# An Introduction to Statistical Learning Theory

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# DigiCosme, Paris-Saclay

Some information on the University of São Paulo, Brazil

- Founded in 1934 in the State of São Paulo
  - 46 million people
  - 12 million in the city of São Paulo (capital)
    - 21 million in the capital and neighborhoods
- 11 Campi
  - Annual budget 1.2 billion Euros
- 96.364 students
  - 58.823 Undergraduation
  - 14.106 Masters
  - 15.894 PhD

# DigiCosme, Paris-Saclay

Some information on the University of São Paulo, Brazil

- Students:
  - 52.28% men and 47.72% women
- Staff members
  - 5.844 Professors
  - 14.866 Administrative positions
- World University Ranking of the Times Higher Education

| Rank | Name | Overall | Teaching | Research | Citations | Industry Income | International Outlook |
|---|---|---|---|---|---|---|---|
| 251–300 | University of São Paulo<br>Brazil | 46.4–49.4 | 55.9 | 53.5 | 37.0 | 39.5 | 32.7 |

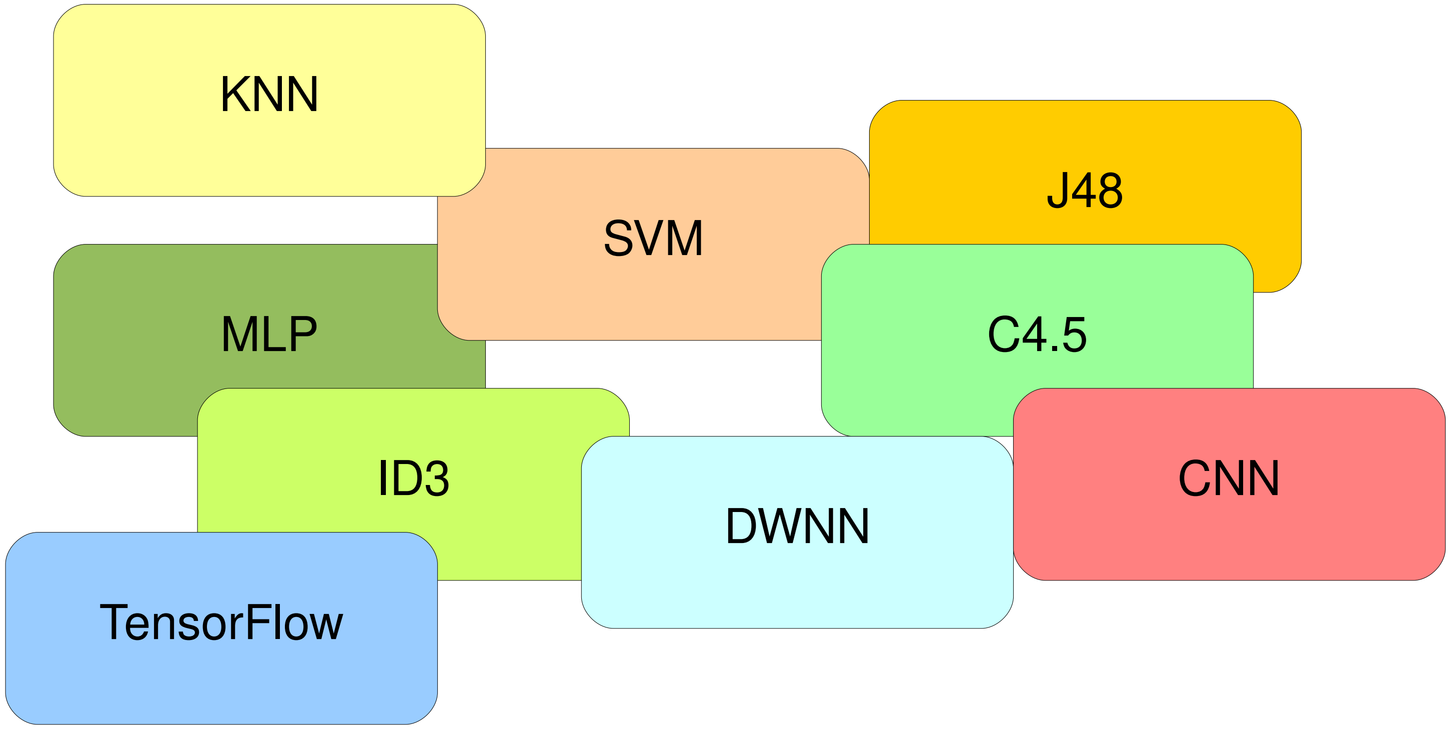
## Basics

- What is Machine Learning?
  - I suppose its two main branches make that easier to explain:
    - Supervised Learning
    - Unsupervised Learning

## Theoretical Aspects

- Interested in Machine Learning?
  - What a better way than starting with the Statistical Learning Theory?

- So many classification algorithms:
  - How can we assess any of those?
    - K-fold cross validation, leave-one-out, ...
  - How can we prove any of those “learn”?



# Statistical Learning Theory

- First of all, what is “learning” in our context?
  - Concept of Generalization by Vapnik

Sample error

Expected error

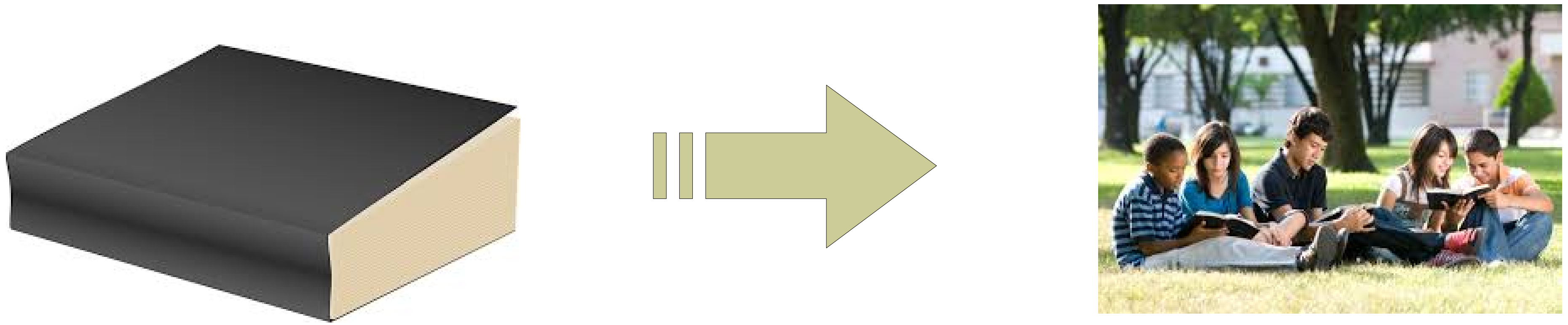
$$G = |R_{\mathrm{emp}}(f) - R(f)|$$

**This is the concept of Generalization**

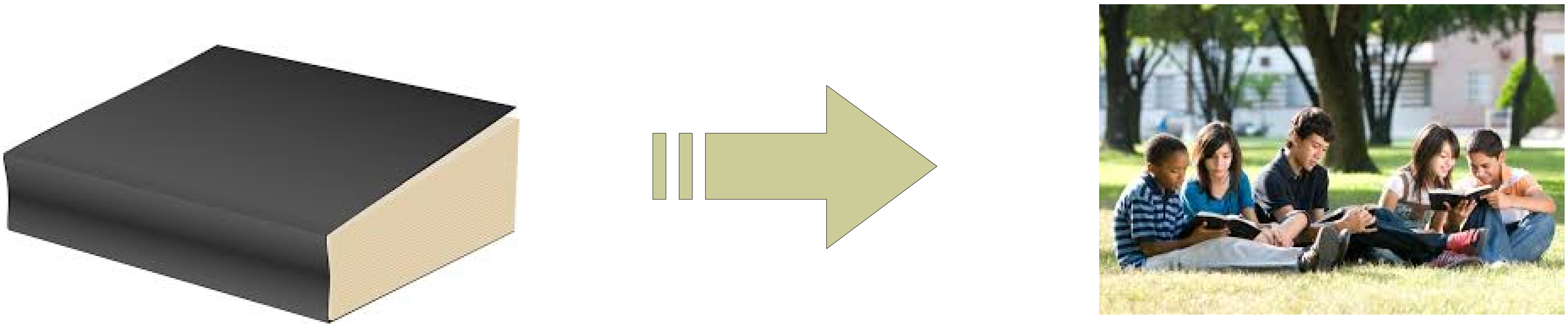
- In addition, the Empirical Risk must be as small as possible

## Statistical Learning Theory

- In practical terms, what is generalization?
  - Consider someone has given you a subject to study:
    - Option 1: You dedicated yourself to know a book by heart



- In practical terms, what is generalization?
  - Consider someone has given you a subject to study:
    - Option 1: You dedicated yourself to know a book by heart
    - Option 2: You decided to study several books, solve some exercises and code some examples



# Statistical Learning Theory: Bias-Variance Dilemma

- This is the same as a **regression problem**:

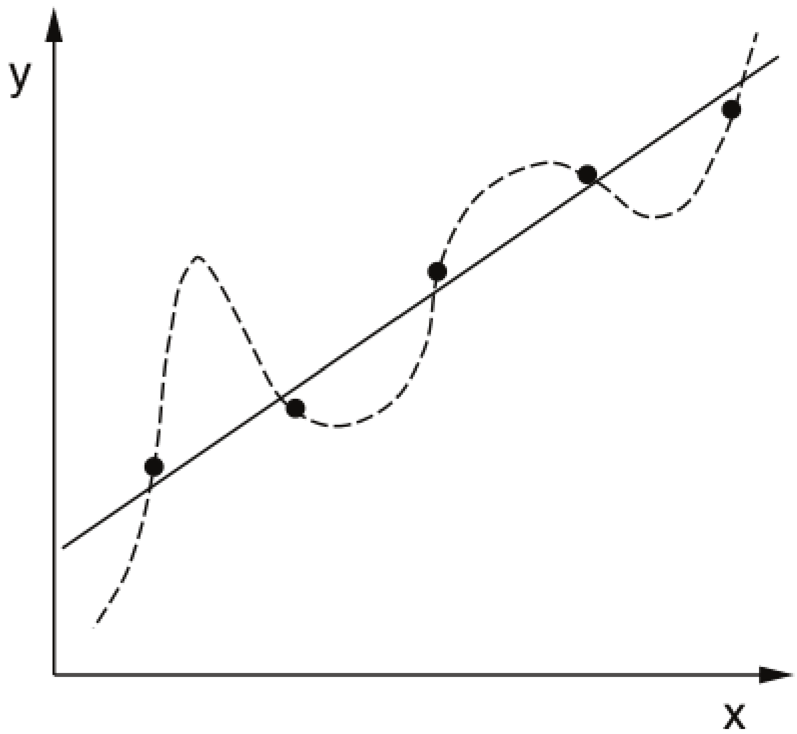



Figure from Luxburg and Scholkopf, Statistical Learning Theory: Models, Concepts, and Results

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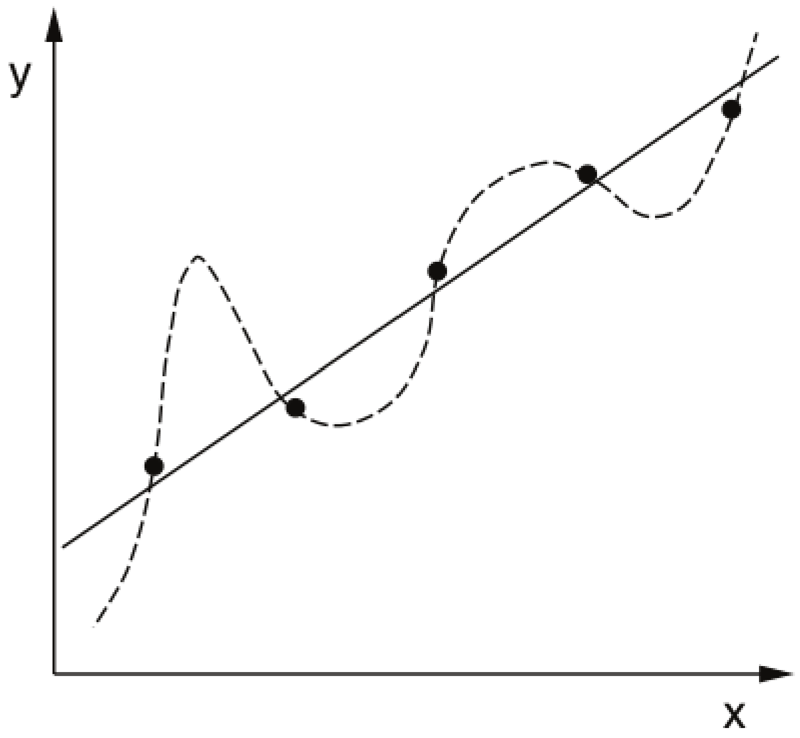


**Are you worried about memorizing the examples given to you??**

Figure from Luxburg and Scholkopf, Statistical Learning Theory: Models, Concepts, and Results

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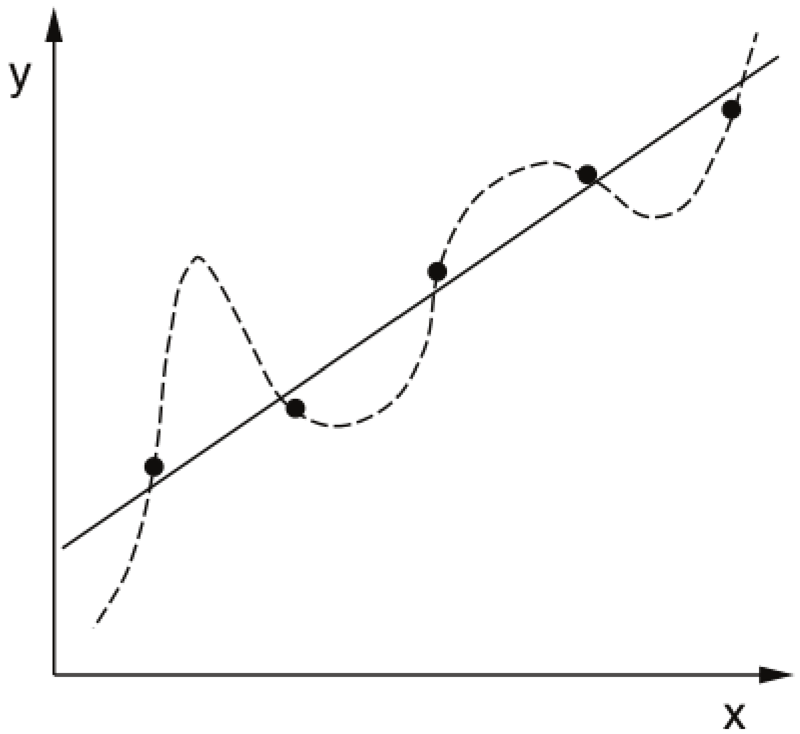


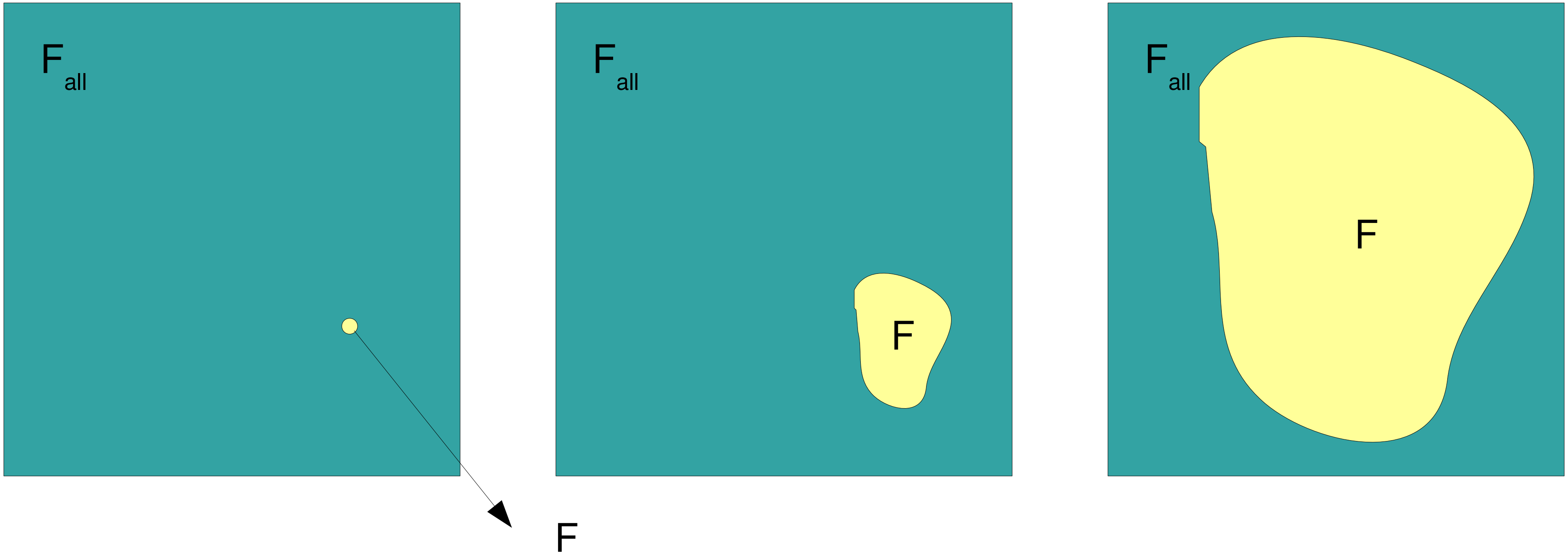

**Are you worried about memorizing the examples given to you??**

**Or are you interested in Generalizing while minizing the Empirical Risk (sample error)?**

Figure from Luxburg and Scholkopf, Statistical Learning Theory: Models, Concepts, and Results

# Statistical Learning Theory: Bias-Variance Dilemma

- The dichotomy associated to the Bias-Variance Dilemma

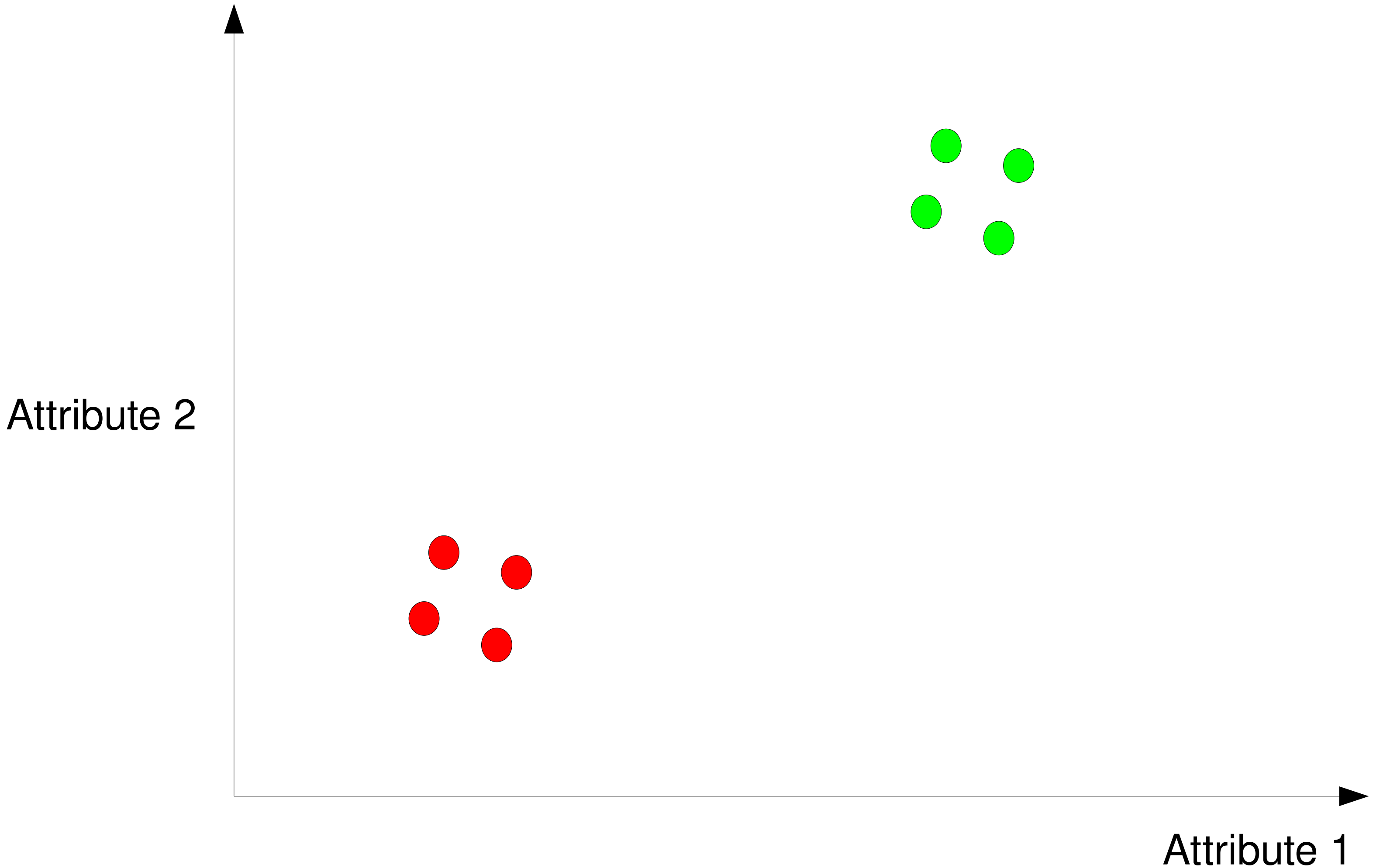



**Three examples of algorithm biases**

## Using the Distance-Weighted Nearest Neighbors to illustrate algorithm biases

# Distance-Weighted Nearest Neighbors

- Based on the same principles as the k-Nearest Neighbors



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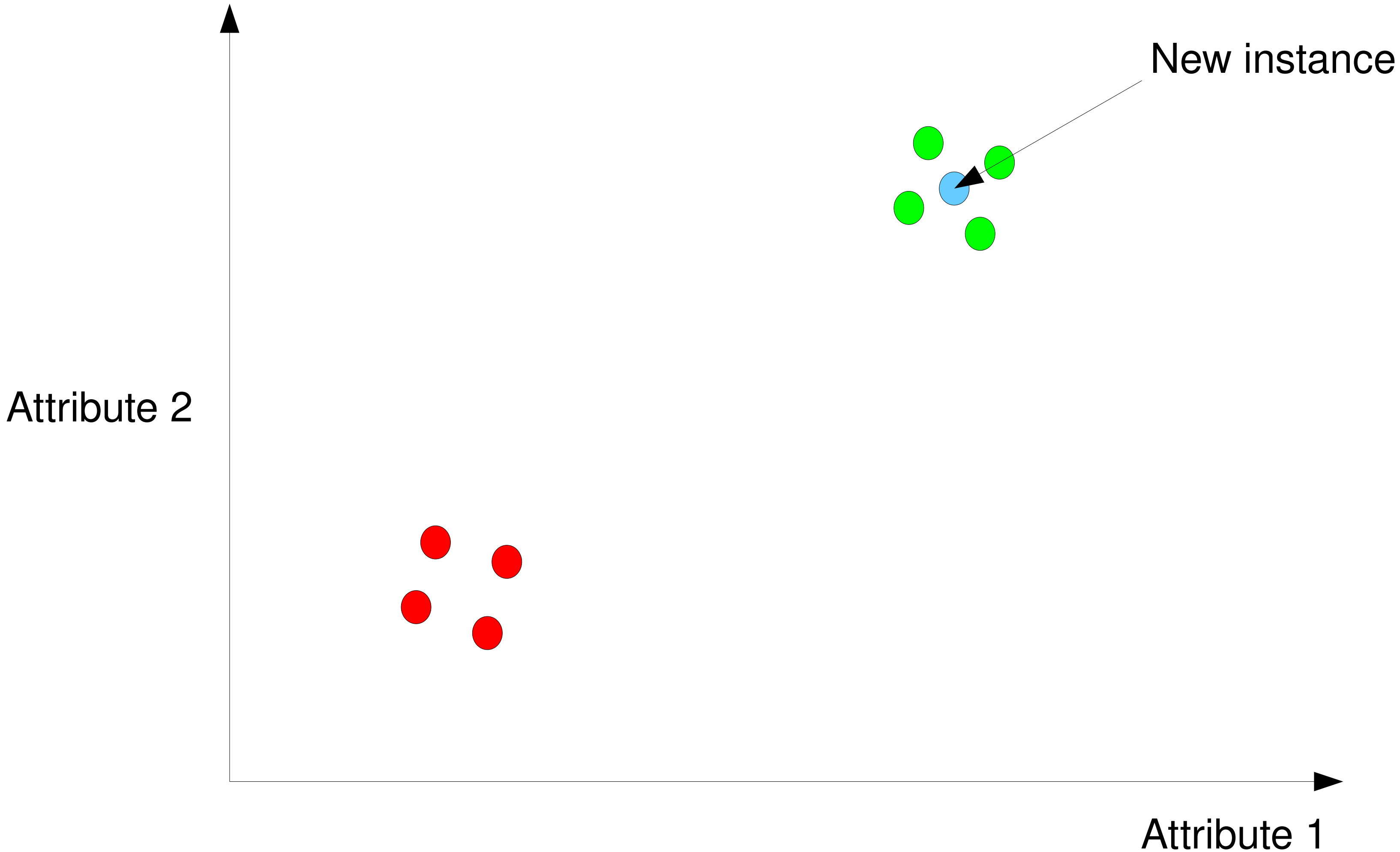

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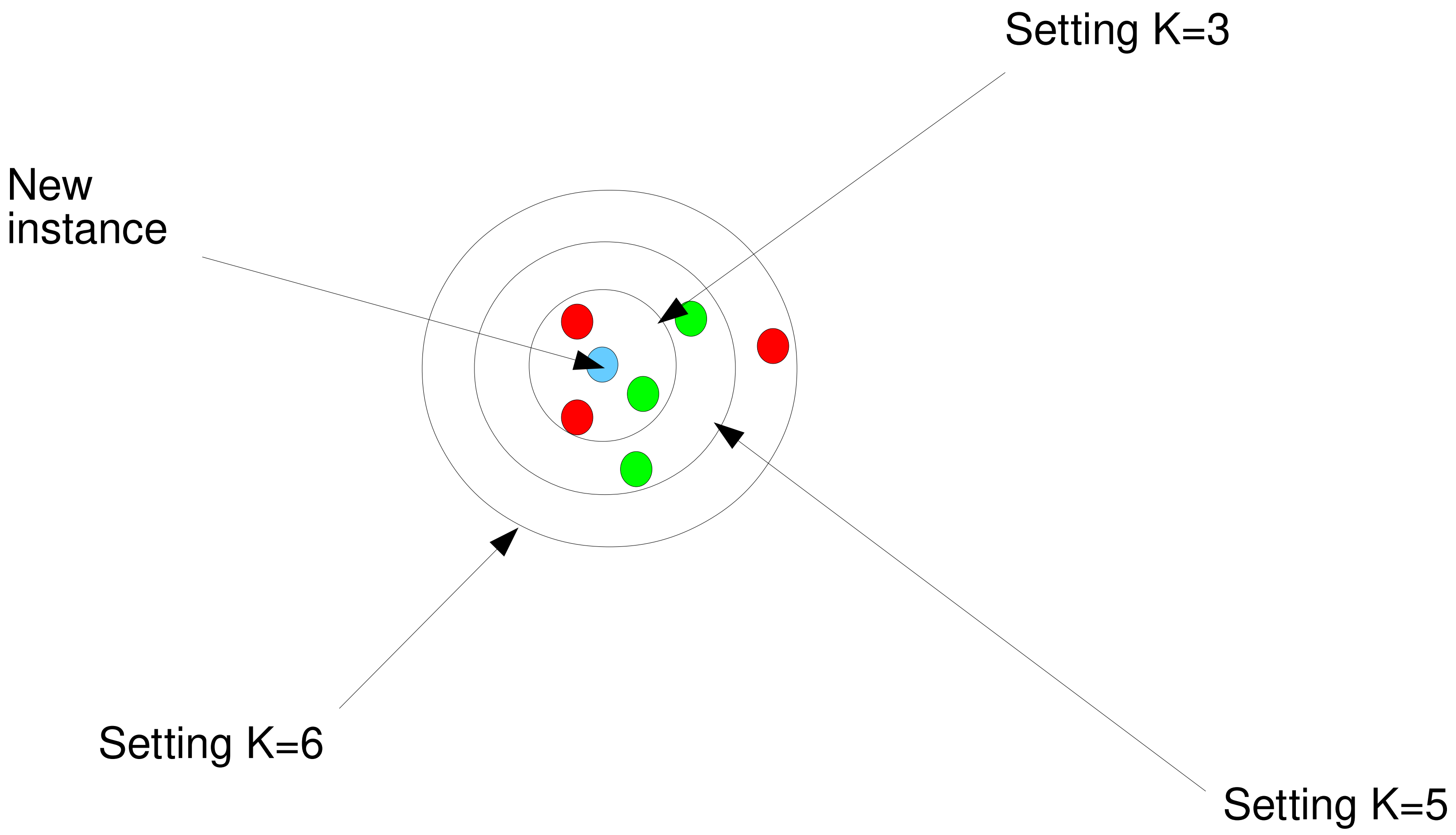


# Distance-Weighted Nearest Neighbors

- It is based on Radial functions centered at the new instance a.k.a. query point

- Classification output:

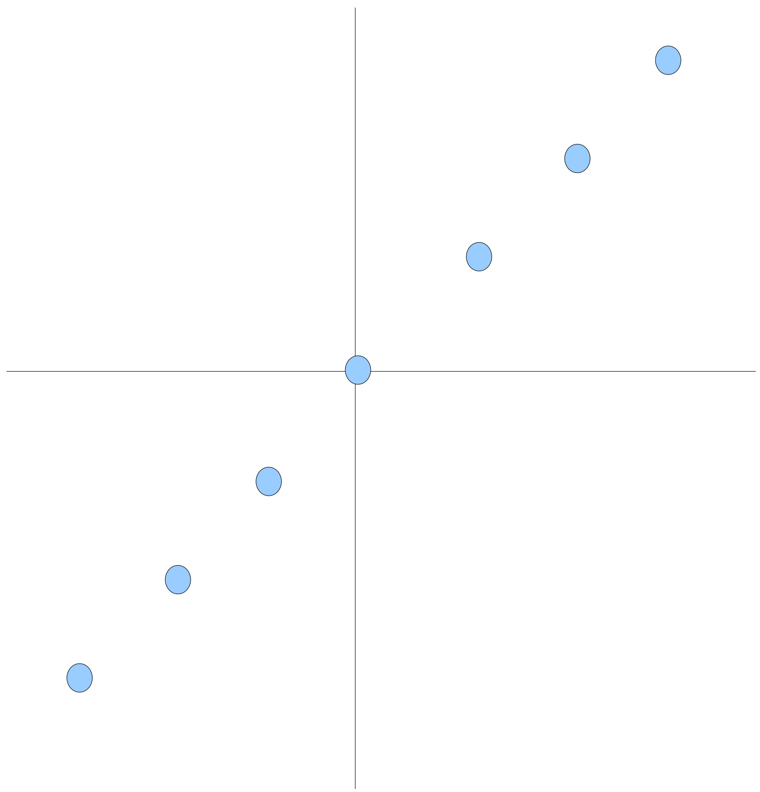
$$f(\mathbf{x}) = \frac{\sum_{i=1}^{n} w_i y_i}{\sum_{i=1}^{n} w_i}$$

- Given the weight function:

$$w_i = \exp - \frac{\left\|\mathbf{x} - \mathbf{x}_i\right\|^2}{2\sigma^2}$$

# Distance-Weighted Nearest Neighbors

- After implementing, test it on this simple example of an identity function:



Two main questions:

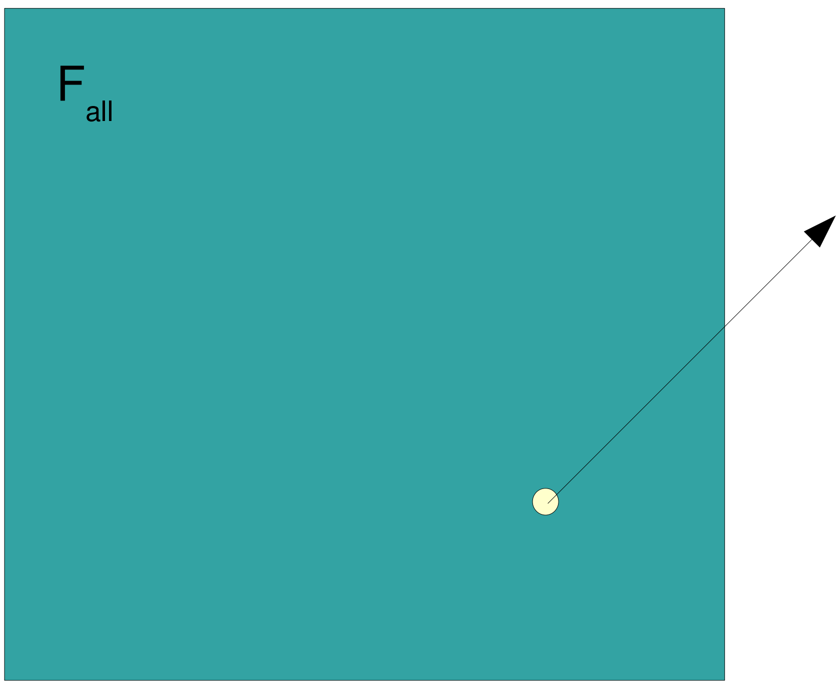
- What happens if sigma is too big?

- What happens if sigma is too small?

So, how can we define the best value for sigma?

# Distance-Weighted Nearest Neighbors

- When sigma tends to infinity

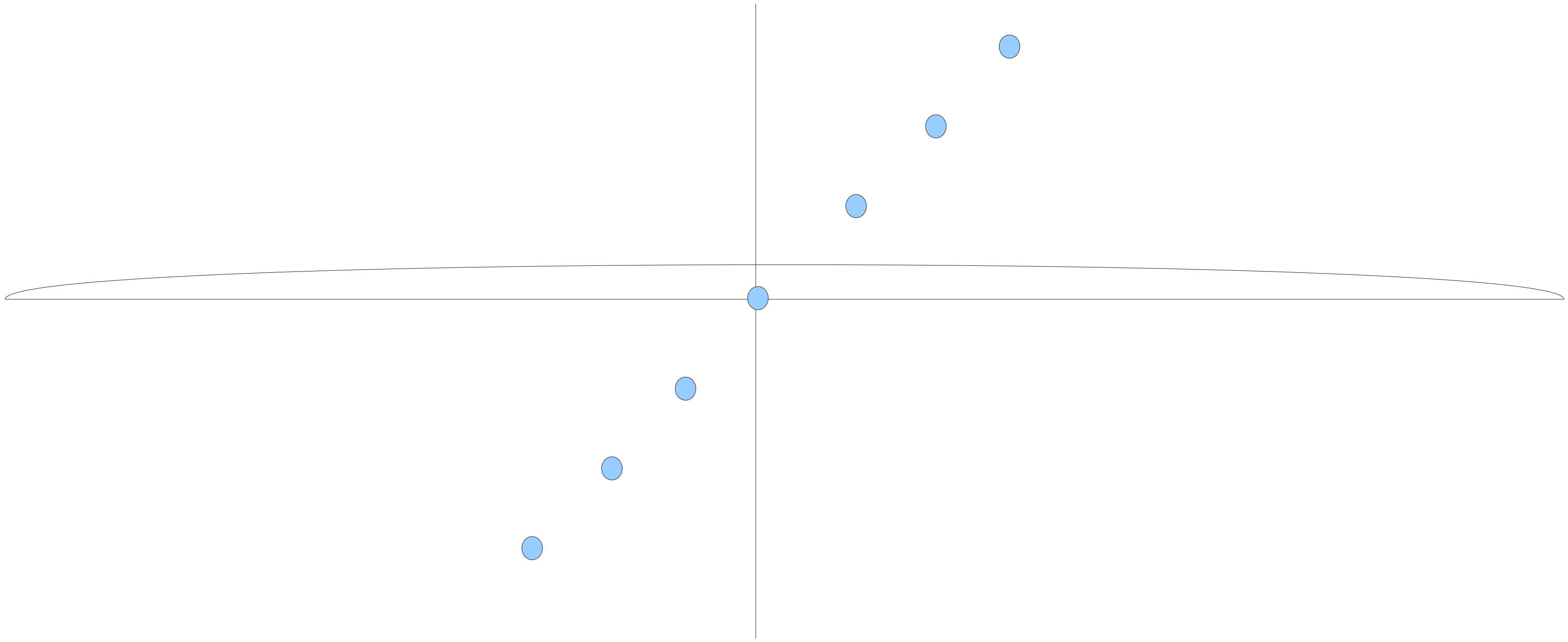



The space of admissible functions (bias) will contain a single function

In this case, the average function

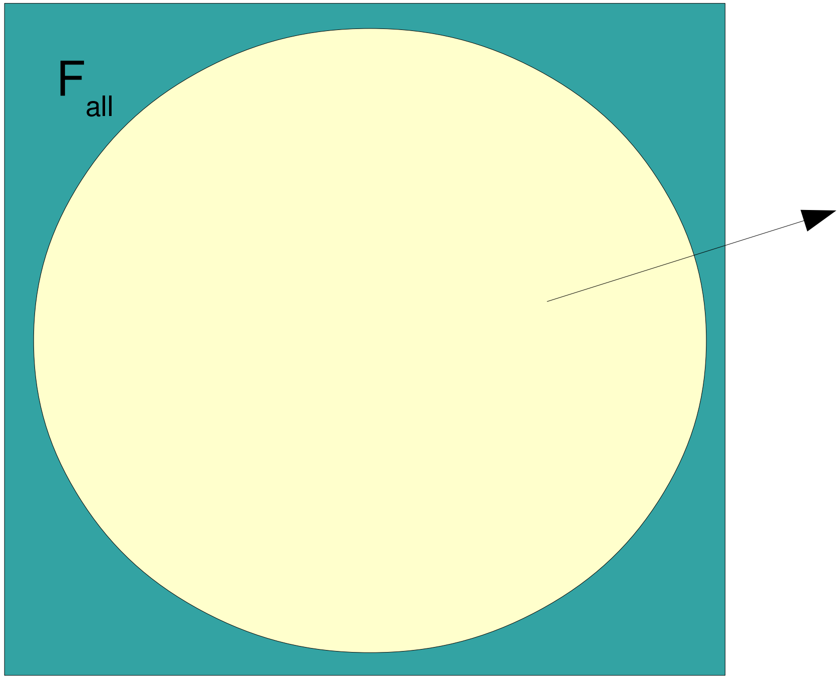
## Distance-Weighted Nearest Neighbors

- When sigma tends to infinity



# Distance-Weighted Nearest Neighbors

- When sigma tends to zero



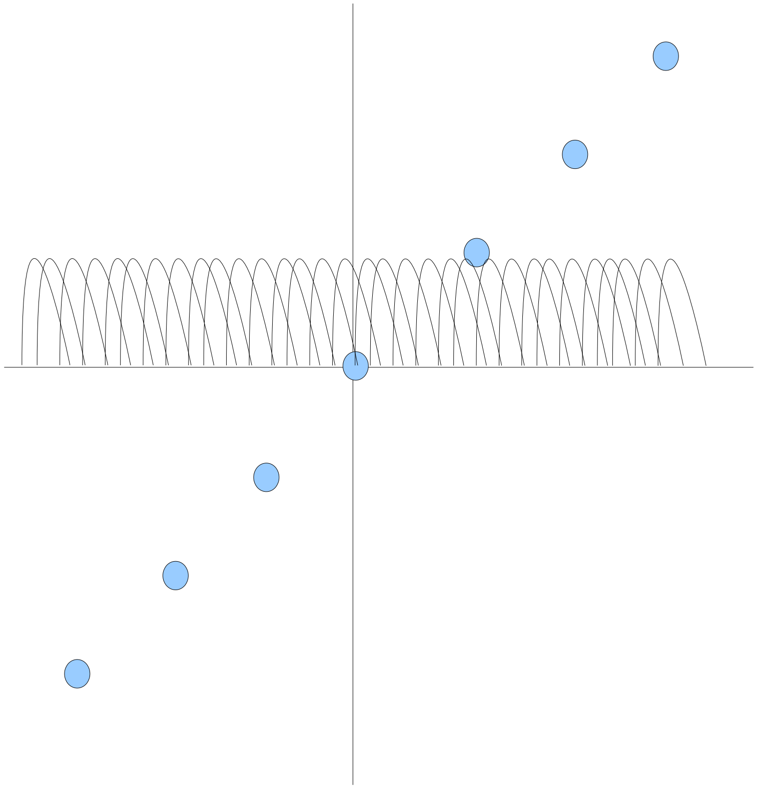

The space of admissible functions (bias) will tend to the whole space

What is the problem with that?

It will most probably contain at least one memory-based classifier

# Distance-Weighted Nearest Neighbors

- When sigma tends to zero



# Distance-Weighted Nearest Neighbors

- Additional:
  - Linear problem
  - Nonlinear problem

# Distance-Weighted Nearest Neighbors

- Some questions:
  - Is DWNN enough to tackle any problem?
    - It can represent the whole space of admissible functions by changing sigma
  - So, why develop new classification and regression algorithms?
    - Improve bias restriction and then learning guarantees

## Understanding the basics about SLT

- Vapnik formulated the great part of the Statistical Learning Theory
  - His basic idea was to prove how some supervised algorithm “learns”
  - That required some formalization
    - Concept of Generalization
    - Reduce the empirical risk as more examples are sampled
  - Took advantage of the Law of Large Numbers

# Understanding the basics about SLT

- Vapnik took advantage of the Law of Large Numbers:

$$P\left(\left|\frac{1}{n}\sum_{i=1}^{n}\xi_i - E(\xi)\right| > \epsilon\right) \leq 2\exp(-2n\epsilon^2)$$

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    - It cannot change along time

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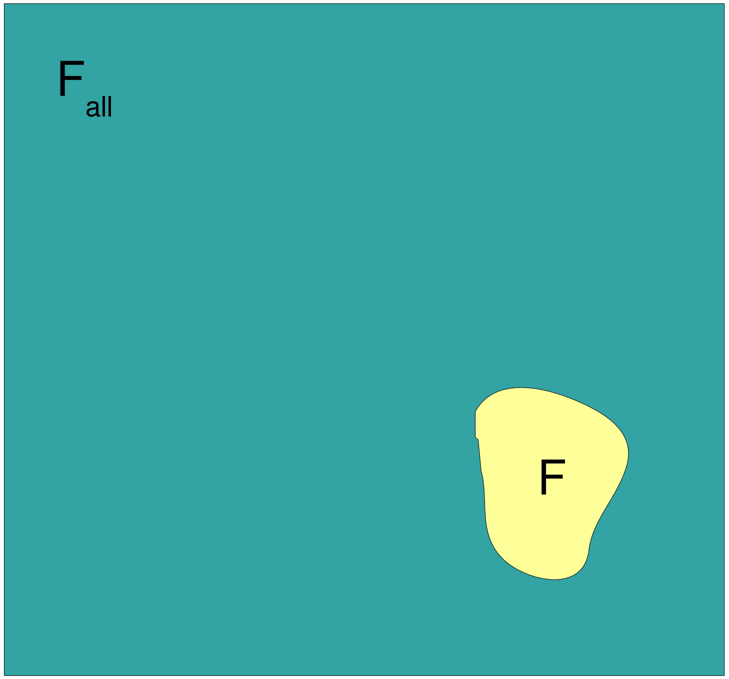
    - It cannot change along time
- Main advantage:
  - We have an upper bound → lets see it!

## Understanding the basics about SLT

- Then Vapnik decided to adapt its problem to be represented by the Law of Large Numbers
  - Problems:
    - Training examples are used to select a function from the algorithm bias (a.k.a. space of admissible functions)
      - Makes the Law inconsistent



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      - Data distribution is static
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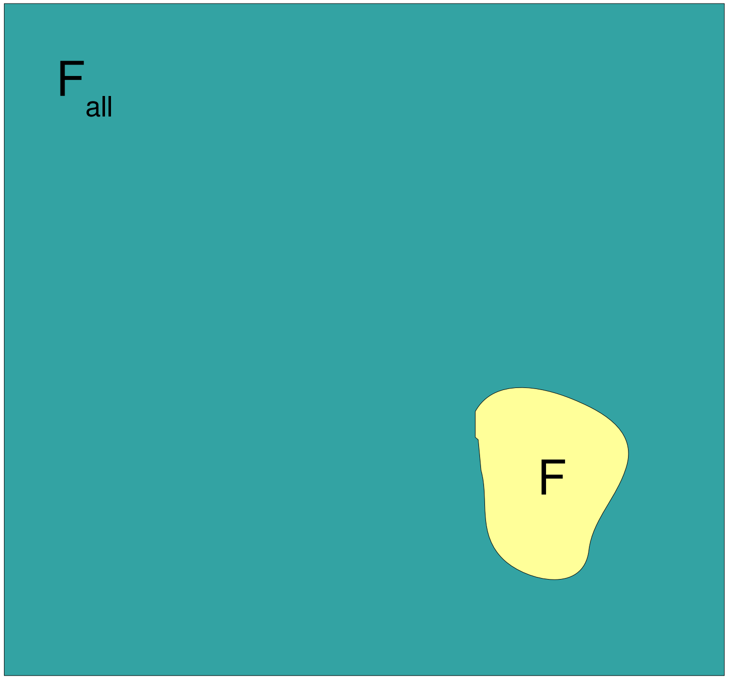

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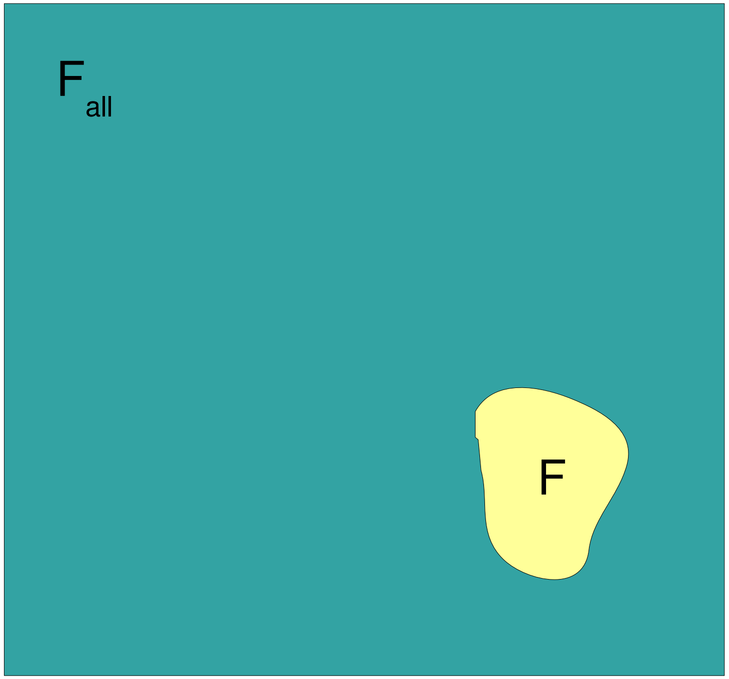
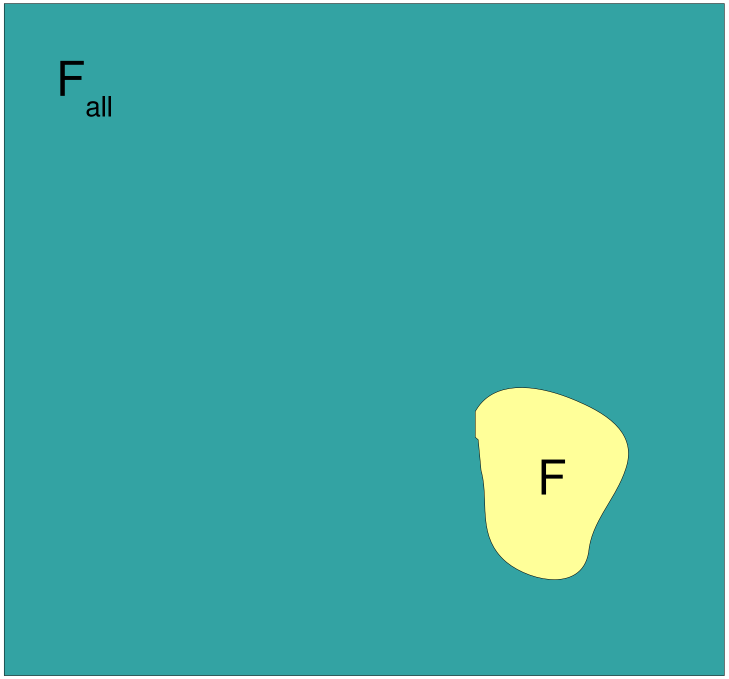
    - So, how to proceed?



- Vapnik had a clever idea:
  - Let us consider any function can be selected
    - In fact, not any but all of them



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- He defined the following:

$$P(|R_{\mathrm{emp}}(f) - R(f)| > \epsilon) \leq 2\exp(-2n\epsilon^2)$$

- In which:

$$R_{\mathrm{emp}}(f) = \frac{1}{n}\sum_{i=1}^{n}\ell(X_i, Y_i, f(X_i))$$

$$R(f) = E(\ell(X, Y, f(X))$$

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- In which:

**But that is valid for a single predefined function f**

# Understanding the basics about SLT

- Vapnik rewrote:

$$P(|R_{\text{emp}}(f) - R(f)| > \epsilon) \leq 2\exp(-2n\epsilon^2)$$

- So, for all functions contained in the algorithm bias:

$$P\Big( |R(f_1) - R_{\text{emp}}(f_1)| > \varepsilon \;\text{ or }\; |R(f_2) - R_{\text{emp}}(f_2)| > \varepsilon \;\text{ or }\; \ldots \;\text{ or }\; |R(f_m) - R_{\text{emp}}(f_m)| > \varepsilon \Big)$$

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- What is bounded as follows:

$$P\Big( |R(f_1) - R_{\mathrm{emp}}(f_1)| > \varepsilon \ \text{ or } \ |R(f_2) - R_{\mathrm{emp}}(f_2)| > \varepsilon \ \text{ or } \ \ldots \ \text{ or } \ |R(f_m) - R_{\mathrm{emp}}(f_m)| > \varepsilon \Big)$$
$$\leq \sum_{i=1}^{m} P(|R(f_i) - R_{\mathrm{emp}}(f_i)| > \varepsilon)$$

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- Vapnik rewrote:

$$P(|R_{\text{emp}}(f) - R(f)| > \epsilon) \leq 2\exp(-2n\epsilon^2)$$

- So

$P$

That is not difficult to see...

- What is bounded as

$$P\Big(\ |R(f_1) - R_{\text{emp}}(f_1)| > \varepsilon \ \text{ or } \ |R(f_2) - R_{\text{emp}}(f_2)| > \varepsilon \ \text{ or } \ \ldots \ \text{ or } \ |R(f_m) - R_{\text{emp}}(f_m)| > \varepsilon\ \Big)$$

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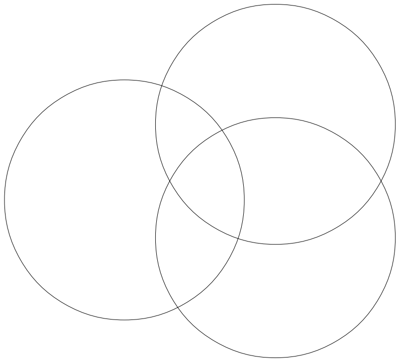
- Suppose we have a set of sets, which could intersect or not:
  - If they intersect:



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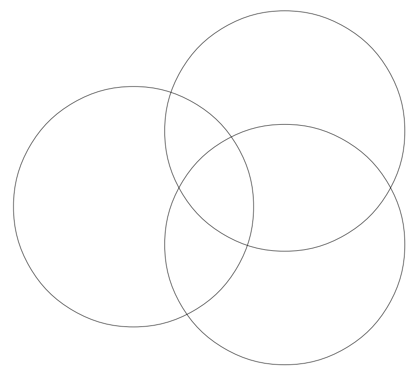
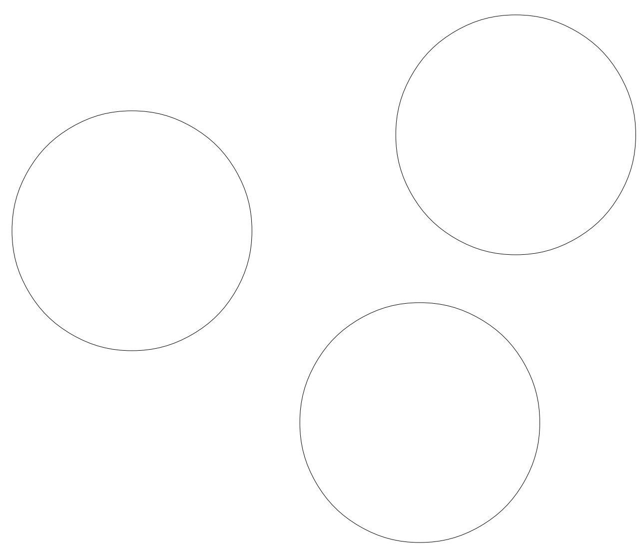


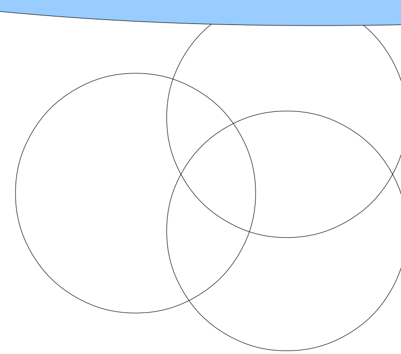
  - If they do not



# Understanding the basics about SLT

- Supp…

**The sum of the union of sets is always smaller than or equal to when they do not intersect!**



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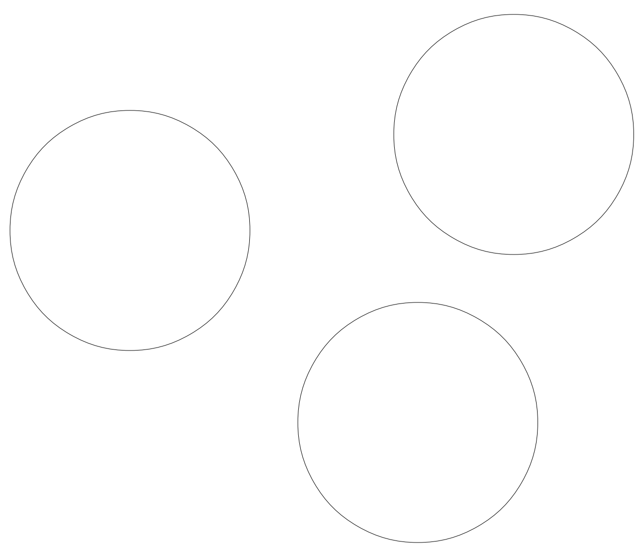

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- Given every function is bounded as follows, according to the Law of Large Numbers:

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- So that Vapnik obtained:

$$\sum_{i=1}^{m} P(|R(f_i) - R_{\text{emp}}(f_i)| > \varepsilon) \;\leq 2m\exp(-2n\varepsilon^2)$$

# Understanding the basics about SLT

- This is one of his main results!

$$\sum_{i=1}^{m} P(|R(f_i) - R_{\text{emp}}(f_i)| > \varepsilon) \ \leq 2m \exp(-2n\varepsilon^2)$$

  - Let us plot it!

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  - But how to define m?
    - Number of different classification/regression functions inside the algorithm bias

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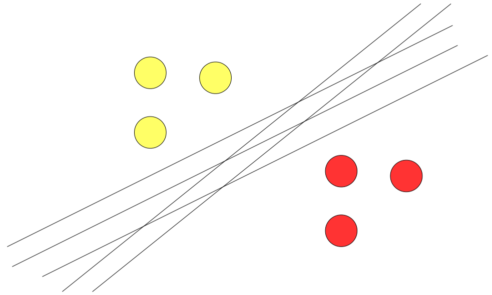
- Let us plot it!
- But how to define m?
  - Number of different classification/regression functions inside the algorithm bias
  - He had a clever idea (once more) of defining similar classifiers according to their outputs

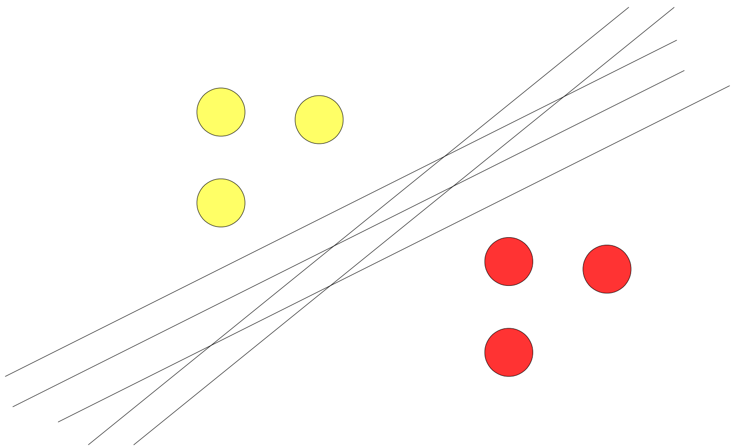


# Understanding the basics about SLT

- Based on that:

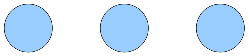
$$\sum_{i=1}^{m} P(|R(f_i) - R_{\text{emp}}(f_i)| > \varepsilon) \leq 2m \exp(-2n\varepsilon^2)$$

- m is a function of n in form:
  - m(n) is referred to as the **Shattering coefficient** or Growth function
  - We can estimate it by finding the maximal number of **distinct** classifiers produced for some problem!



# Understanding the basics about SLT

- For example, consider 3 points in a two-dimensional plane as follows:

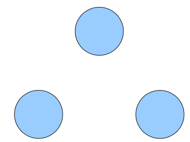


- Suppose linear functions are used to form classifiers:

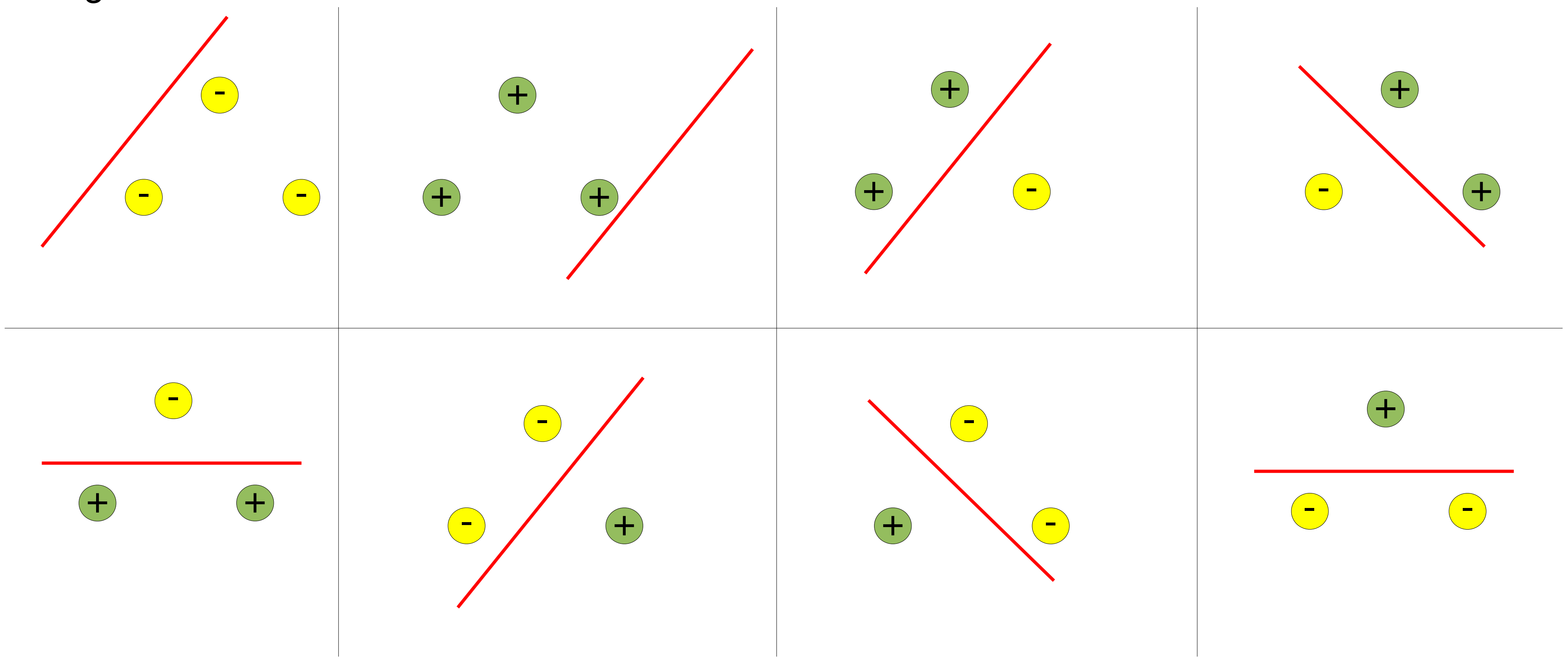

- We could shatter this sample in 4 different ways
  - But is there any other 3-point sample that we could shatter in more ways?

# Understanding the basics about SLT

- Suppose we have the 3 points in different setting (still in $R^2$):



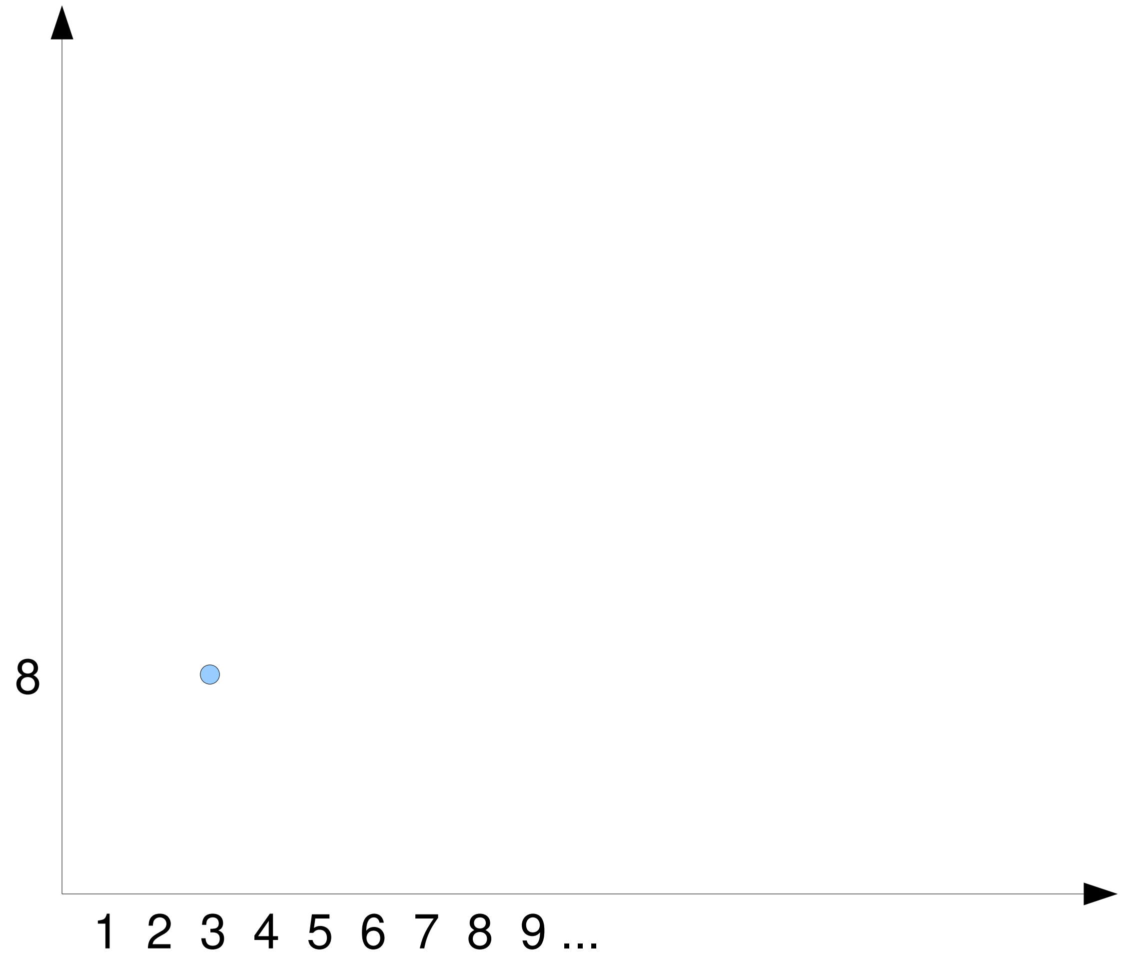
- Again consider F contains all linear functions:




- Observe F was capable of shattering this sample in all $2^n$ possible ways, what take us to the fact that F has a VC dimension at least equal to 3
  - Because there is at least one sample with 3 instances that can be shattered in all possible ways

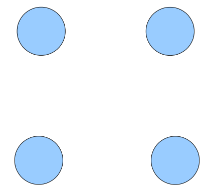
# Understanding the basics about SLT

- In that sense, we conclude that for $R^2$:

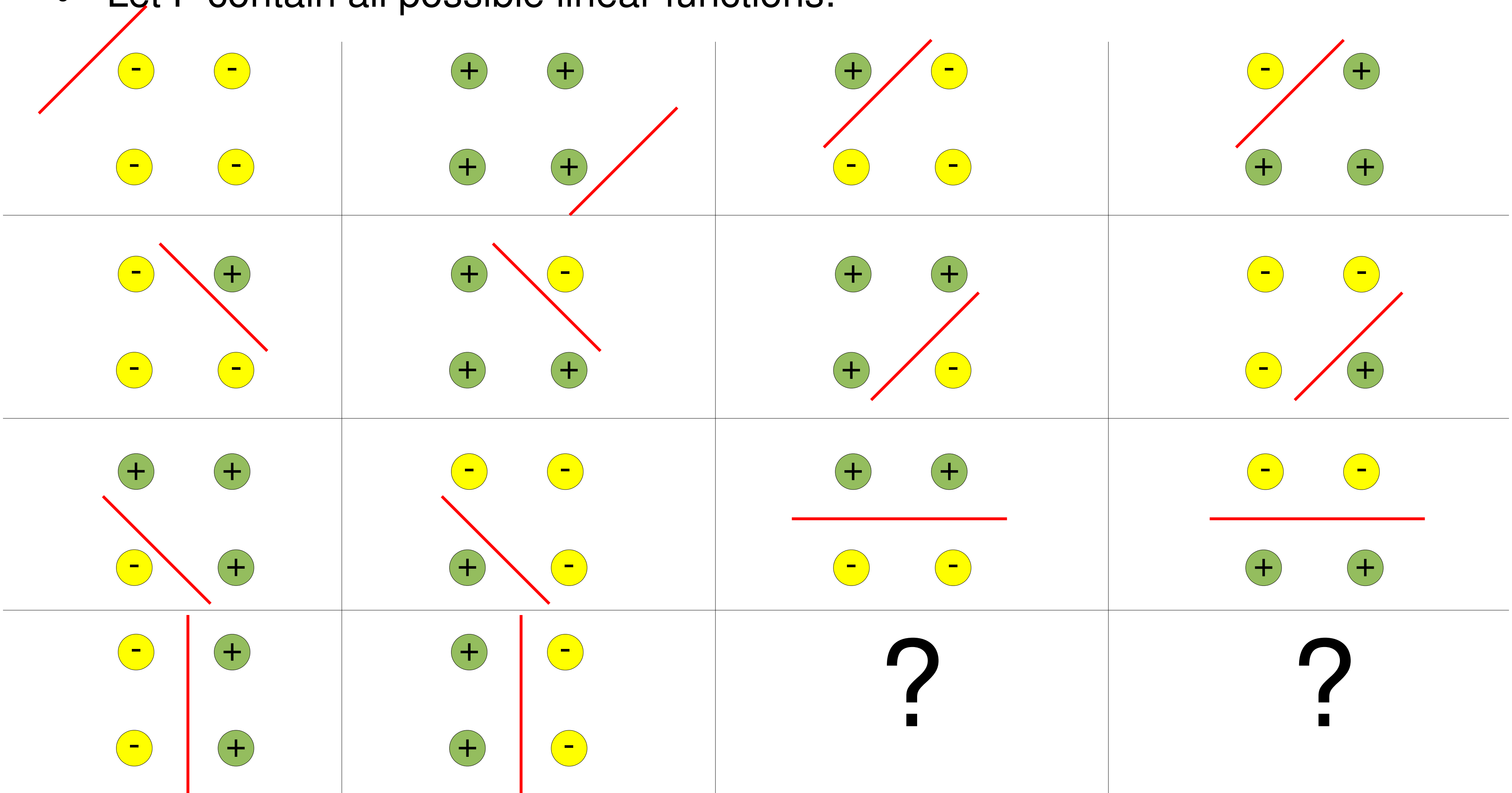


# Understanding the basics about SLT

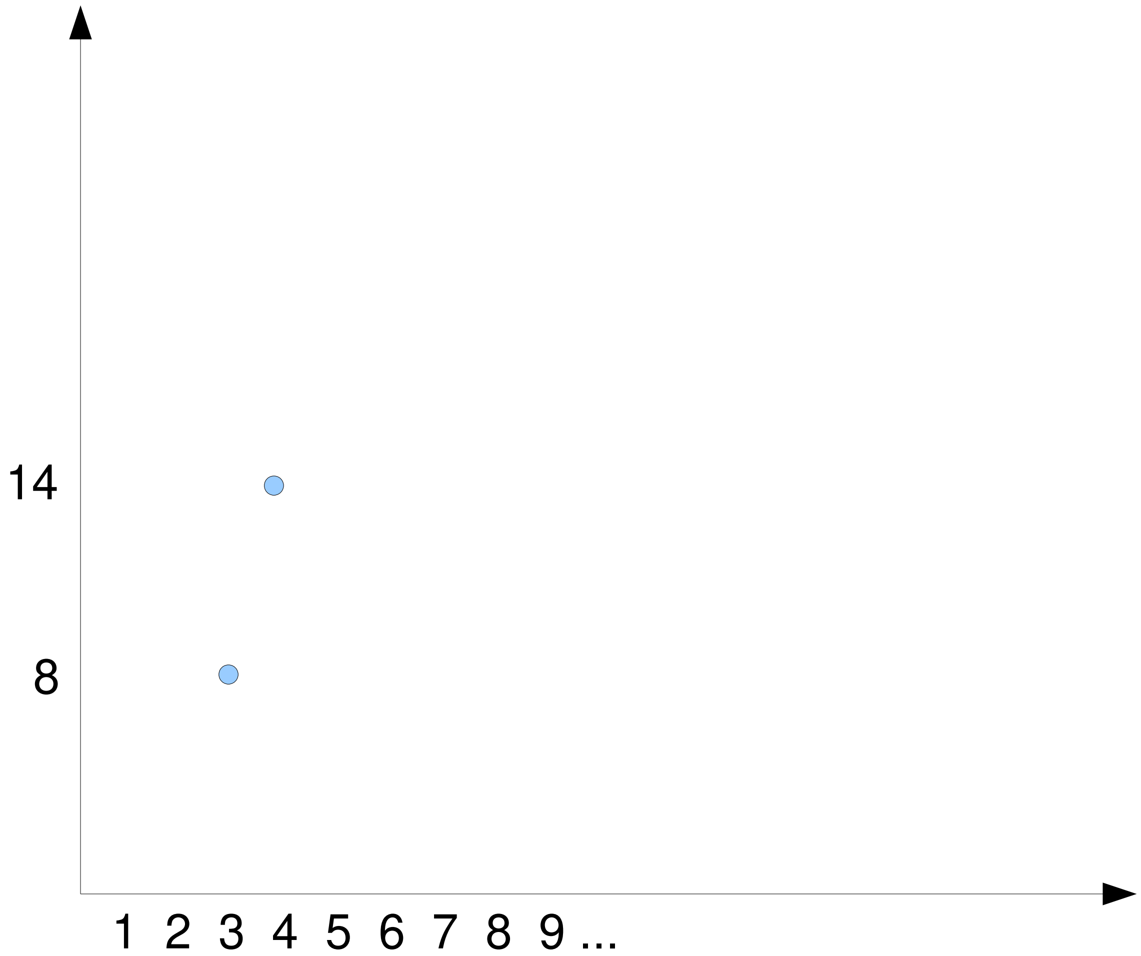
- Let's still consider in $R^2$:



- Let F contain all possible linear functions:

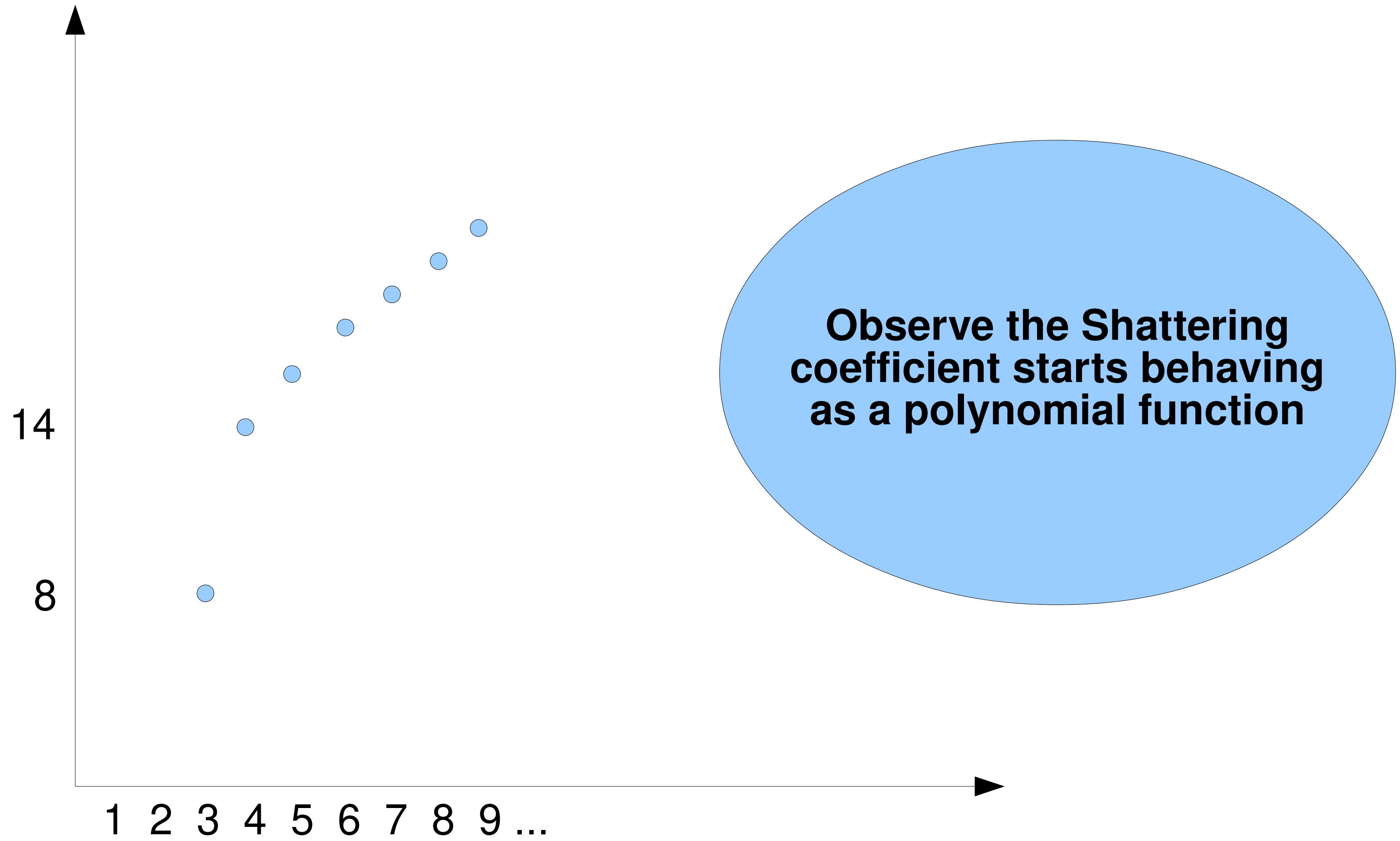


- In that sense, we conclude that for $R^2$:



# Understanding the basics about SLT

- In that sense, we conclude that for $R^2$:



# Understanding the basics about SLT

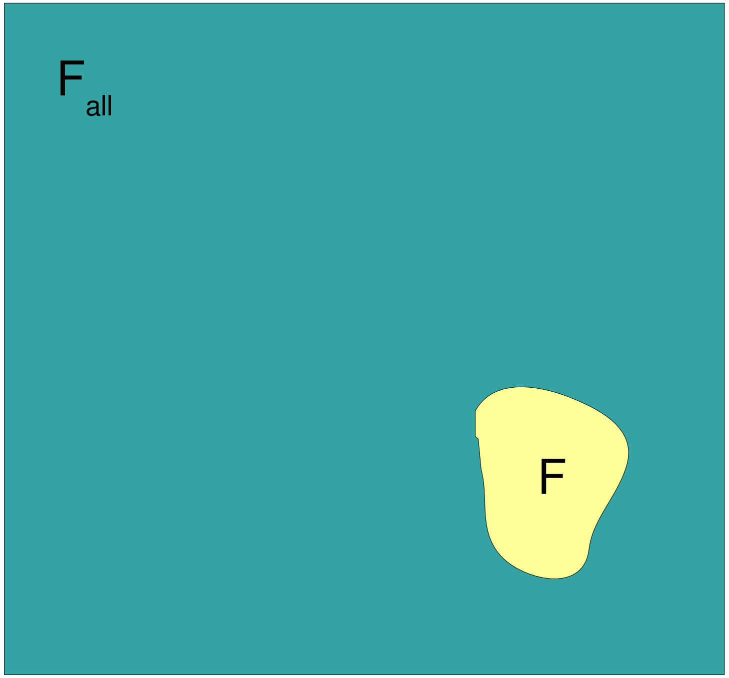
- In fact, Learning is only ensured if m(n) grows polynomially:

$$\sum_{i=1}^{m} P(|R(f_i) - R_{\mathrm{emp}}(f_i)| > \varepsilon) \leq 2m \exp(-2n\varepsilon^2)$$

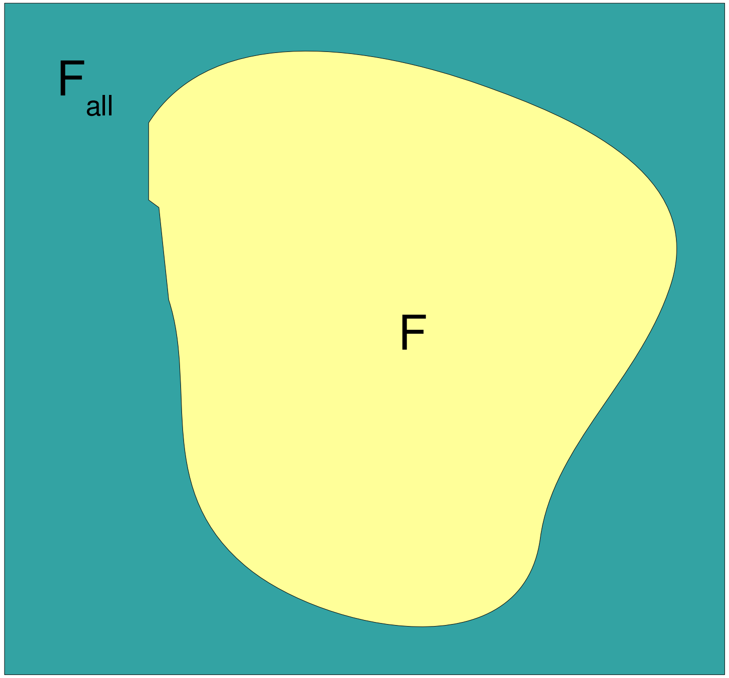
- Let us open the formulation and see what happens:
  - If it is polynomial
  - If it is exponential

# Understanding the basics about SLT

- In this sense:




**Polynomial Shattering coefficient**




**Exponential Shattering coefficient**

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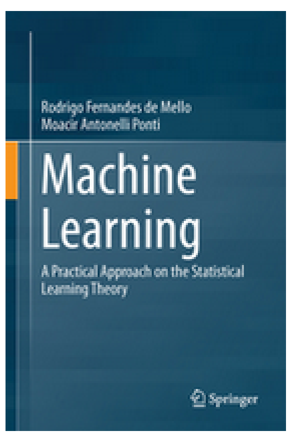




## Machine Learning

A Practical Approach on the Statistical Learning Theory

Authors: **Fernandes de Mello**, Rodrigo, **Antonelli Ponti**, Moacir

# An Introduction to Statistical Learning Theory

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