Cambridge AI+

Linear Regression and Logistic Regression

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Outline

Introduction

Linear Regression

Linear Regression with More than One Feature

Solving Linear Regression: Gradient Descent

Logistic Regression

Applications of Regression

Grade Prediction: Predict exam score of a student based on some data

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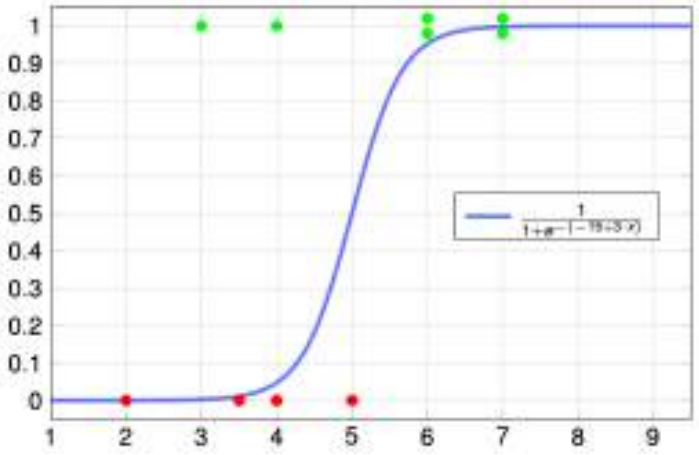

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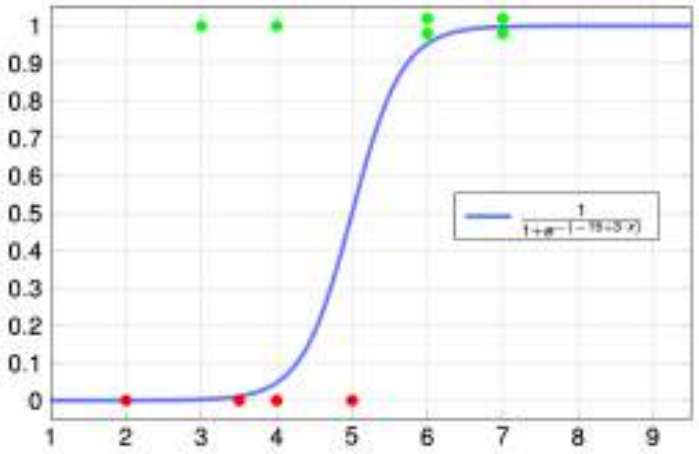

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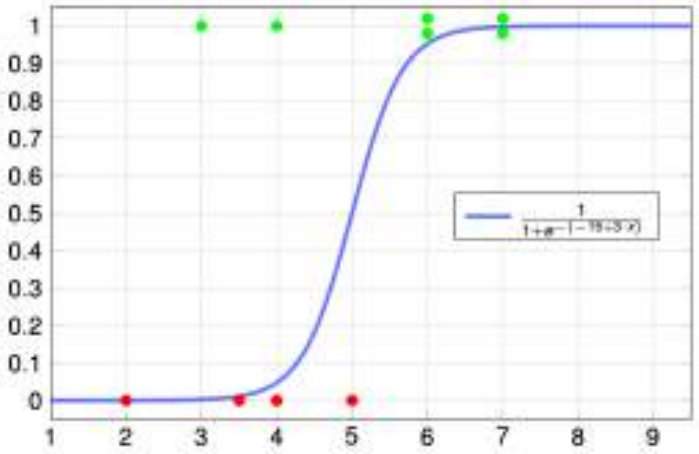

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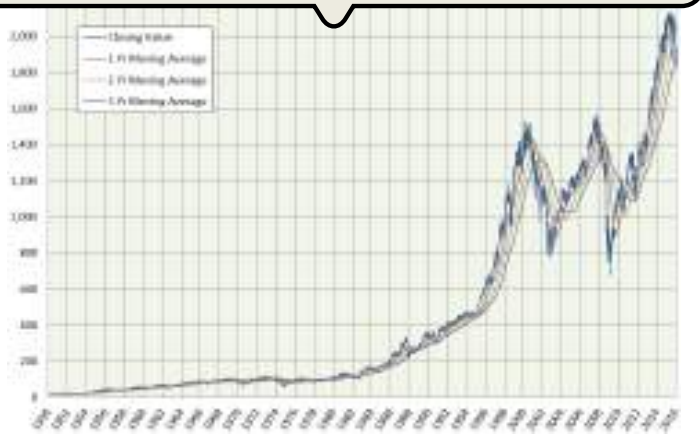

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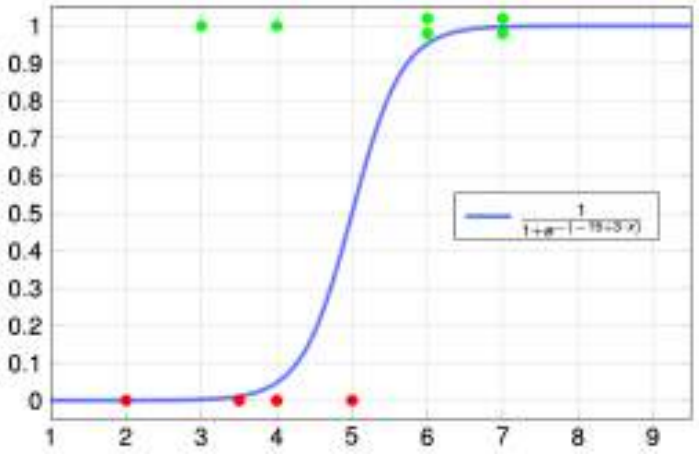

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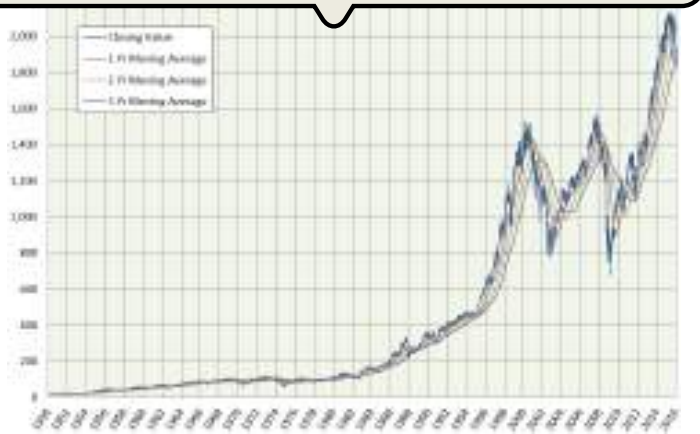

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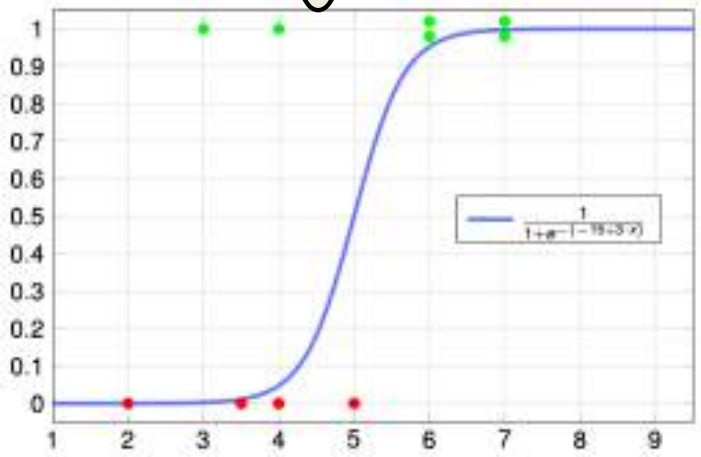
Logistic Regression (next lecture)



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Exercise Question 2

Consider the following data set, which records several phone calls of clients to an e-commerce company.

Client	Call Length	Bought Items
1	13	2
2	17	1
3	32	2
4	36	4
5	45	4
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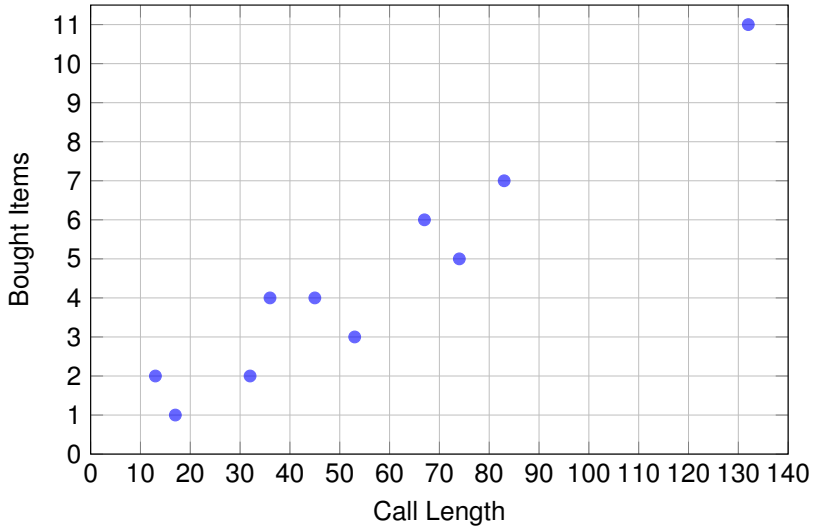

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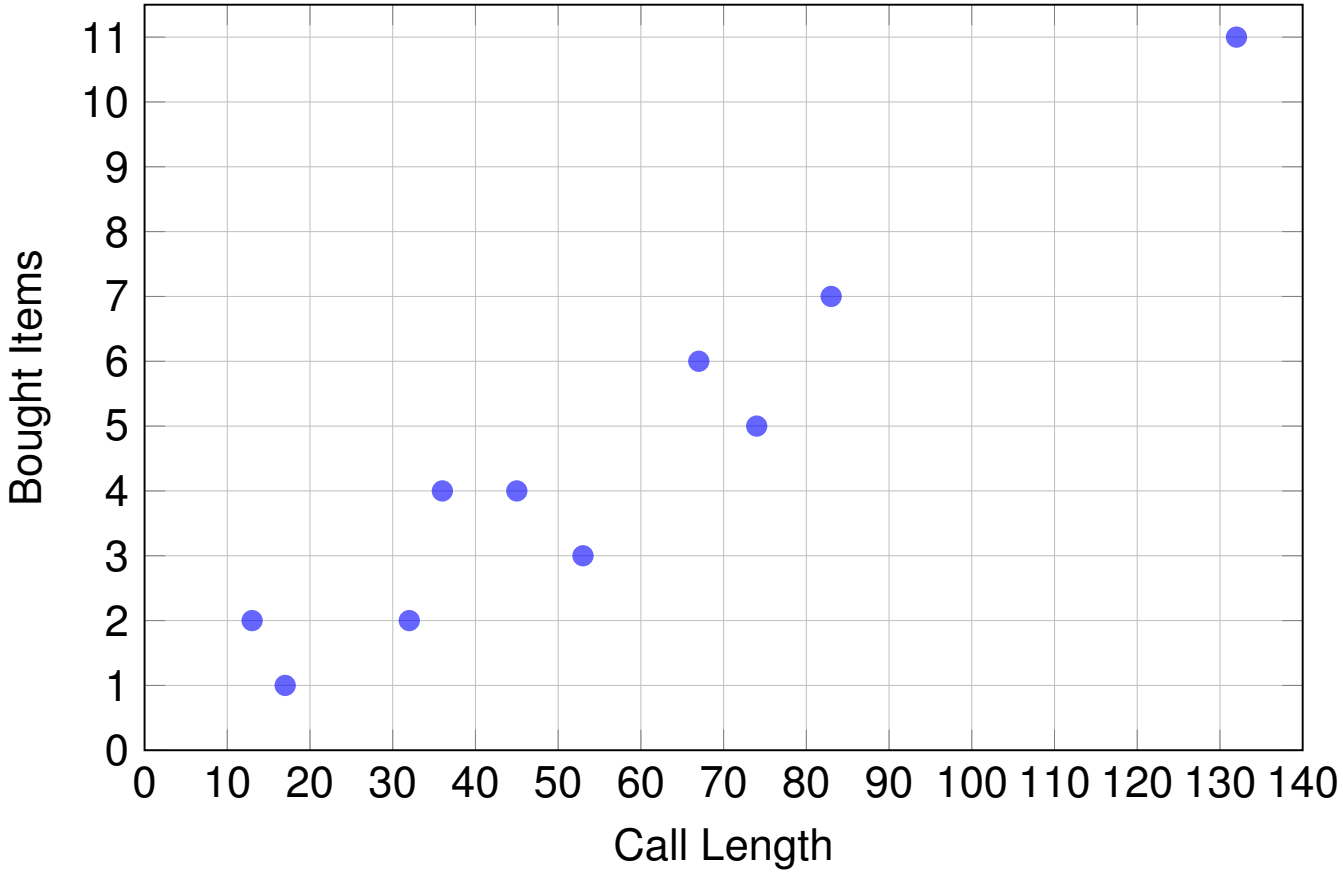

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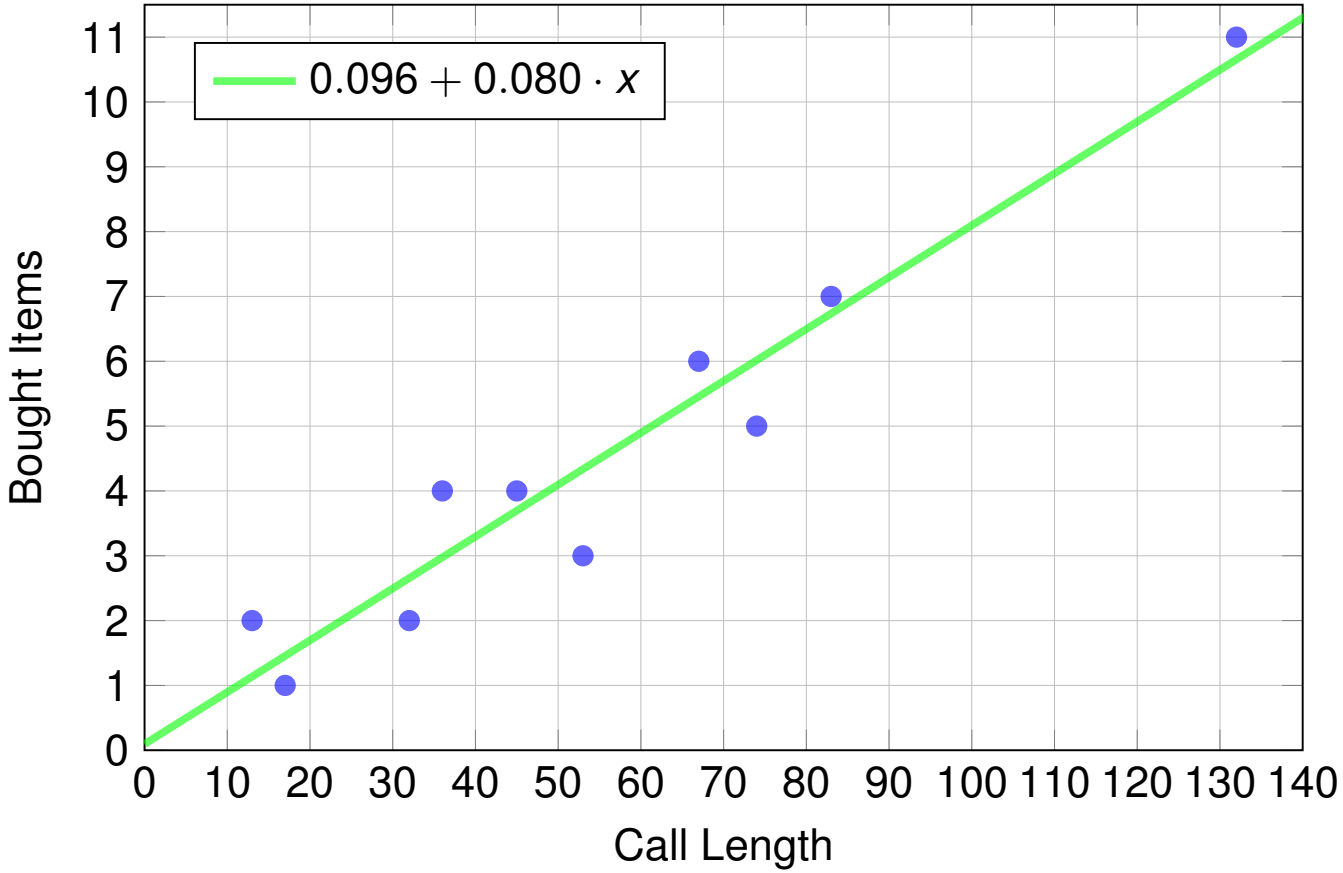

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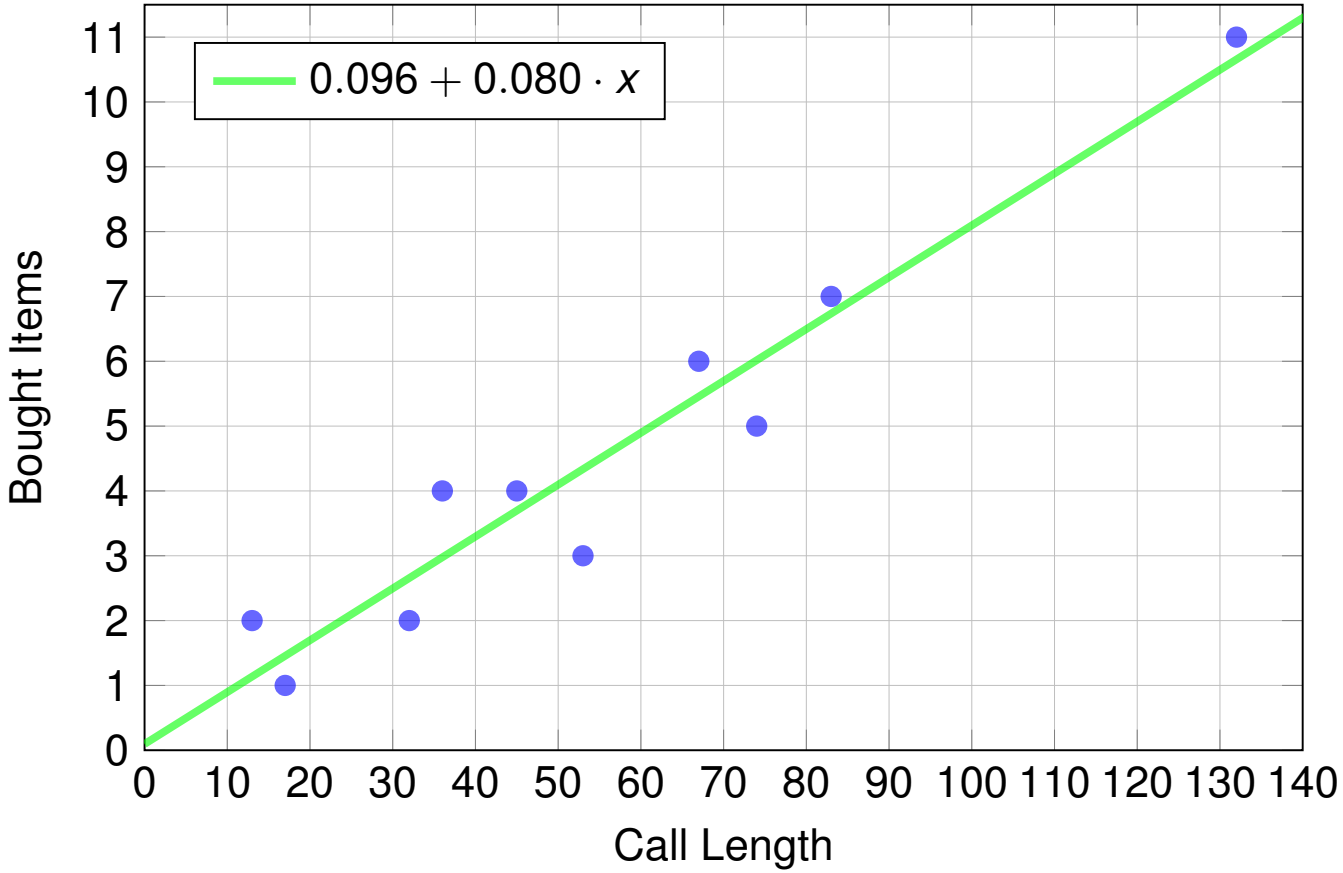

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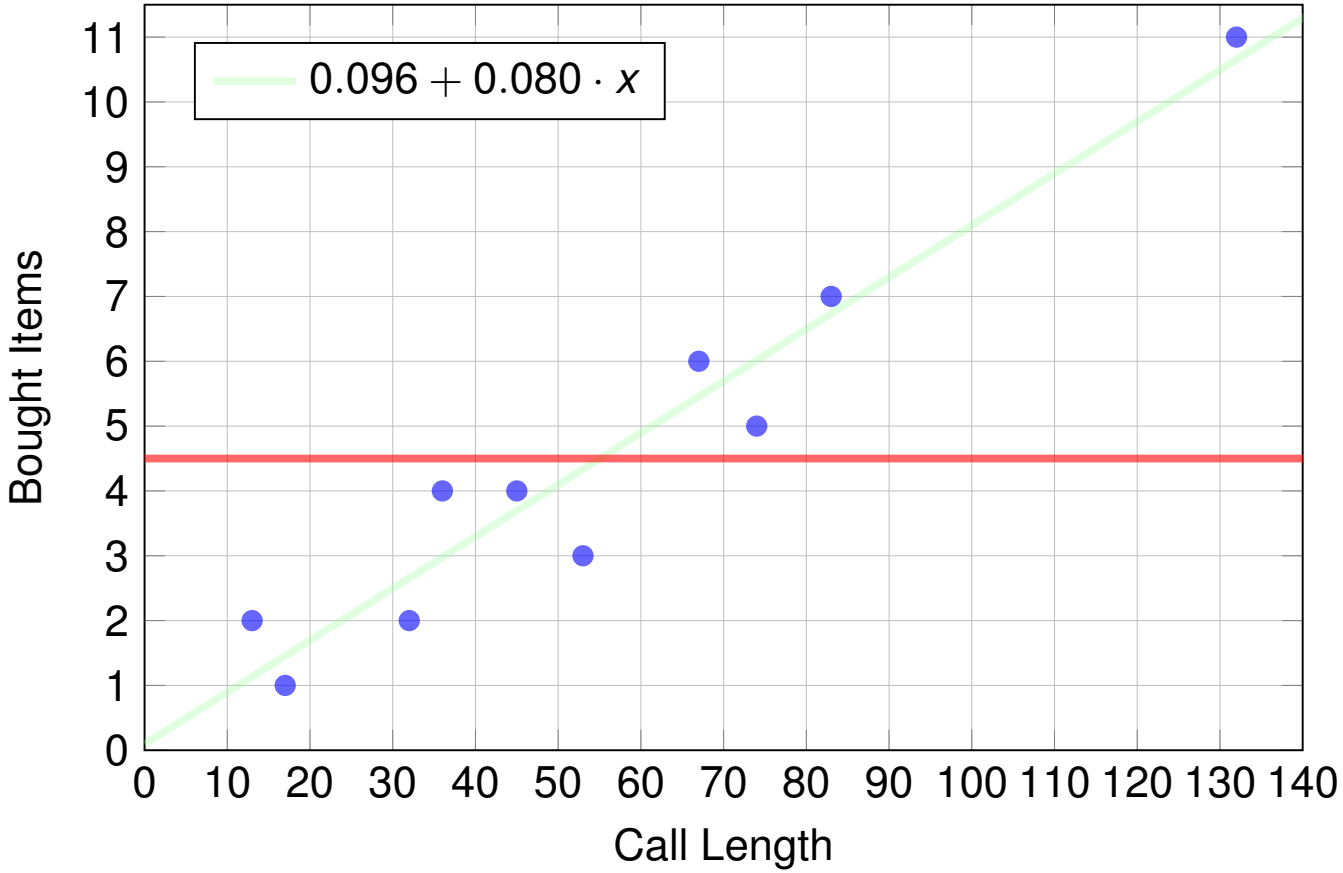

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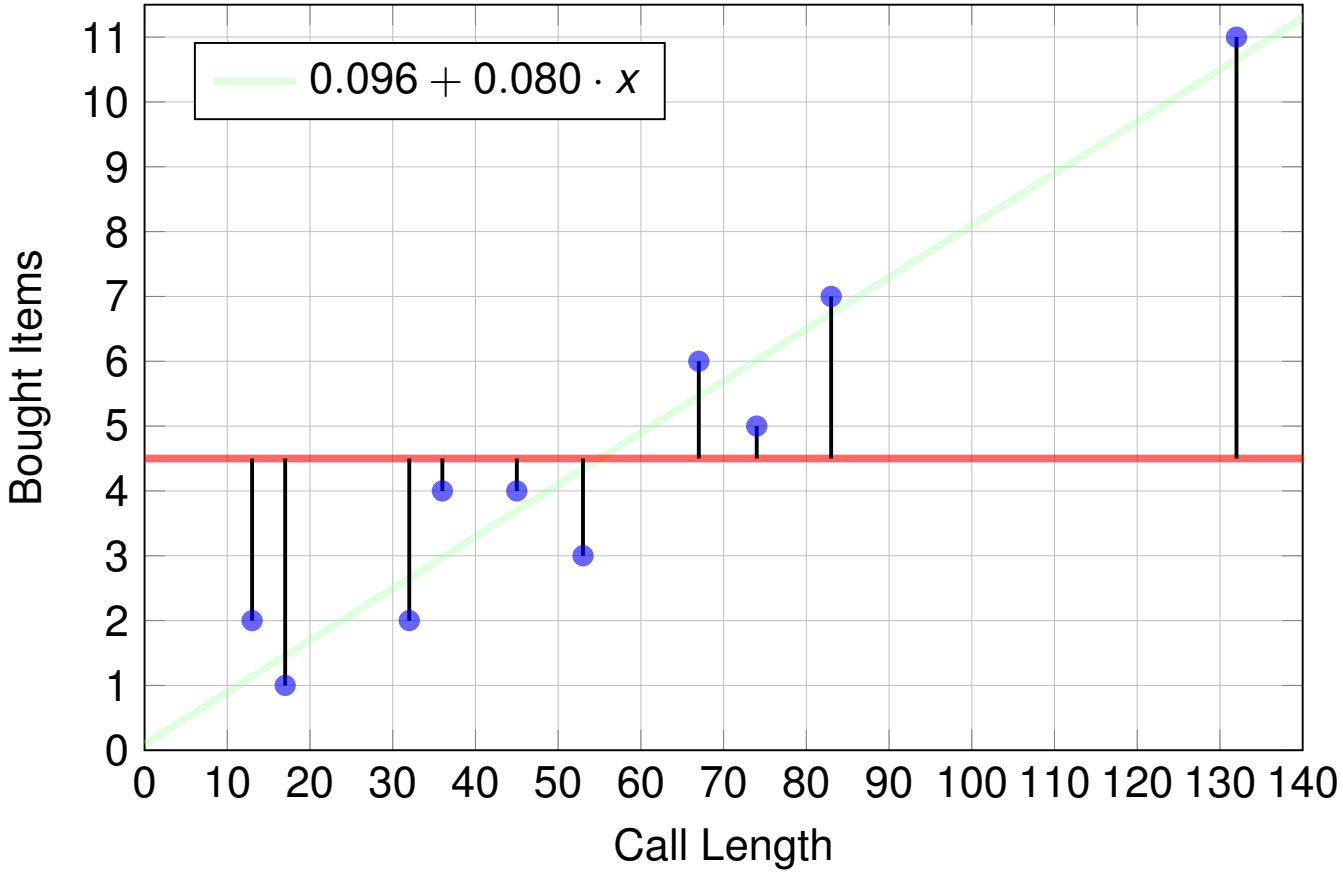

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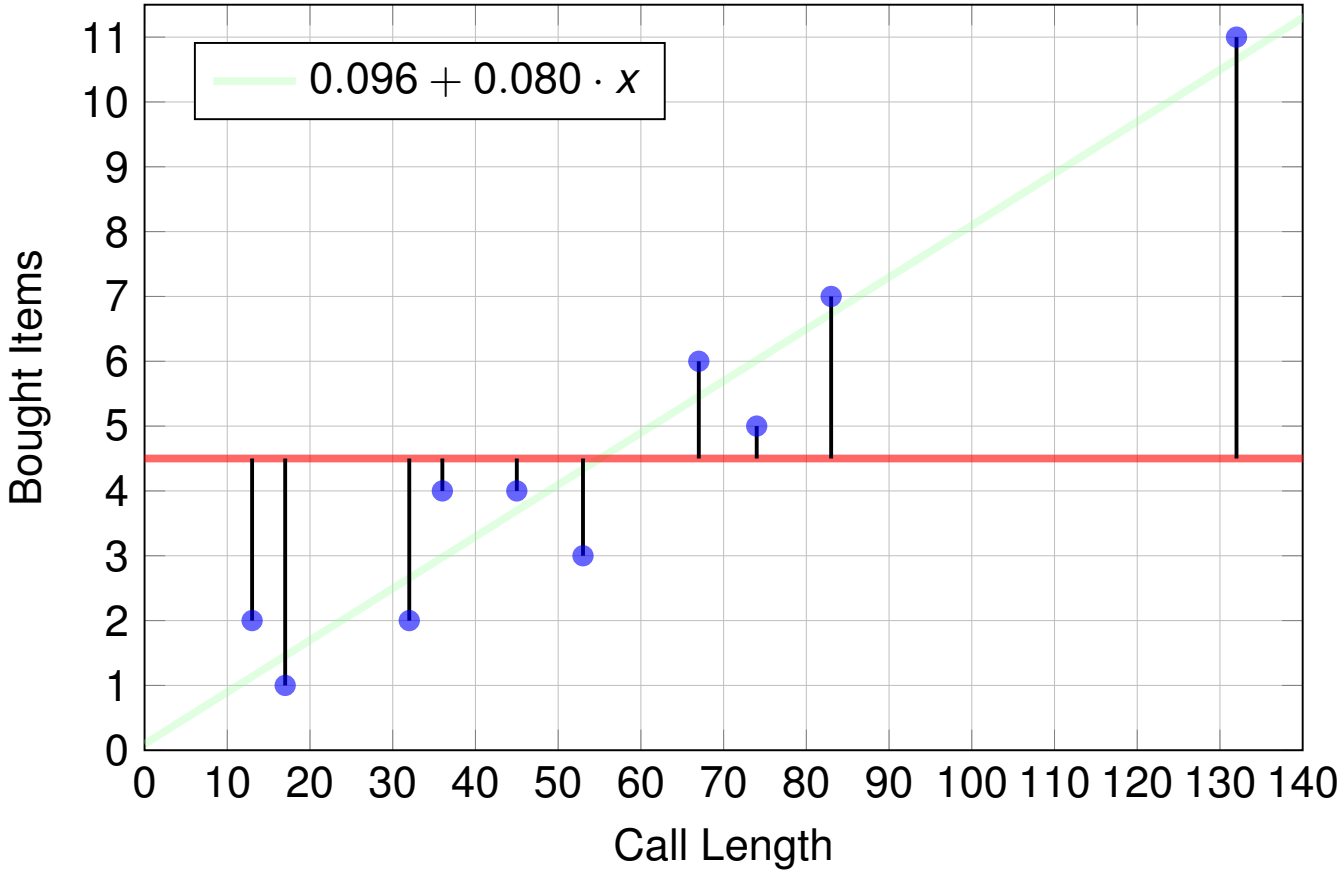

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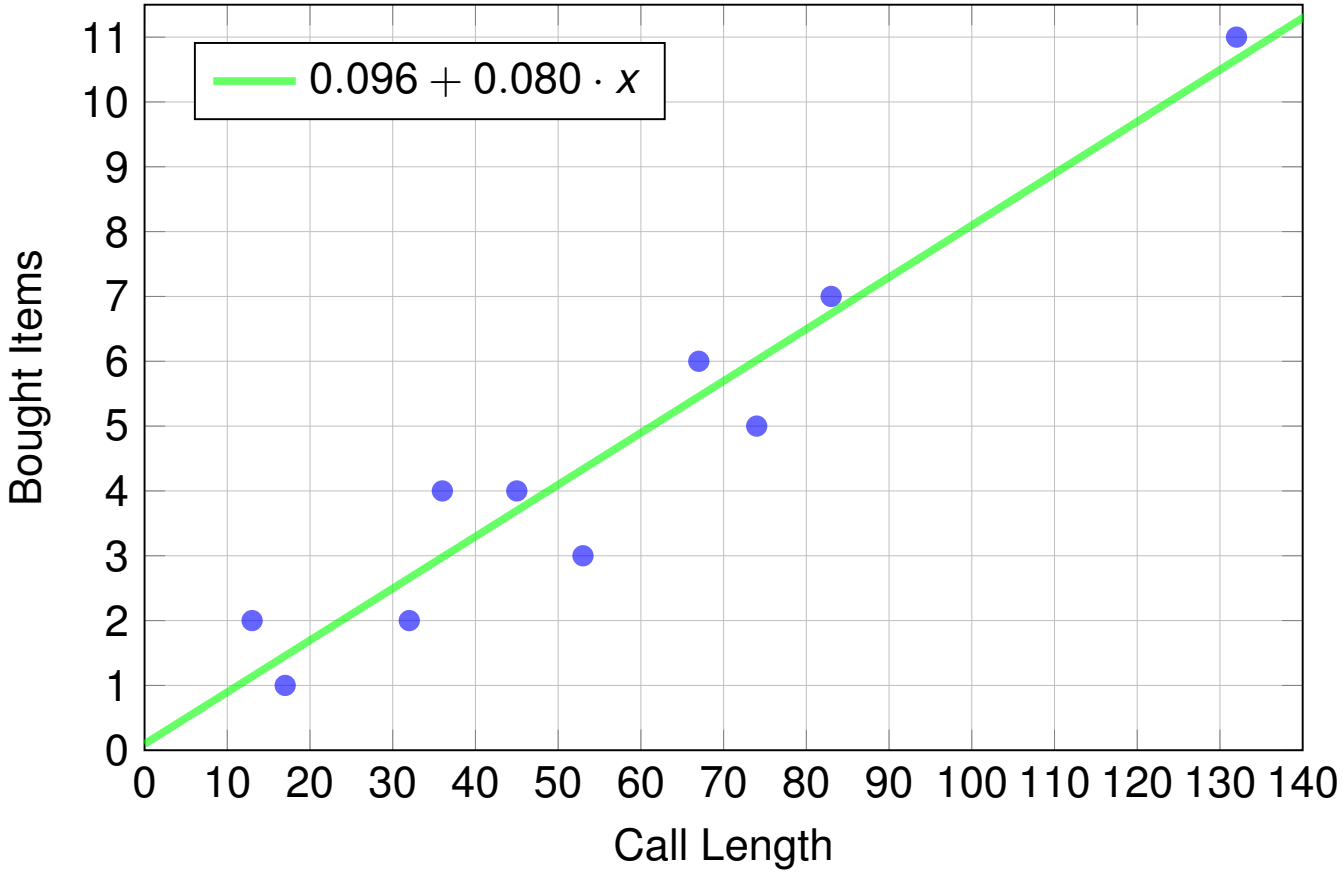

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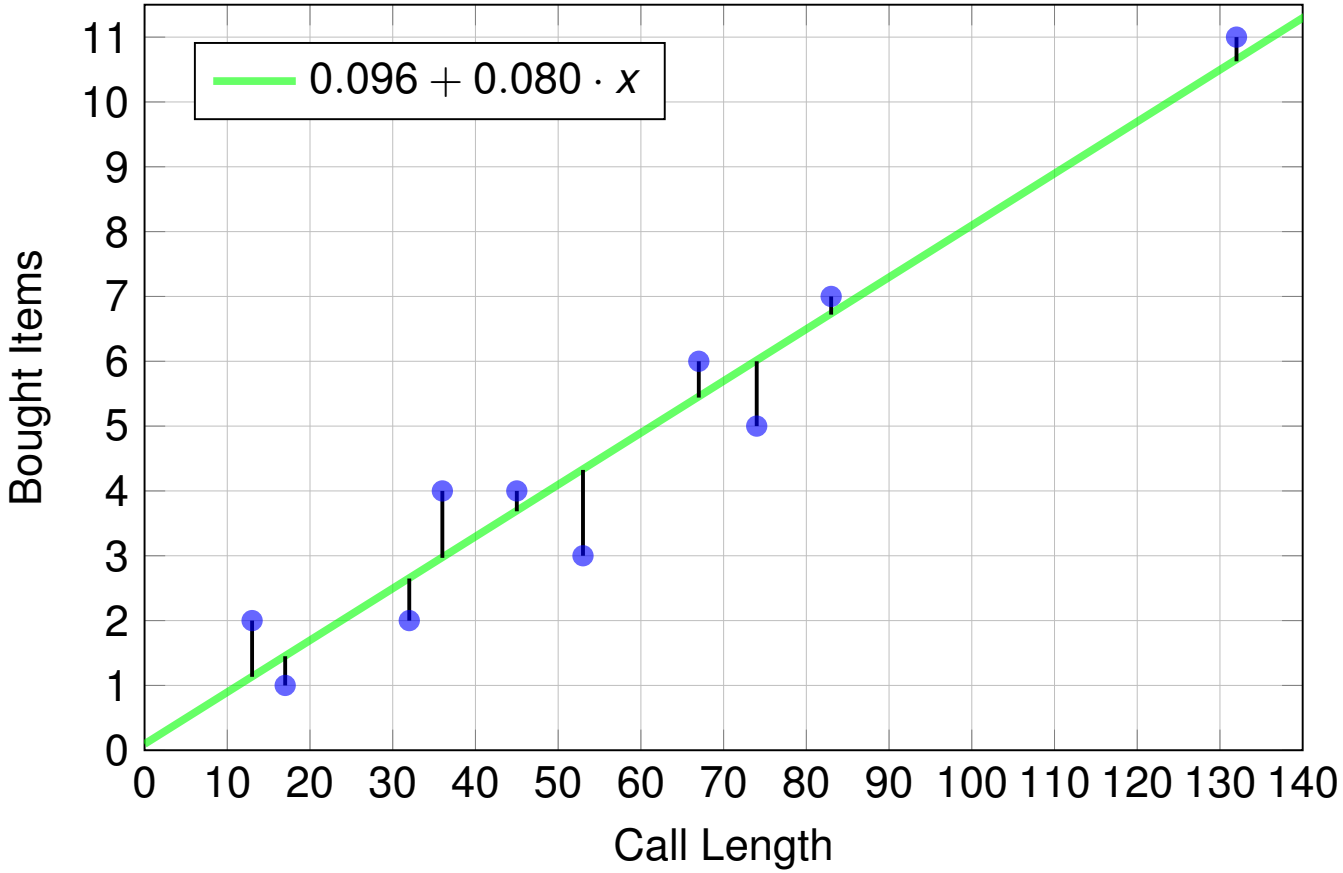

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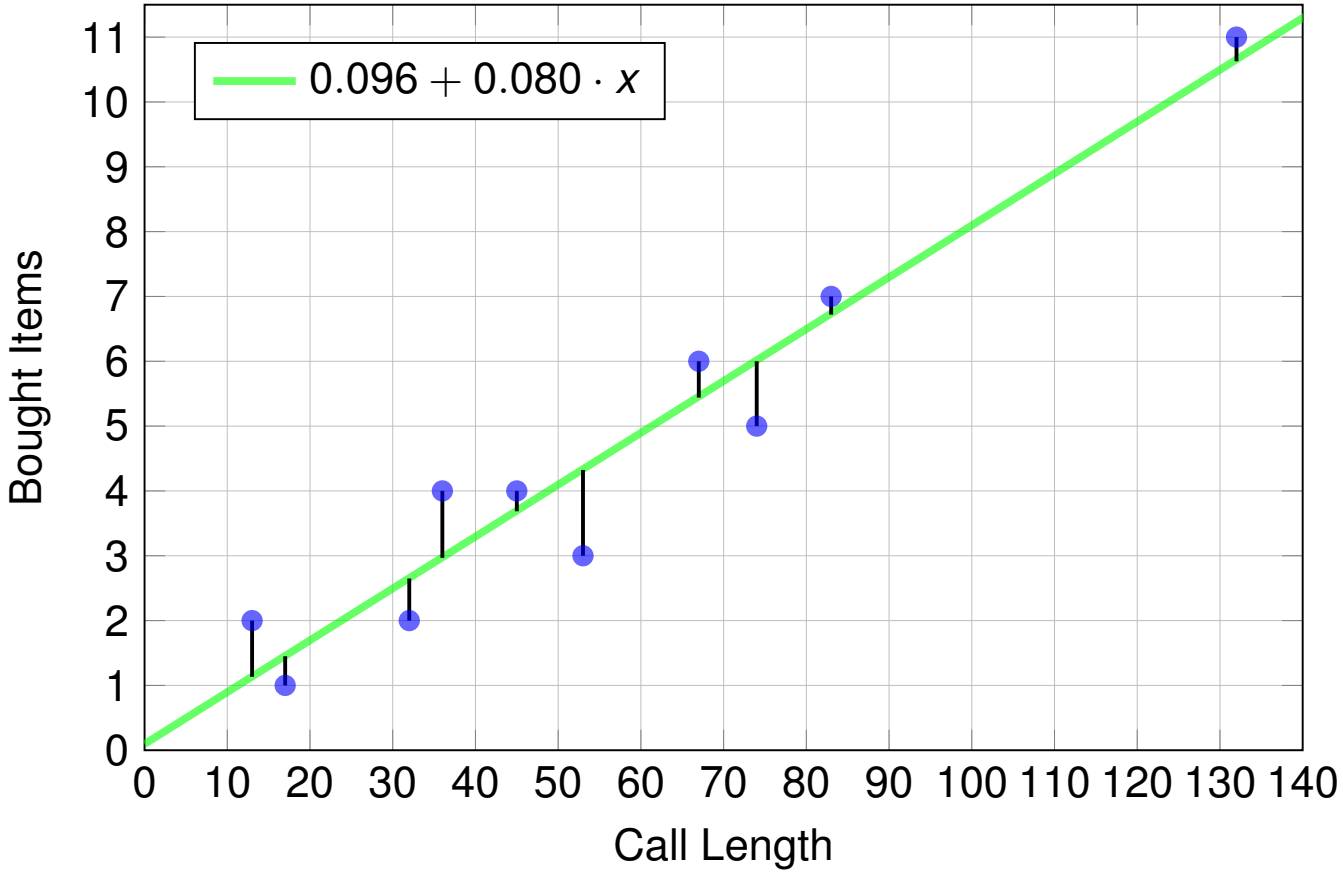

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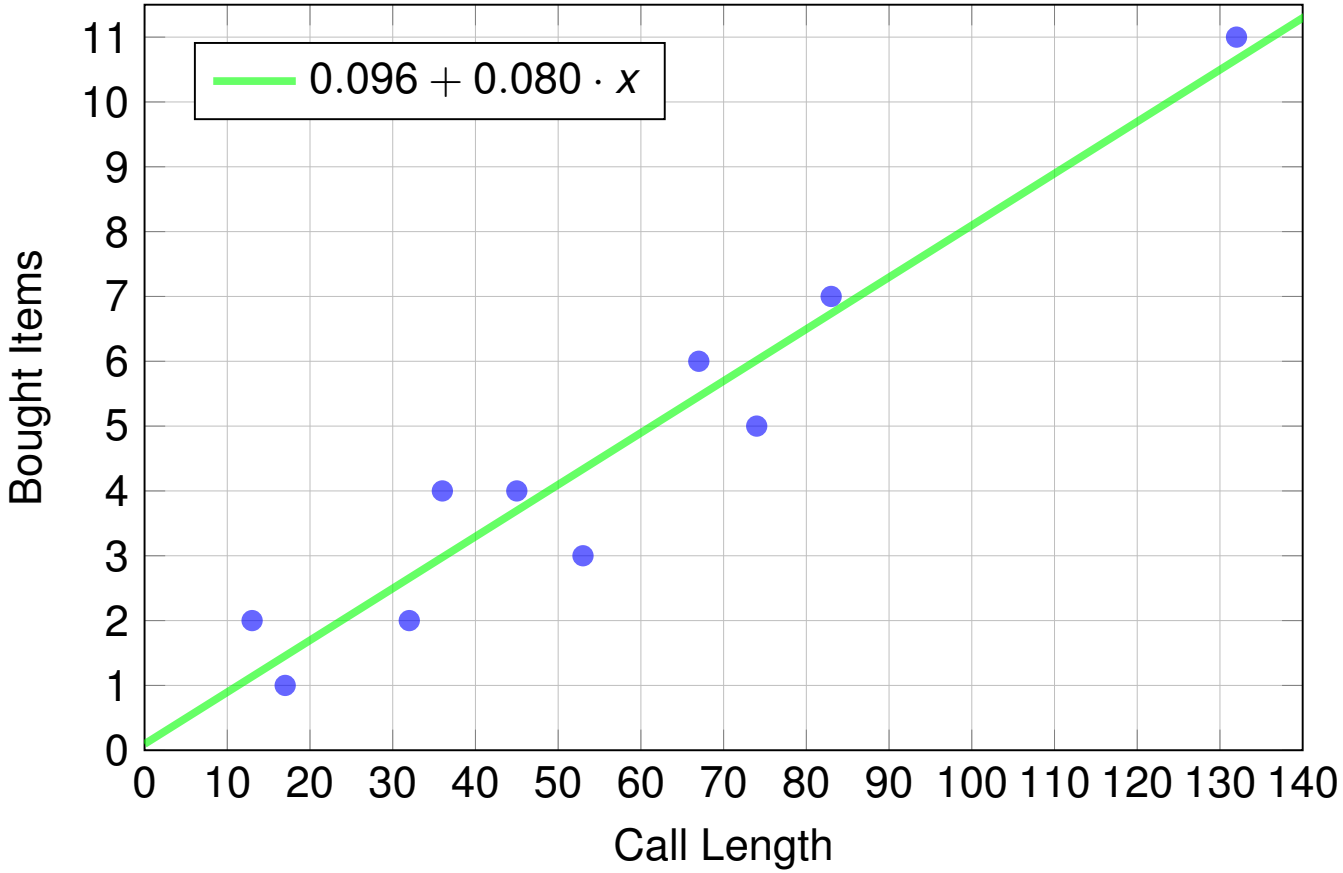

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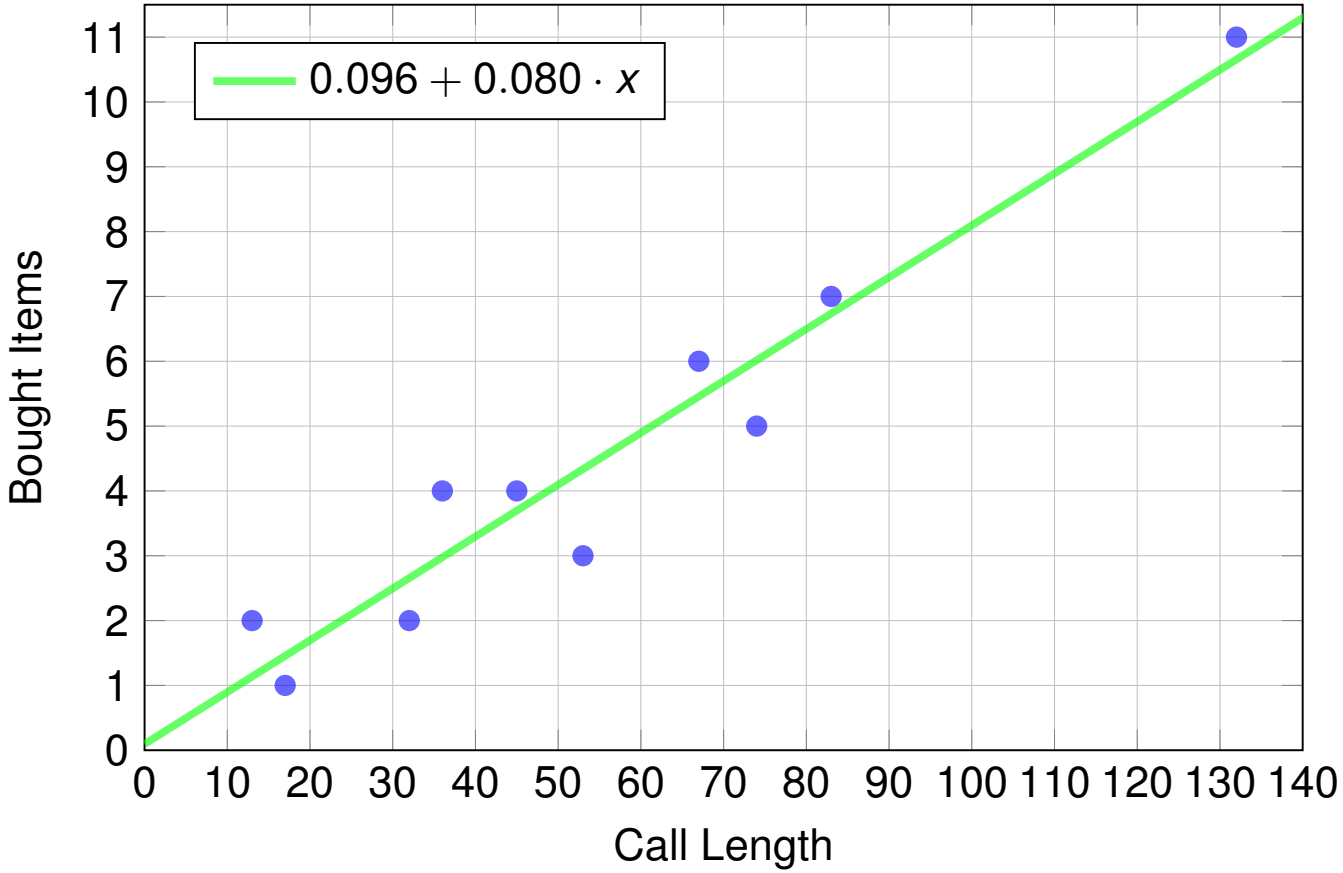

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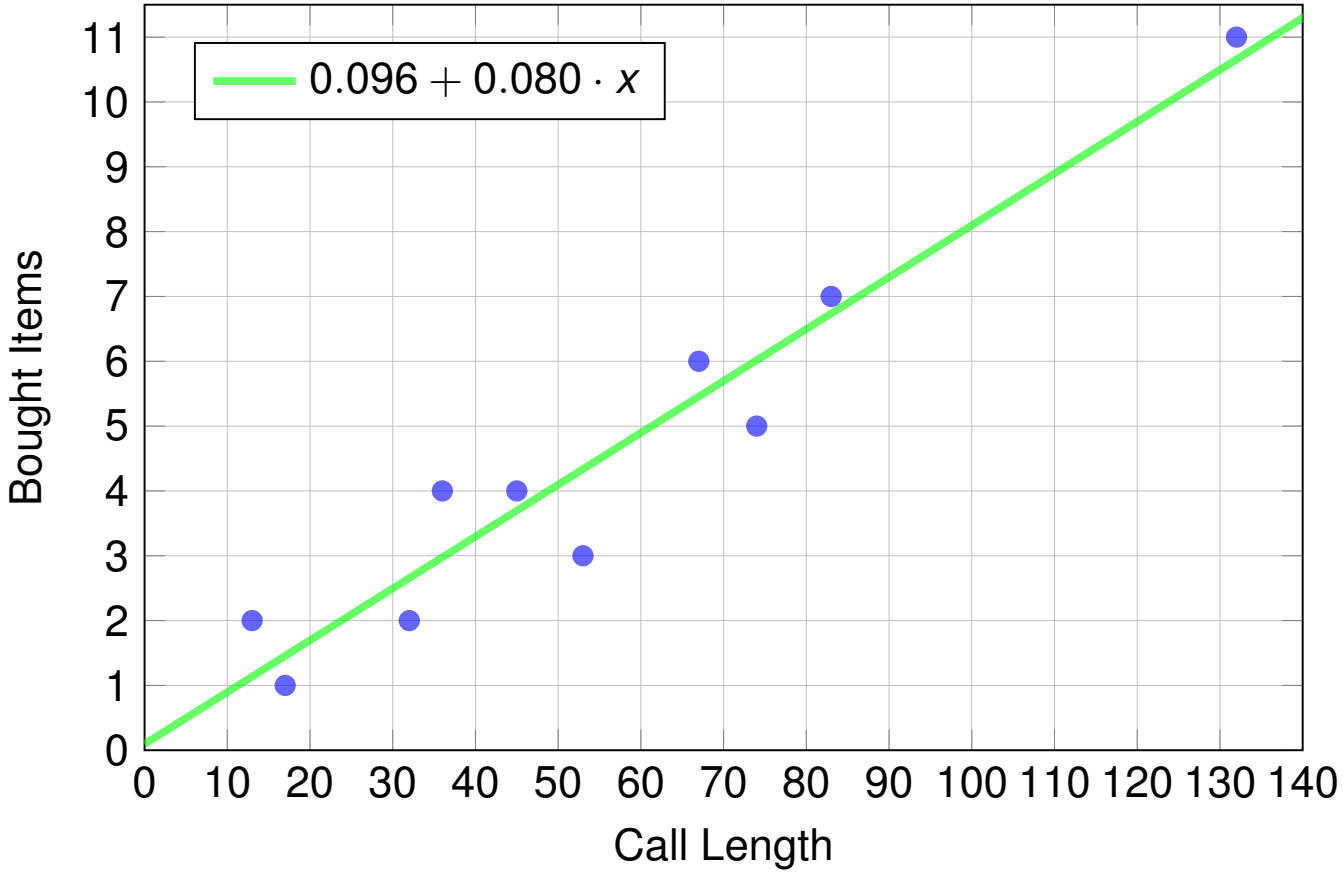

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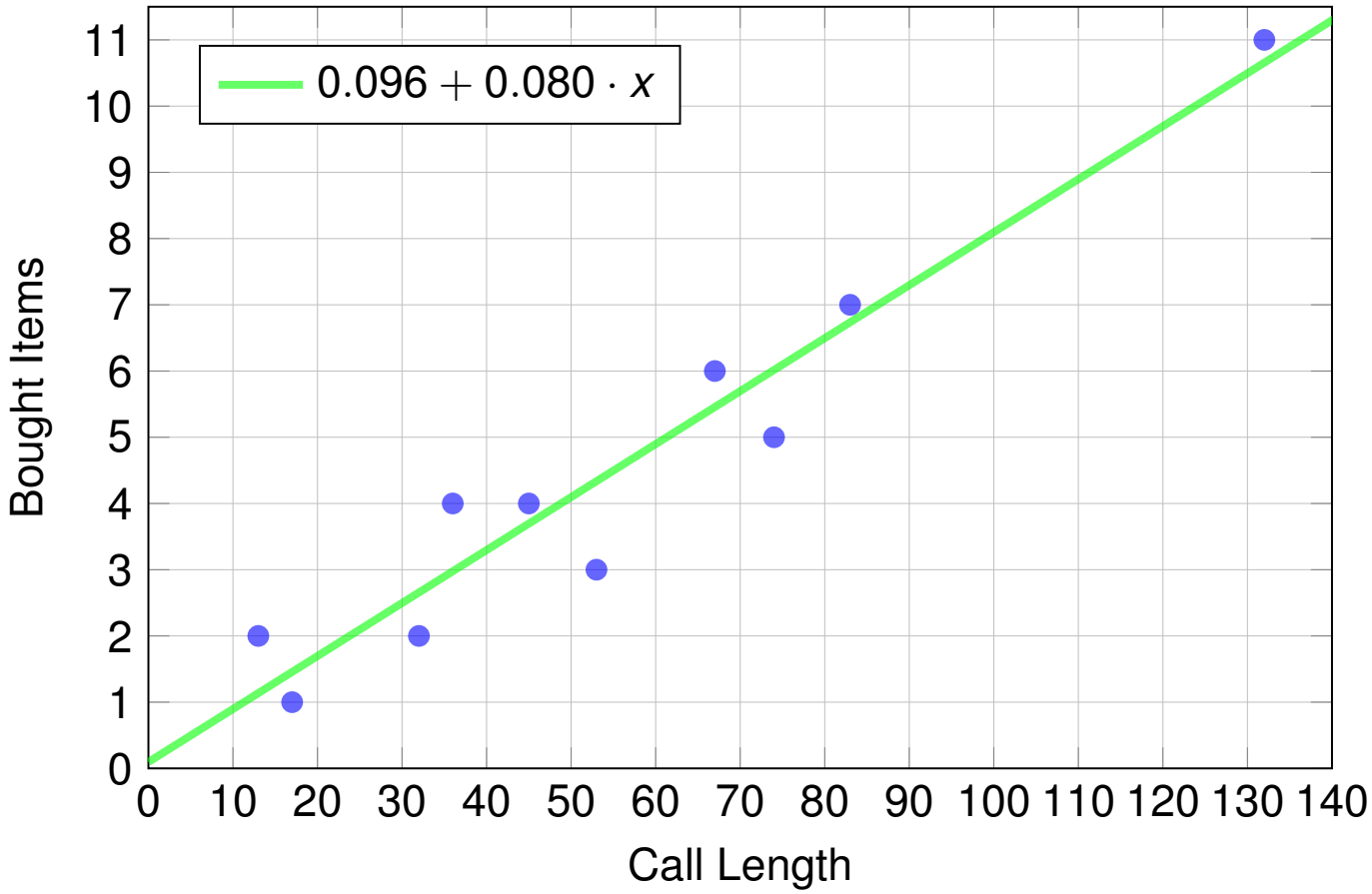
High R^2-value: our regression line is a much better fit than the constant predictor $y = 4.5$!

Step 2: Predicting y for a client

$$y = 0.0964 + 0.0798 \cdot x$$



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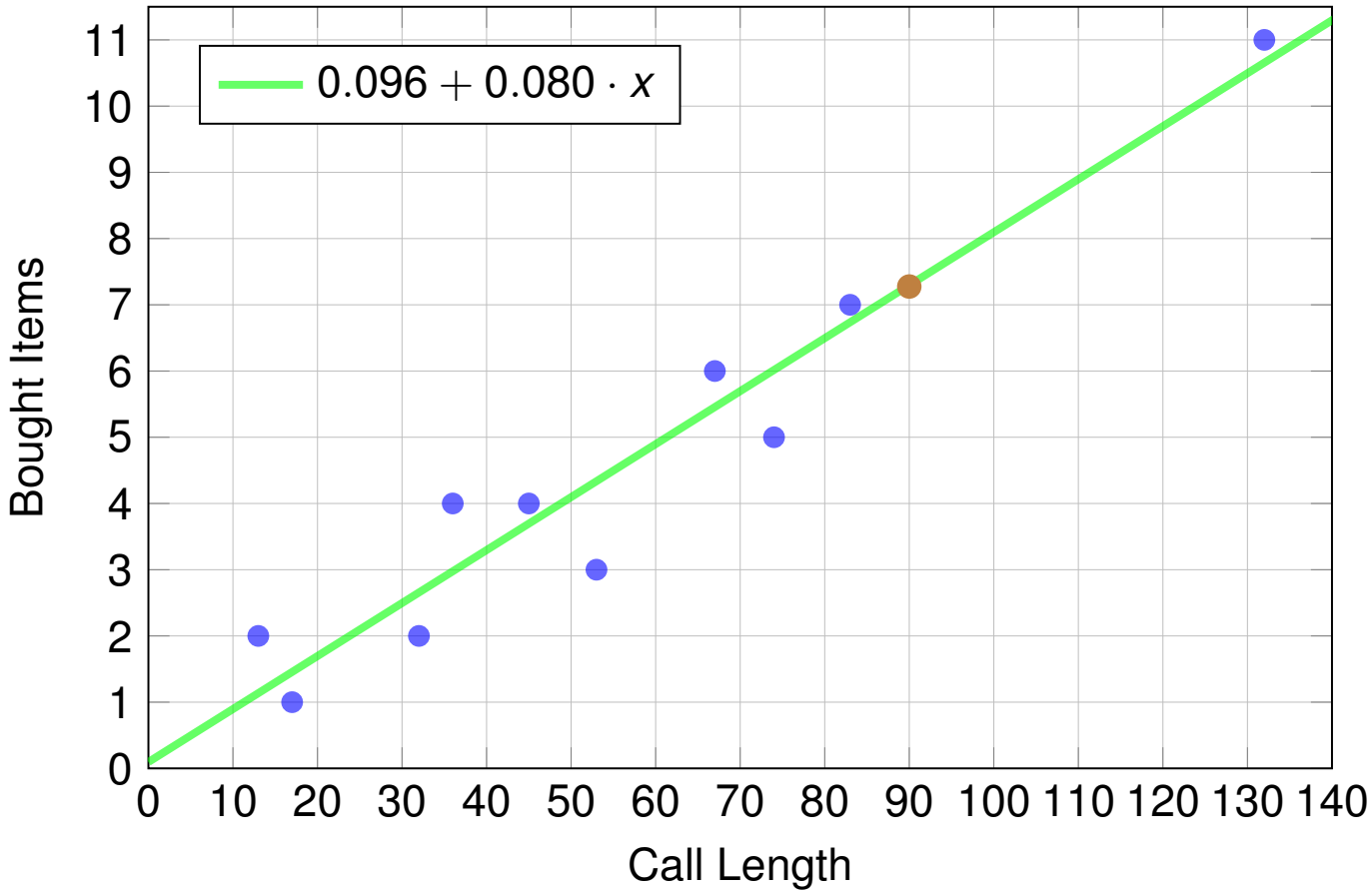
For $x = 90$, we obtain $y(x) = 7.27 \approx 7$



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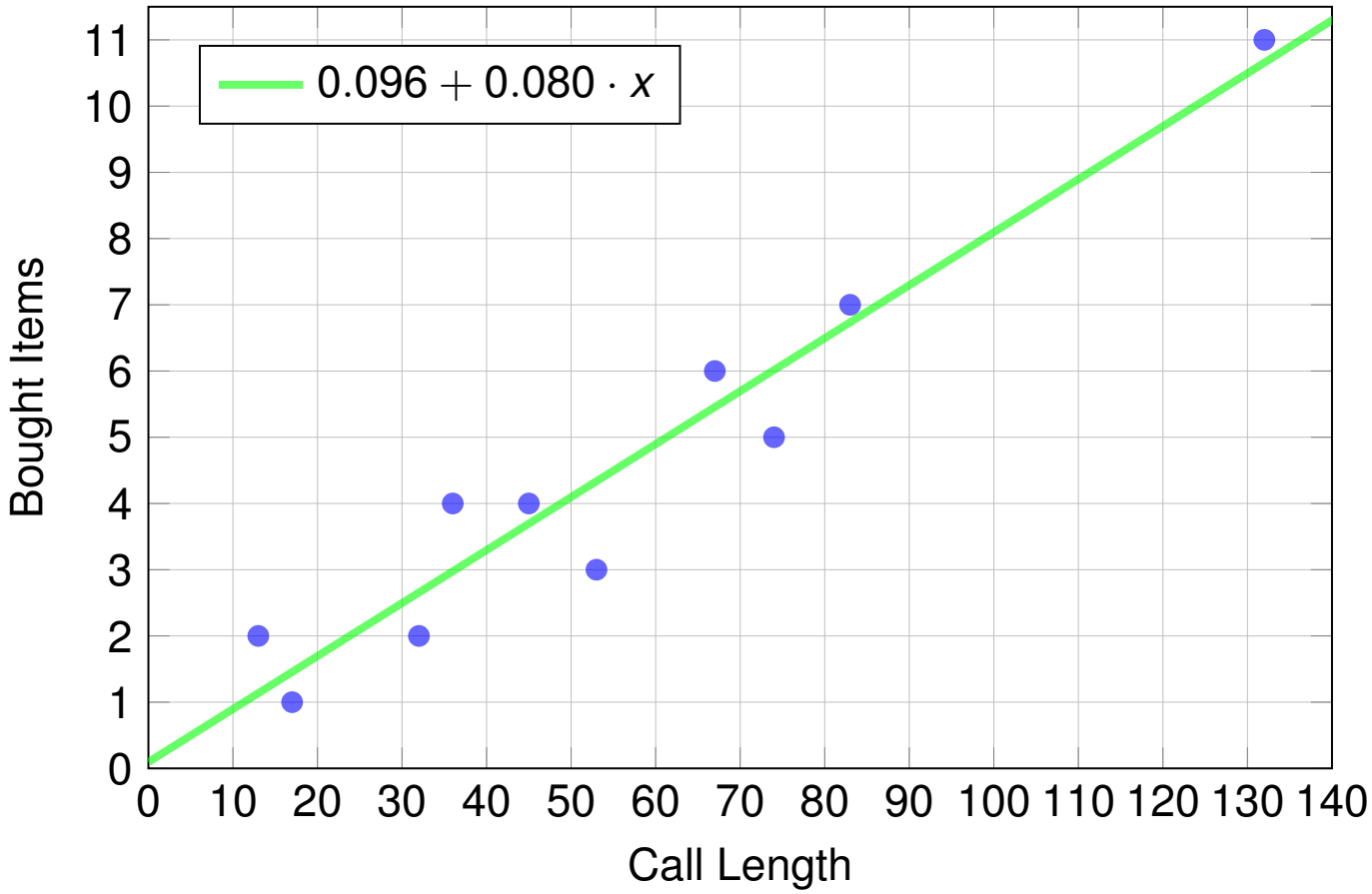

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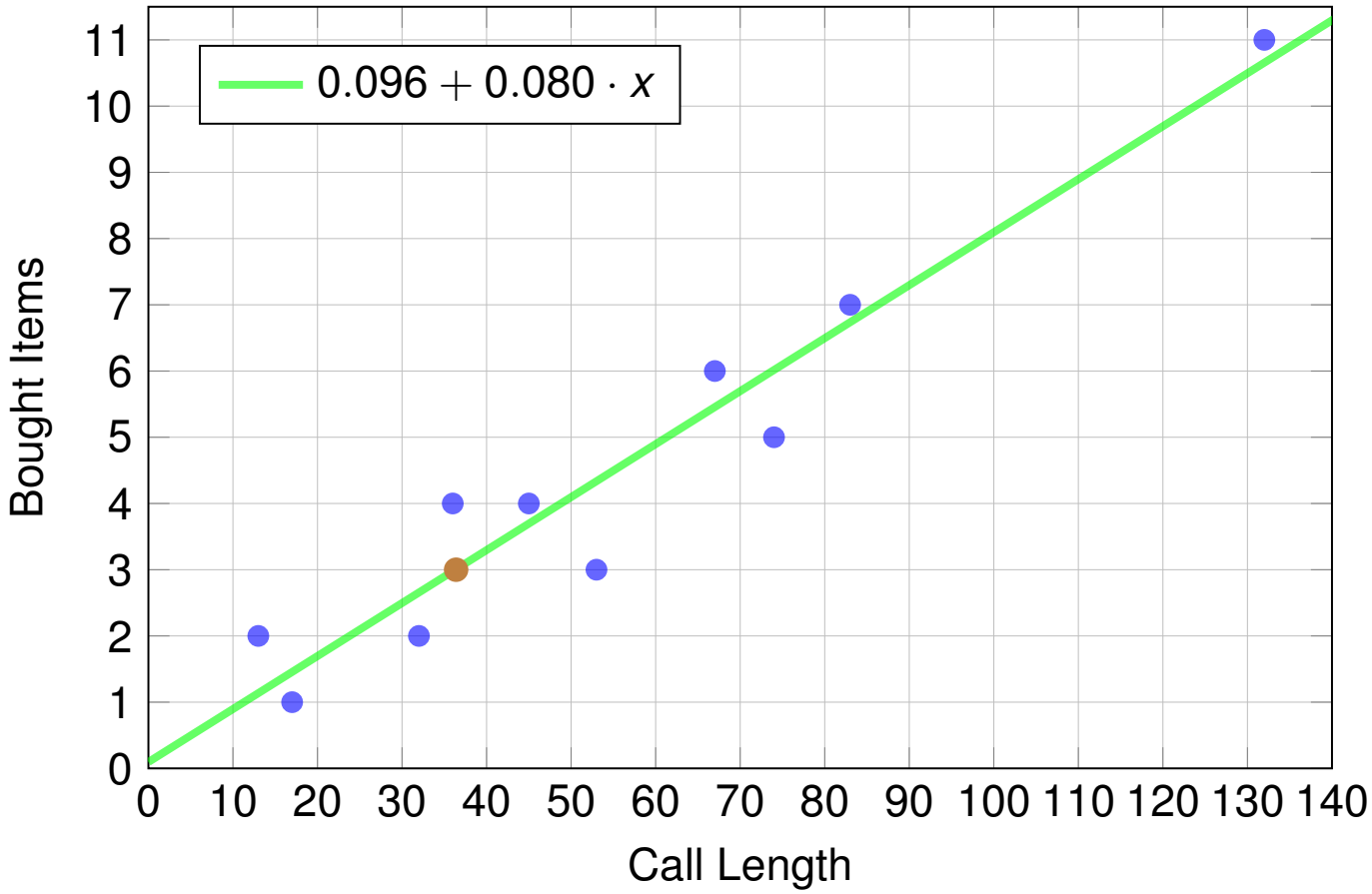
For $y = 3$, we obtain $x(y) = 36.397 \approx 36$



Step 3: Another Approach

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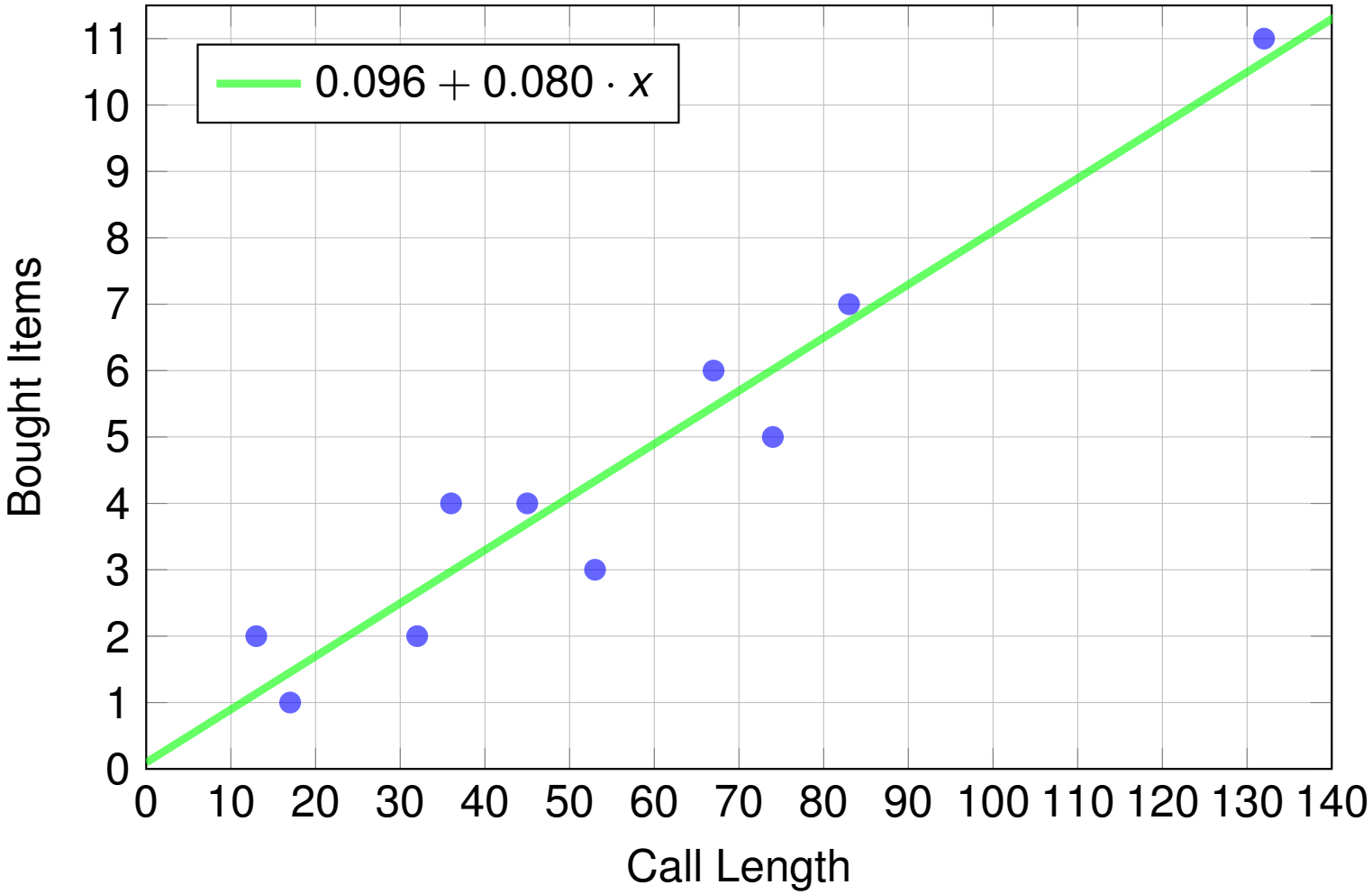
The two Regression Lines



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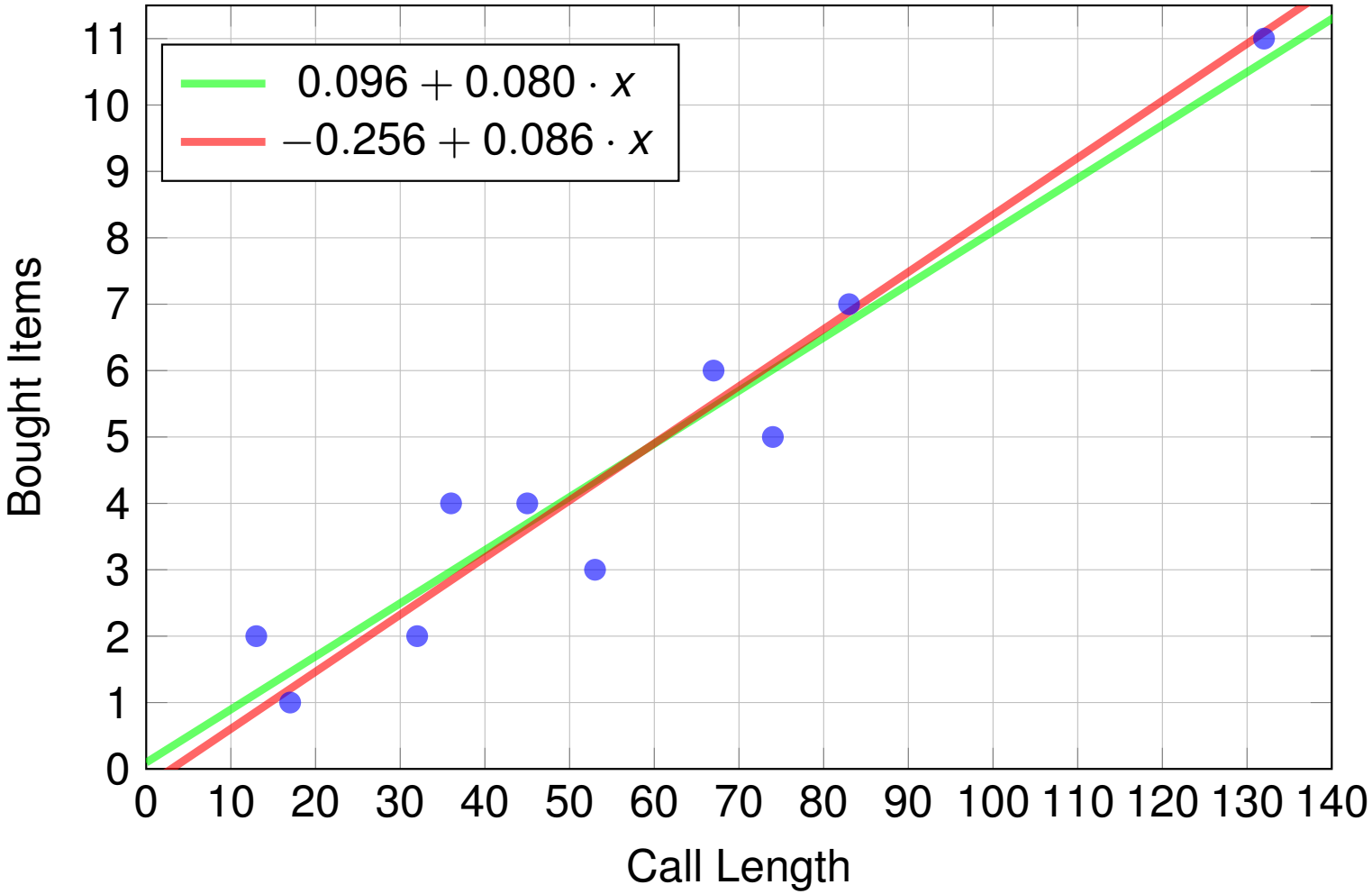
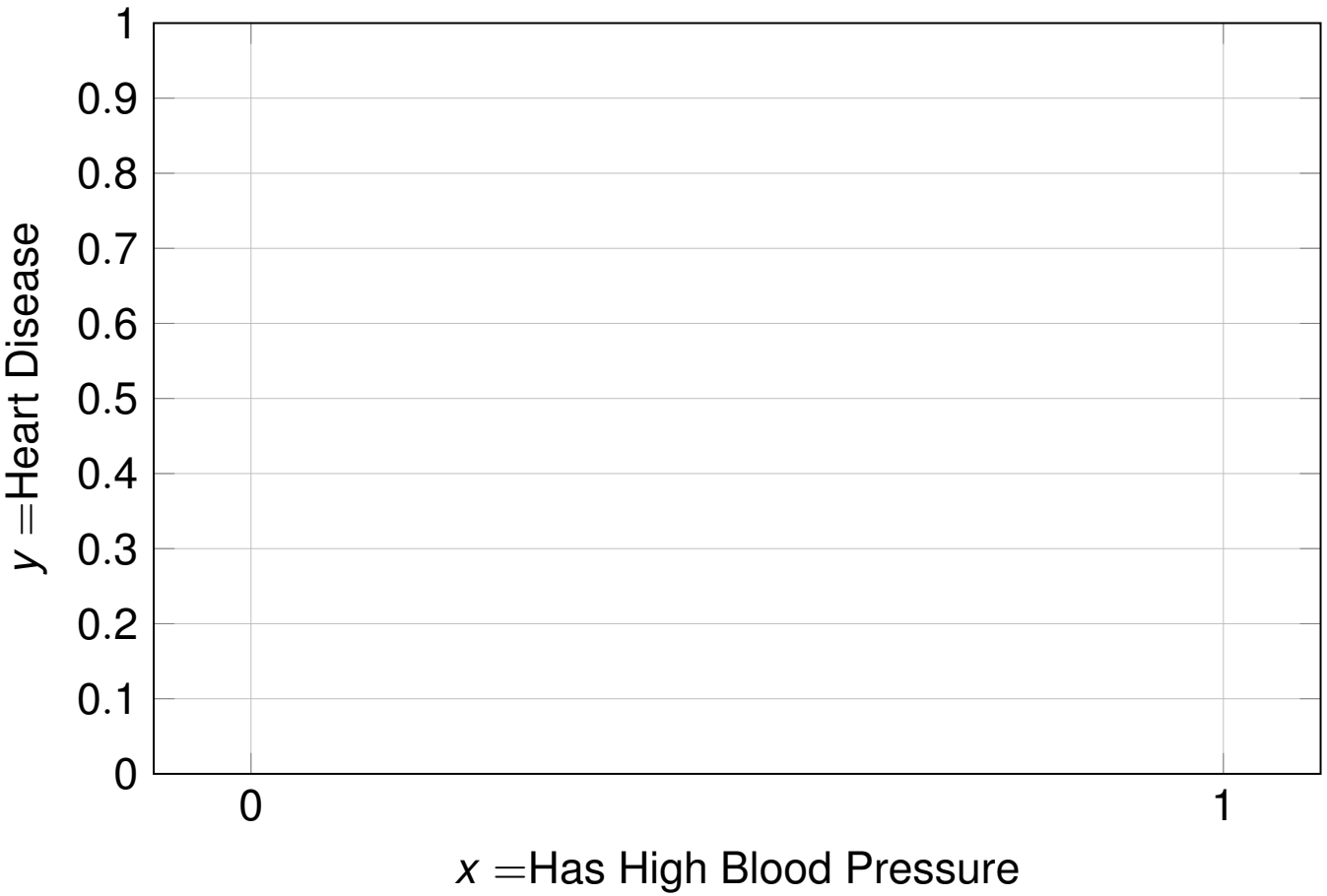


Question 3: Visualising the Data Set

- We have 200 people with **high** blood pressure and no heart disease



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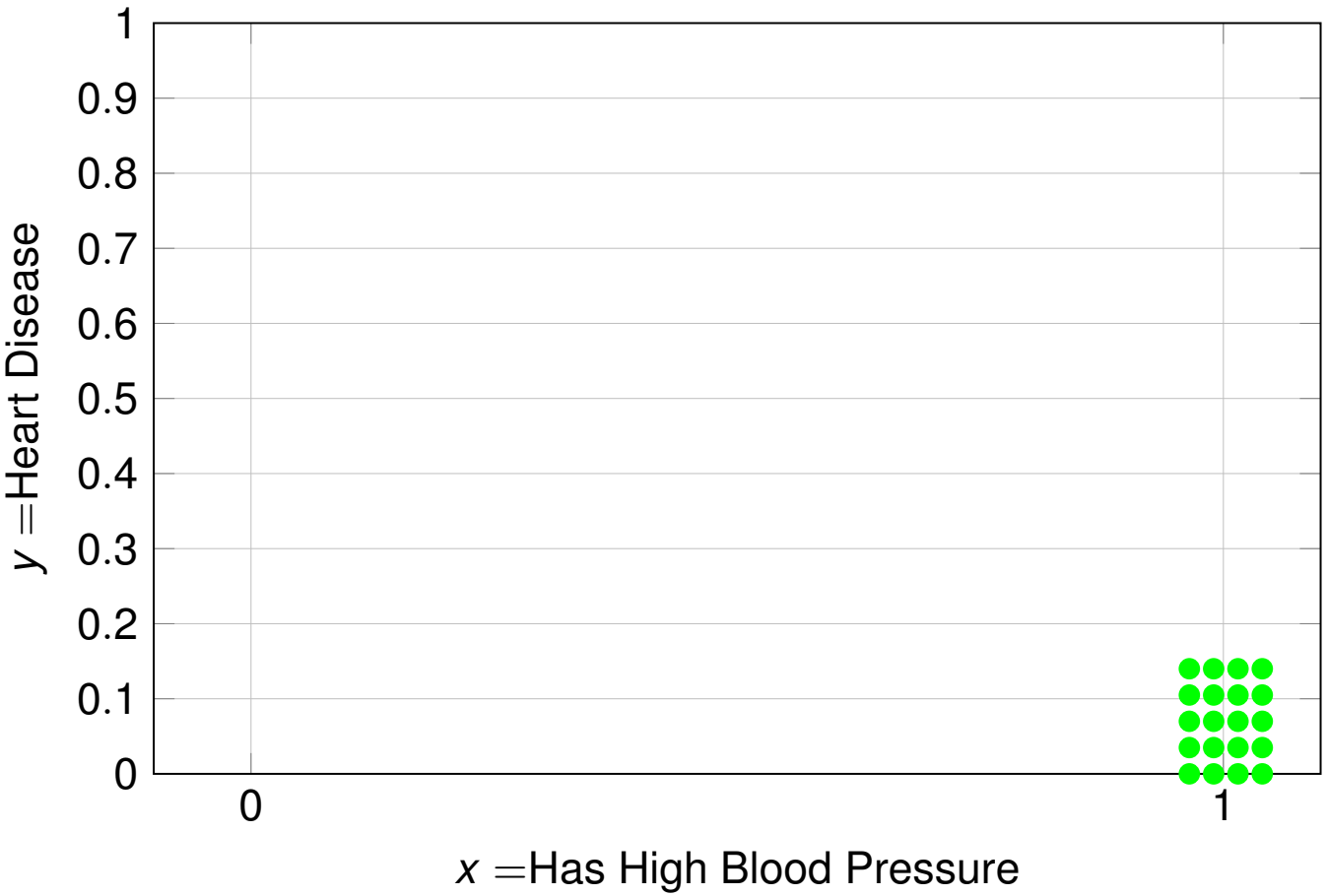

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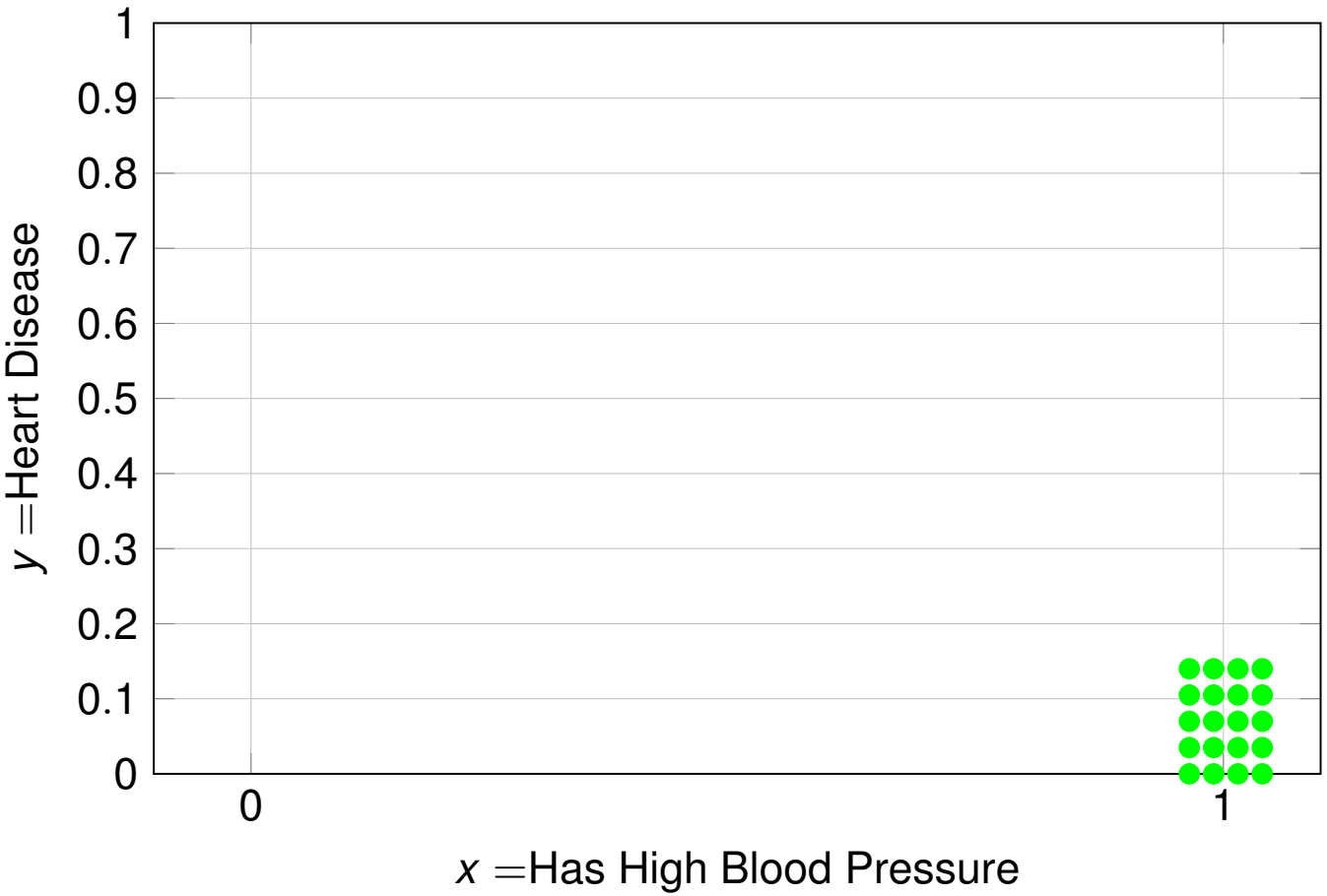

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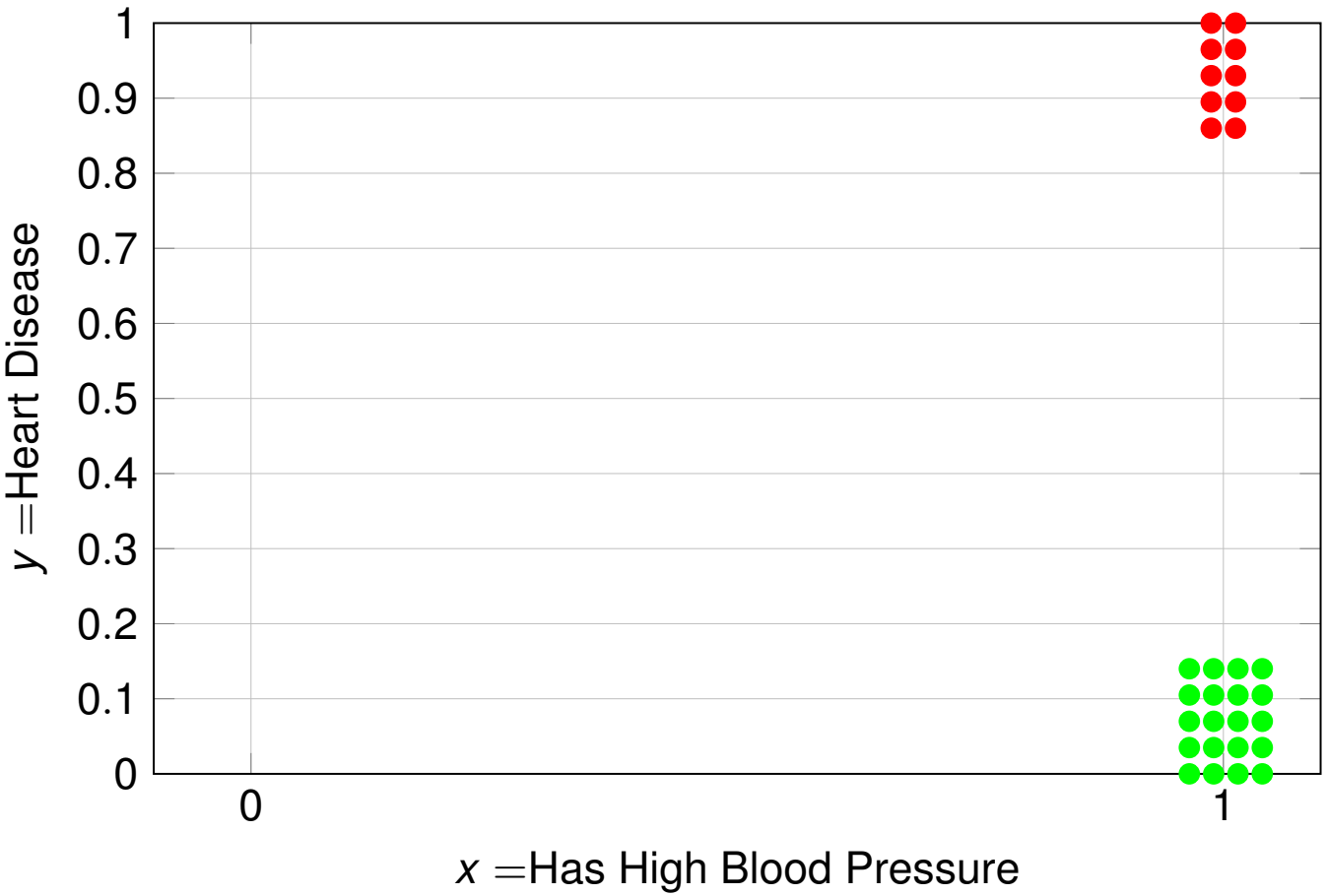

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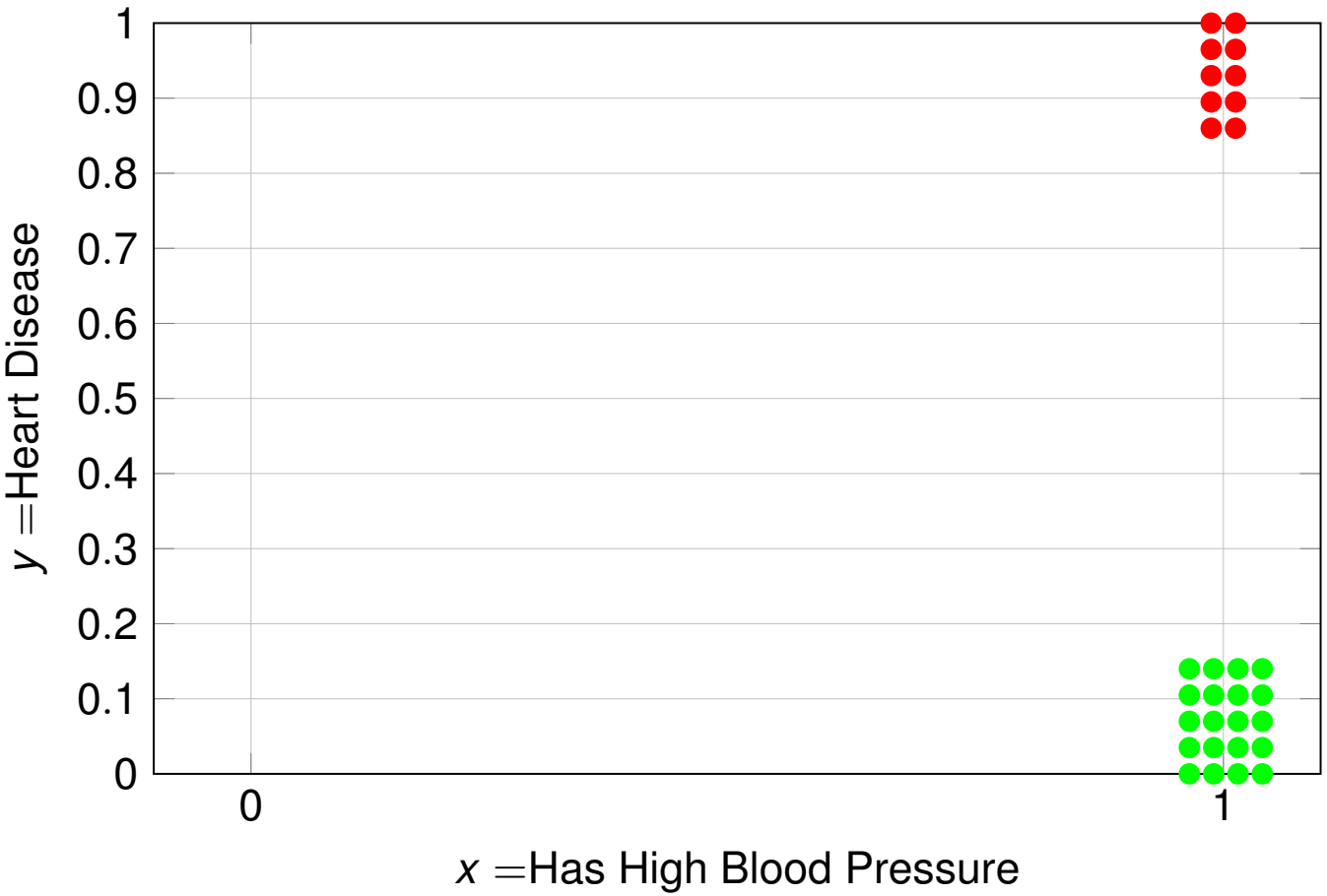

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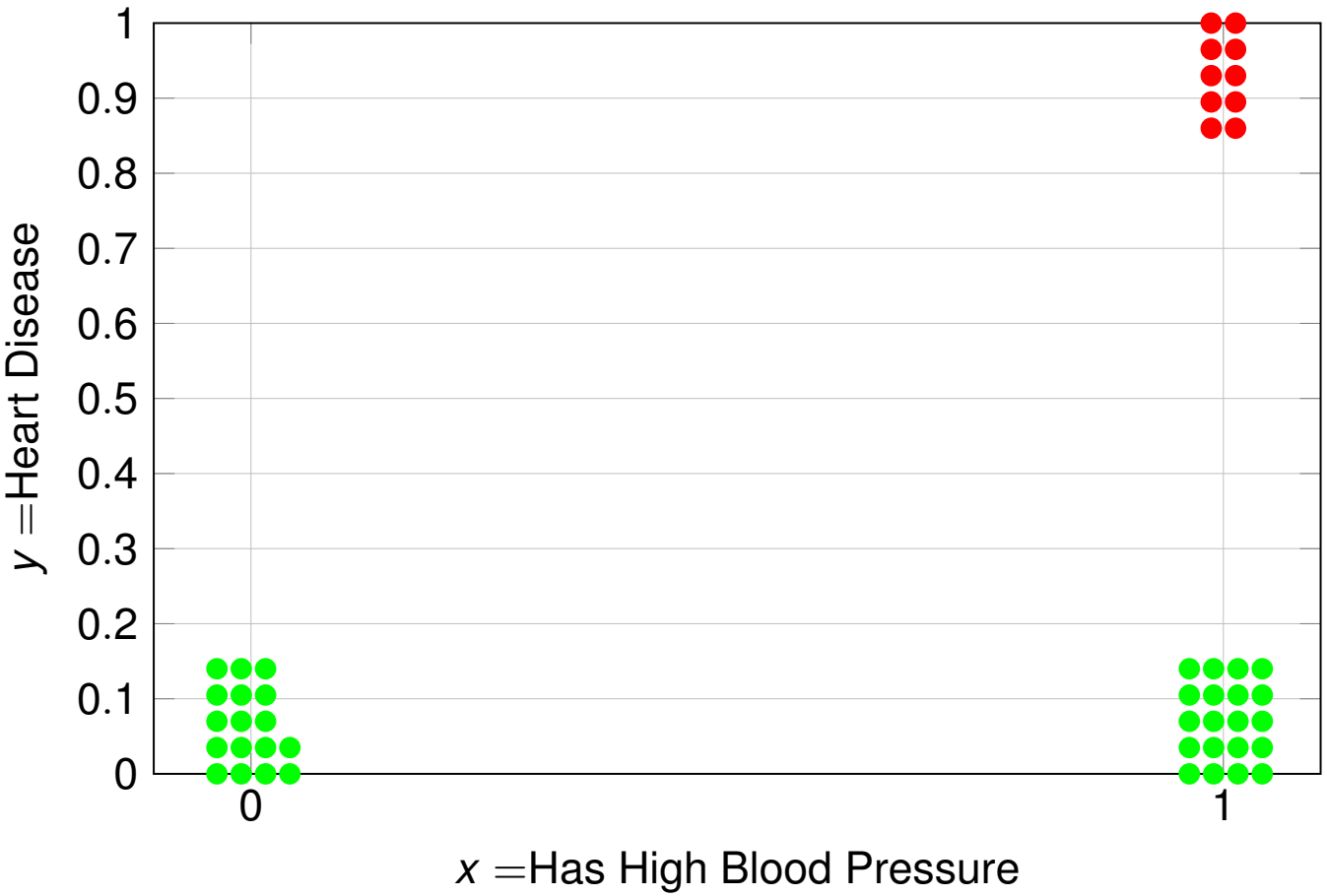

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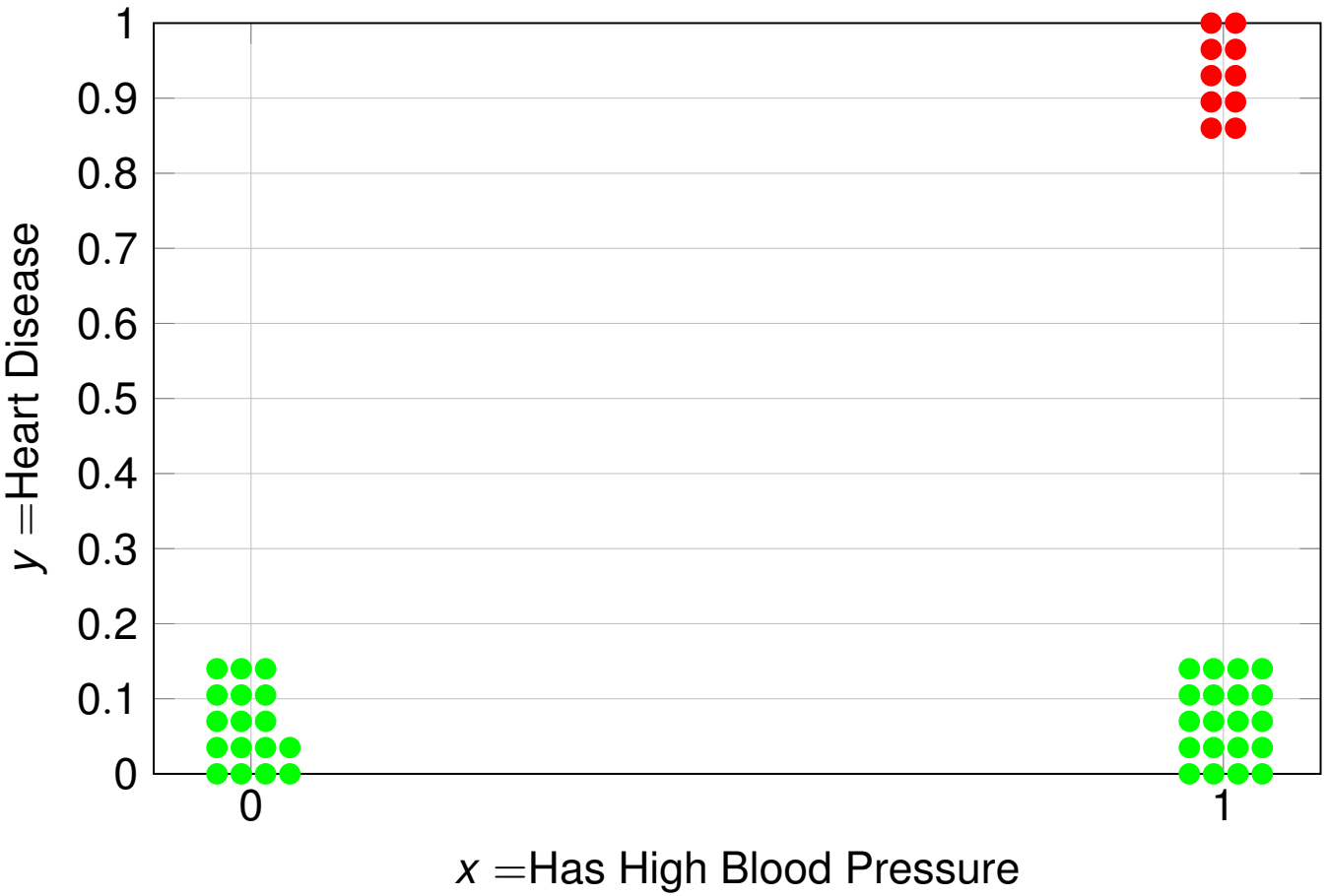

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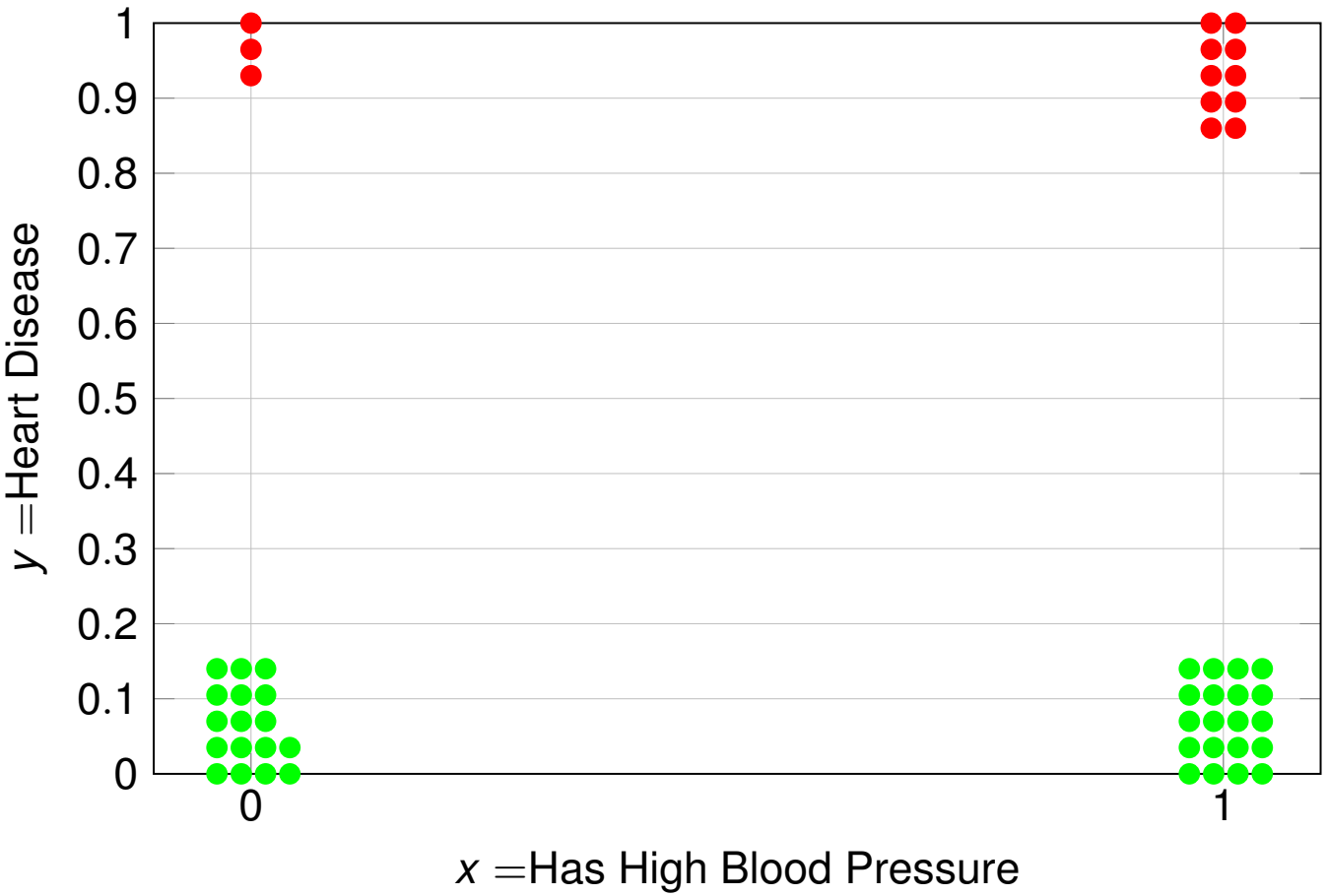

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$$
\begin{aligned}
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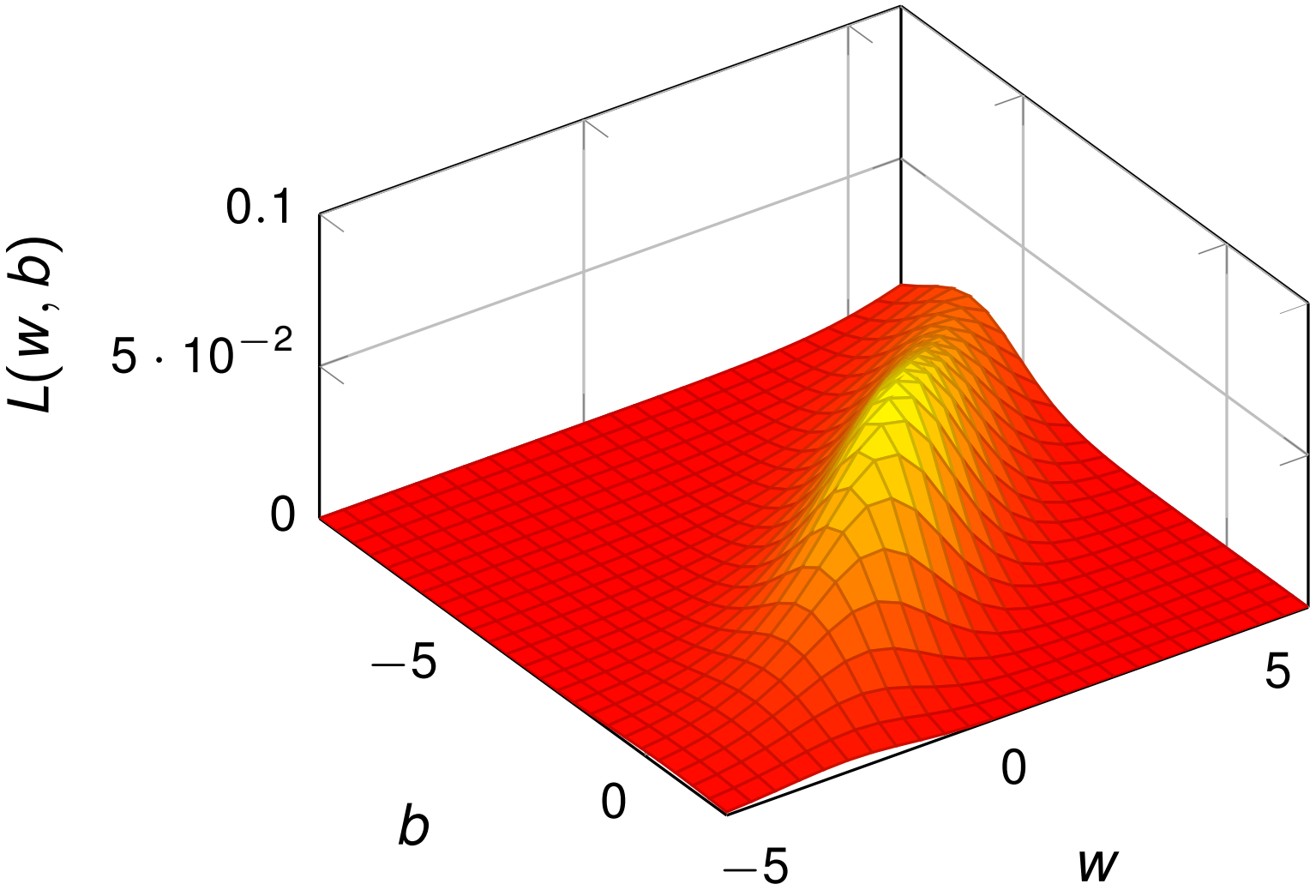
Apply an iterative solver such as Gradient Descent!

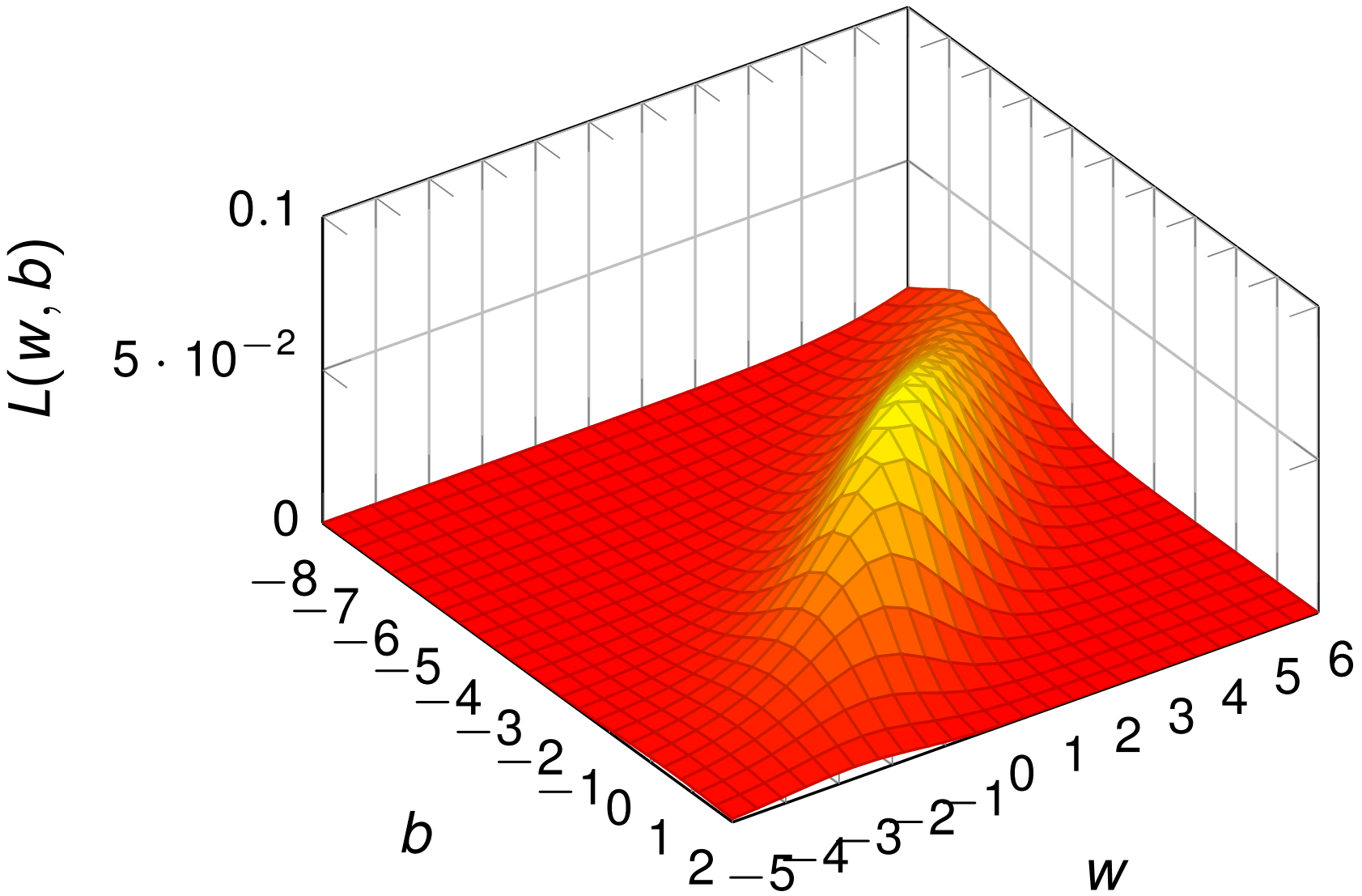
Illustration of the Likelihood Function



Run of Gradient Descent

Iteration	b	w	Likelihood
1	1	1	0.0012
2	0.93	0.96	0.0015
3	0.847	0.91	0.0021
4	0.734	0.843	0.0031
5	0.575	0.75	0.005
10	-1.14	0.28	0.060
20	-1.62	0.90	0.0635
30	-1.718	1.015	0.0636
40	-1.735	1.036	0.0636
50	-1.738	1.040	0.0636
60	-1.739	1.041	0.0636
100	-1.739	1.041	0.0636

Displaying the Optimum



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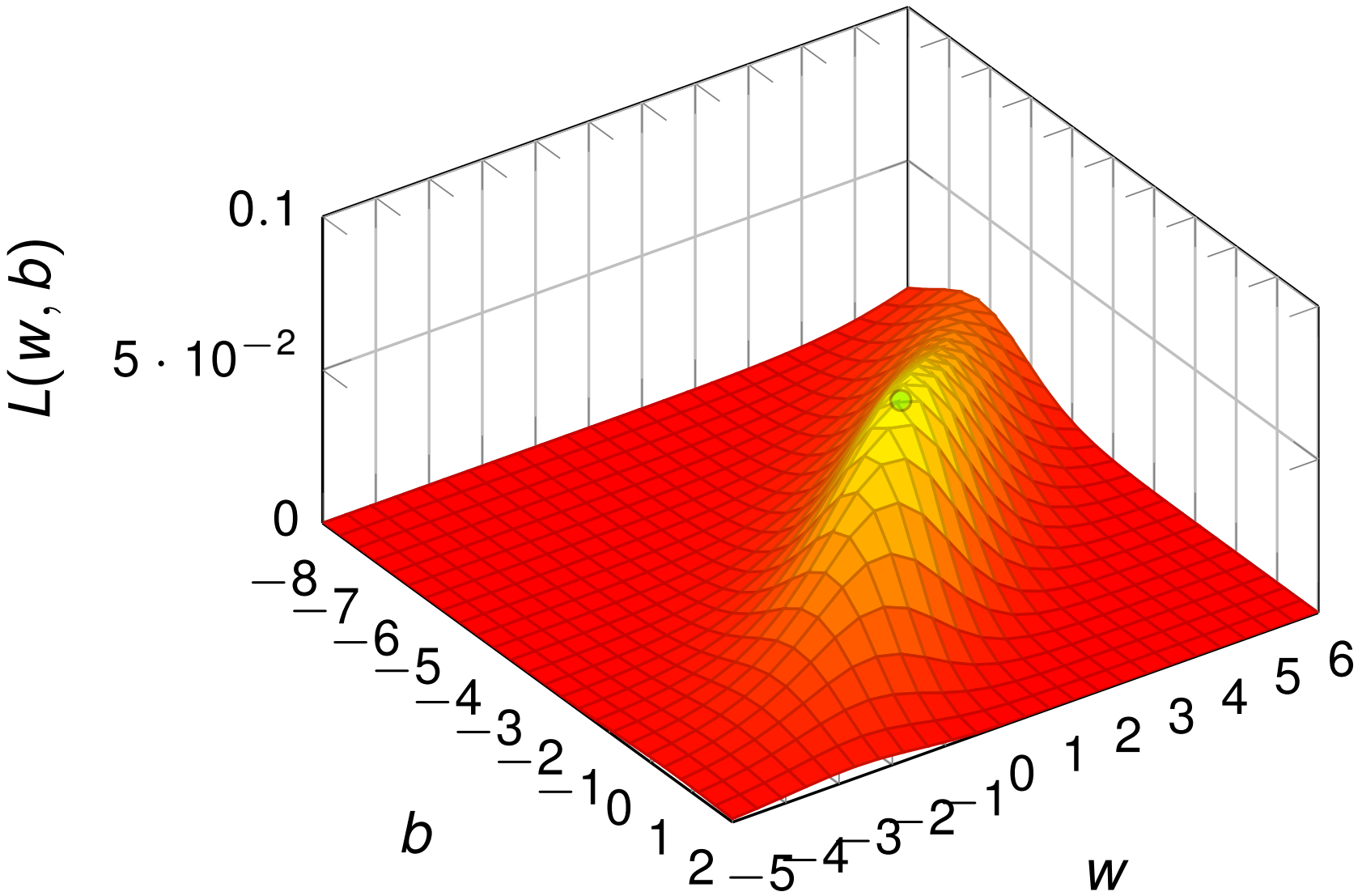

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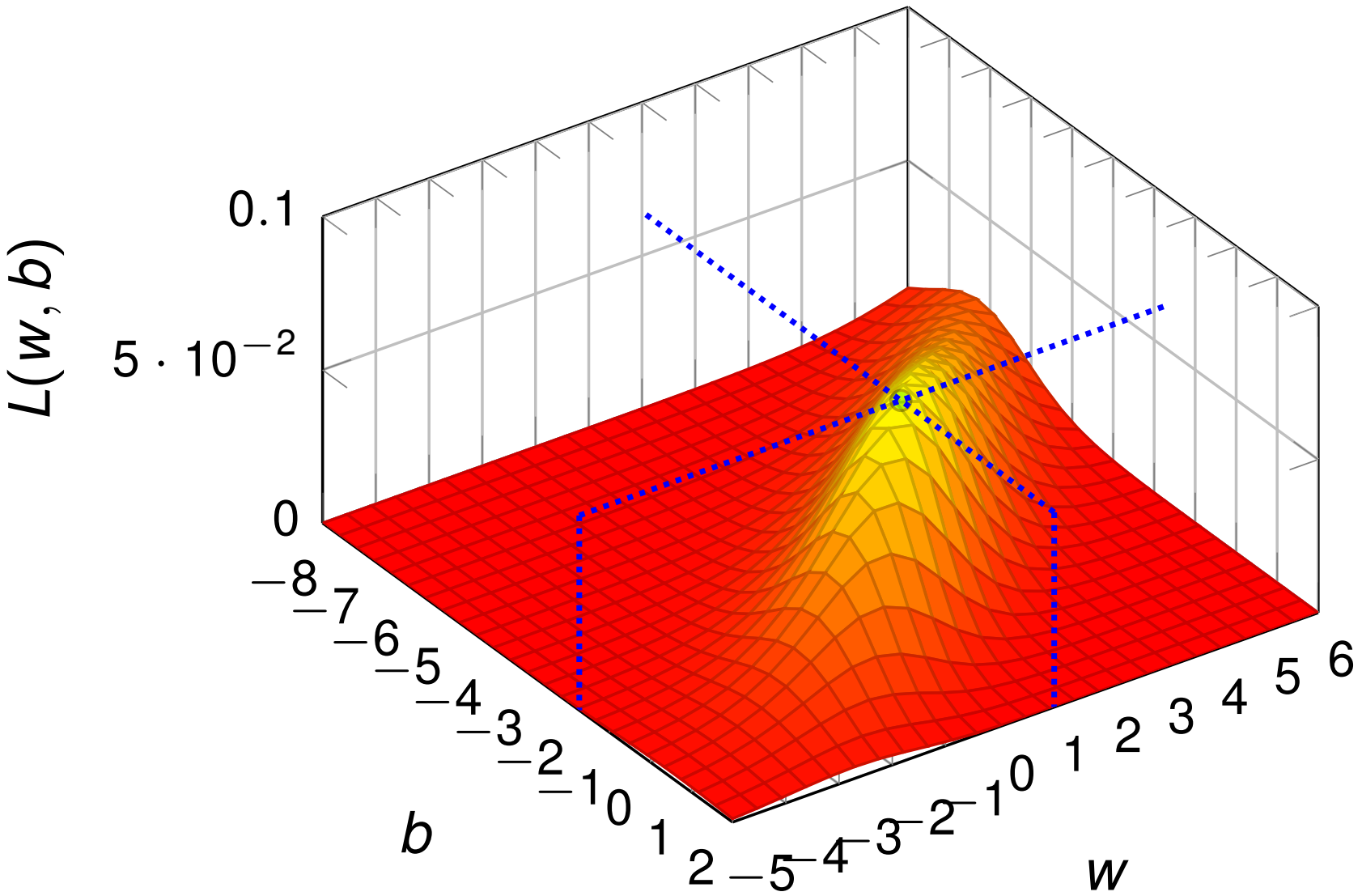

Solution of Logistic Regression

- We have 200 people with **high** blood pressure and no heart disease
- We have 100 people with **high** blood pressure and heart disease
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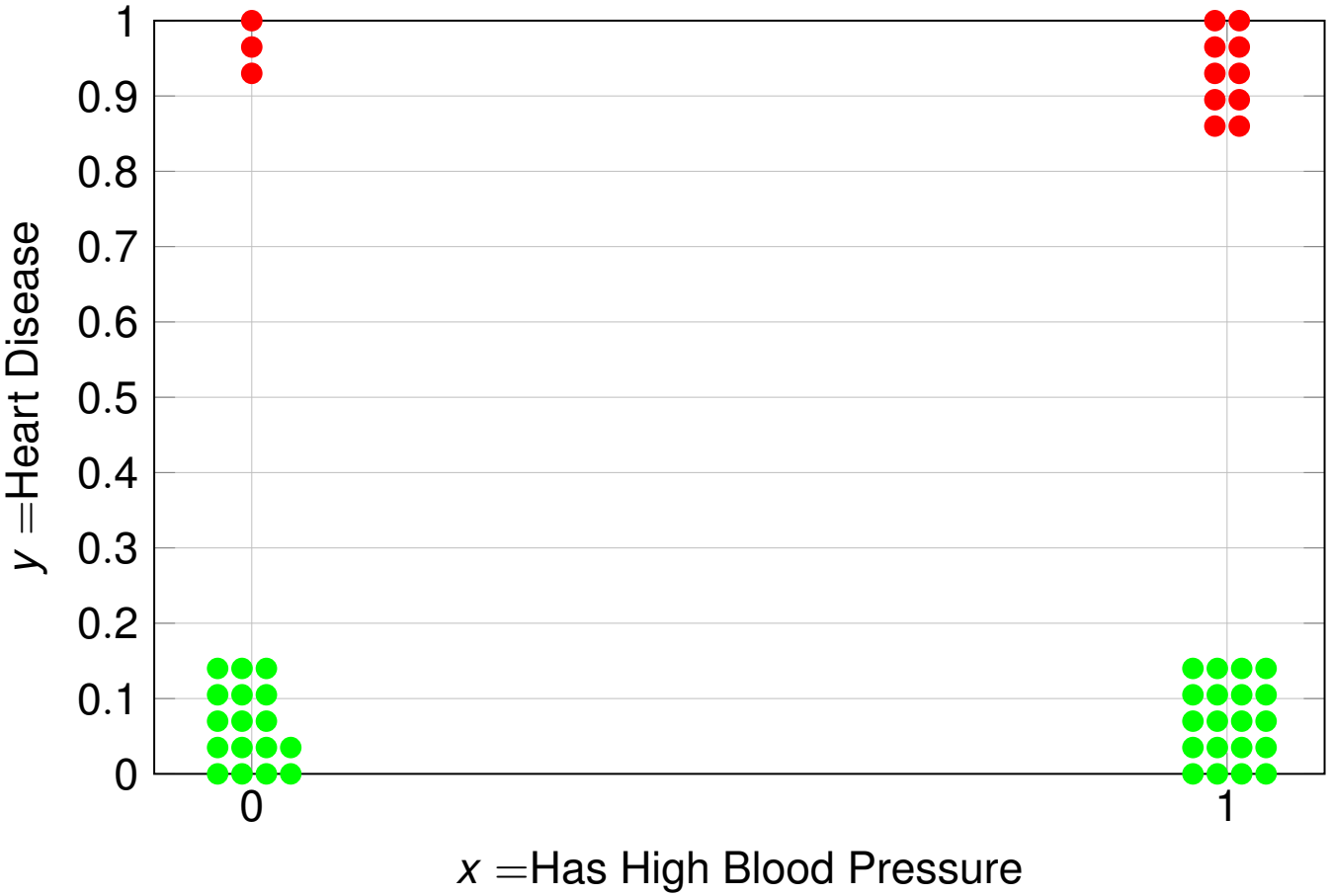

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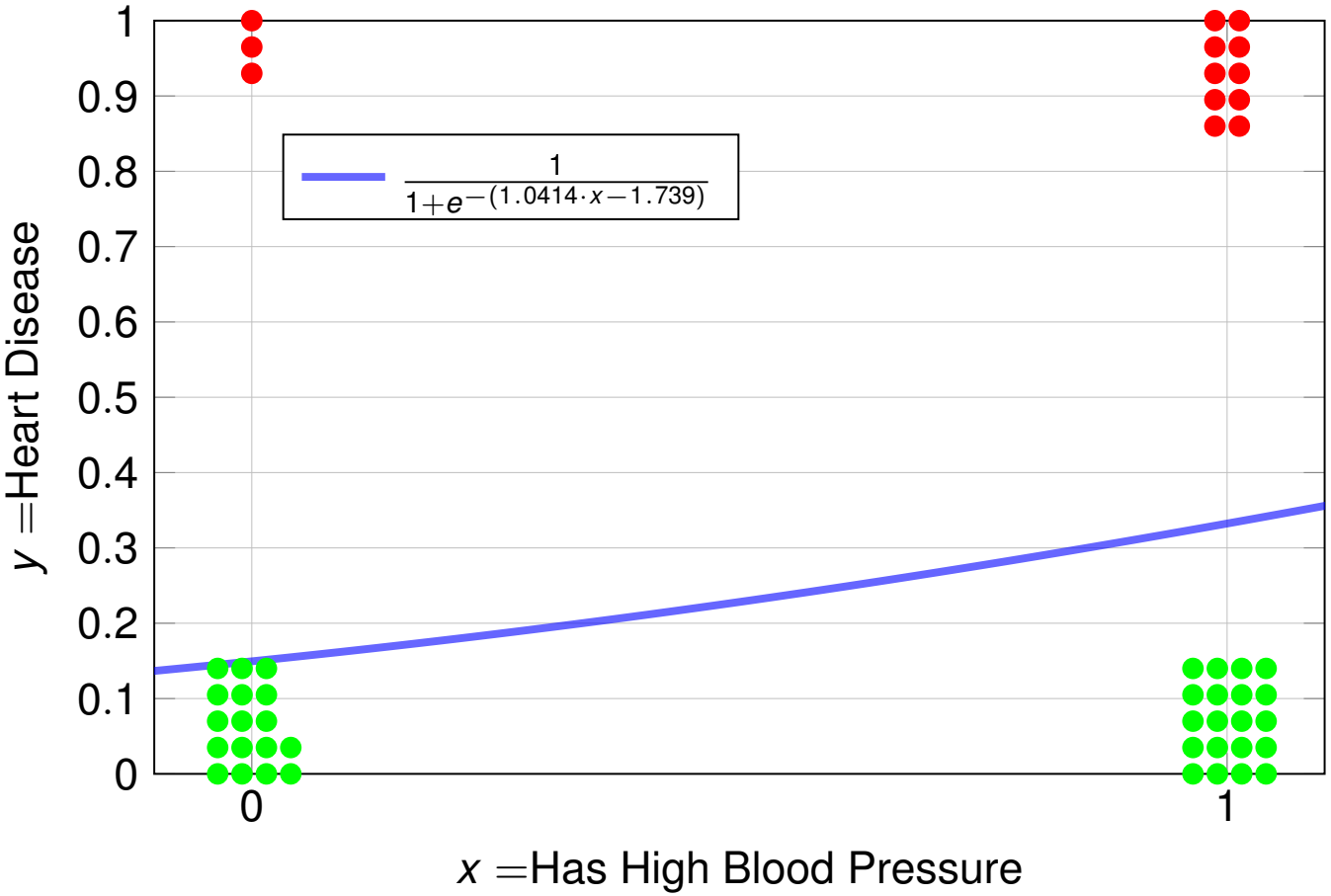

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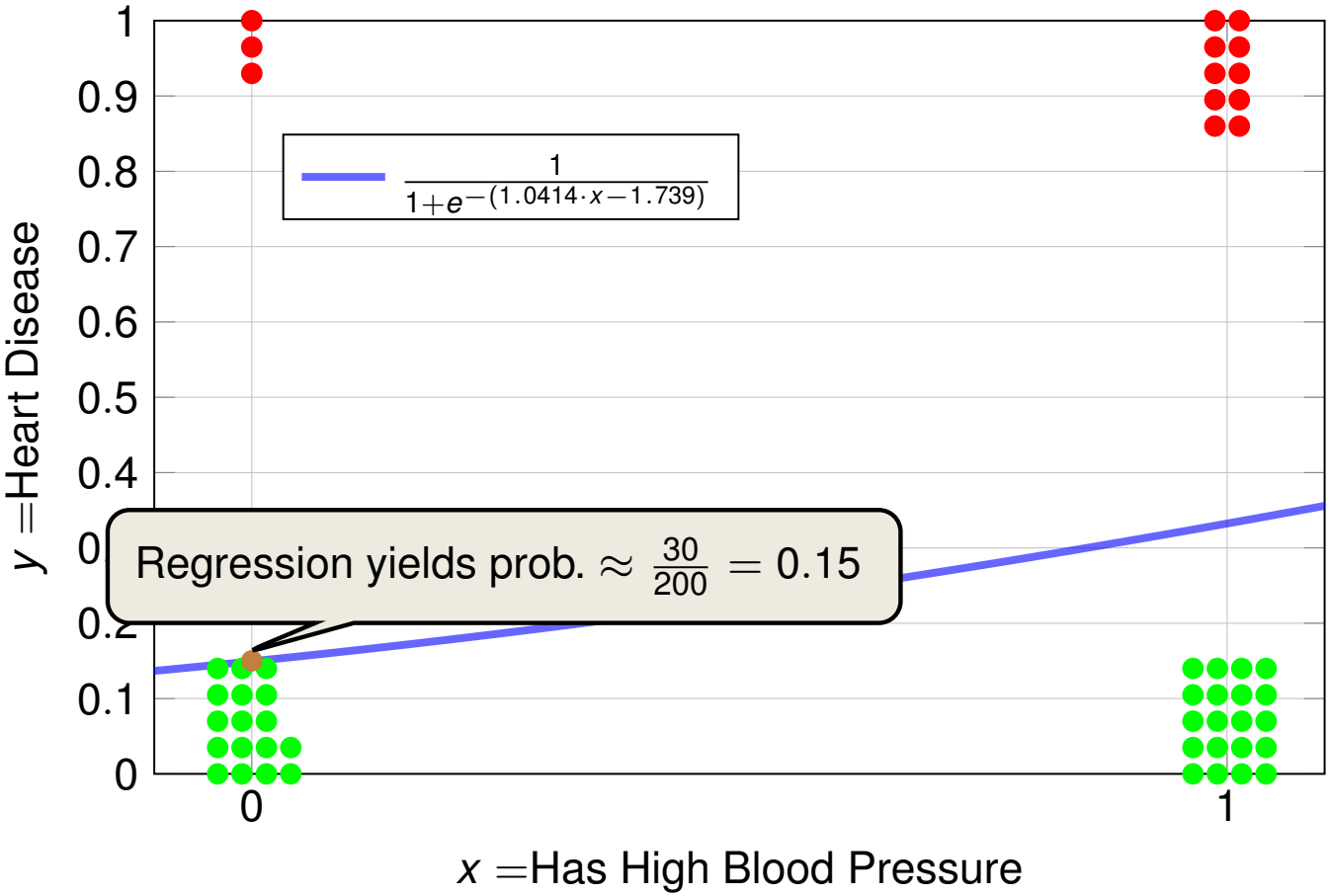

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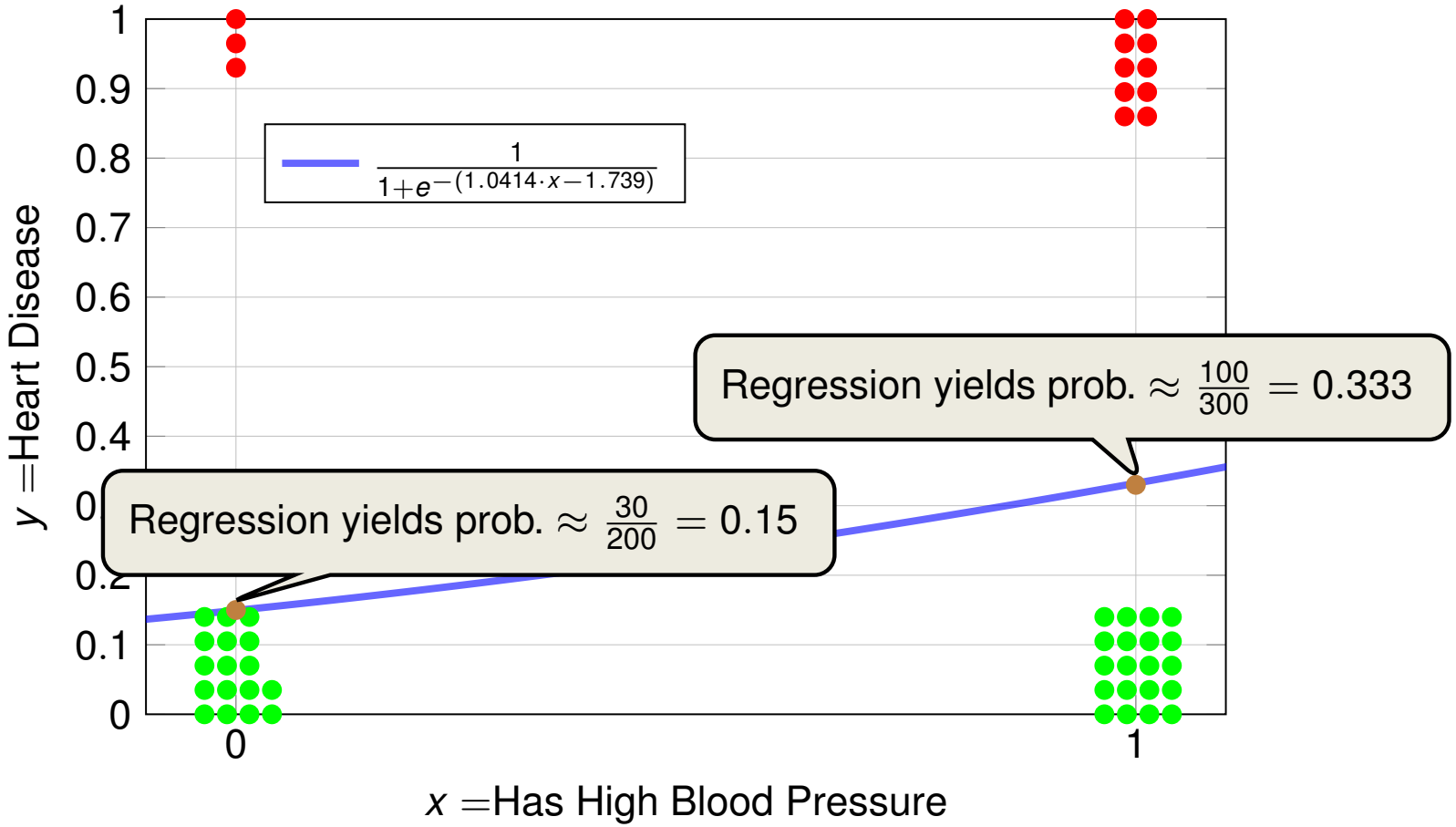

A Simple Example

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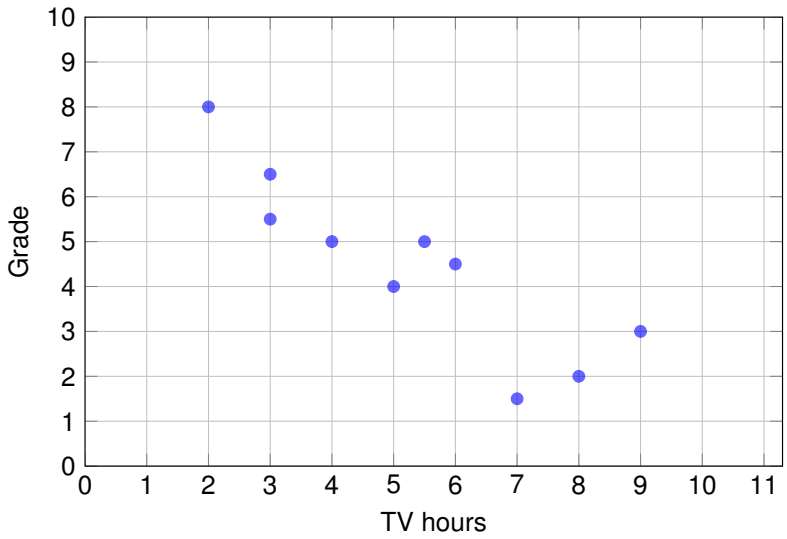

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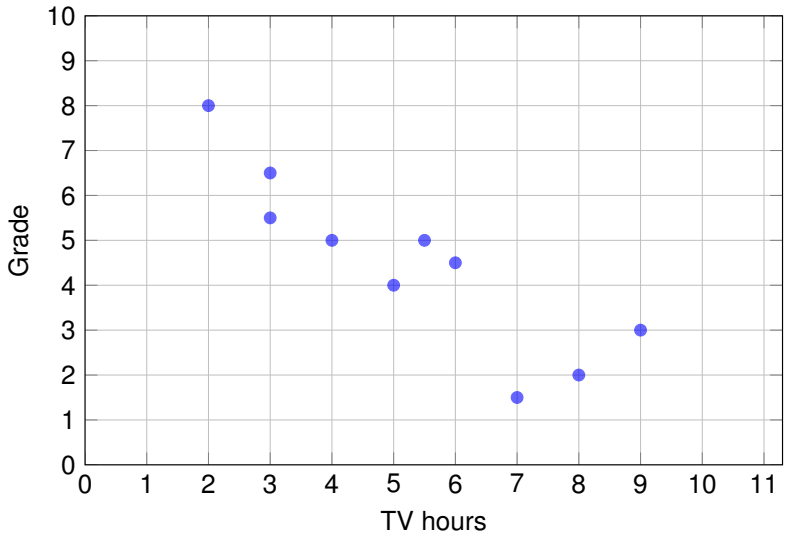

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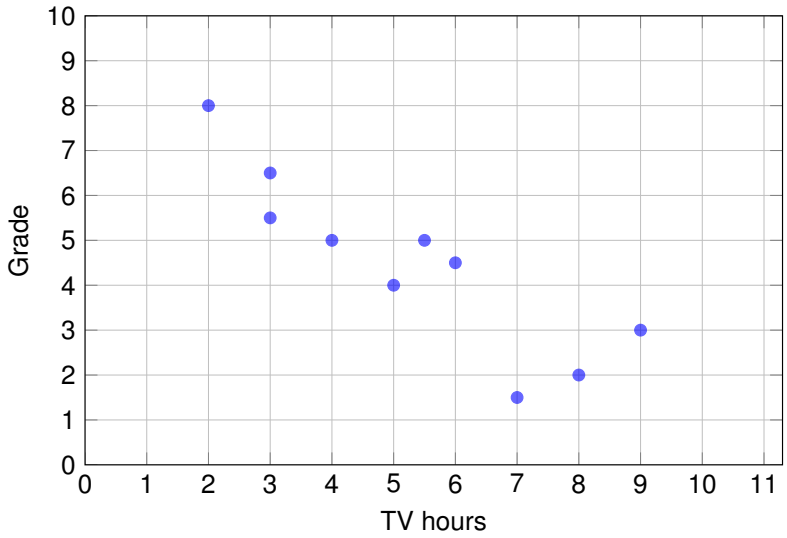

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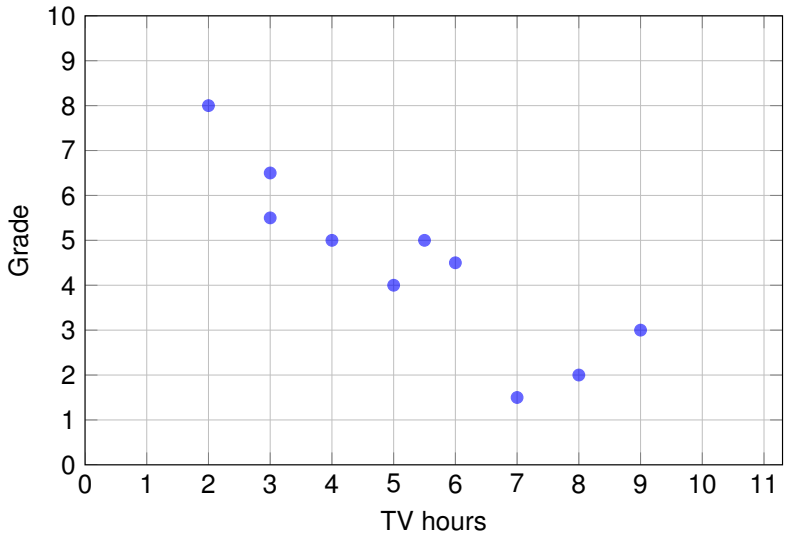

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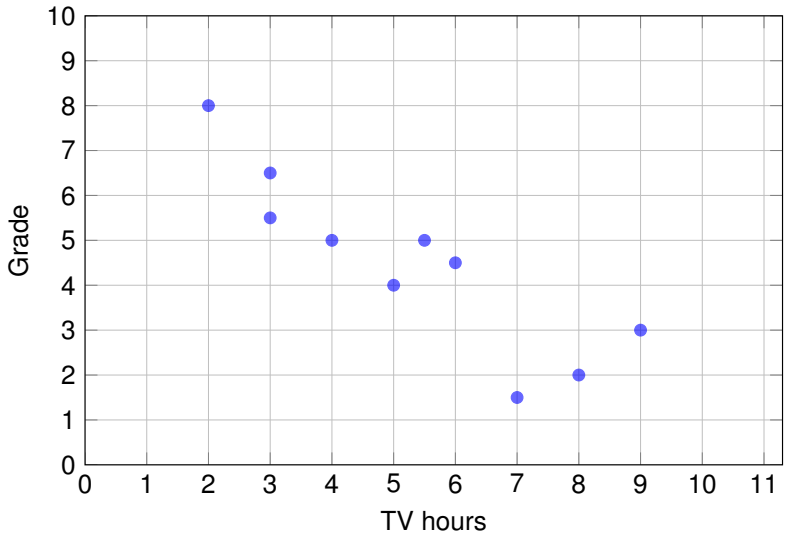

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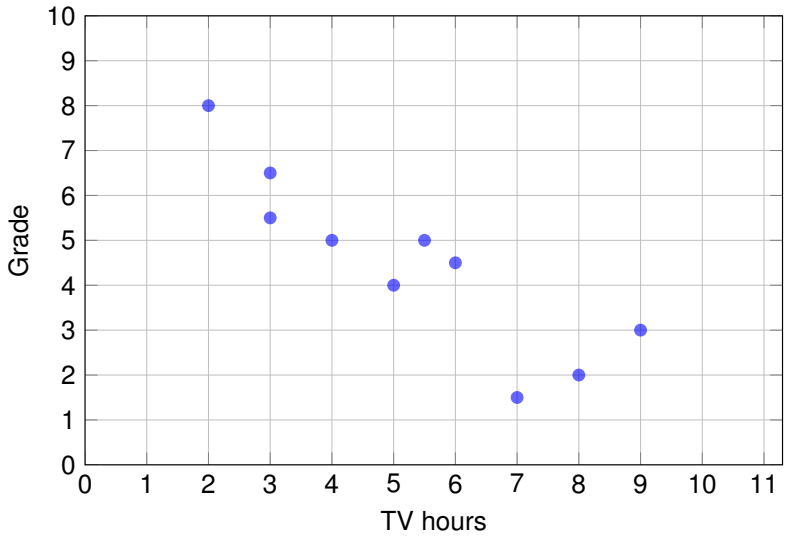

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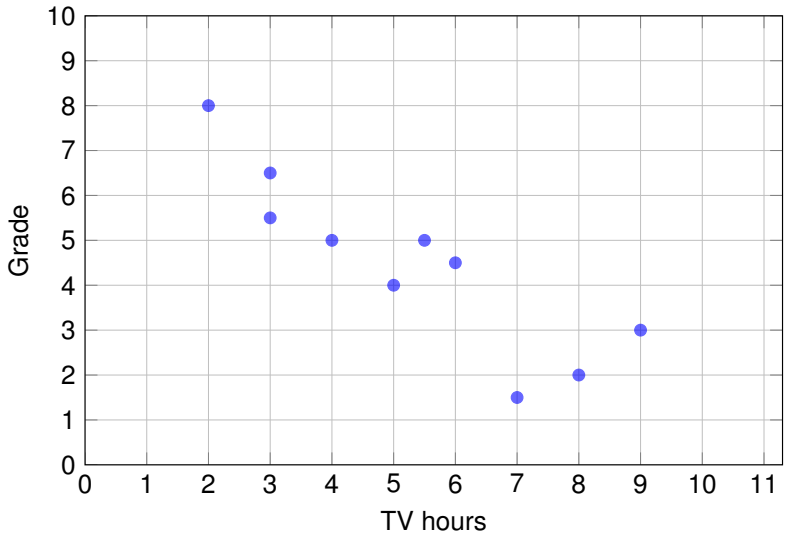

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Any prediction comes with risk and potential error!

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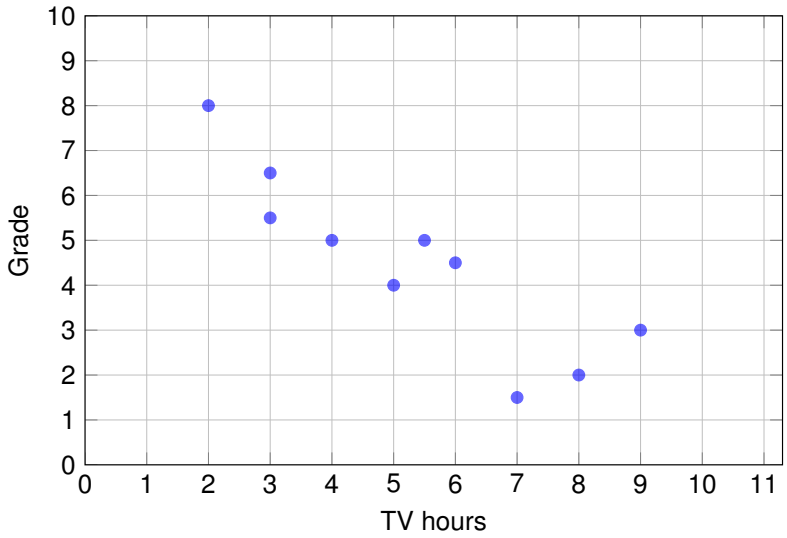

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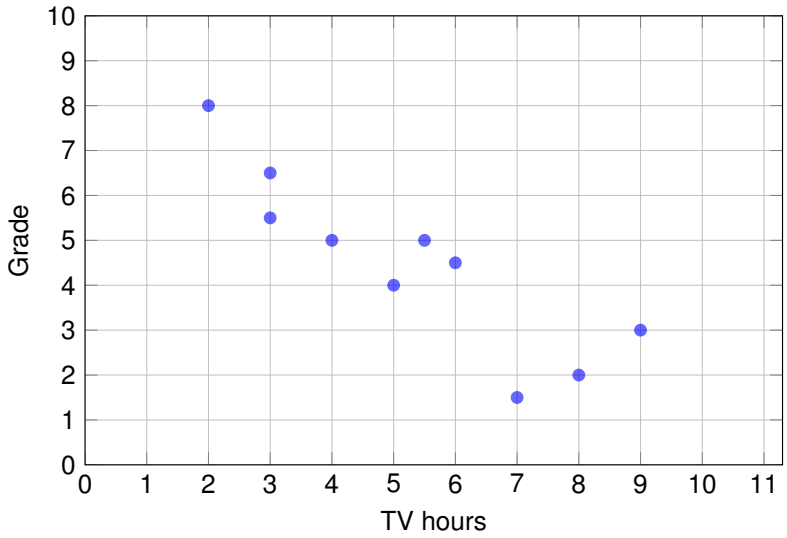

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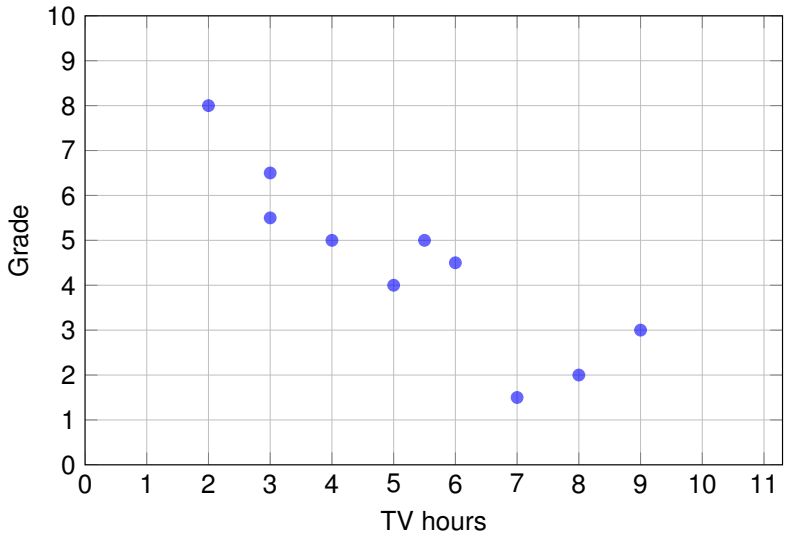

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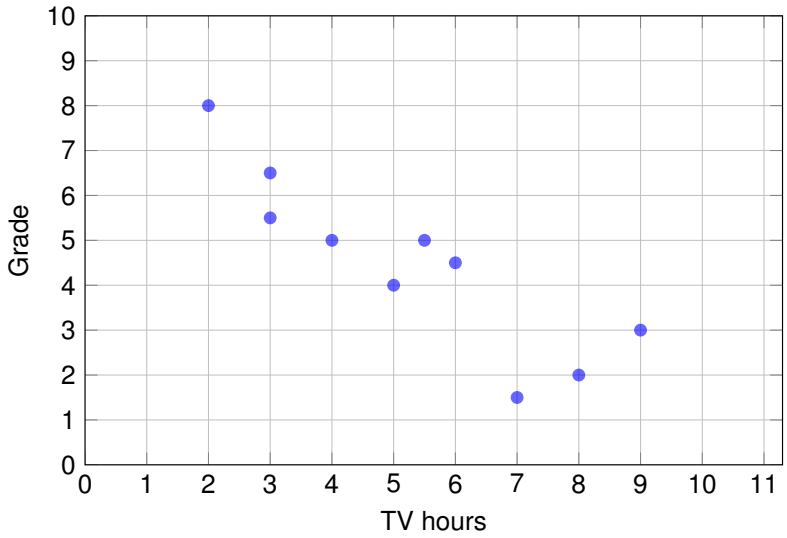

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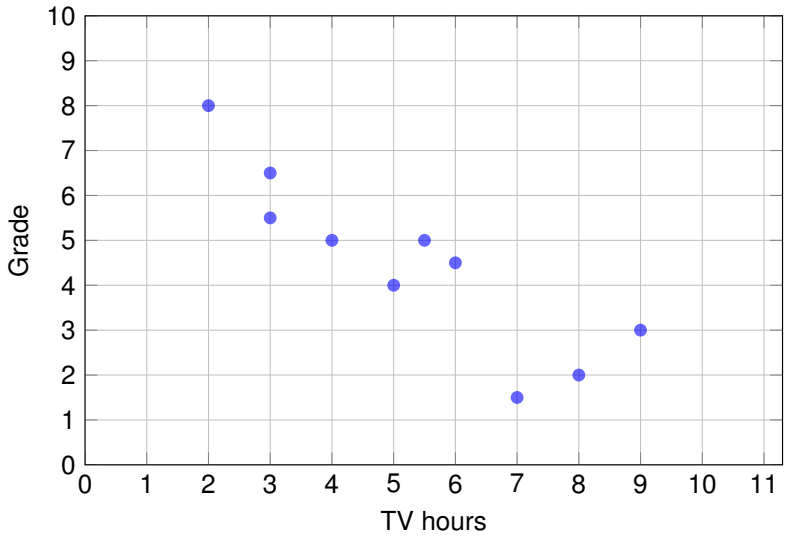

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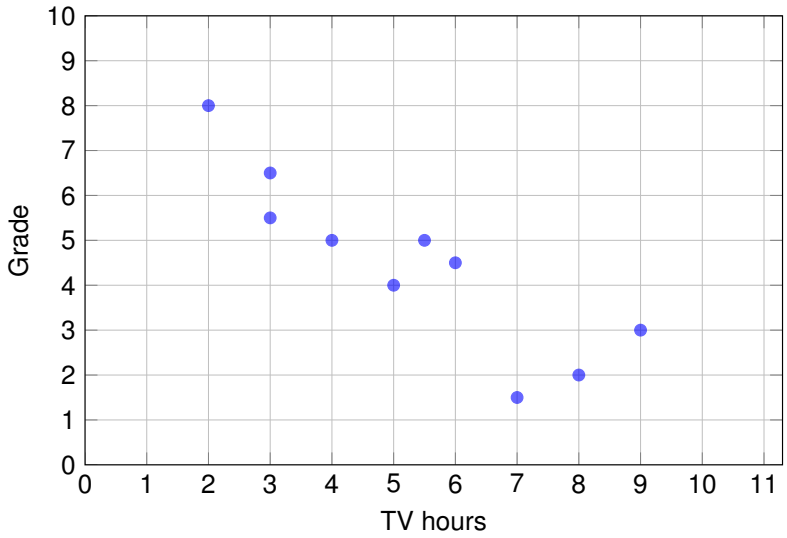

Ex 1: Guess grade for Student 11

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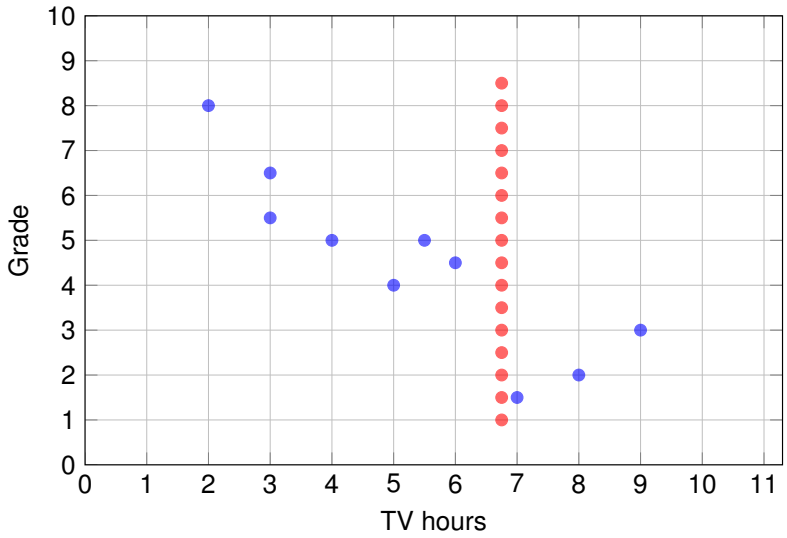

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Outline

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Linear Regression

Linear Regression with More than One Feature

Solving Linear Regression: Gradient Descent

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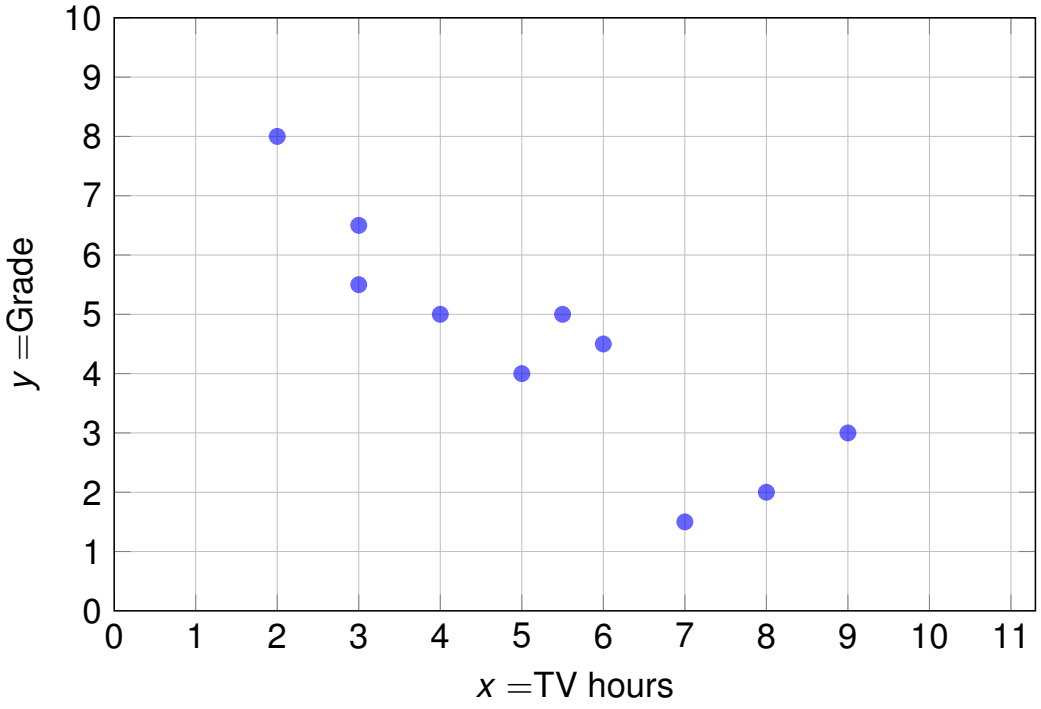
Goal: Find b and w so that $y \approx b + w \cdot x$ for most points.

Example of different Linear Models



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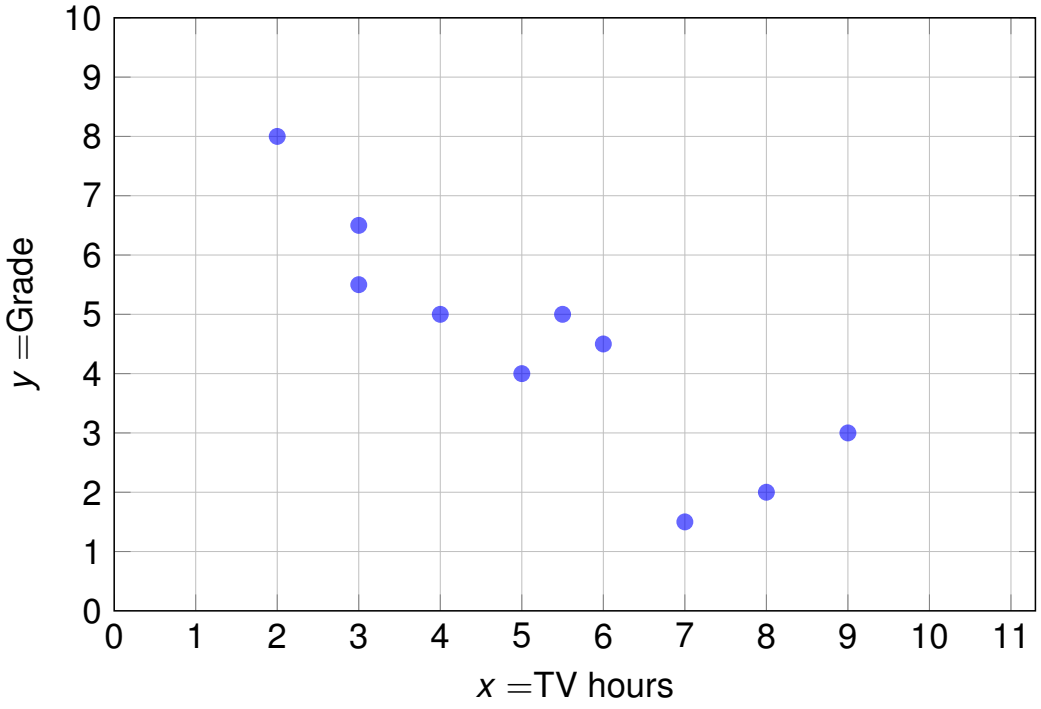

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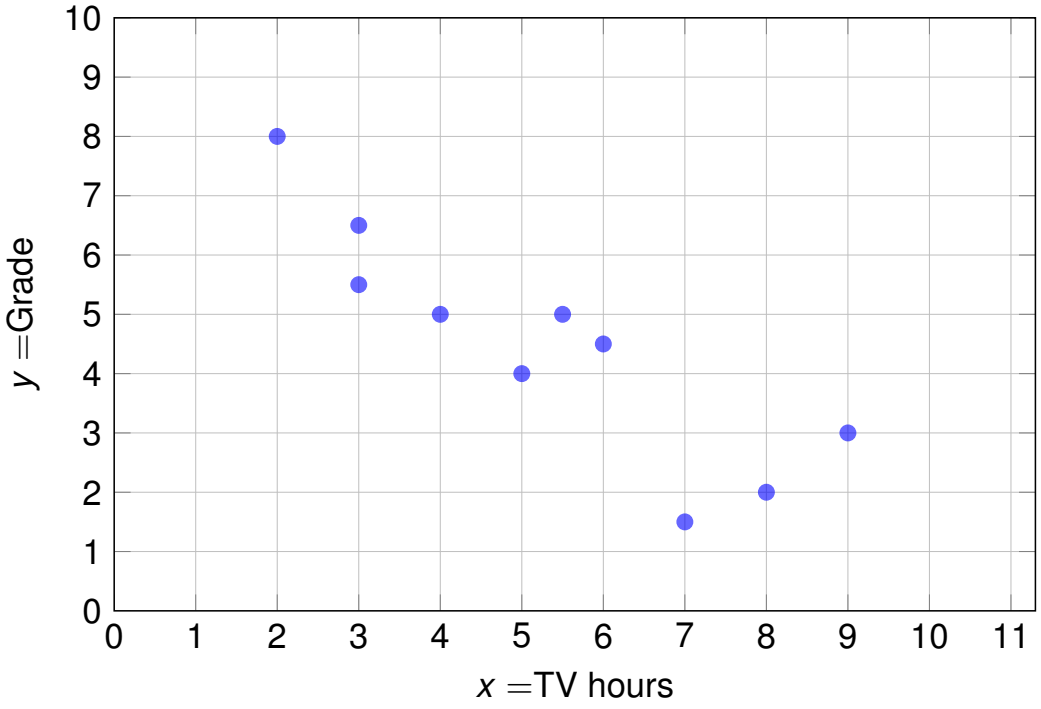

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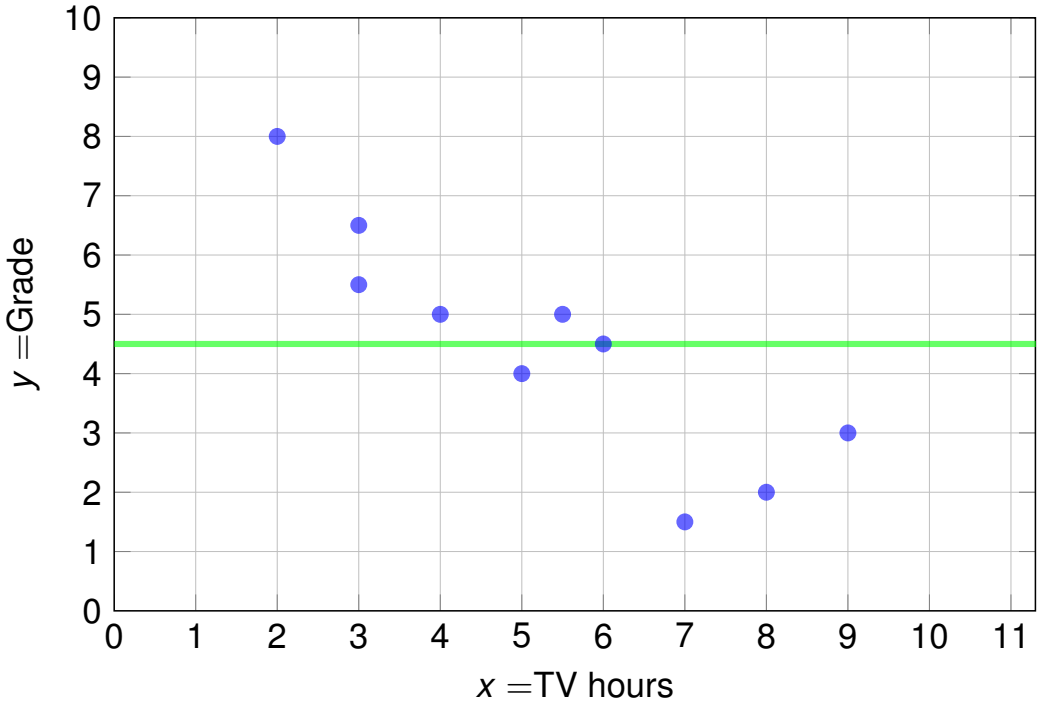

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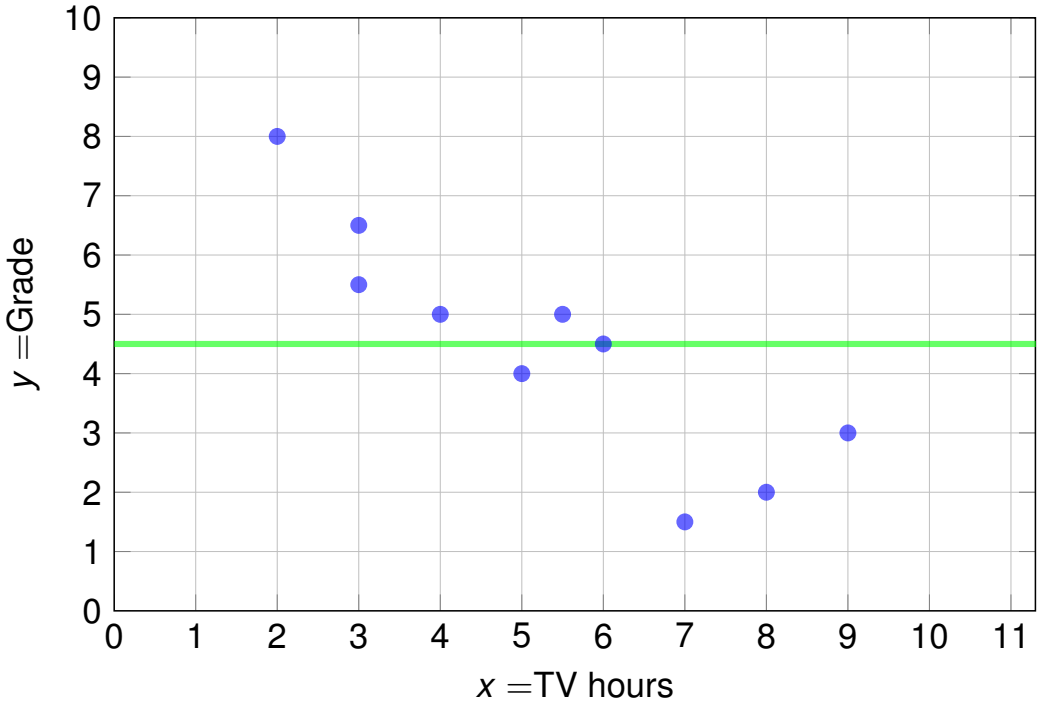

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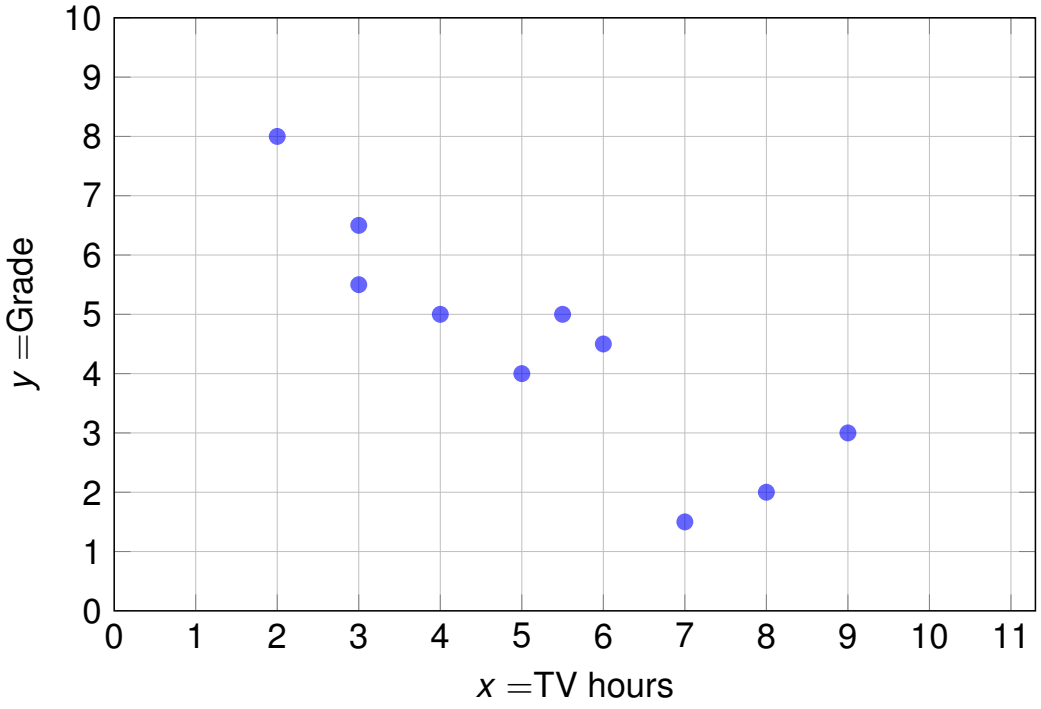

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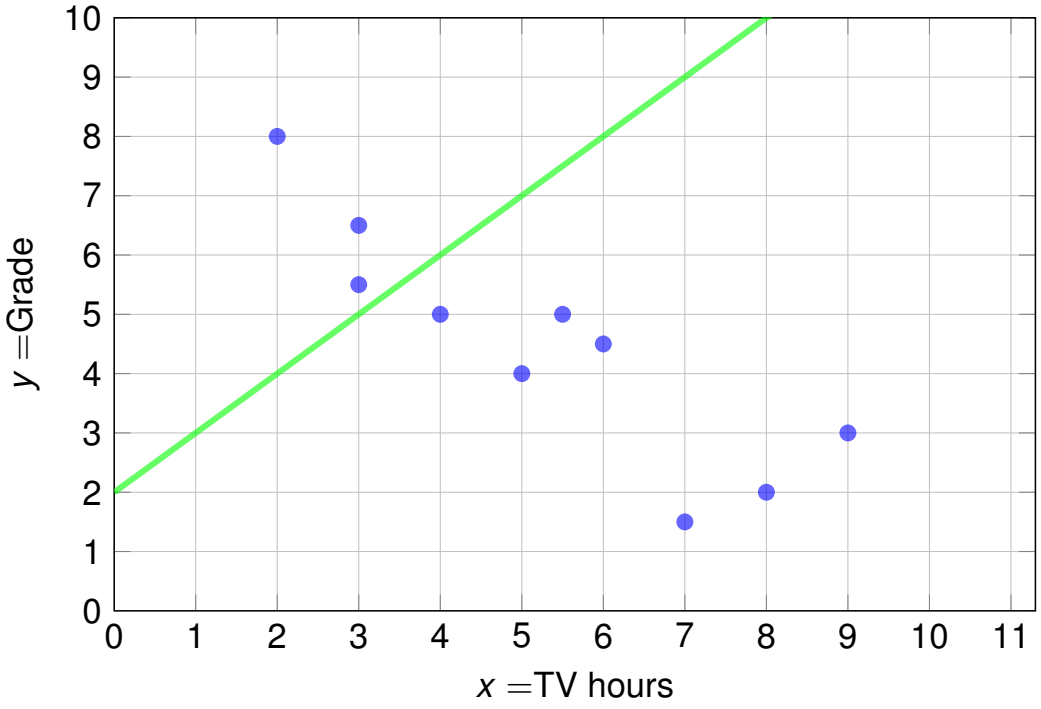

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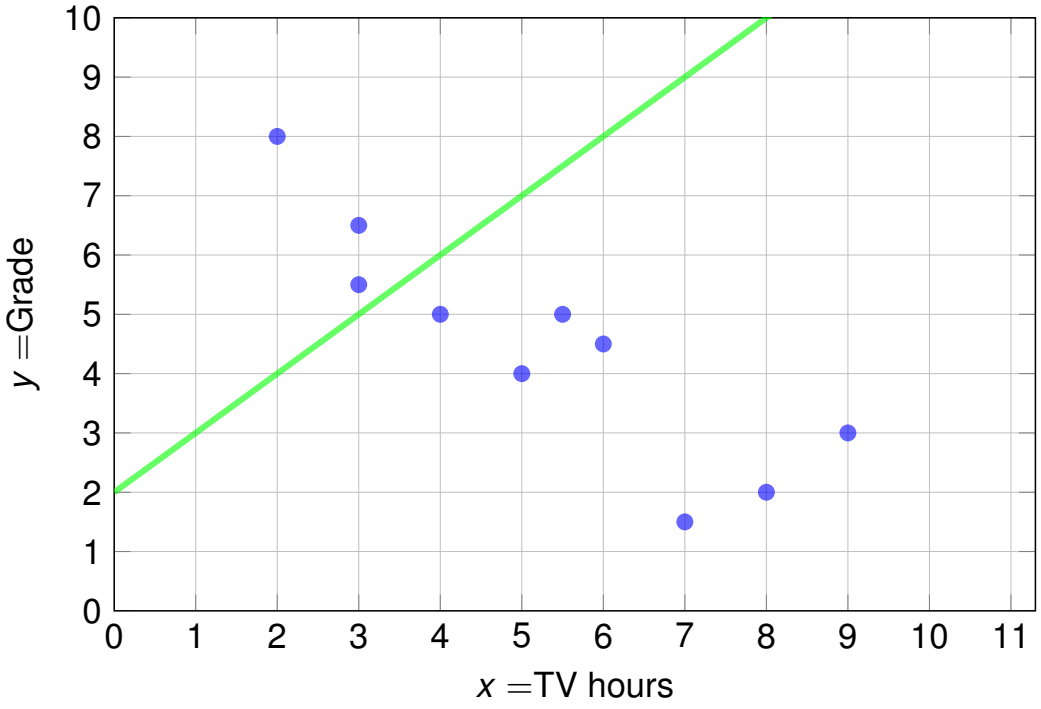

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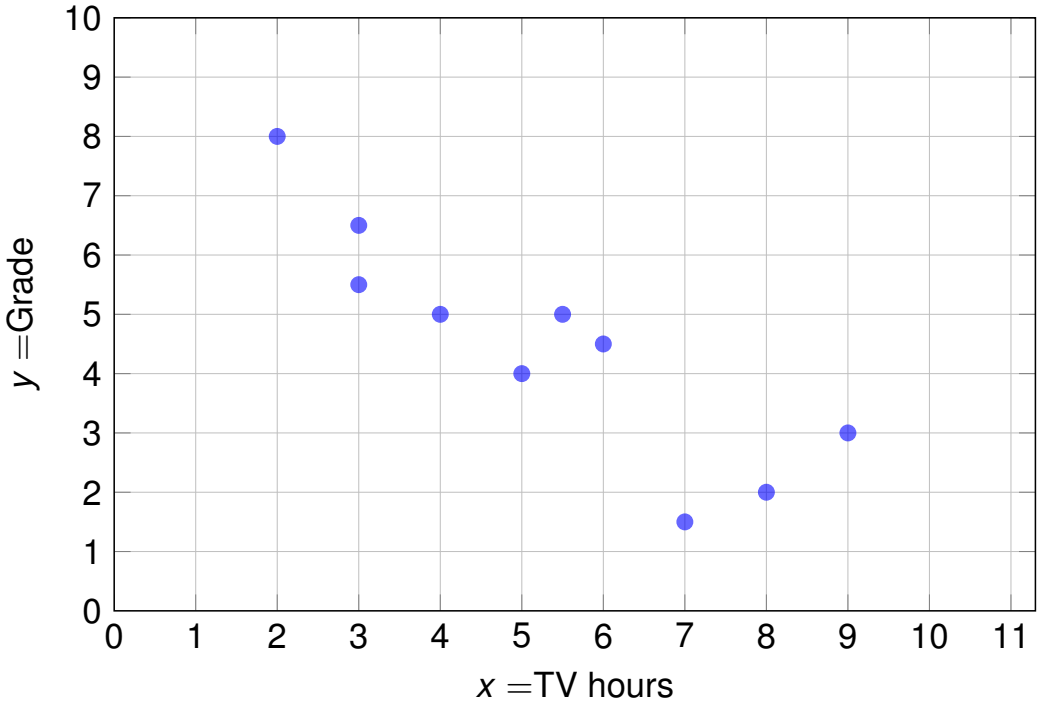

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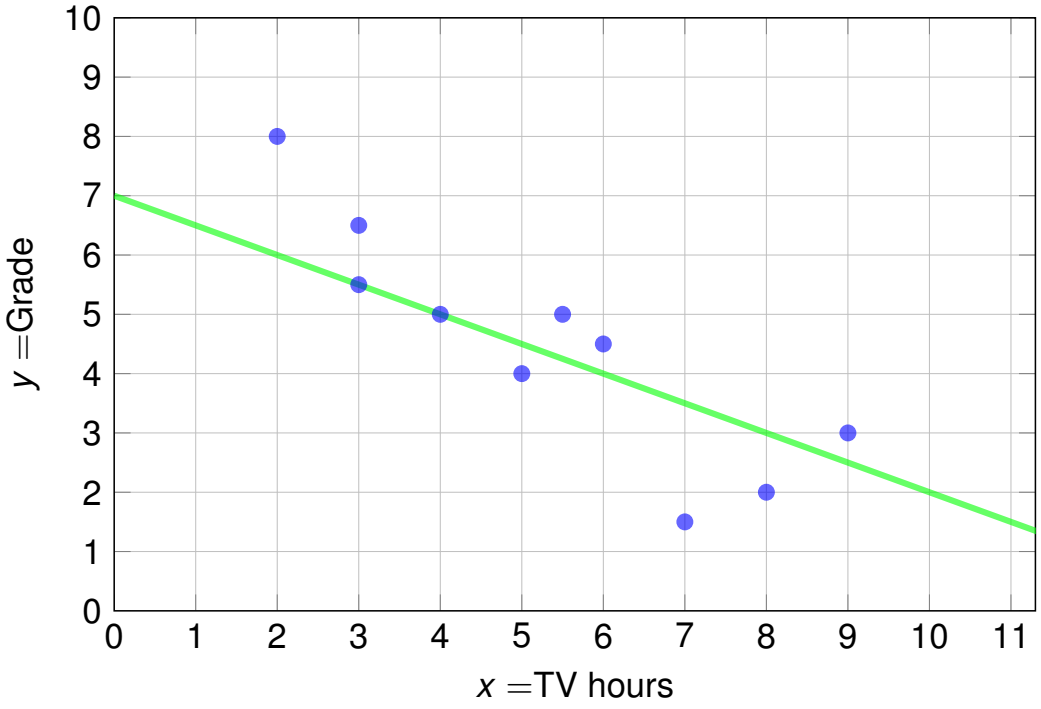

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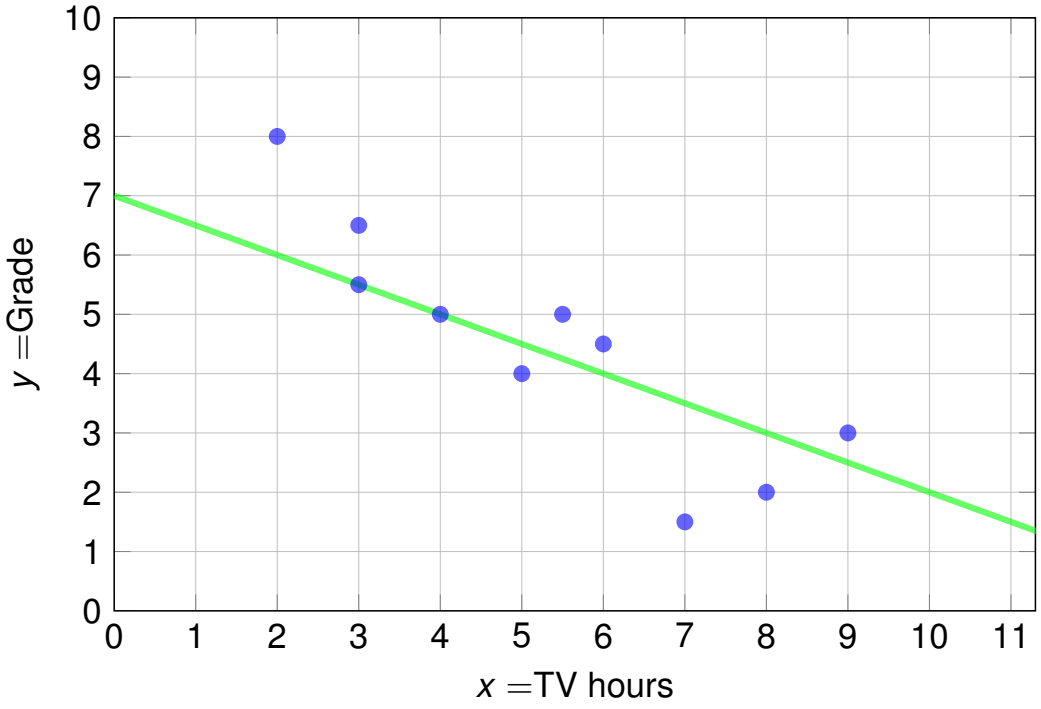

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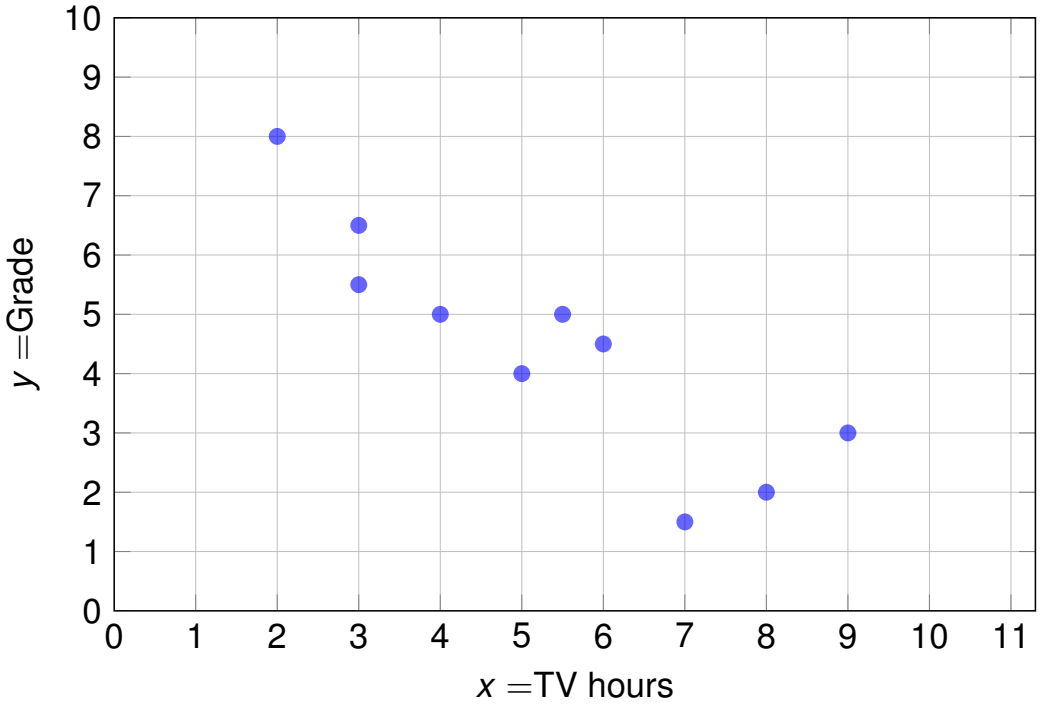

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How do we find a good linear model?

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Find the linear model which achieves the smallest error for the input points.

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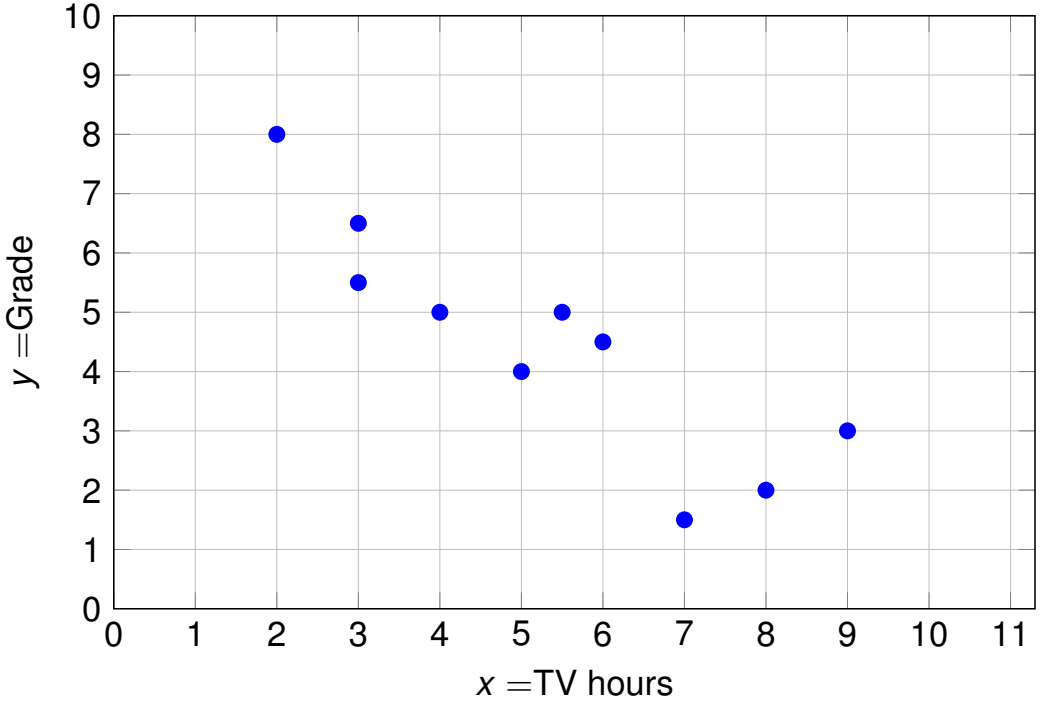

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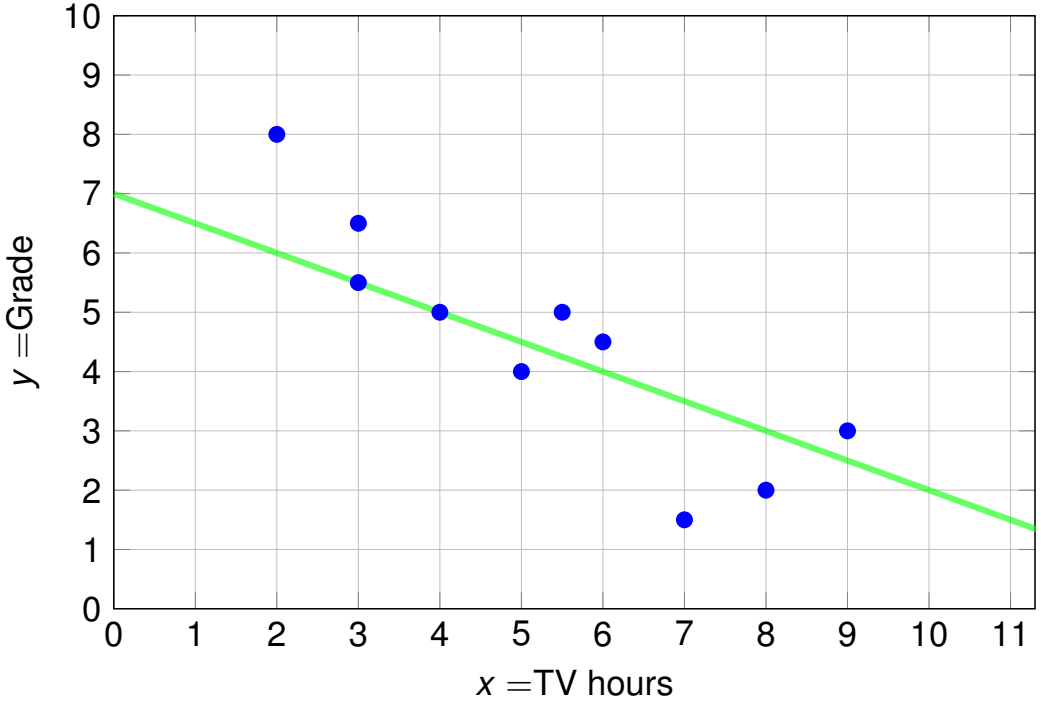

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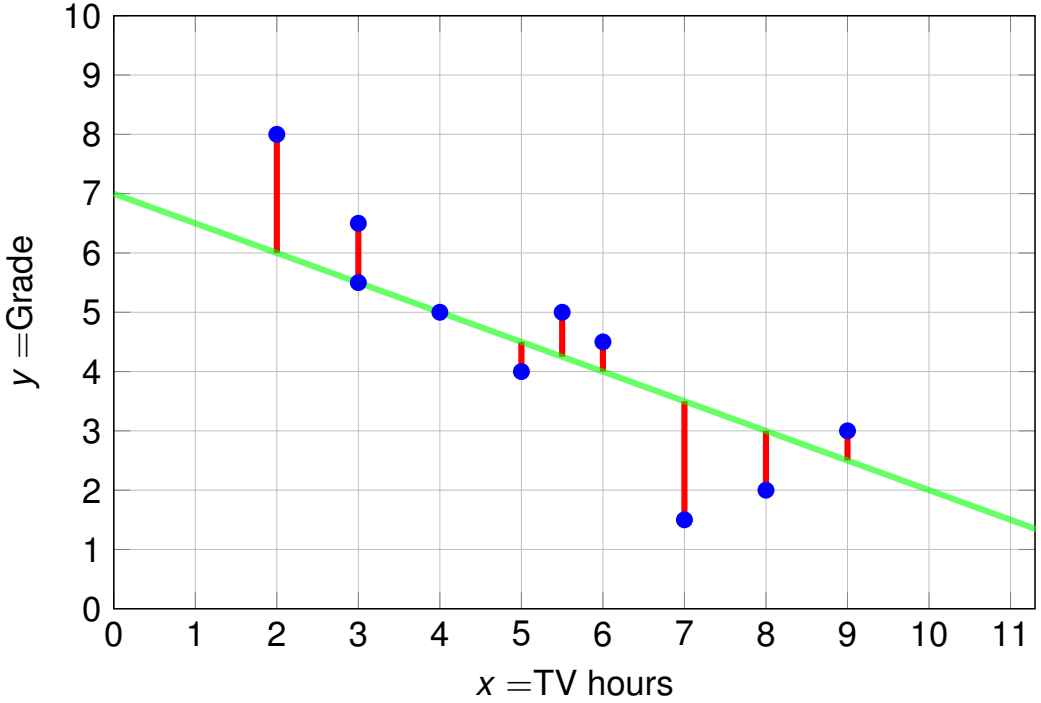

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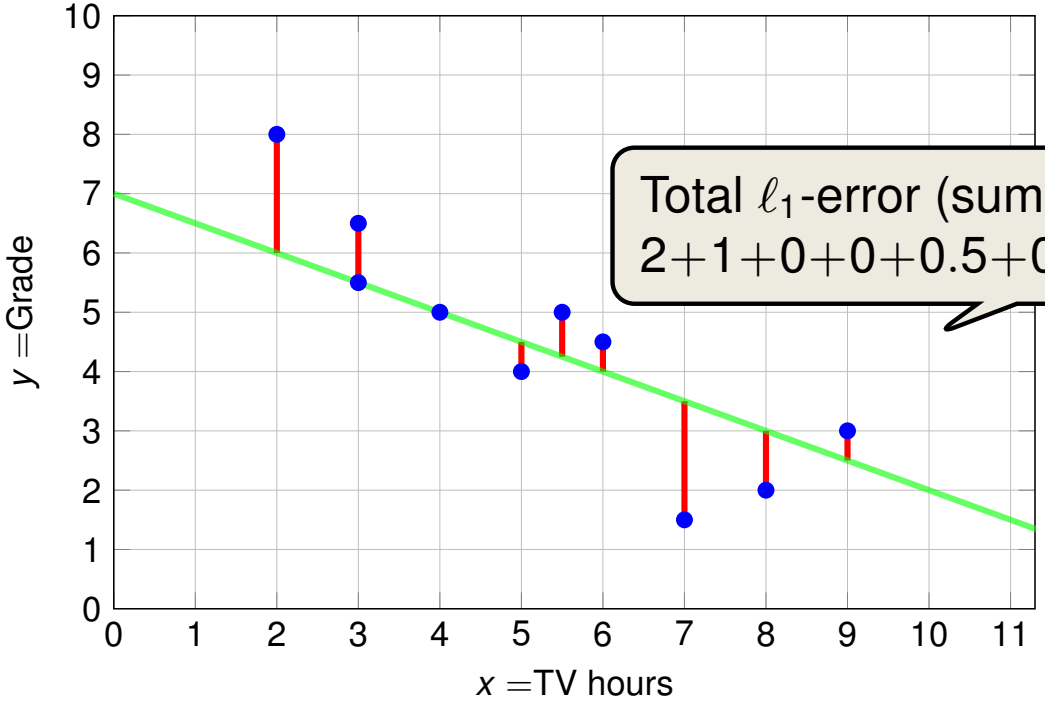

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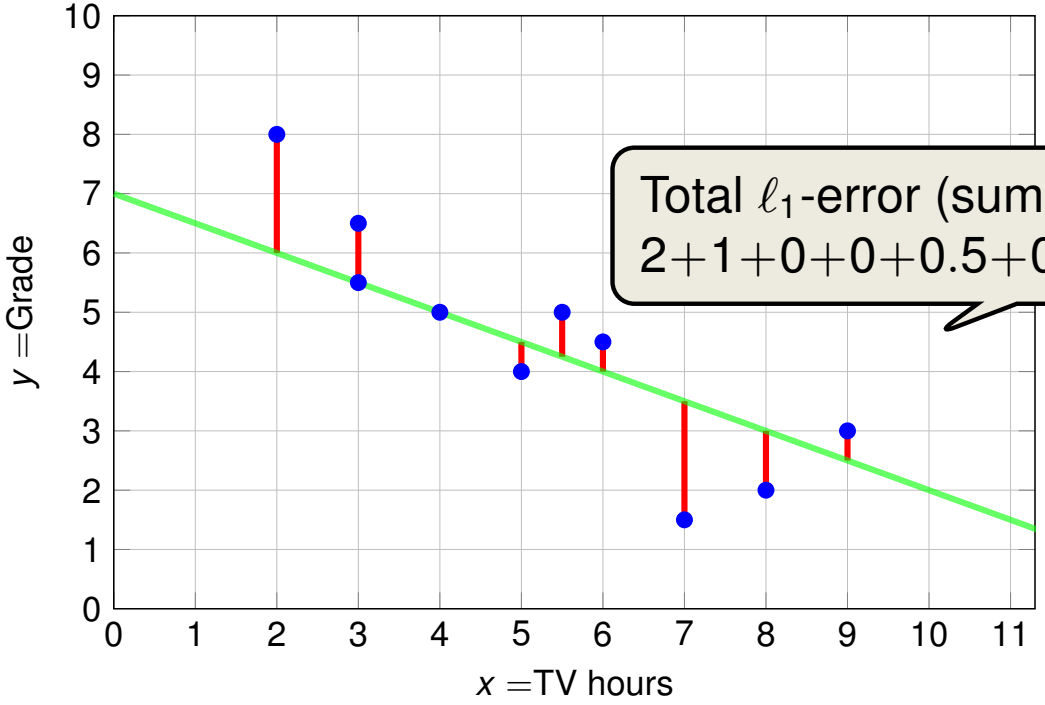

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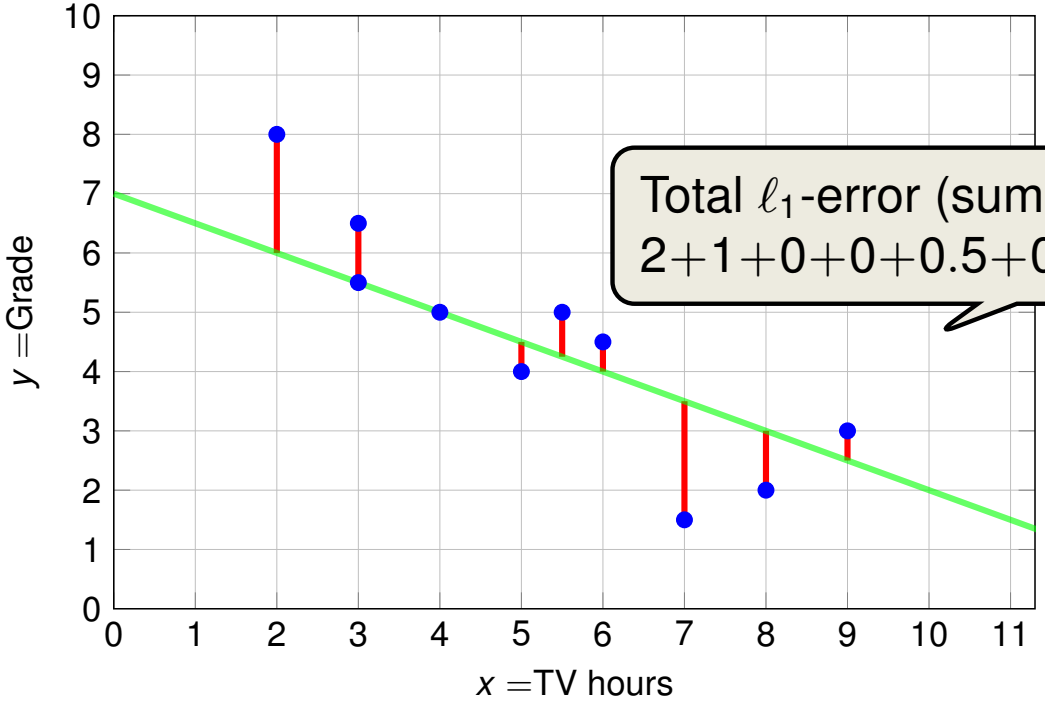

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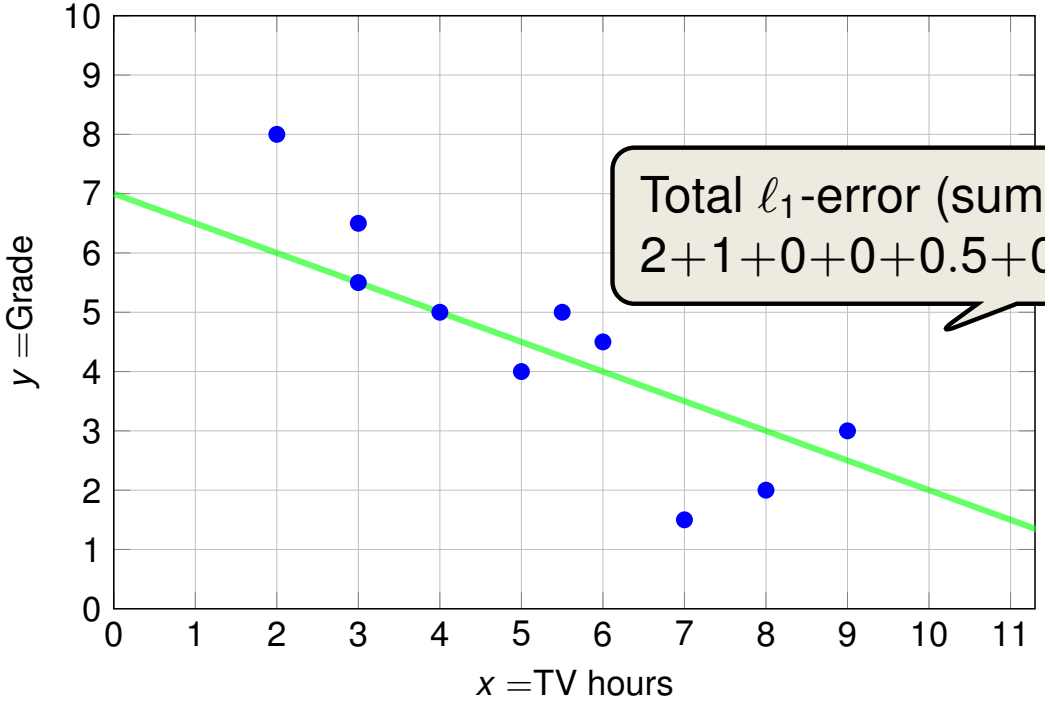

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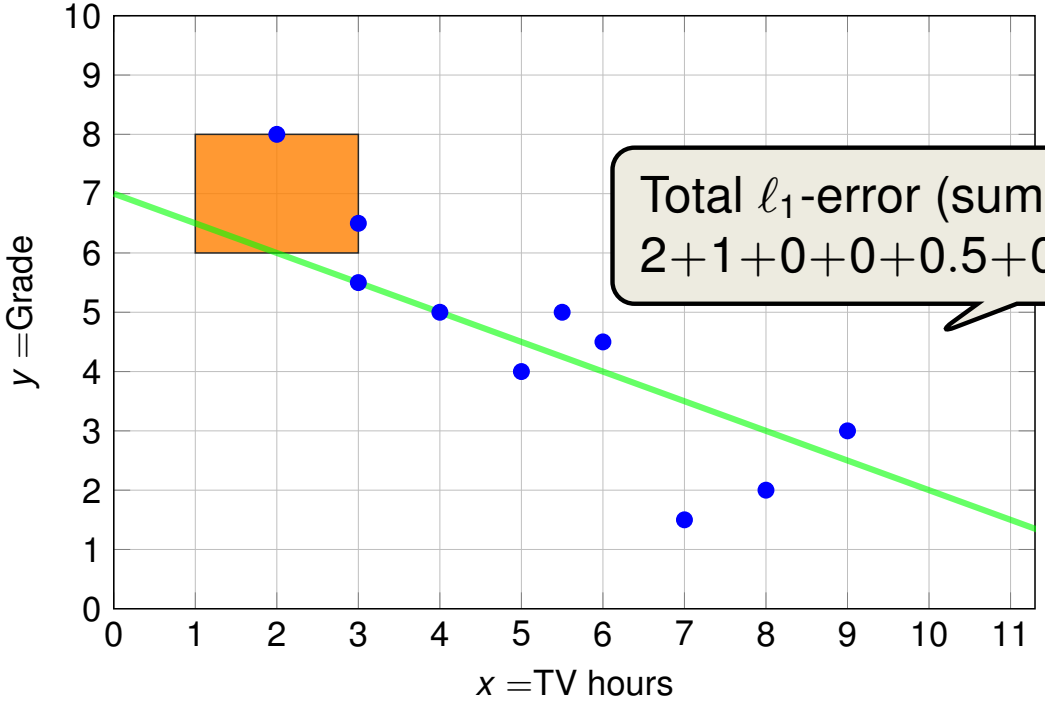

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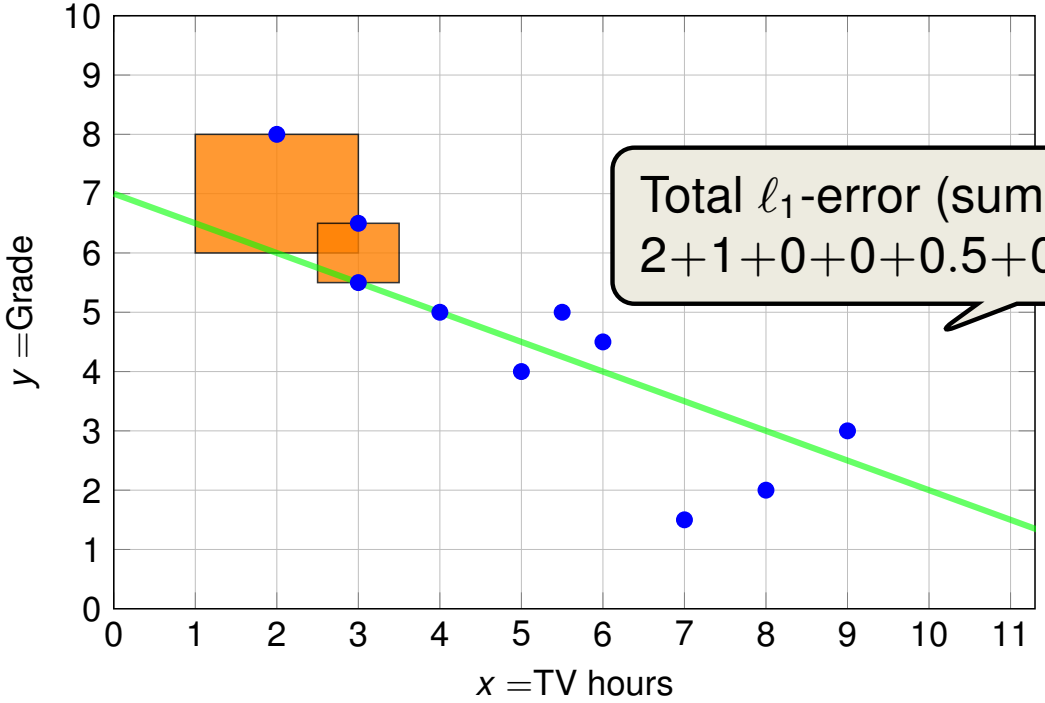

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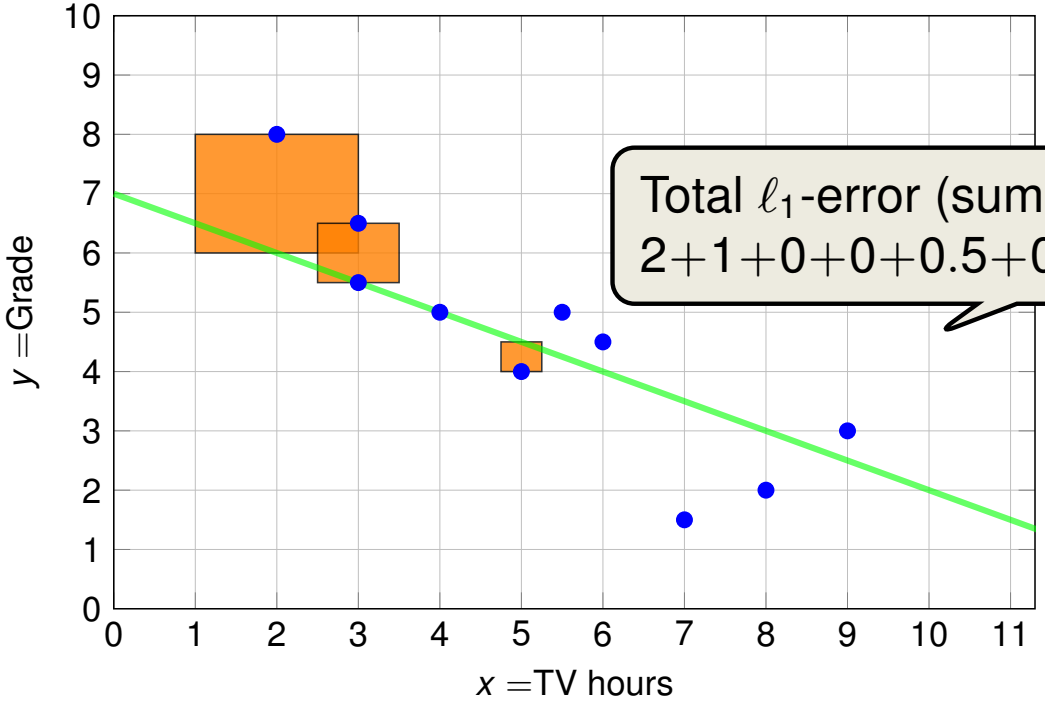

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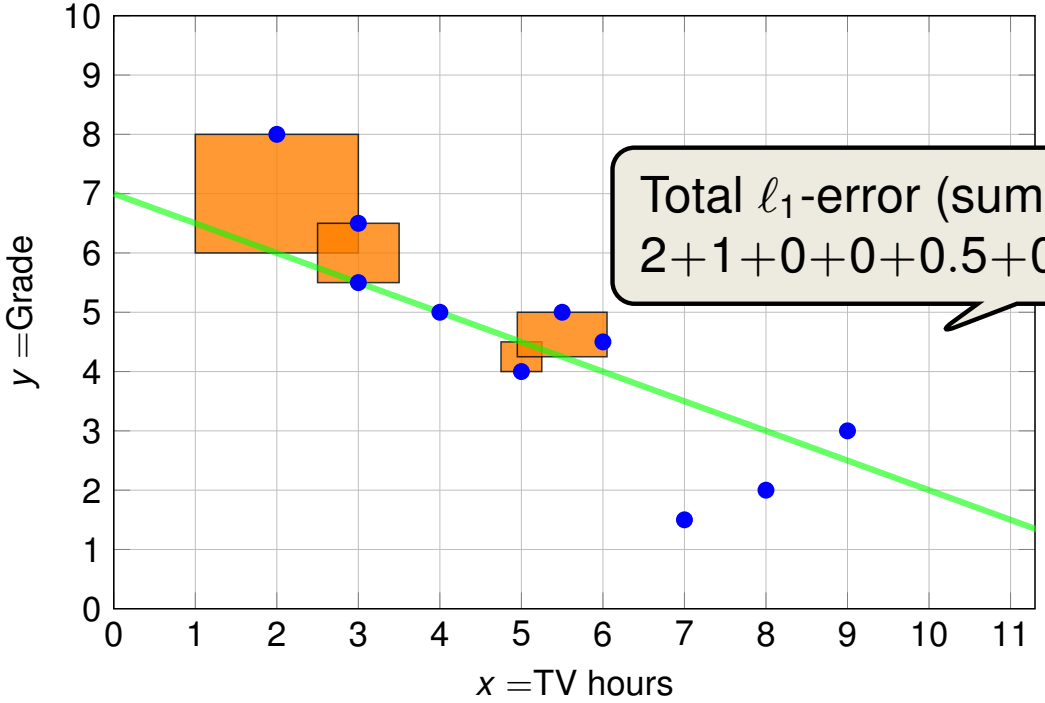

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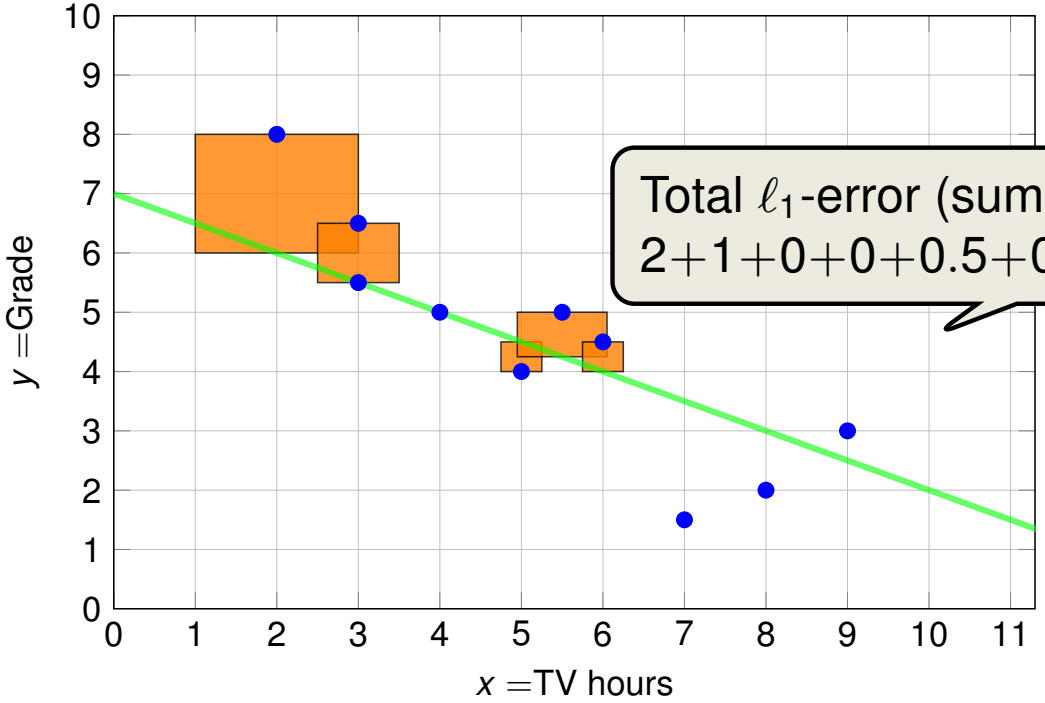

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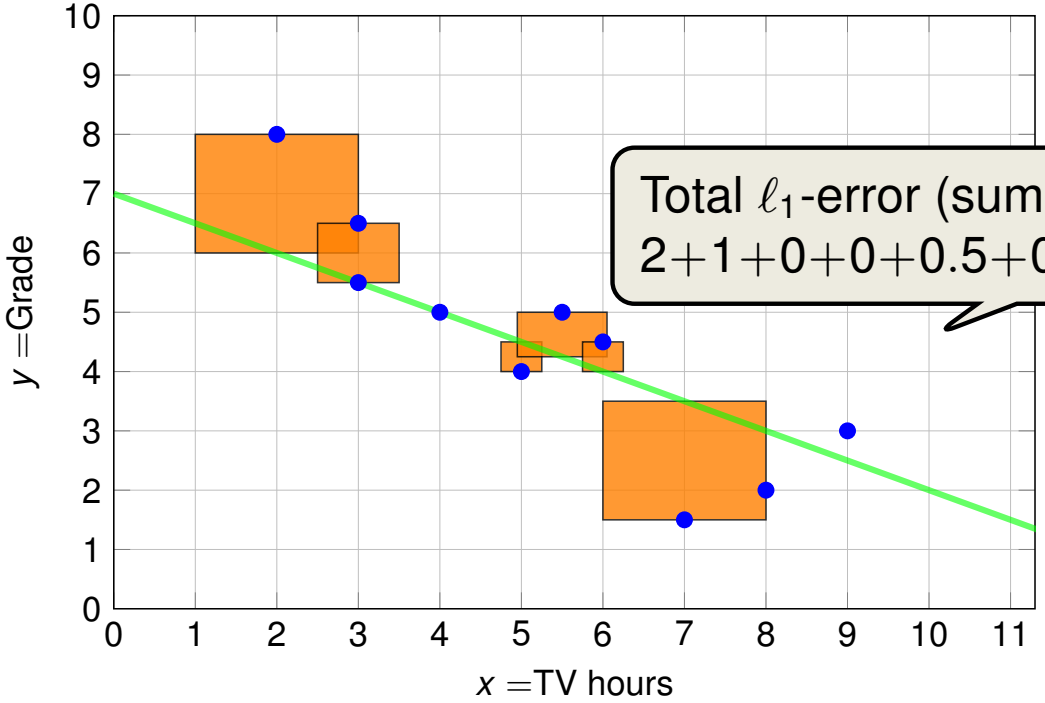

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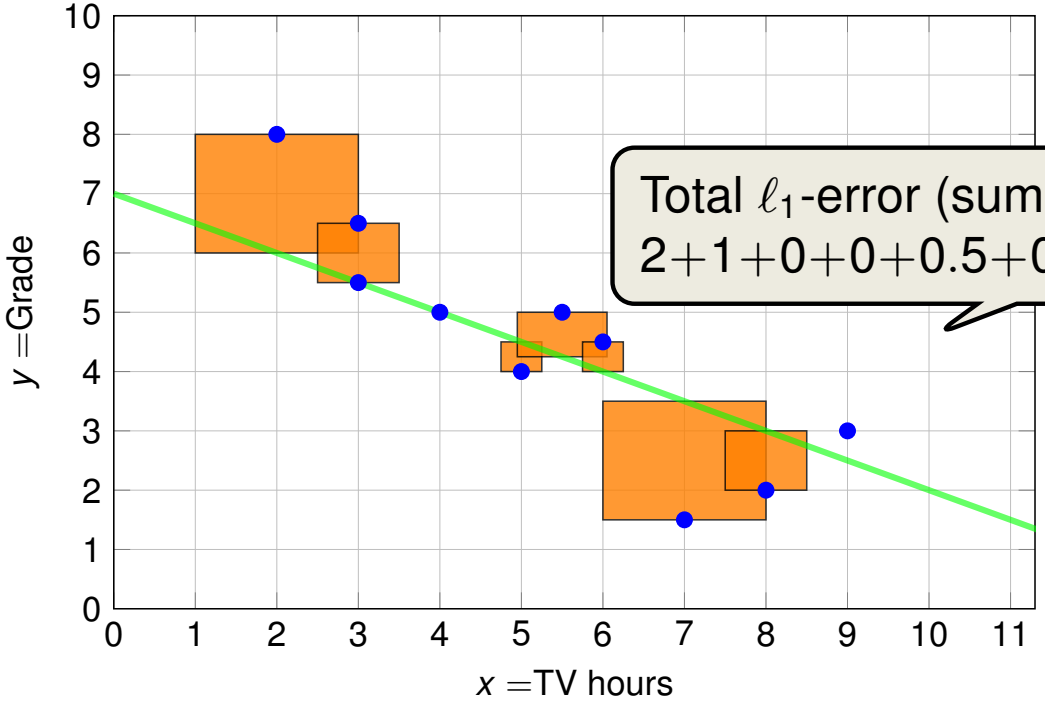

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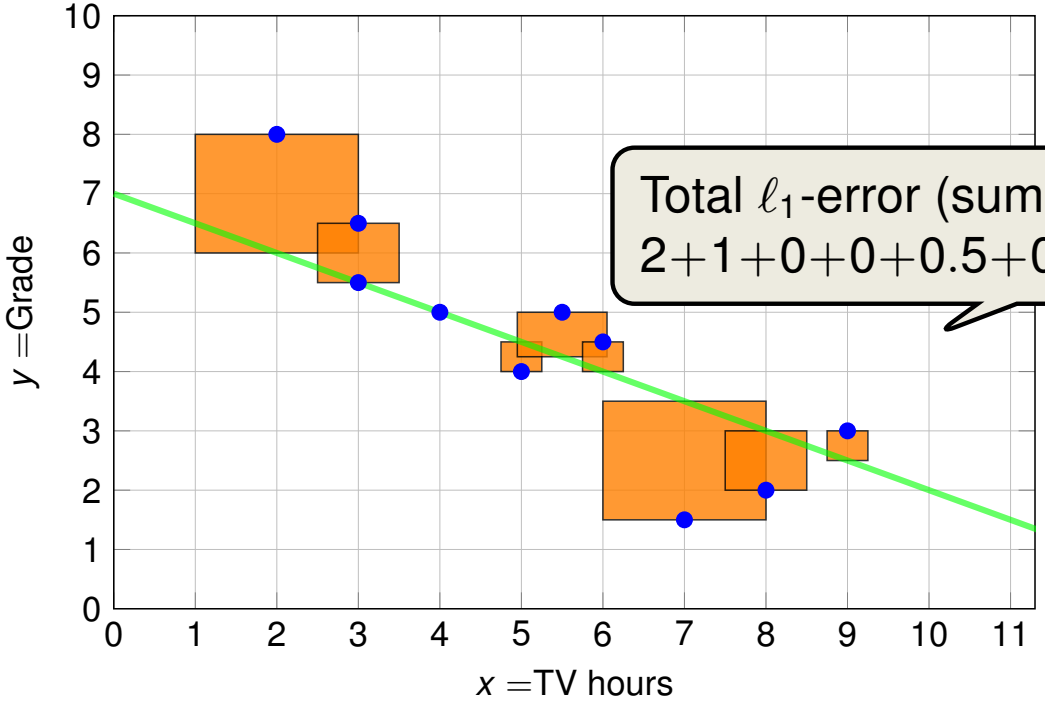

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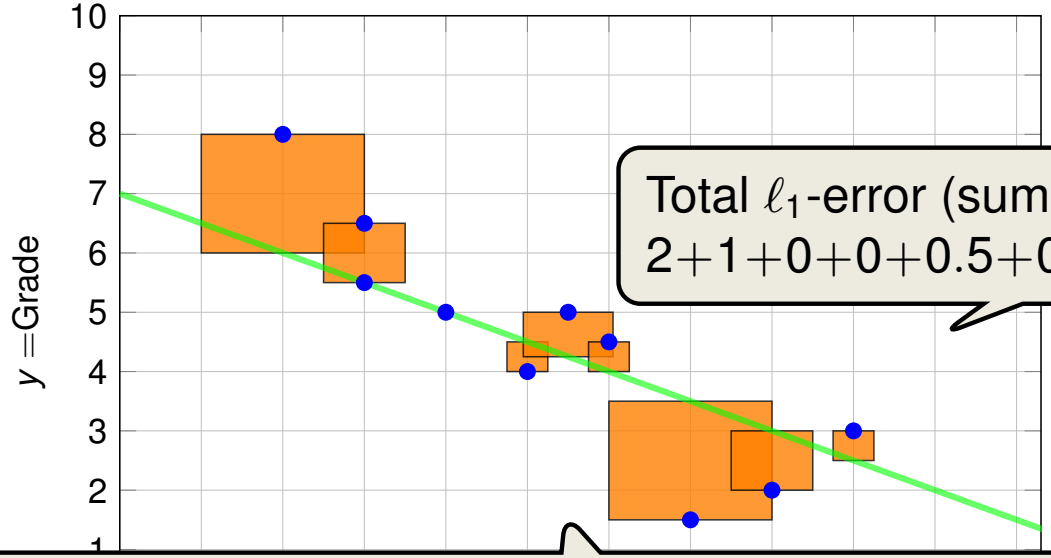

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$2^2+1^2+0+0+0.5^2+0.75^2+0.5^2+2^2+1^2+0.5^2 = 11.3125$

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C. Gauss (1777-1855)

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Direct Solution

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- Then

$$w = \frac{\sum_{i=1}^{n} (x_i - \overline{x}) \cdot (y_i - \overline{y})}{\sum_{i=1}^{n} (x_i - \overline{x})^2}$$

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6	8	2
7	3	6.5
8	5.5	5
9	7	1.5
10	9	3
Mean	5.25	4.5

- Step 1: Compute $\overline{x}$ and $\overline{y}$:

$$\overline{x} = 5.25, \qquad \overline{y} = 4.5$$

- Step 2: Compute slope w:

$$w = \frac{\sum_{i=1}^{10}(x_i - 5.25) \cdot (y_i - 4.5)}{\sum_{i=1}^{10}(x_i - 5.25)^2}$$

Conclusion of Simple Example (1/2)

Direct Solution

- Let $\overline{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$ and $\overline{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$
- Then

$$w = \frac{\sum_{i=1}^{n}(x_i - \overline{x}) \cdot (y_i - \overline{y})}{\sum_{i=1}^{n}(x_i - \overline{x})^2}$$

and $b = \overline{y} - w\overline{x}$.

Stud.	TV	Exam
1	2	8
2	4	5
3	3	5.5
4	5	4
5	6	4.5
6	8	2
7	3	6.5
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- Step 3: Compute intercept b:

$$b = 5.25 + 0.7611 \cdot 5.25$$

Conclusion of Simple Example (1/2)

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Stud.	TV	Exam	Pred.
1	2	8	
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and $b = \overline{y} - w\overline{x}$.

Stud.	TV	Exam	Pred.
1	2	8	6.97
2	4	5	5.45
3	3	5.5	6.21
4	5	4	4.69
5	6	4.5	3.93
6	8	2	2.41
7	3	6.5	6.21
8	5.5	5	4.31
9	7	1.5	3.16
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- Let $\overline{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$ and $\overline{y} = \frac{1}{n}\sum_{i=1}^{n} y_i$
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Total ℓ_2-error is only

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Total ℓ_2-error is only 7.908!

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- Step 3: Compute intercept b:

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Conclusion of Simple Example (2/2)

$$y = 8.496 - 0.7611 \cdot x$$

Student	TV hours	Exam Grade
1	2	8
2	4	5
3	3	5.5
4	5	4
5	6	4.5
6	8	2
7	3	6.5
8	5.5	5
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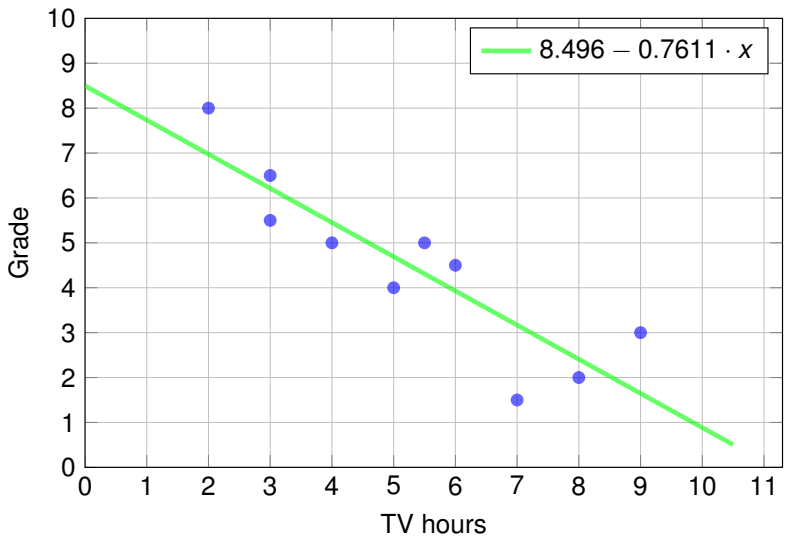

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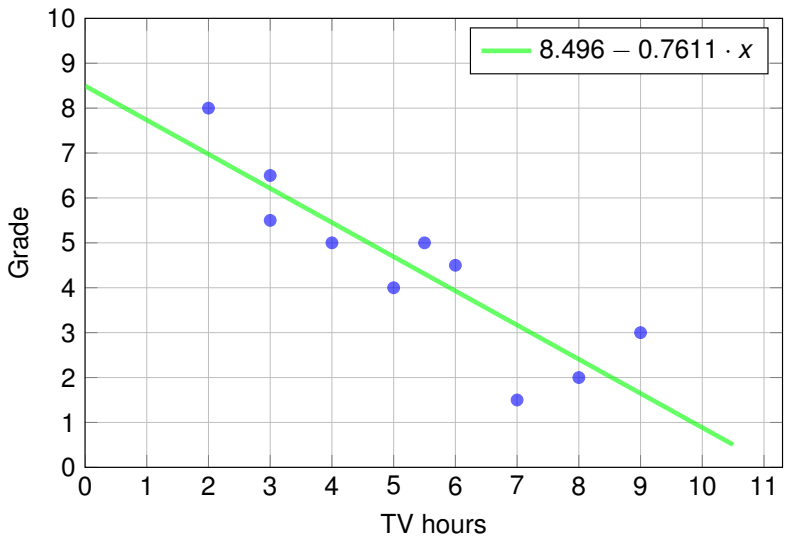
9	7	1.5
10	9	3
11	6.75	??



Which grade do you predict for Student 11?

Conclusion of Simple Example (2/2)

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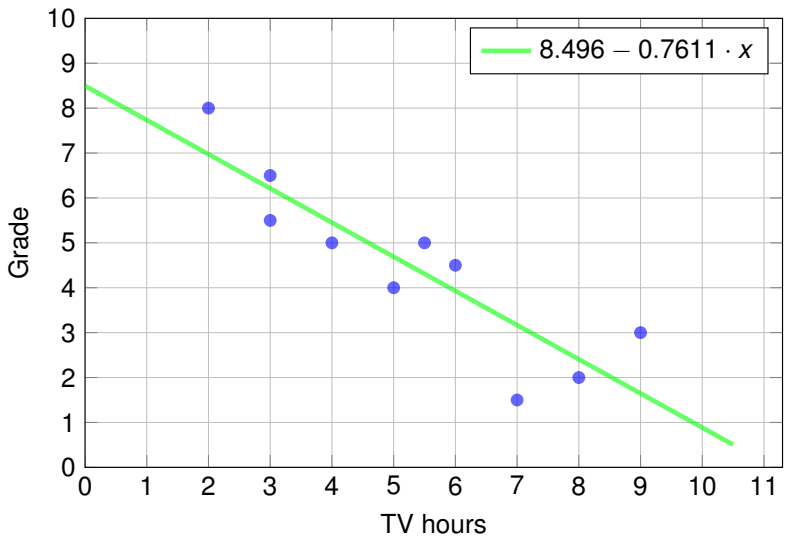

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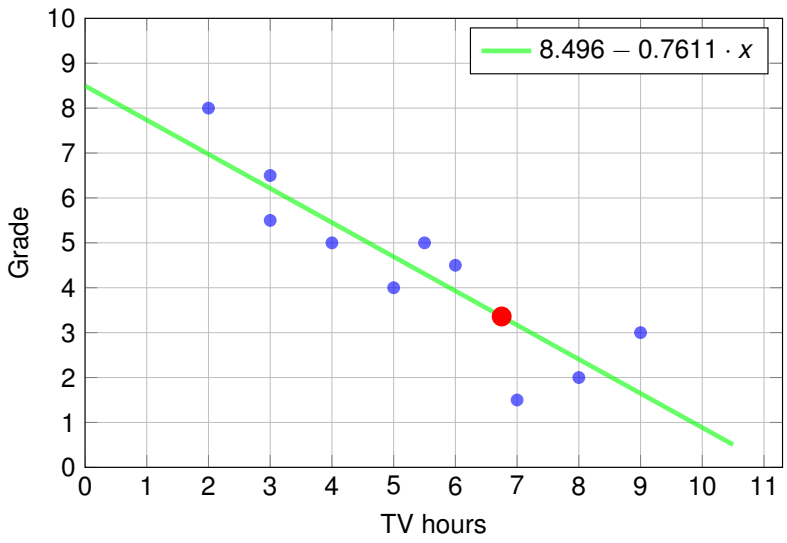

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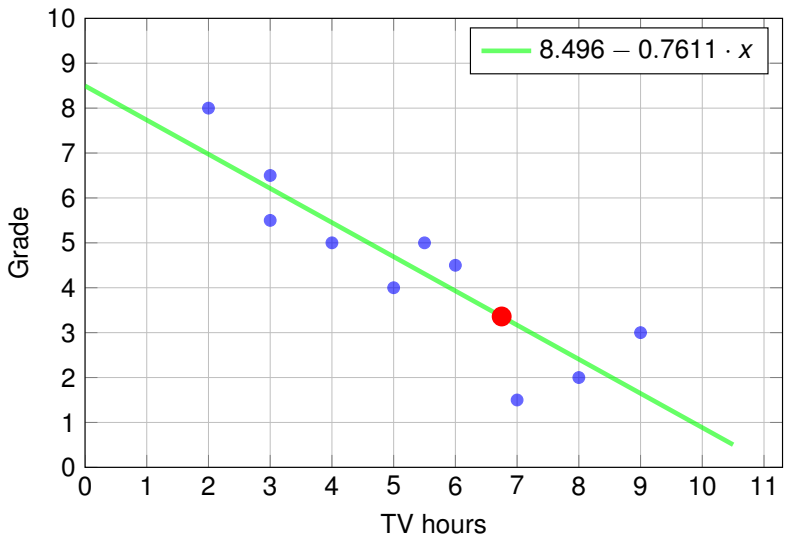

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Is this an accurate answer?

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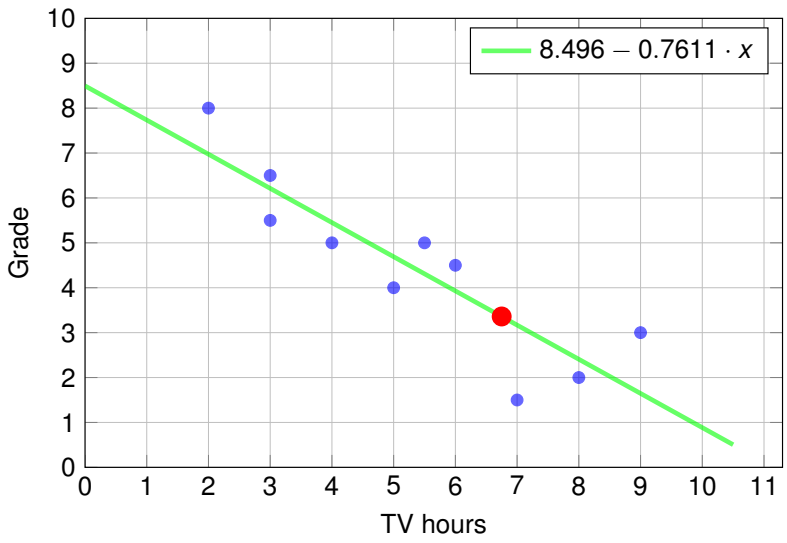

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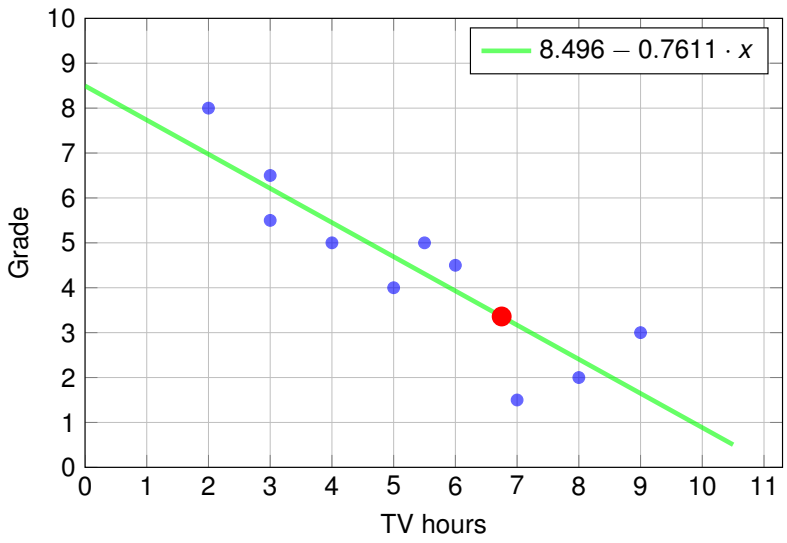

Which grade do you predict for Student 11?

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- Yes (based on the current data and linearity assumption!)
- Methods: A) use test data set for validation

Conclusion of Simple Example (2/2)

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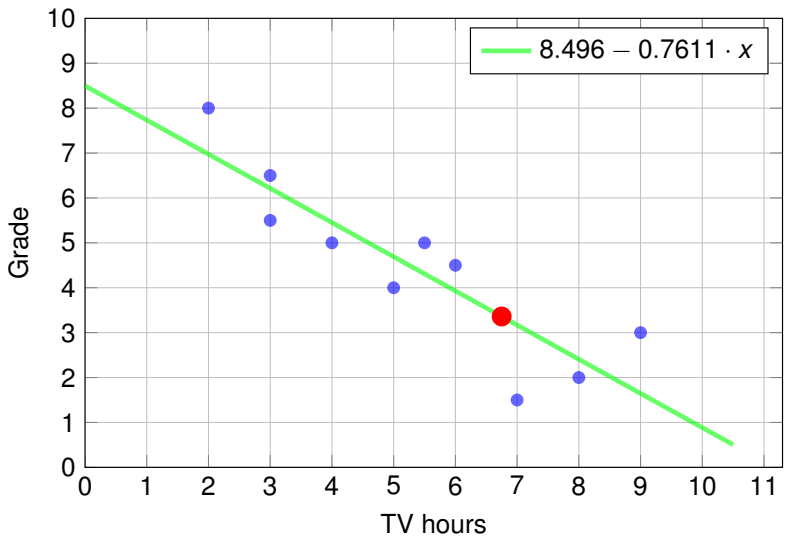

Which grade do you predict for Student 11?

Is this an accurate answer?

- Yes (based on the current data and linearity assumption!)
- Methods: A) use test data set for validation or, B) use probabilistic model $y = b + wx + \mathcal{N}(0, \sigma)$ for some variance σ^2

Conclusion of Simple Example (2/2)

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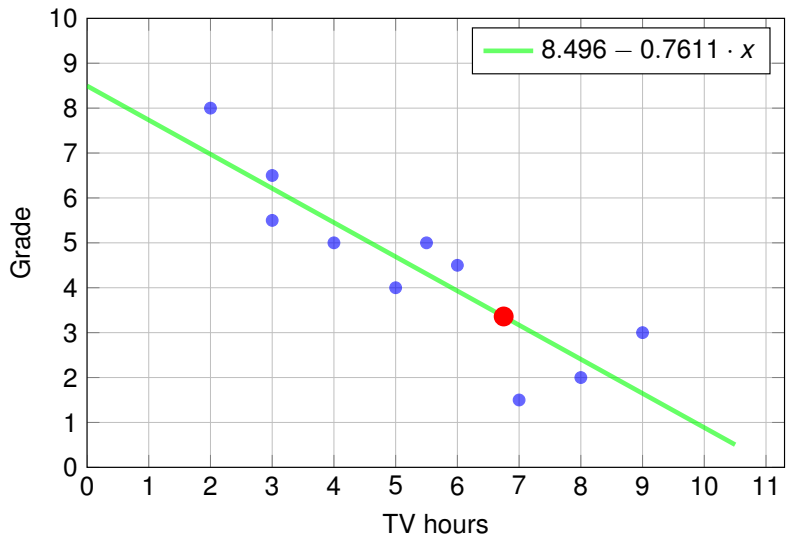

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A) Is our model biased?

Conclusion of Simple Example (2/2)

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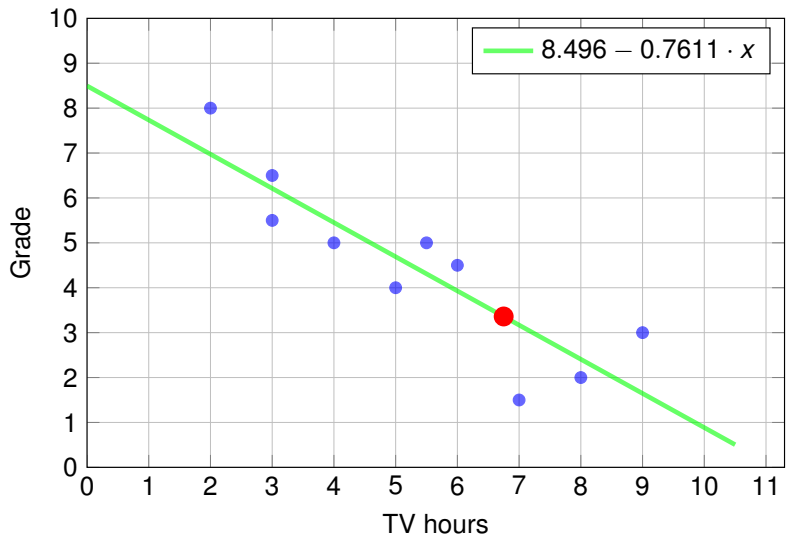

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A) Is our model biased?

B) Is the data too noisy?

Bias versus Variance

In general, predictions by a model could be wrong due to:

Bias versus Variance

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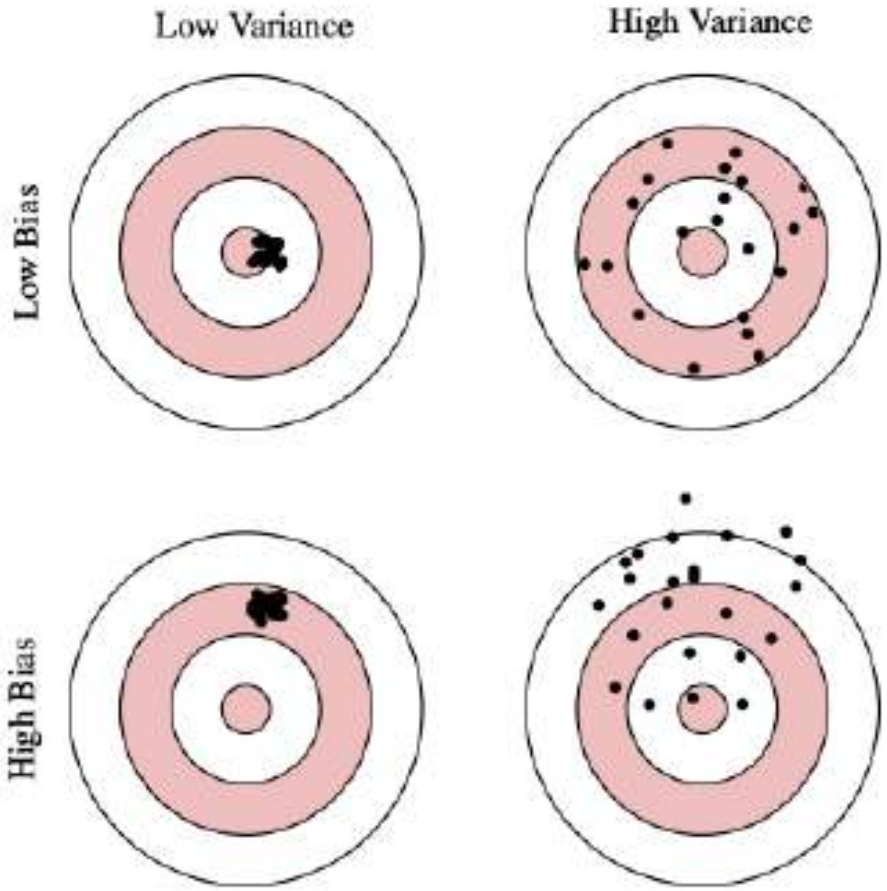
- High Bias: our model does not match the data well

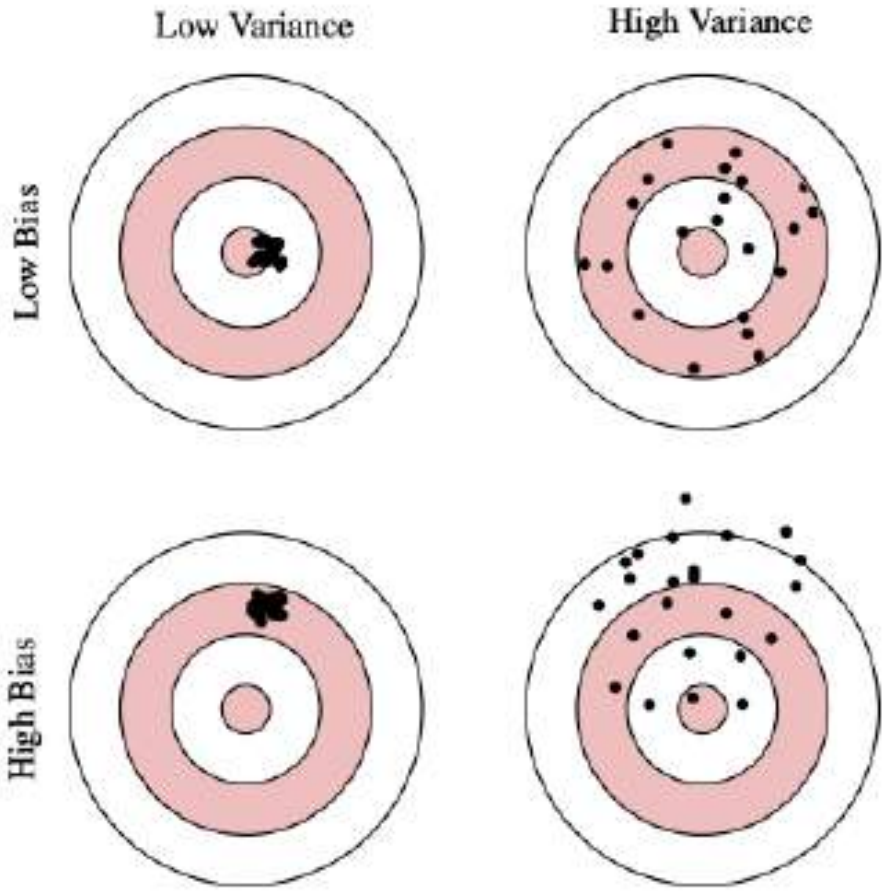


Source: Edwin Leuven (Point Estimation)

Bias versus Variance

In general, predictions by a model could be wrong due to:

- High Bias: our model does not match the data well
- High Variance: data set is inherently noisy, accurate prediction impossible



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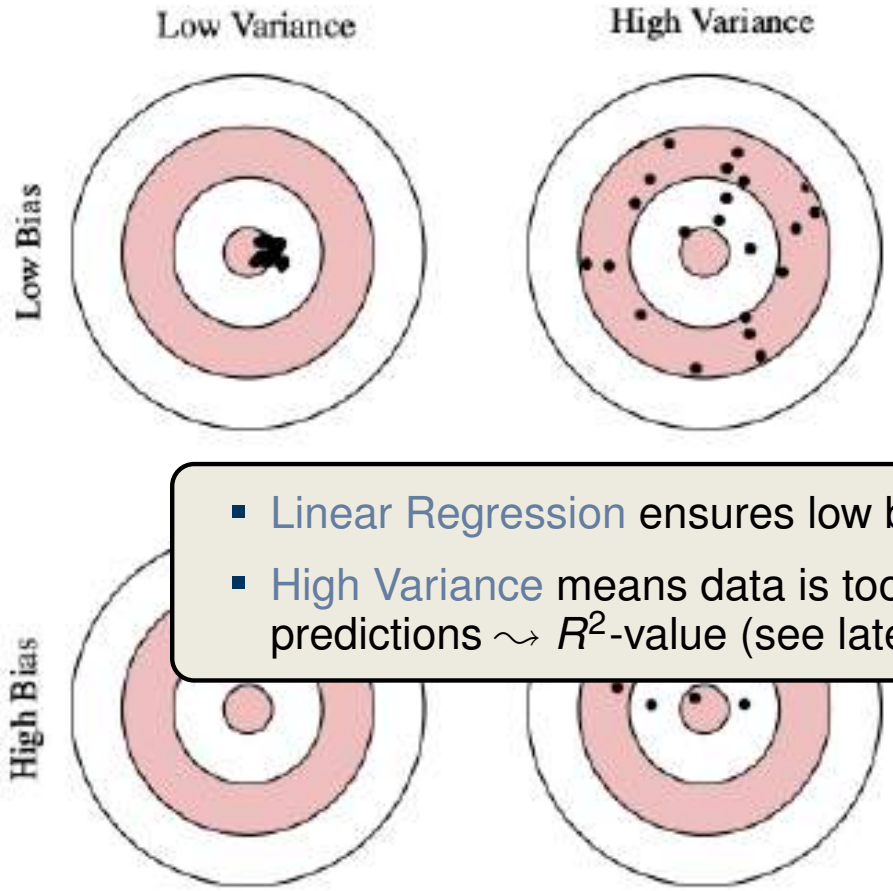

- Linear Regression ensures low bias
- High Variance means data is too noisy for predictions $\rightsquigarrow$ R^2-value (see later)!

Source: Edwin Leuven (Point Estimation)

Outline

Introduction

Linear Regression

Linear Regression with More than One Feature

Solving Linear Regression: Gradient Descent

Logistic Regression

Expanding the Data Set

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1	2	8
2	4	5
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Expanding the Data Set

Student	TV hours	Homework Perf.	Exam Grade
1	2	7	8
2	4	6	5
3	3	4	5.5
4	5	5	4
5	6	3	4.5
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7	3	6	6.5
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7	3	6	6.5
8	5.5	7	5
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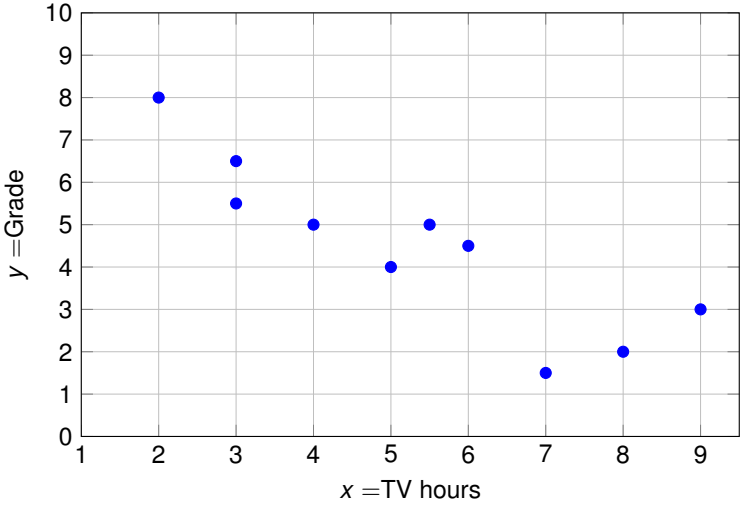
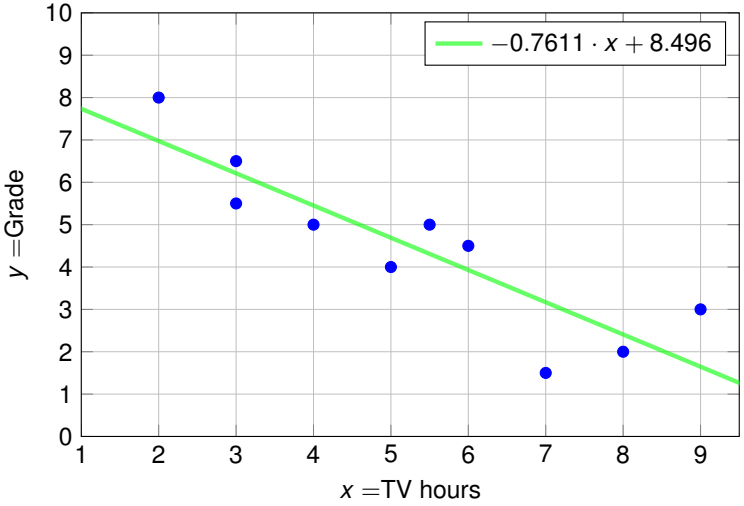
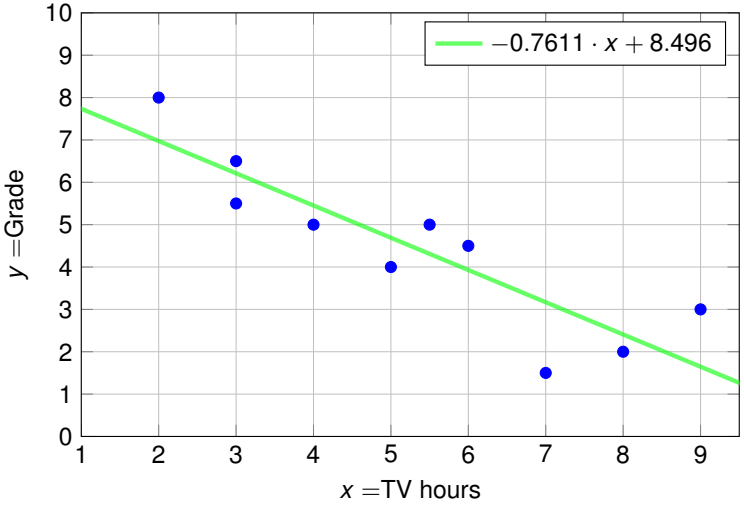
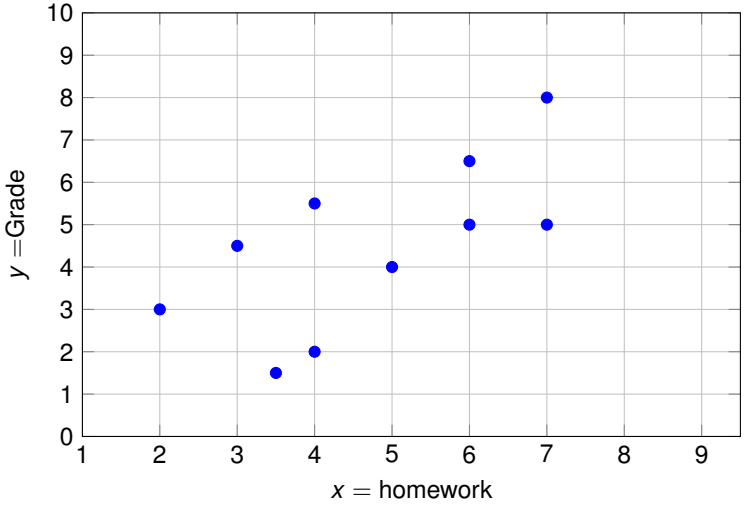
Can we get a better fit with more data?


10
9
8
7
6
5
4
3
2
1
0
1
2
3
4
5
6
7
8
9
y =Grade
x =TV hours



Square Error: 7.908





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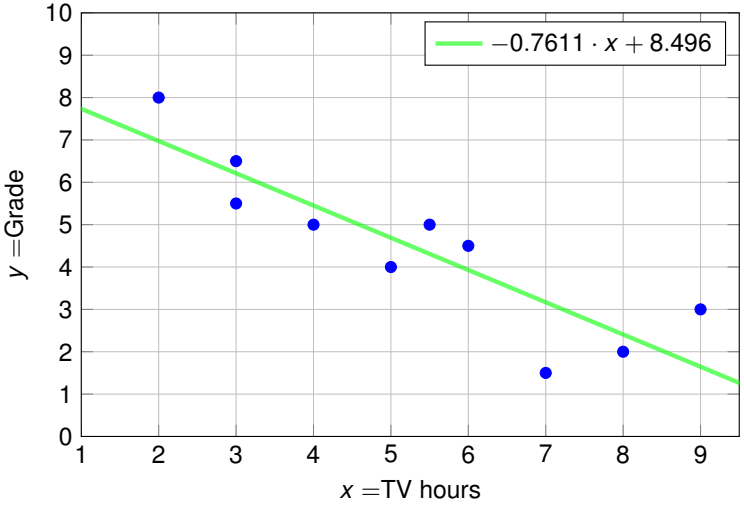

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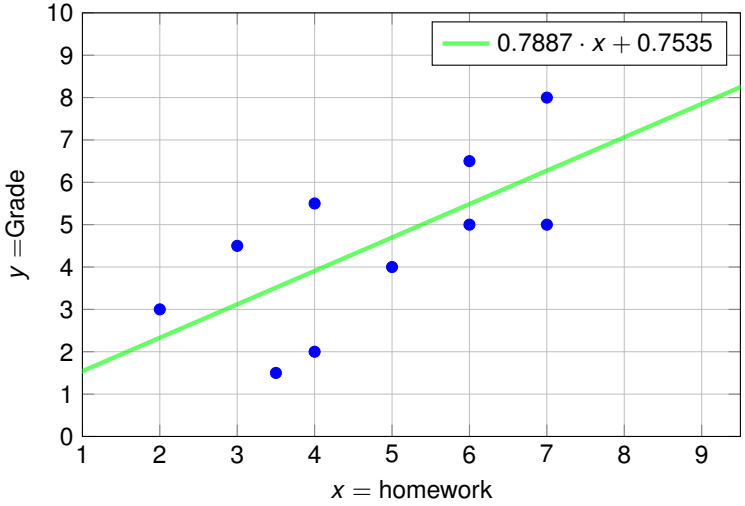

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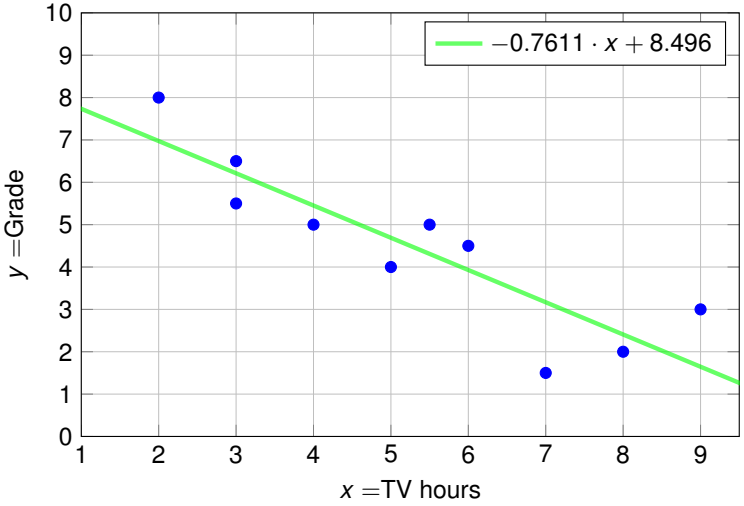

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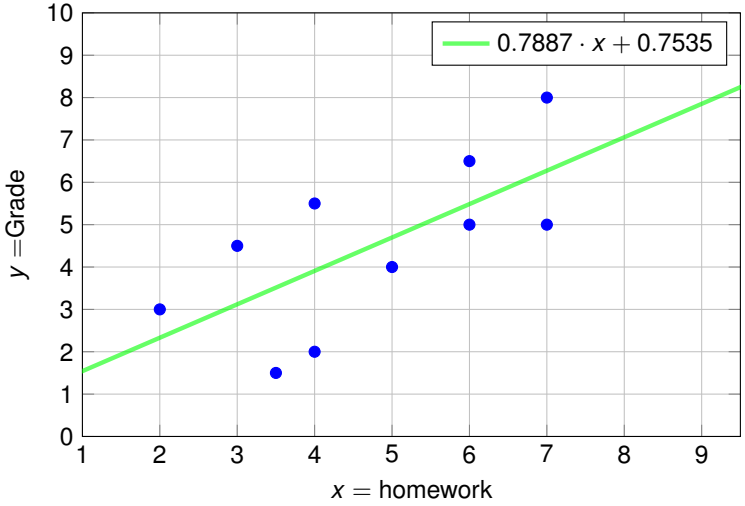
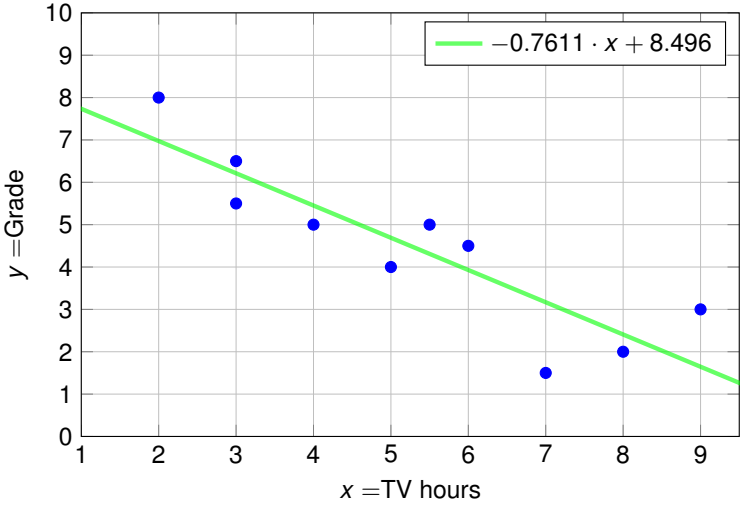
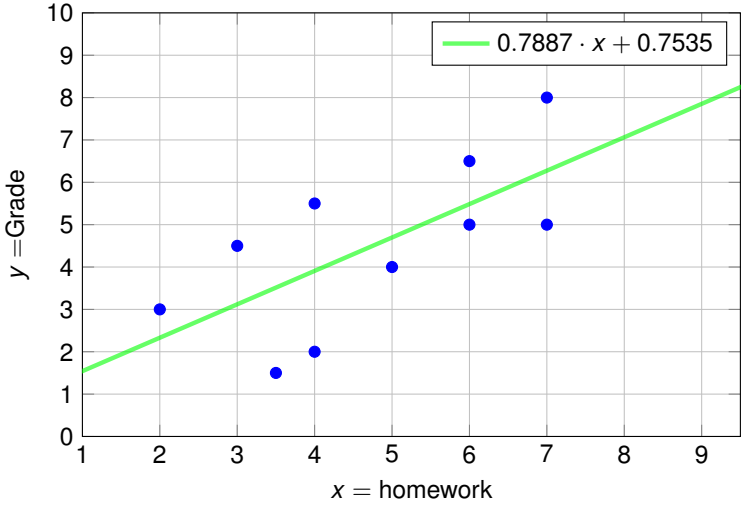


Square Error: 18.93

How to proceed?



Square Error: 7.908



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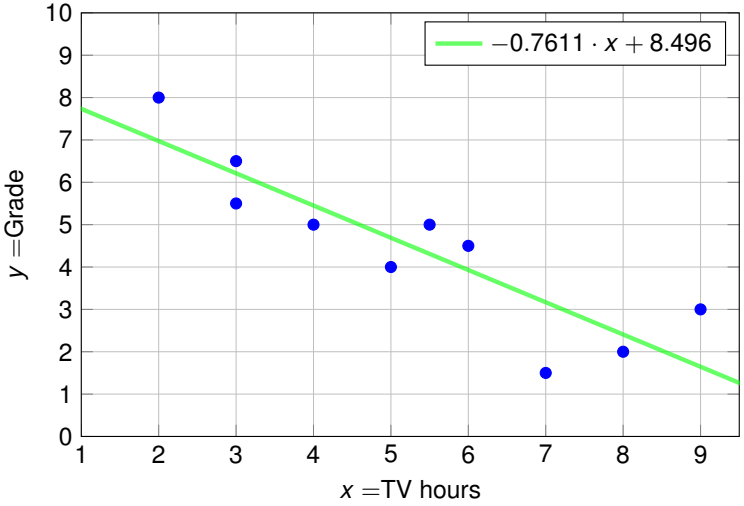
How to proceed?

- take the better of the two fits(?)



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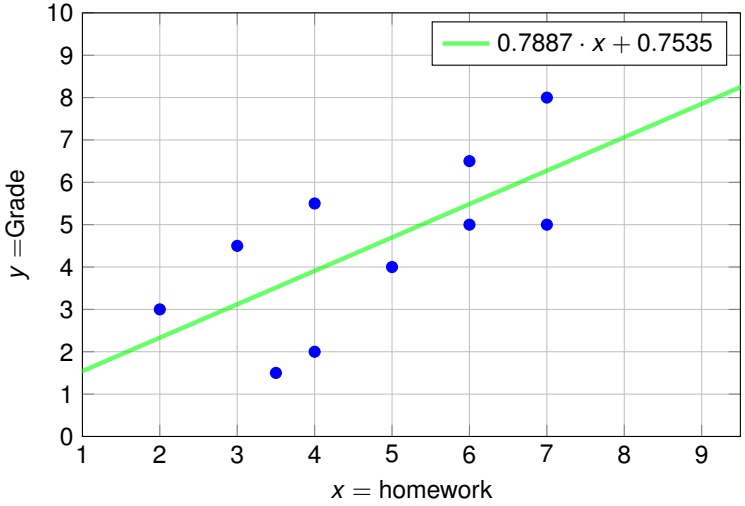

Square Error: 18.93

How to proceed?

- take the better of the two fits(?)
- take the average over the two lines(?) (yields square error: 10.00)

Multiple (Multi-Dimensional) Regression

$$\boxed{y = b + w_1 \cdot x_1 + w_2 \cdot x_2}$$

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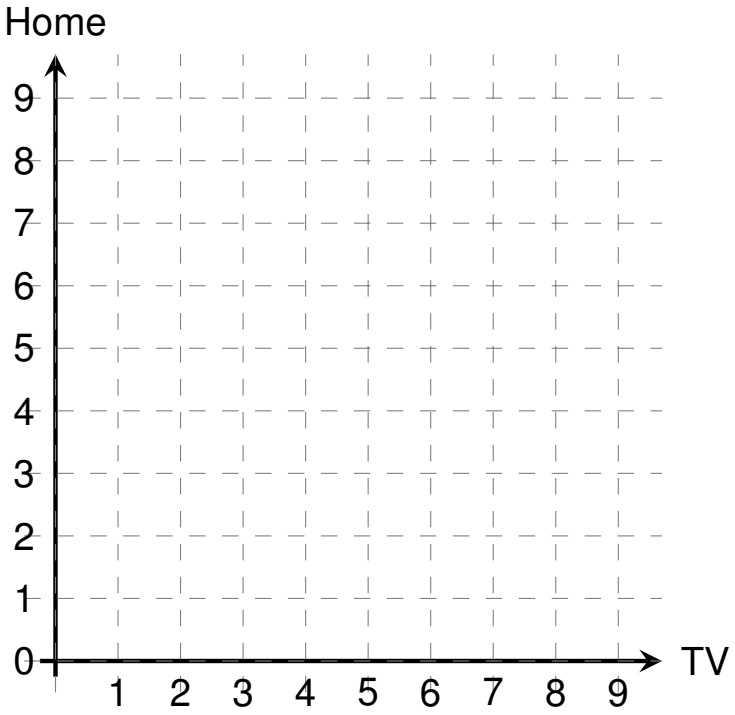

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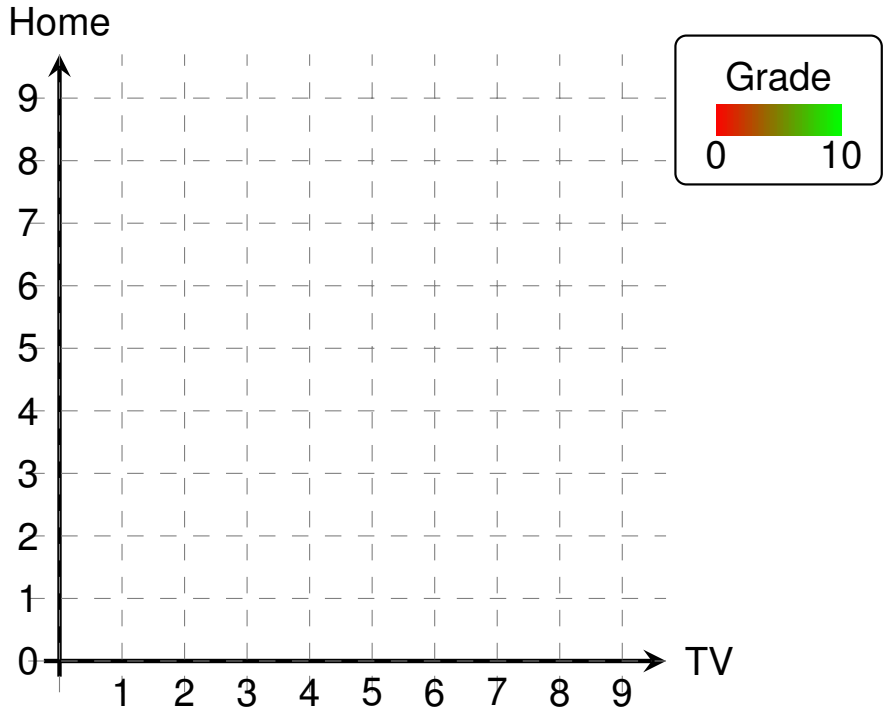

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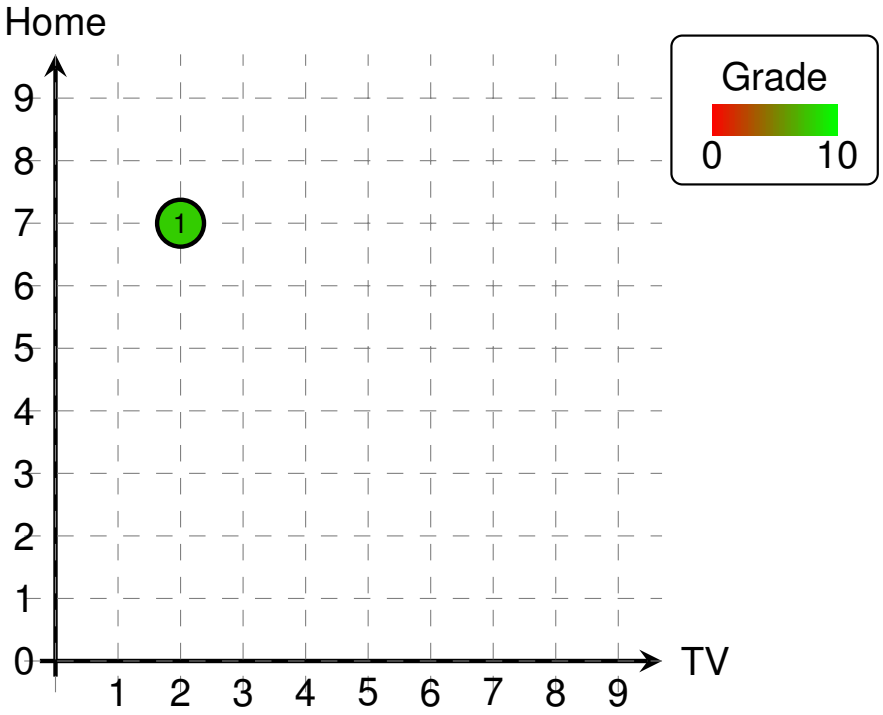

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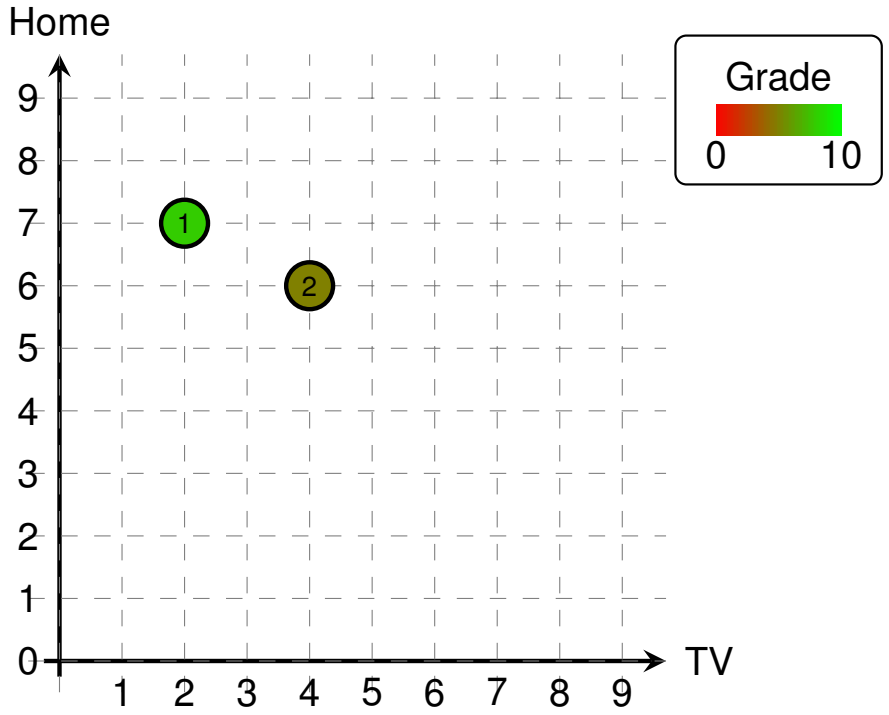

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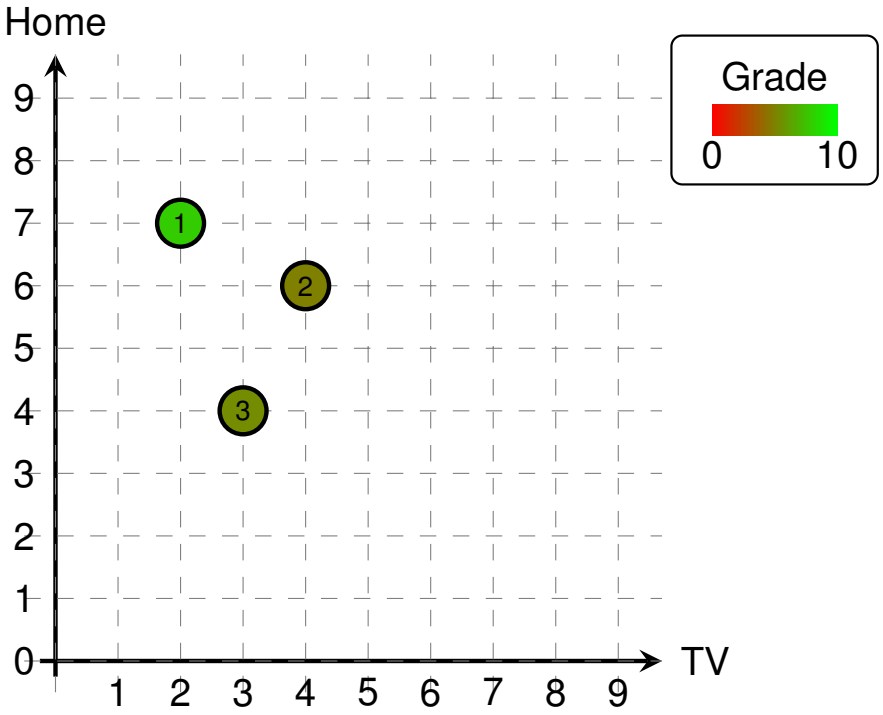

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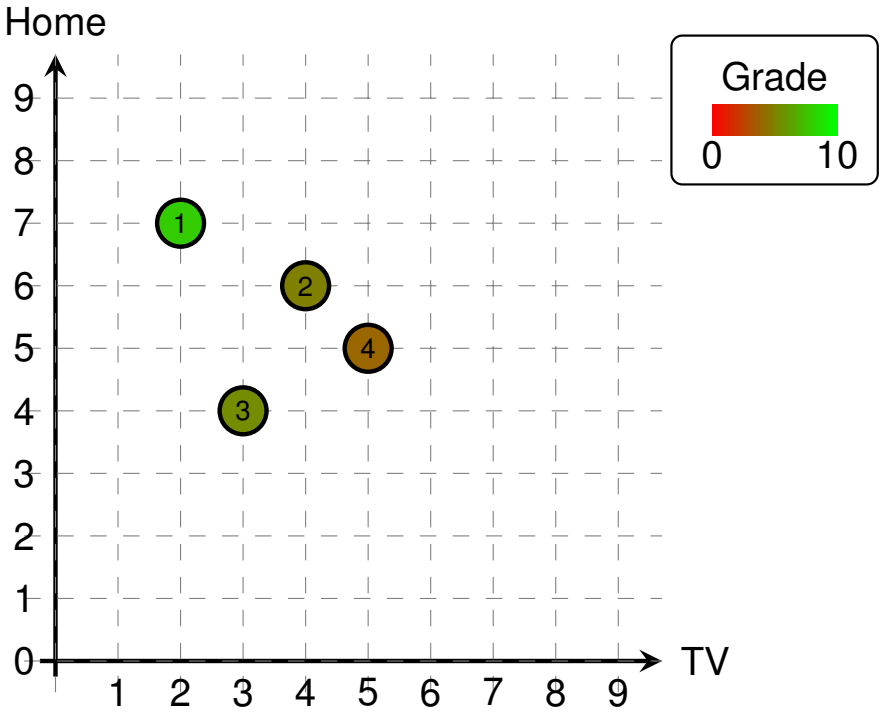

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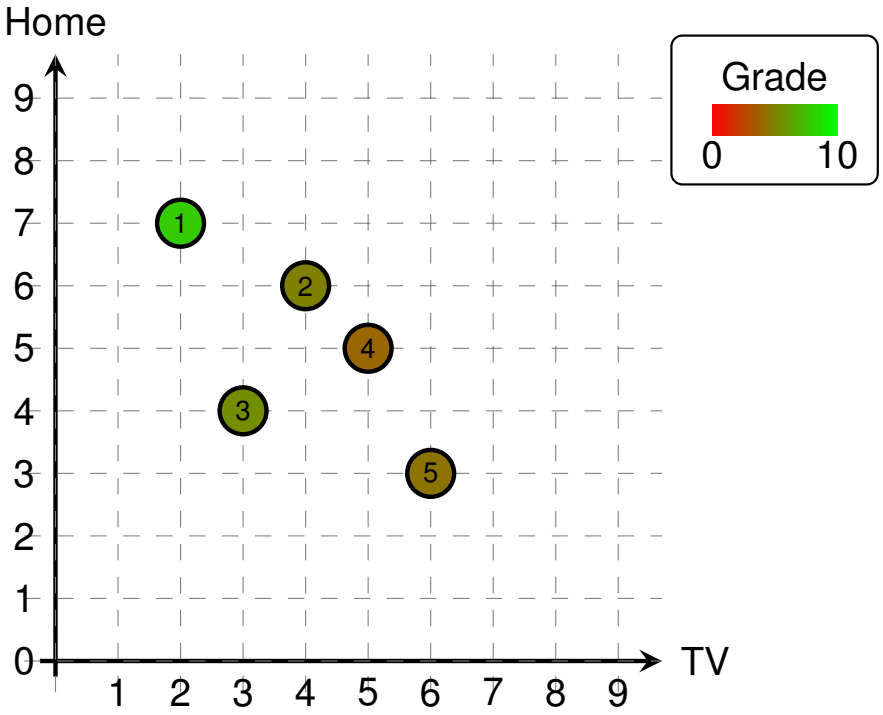

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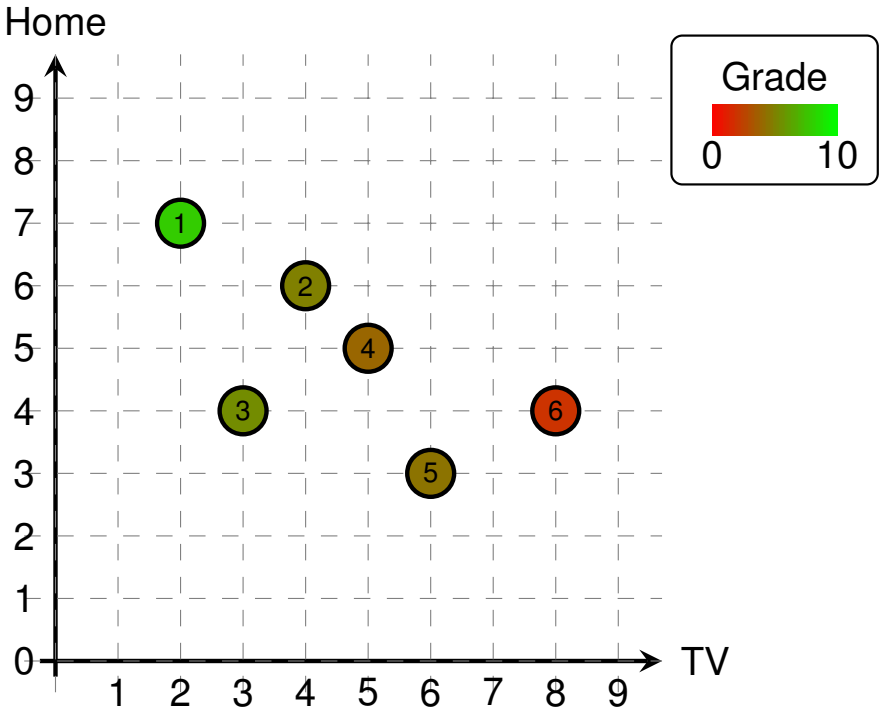

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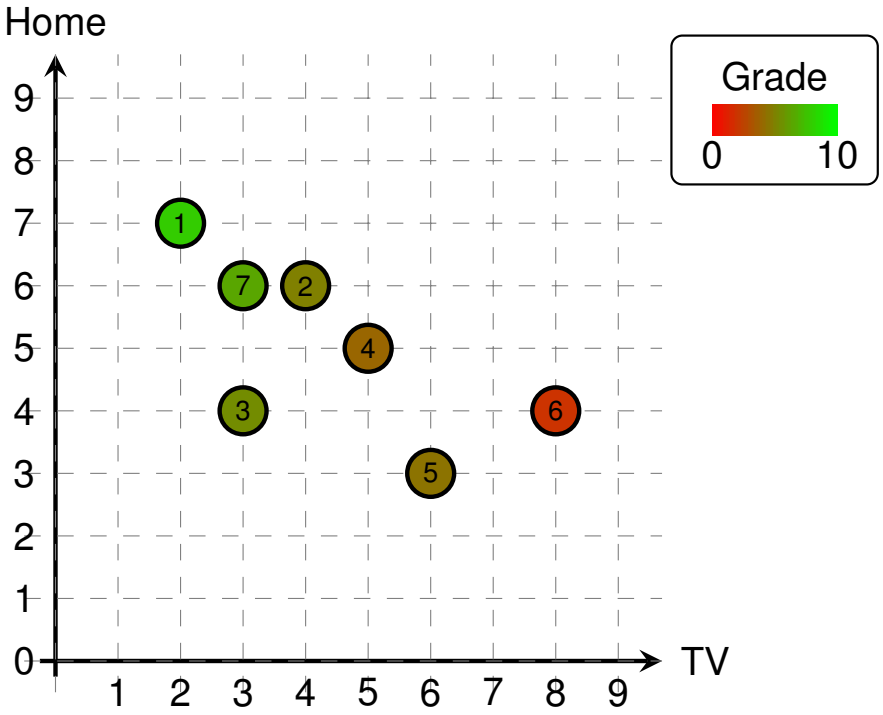

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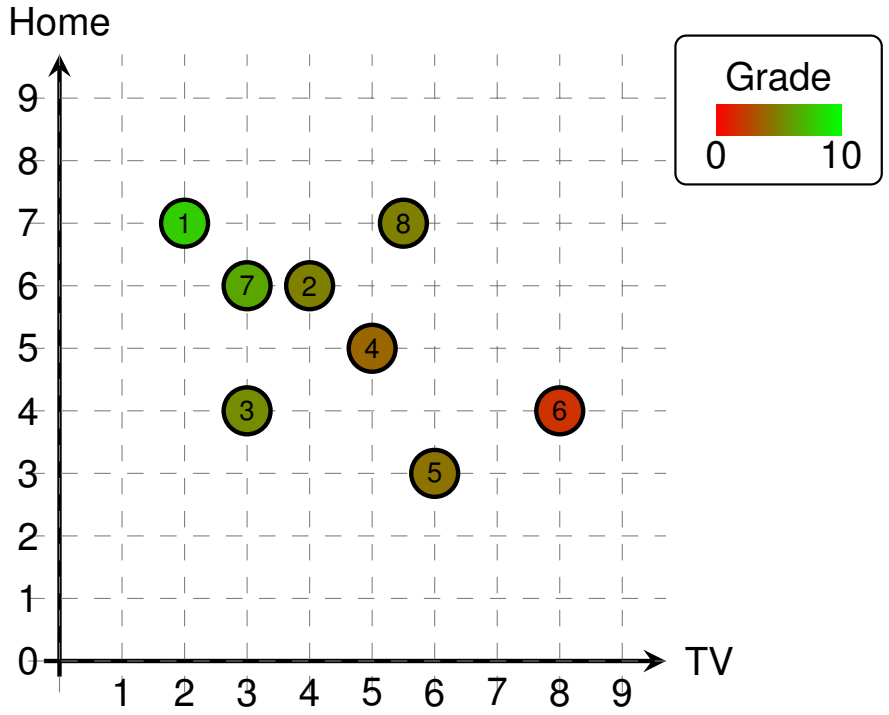

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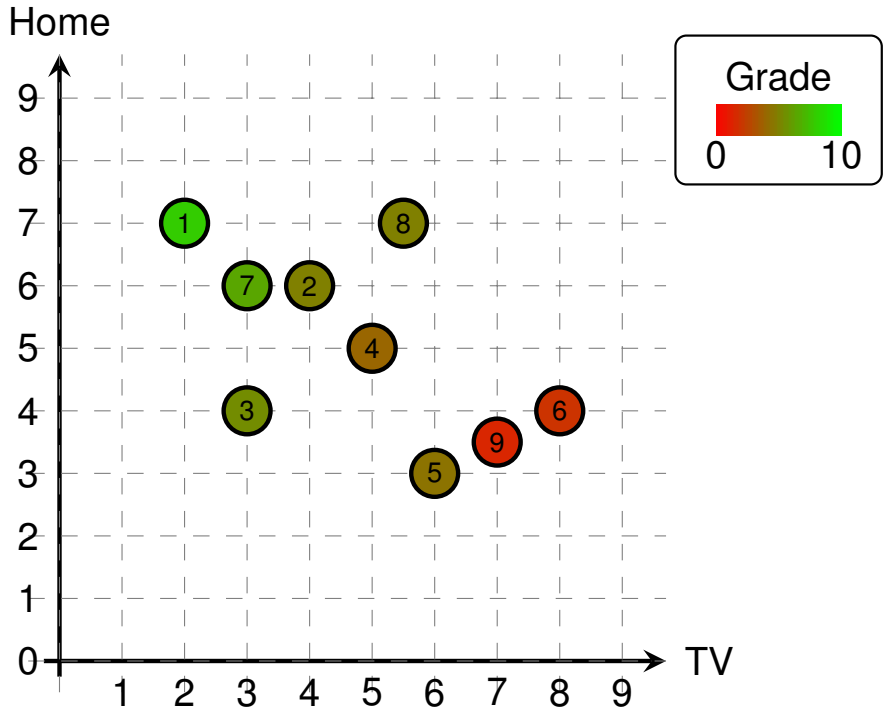

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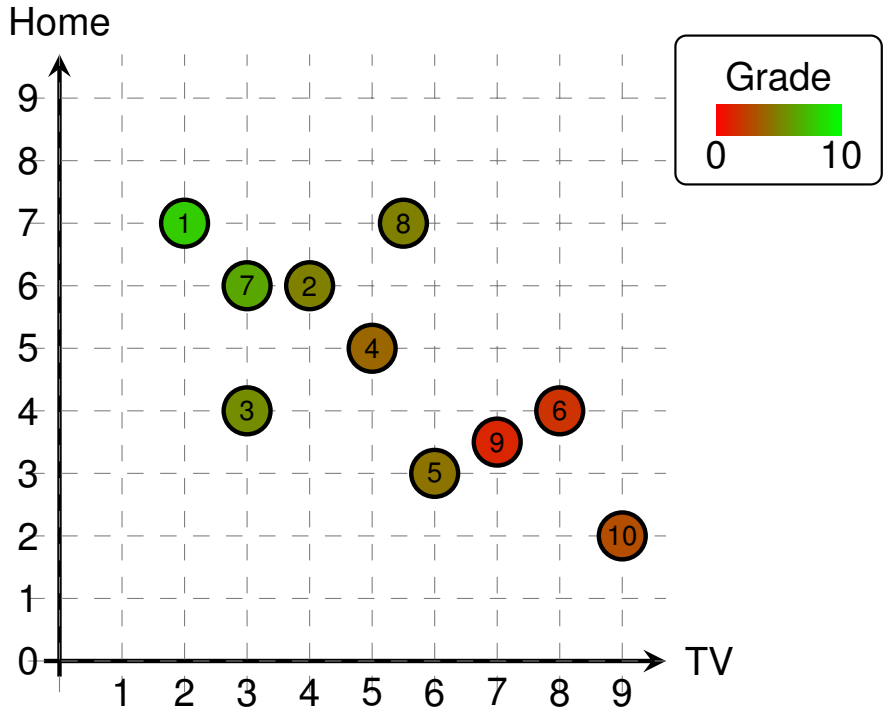

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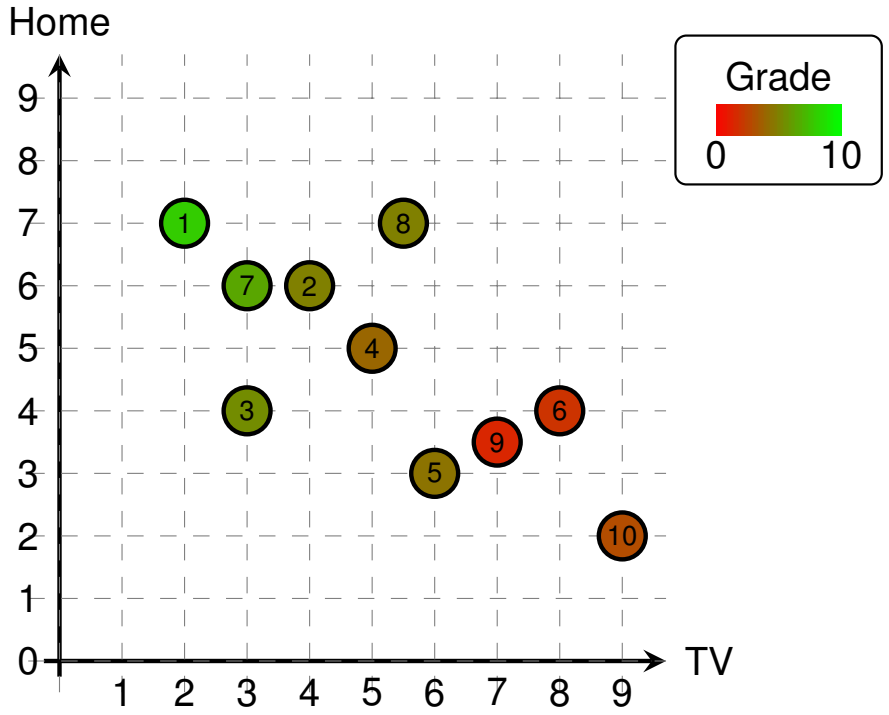
1	2	7	8	7.04
2	4	6	5	5.52
3	3	4	5.5	5.96
4	5	5	4	4.75
5	6	3	4.5	3.75
6	8	4	2	2.50
7	3	6	6.5	6.22
8	5.5	7	5	4.62
9	7	3.5	1.5	3.13
10	9	2	3	1.55



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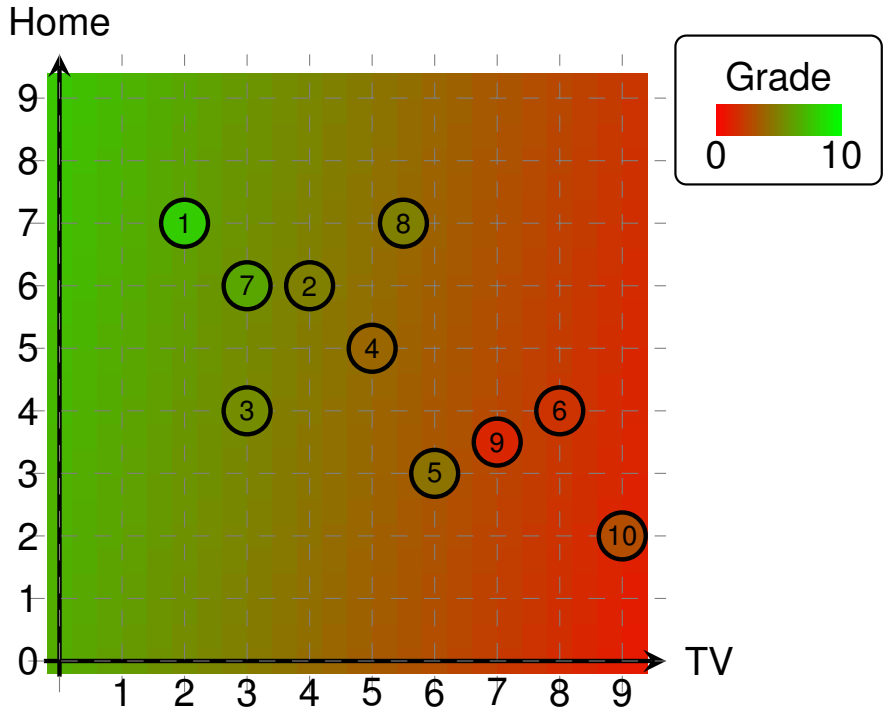

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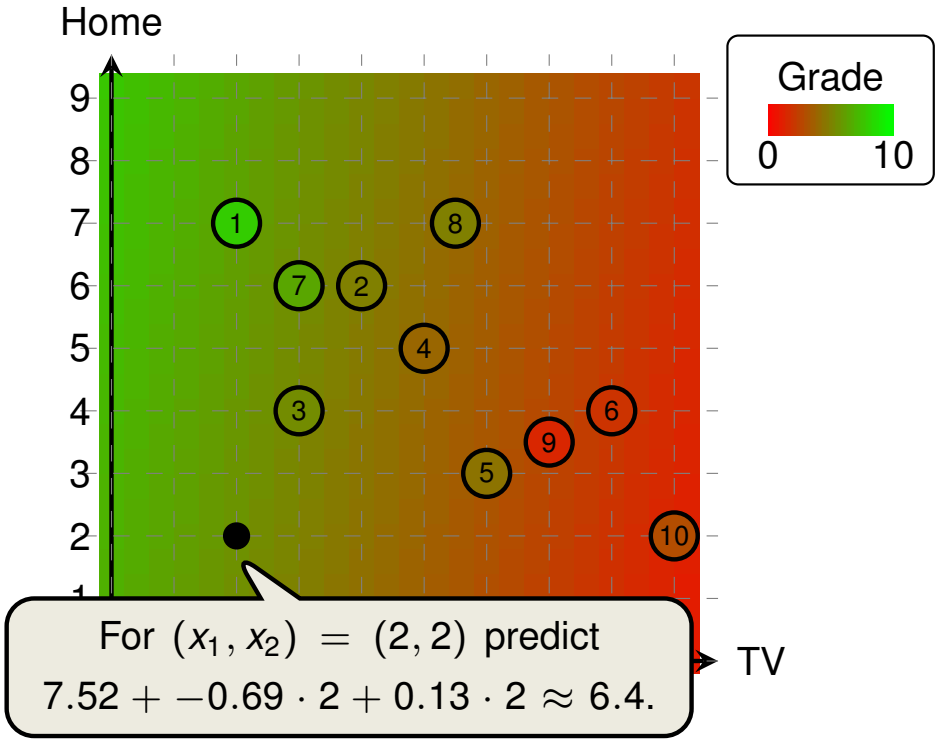

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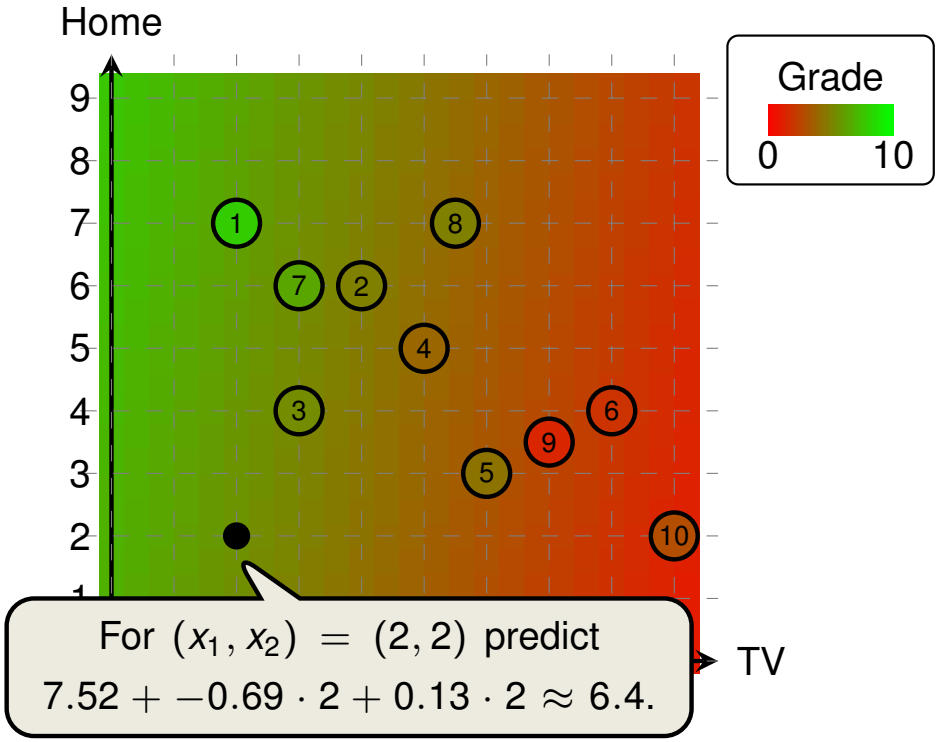
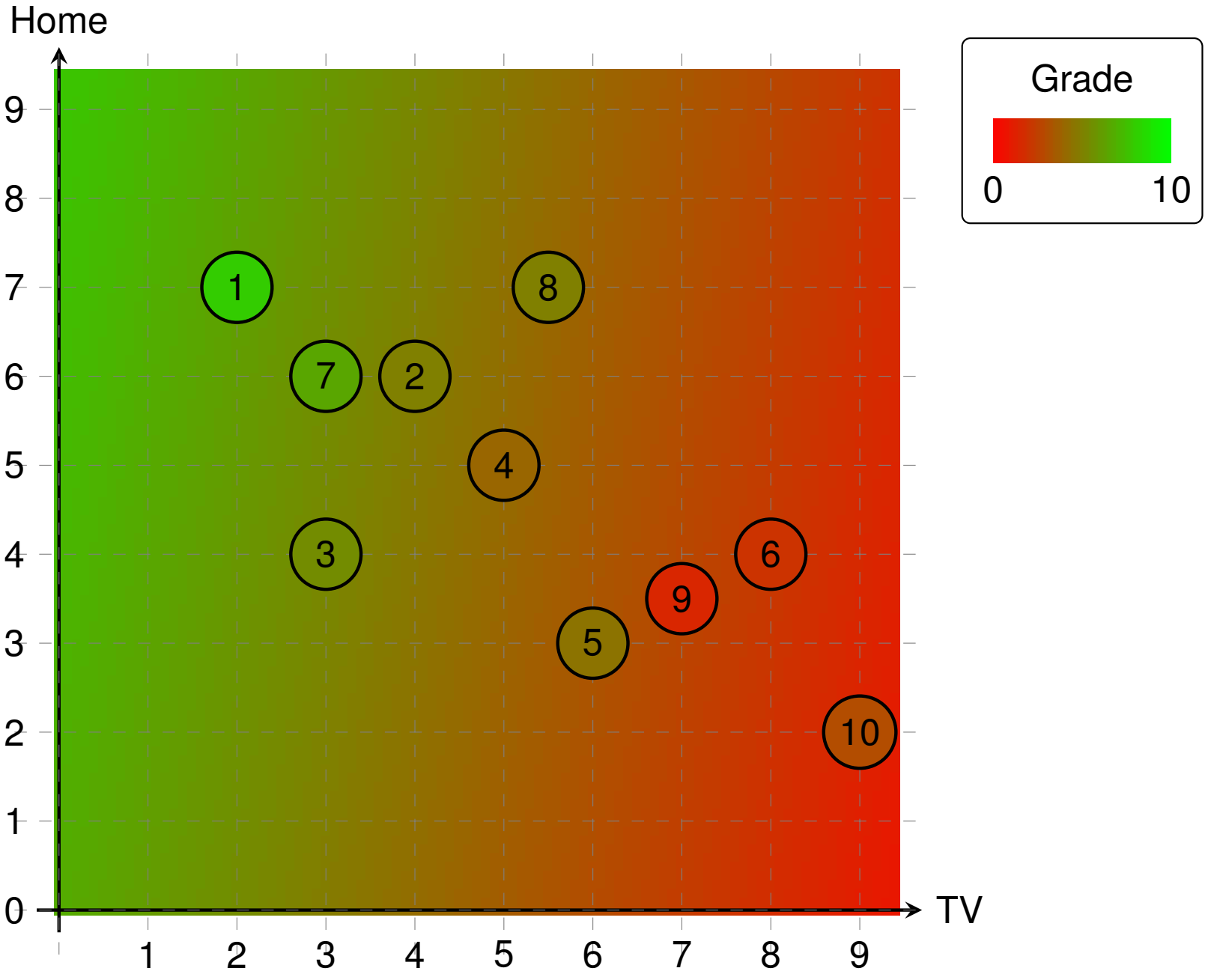
Largest error for Students 9 and 10!




Home
TV
Grade
0
10
0
1
2
3
4
5
6
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9
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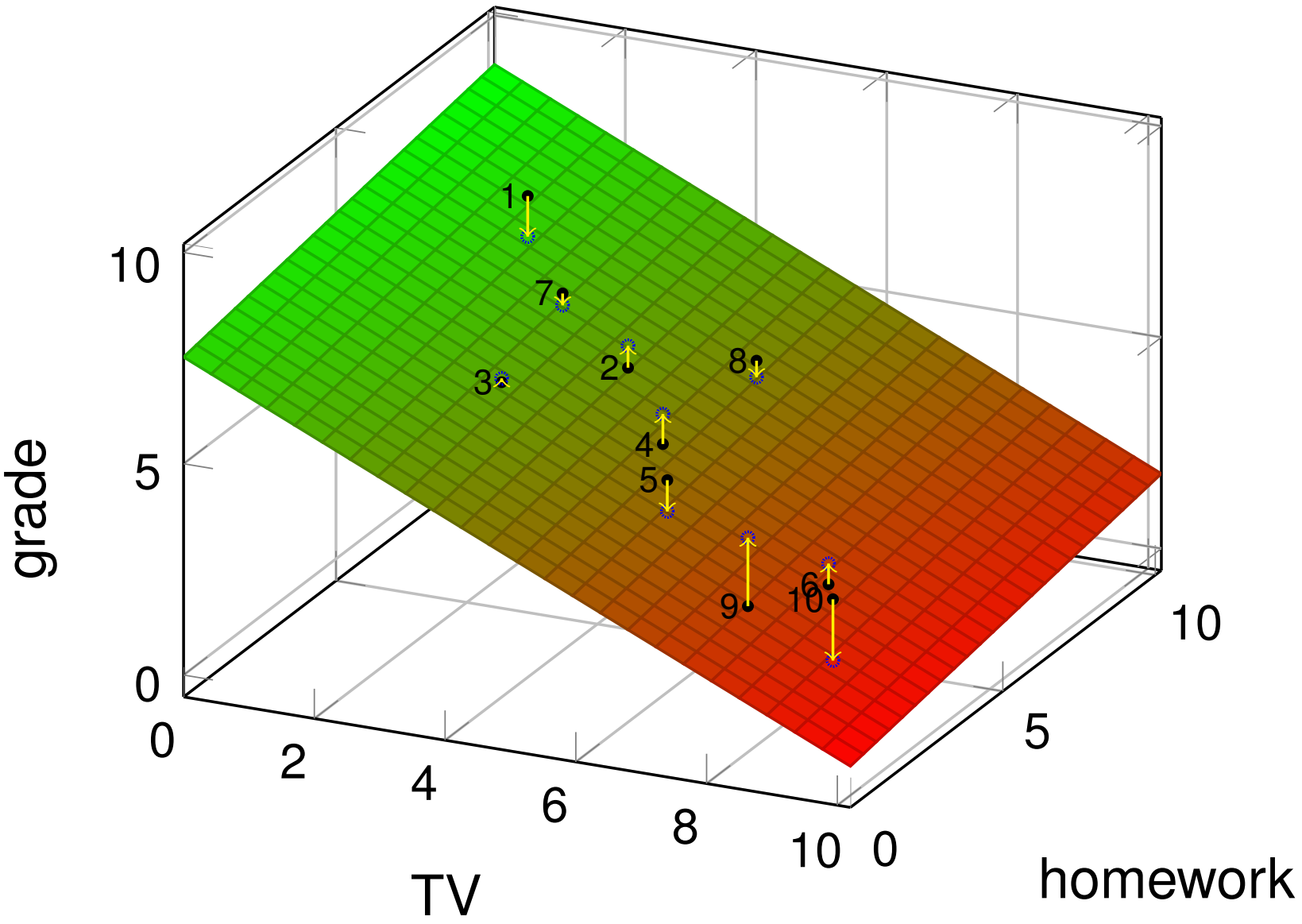
10

$$y = 7.525 - 0.693 \cdot x_1 + 0.129 \cdot x_2$$



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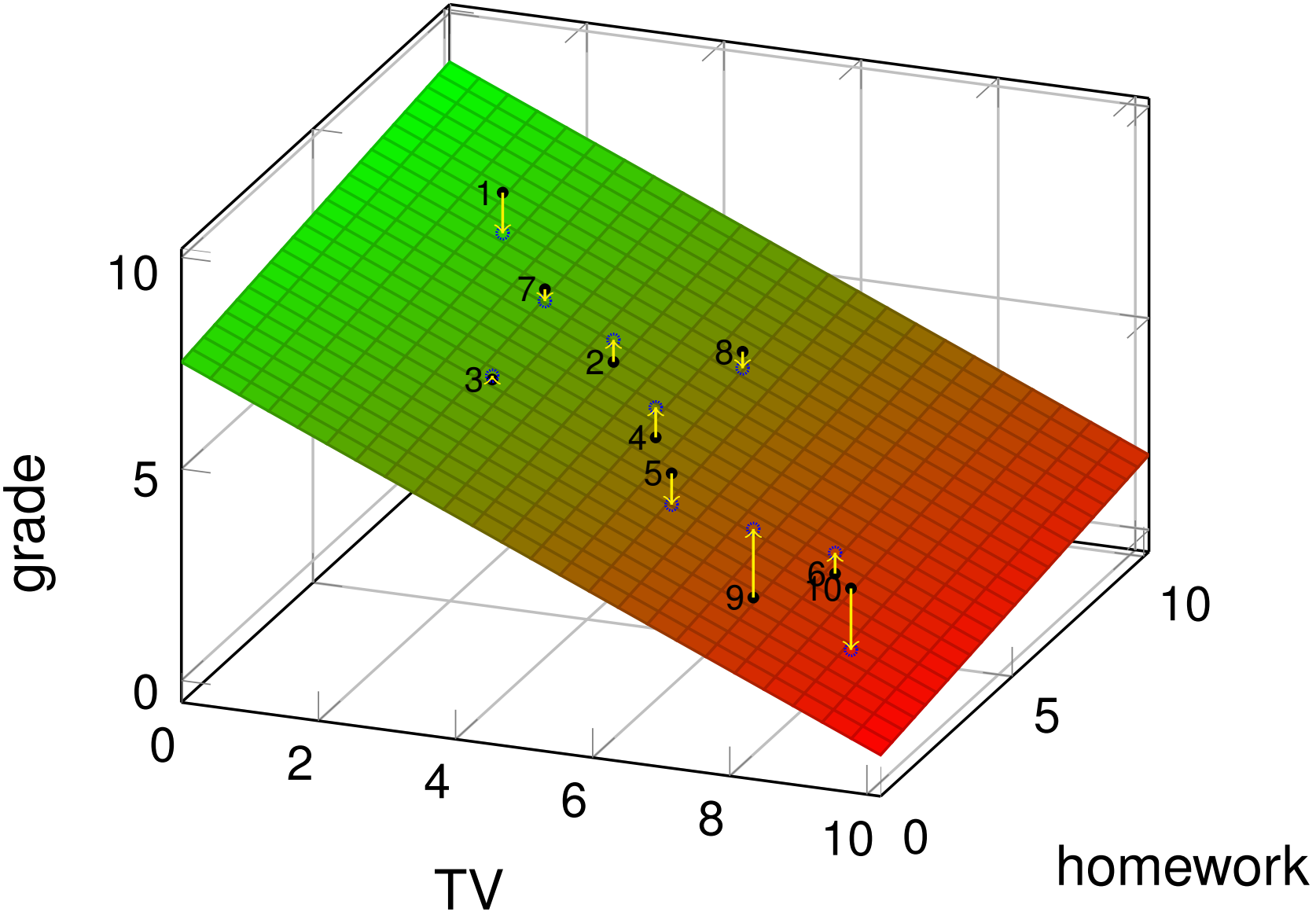

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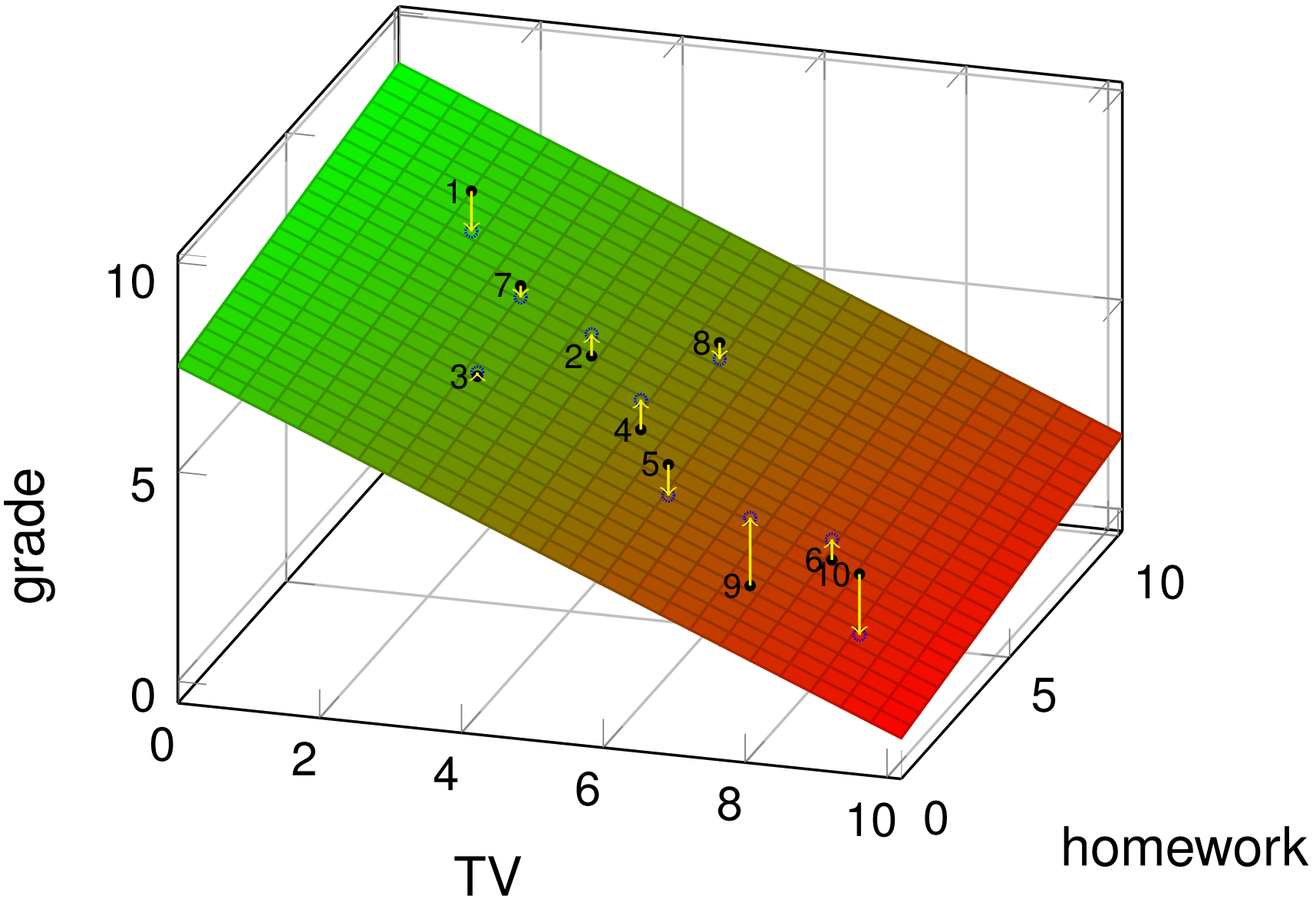

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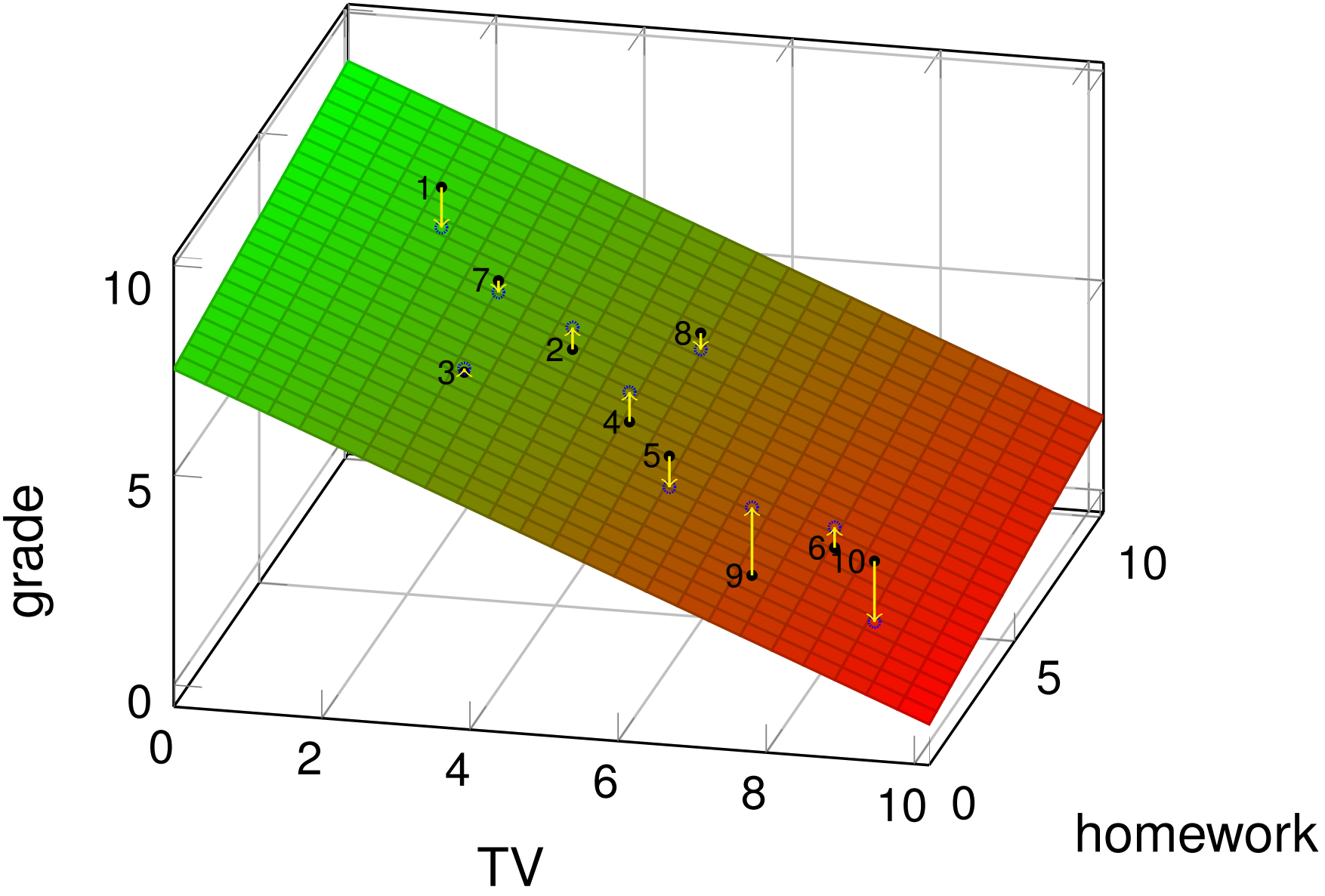

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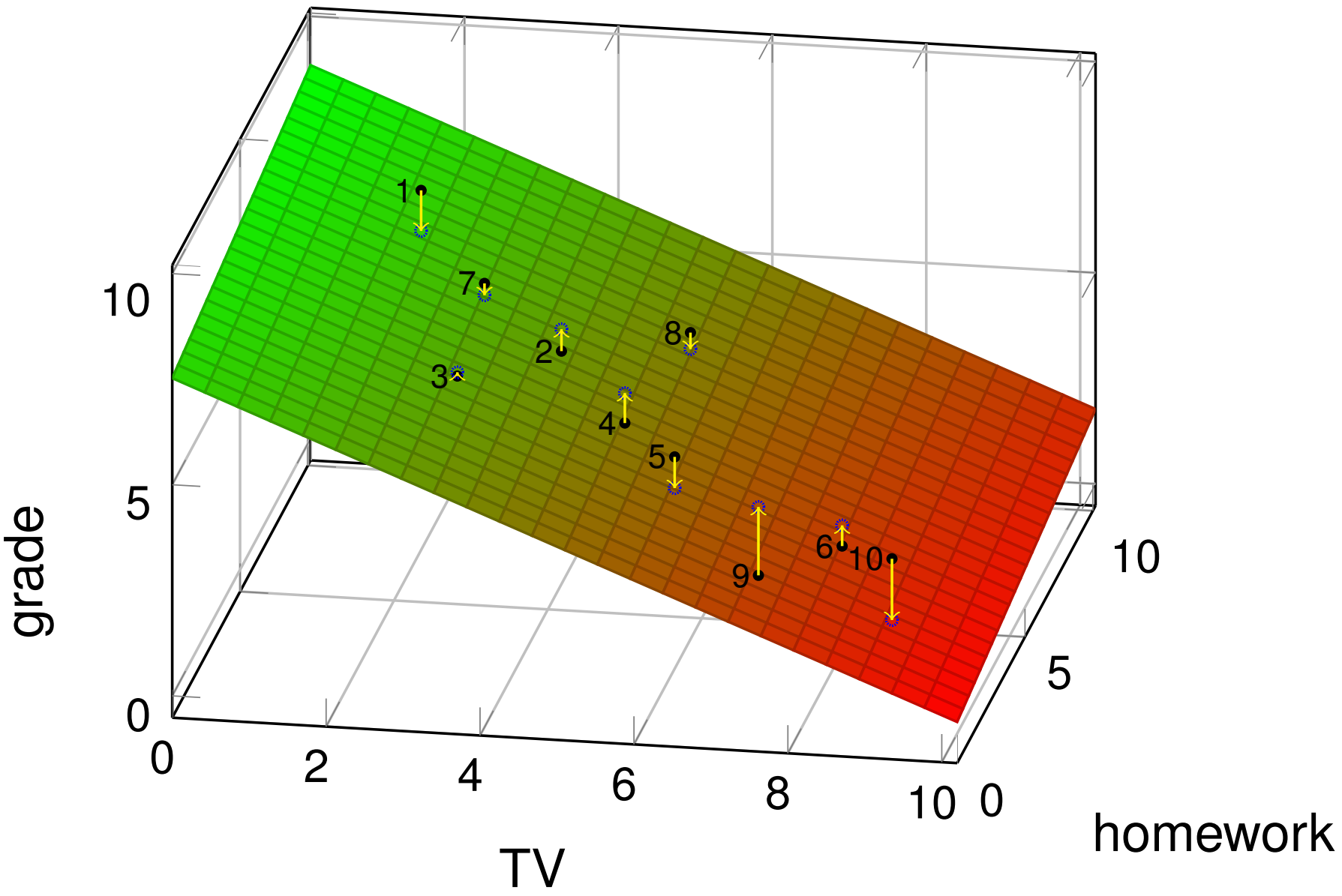

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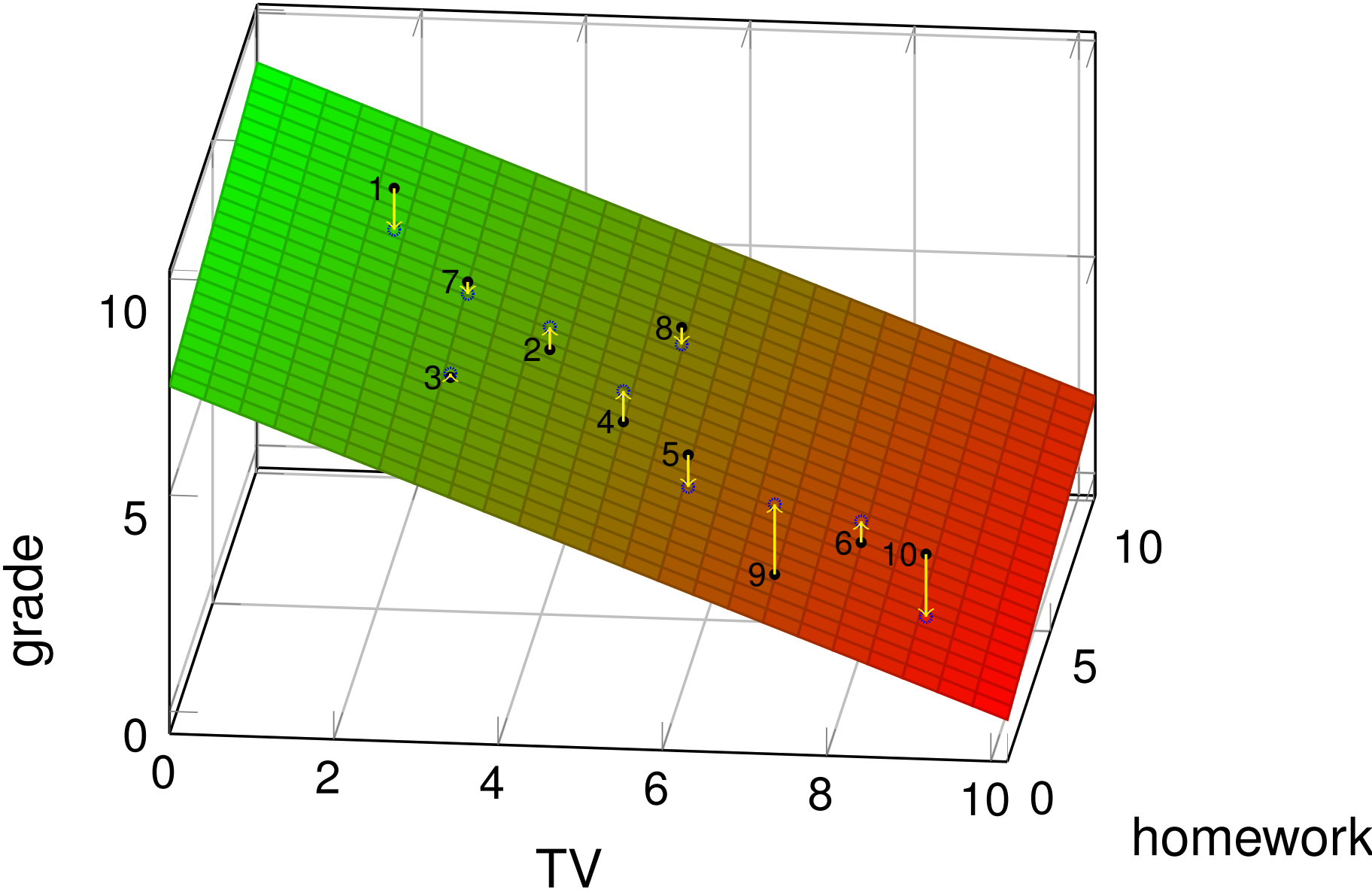

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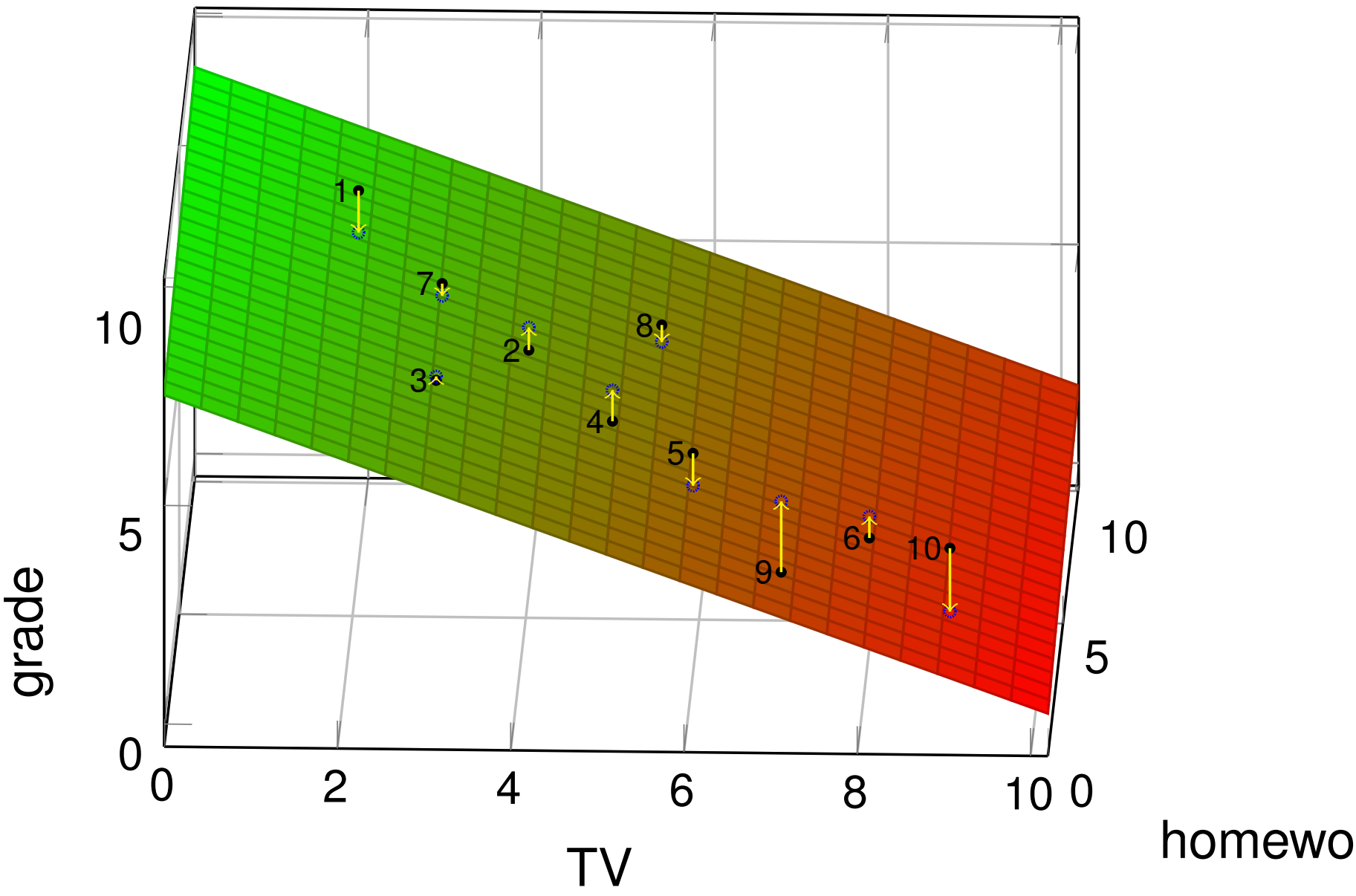

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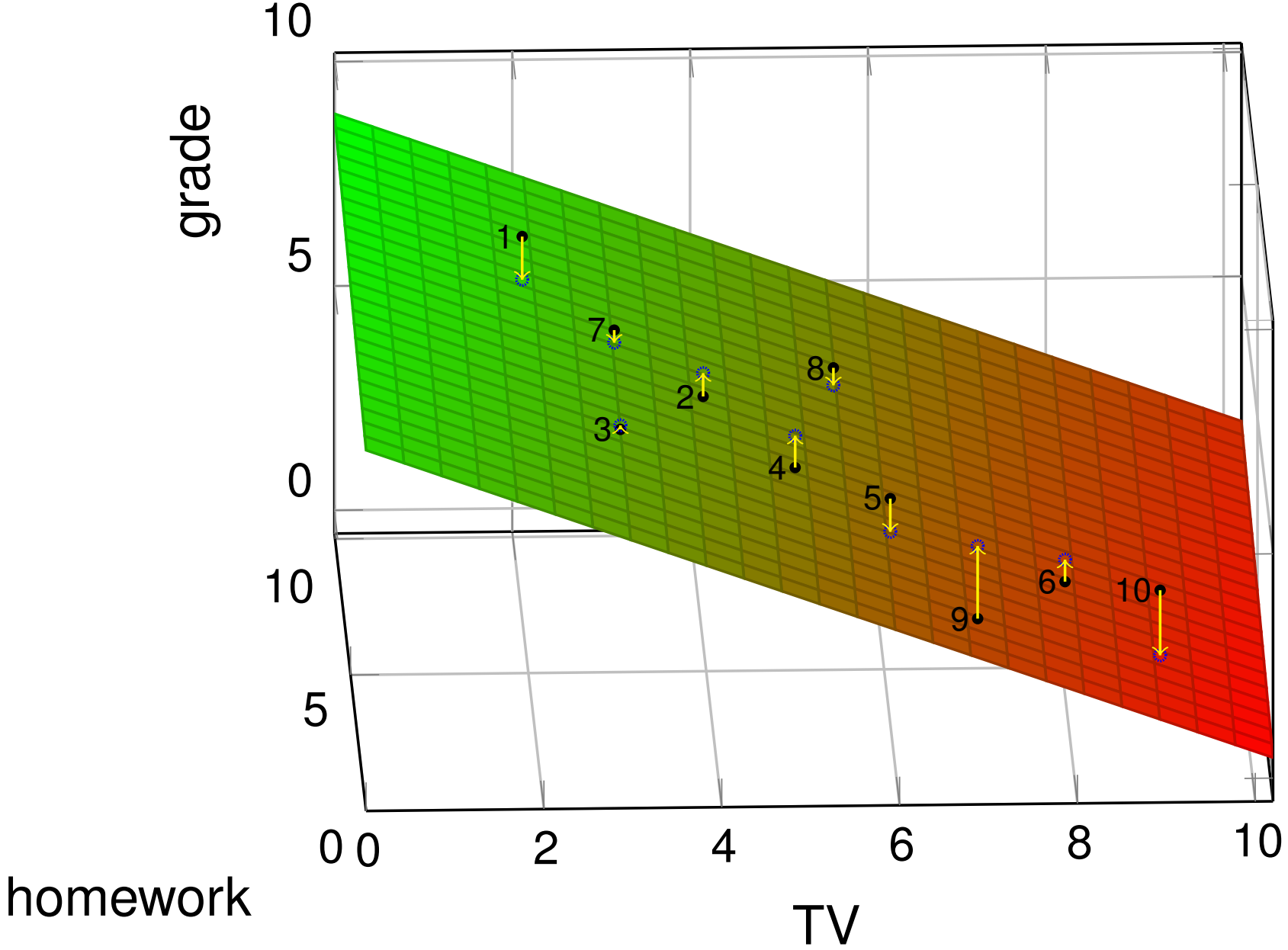

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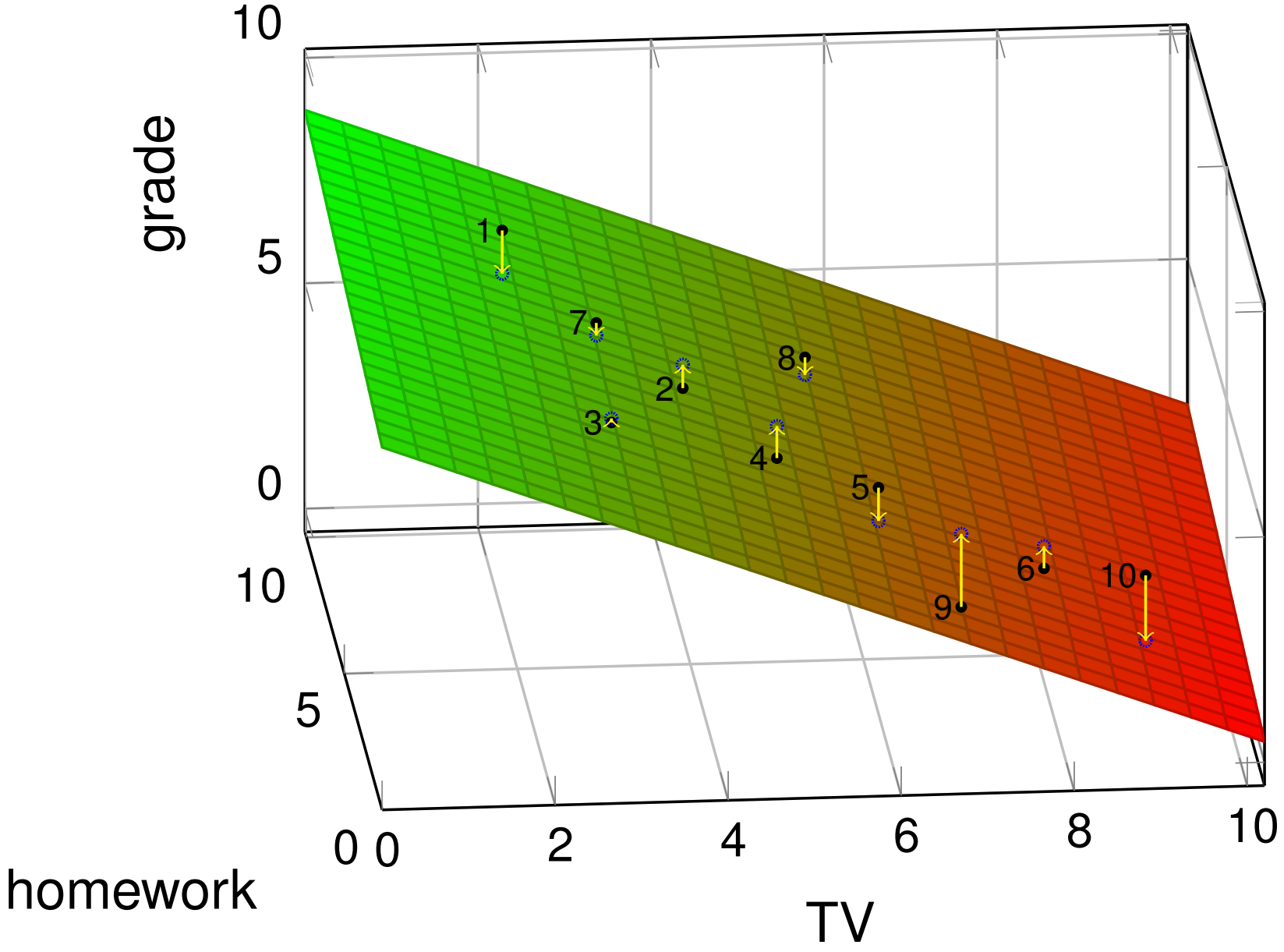

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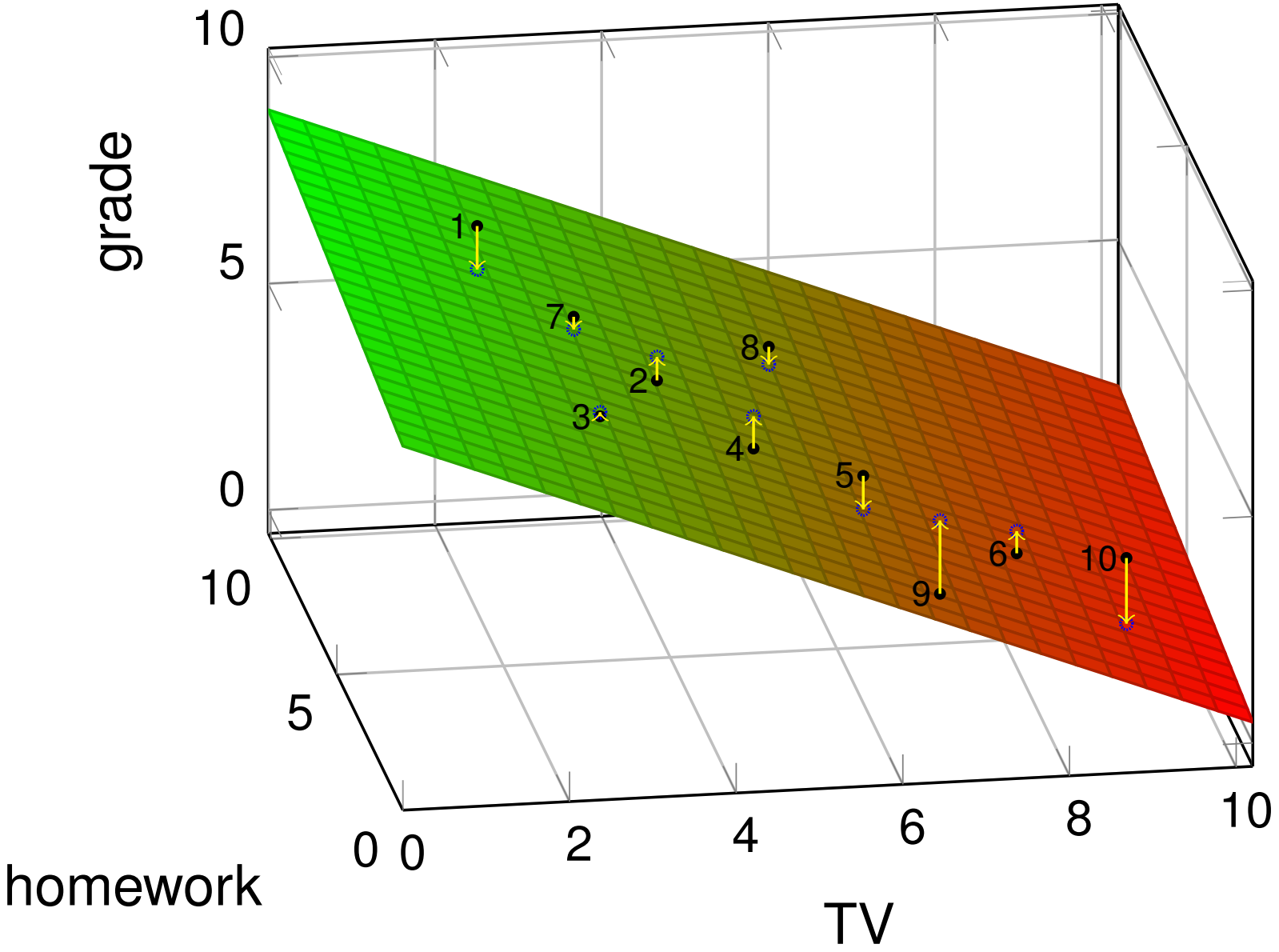

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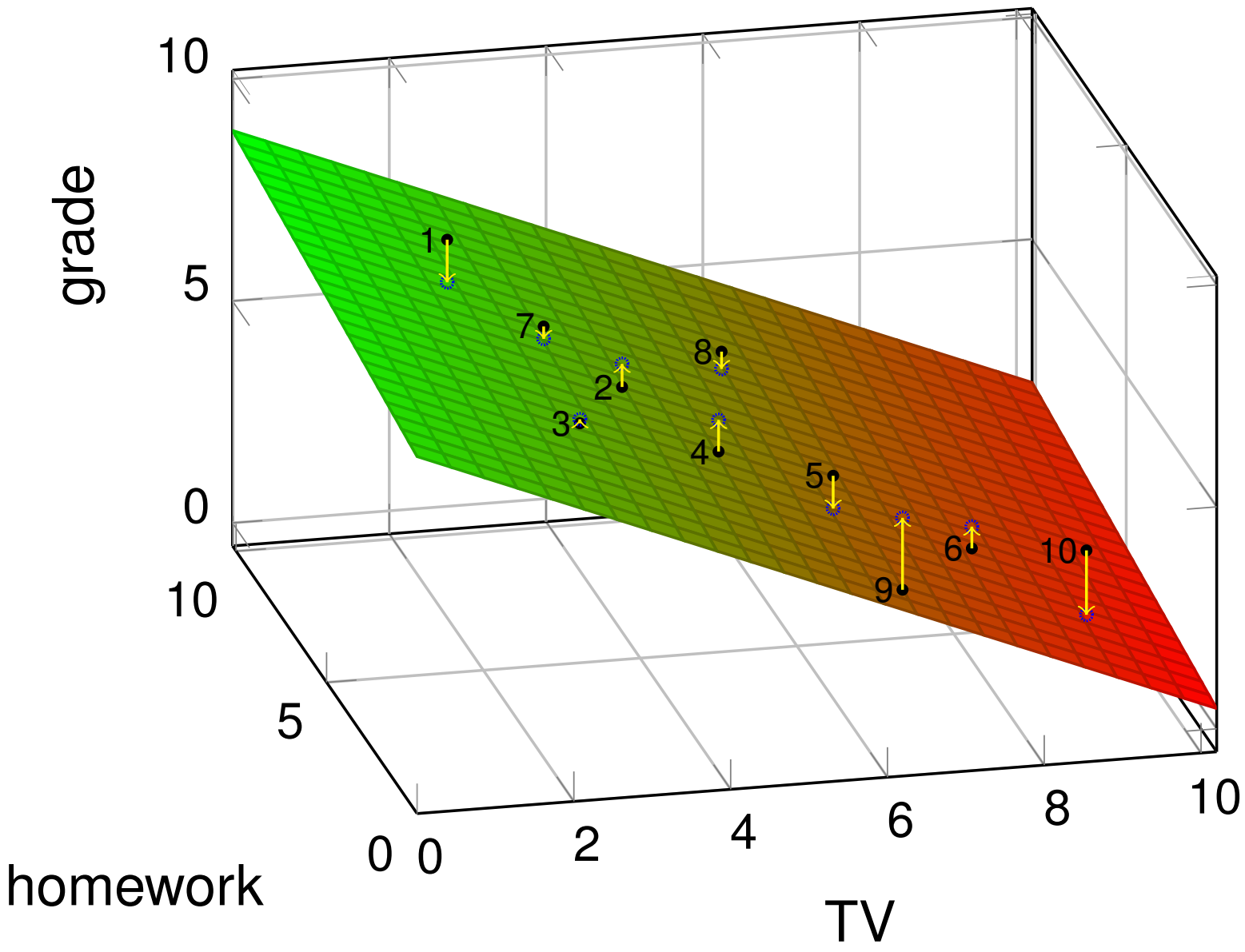

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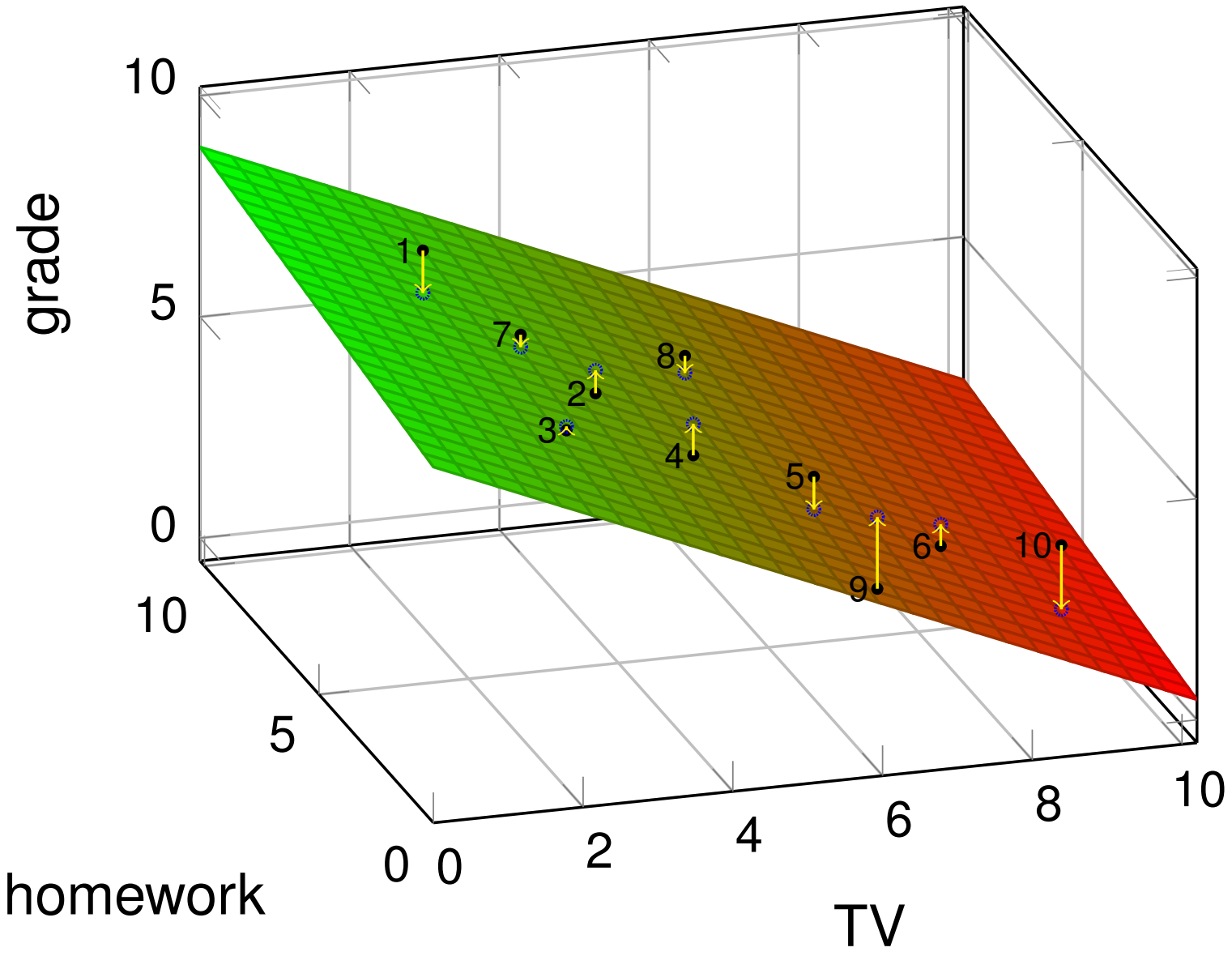

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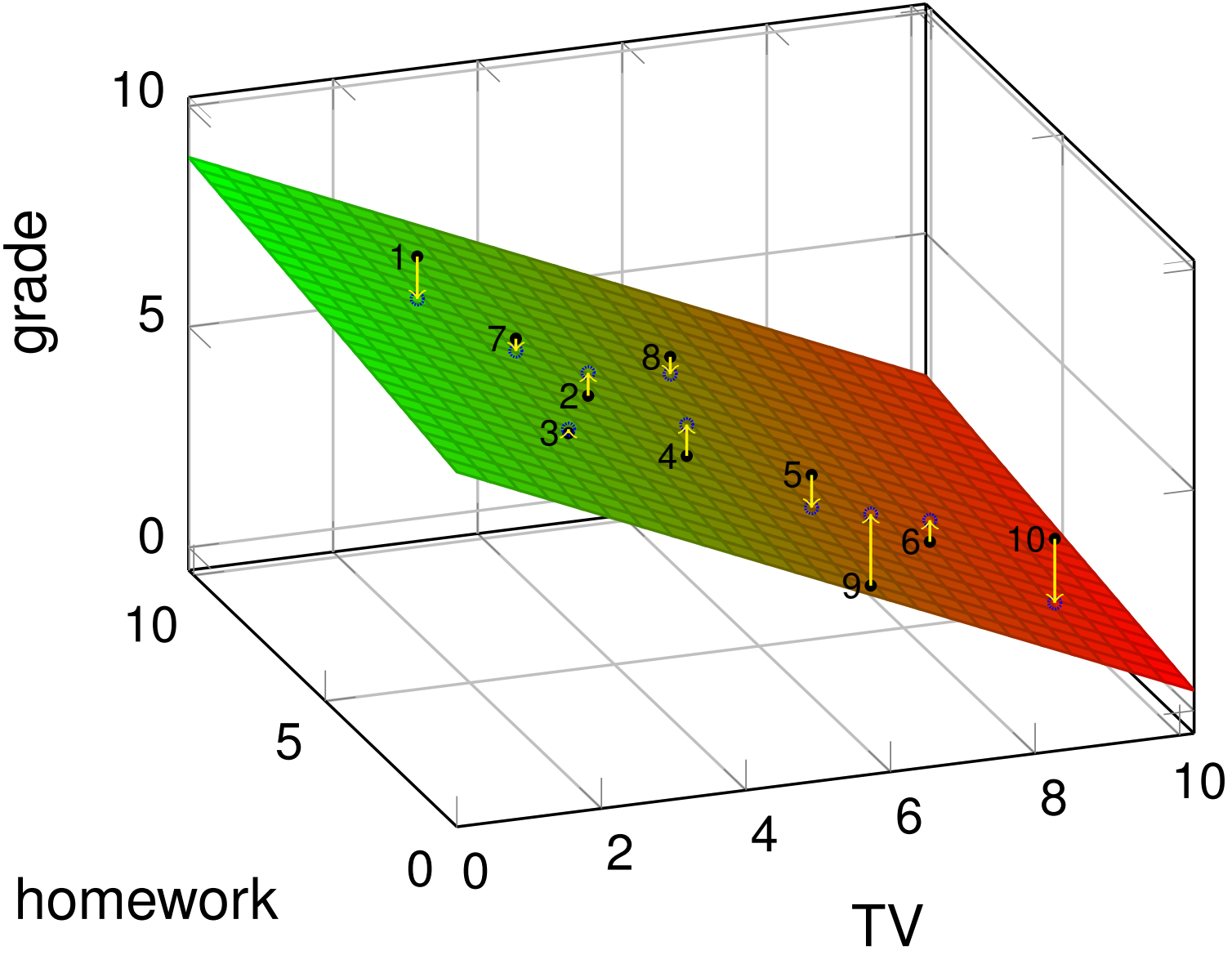

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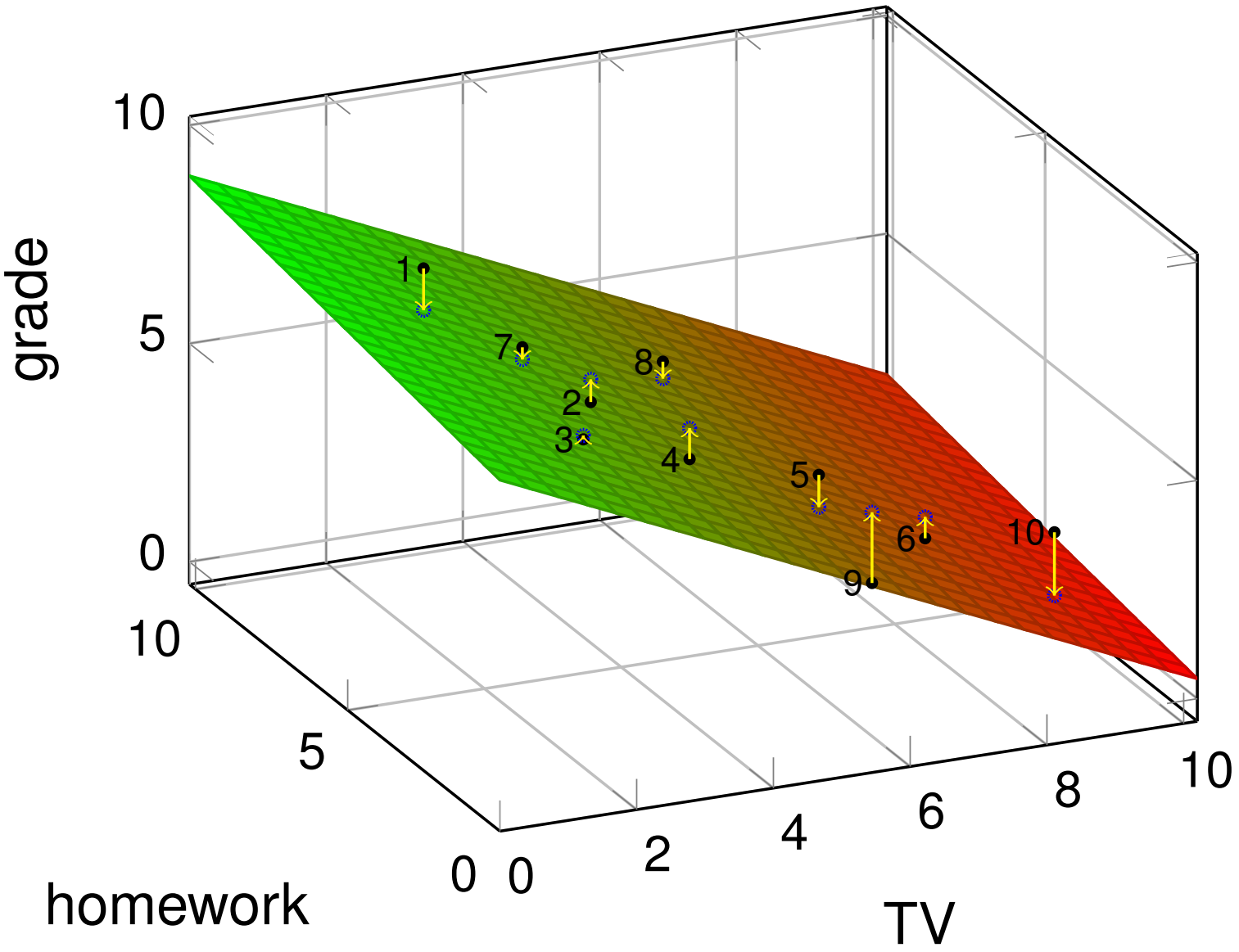

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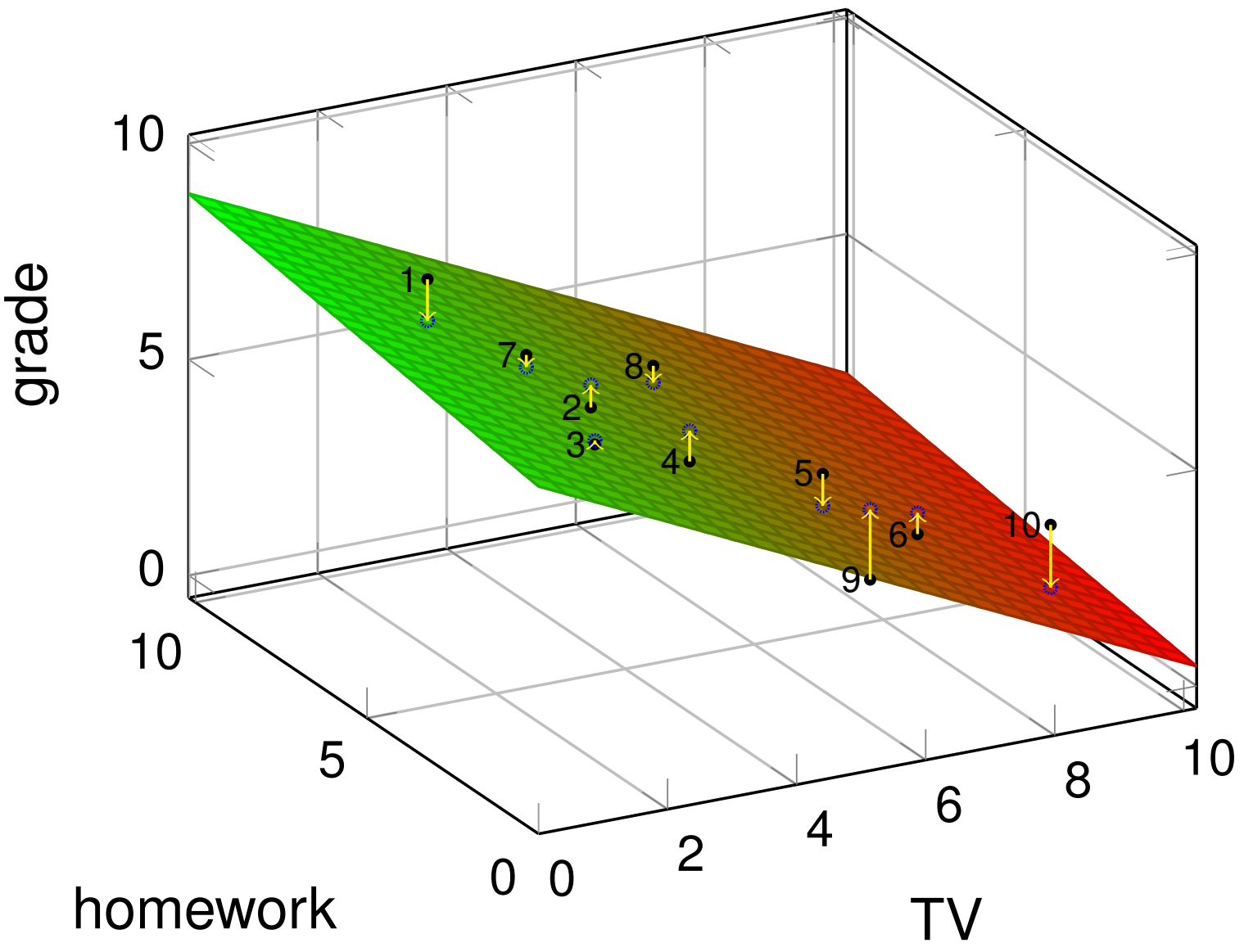

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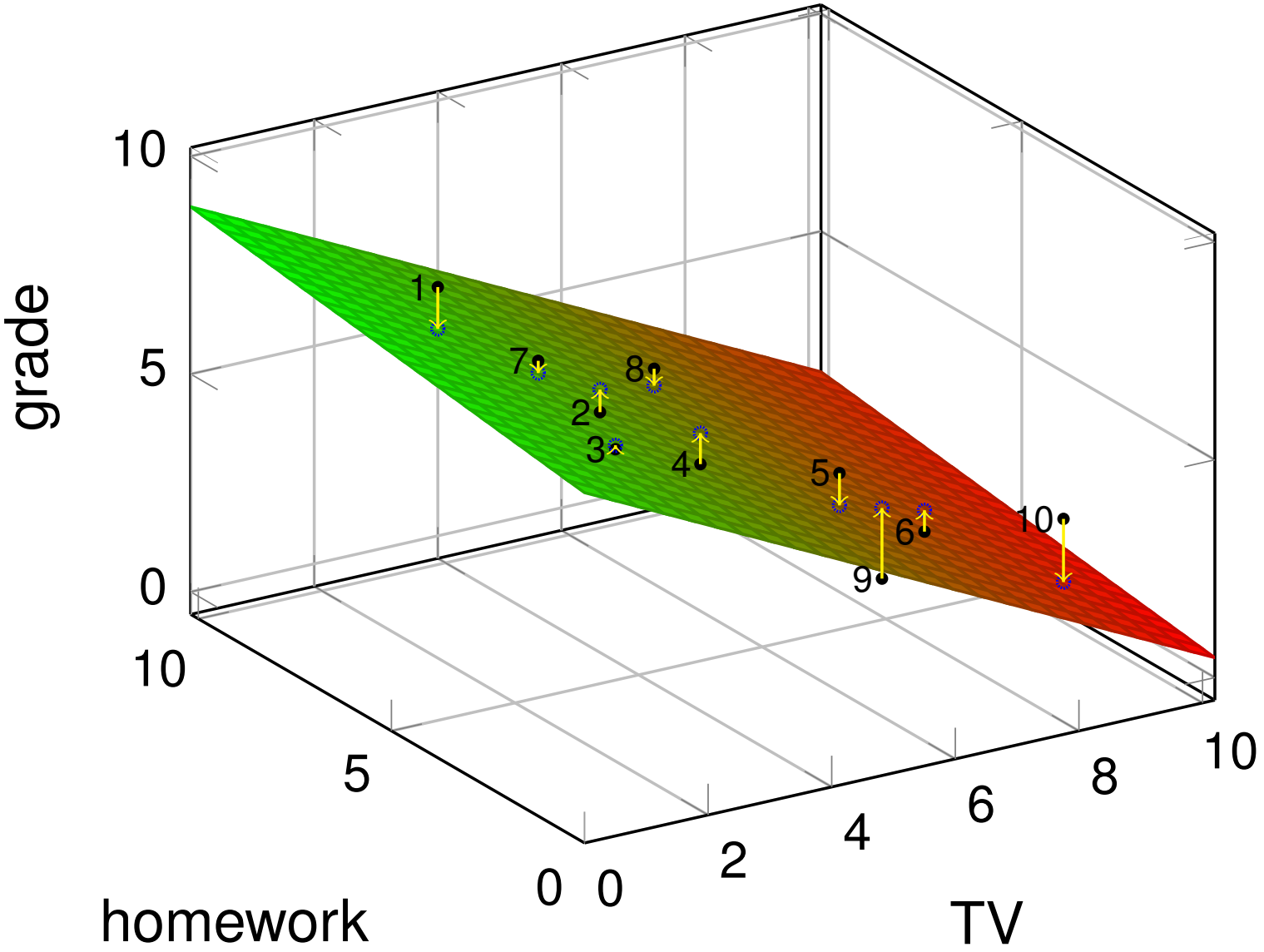

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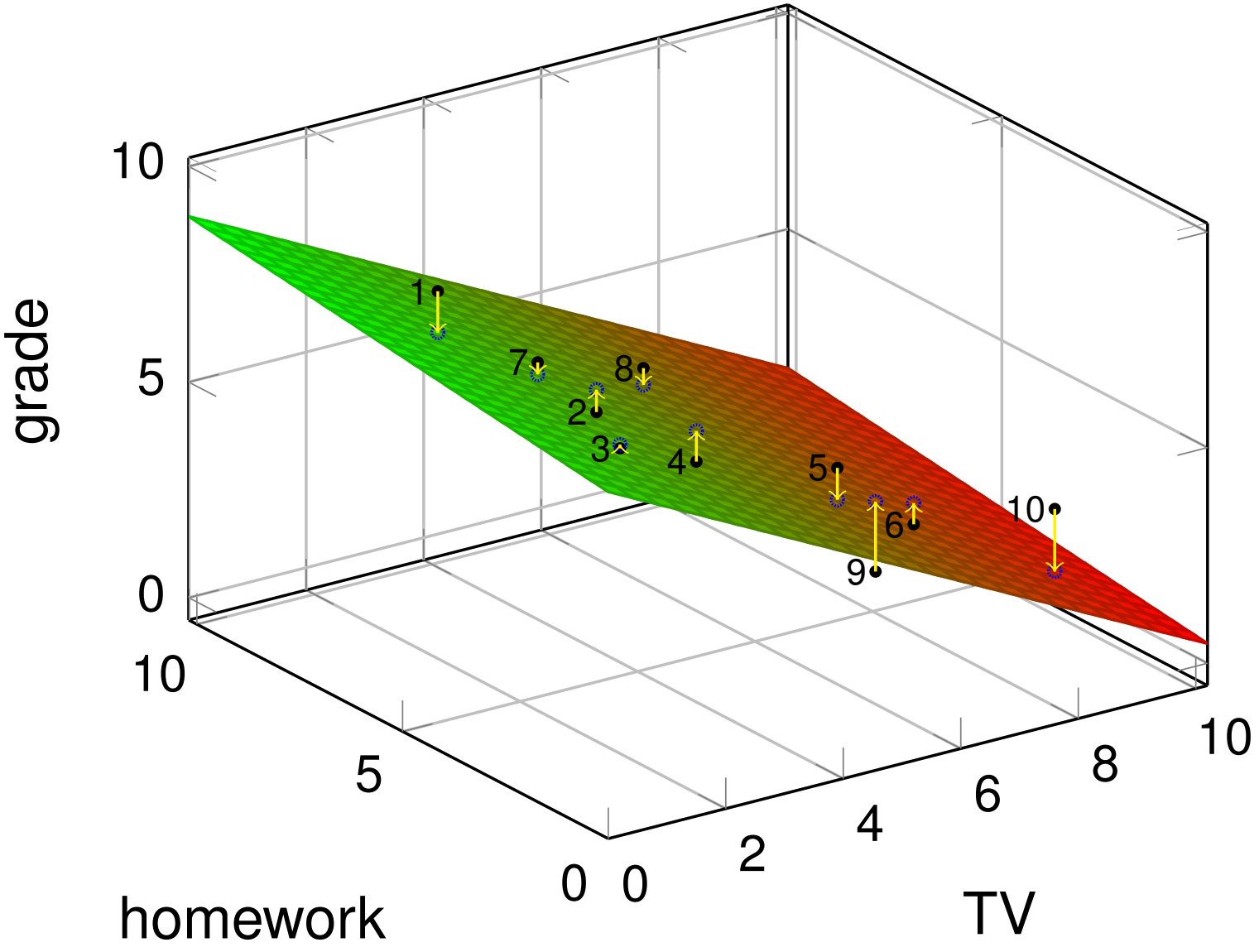

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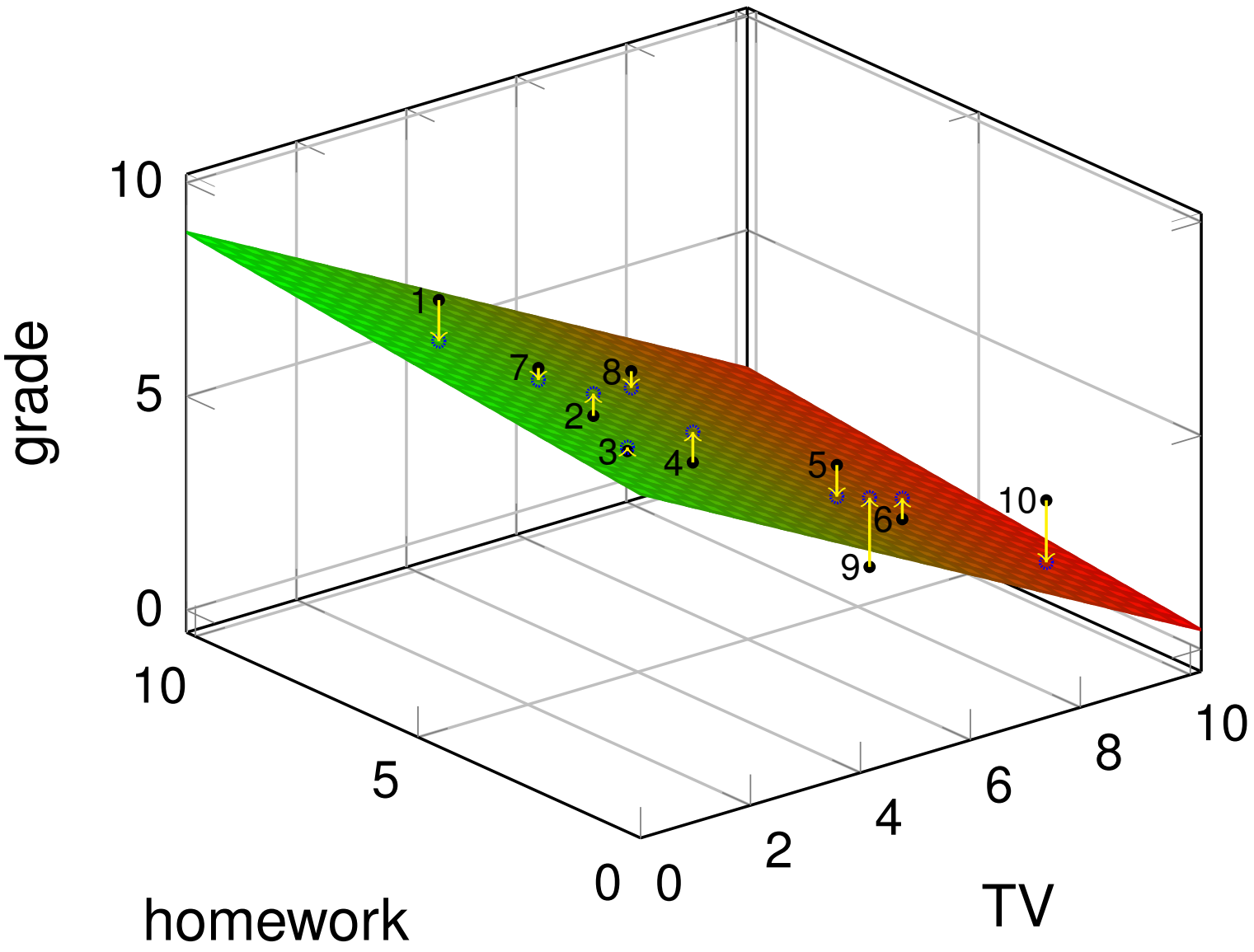

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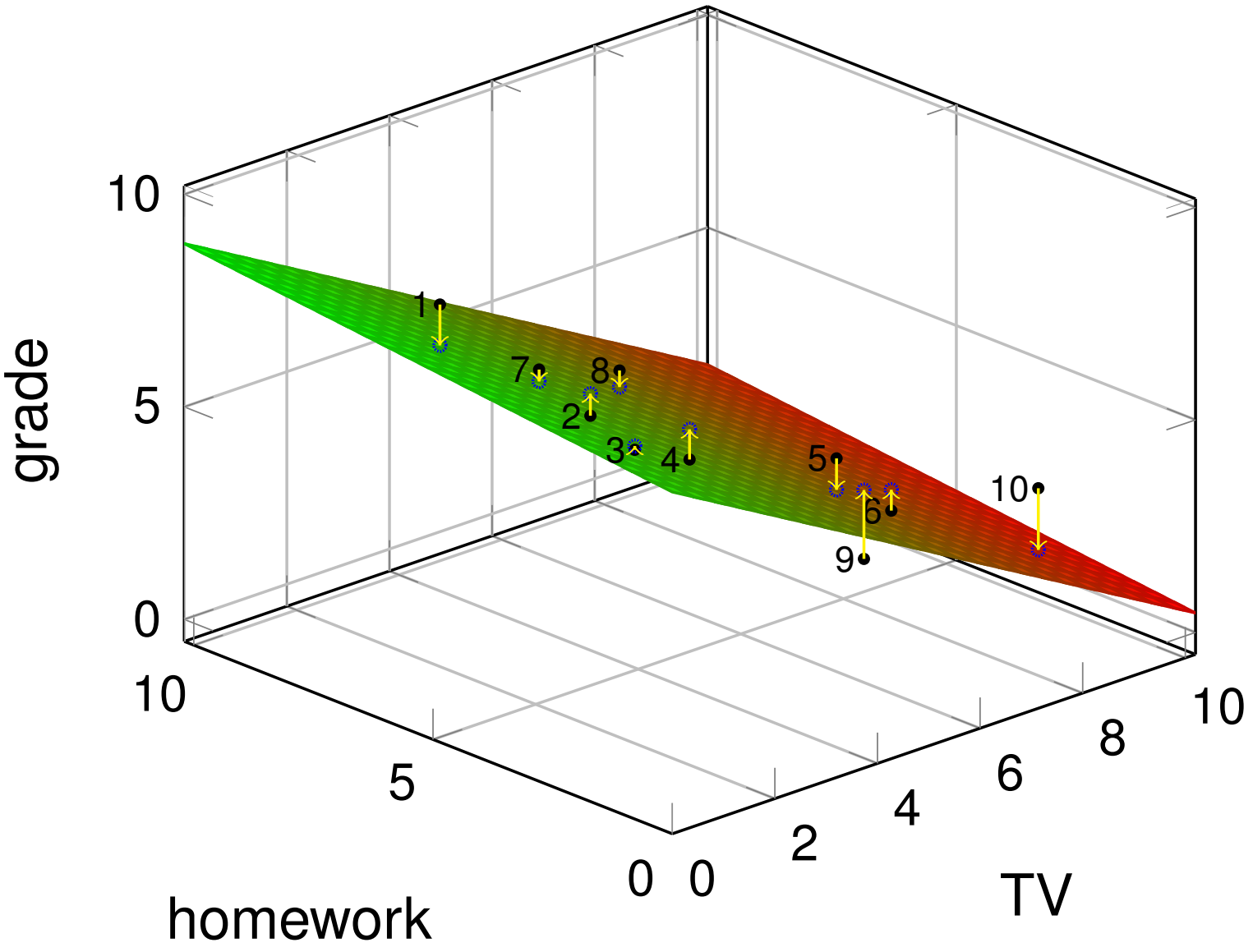

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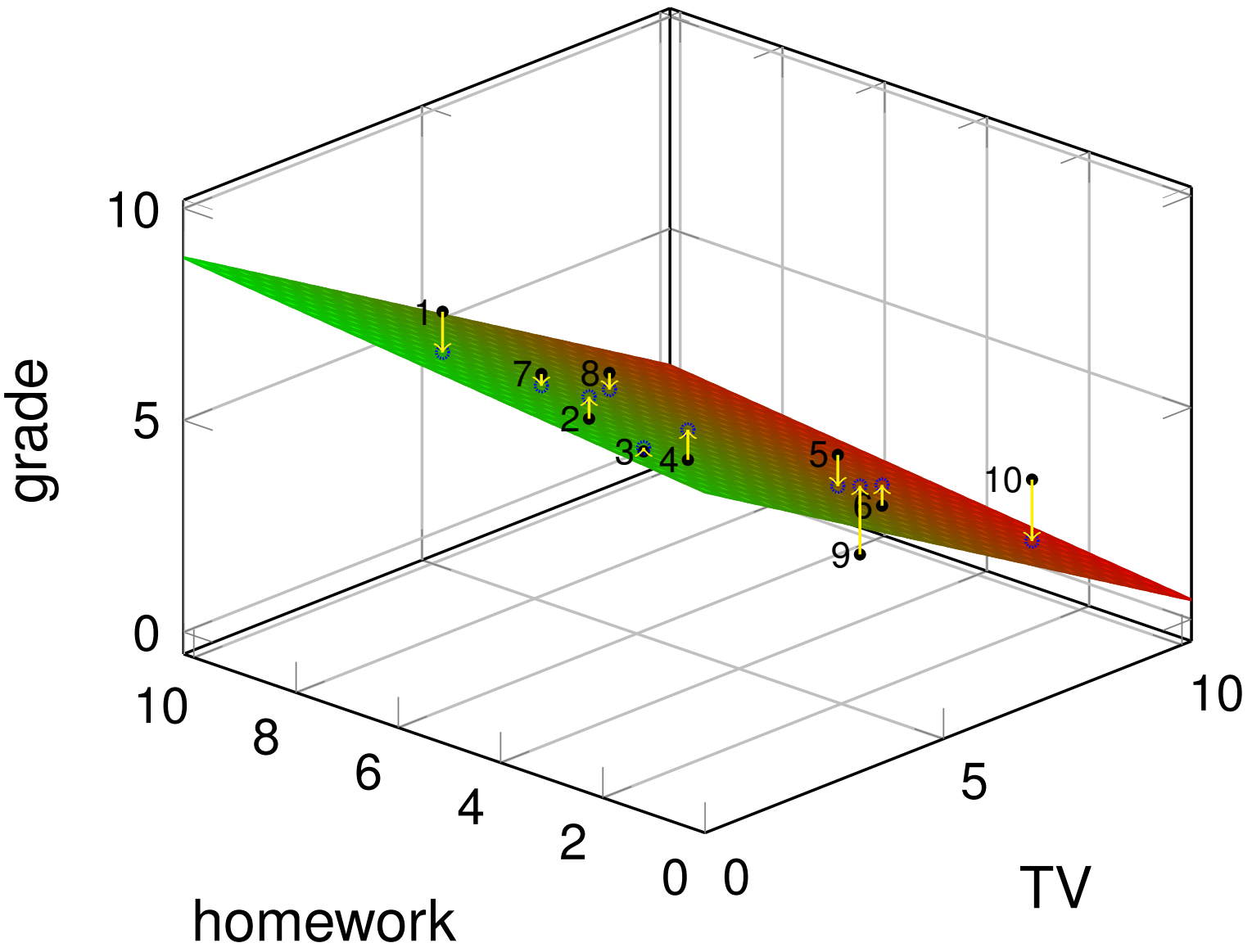

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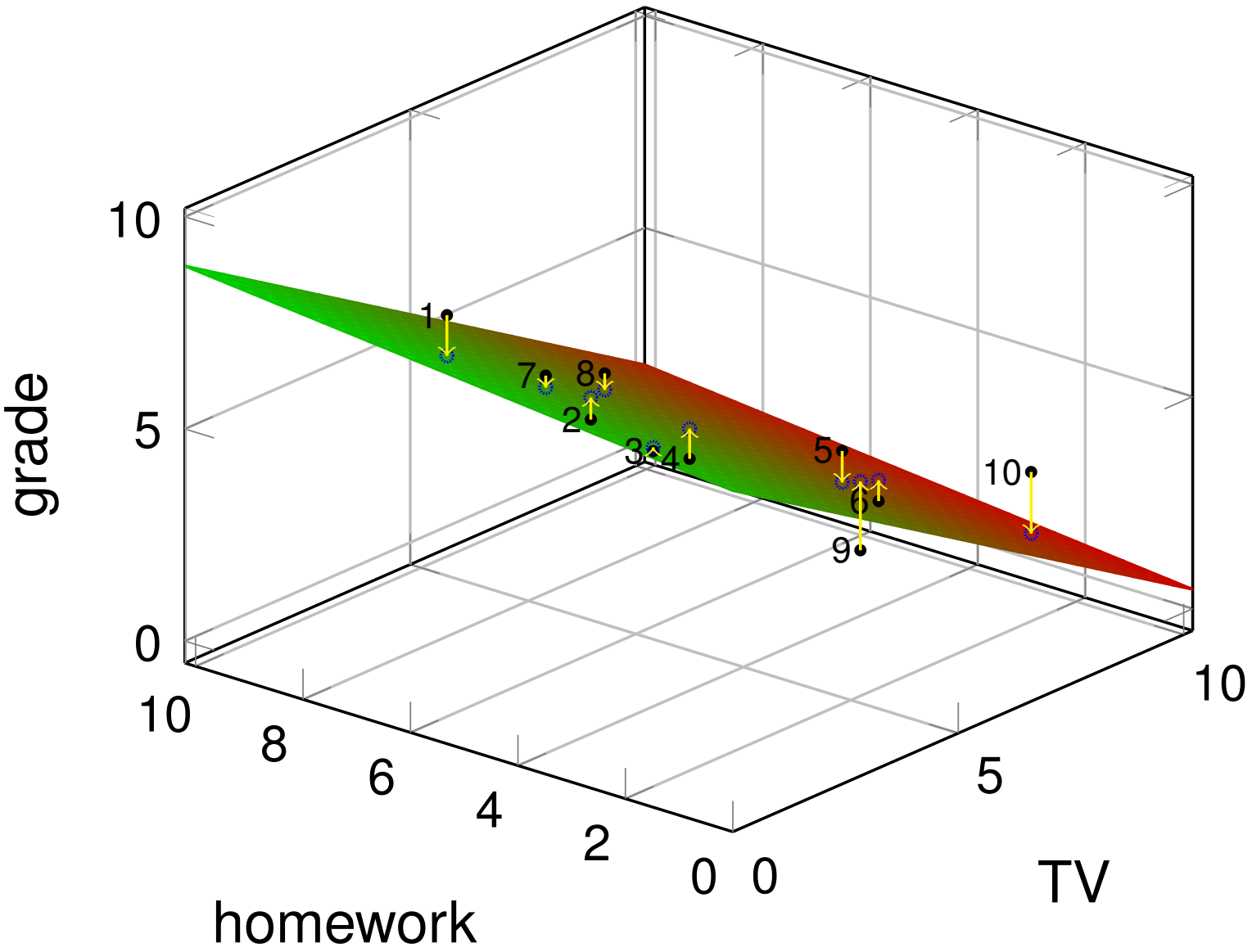

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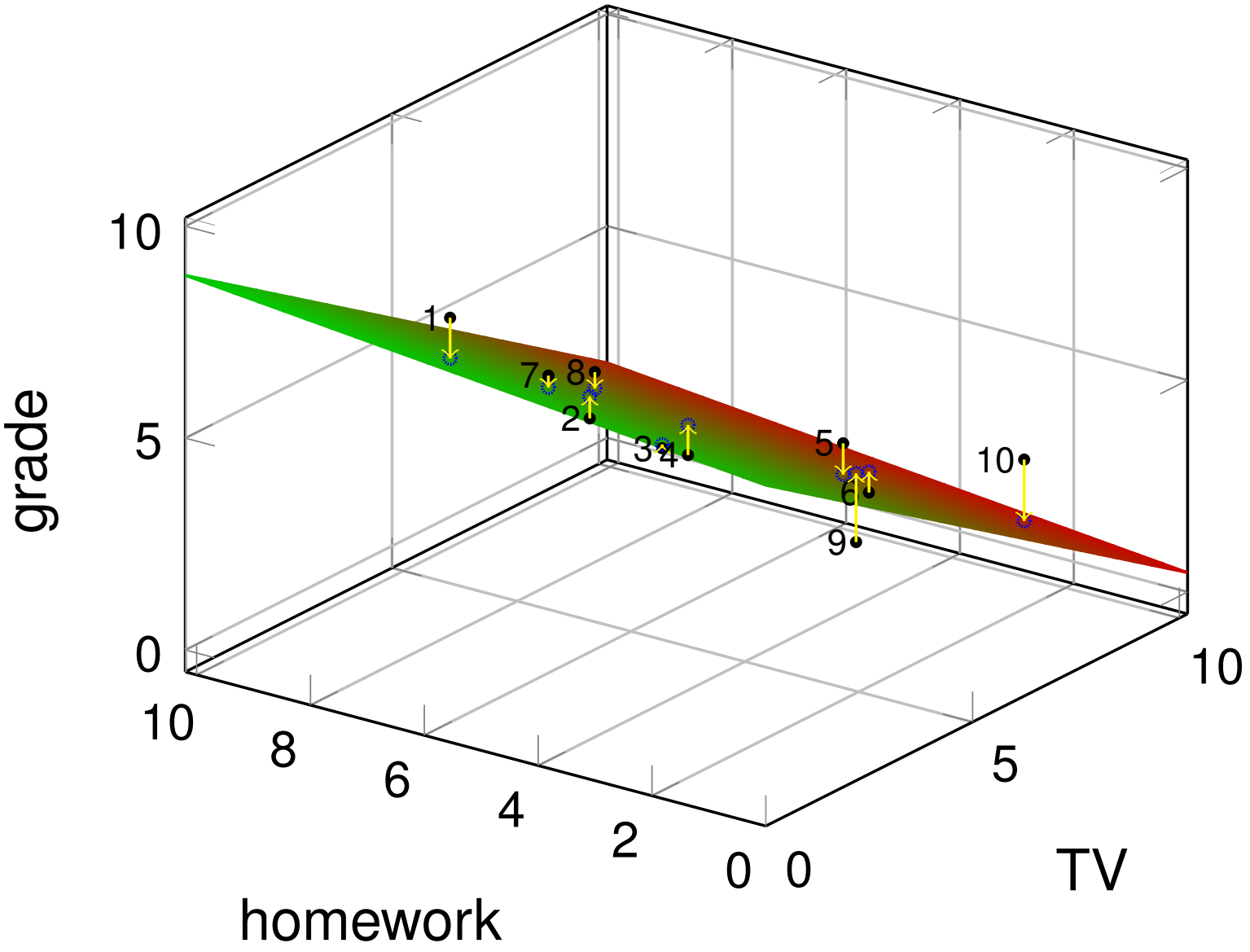

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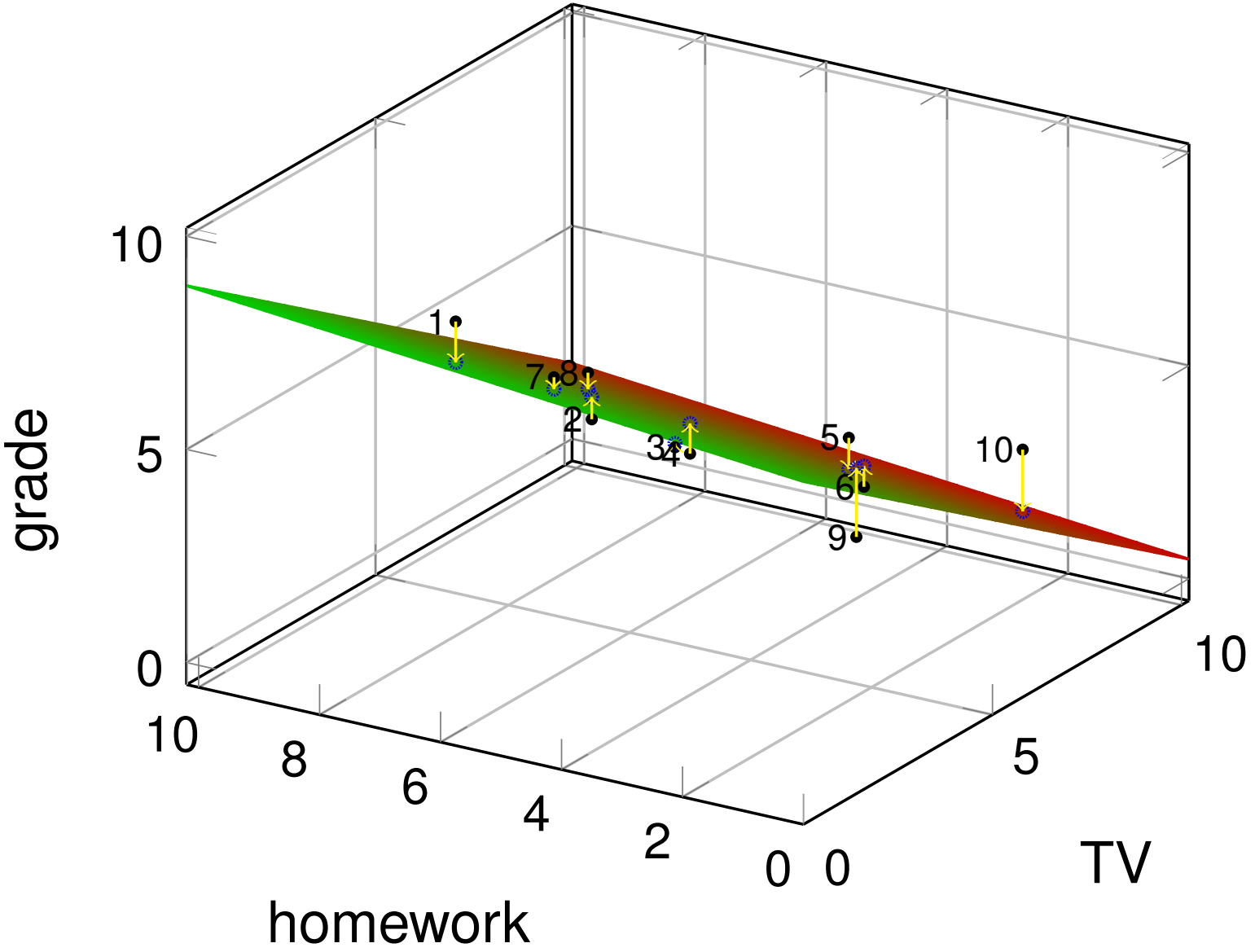

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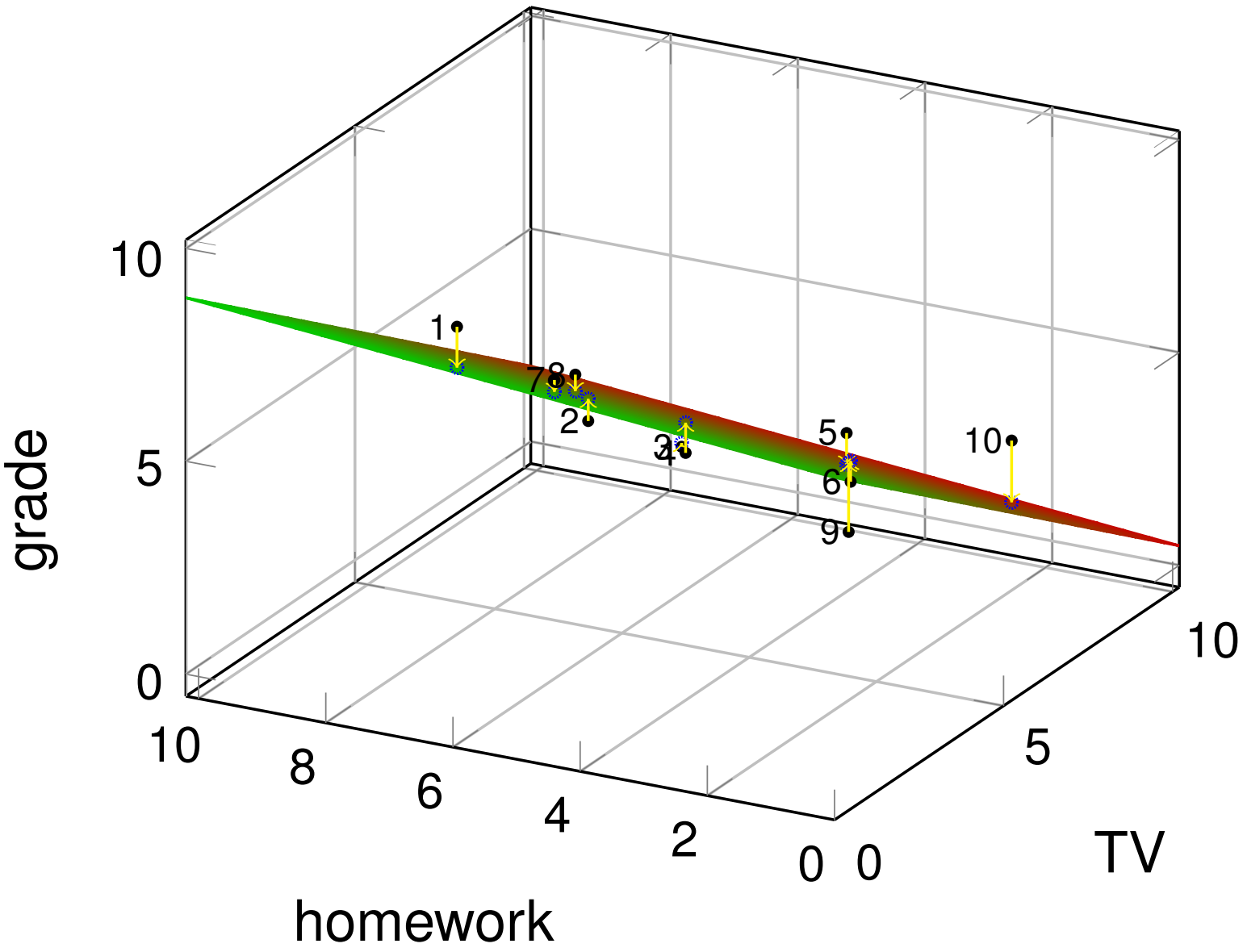

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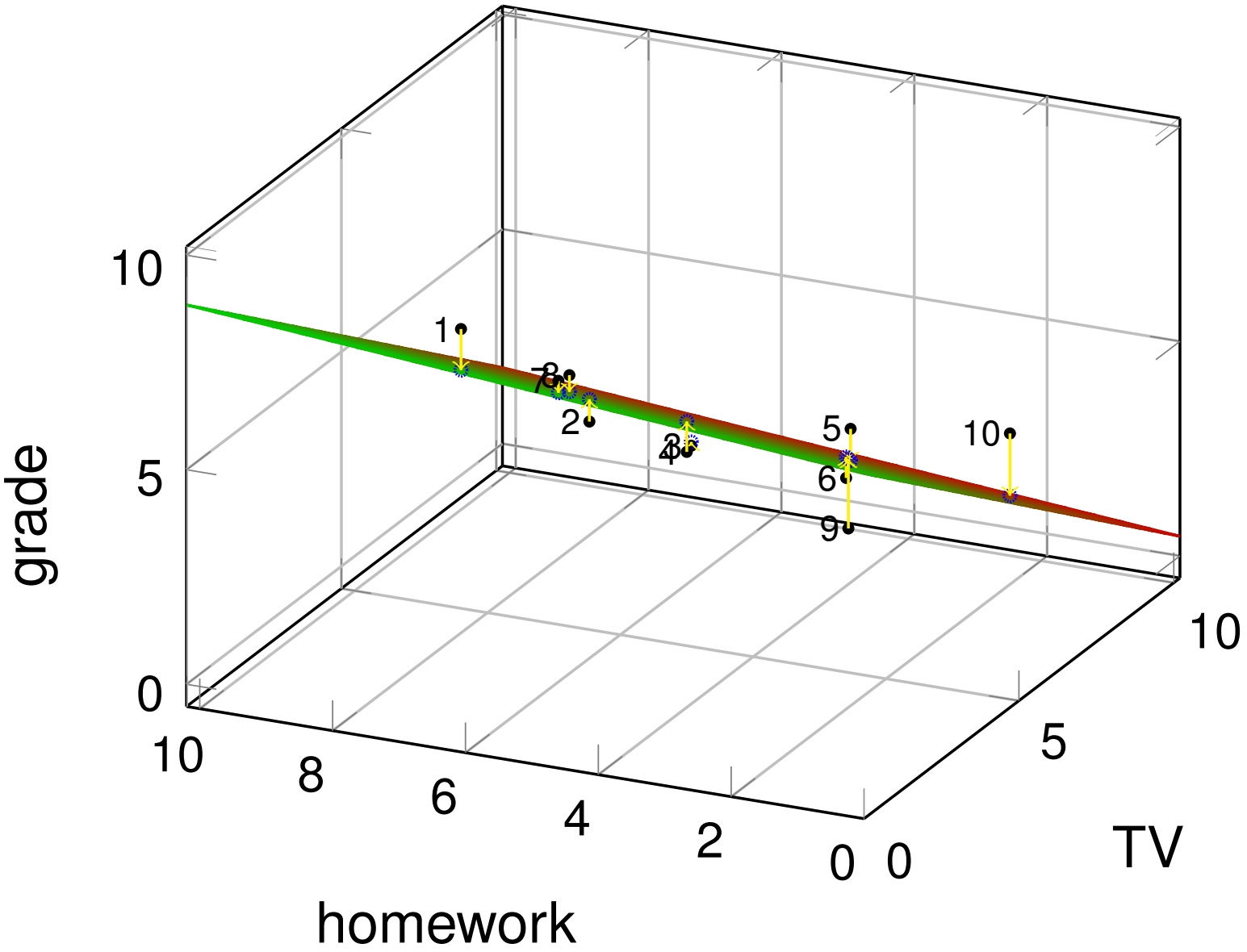

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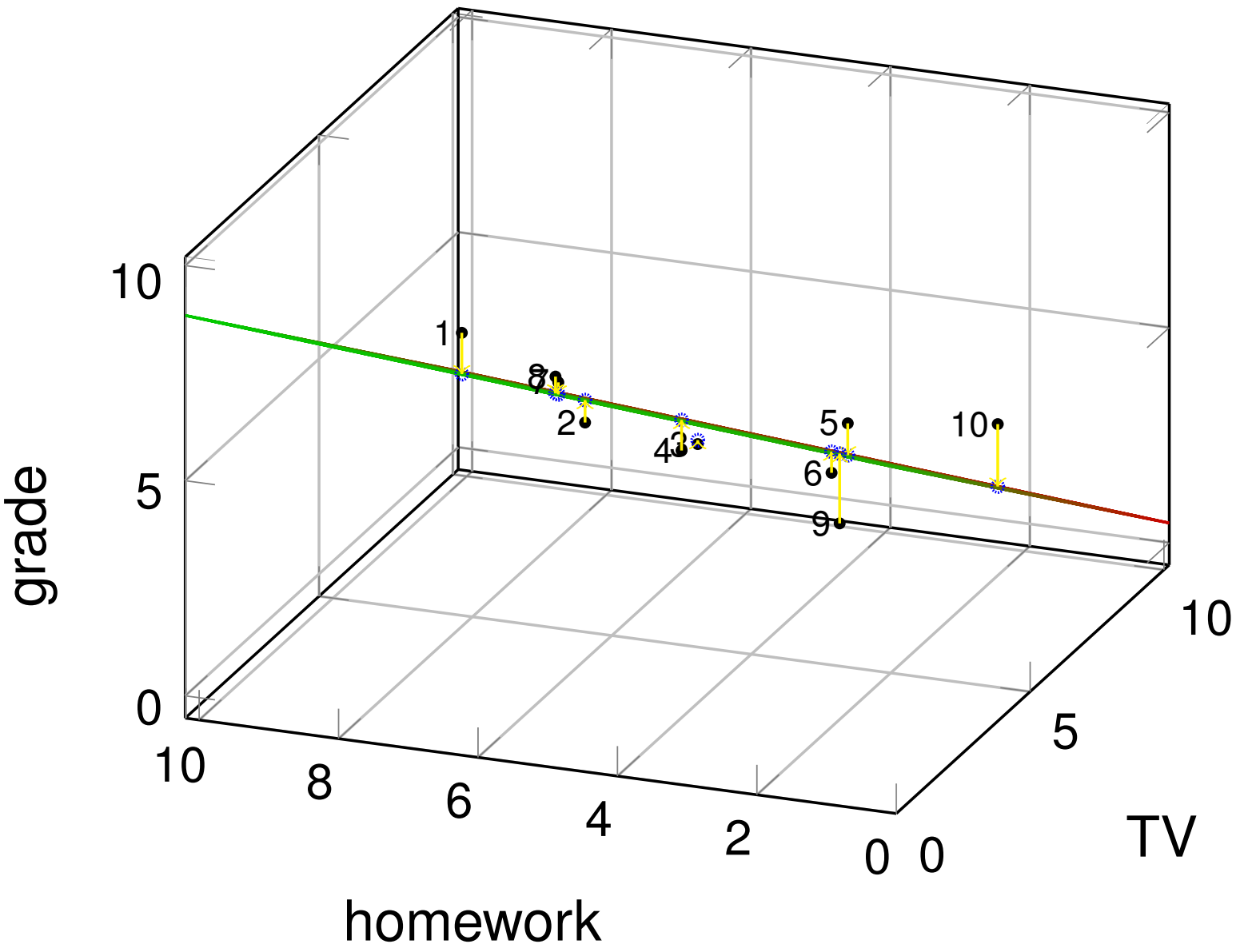

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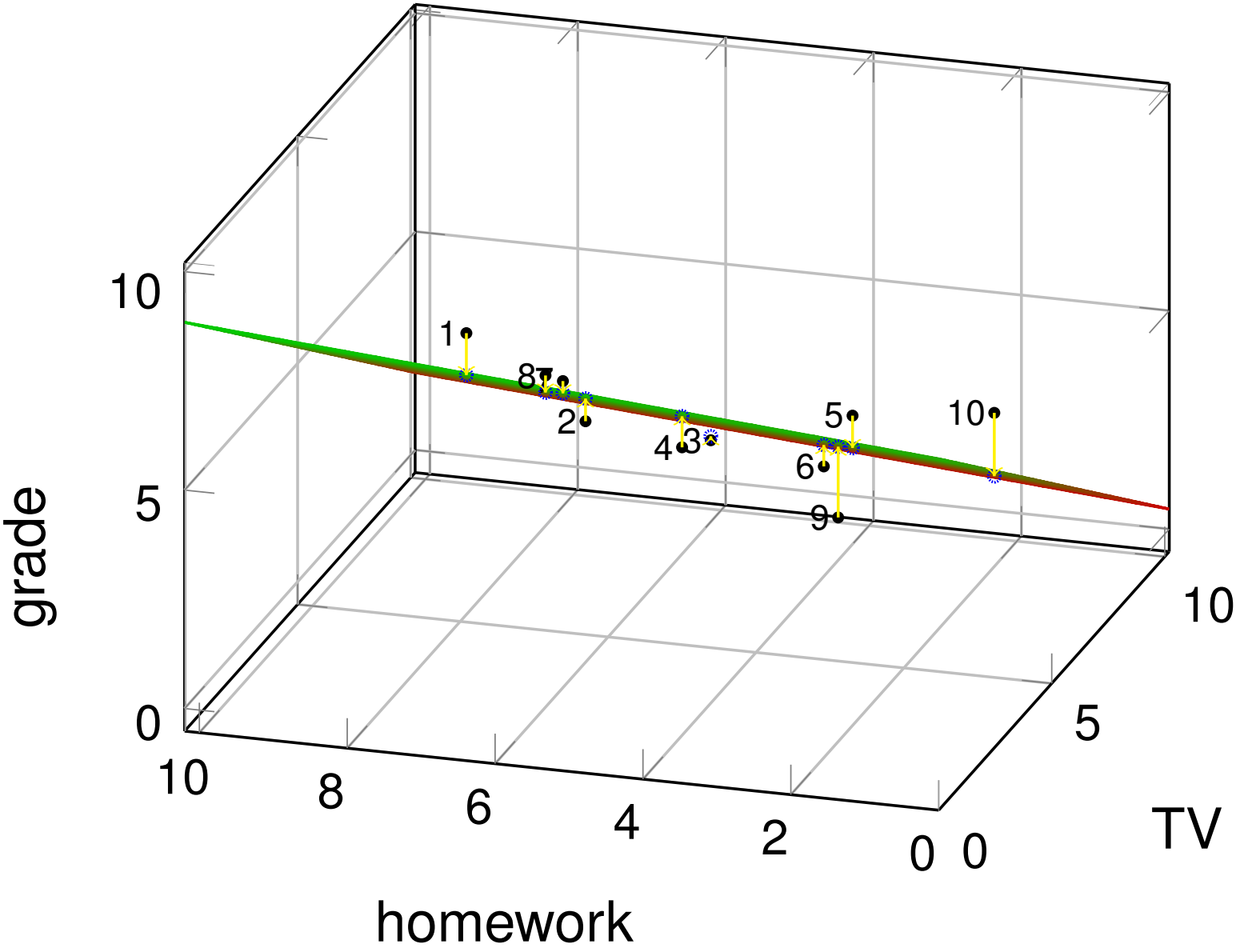

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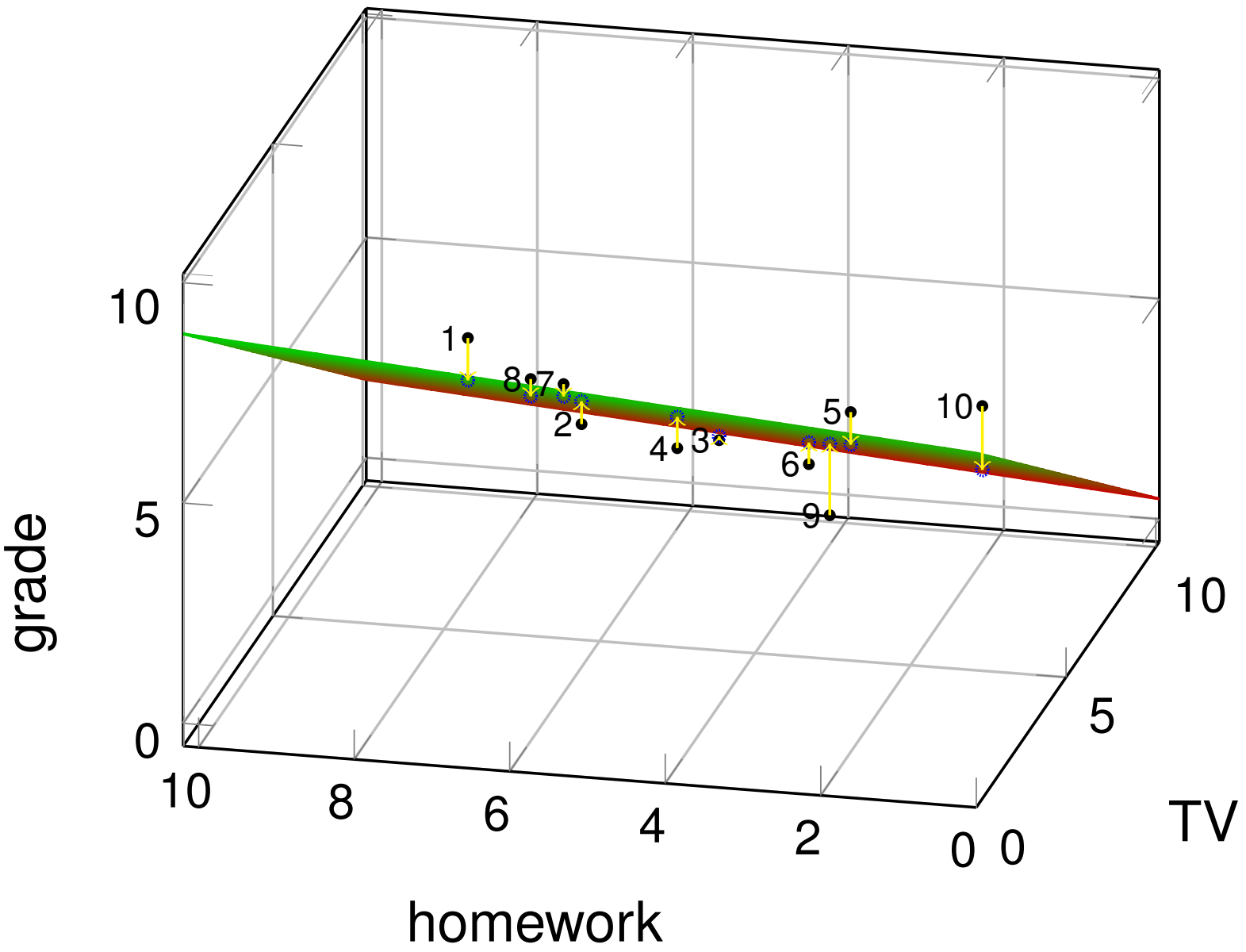

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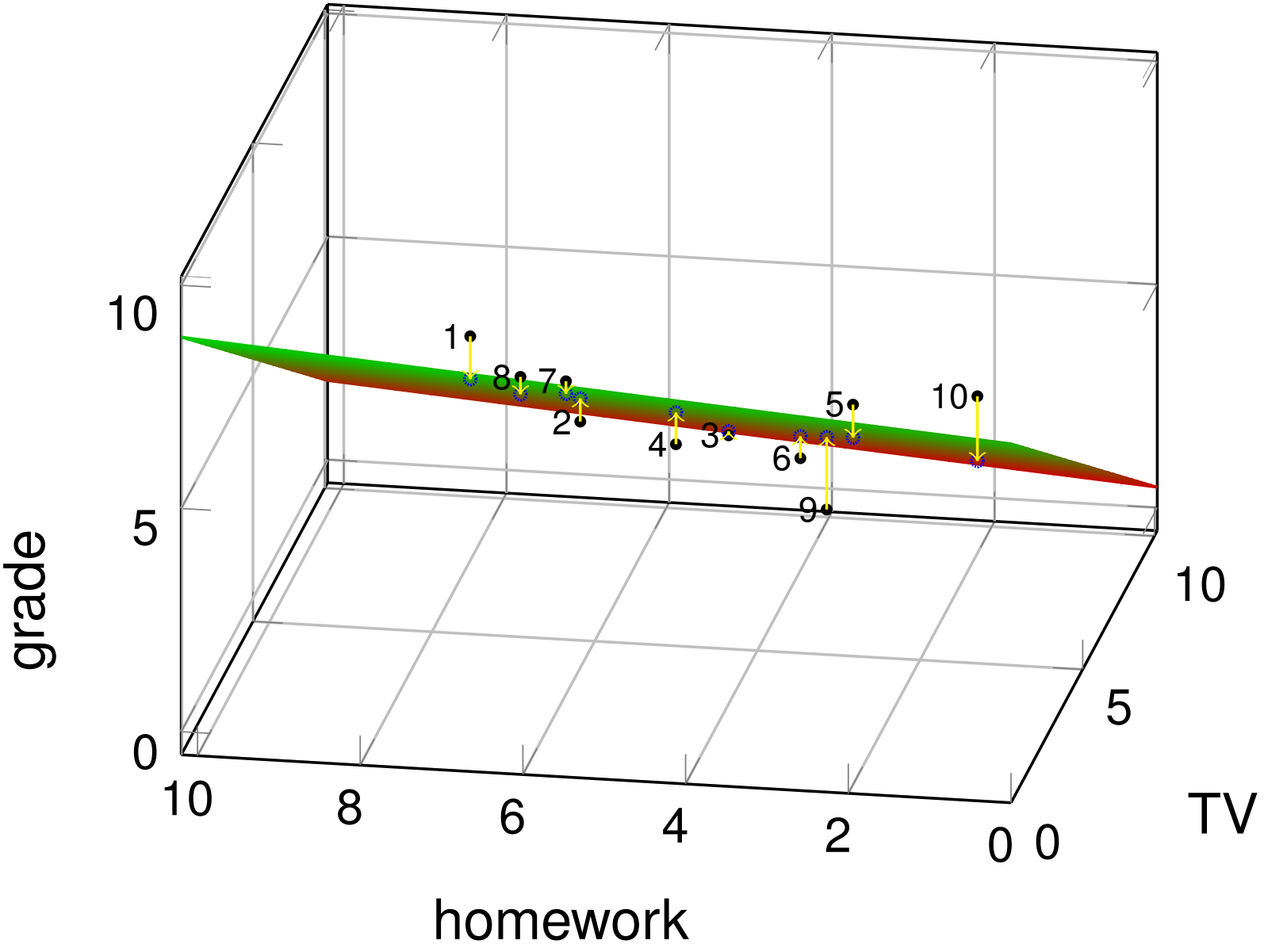

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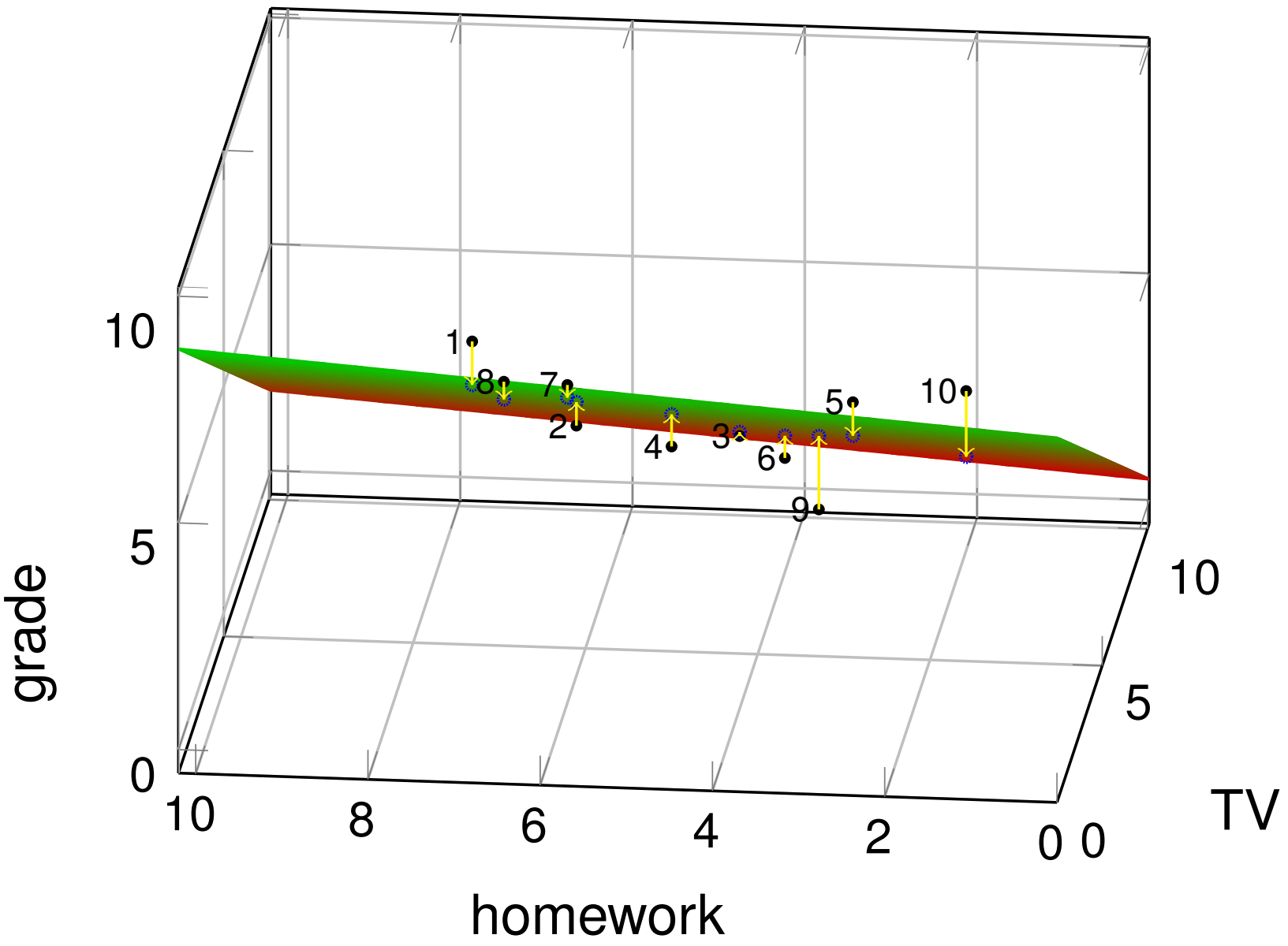

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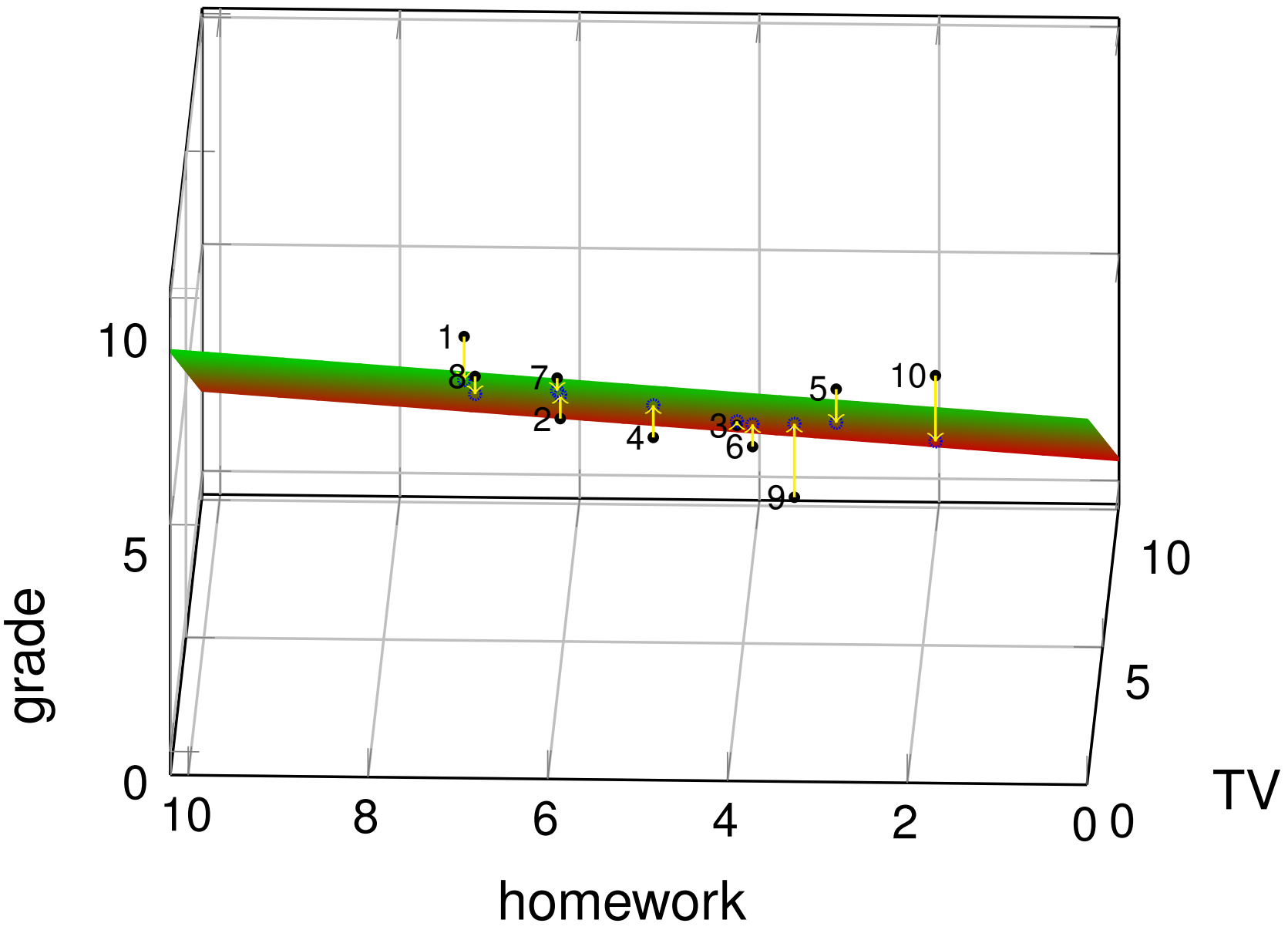

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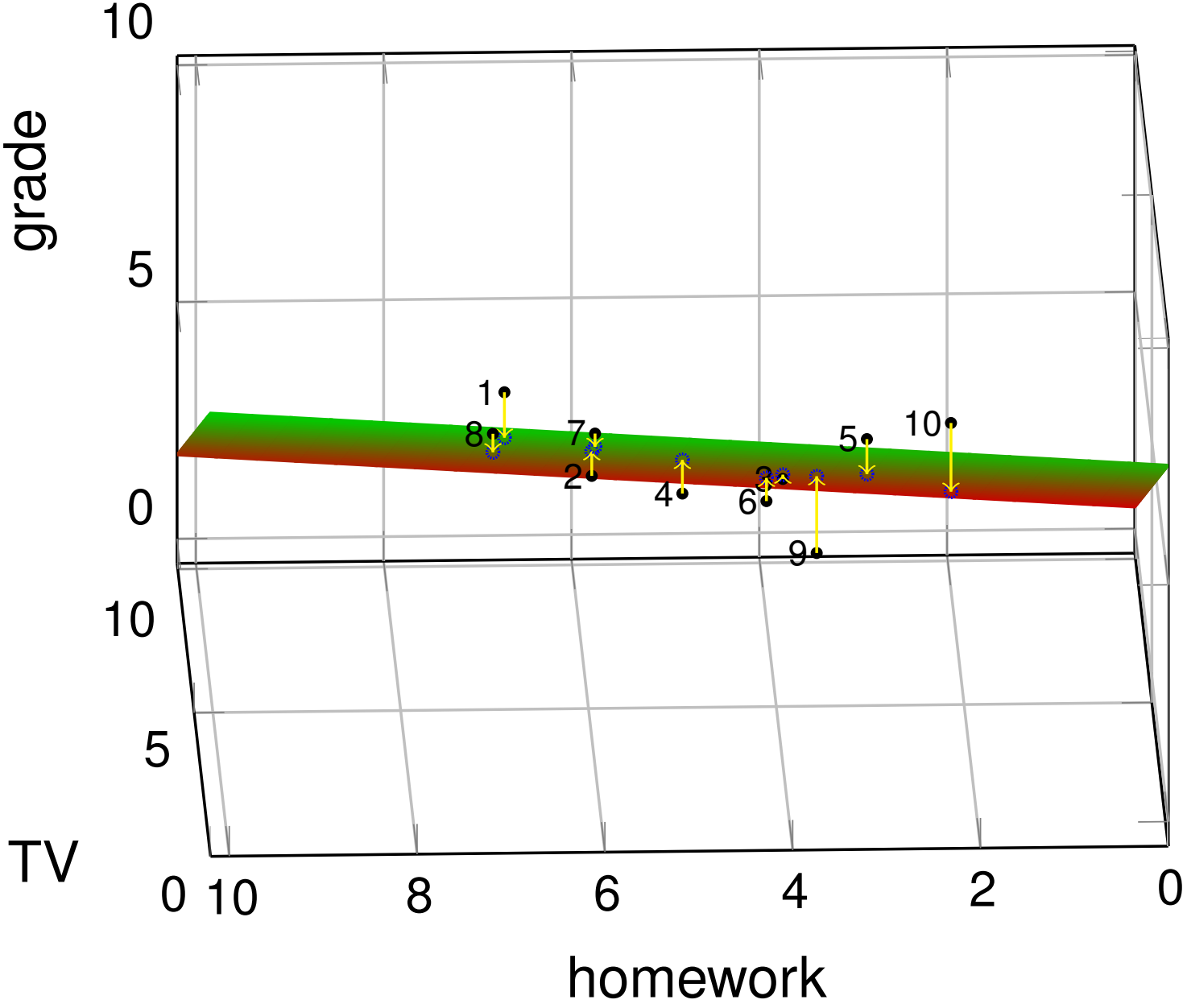

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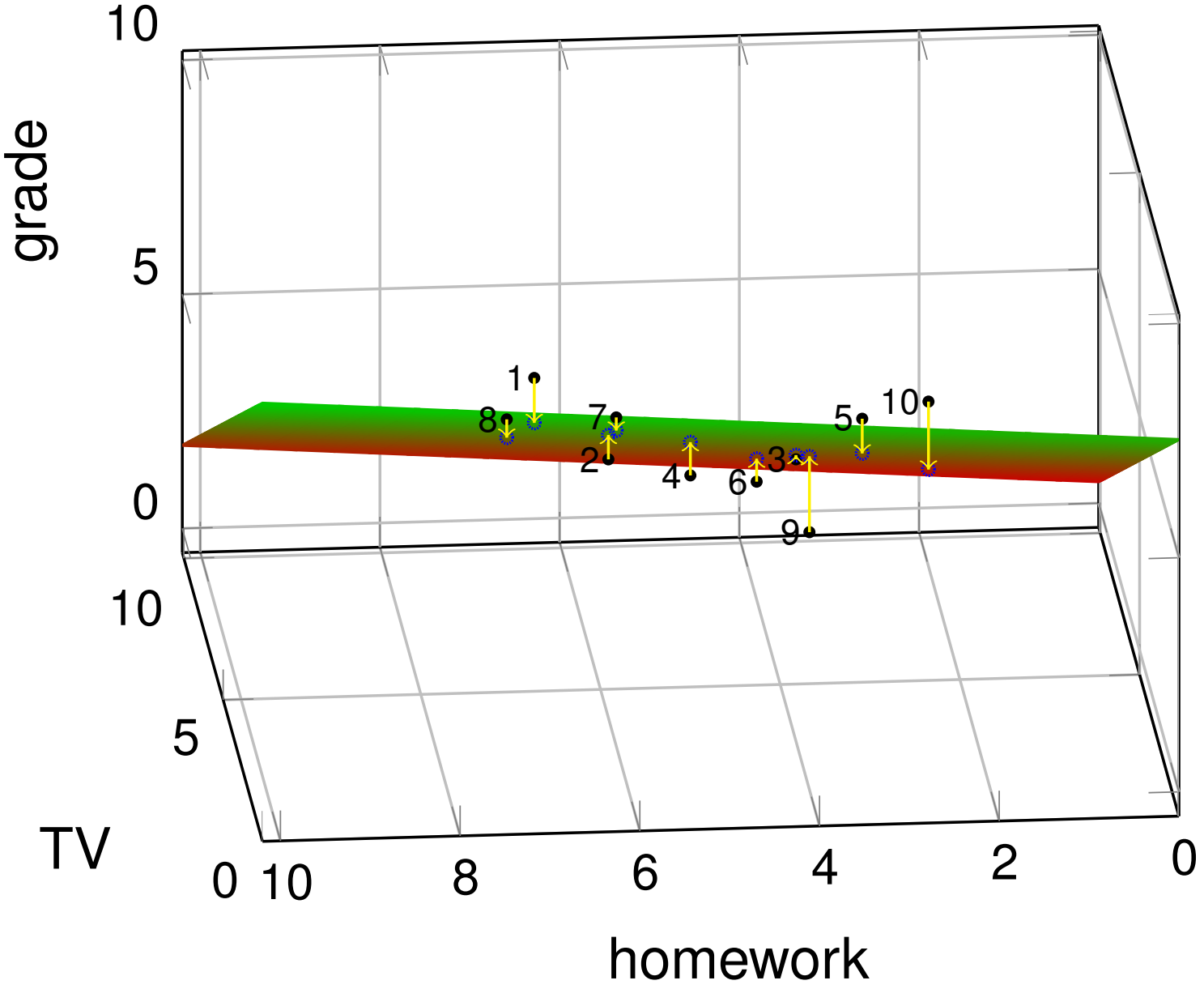

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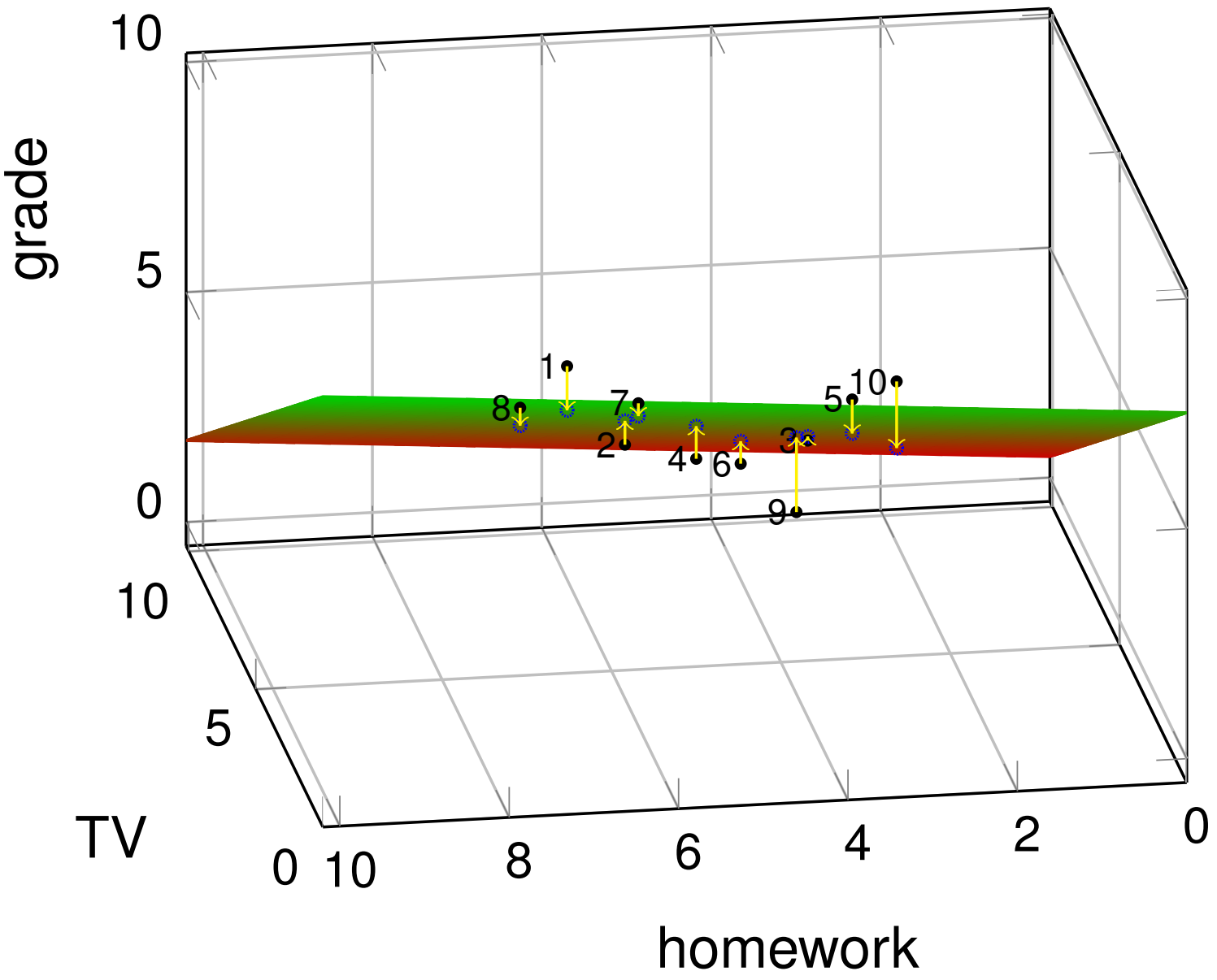

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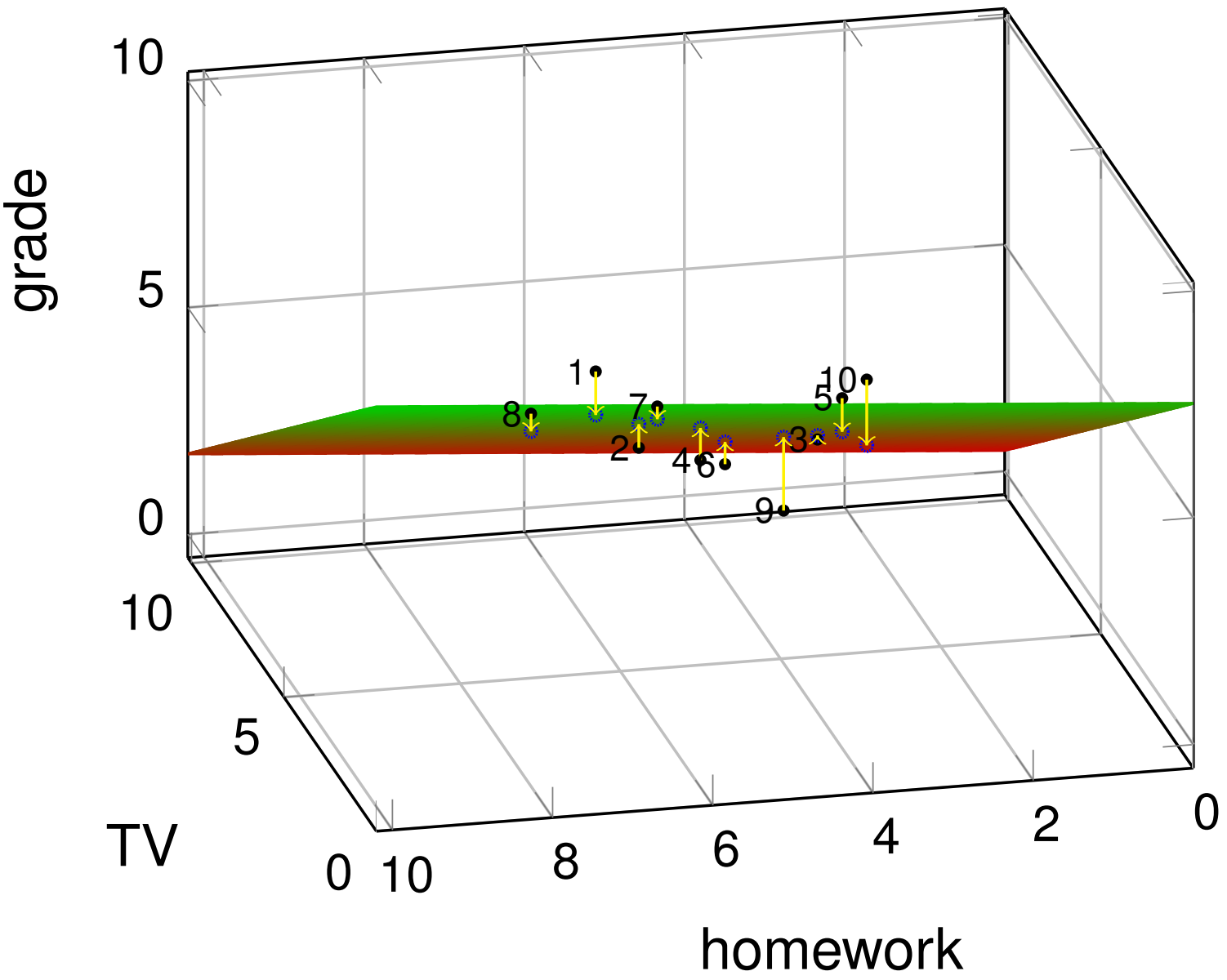

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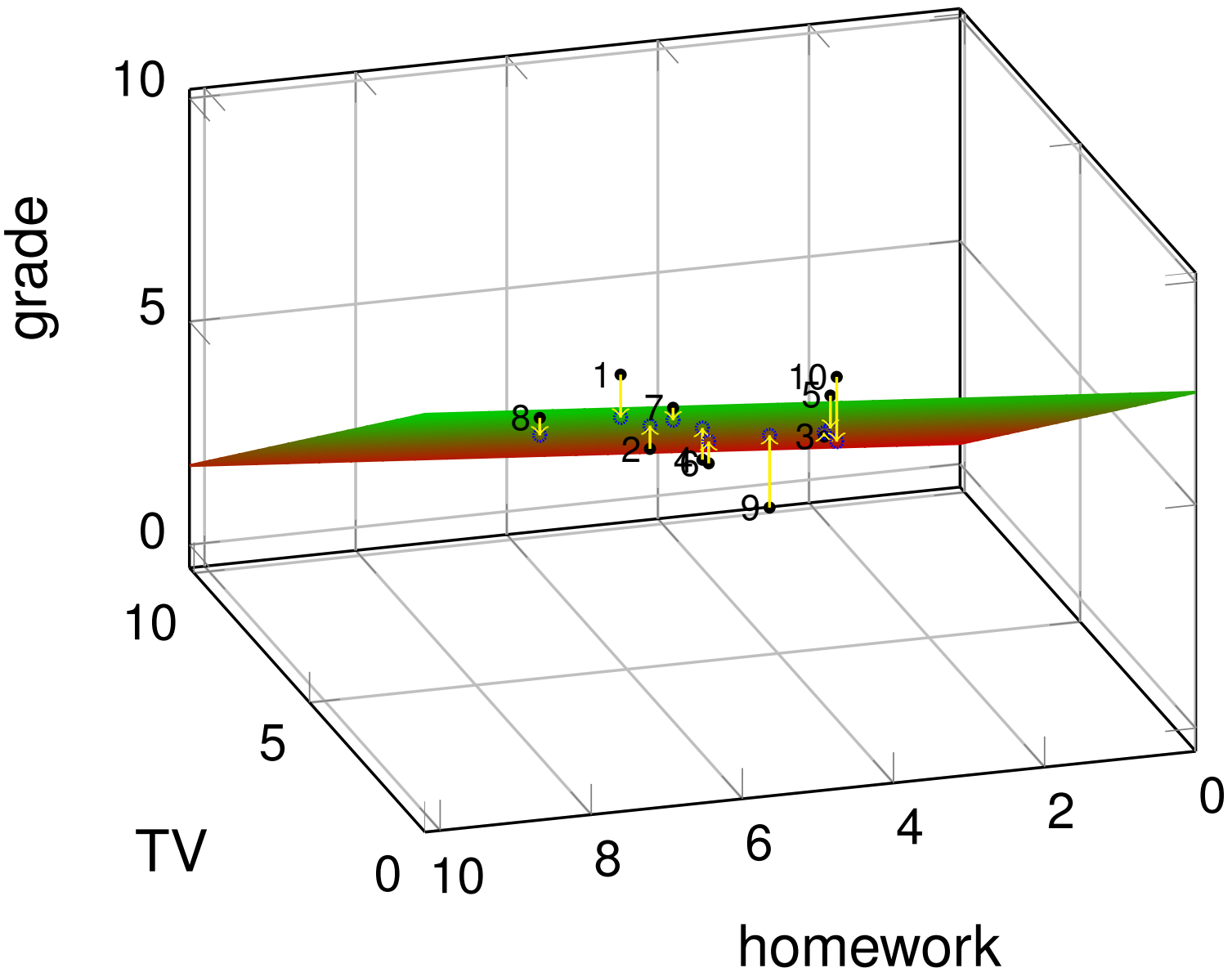

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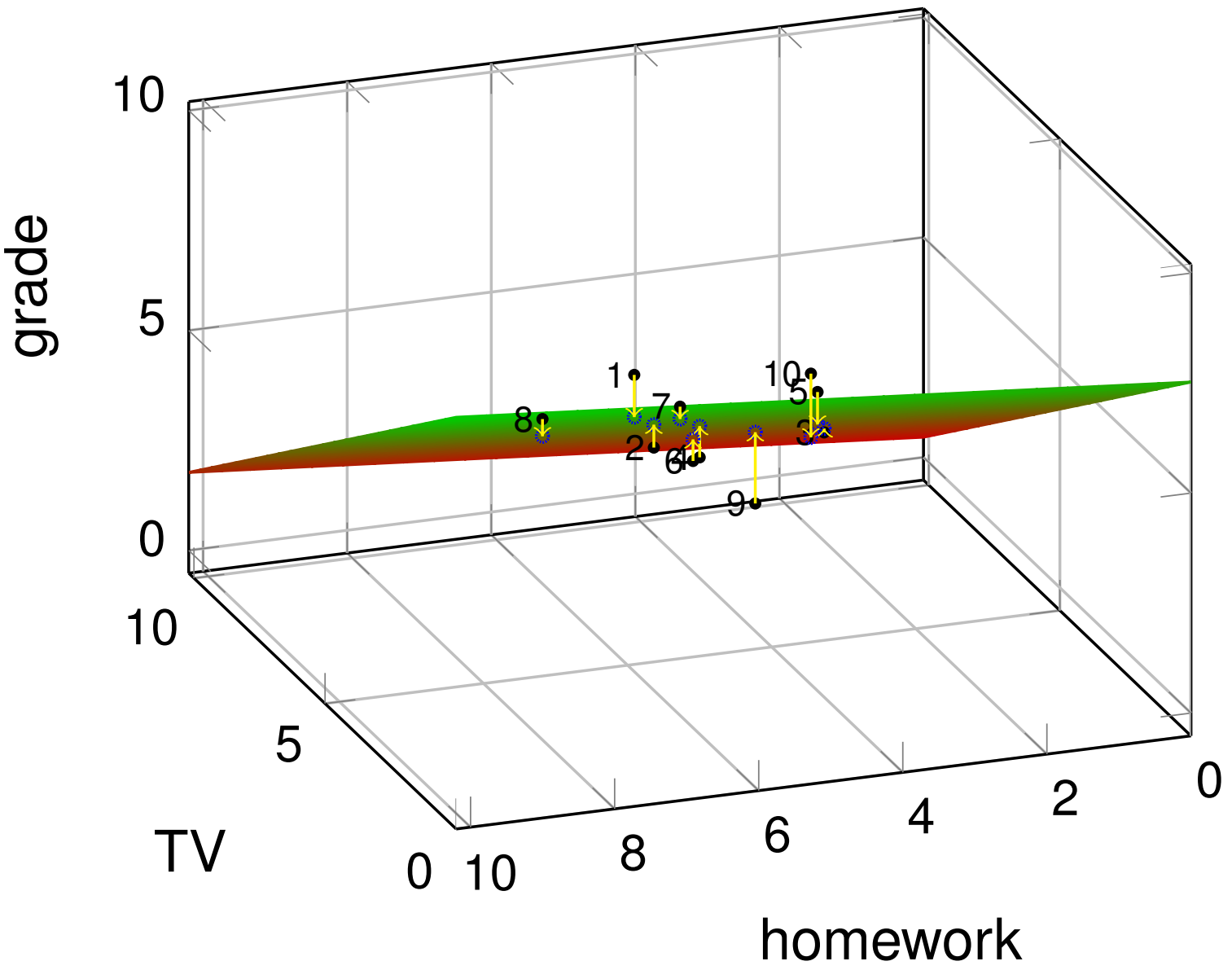

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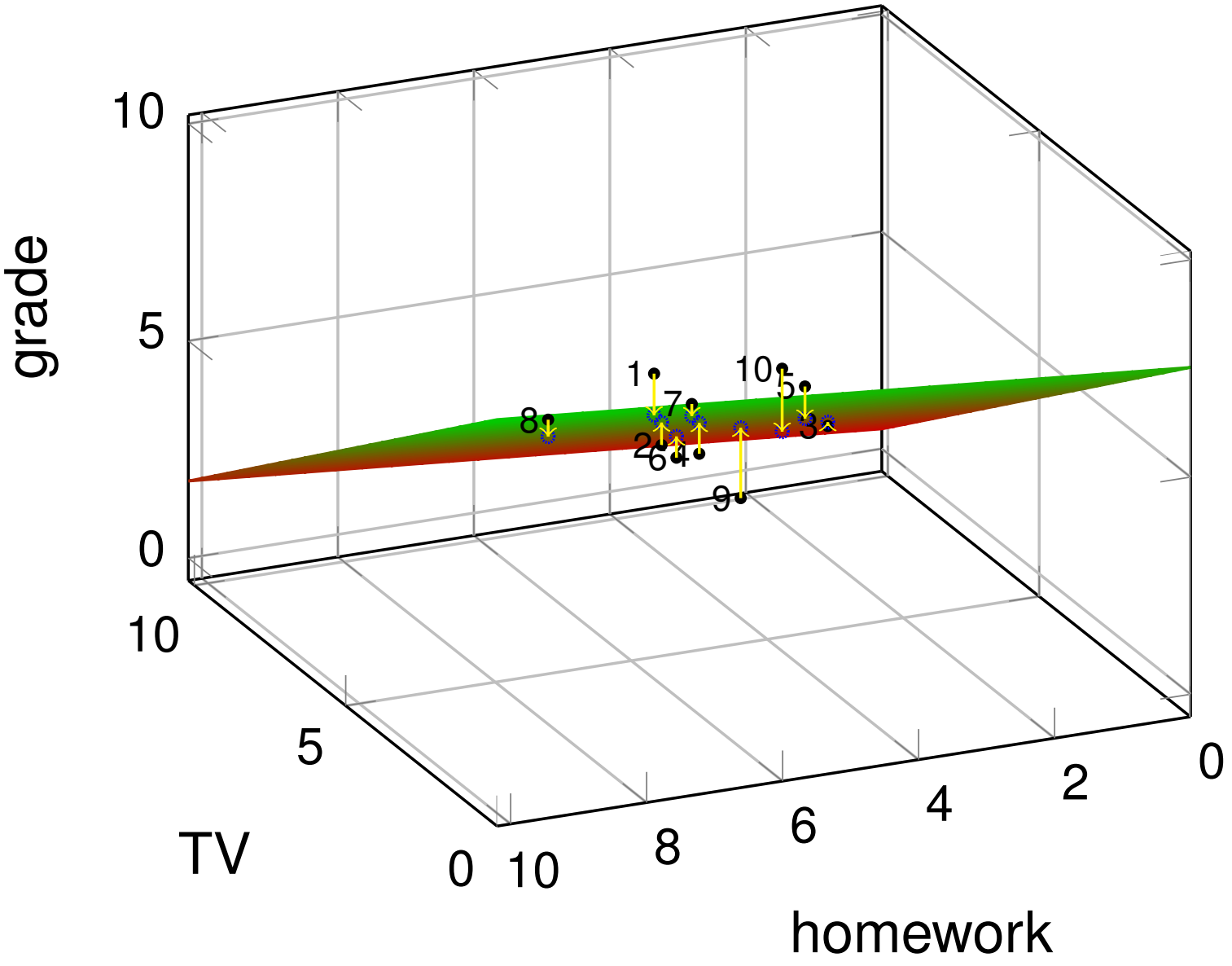

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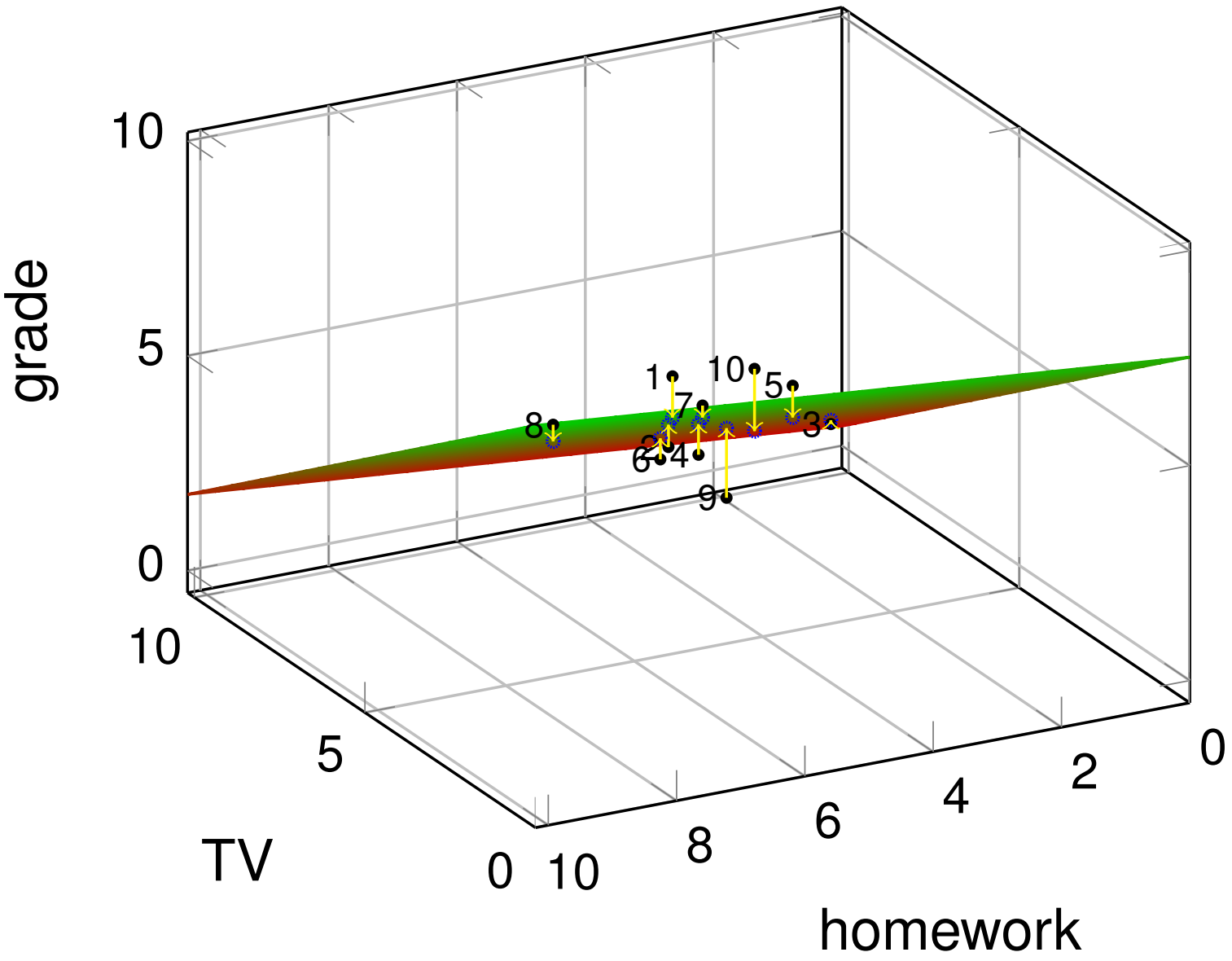

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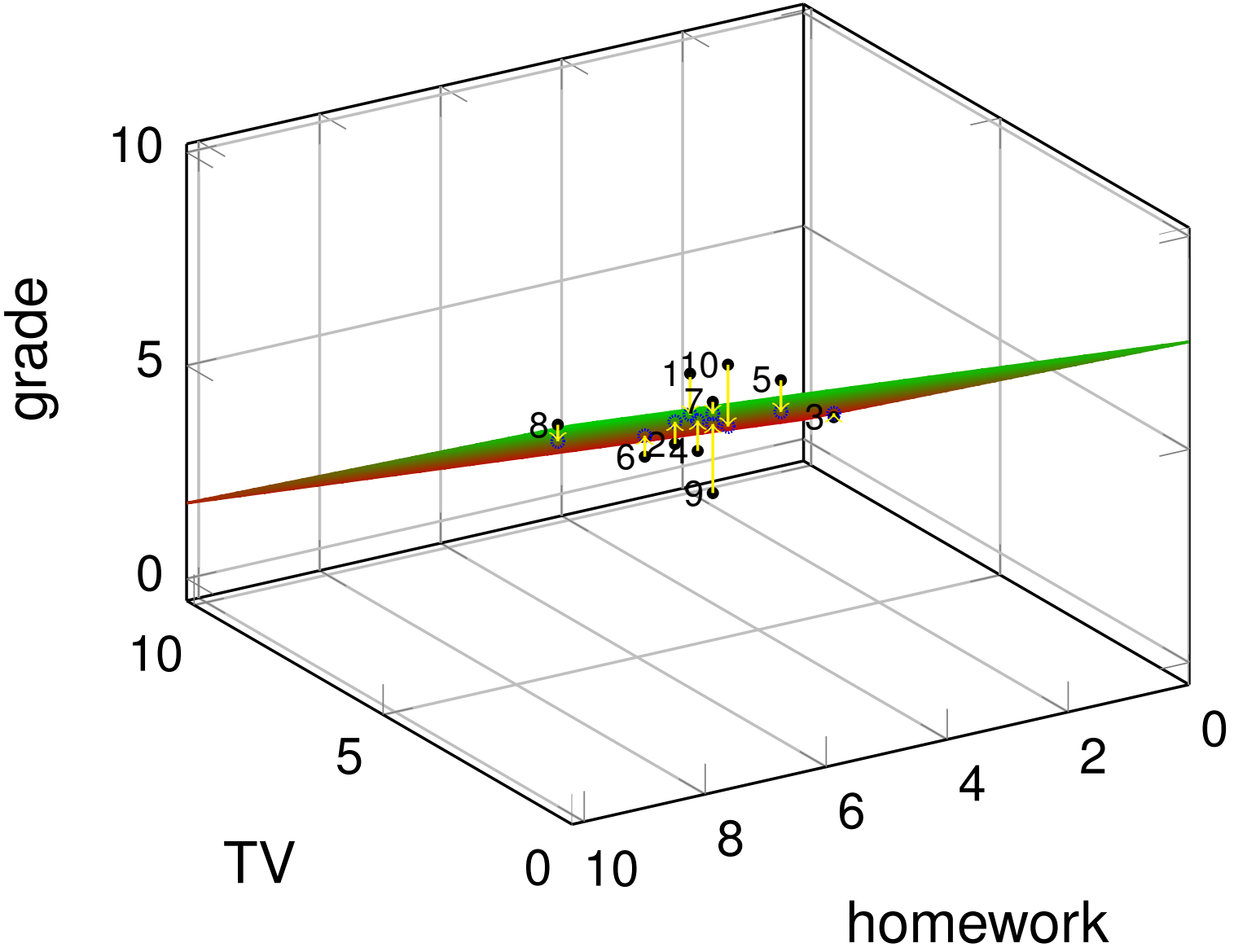

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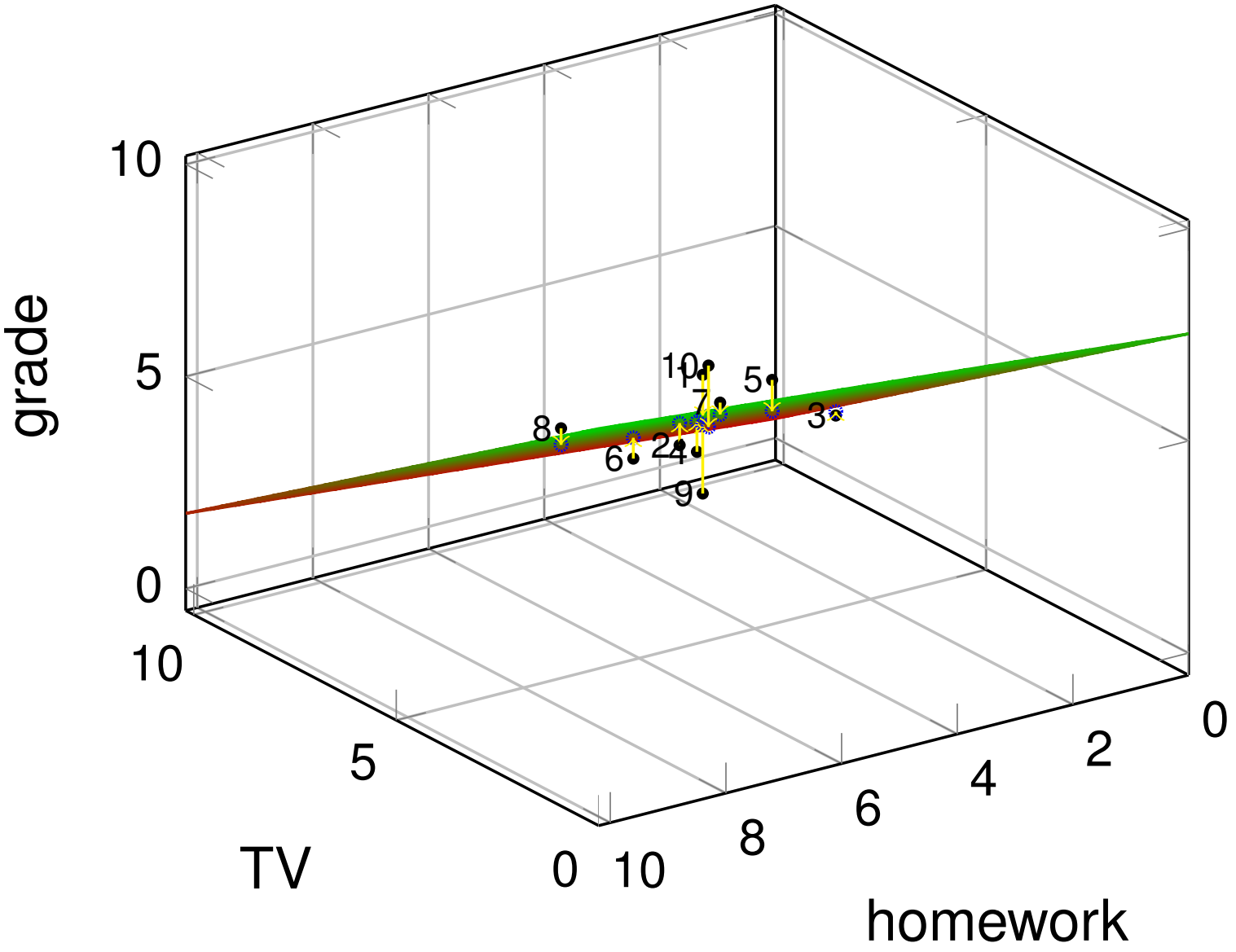

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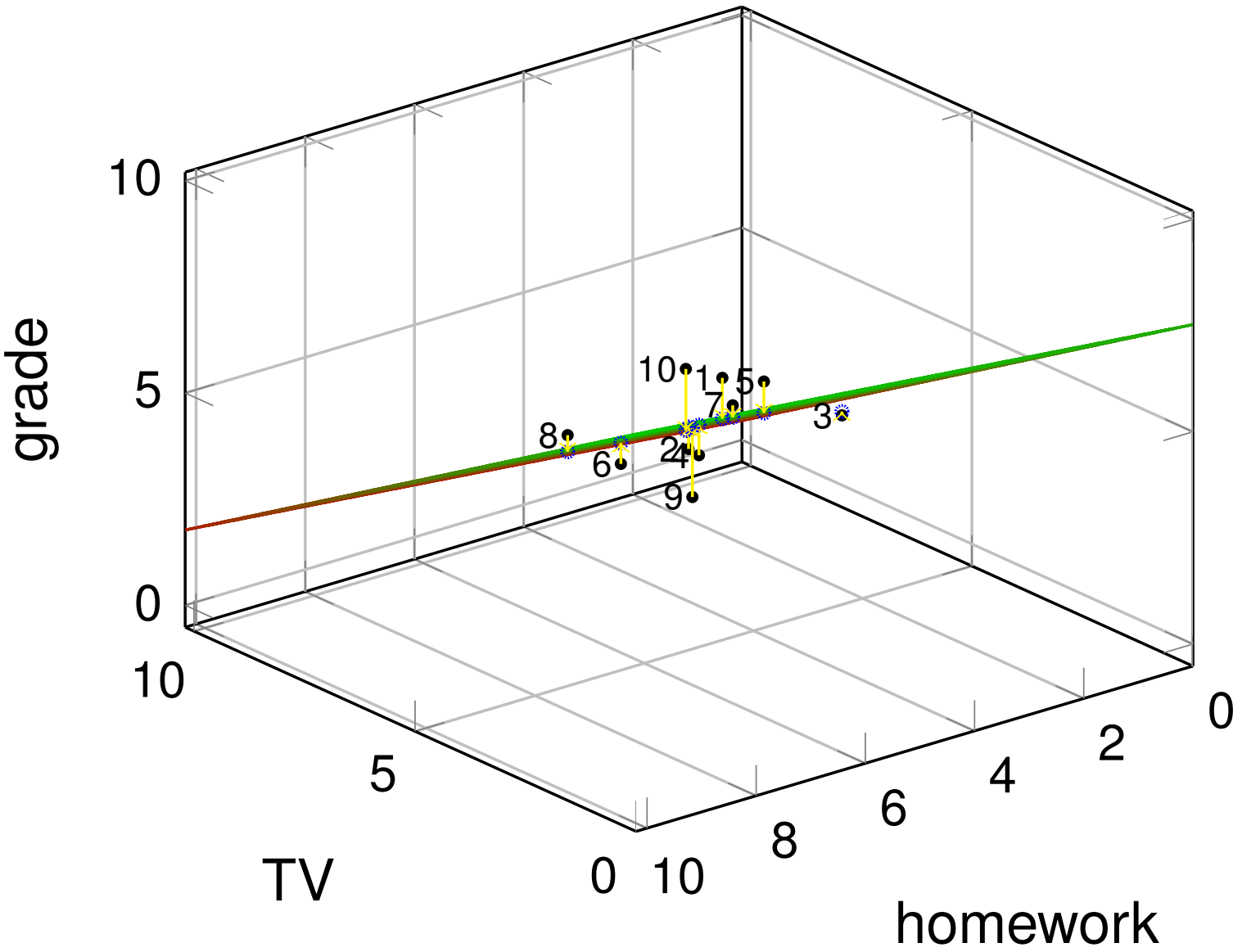

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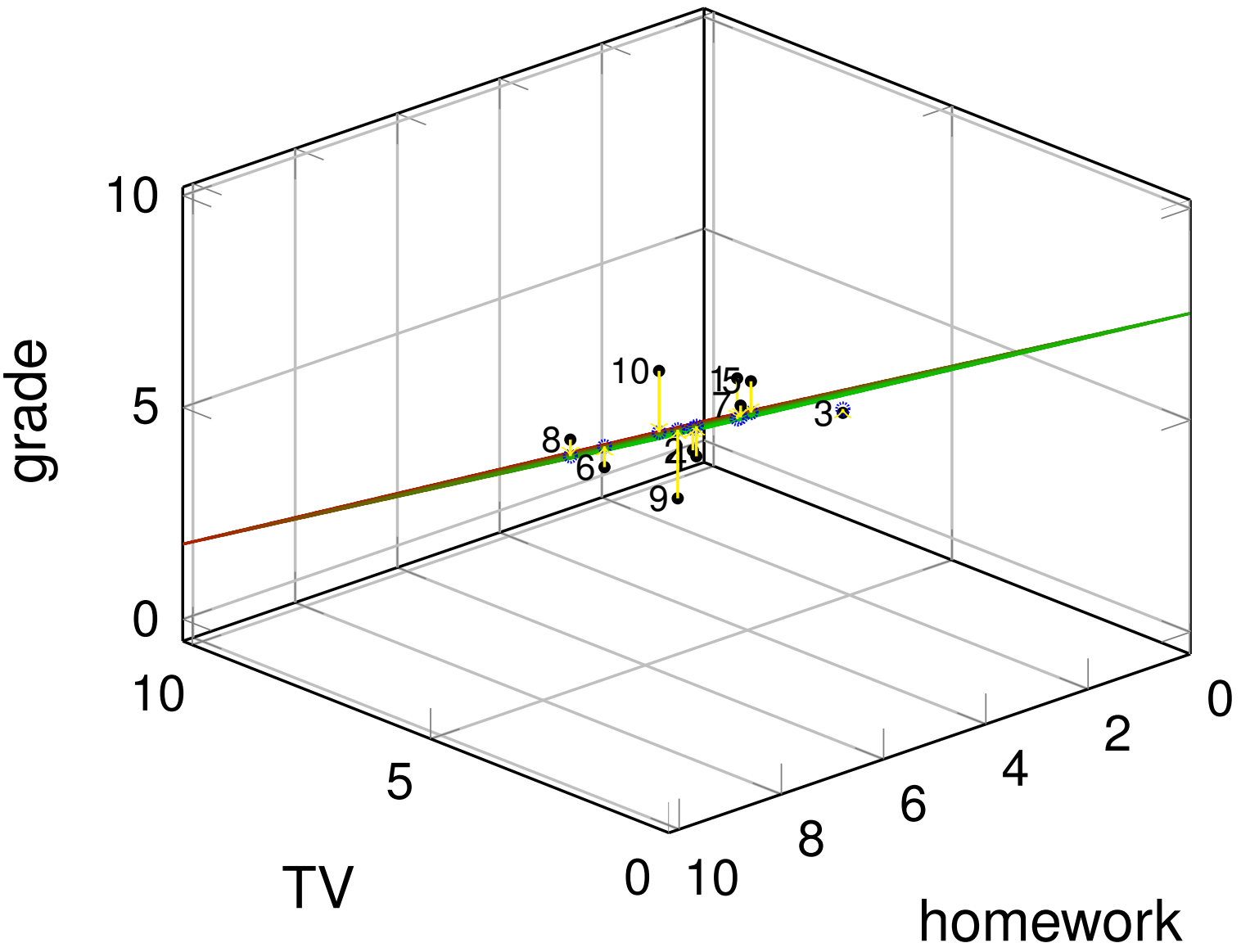

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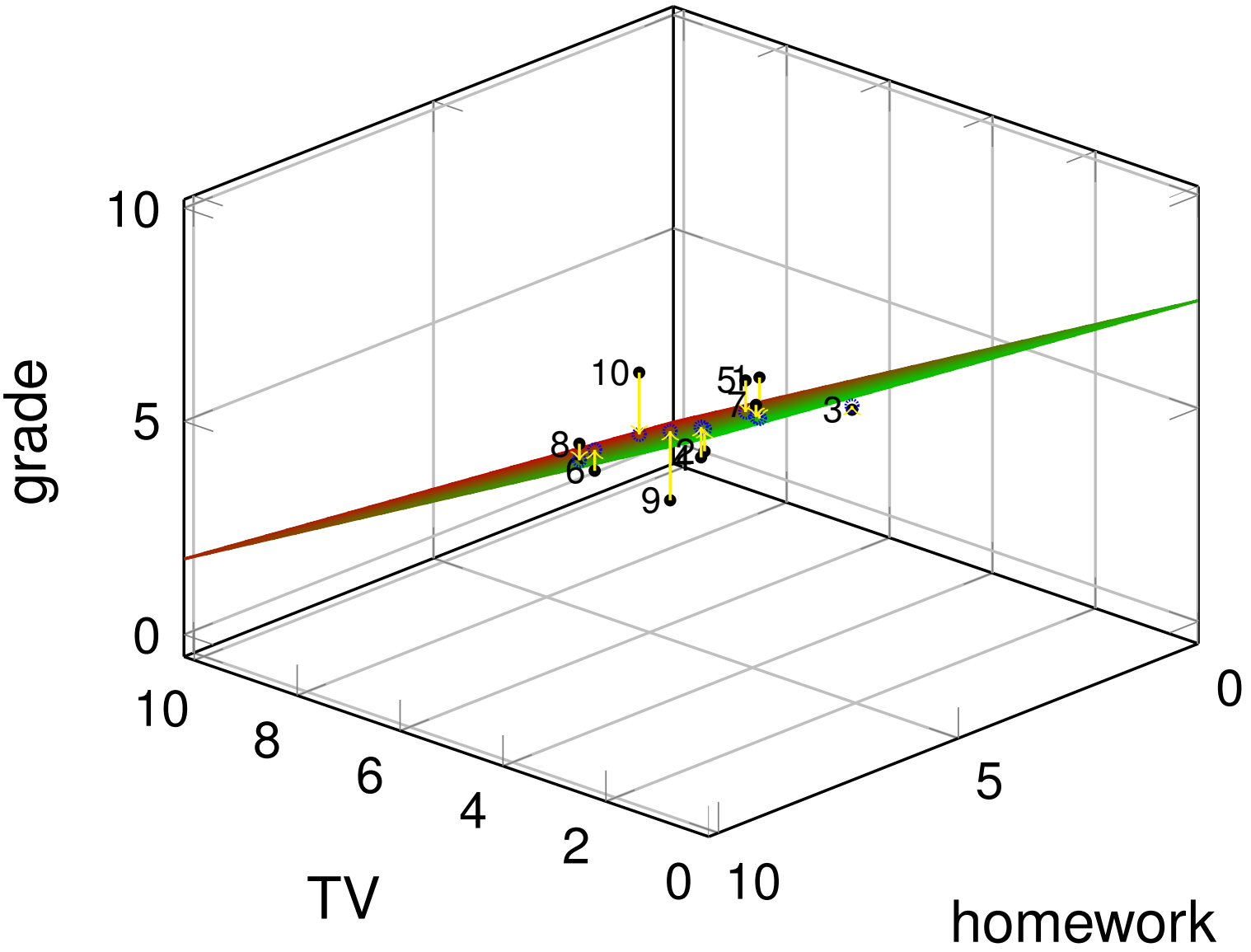

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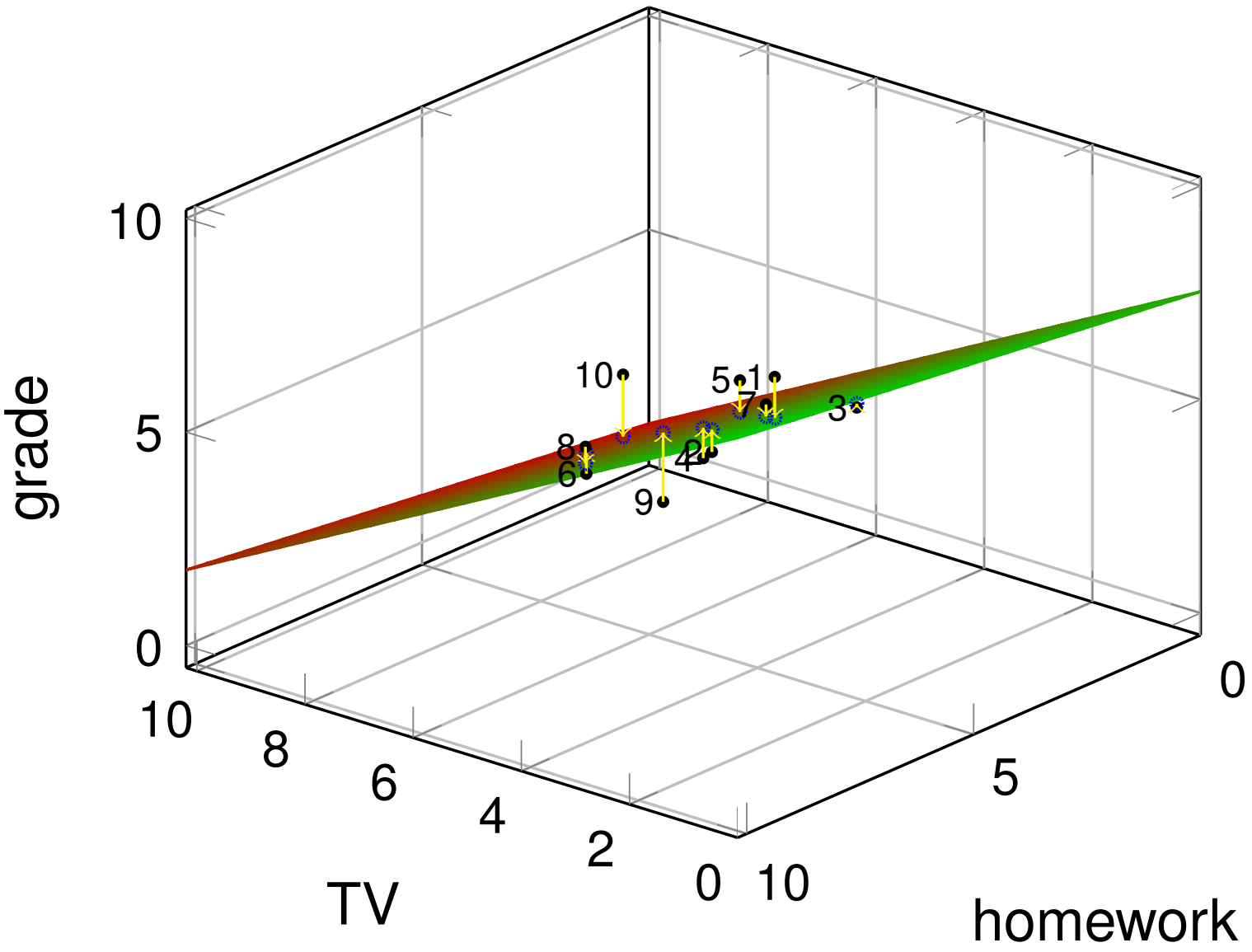

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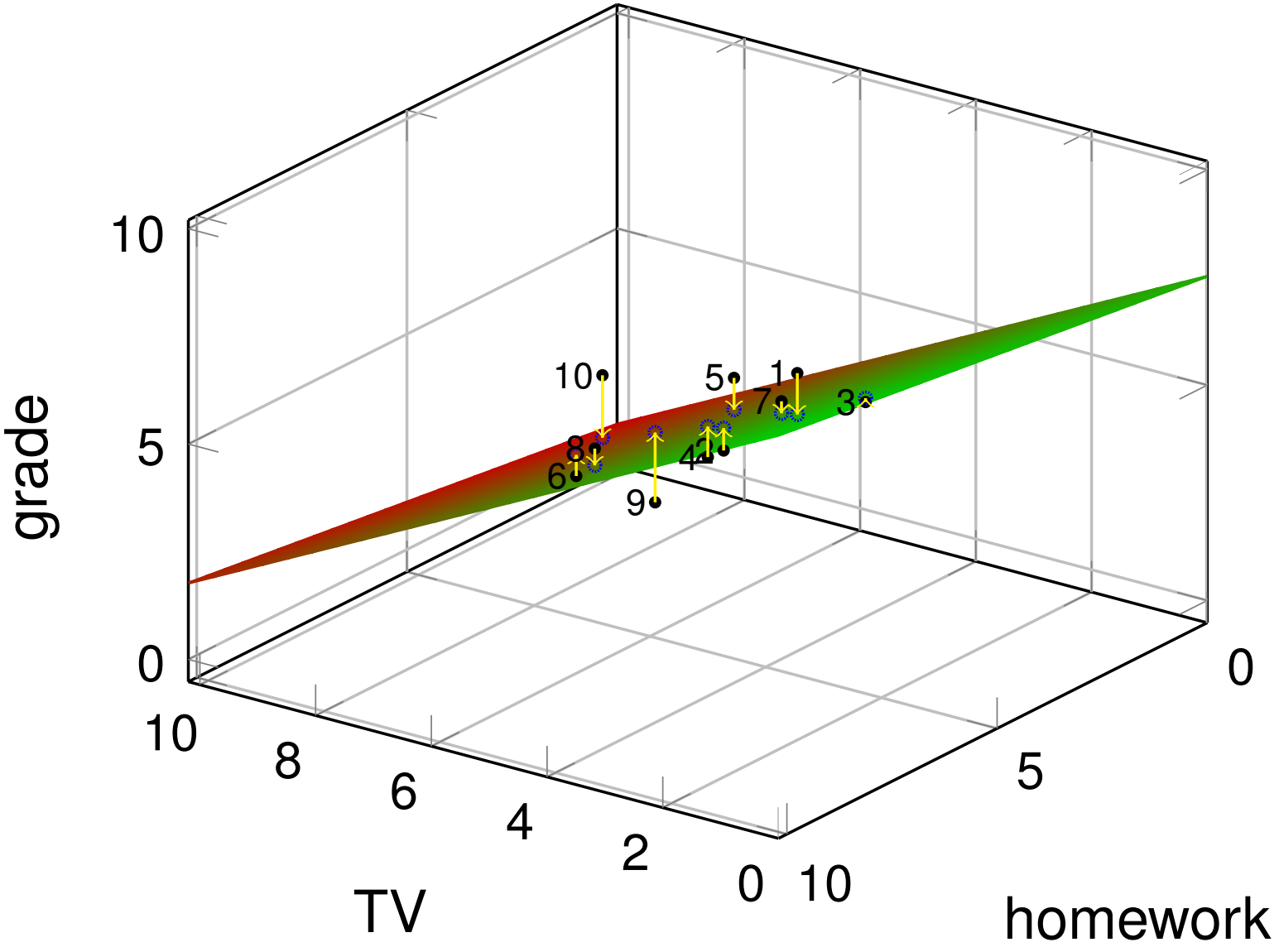

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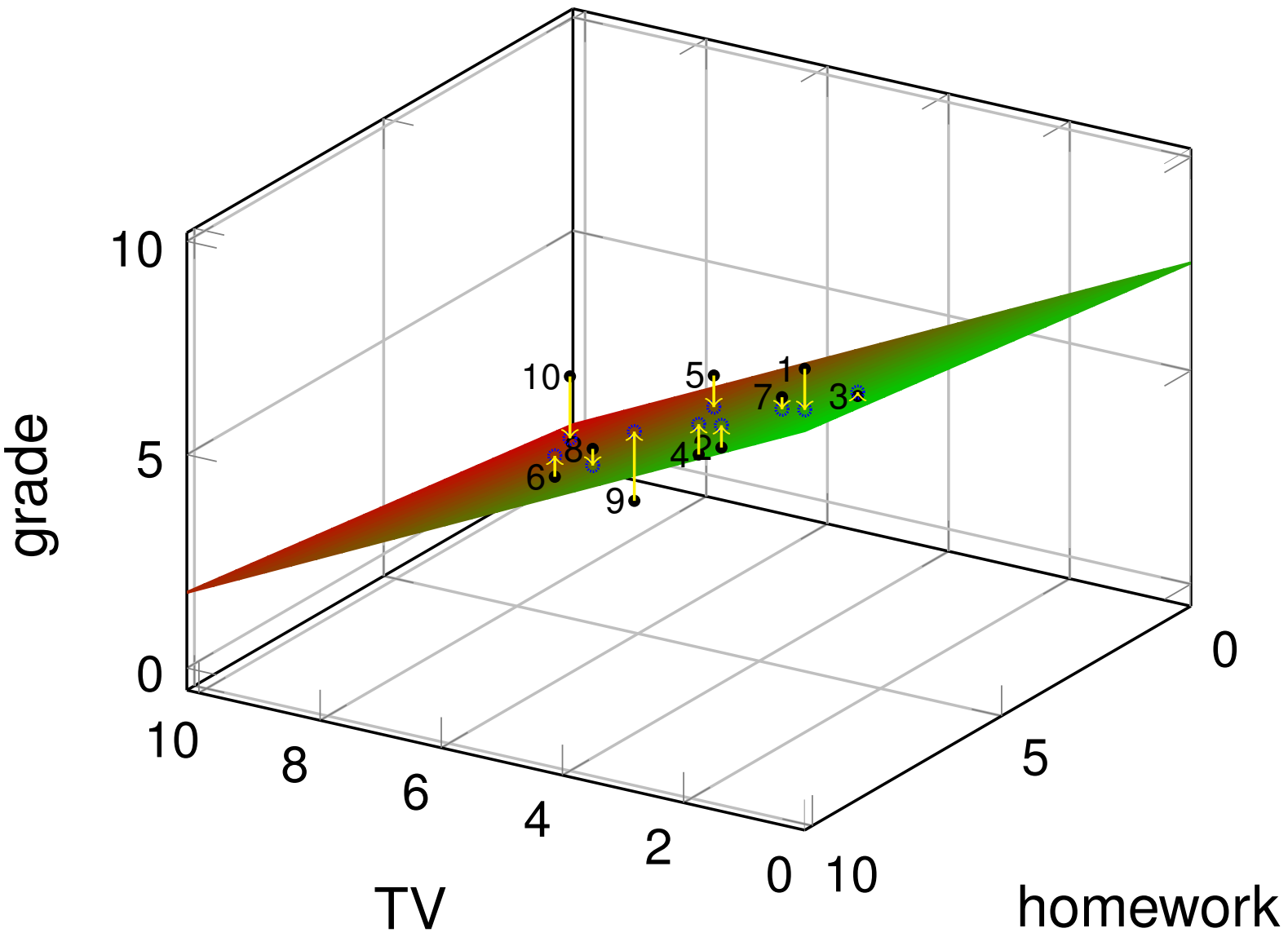

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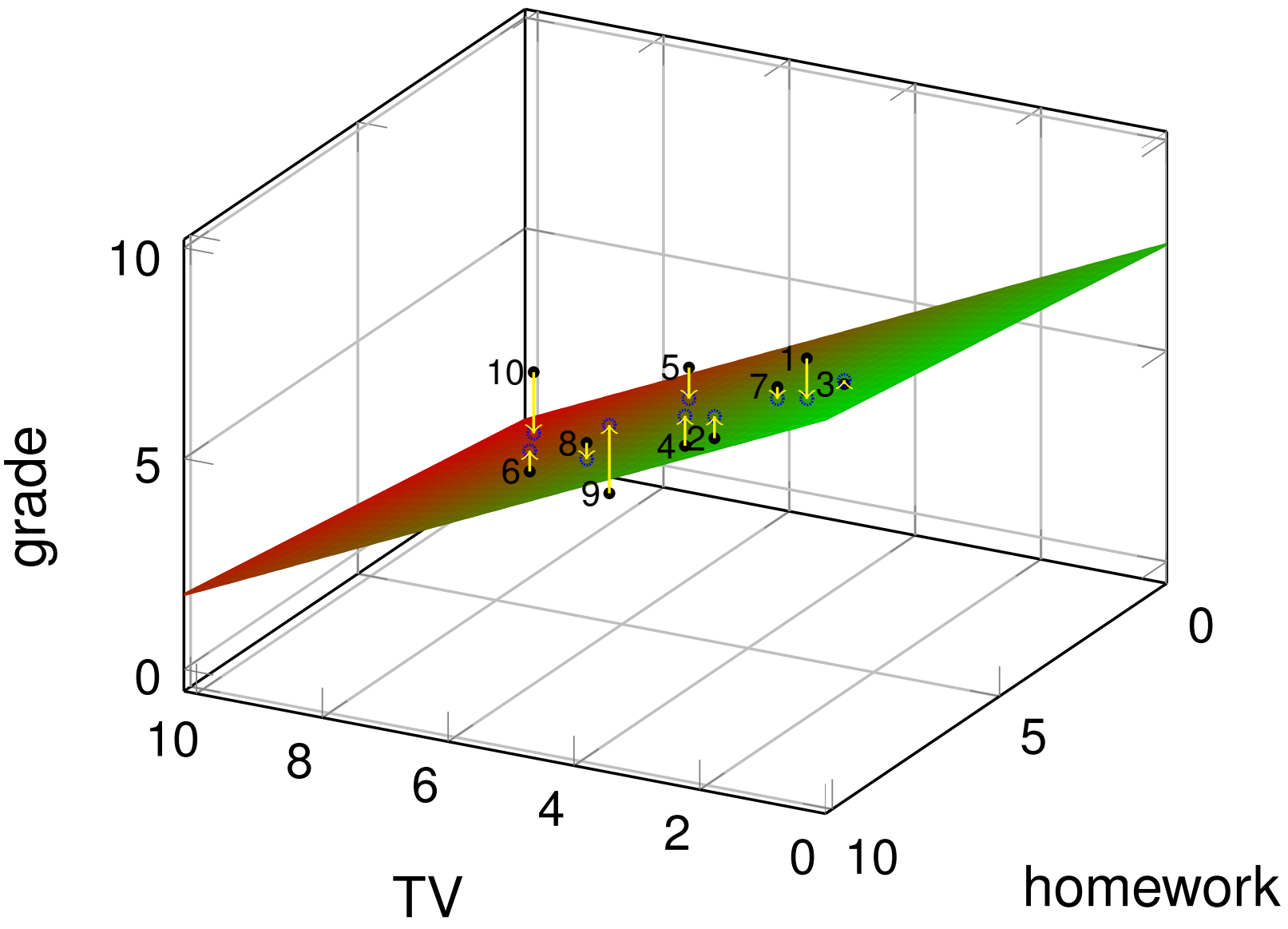

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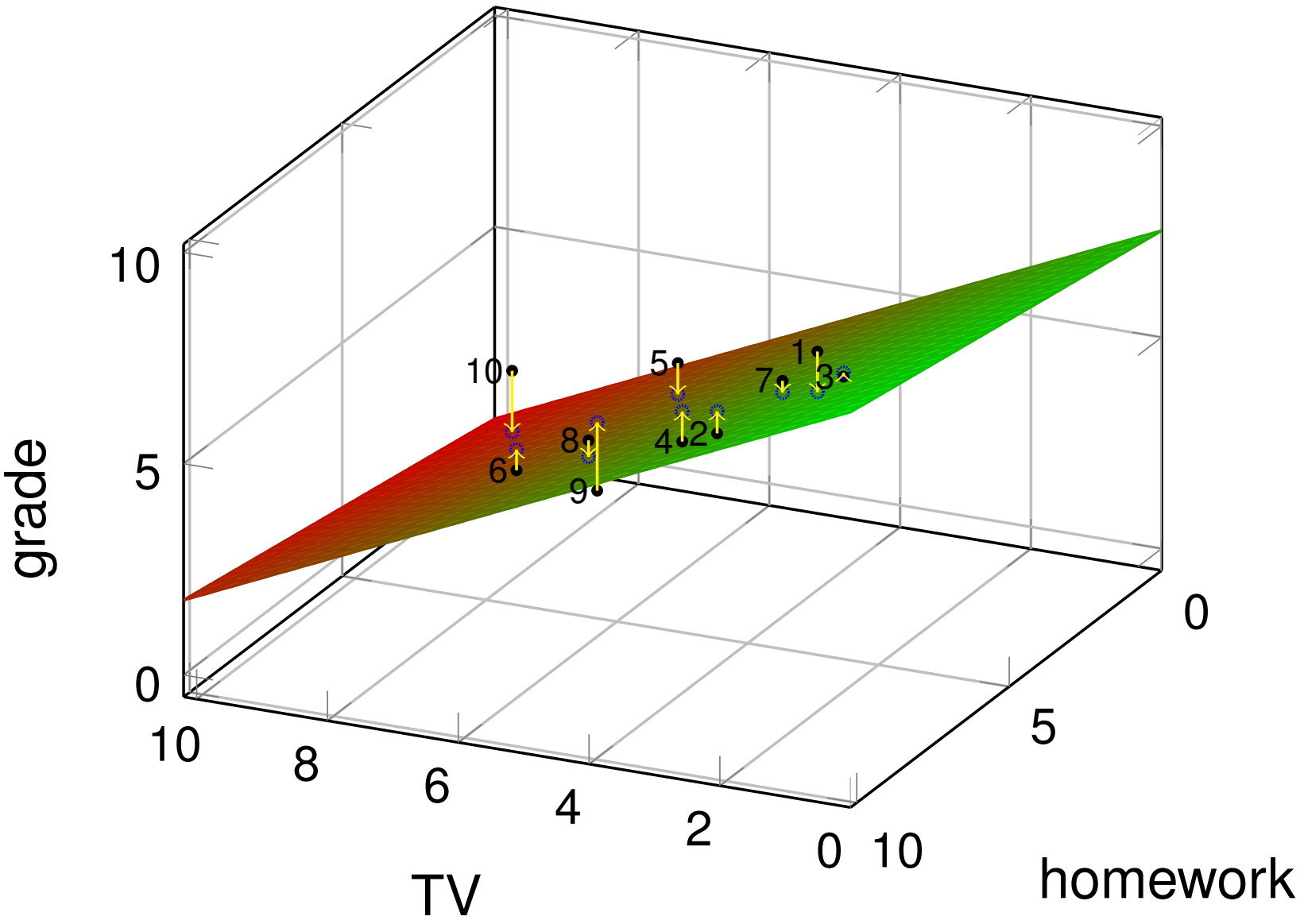

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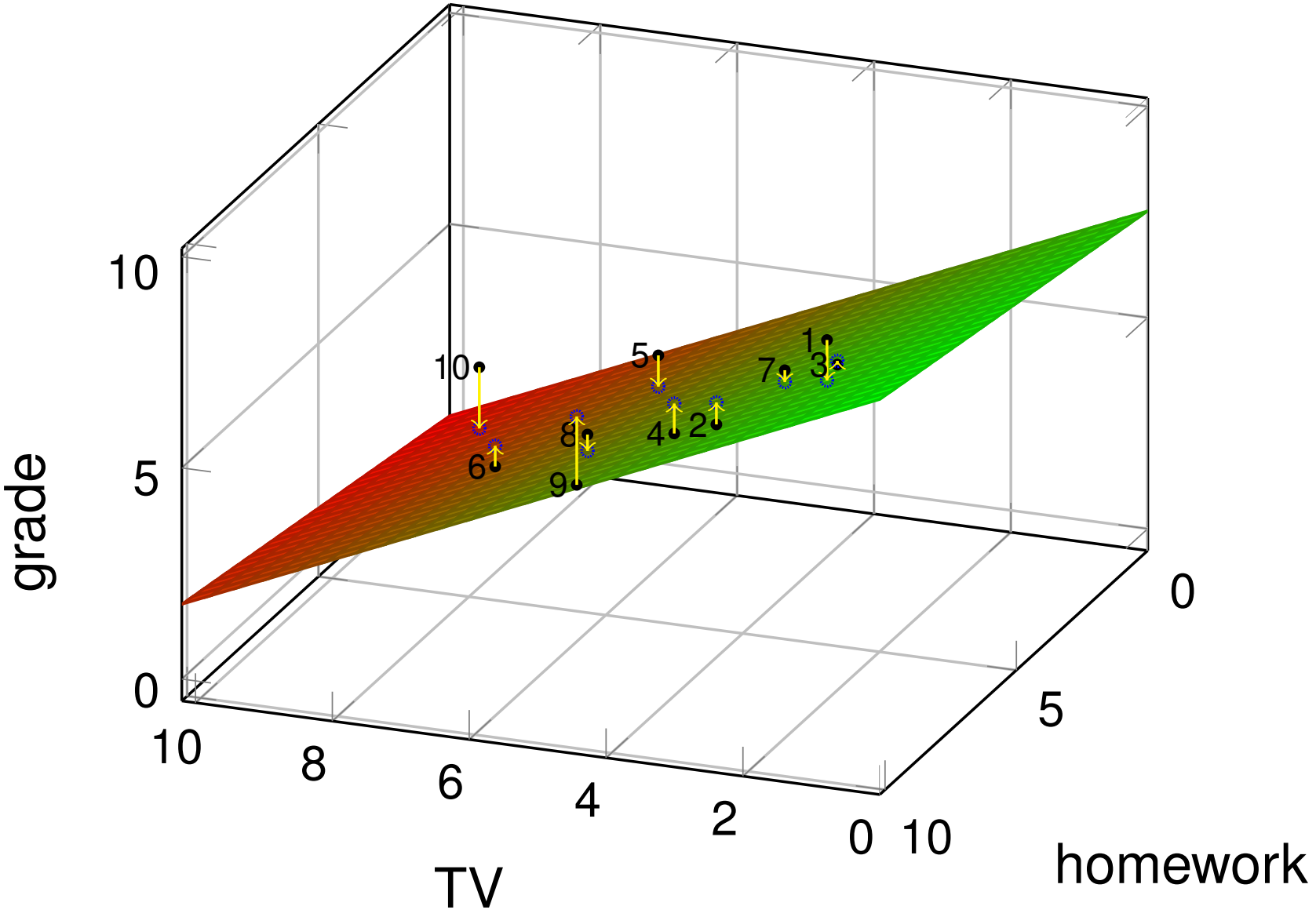

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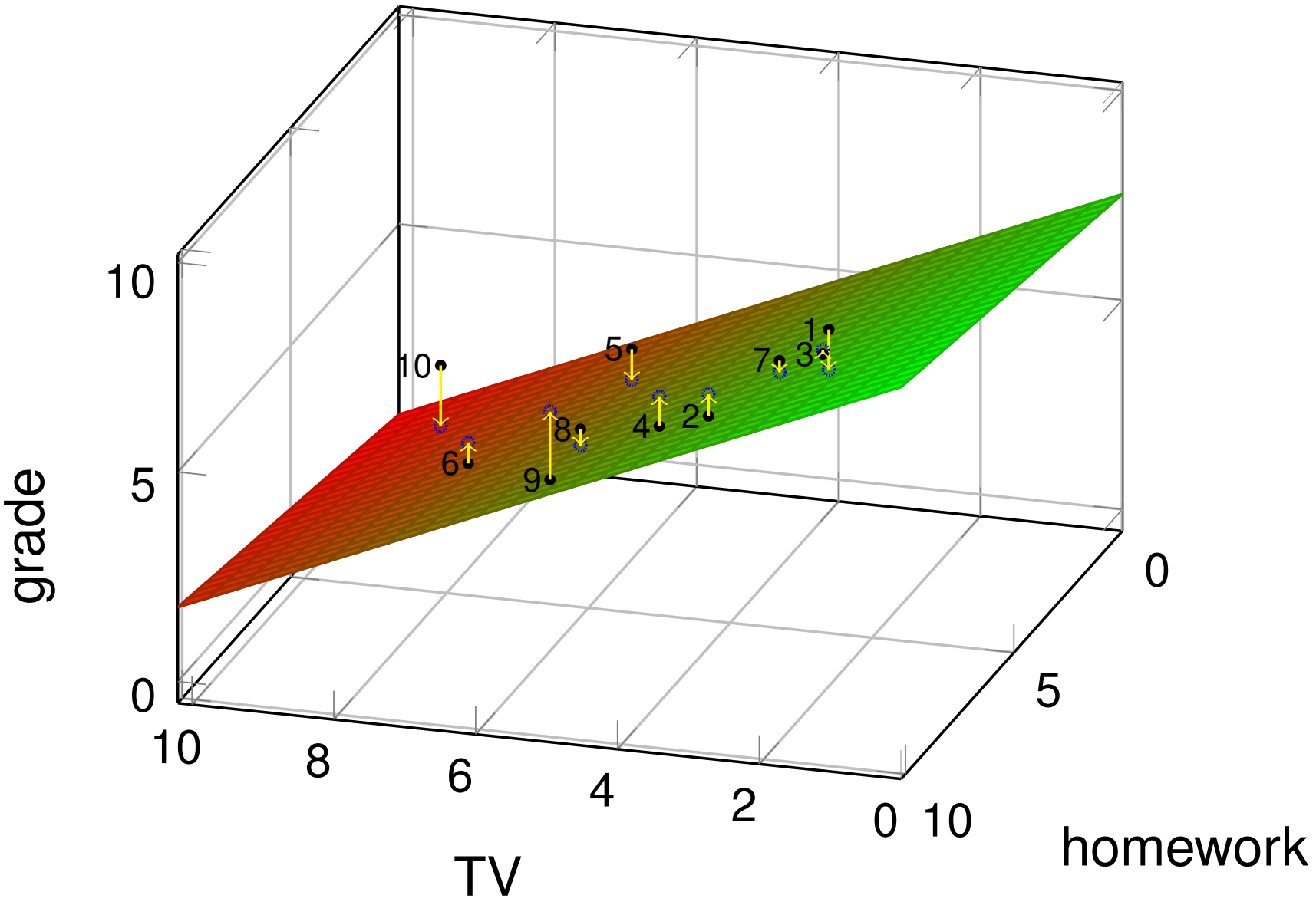

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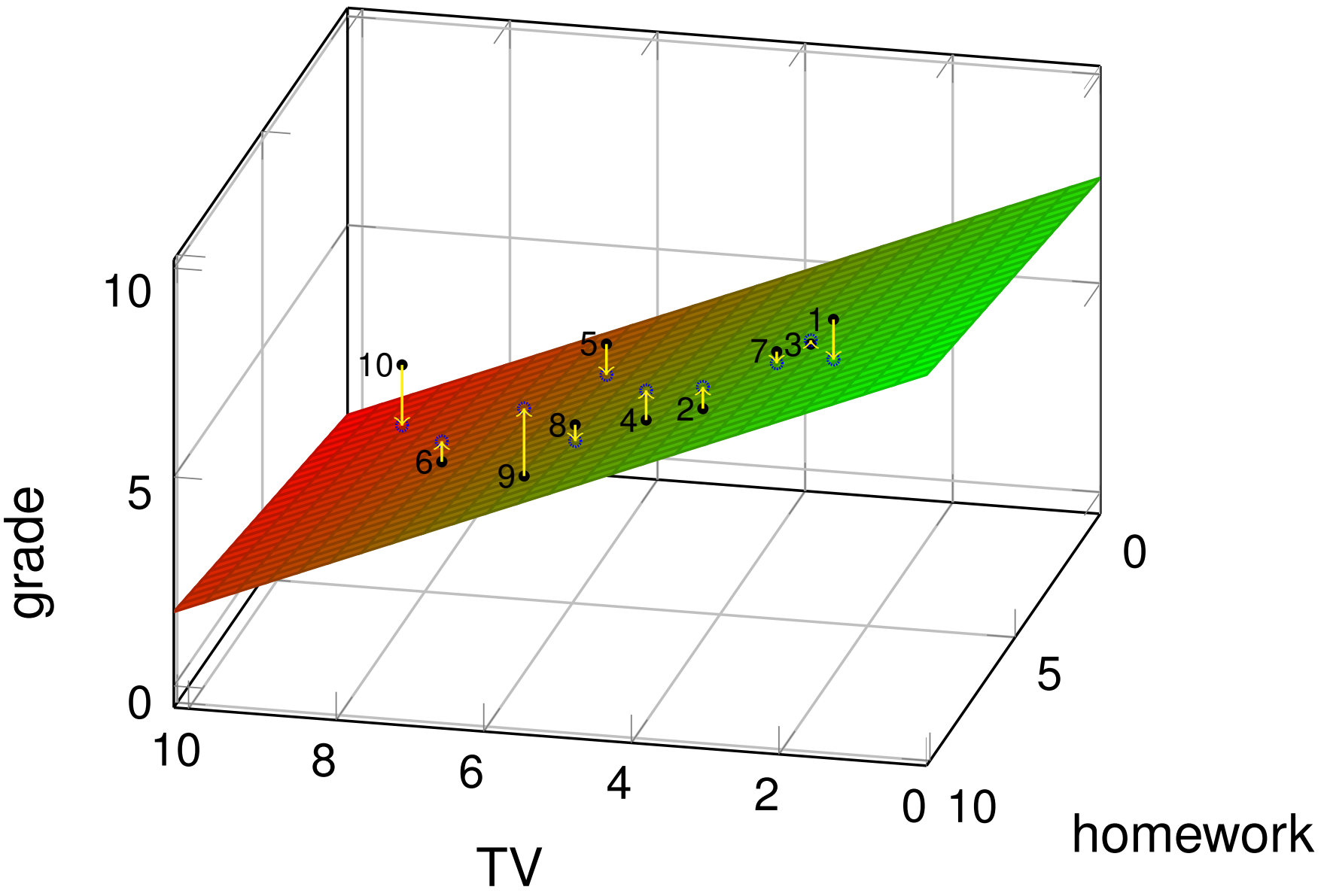

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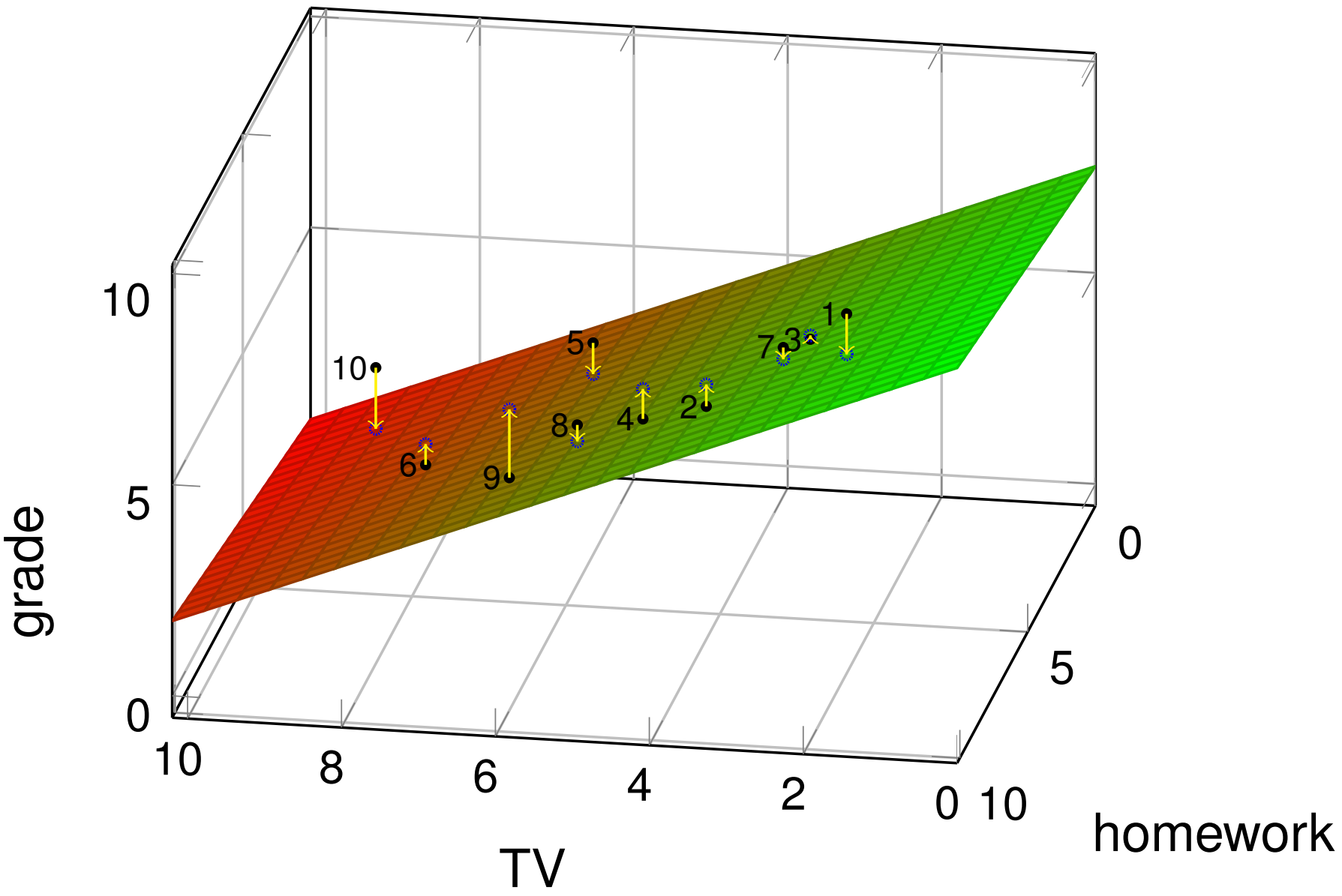

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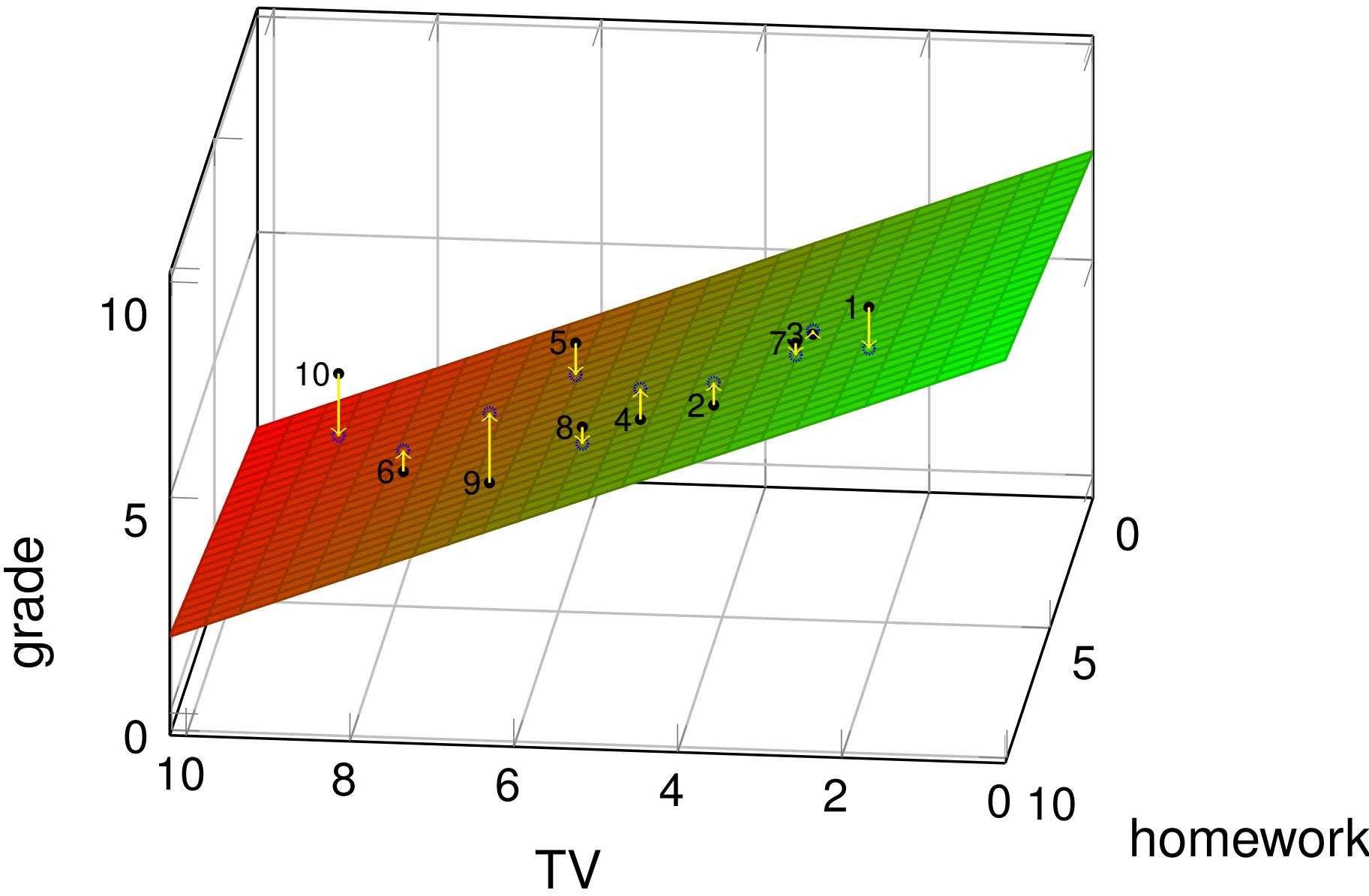

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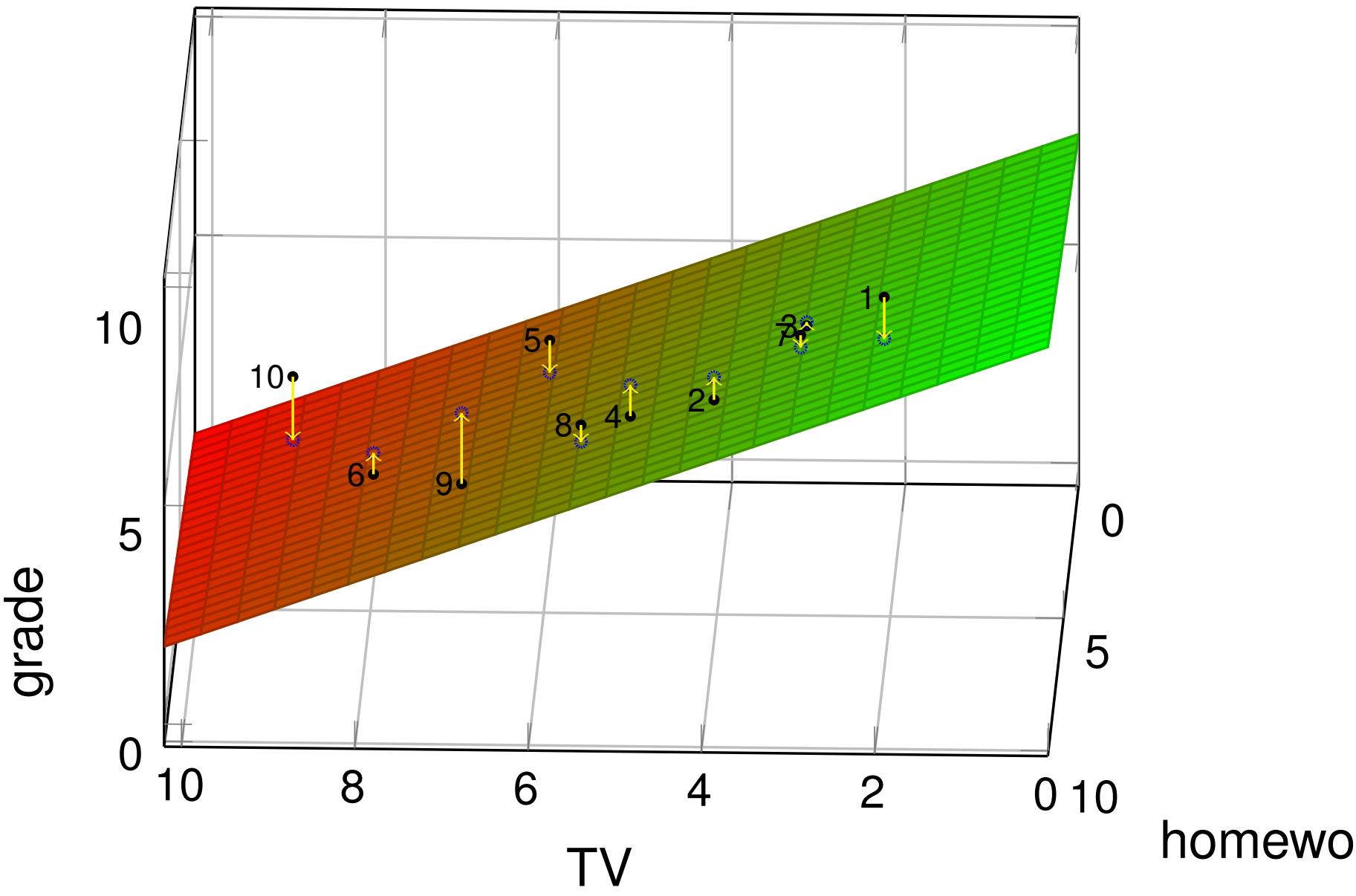

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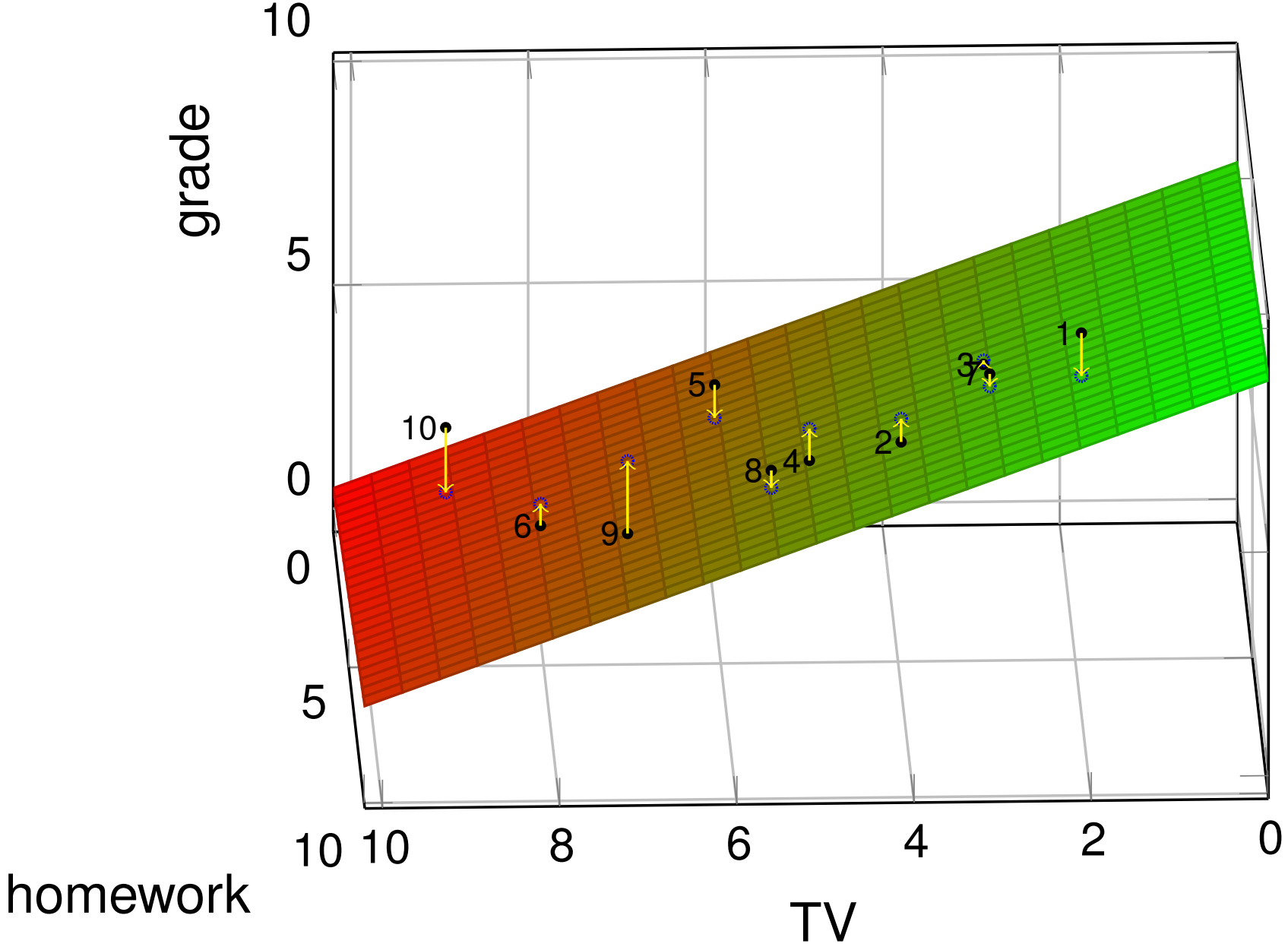

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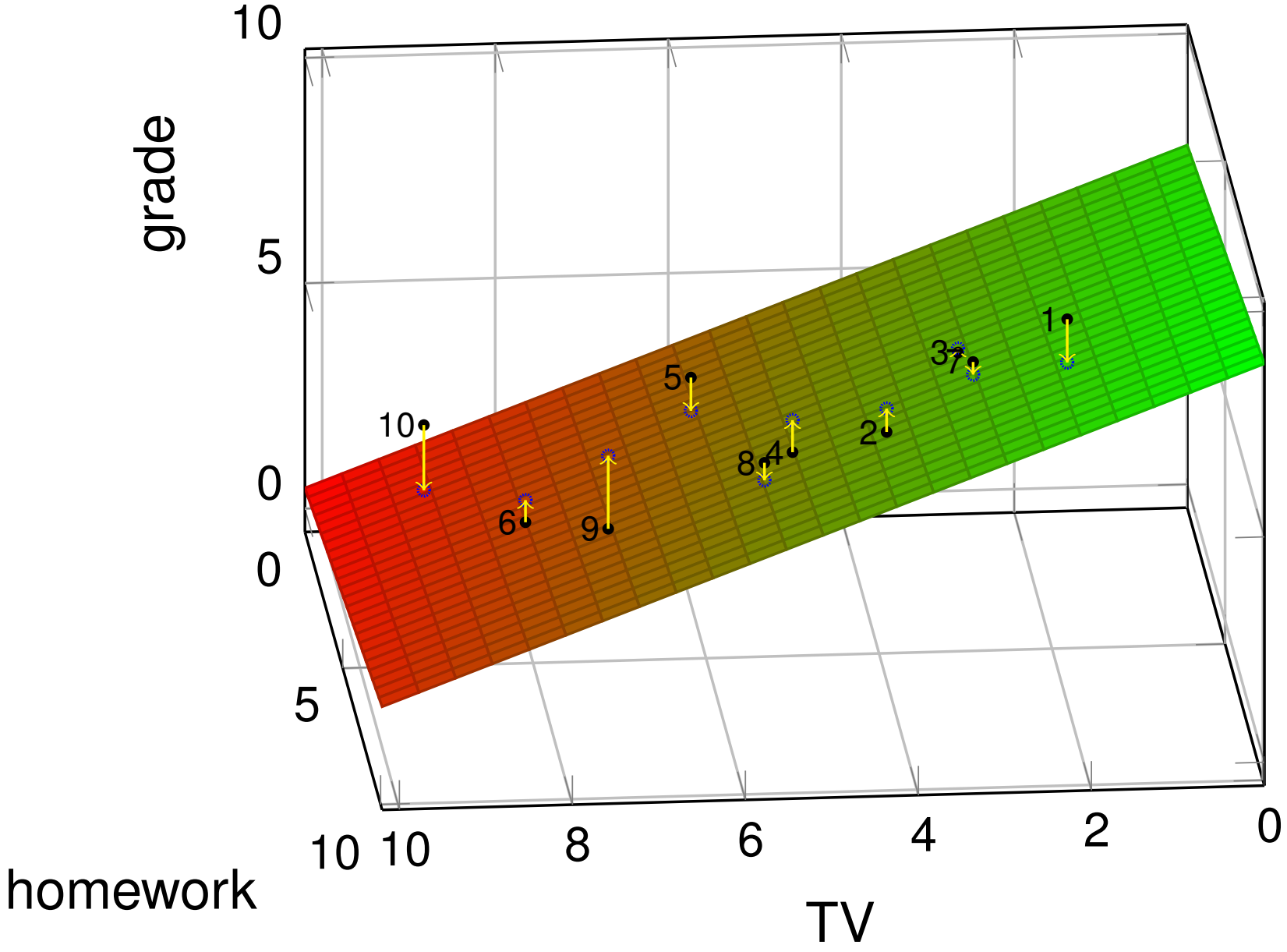

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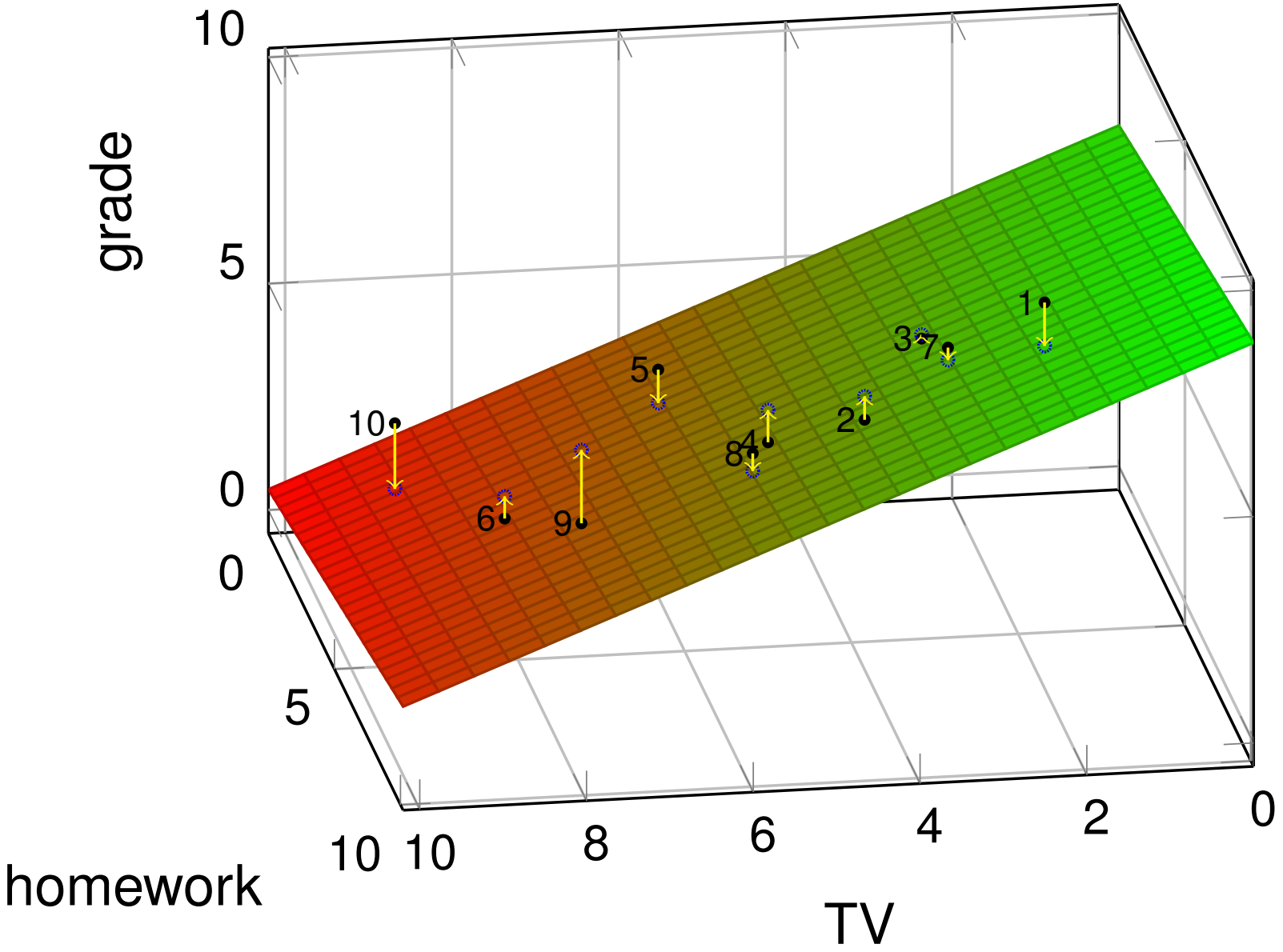

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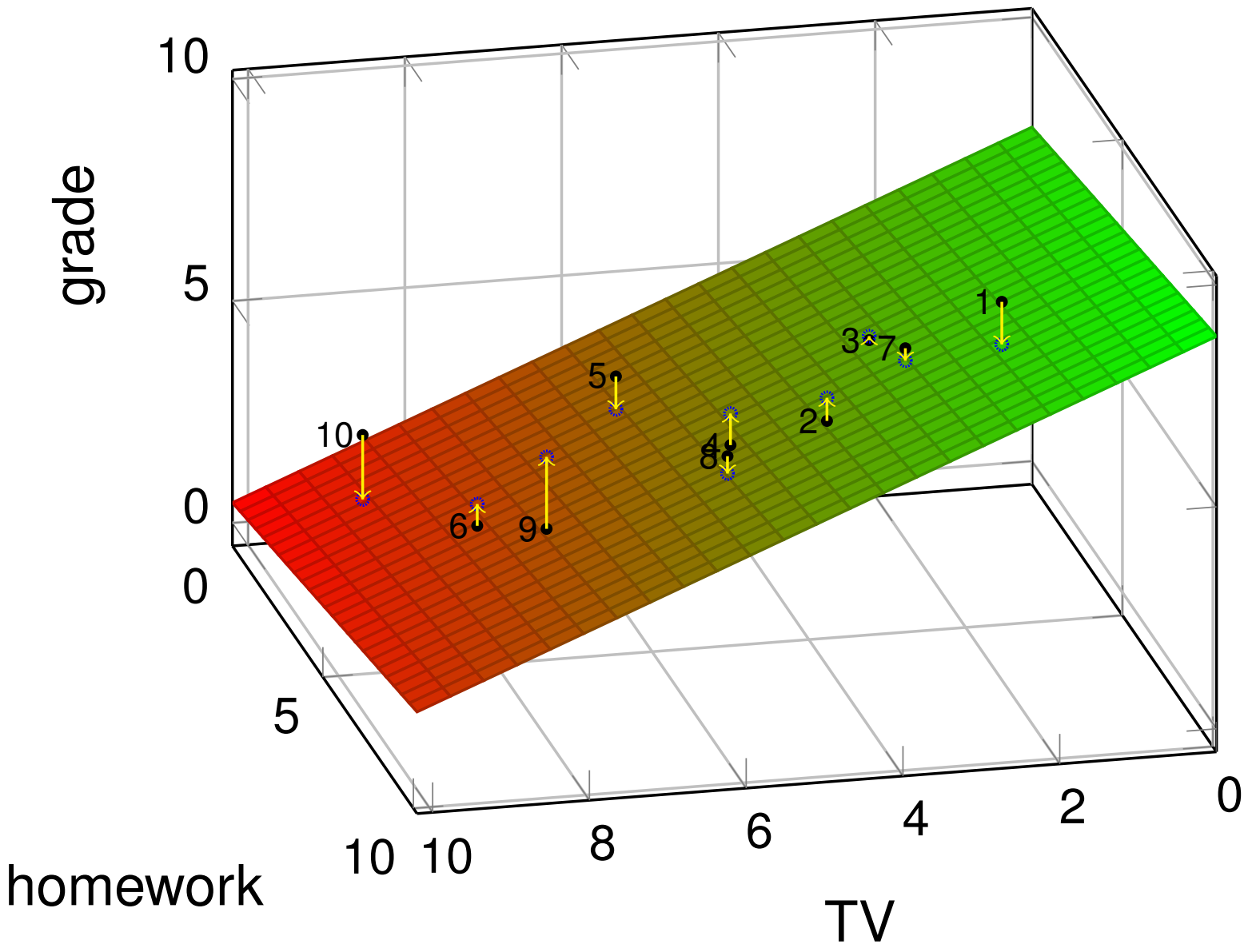

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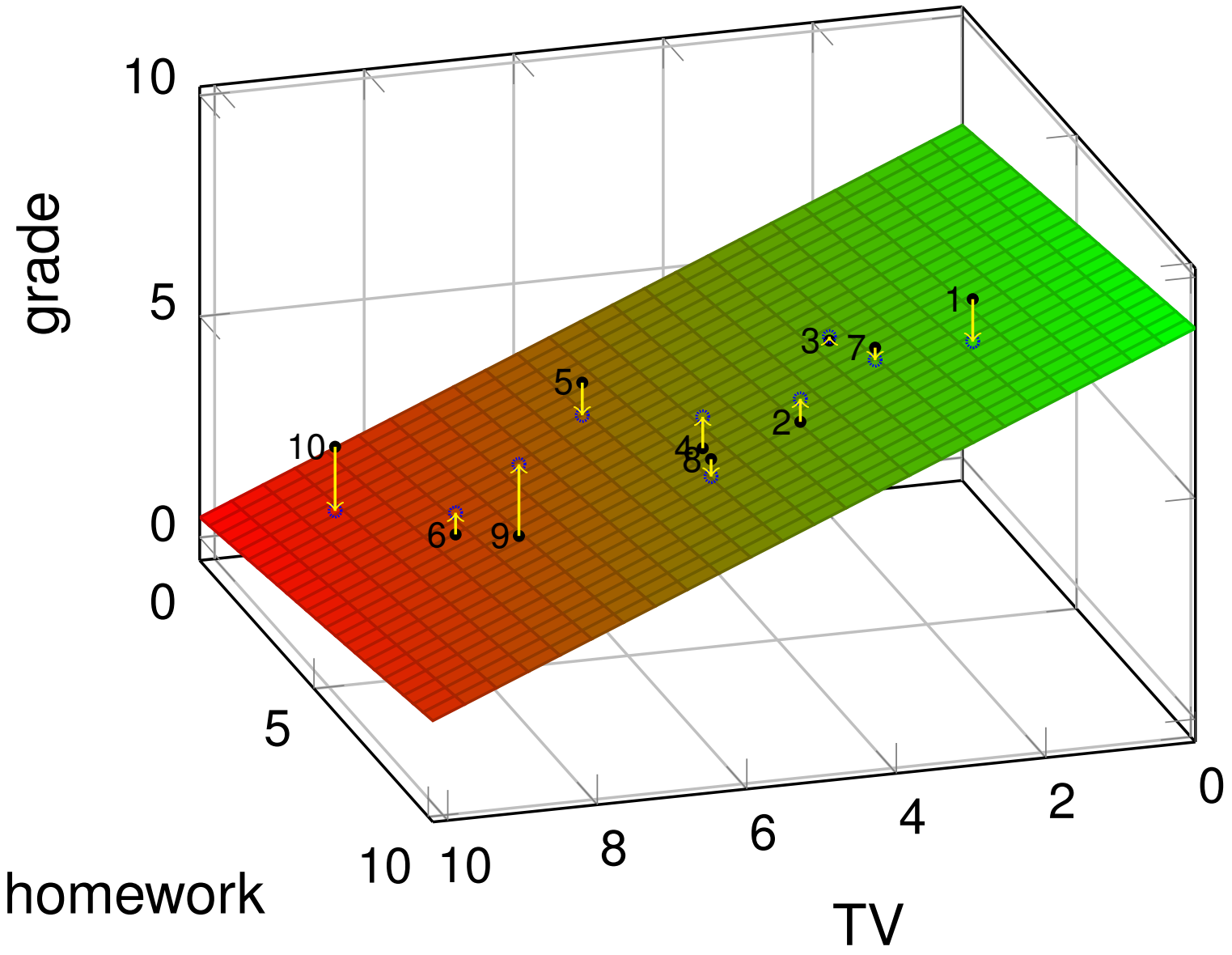

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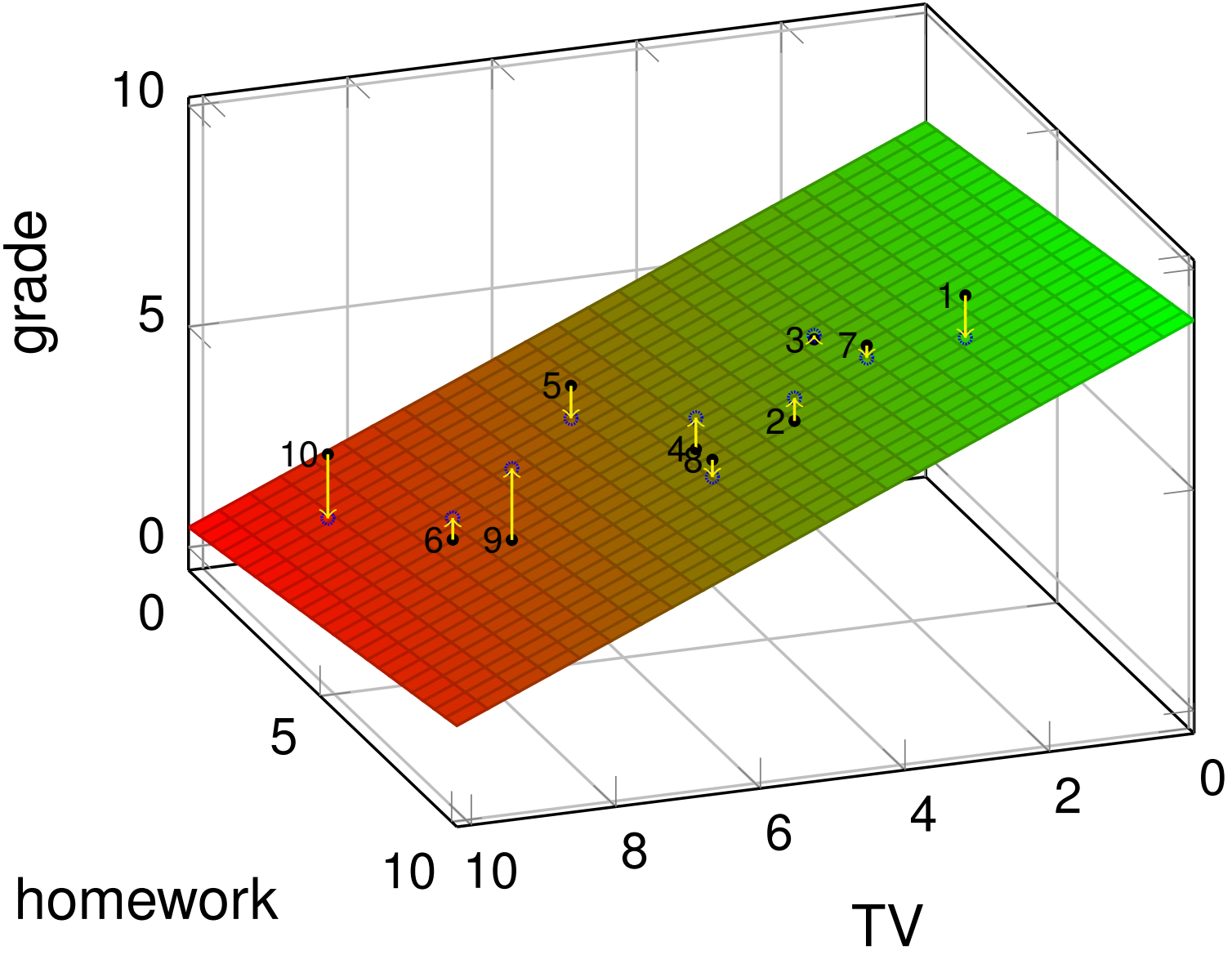

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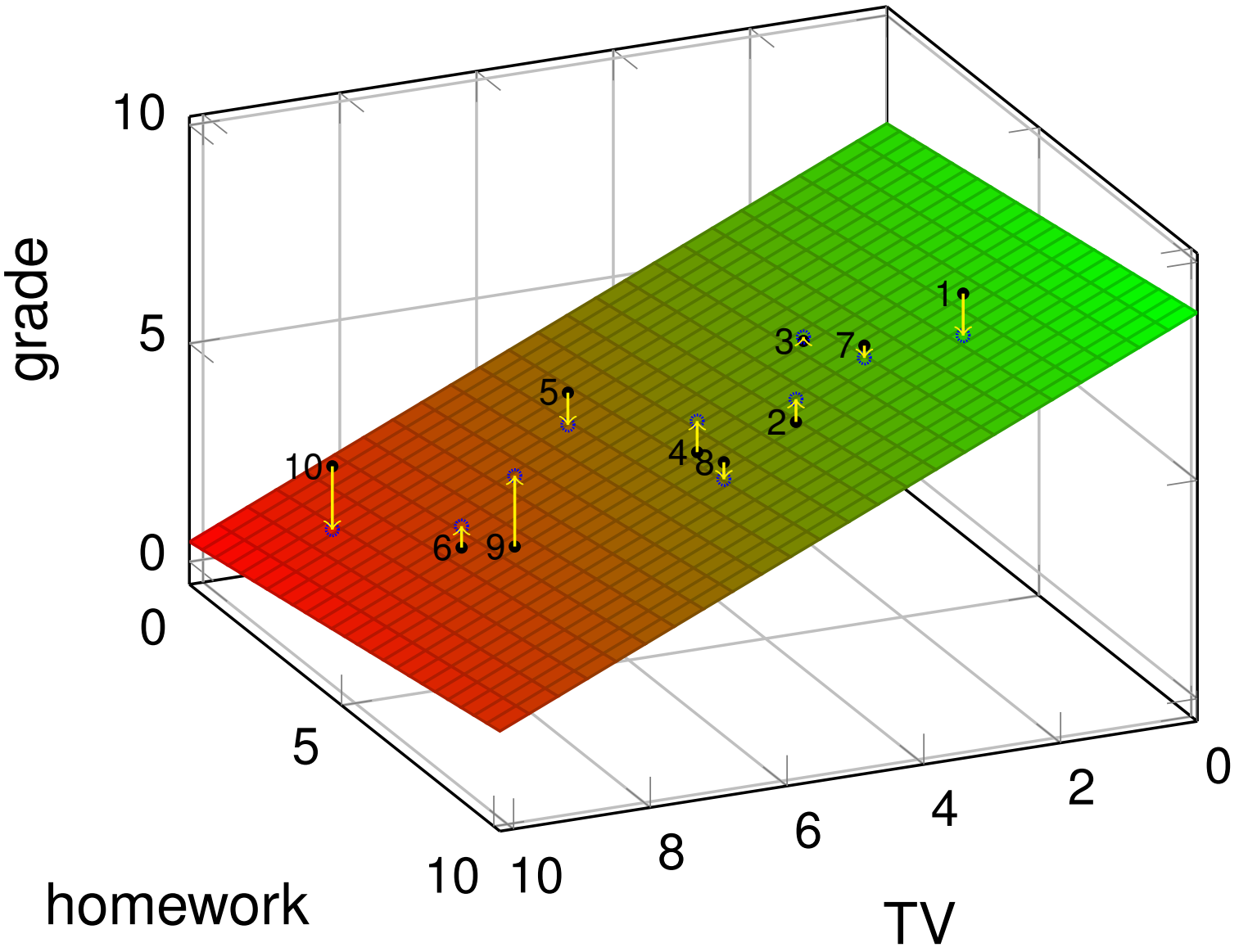

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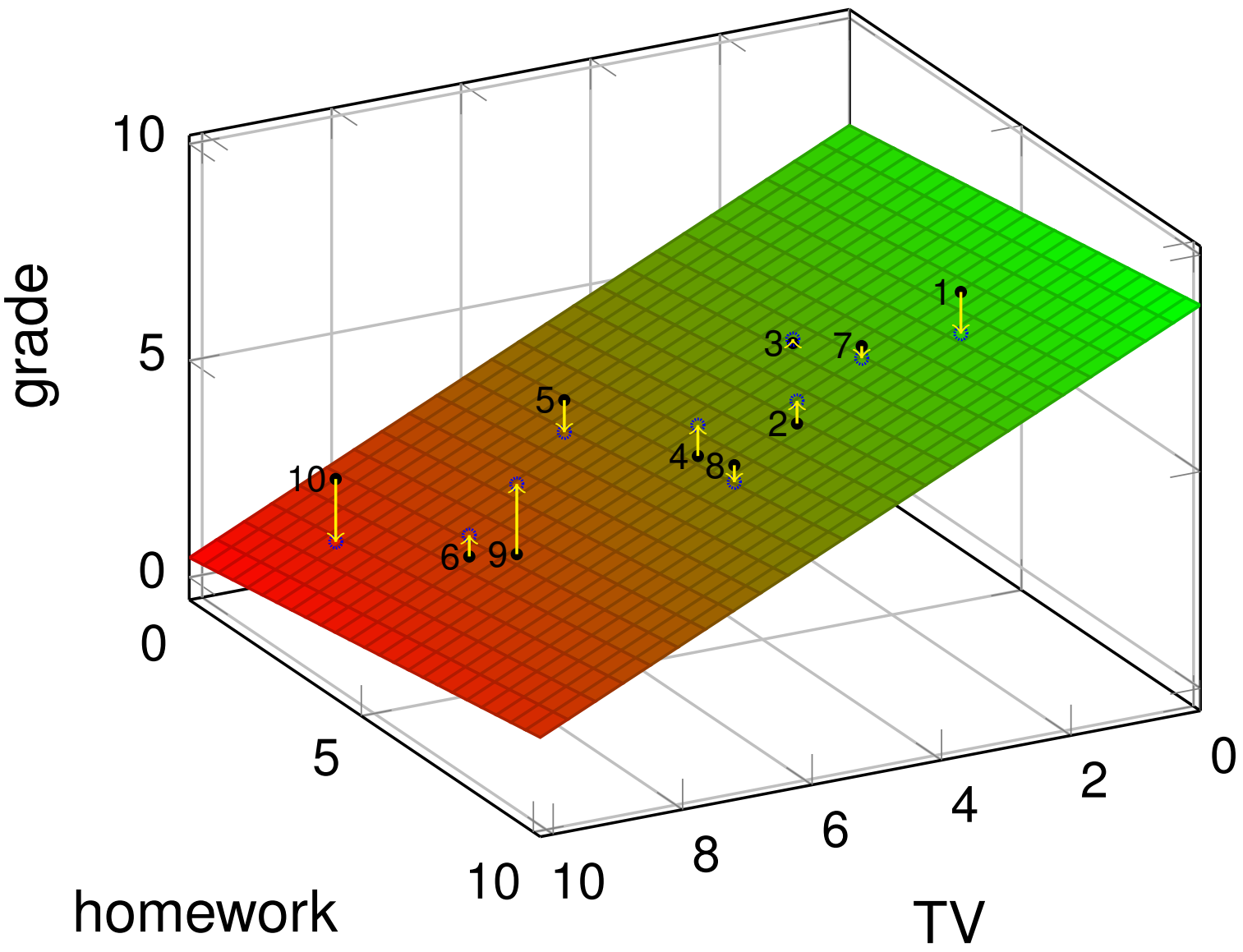

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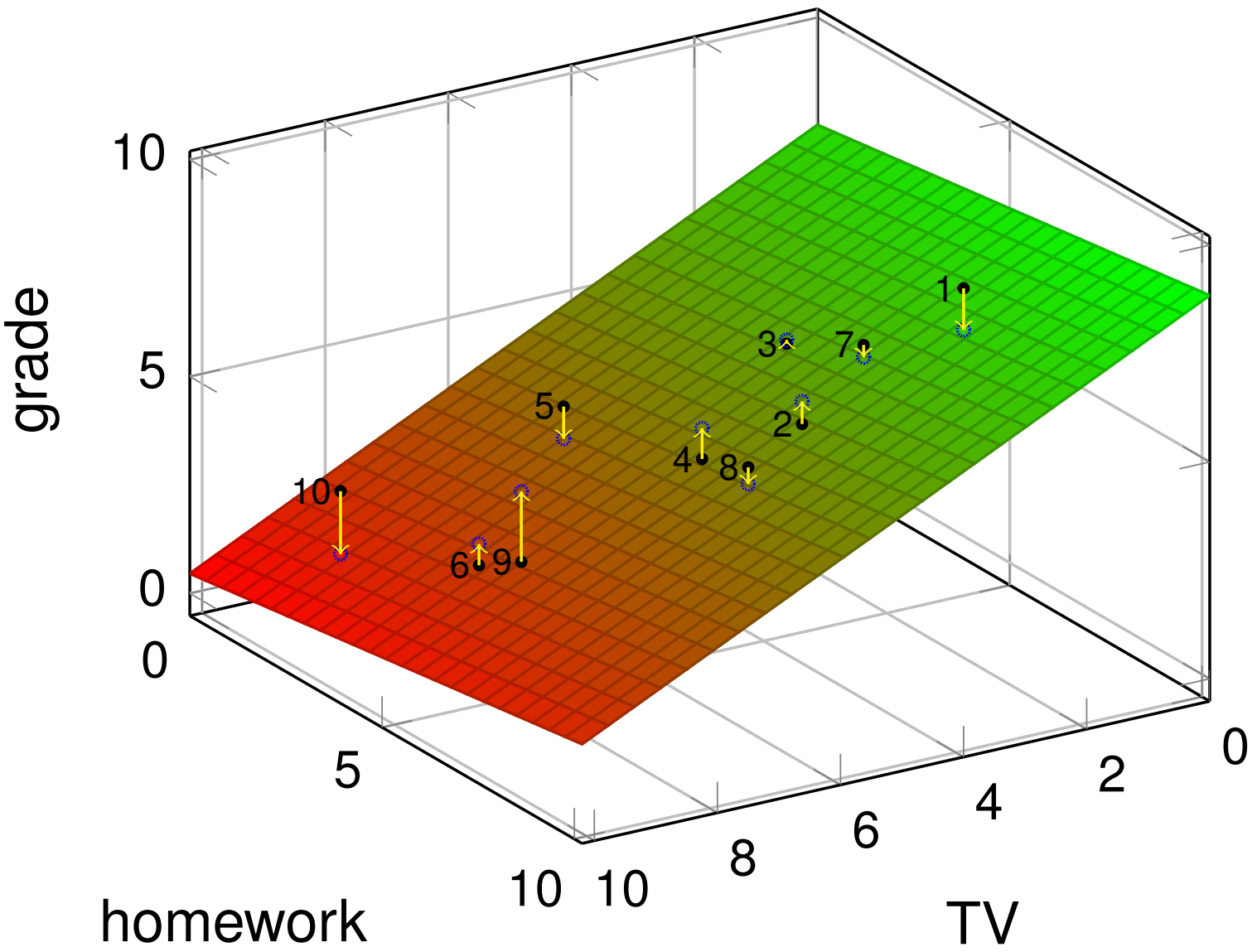

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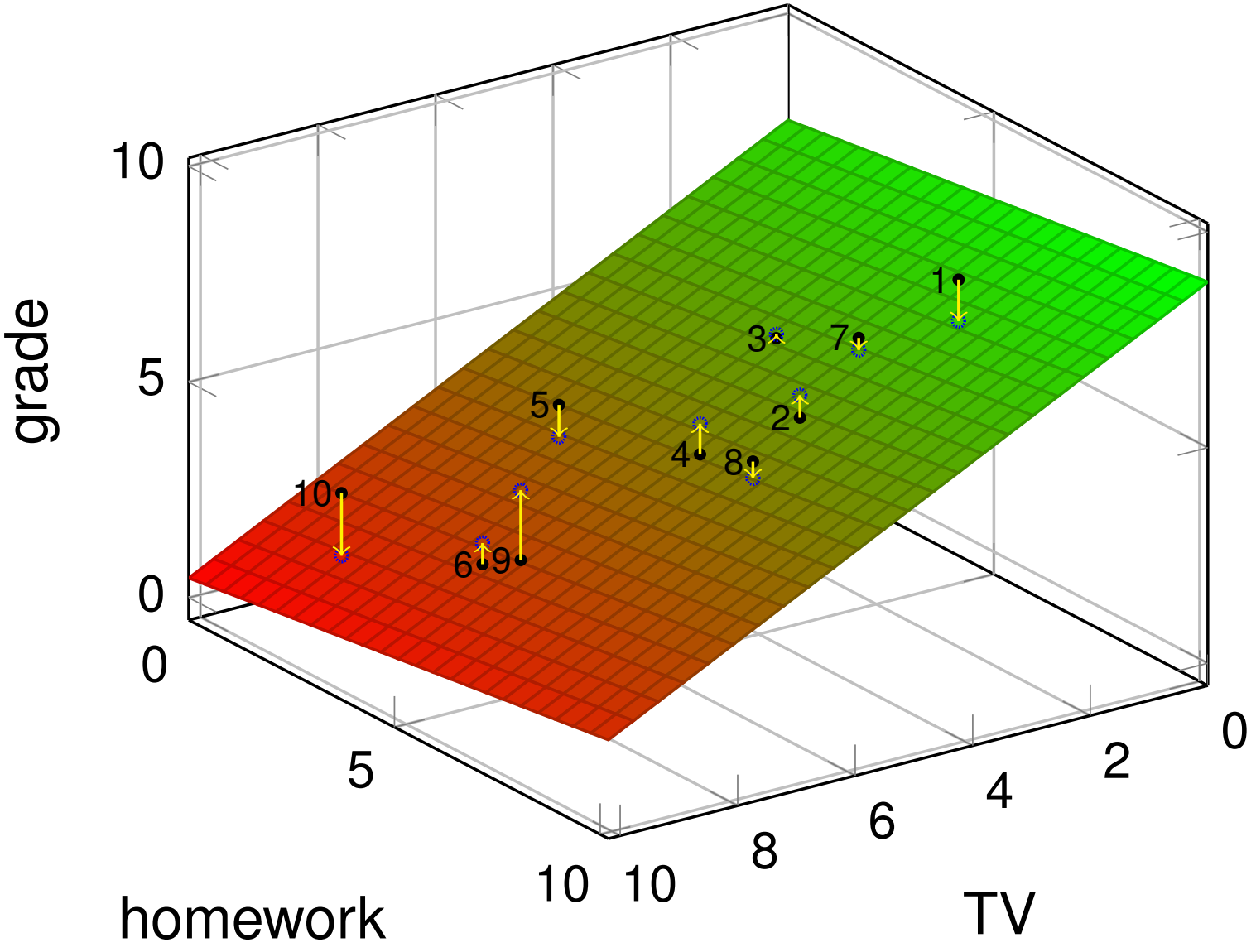

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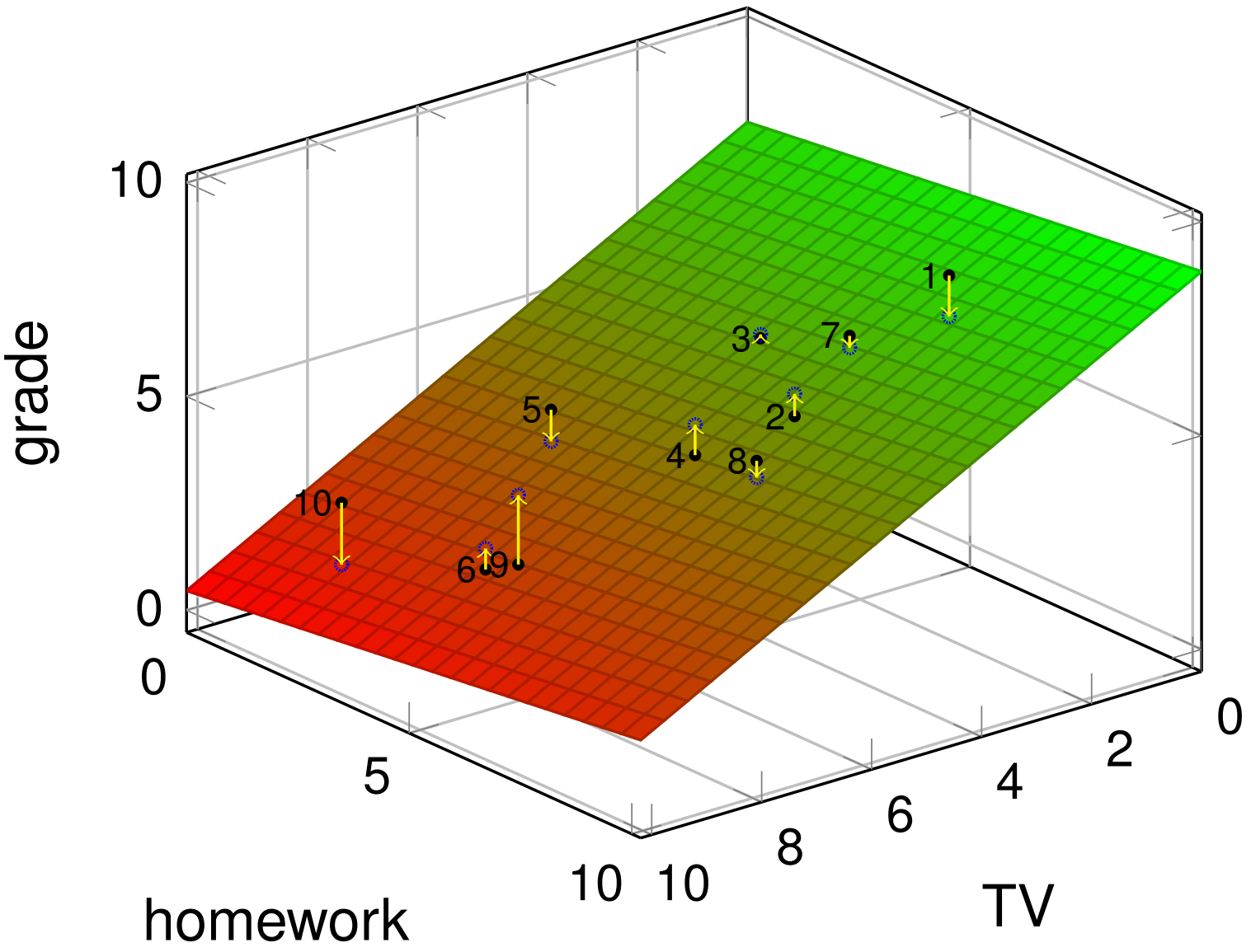

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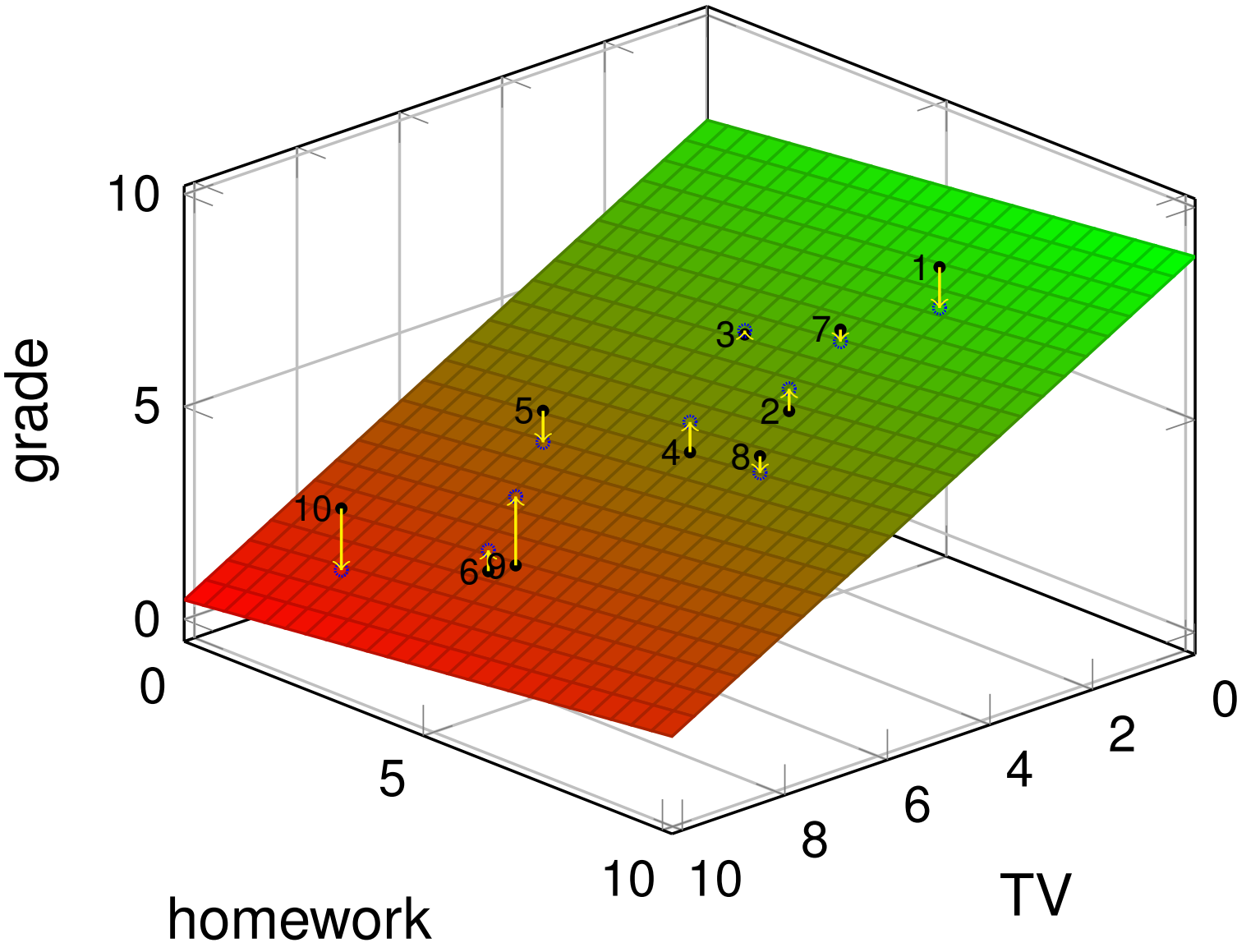

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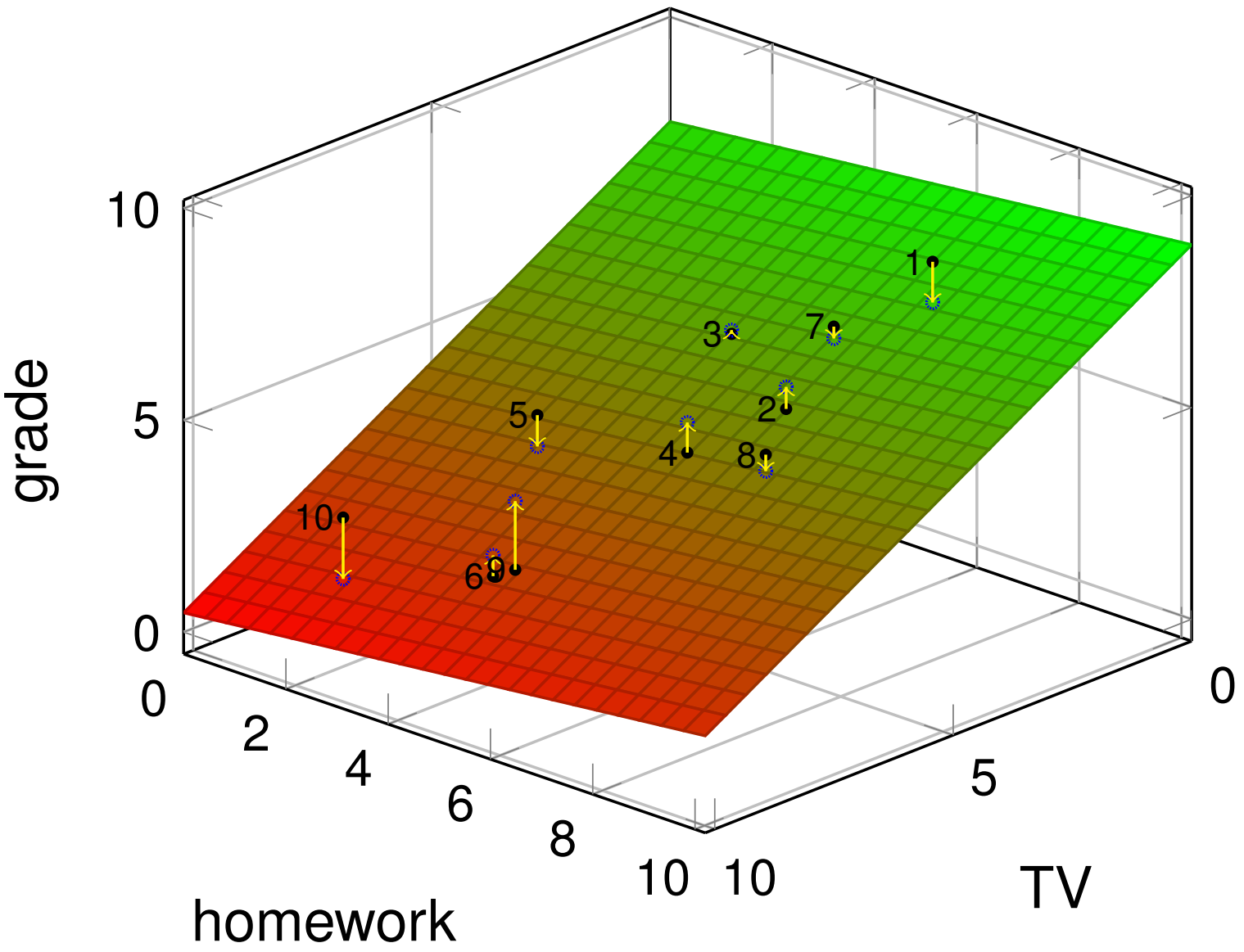

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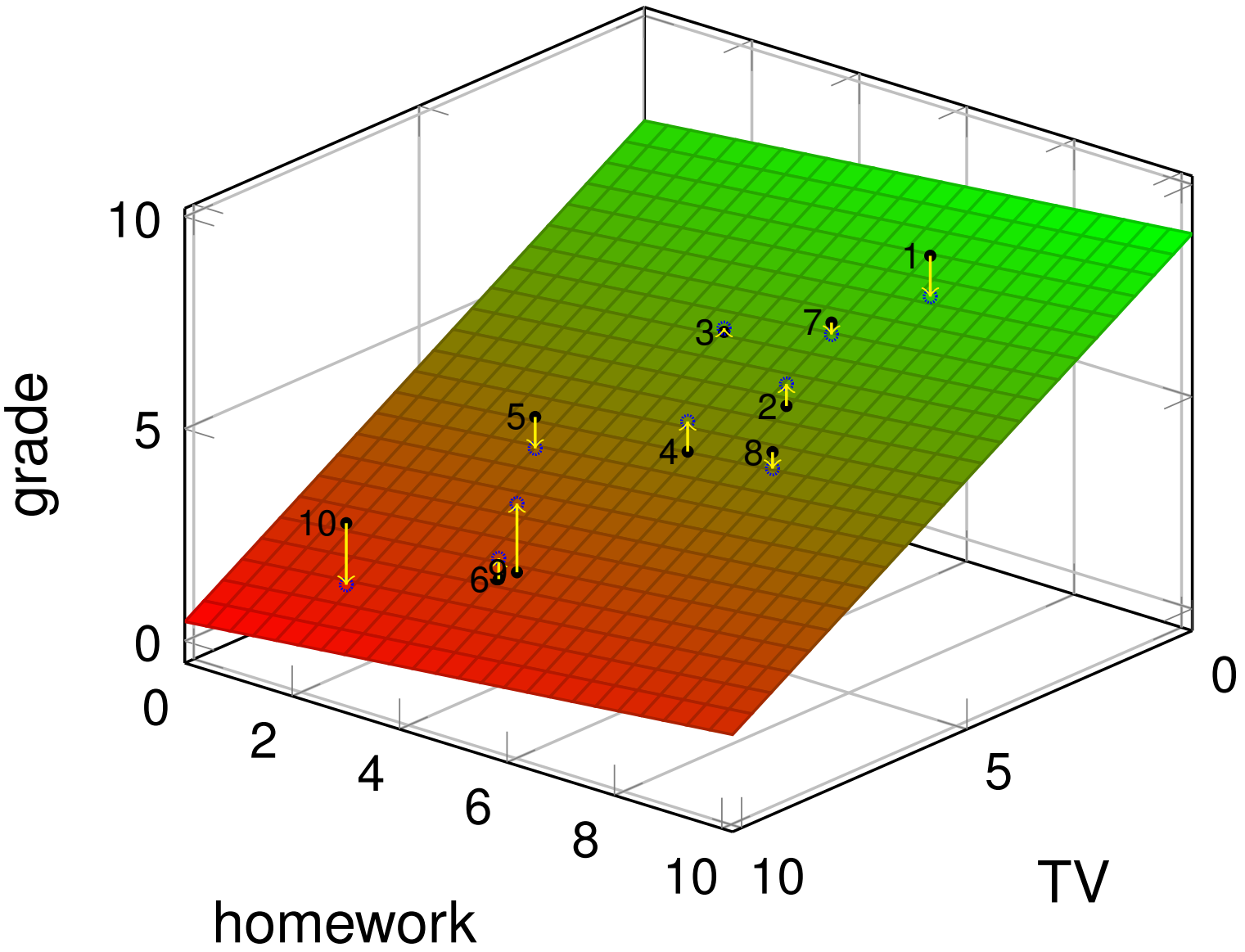

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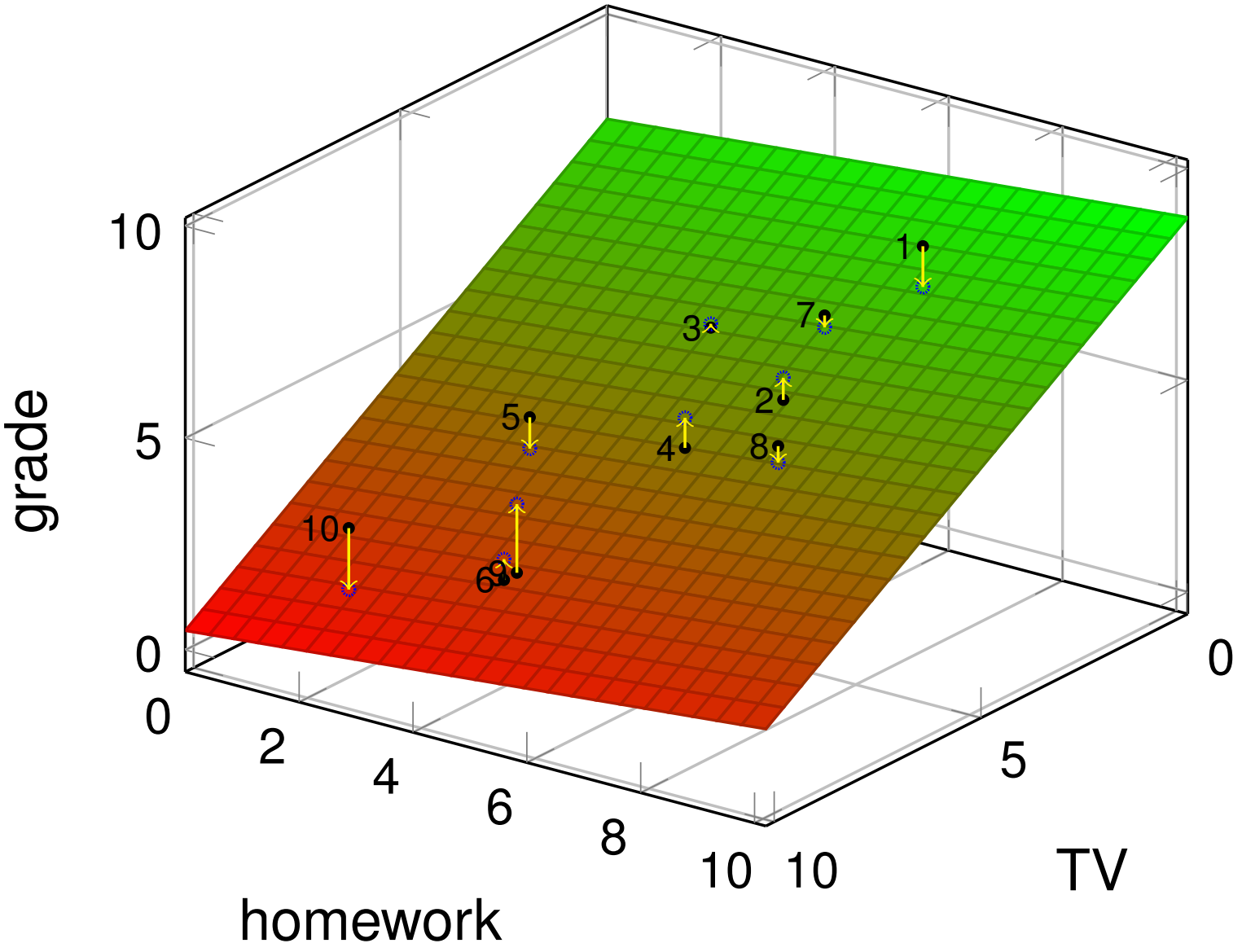

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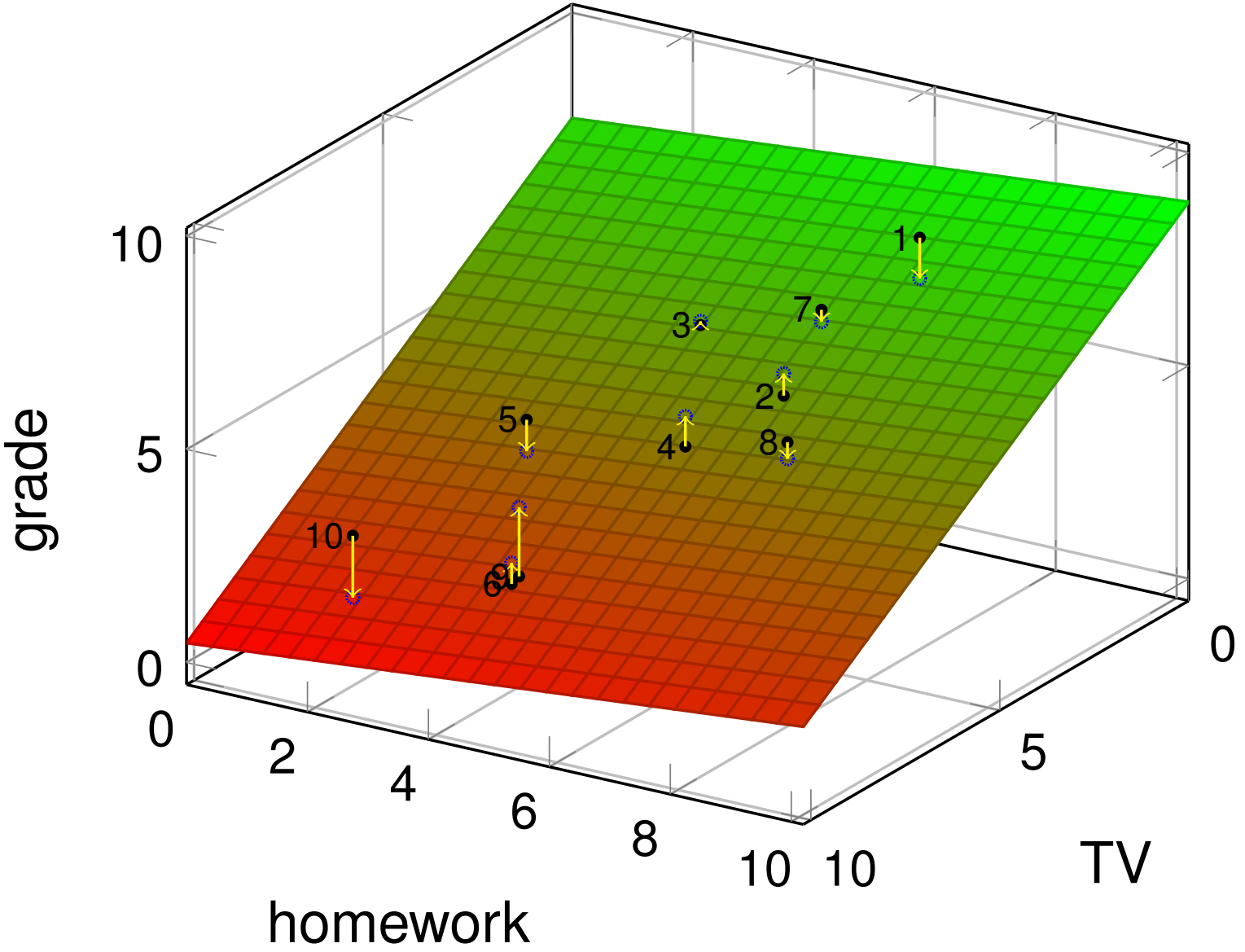

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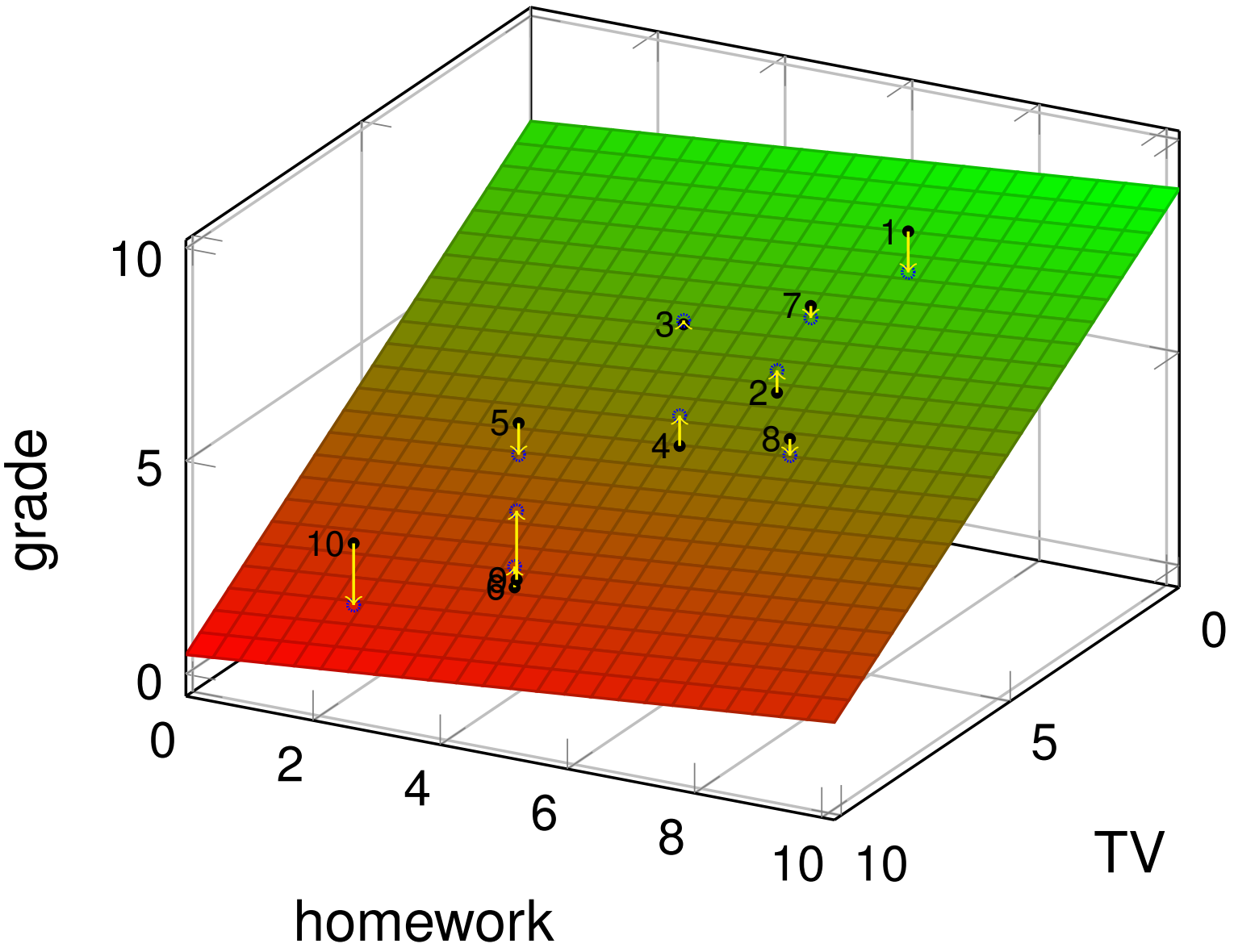

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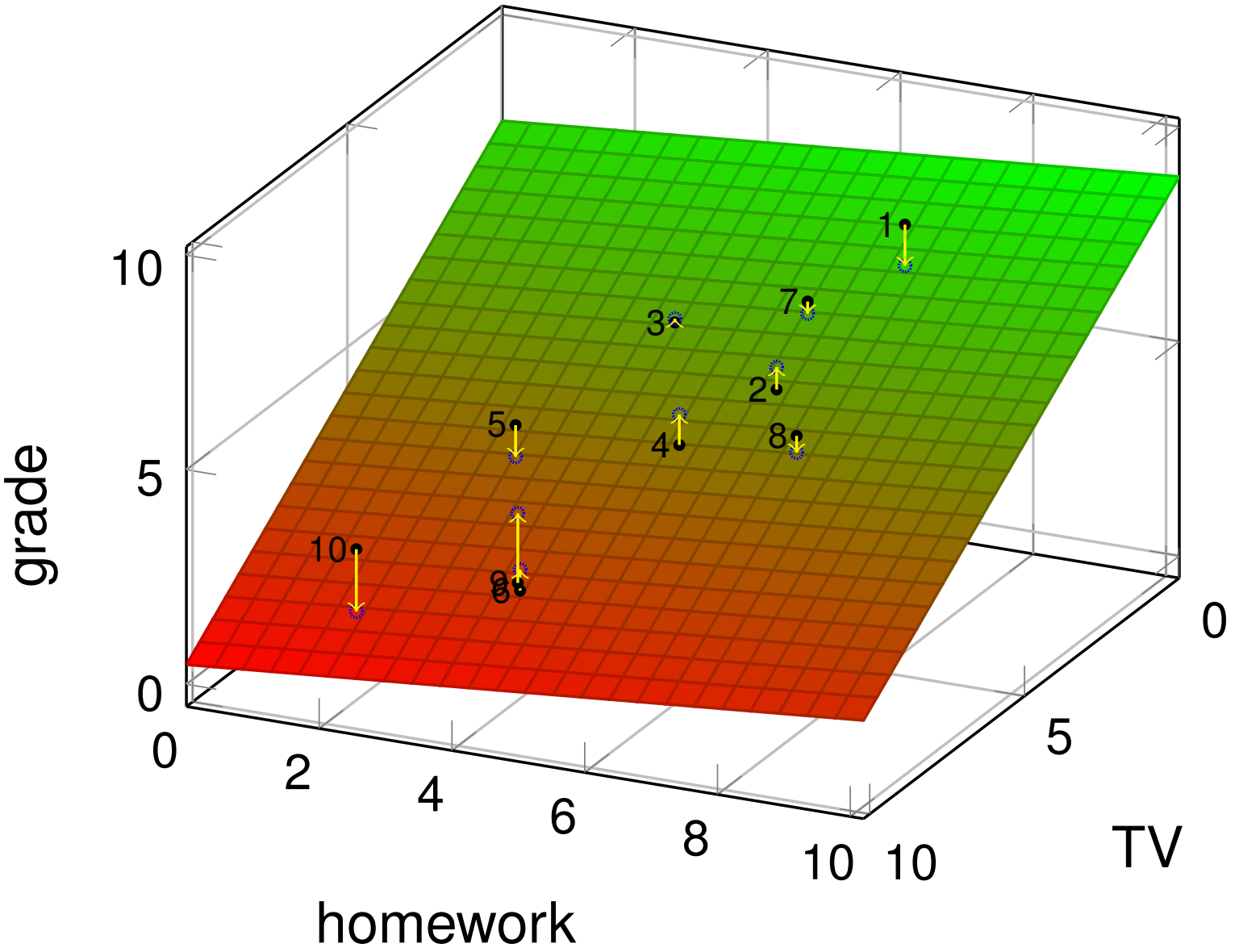

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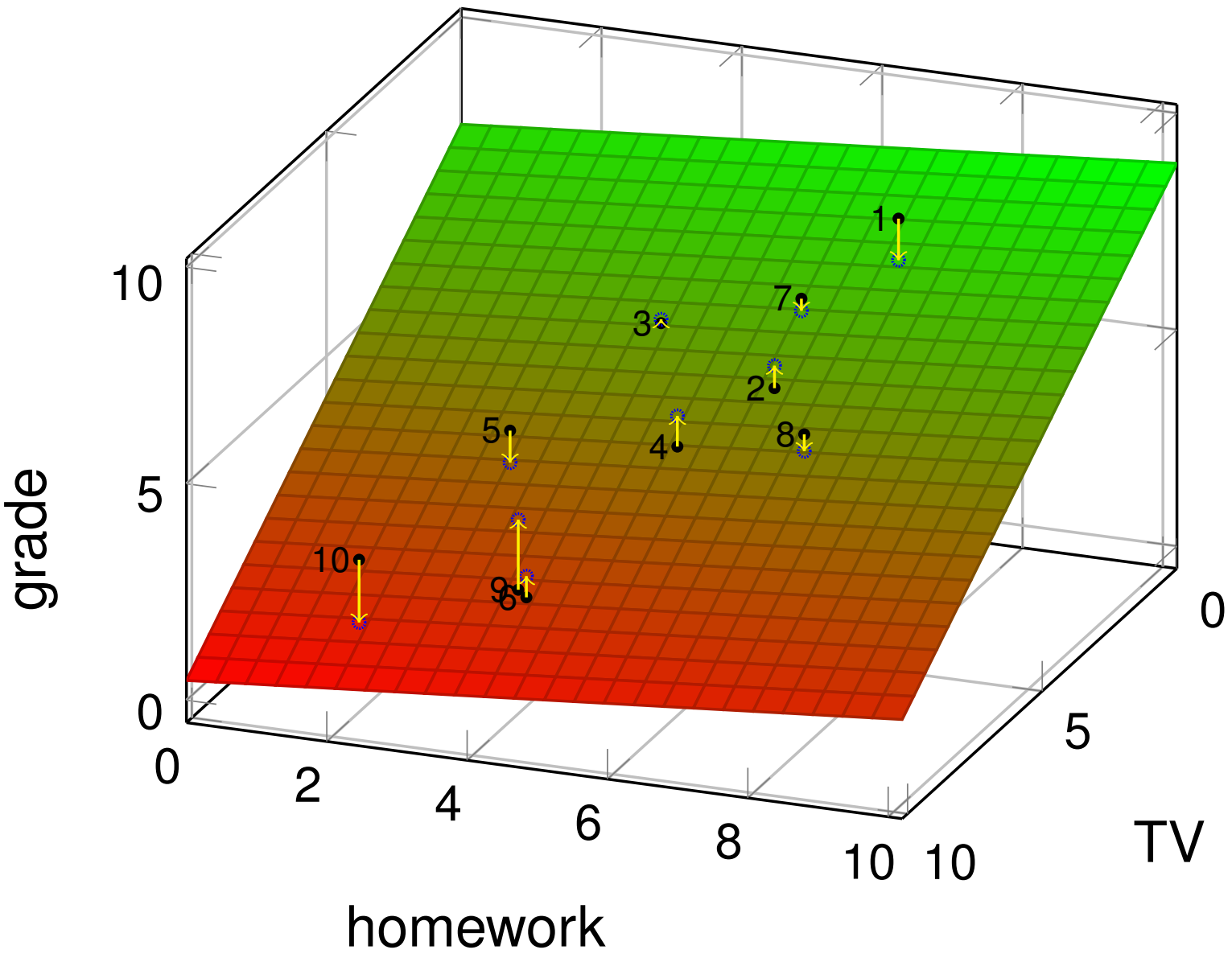

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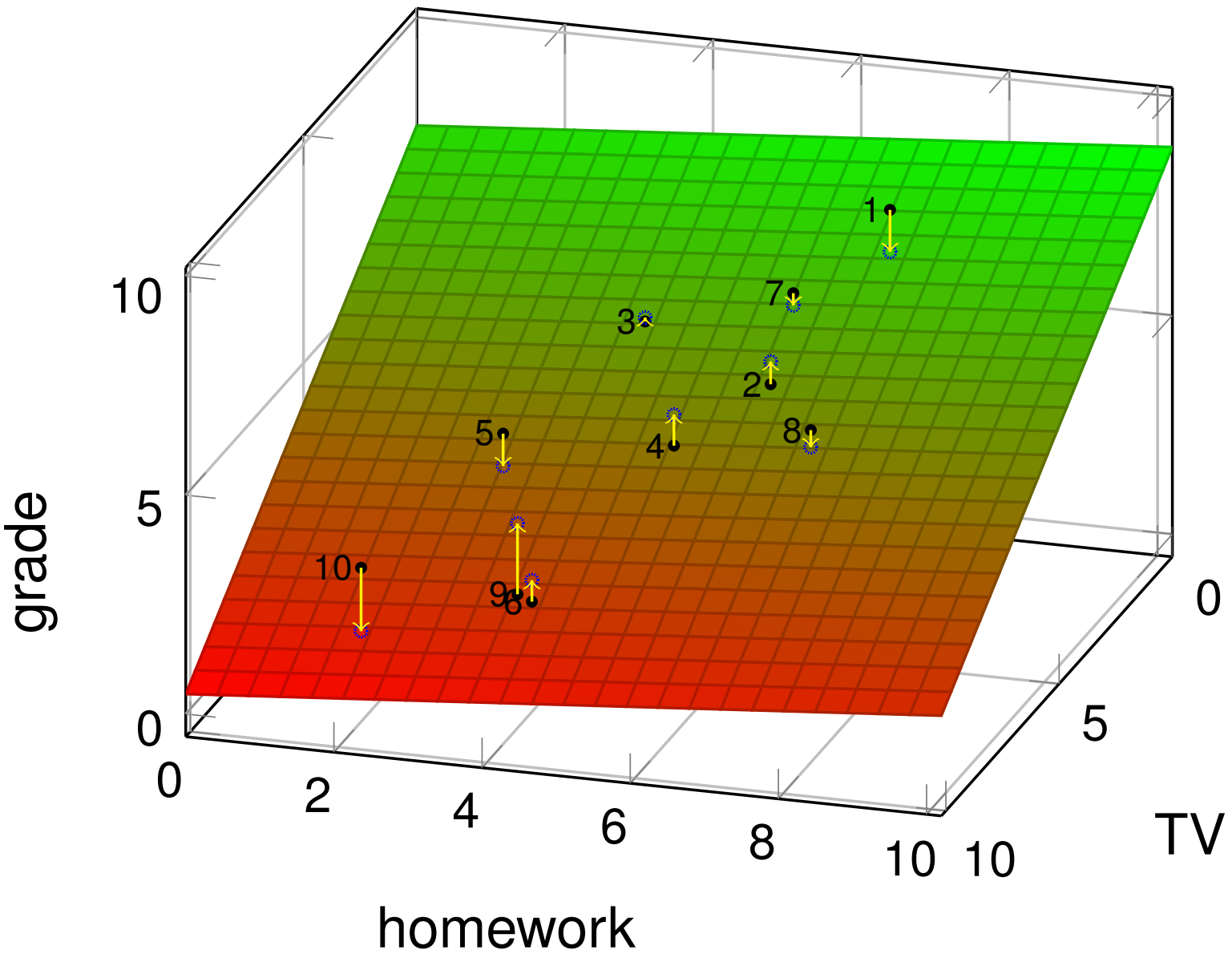

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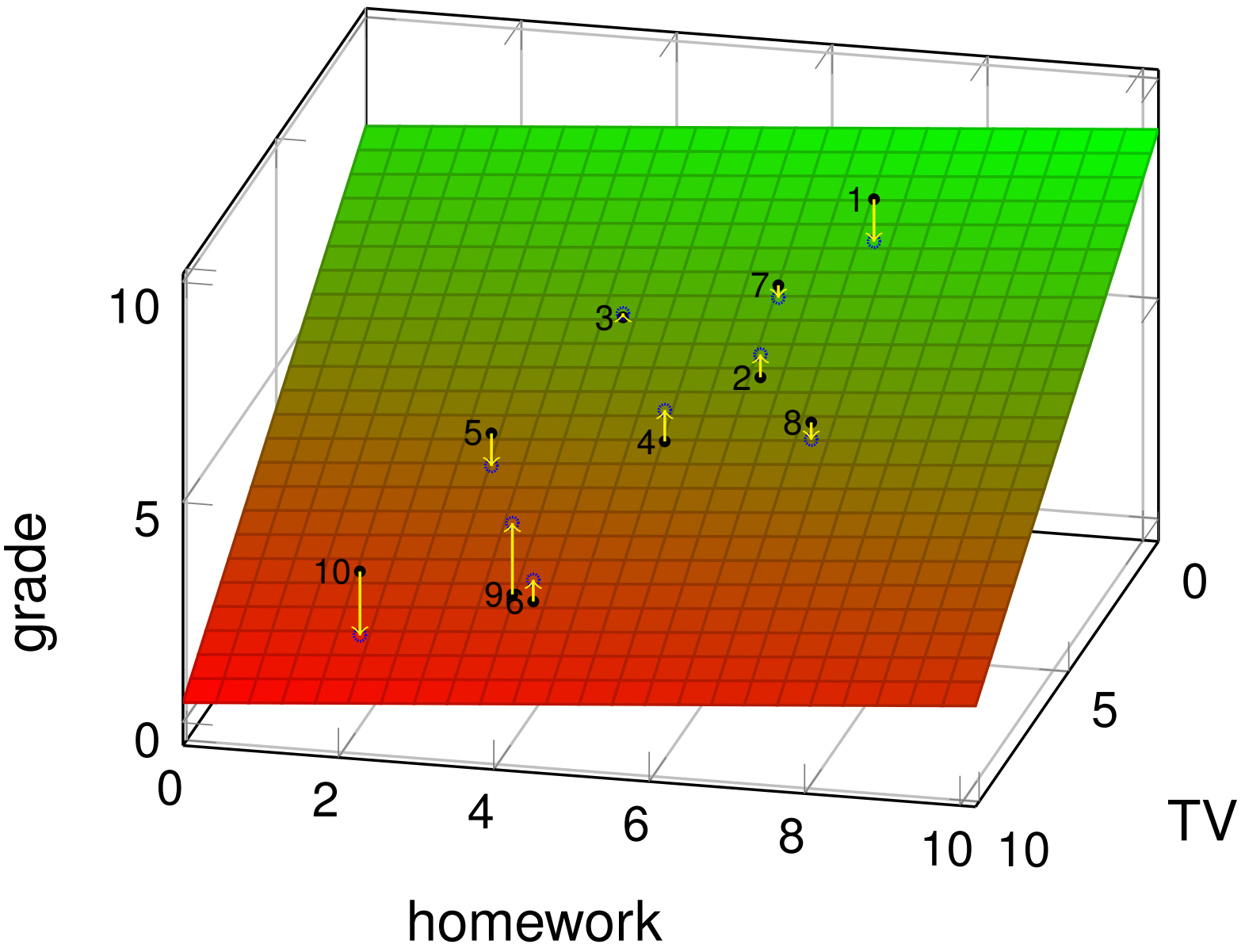

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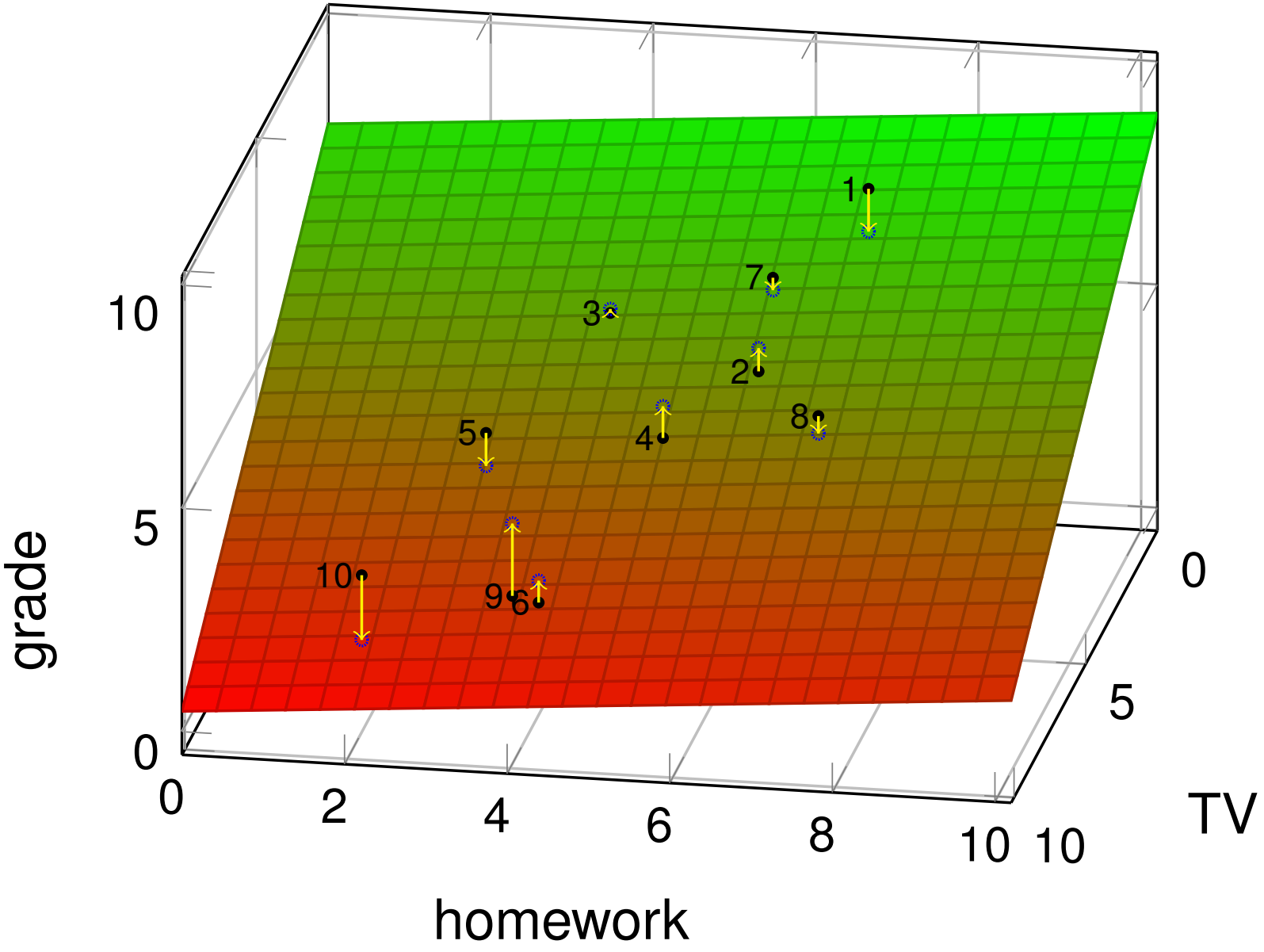

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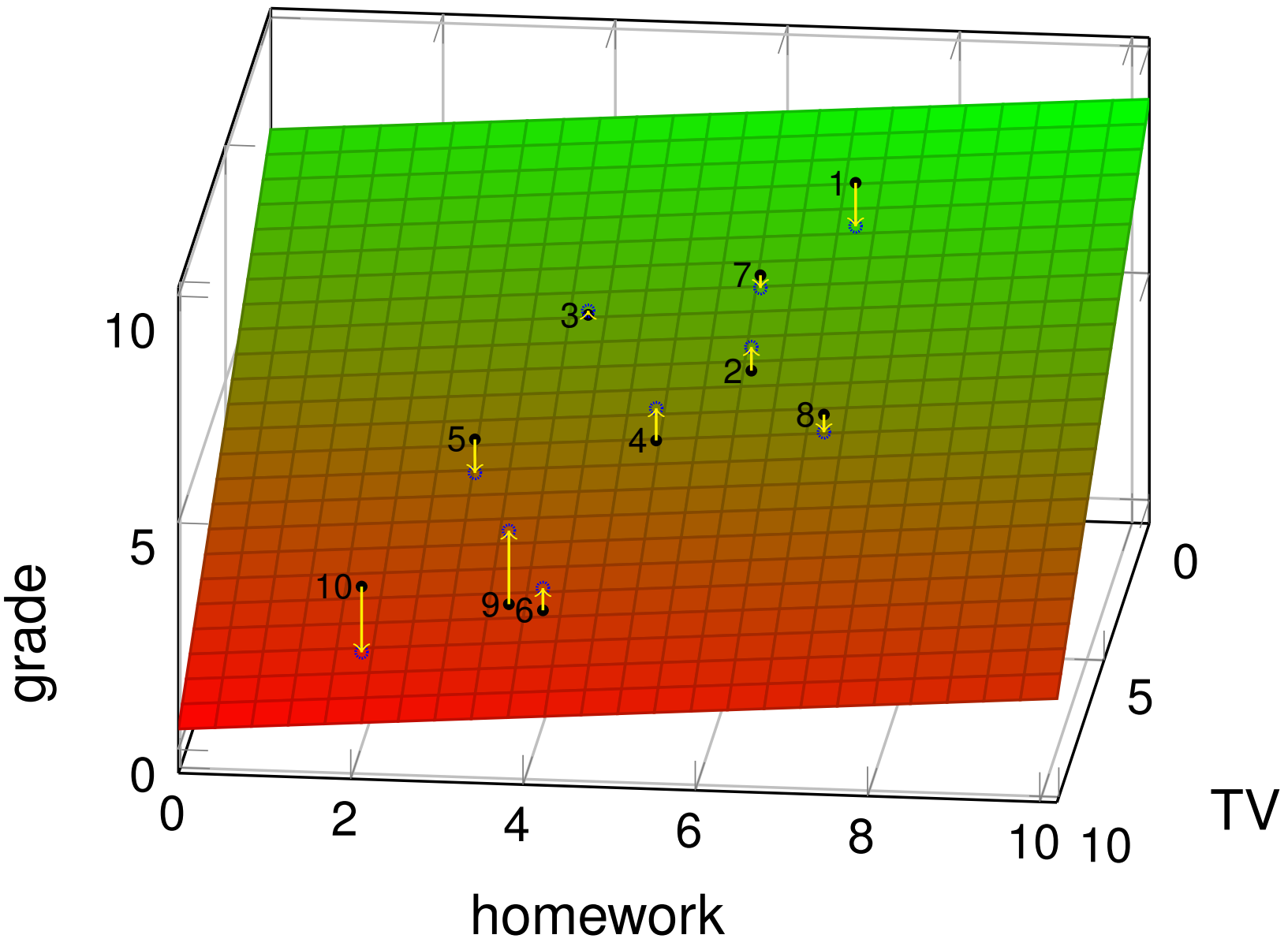

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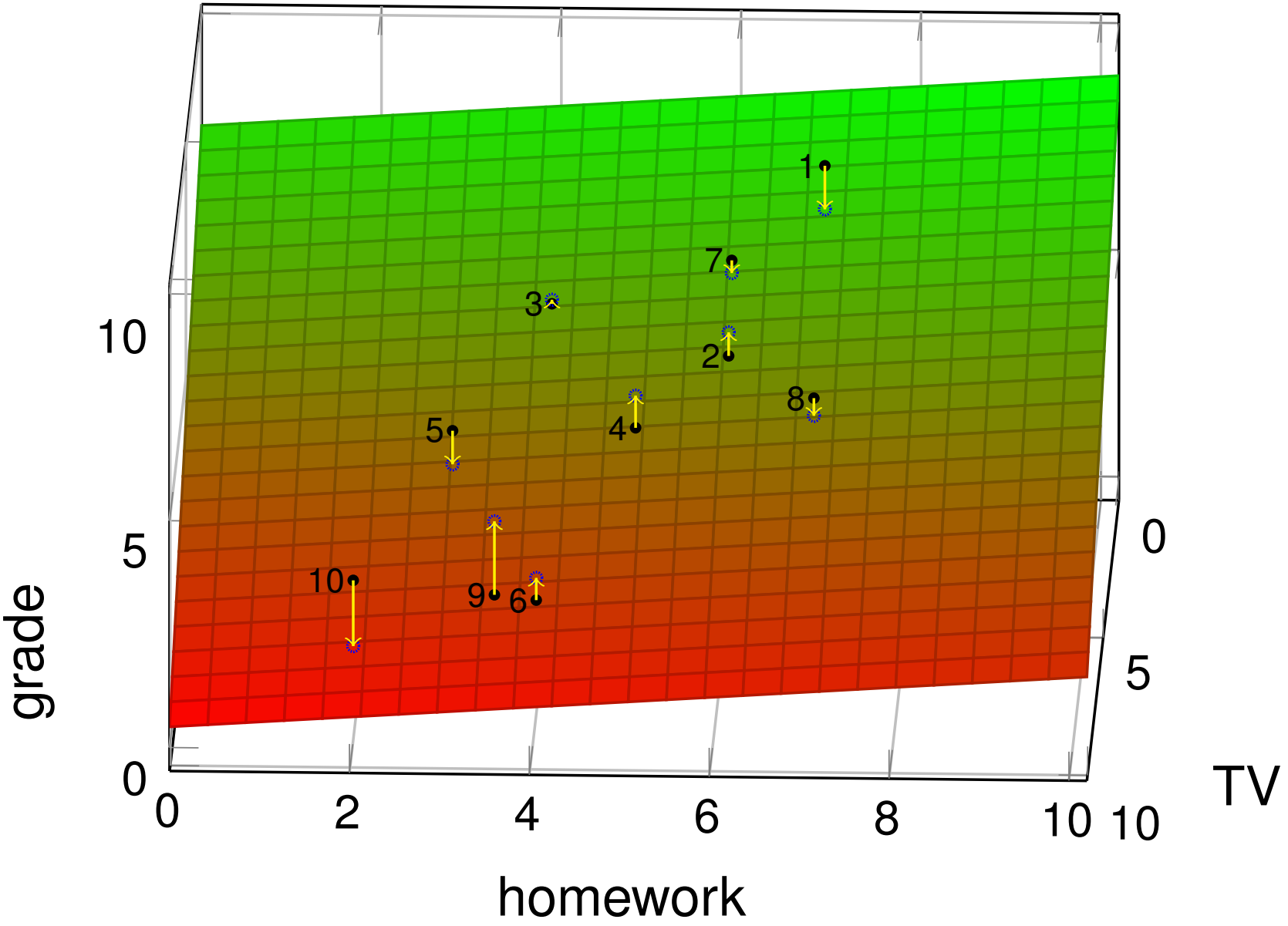

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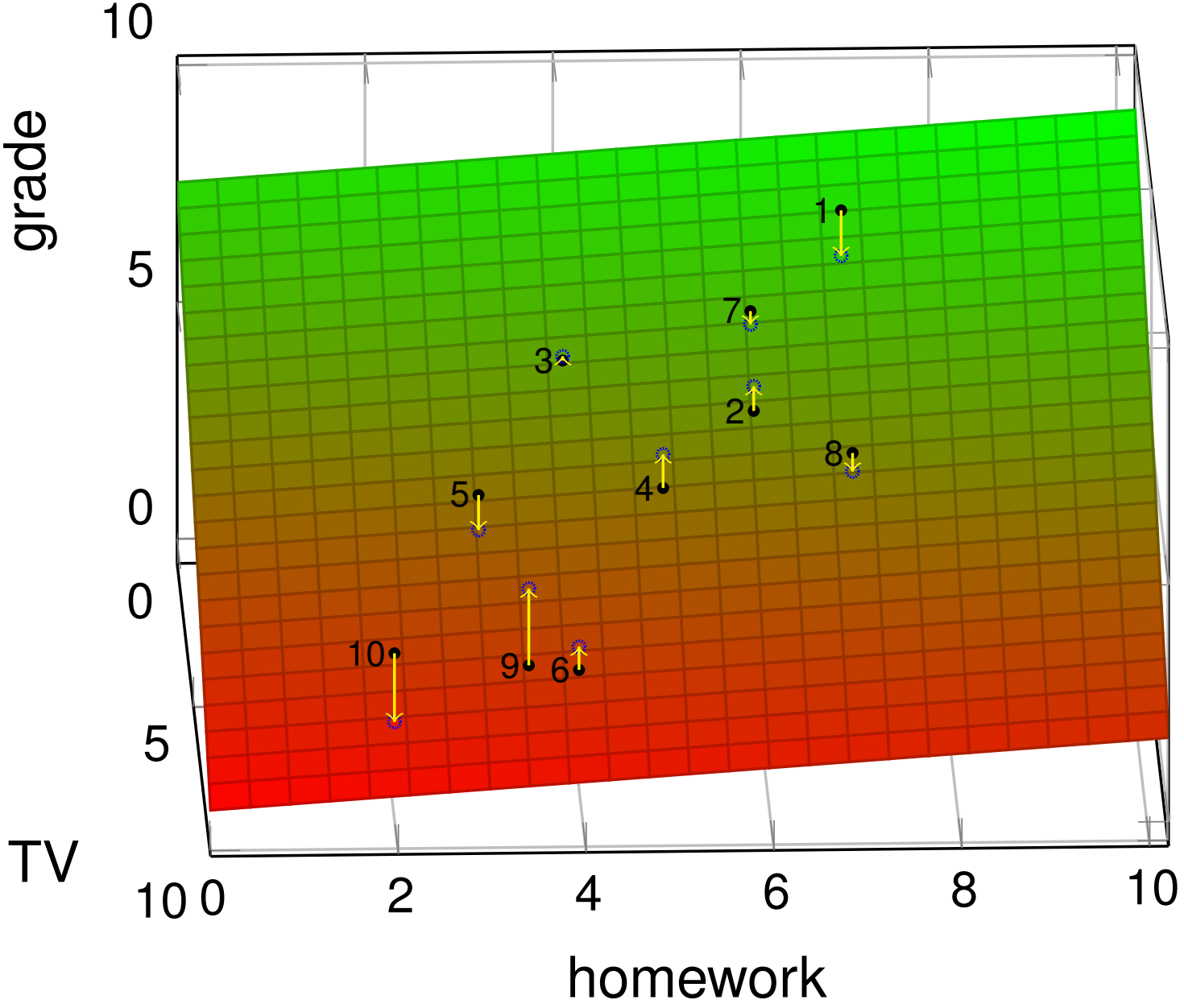

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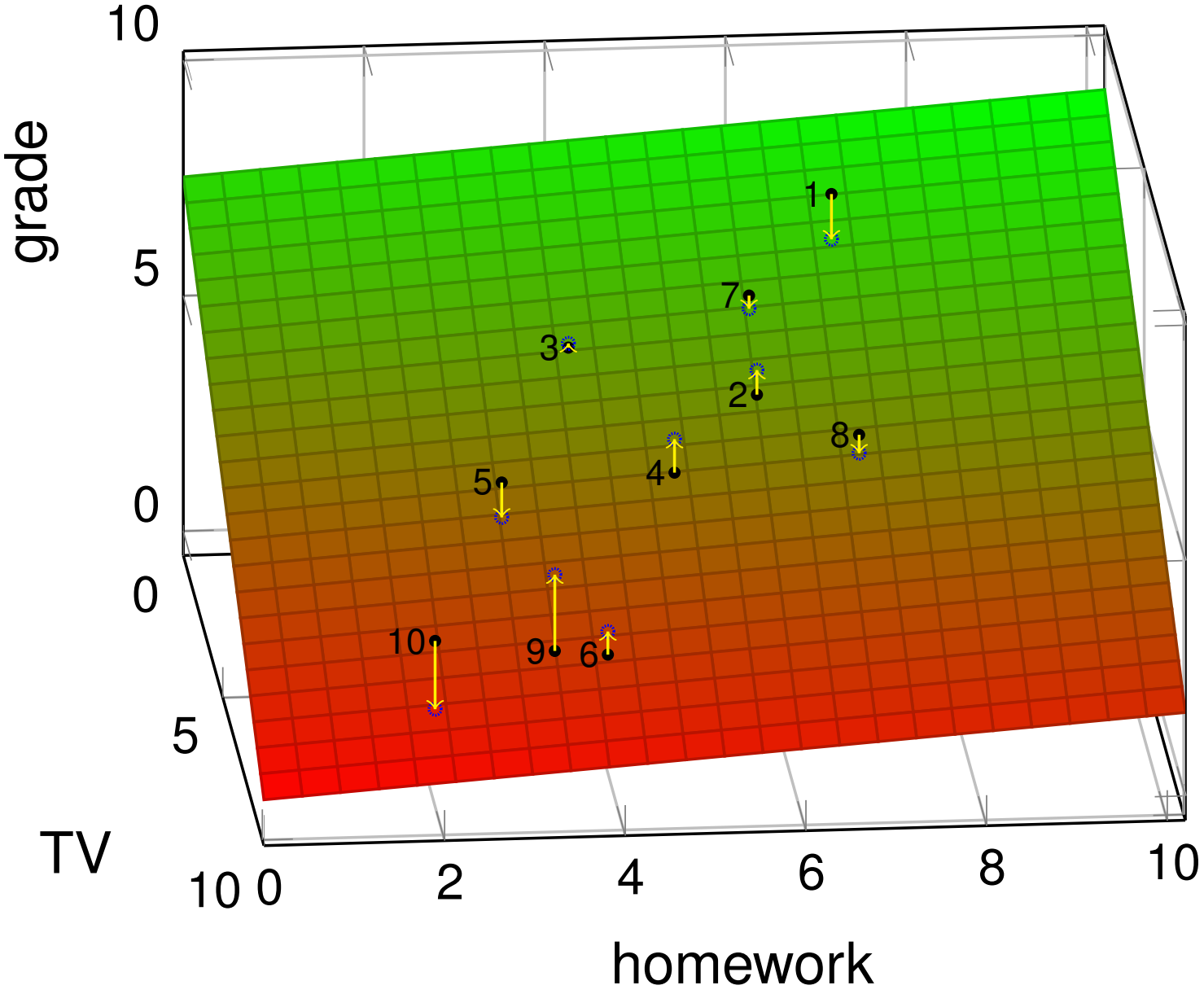

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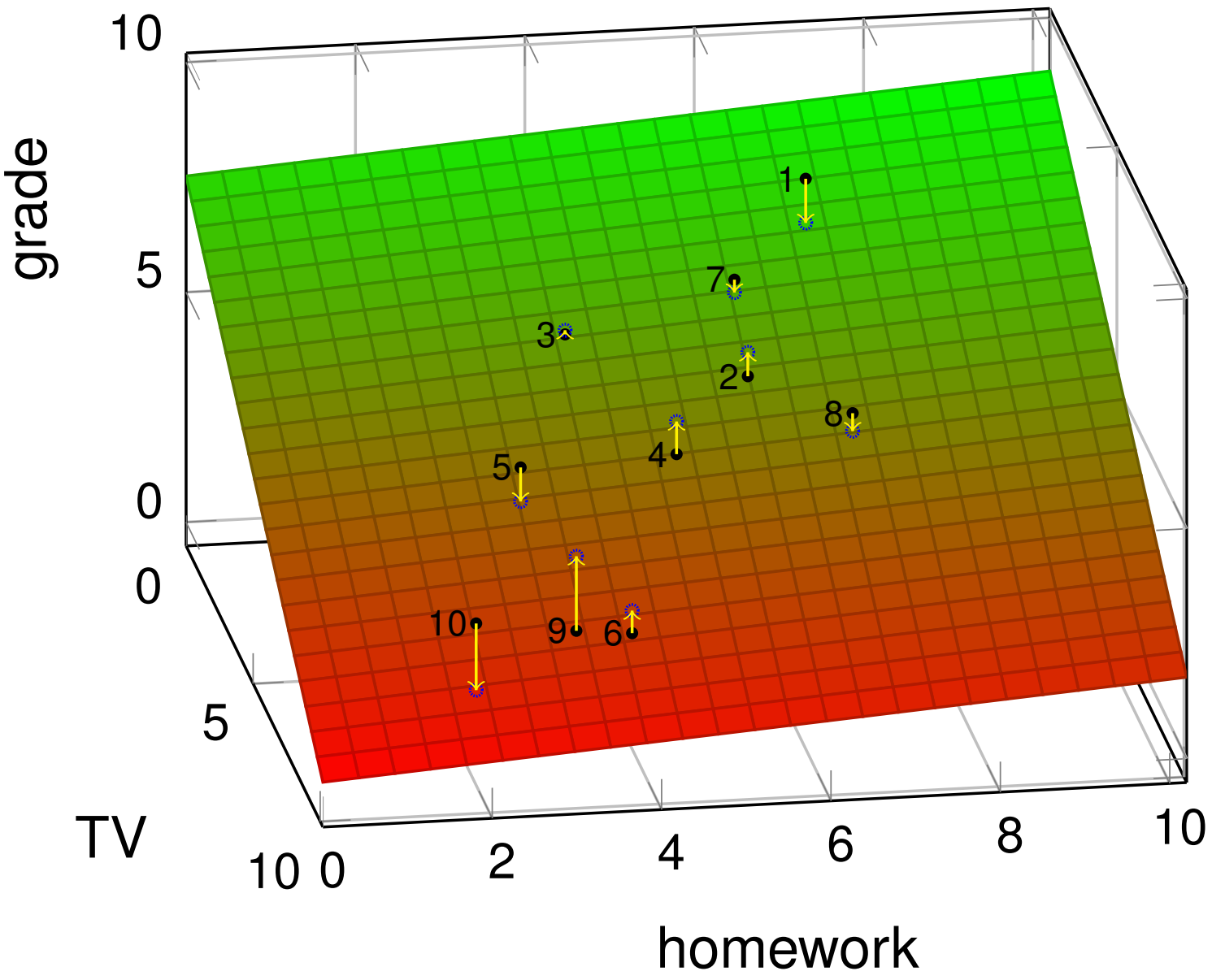

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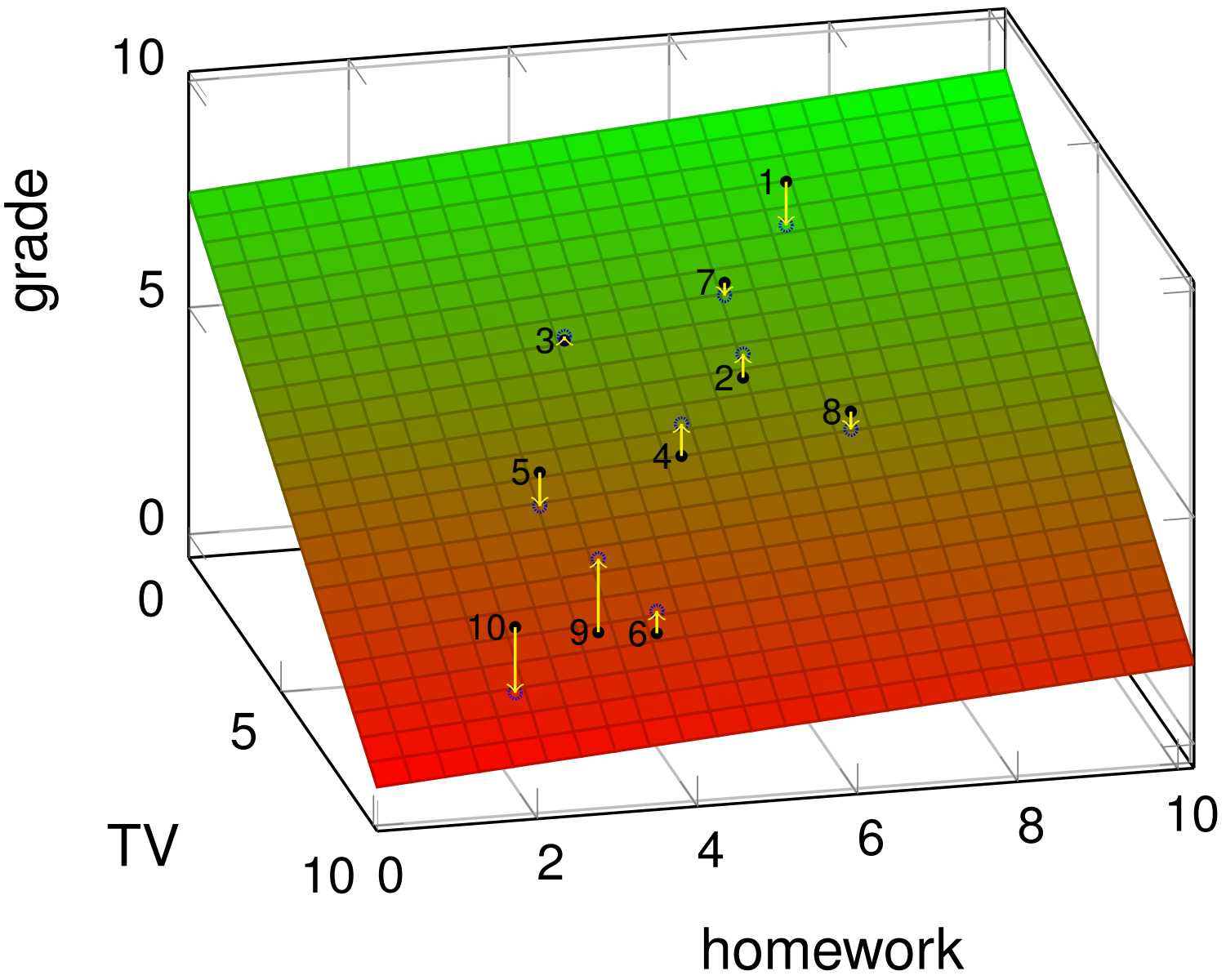

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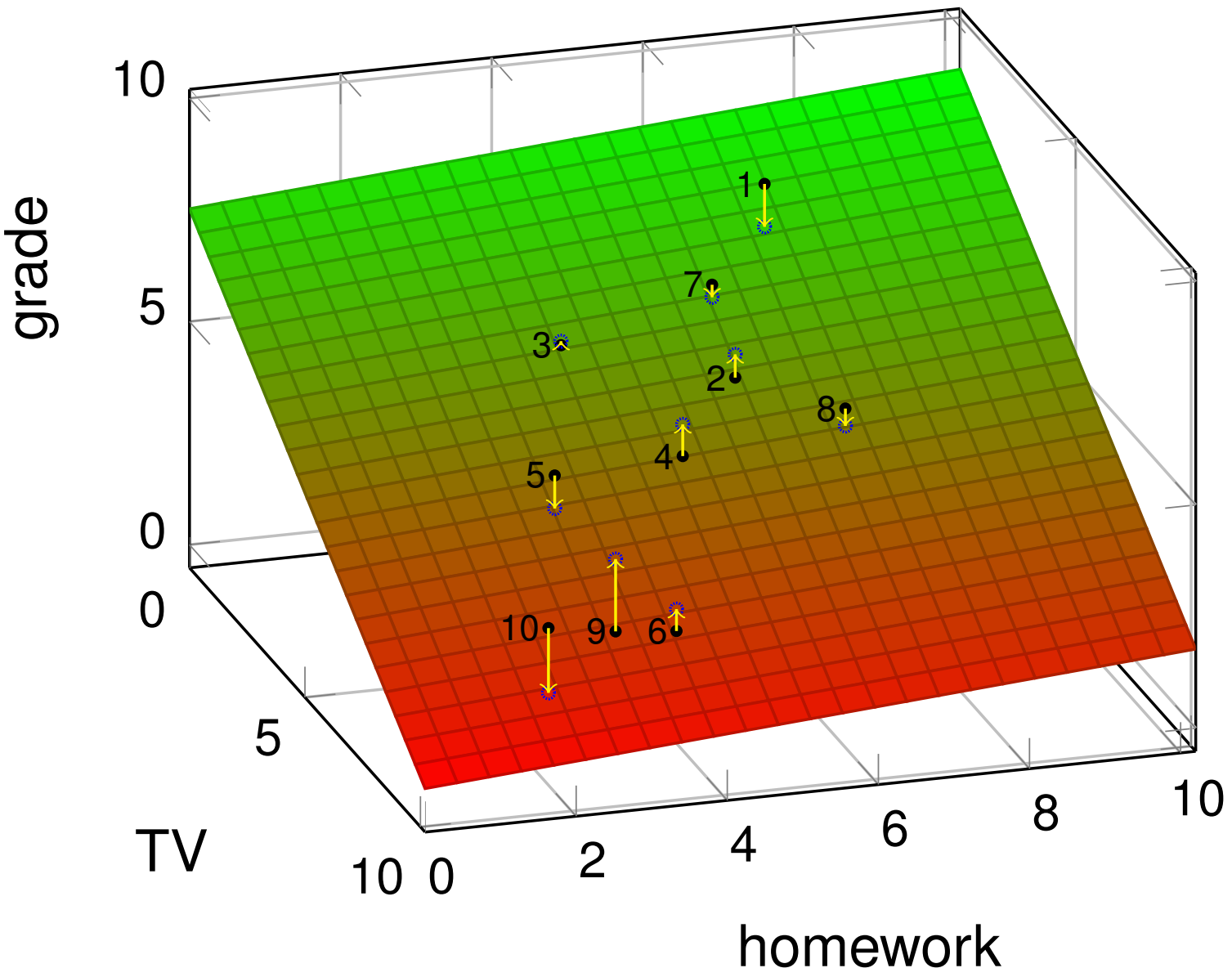

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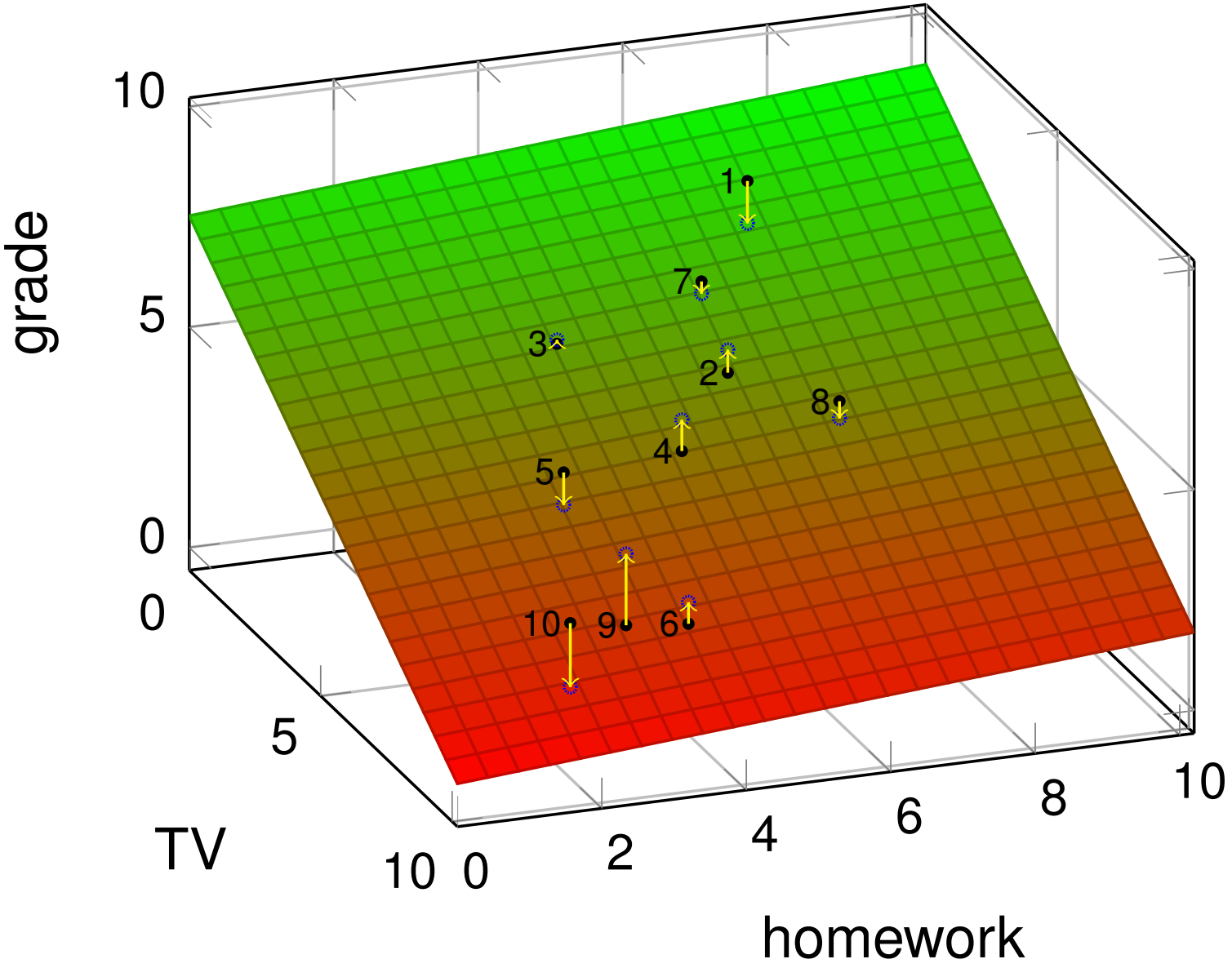

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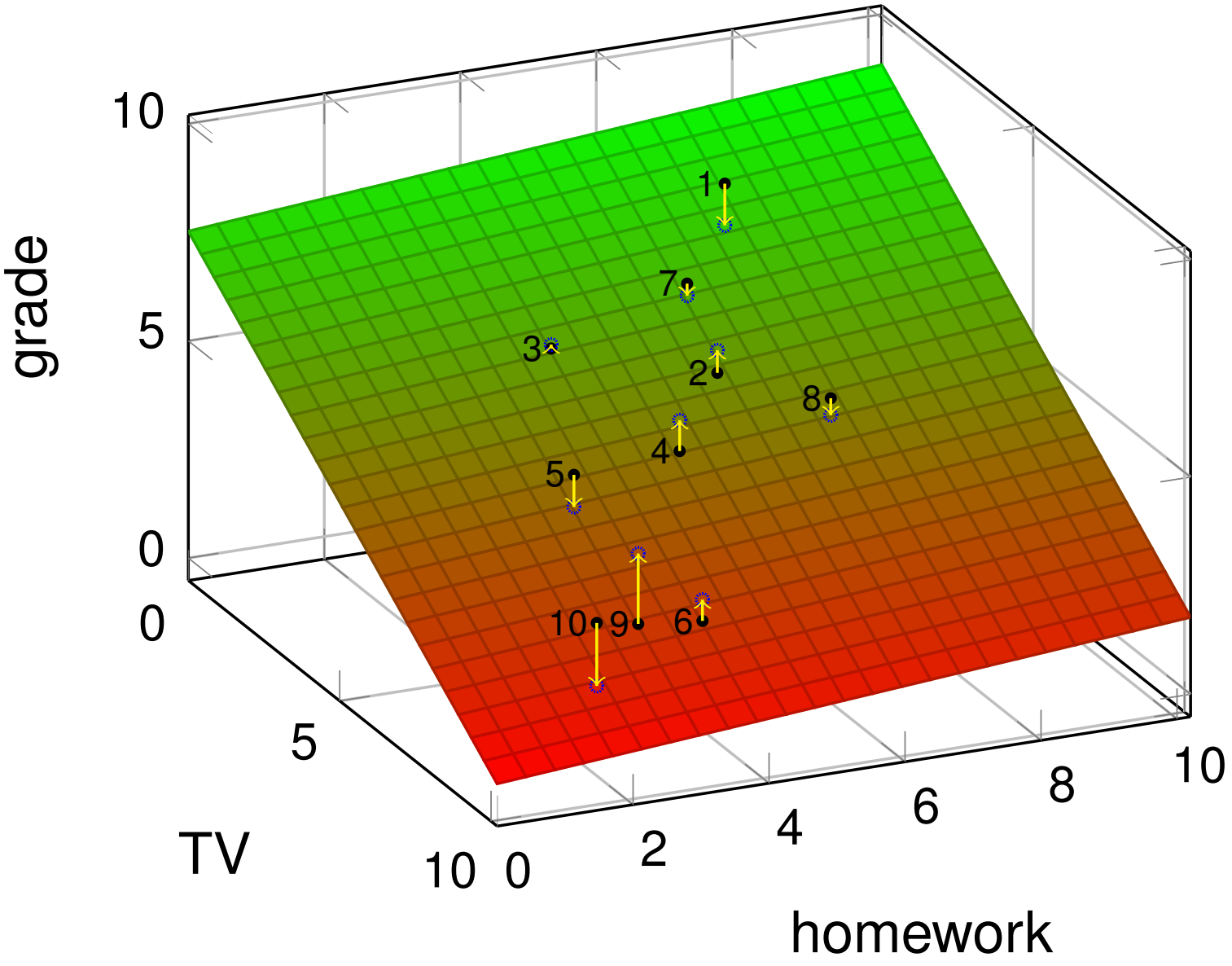

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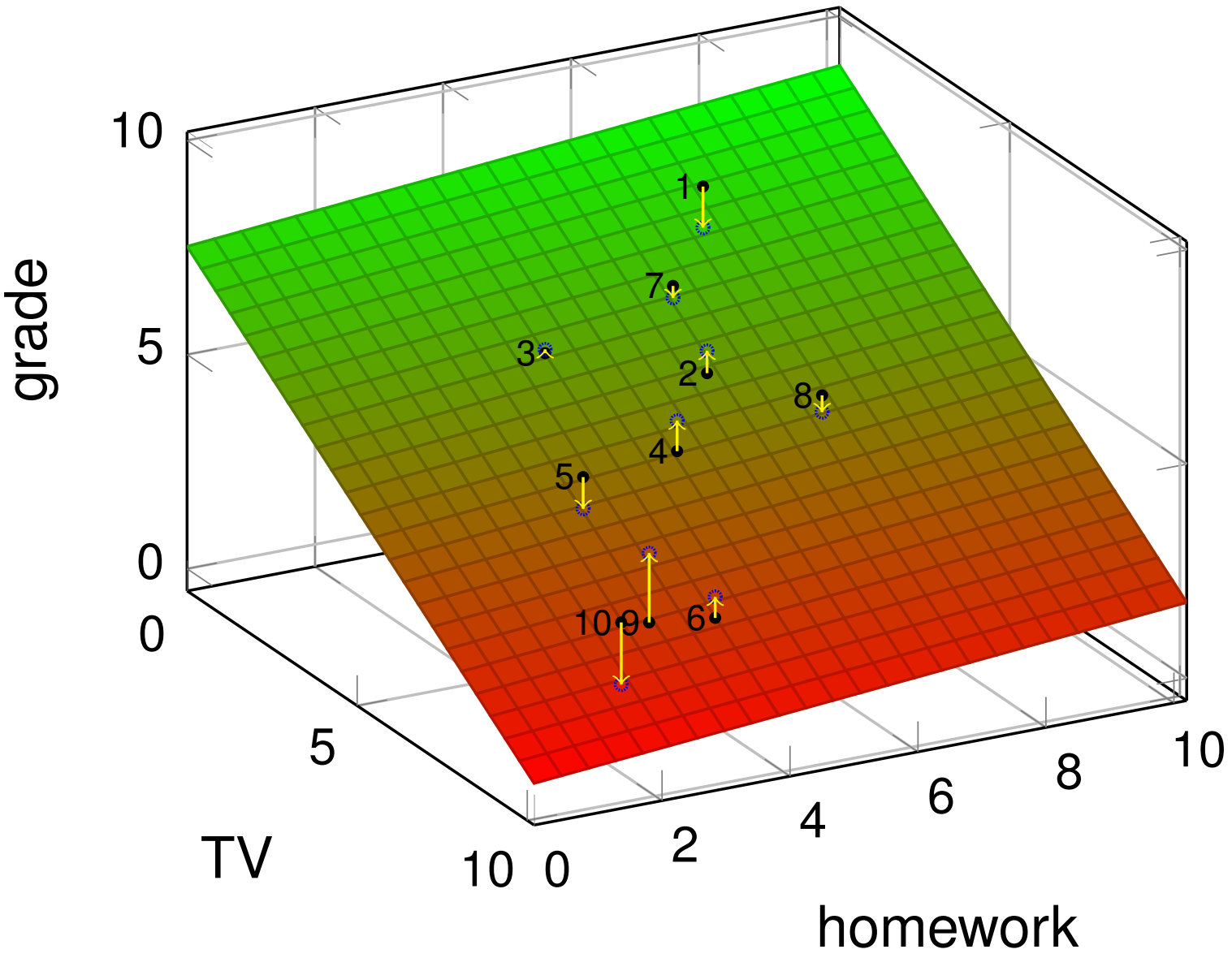

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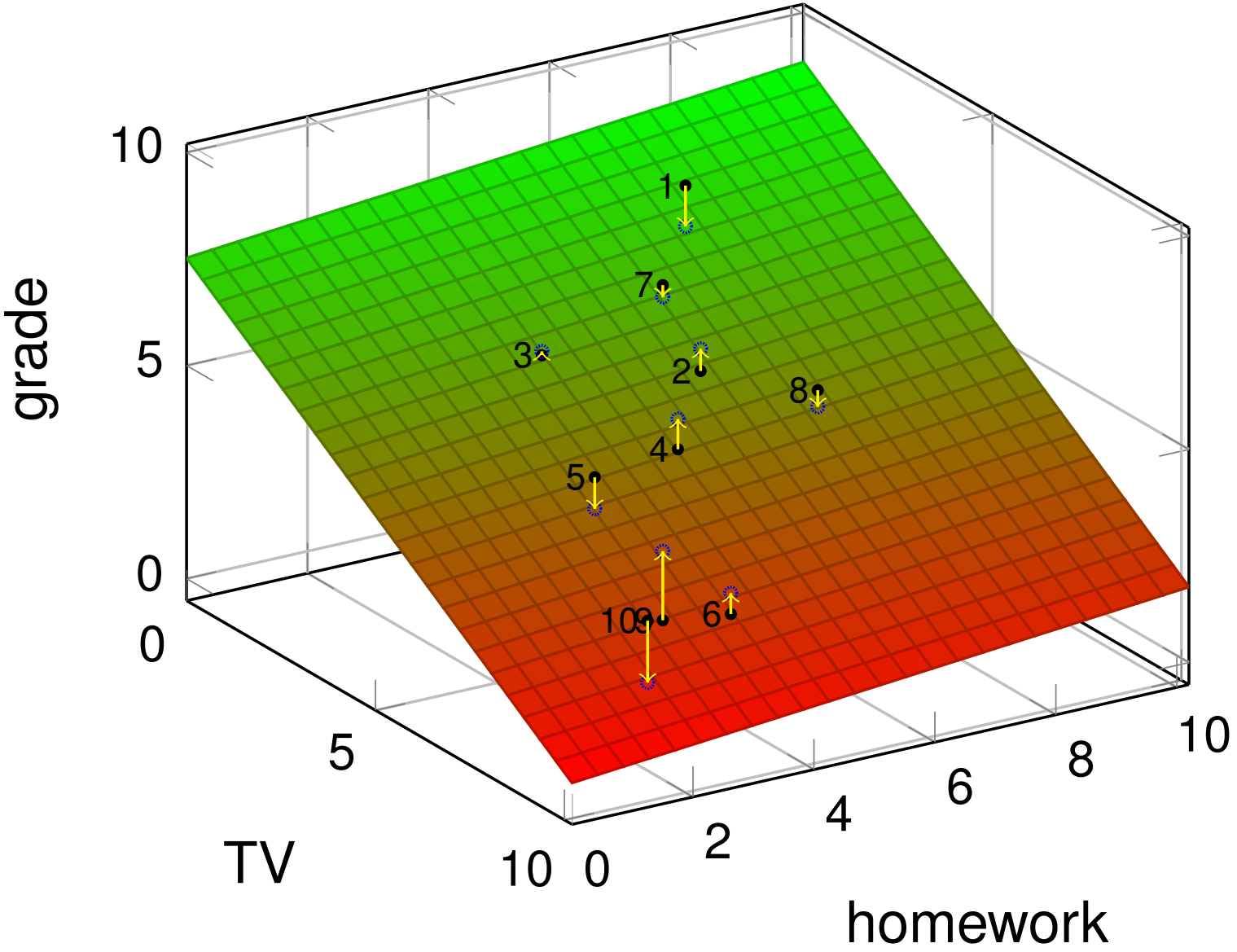

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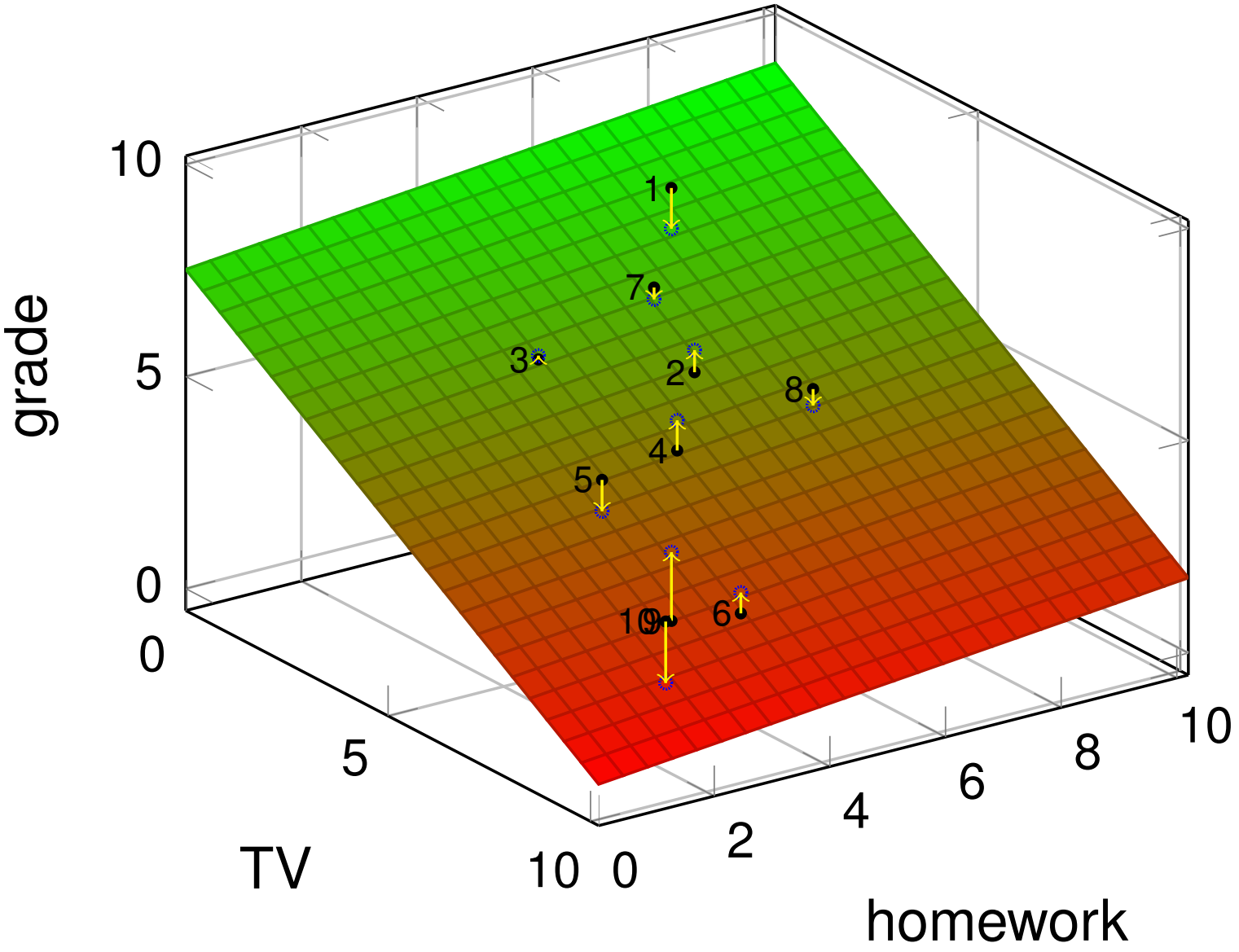

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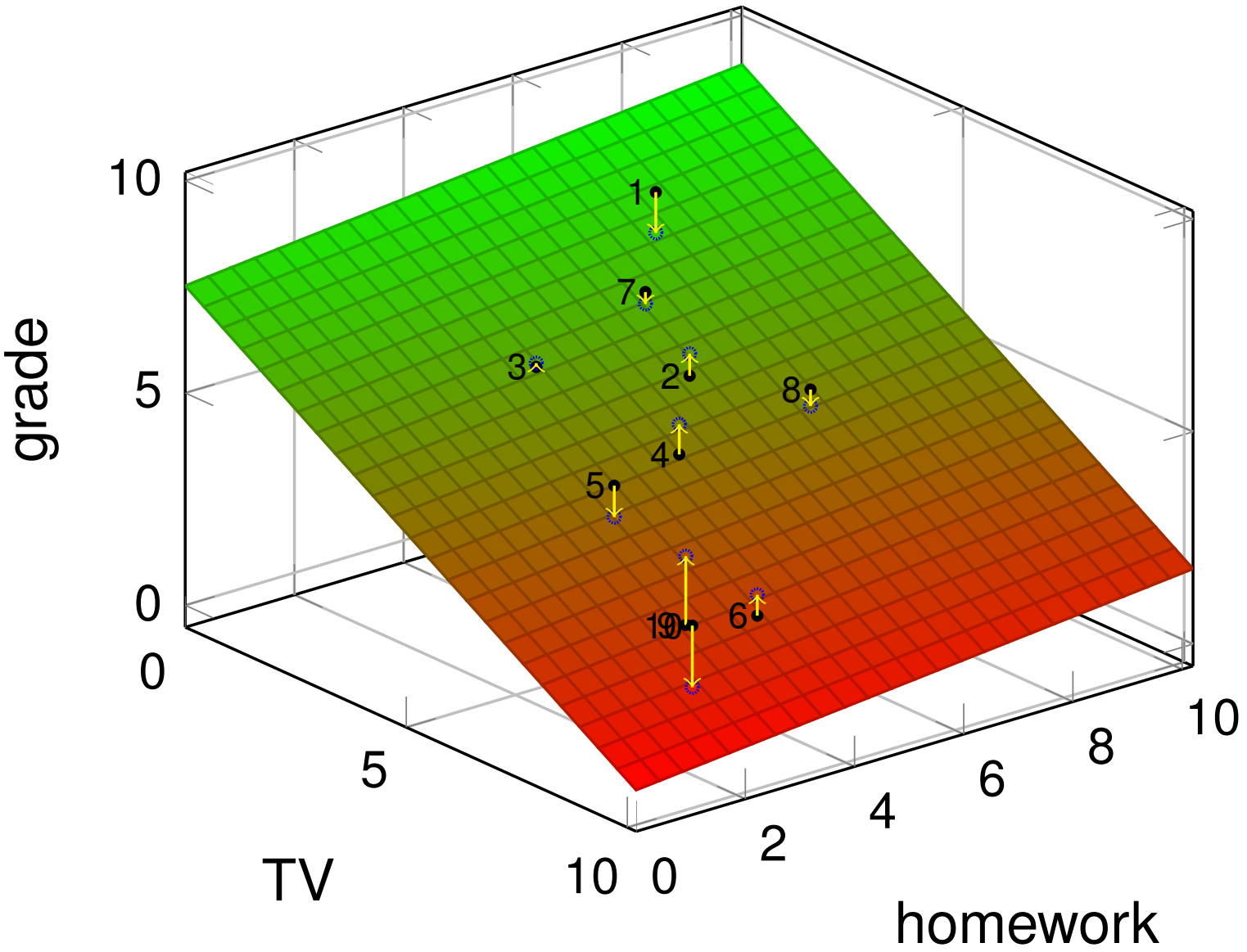

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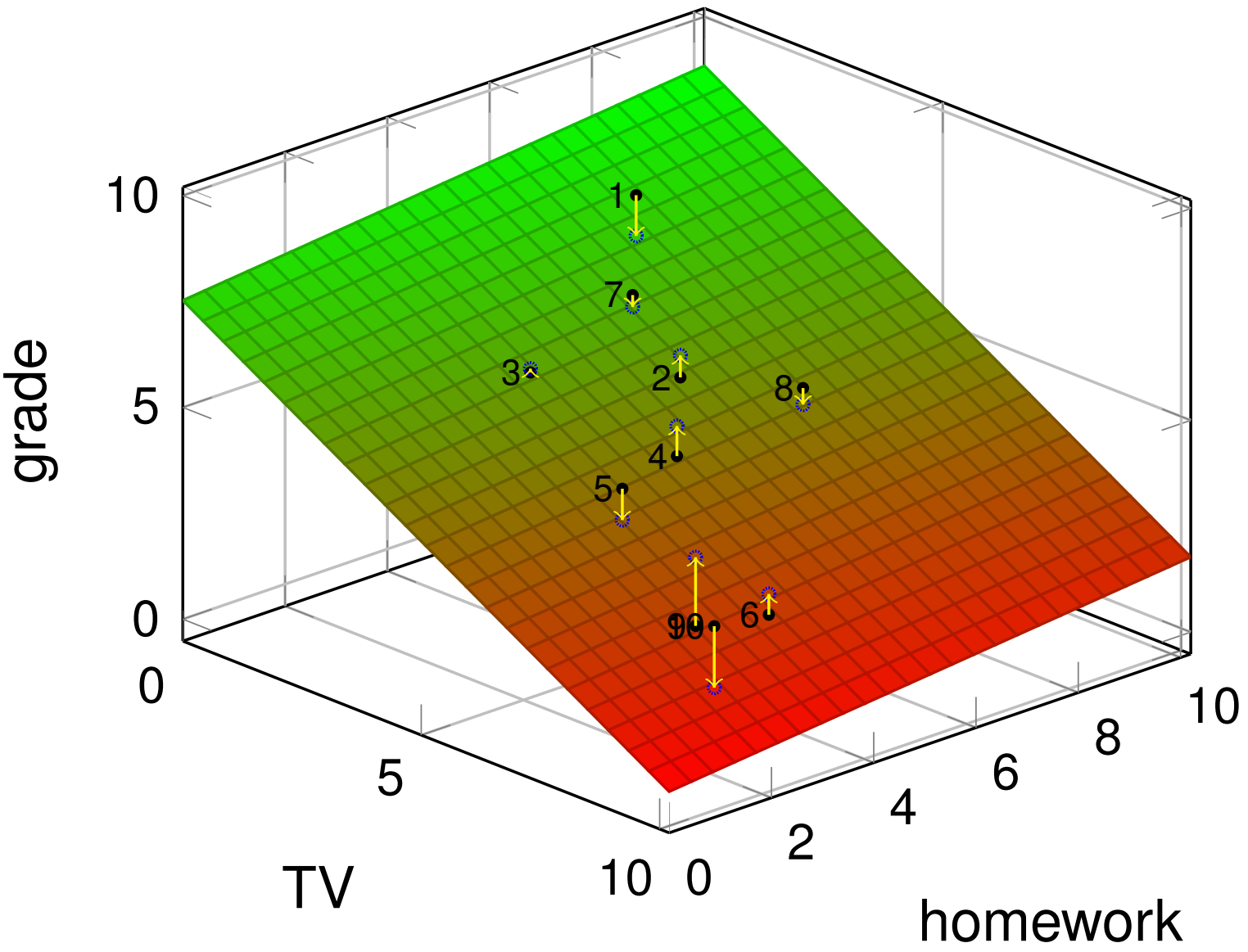

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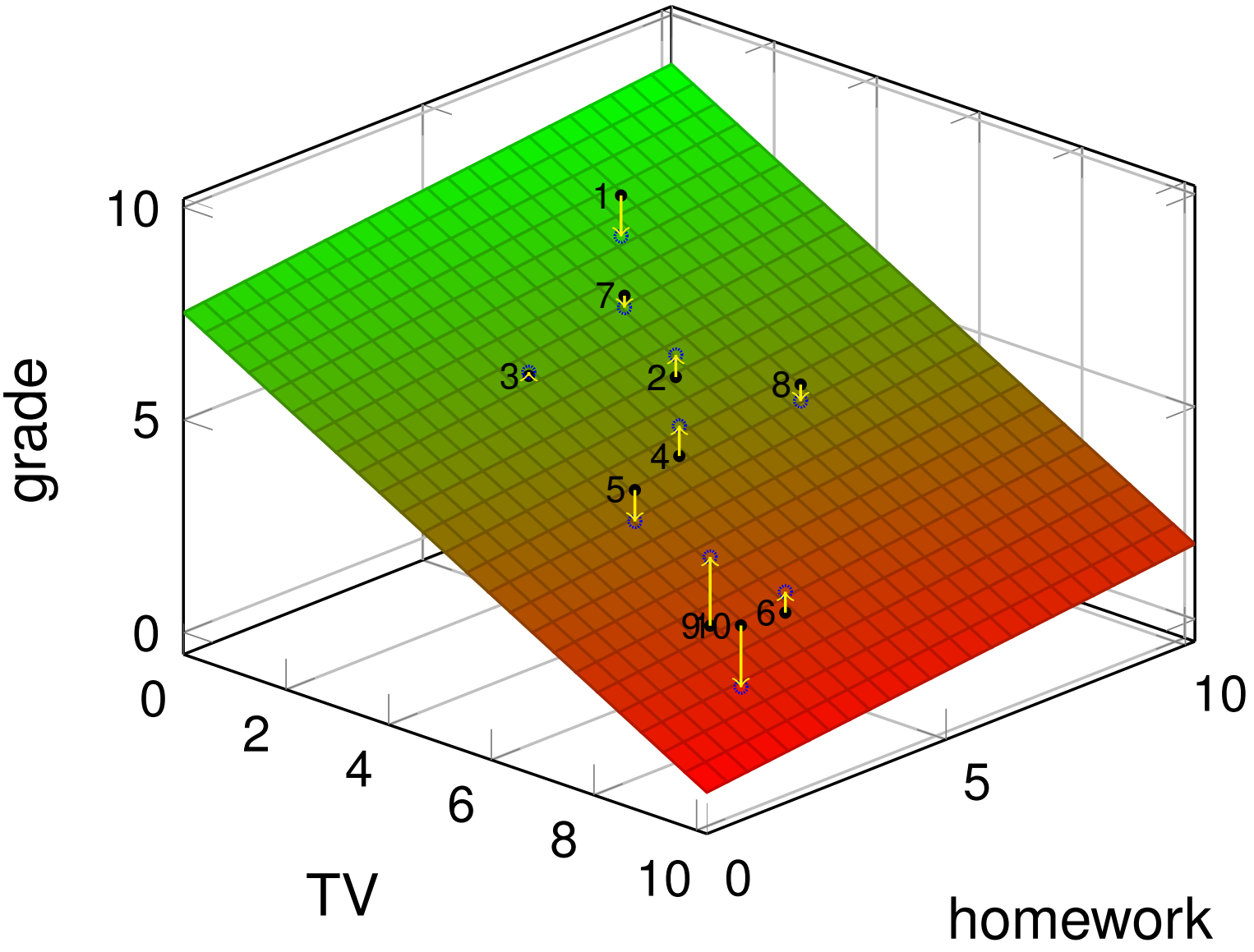

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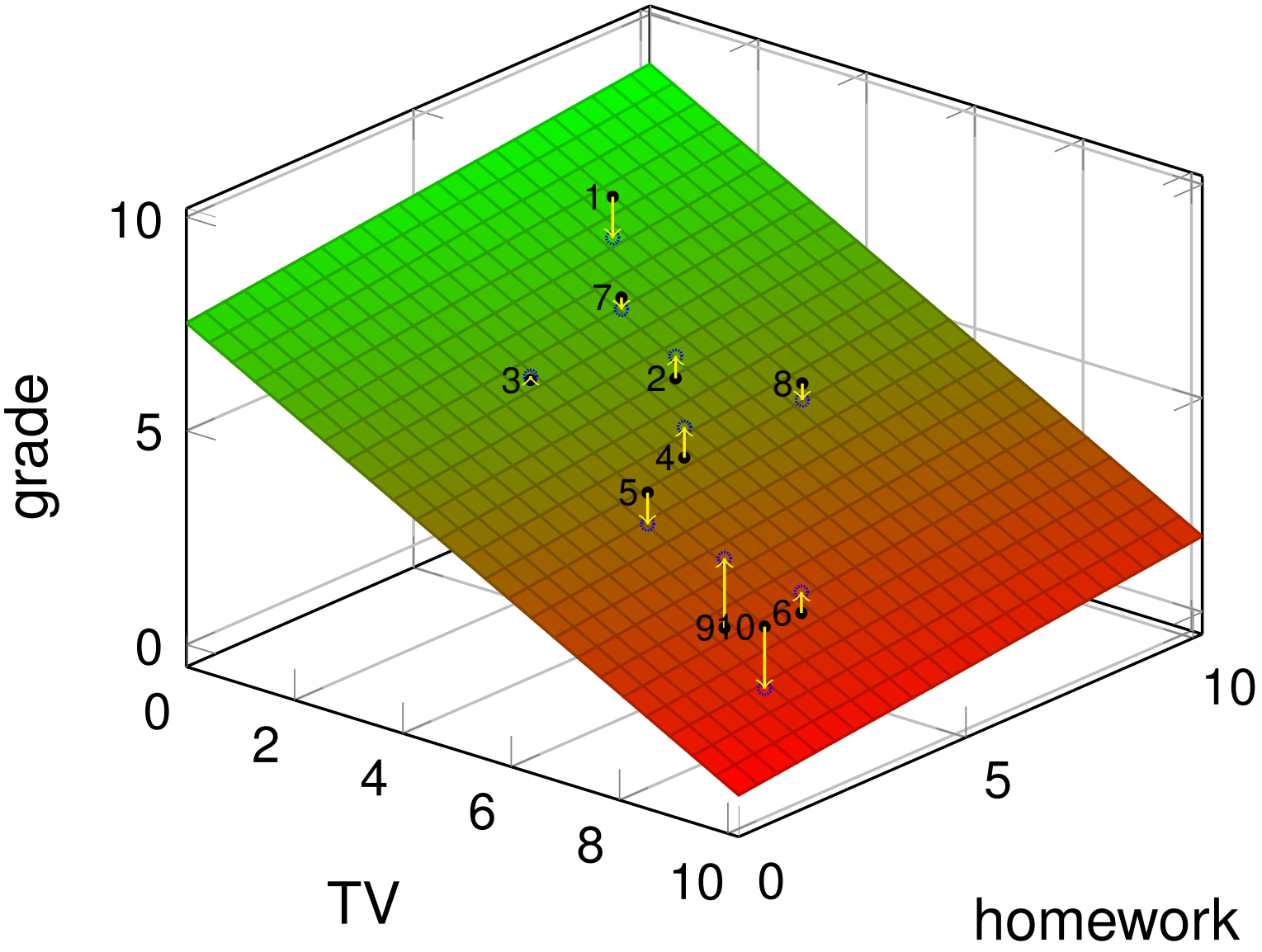

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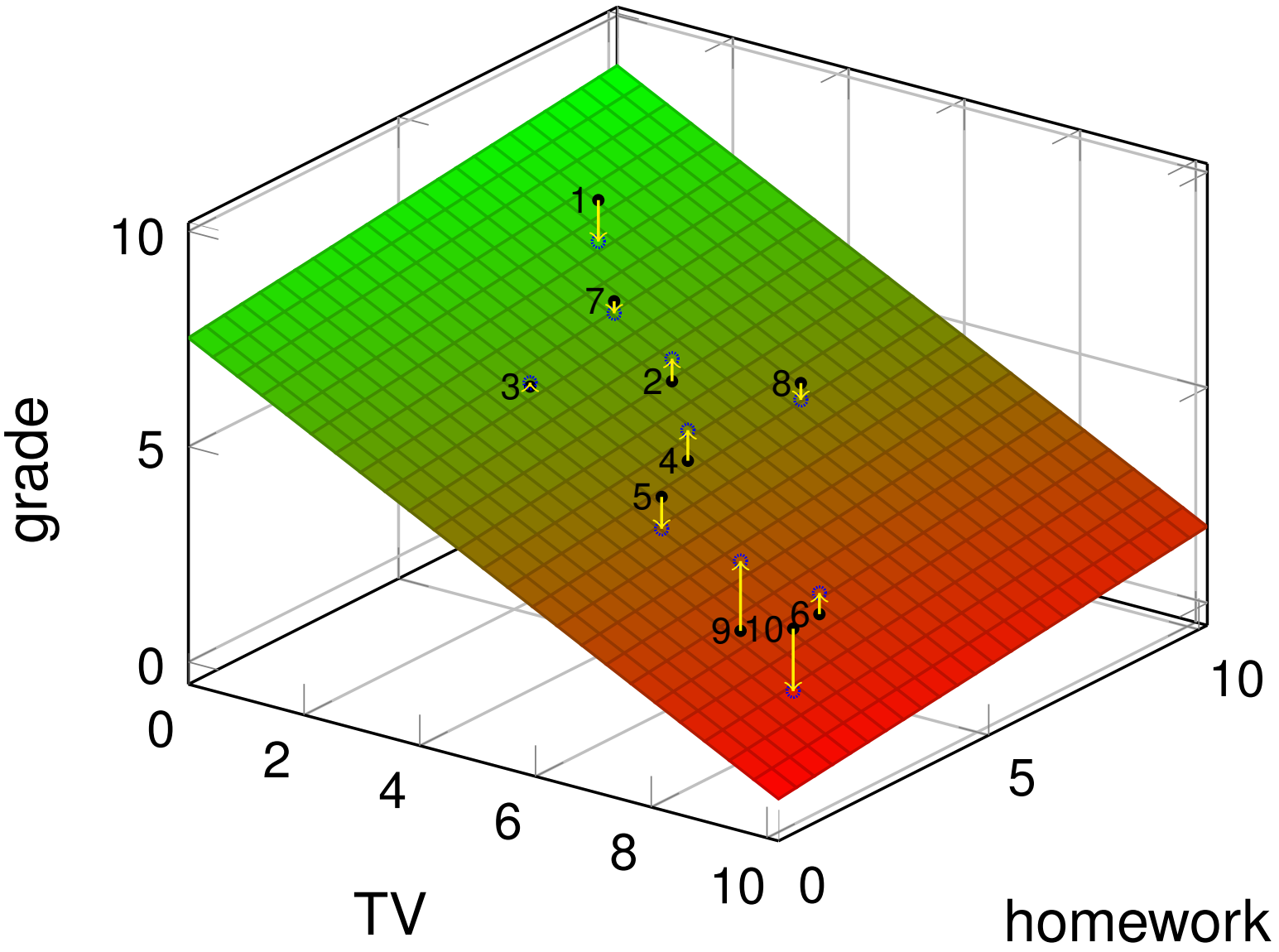

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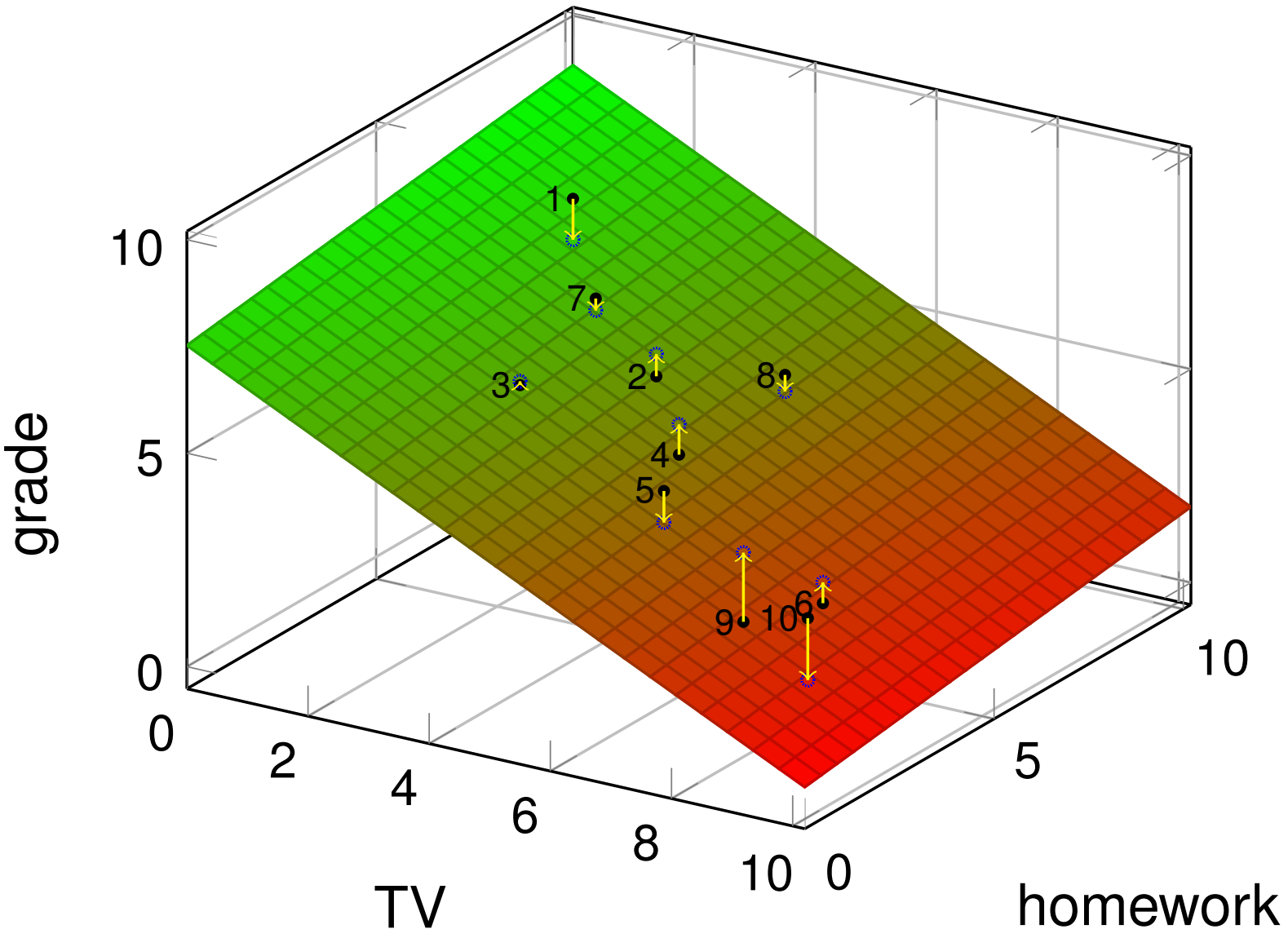

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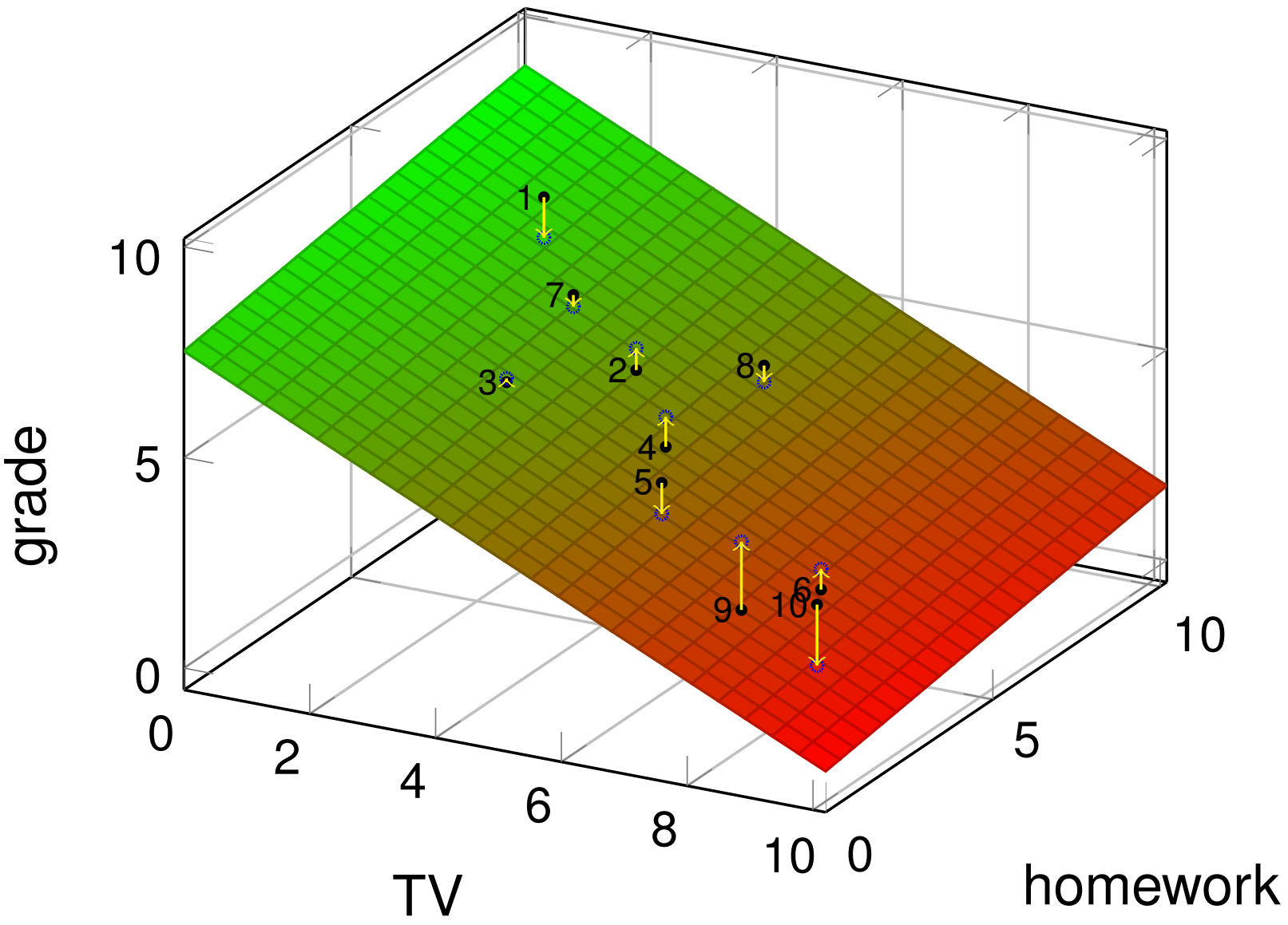
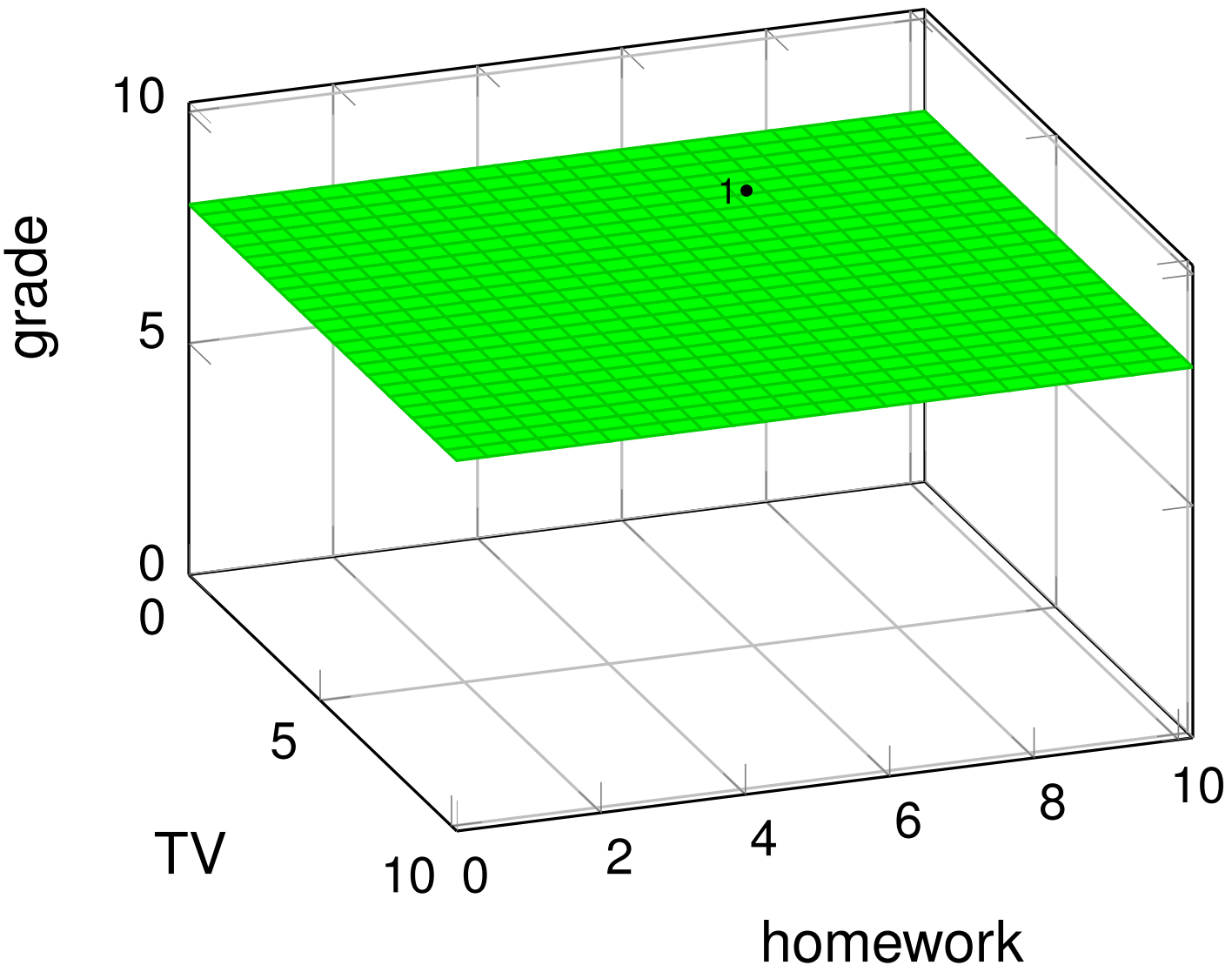
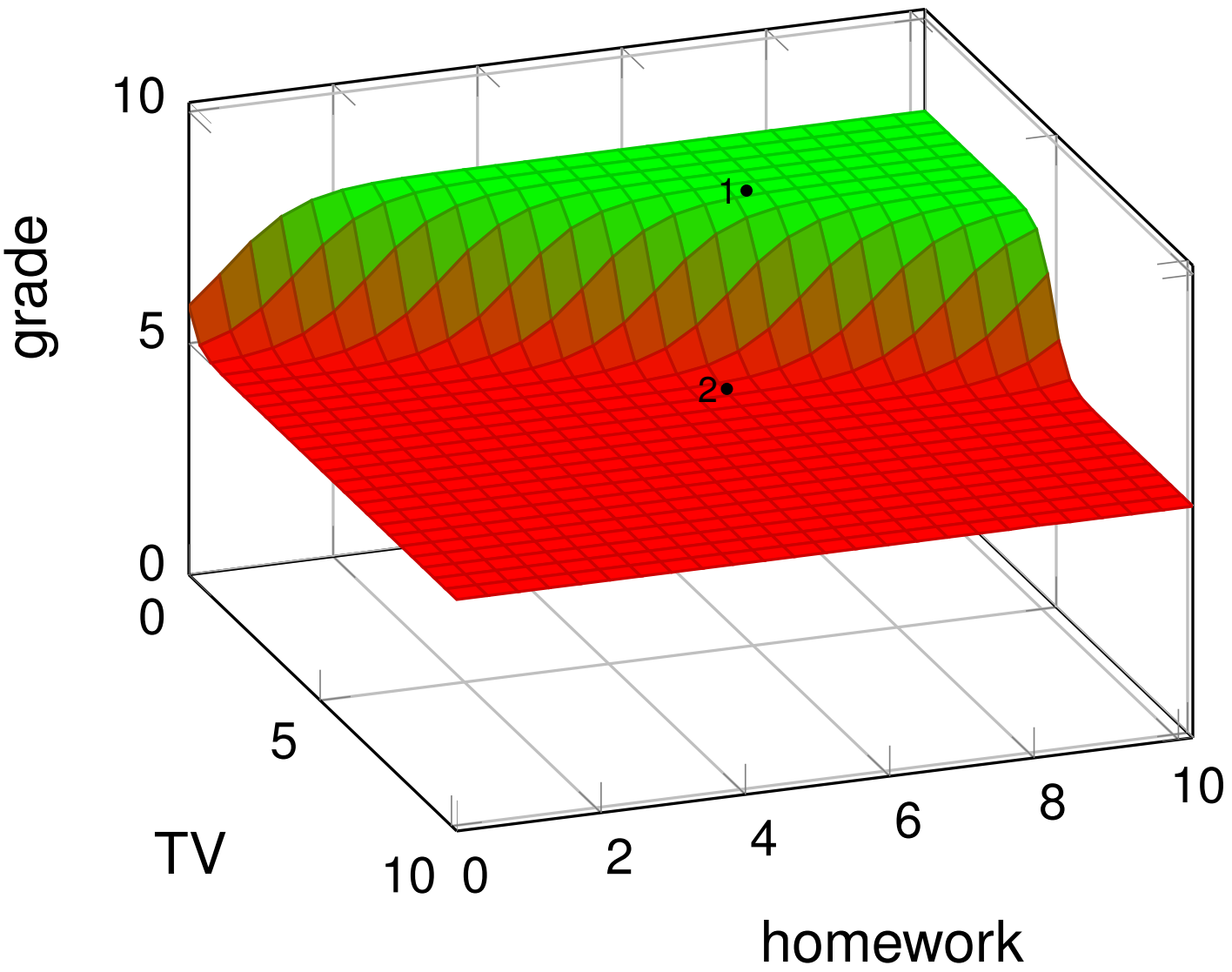


Let us now use k-NN with Gaussian Weighting

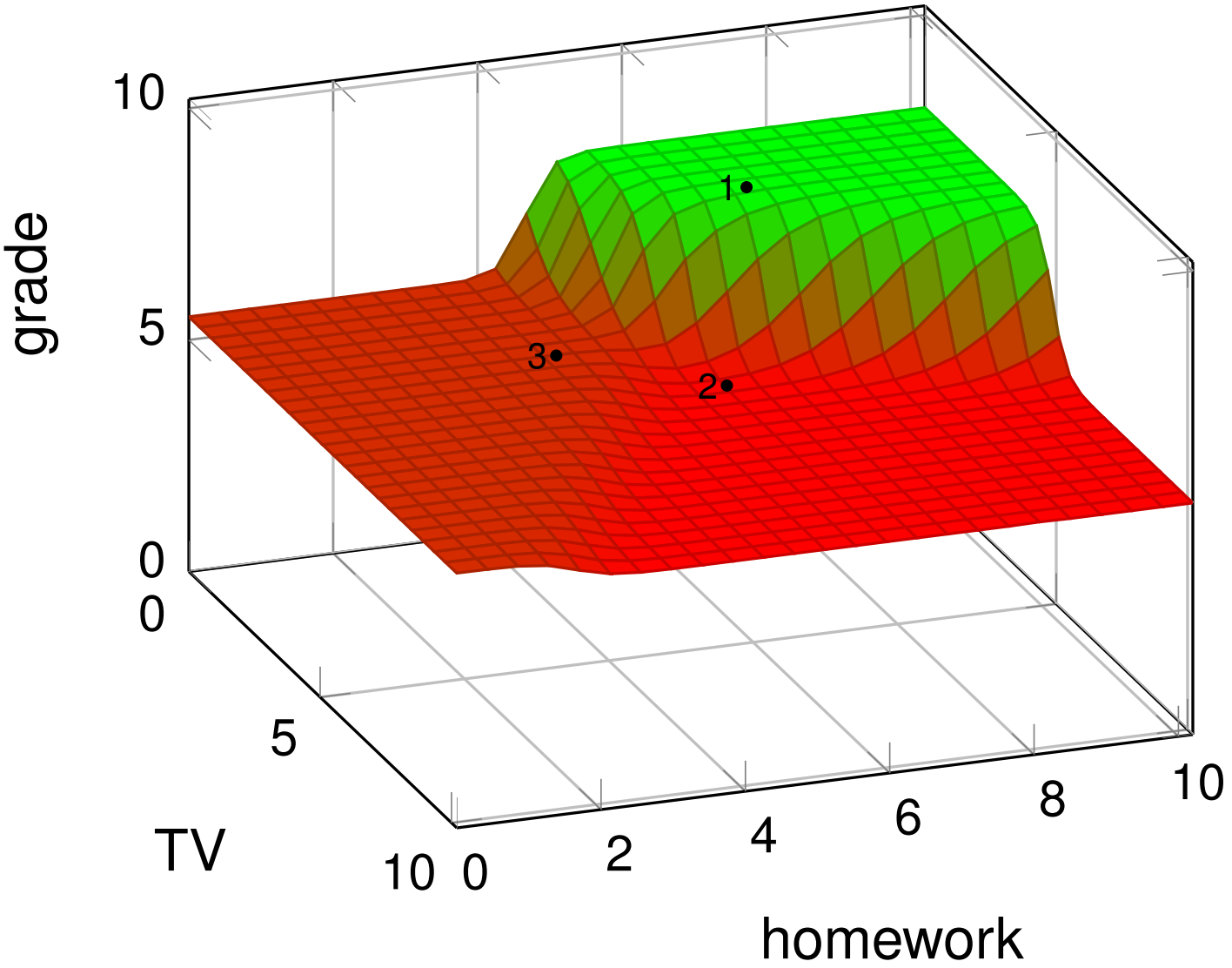
$$y(x) = \frac{\sum_{i=1}^{1} y_i \cdot \exp(-\|x - x_i\|^2)}{\sum_{i=1}^{1} \exp(-\|x - x_i\|^2)}$$



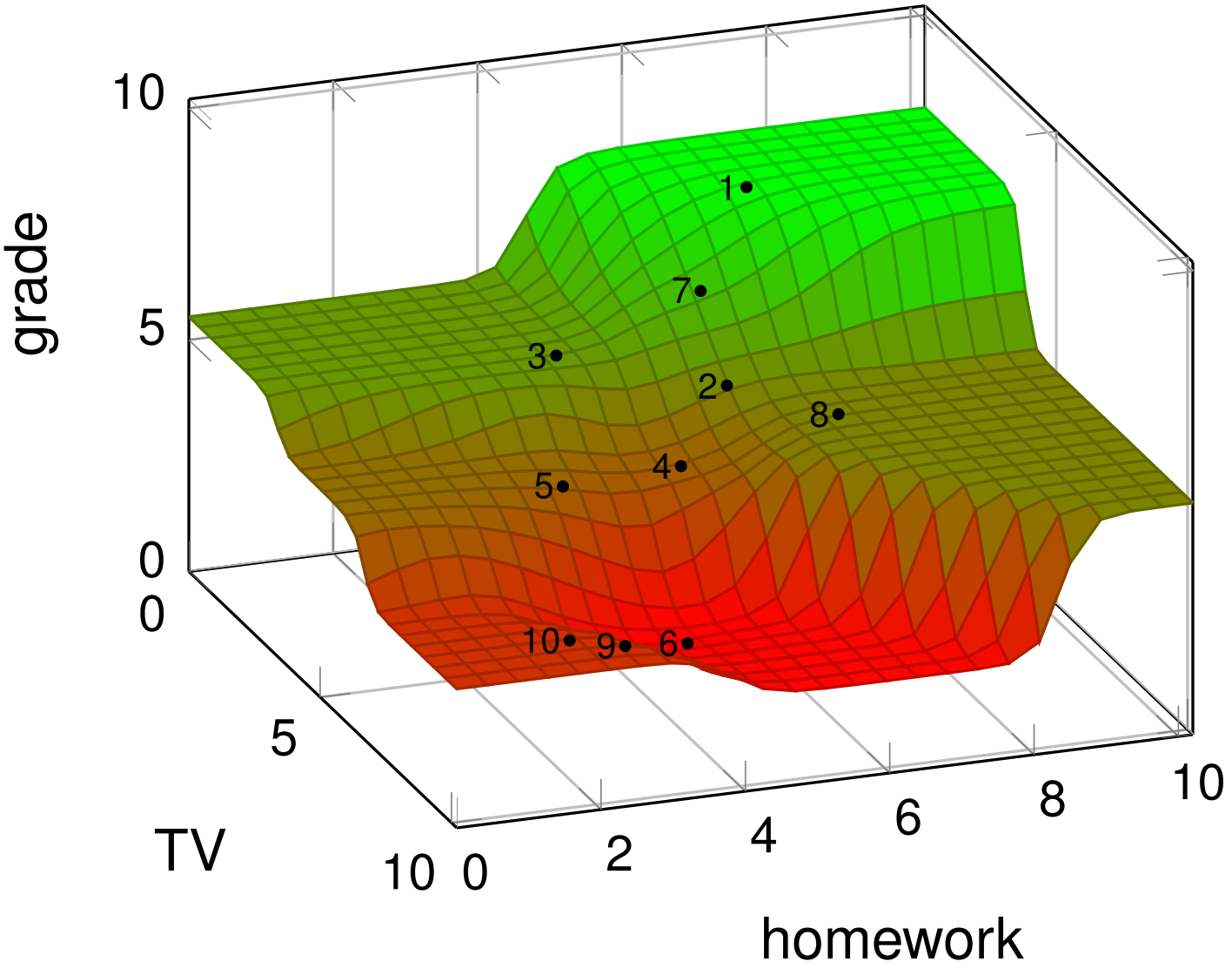
$$y(x) = \frac{\sum_{i=1}^{2} y_i \cdot \exp(-\|x - x_i\|^2)}{\sum_{i=1}^{2} \exp(-\|x - x_i\|^2)}$$



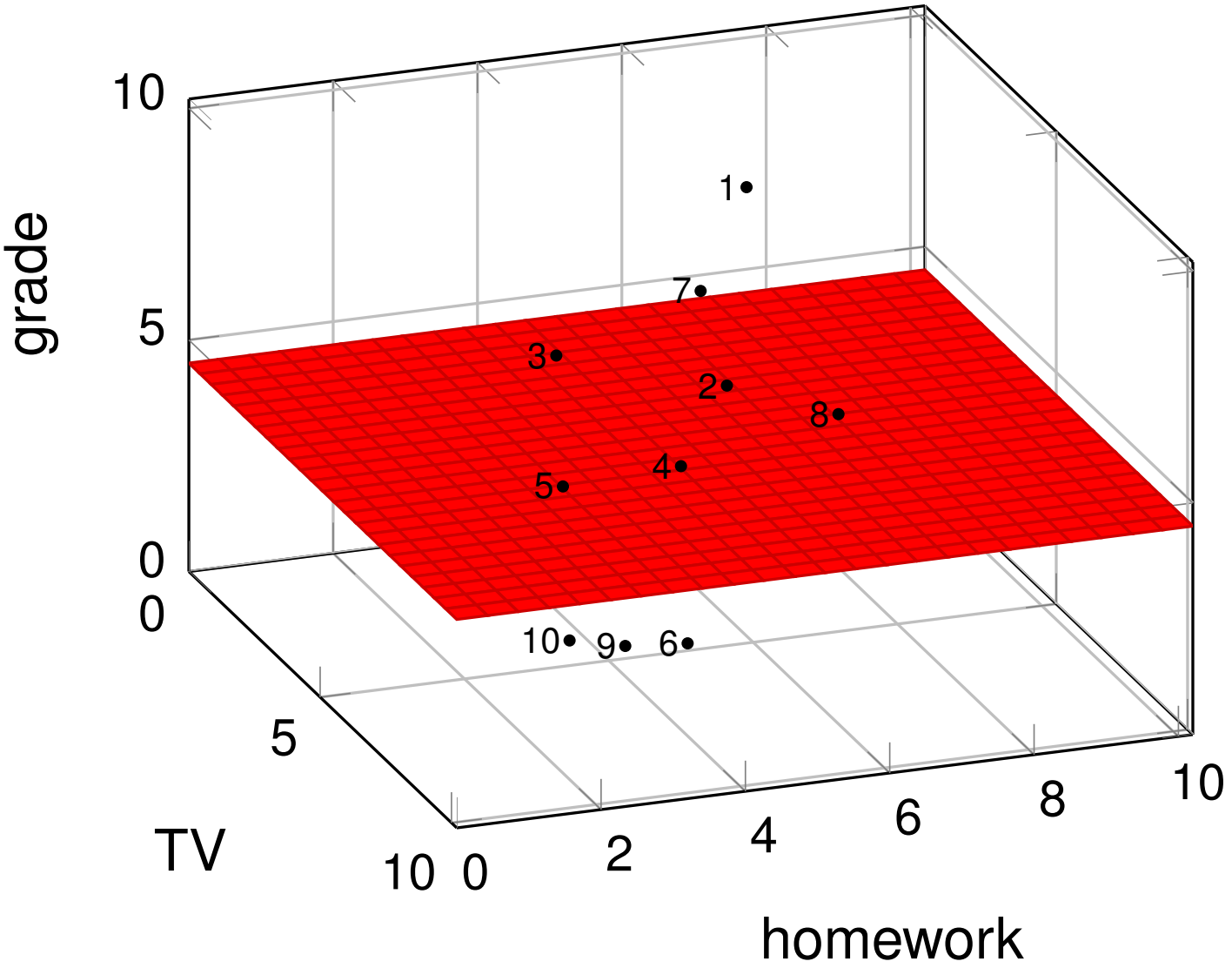
$$y(x) = \frac{\sum_{i=1}^{3} y_i \cdot \exp(-\|x - x_i\|^2)}{\sum_{i=1}^{3} \exp(-\|x - x_i\|^2)}$$



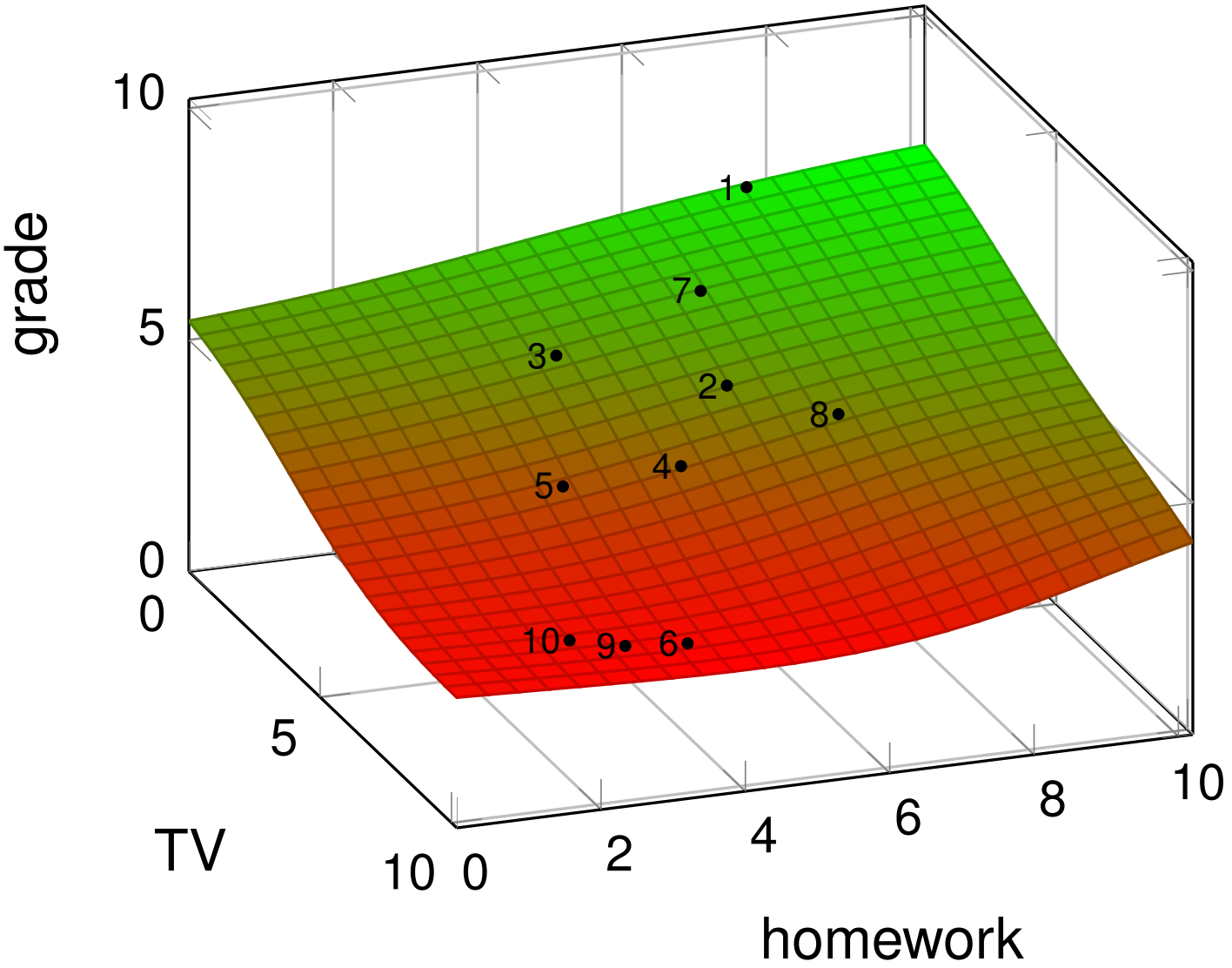
$$y(x) = \frac{\sum_{i=1}^{10} y_i \cdot \exp(-\|x - x_i\|^2)}{\sum_{i=1}^{10} \exp(-\|x - x_i\|^2)}$$



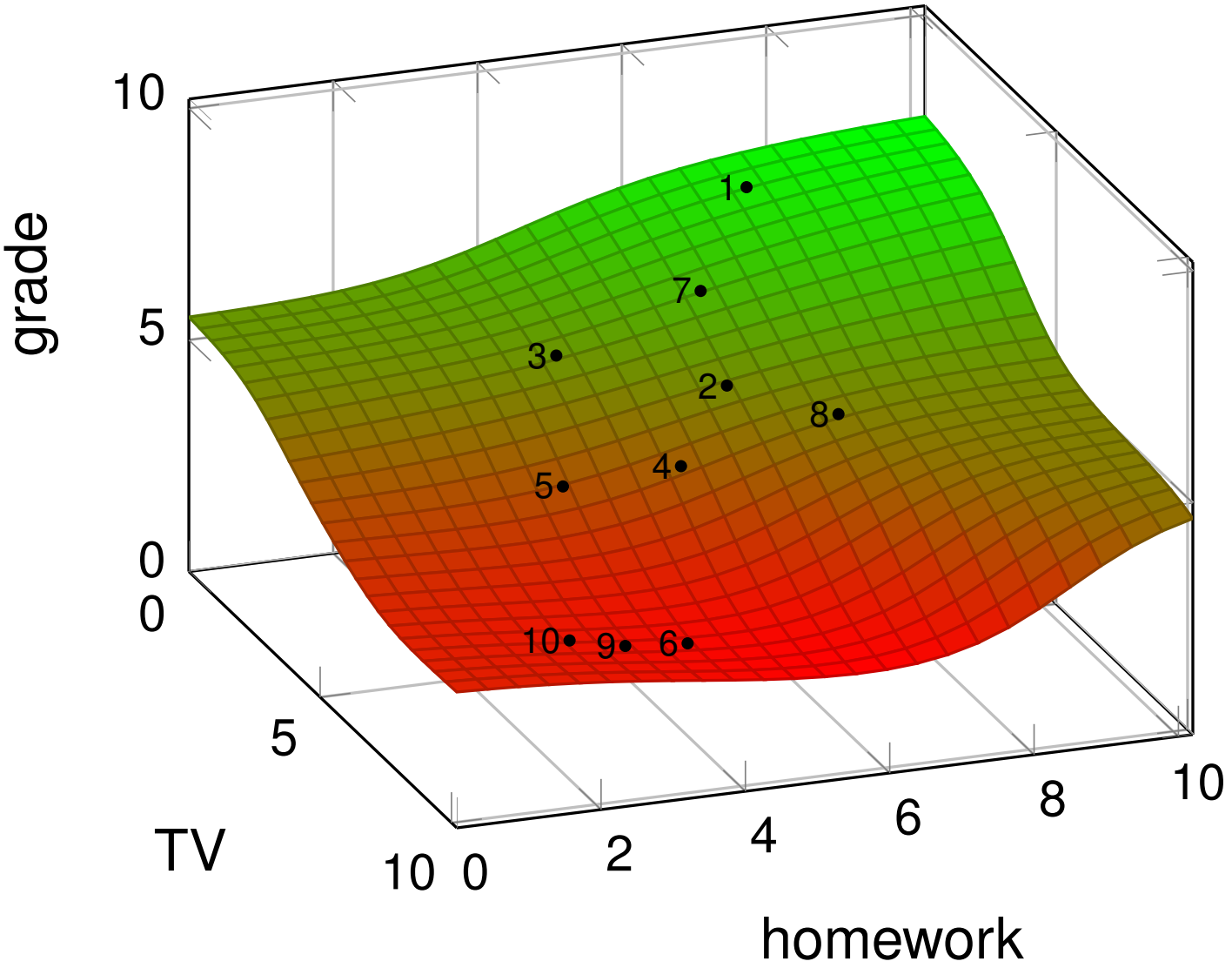
$$y(x) = \frac{\sum_{i=1}^{10} y_i \cdot \exp(-c\|x-x_i\|^2)}{\sum_{i=1}^{10} \exp(-c \cdot \|x-x_i\|^2)}, c = 0.0$$



$$y(x) = \frac{\sum_{i=1}^{10} y_i \cdot \exp(-c\|x-x_i\|^2)}{\sum_{i=1}^{10} \exp(-c \cdot \|x-x_i\|^2)}, c = 0.1$$



$$y(x) = \frac{\sum_{i=1}^{10} y_i \cdot \exp(-c\|x-x_i\|^2)}{\sum_{i=1}^{10} \exp(-c \cdot \|x-x_i\|^2)}, c = 0.2$$



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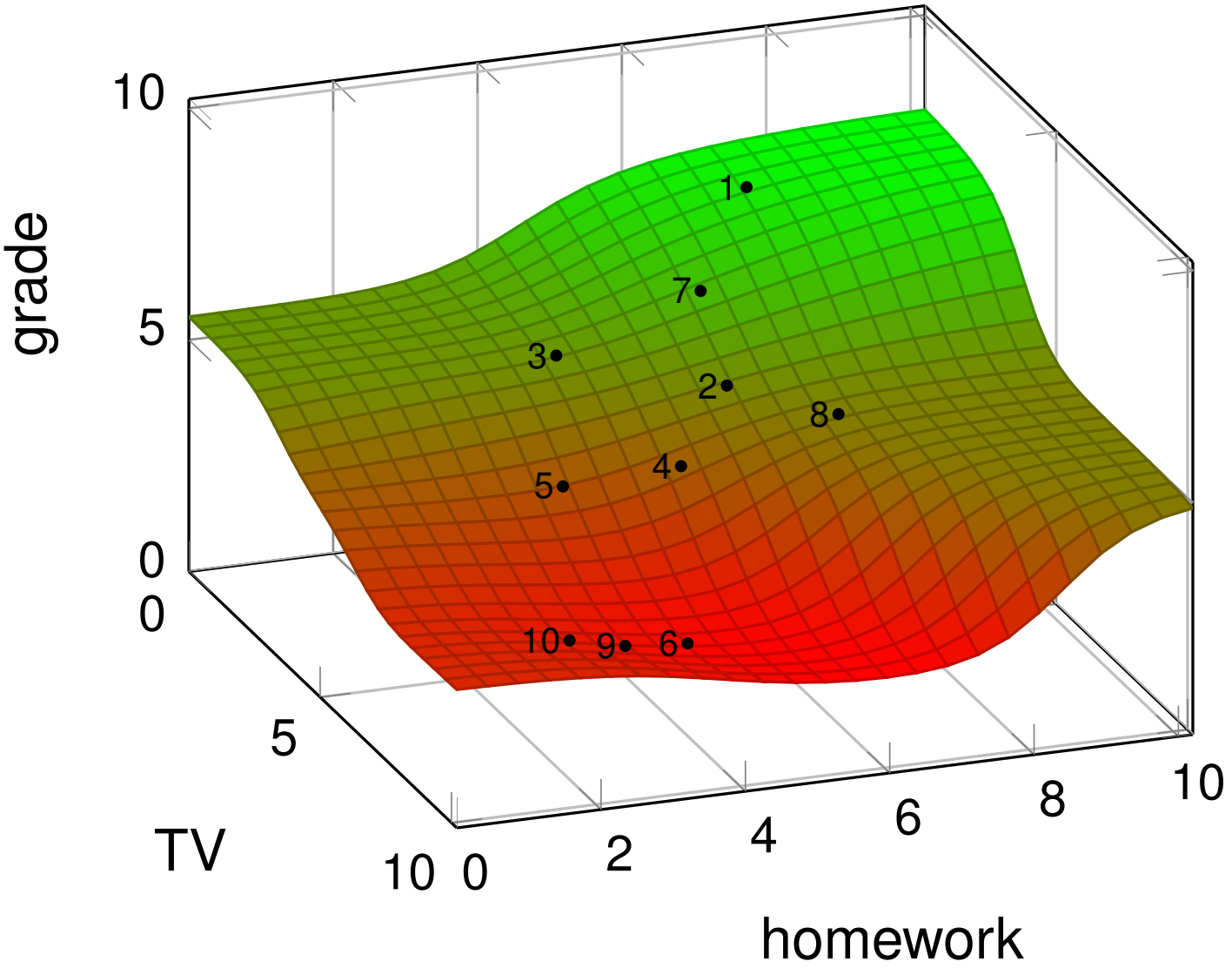
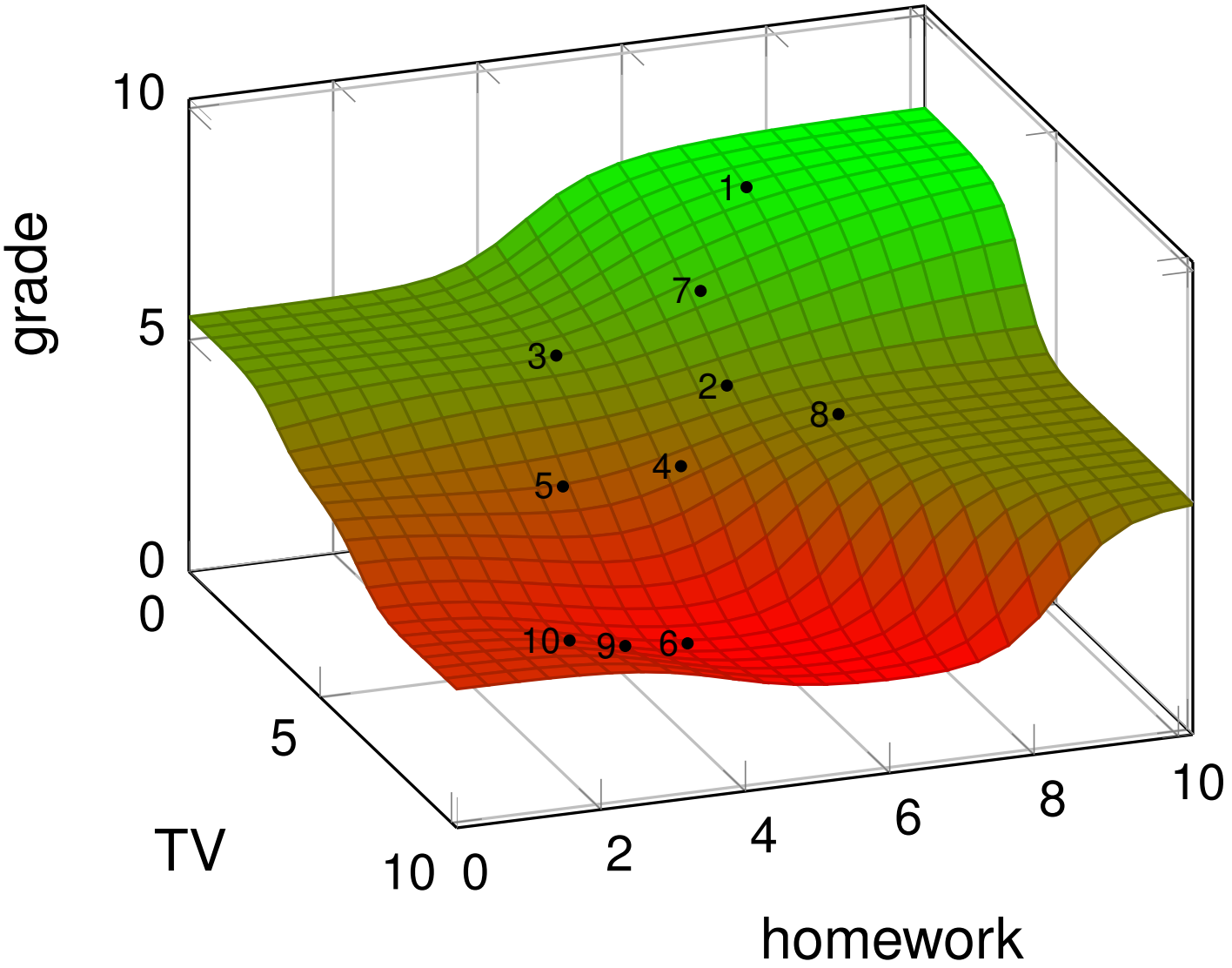
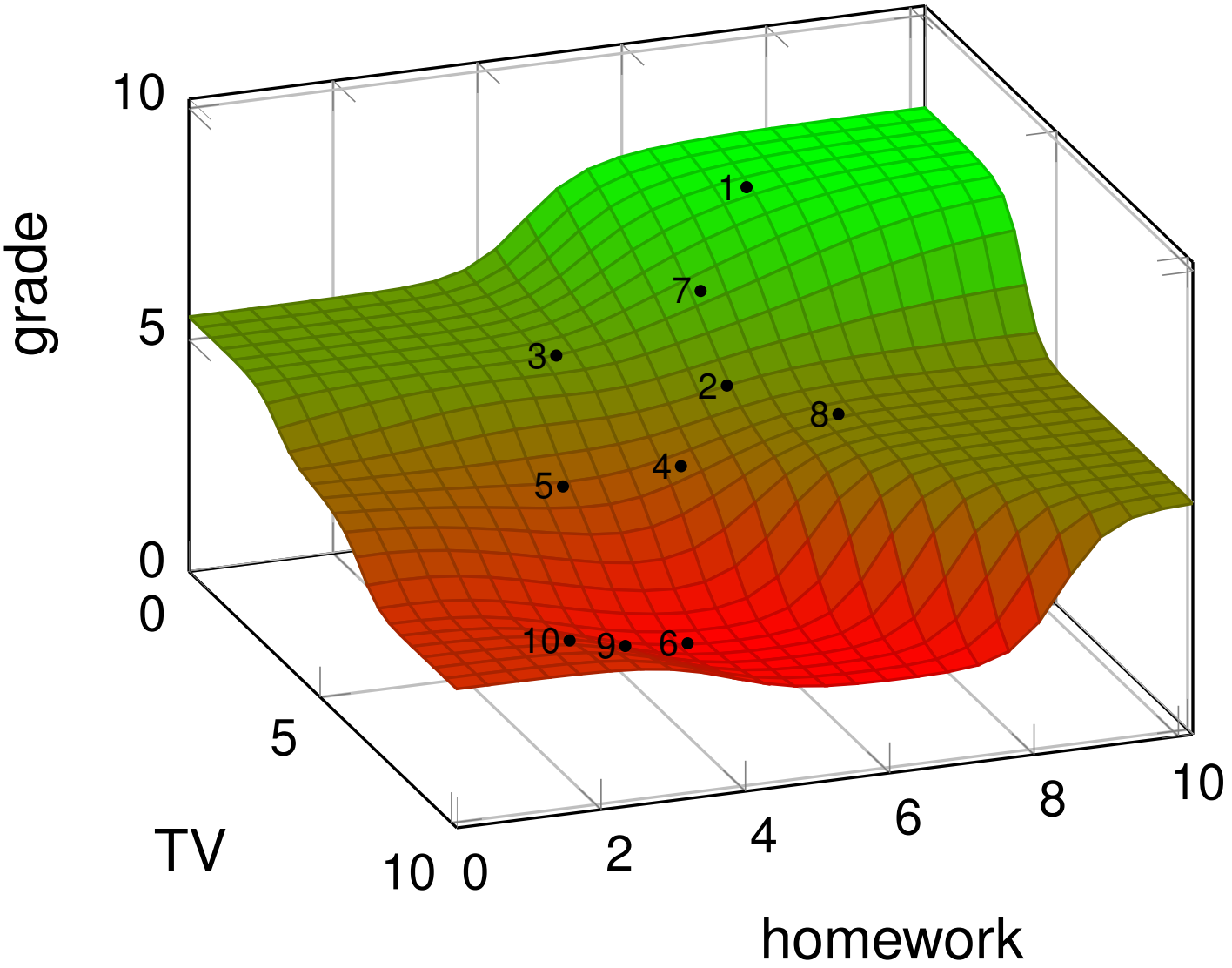


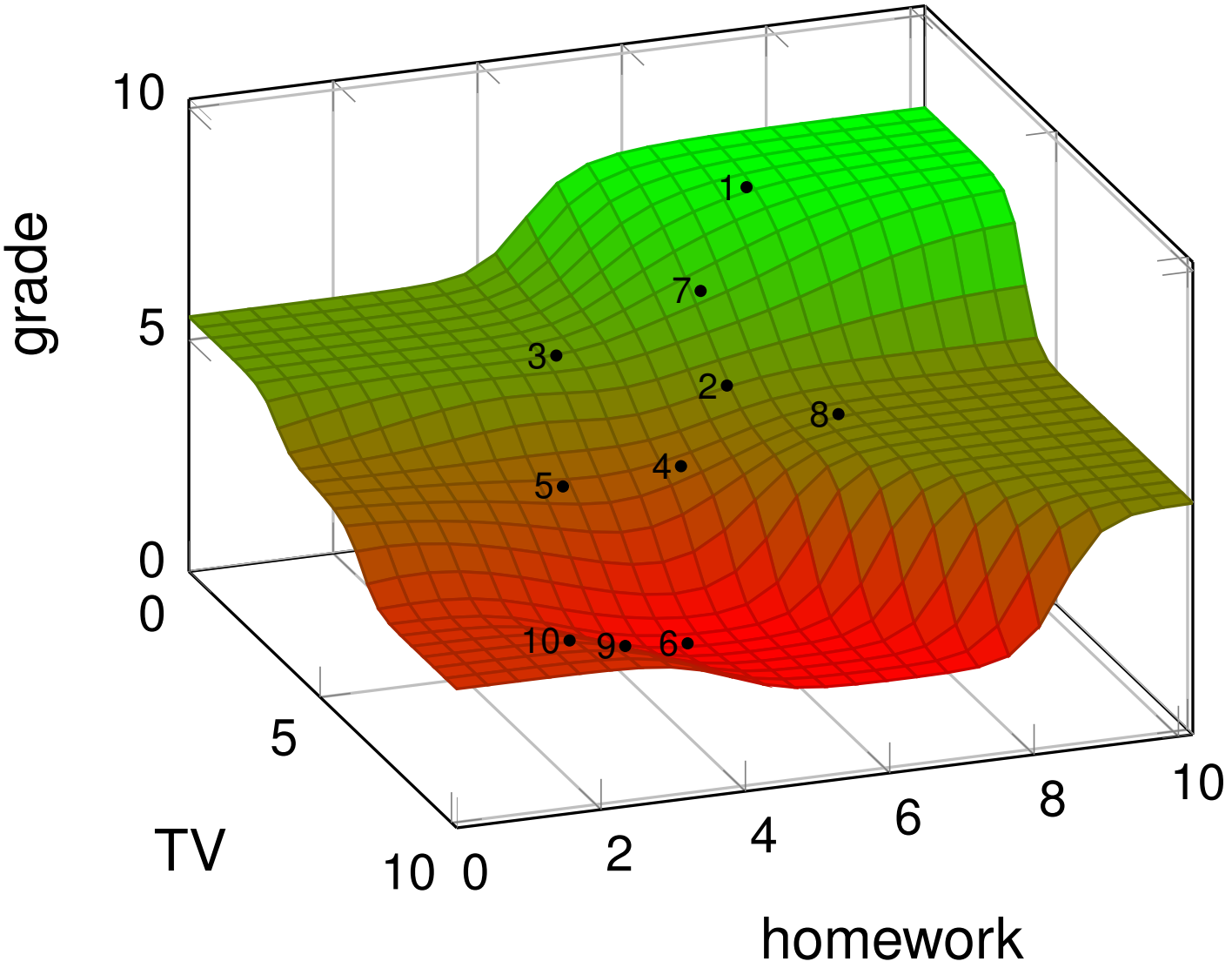
$$y(x) = \frac{\sum_{i=1}^{10} y_i \cdot \exp(-c\|x-x_i\|^2)}{\sum_{i=1}^{10} \exp(-c \cdot \|x-x_i\|^2)}, c = 0.4$$



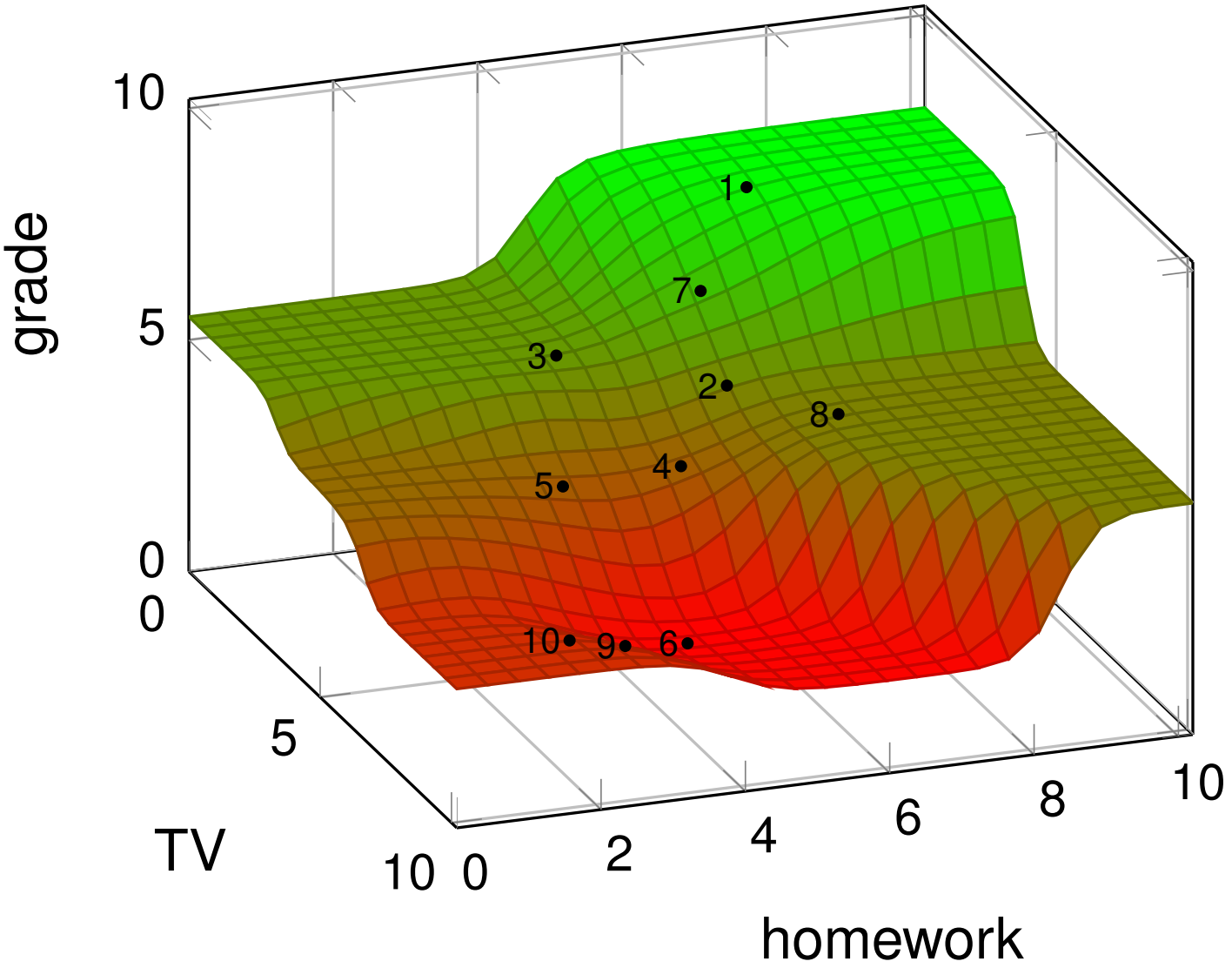
$$y(x) = \frac{\sum_{i=1}^{10} y_i \cdot \exp(-c\|x-x_i\|^2)}{\sum_{i=1}^{10} \exp(-c \cdot \|x-x_i\|^2)}, c = 0.5$$



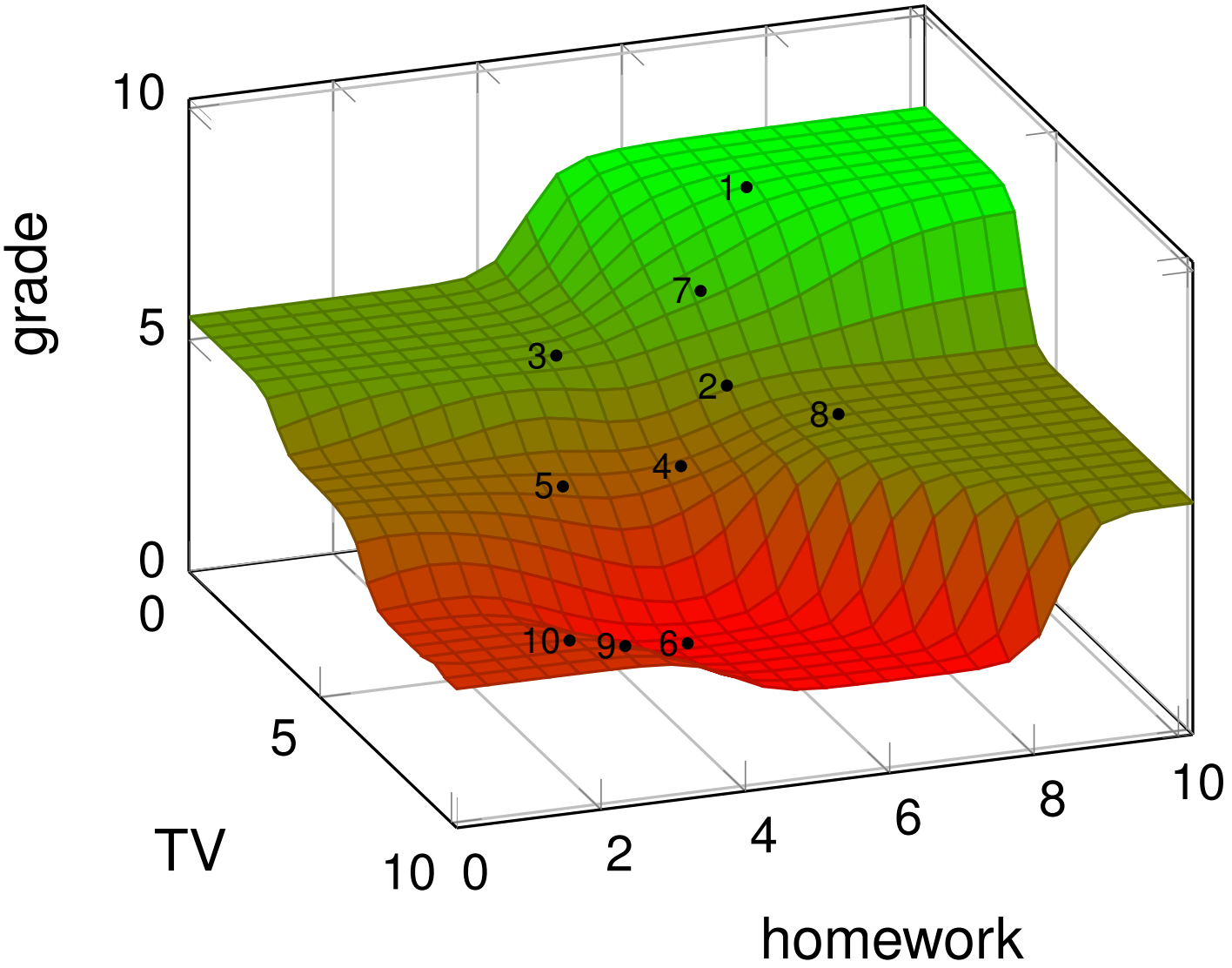
$$y(x) = \frac{\sum_{i=1}^{10} y_i \cdot \exp(-c\|x-x_i\|^2)}{\sum_{i=1}^{10} \exp(-c \cdot \|x-x_i\|^2)}, c = 0.6$$



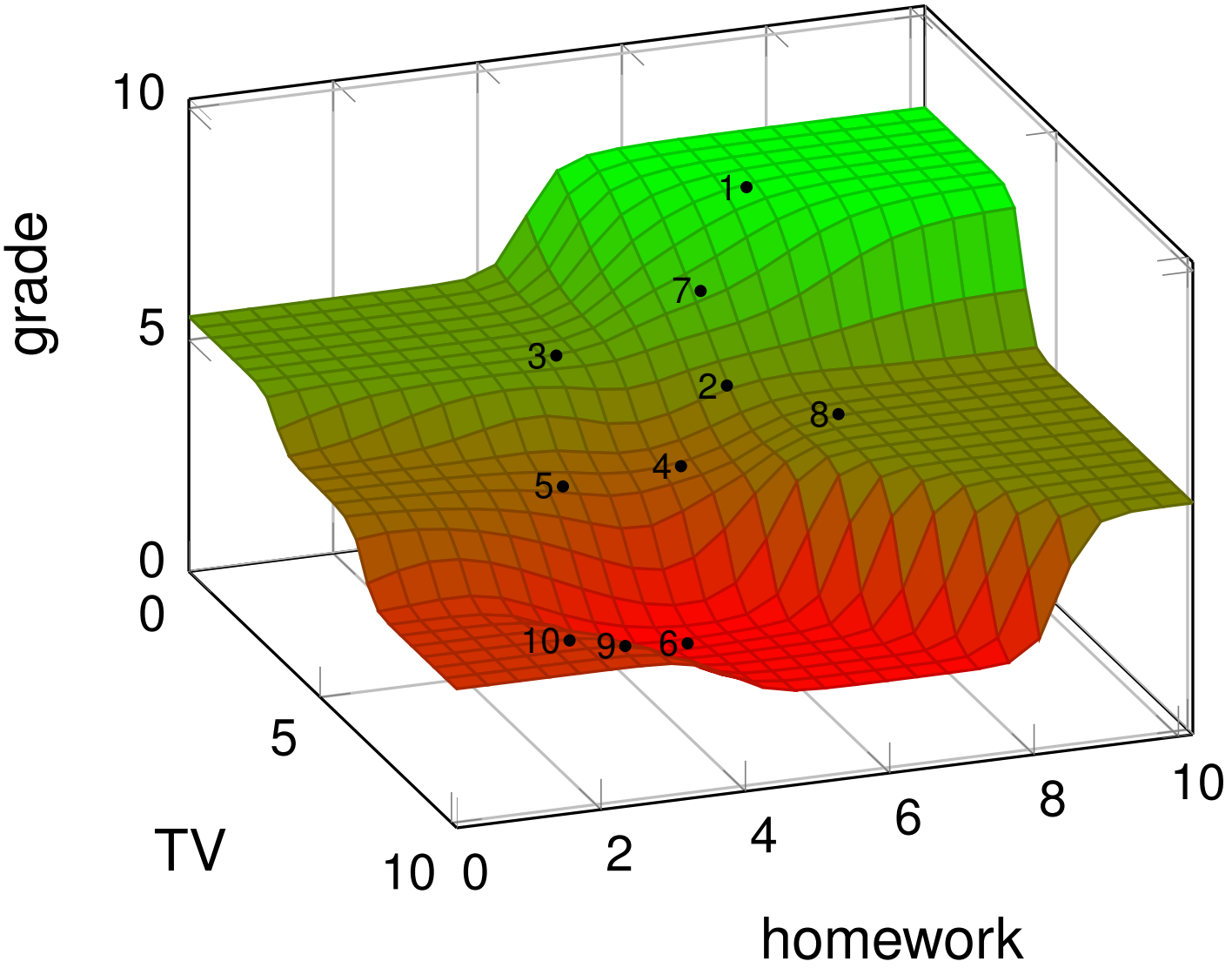
$$y(x) = \frac{\sum_{i=1}^{10} y_i \cdot \exp(-c\|x-x_i\|^2)}{\sum_{i=1}^{10} \exp(-c \cdot \|x-x_i\|^2)}, c = 0.7$$



$$y(x) = \frac{\sum_{i=1}^{10} y_i \cdot \exp(-c\|x-x_i\|^2)}{\sum_{i=1}^{10} \exp(-c \cdot \|x-x_i\|^2)}, c = 0.8$$



$$y(x) = \frac{\sum_{i=1}^{10} y_i \cdot \exp(-c\|x-x_i\|^2)}{\sum_{i=1}^{10} \exp(-c \cdot \|x-x_i\|^2)}, c = 0.9$$



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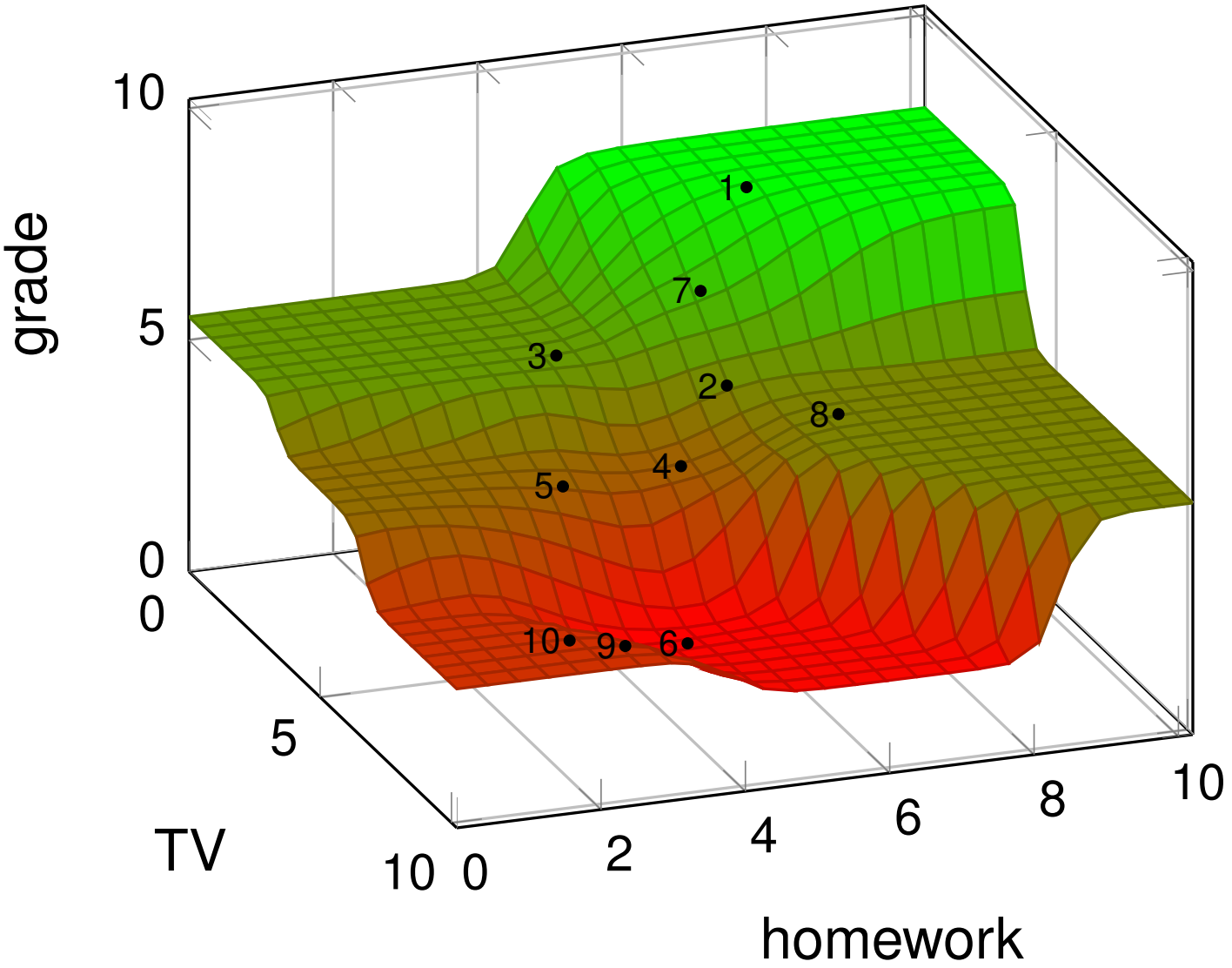
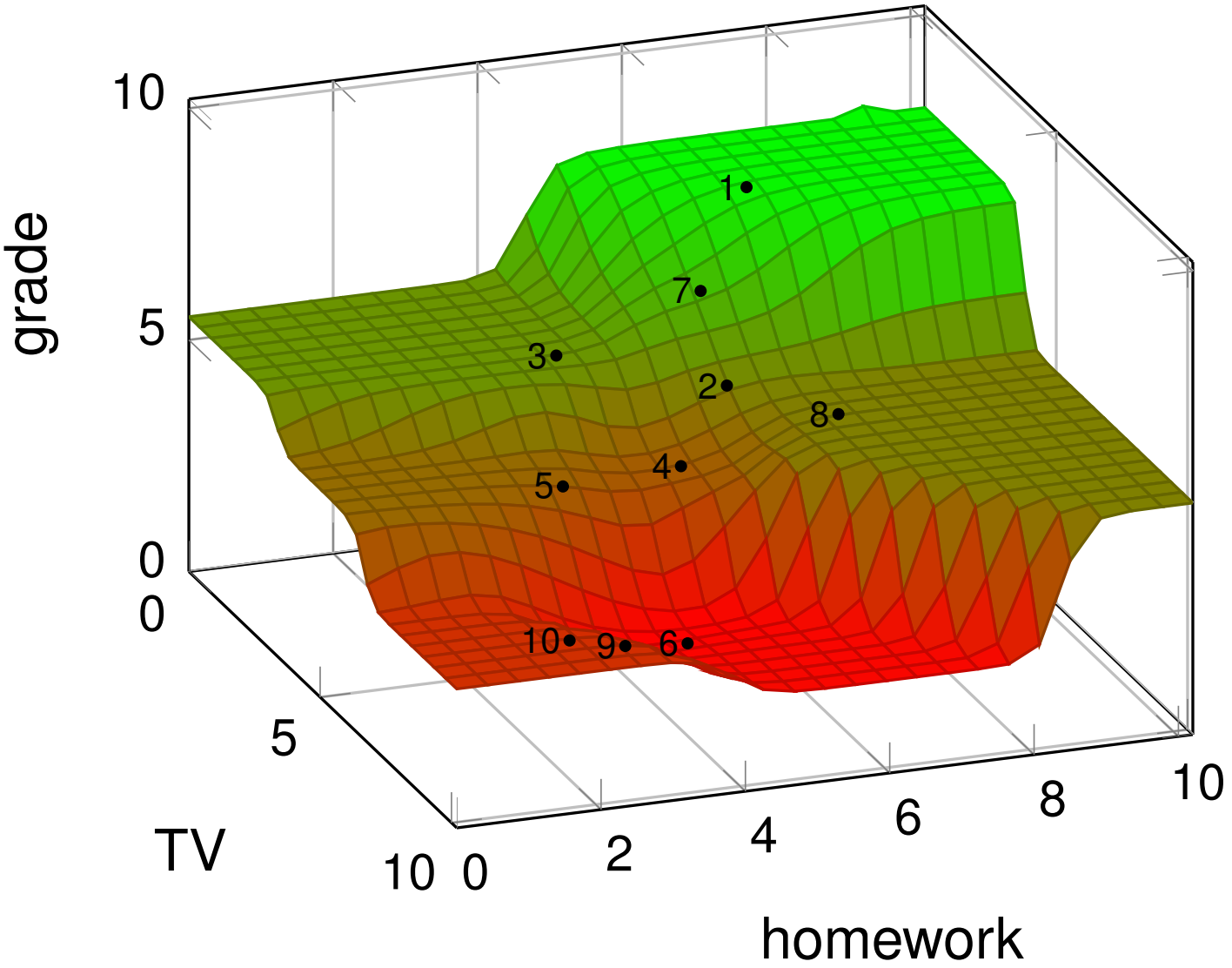


$$y(x) = \frac{\sum_{i=1}^{10} y_i \cdot \exp(-c\|x-x_i\|^2)}{\sum_{i=1}^{10} \exp(-c \cdot \|x-x_i\|^2)}, c = 1.1$$



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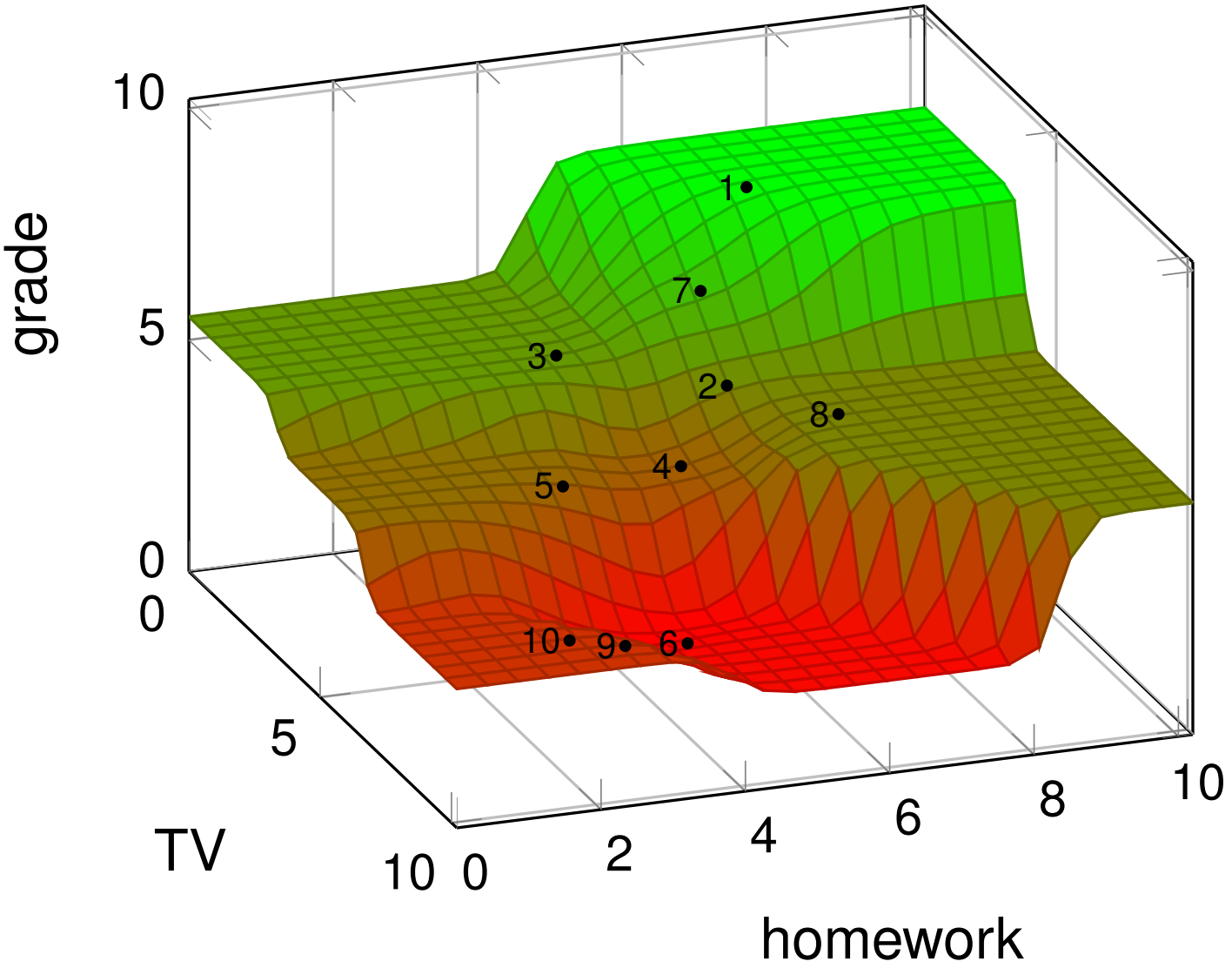

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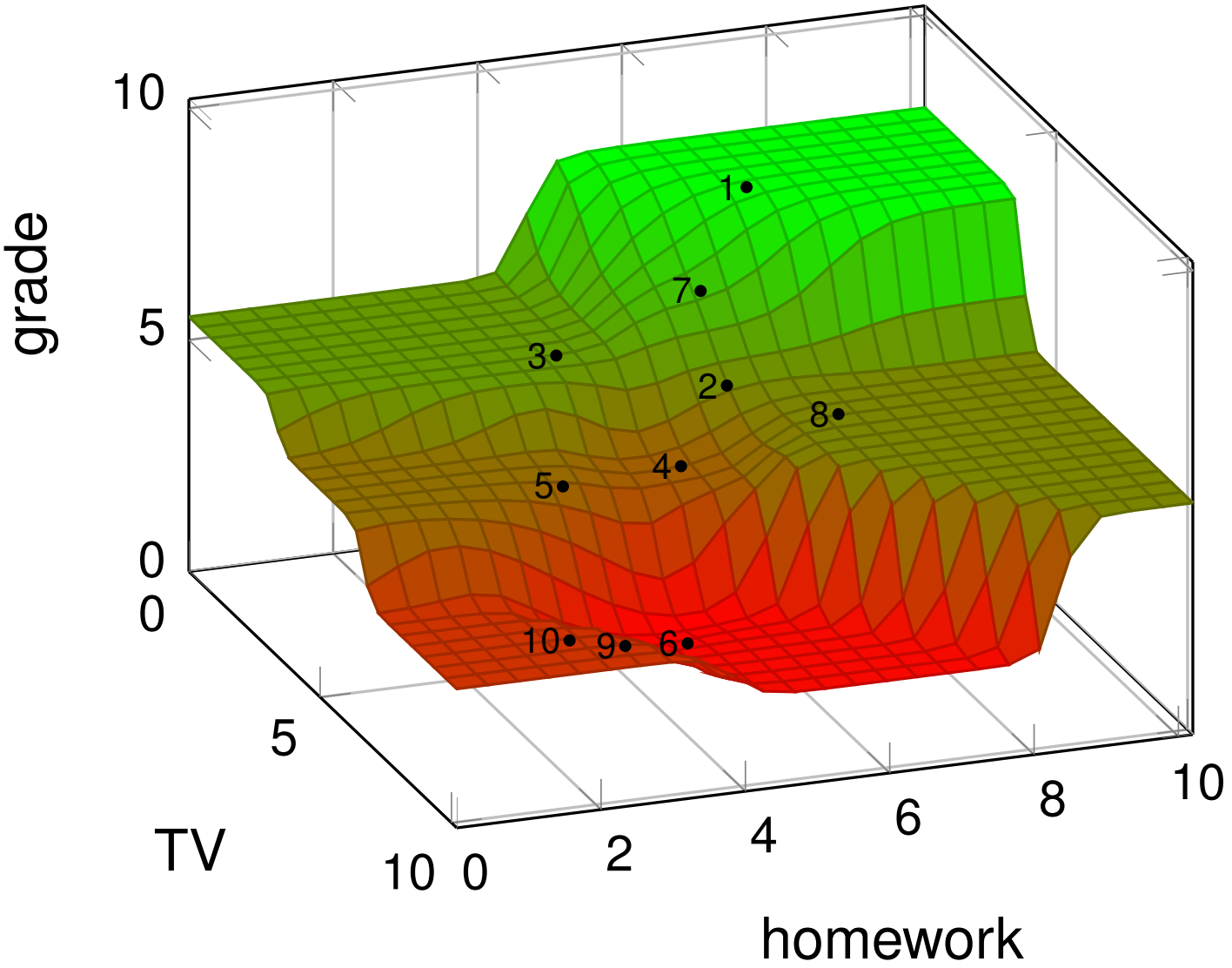

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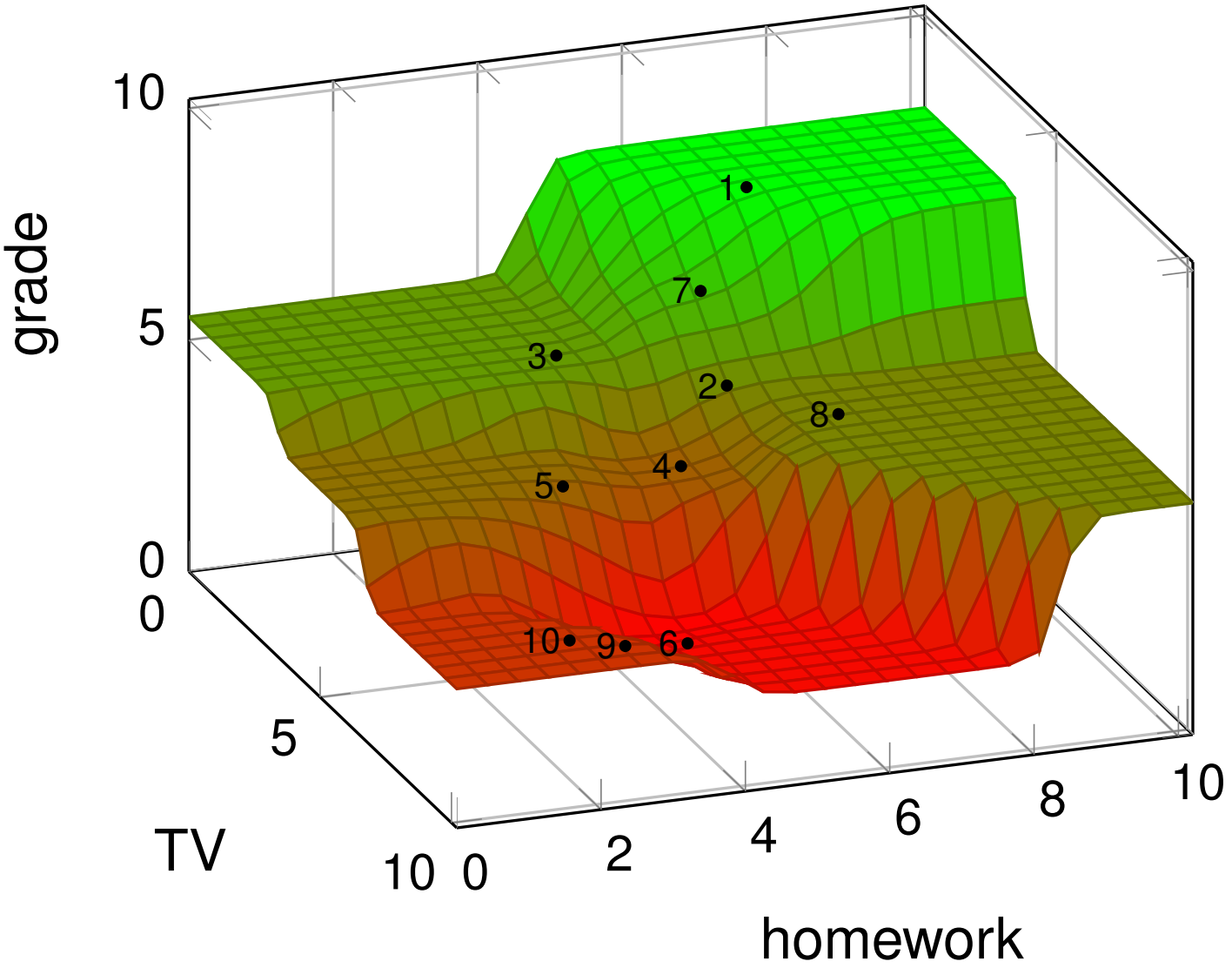

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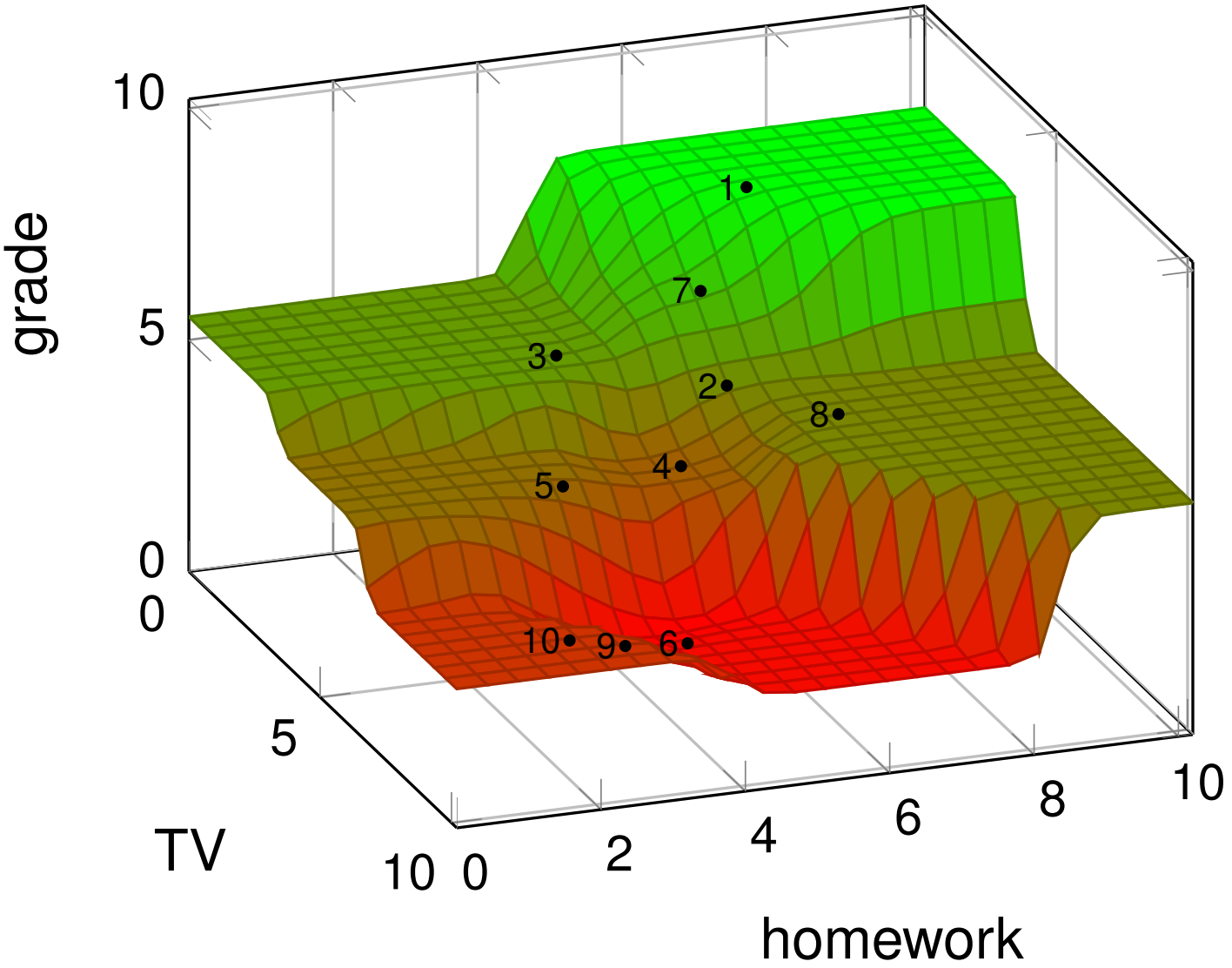

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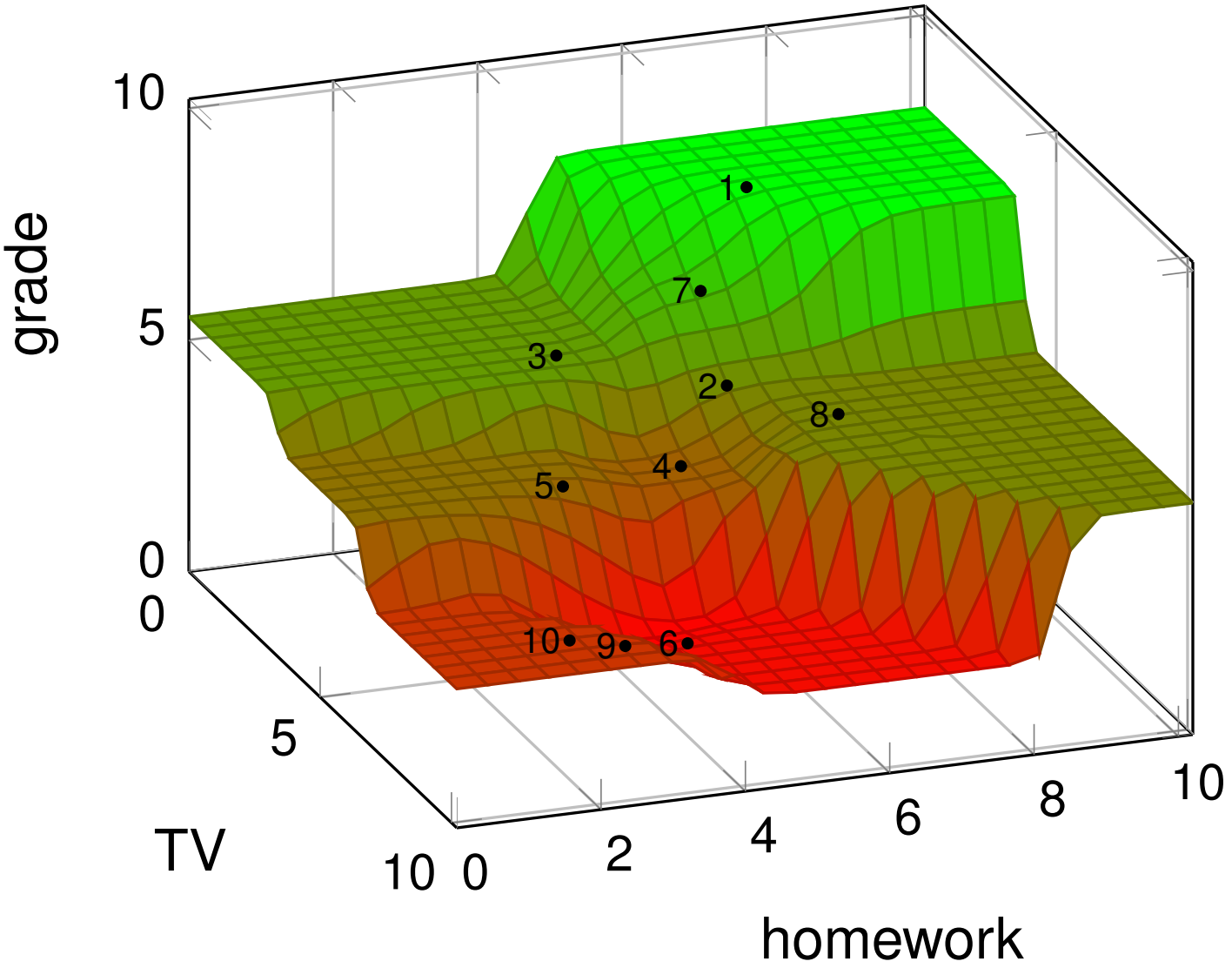

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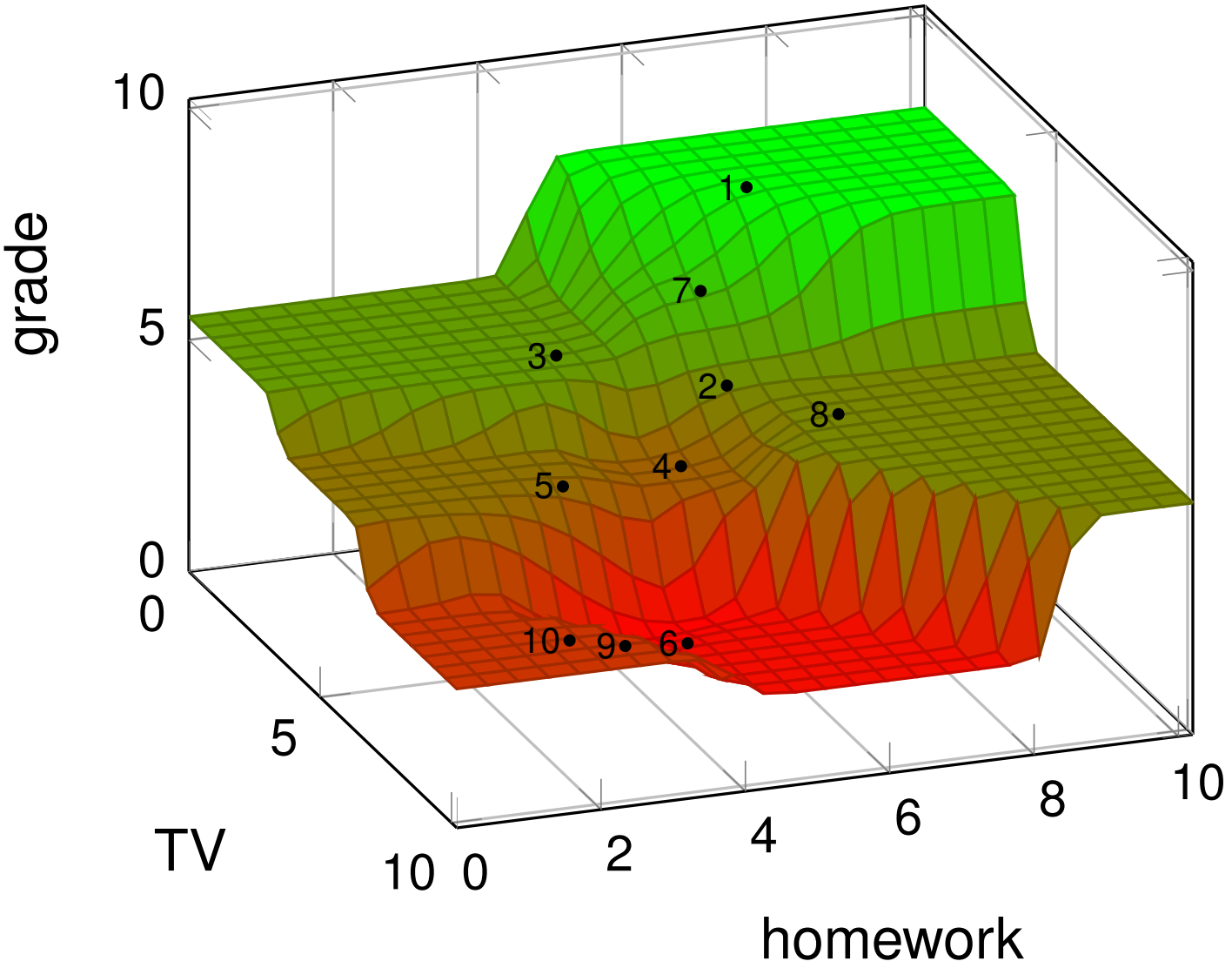

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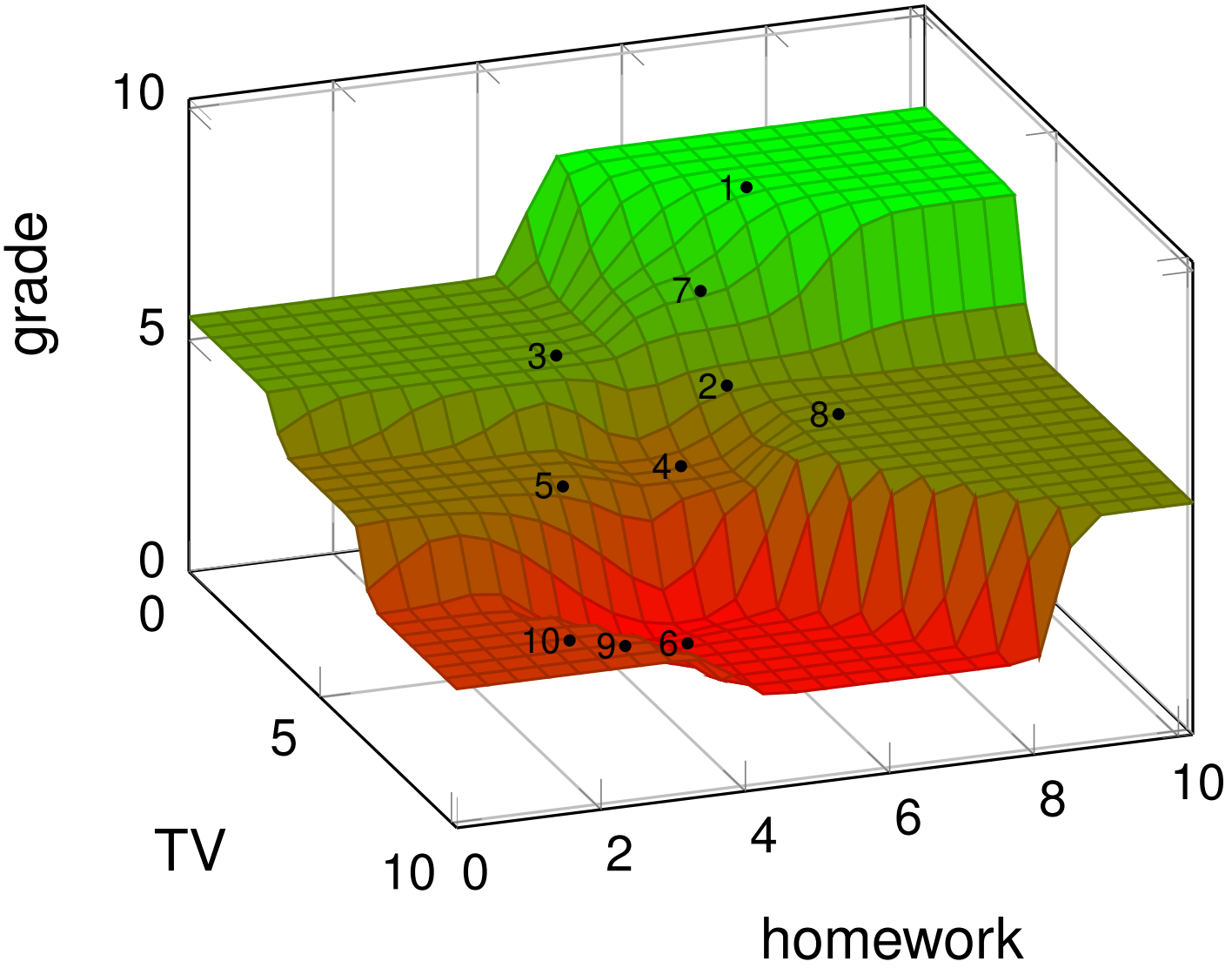

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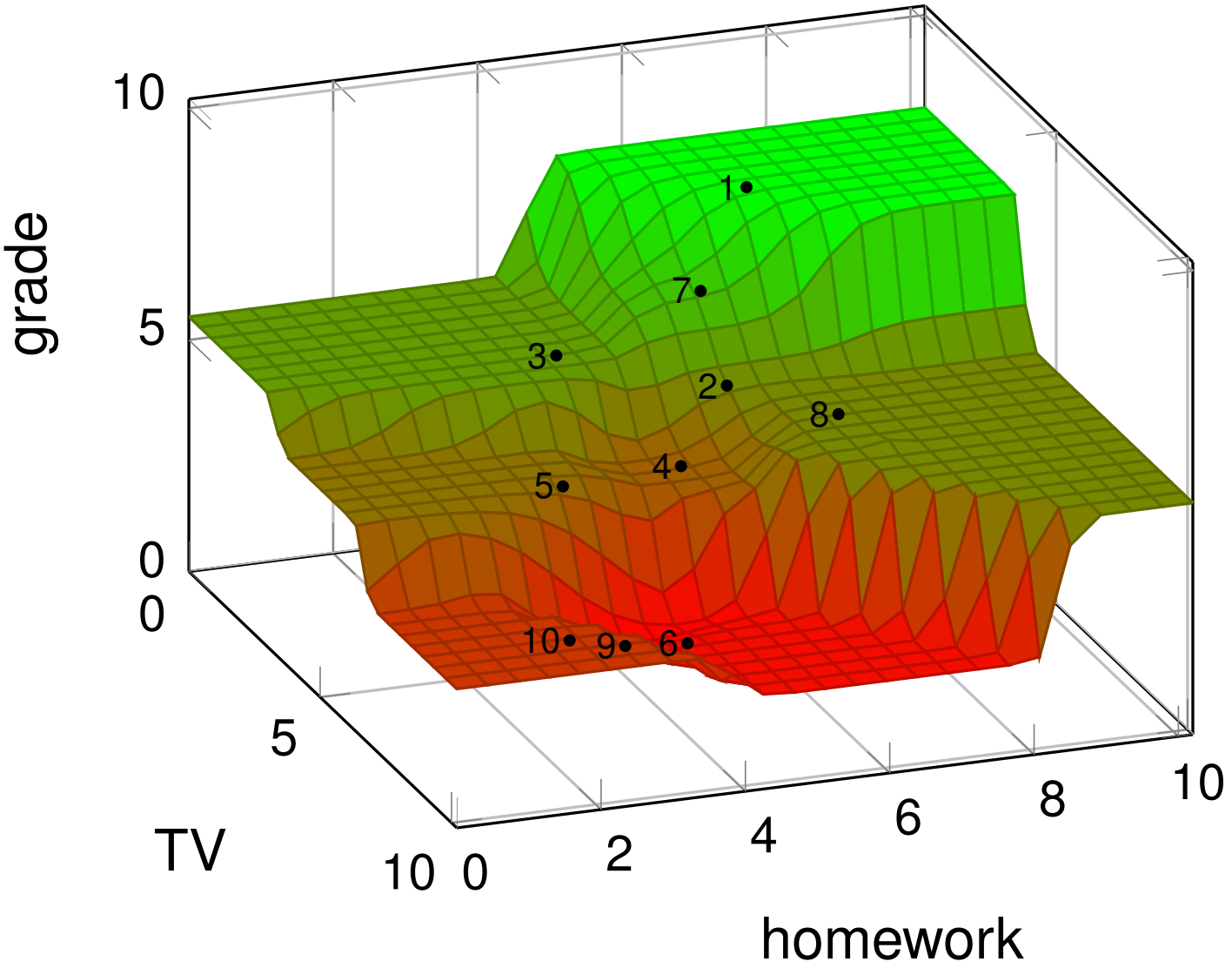

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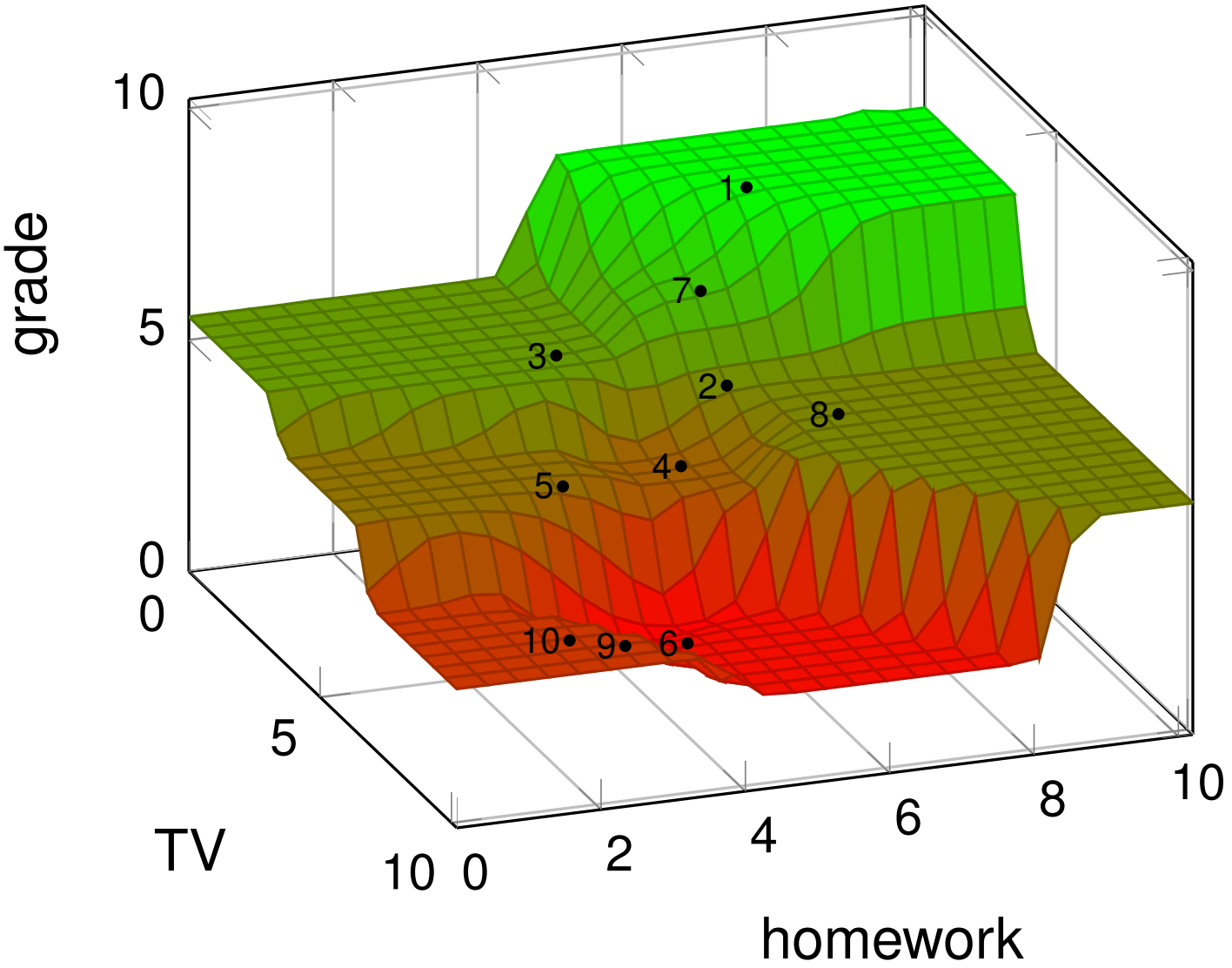

Coefficient of Determination

How to figure out whether our regression model is good? Need a quantity!

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R^2 (coefficient of determination)

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$\overline{y} = 4.5$, $SS_{tot} = 35.5$

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R^2 for our 3 Models

- M1: Use TV to predict exams: $SS_{res} = 7.91 \Rightarrow R^2 = 0.777$
- M2: Use homework to predict exams: $SS_{res} = 18.93$

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- M3: TV & homework to predict exams: $SS_{res} = 7.69$

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Digression: Polynomial Regression Tasks (1/2)

In some learning problems, a polynomial predictor may be more suitable:

$$p(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n.$$

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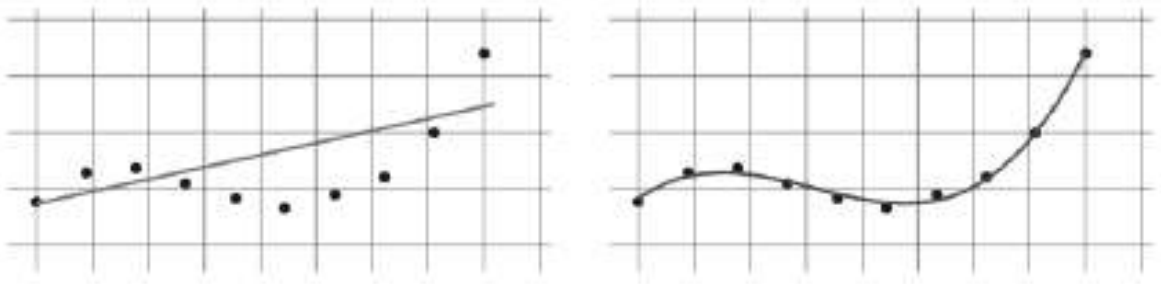

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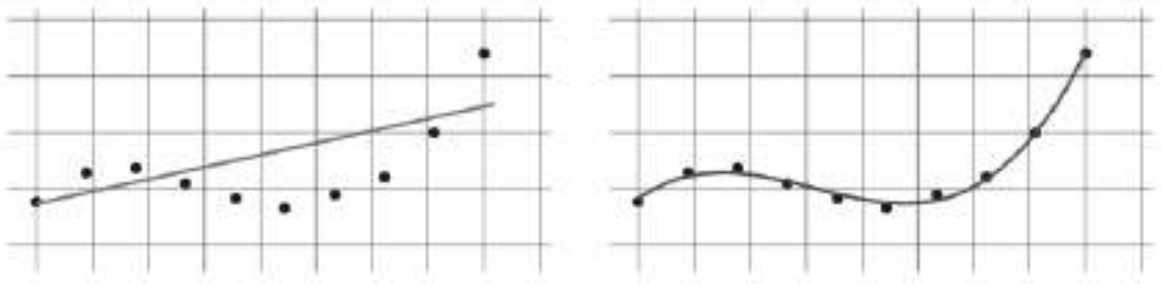

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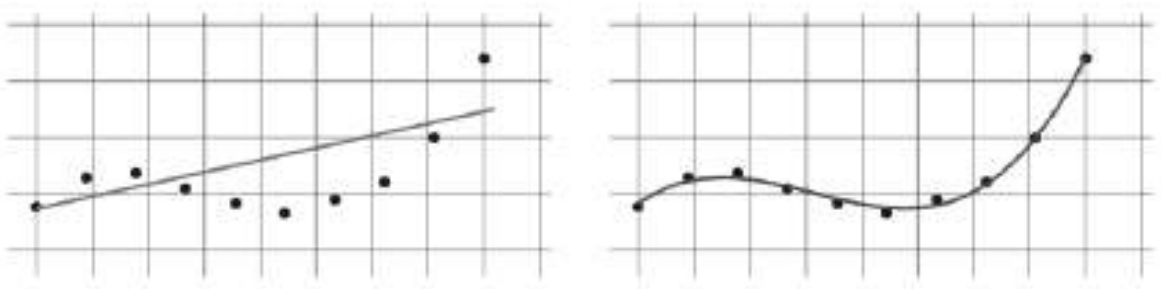

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How can we learn these coefficients? (looks much harder than linear case!)

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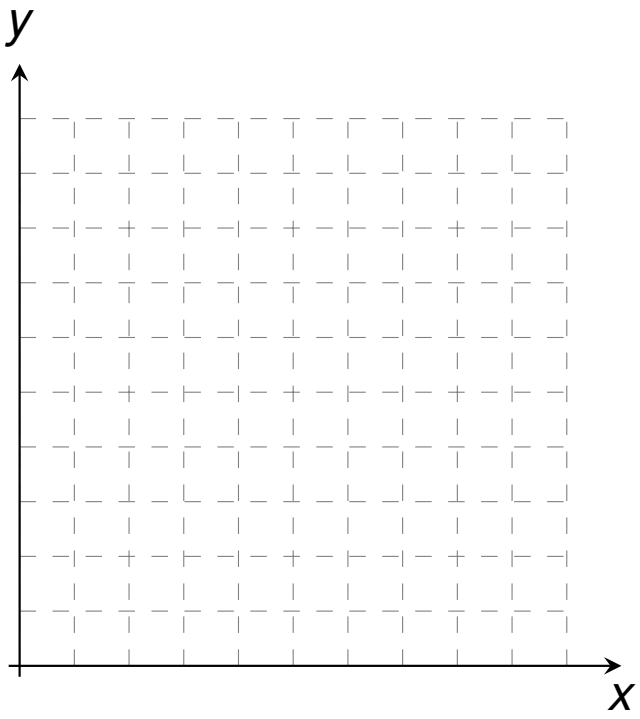

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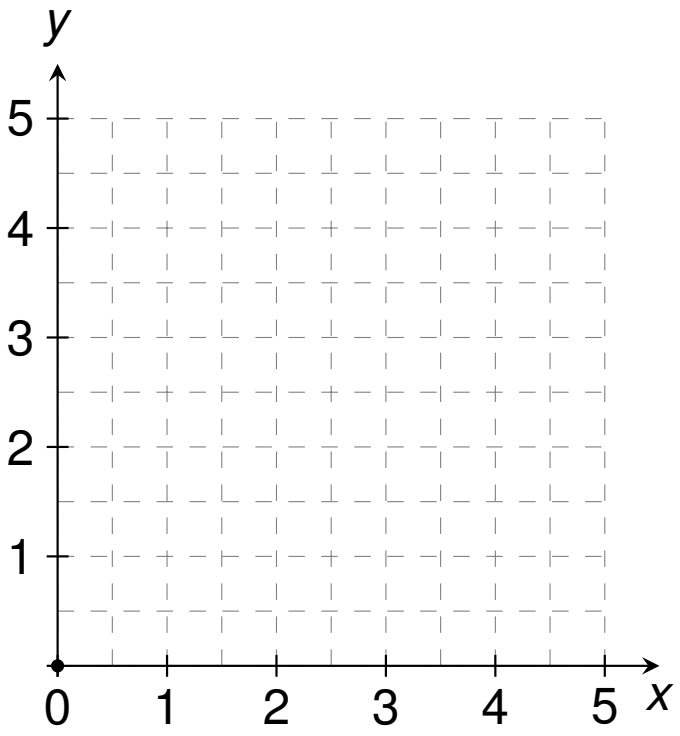

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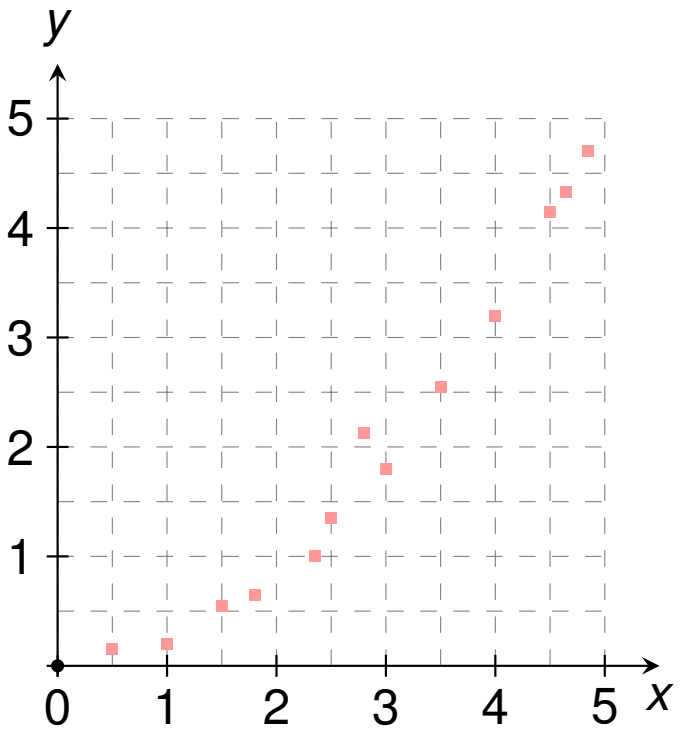

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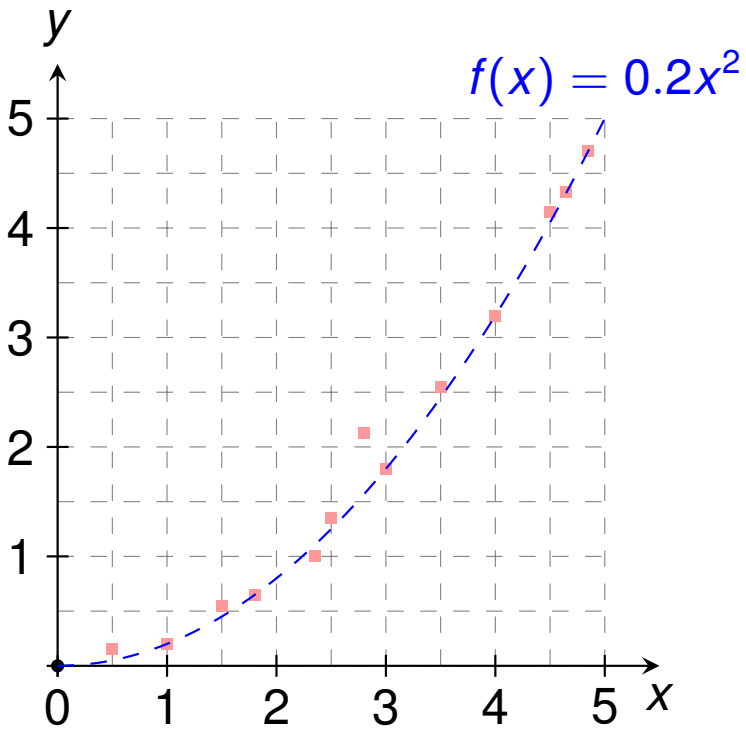

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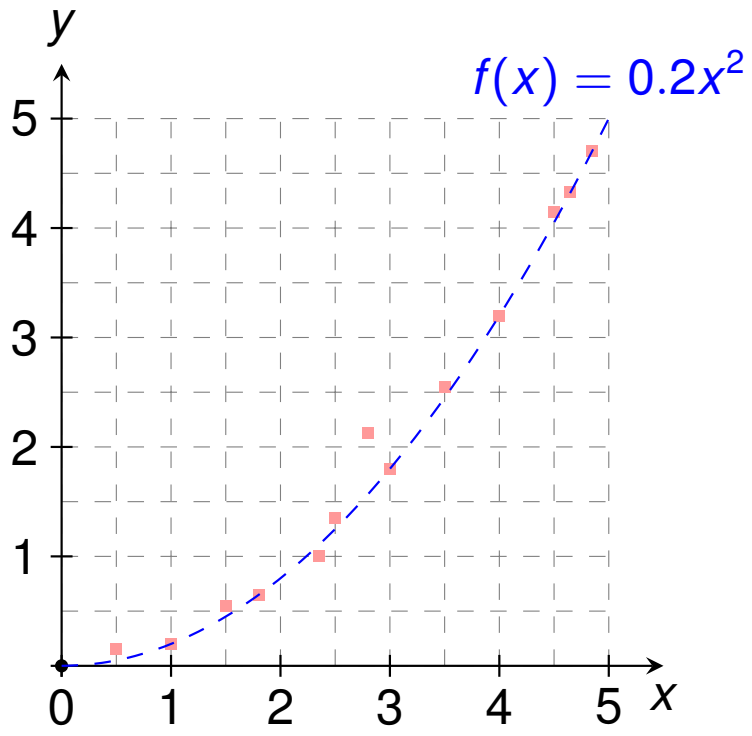

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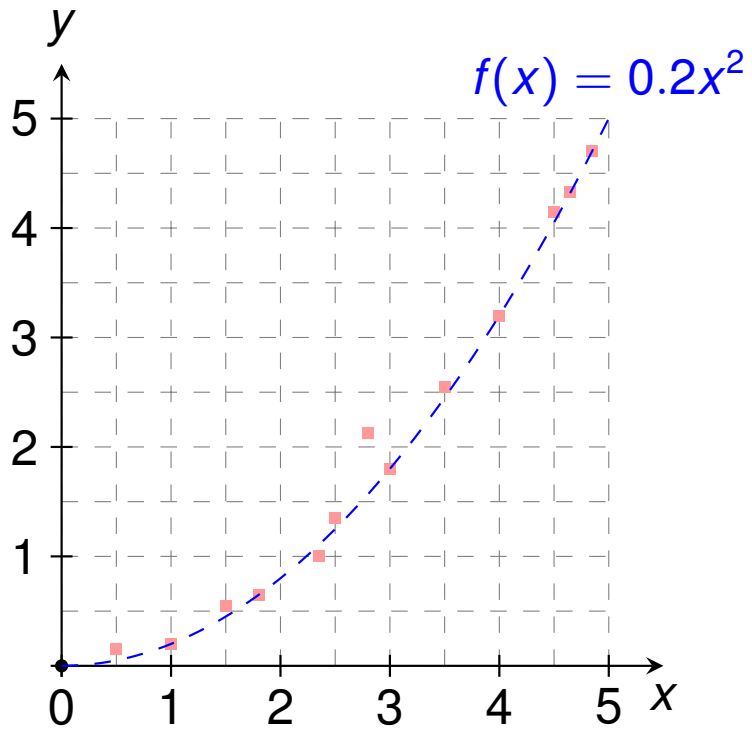

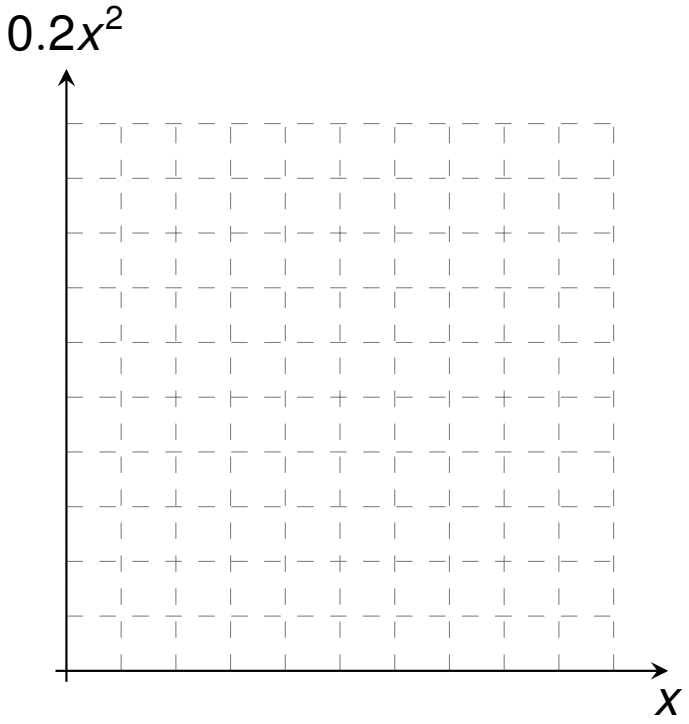

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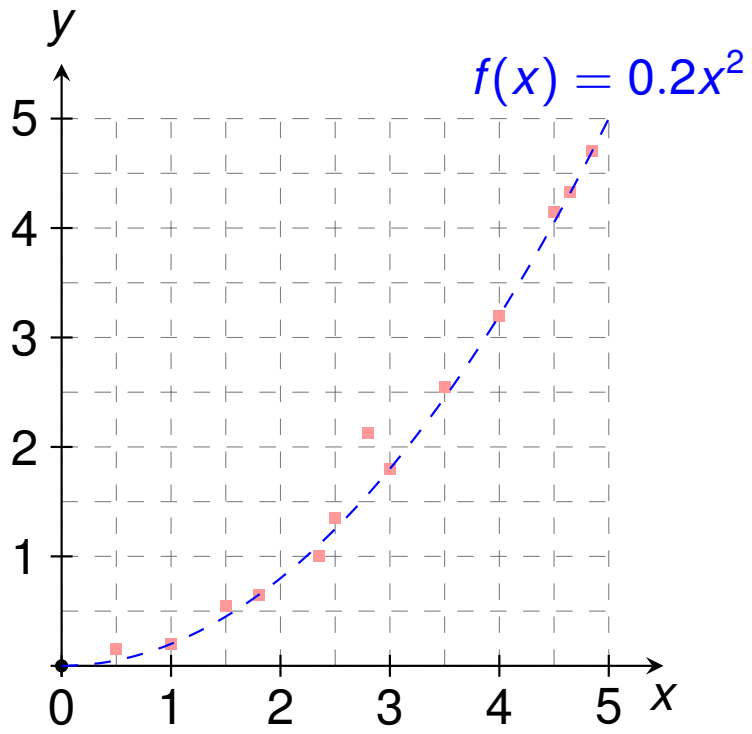

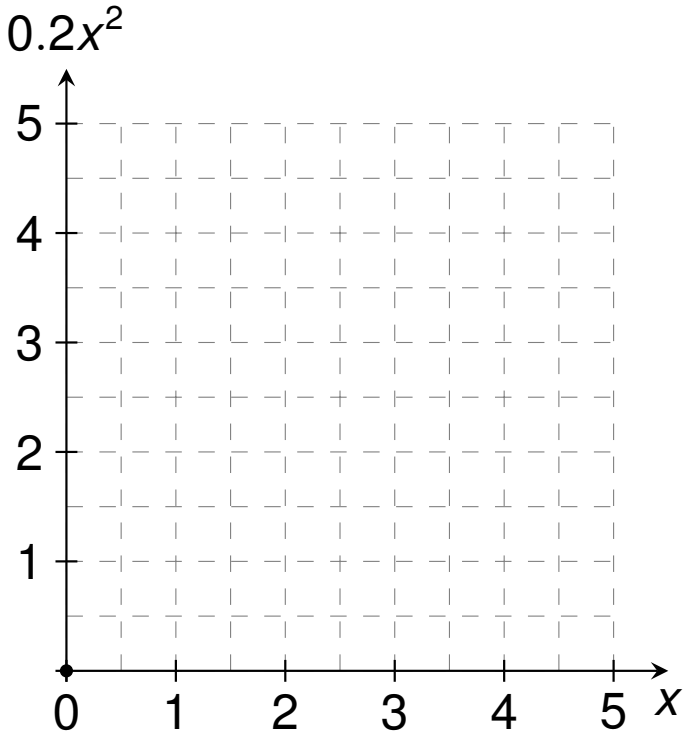

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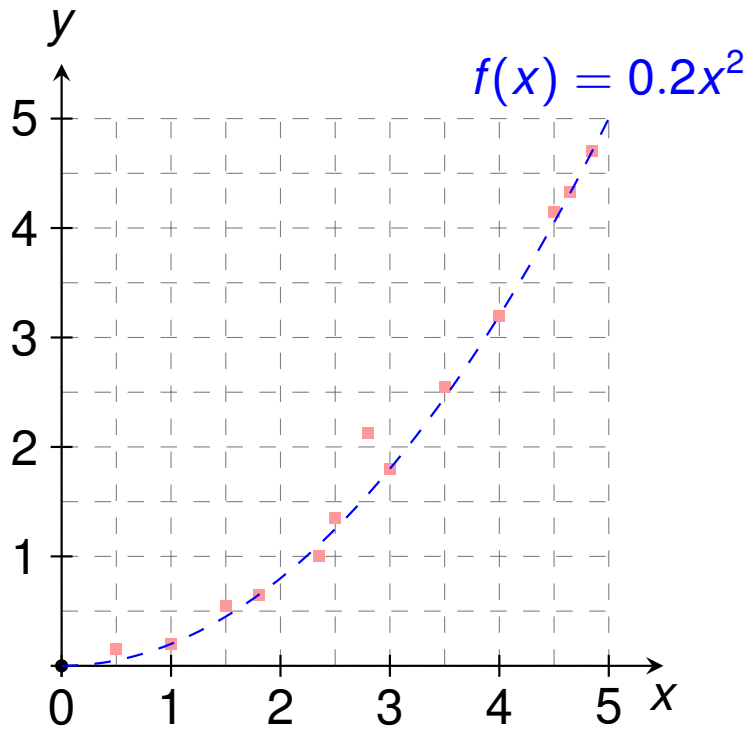

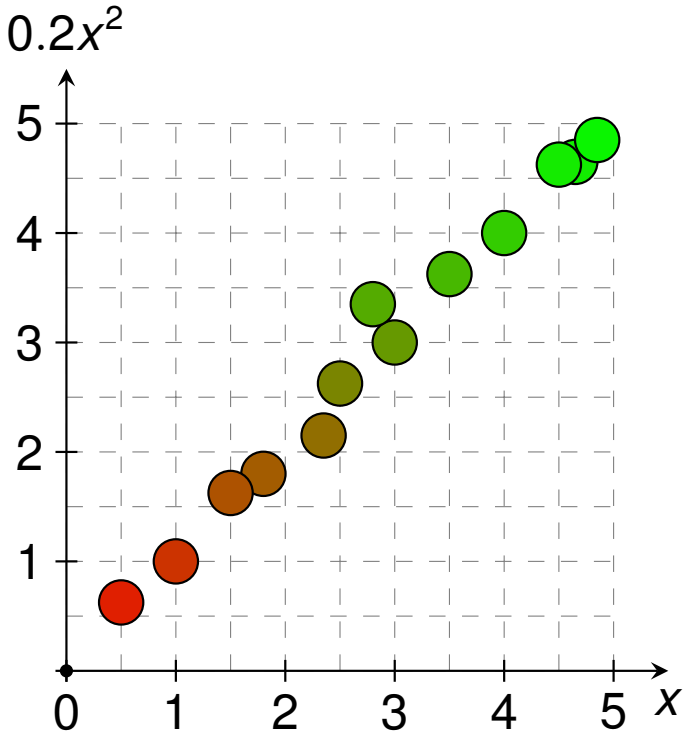

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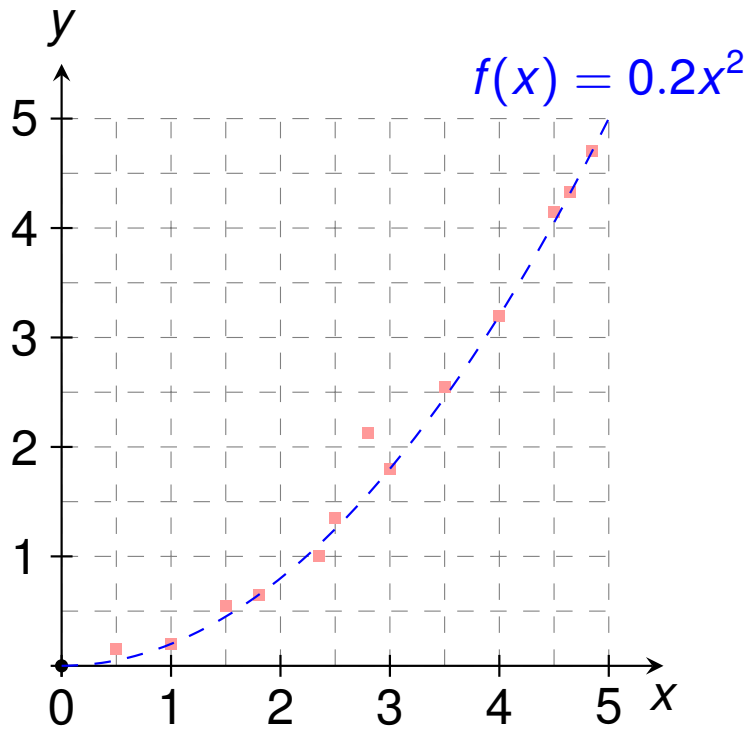

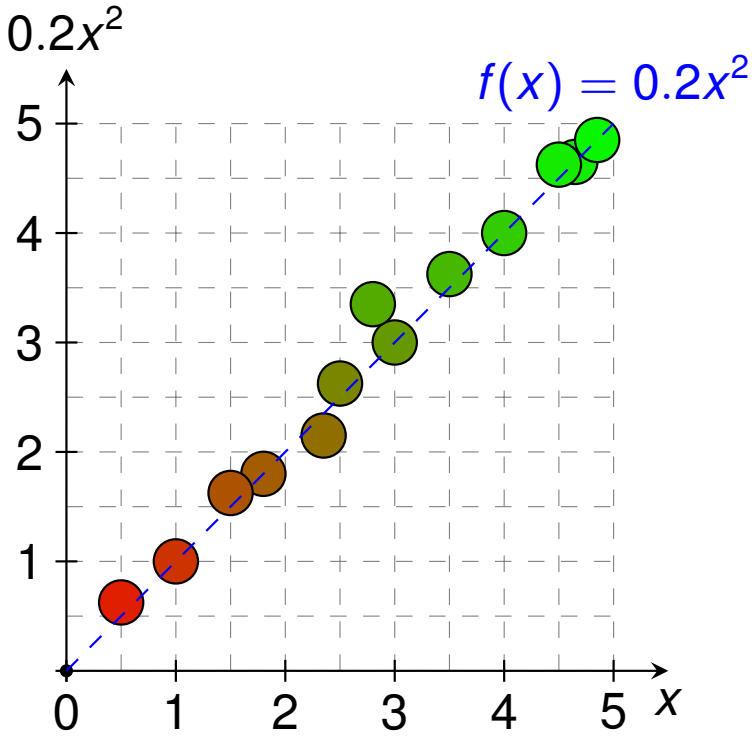

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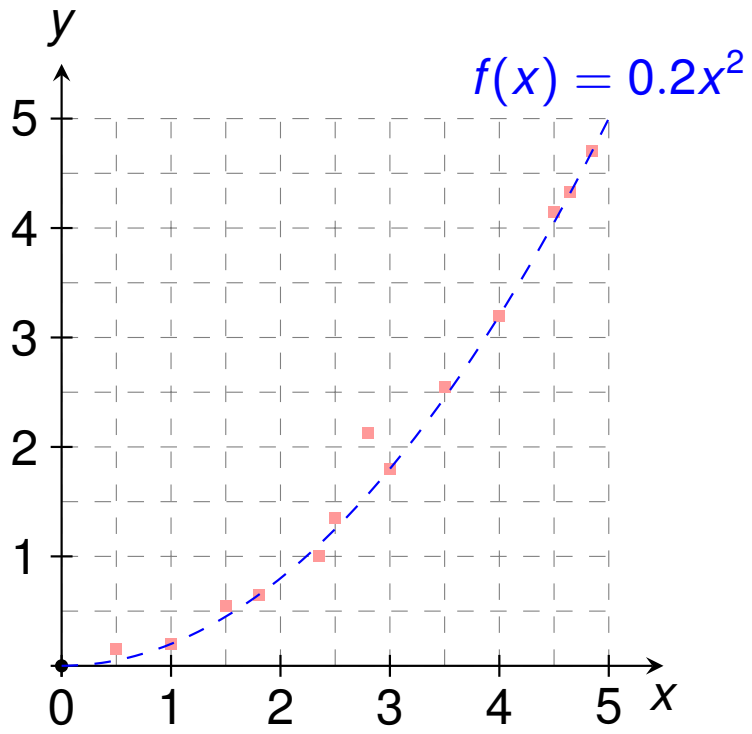

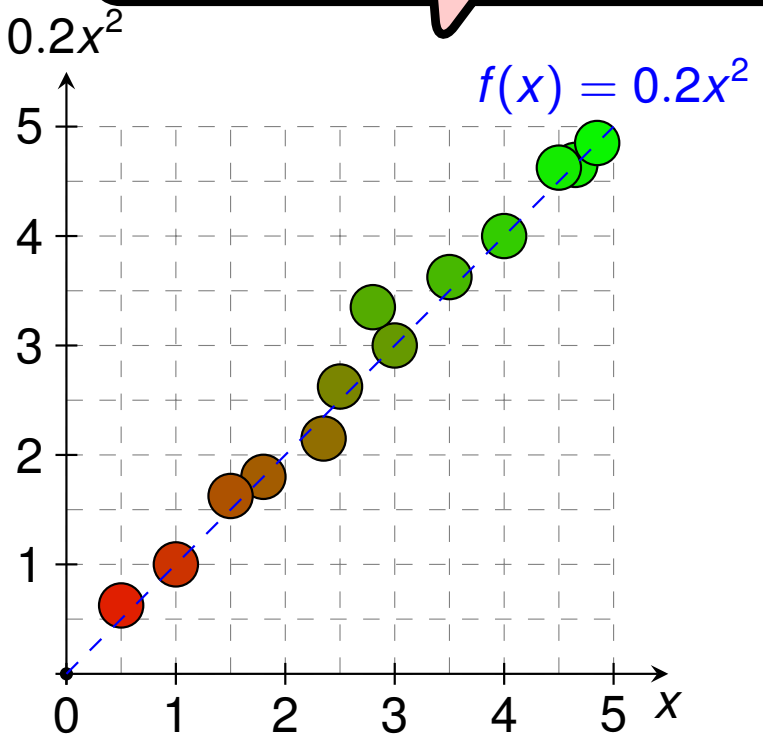

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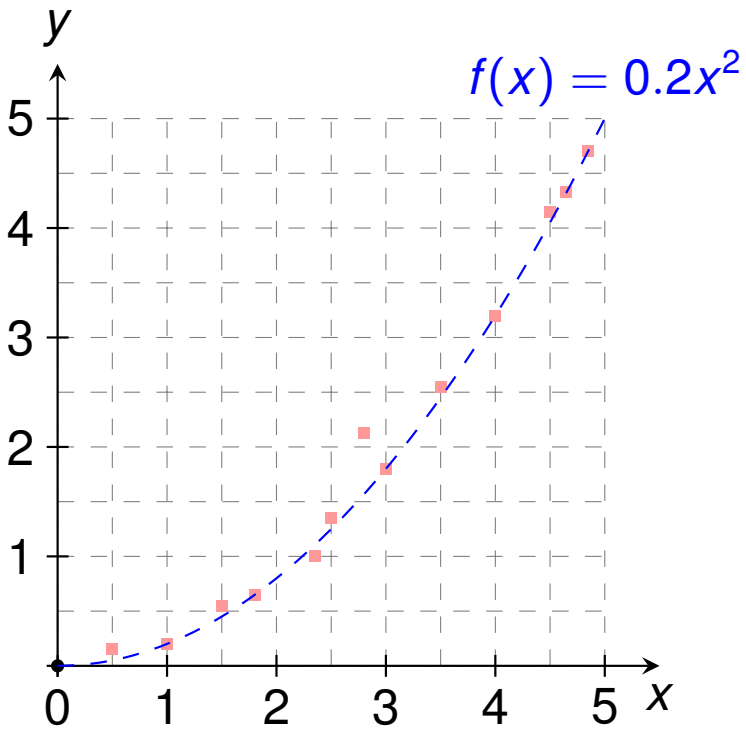

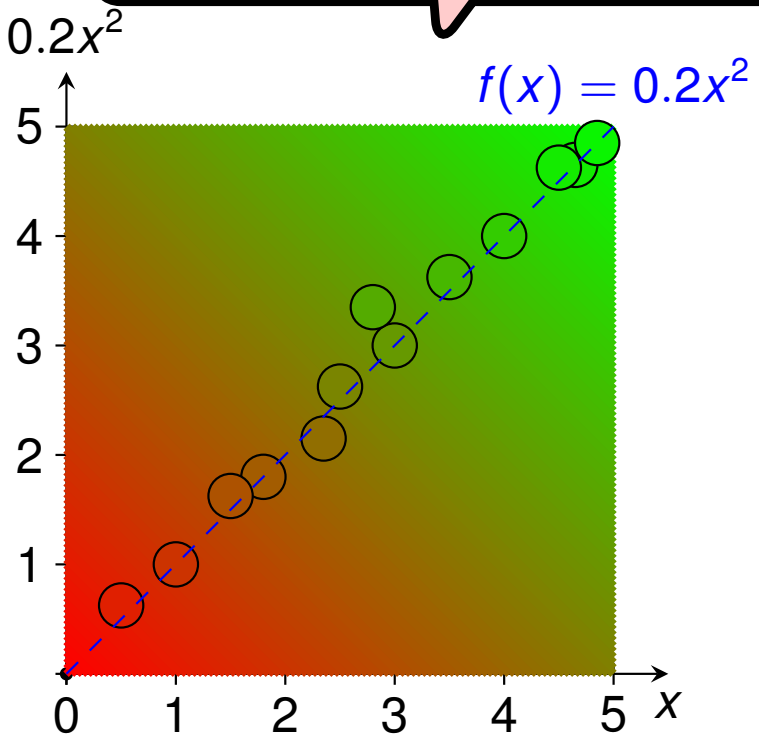

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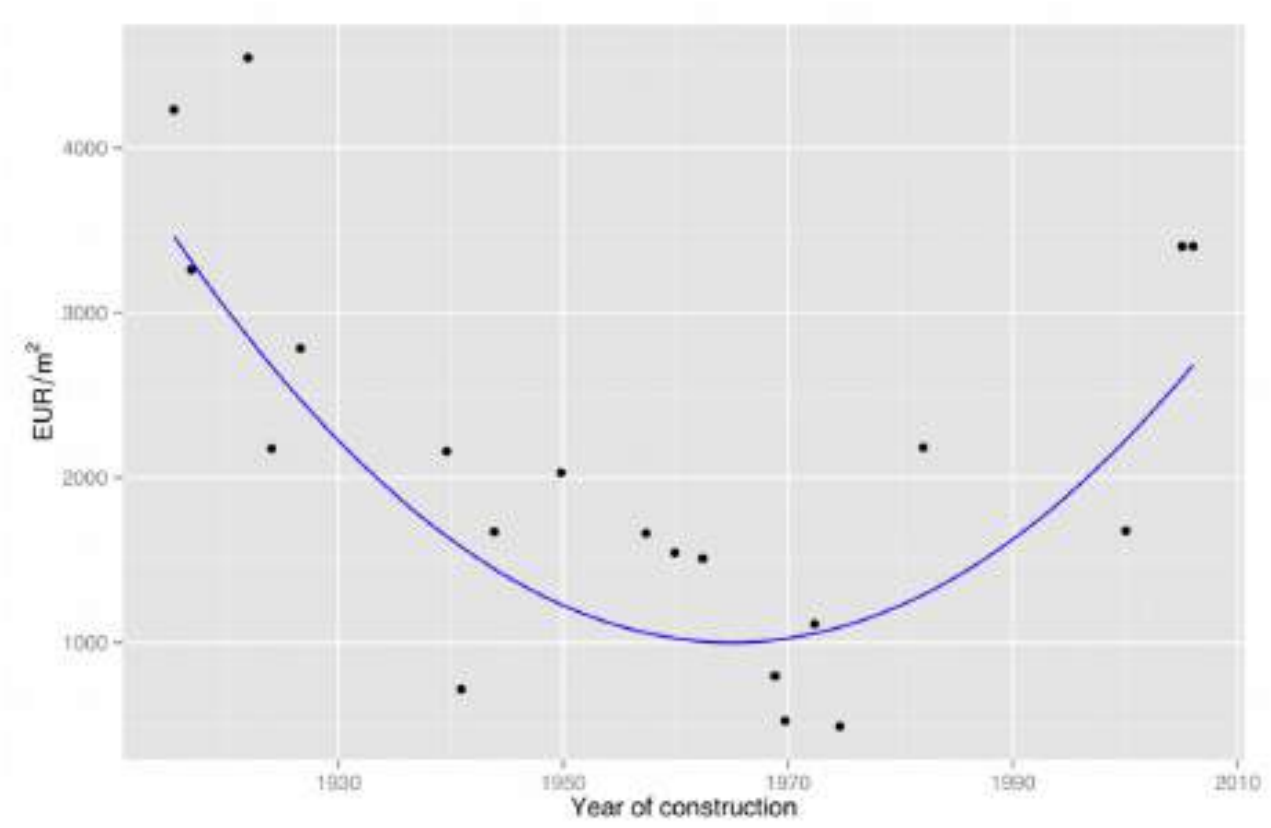

Source: Slides by I. Schuster and P. Jähnichen

Flat Prices in Berlin

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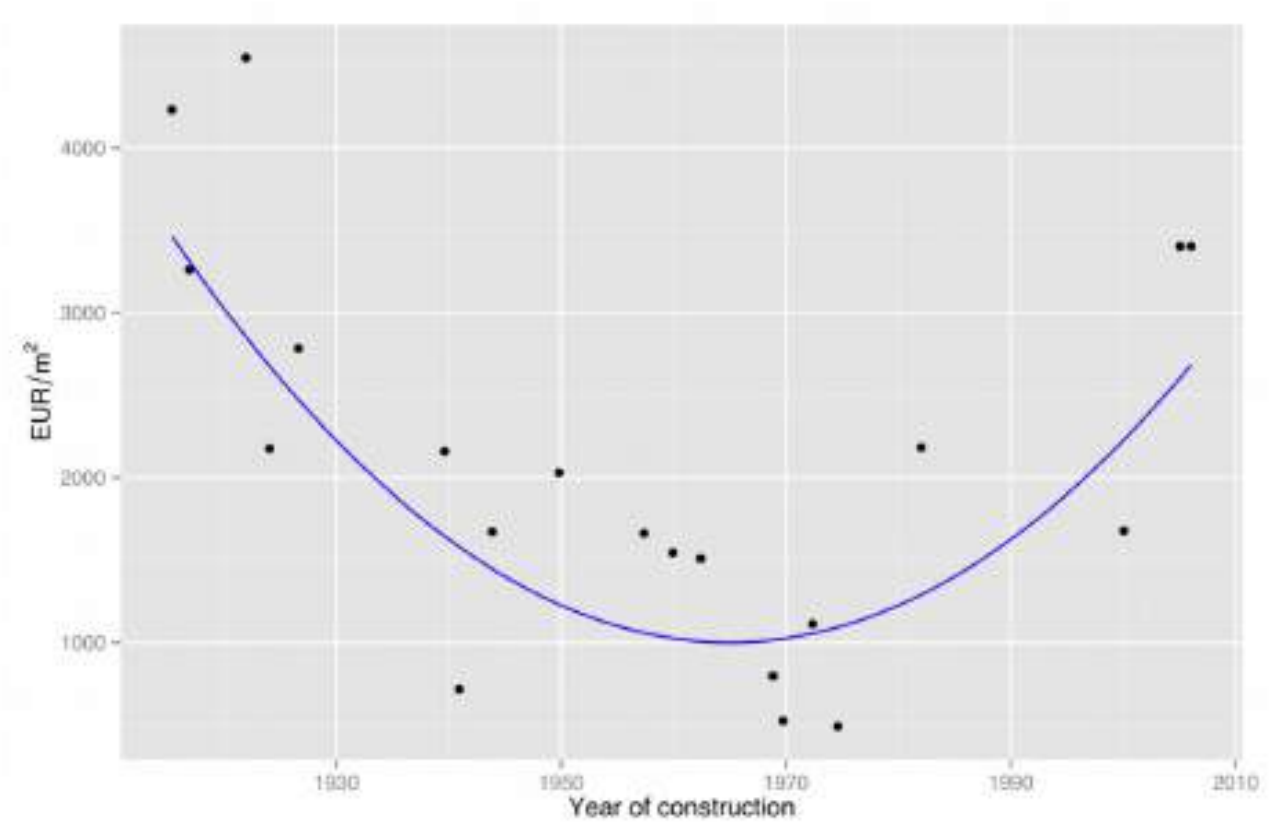

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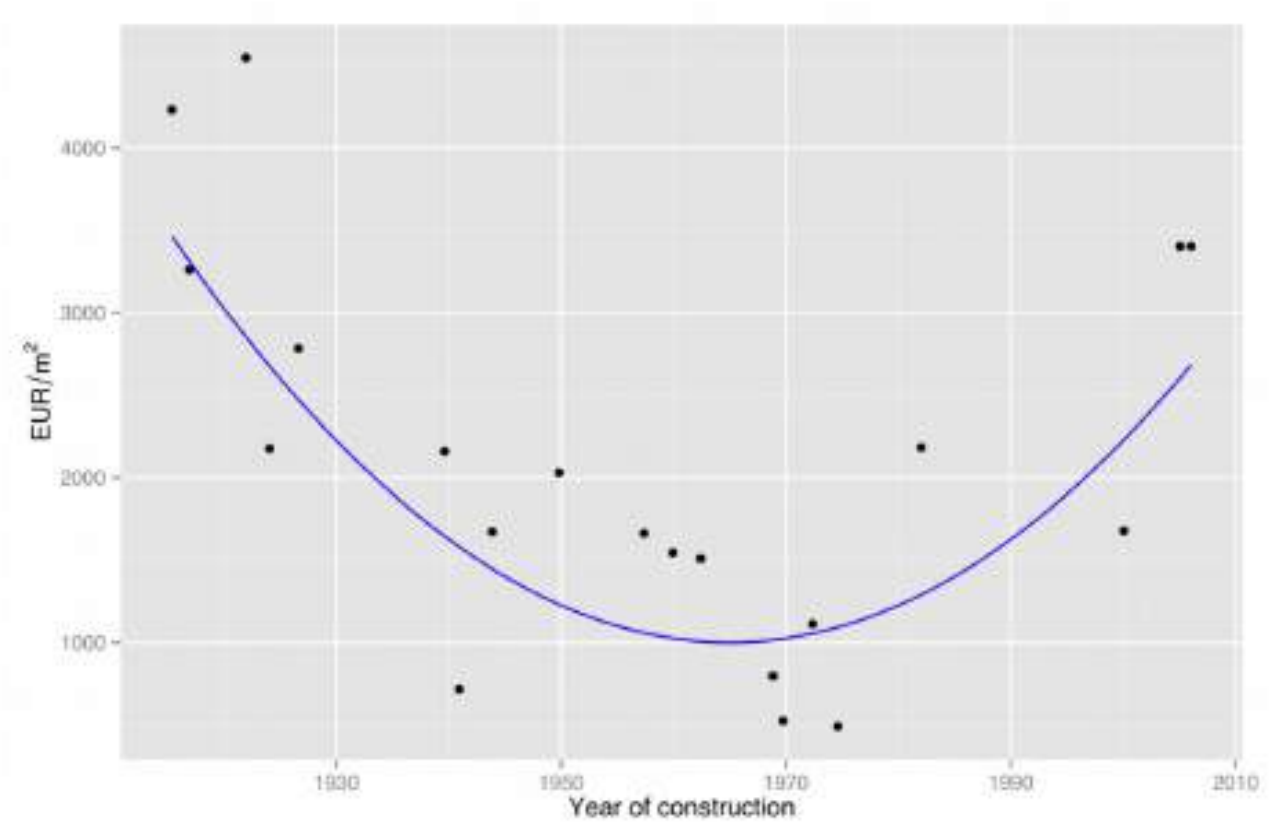

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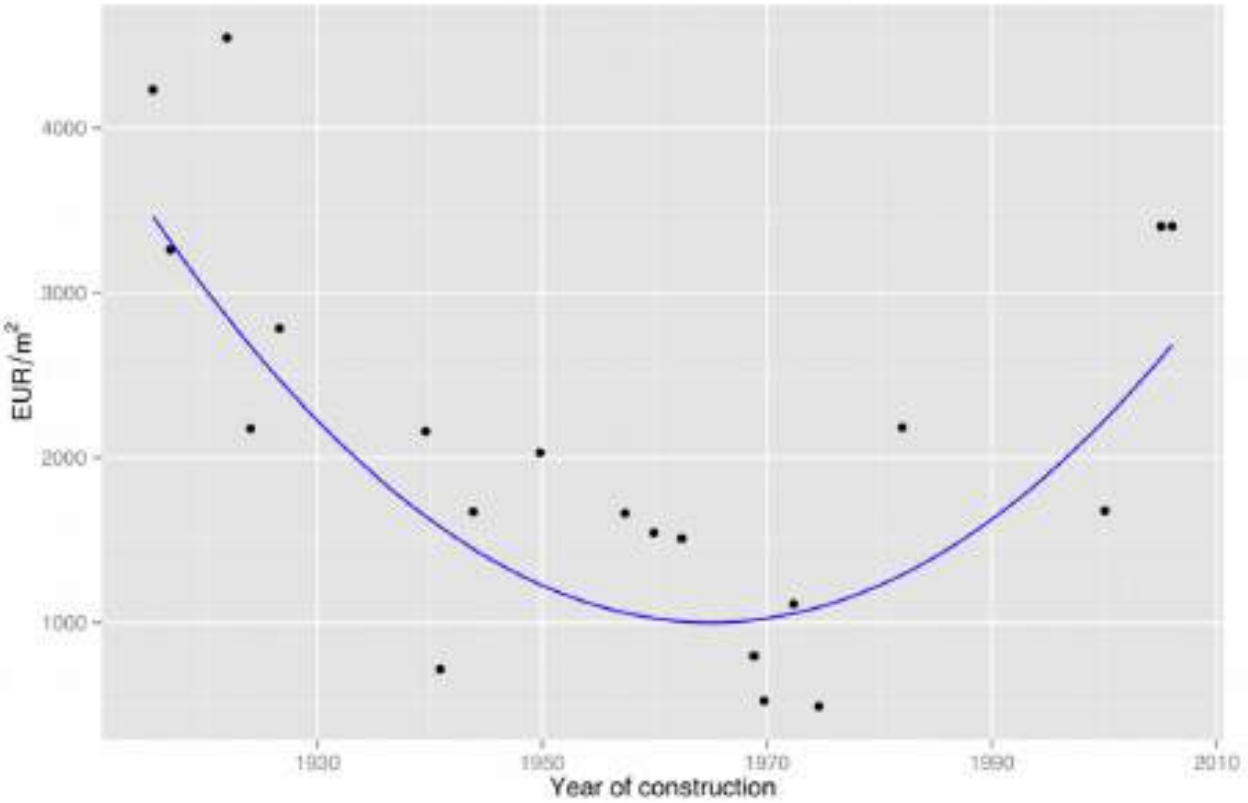

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- flats constructed in the 70s are least attractive (unpopular design?)

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Confounded Features: We can drop one category!

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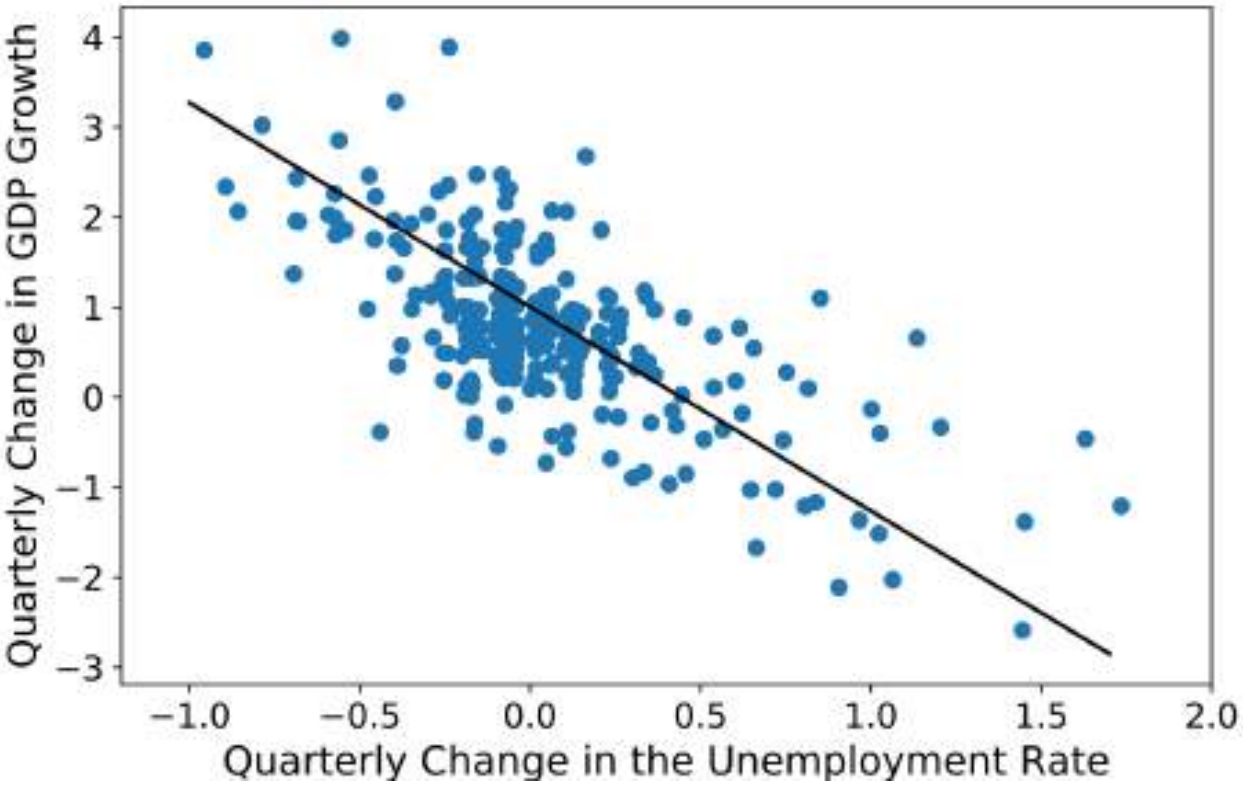
If a student does not study Economics or Physics, then he/she studies Politics ✓

Linear Regression in Practice: Economics

Okun's Law

For every 1% increase in the unemployment rate, a country's GDP will be roughly an additional 2% lower.



Source: Wikipedia

Outline

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Linear Regression

Linear Regression with More than One Feature

Solving Linear Regression: Gradient Descent

Logistic Regression

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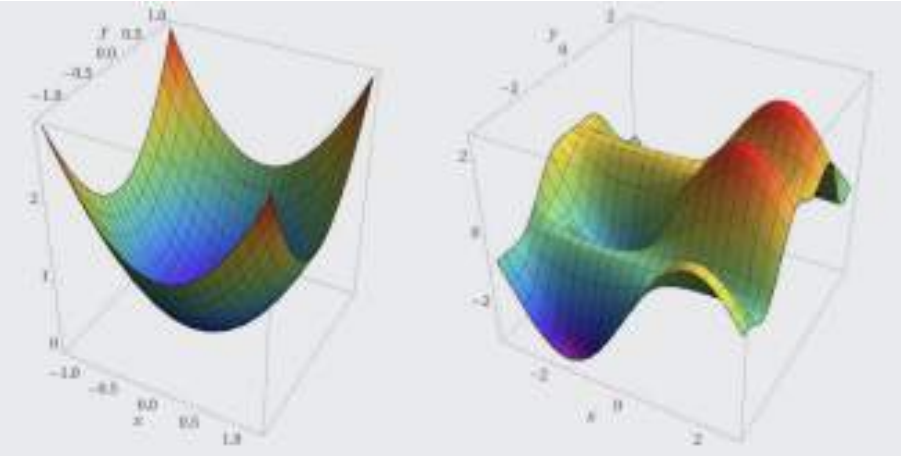

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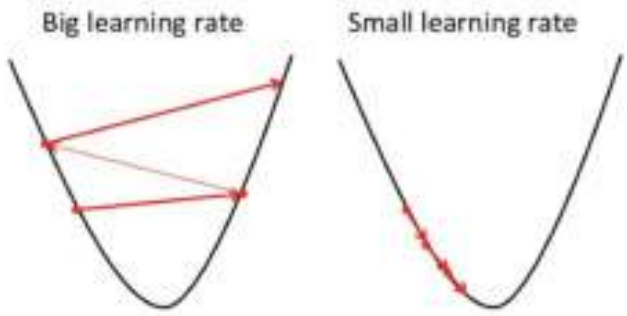

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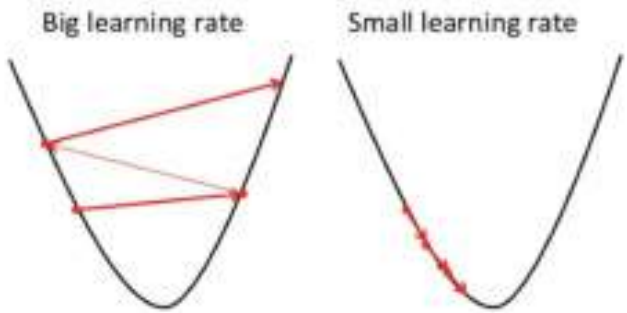

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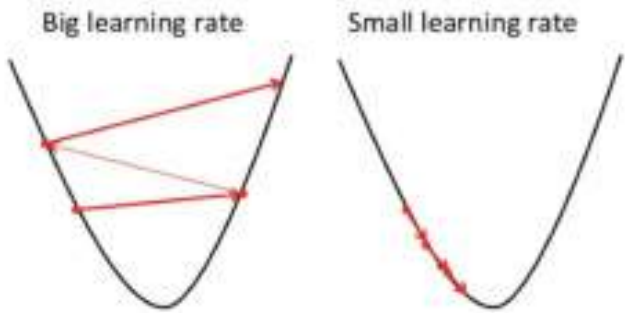

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Problem: In every iteration, we need to recompute $L(\mathbf{w}^{(t)})$, a function over all training examples!

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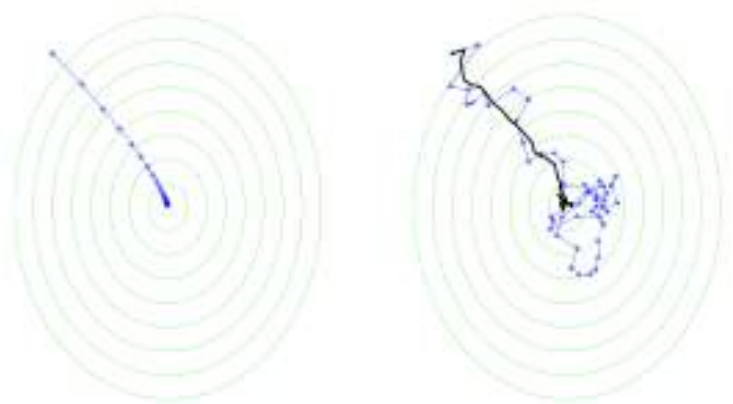

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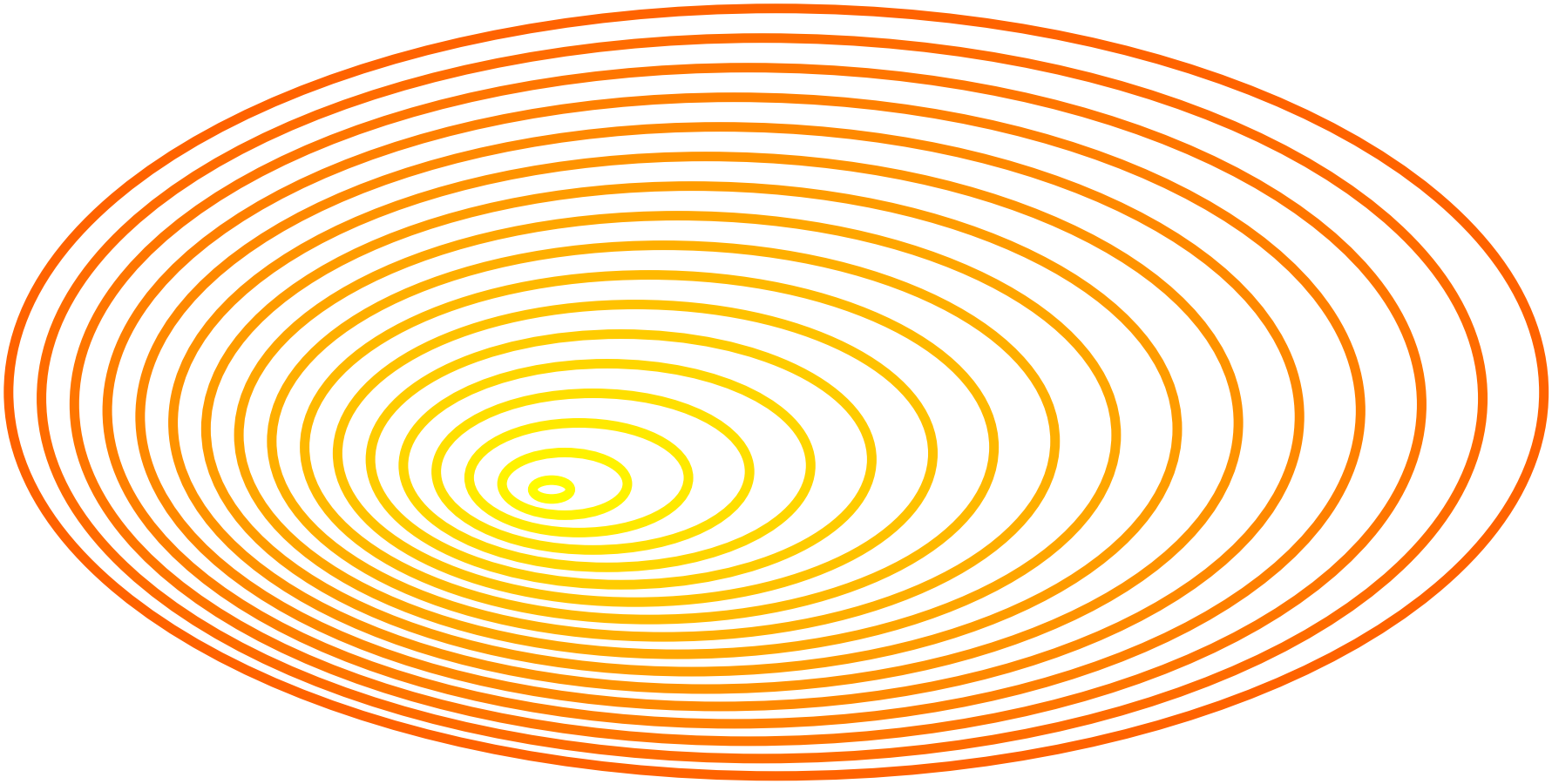

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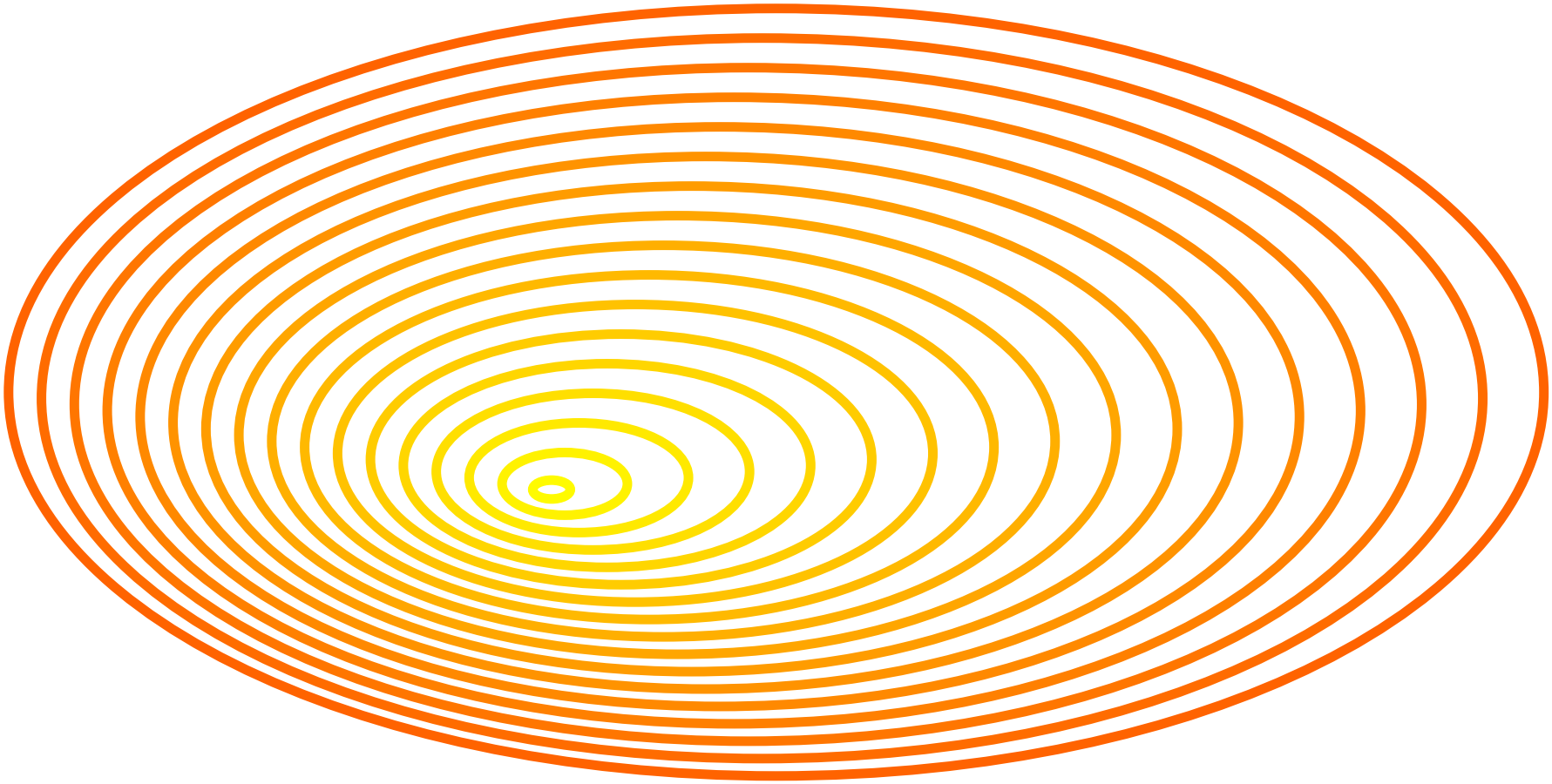

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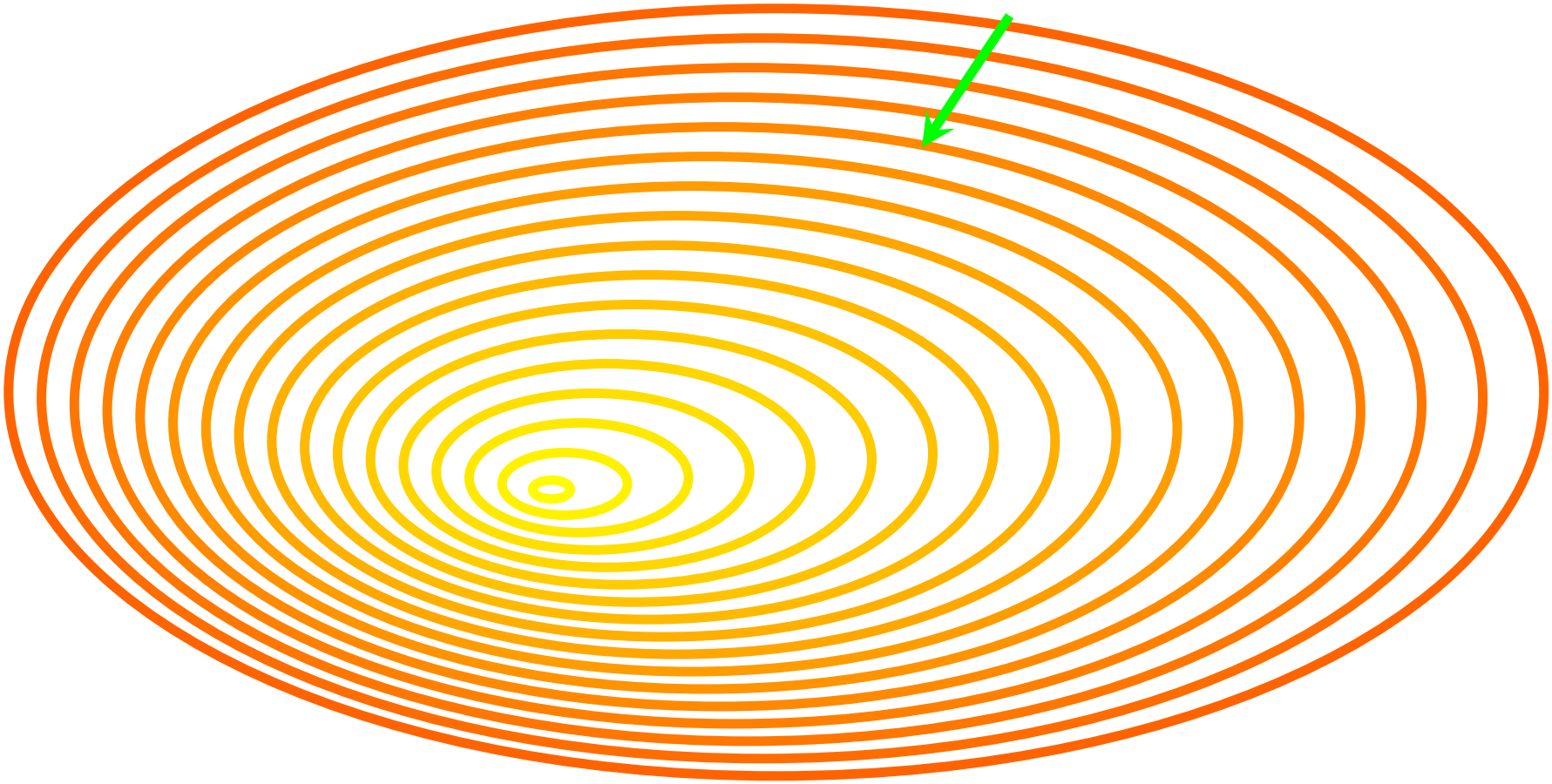

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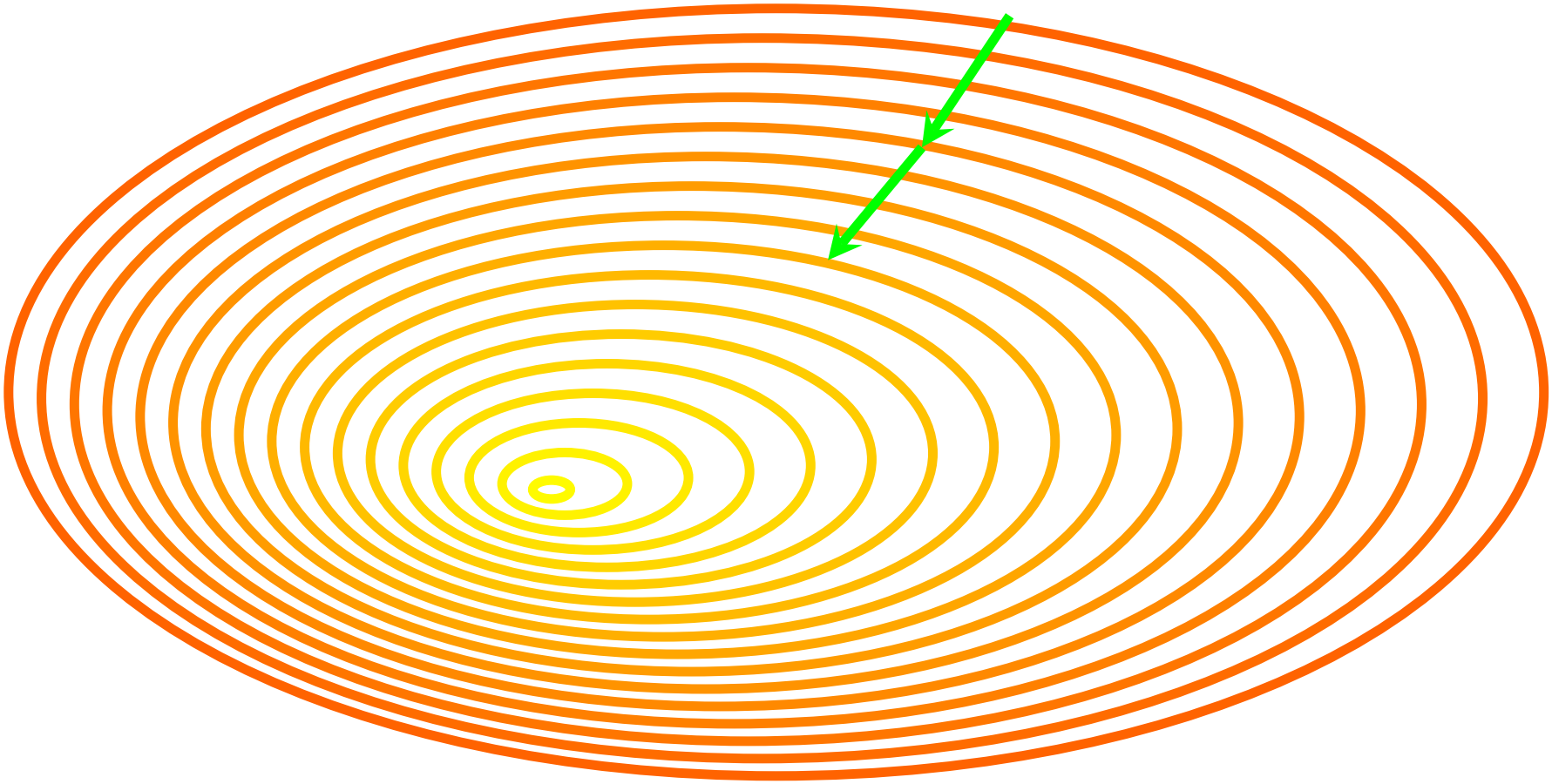

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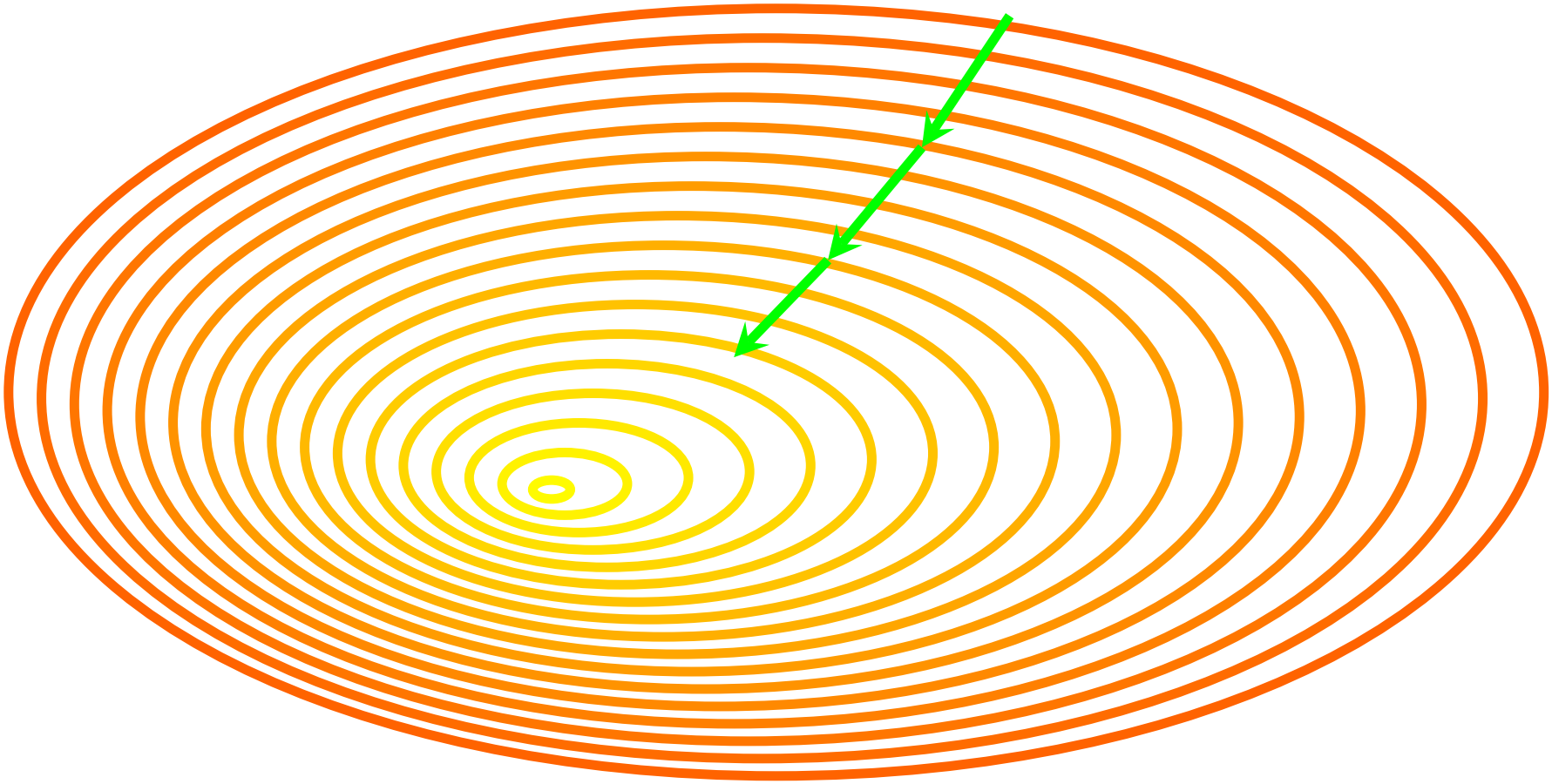

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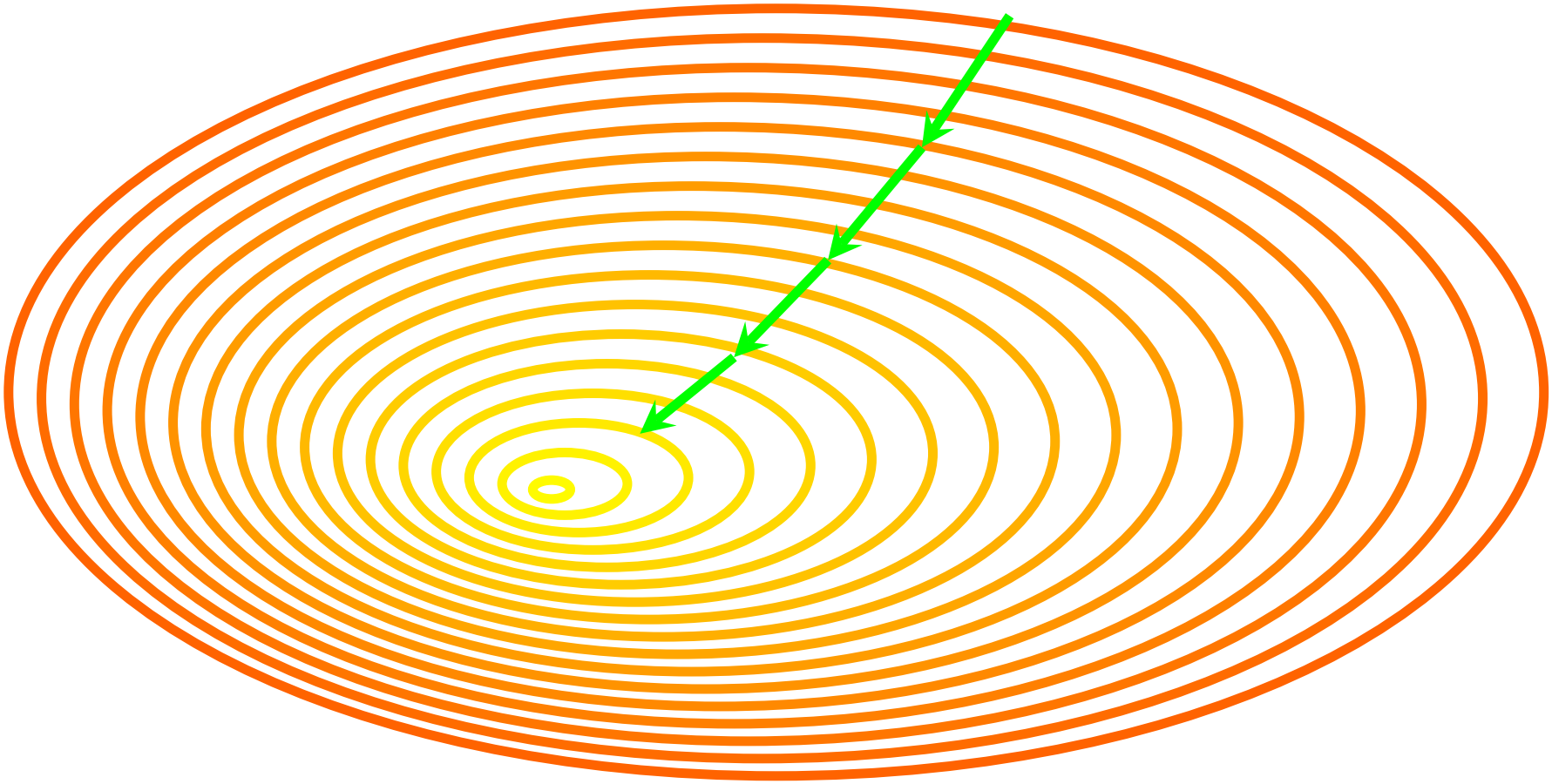

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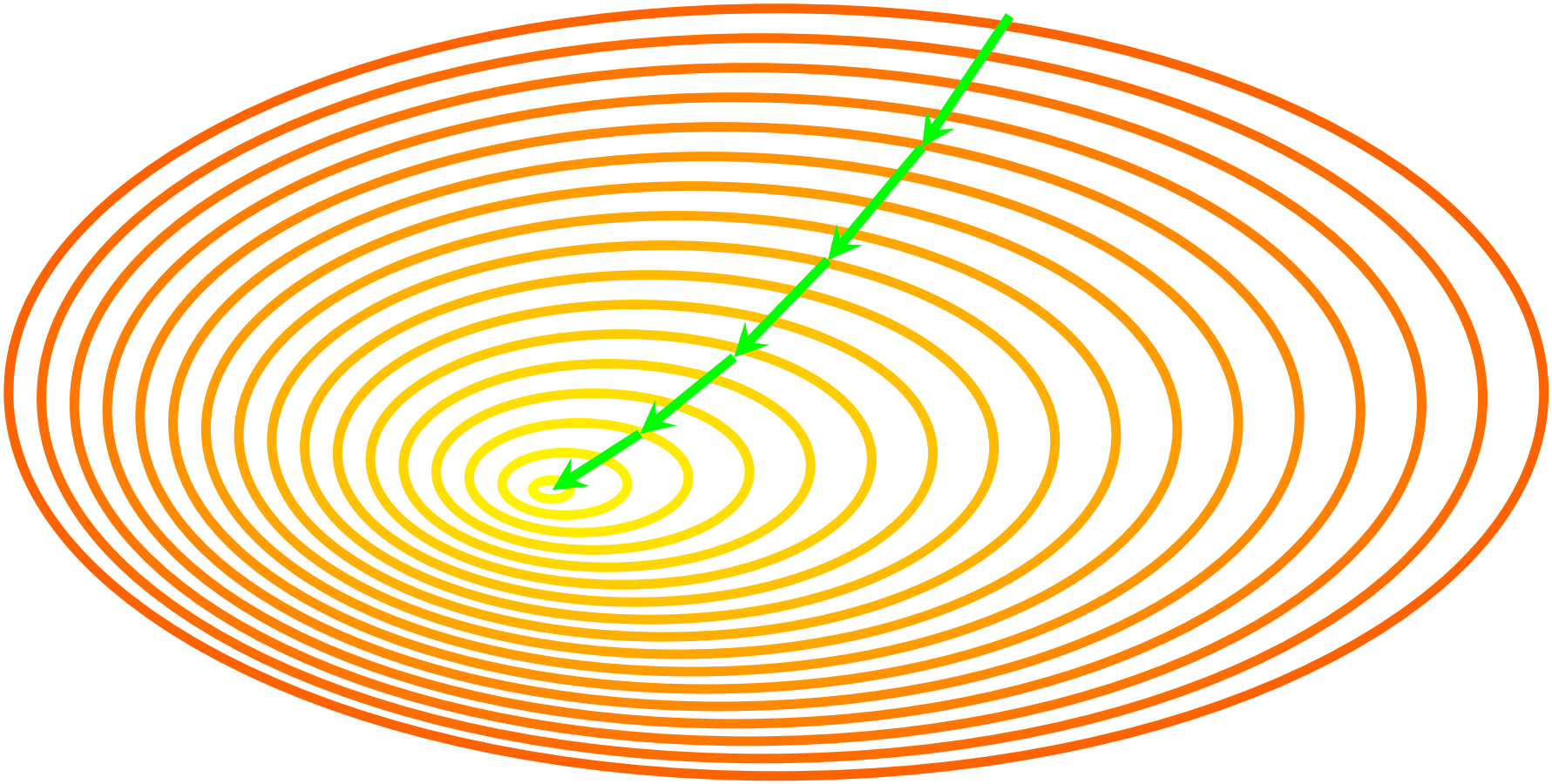

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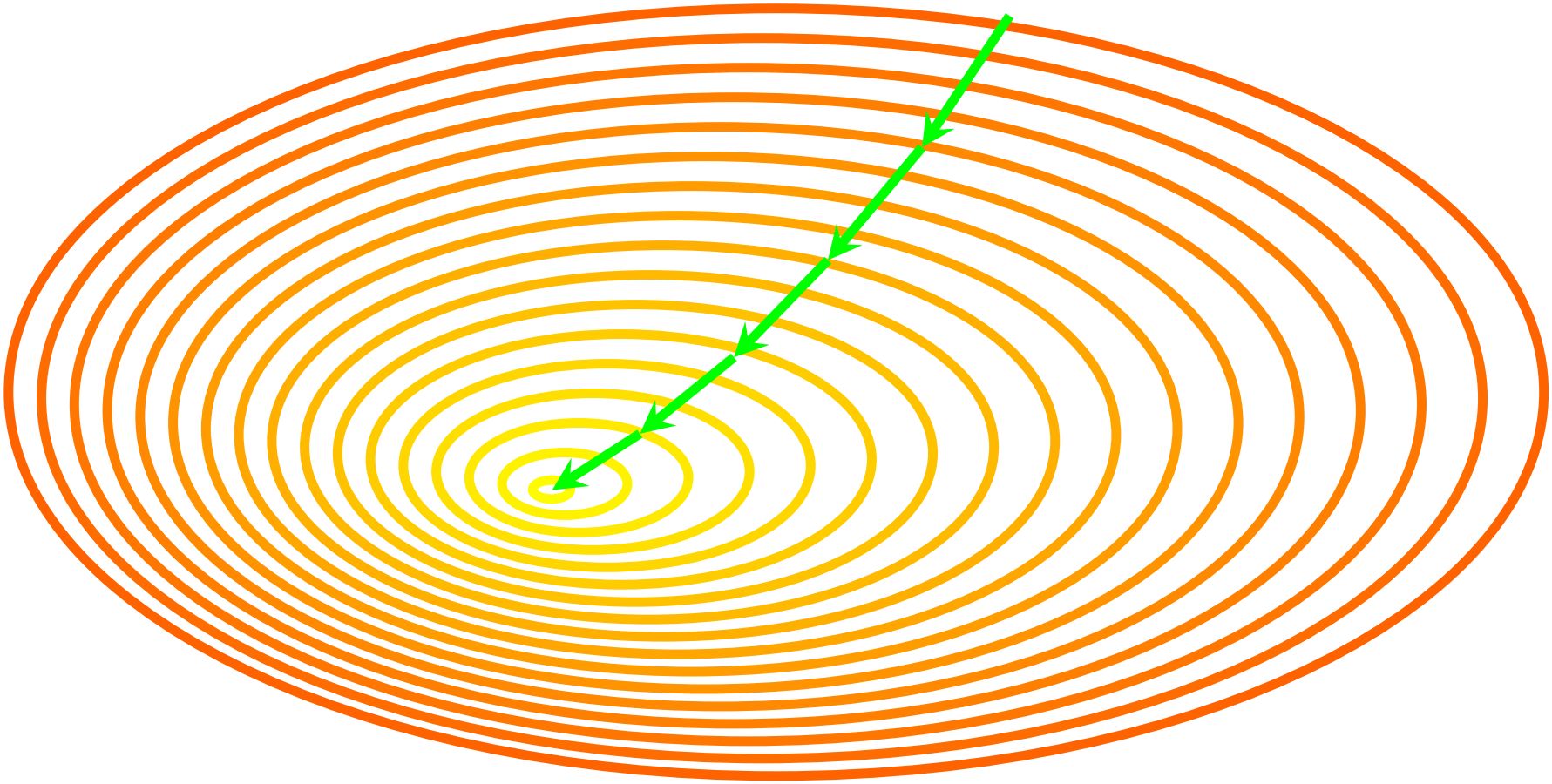

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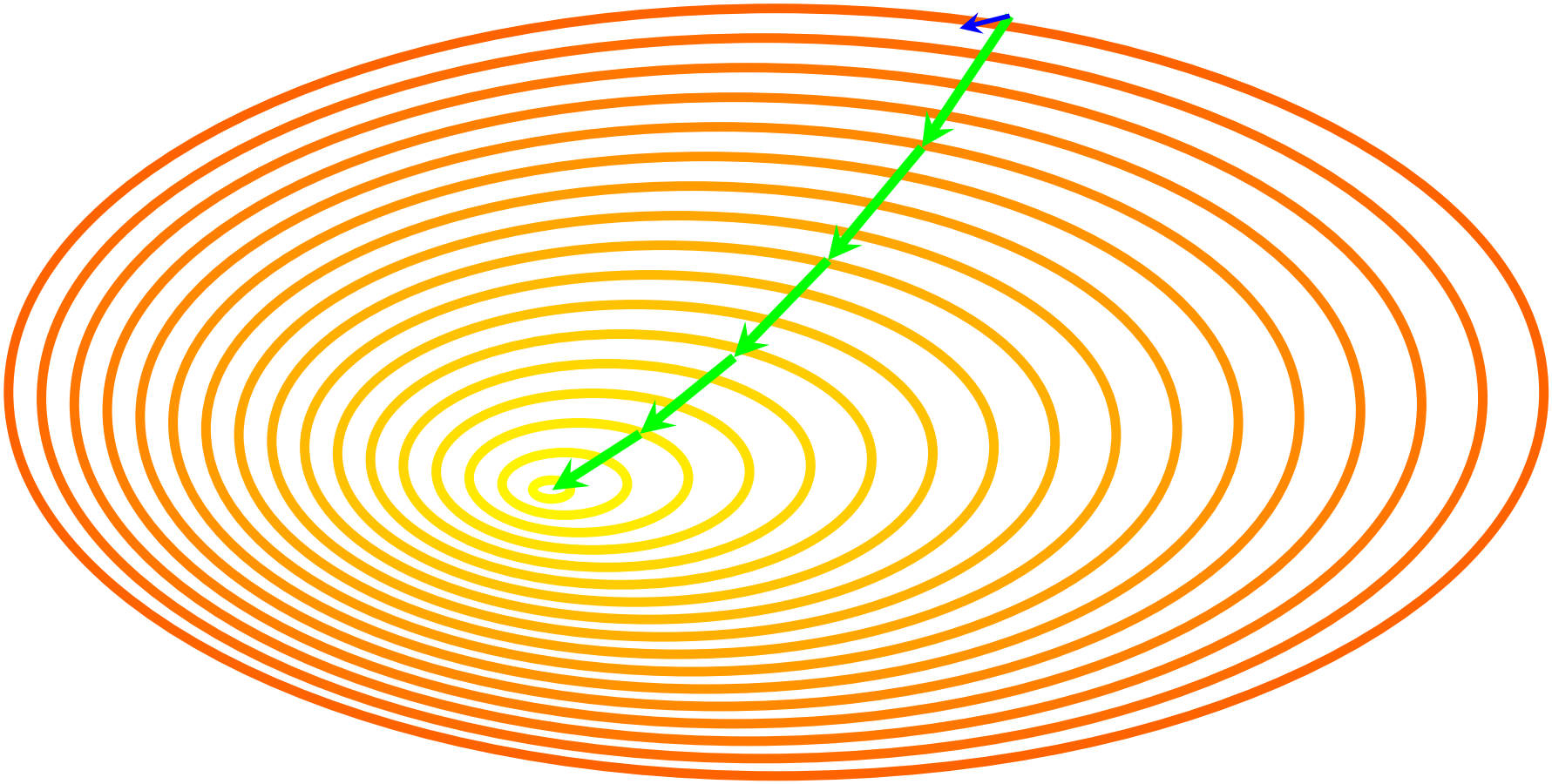

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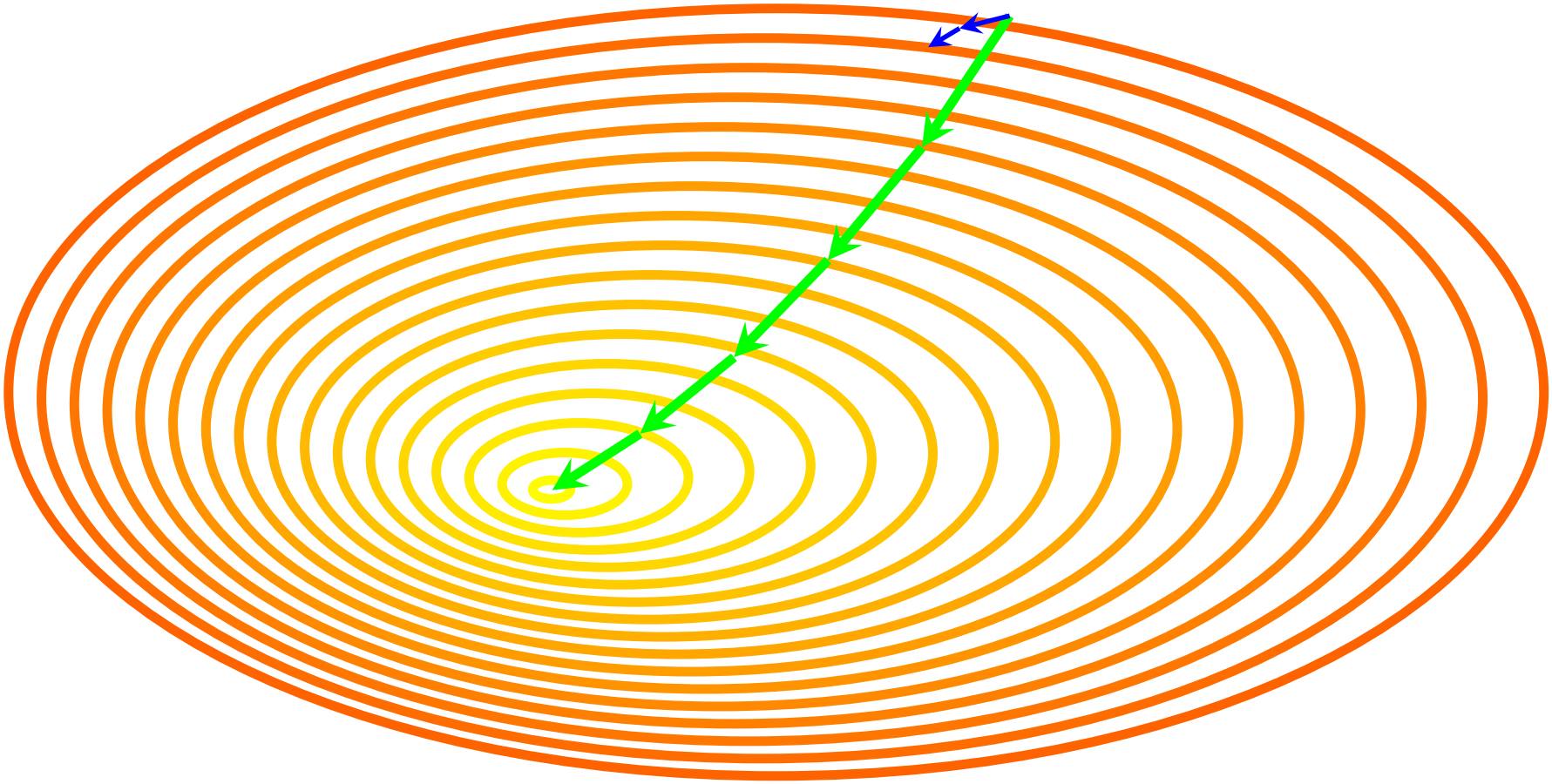

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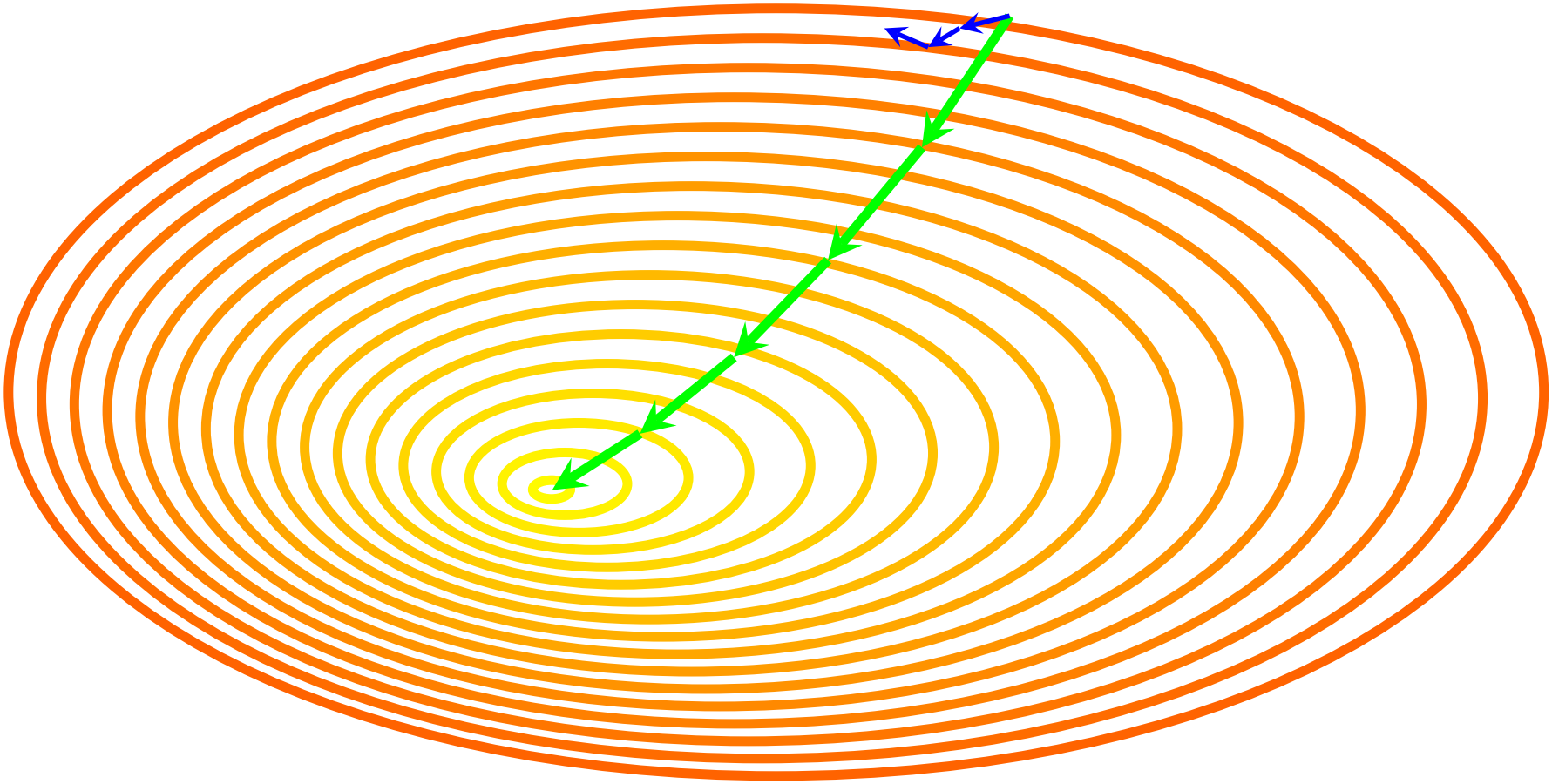

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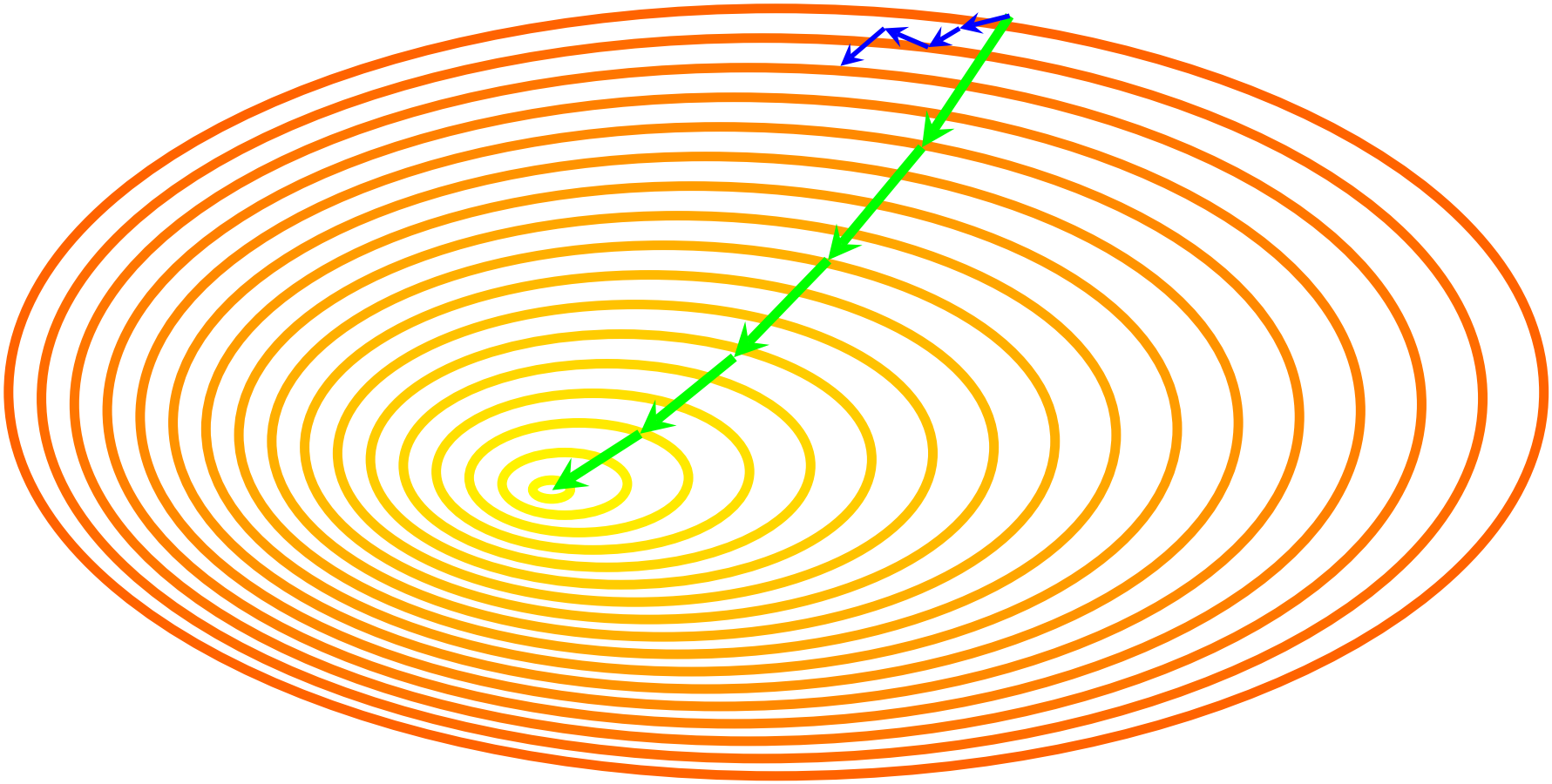

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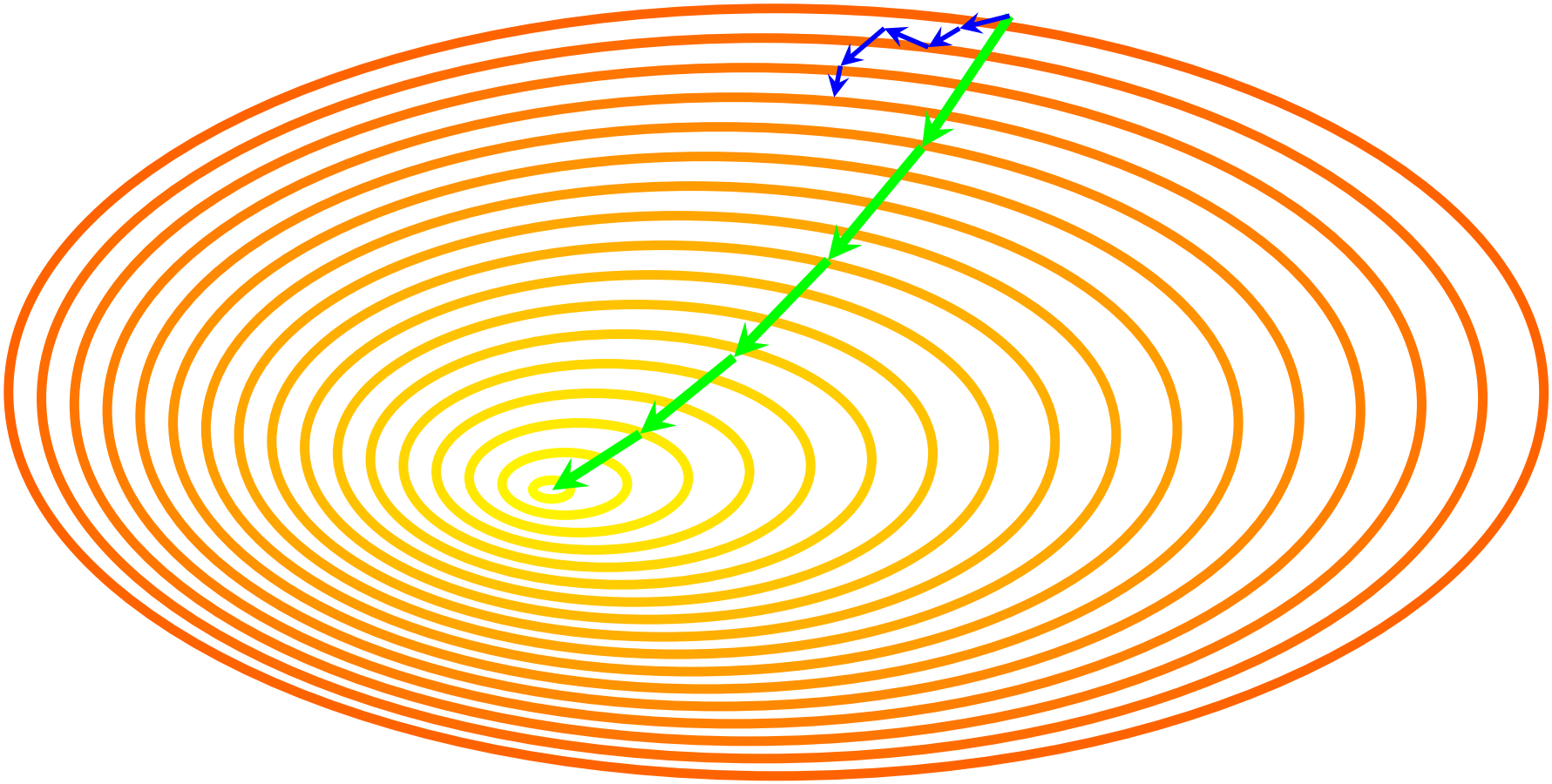

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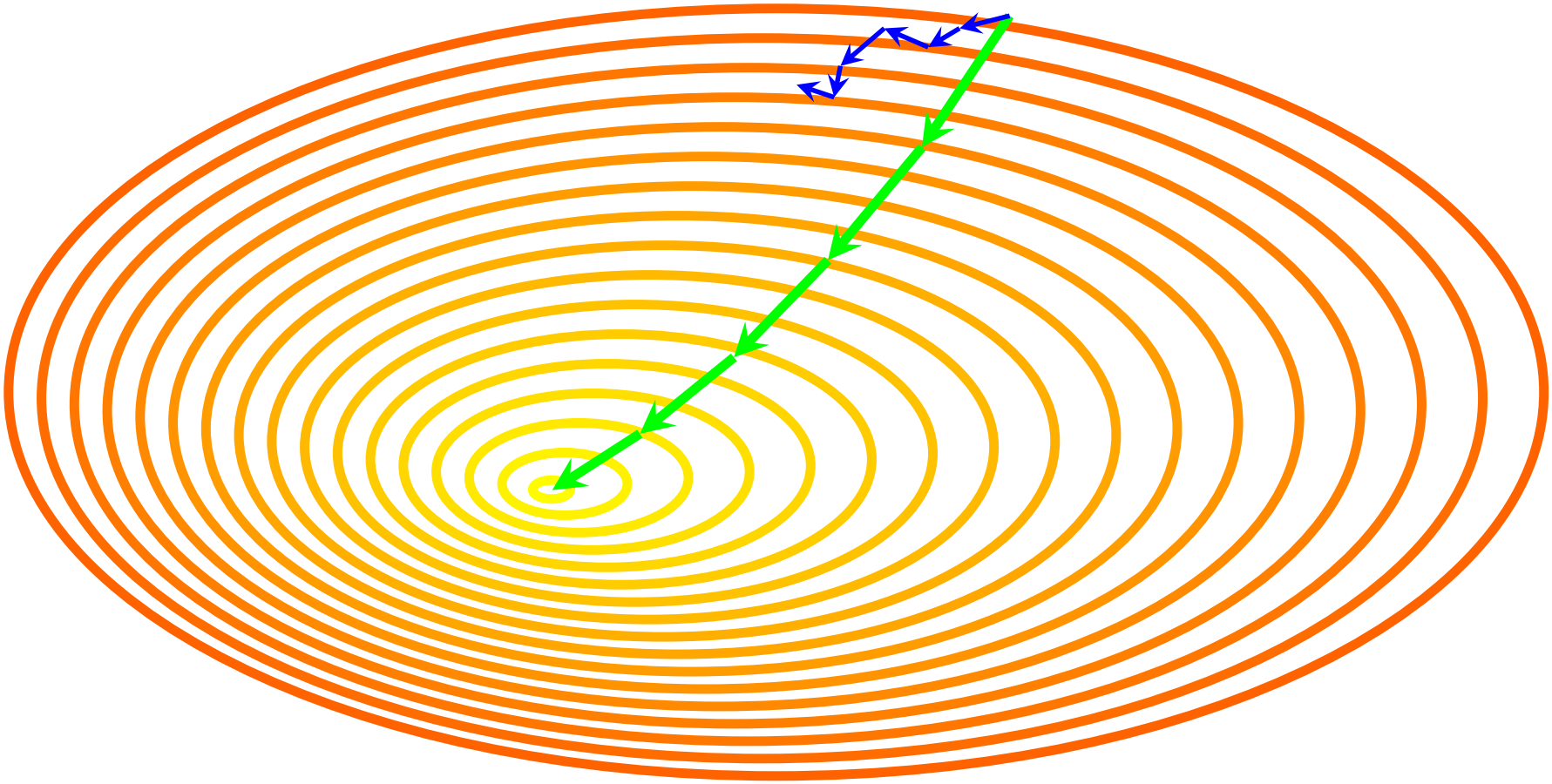

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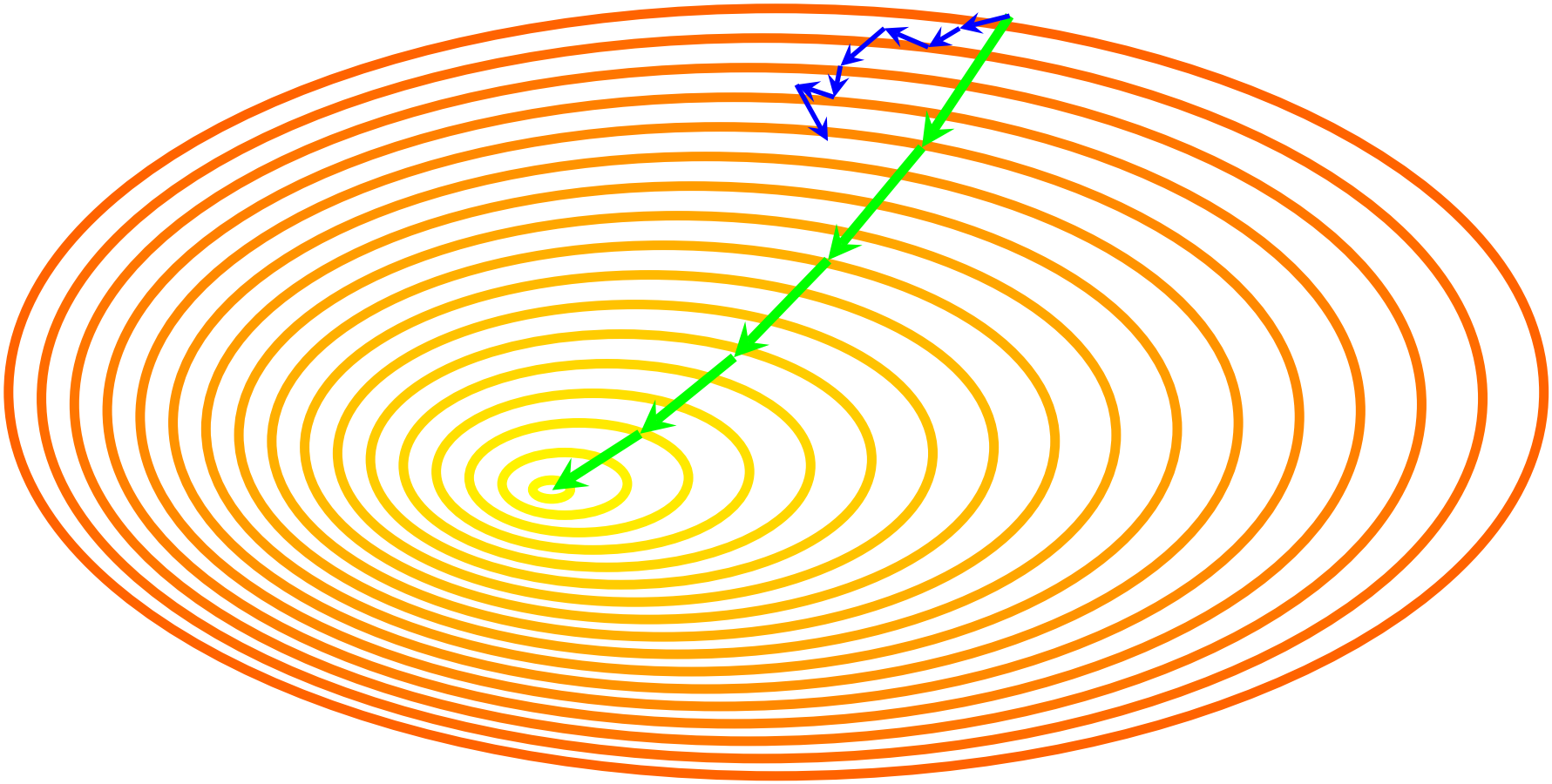

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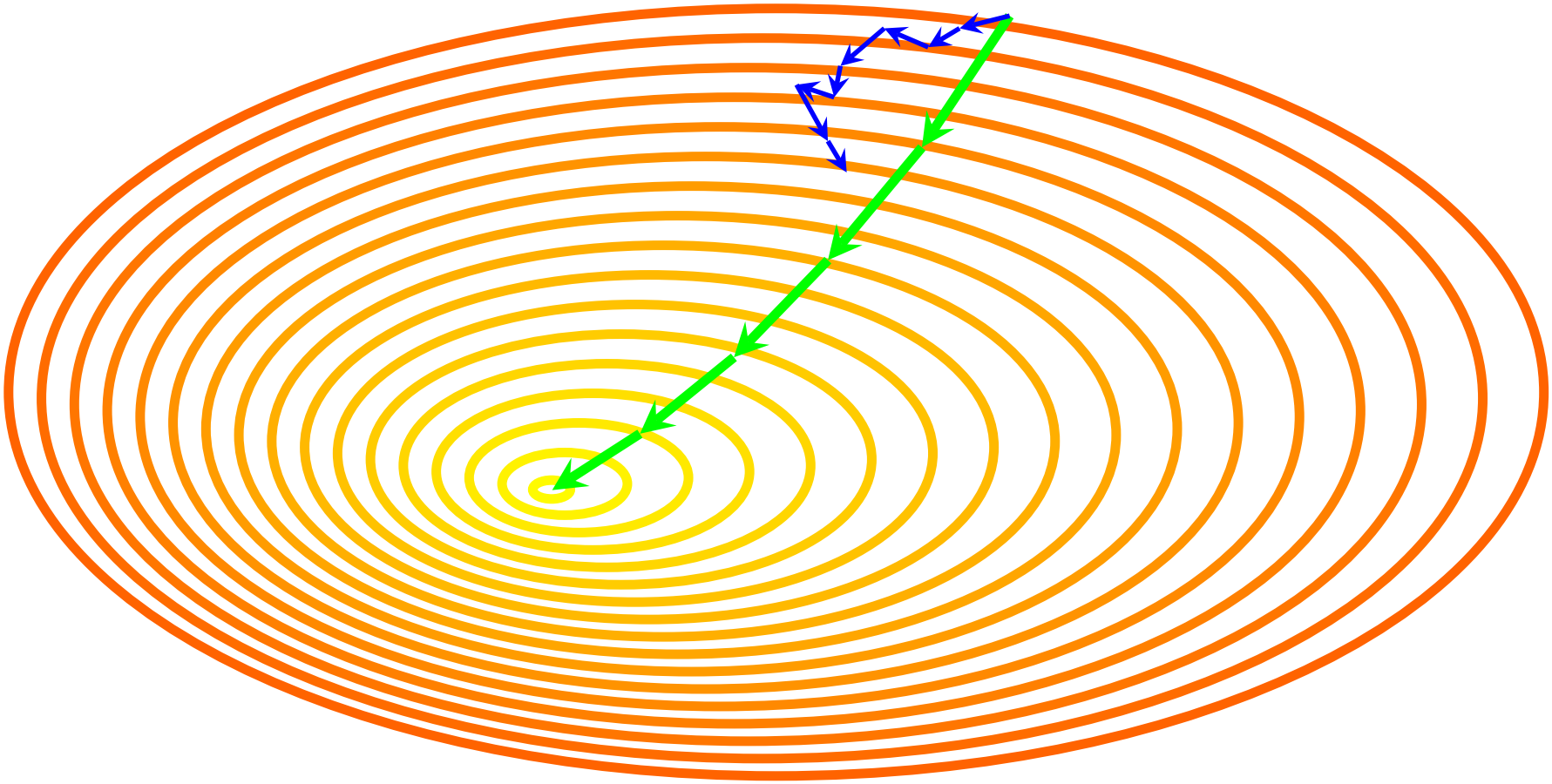

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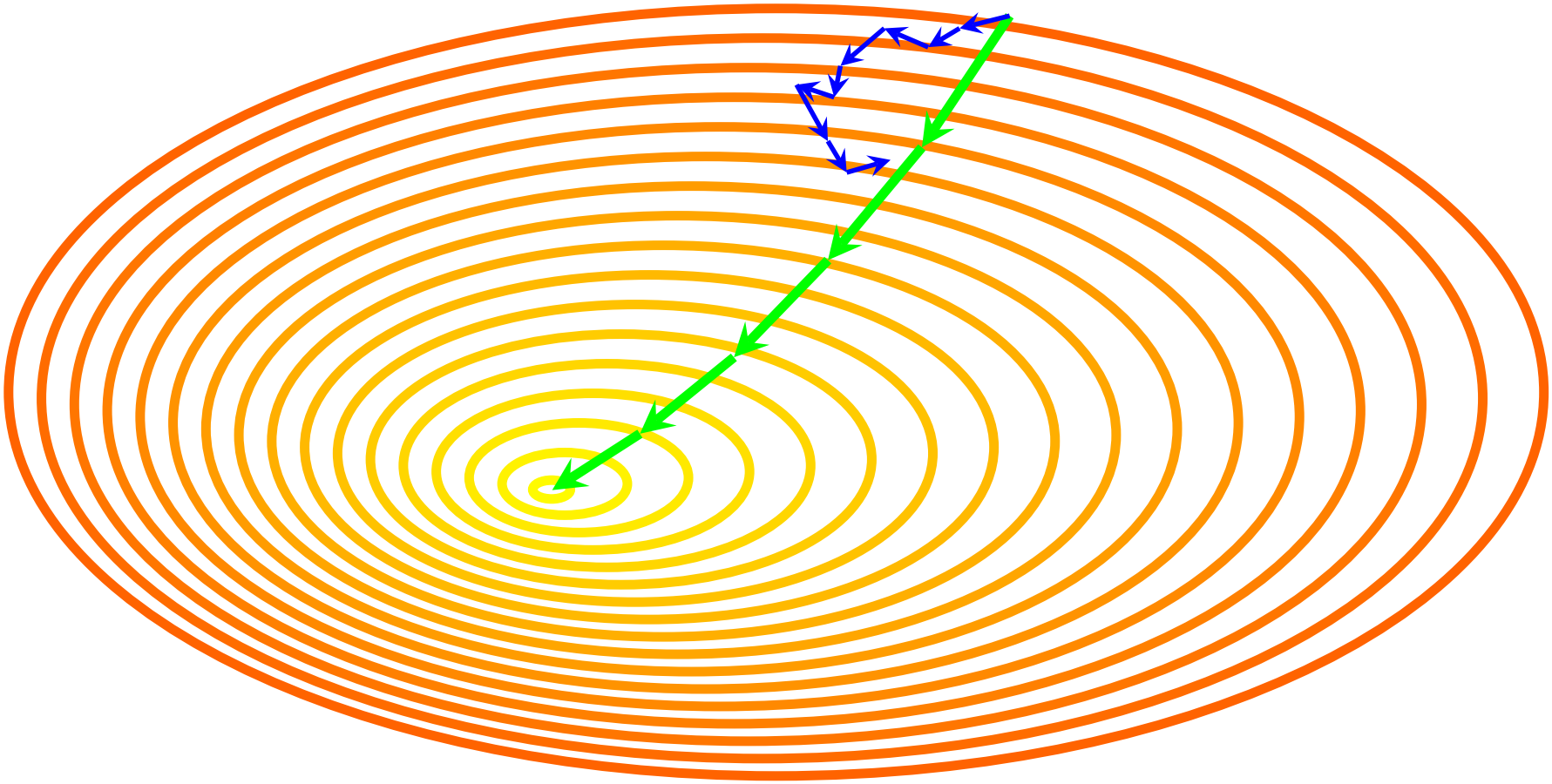

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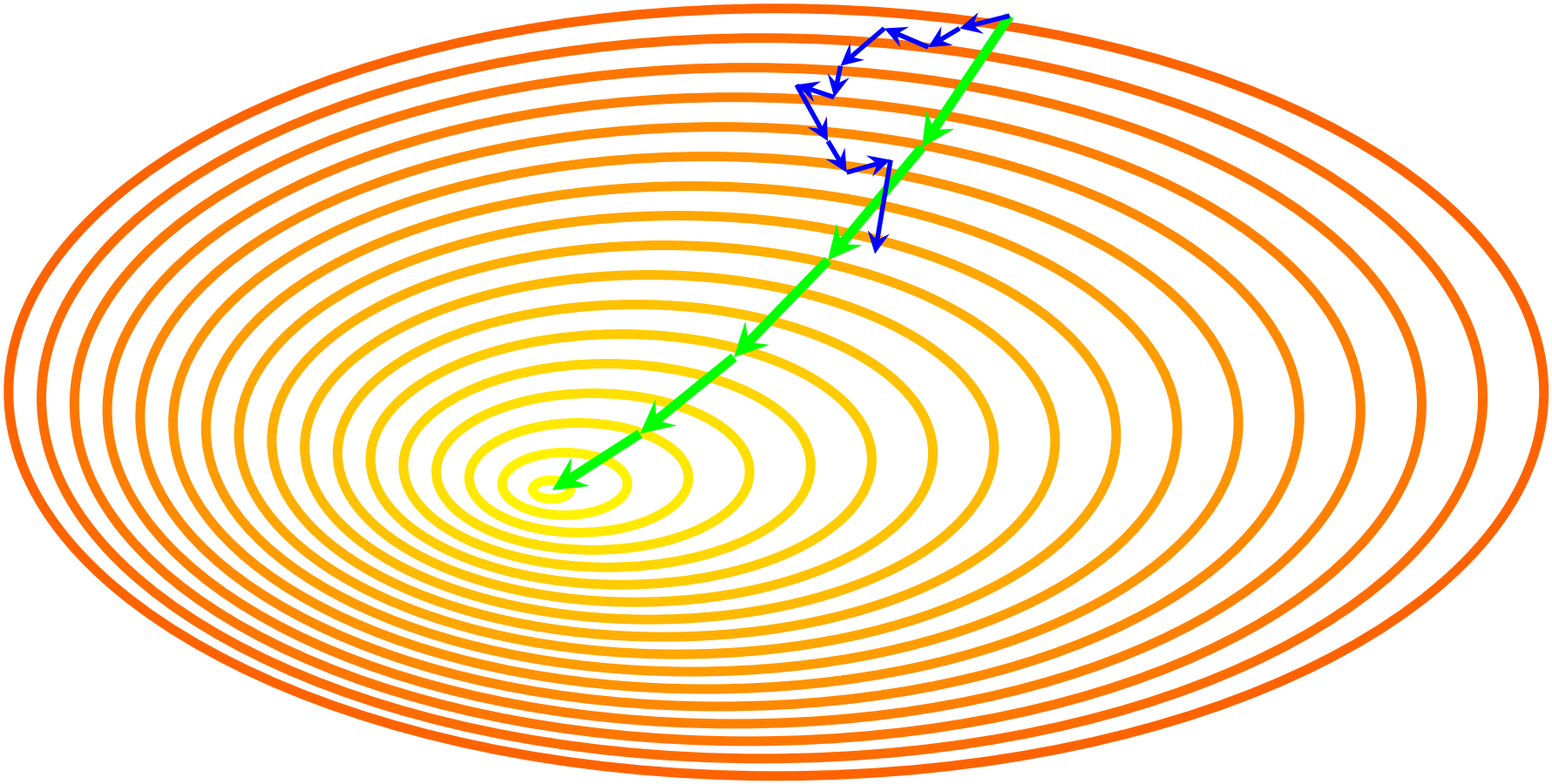

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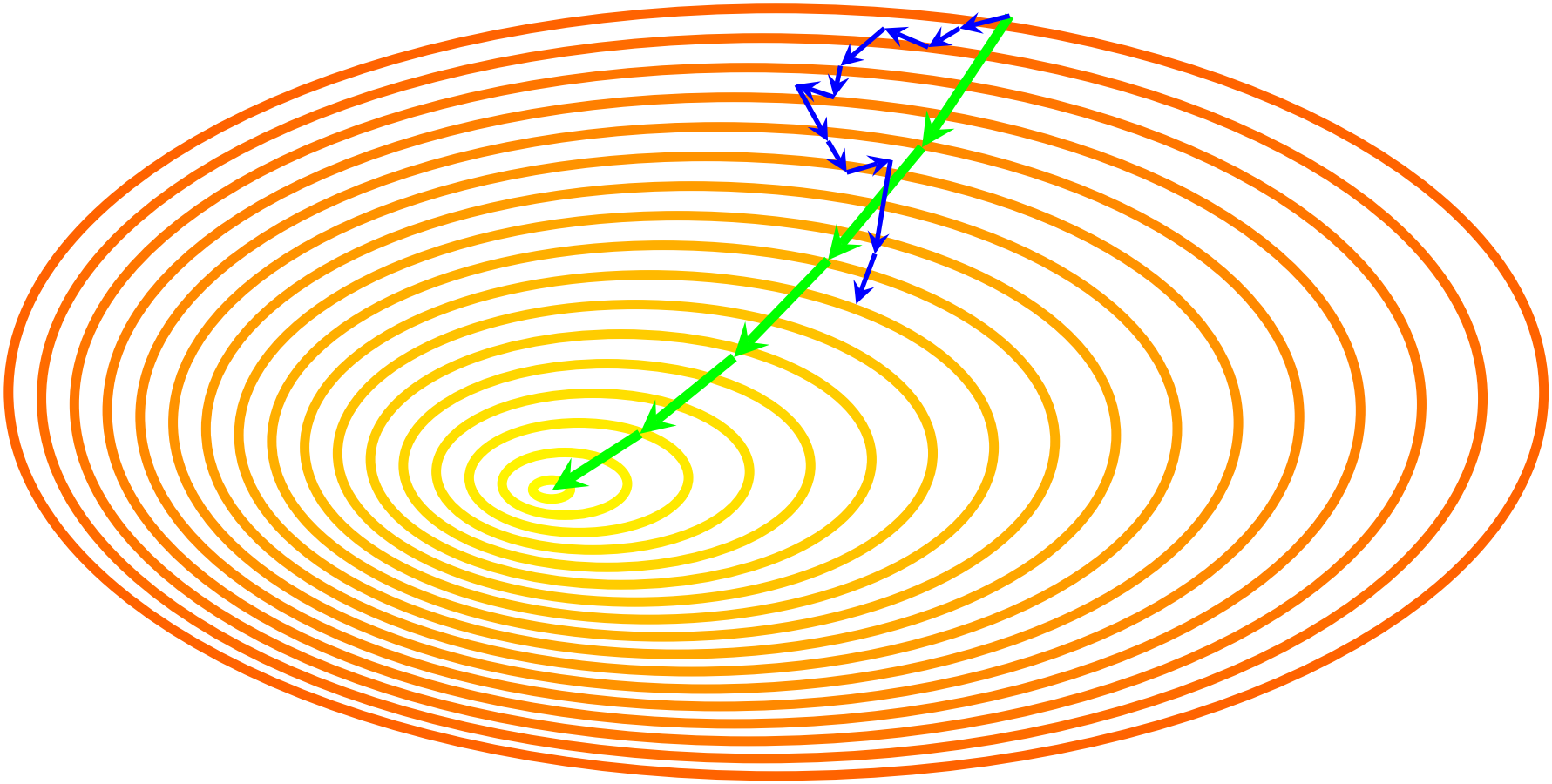

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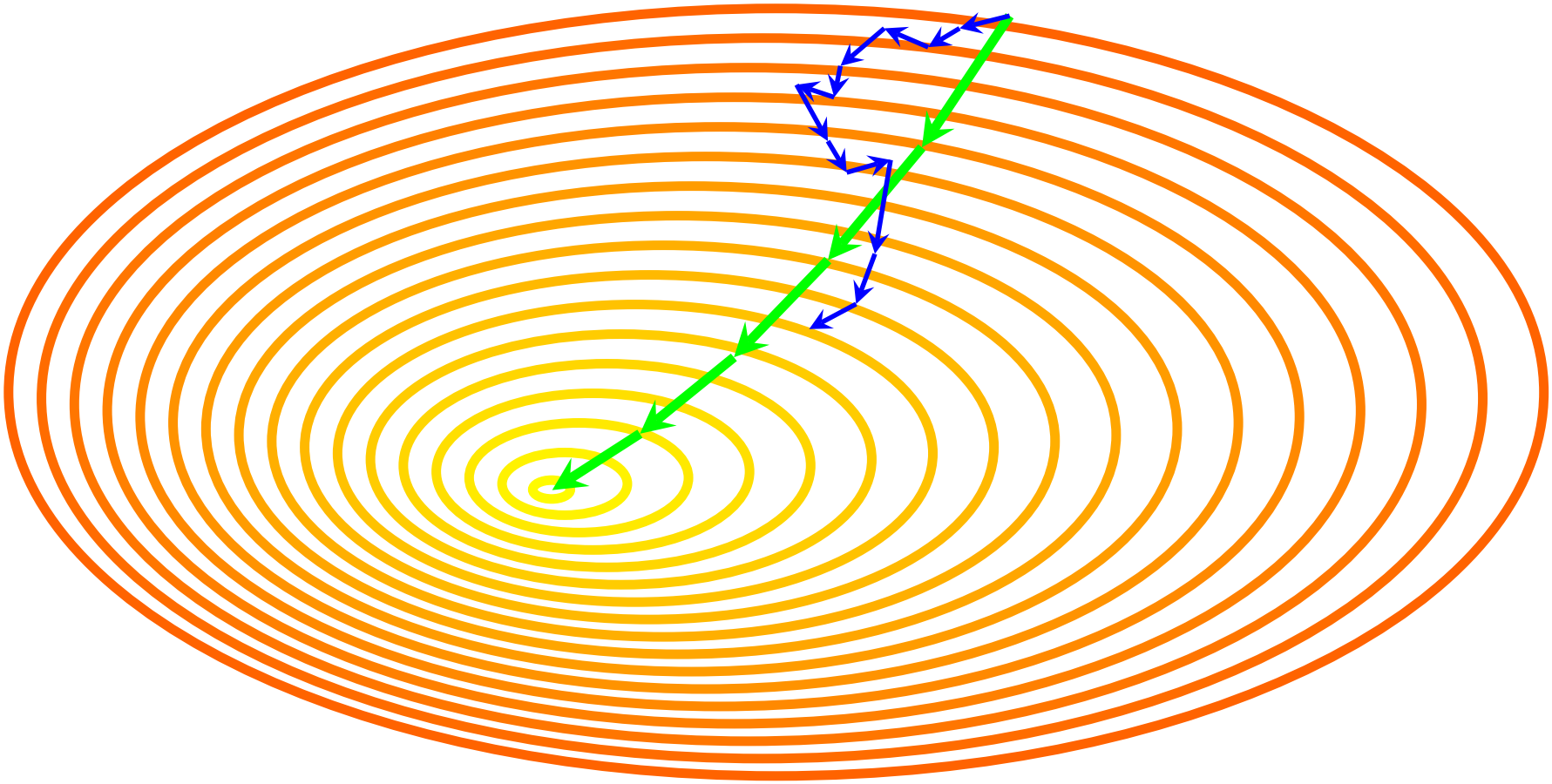

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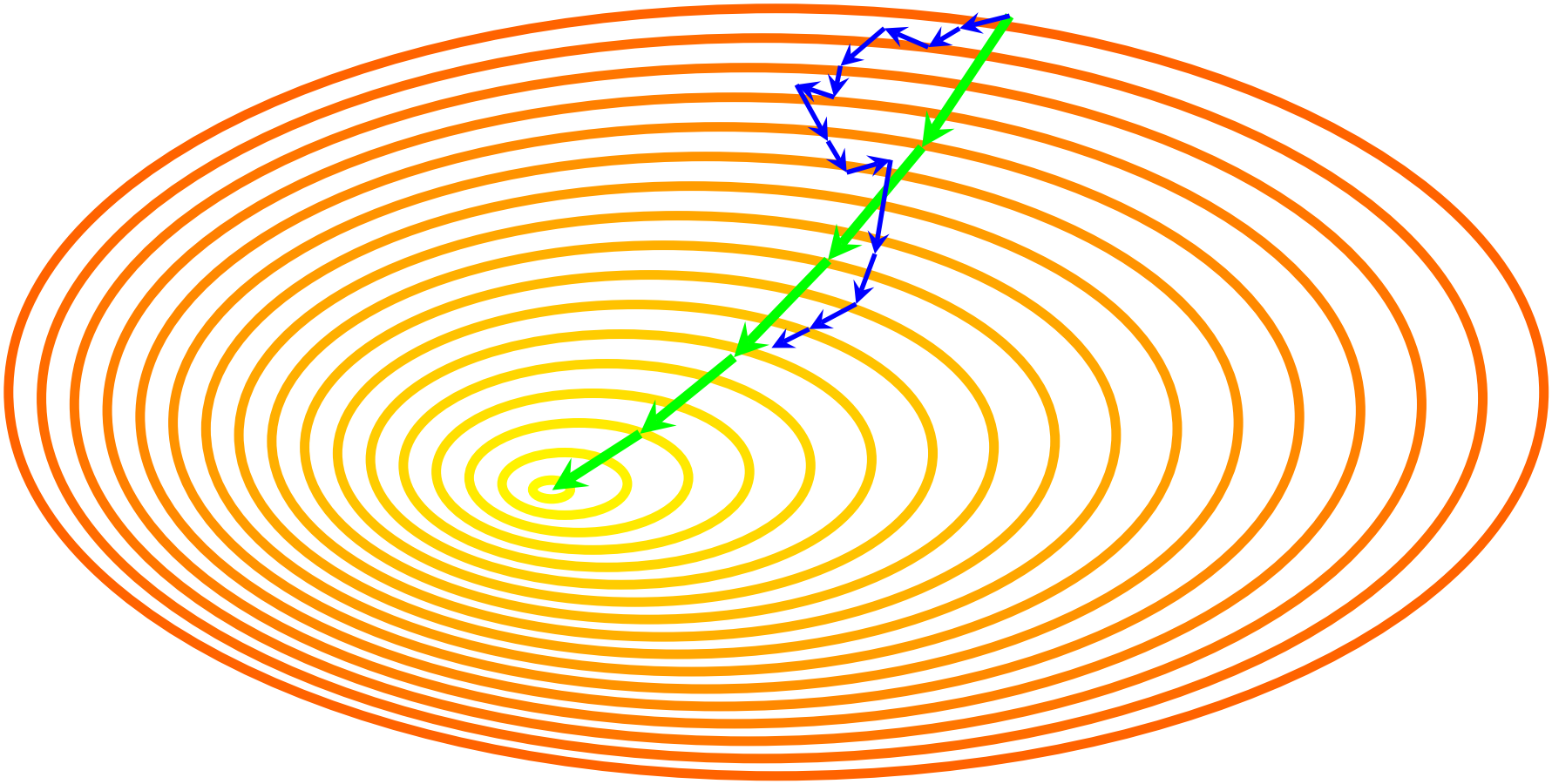

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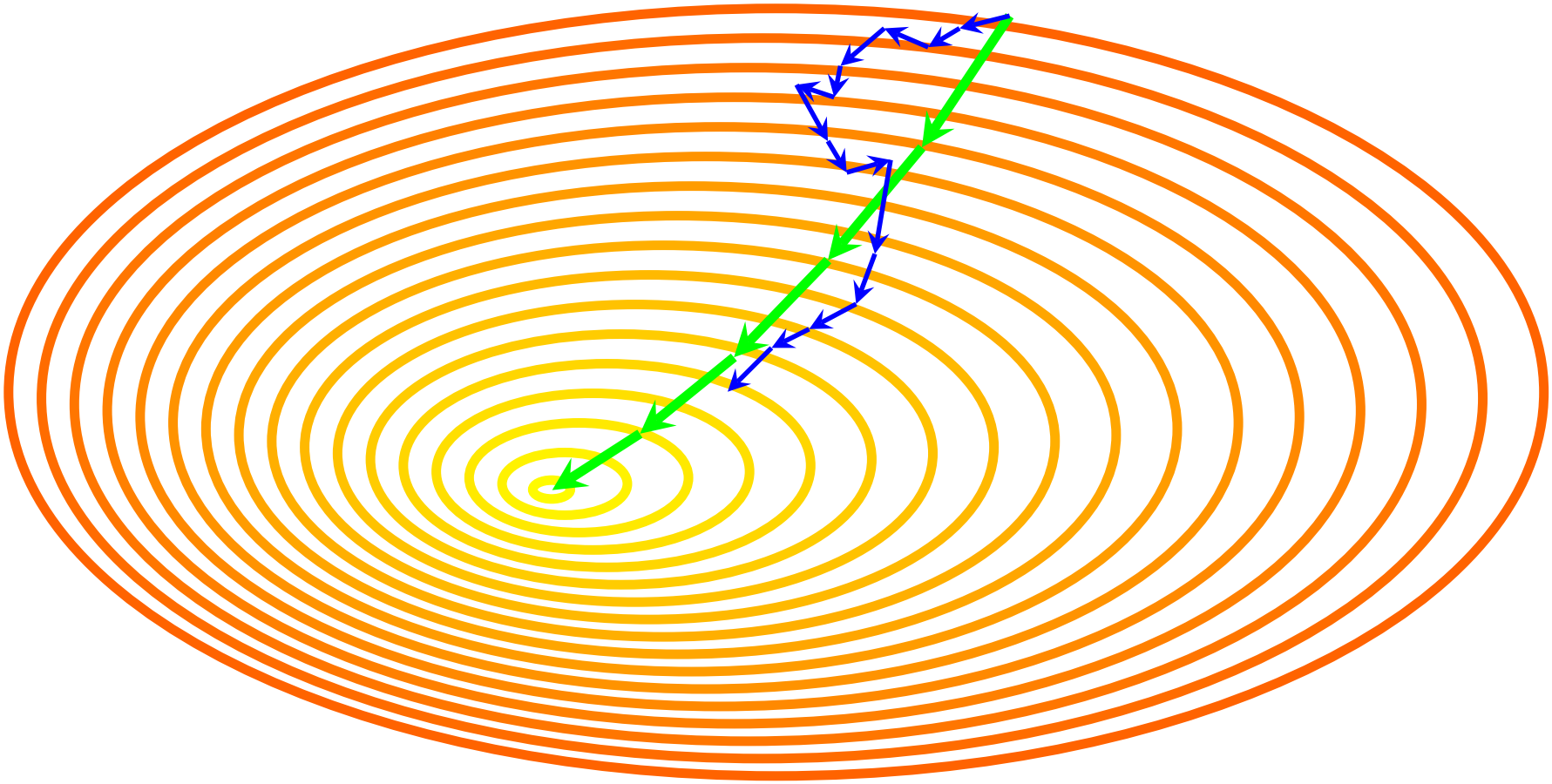

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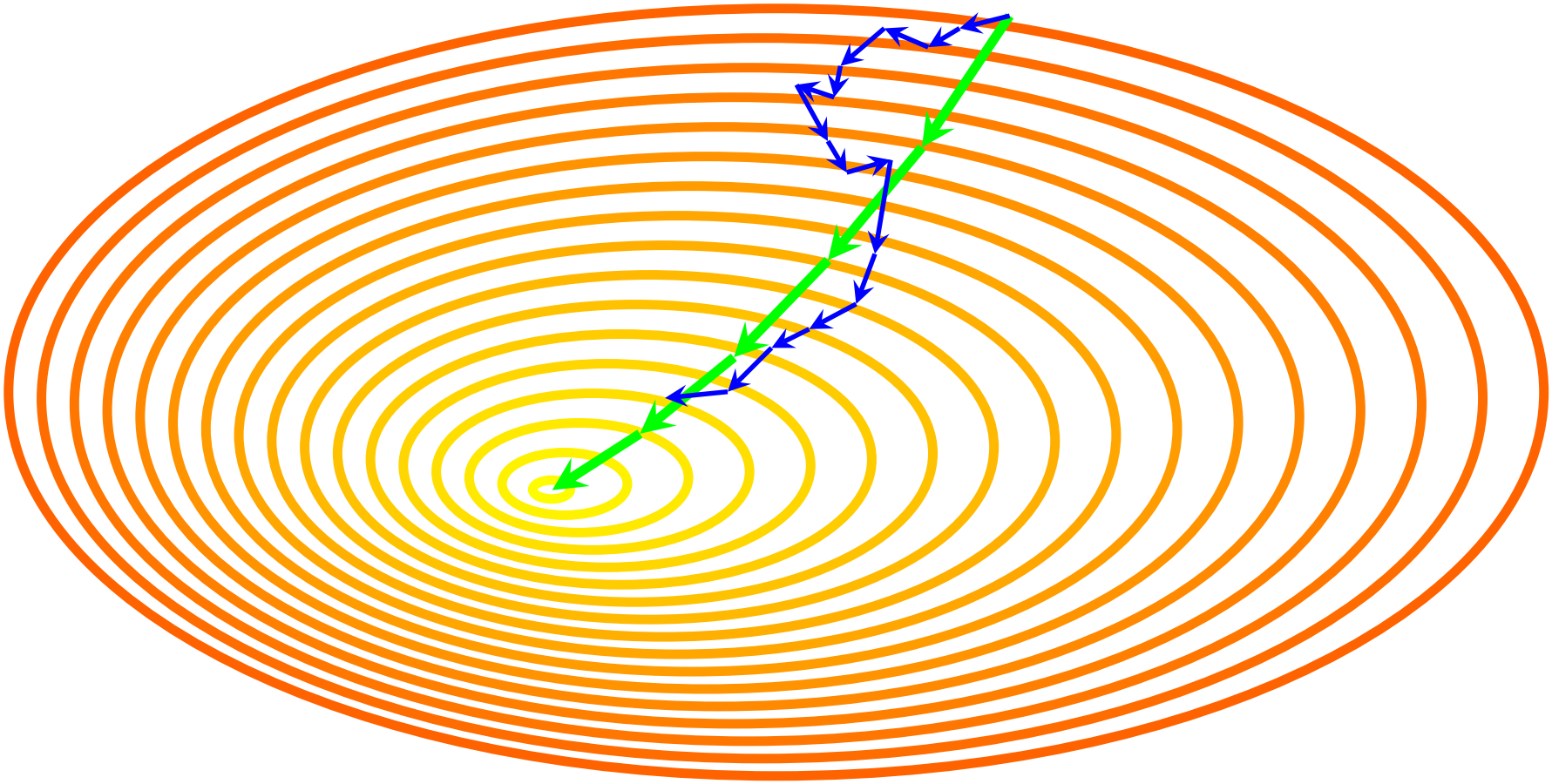

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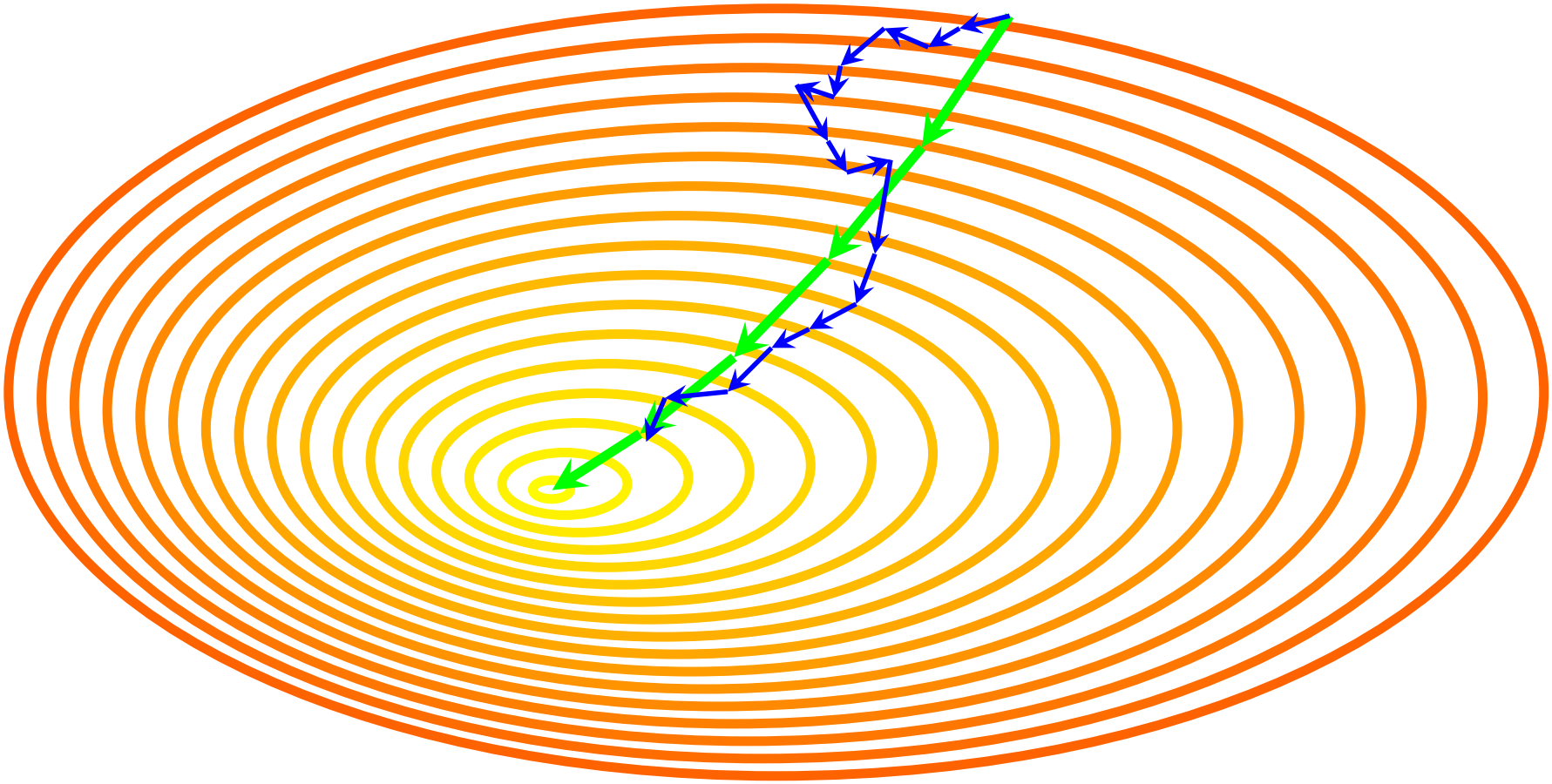

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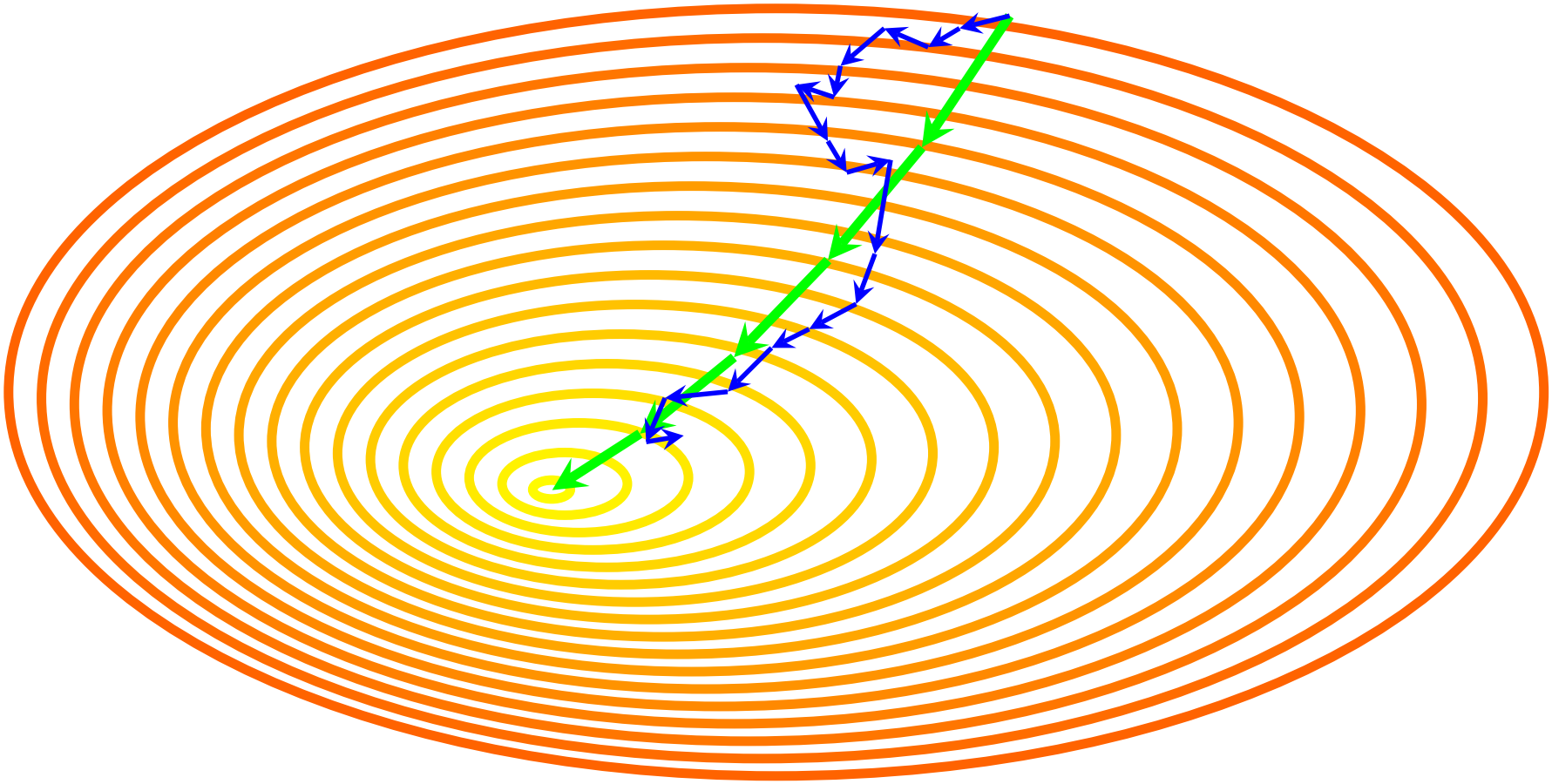

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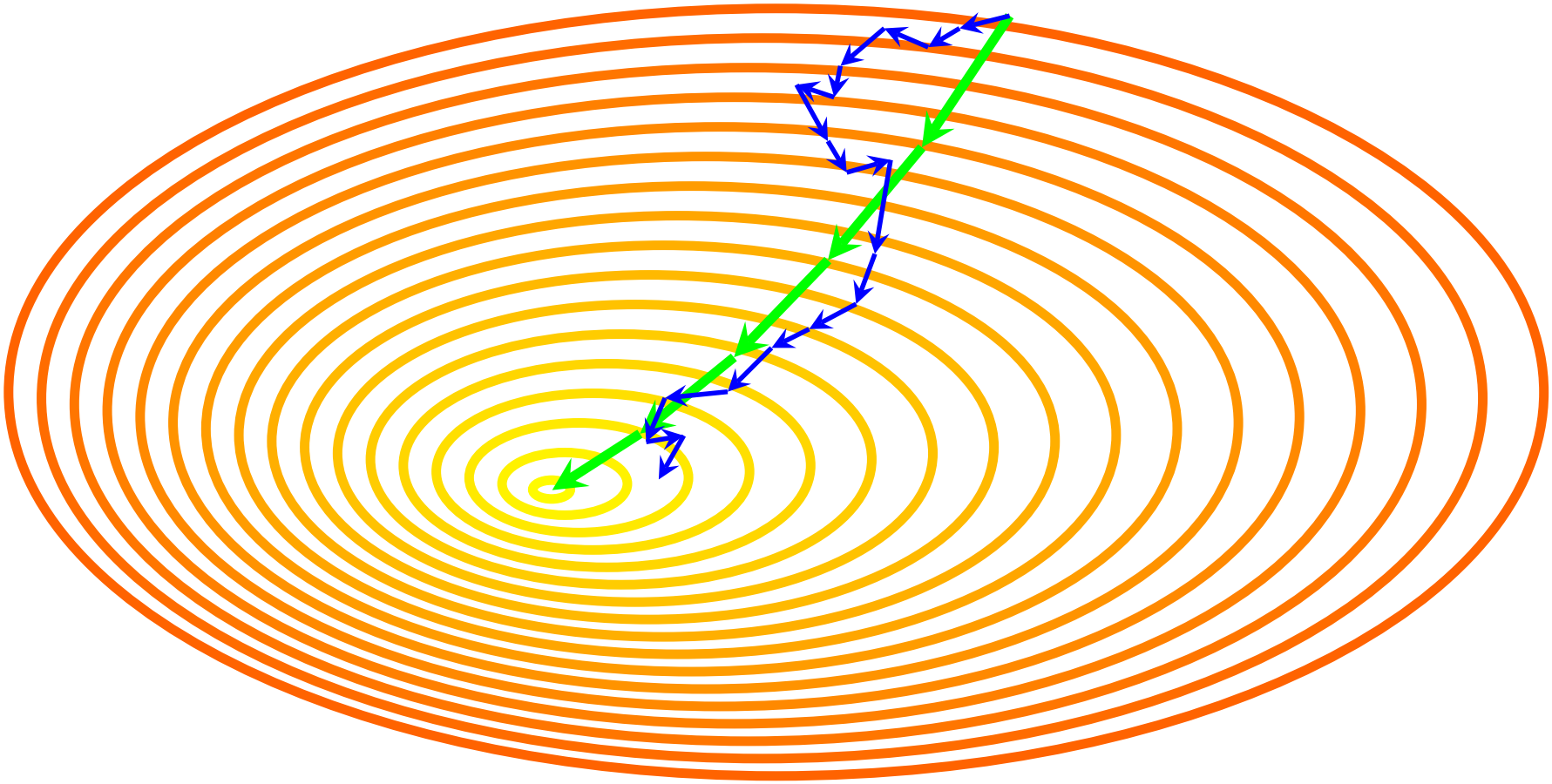

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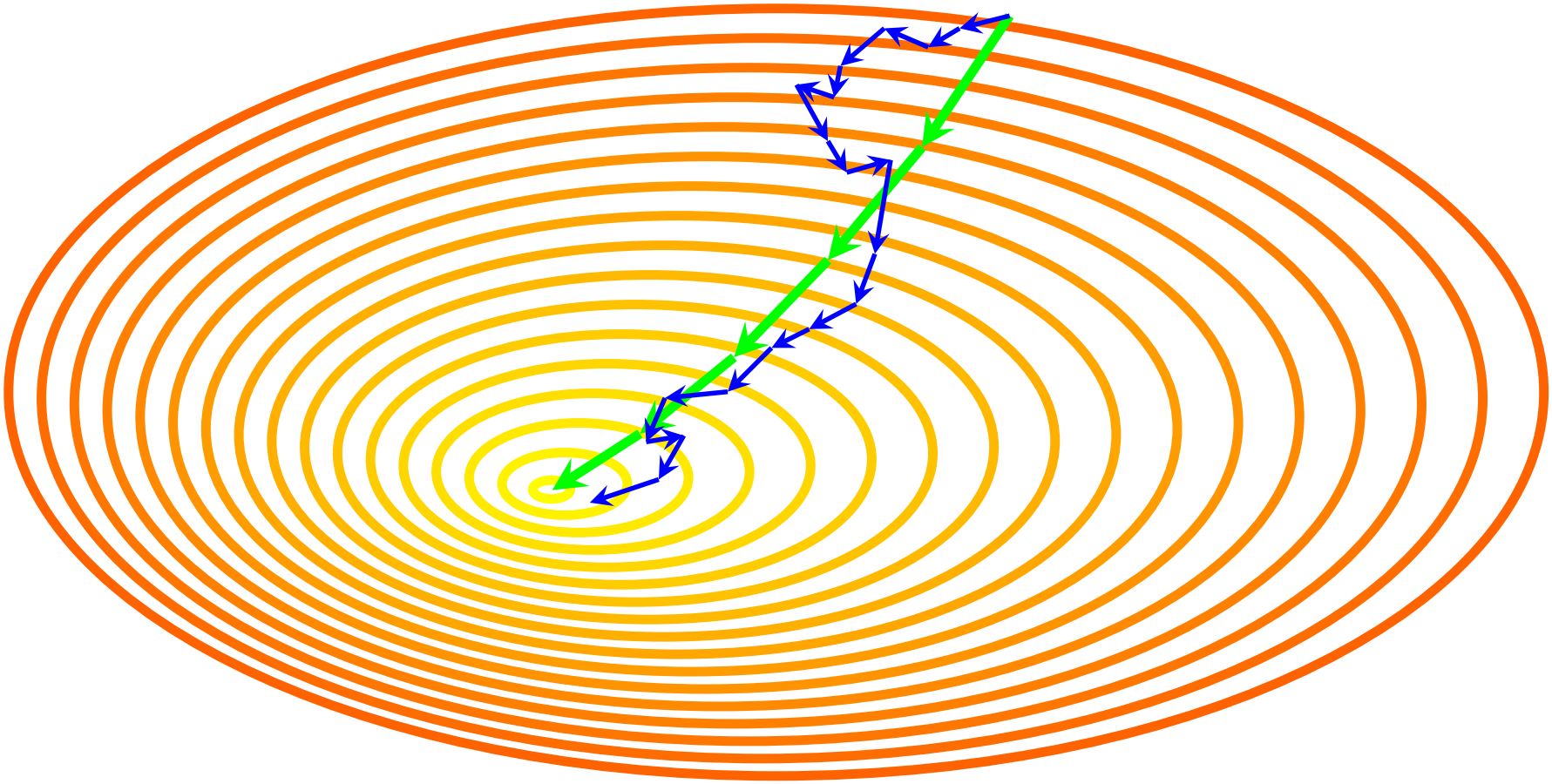

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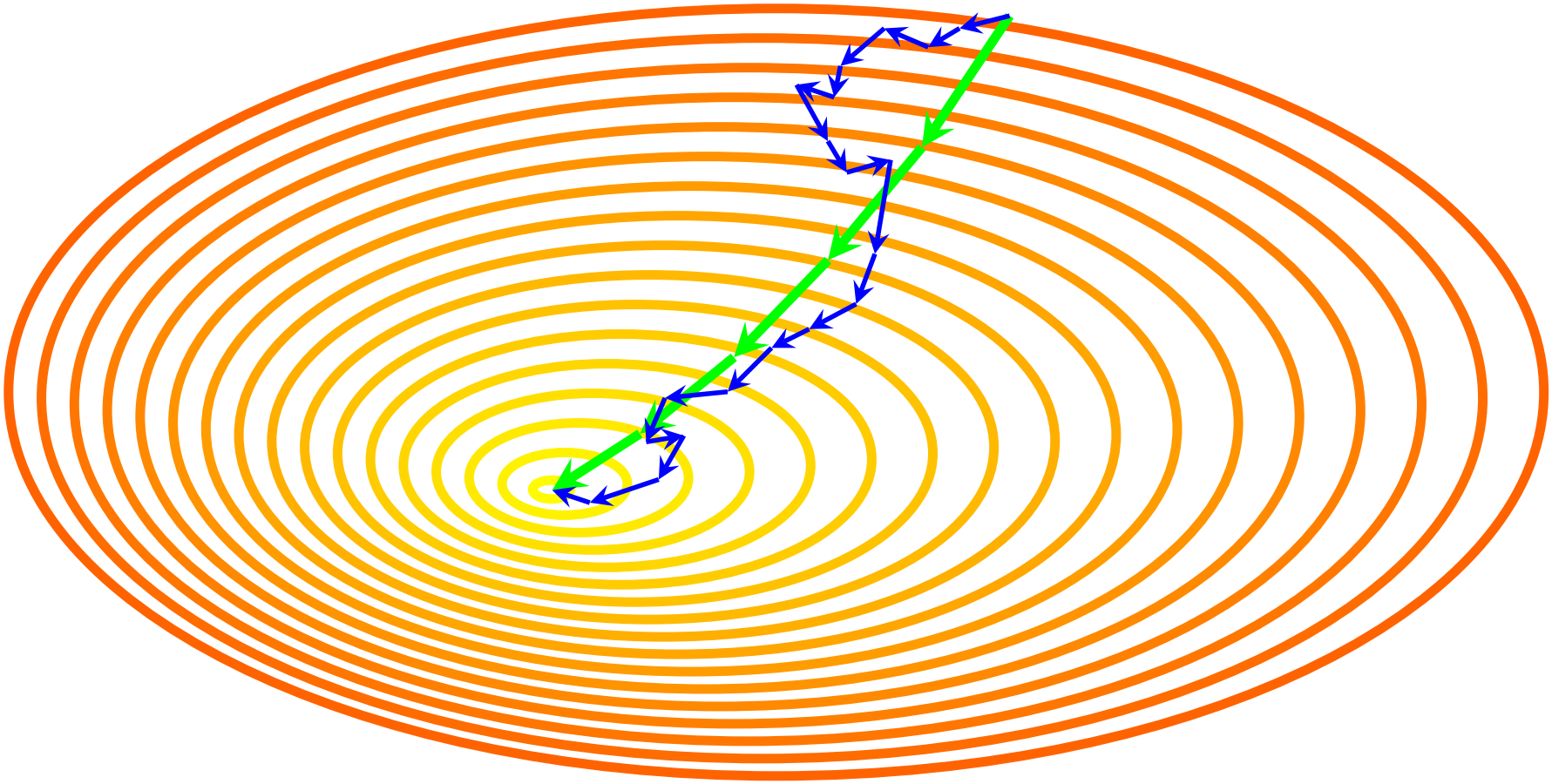

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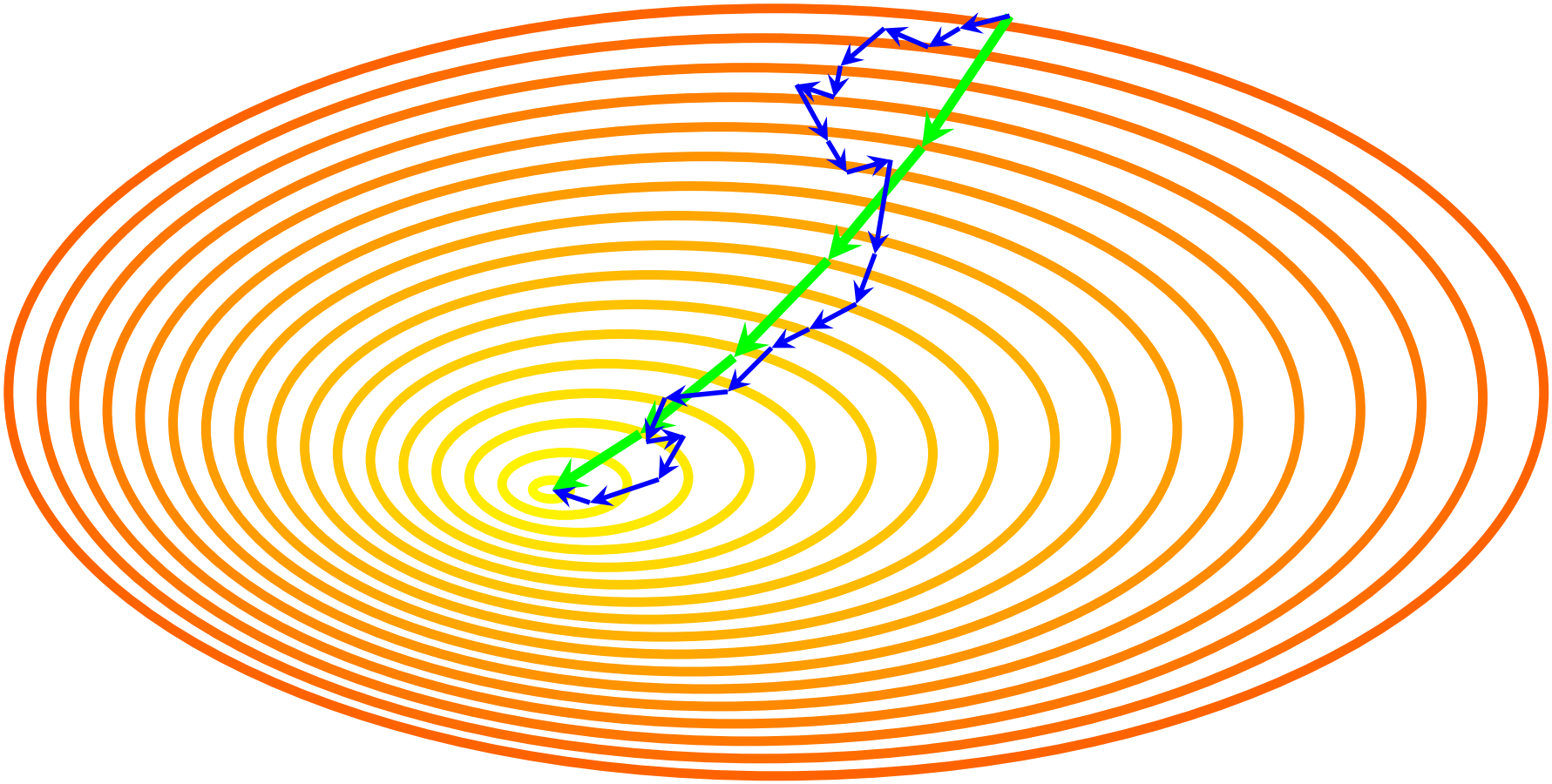

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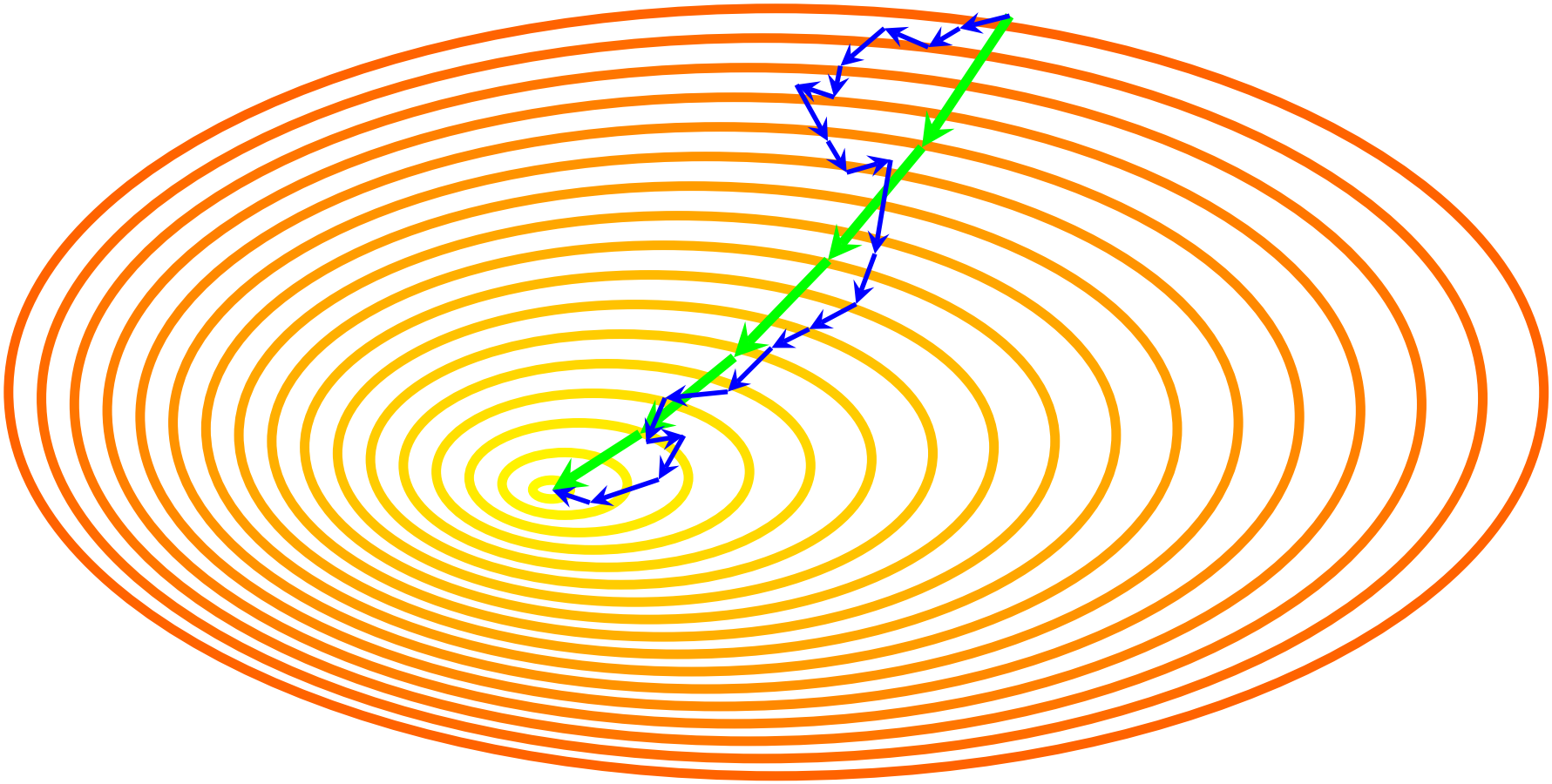
- Stochastic Gradient Descent: may converges more slowly and unsteadily.

Gradient versus Stochastic Gradient



- Gradient Descent: converges quickly and smoothly (usually).
- Stochastic Gradient Descent: may converges more slowly and unsteadily.

But: one iteration of Stochastic Gradient Descent can be computed much more easily!

Recall: One-Dimensional Example

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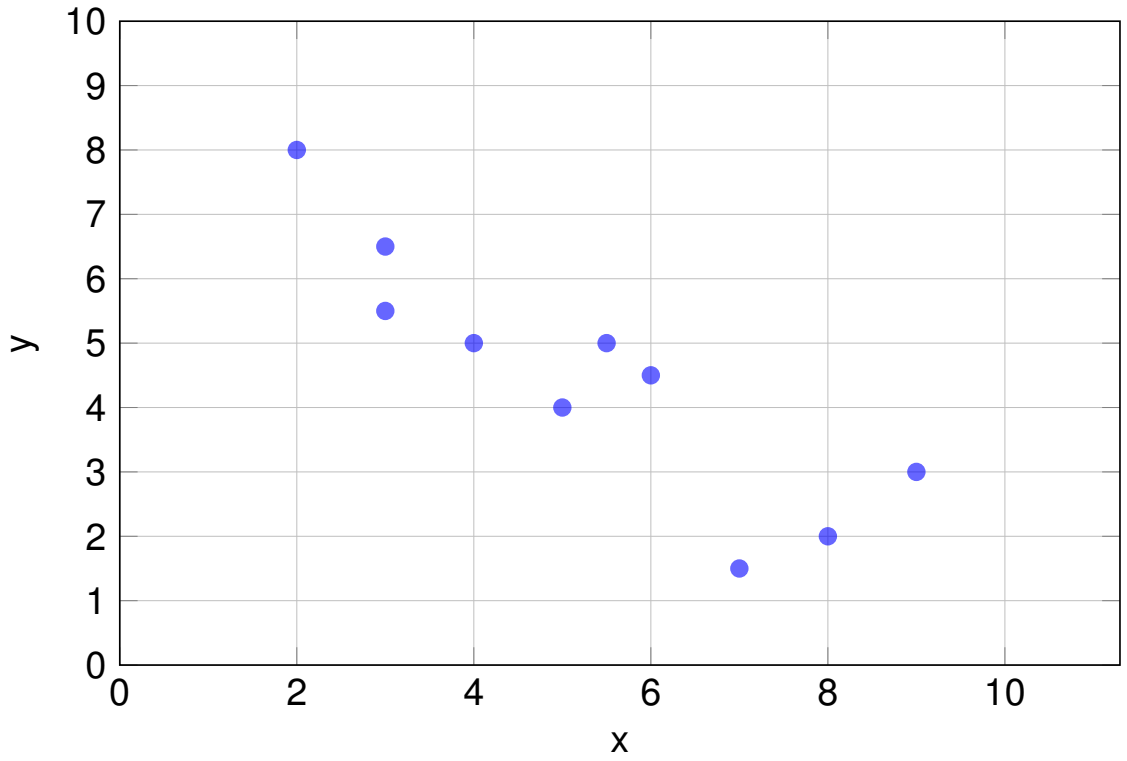

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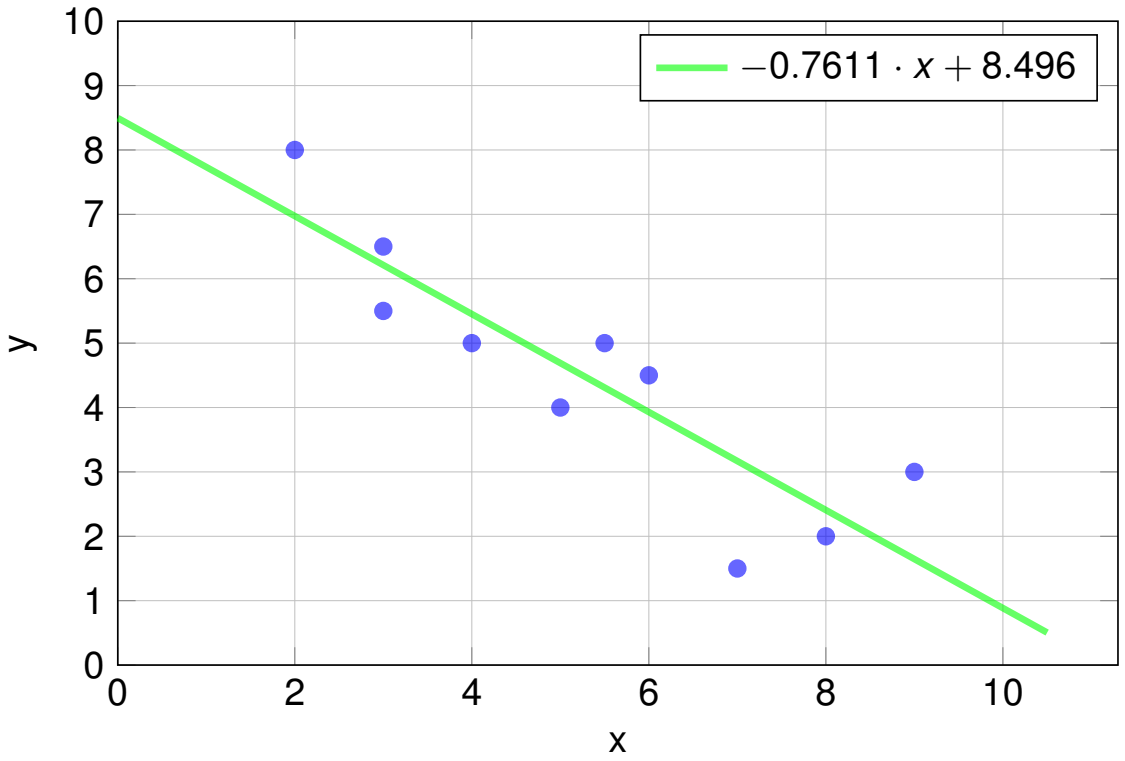

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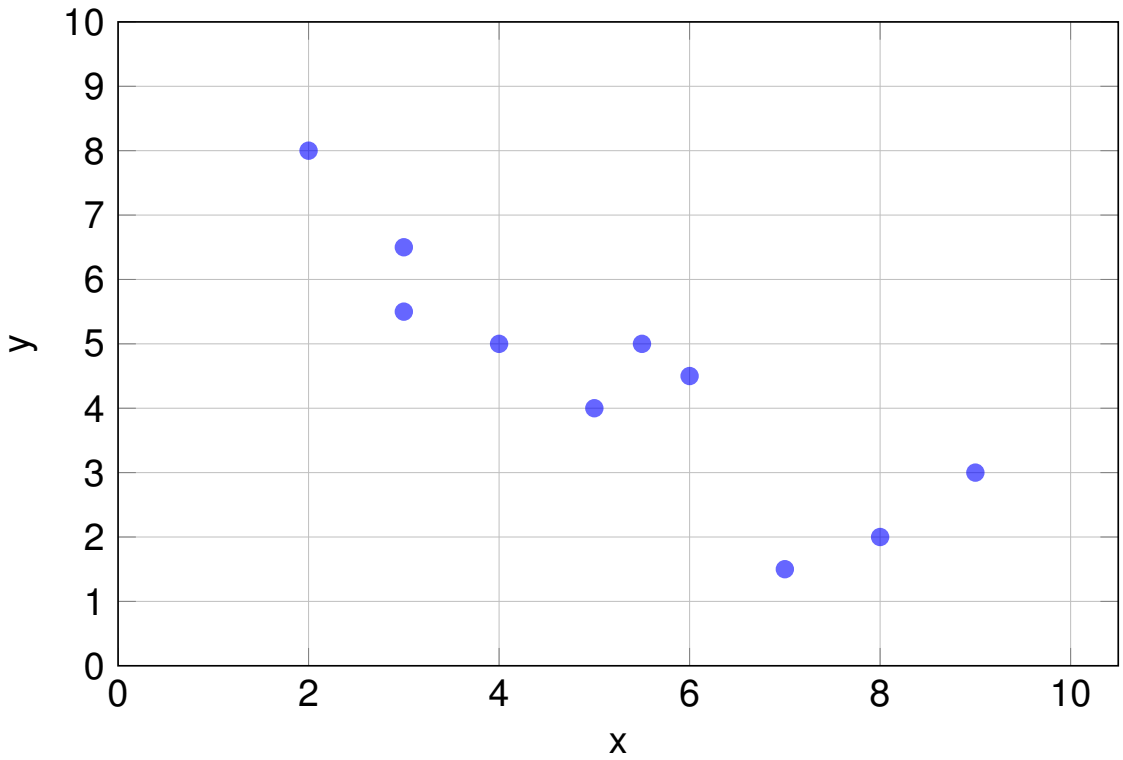

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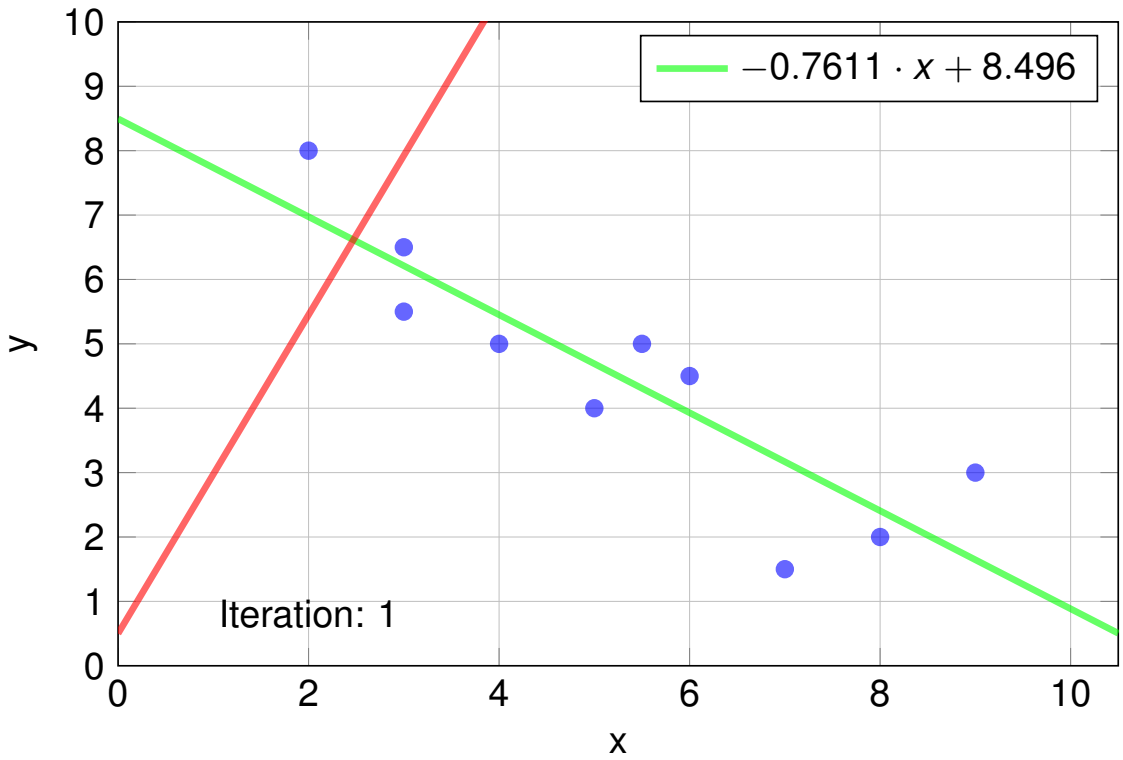

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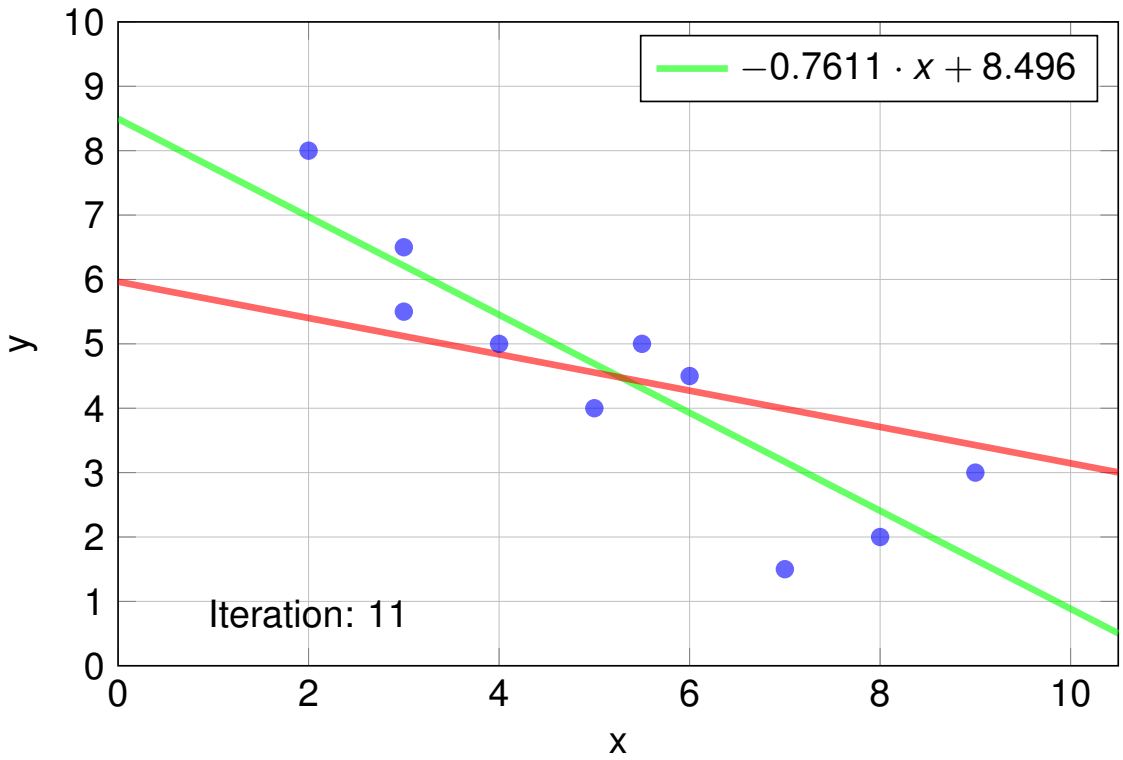

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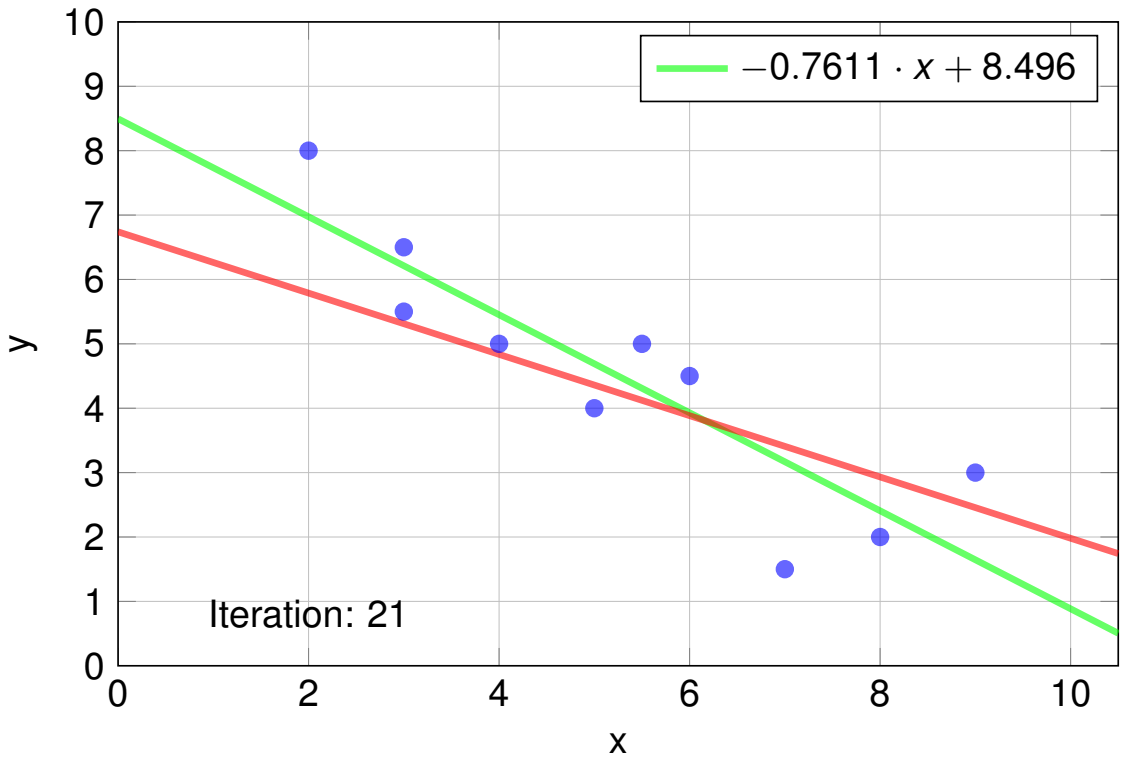

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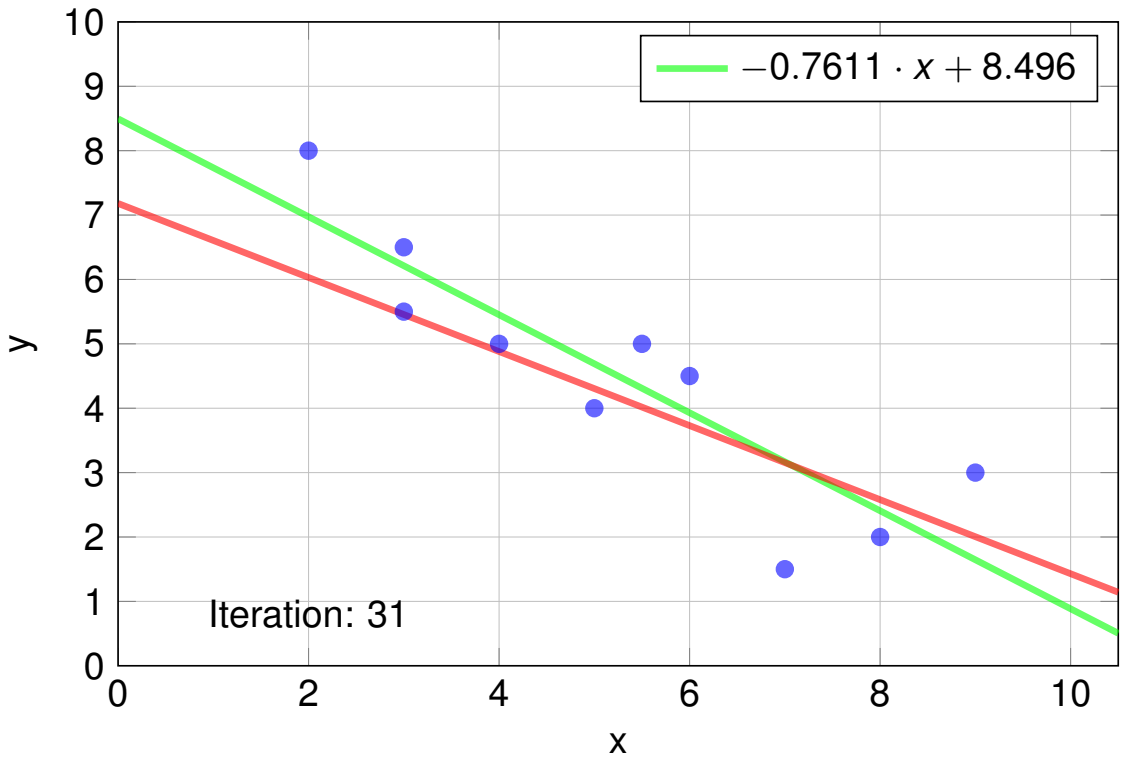

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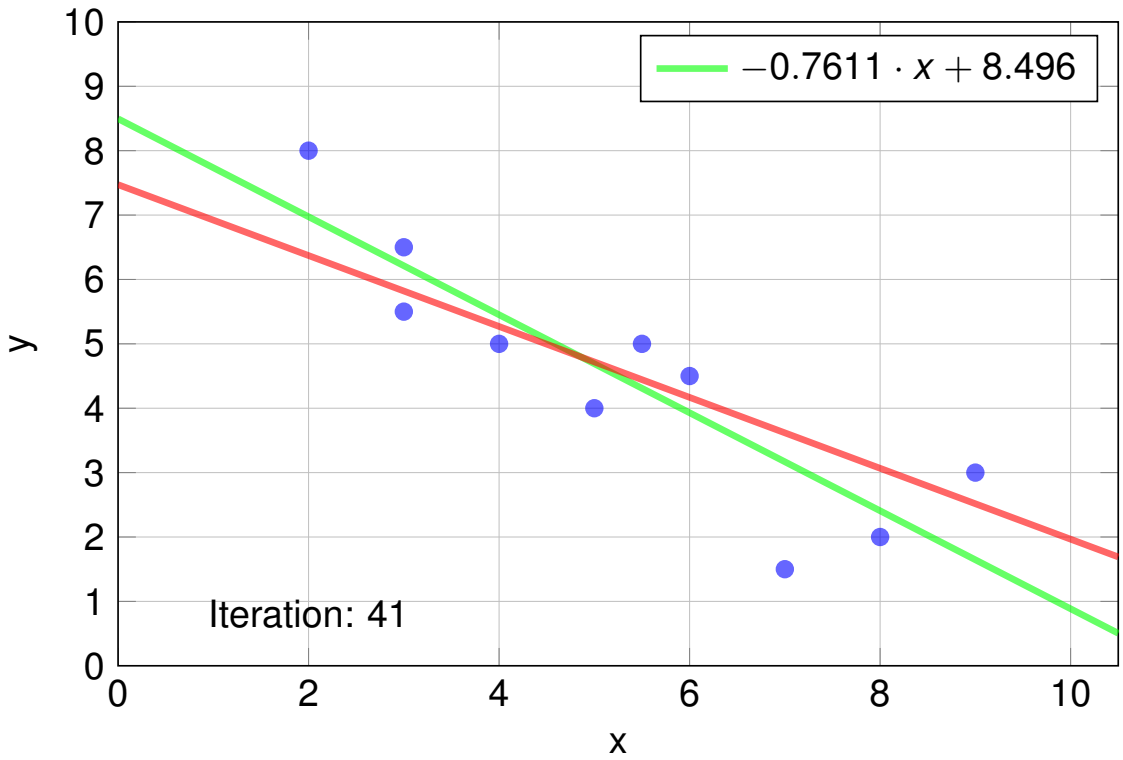

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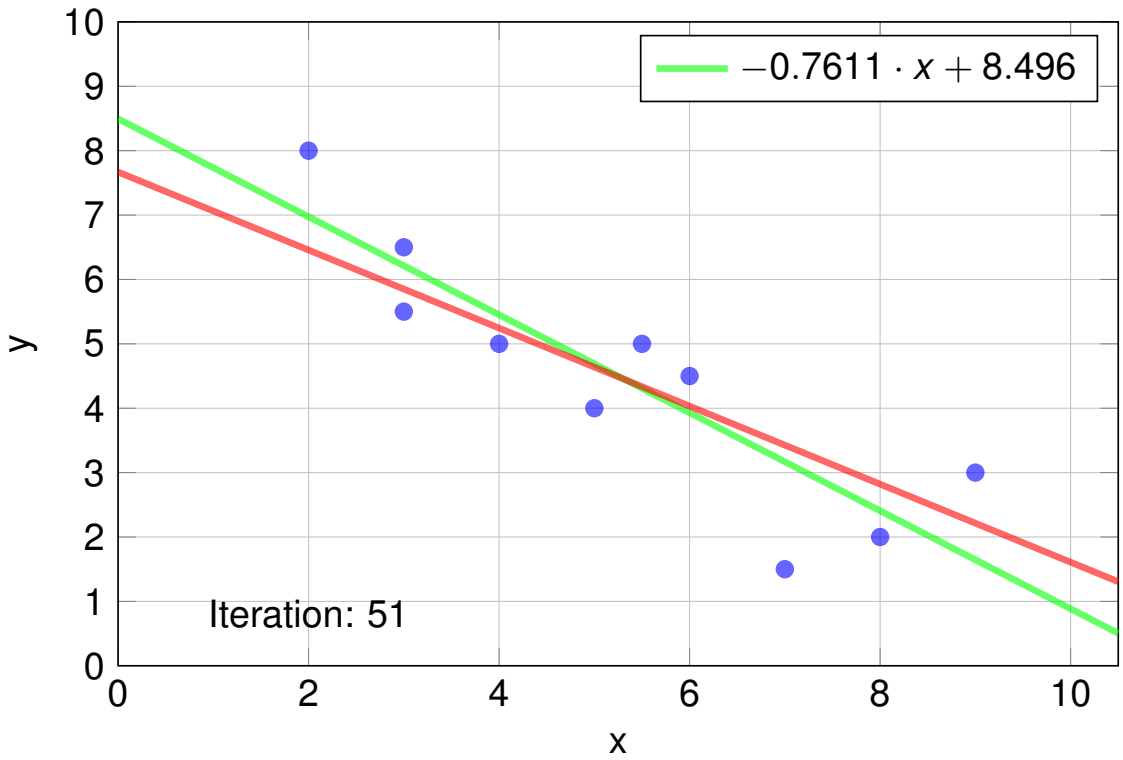

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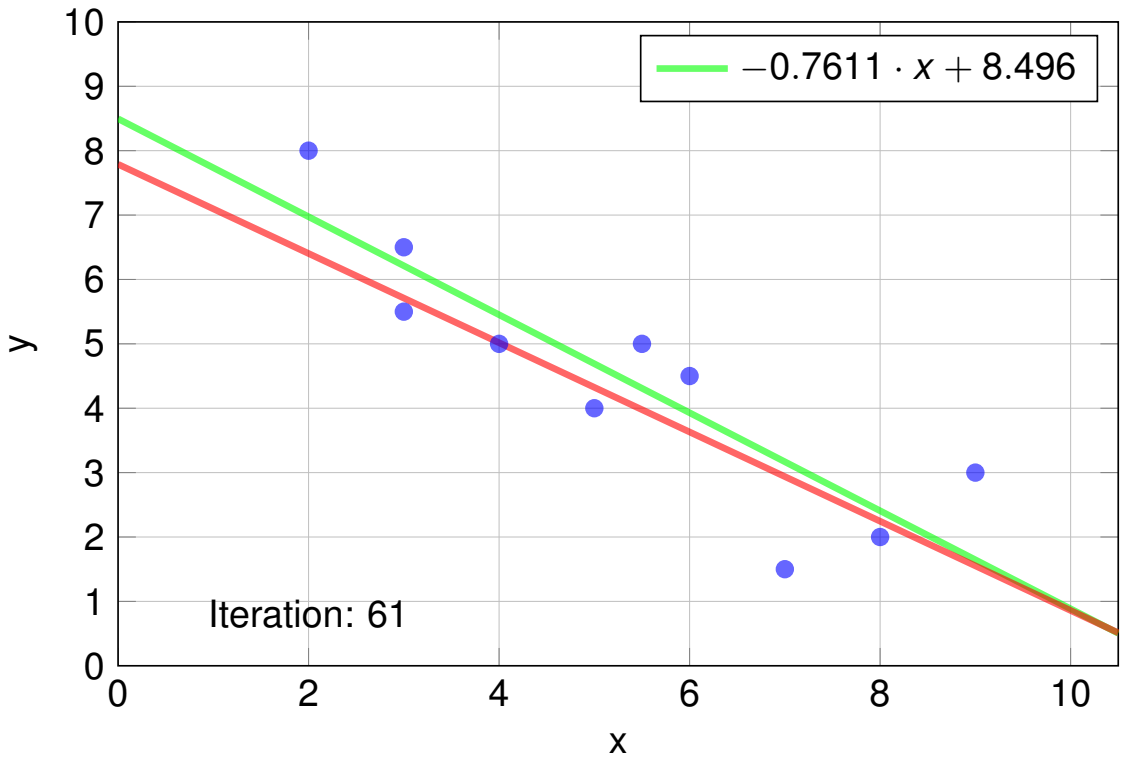

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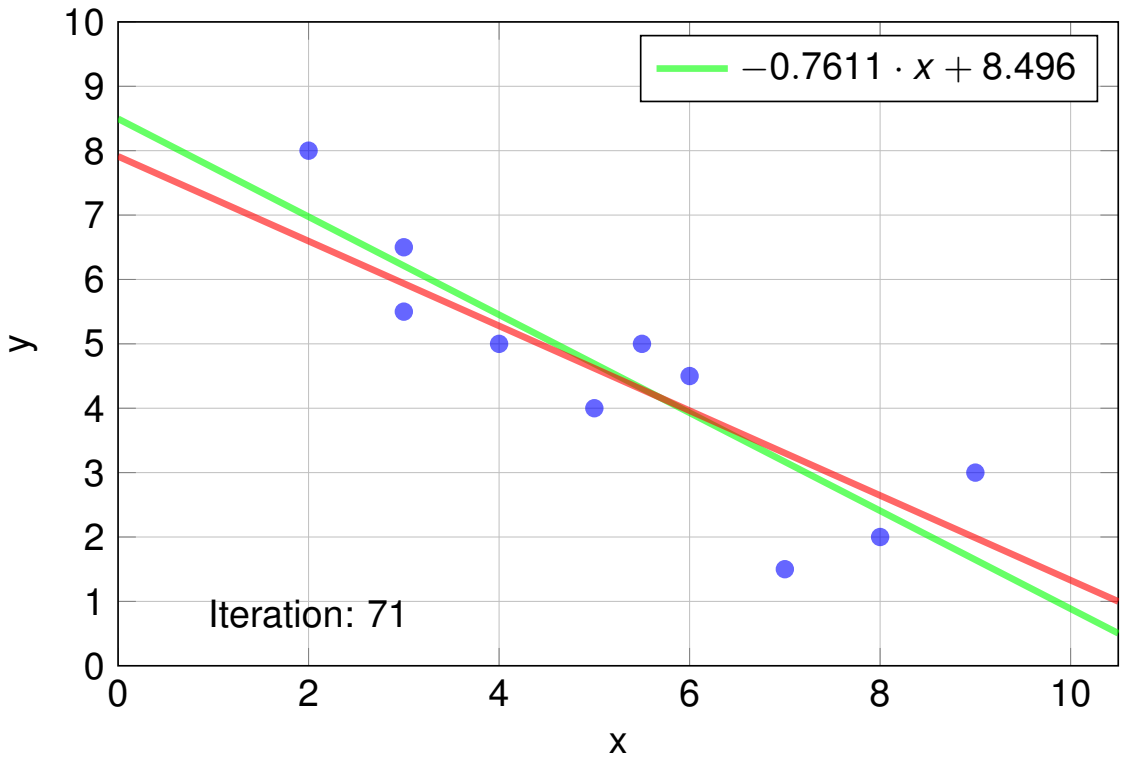

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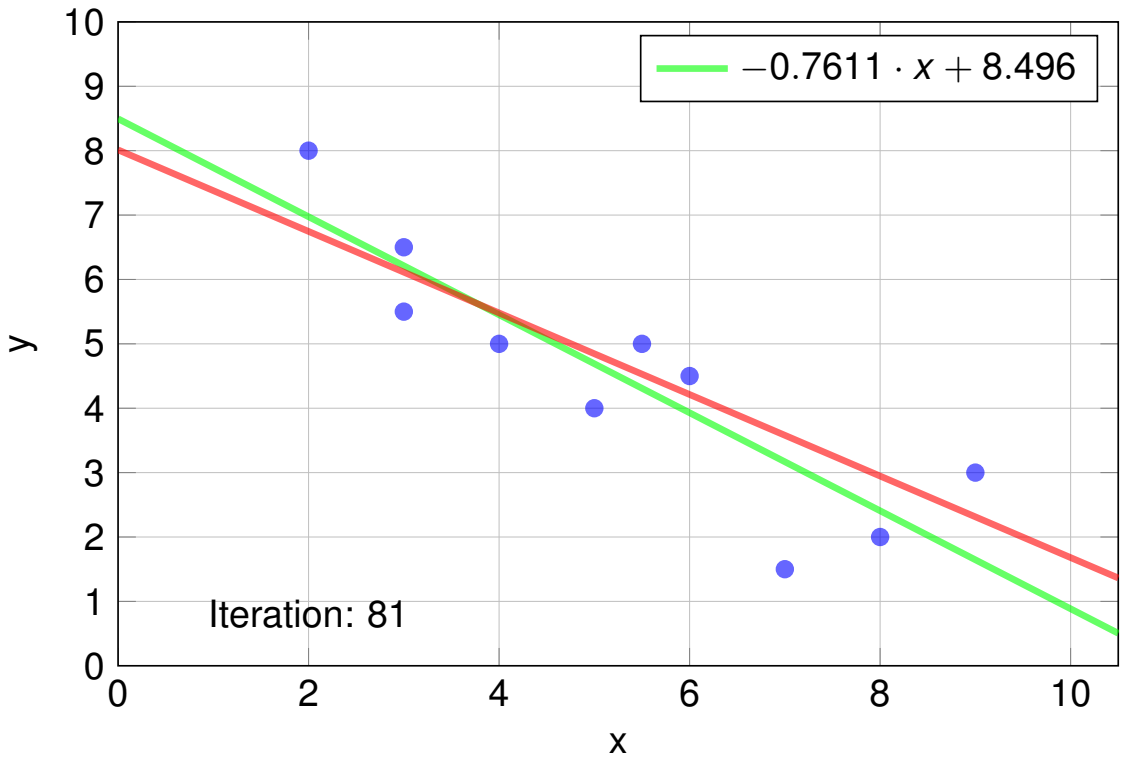

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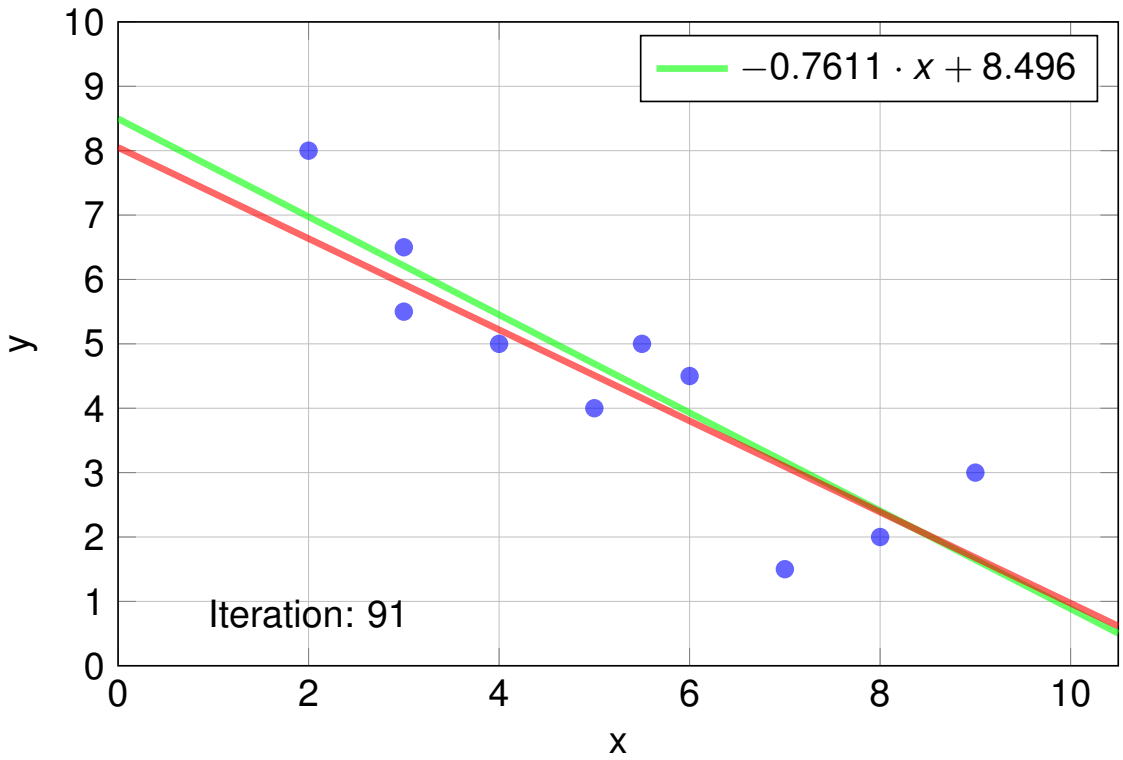

Outline

Introduction

Linear Regression

Linear Regression with More than One Feature

Solving Linear Regression: Gradient Descent

Logistic Regression

Origin of Logistic Regression in Economics

Daniel McFadden (1937–)

James Heckman (1944–)

Nobel Prize of Economics (2000)

"James Heckman and Daniel McFadden have each developed theory and methods that are widely used in the statistical analysis of individual and household behavior, within economics as well as other social sciences."

Motivation: Back to Our Example

- Suppose we only know if student has passed or failed exam
- That is, we do **not** know the grade

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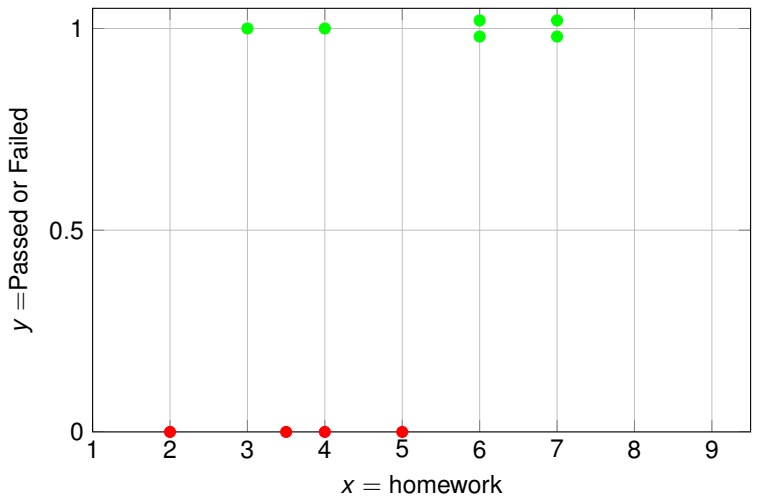

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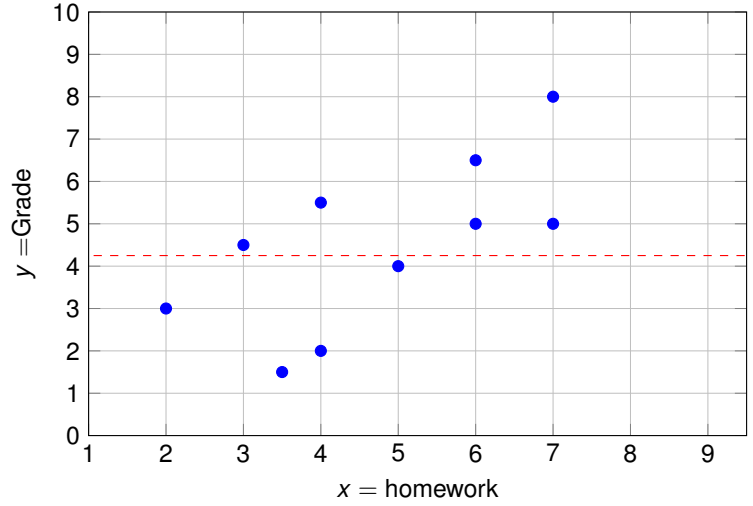

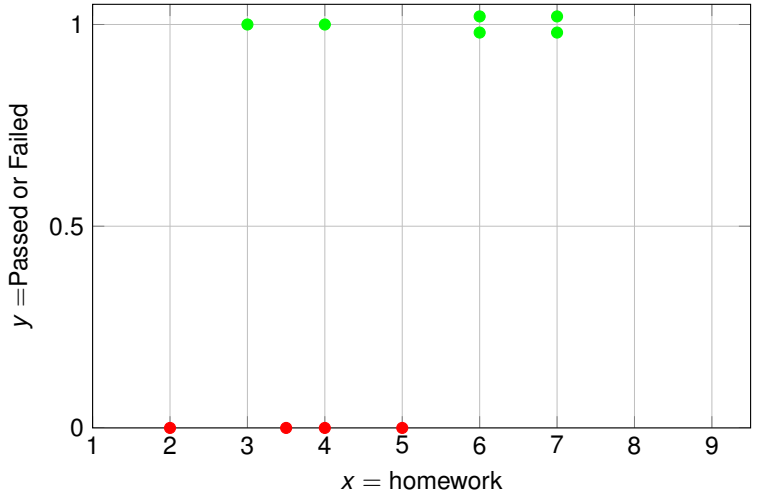

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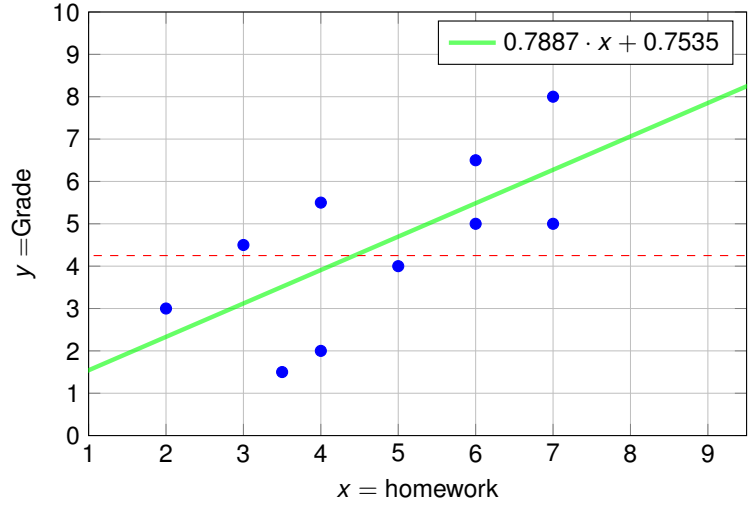

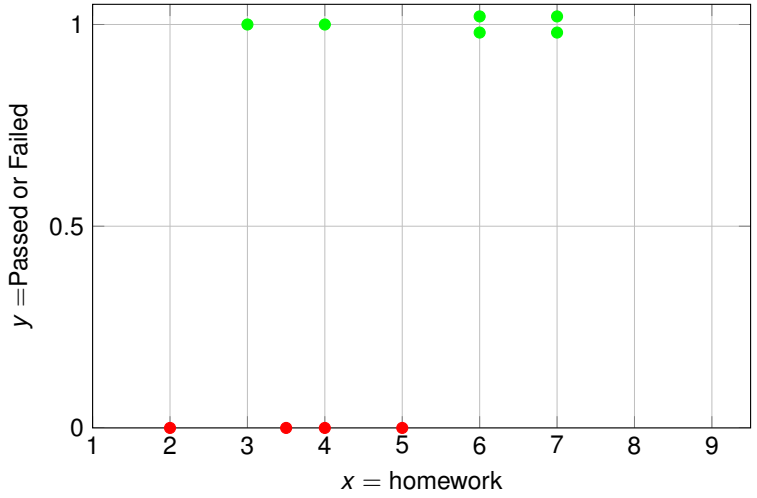

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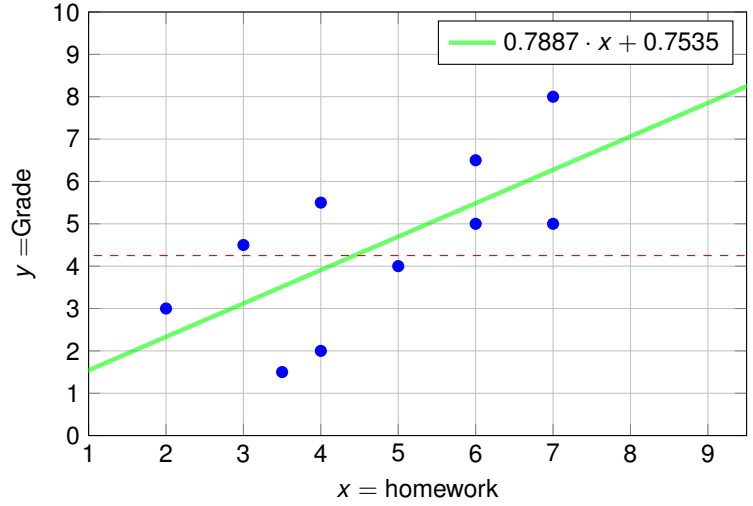

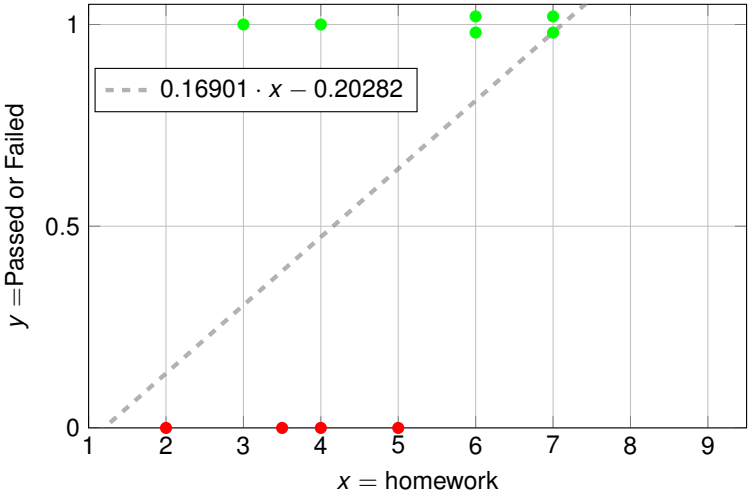

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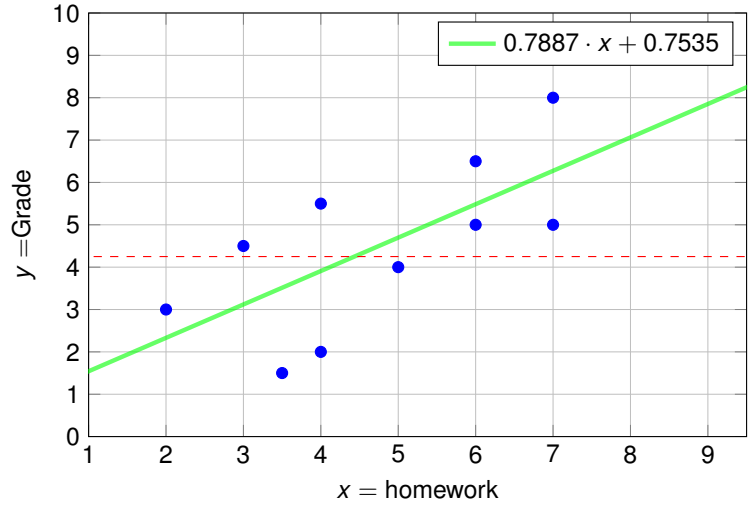

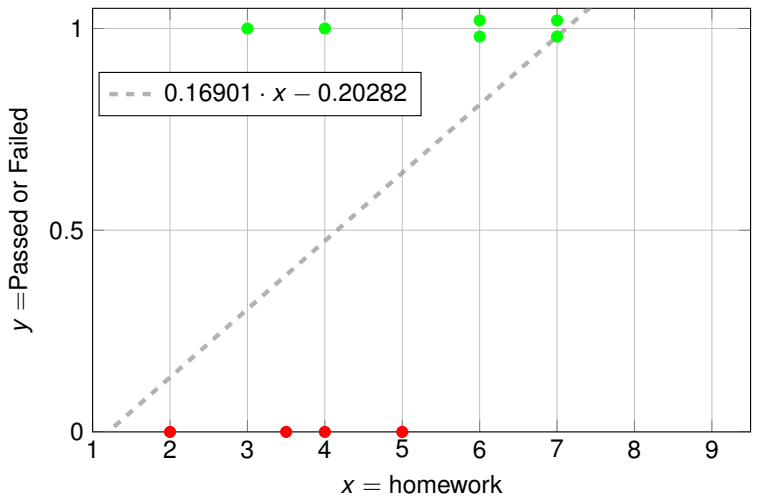

Exercise 3: What are the problems with using the regression line?

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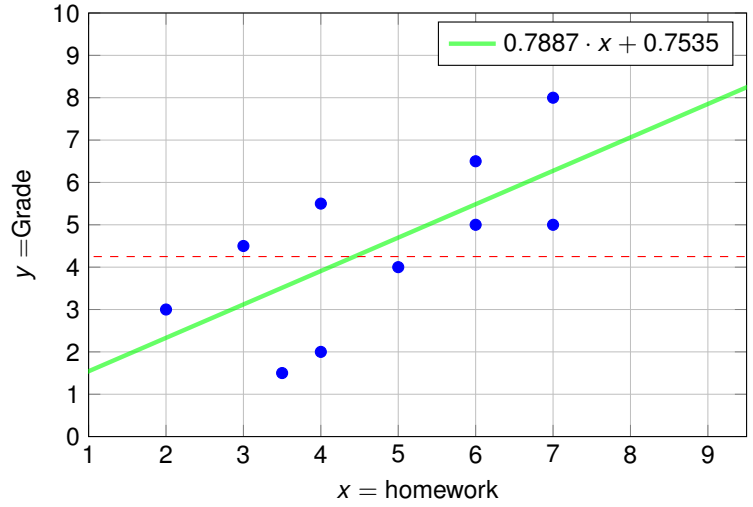

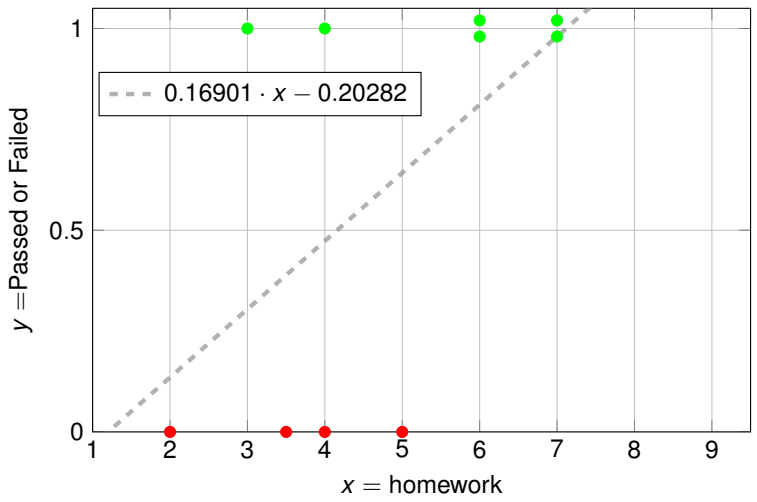

Need a model that assigns only values 1 (passed) and 0 (failed)!

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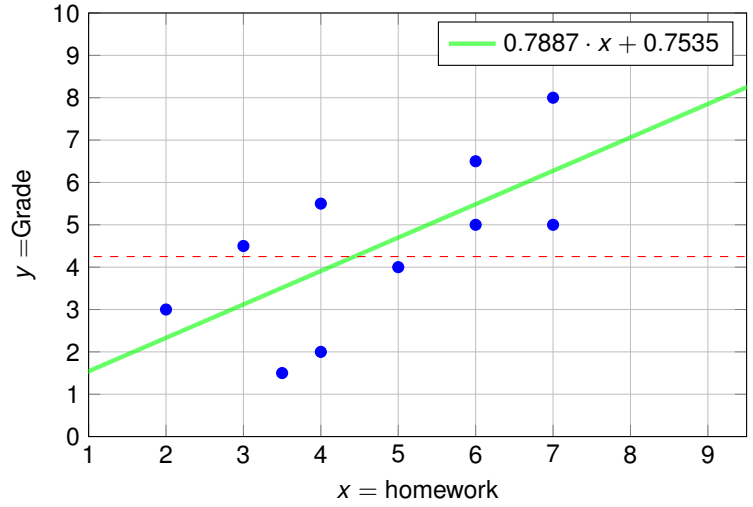
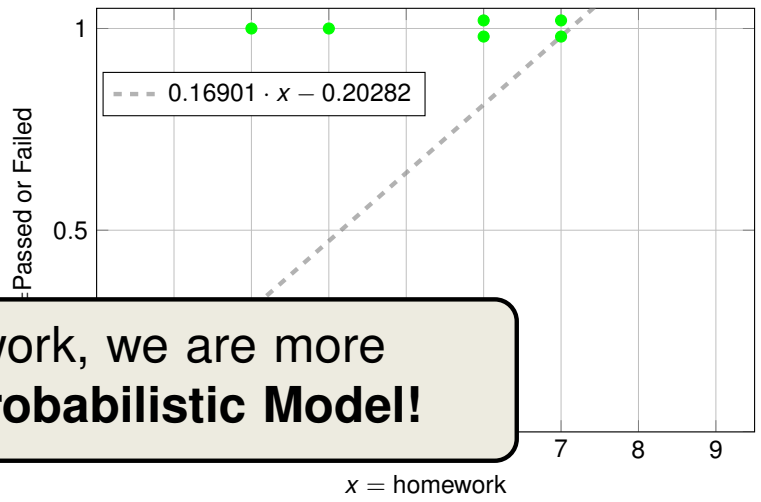
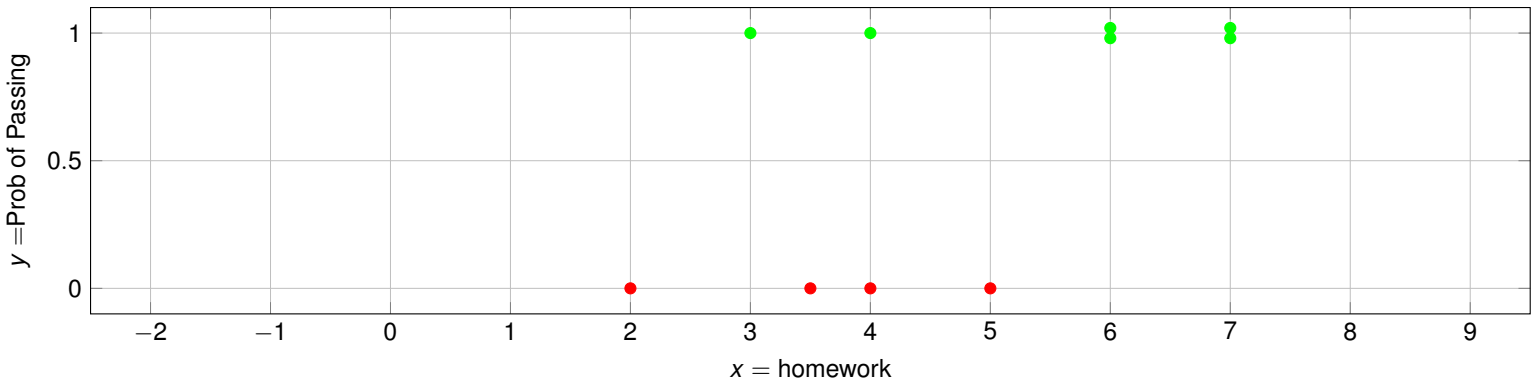




For students that did better on homework, we are more "confident" in predicting a pass! $\rightsquigarrow$ **Probabilistic Model!**

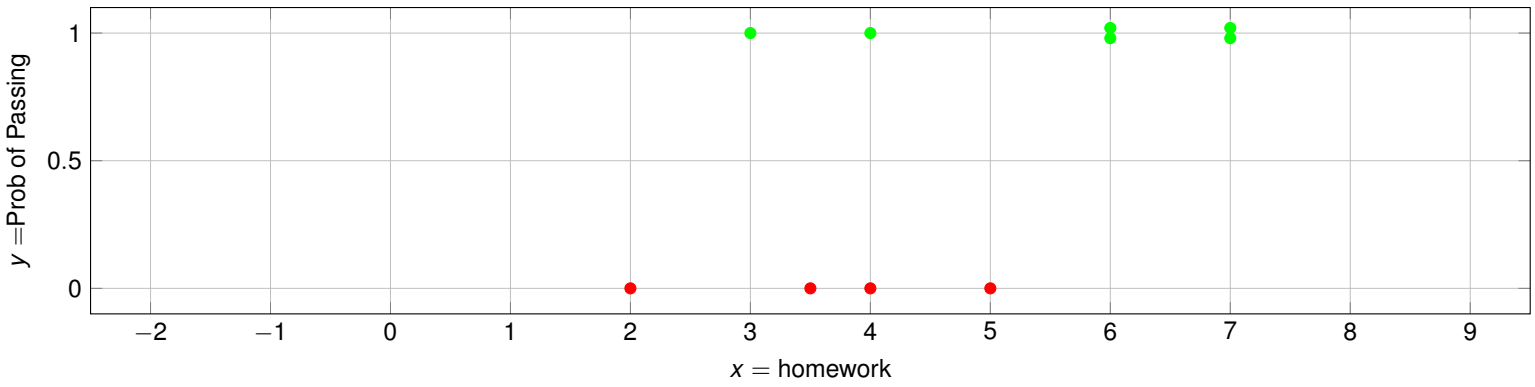
Need a model that assigns only values 1 (passed) and 0 (failed)!

The Logistic Function



- If student did homework very well, then high probability to pass exam

The Logistic Function



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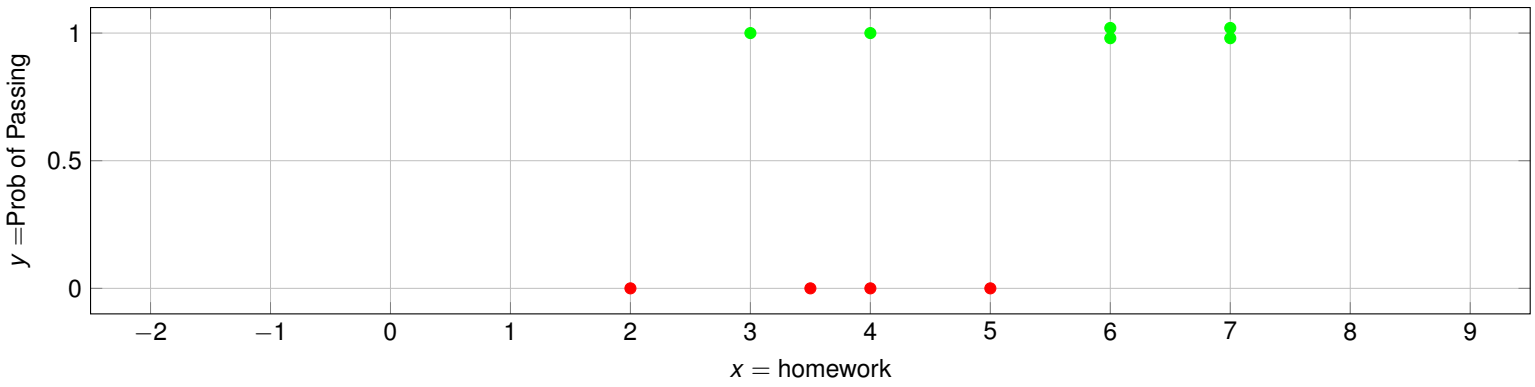

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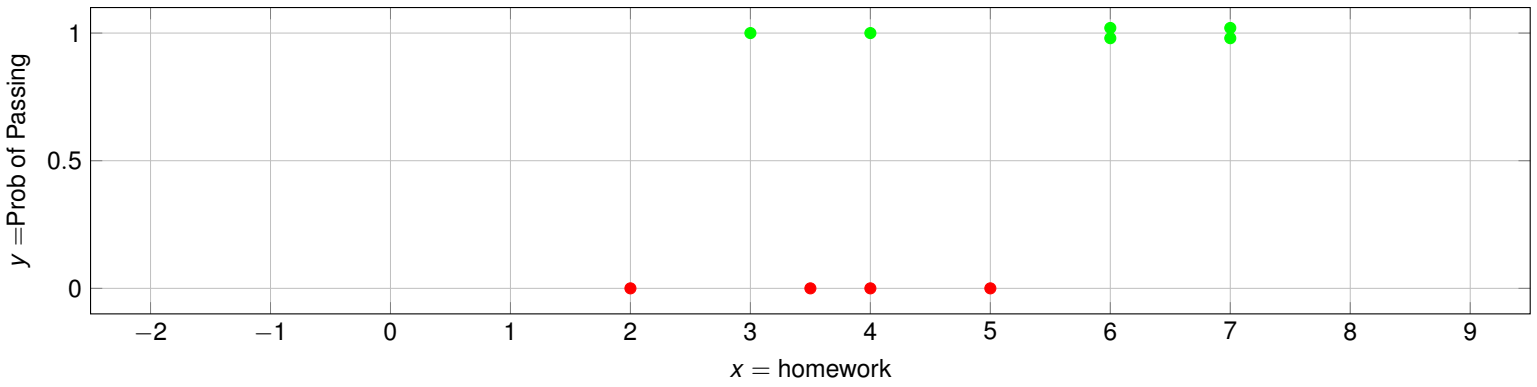

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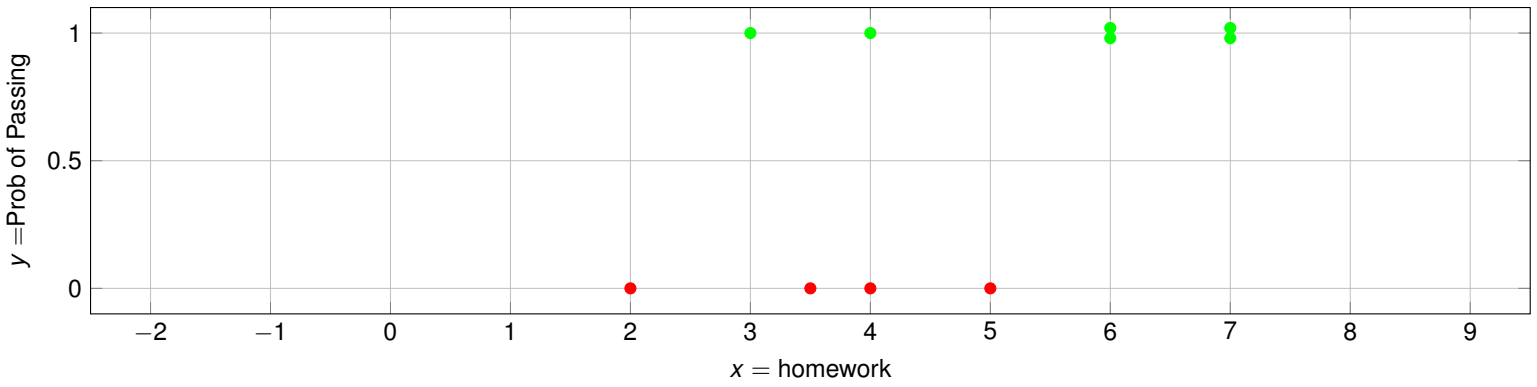

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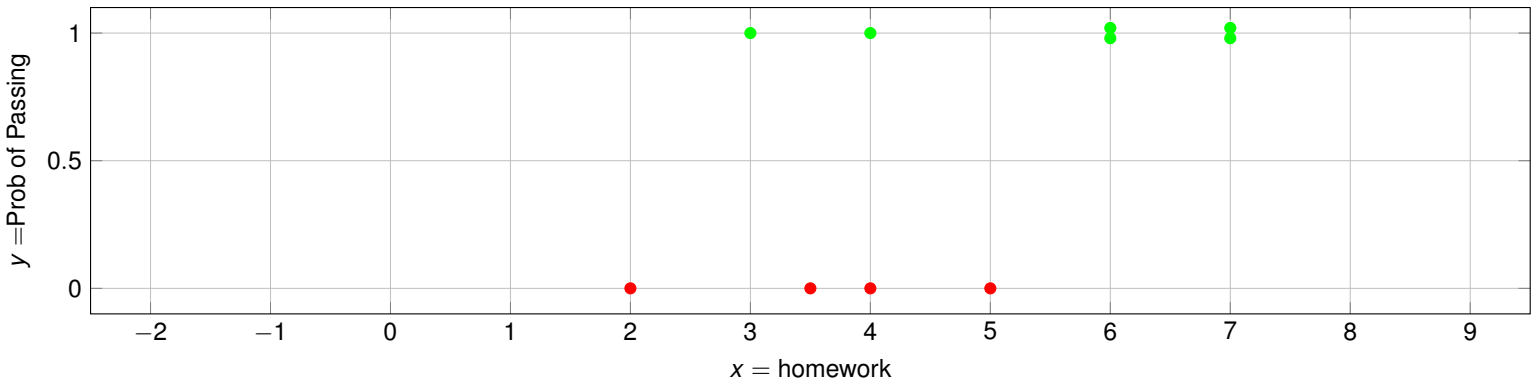

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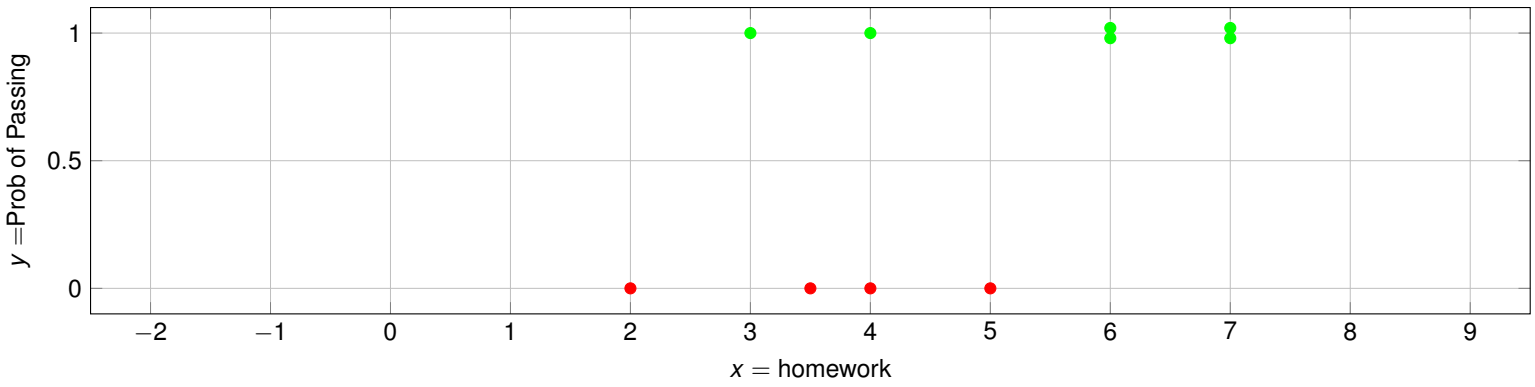

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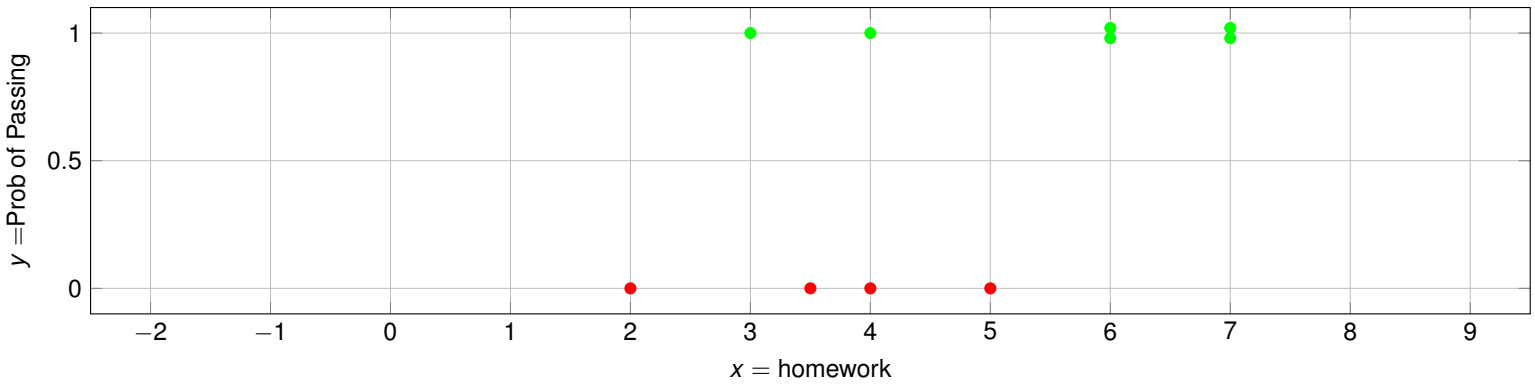

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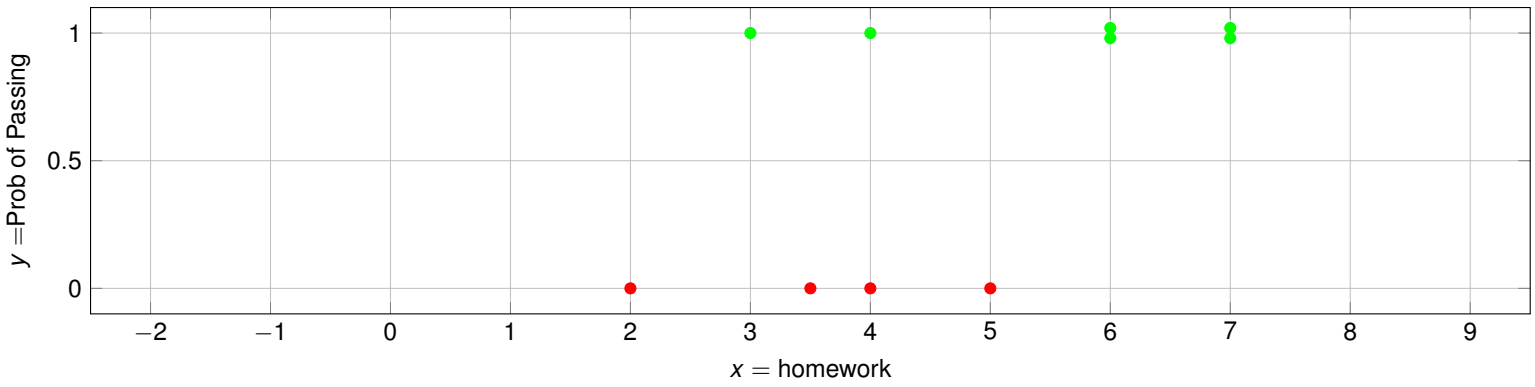

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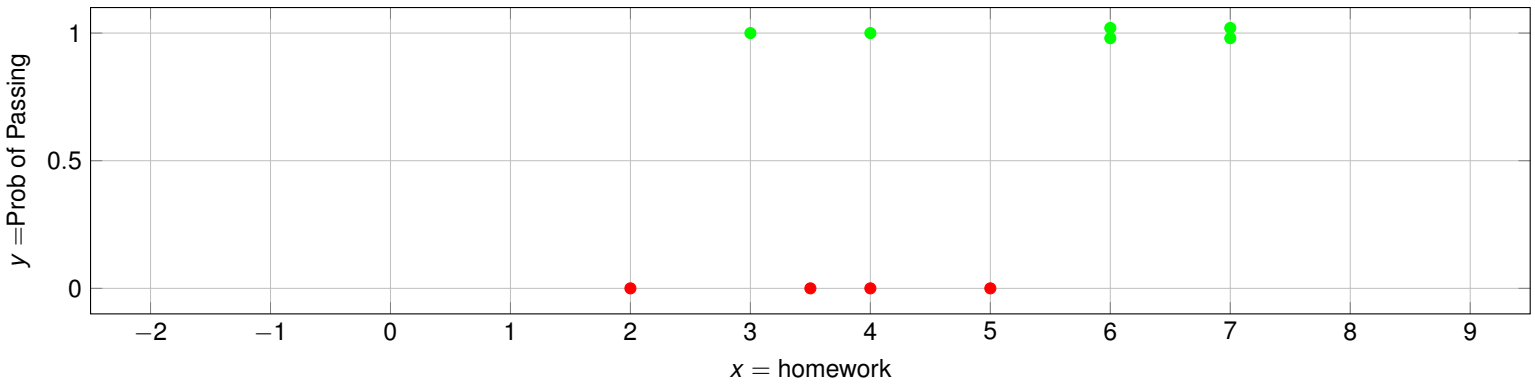

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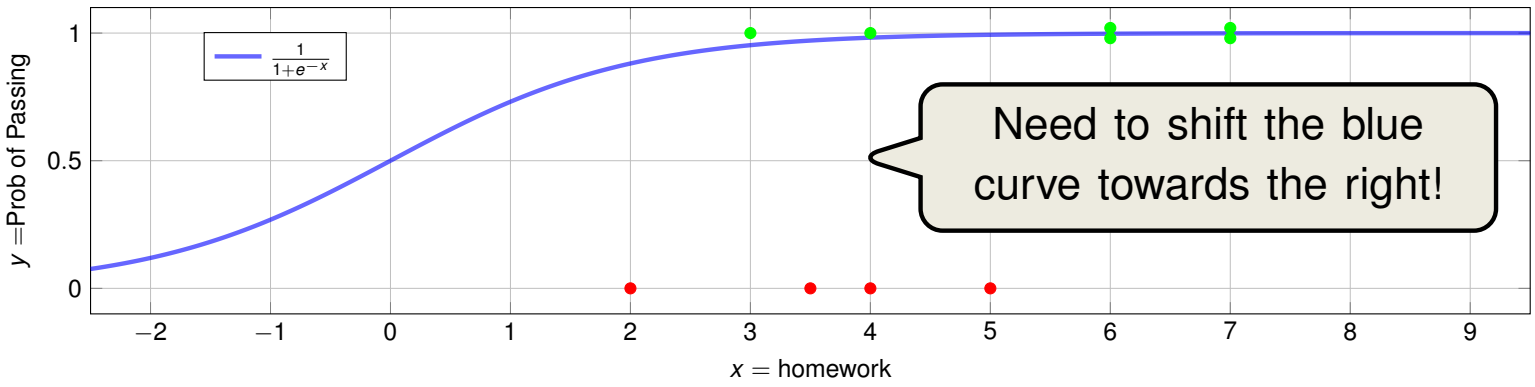

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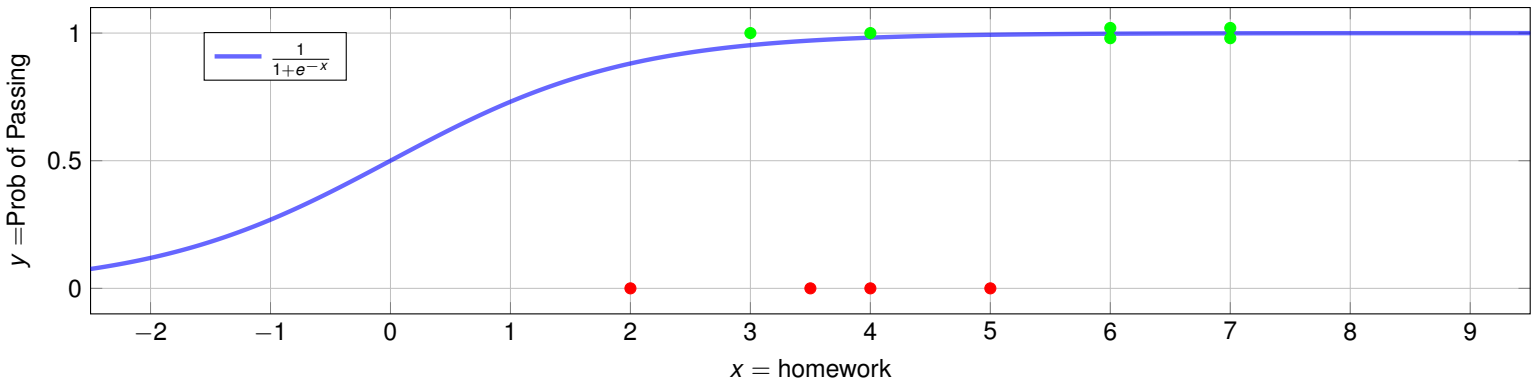

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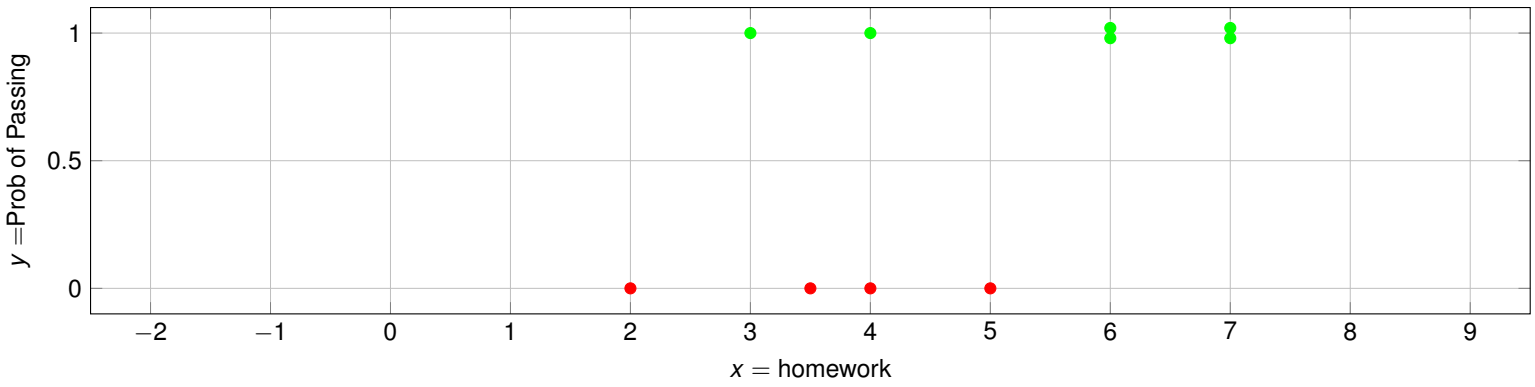

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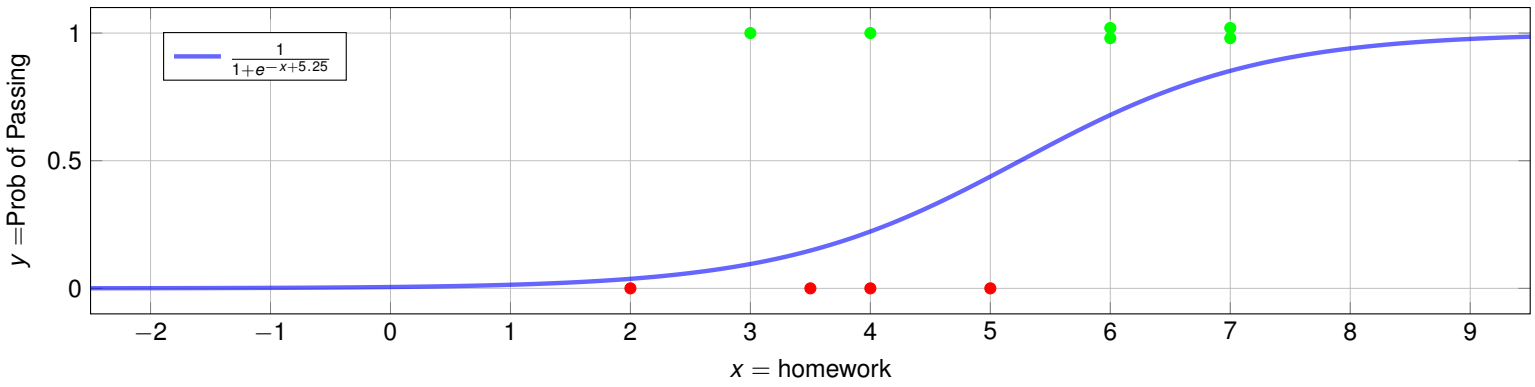

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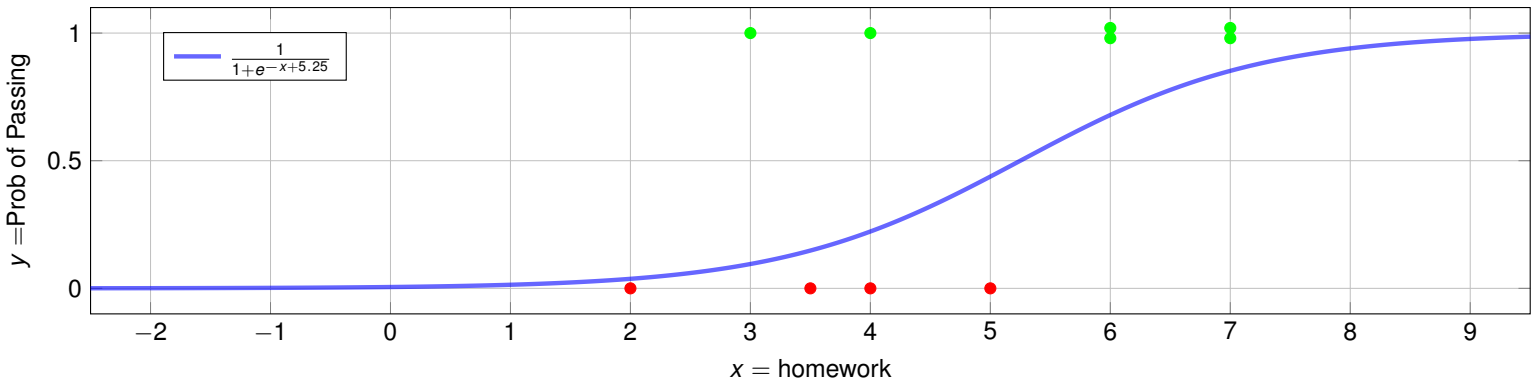

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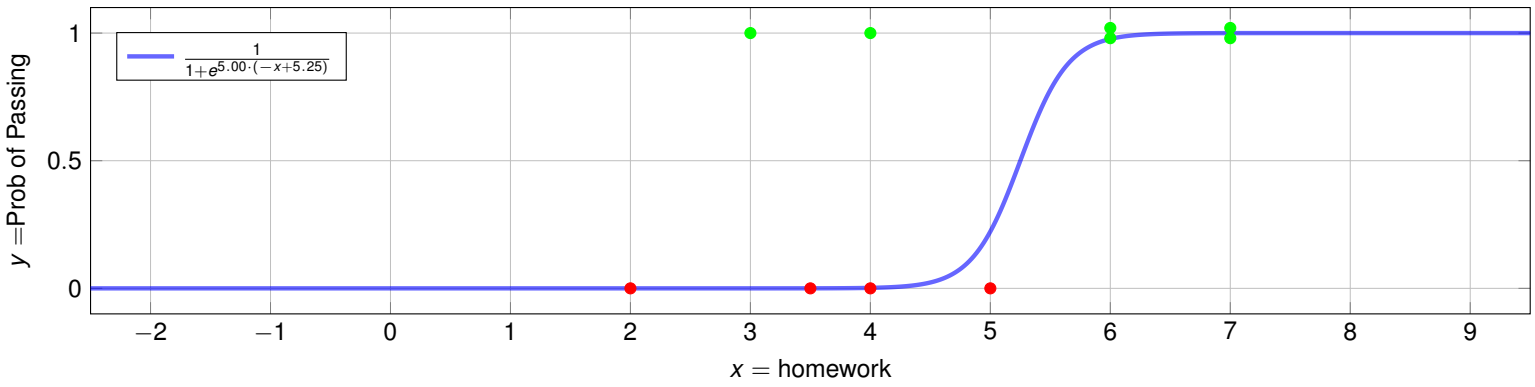

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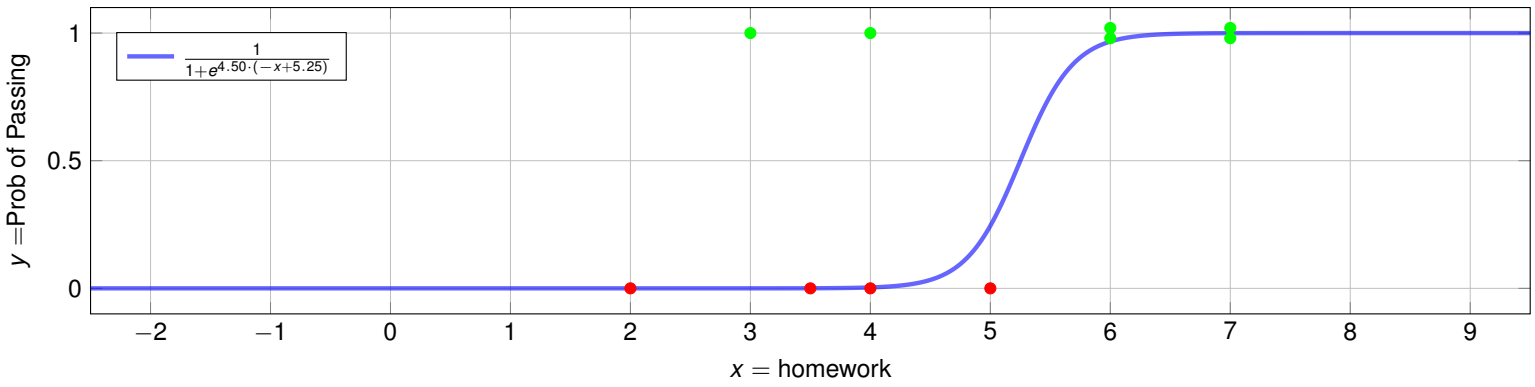

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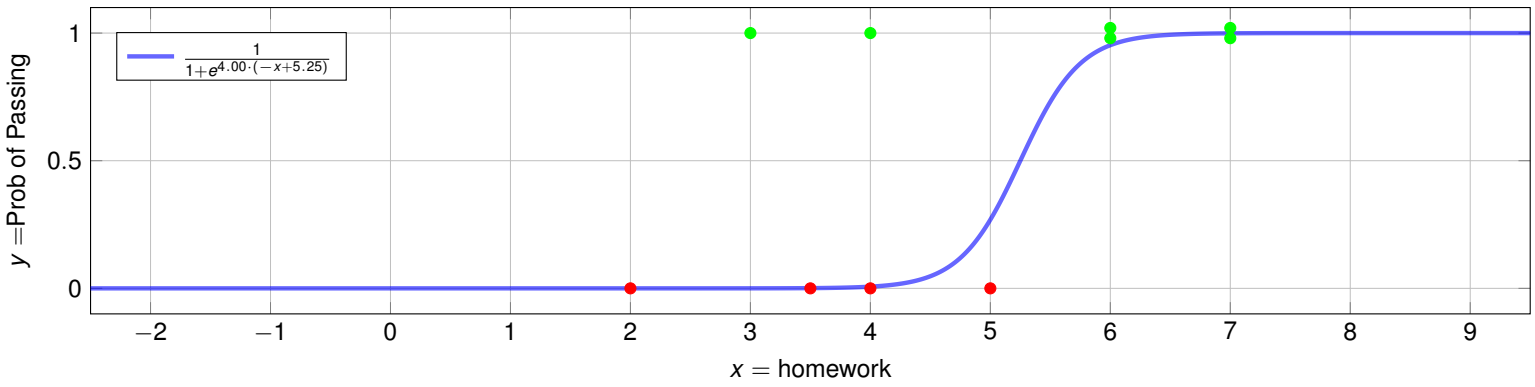

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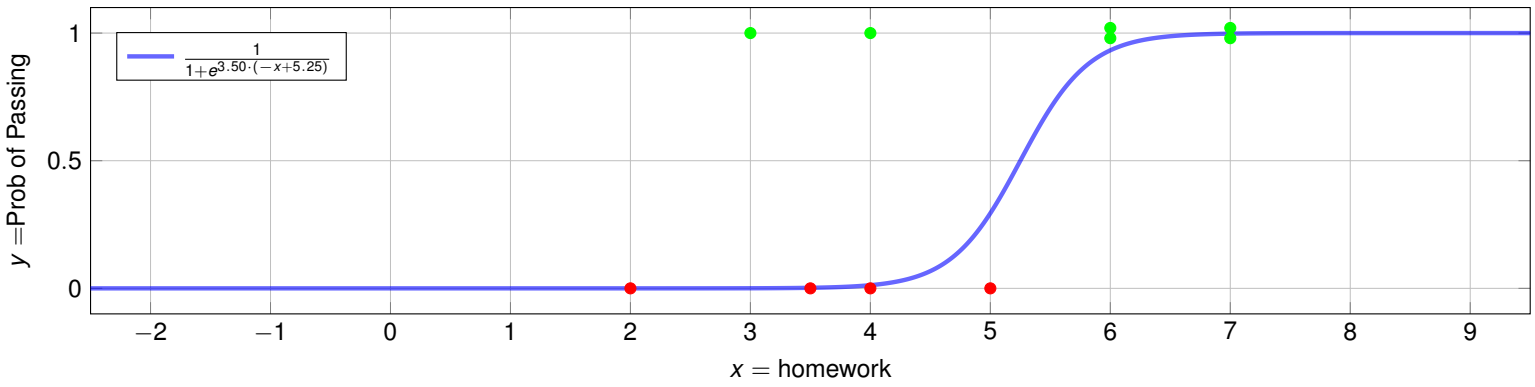

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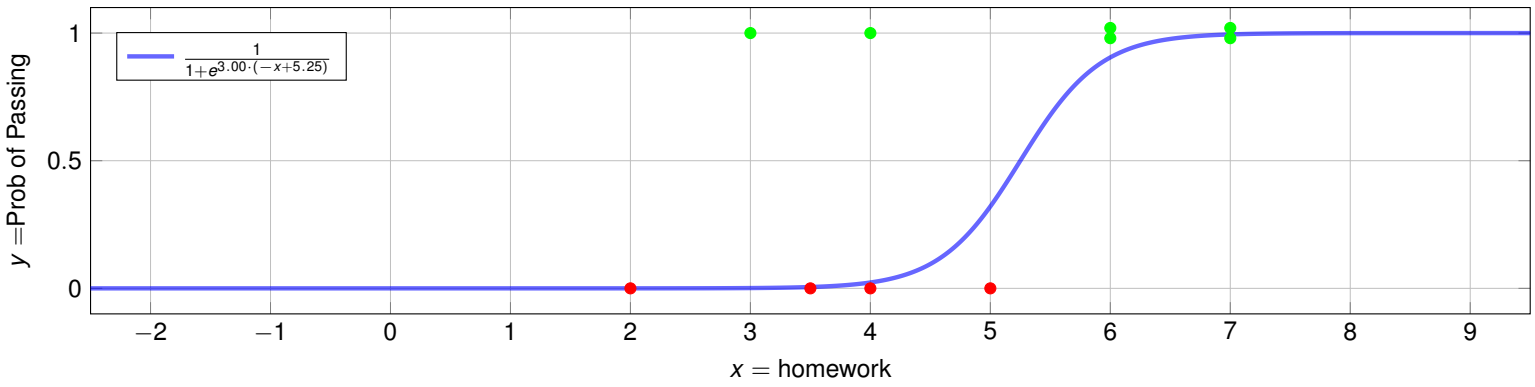

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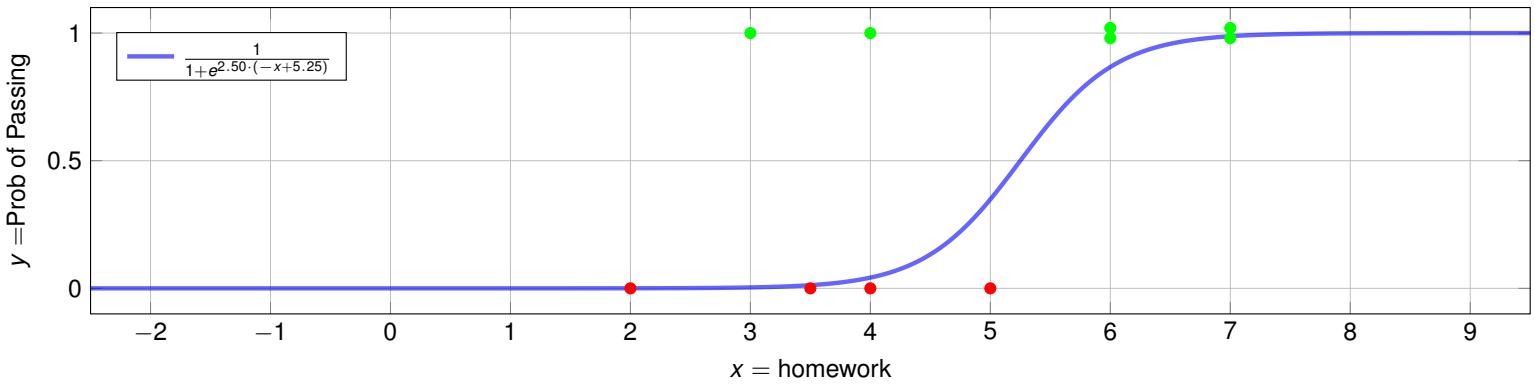

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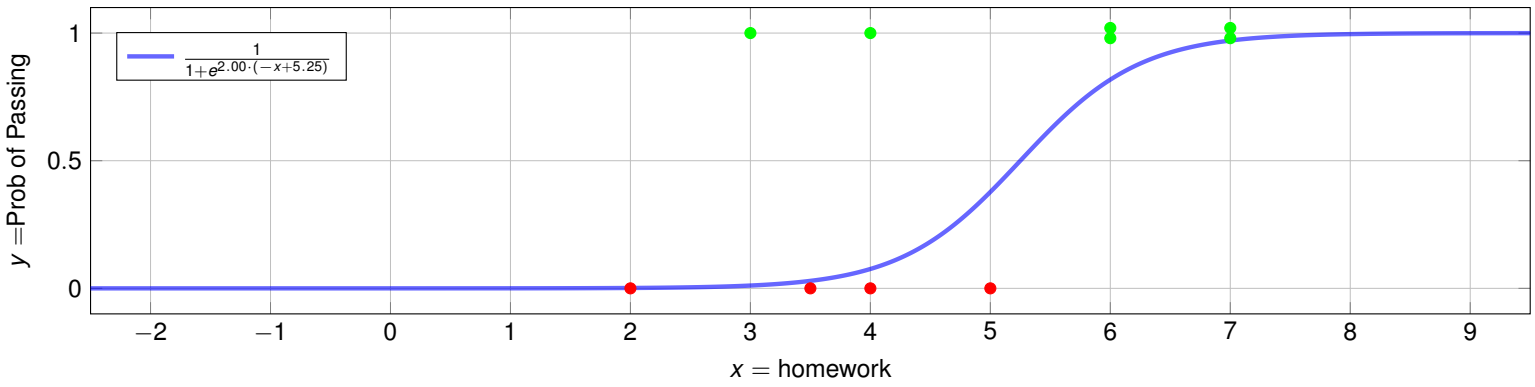

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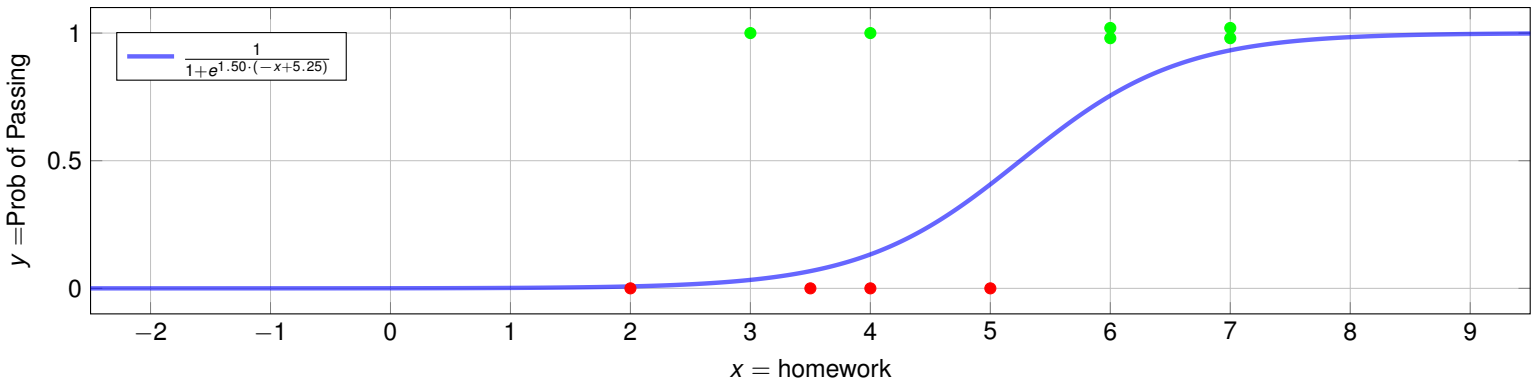

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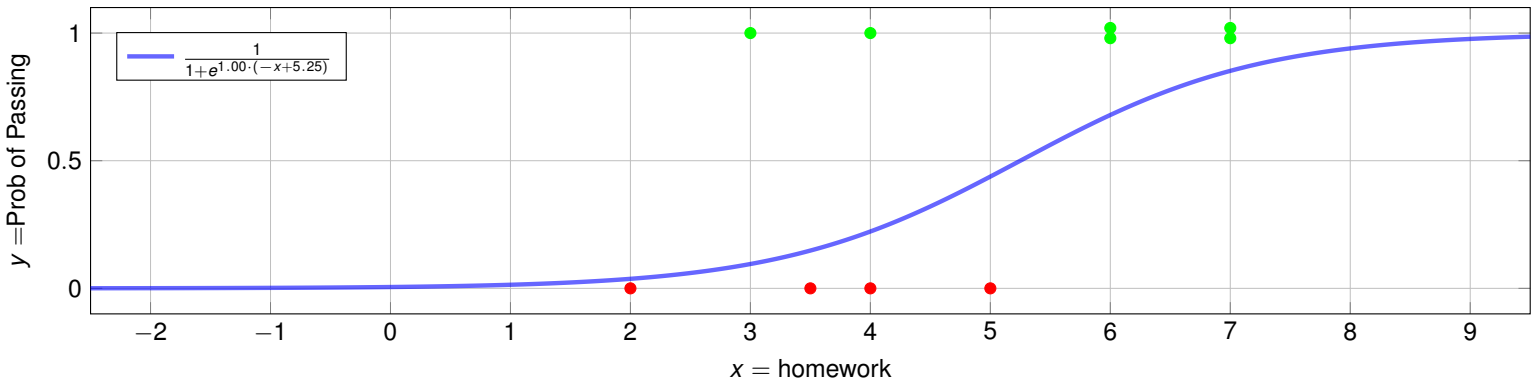

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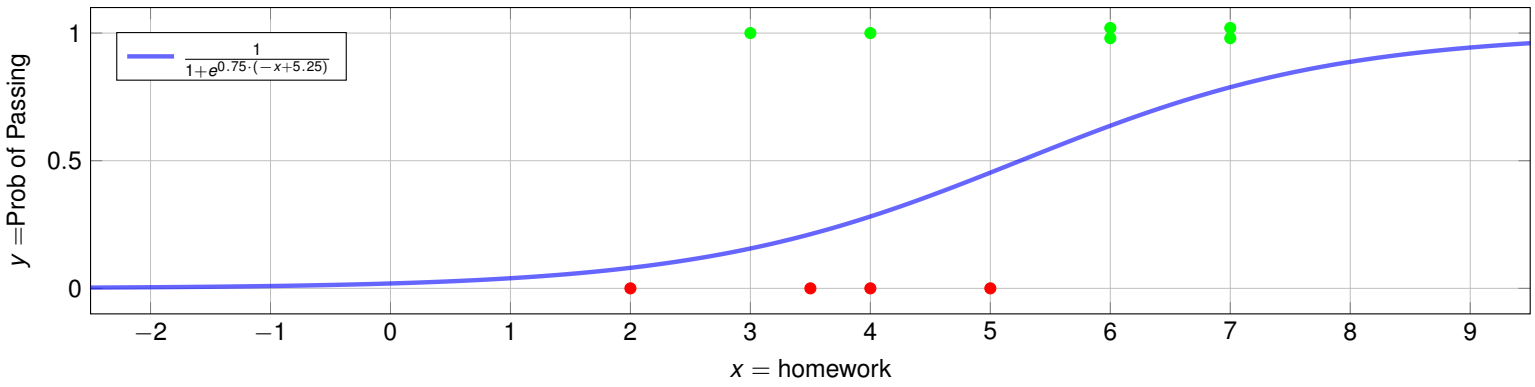

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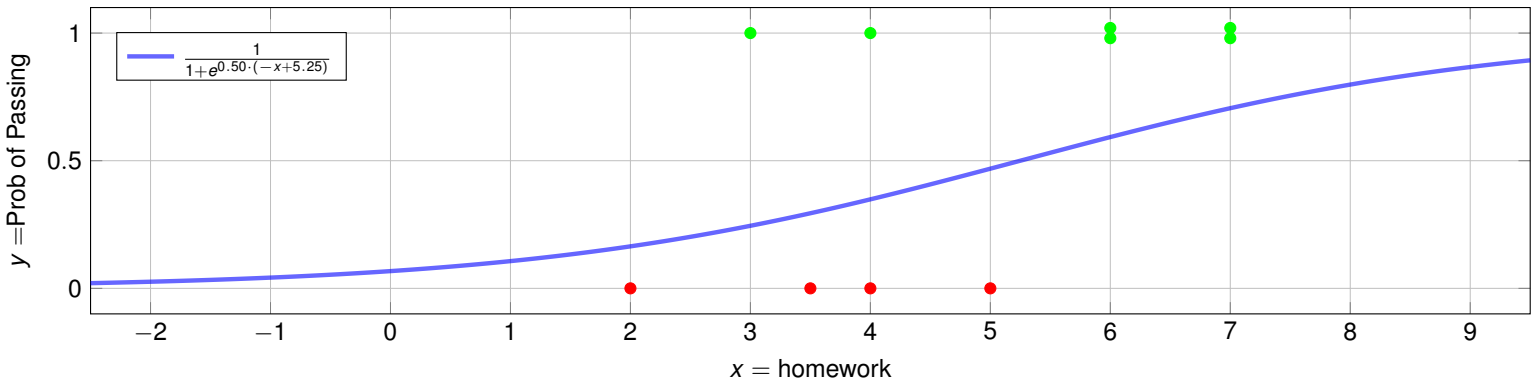

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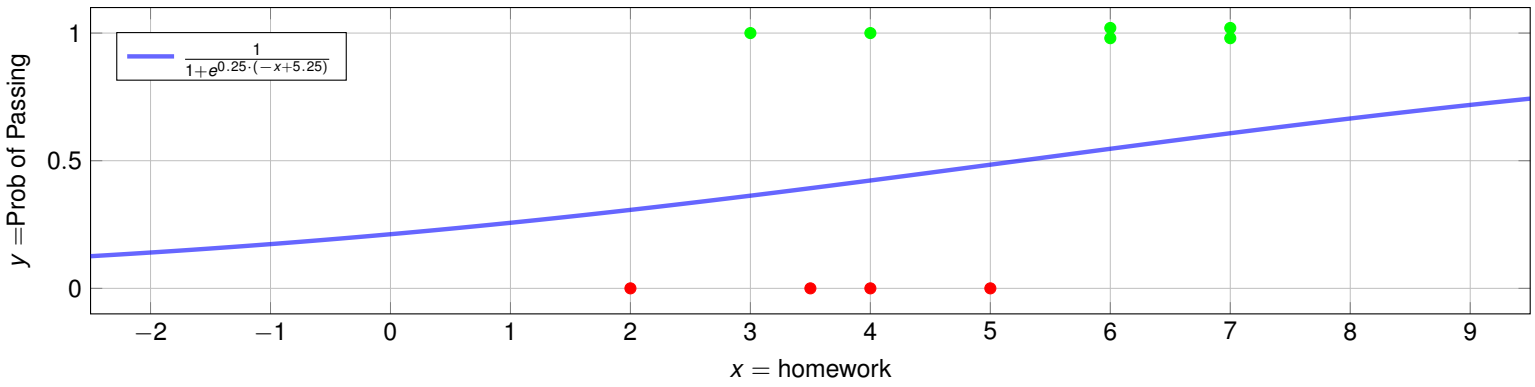

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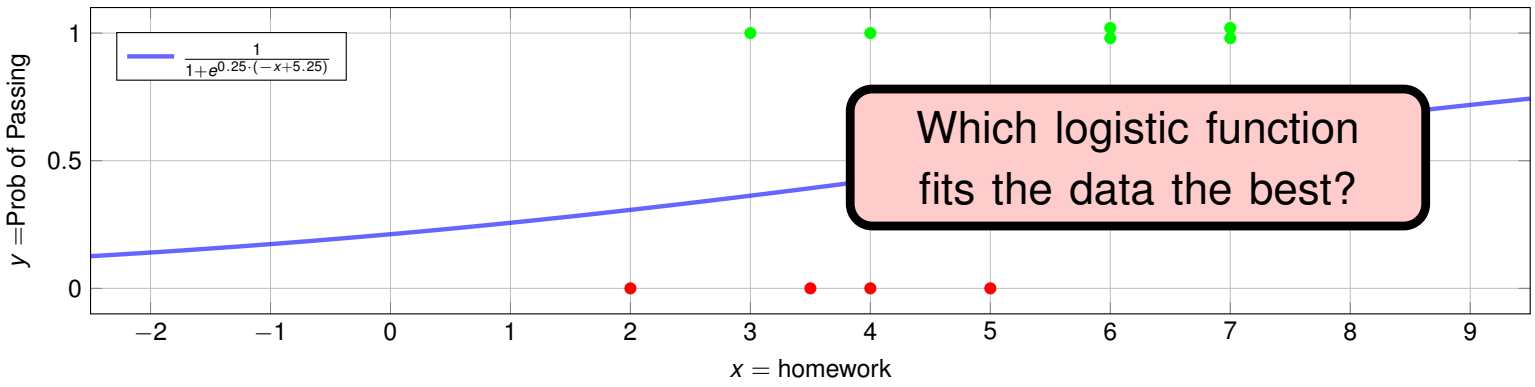

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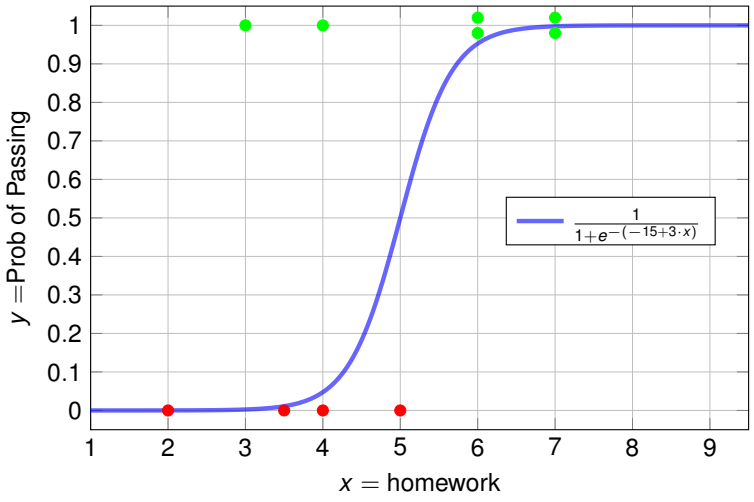

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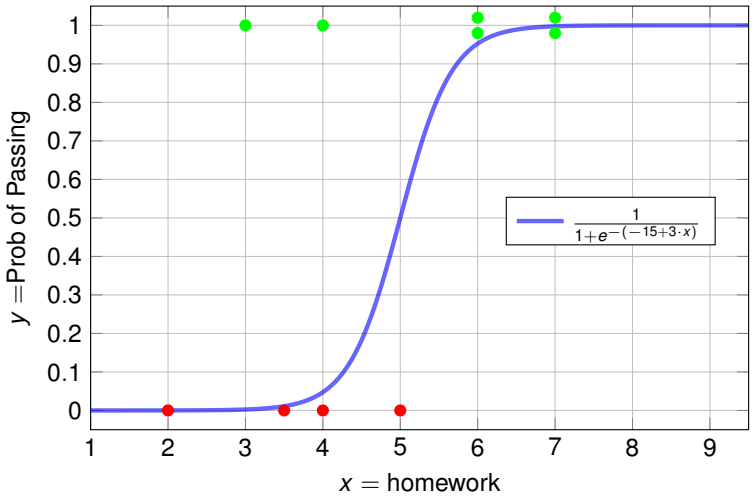
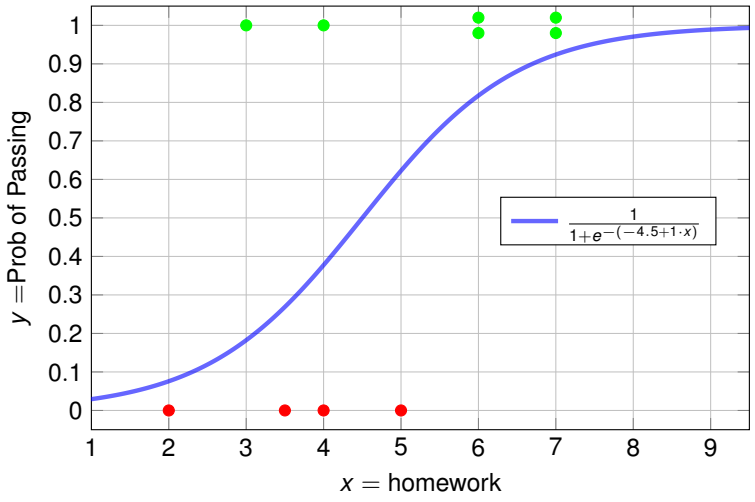
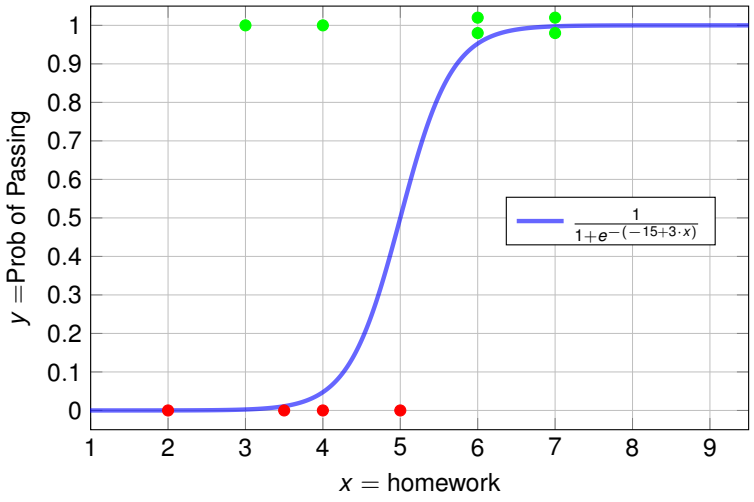
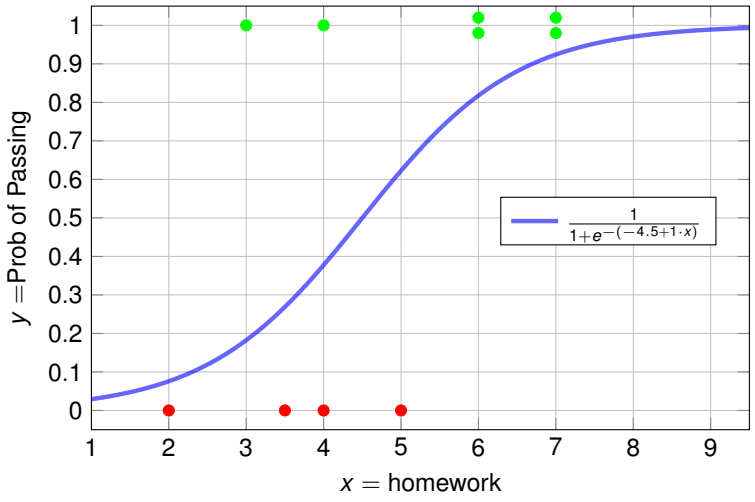




Quantifying the Error

$$y = \frac{1}{1 + \exp\left(-(b + w \cdot x)\right)}$$





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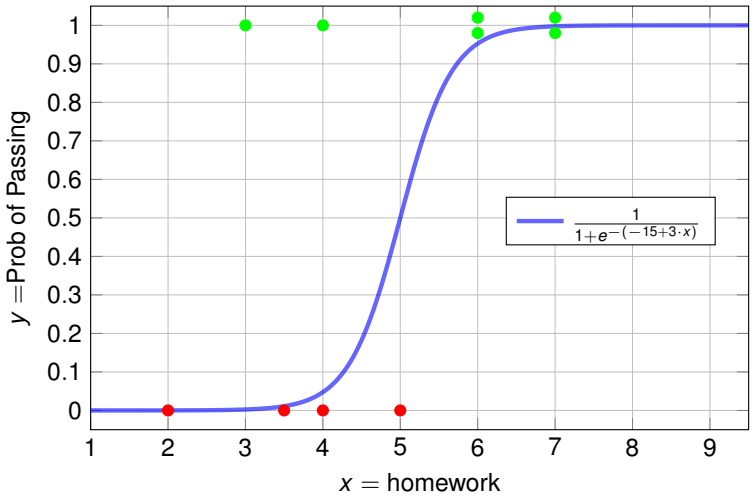

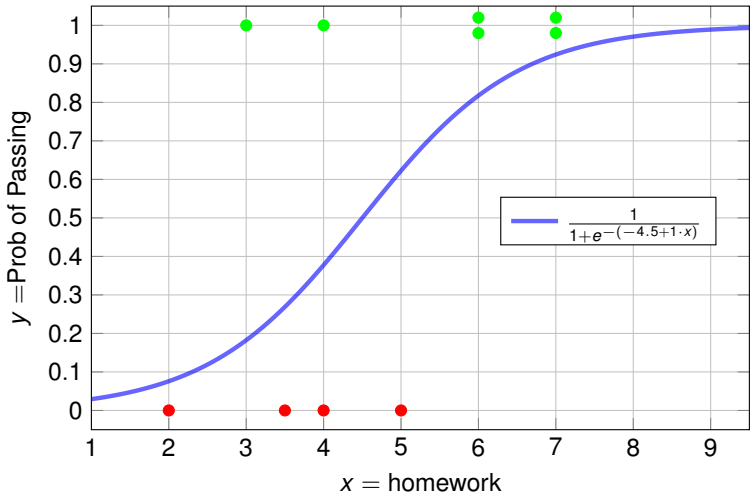

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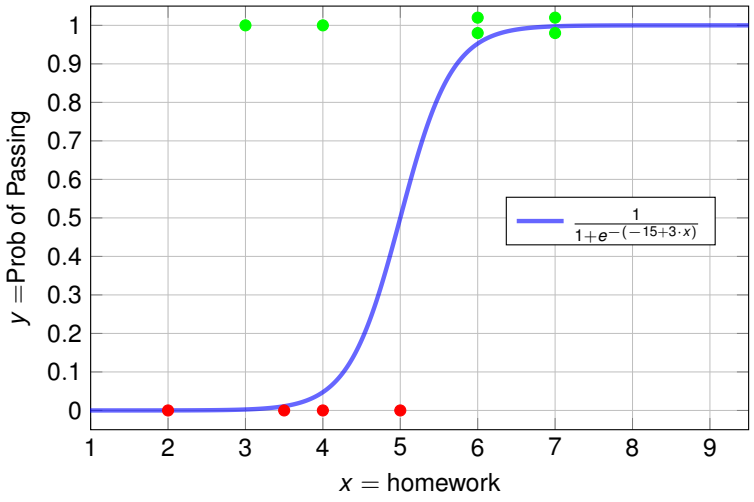

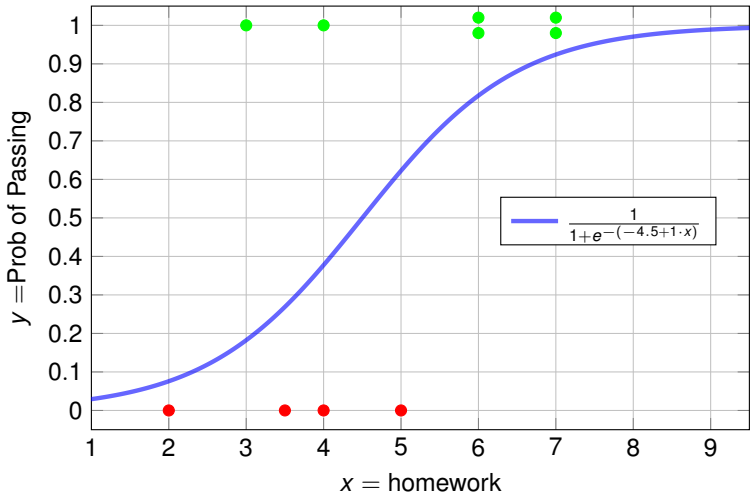

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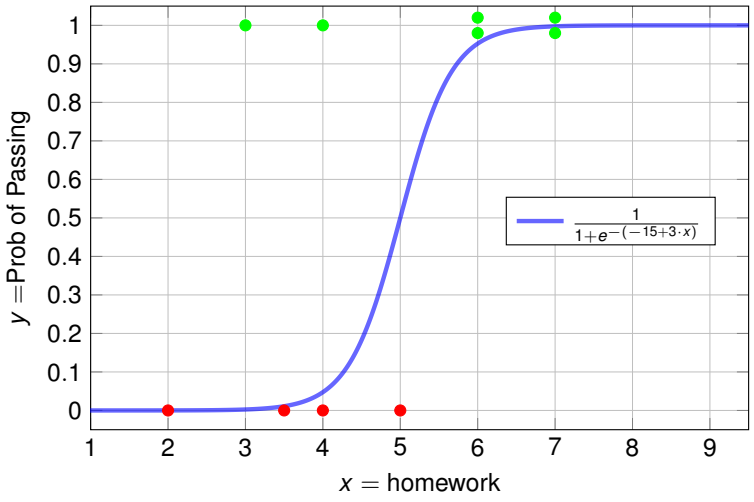

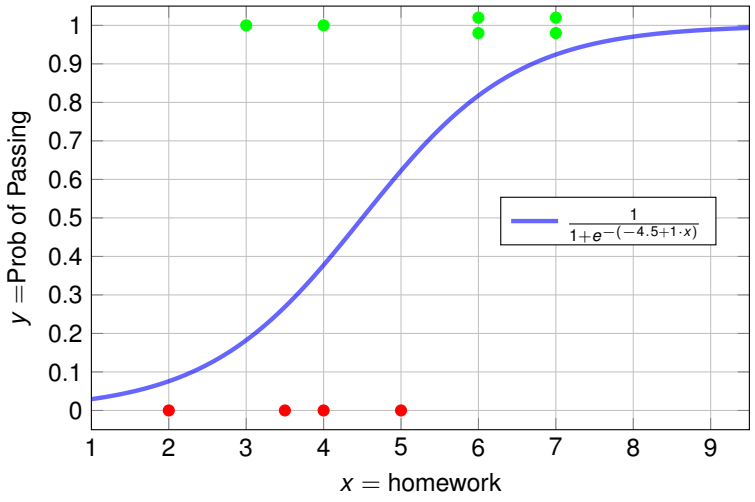

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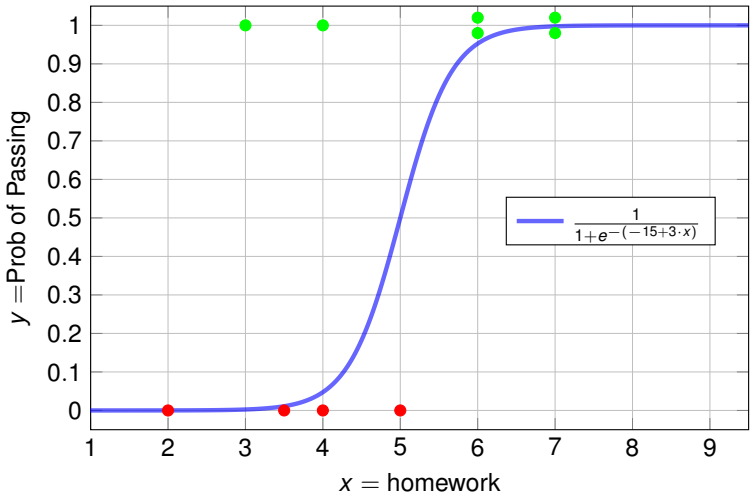

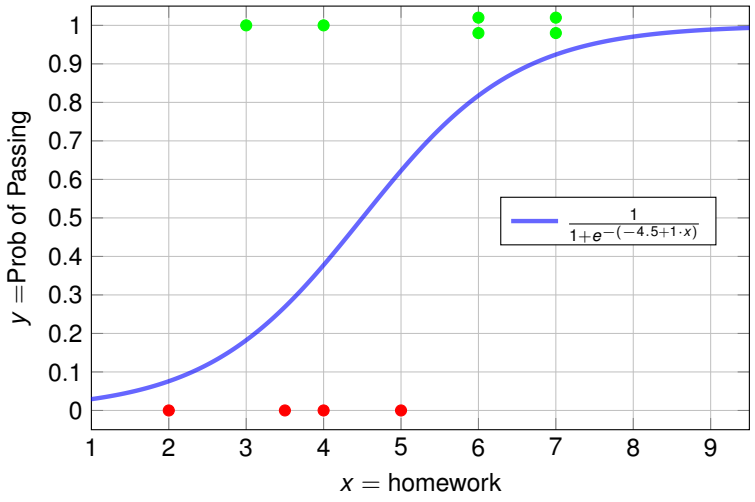

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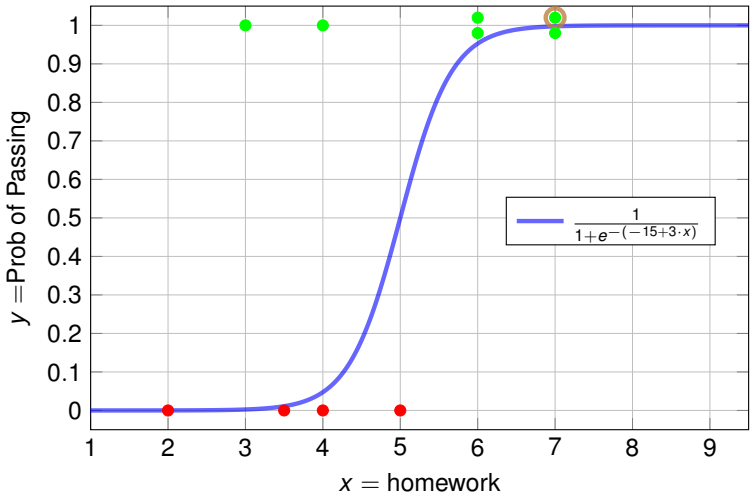

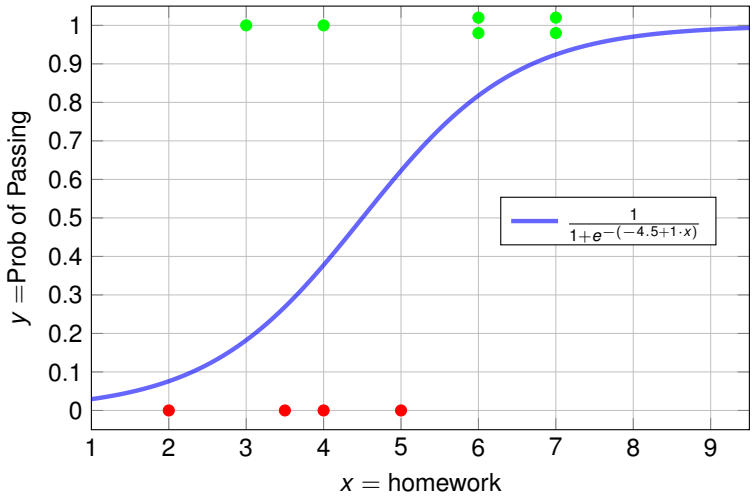

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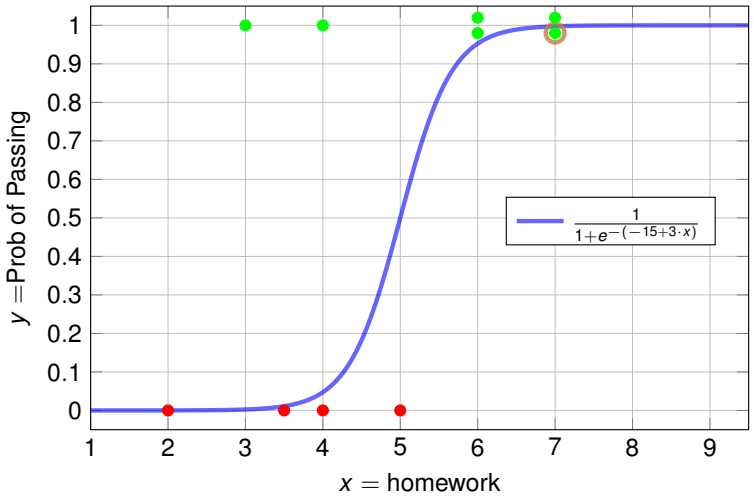

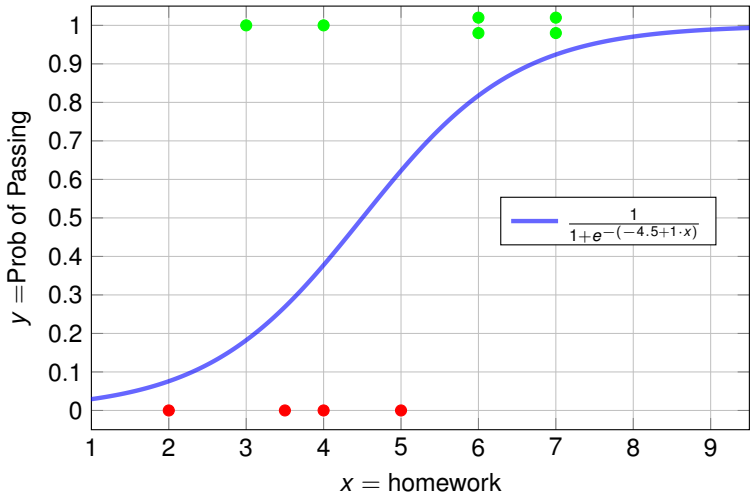

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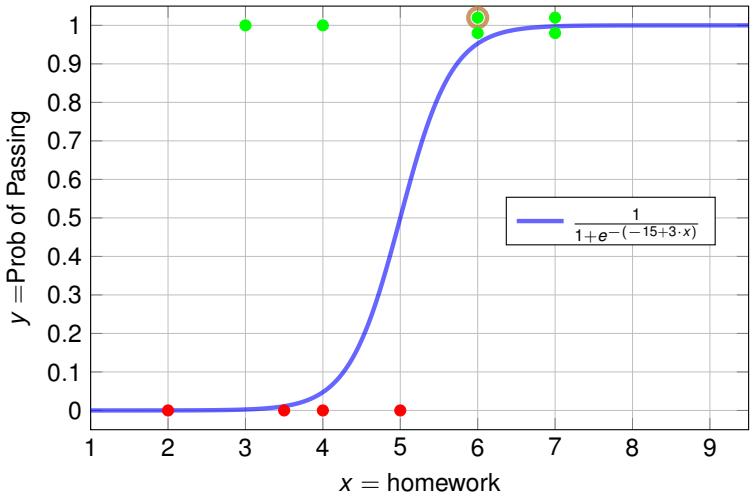

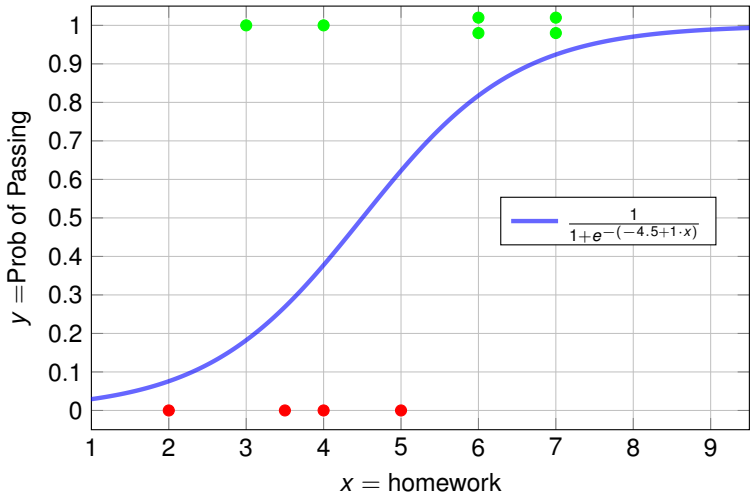

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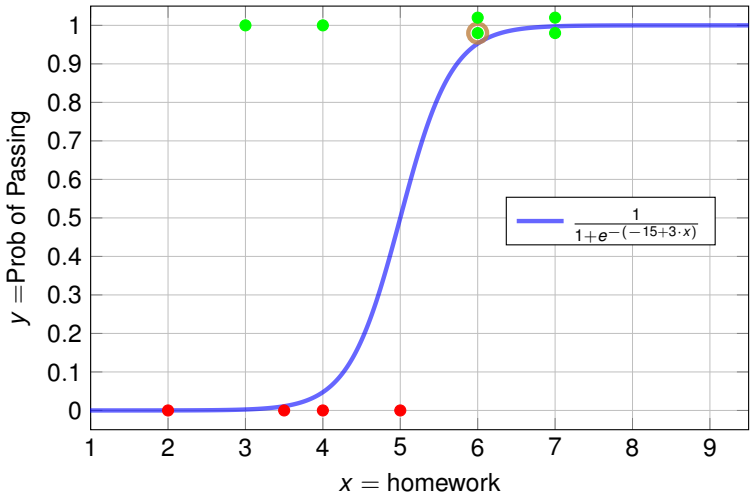

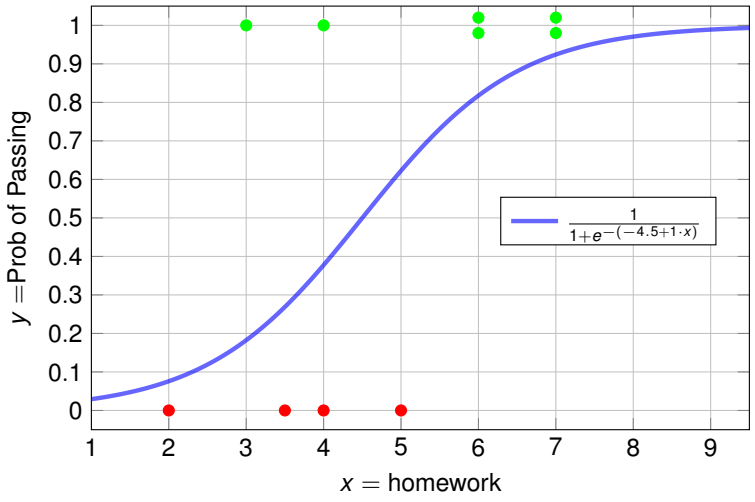

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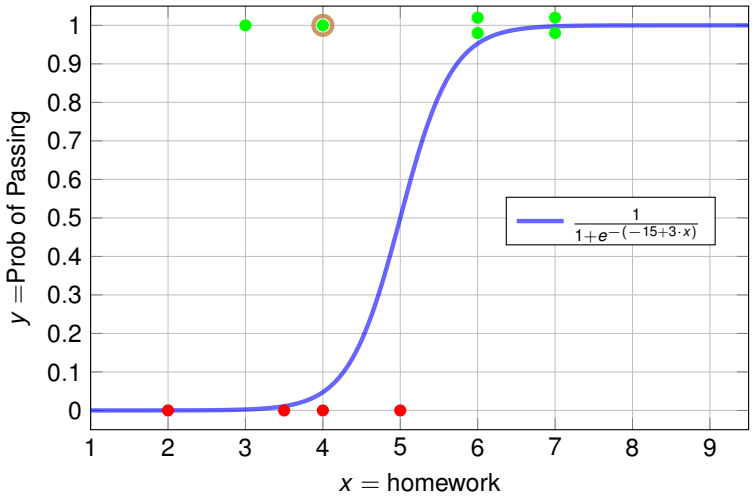

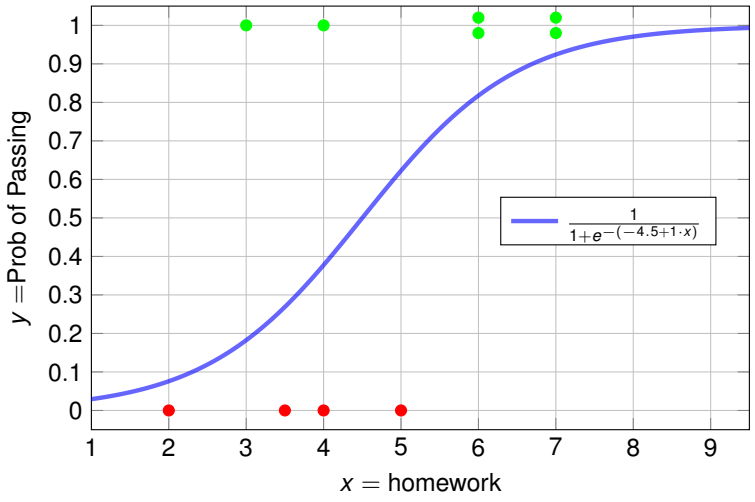

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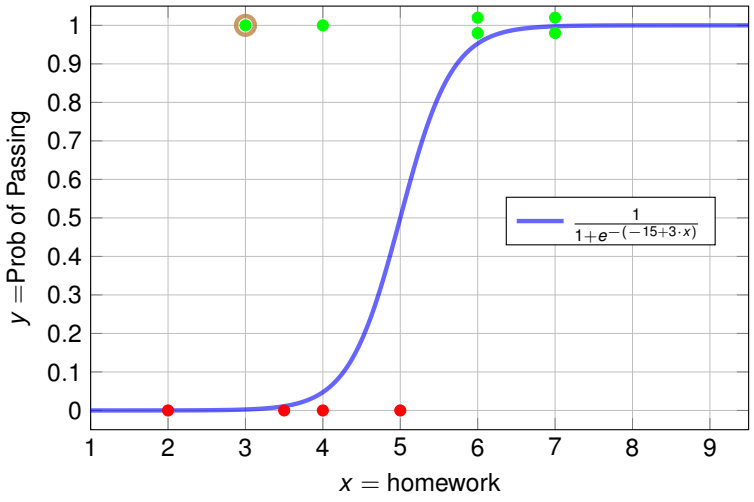

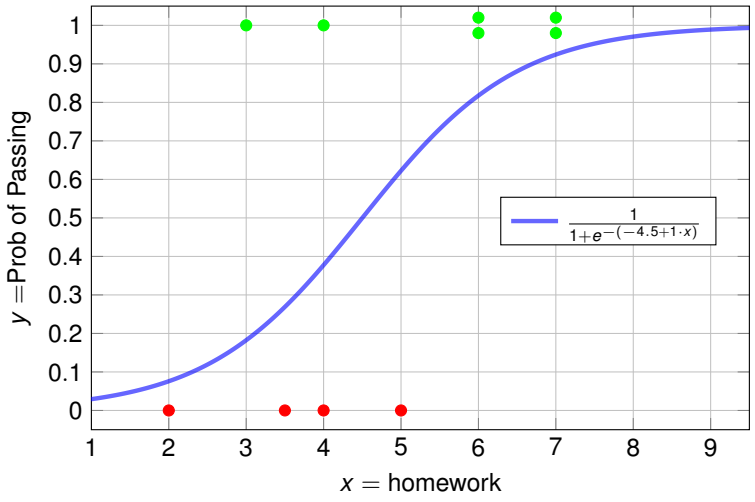

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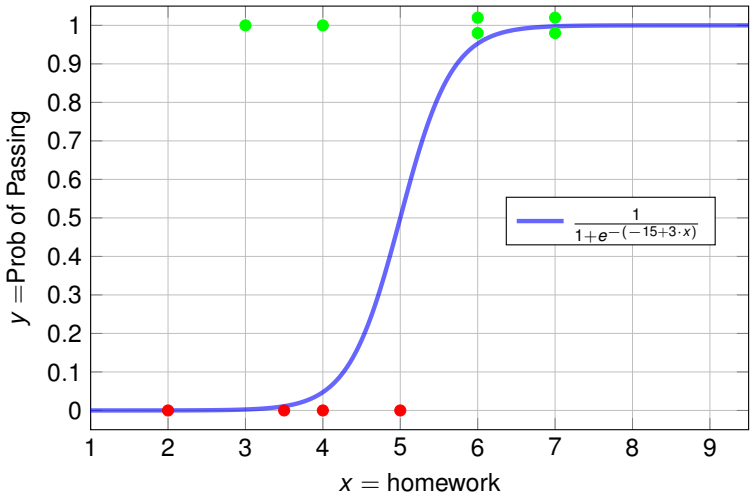

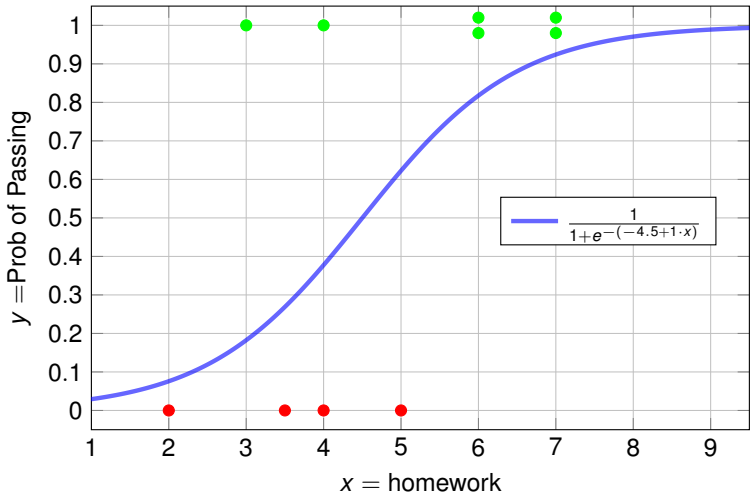

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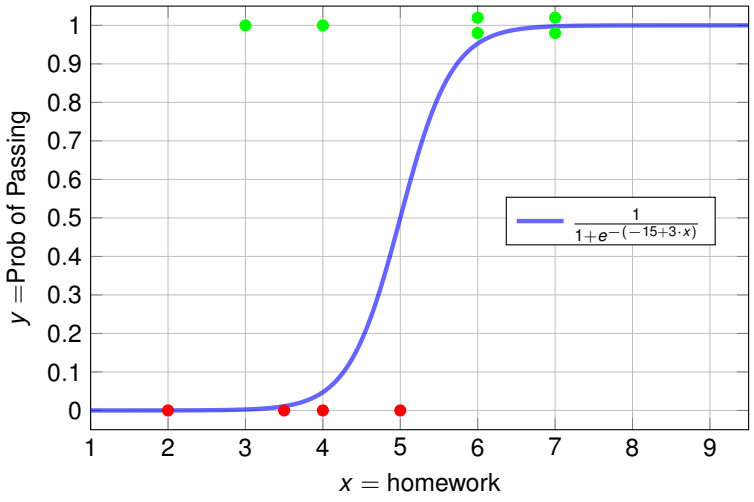

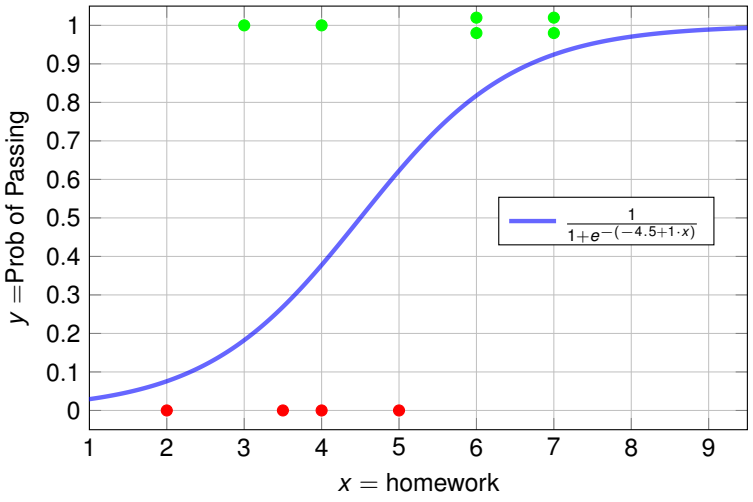

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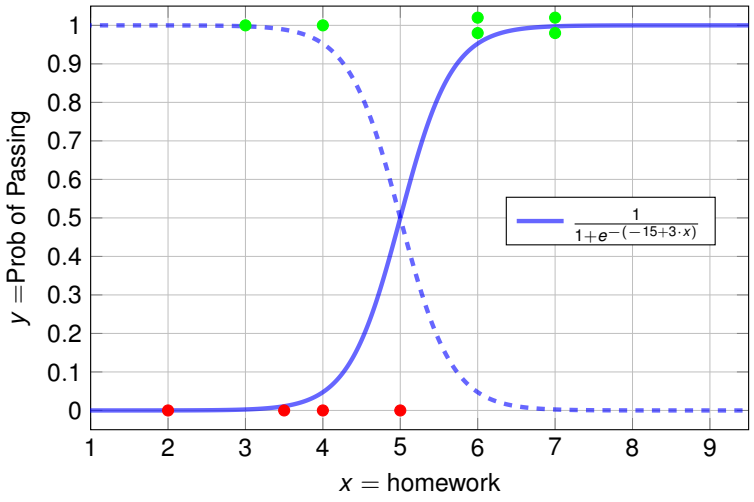

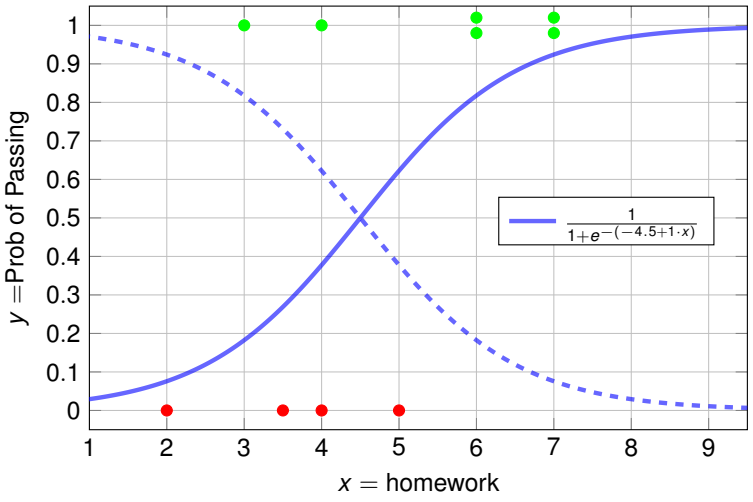

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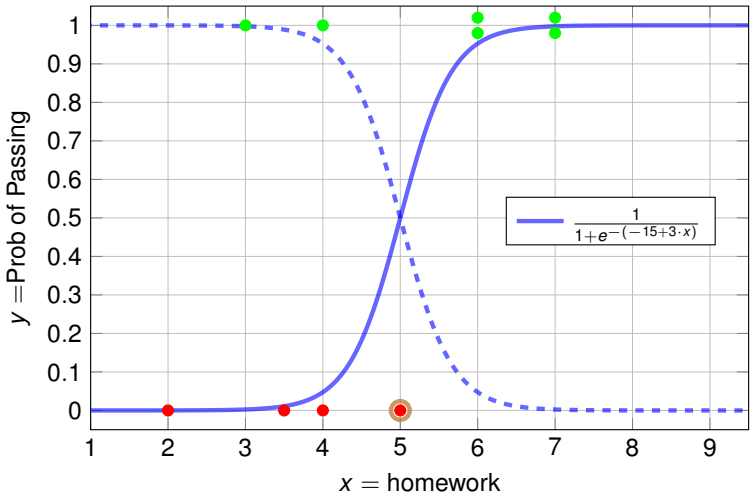

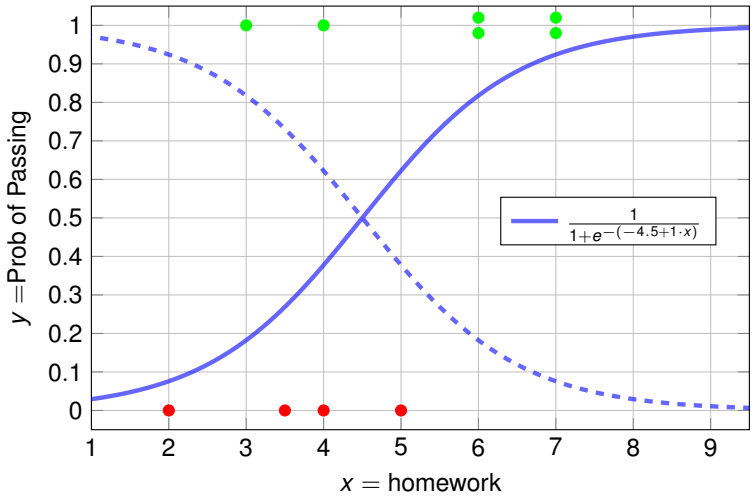

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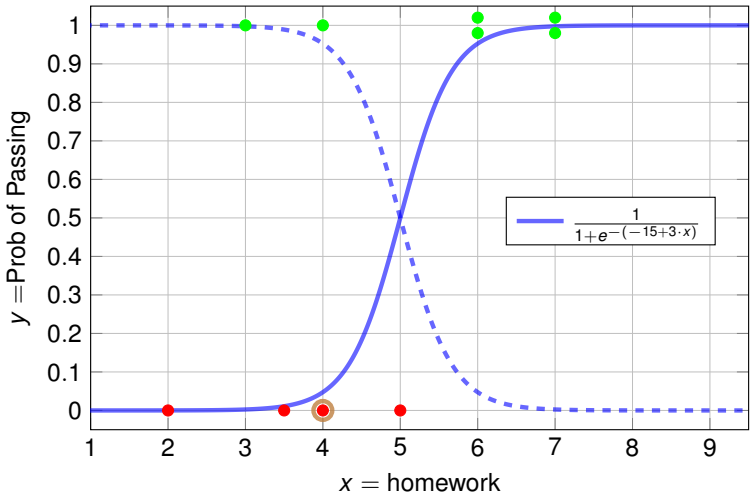

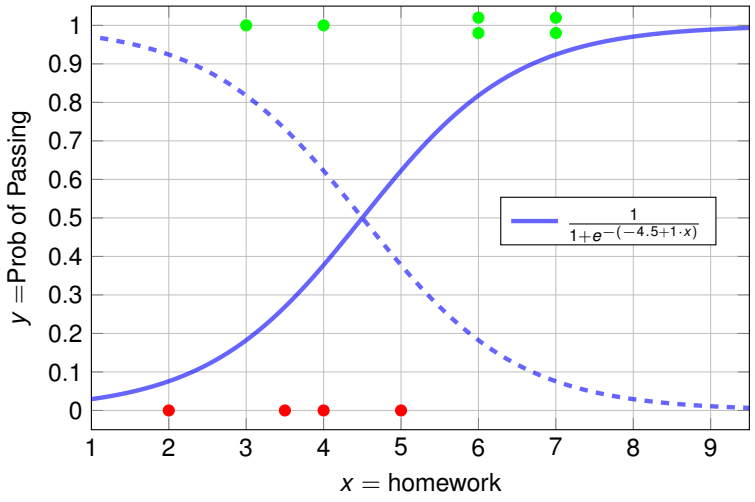

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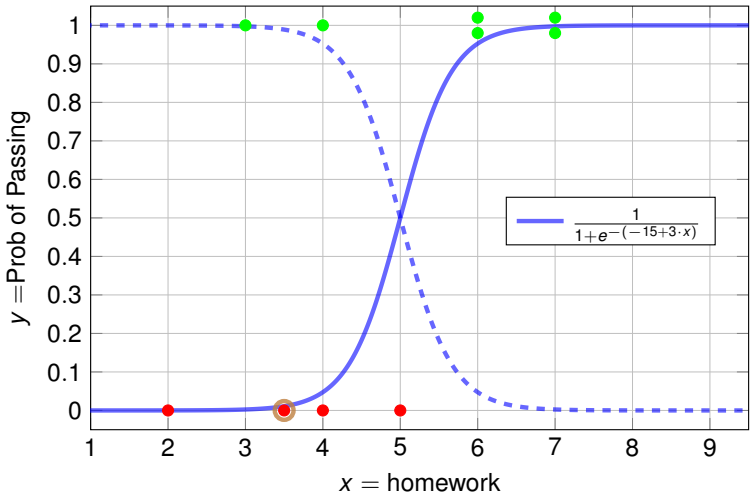

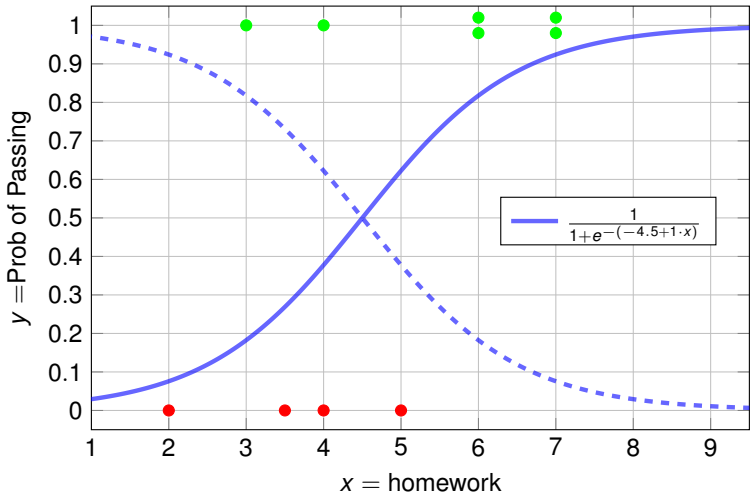

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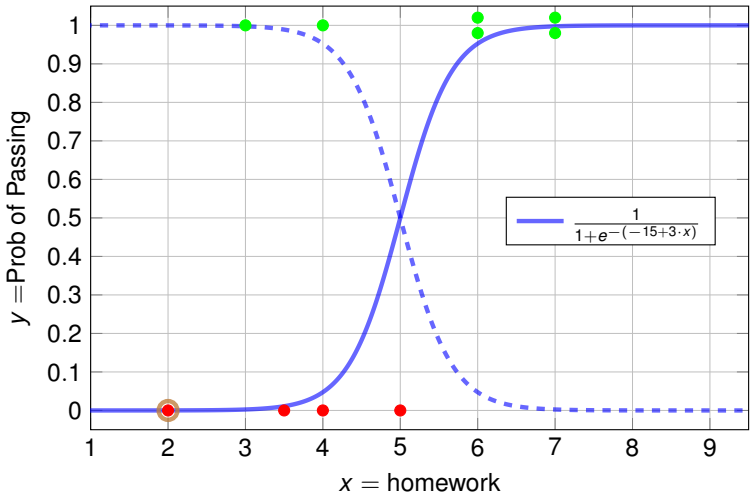

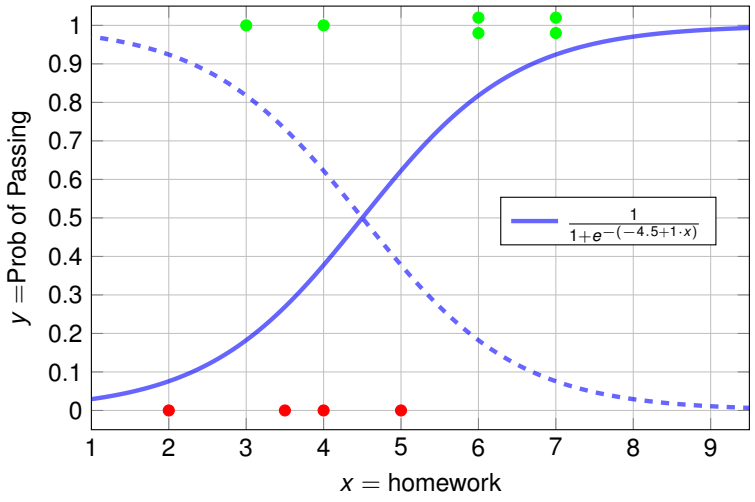

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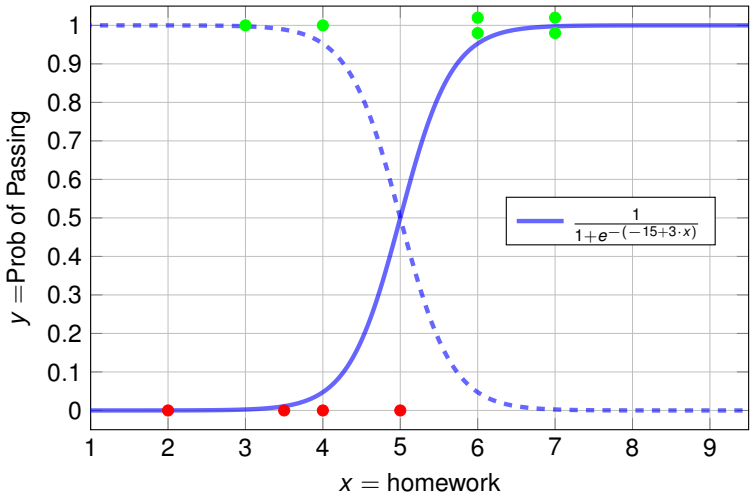

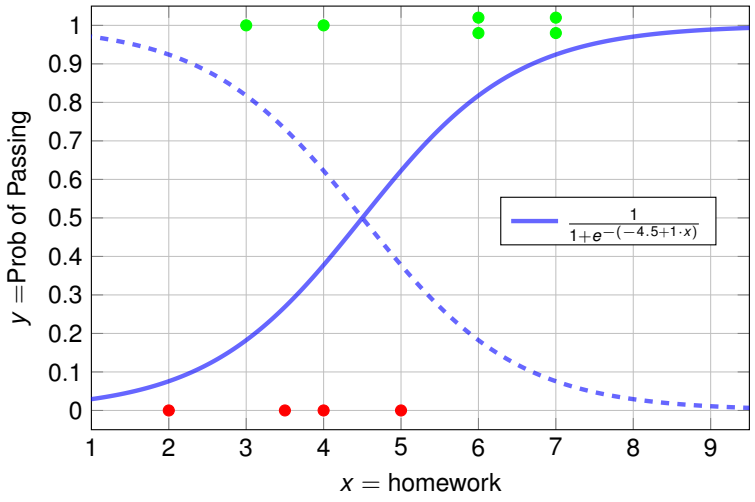

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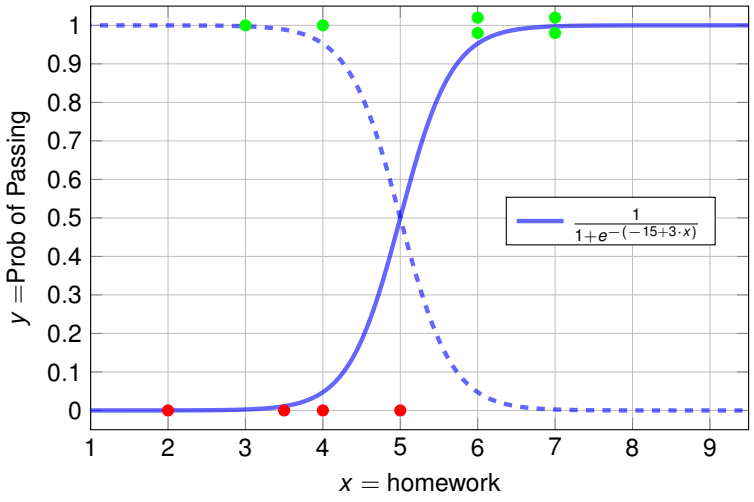
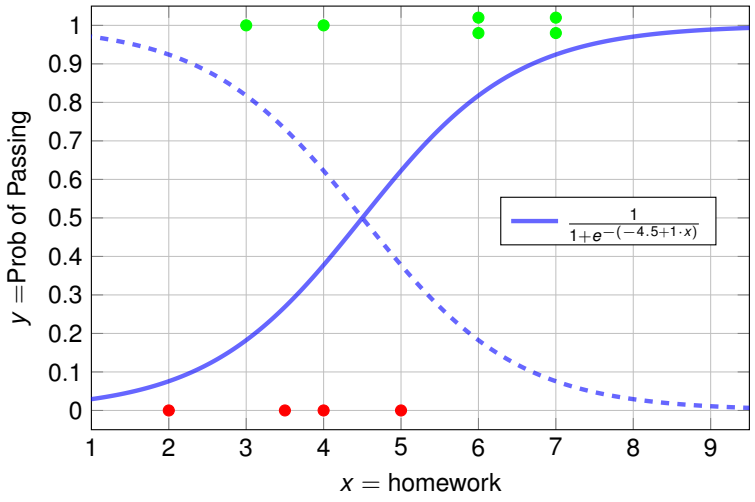
  $\Rightarrow$ overall likelihood is





Quantifying the Error

$$y = \frac{1}{1 + \exp\left(-(b + w \cdot x)\right)}$$

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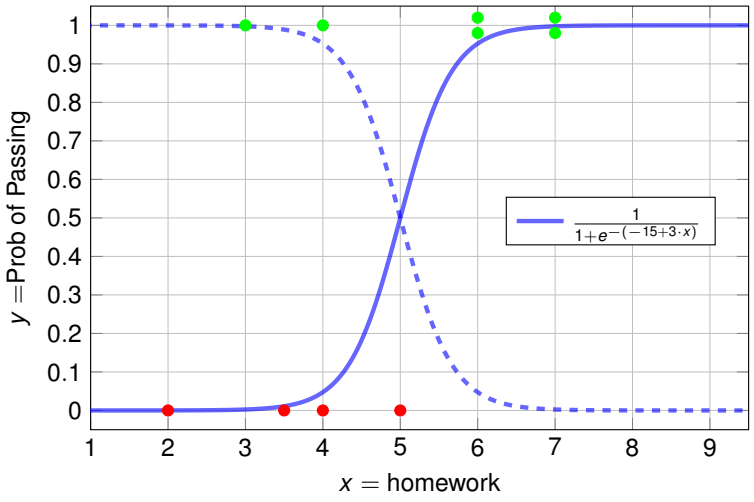
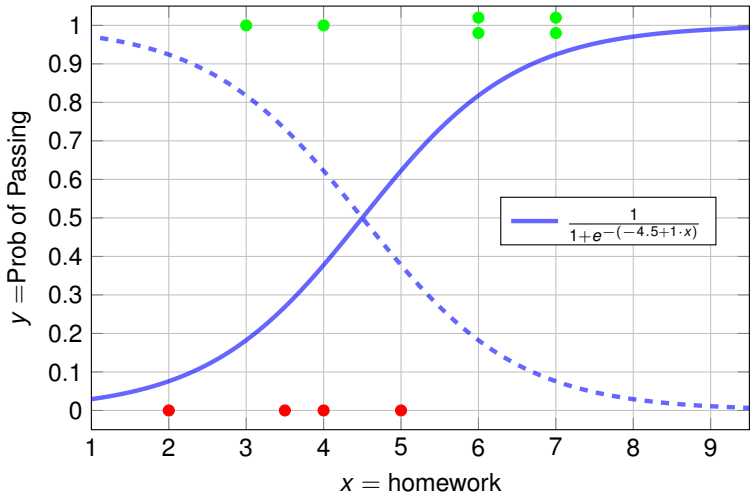
  $\Rightarrow$ overall likelihood is $0.0001 \cdot 0.47 \approx 0.00005$





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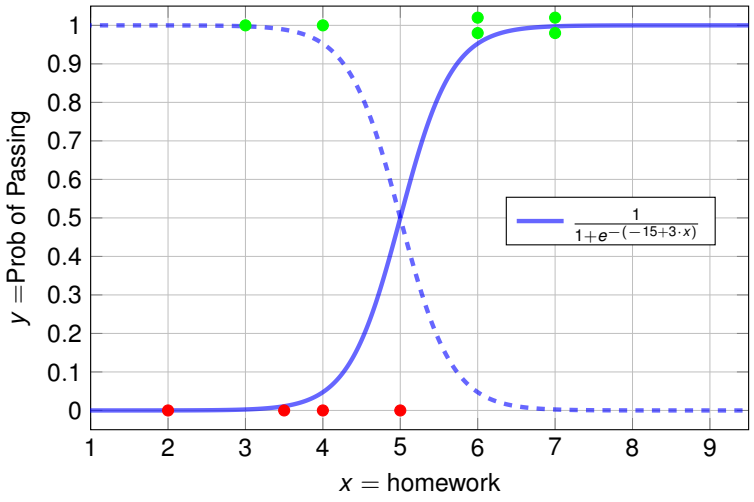

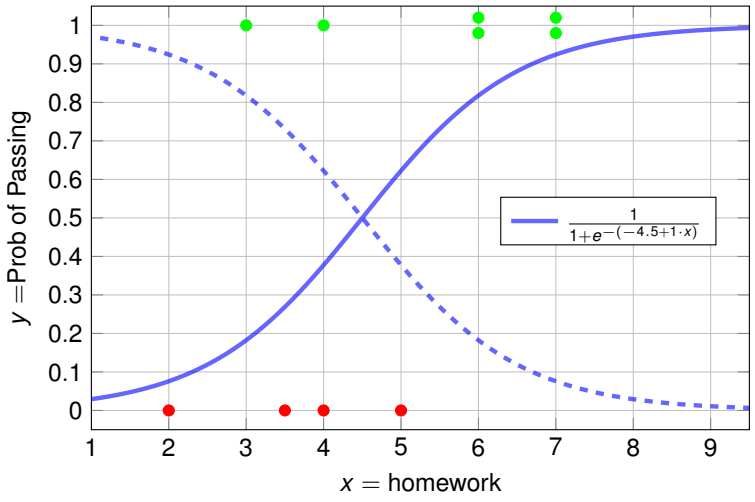

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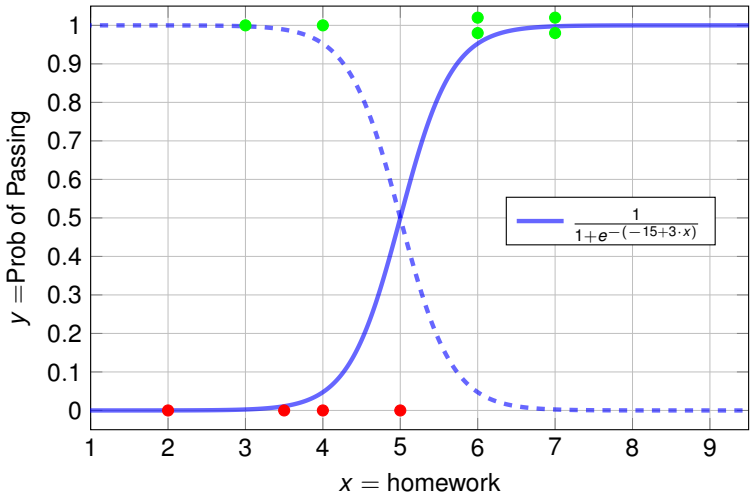
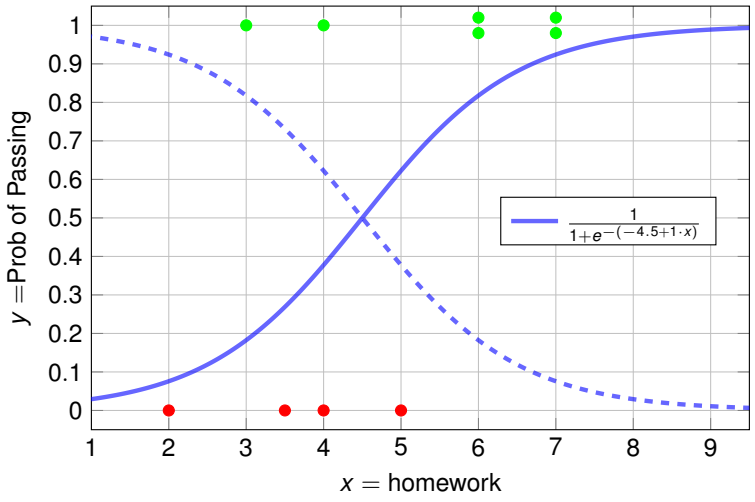


Likelihood ≈ 0.006



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much better model!

Likelihood ≈ 0.00005

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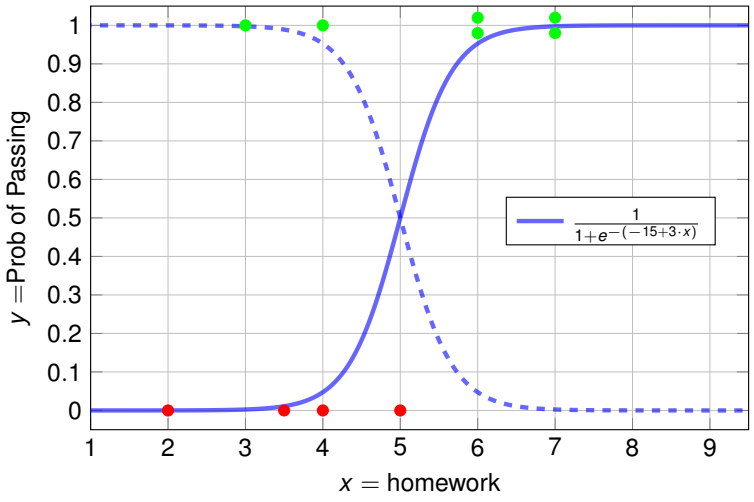

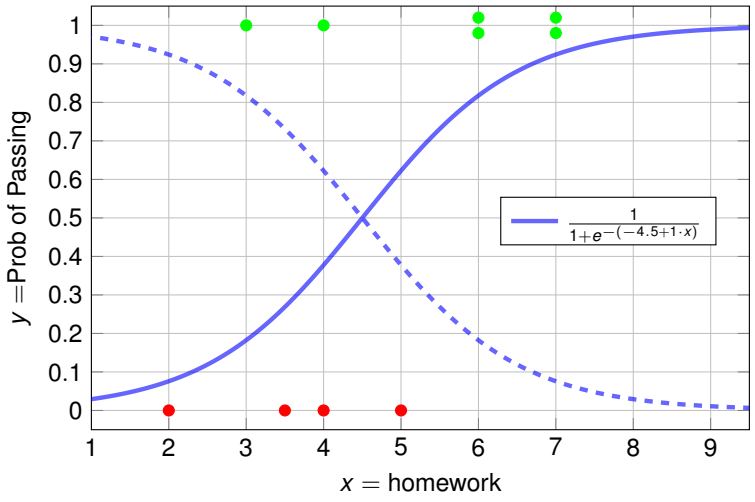

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Optimal Fit

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Optimal Fit

- $b = -3.7349$, $w = 0.914$

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$\Rightarrow$ likelihood of 0.0071.

Plot of the Optimal Model

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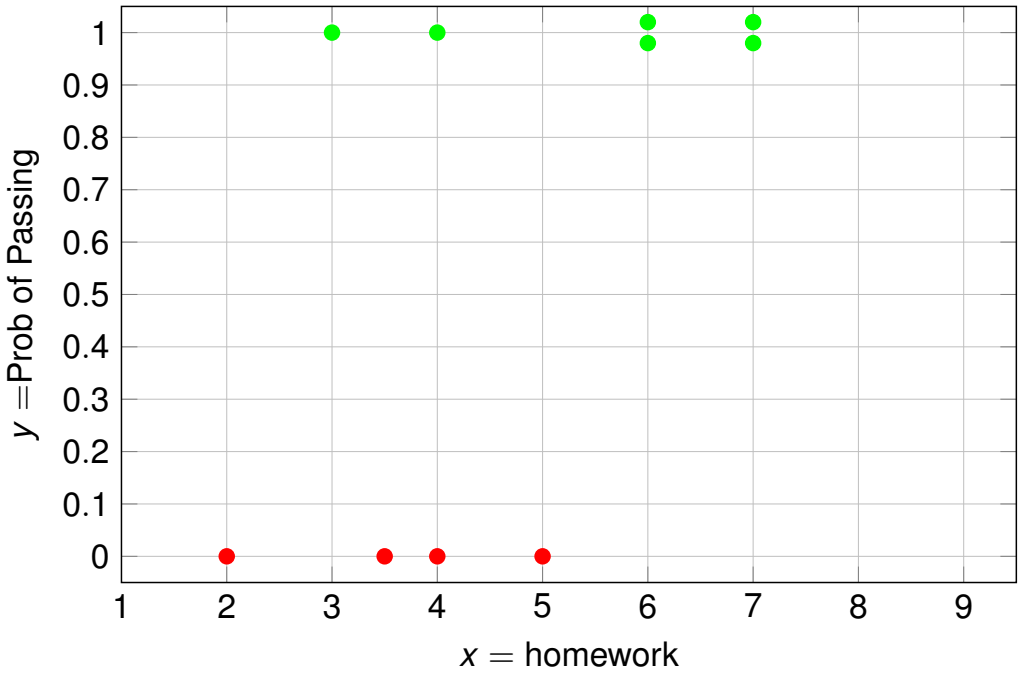

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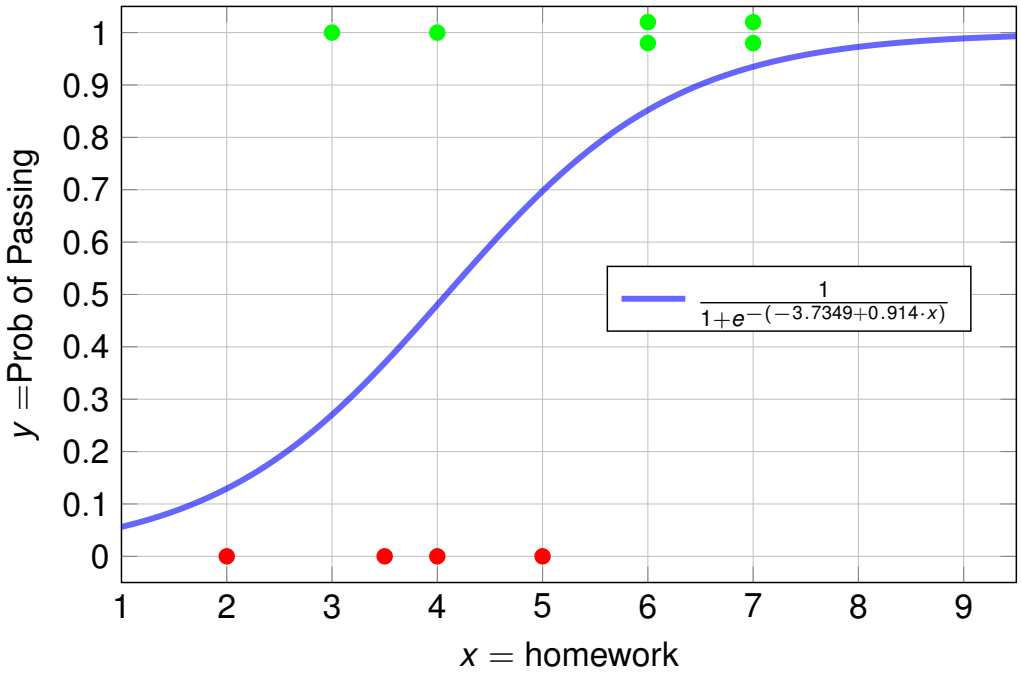

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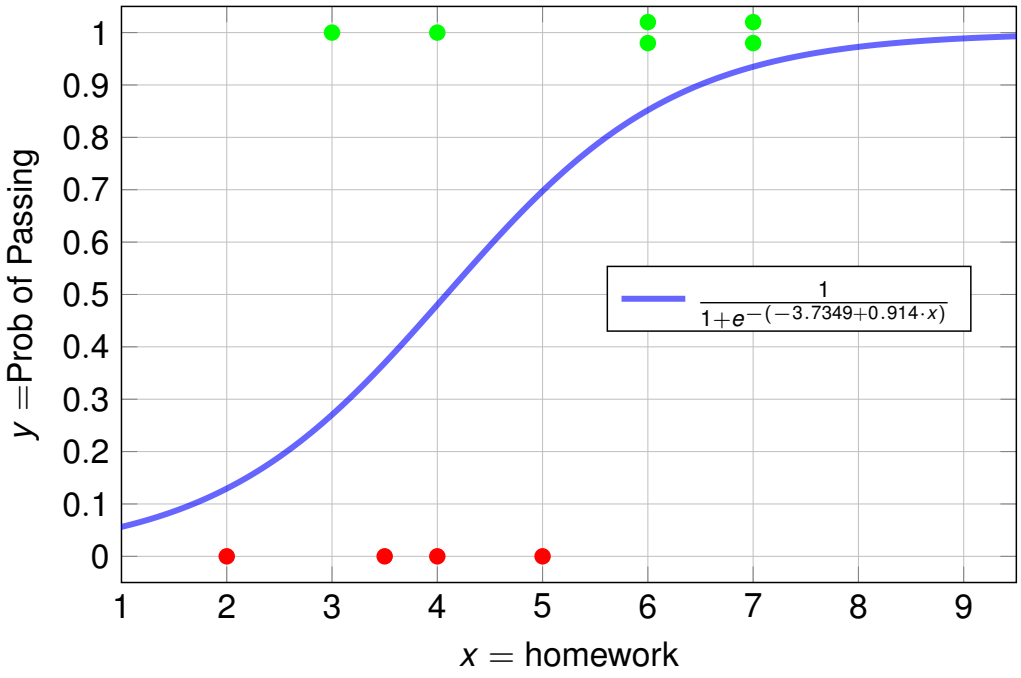

Binary Classification using Logistic Regression

Suppose there is a new student with homework $= 3$ and we have to predict a pass or fail.

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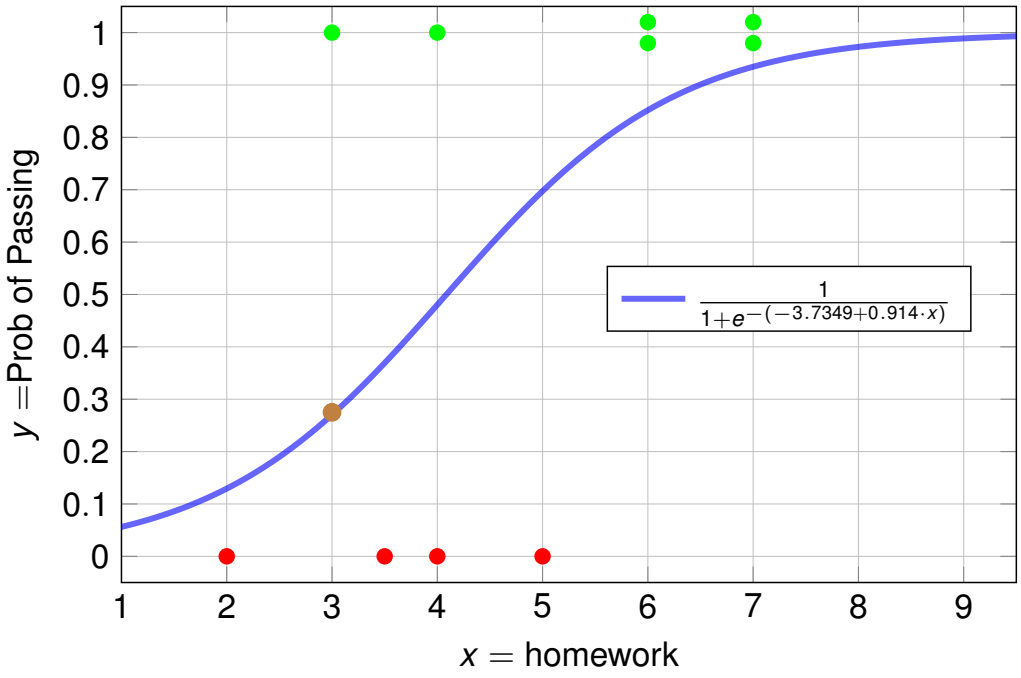

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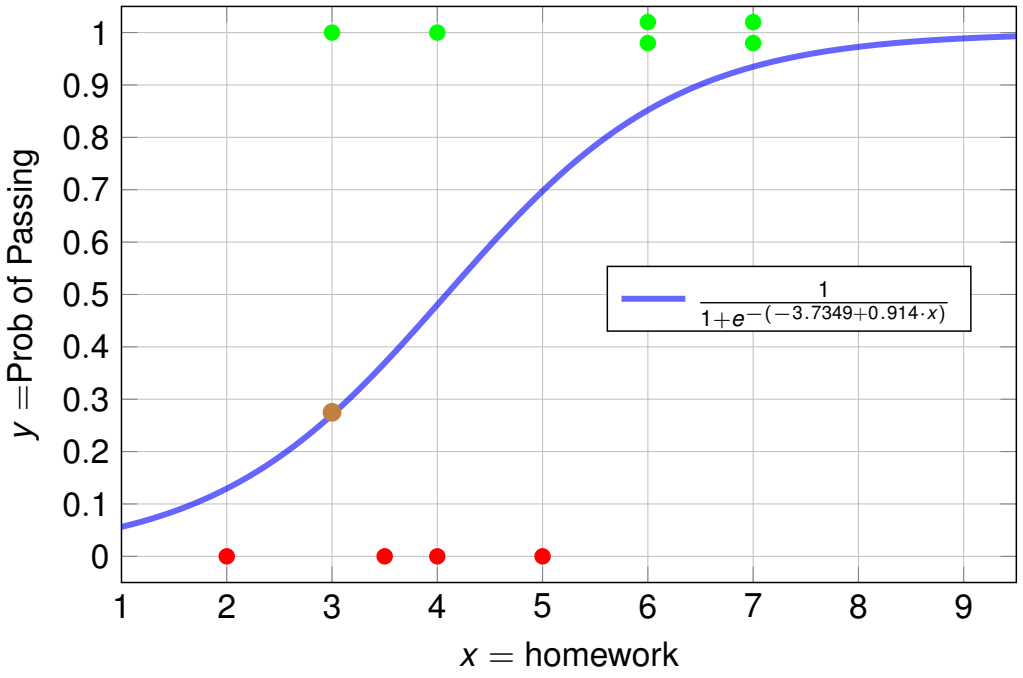

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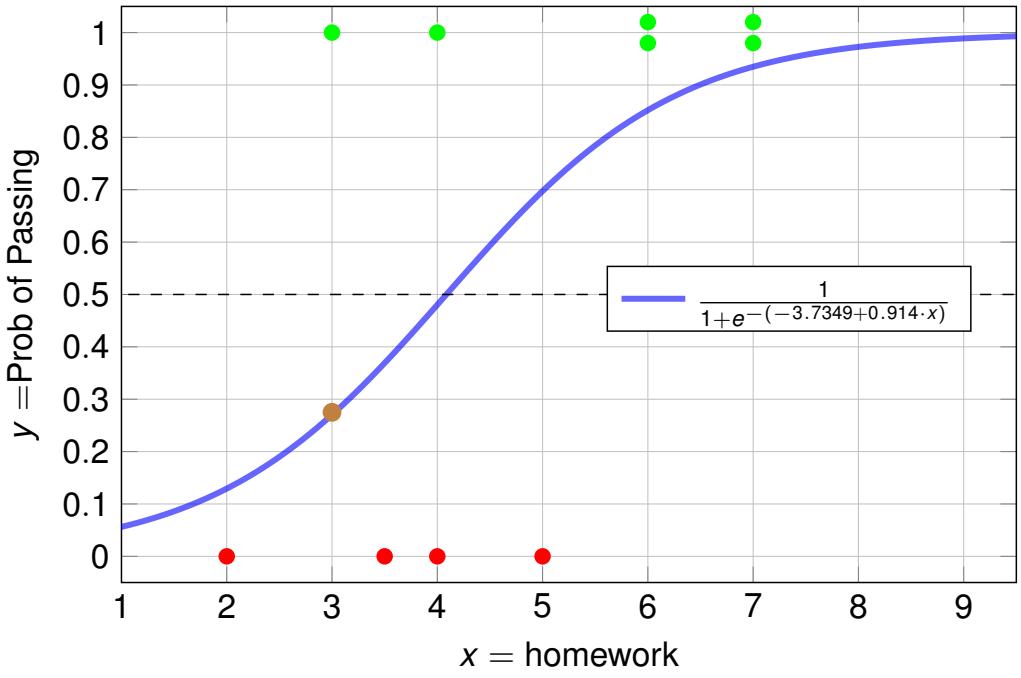

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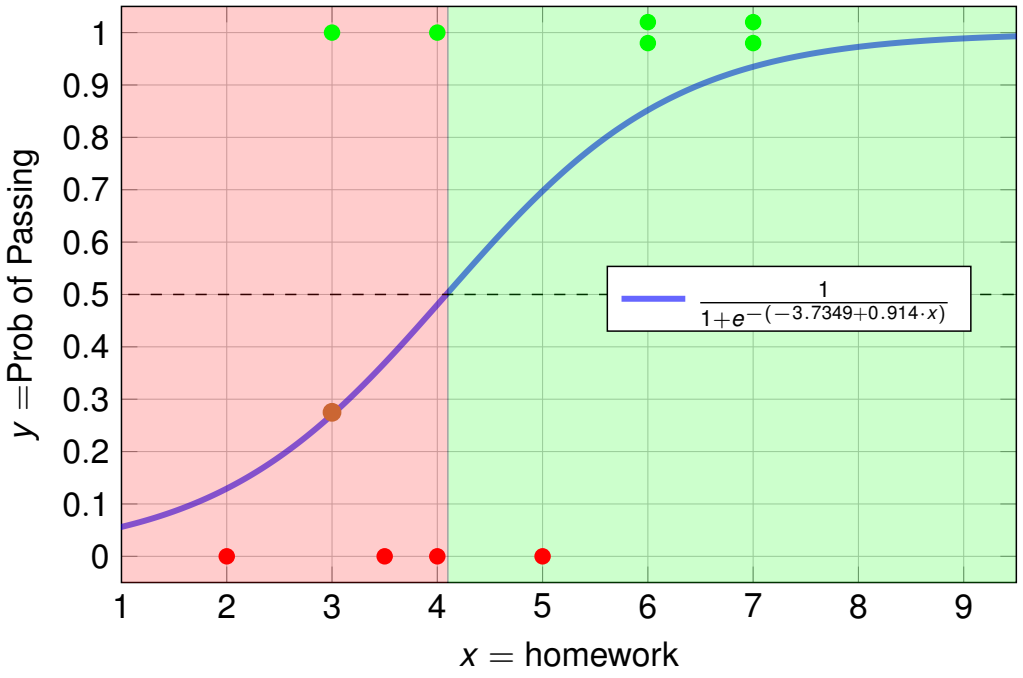

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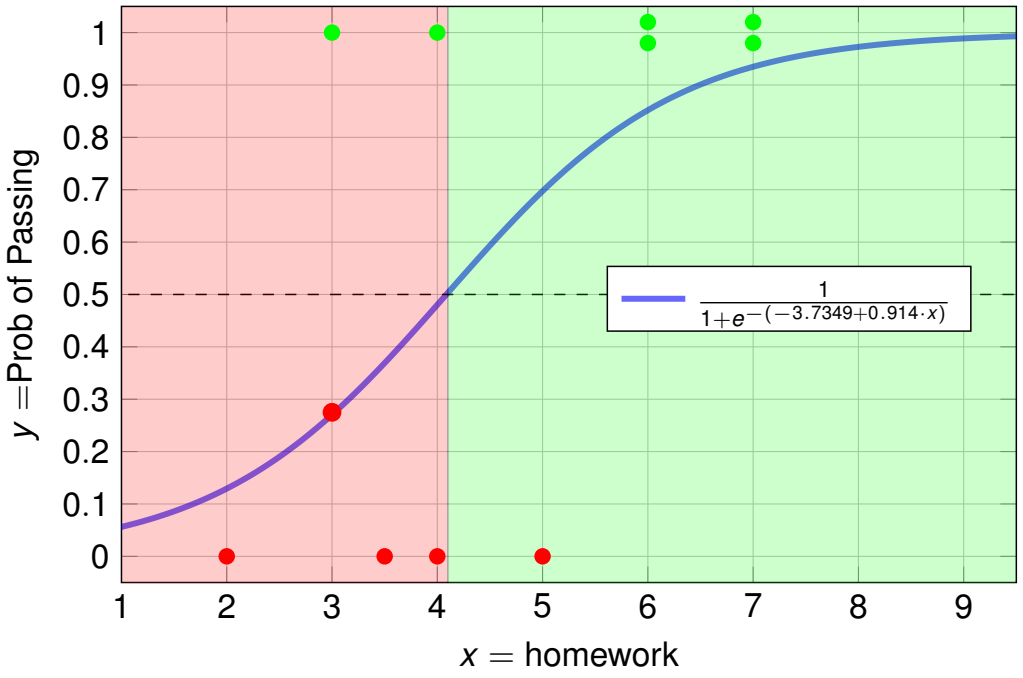

Binary Classification using Logistic Regression

Suppose there is a new student with homework $= 3$ and we have to predict a pass or fail. Model predicts a probability of $< .5 \Rightarrow$ predict fail.

Logistic Regression is a Linear Classifier(!)

- Predict $+1$ iff

$$
\begin{aligned}
& \frac{1}{1+e^{-b-w\cdot x}} \geq 0.5 \\
\Leftrightarrow \quad & 1+e^{-b-w\cdot x} \geq 2 \\
\Leftrightarrow \quad & e^{-b-w\cdot x} \geq 1 \\
\Leftrightarrow \quad & b + w\cdot x \geq 0.
\end{aligned}
$$

Summary: Linear Regression versus Logistic Regression

	Linear Regression	Logistic Regression
Features	numerical or categorical	numerical or categorical
Prediction	numerical	probability, binary (0 or 1)
Optimisation	Least-Squares	Maximum Likelihood
Best-Fit	line/hyperplane	Logistic Function (curve)
Applications	sales forecast	image processing
	grade prediction	spam classification
	...	...

Choice of Logistic Function

Question: Why did we choose the logistic function?

- We could also choose any other function interpolating between 0 and 1, and interpret these values as likelihoods
- The logistic regression function is natural and appears if we assume the Gaussian Naive Bayes model (which we cover in a later lecture)