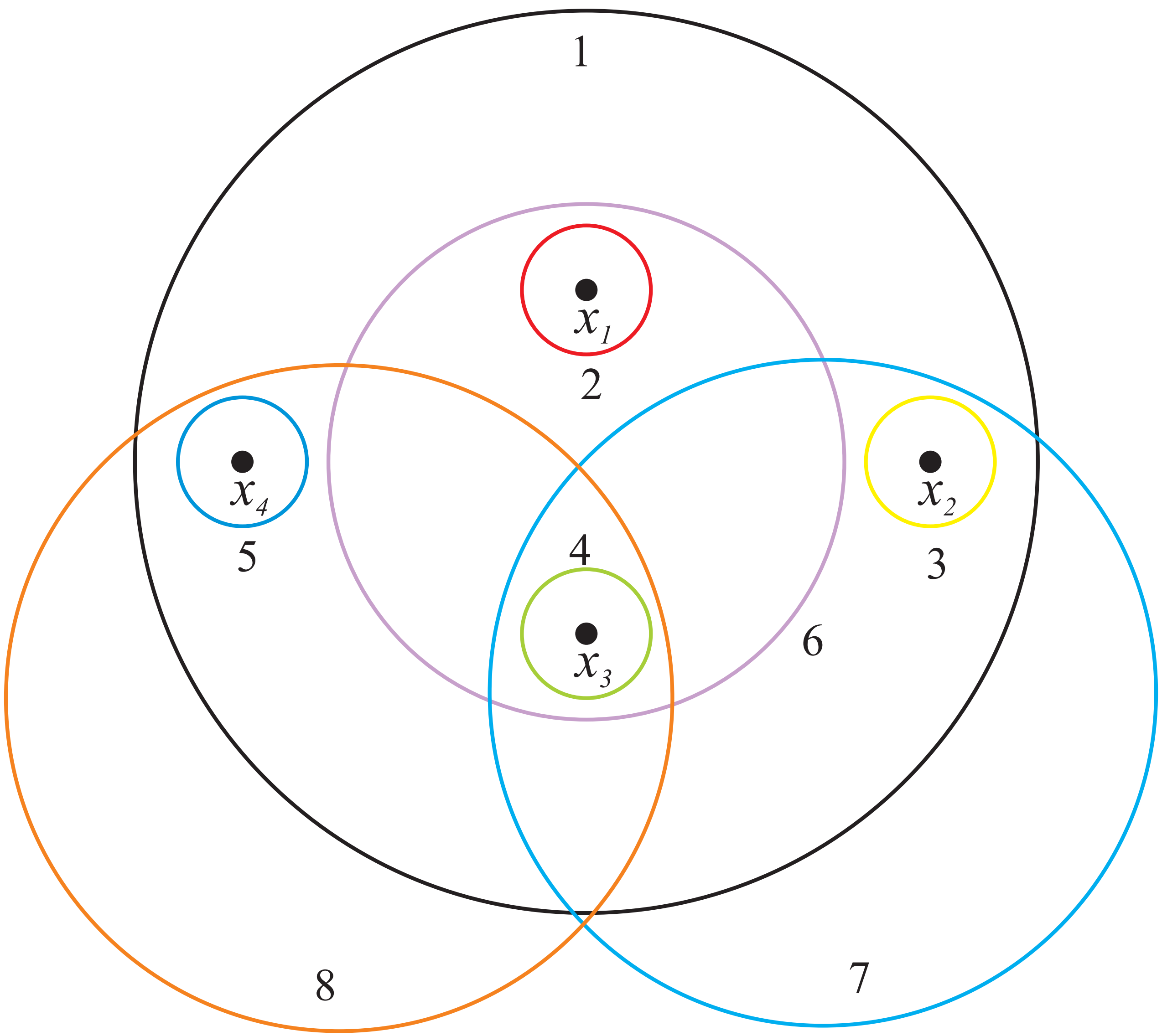
VC-dimension = 3.

Generalization to n-dimensions for linear classifiers

- A hyperplane in the space $\mathbb{R}^n$ shatters any set of $h = n + 1$ linearly independent points.
- Consequently, VC-dimension of linear decision strategies is $h = n + 1$.

VC-dimension in a 2D space for a circular strategy

Maximally 4 data points in $\mathbb{R}^2$ can be shattered in 8 possible ways
$\Rightarrow$ VC-dimension $h = 4$.

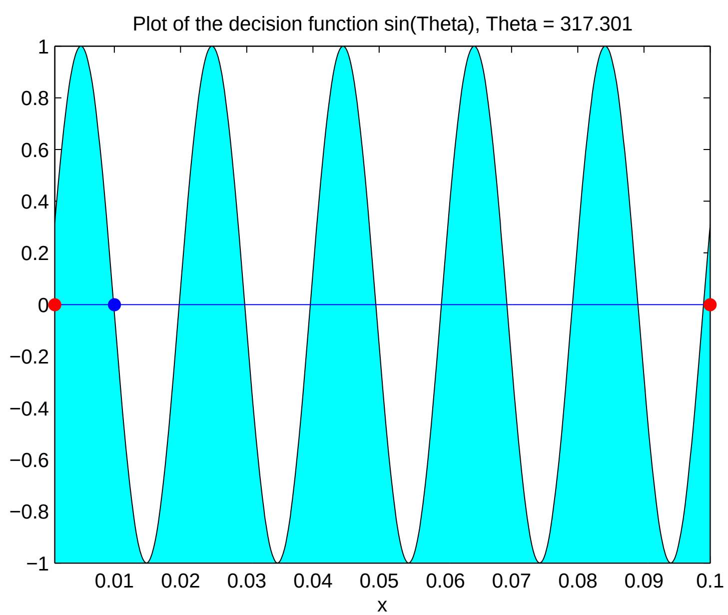


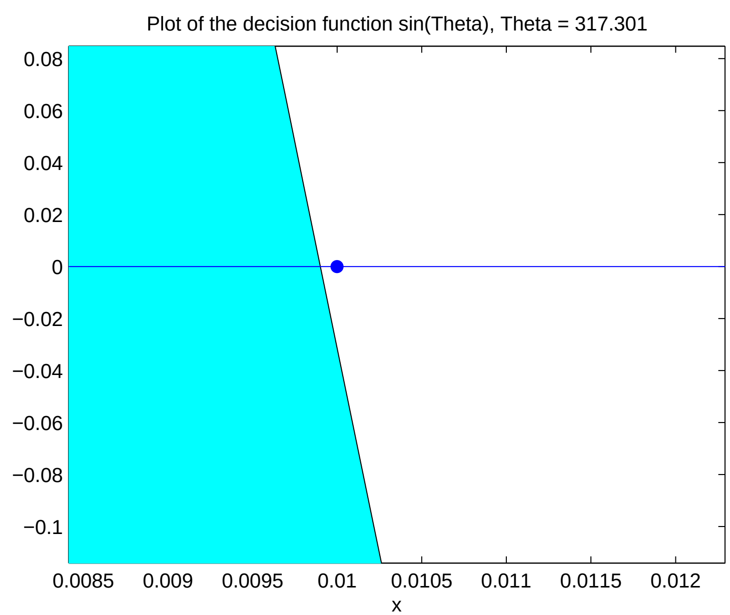
Small # of parameters, VC-dimension=∞

Counterexample by E. Levin, J.S. Denker (Vapnik 1995):

- A sinusoidal 1D classifier, $q(x, \Theta) = sign(\sin(\Theta x))$, $x, \Theta \in \mathbb{R}$.
- For any given number $L \in \mathbb{N}$, the points $x_i = 10^{-i}$, $i = 1, \ldots, L$ and be found and arbitrary labels y_i, $y_i \in \{-1, 1\}$ can assigned to x_i.
- Then $q(x, \Theta)$ is the correct labelling if $\Theta = \pi \left(1 + \sum_{i=1}^{L} \frac{(1-y_i)\, 10^i}{2}\right)$.

  Example: $L = 3$, $y_1 = -1$, $y_2 = 1$, $y_3 = -1$.



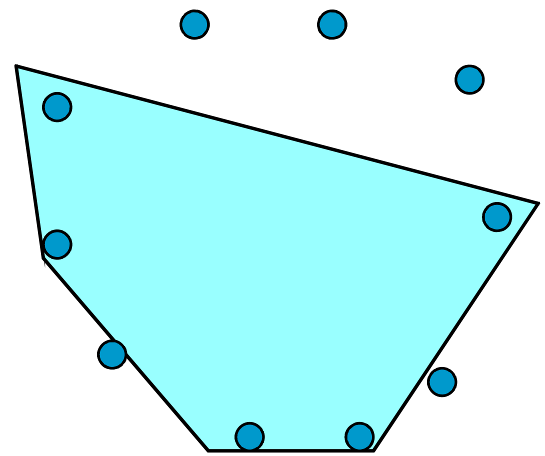


- Thus the VC dimension of this decision strategy is infinite.

Examples of other VC-dimension $= \infty$ strategies

- Nearest-neighbor classifier – any number of observations, labeled arbitrarily, will be classified. Thus VC-dimension $= \infty$. Also $R_{emp} = 0$. The VC-dimension provides no information in this particular case.

- Convex polygons classifying observation lying on a circle, VC-dimension $= \infty$.



- SVM classifiers with Gaussian (or RBF . . .) kernel, VC-dimension $= \infty$.

Structural risk minimization

- Minimize guaranteed risk $J(\Theta)$, that is the upper bound

$$R(\Theta) \leq J(\Theta) = R_{\mathrm{emp}}(\Theta) + \sqrt{\frac{h\left(\log\left(\frac{2L}{h}\right)+1\right) - \log\left(\frac{\eta}{4}\right)}{L}}\,.$$

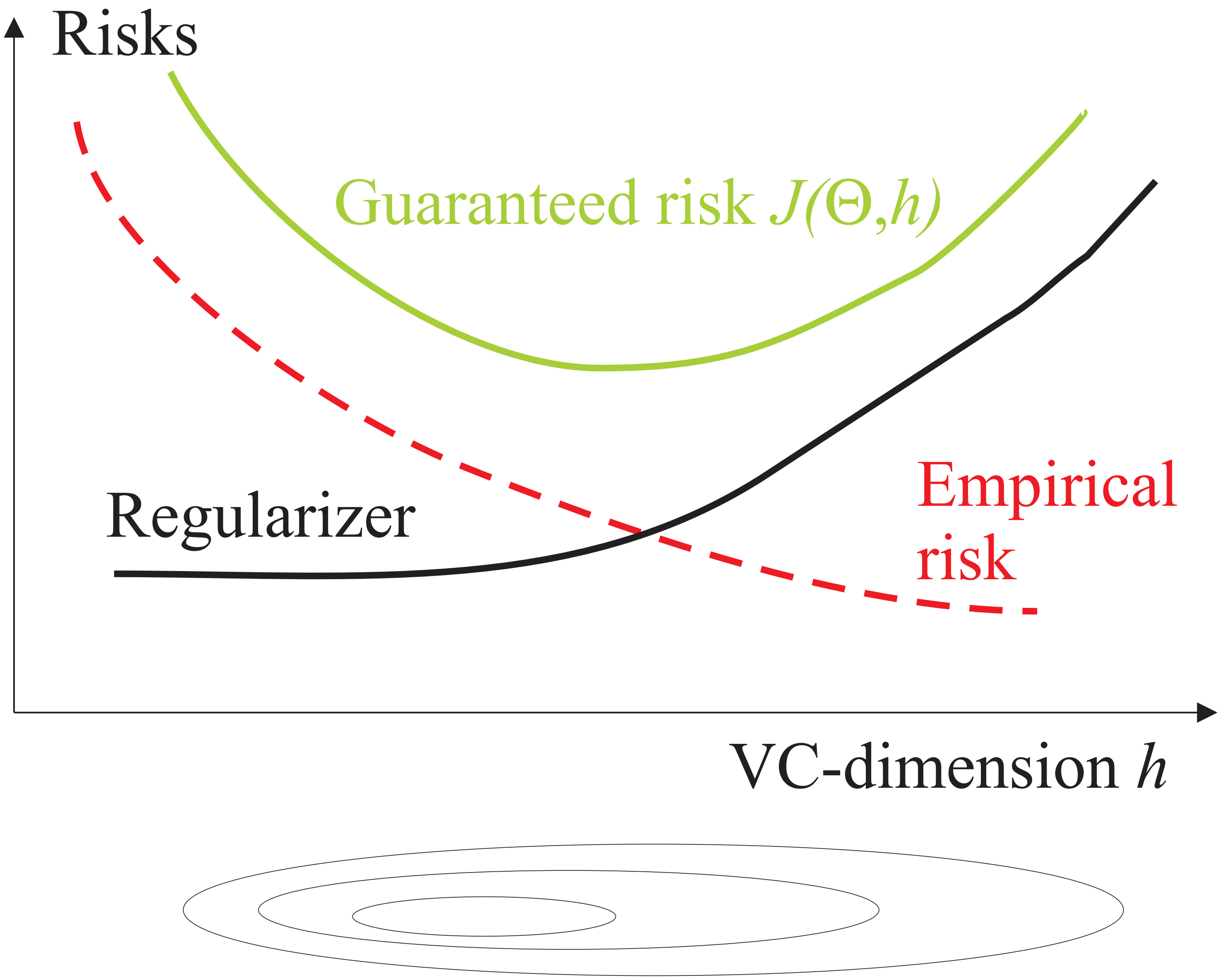
For each model i in the list of hypotheses

  - Compute its VC-dimension h_i.
  - $\Theta_i^* = \operatorname*{argmin}_{\Theta_i} R_{\mathrm{emp}}(\Theta_i)$.
  - Compute $J_i(\Theta_i^*, h_i)$.

Choose the model with the lowest $J_i(\Theta_i^*, h_i)$.

- Preferably, optimize directly over both $(\Theta^*, h^*) = \operatorname*{argmin}_{\Theta, h} J(\Theta, h)$.
- Gap tolerant linear classifiers minimize $R_{\mathrm{emp}}(\Theta)$ while maximizing margin. Support Vector Machine does just that.

Structural risk minimization pictorially



Space of nested hypotheses with decreasing h

VC-dimension, a practical view

Bad news: Computing the guaranteed risk is useless in many practical situations.

- VC dimension cannot be accurately estimated for non-linear models such as neural networks.
- Structural Risk Minimization may lead to a non-linear optimization problem.
- VC dimension may be infinite (e.g., for a nearest neighbor classifier), requiring infinite amount of training data.

Good news: Structural Risk Minimization can be applied for linear classifiers.

- Especially useful for Support Vector Machines.

Empirical risk minimization, notes

Is then empirical risk minimization = minimization of training set error, e.g., neural networks with backpropagation, dead ? **No!**

– Guaranteed risk J may be so large that this upper bound becomes useless.

Find a tighter bound and you will be famous! It is not impossible!

+ Vapnik, Chervonenkis suggest learning with progressively more complex classes of the decision strategies Q.

+ Vapnik & Chervonenkis' theory justifies using empirical risk minimization on classes of functions with a reasonable VC dimension.

+ Empirical risk minimization is computationally hard (impossible for large L). Most classes of decision functions Q for which the empirical risk minimization (at least locally) can be efficiently organized are often useful.

Where does the nearest neighbor classifier fit in the picture?