Introducción a la Inteligencia Artificial

Clase 4

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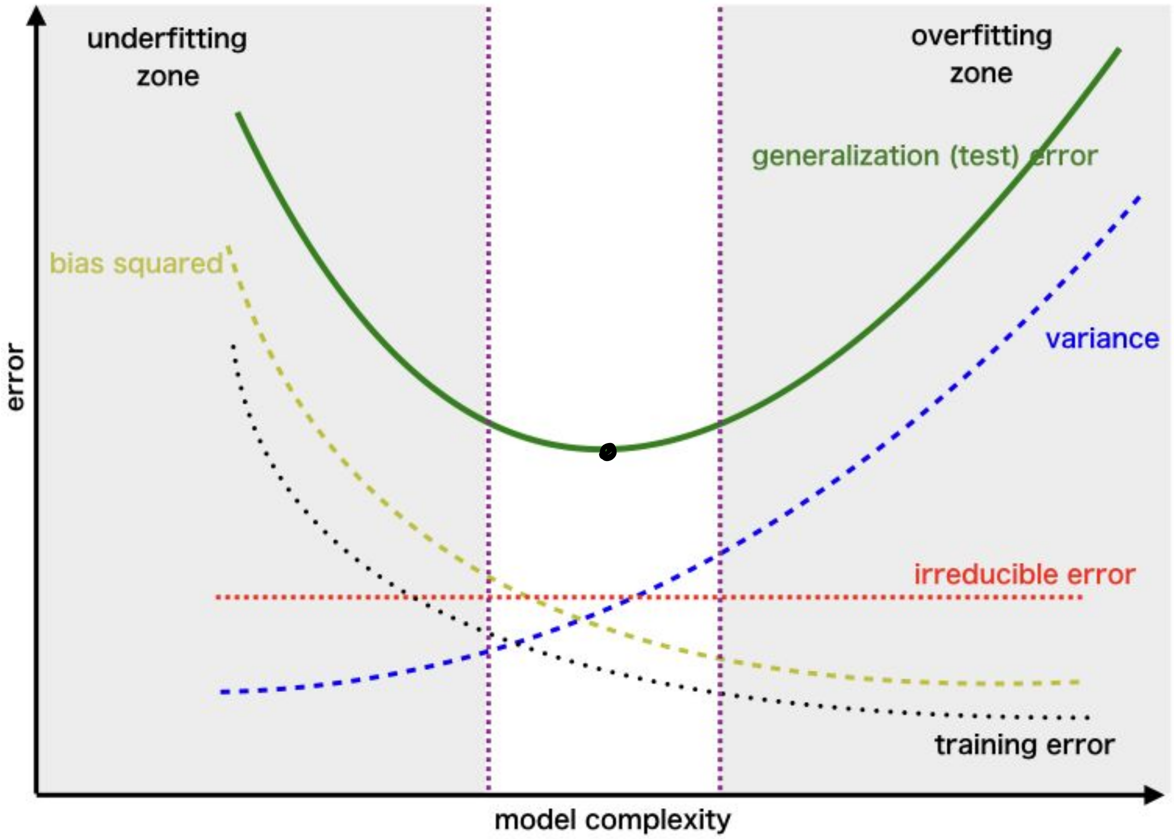
Índice

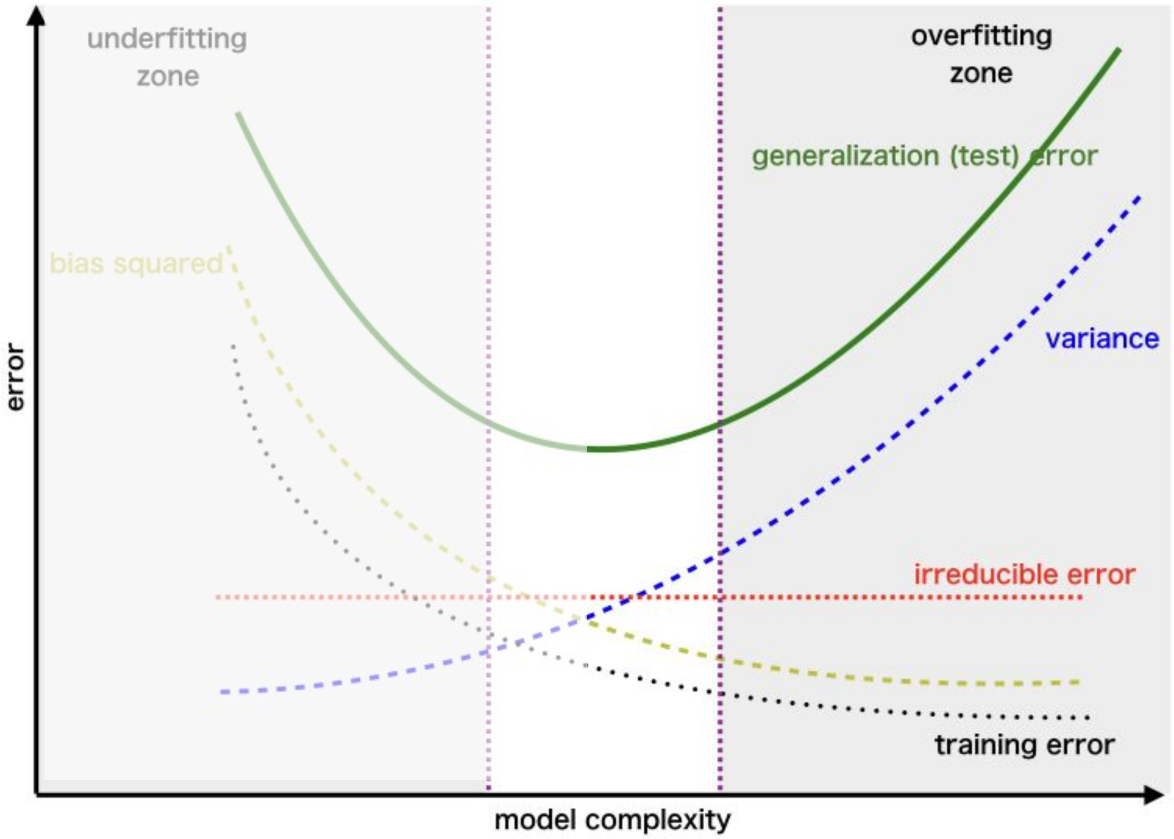
Clase ~~3~~ 4

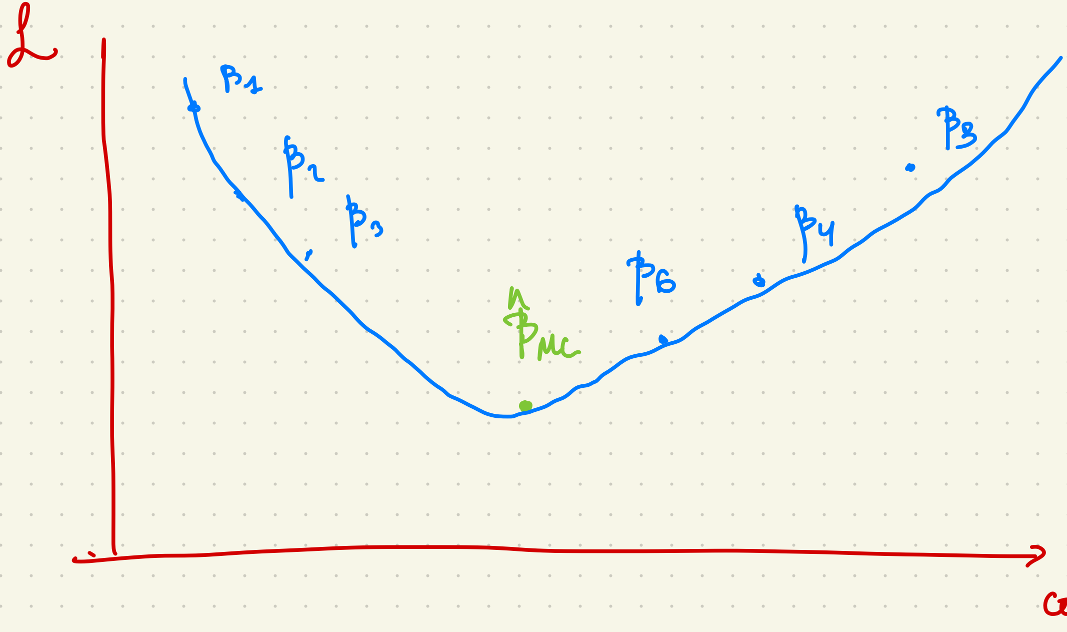
0. Riesgo Empírico
1. Regularización
   a. Caso general
   b. Ridge
   c. Lasso
2. Gradient descent
   a. GD
   b. GD Estocástico
   c. GD Mini-Batch
3. Entrenamiento de modelos
   a. Selección de modelos
   b. Cross-Validation

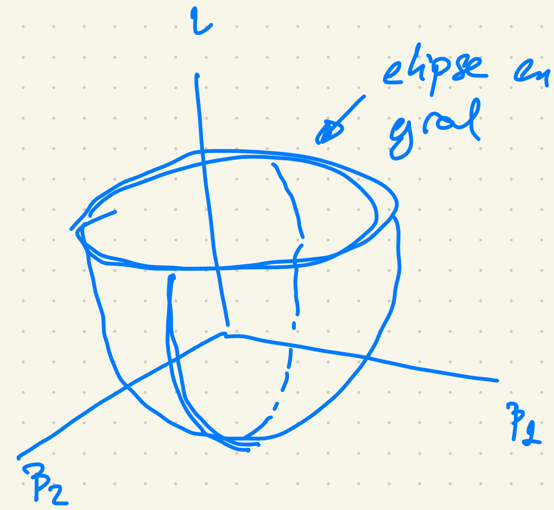
Regularización



Regularización

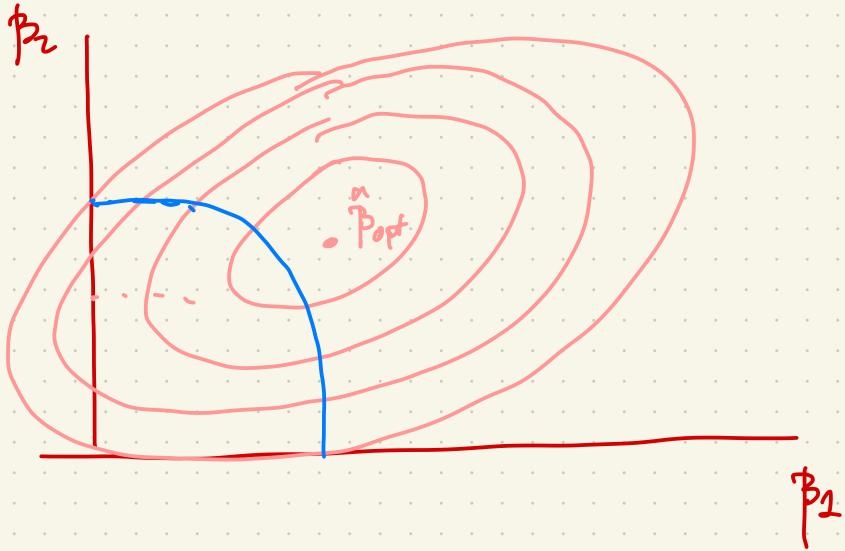






calculando $\hat{\beta}_{ML}$ obtengo un punto

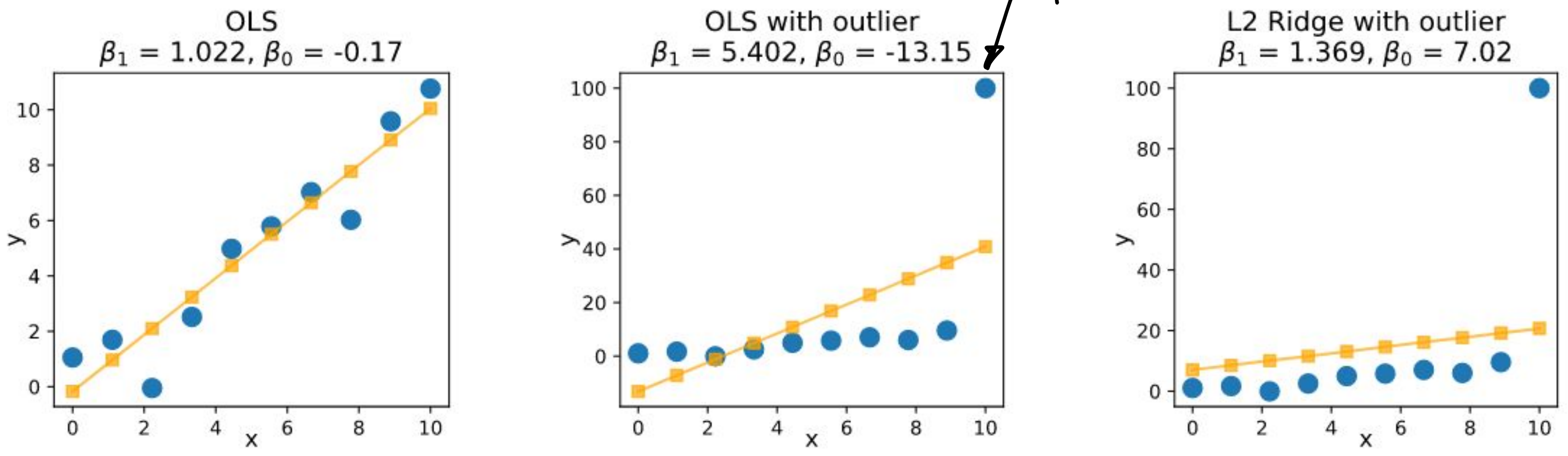
si yo planteo $\beta_i \in [-1, 1]$ pruebo con 100 β's en ese intervalo



β_2
$\hat{\beta}_{opt}$
β_1

Regularización - Motivación

outliers pesados ó high leverage points



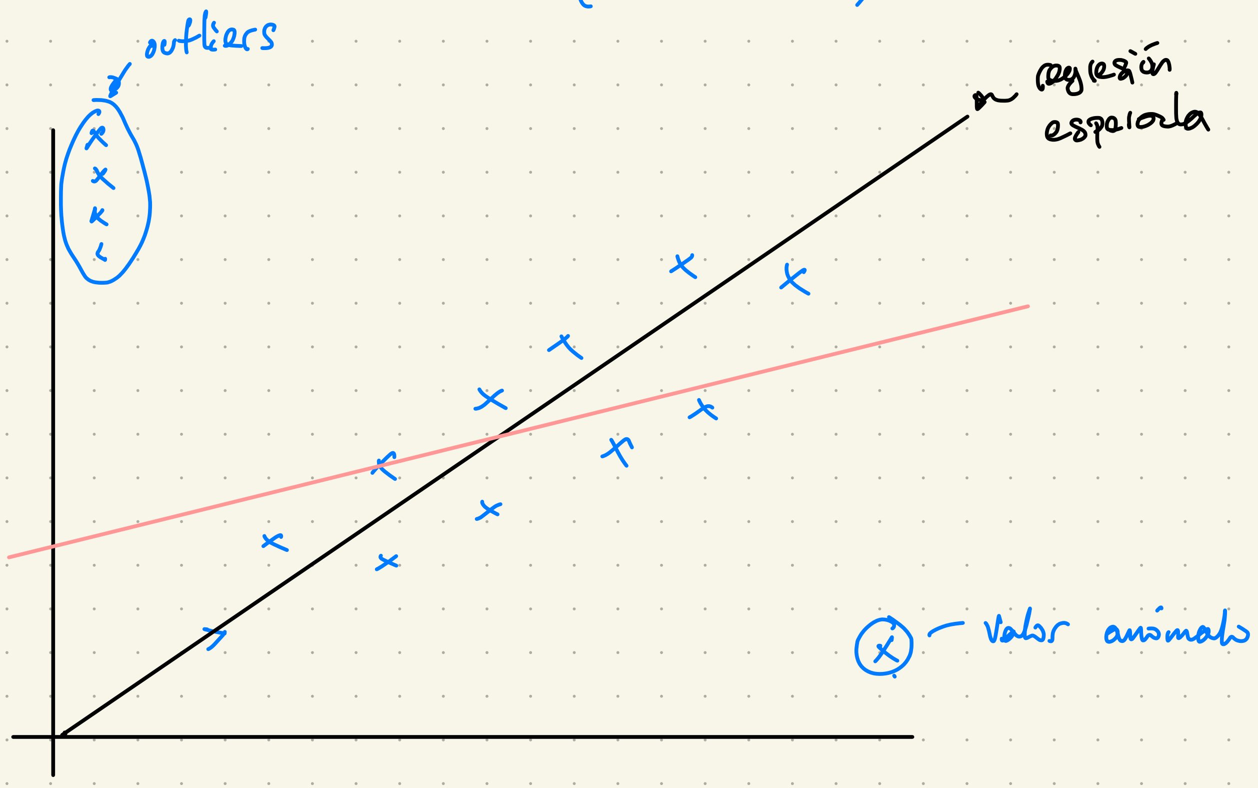
Regularización: analiza $\bar{\beta}$'s. → mejora* por restricción

Riesgo Empírico: analiza la perdida. → mejora* por construcción

Riesgo Empírico

$$R(f) = \mathbb{E}\big(\underbrace{L(f, \hat{f})}_{\text{función de pérdida (loss function)}}\big) \rightsquigarrow L(f, \hat{f}) = (f - \hat{f})^2$$

fn. de pérdida L2

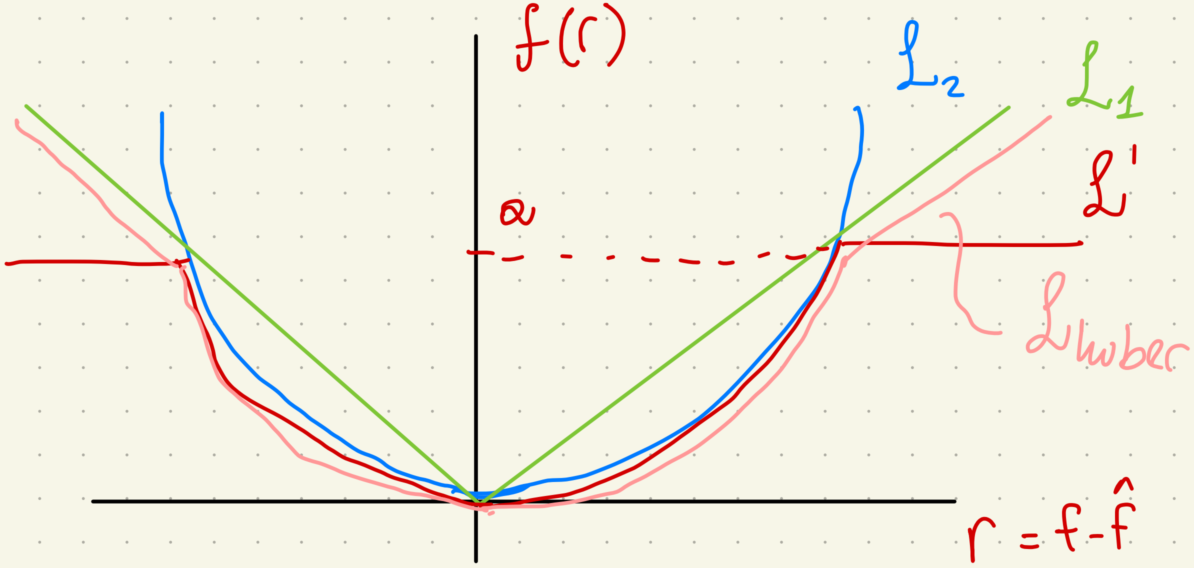


$$L' = \begin{cases} (f - \hat{f})^2 & \text{si } |f - \hat{f}| \leq c \\ a & \text{o.w.} \end{cases}$$

¿Cómo podemos mejorar mi reg. lineal?

1. Cambiar L
   - $L_1 = |f - \hat{f}|$
   - $L_2 = (f - \hat{f})^2$
   - $L_{\mathbb{I}} = \mathbb{I}_{|f - \hat{f}| \leq c}$
   - L_{huber}
   - L_{Tukey}

   $\left.\begin{matrix} L_{huber} \\ L_{Tukey} \end{matrix}\right\}$ Estimadores robustos de la pérdida (multiparamétricos)



$$\mathcal{L}_{huber} = \begin{cases} \frac{1}{2} r^2 & |r| \leq \delta \\ \delta\left(|r| - \frac{1}{2}\delta\right) & o.w. \end{cases}$$

$$\mathcal{L}_{Tukey} = \begin{cases} \frac{c^2}{6}\left(1 - \left[1 - \left(\frac{r}{c}\right)^2\right]^3\right) & \text{para } |r| \leq c \\ \frac{c^2}{6} & o.w. \end{cases}$$

'huber regressor' en sklearn

robust regressor en stat models.

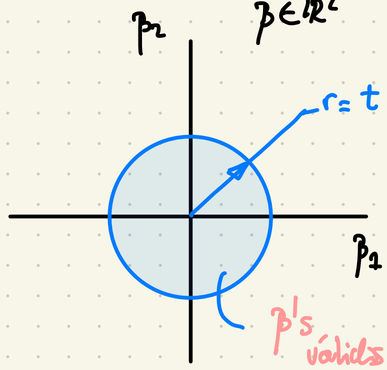
nosotros siempre busamos minimizar R de la forma más sencilla, a veces cambiar L no es barato o peor no es útil $\longrightarrow$ probamos regularizar

2. Regularización.

Con reg. busamos min R al mismo tiempo que restringimos (limitamos) el comp. de los parámetros (parameter shrinking).

partimos de

$$\begin{cases} \hat{y} = \beta_0 + \sum_i \beta_i x_i \\ \hat{\beta} = \underset{\beta}{\arg\min} \left(\sum_i y_i - \sum_j \beta_j x_{ij} \right)^2 \\ \frac{1}{q} \sum_j \beta_j^{q} \leq t \qquad \left(\|\beta\|^{q} \leq t \right) \end{cases}$$



Espacio de parámetros

$$q=2 \longrightarrow \hat{\beta} = \underset{\beta}{\arg\min} \left(\sum_i y_i - \sum_j \beta_j x_{ij} \right)^2 - \lambda \sum_j \beta_j^2$$

Termino de regularización (Weigth decay)

parámetro de complejidad

Regularización

Expectation - maximization
Algoritmo (E-M)

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

Observado - Predicción

↓

w está "libre"

en este caso $\bar{w} = \bar{\beta}$

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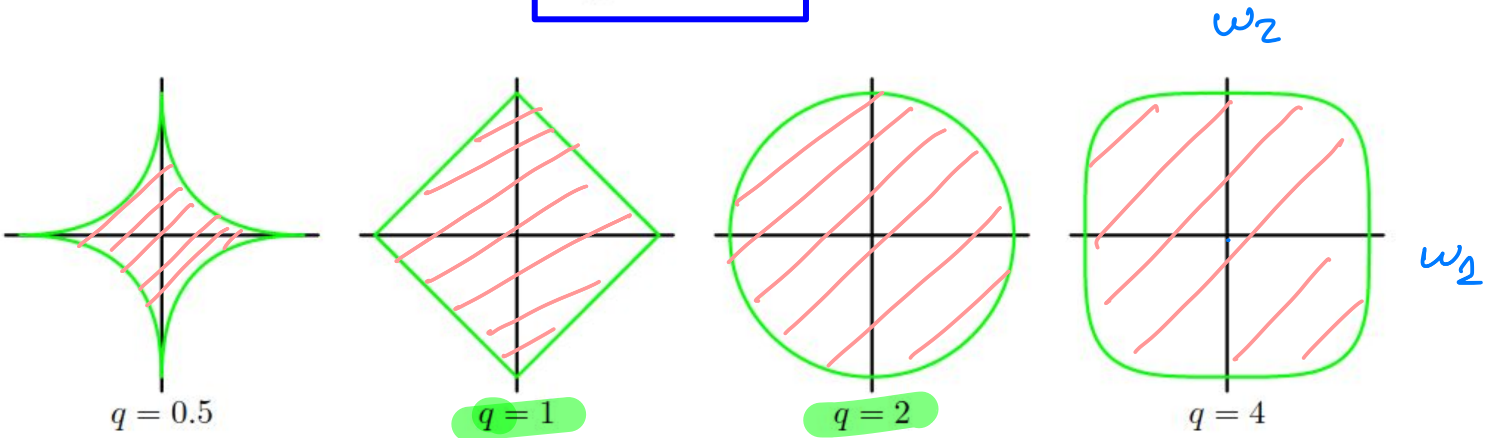
Regularización

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

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



valores validos de $\|w\|_2$

Lasso

penalidad L1

Ridge

pen L2

(w_1, w_2)

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

Maximum A Posteriori como regularización

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

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

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

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

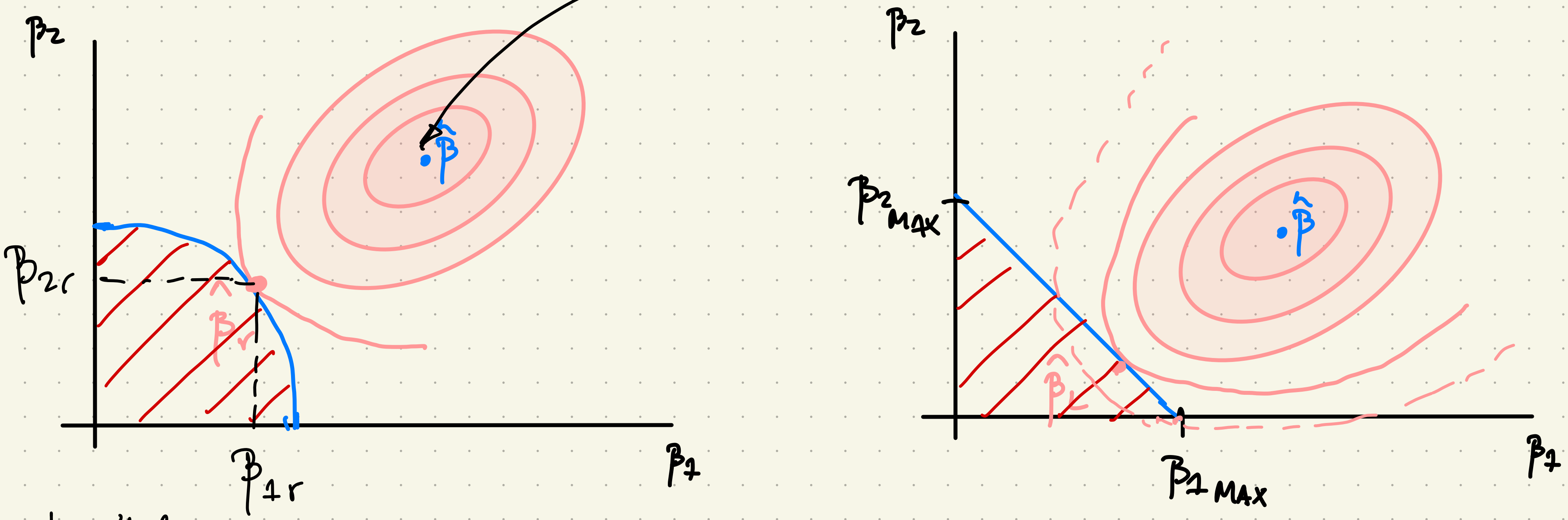
$p(w)$

$p(\beta)$

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

Gaussian prior con varianza b2

Representación gráfica: $\hat{\beta}$: Es el mejor $\hat{\beta}$ posible



▨ β's válidos

Ridge $\quad\quad -\lambda \sum_j |\beta_j|^q \quad\quad$ Lasso

↓ (Ridge) porque enrobustece mi sist.

↓ (Lasso) porque hace un proceso de selección de variables

Recordemos que $\hat{\beta}$ en gral tiene curvas de nivel elípticas (por construcción del estimador).

Pero, regularizar viene a costo de alejarnos del óptimo.

¿Cómo funciona?

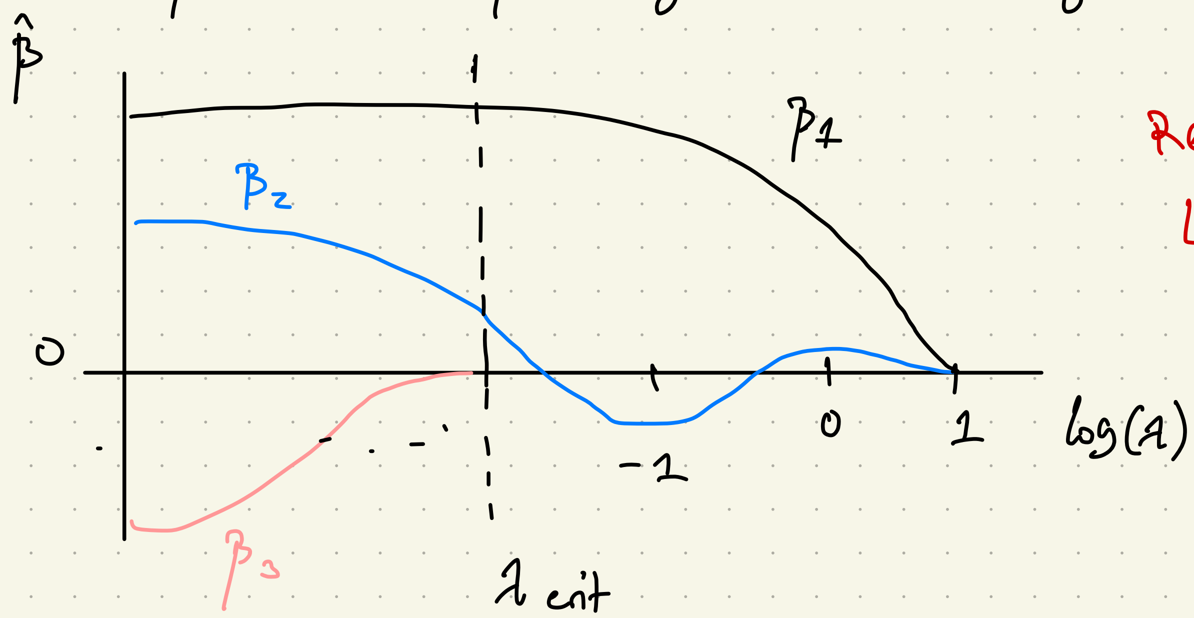
1. Elegir q (Lasso: 1, Ridge: 2)

2. Voy a elegir un vector de λ's "apropiado" ($\lambda\uparrow$ más $\uparrow$ penalidad)

3. optimizo para λ_i mas $RSS(\lambda; q) = \|y - X\beta\|^q + \lambda\|\beta\|_q$

4. calcular las métricas (Error de representación, bondad, algún criterio externo).

5. Comparamos y elegimos el mejor:



Regresión Lasso típica

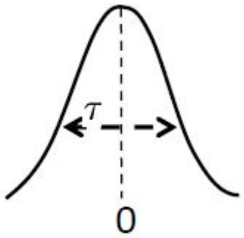
Regularización

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

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



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

Ridge Regression

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

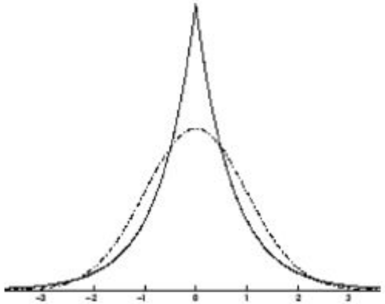
Machine Learning 10-315, Carnegie Mellon

Maximum A Posteriori como regularización - LASSO (L1)

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

II) Laplace Prior

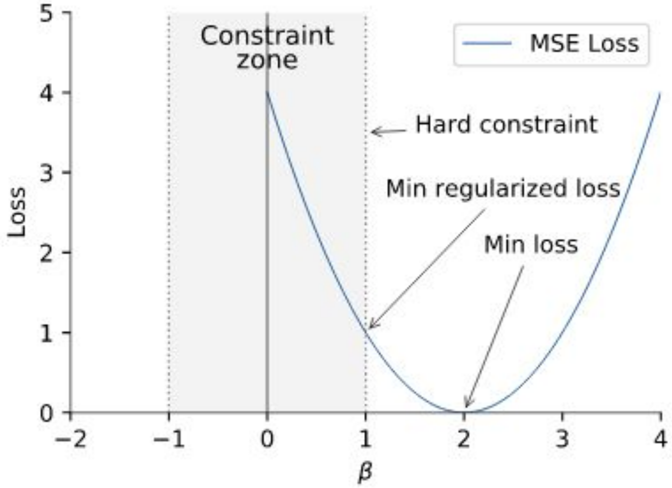
$$\beta_i \overset{iid}{\sim} \text{Laplace}(0, t) \qquad\qquad p(\beta_i) \propto e^{-|\beta_i|/t}$$

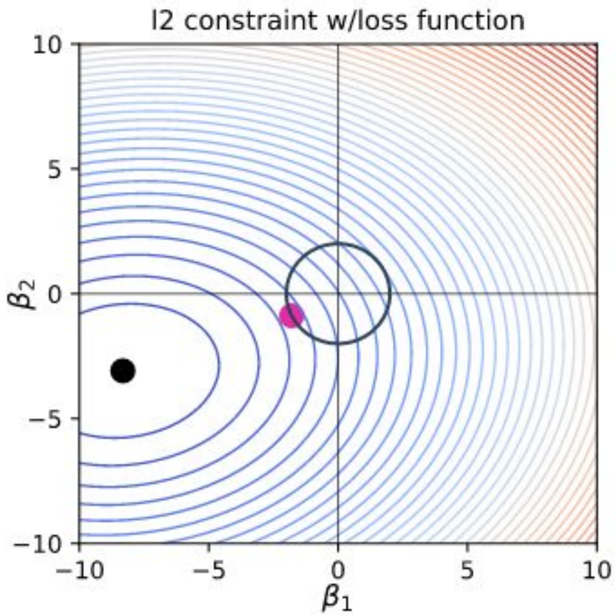


$$\widehat{\beta}_{\mathrm{MAP}} = \arg\min_{\beta} \sum_{i=1}^{n} (Y_i - X_i\beta)^2 + \underset{\downarrow \atop \text{constant}(\sigma^2, t)}{\lambda} \|\beta\|_1$$

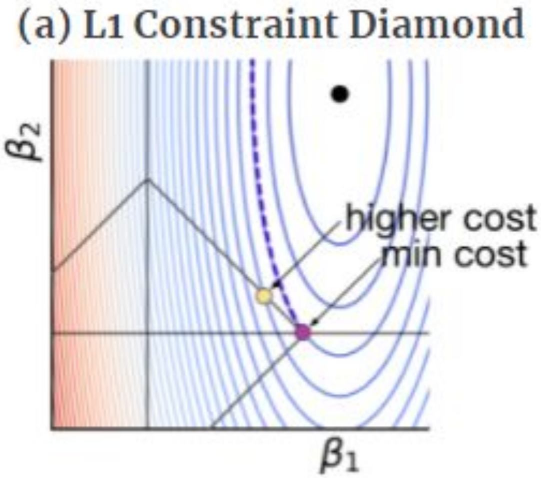
Lasso

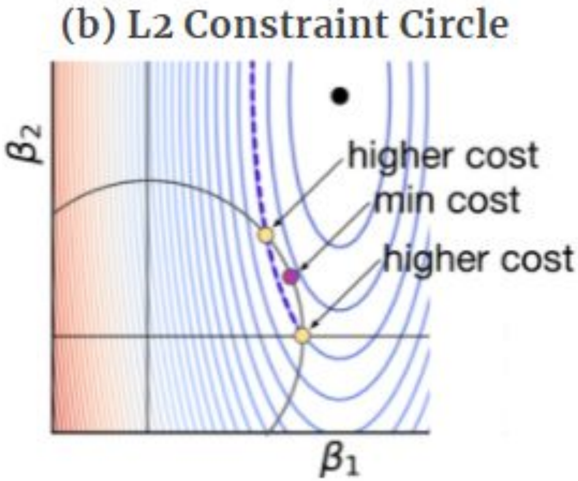
Regularización





Regularización





ElasticNet

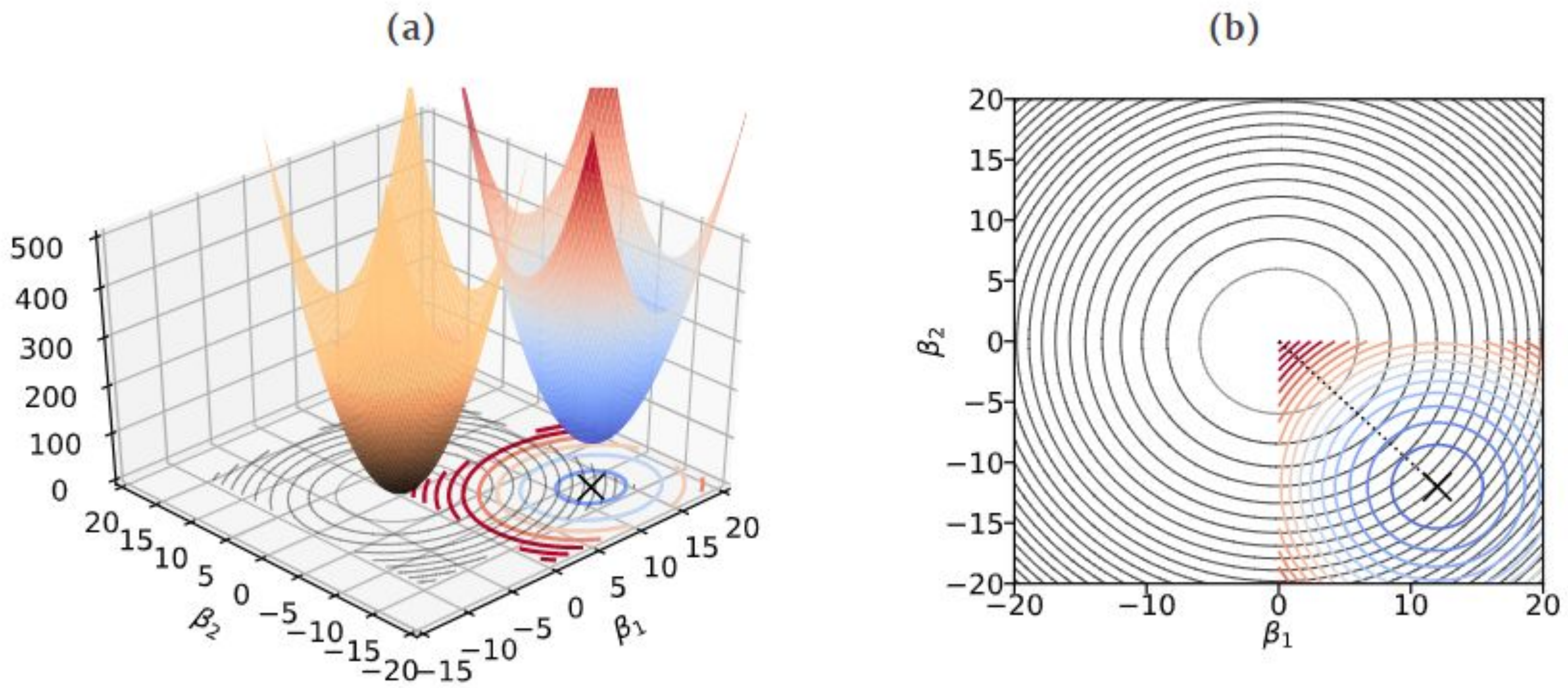
λ término de complejidad

¿Qué β se reduce más?

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

α parametro de elasticnet

Regularización



Cross-Validation

parametros n_folds

folds en gral son subdivisiones random del dataset

lasso

$\lambda \in [-10, 5]$

$X_{t1}\ Y_t$

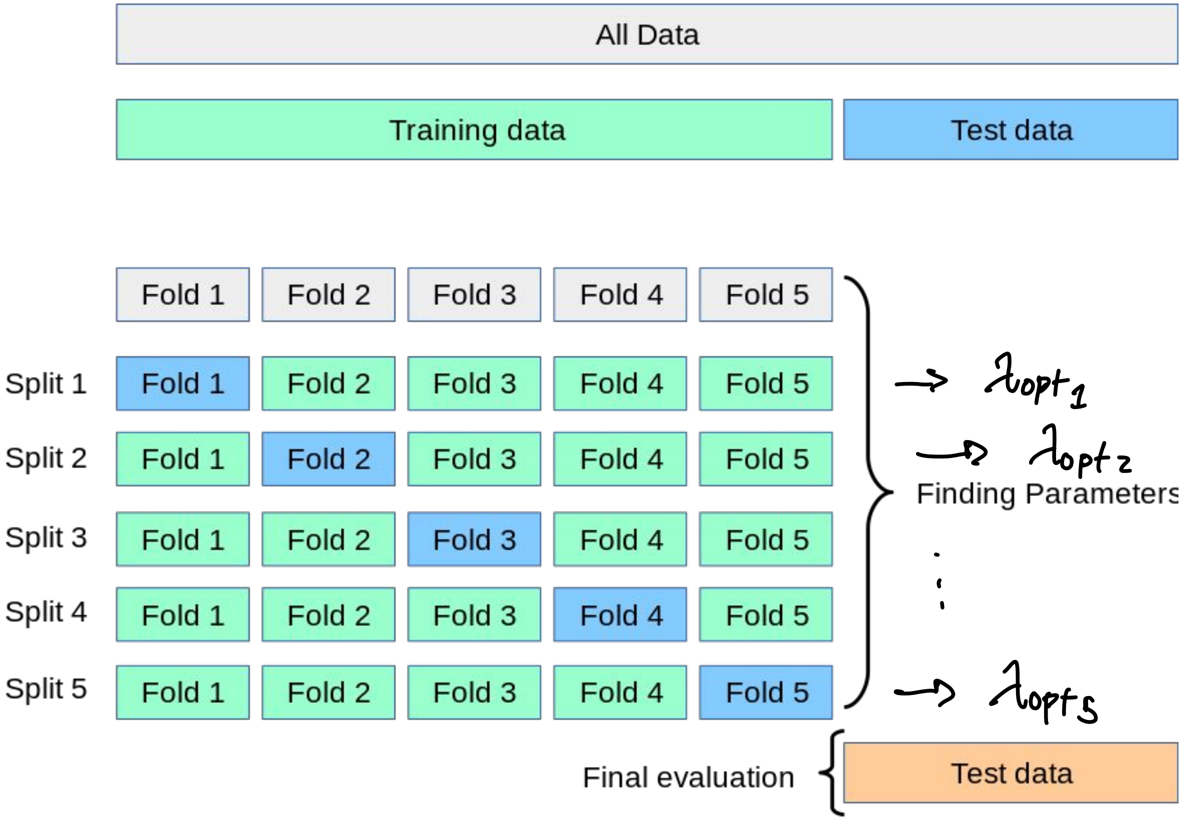
X_{t1} X_{te}'

X_{t2}

X_{t3} X_t'

X_{t4}

X_{t5}



$\to \lambda_{opt1}$

$\to \lambda_{opt2}$

$\vdots$

$\to \lambda_{opt5}$

$\bar{\lambda}_{opt}$

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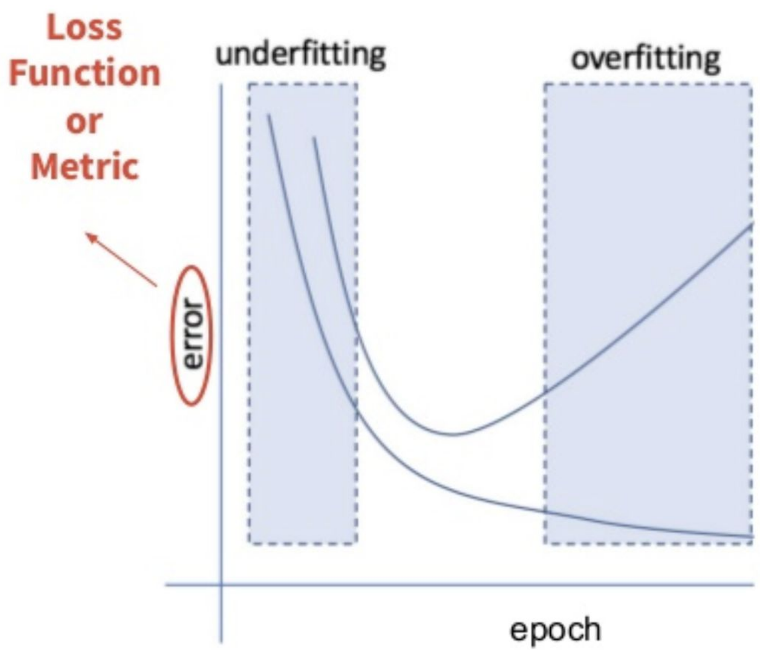
Entrenamiento numérico del modelo seleccionado - Obtención de parámetros

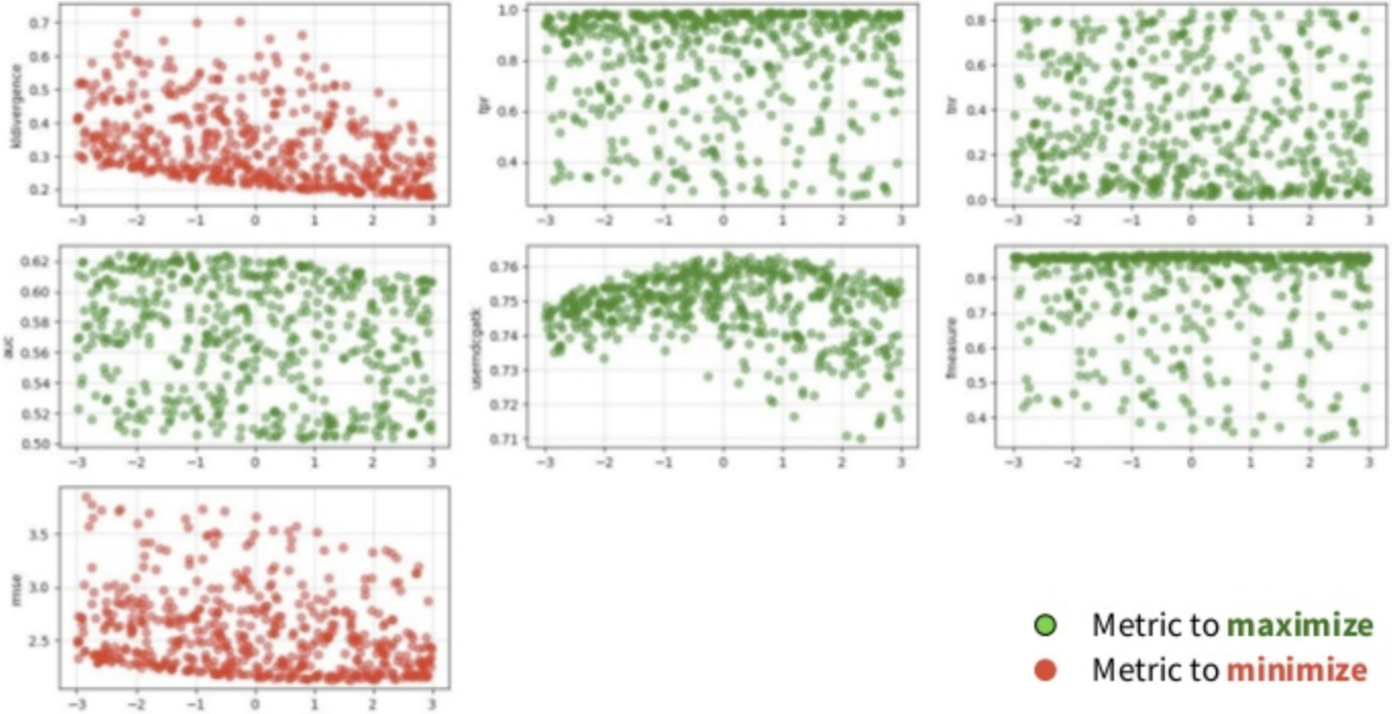


Mini-Batch Gradient Descent

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

Selección de los hiper parámetros



Grid Search

Random Search

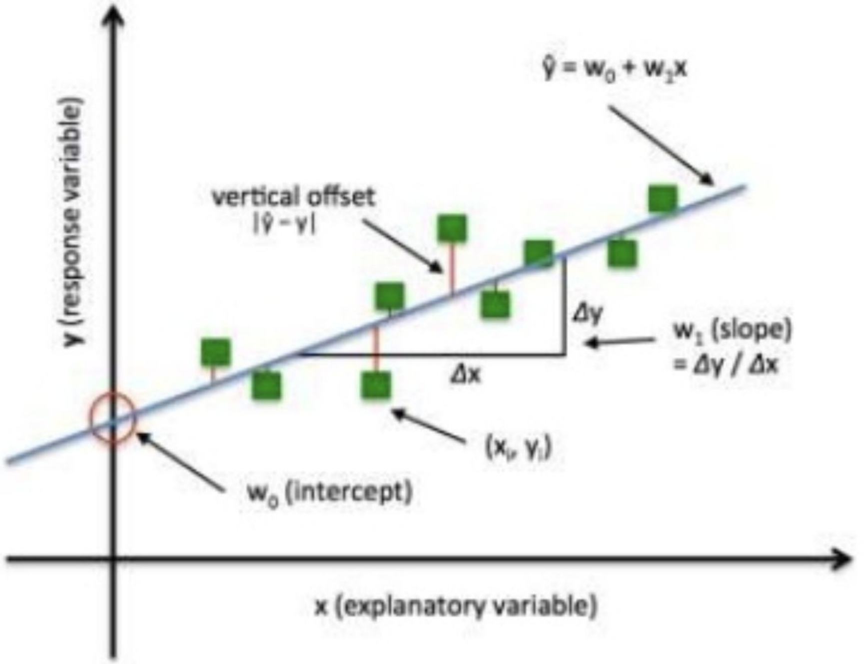
Gradiente Descendente

Implementación de Gradiente Descendente

Solucion analitica

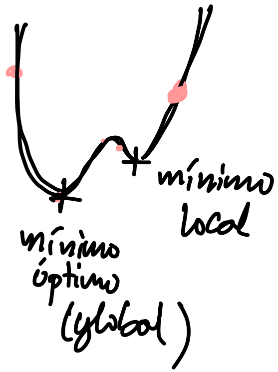
$$\min_W \|Y - XW\|_2^2$$

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



Implementación de Gradiente Descendente

$GD(\alpha, w_0)$



Solución numérica

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

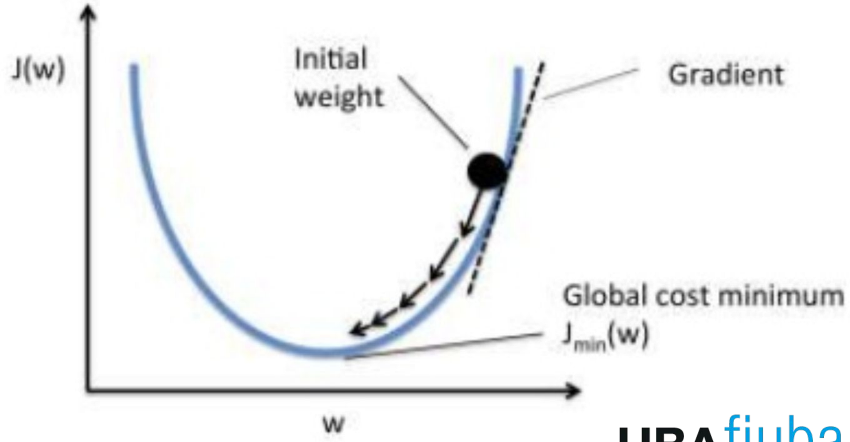
cond inicial

W_0

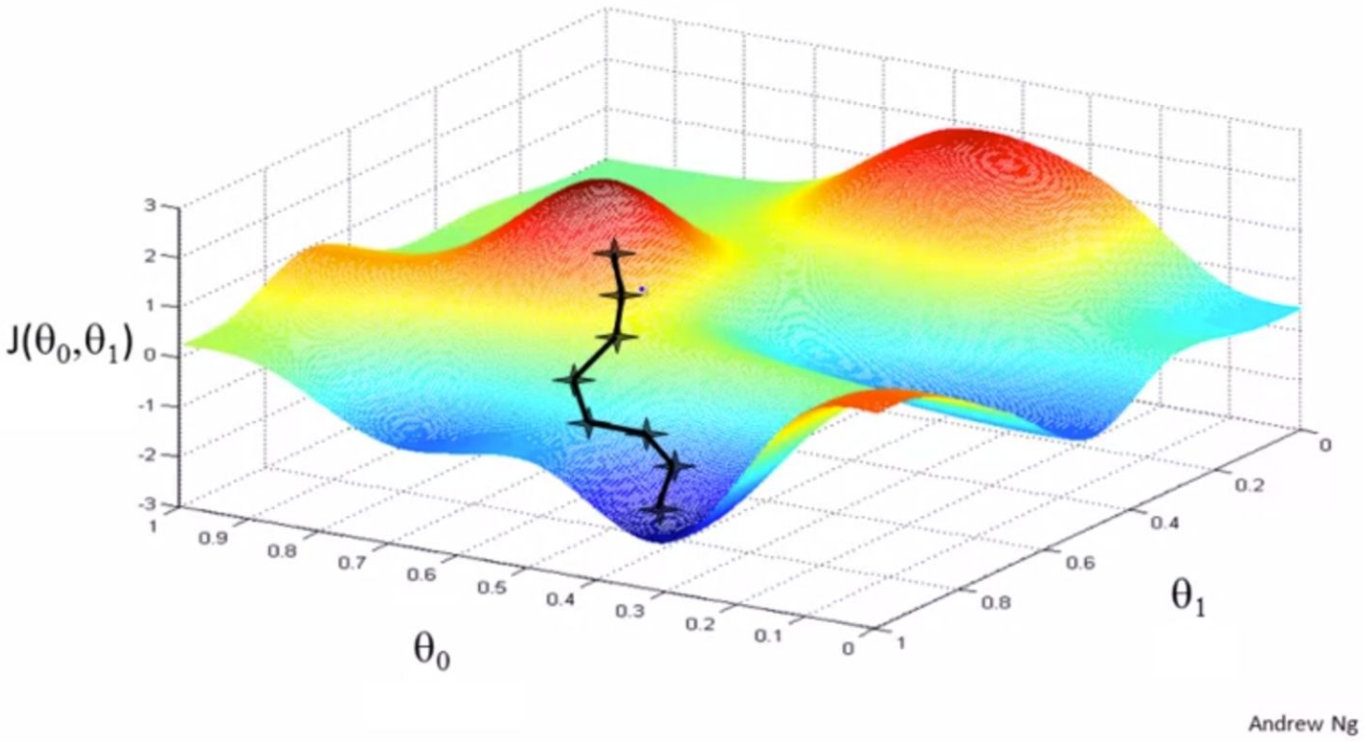
$$W_{n+1} \leftarrow W_n \underbrace{- \alpha \nabla \left(\sum_i (y_i - X_i \cdot W)^2 \right)}_{\text{"evolución"}}$$

learning rate

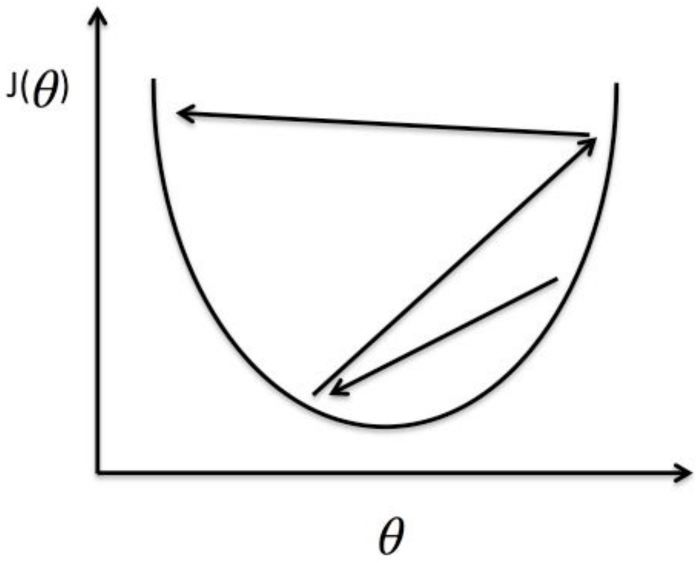
$\hookrightarrow \alpha \in \mathbb{R}^+$



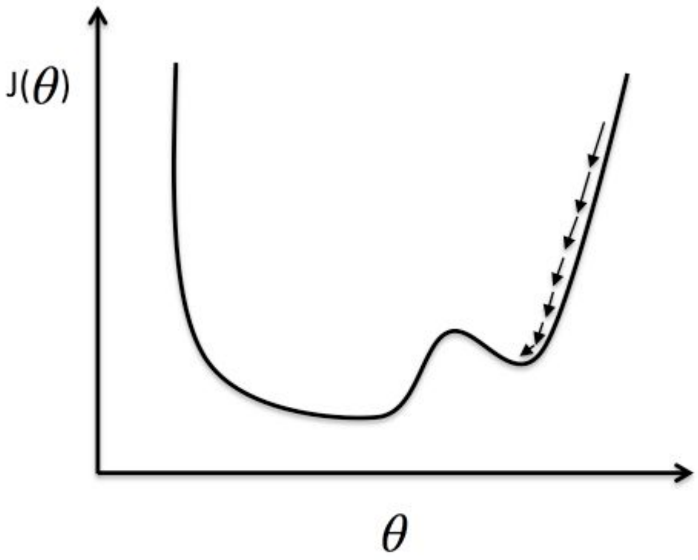
Gradiente Descendente



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

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

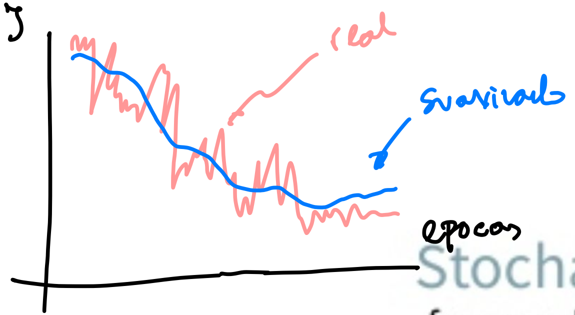
Gradient Descent algorithm

for epoch in n_epochs: Alternativa while e < tol || n_epoch < 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



$i \subset K$

es la cant. total de muestras

es un subset

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

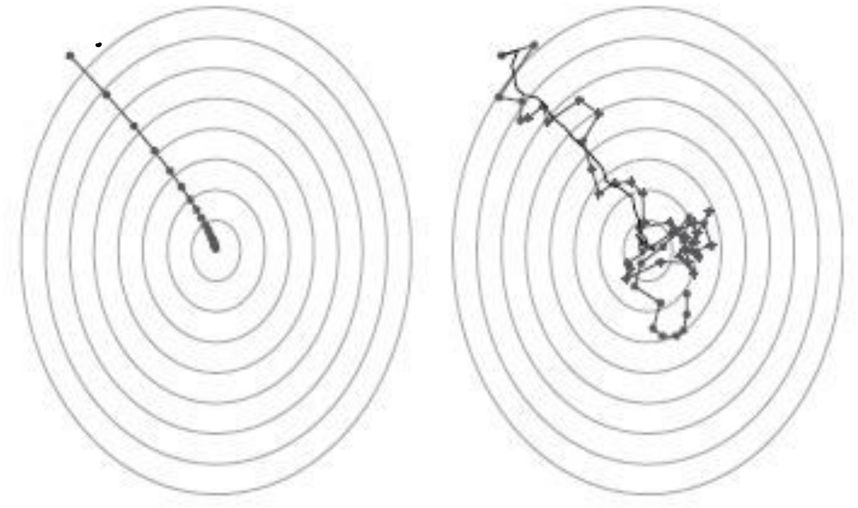
Stochastic Gradient Descent algorithm

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

B_1	B_2	B_3	B_4	B_5

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

e_1 B_5 B_3 B_1 B_4 B_2

e_2 B_1 B_4 B_3 B_5 B_2

Mini-Batch Gradient Descent algorithm

n_epoch, n_batch, batch_size

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

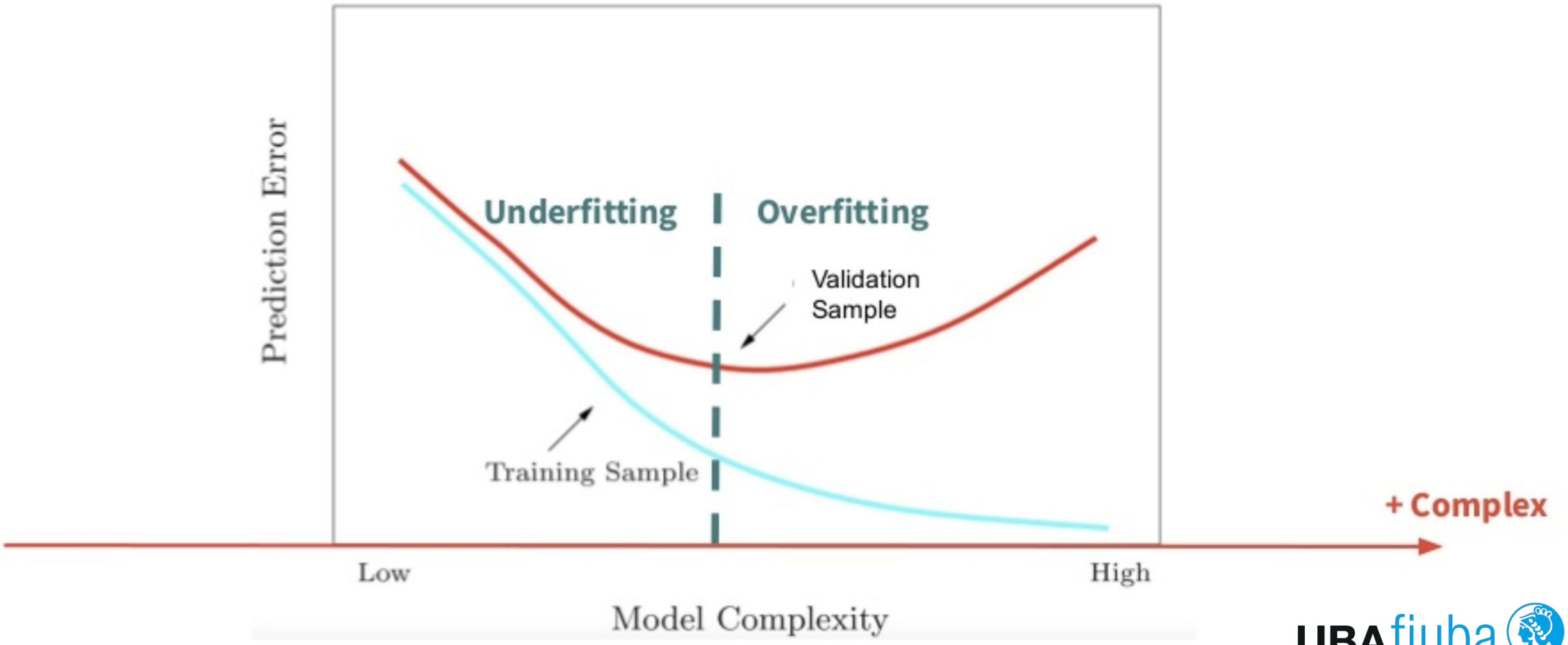
\sum_i \Big(-2 (y_i - \hat{y}_i) x_{ij}
\Big)

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



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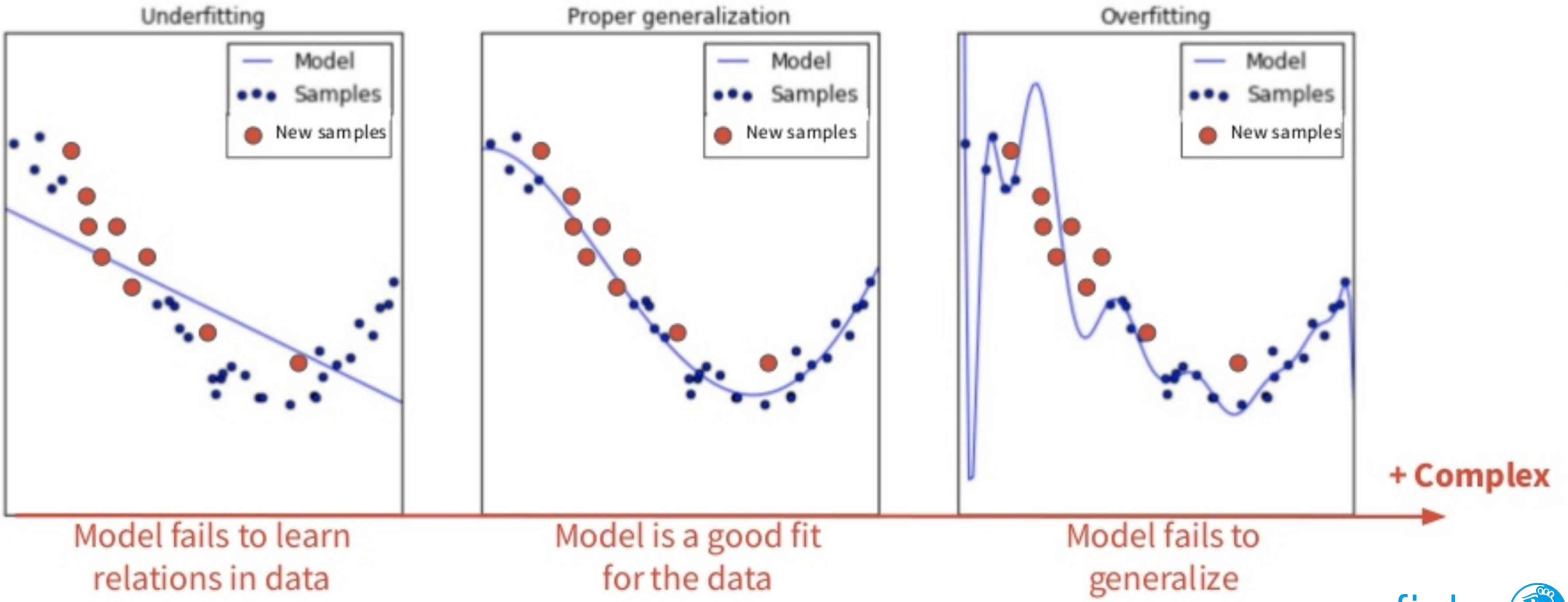

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