# Introducción a la Inteligencia Artificial

Clase 5

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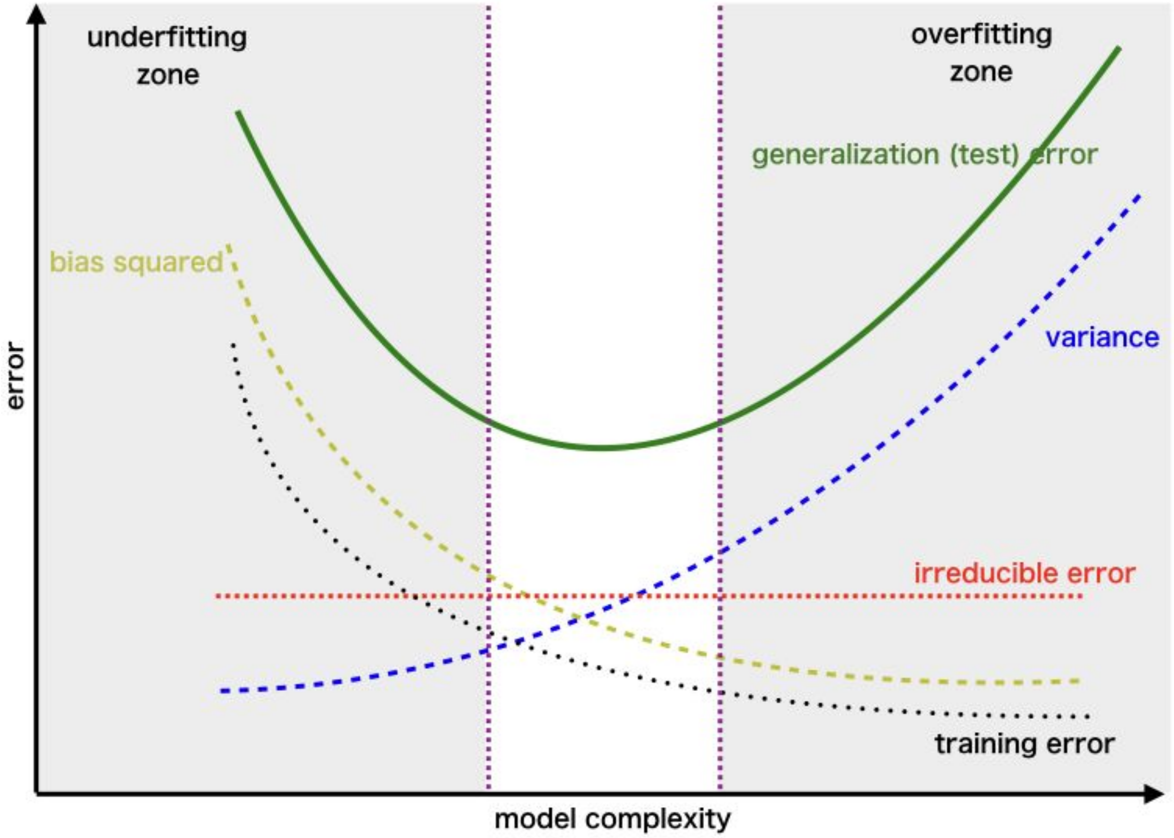
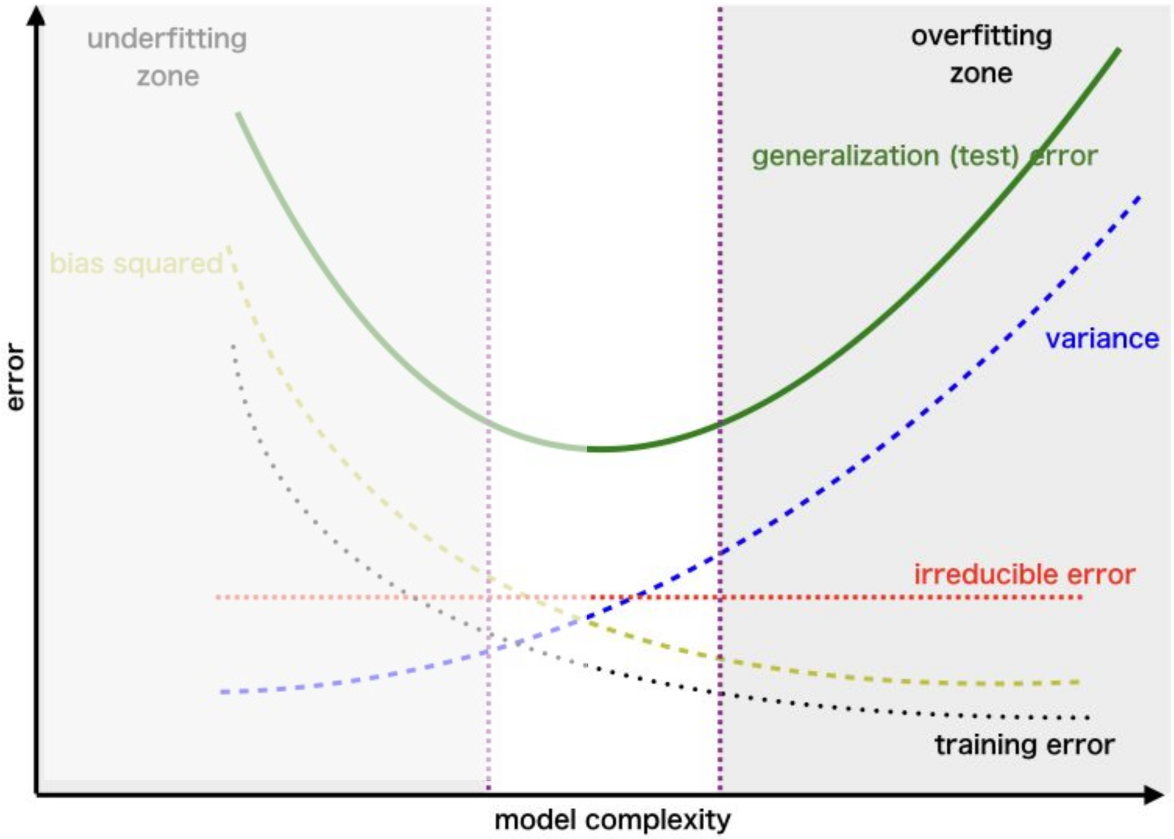
# Índice

## Clase 5

# Regularización



# Regularización

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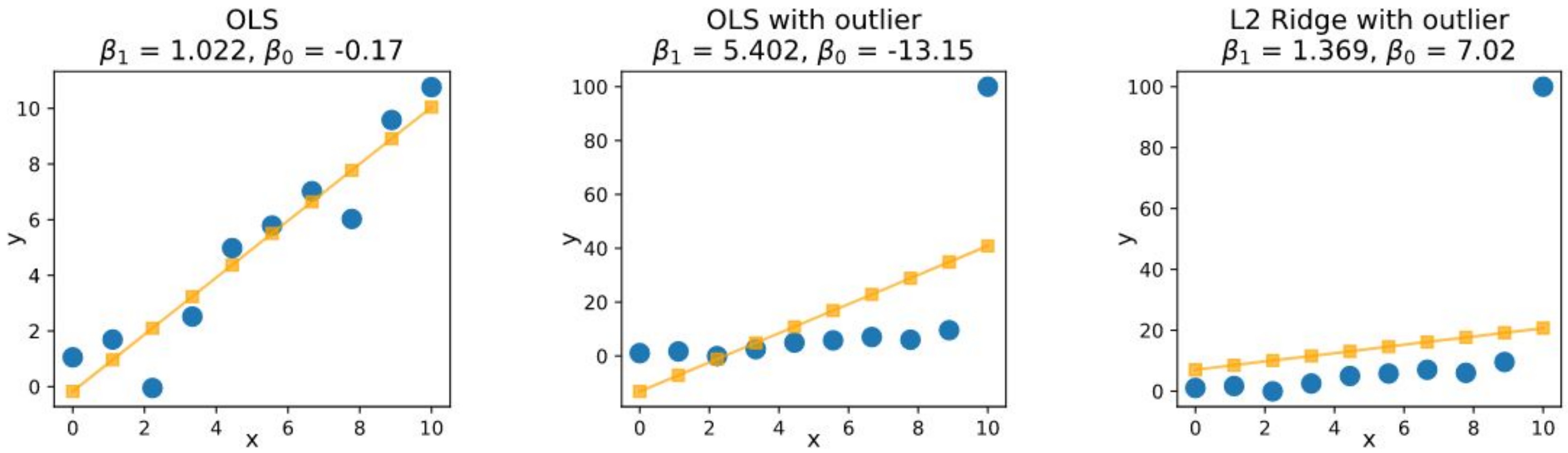
## Regularización - Motivación



# Regularización

$$E_D(\mathbf{w}) = \frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n)\}^2$$

Observado **-** Predicción

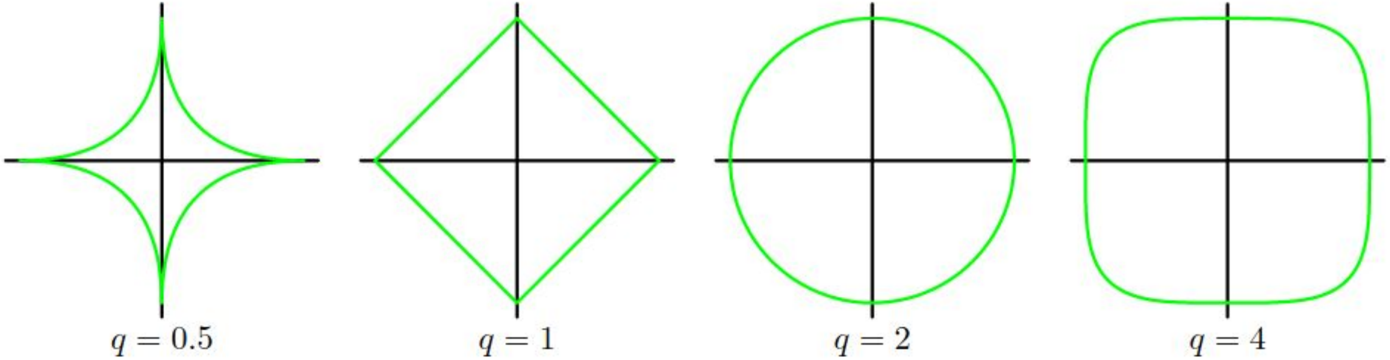
↓

w está “libre”

# Regularización

$$\frac{1}{2}\sum_{n=1}^{N}\{t_n - \mathbf{w}^{\mathrm{T}}\phi(\mathbf{x}_n)\}^2 + \boxed{\frac{\lambda}{2}\sum_{j=1}^{M}|w_j|^q}$$

Término de regularización "weight decay" → w afecta la pérdida




Lasso

Ridge

$$w = (\Phi^T\Phi + \lambda I)^{-1}\Phi^T y$$

## Maximum A Posteriori como regularización

Distribución “a priori” de los parámetros → Observar data → Actualizar distribución (Posterior)

$$p(w) \sim D(\theta)$$

$$(\mathcal{X}, \mathcal{Y})$$

$$p(w|\mathcal{X}, \mathcal{Y}) = \frac{p(\mathcal{Y}|\mathcal{X}, w)p(w)}{p(\mathcal{Y}|\mathcal{X})}$$

$$w_{map} = (\Phi^T\Phi + \frac{\sigma^2}{b^2}I)^{-1}\Phi^T y$$

Gaussian prior con varianza b2

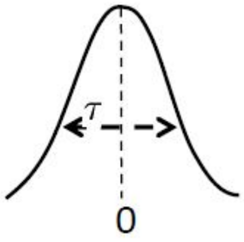
# Regularización

## Maximum A Posteriori como regularización - Ridge (L2)

$$\widehat{\beta}_{\text{MAP}} = \arg\max_{\beta} \underbrace{\log p(\{Y_i\}_{i=1}^n | \beta, \sigma^2, \{X_i\}_{i=1}^n)}_{\text{Conditional log likelihood}} + \underbrace{\log p(\beta)}_{\text{log prior}}$$

I) Gaussian Prior

$$\beta \sim \mathcal{N}(0, \tau^2 \mathbf{I}) \qquad p(\beta) \propto e^{-\beta^T \beta / 2\tau^2}$$




$$\widehat{\beta}_{\text{MAP}} = \arg\min_{\beta} \sum_{i=1}^{n} (Y_i - X_i \beta)^2 + \underset{\substack{\downarrow \\ \text{constant}(\sigma^2, \tau^2)}}{\lambda} \|\beta\|_2^2$$

Ridge Regression

$$\widehat{\beta}_{\text{MAP}} = (\boldsymbol{A}^\top \boldsymbol{A} + \lambda \boldsymbol{I})^{-1} \boldsymbol{A}^\top \boldsymbol{Y}$$

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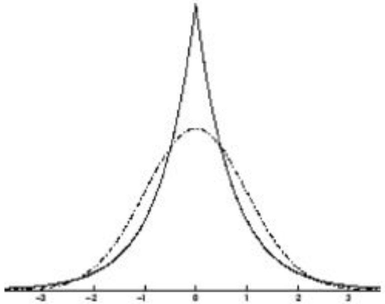
# Regularización

## Maximum A Posteriori como regularización - LASSO (L1)

$$\widehat{\beta}_{\text{MAP}} = \arg\max_{\beta} \underbrace{\log p(\{Y_i\}_{i=1}^{n} | \beta, \sigma^2, \{X_i\}_{i=}^{n}}_{\text{Conditional log likelihood}} + \underbrace{\log p(\beta)}_{\text{log prior}}$$

II) Laplace Prior

$$\beta_i \overset{iid}{\sim} \text{Laplace}(0, t) \qquad\qquad p(\beta_i) \propto e^{-|\beta_i|/t}$$



$$\widehat{\beta}_{\text{MAP}} = \arg\min_{\beta} \sum_{i=1}^{n} (Y_i - X_i\beta)^2 + \underset{\substack{\downarrow \\ \text{constant}(\sigma^2, t)}}{\lambda} \|\beta\|_1$$

Lasso

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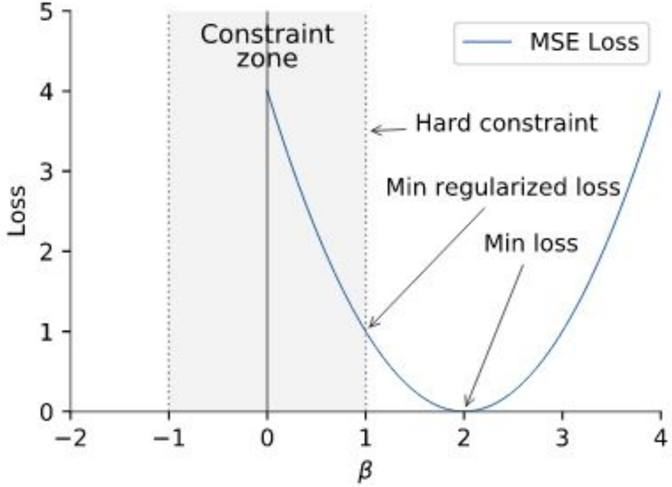
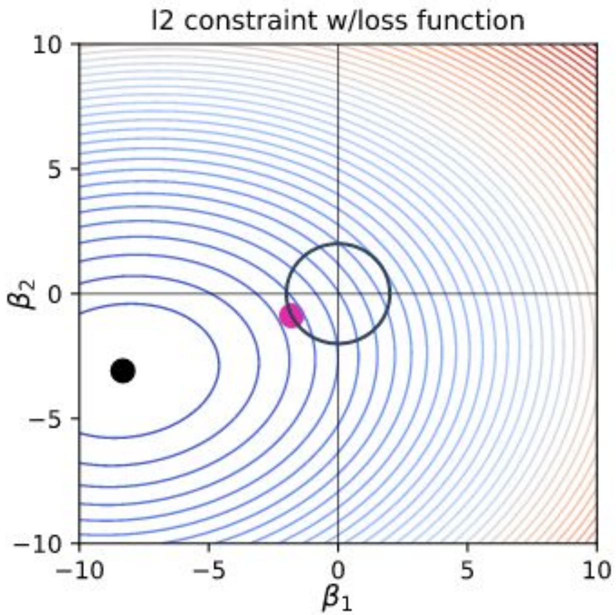
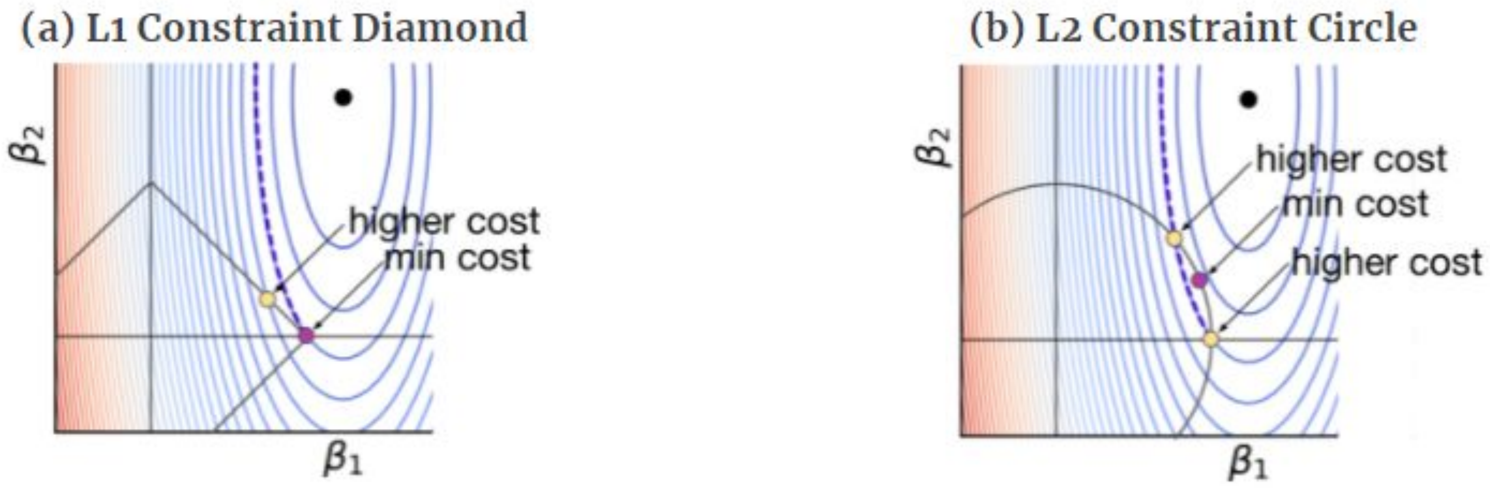
# Regularización



# Regularización

## Regularización

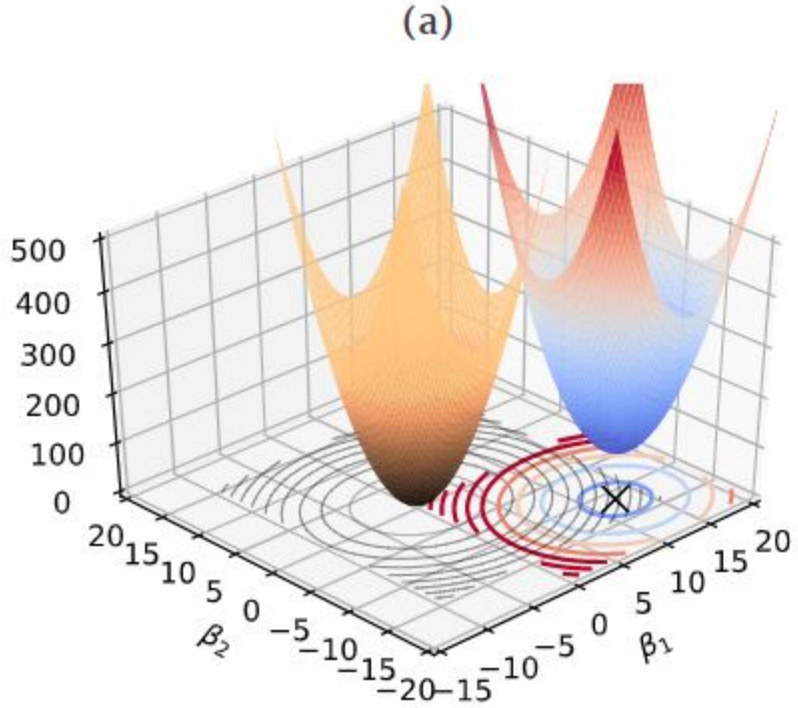


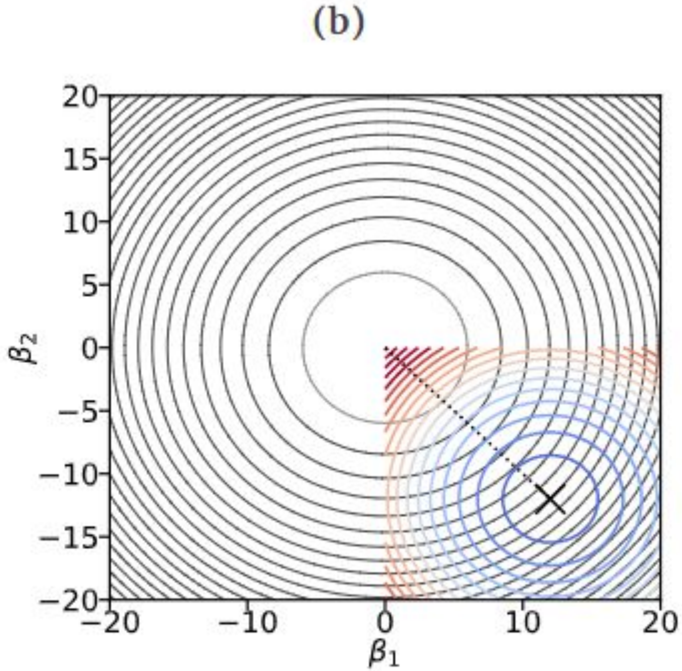

## ElasticNet

$$(\alpha\lambda||\beta||_1 + \tfrac{1}{2}(1-\alpha)||\beta||_2^2)$$

¿Qué β se reduce más?

# Regularización



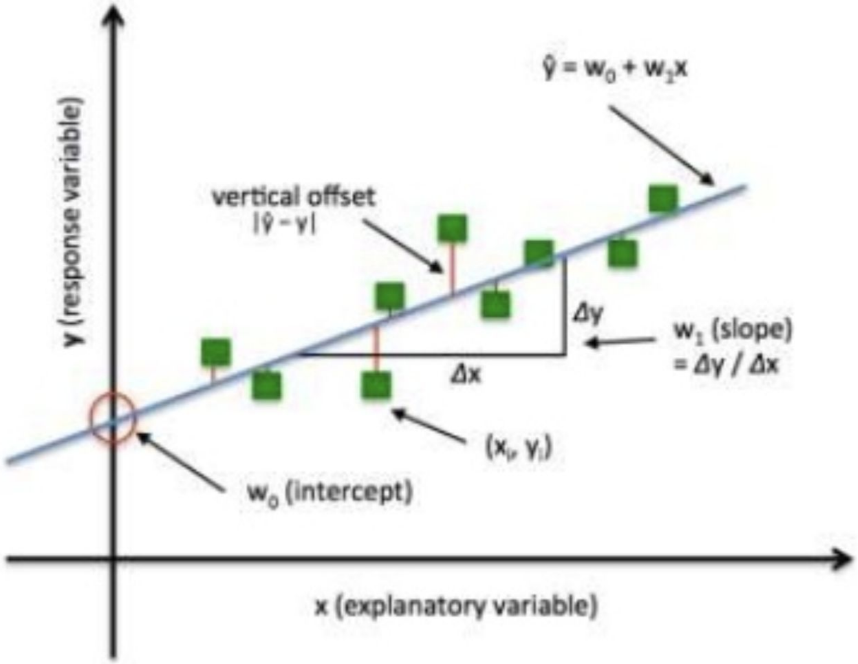
# Gradiente Descendente

## Implementación de Gradiente Descendente

Solucion analitica

$$\min_{W} \|Y - XW\|_2^2$$

$$W = (X^T X)^{-1} X^T Y$$

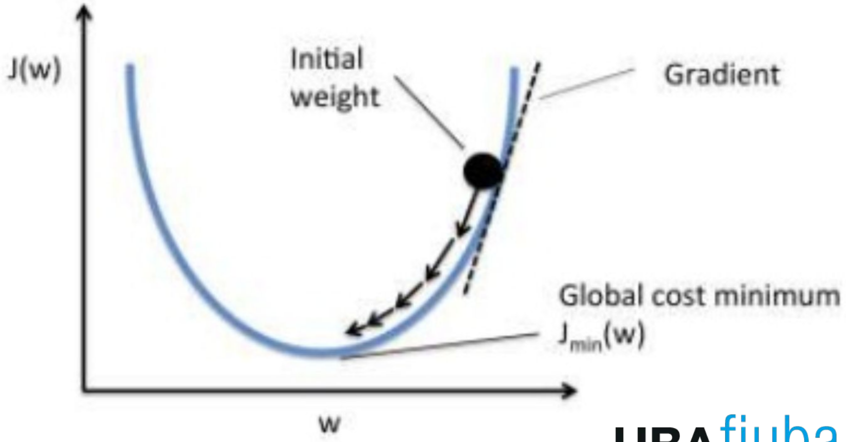


## Implementación de Gradiente Descendente

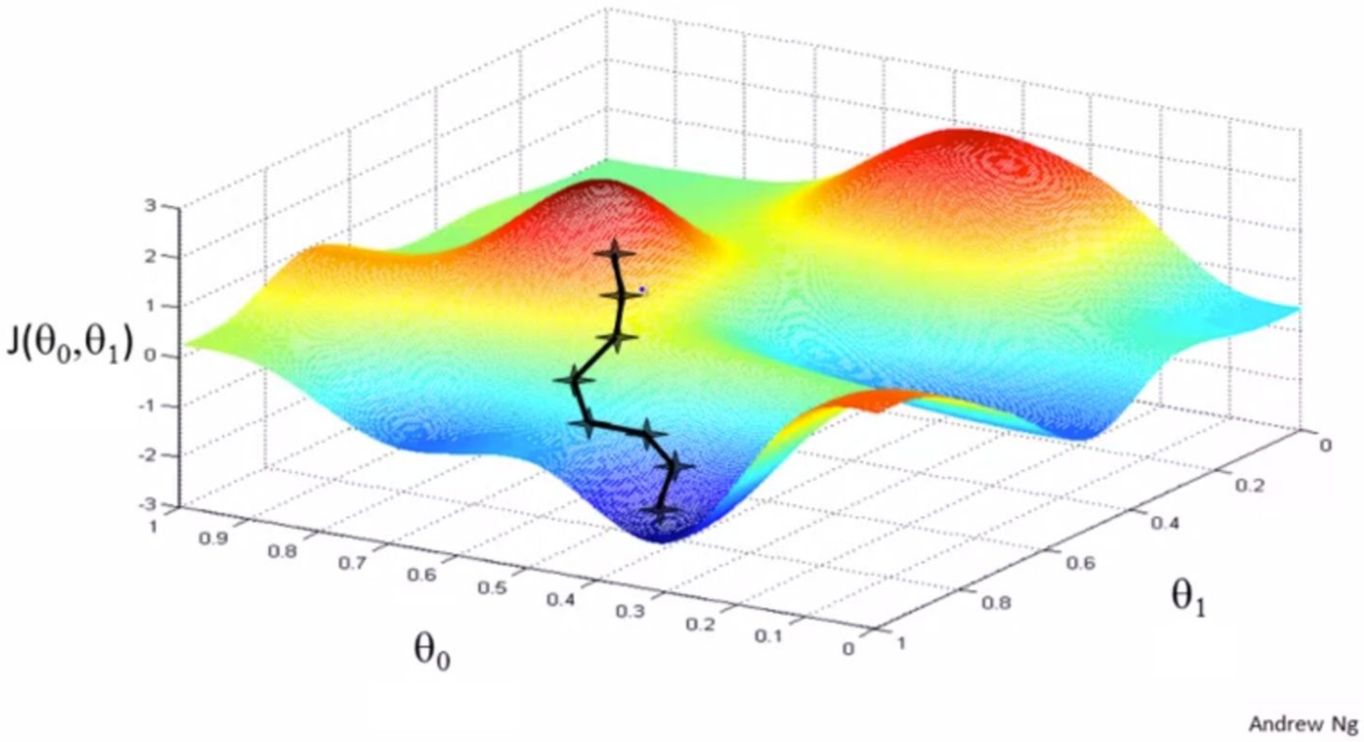
Solución numérica

$$\min_W \|Y - XW\|_2^2 \implies \min_W \sum_i (y_i - X_i \cdot W)^2$$

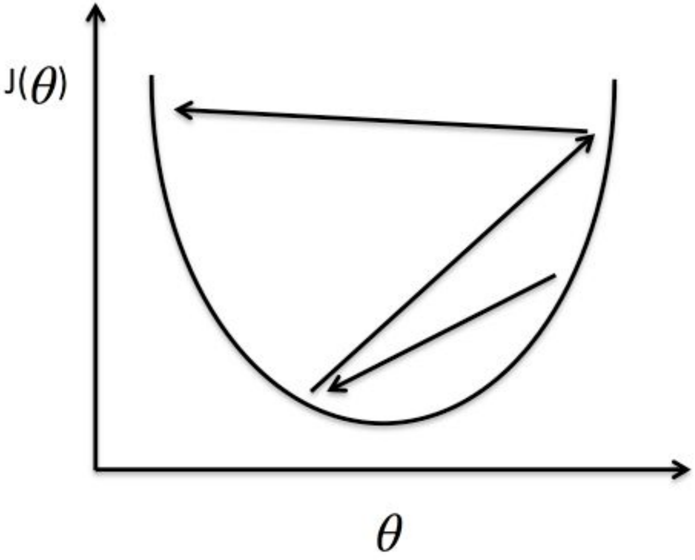
$$W \longleftarrow W - \alpha \nabla \left( \sum_i (y_i - X_i \cdot W)^2 \right)$$



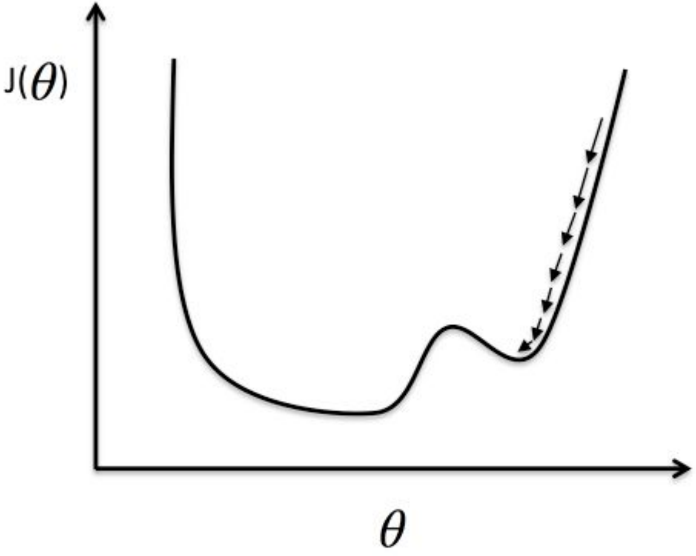
## Gradiente Descendente



## Gradiente Descendente




Large learning rate: Overshooting.




Small learning rate: Many iterations until convergence and trapping in local minima.

## Implementación de Gradiente Descendente

Solución numérica

$$
\begin{aligned}
\nabla_w J(w) &= \nabla_w \Big( \sum_i (y_i - X_i W)^2 \Big) \\
&= \sum_i \Big( \nabla_w (y_i - X_i W)^2 \Big) \\
&= \sum_i \Big( \nabla_w (y_i - (x_{i1} w_1 + x_{i2} w_2 + \cdots + x_{im} w_m))^2 \Big) \\
&= \sum_i \Big( -2(y_i - \hat{y}_i) x_{ij} \Big) \qquad \forall j \in (1 \cdots m)
\end{aligned}
$$

**Implementación de Gradiente Descendente**

Solución numérica

$$\nabla \left( \sum_{\text{all samples}} (y_i - f_W(X_i))^2 \right)$$

## Gradient Descent algorithm

for epoch in n_epochs:

- compute the predictions for **all the samples**
- compute the error between truth and predictions
- compute the gradient using **all the samples**
- update the parameters of the model

## Implementación de Gradiente Descendente Estocástico

Solución numérica

$$\nabla \left( (y_i - f_W(X_i))^2 \right)$$

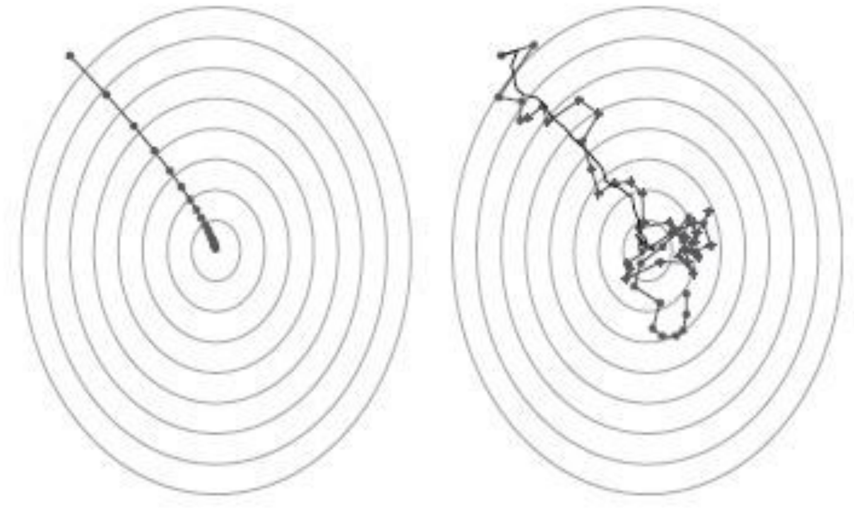
### Stochastic Gradient Descent algorithm

for epoch in n_epochs:

- shuffle the samples
- **for sample in n_samples:**
  - compute the predictions for **the sample**
  - compute the error between truth and predictions
  - compute the gradient using **the sample**
  - update the parameters of the model

## Implementación de Gradiente Descendente Estocástico

Solución numérica



## Implementación de Gradiente Descendente Mini-Batch

Solución numérica

$$\nabla \left( \sum_{\text{batch samples}} (y_i - f_W(X_i))^2 \right)$$

### Mini-Batch Gradient Descent algorithm

for epoch in n_epochs:

- shuffle the batches
- **for batch in n_batches:**
  - compute the predictions for **the batch**
  - compute the error for the batch
  - compute the gradient for **the batch**
  - update the parameters of the model

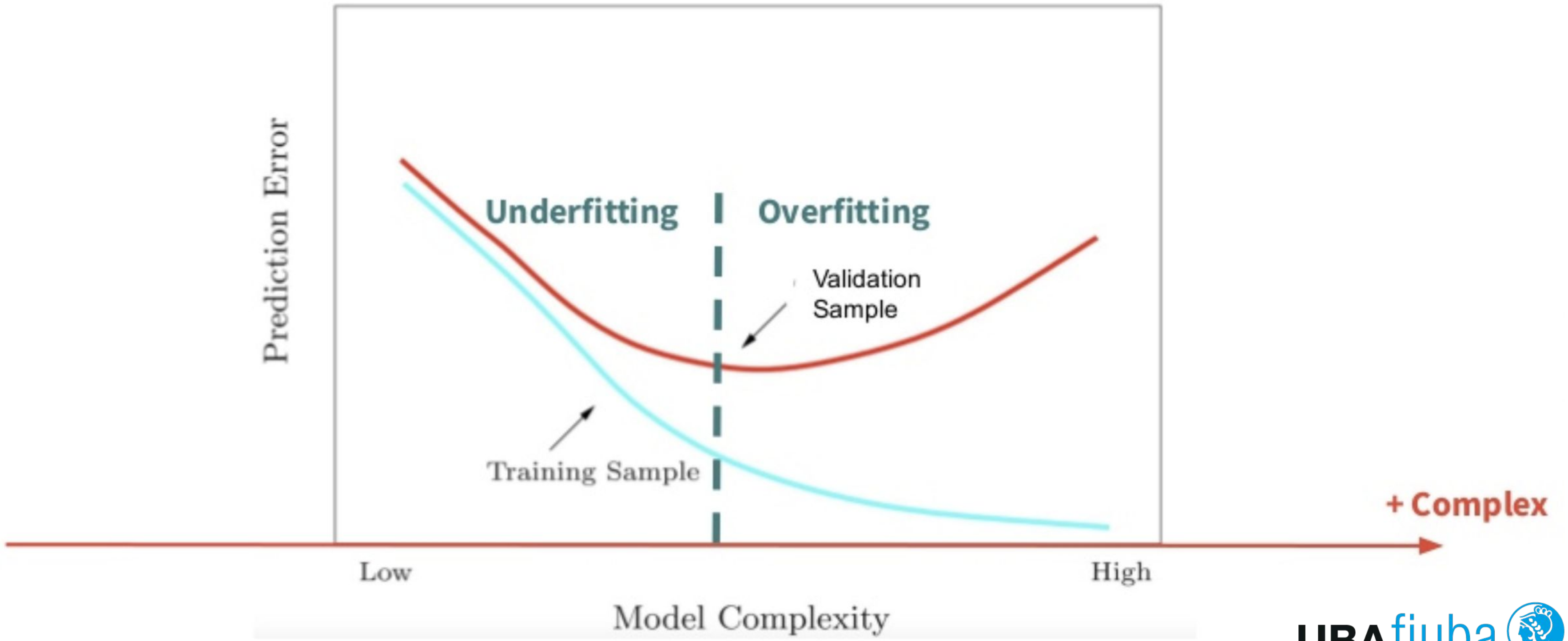
$\sum_i \Big( -2 (y_i - \hat{y}_i) x_{ij} \Big)$

## Comparativa de gradientes

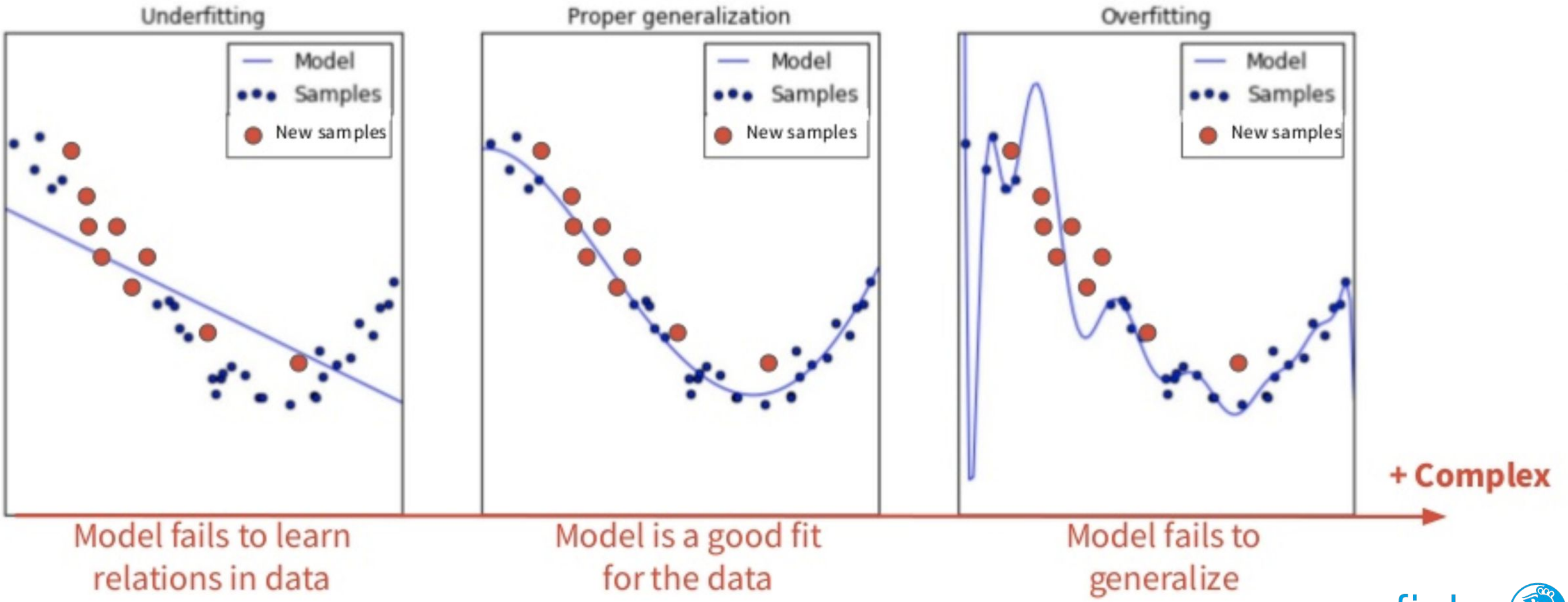
| | Gradient Descent | Stochastic Gradient Descent | Mini-Batch Gradient Descent |
|---|---|---|---|
| **Gradient** | $\nabla \left( \sum_{\text{all samples}} (y_i - f_W(X_i))^2 \right)$ | $\nabla \left( (y_i - f_W(X_i))^2 \right)$ | $\nabla \left( \sum_{\text{batch samples}} (y_i - f_W(X_i))^2 \right)$ |
| **Speed** | Very Fast (vectorized) | Slow (compute sample by sample) | Fast (vectorized) |
| **Memory** | O(dataset) | O(1) | O(batch) |
| **Convergence** | Needs more epochs | Needs less epochs | Middle point between GD and SGD |
| **Gradient Stability** | Smooth updates in params | Noisy updates in params | Middle point between GD and SGD |

# Selección de modelos

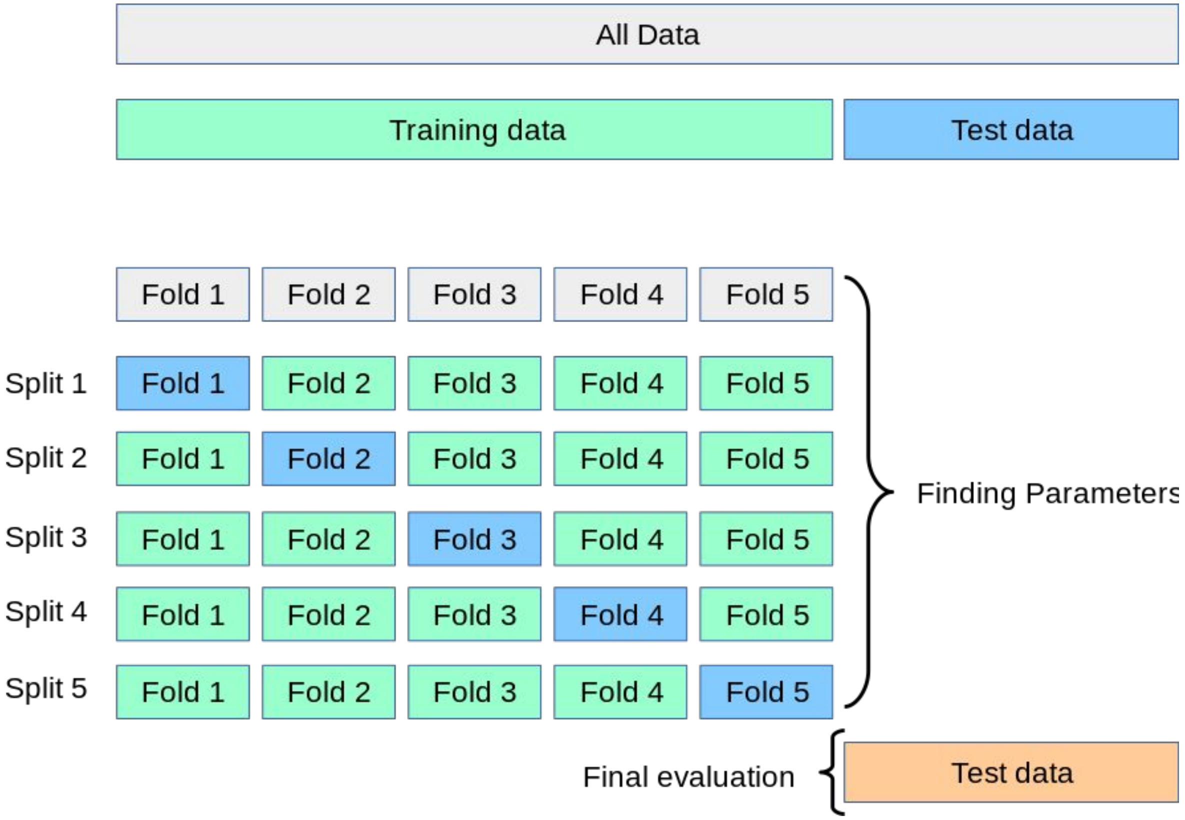
## Selección de modelos



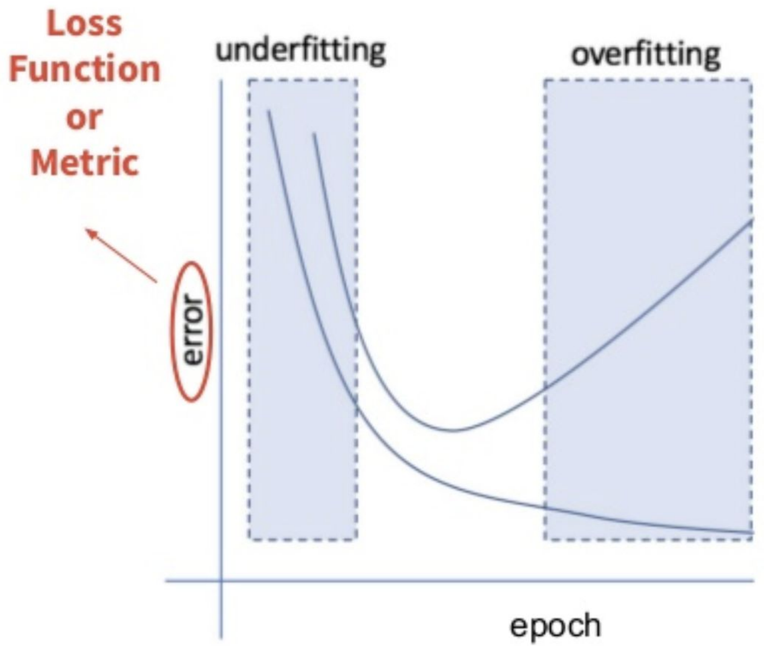
## Selección de modelos



## Cross-Validation



## Entrenamiento numérico del modelo seleccionado - Obtención de parámetros



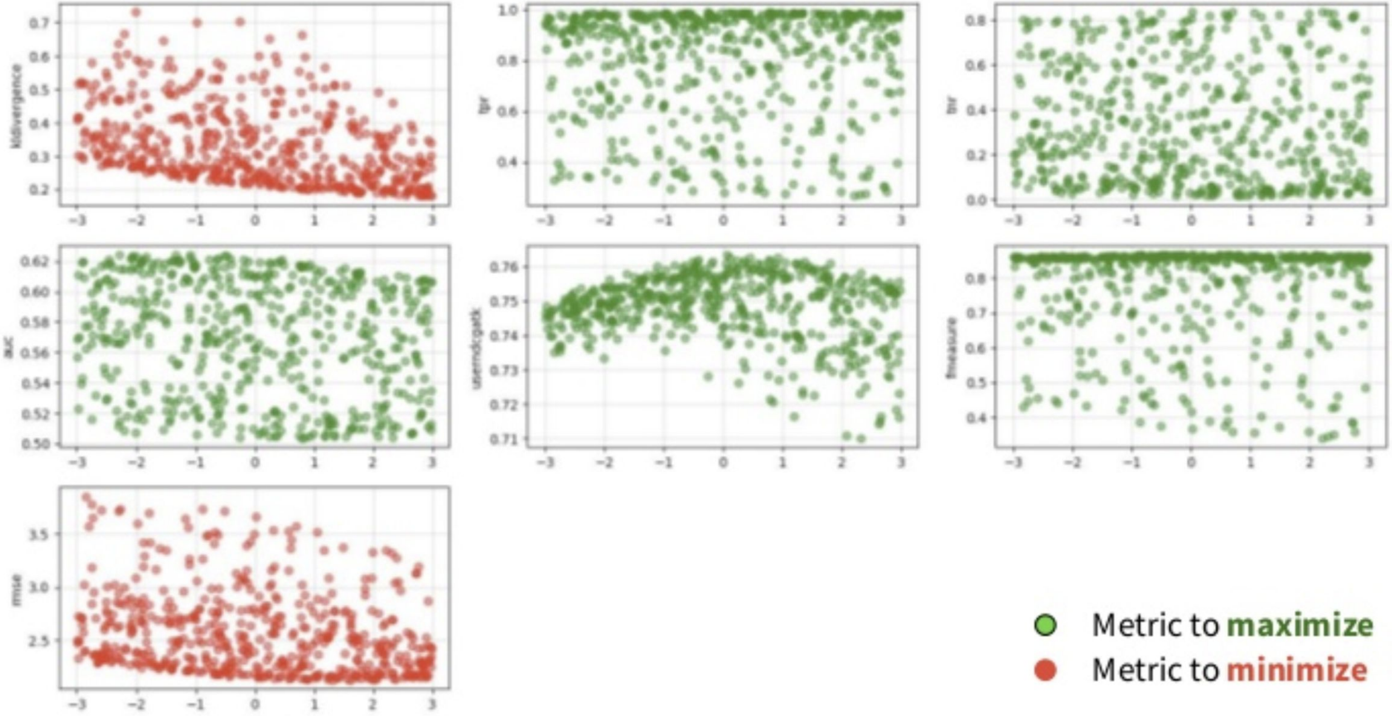

### Mini-Batch Gradient Descent

for epoch in n_epochs:

- shuffle the batches
- for batch in n_batches:
  - compute the predictions for the batch
  - compute the error for the batch
  - compute the gradient for the batch
  - update the parameters of the model
- plot error vs epoch

# Entrenamiento de modelos - Hiper parámetros

## Selección de los hiper parámetros




**Grid Search**

**Random Search**

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