# Advanced Machine Learning

## *Over-Fitting*

*Overfitting, regularisation, feature selection*

# Outline

1. **Over-fitting?**
2. Controlling Complexity
3. Hidden structure
4. Regularisation

# Over-fitting

- Complex machine can **over-fit**

  ***over-fitting**: fitting the training data well at the cost of getting poorer generalisation performance*

- Three red cars. . .

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# Binary Classification Task for You

Class 1

Class 2

# Which Category?

- Which category does the following image belong to?

# Spurious Rules

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# All Binary Functions

$$\boldsymbol{x}_0 = 0\,0\,0 \quad y_0 = \left\{ \begin{array}{c} 0 \\ 1 \end{array} \right.$$

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- Would an MLP that could approximate any function be useful?
- **Absolutely not!**

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2. **Controlling Complexity**
3. Hidden structure
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# Controlling Complexity

- Infinitely flexible machine don't generalise

- **Machine learning only works because there is some structure in the data**

- A successful machine should capture this structure

- Even deep learning machines with millions of parameters only work because they successfully capture the structure of images or text

- Different learning machines have different performance on different problems because the data has different structure

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# Training Examples

- As we increase the number of training examples, we make it hard to find a spurious rule
- Bigger data sets allow us to use more complicated machines
- Part of the success of deep learning is because they use huge training sets
- (Labelled) data is often expensive to collect so we sometimes have no choice but to use a small training set
- One of the limitations of using deep learning comes because we often have limited data

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# Identifying Structure

- In some cases we know *a priori* some of the structure in the data
- In images we believe the identity of an object is invariant to translation and scaling
- The success of *convolutional neural networks* (CNNs) in deep learning is in large part because the convolutions respect translational invariance

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# Preprocessing

- Structure might often be obscure to the learning machine
- If we are trying to predict the spread of disease then a list of place names might be a lot less useful than their coordinates
- Imposing an ordering on an unordered set might **not** be useful

$$\{\text{“blue”} : 0,\ \text{“brown”} : 1,\ \text{“green”} : 2,\ \text{“black”} : 3\}$$

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# Automatic Preprocessing

- One view of deep learning is that each layer (particularly in CNNs) acts as a preprocessor
- That is, it finds filters that captures features salient to the problem being tackled
- For both images and texts we expect salient features to be spatially localised
- The deep structure allows ever more complicated features to be captured—that is, we can find spatially localised features on different scales
- Having very large datasets and simple filters (the number of weights in the CNN layers tends to be small) stops overfitting

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# Outline

1. Over-fitting?
2. Controlling Complexity
3. **Hidden structure**
4. Regularisation

# Hidden Structure

- Often the structure of data is invisible to us
- A very successful strategy is to try many different machine learning techniques and choose the best
- Often learning machines have adjustable parameters (hyper-parameters) that we have to set (they are the same for all input data, but change with the problem)
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- We need to choose the hyper-parameters to fit the data in our problem
- Fine tuning hyper-parameter is important and almost always required (true in SVMs, MLP, deep learning)

# Measuring Generalisation Performance

- Recall, we want to predict **unseen** data
- **You cannot use data that you have trained on!**

- Need to split your data up into training and validation set
- Use the validation set to choose the hyper-parameters
- You need a separate testing set if you want to measure your generalisation performance

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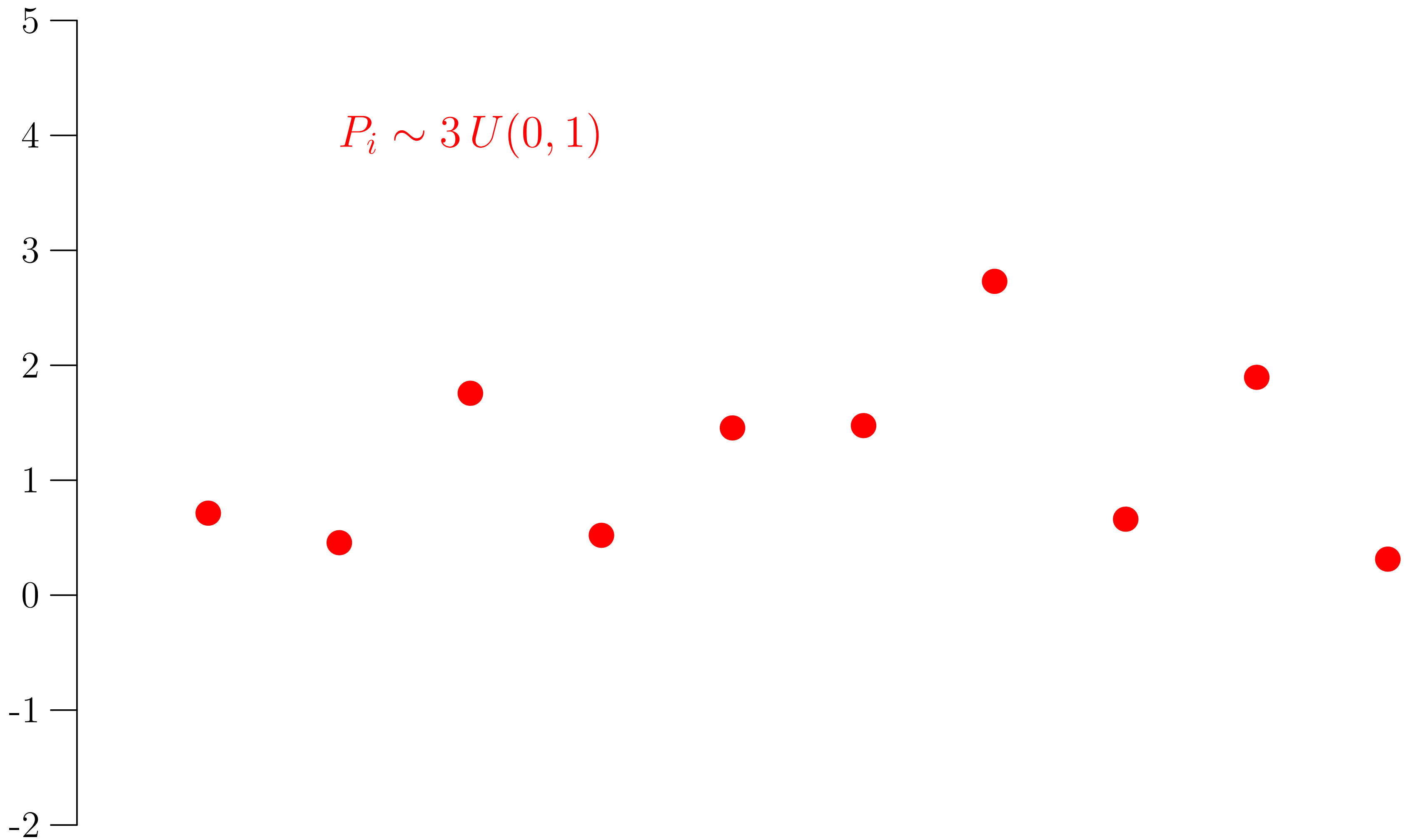

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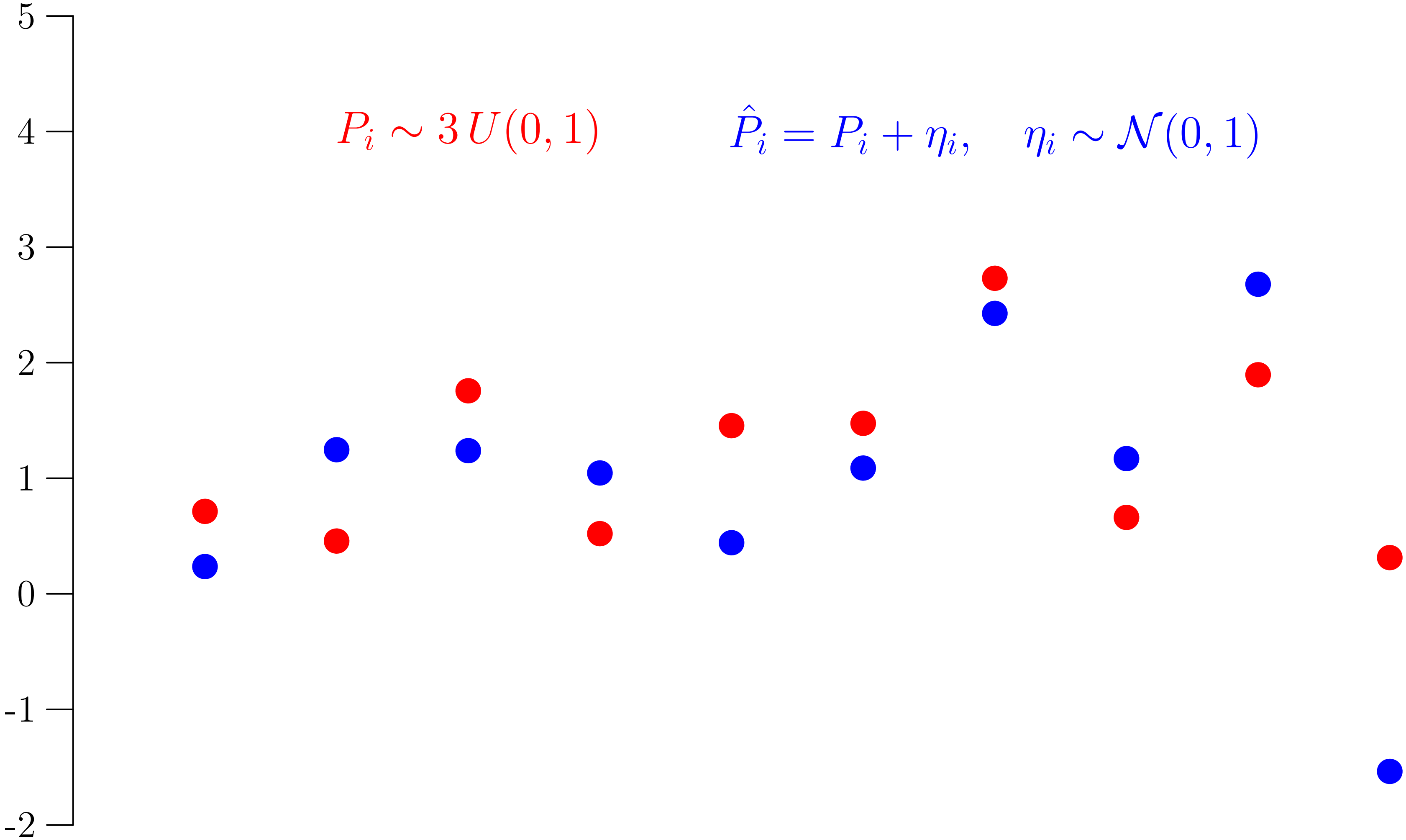

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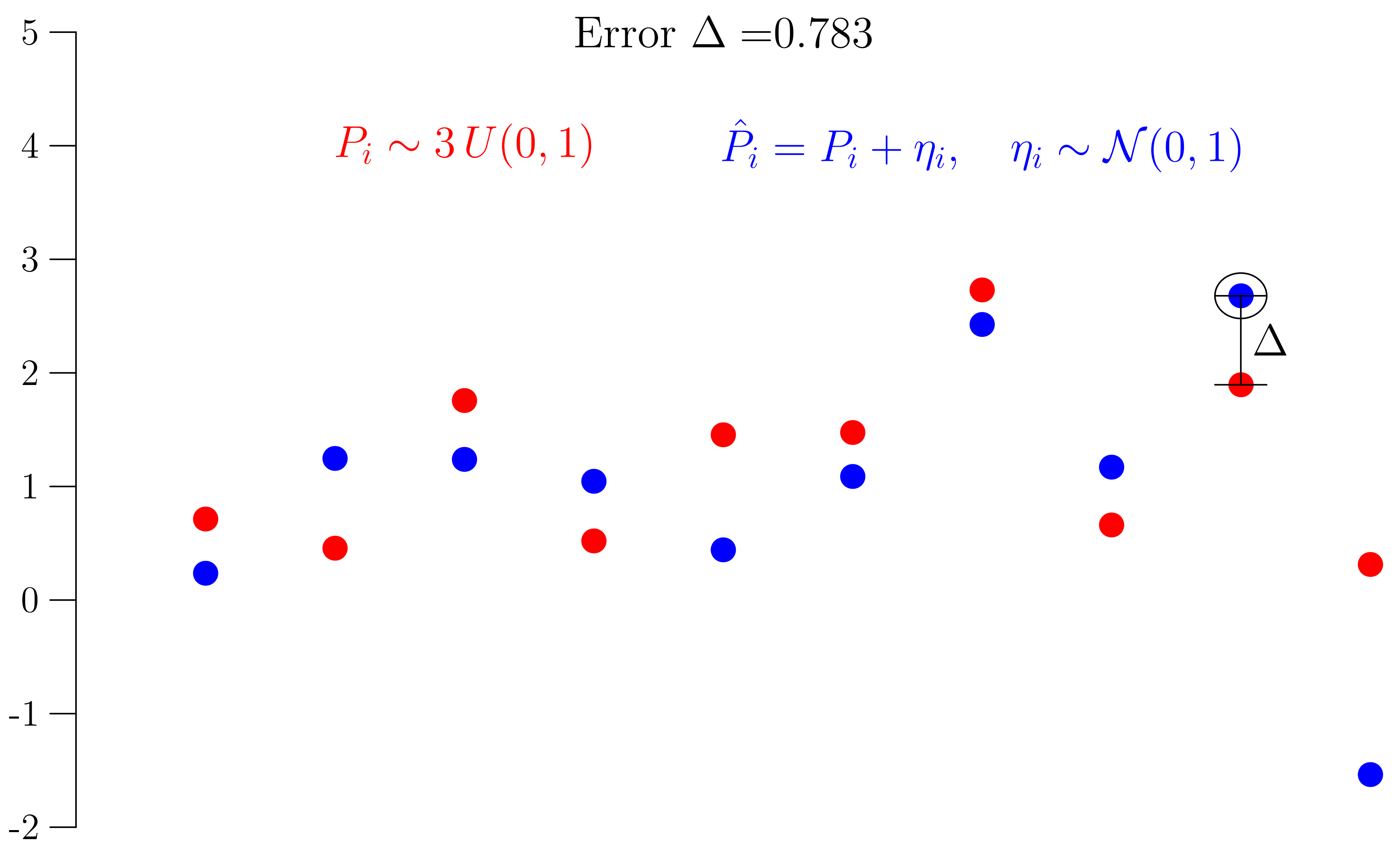

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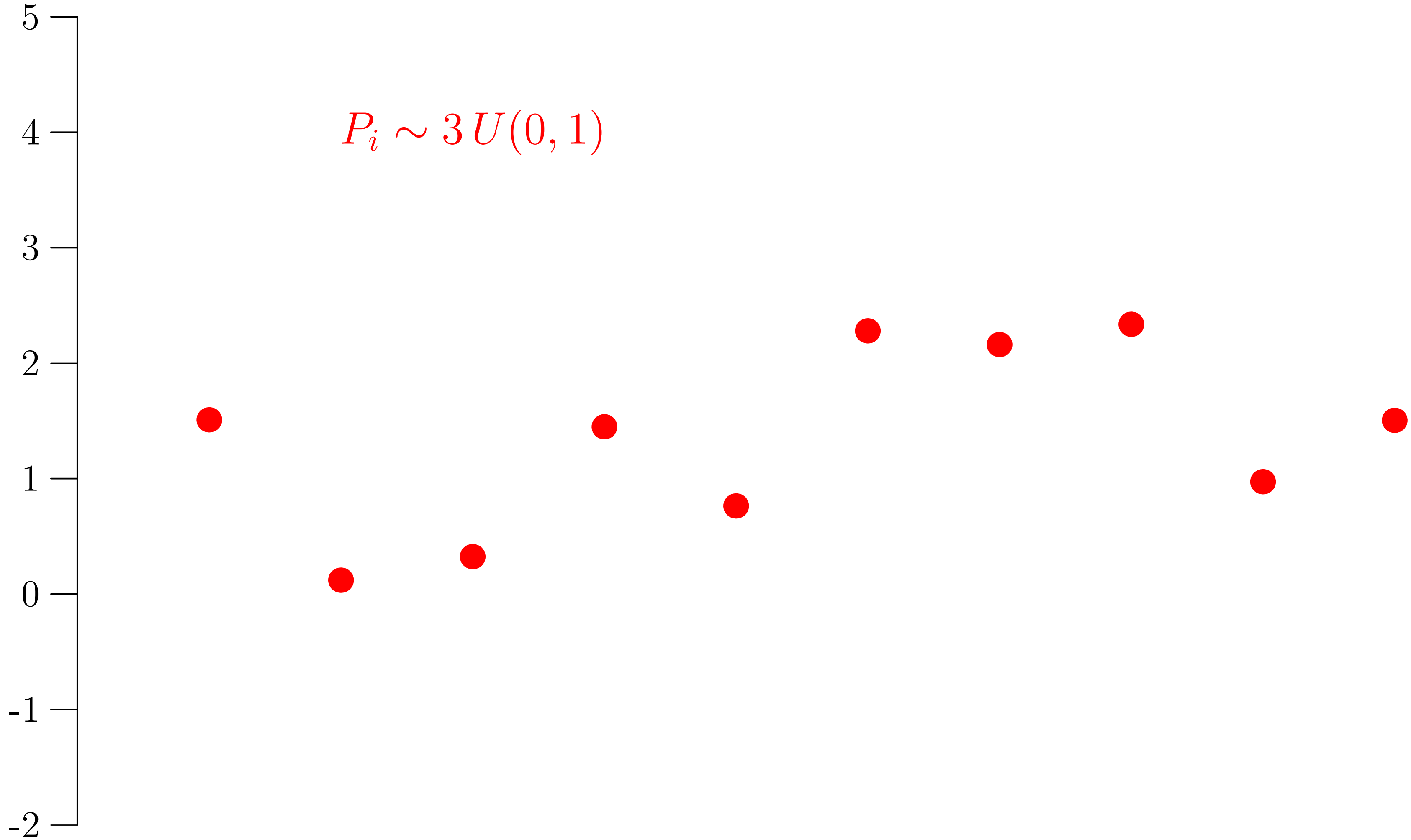

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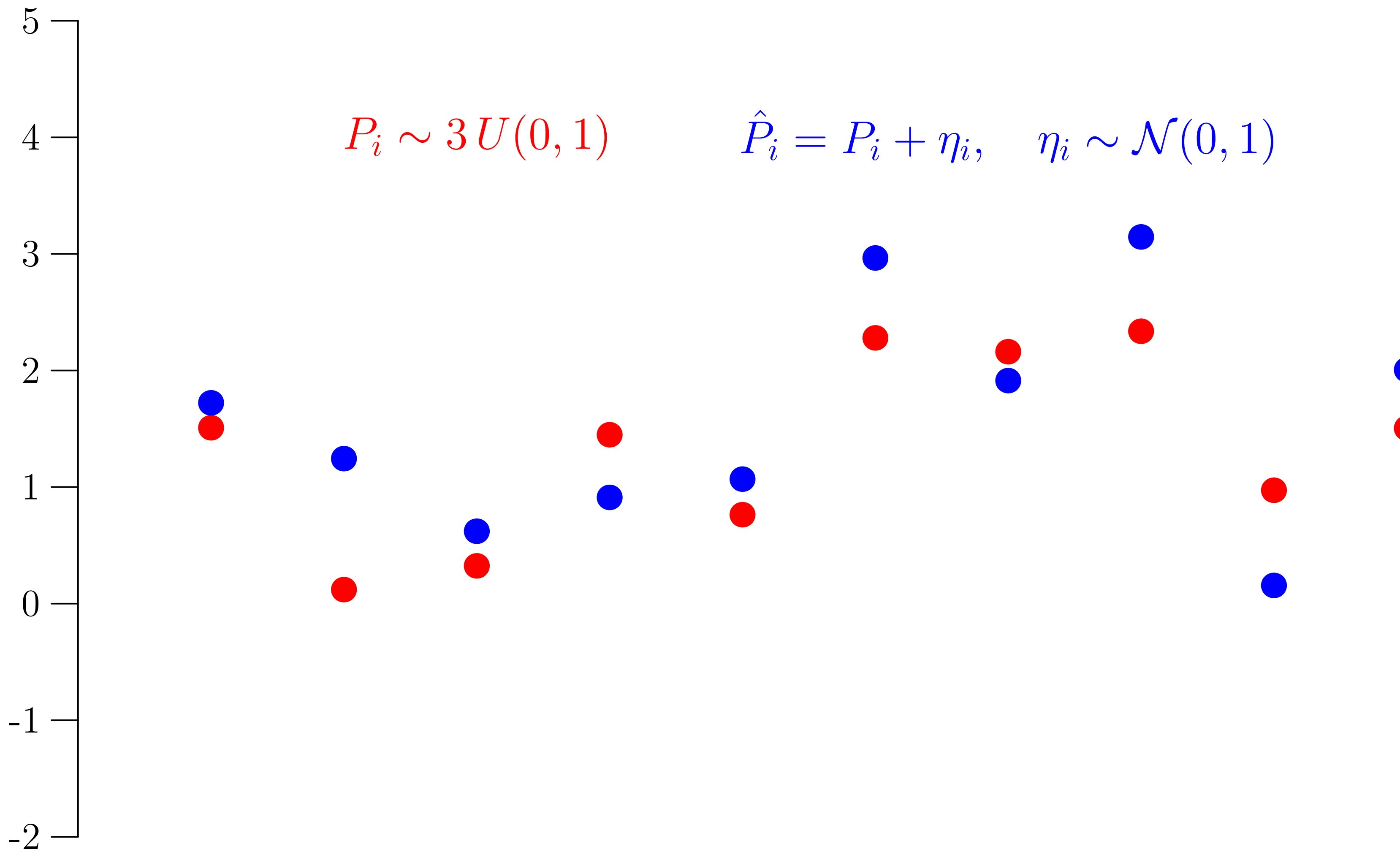

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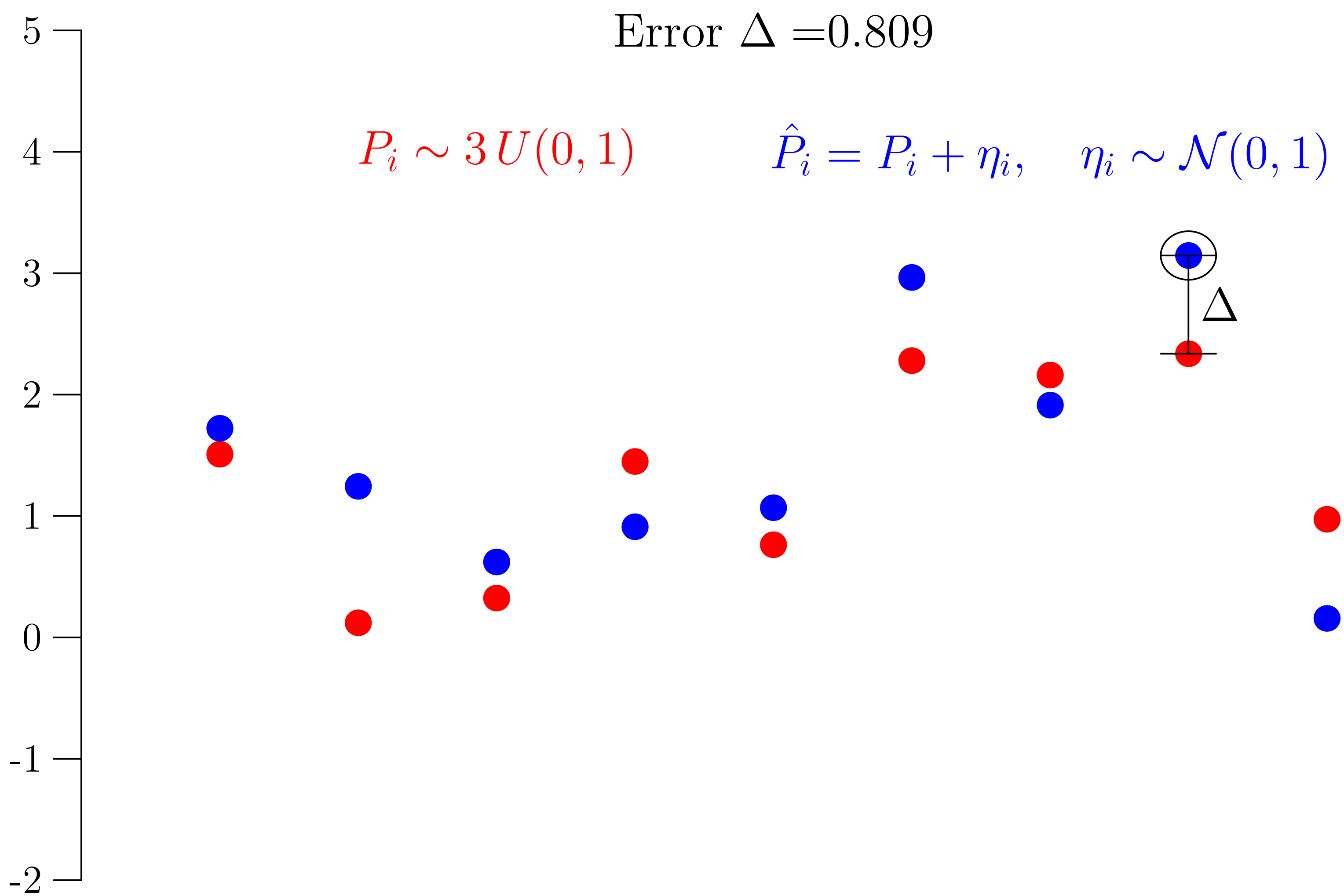

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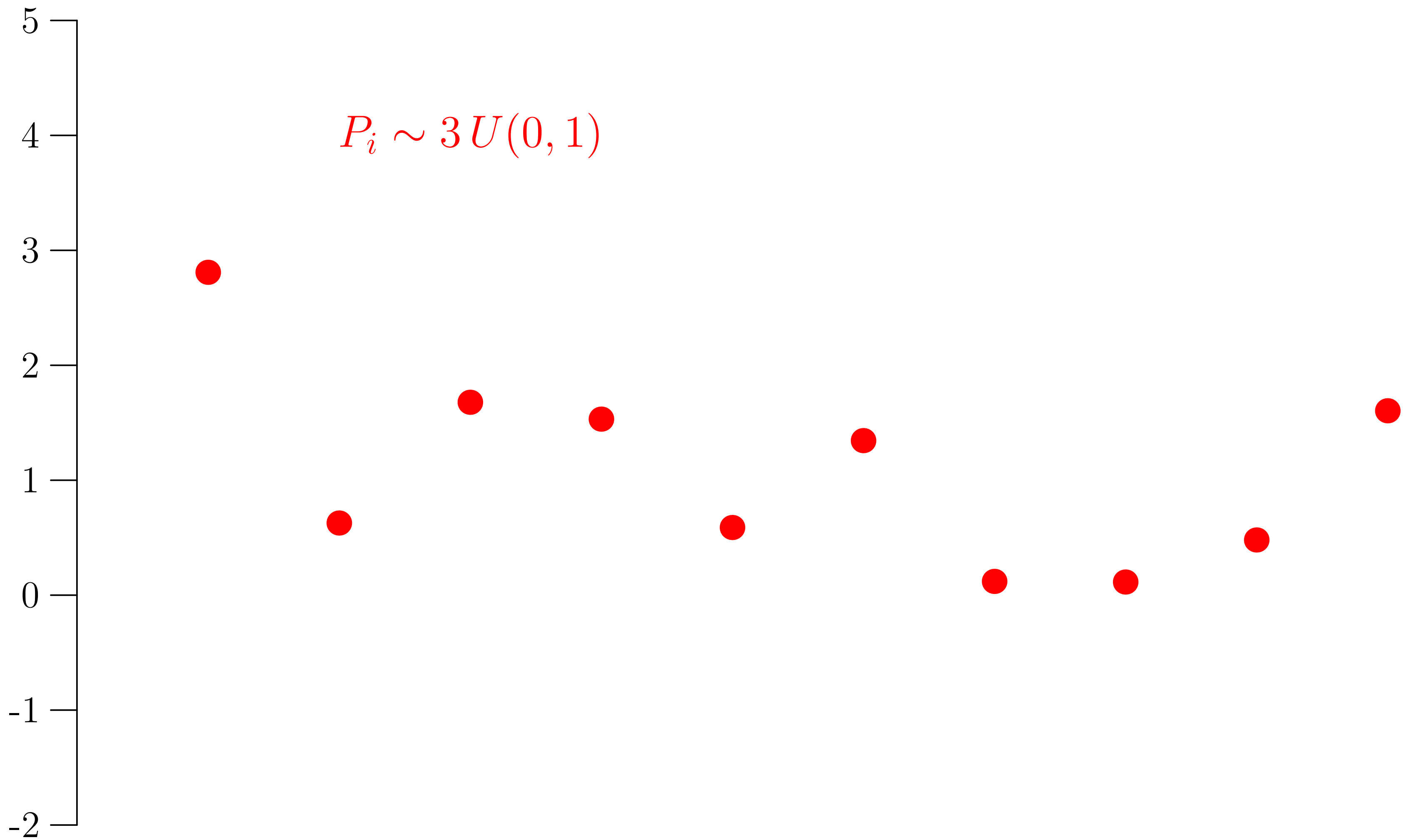

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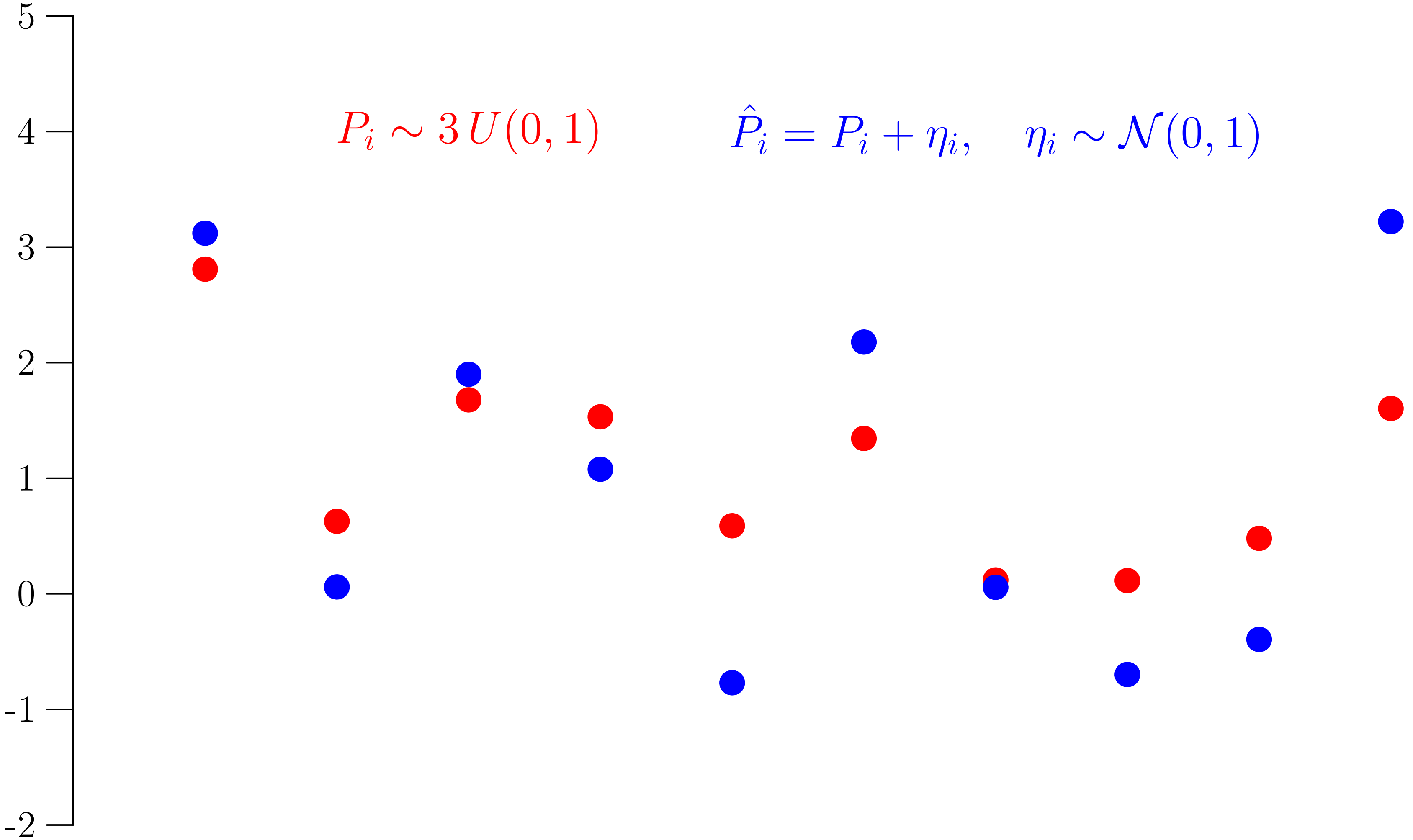

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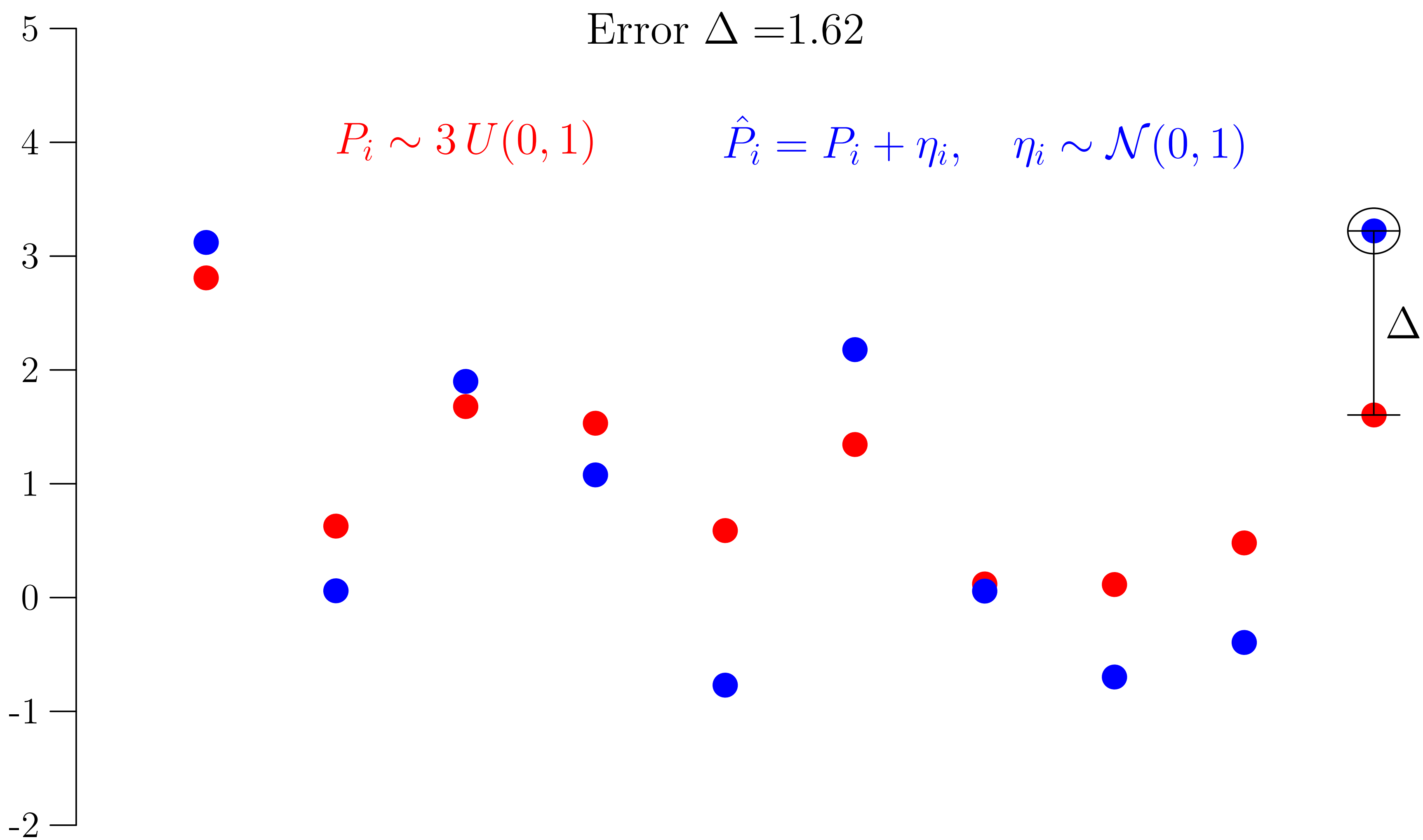

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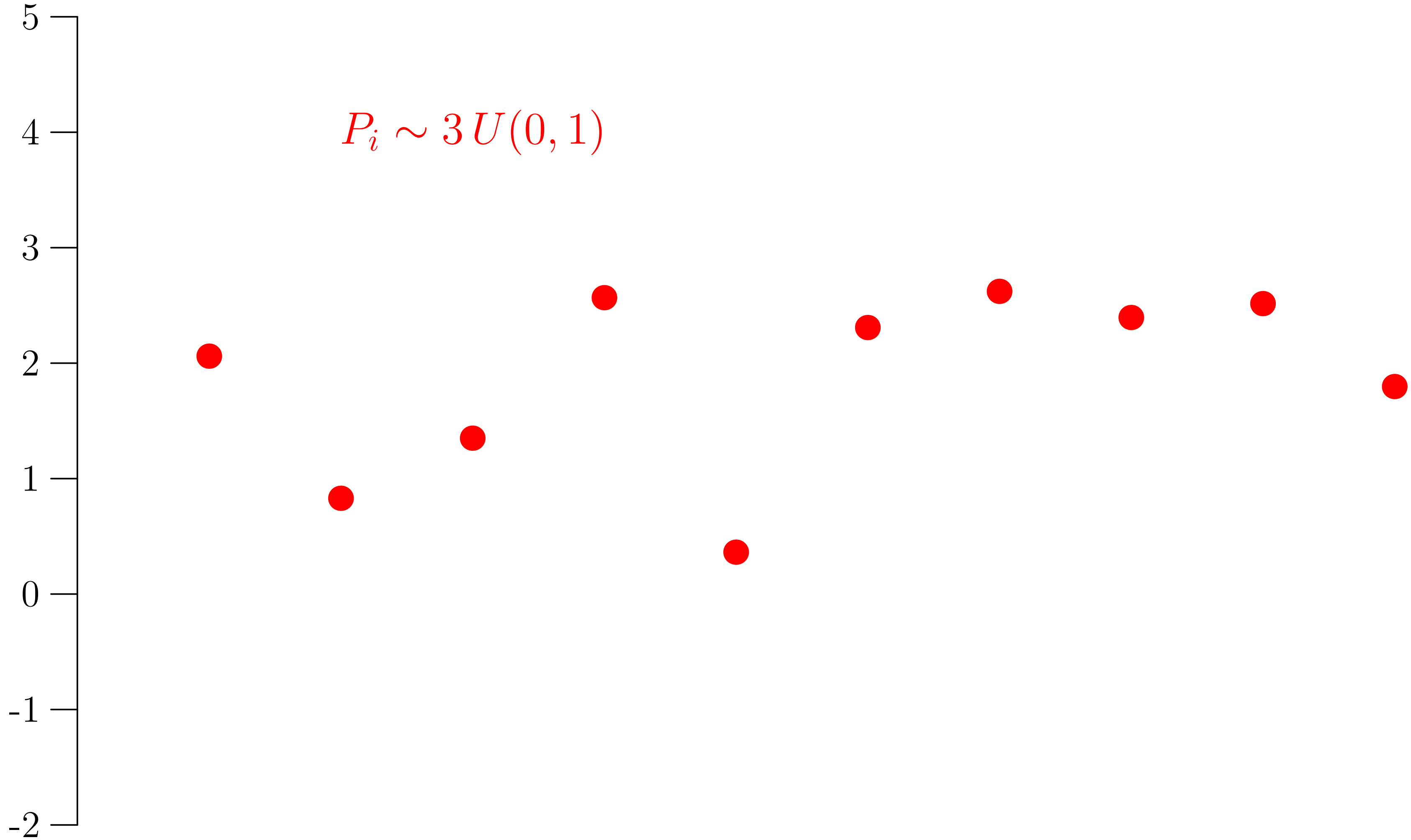

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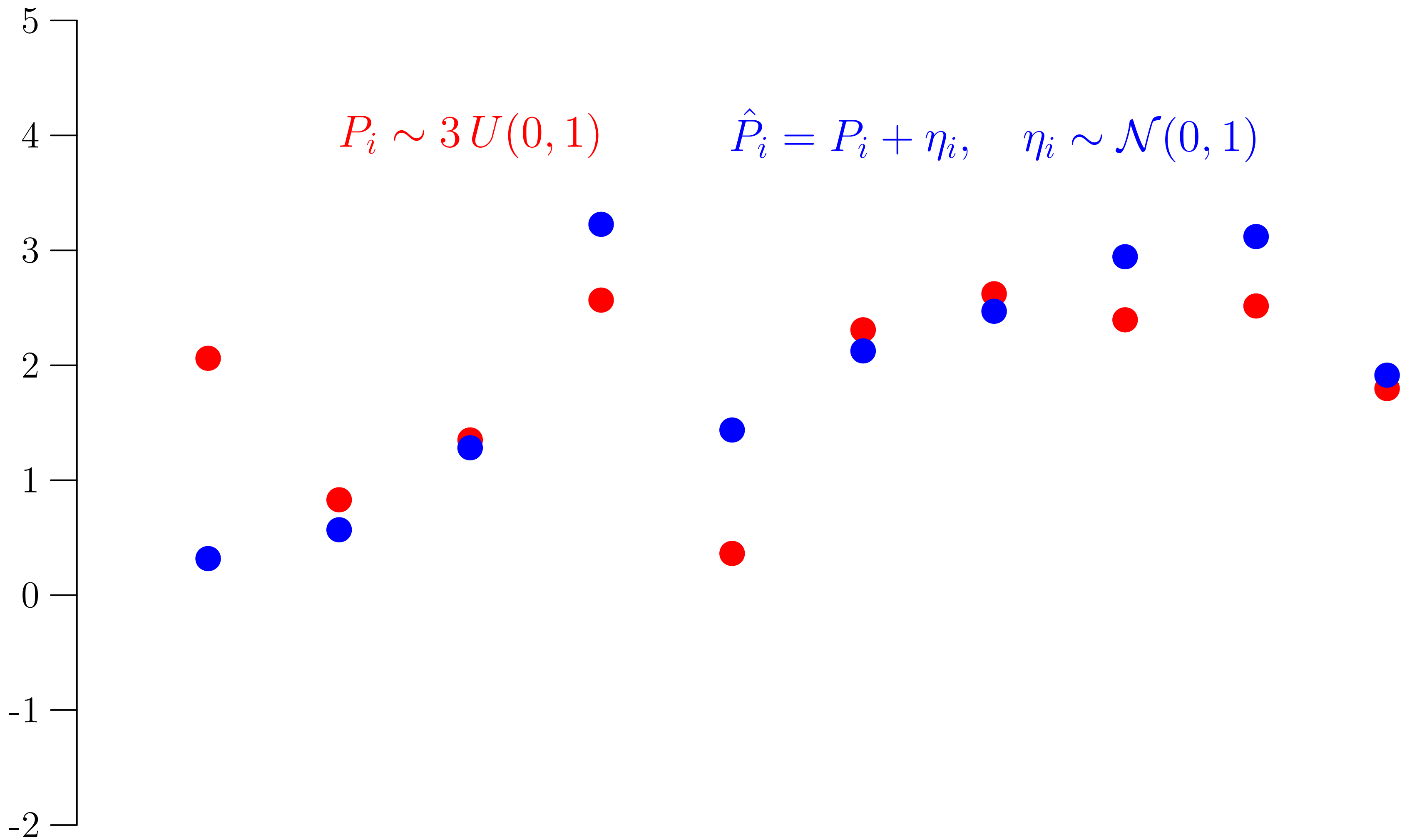
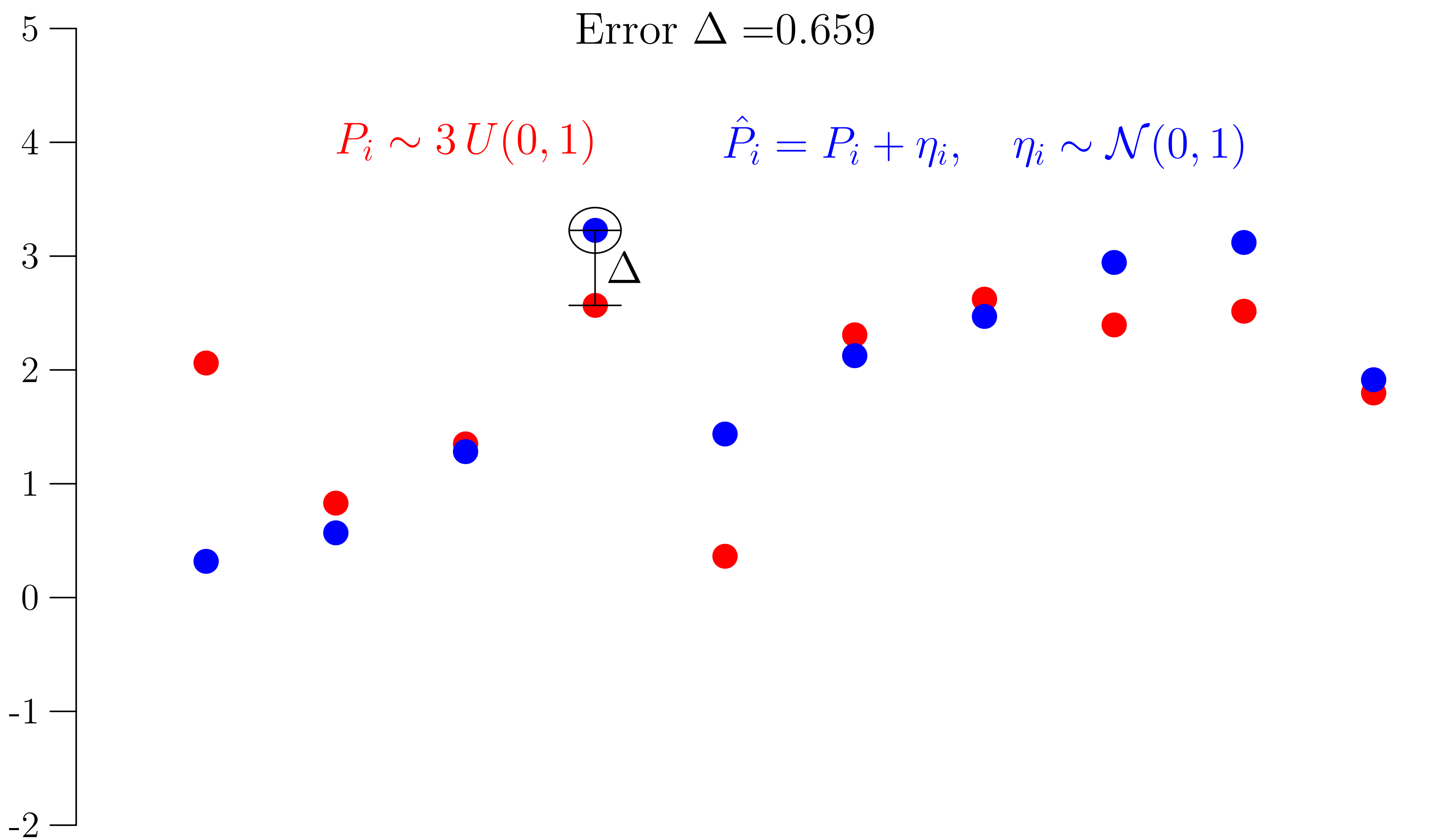
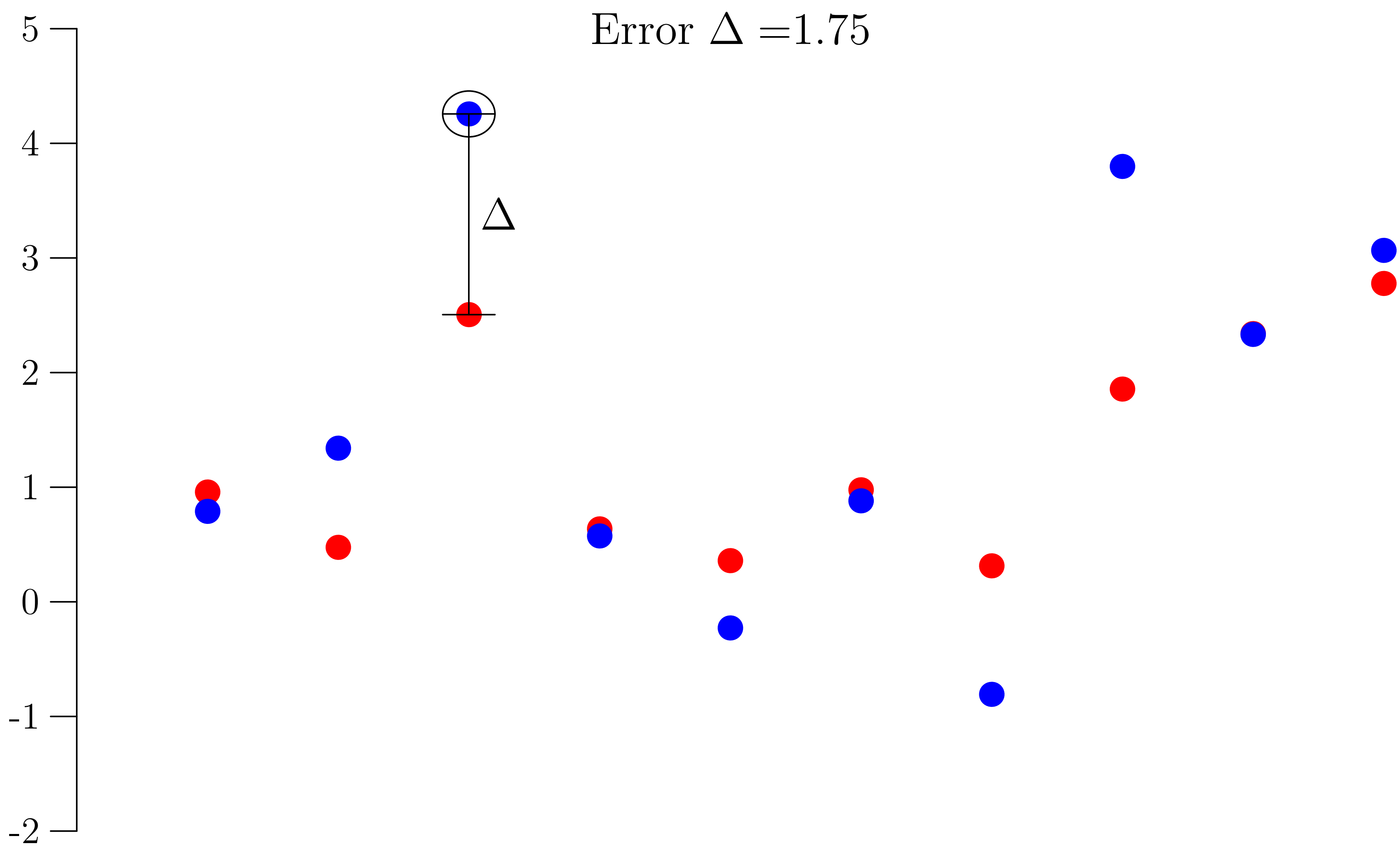


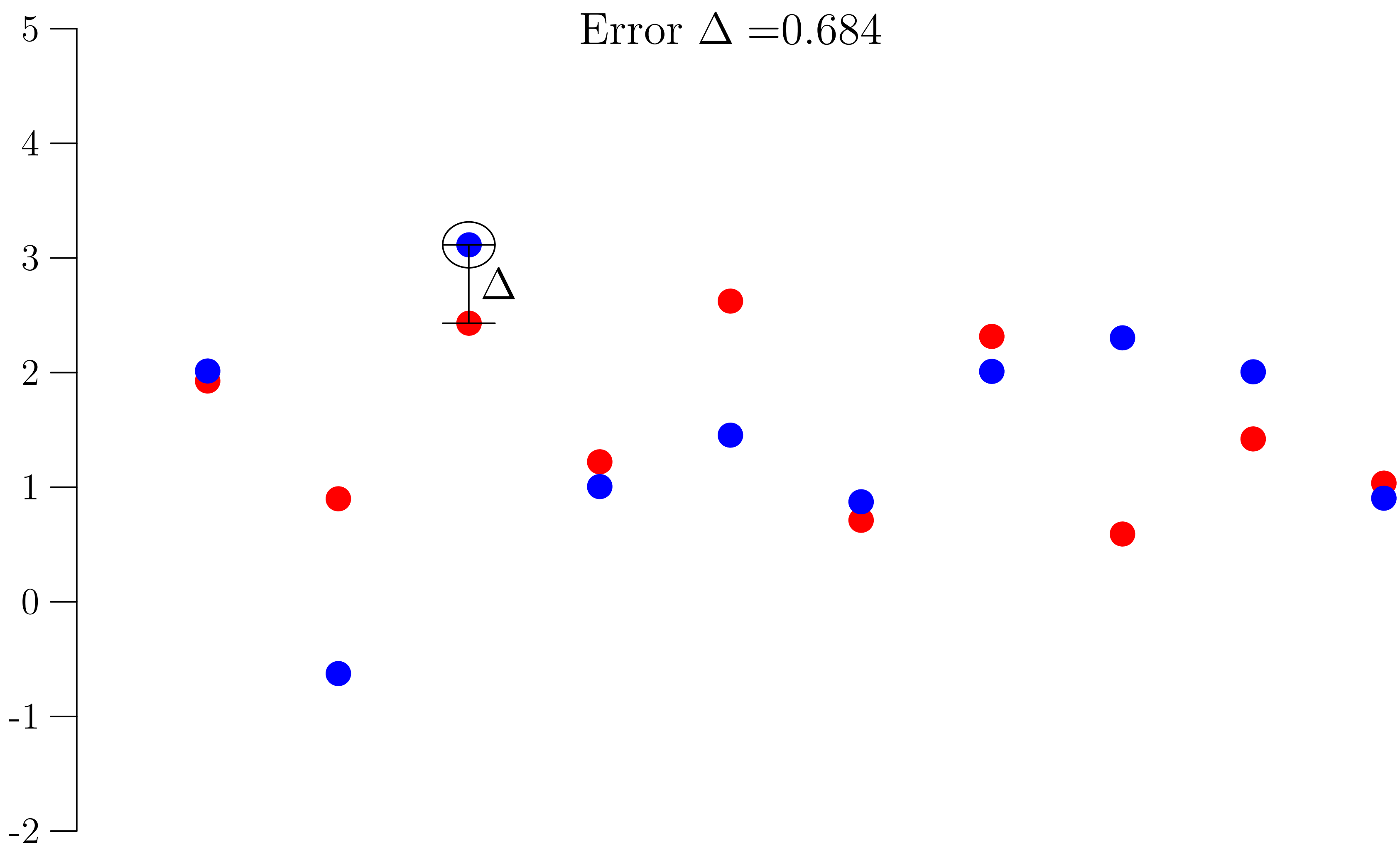
# The Overfitting Game



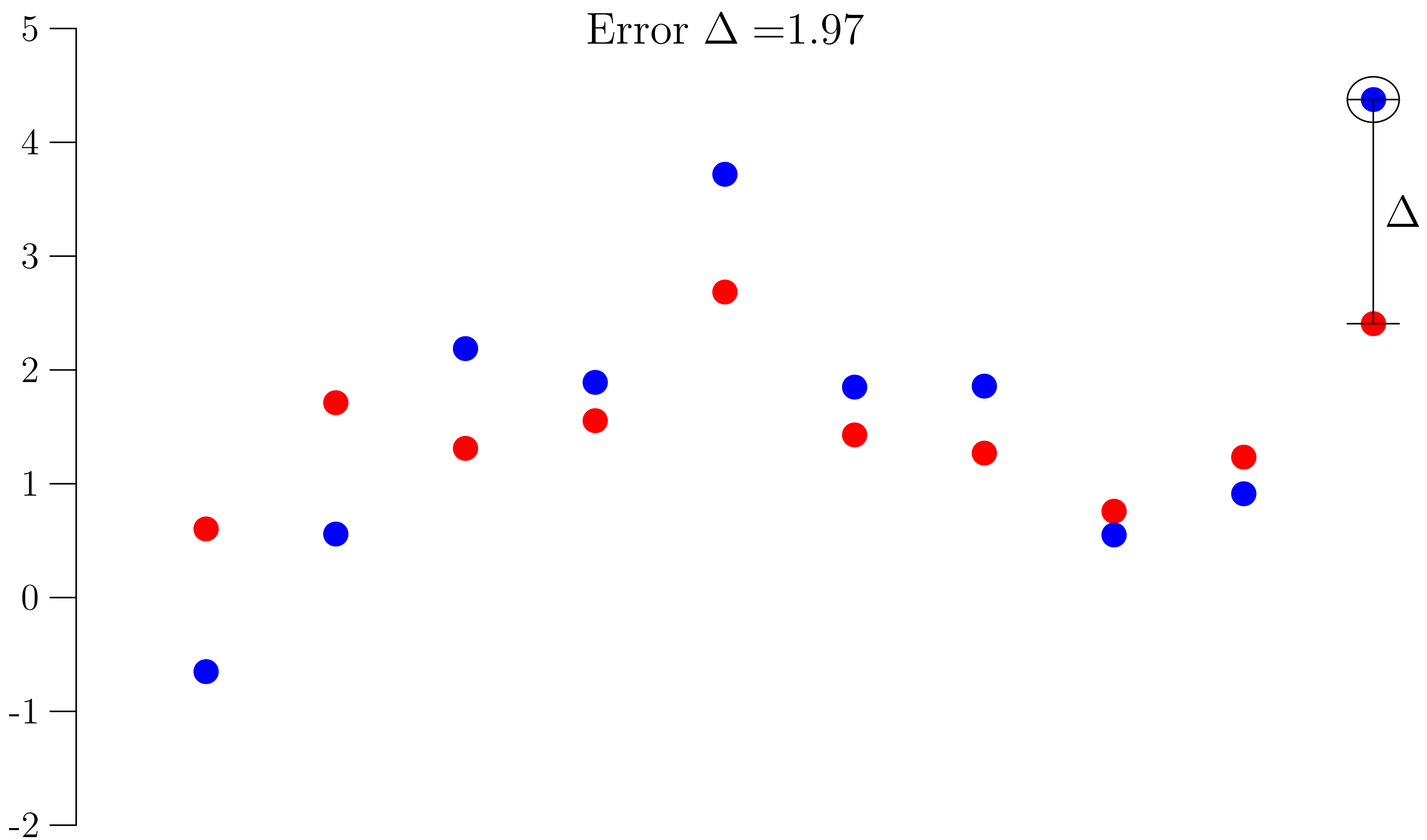
# The Overfitting Game



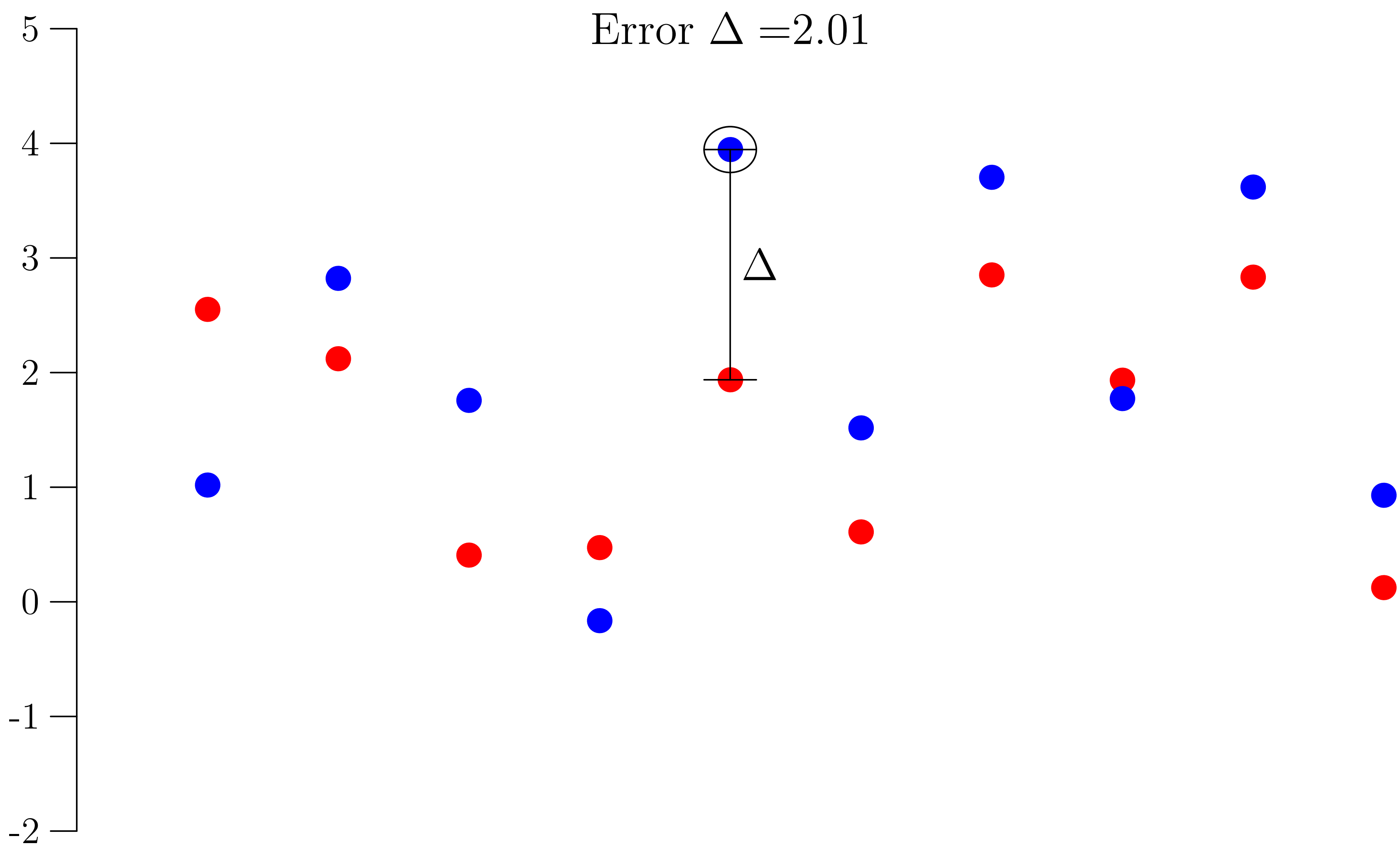
# The Overfitting Game



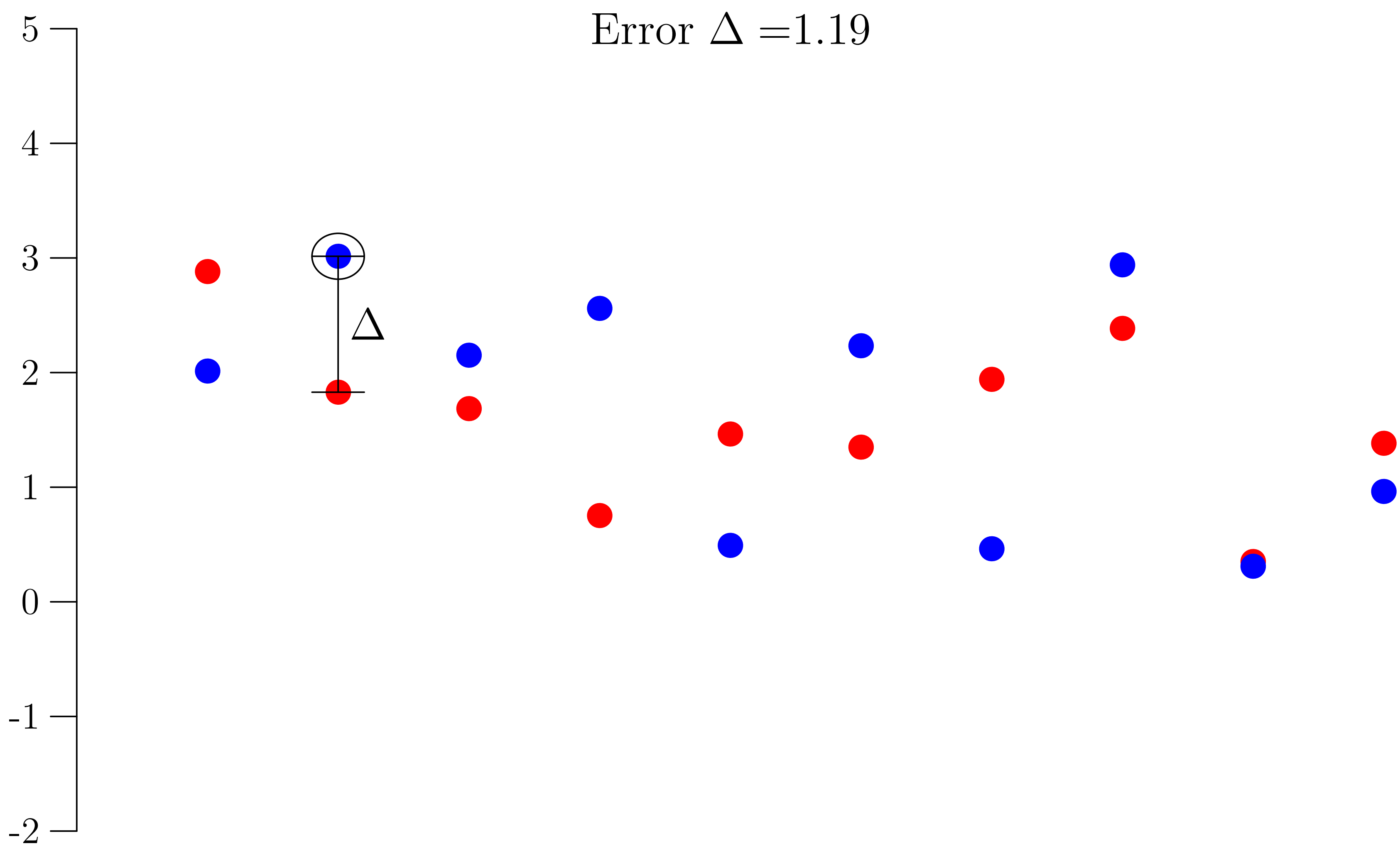
# The Overfitting Game



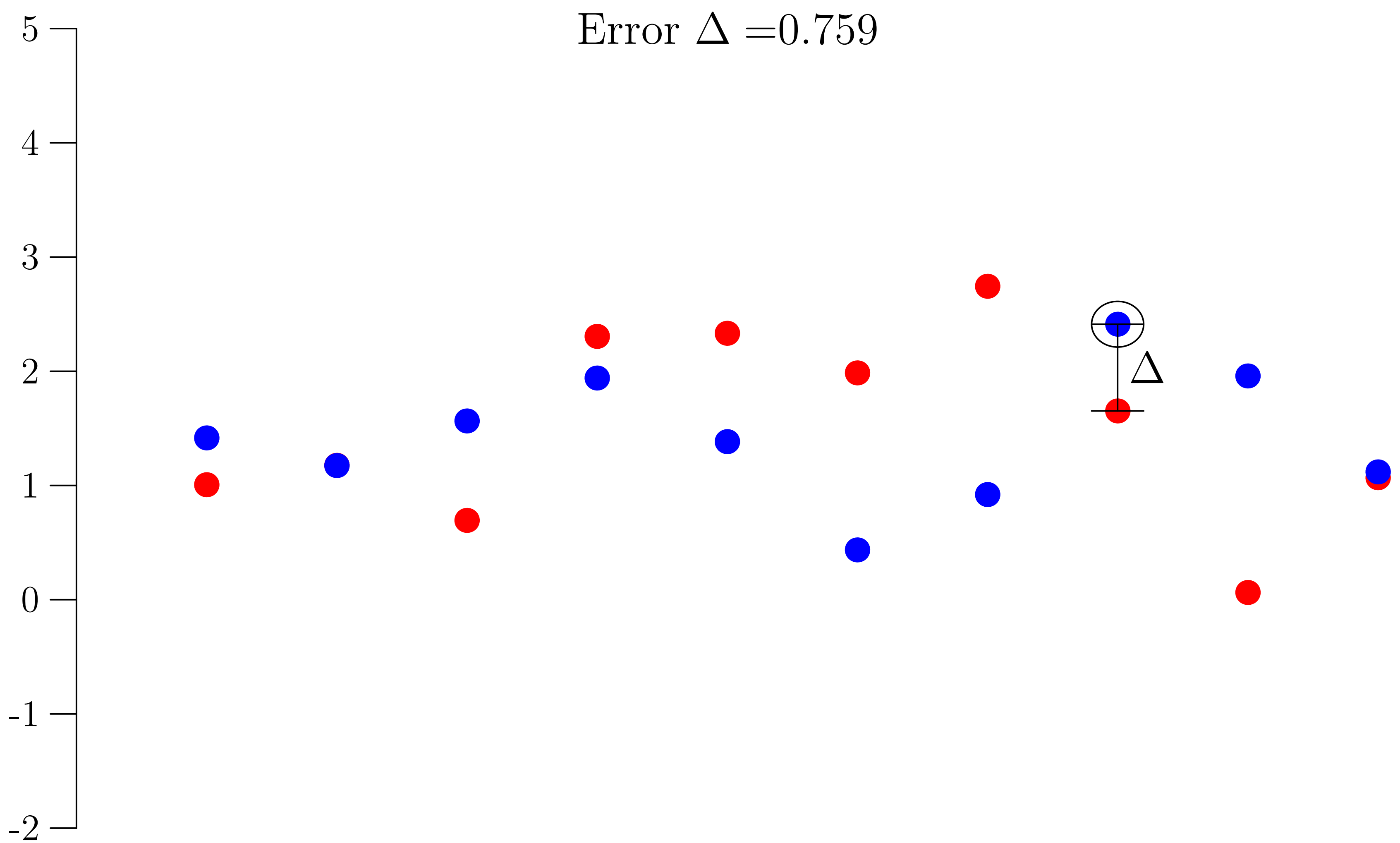
# The Overfitting Game



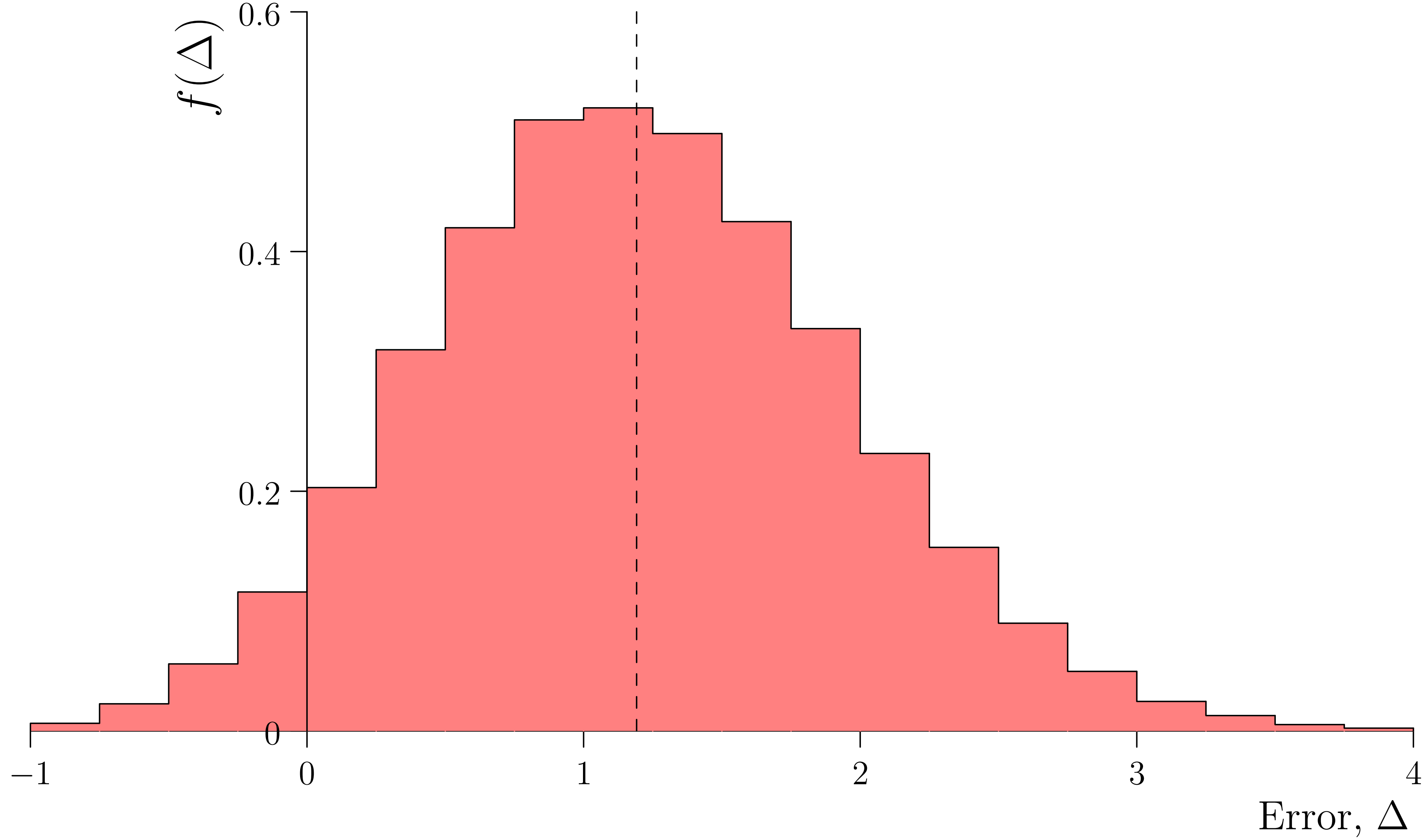
# The Overfitting Game



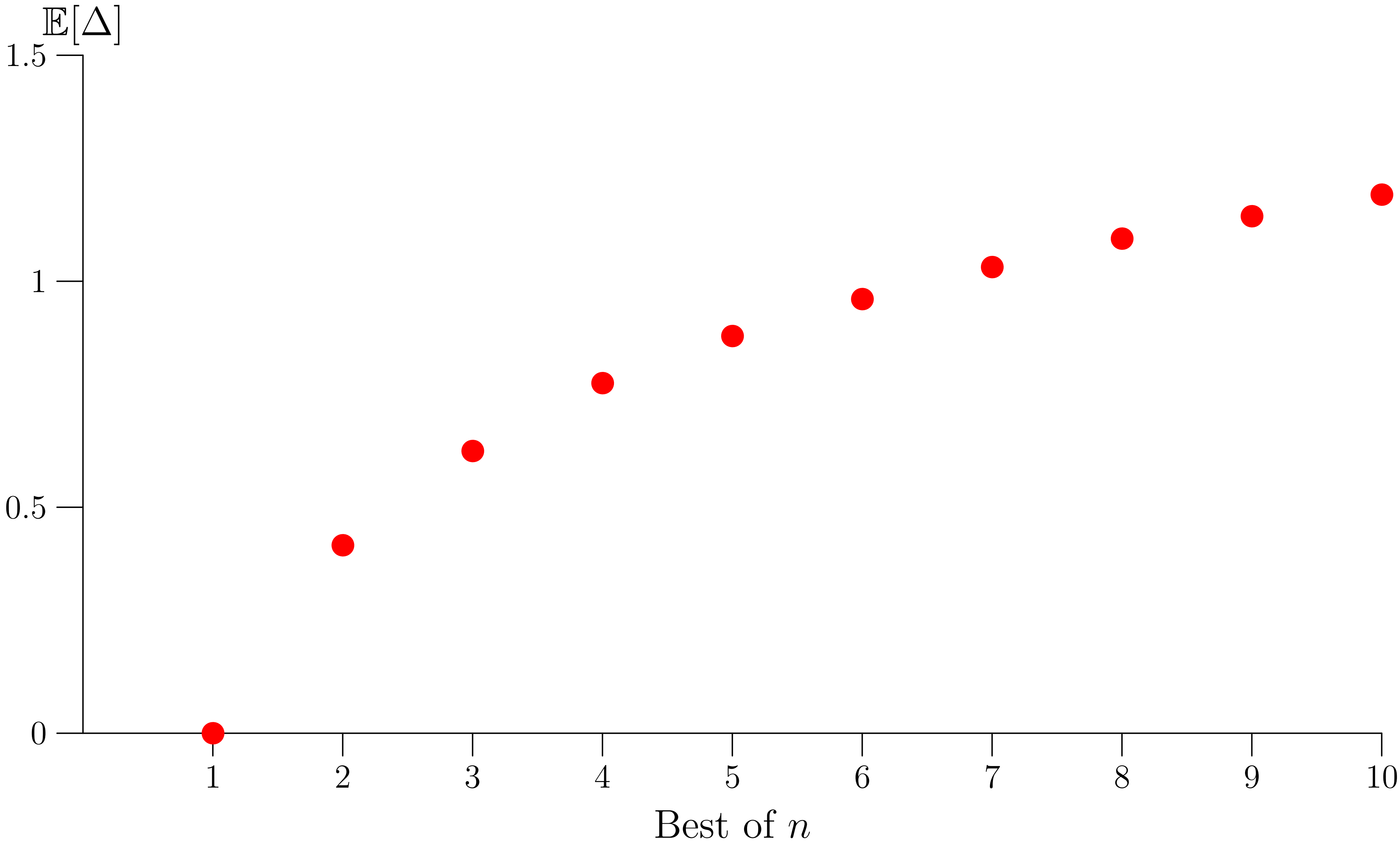
# The Overfitting Game



# The Overfitting Game



# The Overfitting Game



# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \qquad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |

# Cross Validation

- If you want to use more data for training then you can use cross validation
- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \quad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |

# Cross Validation

- If you want to use more data for training then you can use cross validation
- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \qquad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |

Test Set Training Set

5-fold cross-validation

$E_g =$ 5.1

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \qquad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |

Training Set  Test Set  Training Set

5-fold cross-validation

3.7

$E_g =$

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \qquad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |

Training Set　　Test Set　　Training Set

5-fold cross-validation

$$E_g = \qquad 4.6$$

# Cross Validation

- If you want to use more data for training then you can use cross validation
- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \quad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |

Training Set Test Set Training Set

5-fold cross-validation

$E_g =$

4.6

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \qquad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |

Training Set Test Set

5-fold cross-validation

$E_g =$ 3.3

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \qquad D_i = (\mathbf{x}_i, y_i)$$

| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|

$$\langle E_g \rangle = \frac{5.1 \quad + \quad 3.7 \quad + \quad 4.6 \quad + \quad 4.6 \quad + \quad 3.3}{5} = 4.3$$

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \quad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |

Test Set Training Set

10-fold cross-validation

$$E_g = \quad 5.8$$

# Cross Validation

- If you want to use more data for training then you can use cross validation
- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \qquad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |

Test Set Training Set

10-fold cross-validation

$$E_g = \quad 1.8$$

# Cross Validation

- If you want to use more data for training then you can use cross validation
- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \qquad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |

Training Set Test Set Training Set

10-fold cross-validation

$E_g =$ 4.8

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \qquad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |

Training Set Test Set Training Set

10-fold cross-validation

$$E_g = \qquad 3.6$$

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \qquad D_i = (\mathbf{x}_i, y_i)$$

| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|

Training Set Test Set Training Set

10-fold cross-validation

$$E_g = \qquad 7.4$$

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \quad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |

Training Set Test Set Training Set

10-fold cross-validation

$$E_g = \qquad 0.99$$

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \qquad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |

Training Set Test Set Training Set

10-fold cross-validation

$E_g =$ 4.5

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \qquad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |

Training Set Test Set Training Set

10-fold cross-validation

$E_g =$ 5.4

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \qquad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |

Training Set　　　Test Set

10-fold cross-validation

$E_g =$　　　6.2

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \quad D_i = (\mathbf{x}_i, y_i)$$

| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|

Training Set Test Set

10-fold cross-validation

$E_g =$ $2.7$

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \qquad D_i = (\mathbf{x}_i, y_i)$$

| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|

$$\langle E_g \rangle = \frac{5.8 + 1.8 + 4.8 + 3.6 + 7.4 + 0.99 + 4.5 + 5.4 + 6.2 + 2.7}{10} = 4.3$$

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \qquad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |
| Test | | | | | | | | | | | | | | | | | | | |

Leave-one-out cross-validation

$$E_g = {}^{5}$$

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \qquad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |
| | Test | | | | | | | | | | | | | | | | | | |

Leave-one-out cross-validation

$$E_g = \quad 3.7$$

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \qquad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |
| | | Test | | | | | | | | | | | | | | | | | |

Leave-one-out cross-validation

$$E_g = \quad 5$$

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \quad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |
| | | | Test | | | | | | | | | | | | | | | | |

Leave-one-out cross-validation

$$E_g = \quad 2.2$$

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \quad D_i = (\mathbf{x}_i, y_i)$$

| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |
| | | | | Test | | | | | | | | | | | | | | | |

Leave-one-out cross-validation

$$E_g = \quad 3.8$$

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \quad D_i = (\mathbf{x}_i, y_i)$$

| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|

$\langle E_g \rangle = 6.5$

# Cross Validation

- If you want to use more data for training then you can use cross validation

- $K$-fold cross validation splits the data into $K$ groups

$$\mathcal{D} = \{D_i\}_{i=1}^{P} \quad D_i = (\mathbf{x}_i, y_i)$$

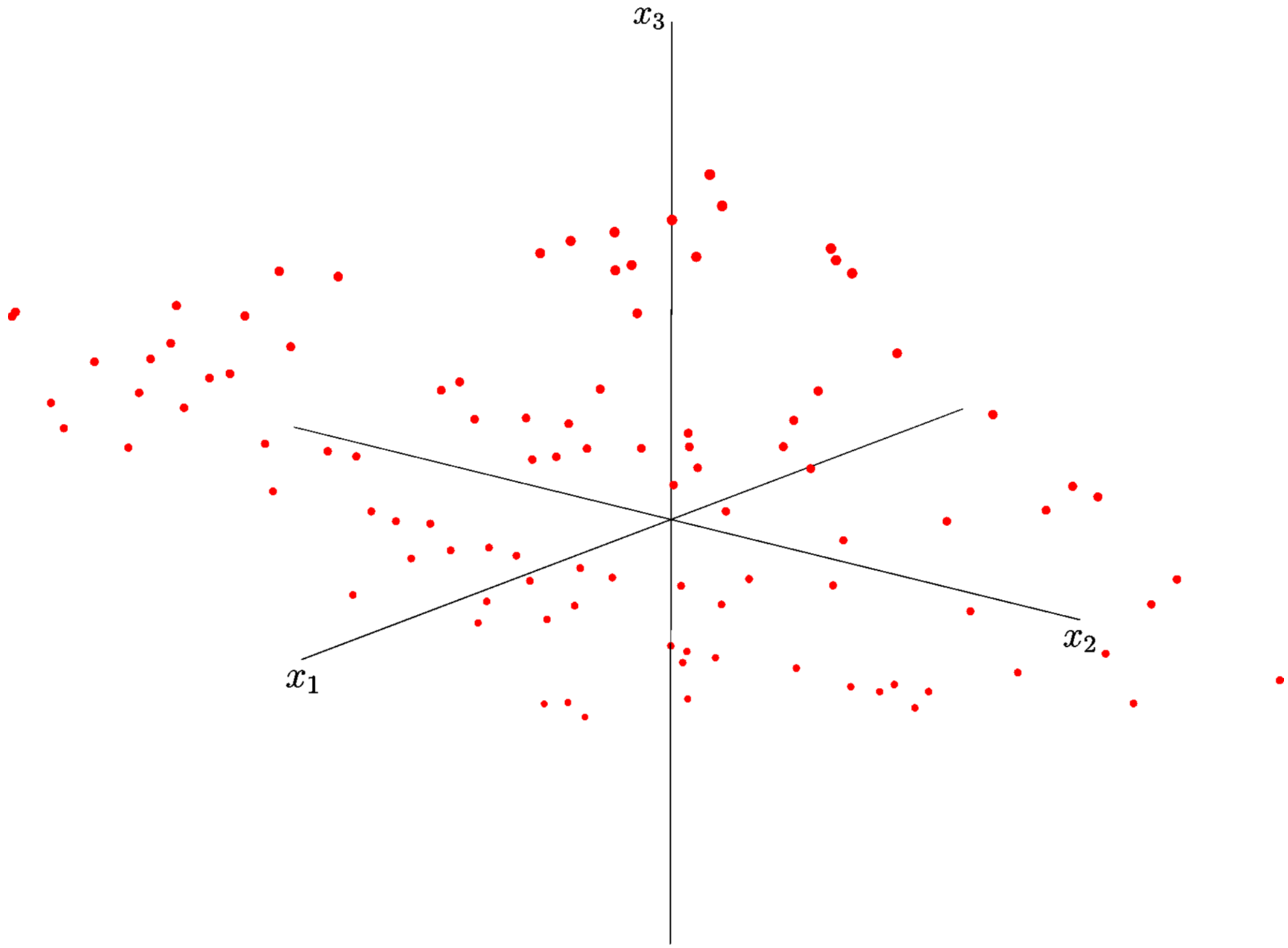
| | | | | | | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $D_1$ | $D_2$ | $D_3$ | $D_4$ | $D_5$ | $D_6$ | $D_7$ | $D_8$ | $D_9$ | $D_{10}$ | $D_{11}$ | $D_{12}$ | $D_{13}$ | $D_{14}$ | $D_{15}$ | $D_{16}$ | $D_{17}$ | $D_{18}$ | $D_{19}$ | $D_{20}$ |

$\langle E_g \rangle = 6.5$

- Leave-one-out cross-validation is extreme case

# Hidden Structure

Can't spot low dimensional data by looking at numbers



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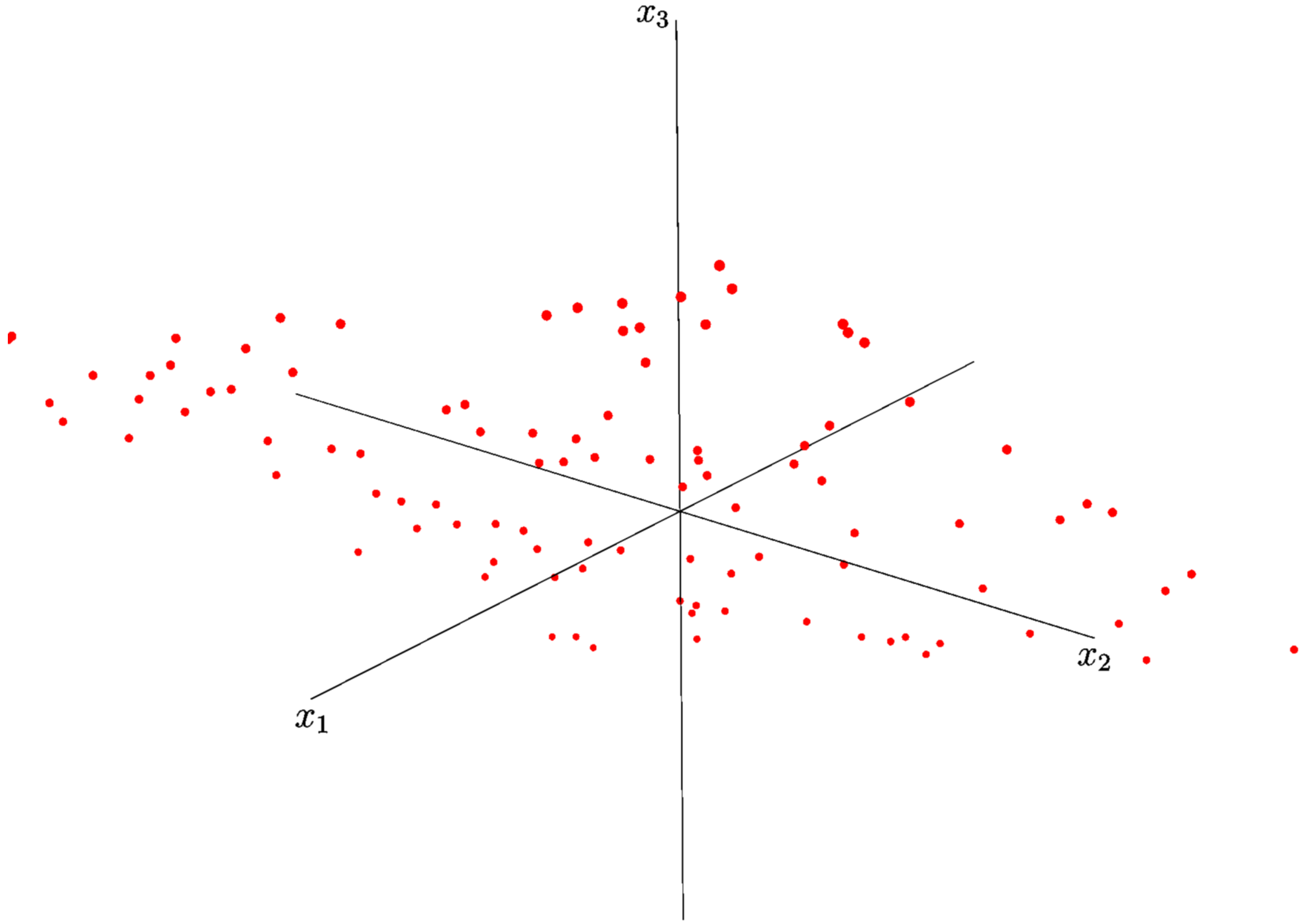

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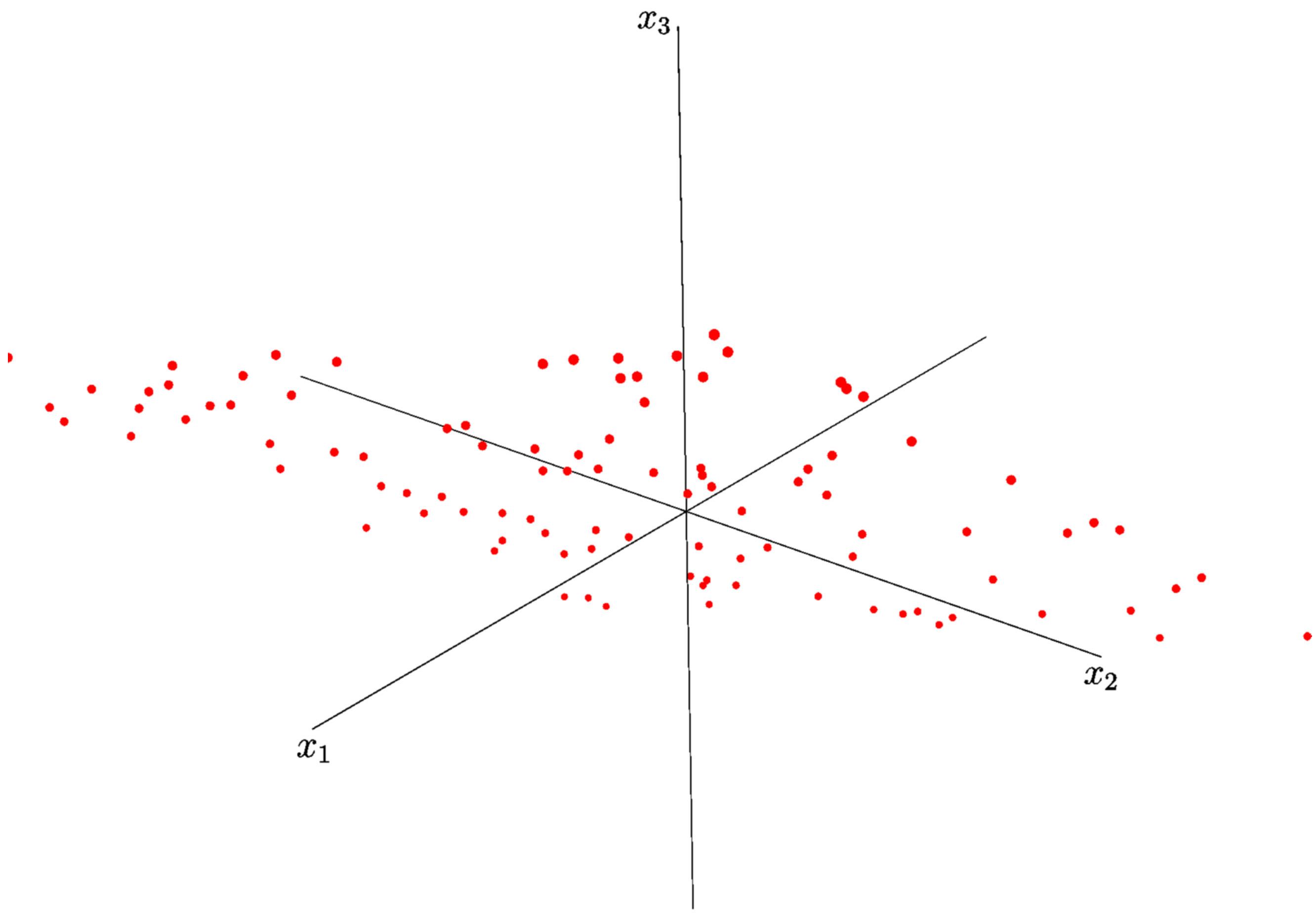

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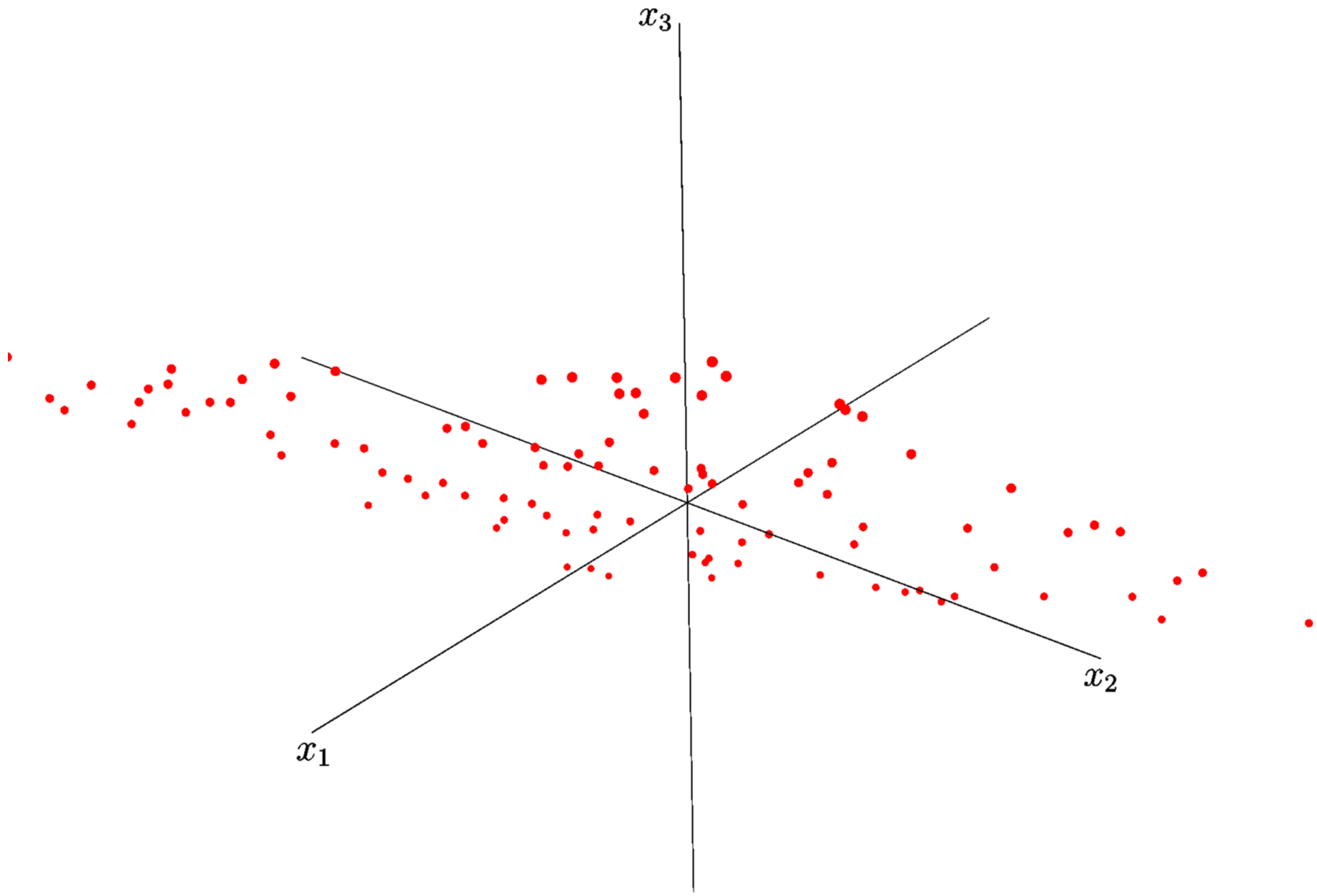

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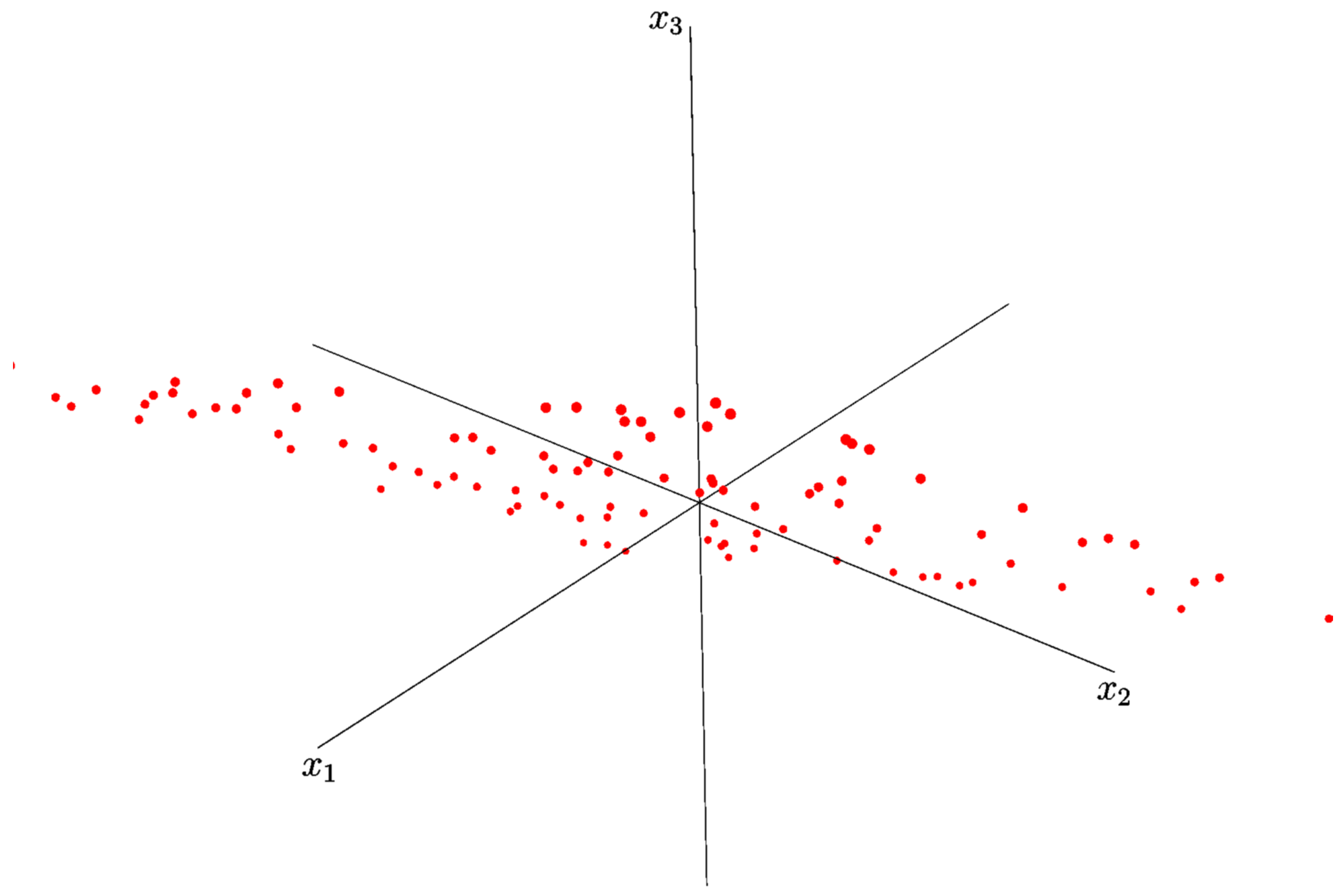

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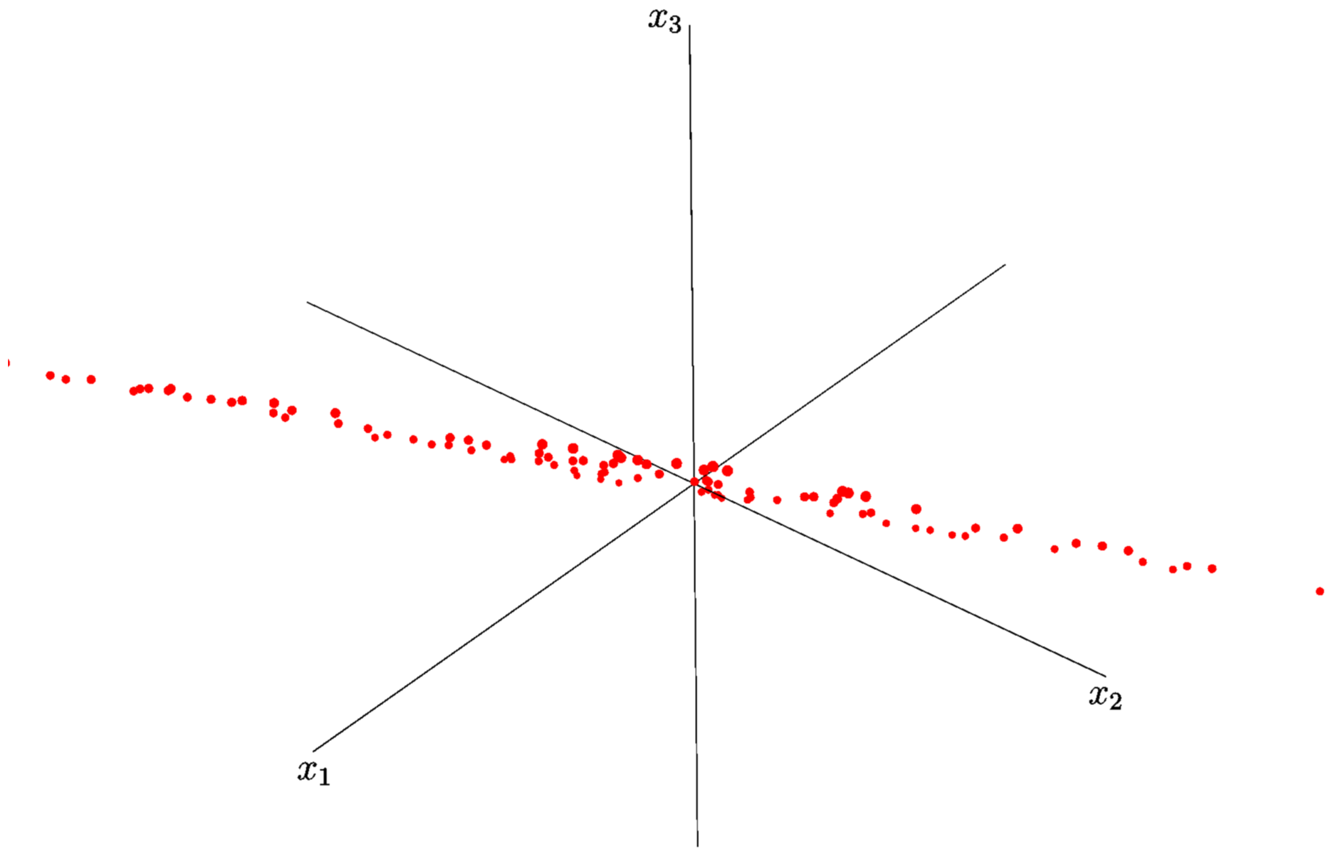

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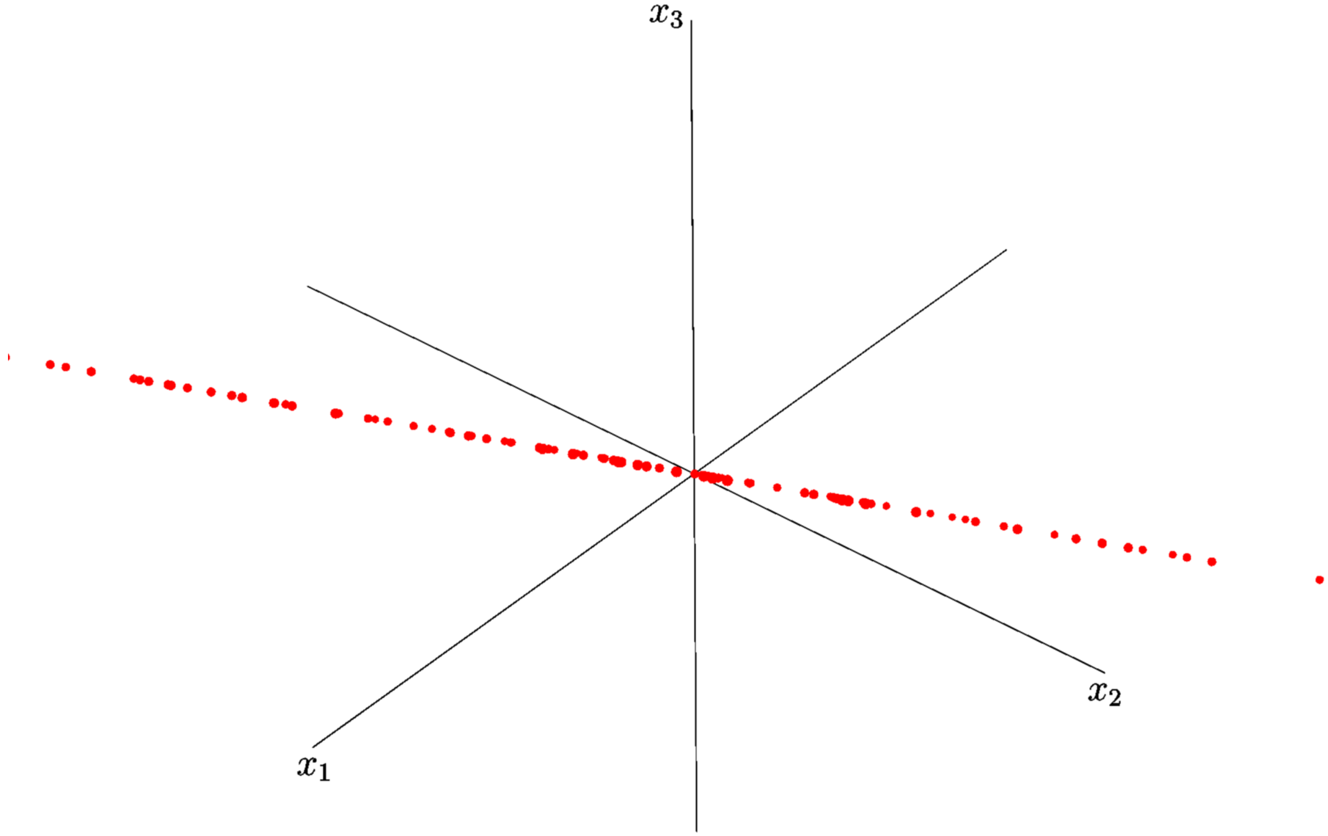

# Dimensionality Reduction

- We can sometimes simplify our machines by using less features
- We can project our data onto a lower dimensional sub-space (e.g. one with the maximum variation in the data: PCA)
- We can use clustering to find exemplars and recode our data in terms of distances from the exemplars (radial basis functions)
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# Feature Selection

- Spurious features will allow us to find spurious rules (**over-fitting**)
- We can try different combinations of features to find the best set, although it rapidly becomes intractable to do this in all ways
- We can use various heuristics to decide which features to keep, but no heuristic is fail-safe method to find the best set of features
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# Normalising Features

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$$x_i^\alpha \leftarrow \frac{x_i^\alpha - \hat{\mu}_i}{\hat{\sigma}_i}, \quad \hat{\mu} = \frac{1}{m}\sum_{\beta=1}^{m} x_i^\beta, \quad \hat{\sigma}_i^2 = \frac{1}{m-1}\sum_{\beta=1}^{m}(x_i^\beta - \hat{\mu}_i)^2$$

# Outline

1. Over-fitting?
2. Controlling Complexity
3. Hidden structure
4. **Regularisation**

# Explicit Regularisation

- As you've seen in the foundations of ML course, we can modify our error function to choose smoother functions

$$L = \sum_{k=1}^{m} \left( \boldsymbol{w}^\mathsf{T} \boldsymbol{x}_k - y_k \right)^2$$

- Second term is minimised when $w_i = 0$
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$$f(\boldsymbol{x}|\boldsymbol{w}) = \boldsymbol{w}^\mathsf{T} \boldsymbol{x}$$

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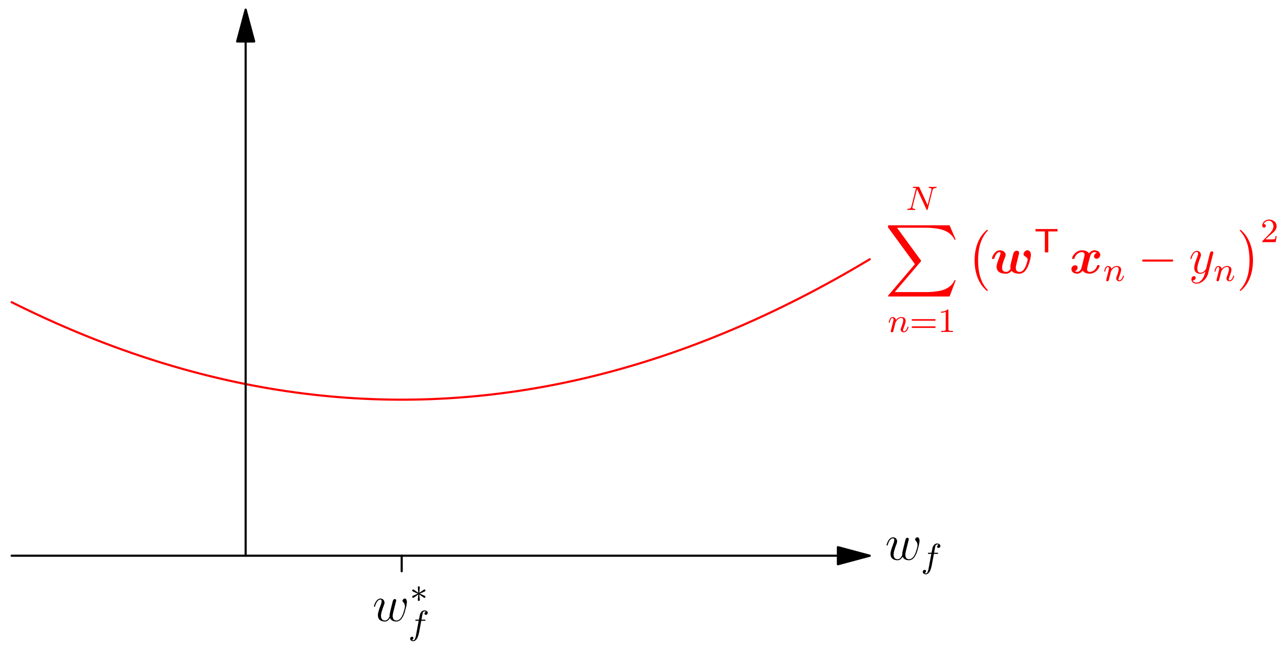

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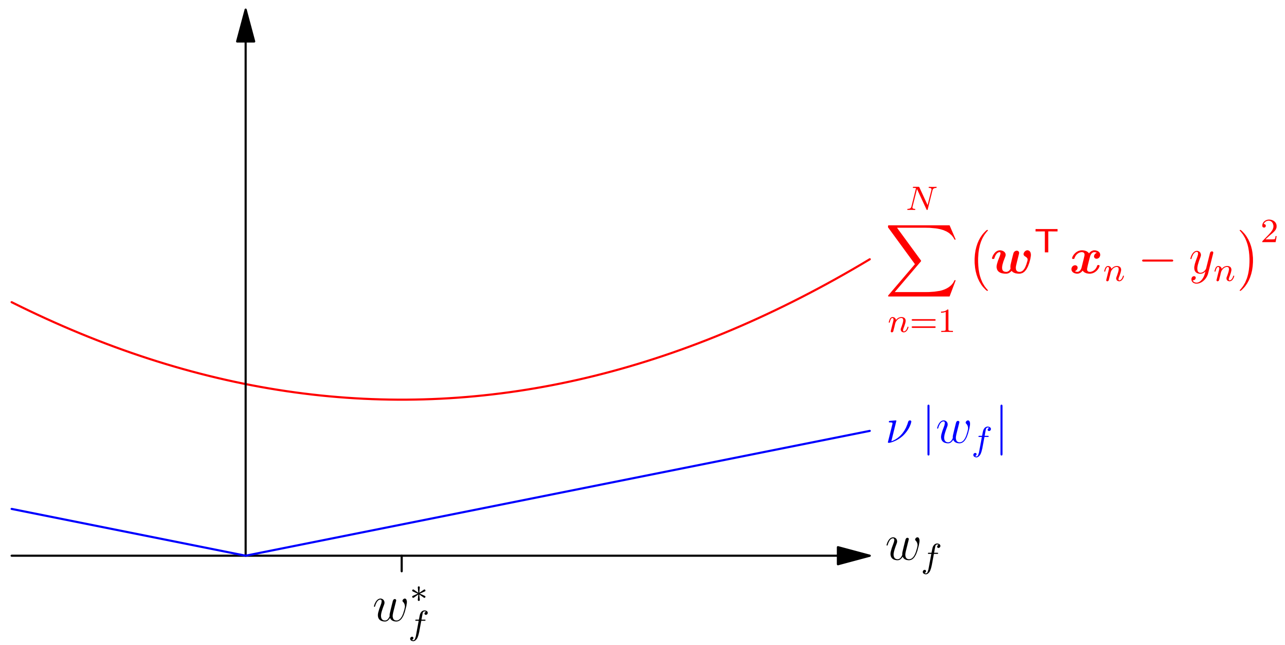

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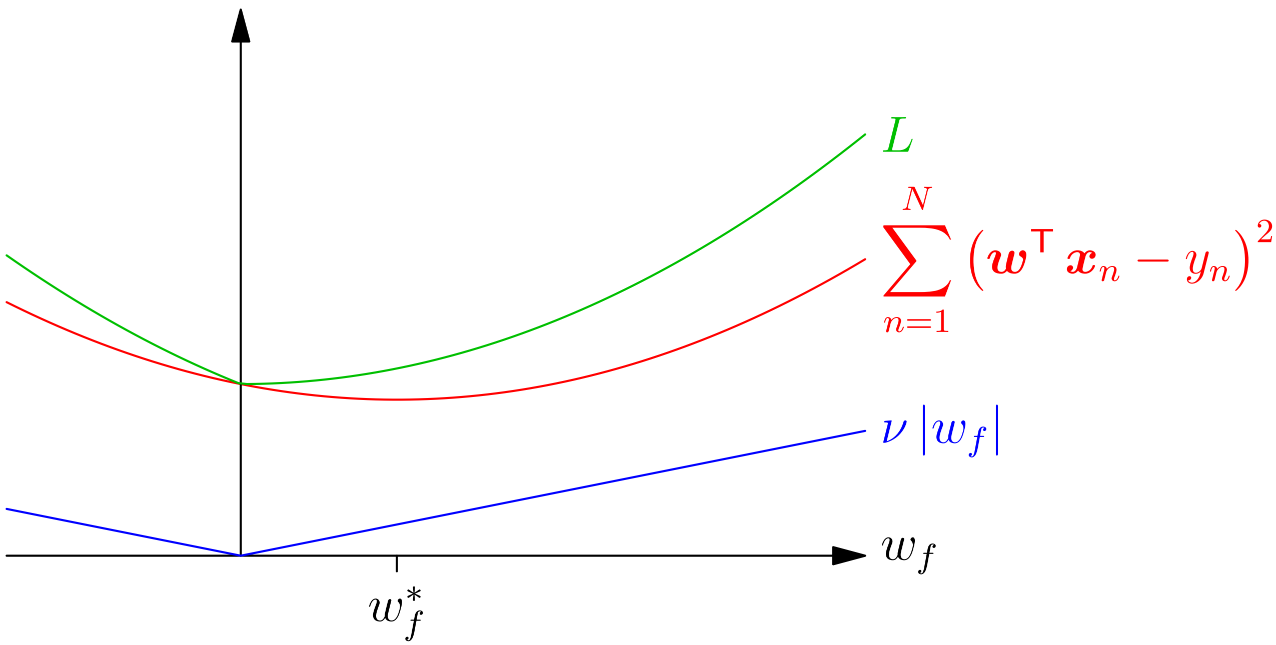

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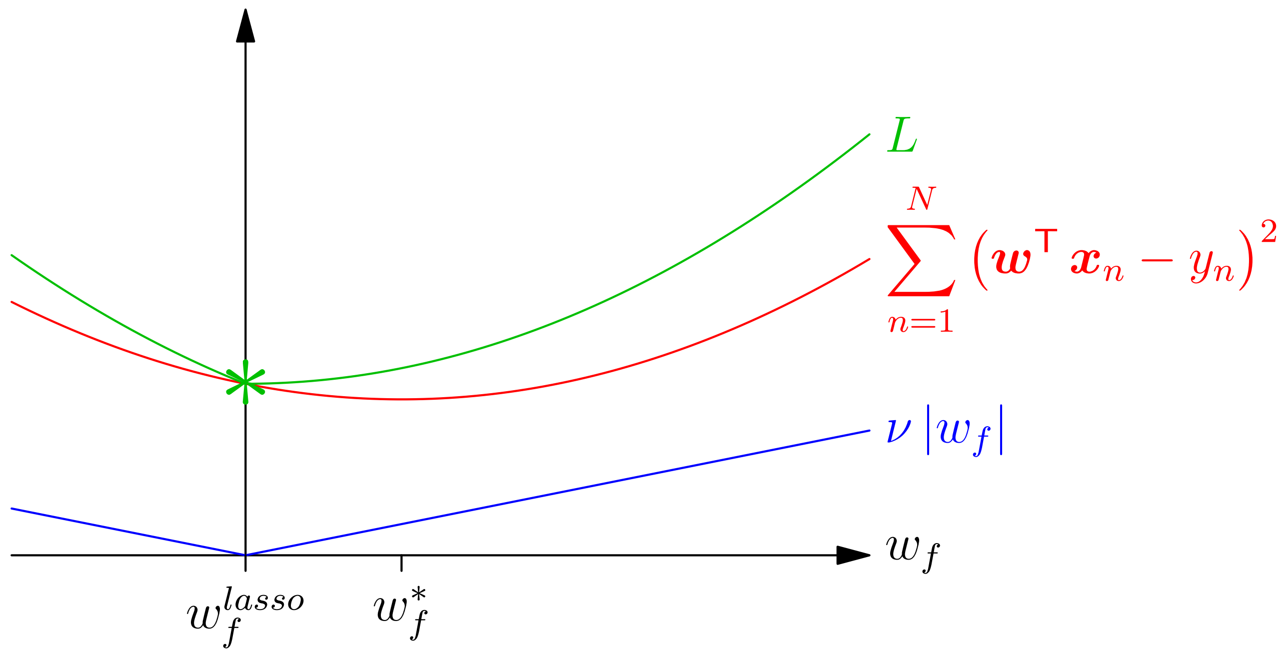

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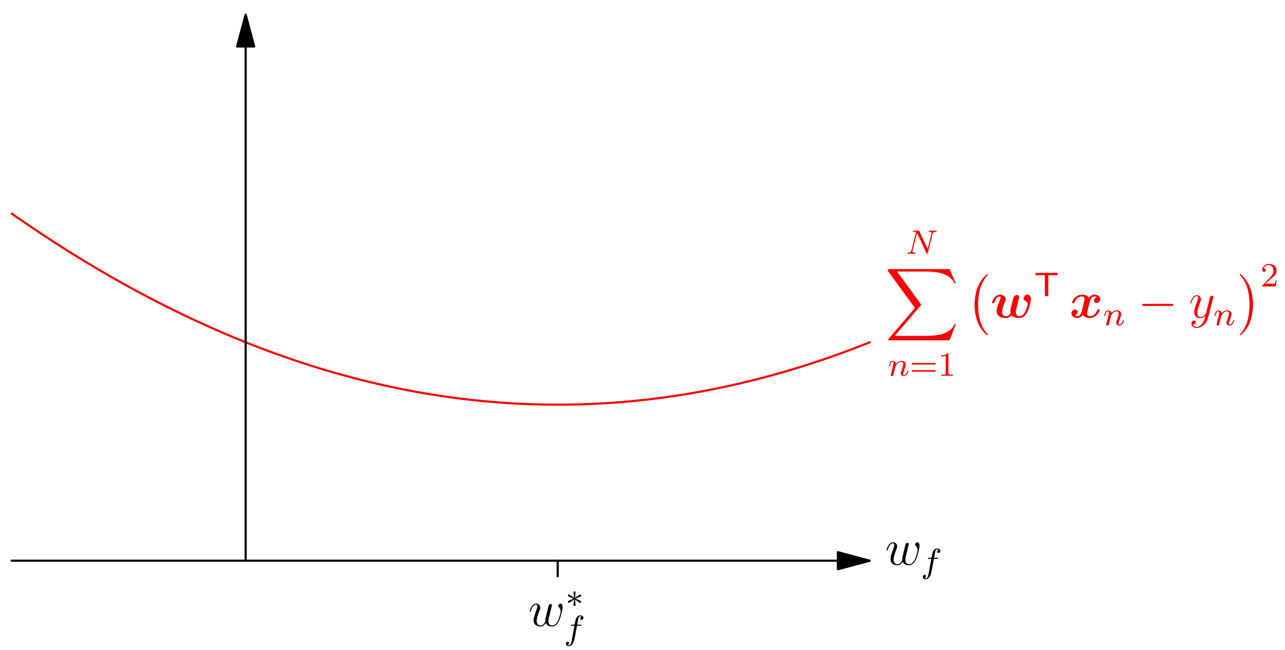

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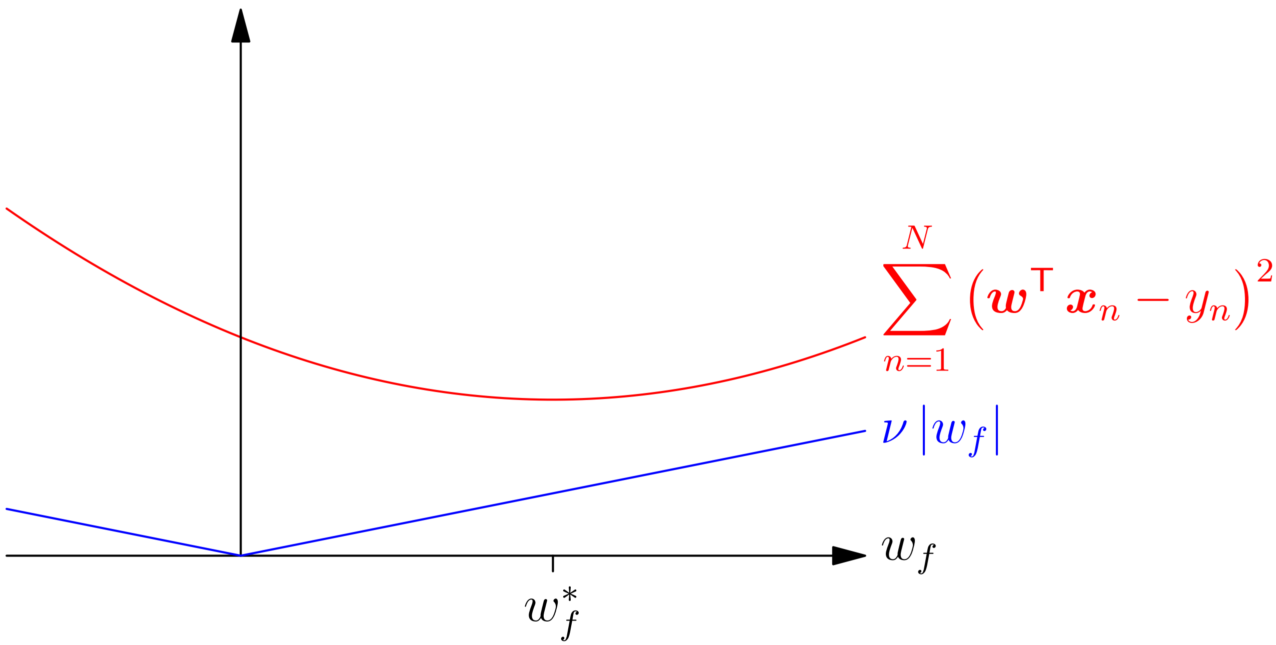

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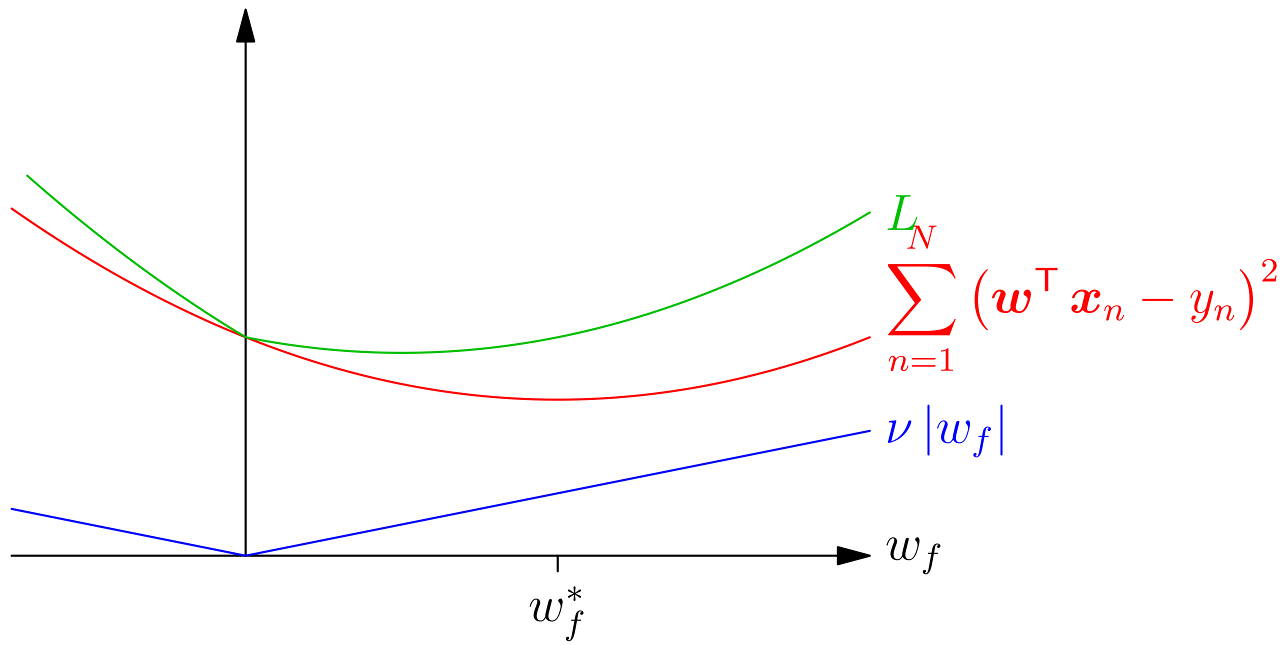

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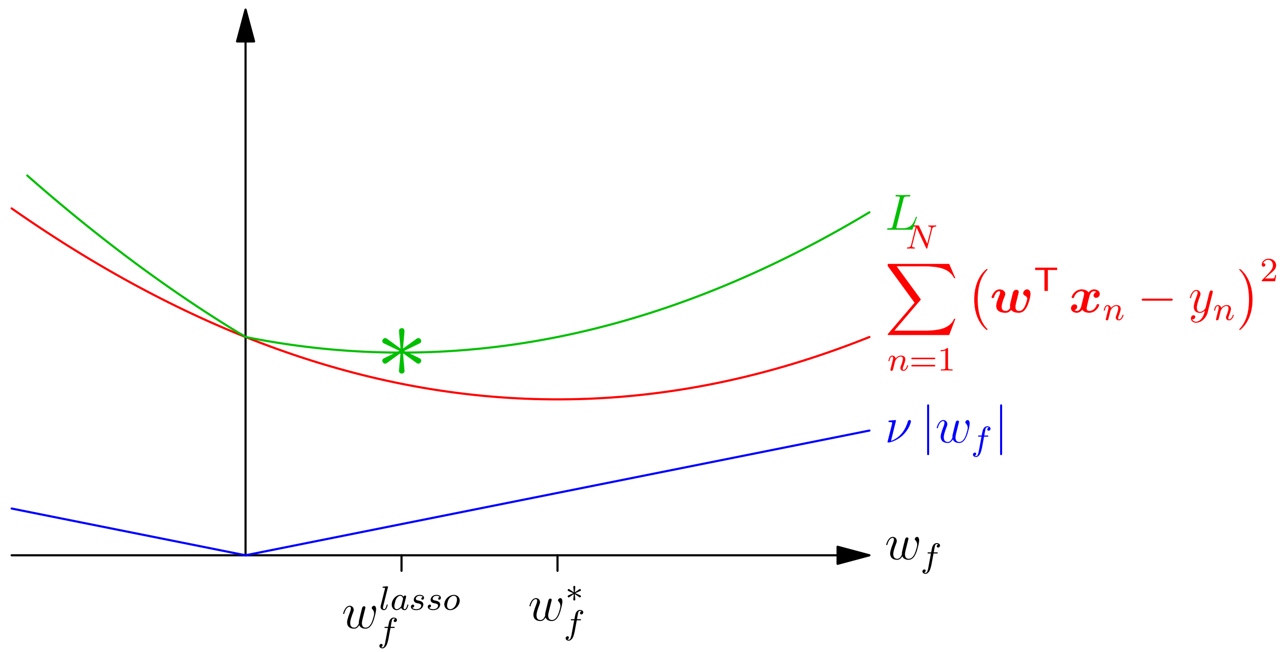

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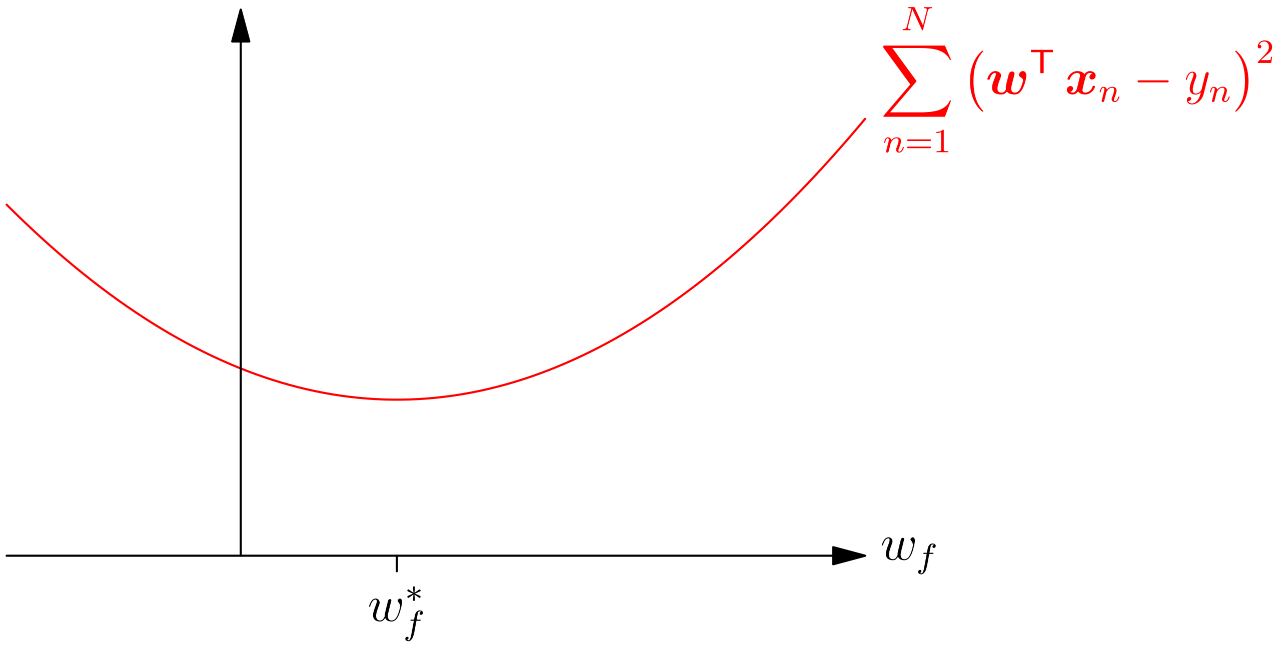

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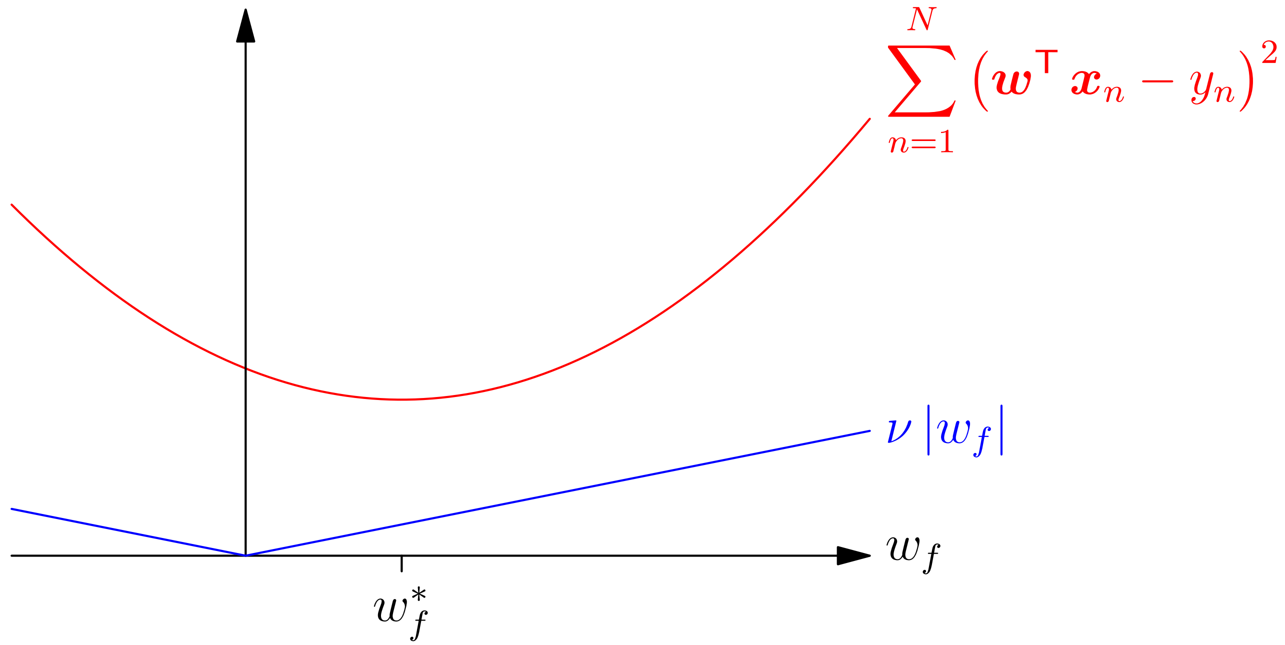

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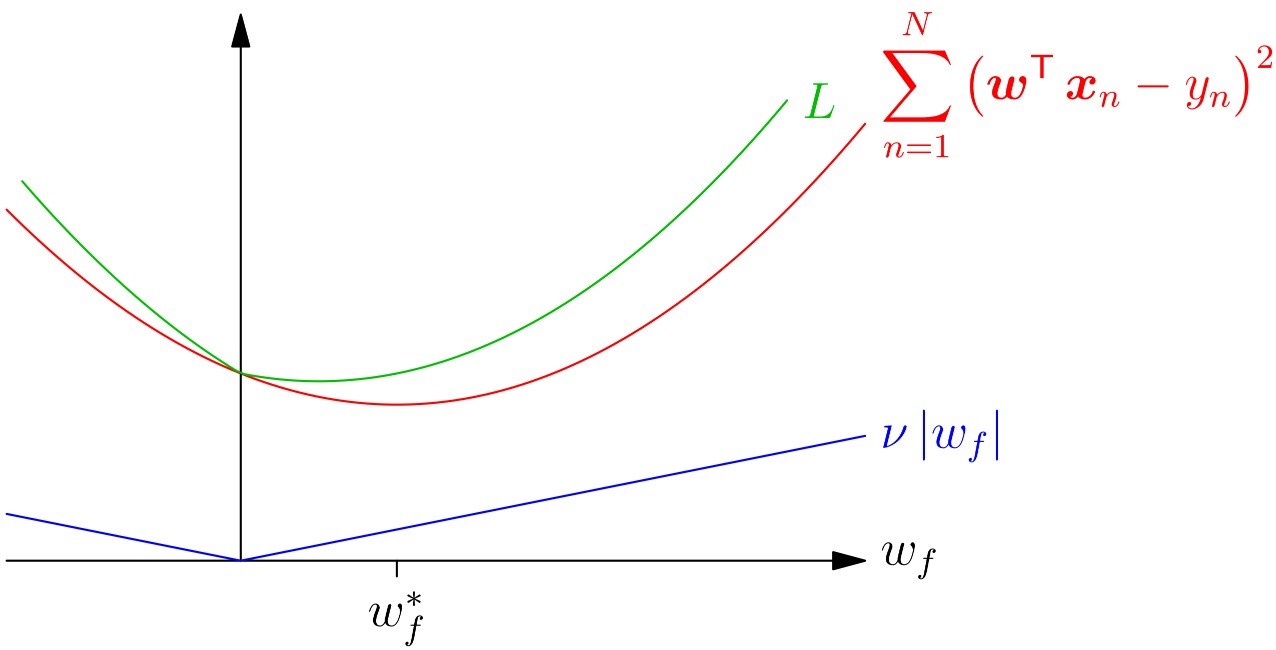

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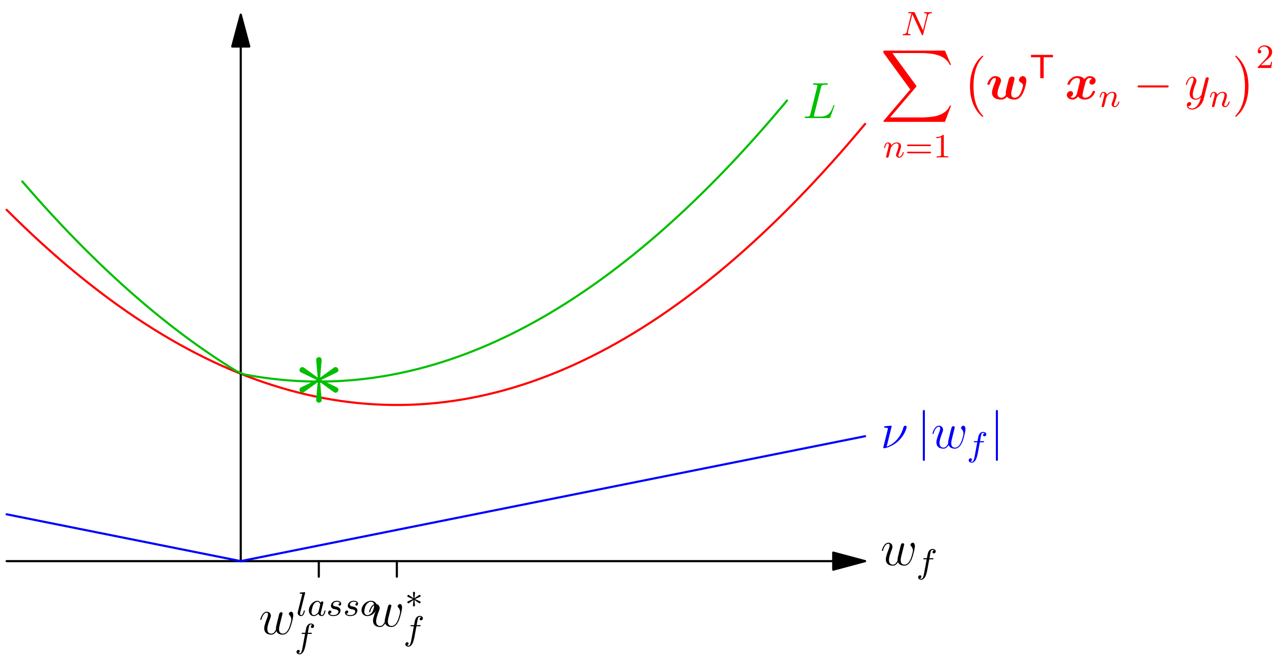

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- Some deep learning architectures do subtle averaging
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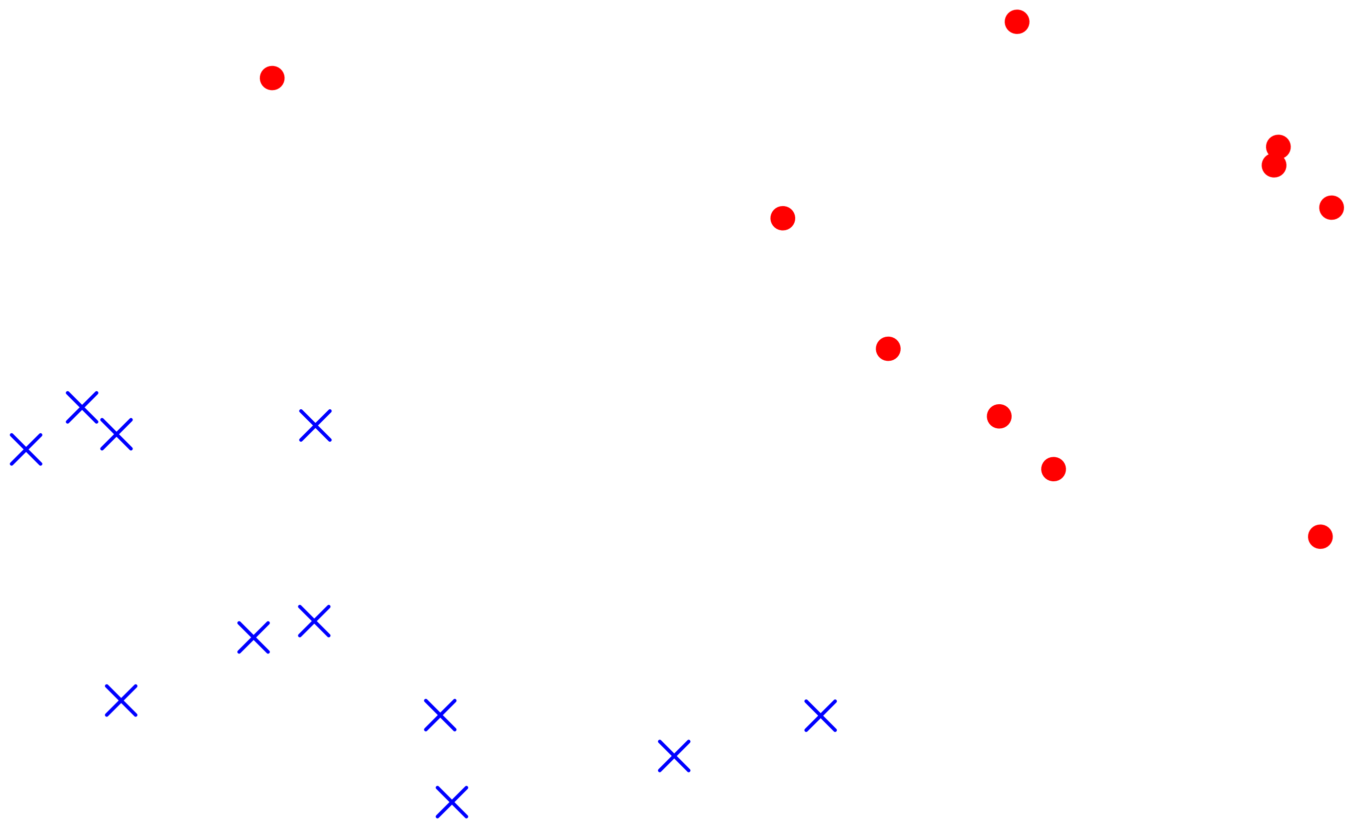

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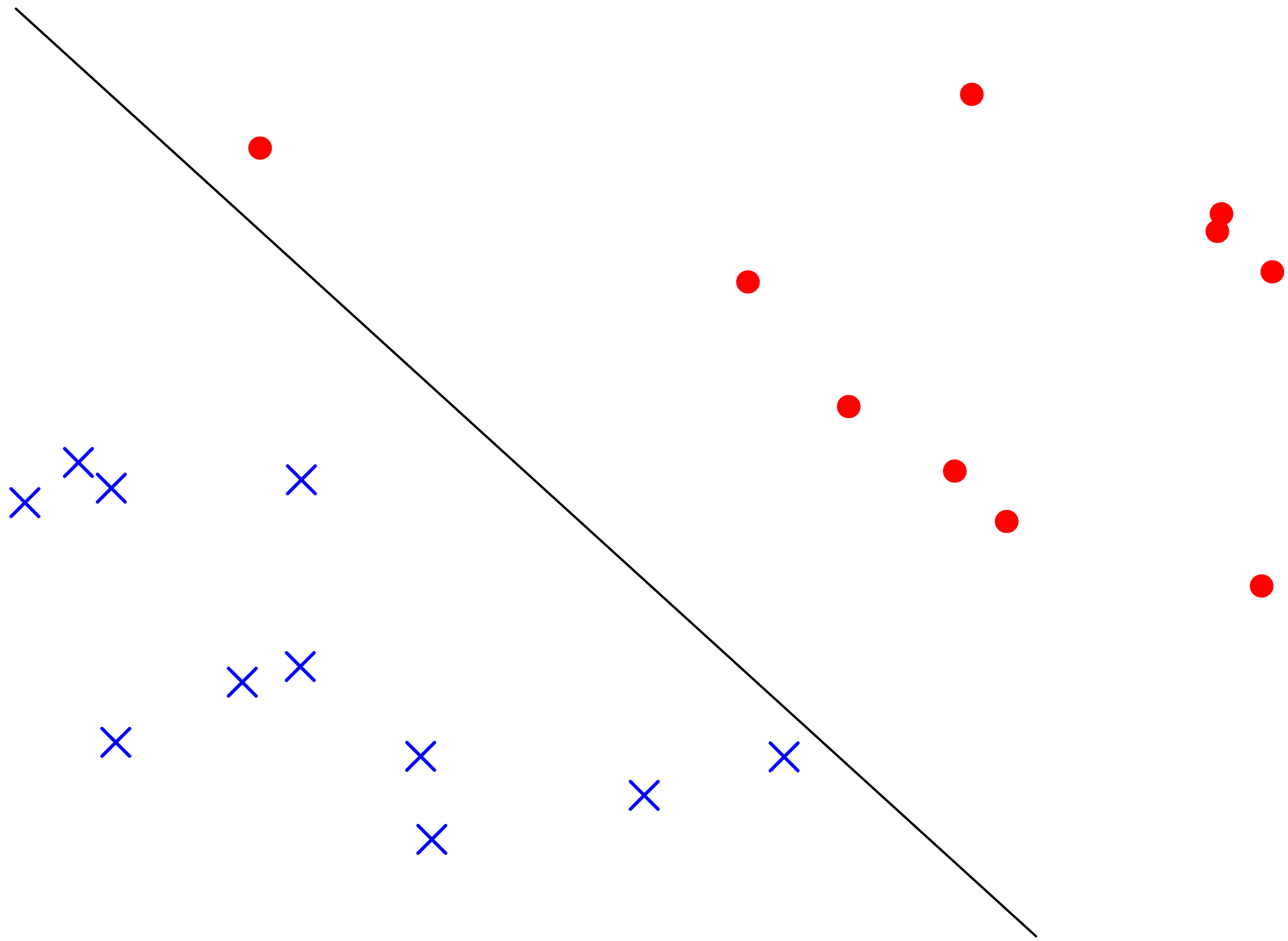

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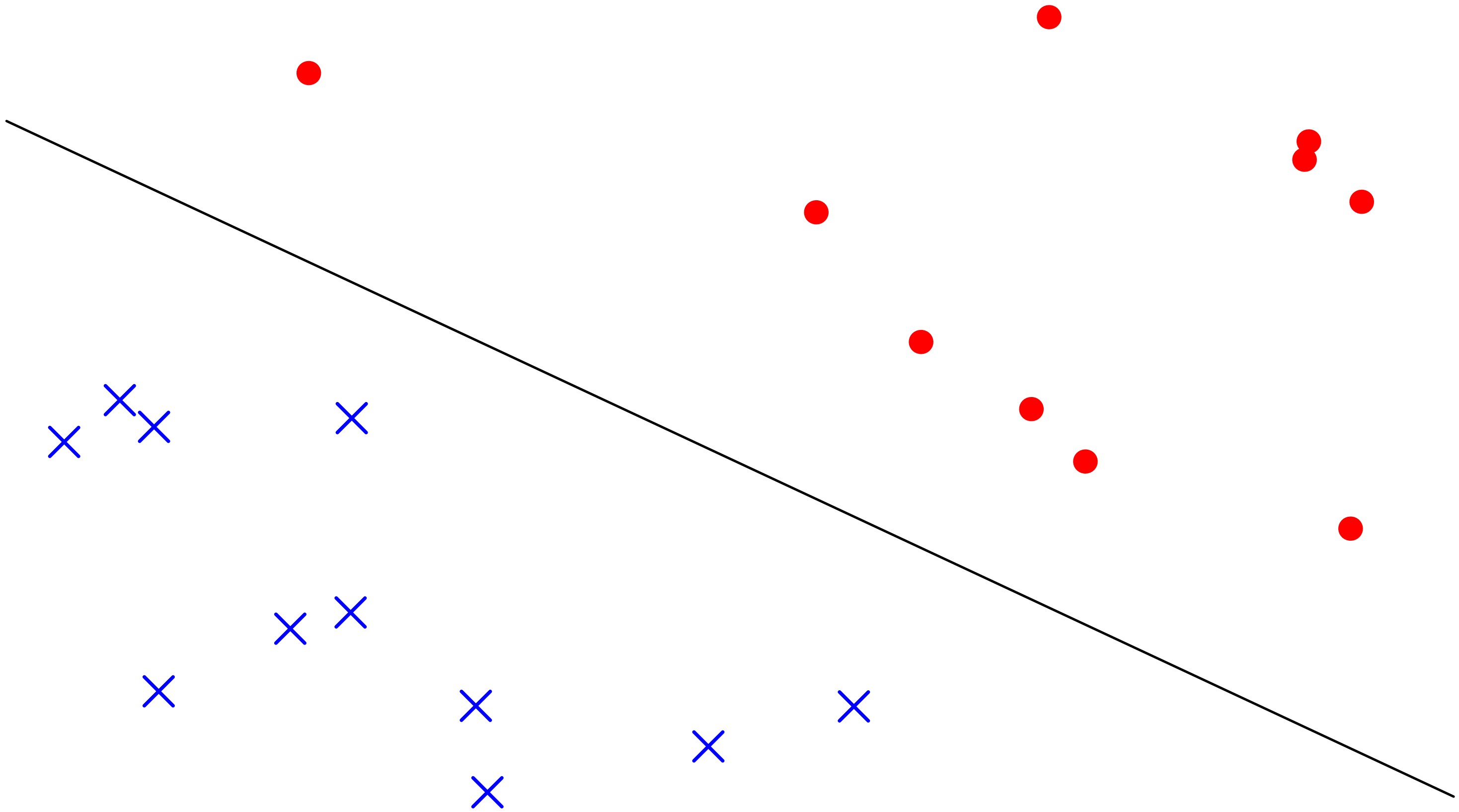

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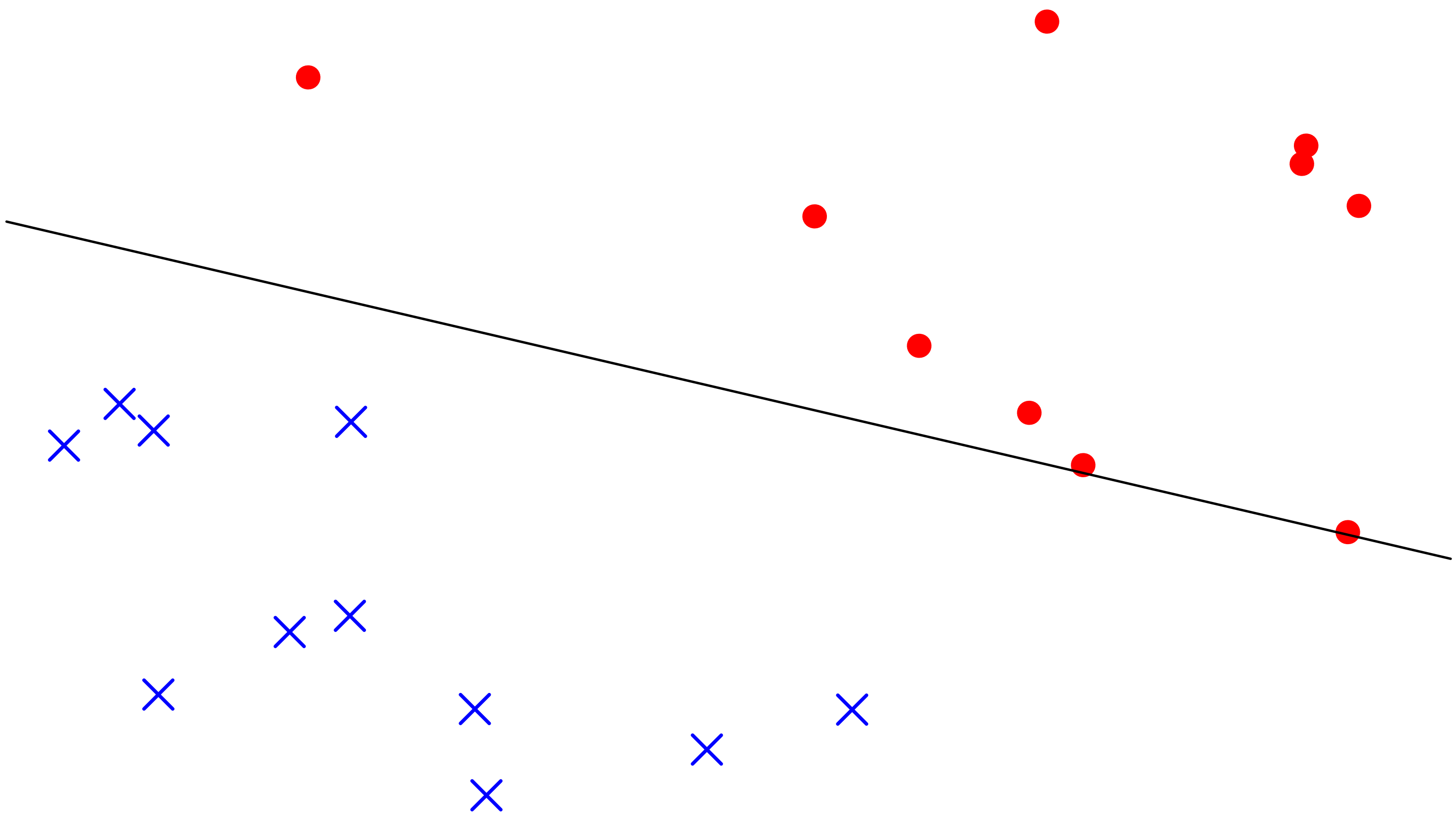

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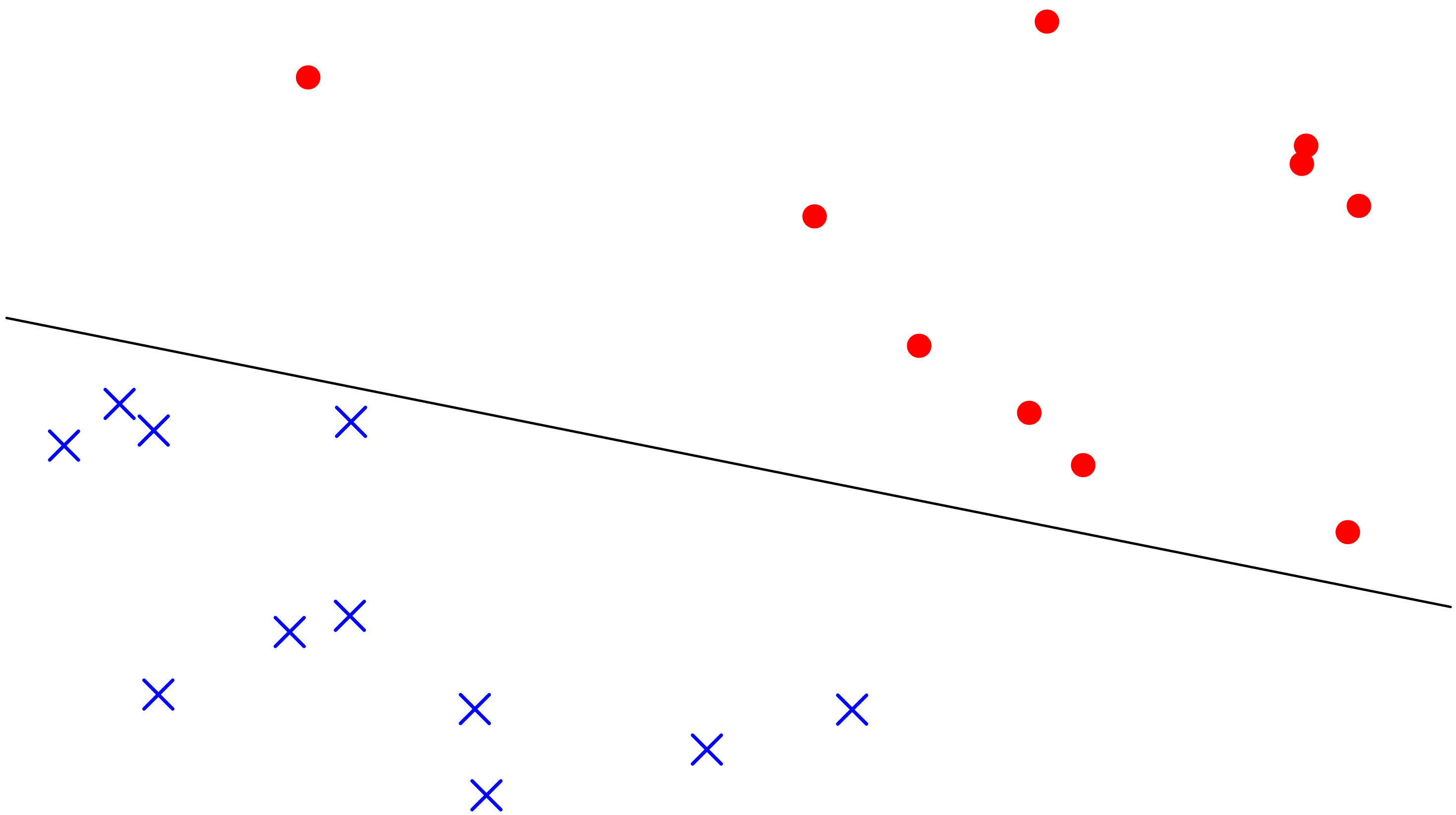

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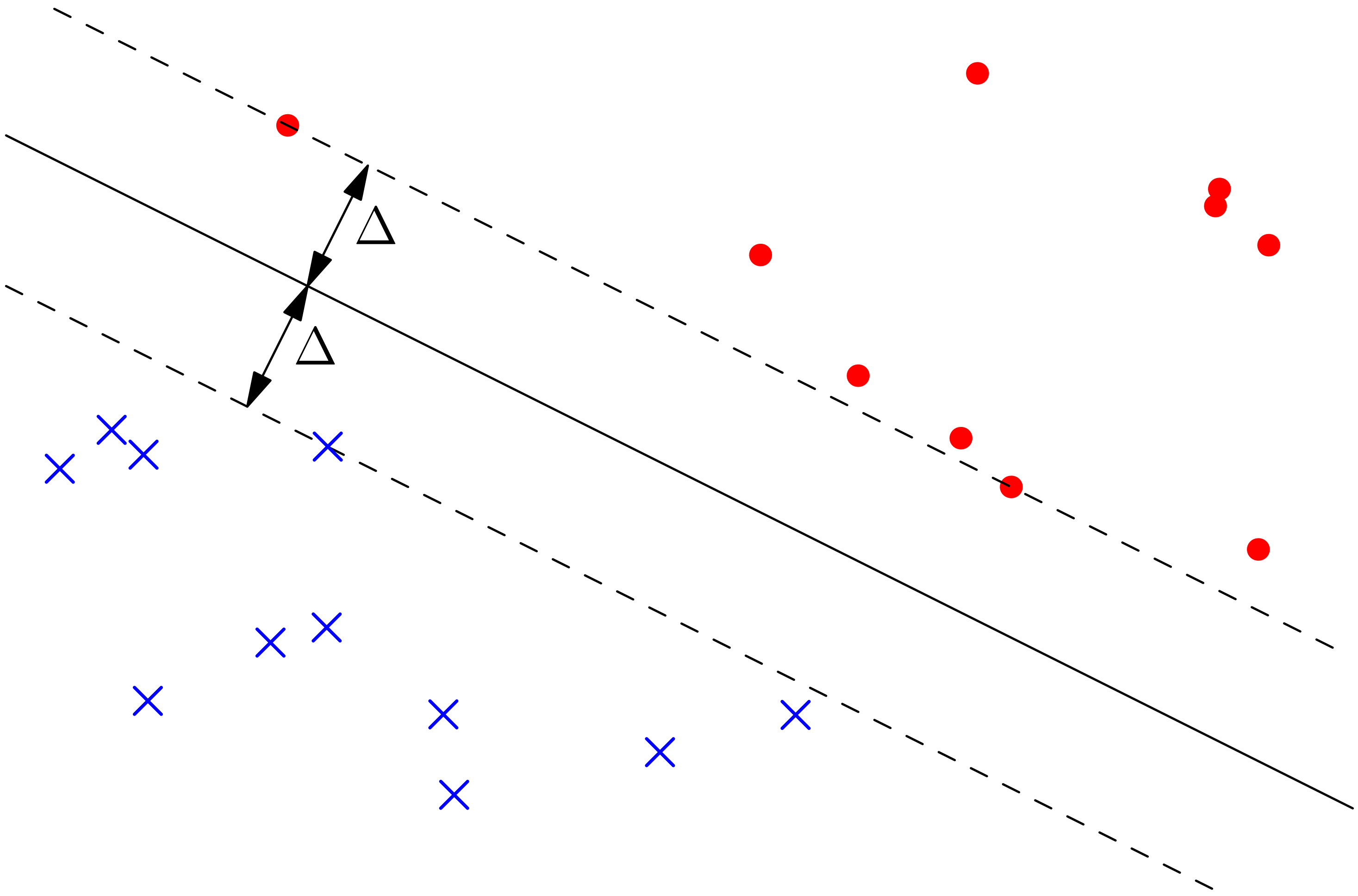

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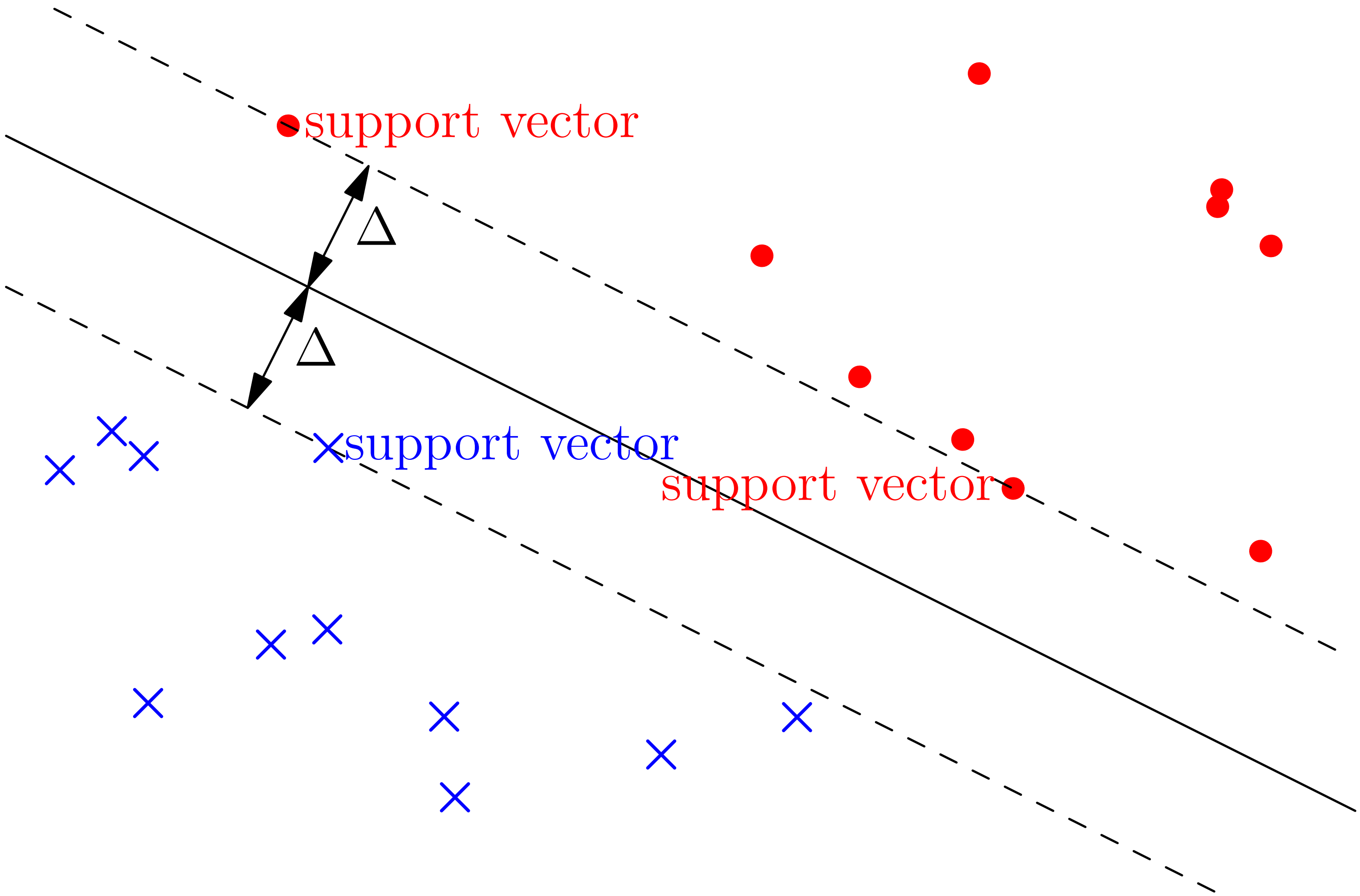

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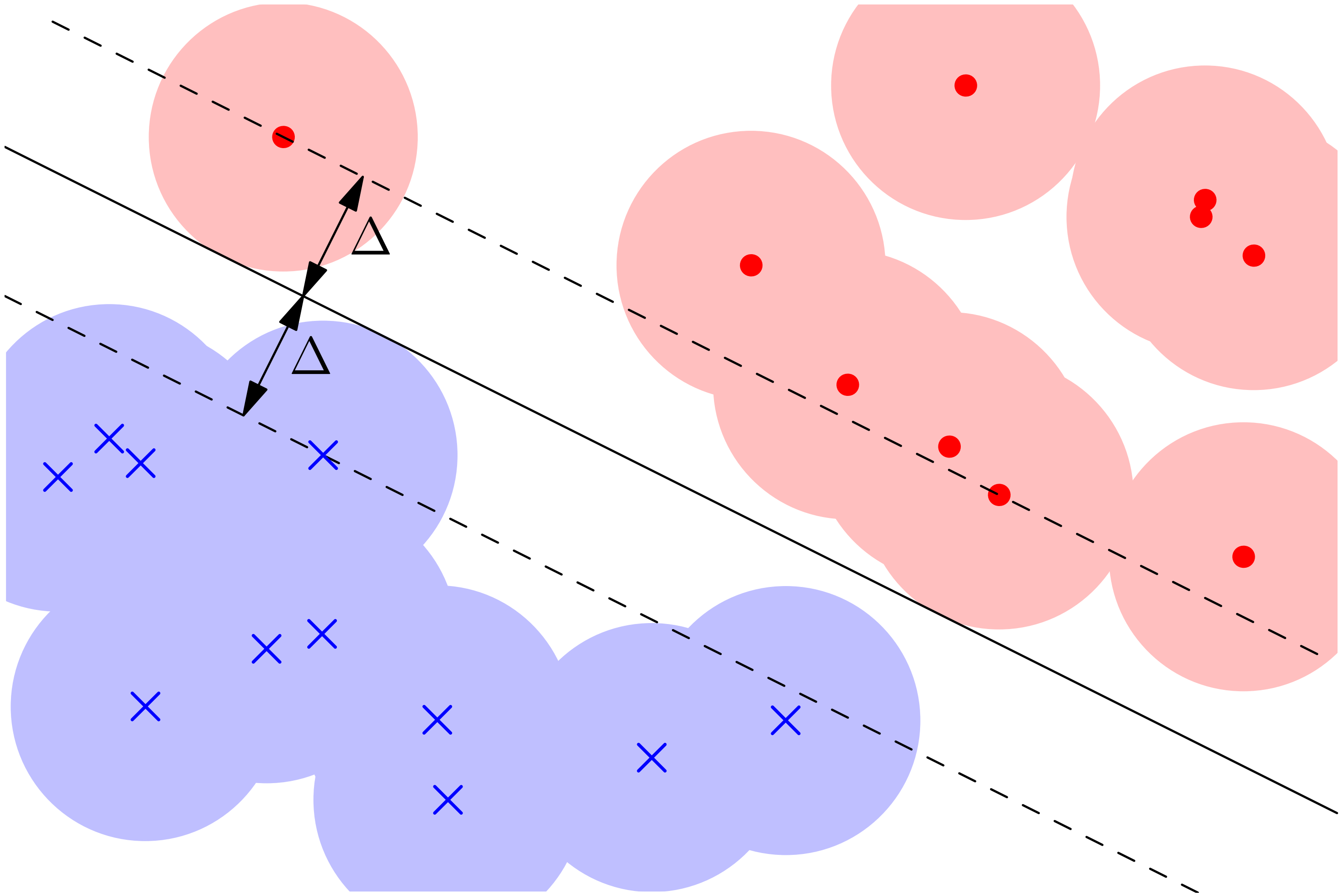

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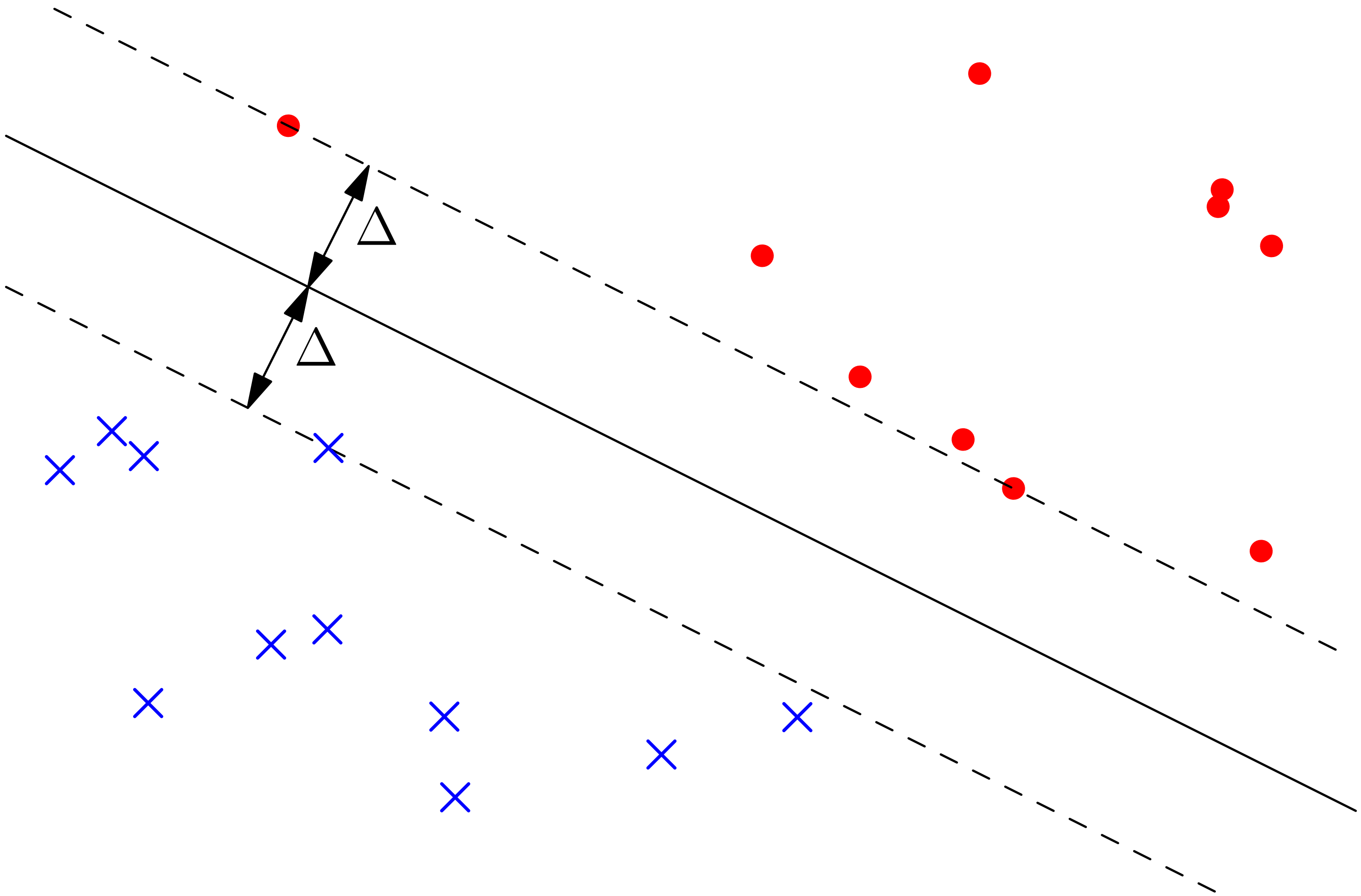

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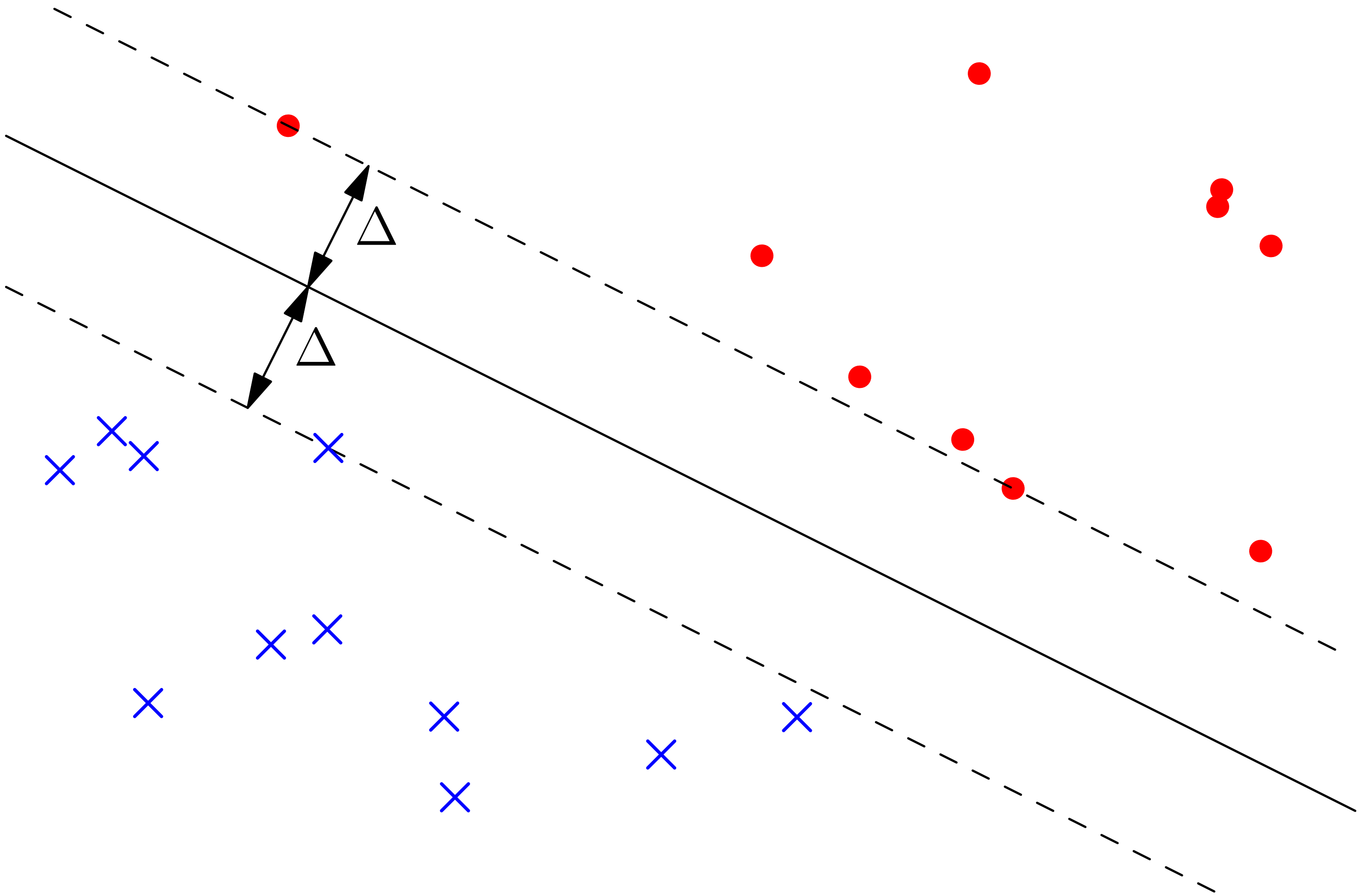


- SVMs choose the machine with the biggest margins

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- But you still need to normalise the features
- You also need to tune its hyper-parameters ($C$ and sometimes $\gamma$)

# Lessons

- Machine learning isn't magic
- It works when the learning machine is well attuned to the problem
- Sometimes you can help by preprocessing your data
- Sometimes there is a regularisation term that helps select a simpler machine
- Most machines have hyper-parameter that you tune to match the machine to the data
- Really clever machines try to do this matching automatically

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