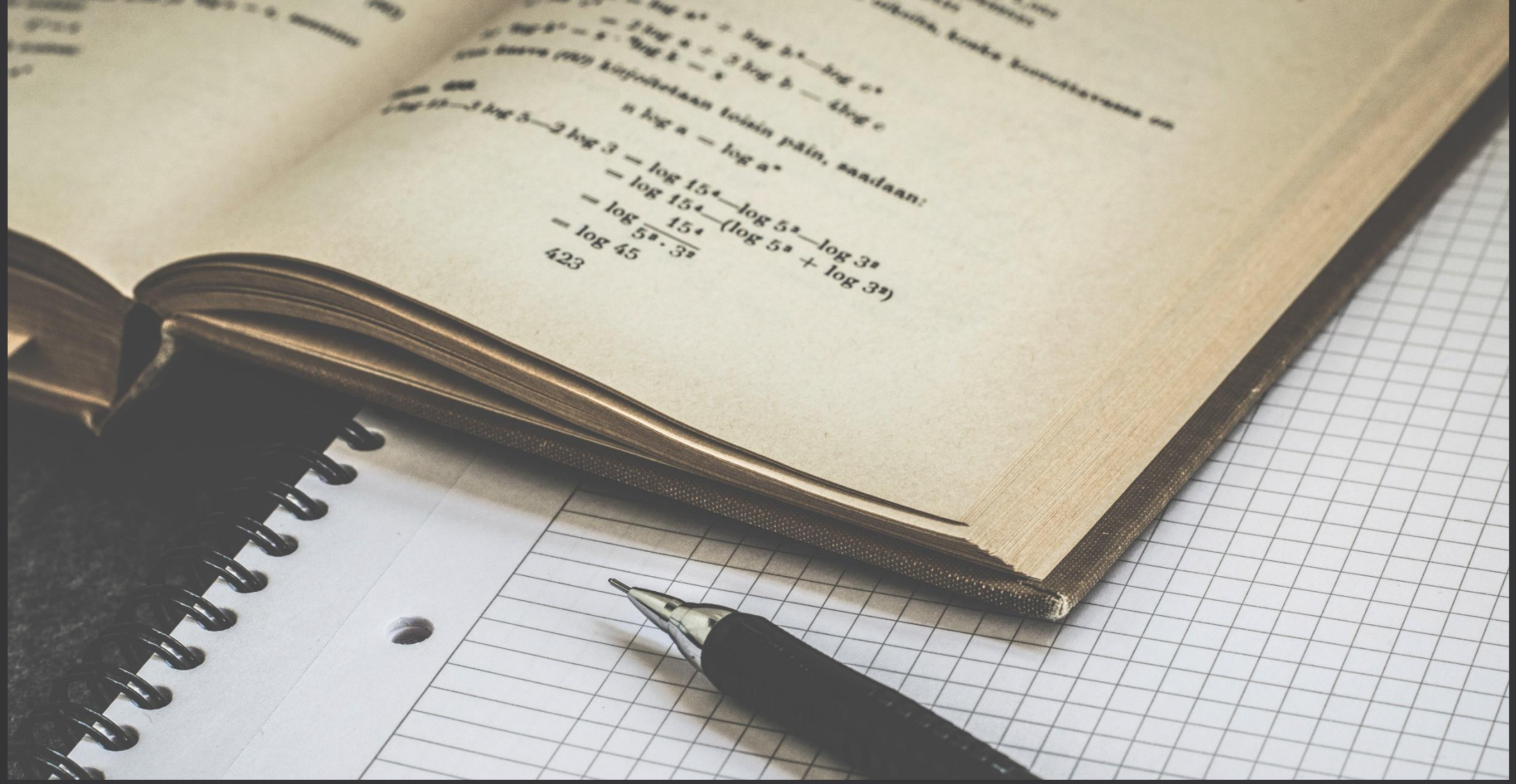

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Introduction to Machine Learning

Machine Learning is a form of statistics

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Machine Learning is a form of statistics

Work with data

Machine Learning is a form of statistics

Use applied mathematics to understand the data

Machine Learning is a form of statistics

Measure your understanding quantitatively

Machine Learning is a form of **automated** statistics

Teach your computer to do it all for you

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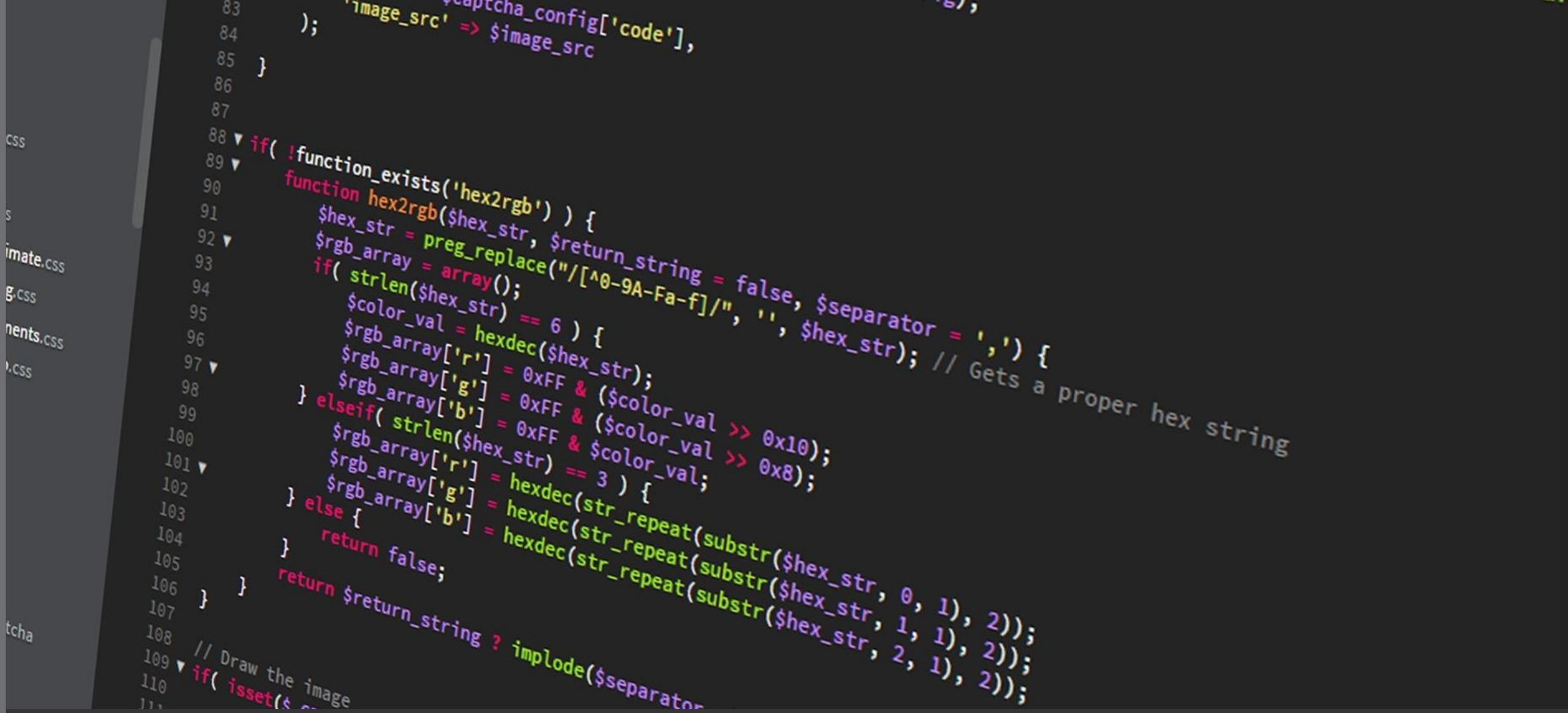

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Introduction to Machine Learning

Setting up an ML and DS problem

Ingredients

Photo by Calum Lewis on Unsplash (retrieved 2023-04-02)

Setting up an ML and DS problem

Ingredients

1. Dataset X
2. Target / label data y

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Setting up an ML and DS problem

Ingredients

1. Dataset X
2. Target / label data y
3. ML model $\hat{y}(w)$
4. Parameters w

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Instructions

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2. Clean / process X and y

Photo by Calum Lewis on Unsplash (retrieved 2023-04-02)

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3. Engineer features of X
4. Split X and y into train, test and validation sets

Photo by Calum Lewis on Unsplash (retrieved 2023-04-02)

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4. Split X and y into train, test and validation sets
5. Set up and train $\hat{y}(w)$
6. Measure $E(y, \hat{y}(w))$ on train and test sets

Photo by Calum Lewis on Unsplash (retrieved 2023-04-02)

Setting up an ML and DS problem

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7. Tune hyperparameters of $\hat{y}(w)$
8. Best $\hat{y}(w)$ minimizes $E(y, \hat{y}(w))$

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5. Set up and train $\hat{y}(w)$
6. Measure $E(y, \hat{y}(w))$ on train and test sets
7. Tune hyperparameters of $\hat{y}(w)$
8. Best $\hat{y}(w)$ minimizes $E(y, \hat{y}(w))$
9. Run final measurement on the validation set

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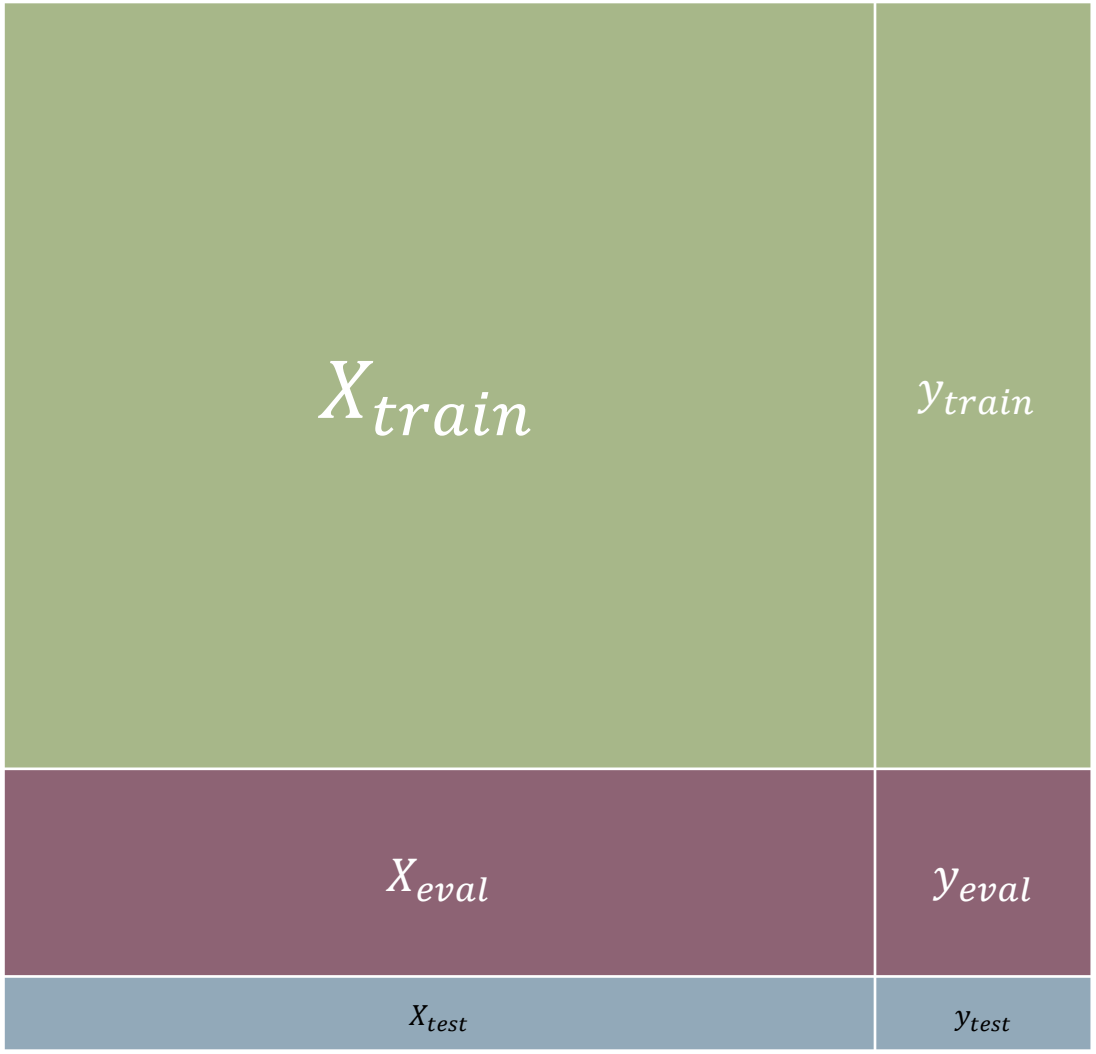
Setting up an ML and DS problem

Describing vs Predicting

Setting up an ML and DS problem

Describing vs **Predicting**



Error function

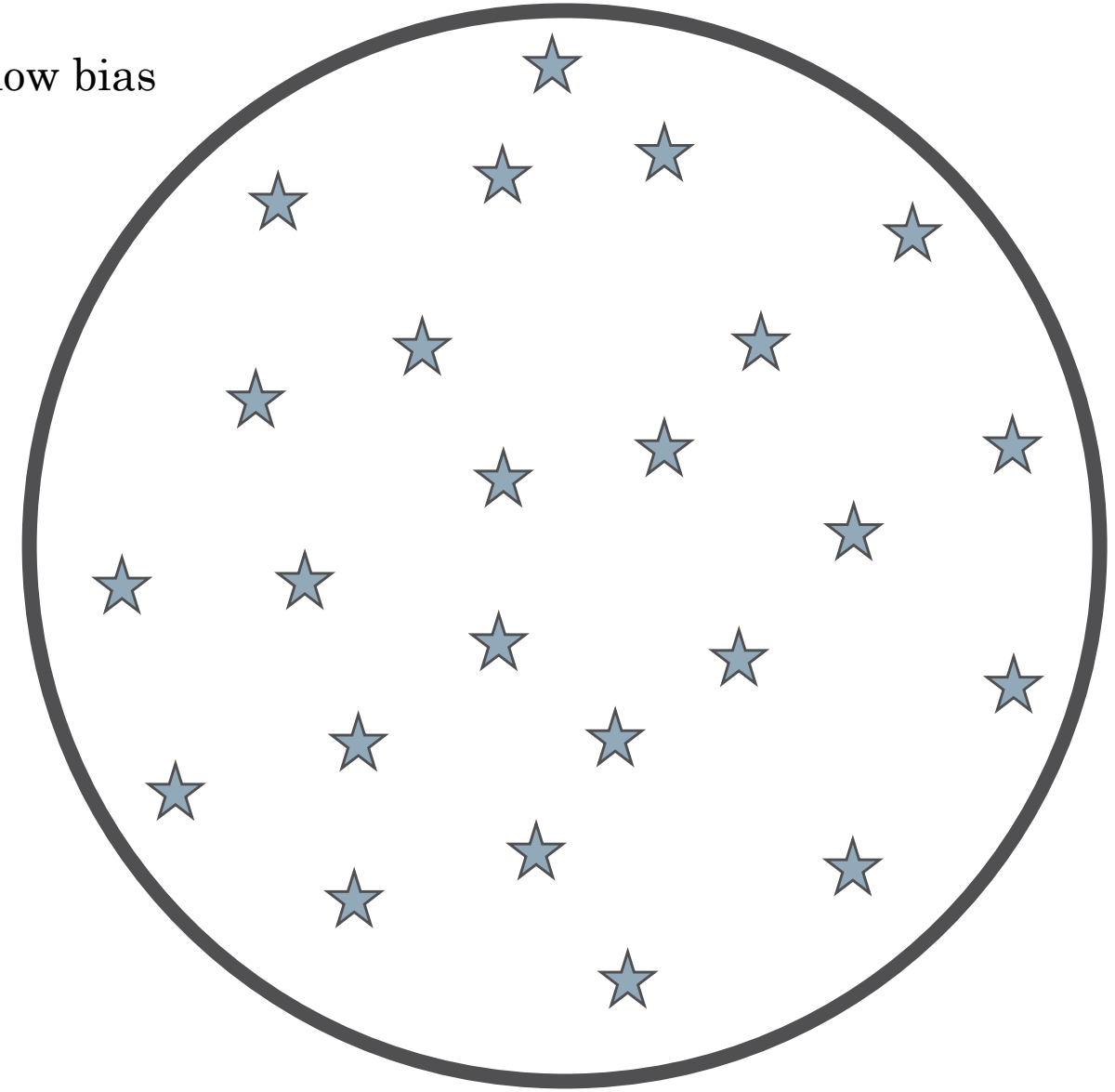
$$E = \sum_i |y_i - \hat{y}_i|$$

Overfitting vs underfitting

This is what **regularization** is for

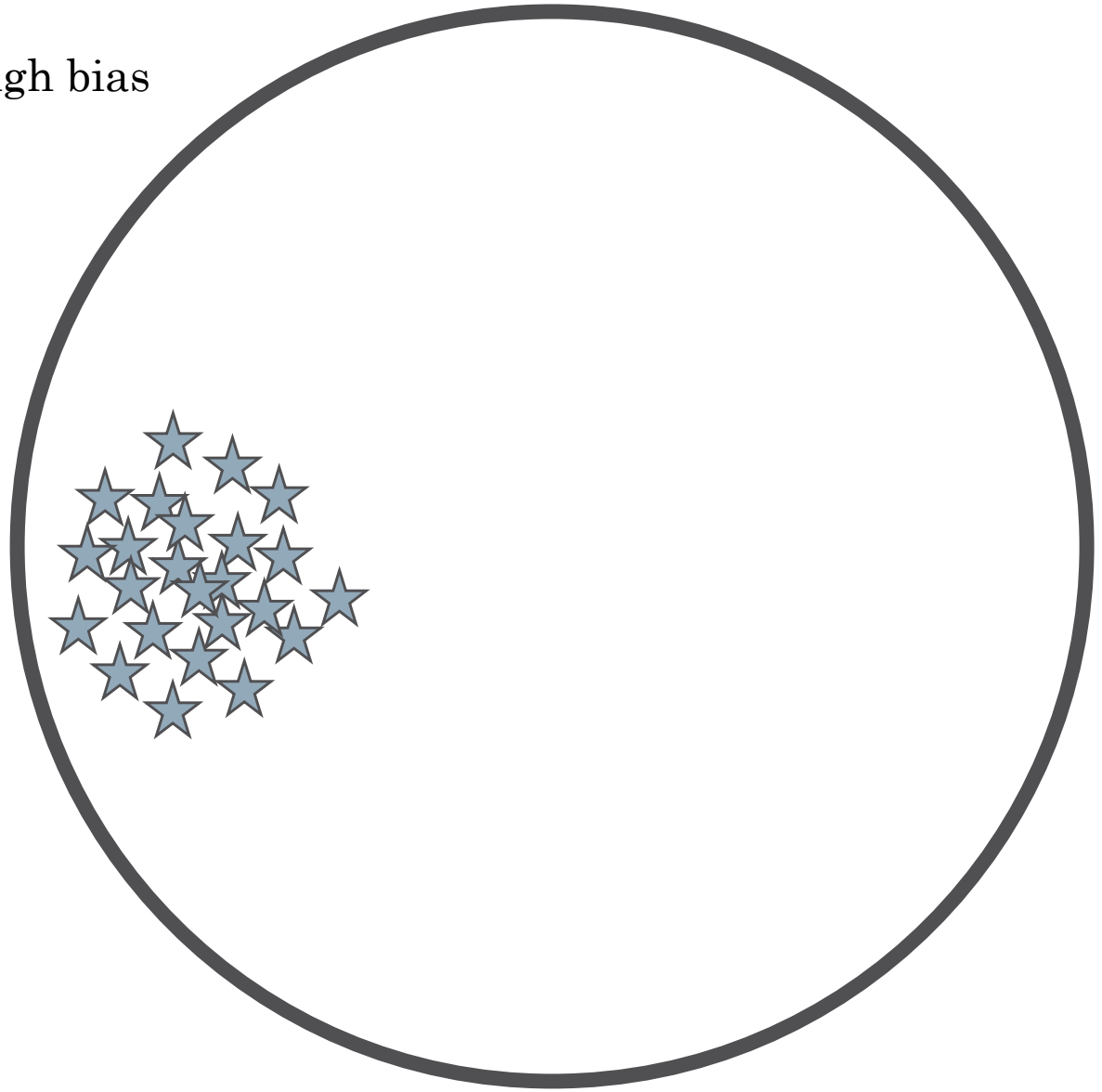
Bias vs variance

High variance, low bias



Bias vs variance

Low variance, high bias



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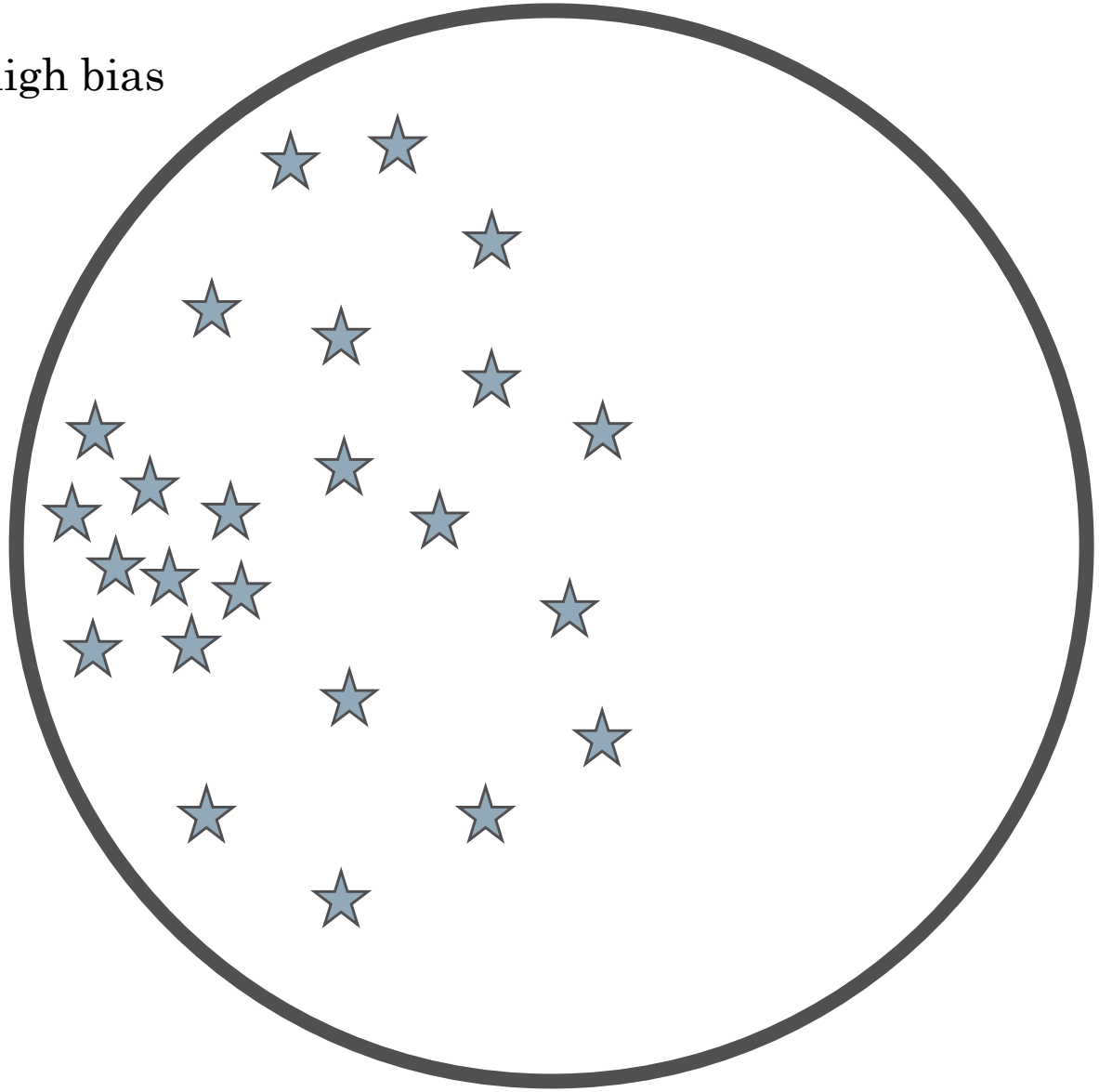

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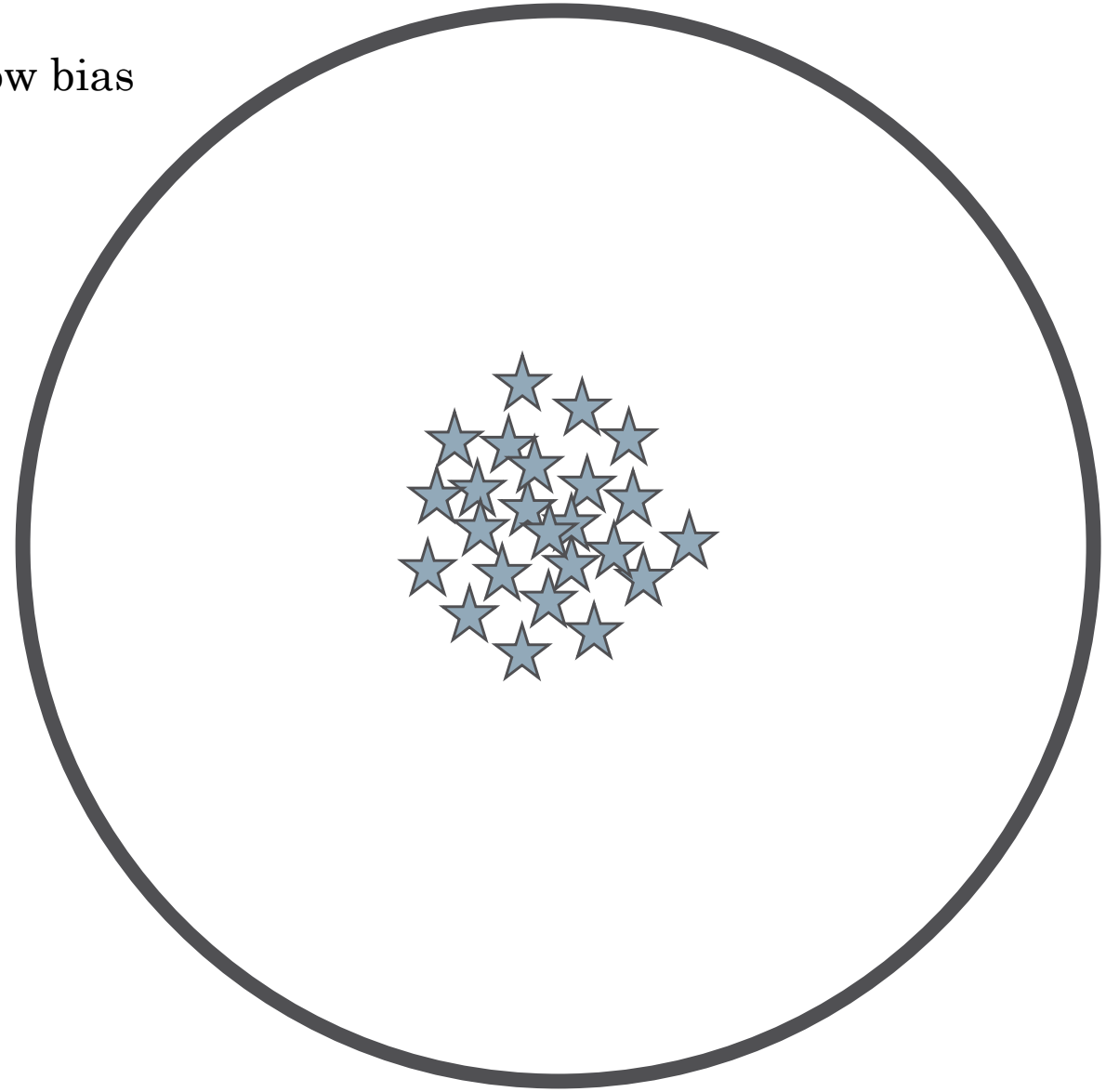
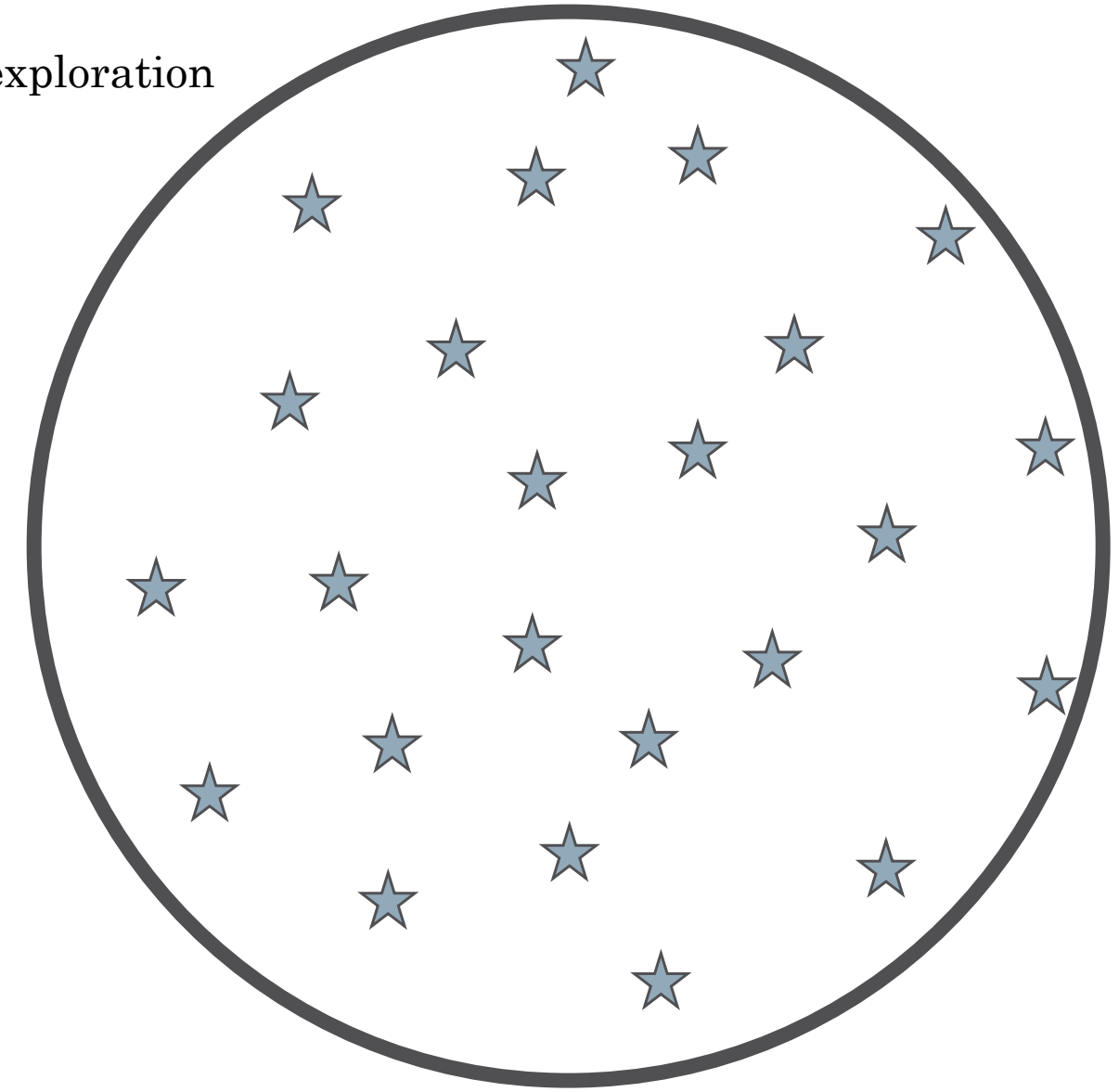


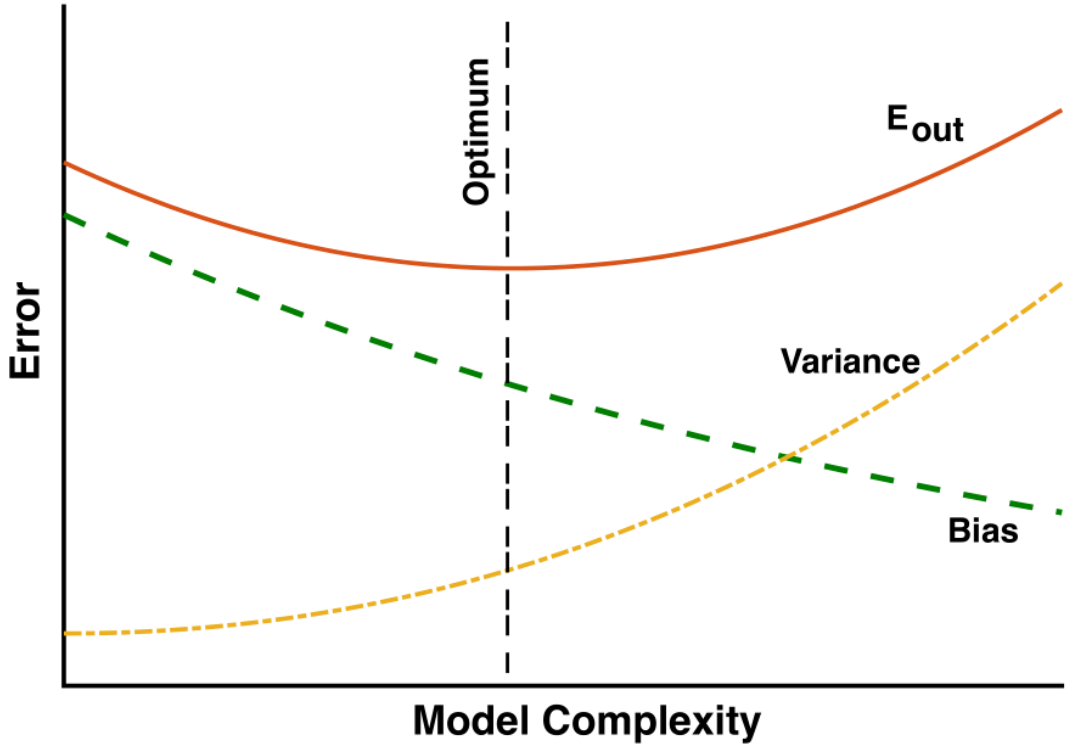
Bias vs variance

Exploitation vs exploration



Reducing bias or variance

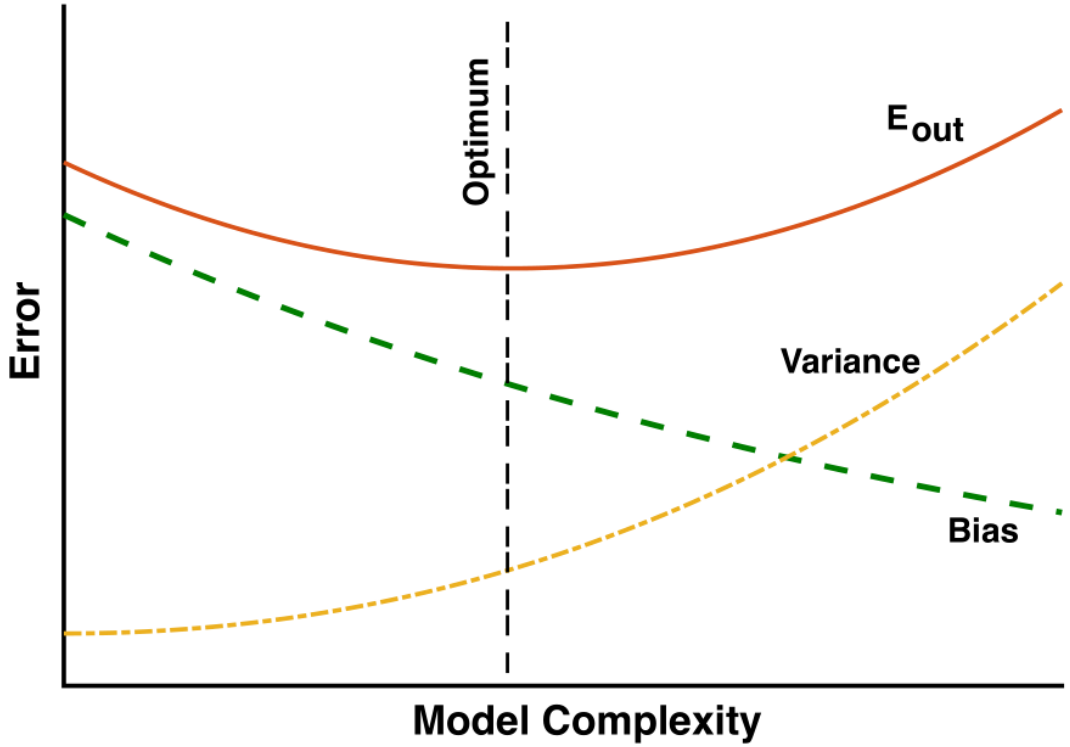
Model complexity



Mehta *et al.*, Physics reports **810**, 1-124 (2019)

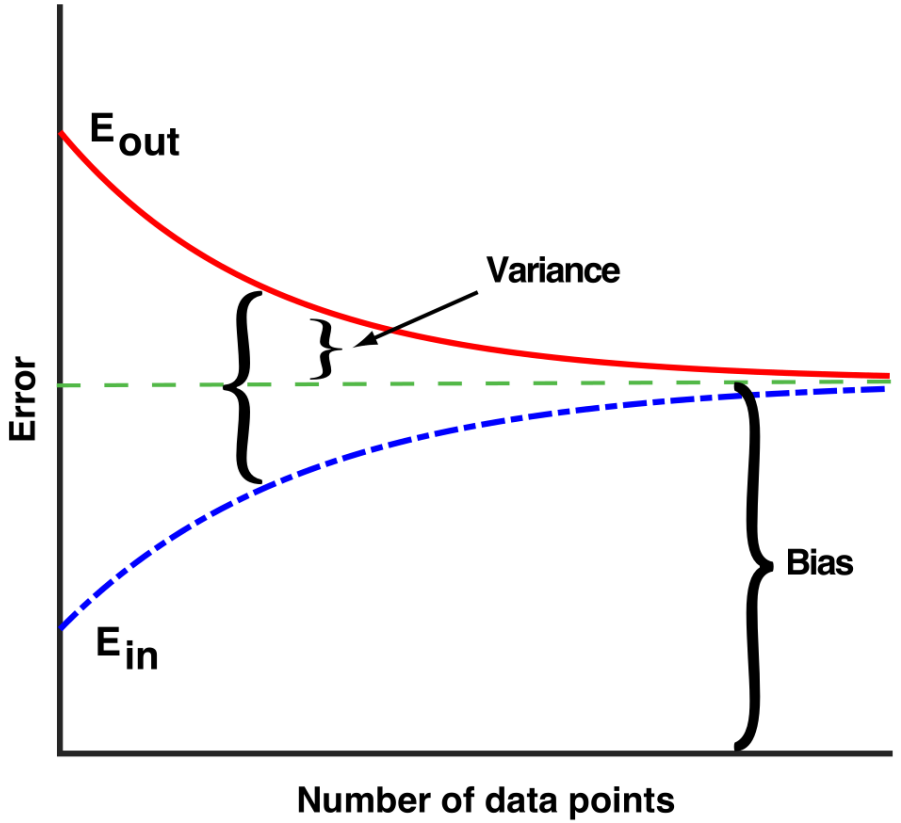
Reducing bias or variance

Model complexity



Mehta *et al.*, Physics reports **810**, 1-124 (2019)

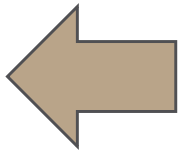
Data set size



Mehta *et al.*, Physics reports **810**, 1-124 (2019)

Gradient descent

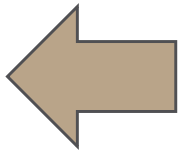
$$E = \sum_i |y_i - \hat{y}_i|$$



How to reduce the error function?

Gradient descent

$$E(w) = \sum_i |y_i - \hat{y}(w)_i|$$

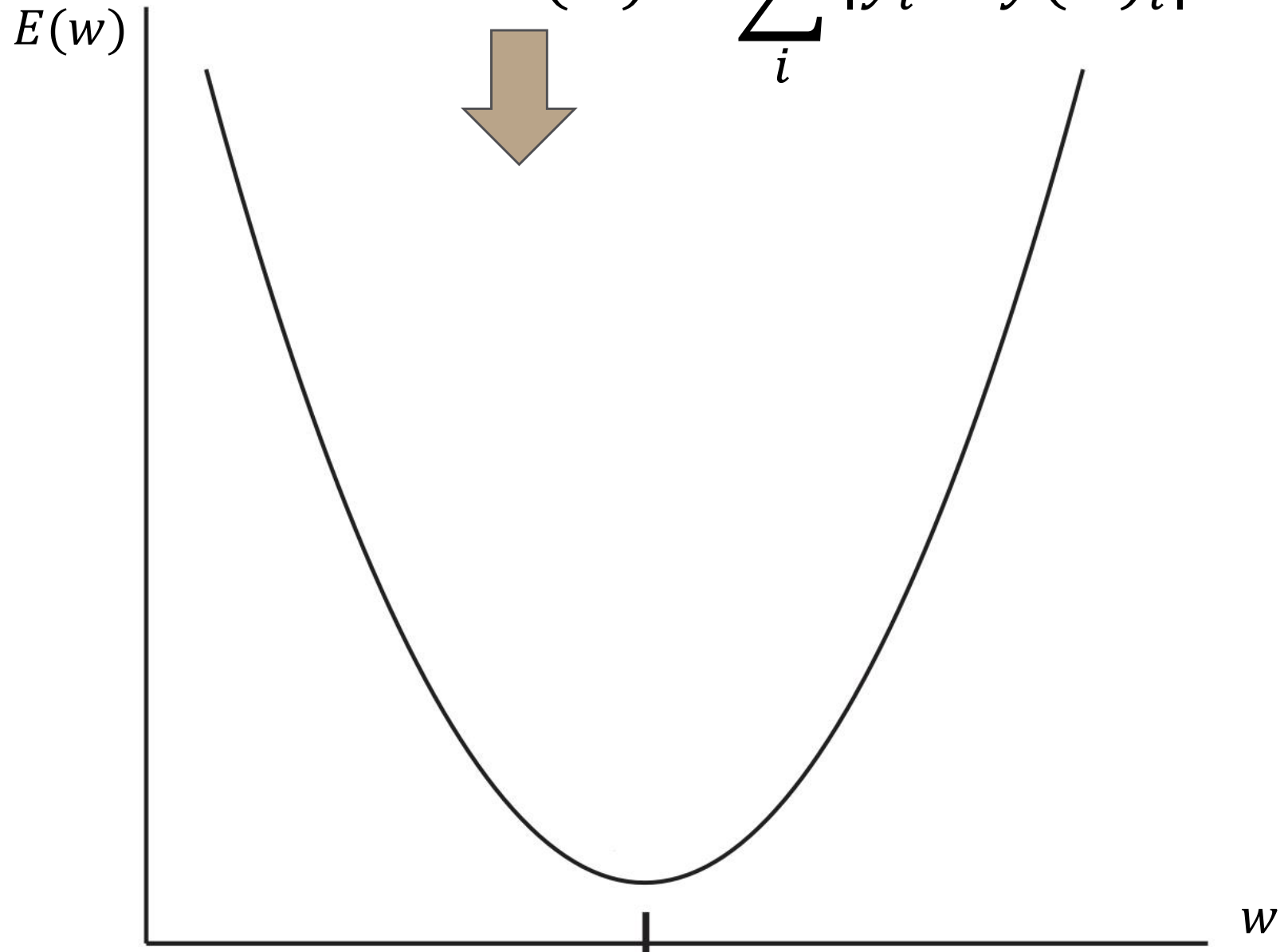


How to reduce the error function?

Gradient descent

$$E(w) = \sum_i |y_i - \hat{y}(w)_i|$$

How to reduce the error function?



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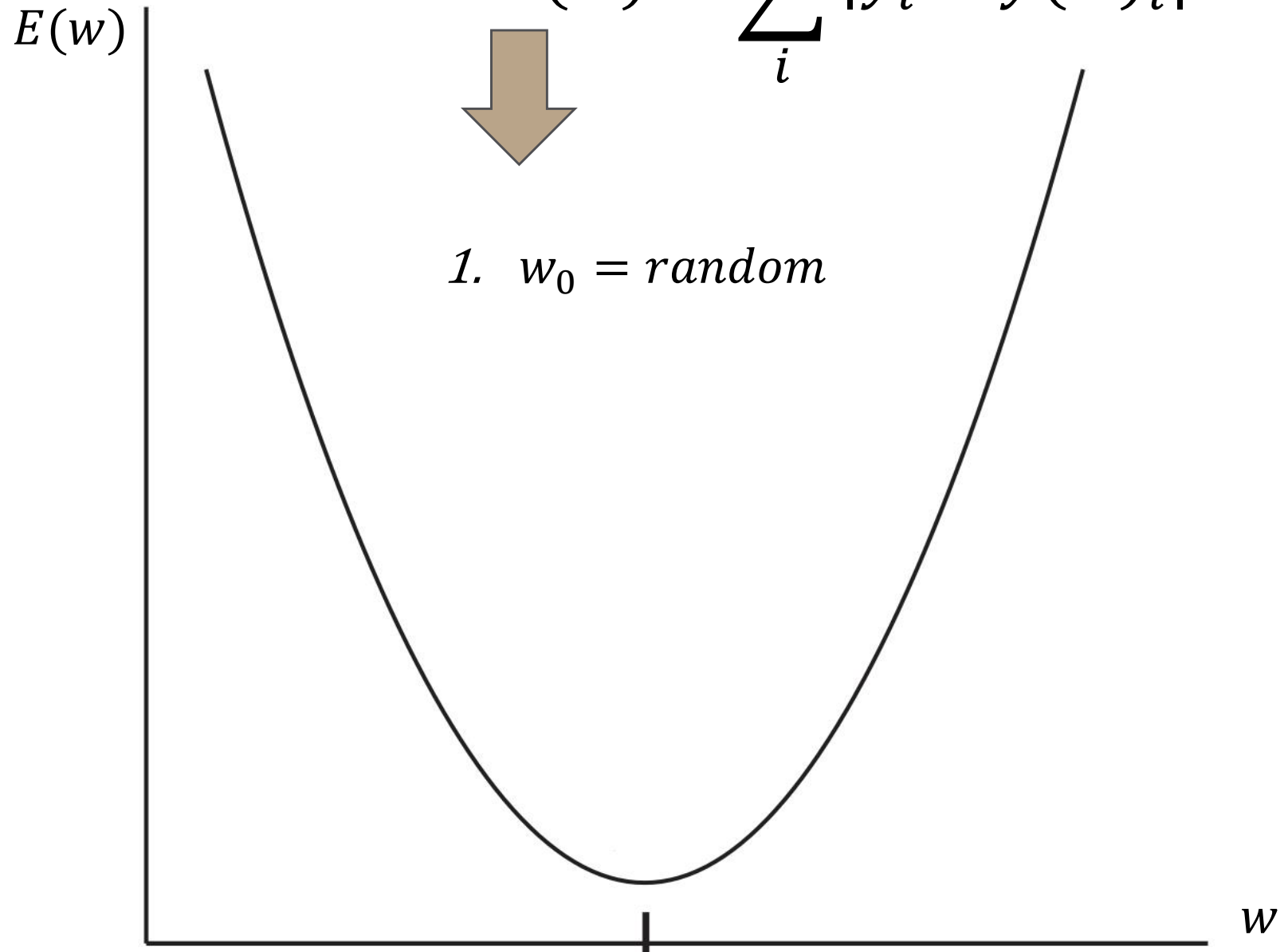
How to reduce the error function?

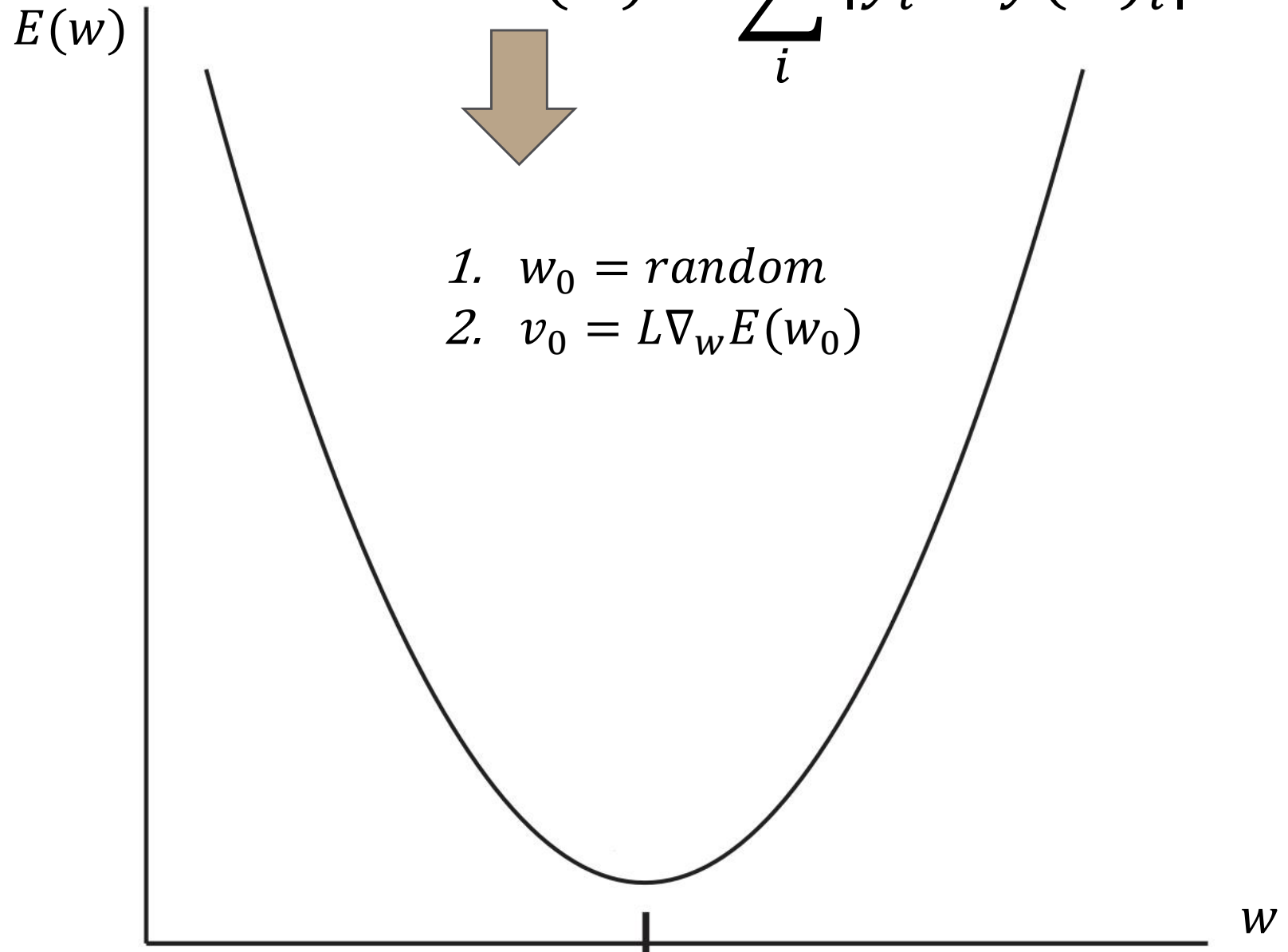


1. $w_0 = random$

Gradient descent

$$E(w) = \sum_i |y_i - \hat{y}(w)_i|$$

How to reduce the error function?

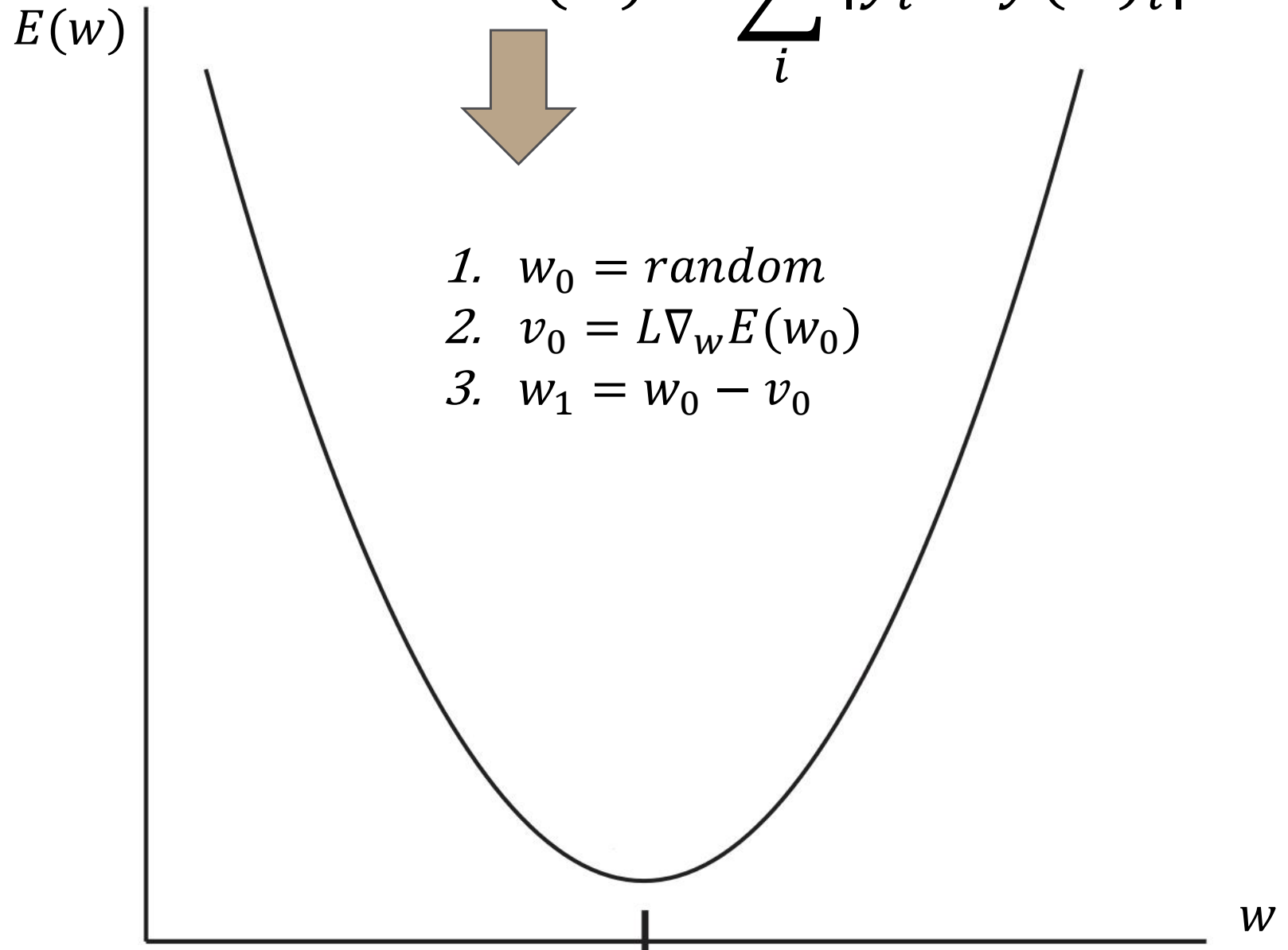


1. $w_0 = random$
2. $v_0 = L\nabla_w E(w_0)$

Gradient descent

$$E(w) = \sum_i |y_i - \hat{y}(w)_i|$$

How to reduce the error function?

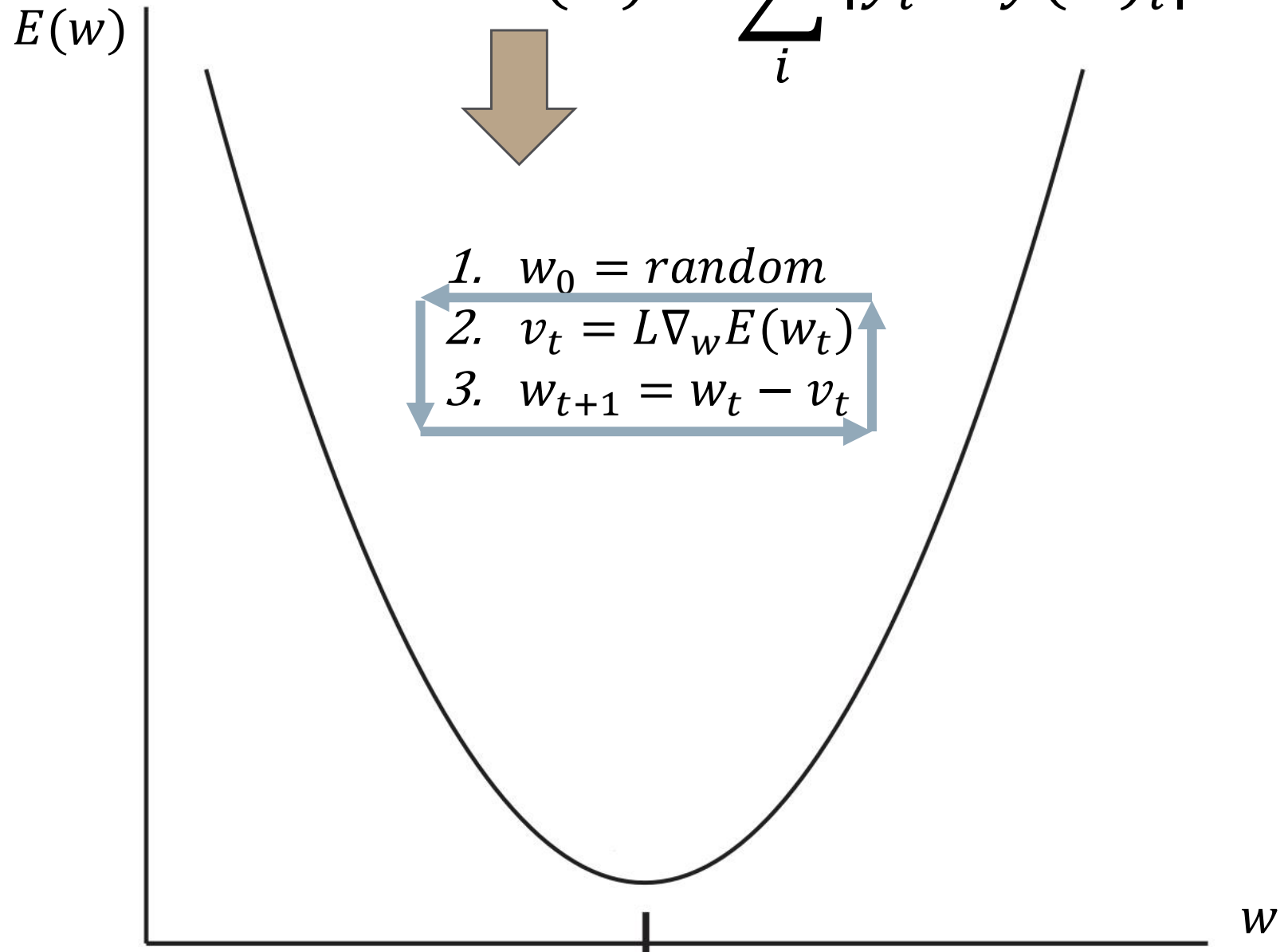


1. $w_0 = random$
2. $v_0 = L\nabla_w E(w_0)$
3. $w_1 = w_0 - v_0$

Gradient descent

$$E(w) = \sum_i |y_i - \hat{y}(w)_i|$$

How to reduce the error function?

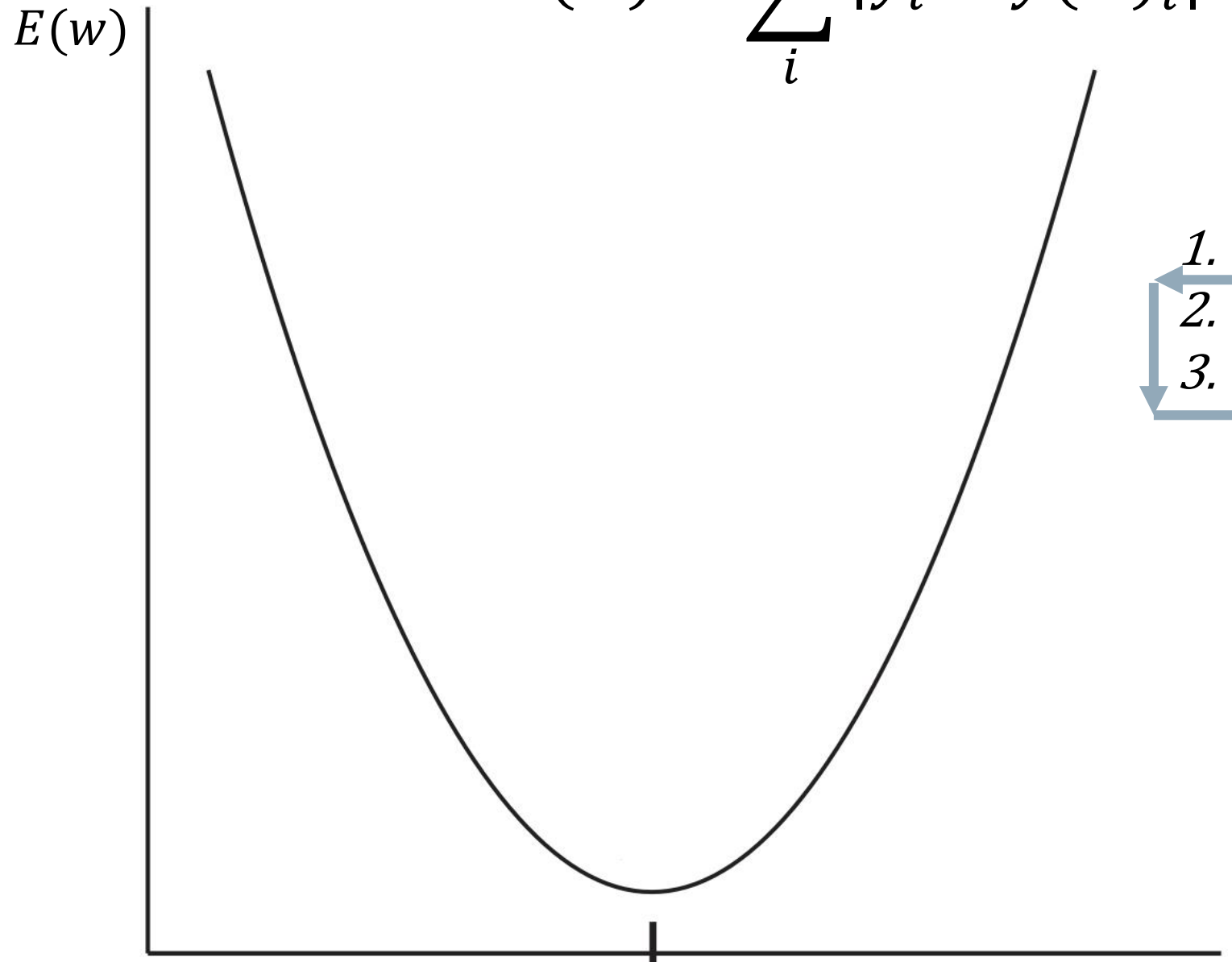


1. $w_0 = random$
2. $v_t = L\nabla_w E(w_t)$
3. $w_{t+1} = w_t - v_t$

Gradient descent

$$E(w) = \sum_i |y_i - \hat{y}(w)_i|$$

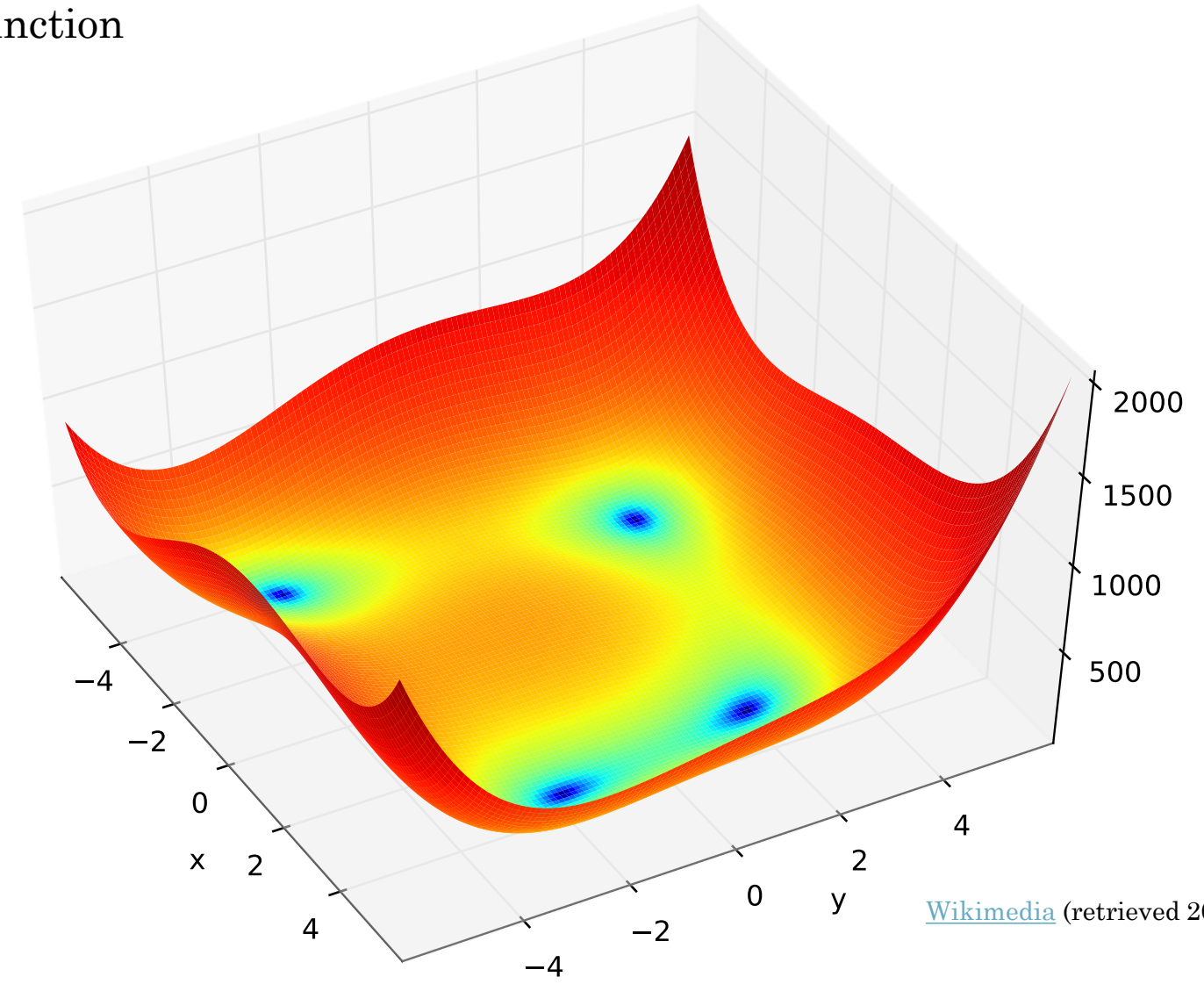
How to reduce the error function?



1. $w_0 = random$
2. $v_t = L\nabla_w E(w_t)$
3. $w_{t+1} = w_t - v_t$

Real-world error functions

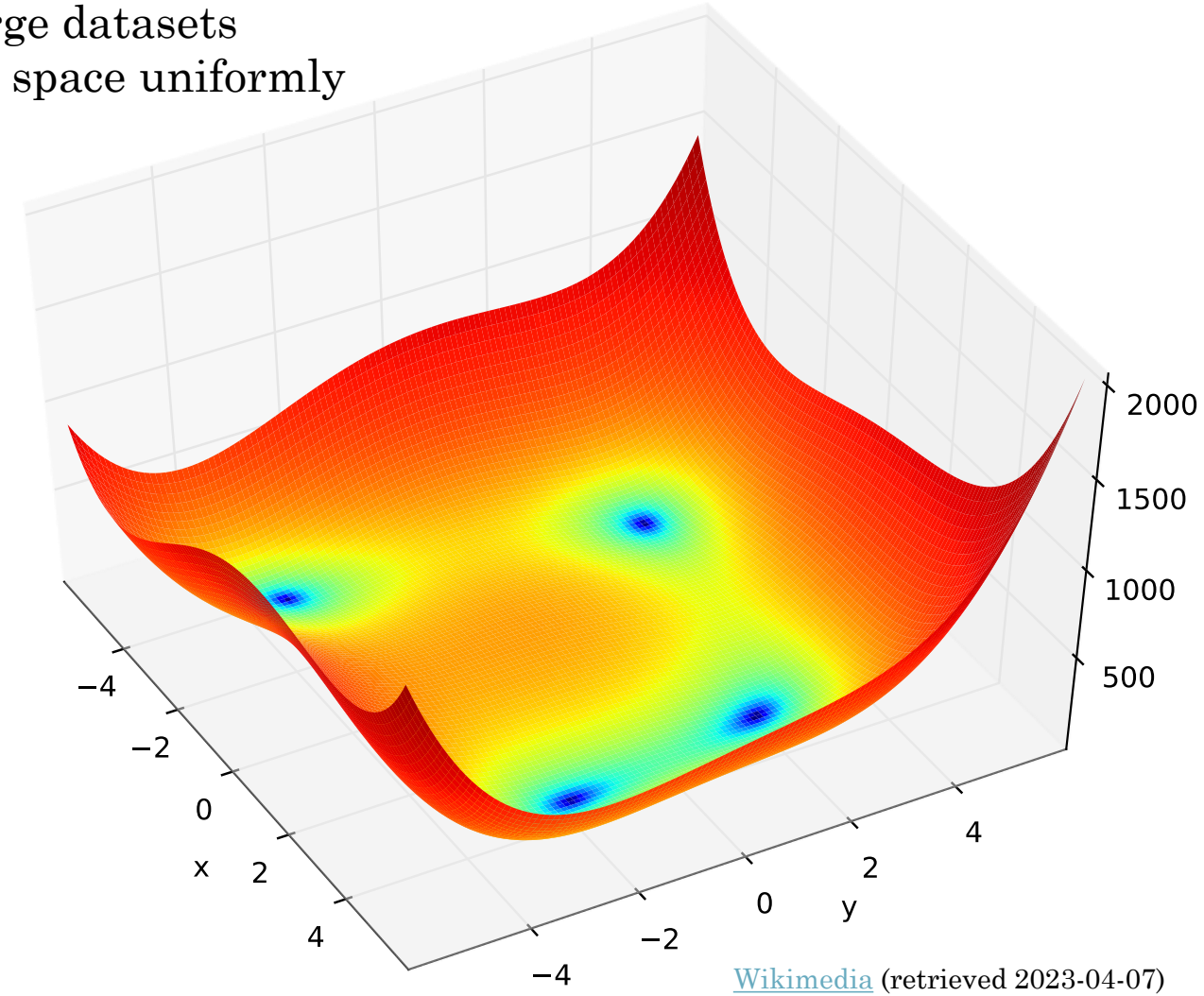
Himmelblau's function



Wikimedia (retrieved 2023-04-07)

Weeknesses of the gradient descent

- GD finds local minima of the cost function
- Computationally expensive for large datasets
- Treats all directions in parameter space uniformly
- Sensitive to L
- Sensitive to w_0



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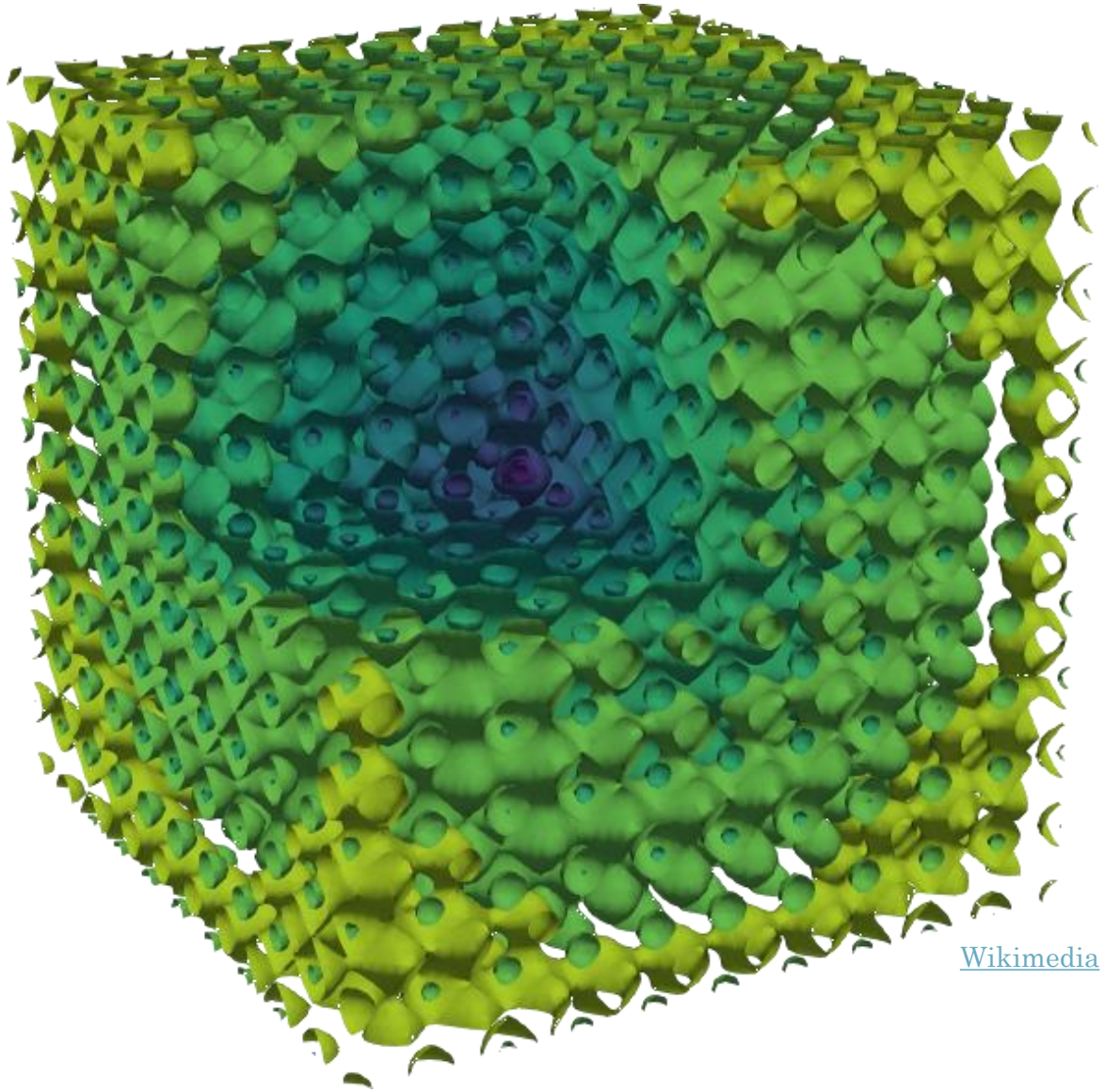
Real-world error functions

Ackley function



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Stochastic gradient descent

$$E(w) = \sum_{i \in B_k} |y_i - \hat{y}(w)_i|$$

Photo by Mark Stebnicki from Pexels retrieved 2023-04-02)

Stochastic gradient descent

$$E_{\boldsymbol{B}}(w) = \sum_{i \in B_k} |y_i - \hat{y}(w)_i|$$

- ✓ Less prone to getting stuck in local minima
- ✓ Less computationally expensive
- • Treats all directions in parameter space uniformly
- • Sensitive to L
- ✓ Less sensitive to w_0

1. $w_0 = random$
2. $v_t = L\nabla_w E_B(w_t)$
3. $w_{t+1} = w_t - v_t$

Photo by Mark Stebnicki from Pexels (retrieved 2023-04-02)

Stochastic gradient descent

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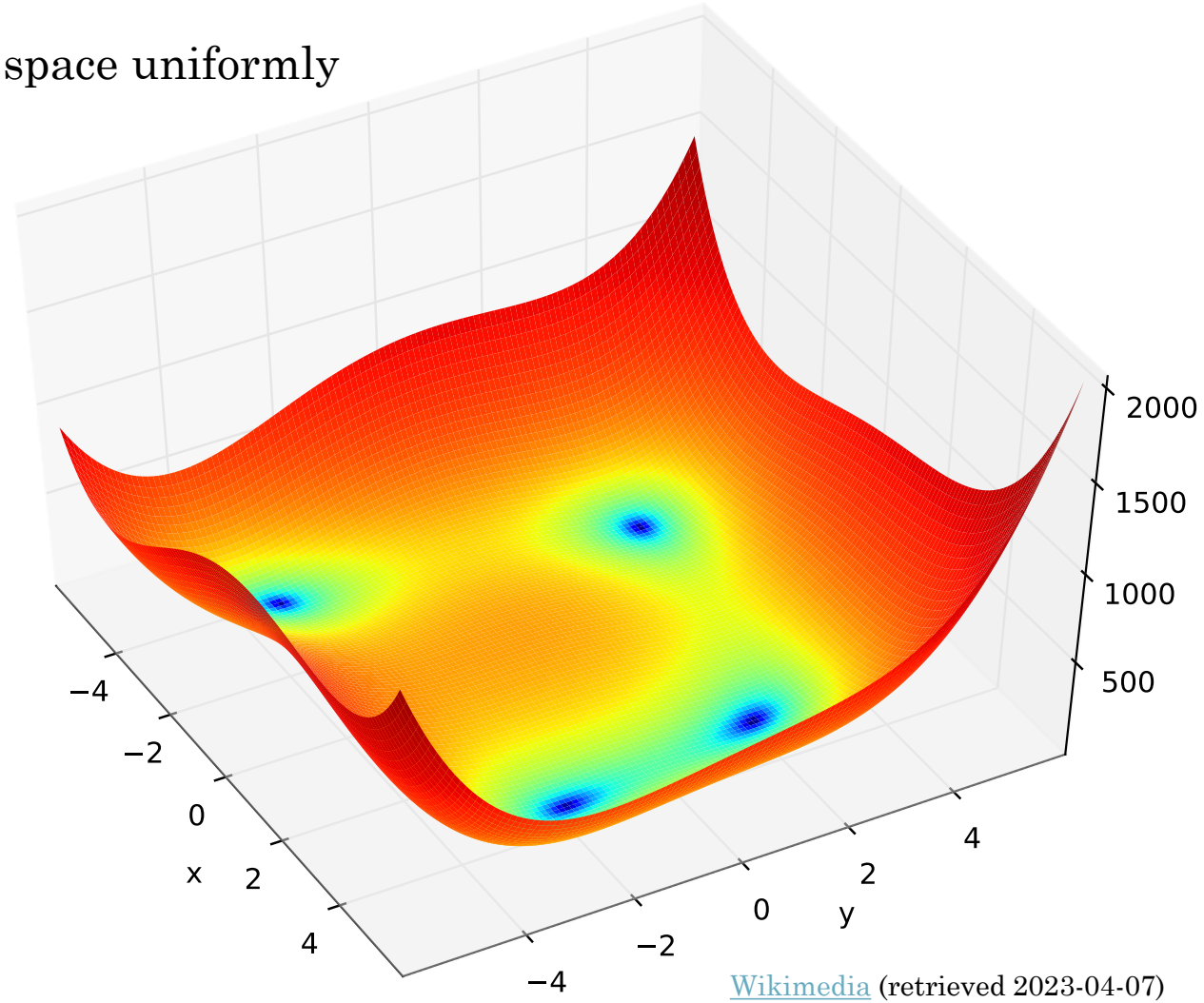

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Adam

$$E_B(w) = \sum_{i \in B_k} |y_i - \hat{y}(w)_i|$$

- ✓ Less prone to getting stuck in local minima
- ✓ Less computationally expensive
- ✓ Doesn't treat all directions in parameter space uniformly
- ✓ Less sensitive to L
- ✓ Less sensitive to w_0

1. $w_0 = random$
2. $v_t = L\frac{m_t}{\sqrt{s_t}+\epsilon}$
3. $w_{t+1} = w_t - v_t$

Photo by Ketut Subiyanto from Pexels (retrieved 2023-04-02)

Adam

$$E_B(w) = \sum_{i \in B_k} |y_i - \hat{y}(w)_i|$$

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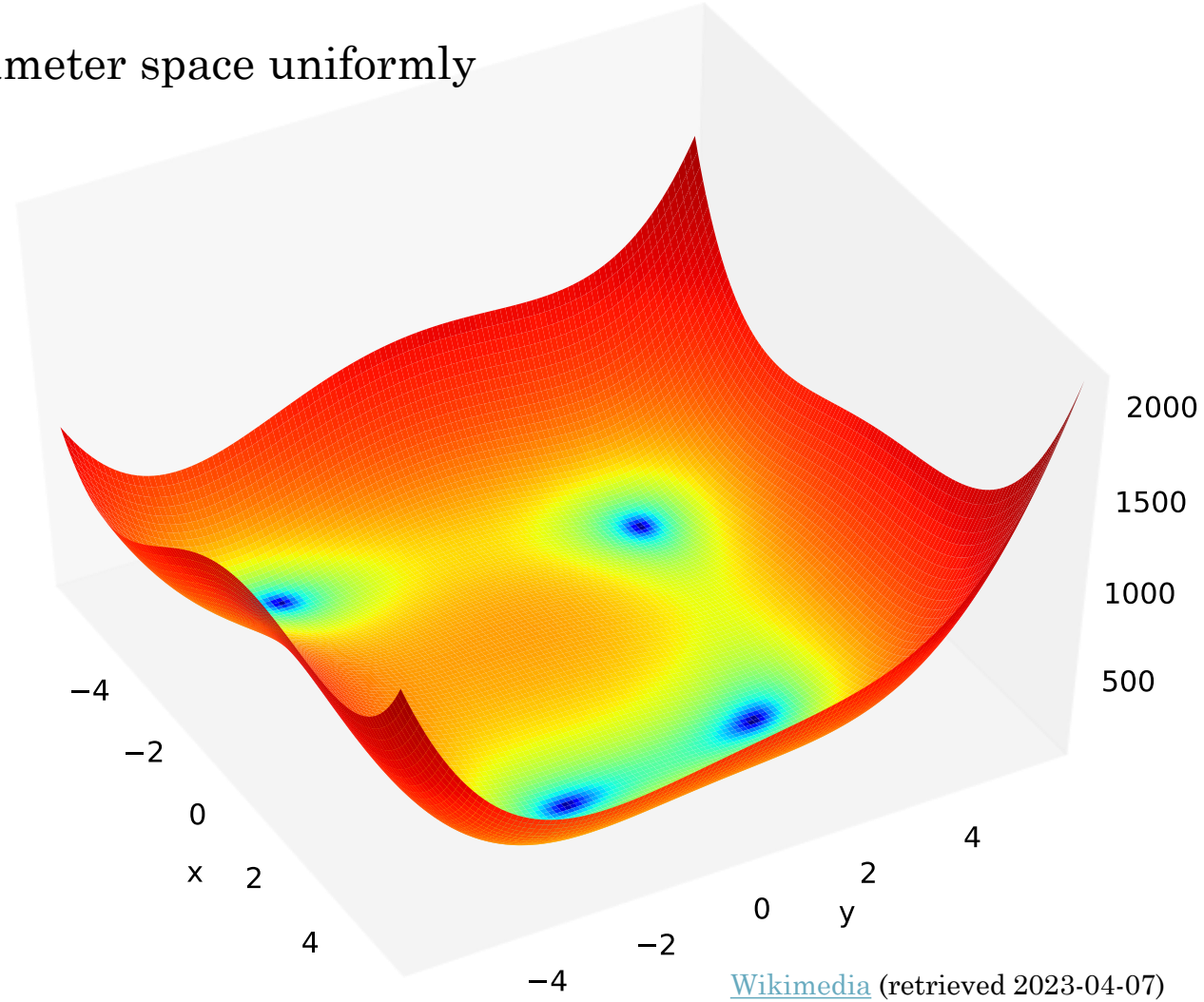

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Regression vs classification

Regression	Classification

Classification: sigmoid and softmax

Sigmoid
- output is a vector of elements in (0,1)
- each element evaluated separately

$$f(x_i) = \frac{e^{x_i}}{e^{x_i} + 1}$$

$$\begin{pmatrix} 3 \\ 5 \\ 8 \\ 2 \\ 3 \\ 4 \end{pmatrix} \rightarrow ML \rightarrow sigmoid \rightarrow round \rightarrow \begin{pmatrix} 1 \\ 1 \\ 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}$$

Softmax
- output is a vector of elements in (0,1)
- "survival of the fittest"

$$f(x_i) = \frac{e^{x_i}}{\sum_j e^{x_j}}$$

$$\begin{pmatrix} 3 \\ 5 \\ 8 \\ 2 \\ 3 \\ 4 \end{pmatrix} \rightarrow ML \rightarrow softmax \rightarrow round \rightarrow \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

Classification: cross-entropy

The go-to error function for classification

$$P = \prod_i f(x_i, w)^{y_i} (1 - f(x_i, w))^{1-y_i}$$

Classification: cross-entropy

The go-to error function for classification

$$P = \prod_i f(x_i, w)^{y_i}(1 - f(x_i, w))^{1-y_i}$$

$$l = \sum_i y_i \log(f)(1 - y_i)\log(1 - f)$$

Classification: cross-entropy

The go-to error function for classification

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$$\hat{w} = argmax_w\ (l)$$

Classification: cross-entropy

The go-to error function for classification

$$P = \prod_i f(x_i, w)^{y_i}(1 - f(x_i, w))^{1-y_i}$$

$$l = \sum_i y_i \log(f)(1 - y_i)\log(1 - f)$$

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Classification: cross-entropy

The go-to error function for classification

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$$l = \sum_i y_i \log(f)(1 - y_i)\log(1 - f)$$

$$\hat{w} = argmax_w\ (l) = argmin_w\ (-l)$$

cross-entropy $= -\sum_i y_i \log(f)(1 - y_i)\log(1 - f)$

Bagging and boosting

- BAGGing = Bootstrap AGGregation
- Bootstrapping: sampling data with replacement (not to confuse with *batching*)

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Bagging and boosting

- BAGGing = Bootstrap AGGregation
- Bootstrapping: sampling data with replacement
- Approach:
  1. Bootstrap various data samples
  2. Create a weak classifier for each bootstrapped sample
  3. Aggregate the weak classifiers into one "collectively" strong classifier

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Bagging and boosting

- BAGGing = Boostrap AGGregation
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Bagging and boosting

- BAGGing = Boostrap AGGregation
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- Approach:
  1. Bootstrap various data samples
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  3. Apply a weight to each weak classifier (=**boosting**)
  4. Aggregate the weak classifiers into one "collectively" strong classifier

- Bagging reduces variance but increases bias
- Best practice: use with "unstable" ML models

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Types of learning

Supervised

Photo by Andrea Piacquadio from Pexels (retrieved 2023-04-07)

Types of learning

Supervised

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Data 1	Data 2	Data …	Data 100	Labels
x11	x21	…	x1001	0
x12	x22	…	x1002	1
x13	x23		x1003	0
x14	x24		x1004	0
x15	x25		x1005	1

Types of learning

Unsupervised

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Types of learning

Unsupervised

Examples:
- Clustering
- Dimensionality reduction
- Generative modeling

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Types of learning

Reinforcement

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Types of learning

Reinforcement

- Agent interacting with the environment.
- Updating behavior based on reward
- Often used in games and robotics

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