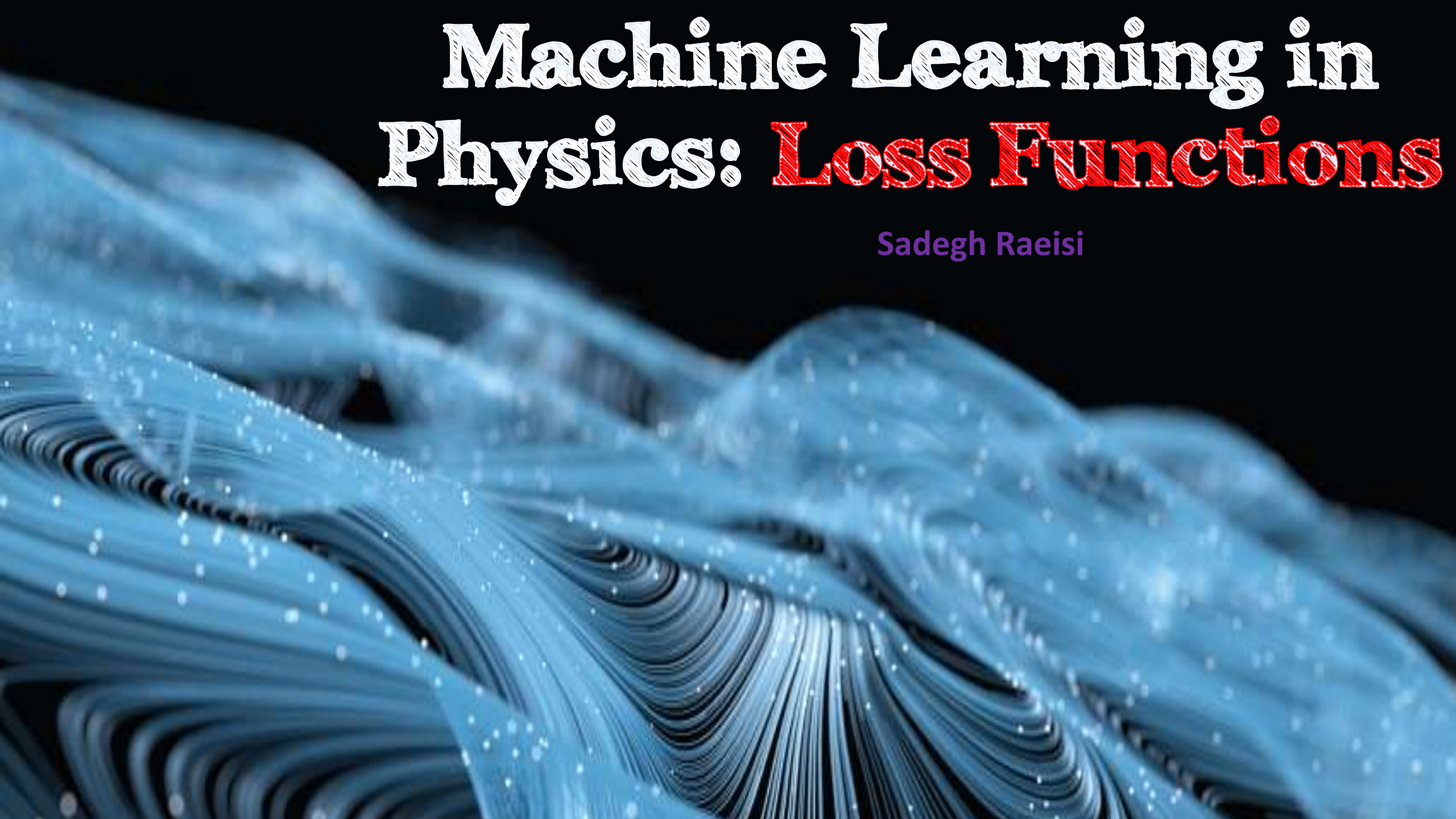
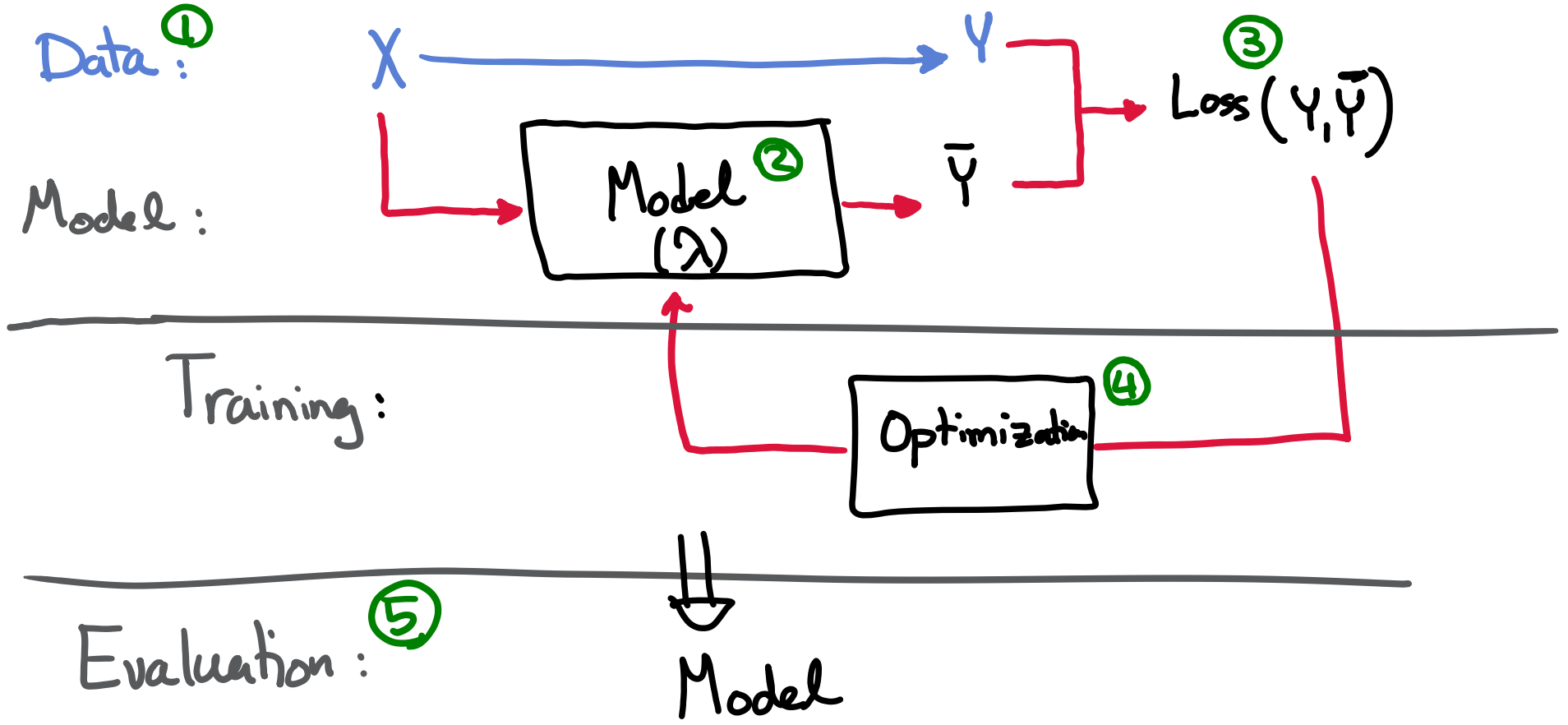
Machine Learning in Physics: Loss Functions

Sadegh Raeisi

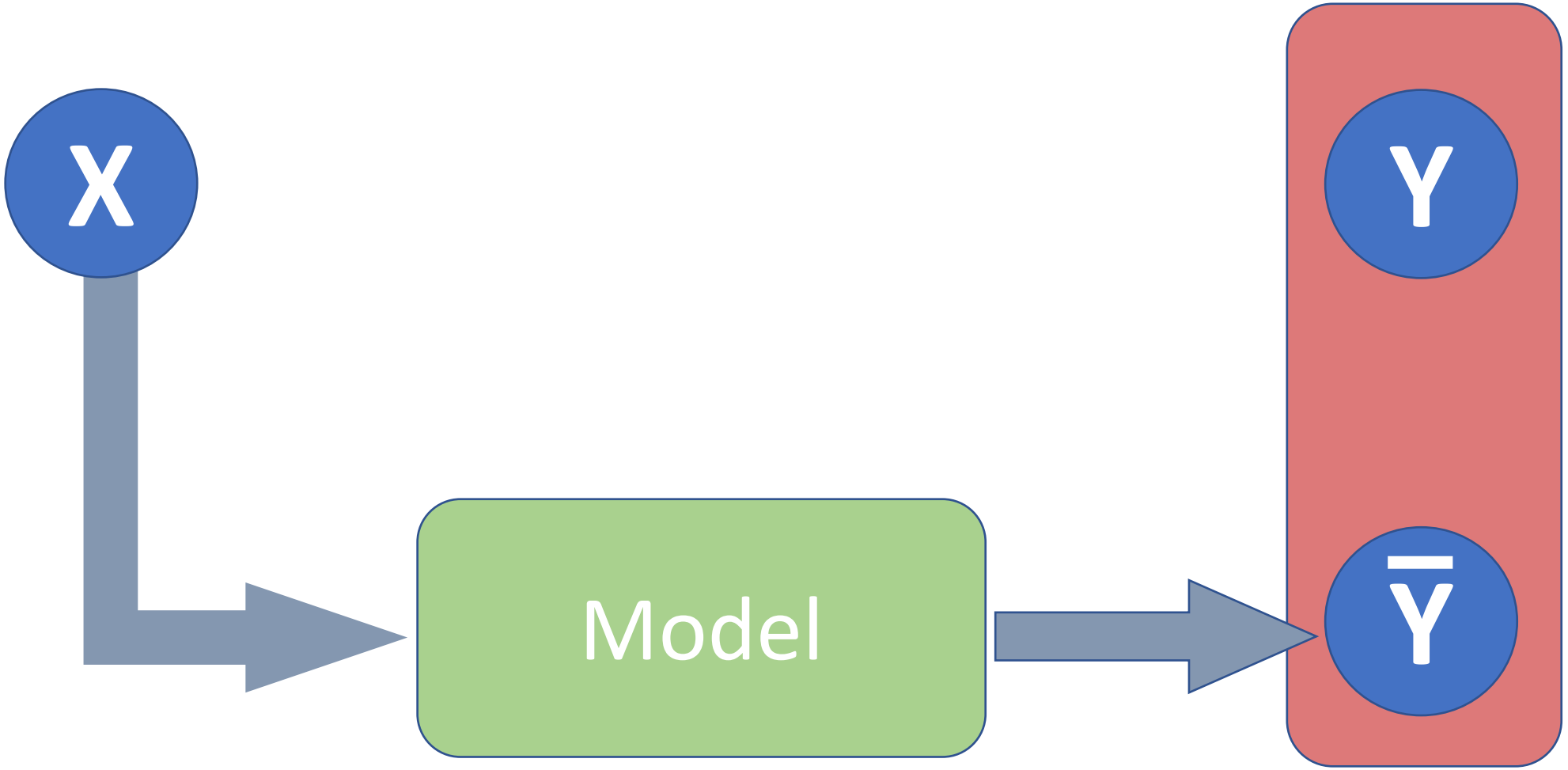


Supervised: Ingredients

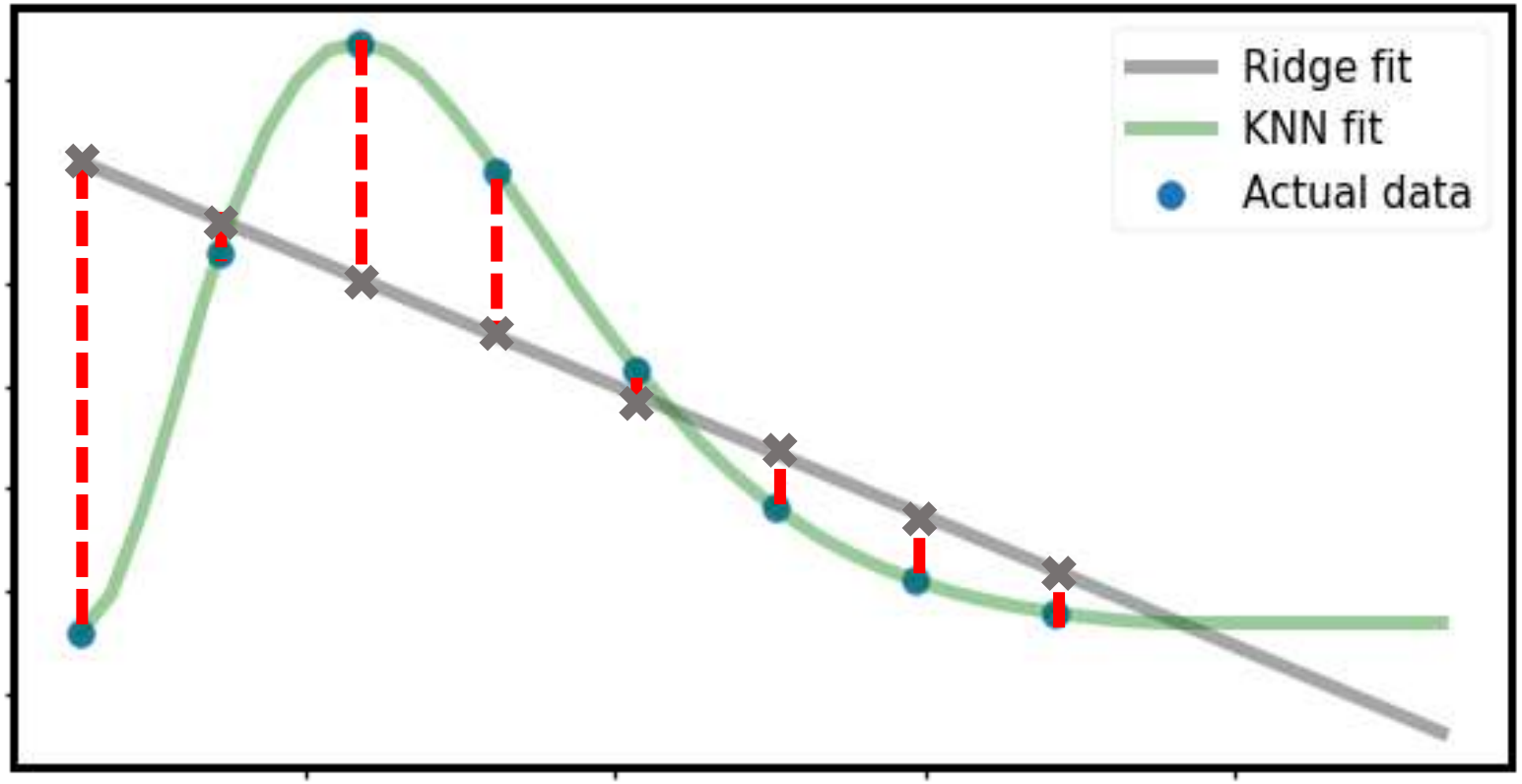


Outline

Concept


X
Model
Y
Ȳ

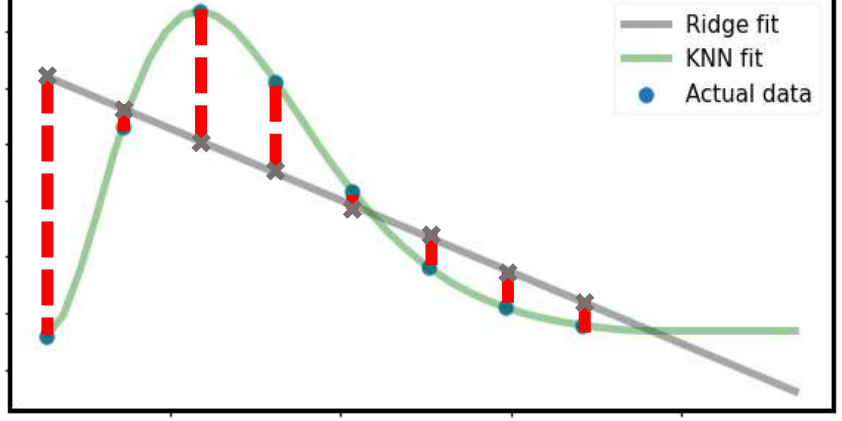
How close are the predictions?



How can we quantify the difference?

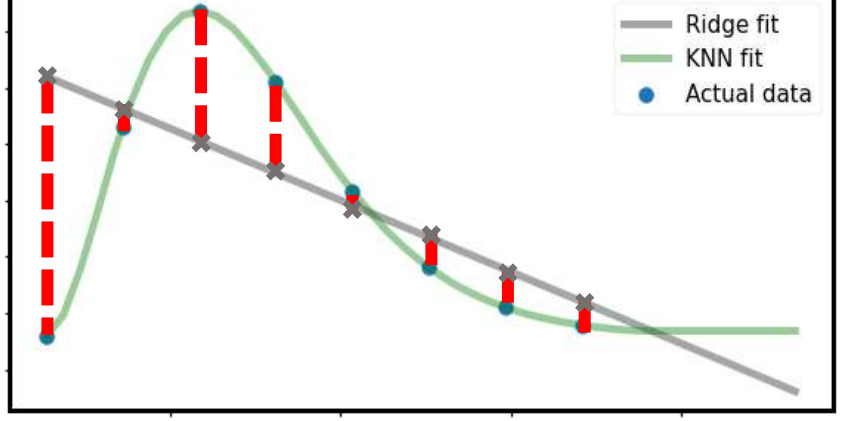
Regression

Minkowski distance



$$D(Y, \bar{Y}) = \left(\sum_i |Y^i - \overline{Y^i}|^p \right)^{\frac{1}{p}}$$

Minkowski distance



$$D_1(Y, \bar{Y}) = \sum_i \left| Y^i - \bar{Y}^i \right|$$

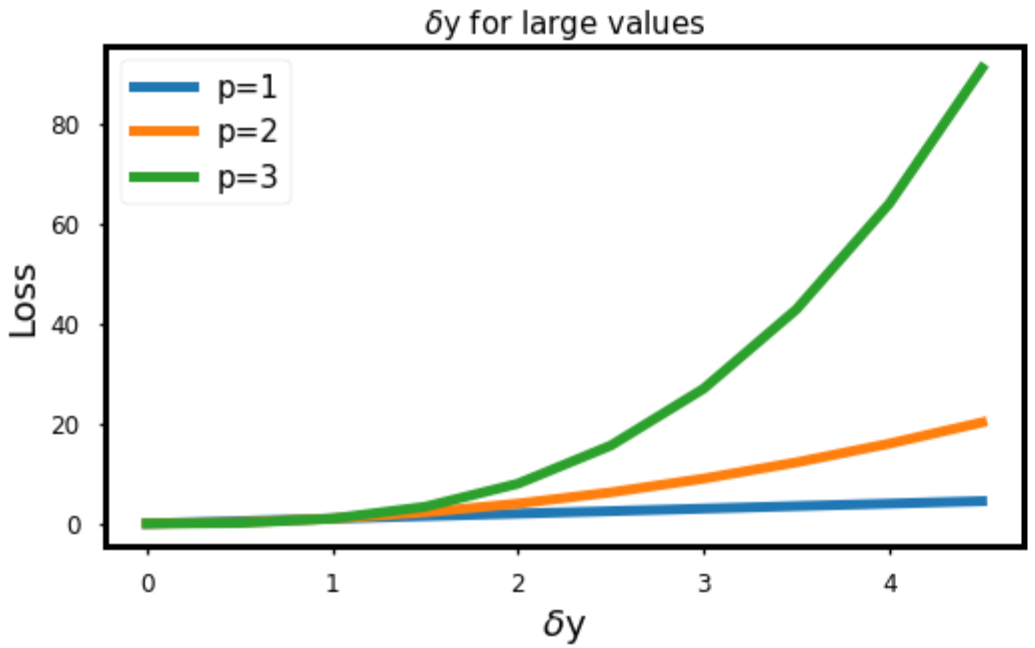
$$D_2(Y, \bar{Y}) = \sqrt{\sum_i \left| Y^i - \bar{Y}^i \right|^2}$$

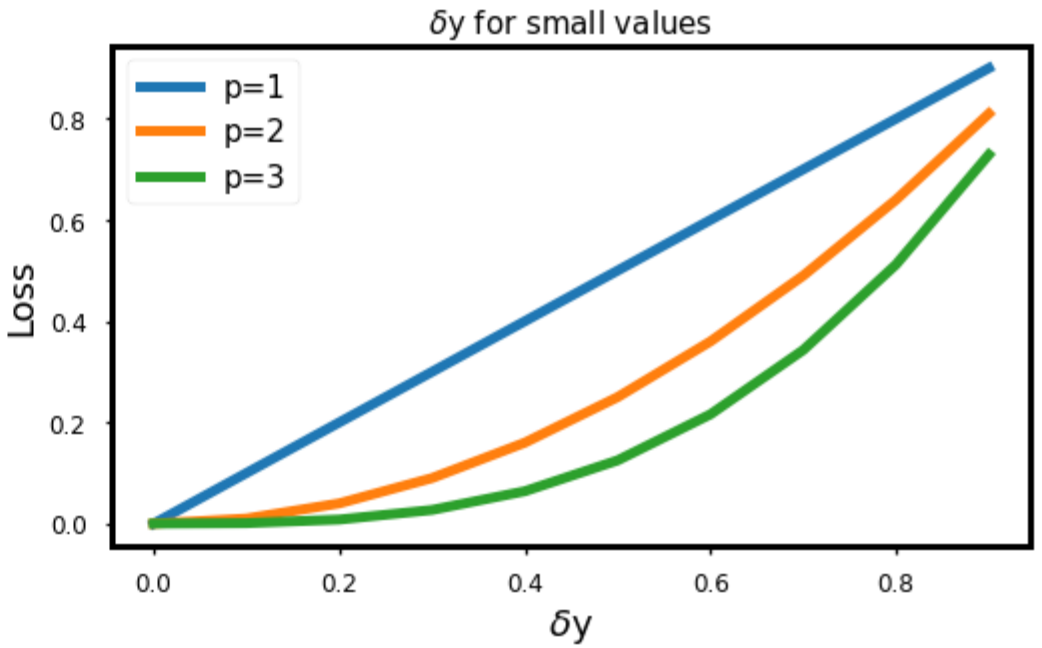
→ Penalizes larger deviations more

$$D_\infty(Y, \bar{Y}) = \max_i \left| Y^i - \overline{Y^i} \right|$$

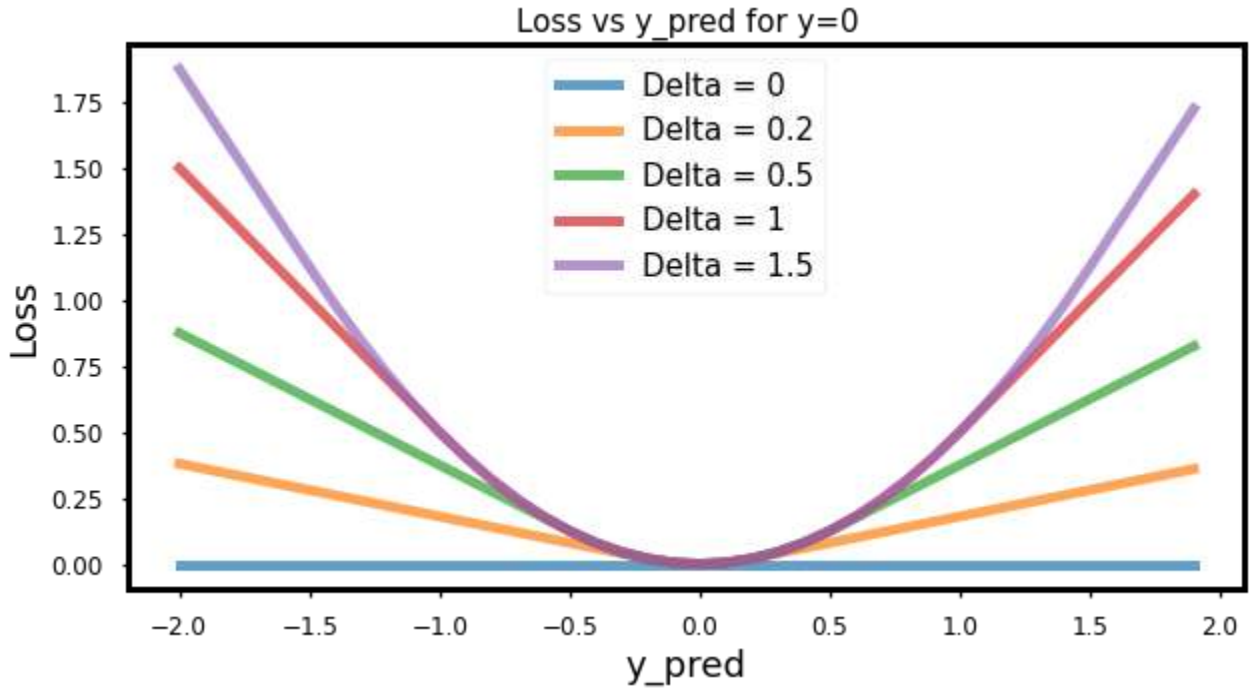
→ Worst case

Minkowski distance





Huber: the best of both worlds

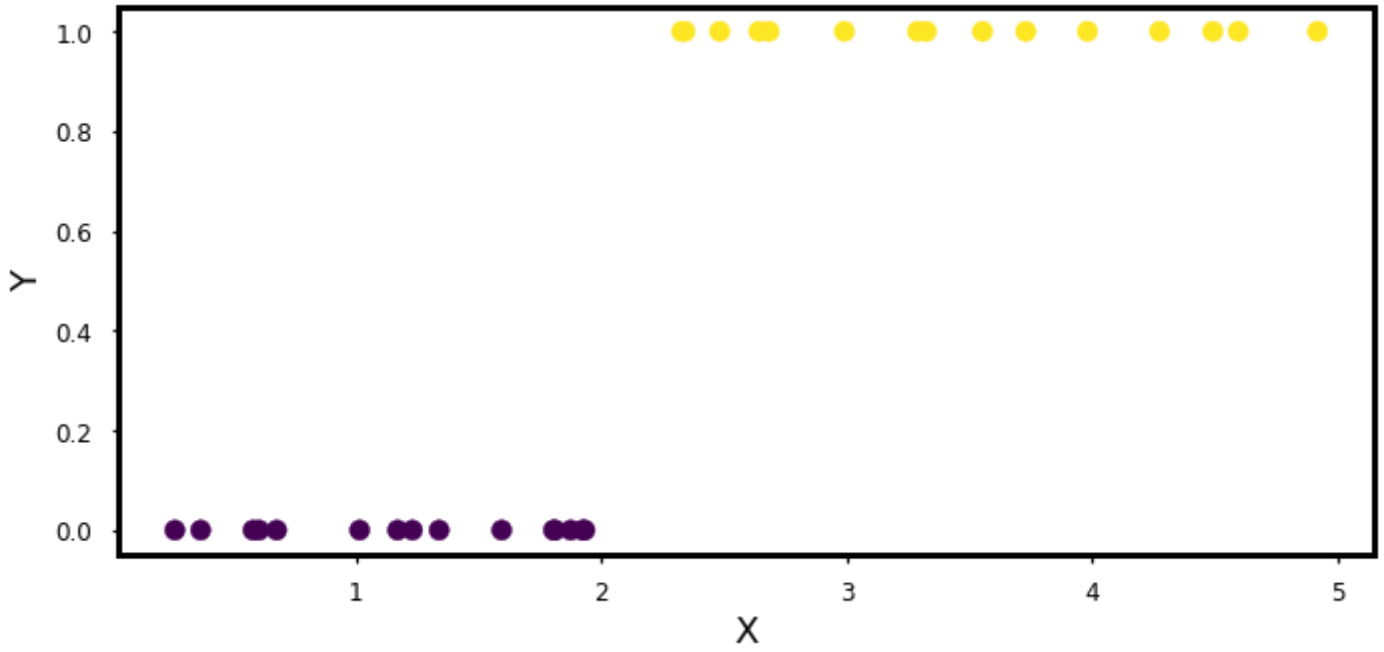


What other functions?

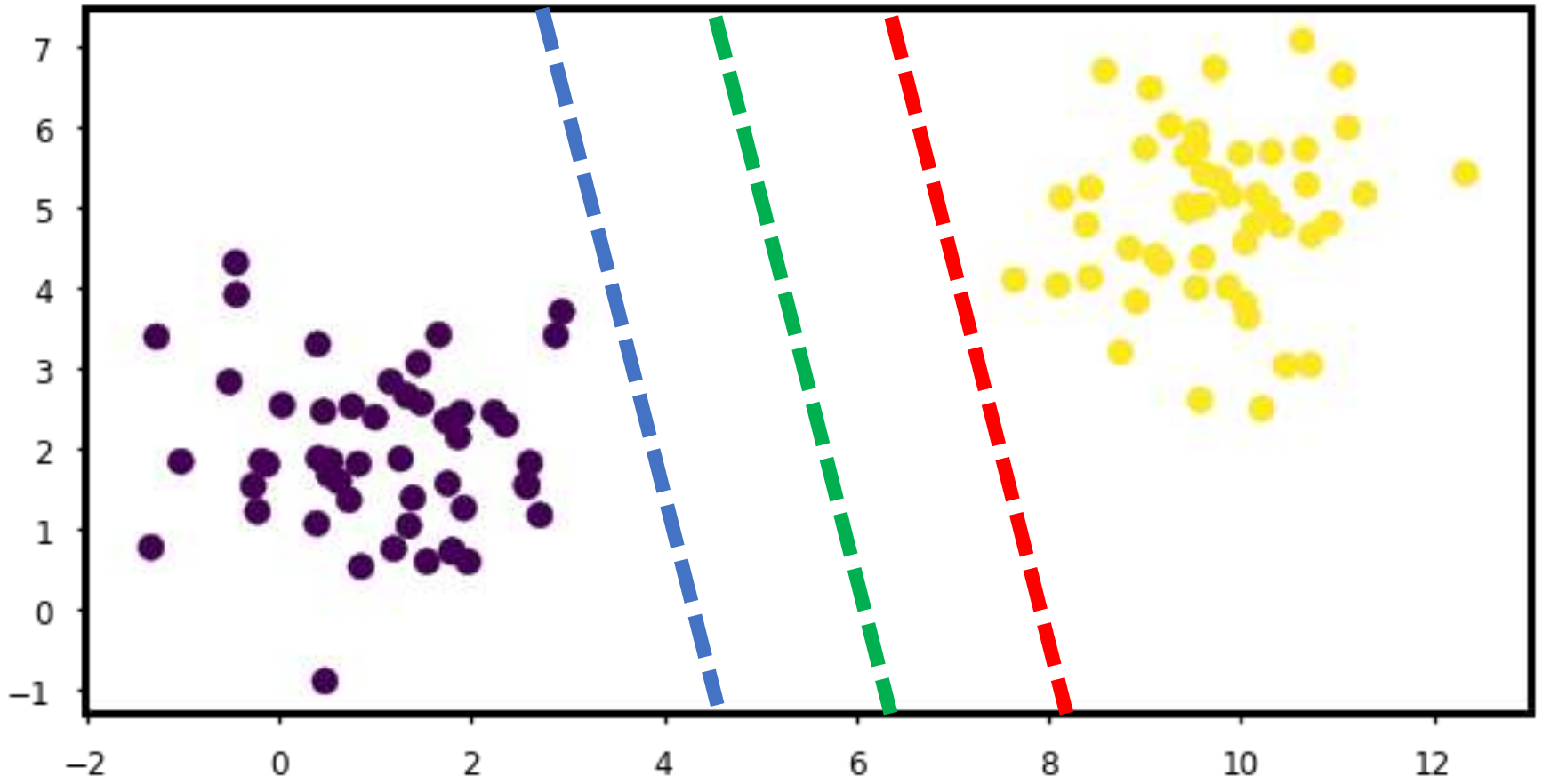
Take a look at scikit-learn!

Classification

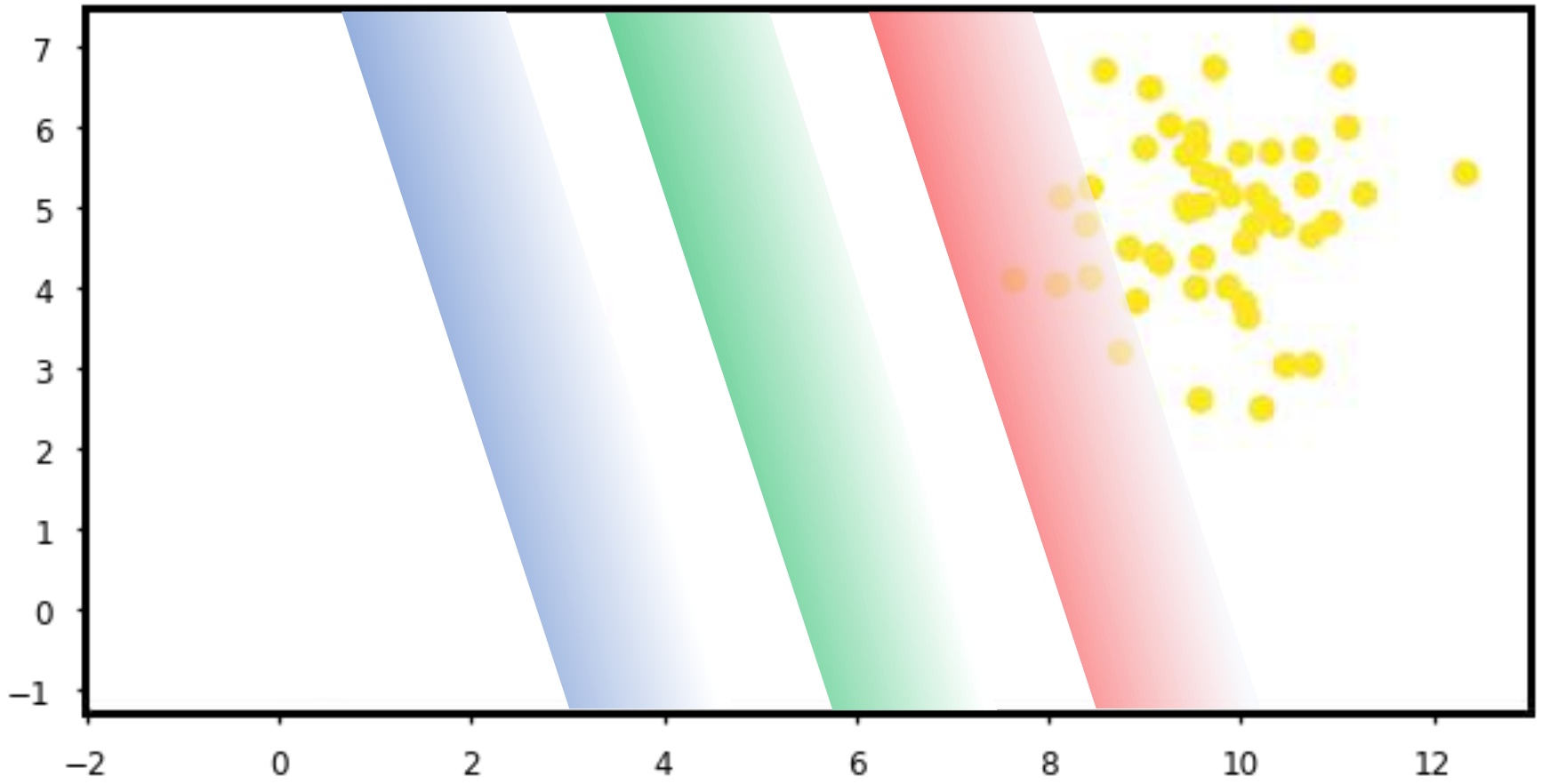
We can use regression loss functions



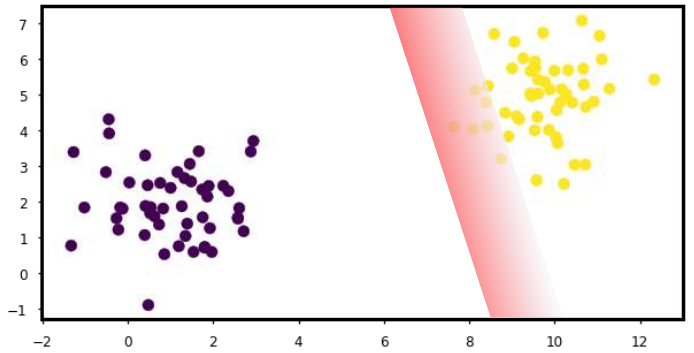
Hinge

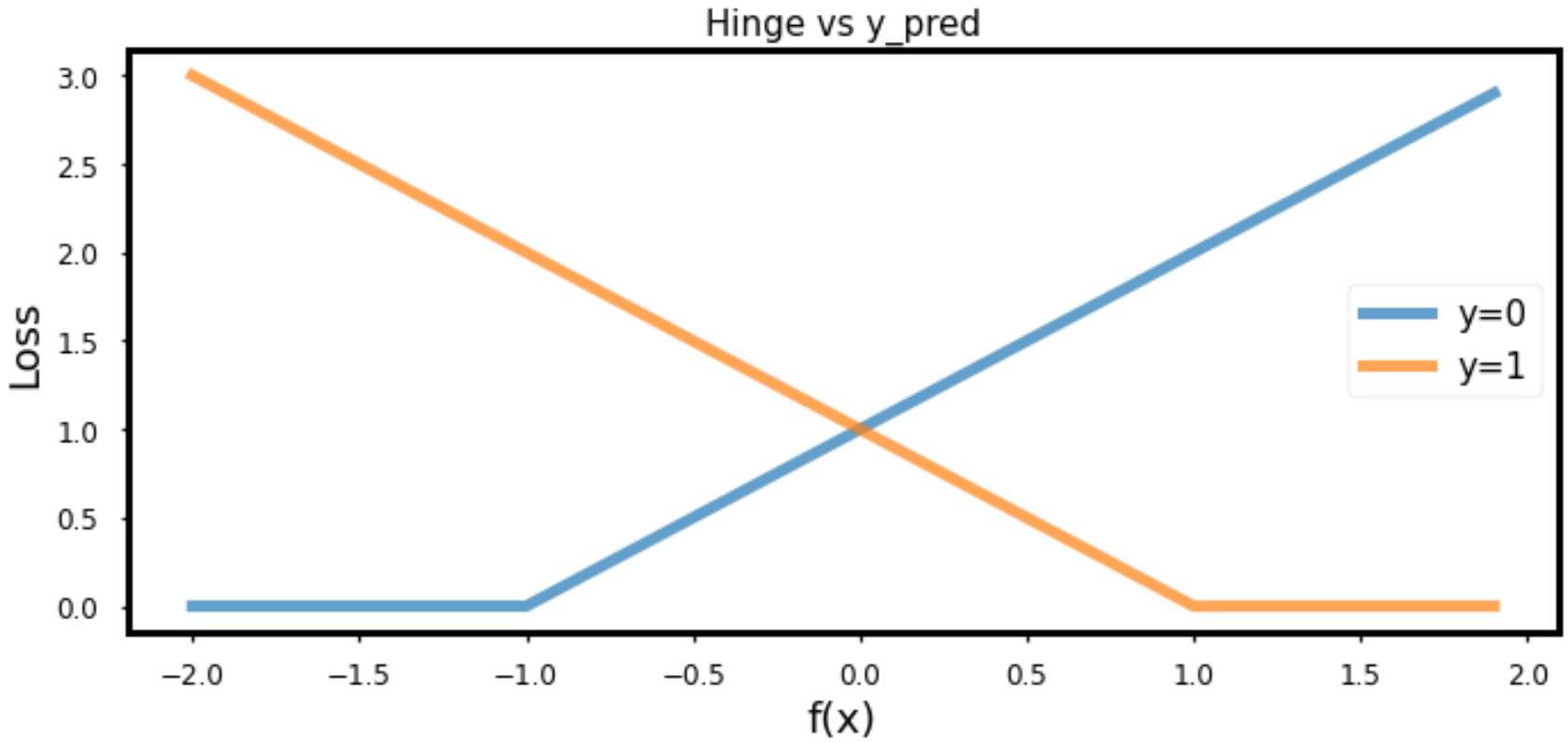


Hinge

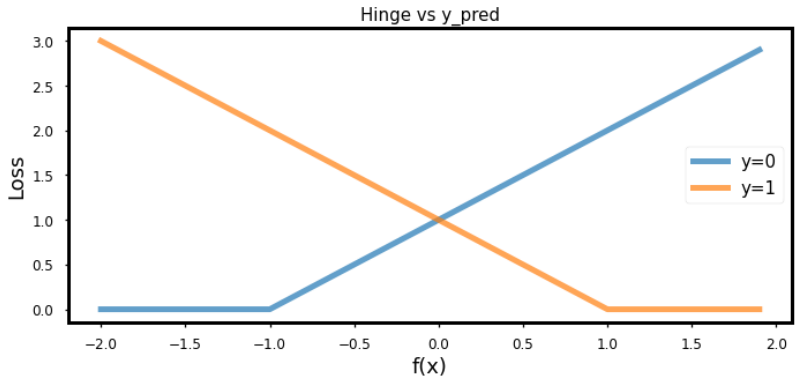


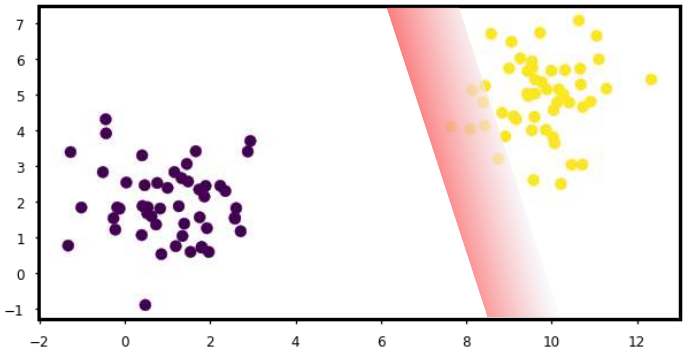
Hinge


7
6
5
4
3
2
1
0
−1
−2
0
2
4
6
8
10
12


Hinge vs y_pred
Loss
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−2.0
−1.5
−1.0
−0.5
0.0
0.5
1.0
1.5
2.0
f(x)
y=0
y=1

Hinge





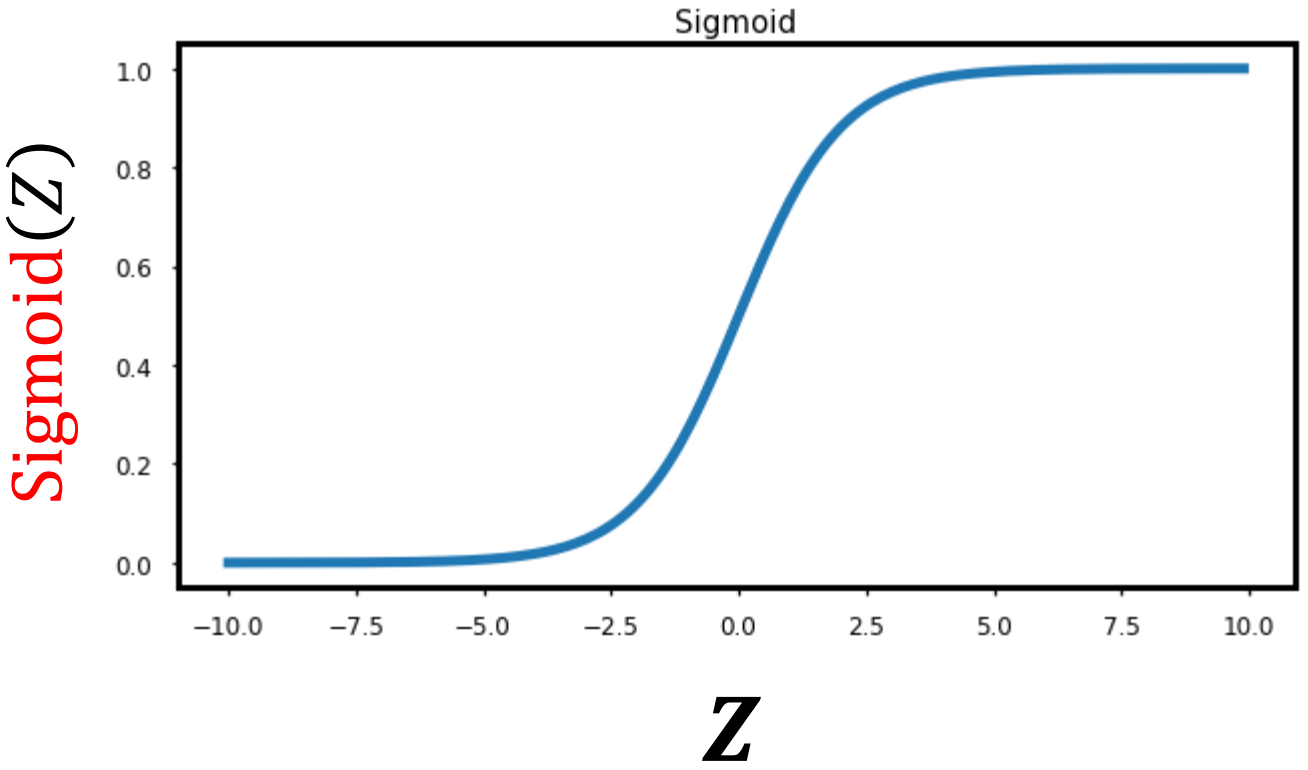
$$D_h(Y, \bar{Y}) = \max(0, 1 - Y^i * f_w(X^i))$$

Note that $\boldsymbol{f_w}$ is the decision boundary, not the class.

Also note that $Y^i = \pm 1$ and not $\{0,1\}$.

Probability:

Logistic Regression



Probability: Cross-entropy

$$D_{CE}(Y, \bar{Y}) = -\sum_i Y^i \log \bar{Y}^i + (1 - Y^i) \log(1 - \bar{Y}^i)$$

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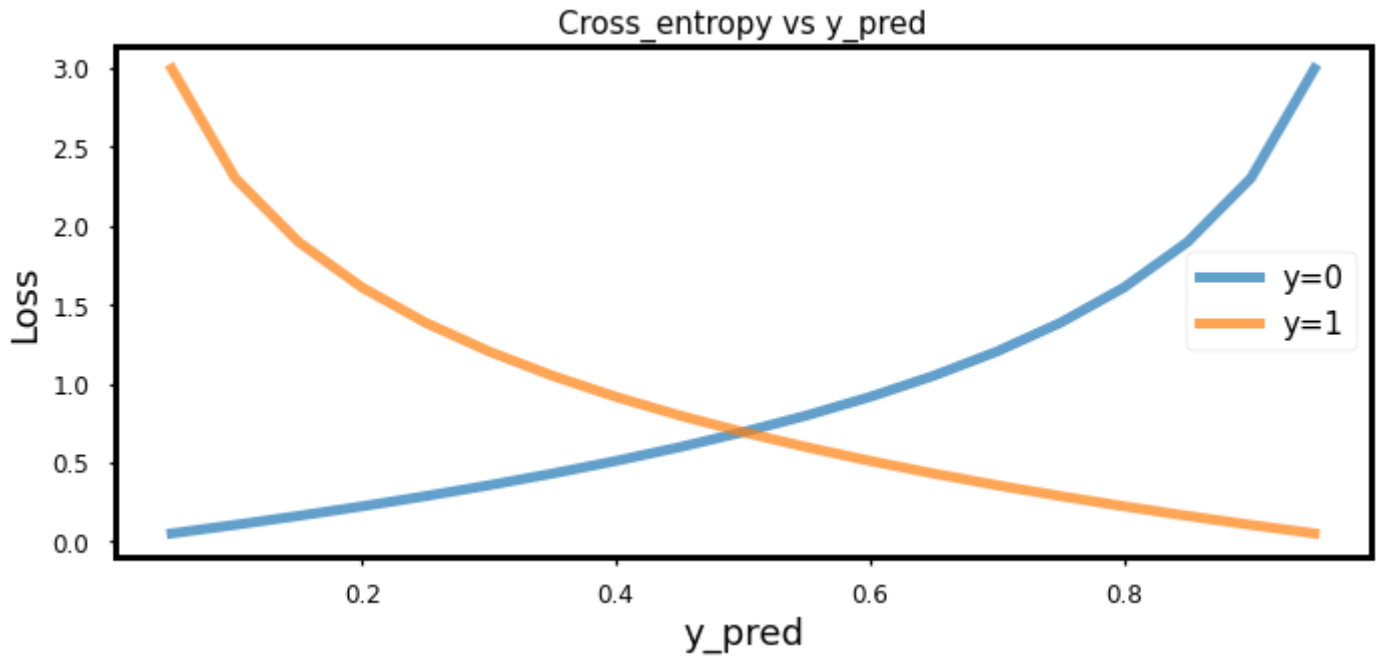
$$D_{CE}(Y, \bar{Y}) = -\sum_i Y^i \log \bar{Y}^i + (1 - Y^i) \log(1 - \bar{Y}^i)$$



Other loss functions

What would be a good loss function for a multi-class problem?

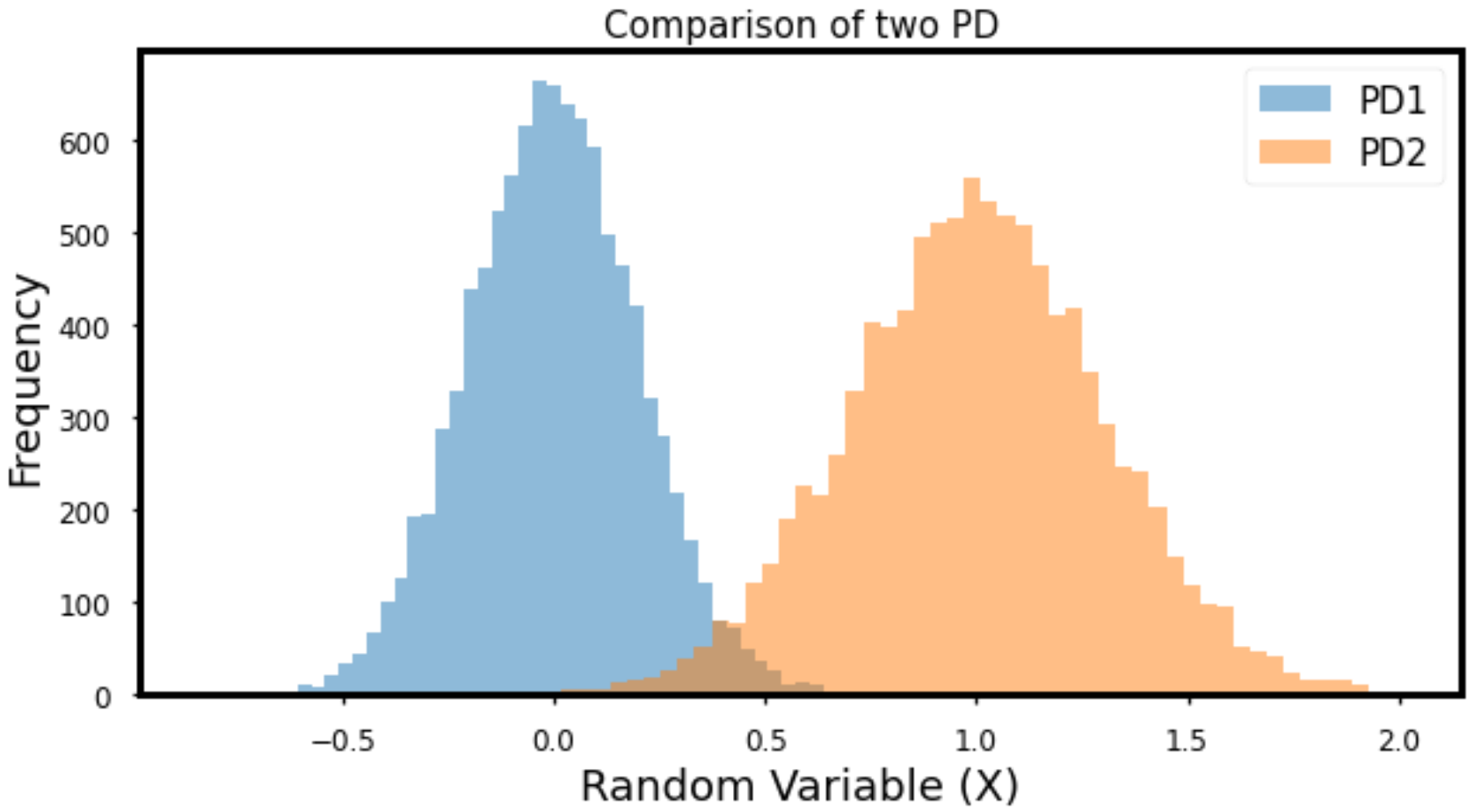
- $Y \in \{-1, 0, 1\}$

What would be a good loss function for $Y \in \{0,1\}^{\otimes n}$?

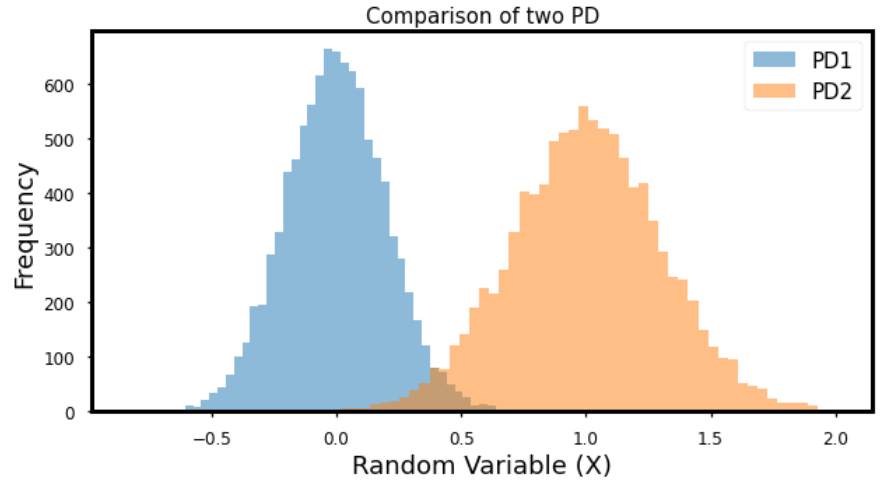
Example:

$$Y^1 = (0,0,1,0,1)$$

Probability Distributions



Probability Distributions



- Kullback–Leibler divergence (Relative Entropy)

$$D_{KL}(PD_1||PD_2) = \sum_X PD_1(X)\log(\frac{PD_1(X)}{PD_2(X)})$$

What would be a good loss function for clustering?

The right choice for the Loss function

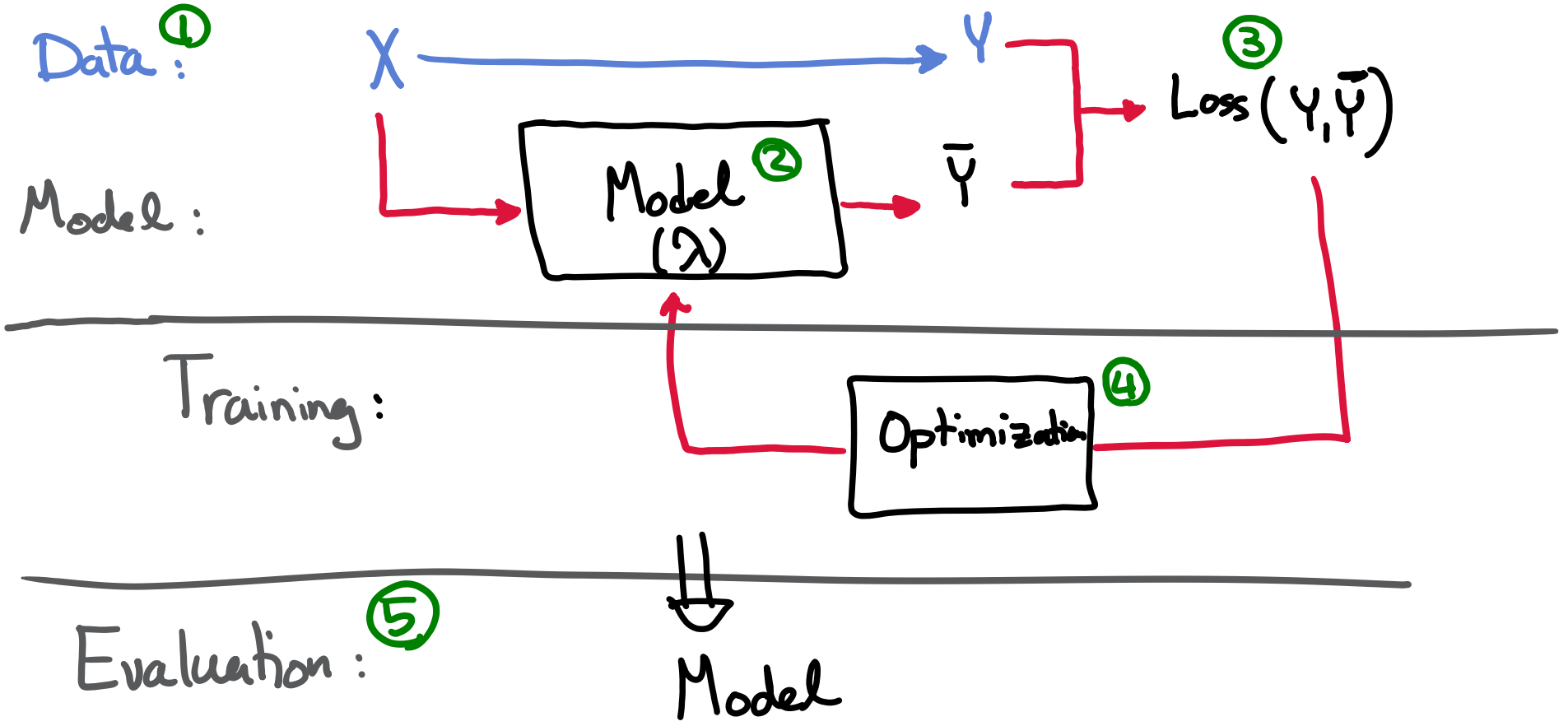
How do we choose the right loss function?

- Convexity
- Objective

How does this choice affect the model?

See the NB.

So far …


Data: ①
X
Y
③
Loss(Y, Ŷ)
Model:
Model (λ) ②
Ŷ
Training:
④
Optimization
Evaluation: ⑤
Model