

# Implementación de Métodos de Aprendizaje Automatizado en problemas colisionales

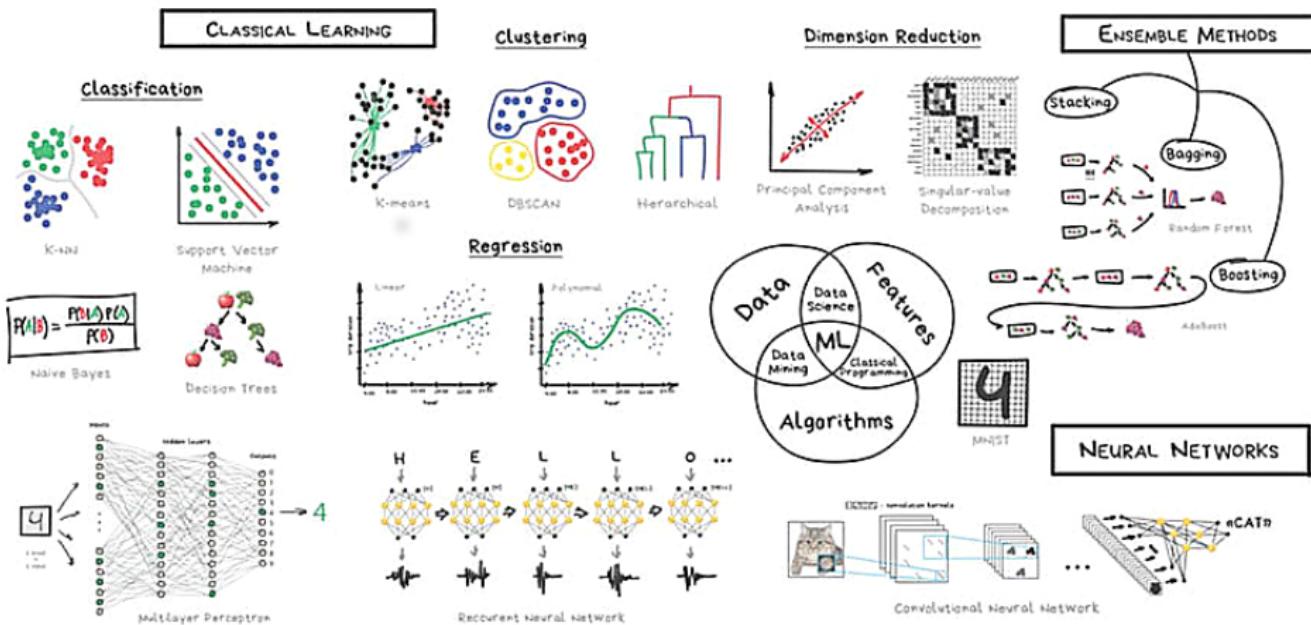
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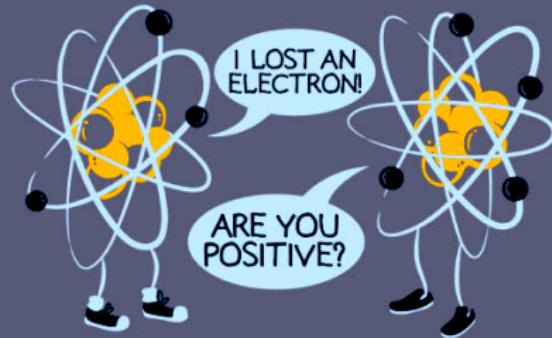
3 de Septiembre – Buenos Aires



# Machine Learning

# Problema 1:

## Potenciales efectivos (DIM)



# Método de Inversión Depurada (DIM)

$$\left[ -\frac{1}{2} \frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + V_{nl}(r) \right] P_{nl}(r) = E_{nl} P_{nl}(r)$$

# Método de Inversión Depurada (DIM)

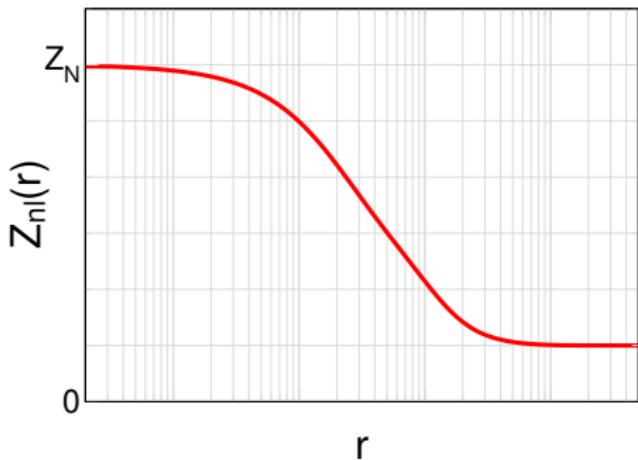
$$\left[ -\frac{1}{2} \frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + V_{nl}(r) \right] P_{nl}(r) = E_{nl} P_{nl}(r)$$

$$V_{nl}(r) = \frac{1}{2} \frac{P''_{nl}(r)}{P_{nl}(r)} - \frac{l(l+1)}{2r^2} + E_{nl}$$

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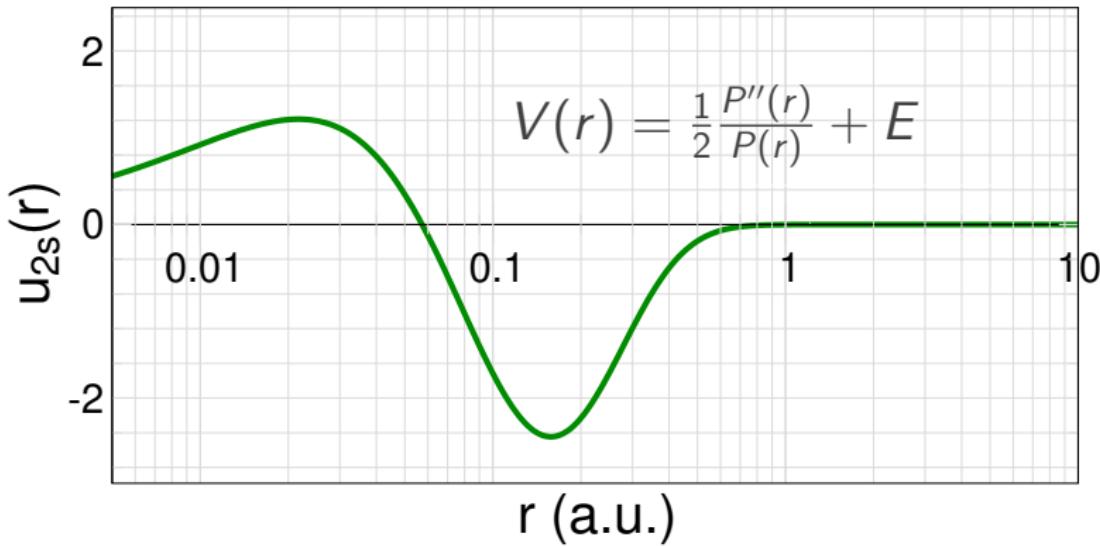
$$V_{nl}(r) = \frac{1}{2} \frac{P''_{nl}(r)}{P_{nl}(r)} - \frac{l(l+1)}{2r^2} + E_{nl}$$



$$V(r) = -\frac{Z(r)}{r}$$

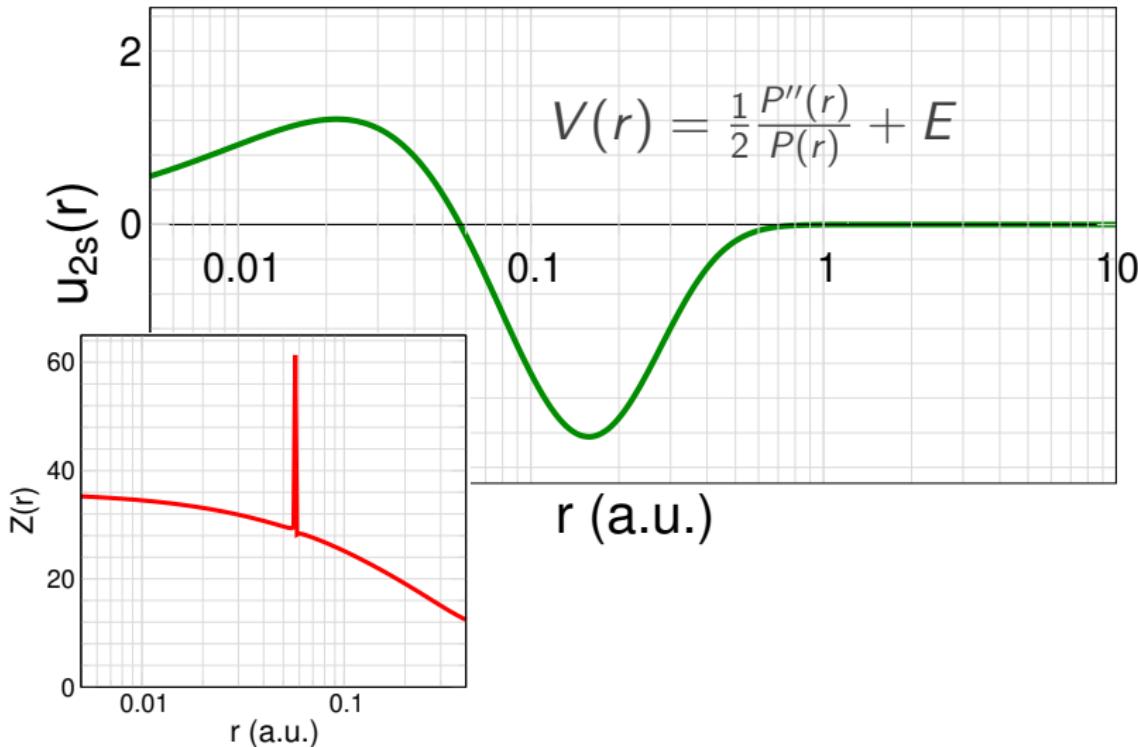
# Houston, we have a problem!

Kr



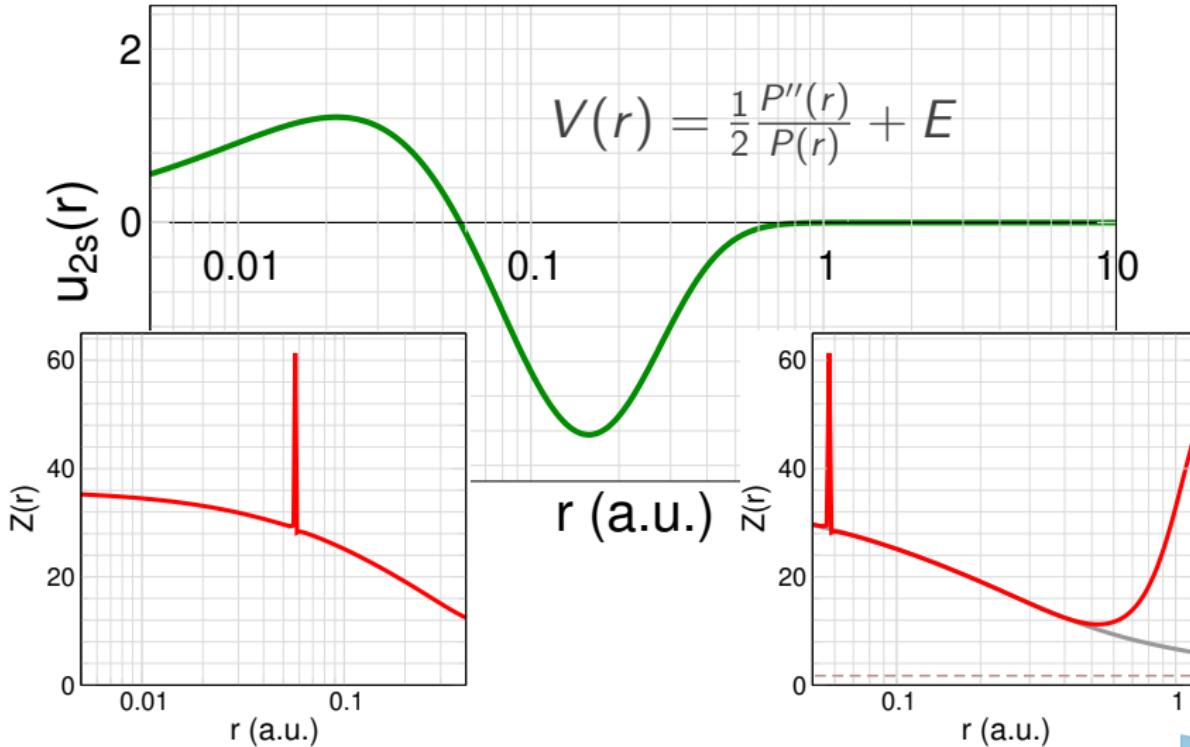
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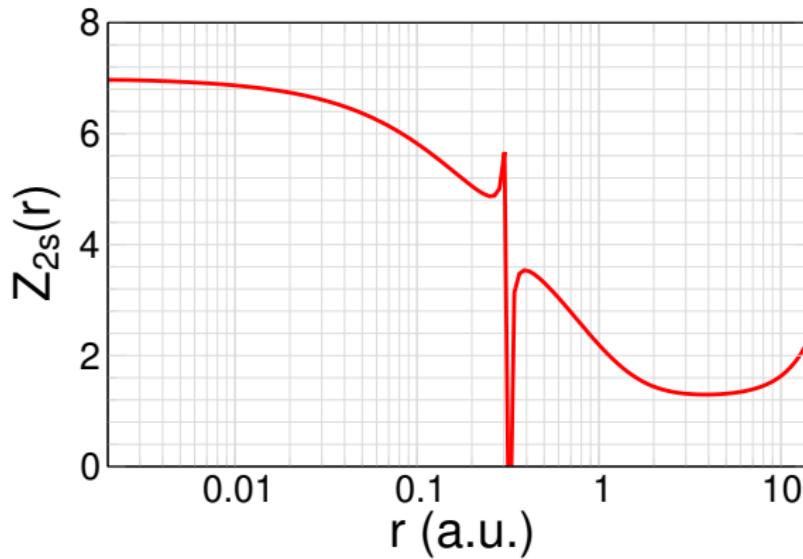
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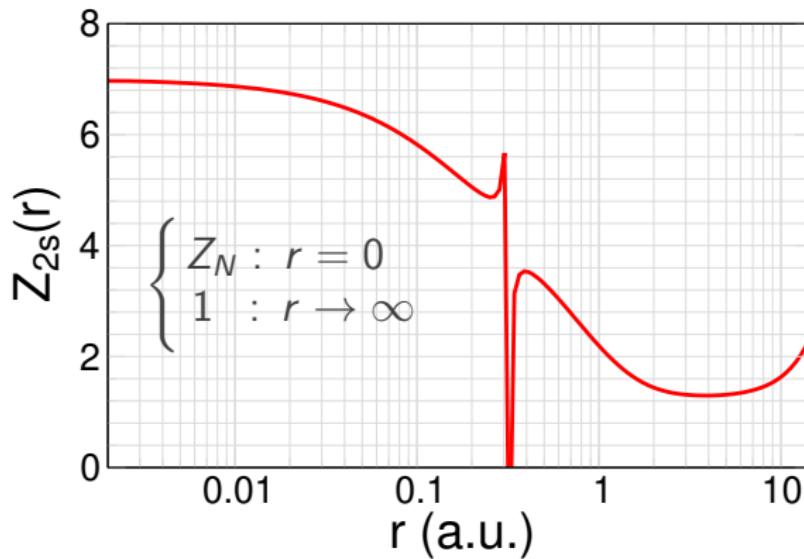
# Depuración

N



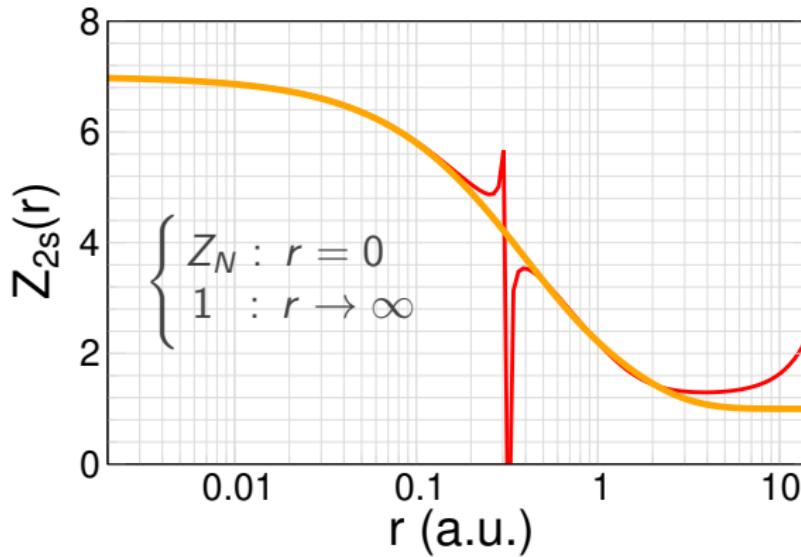
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N



# Depuración

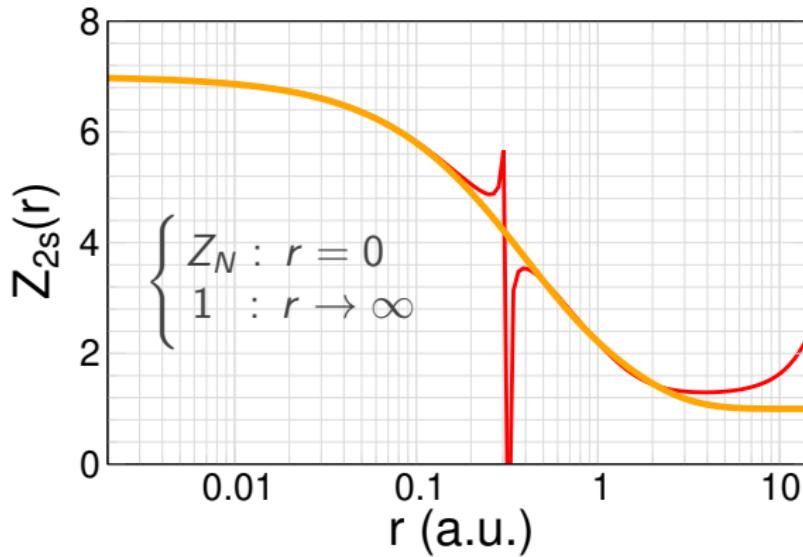
N



$$Z(r) = 1 + \sum_j \alpha_j e^{-\beta_j r}$$

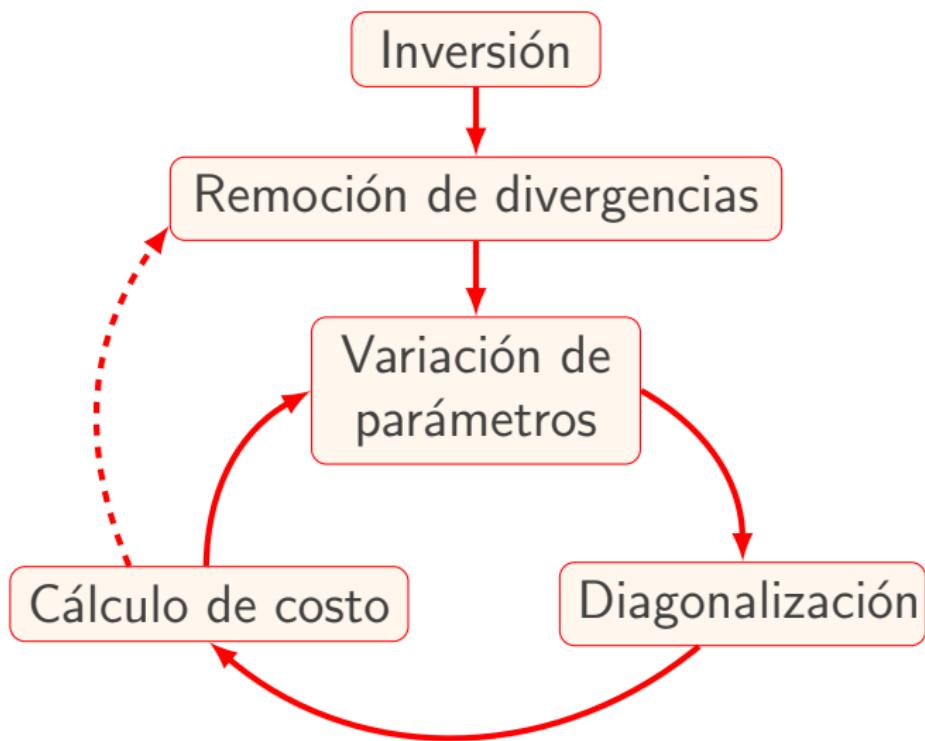
# Depuración

N



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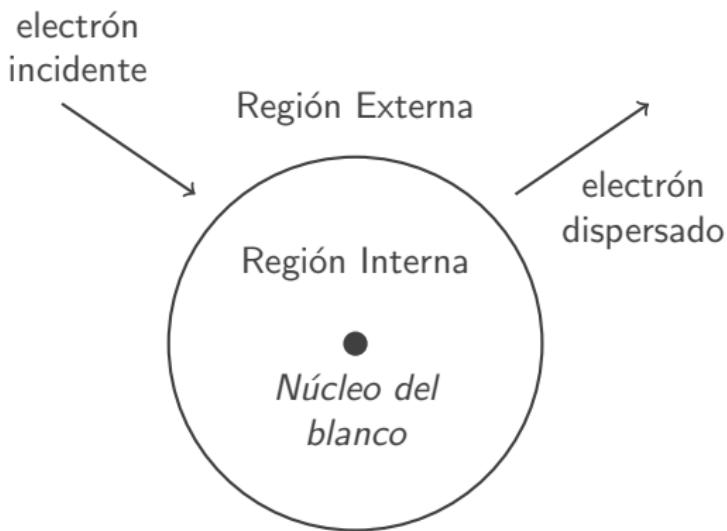
# Procedimiento



# Problema 2:

## Cálculos colisionales (R-Matrix)

# R-Matrix



Estructura del blanco

AUTOSTRUCTURE



Región Interna

RMATRXI



Región Externa

STGF

# Descripción del blanco

$$\Psi_i(\mathbf{r}) = \sum_j^N c_{ji} \Phi_j(\mathbf{r})$$

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*N*

*Configuraciones*

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*N*

Configuraciones

$$\left[ \frac{1}{2} \frac{d^2}{dr^2} - \frac{l(l+1)}{2r^2} + V_{nl}^{\text{eff}}(\lambda_{nl}, r) + E_{nl} \right] P_{nl}(r) = 0$$

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- Slater-Type-Orbital de Burgess

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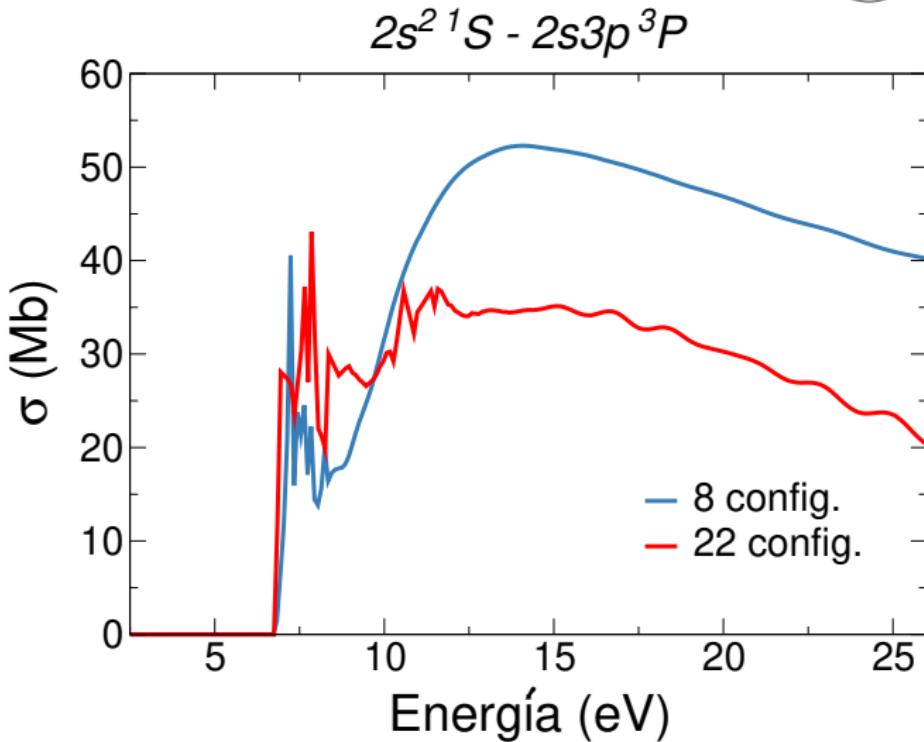
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*Parámetro de escaleo*

- Thomas–Fermi–Dirac–Amaldi
- Slater-Type-Orbital de Burgess

# Dependencia de CI ( $N$ )

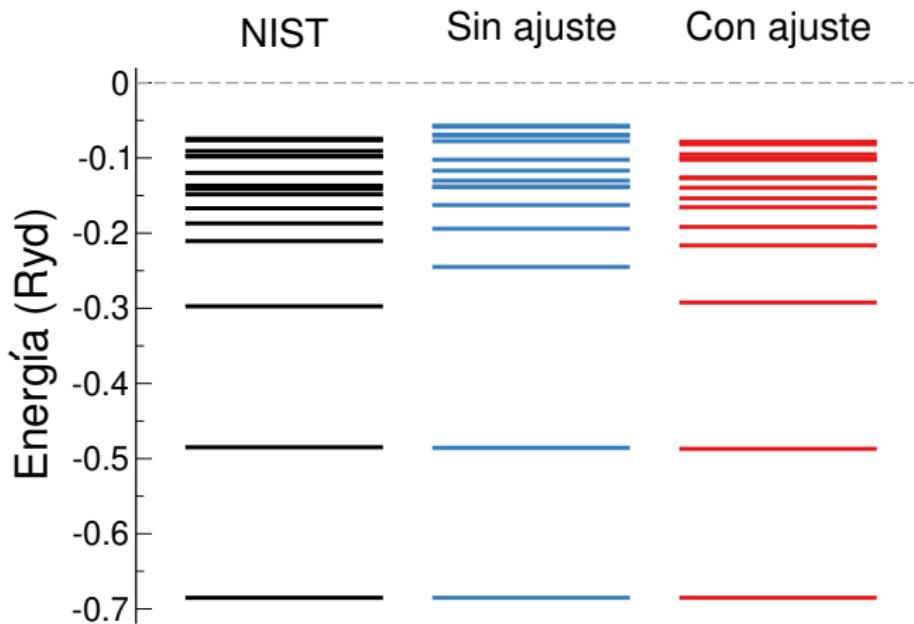
$1s^2 2s^2$   
 $1s^2 2snl$   
 $1s^2 2p^2$   
 $1s^2 2pnl$



Be

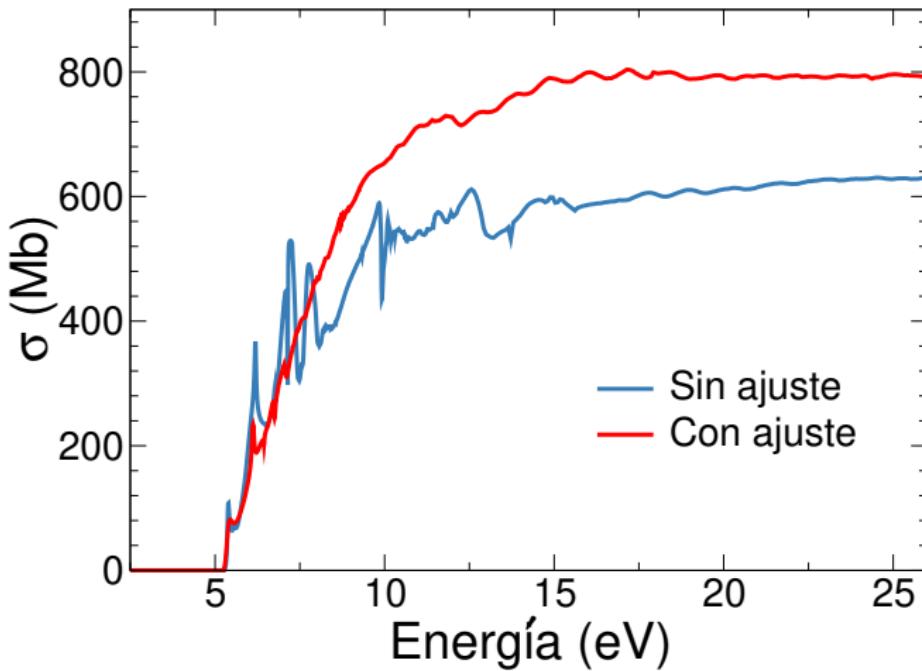
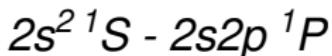
# Dependencia de escaleo ( $\lambda_{nl}$ )

Be

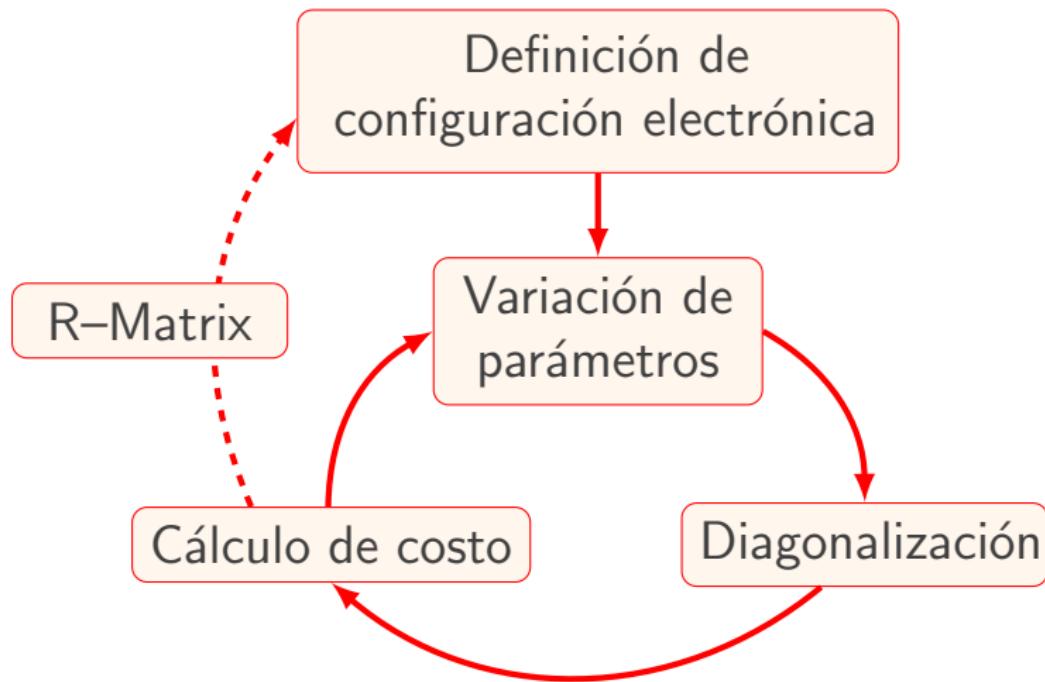


# Dependencia de escaleo ( $\lambda_{nl}$ )

Be



# Procedimiento



# Síntesis del problema

Función de costo:

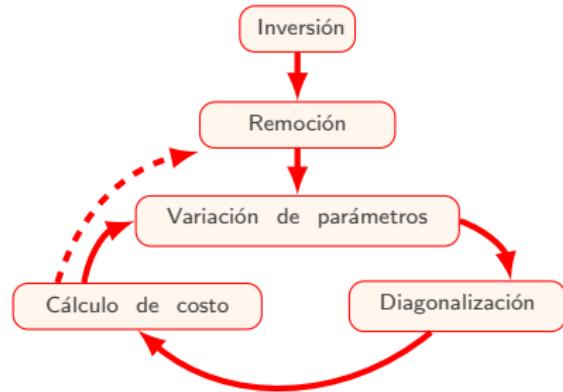
$$J = \sum_j \left| \frac{\tilde{E}_j(\xi) - E_j}{E_j} \right|$$

- DIM:  $\xi = \{\mathbf{R}, \alpha, \beta\}$
- R-Matrix:  $\xi = \{N, \lambda\}$

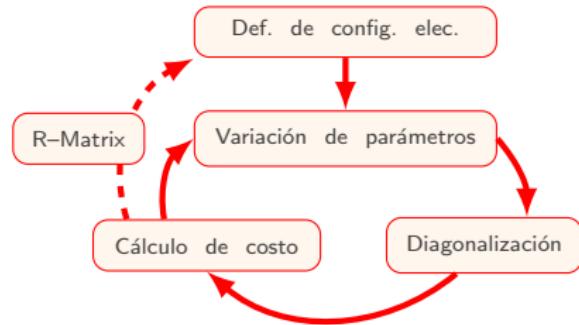
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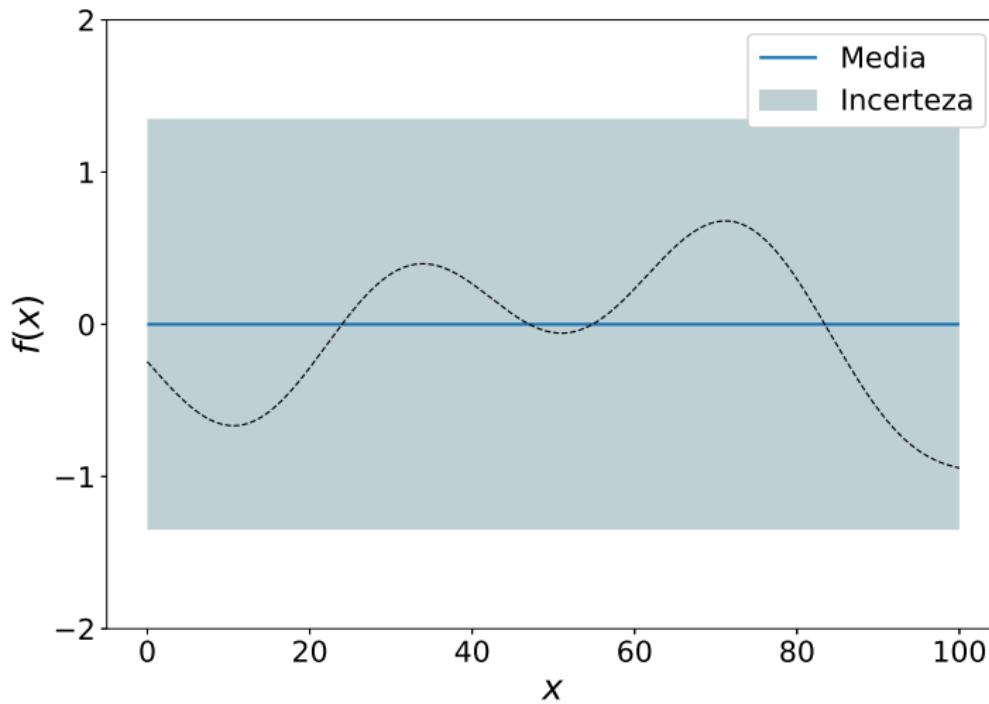


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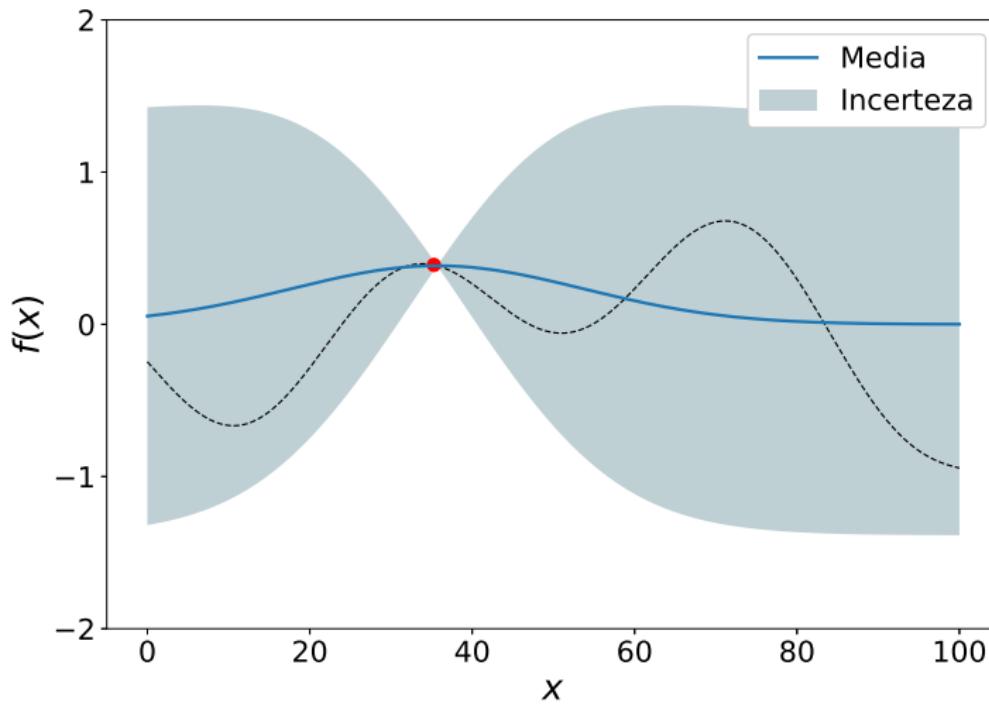


# Optimización Bayesiana con Procesos Gaussianos

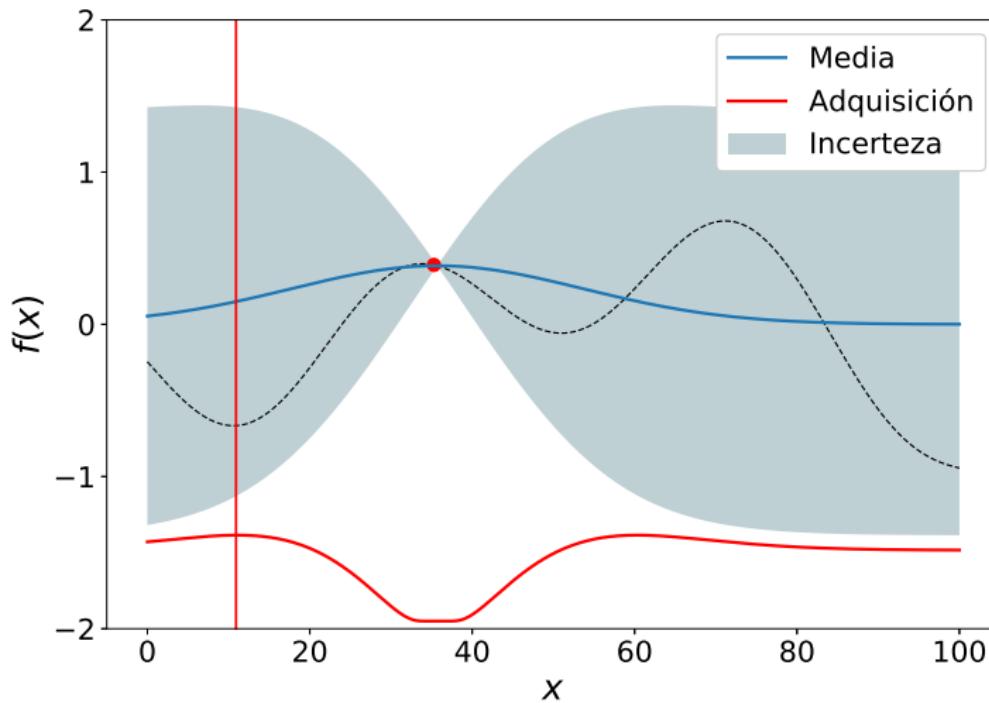
# Procesos Gaussianos



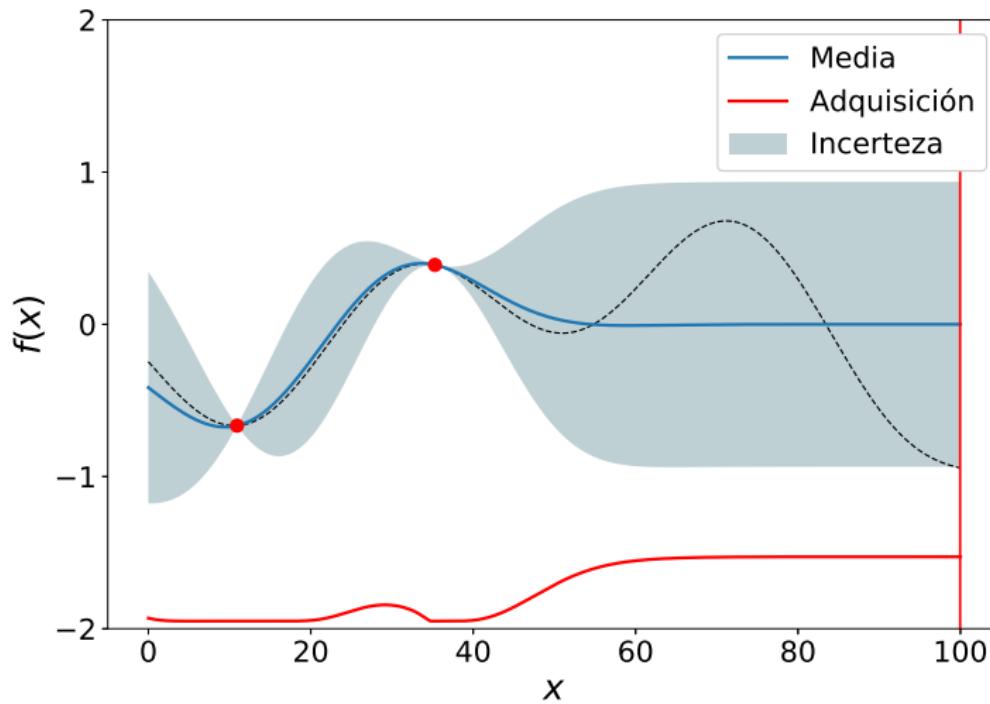
# Procesos Gaussianos



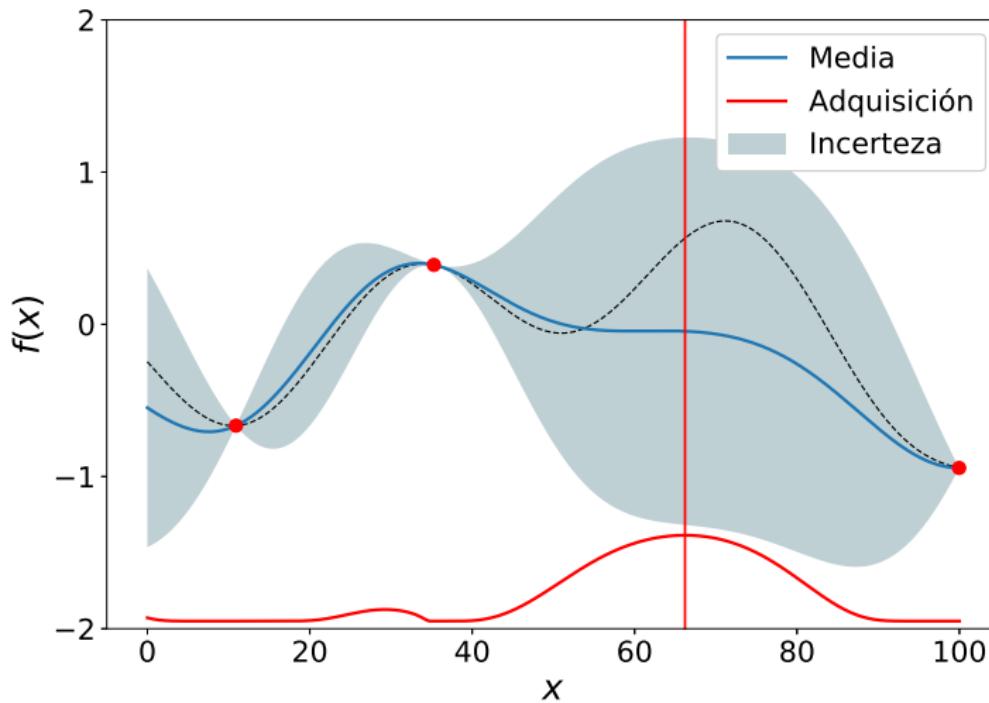
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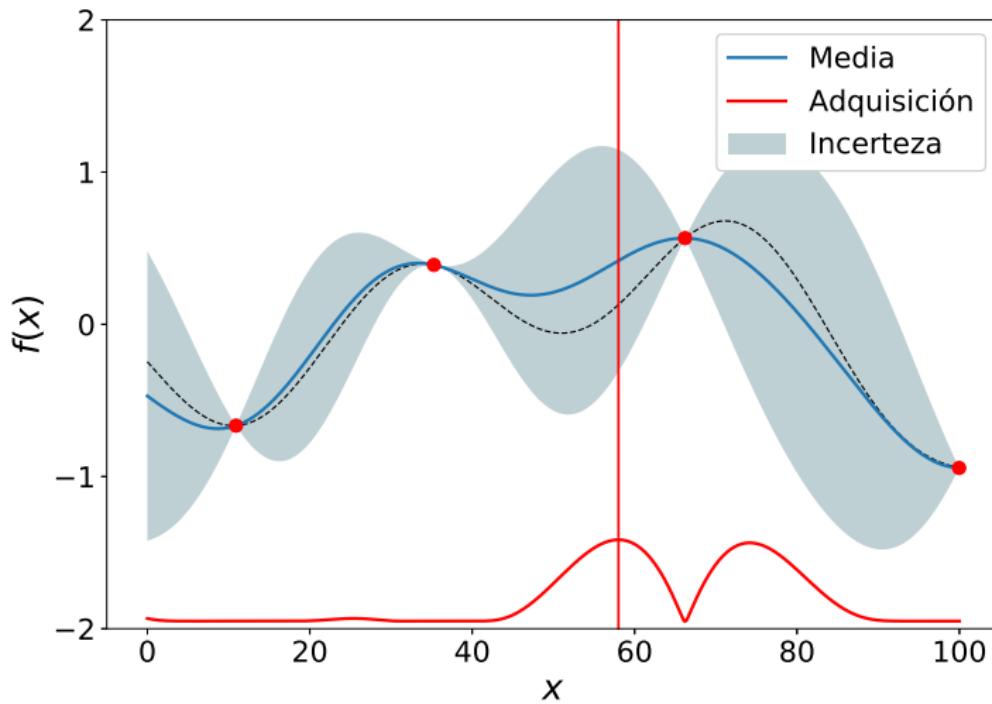
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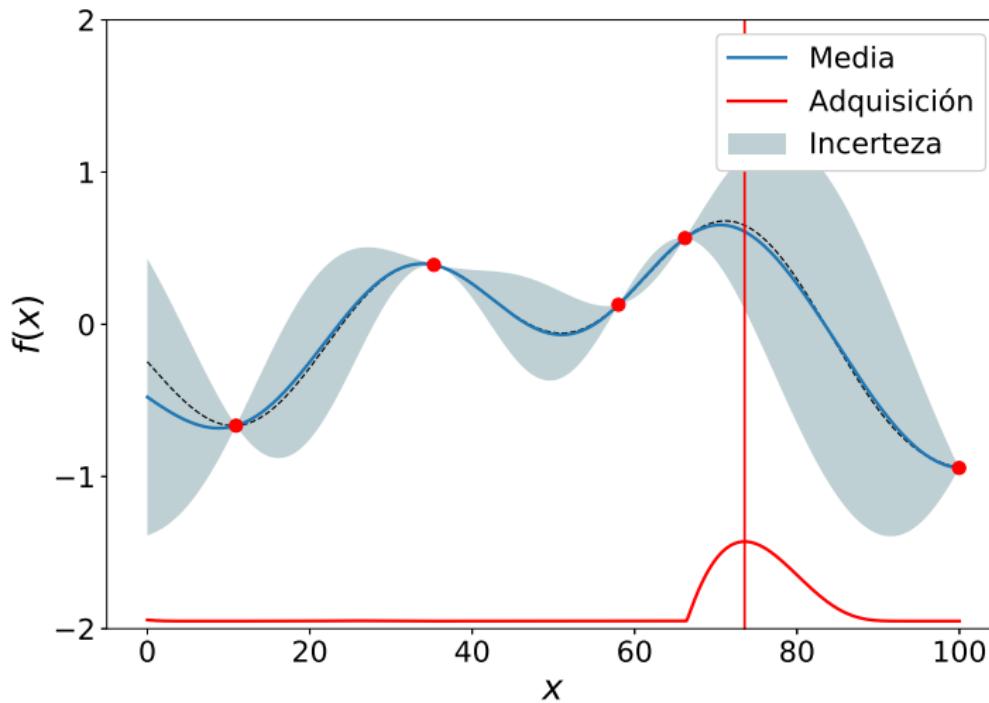
# Procesos Gaussianos



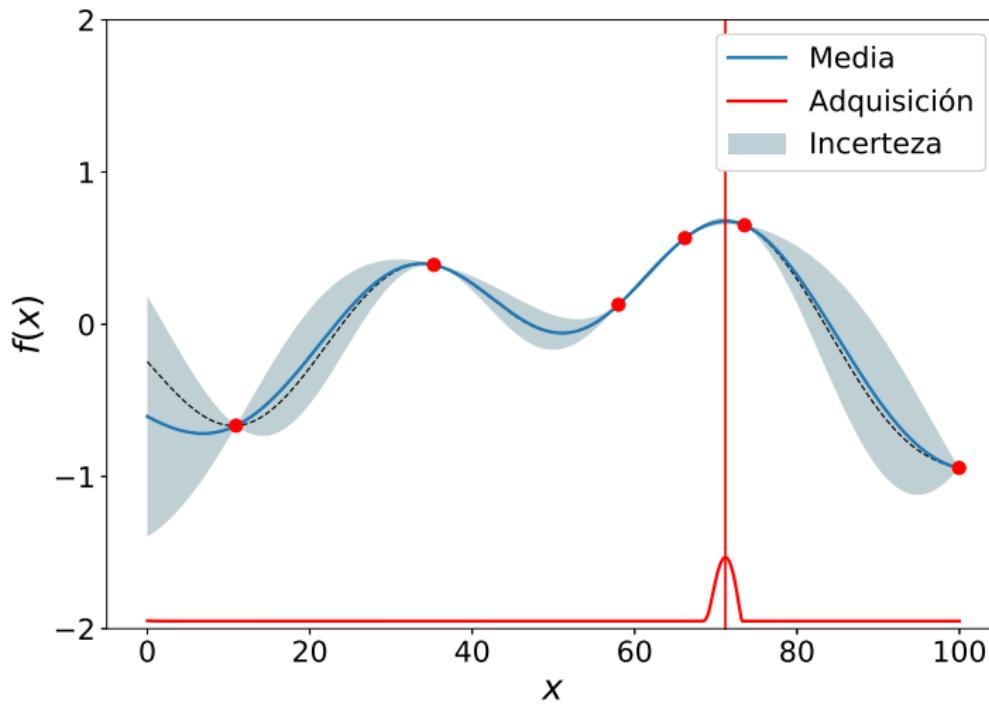
# Procesos Gaussianos



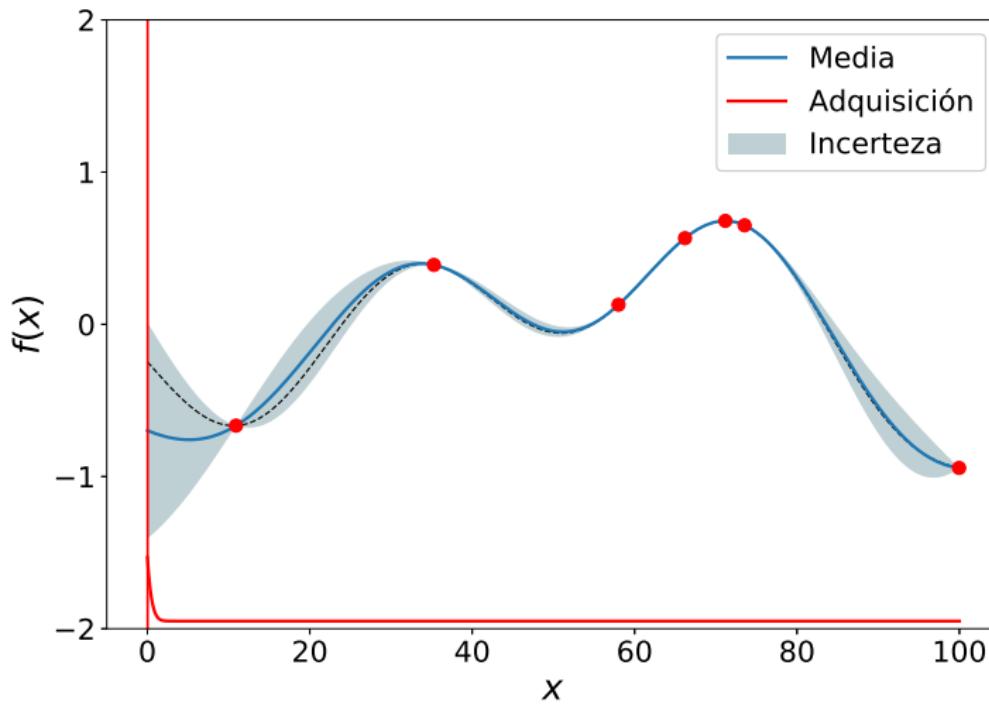
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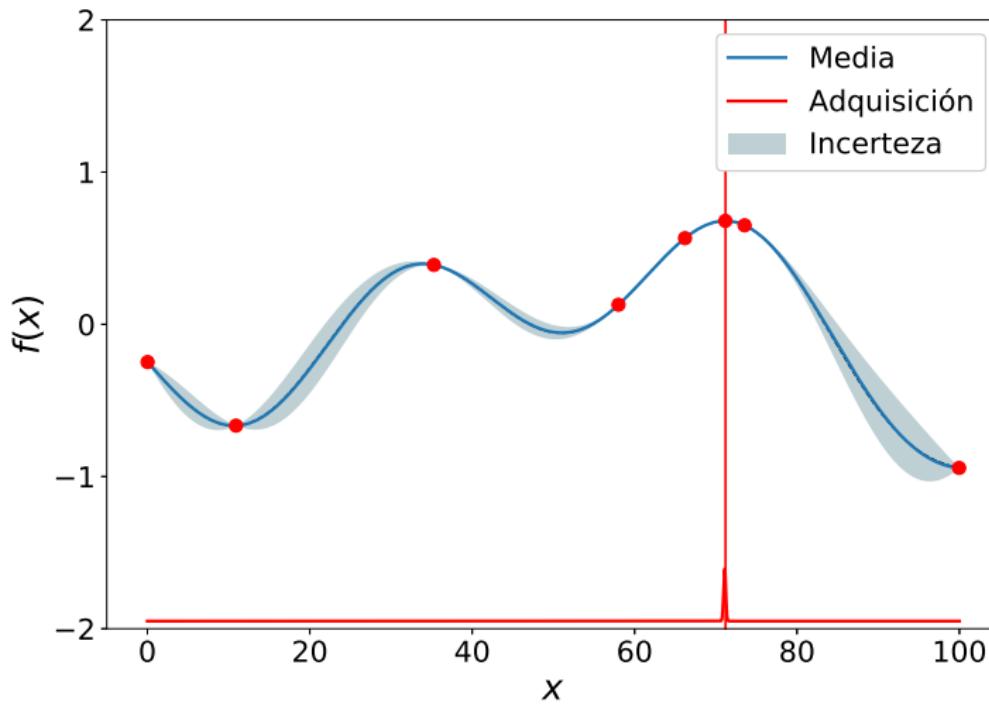
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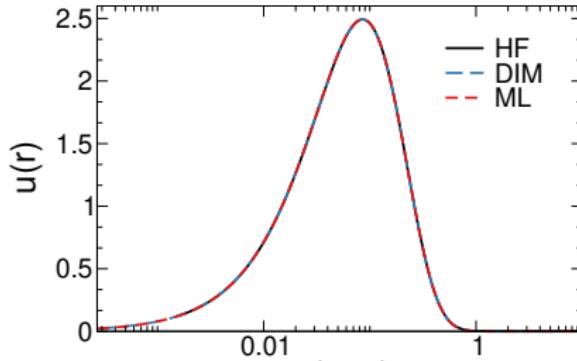
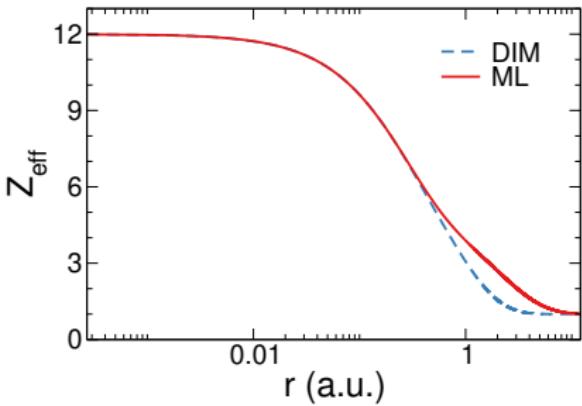


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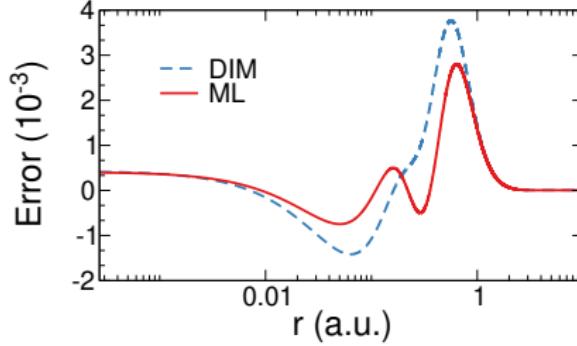


# Resultados

# DIM: Mg



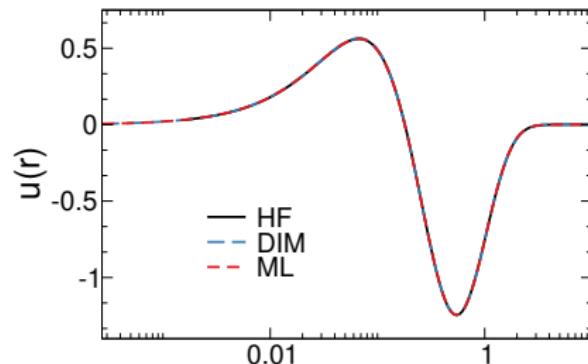
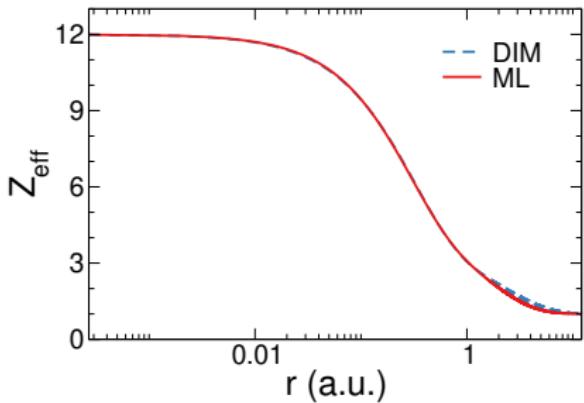
$E$  ✓  
 $\langle r \rangle$   $10^{-2} \%$   
 $\langle 1/r \rangle$



1s

# DIM: Mg

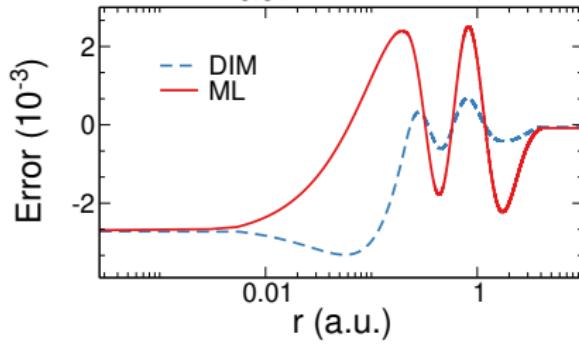
2s



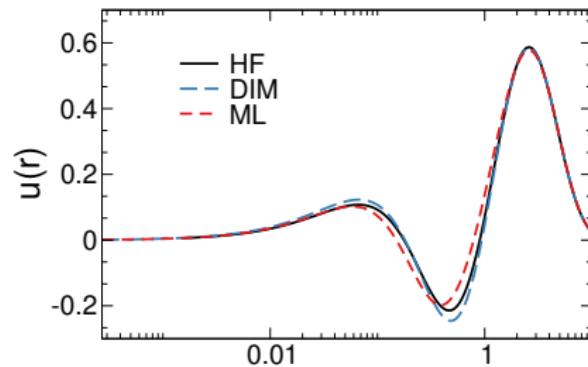
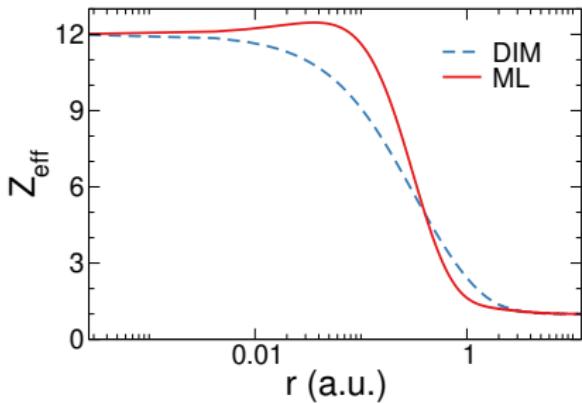
$$\begin{array}{c} E \\ \langle r \rangle \\ \langle 1/r \rangle \end{array}$$

✓

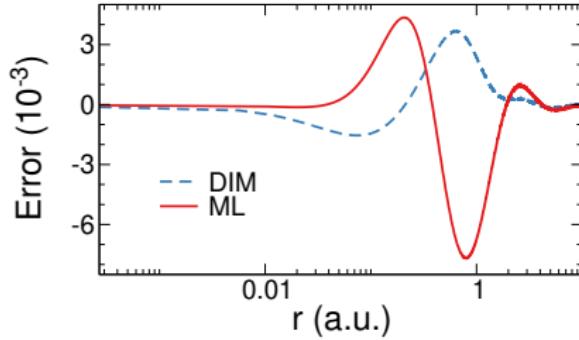
$10^{-2} \%$



# DIM: Mg

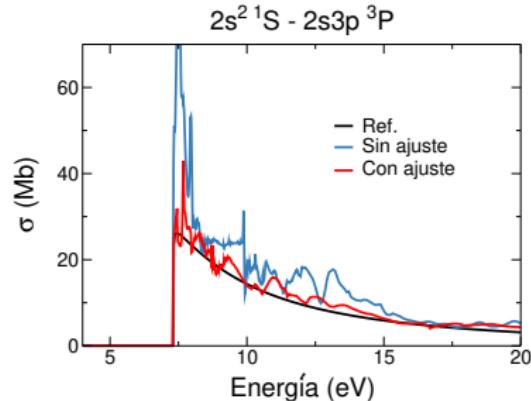
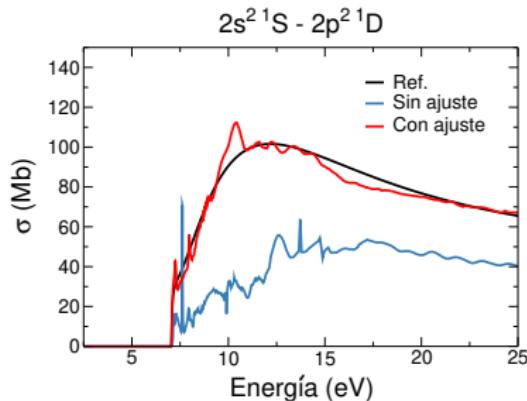
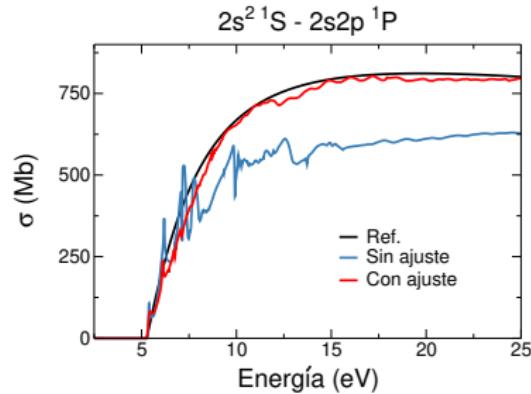
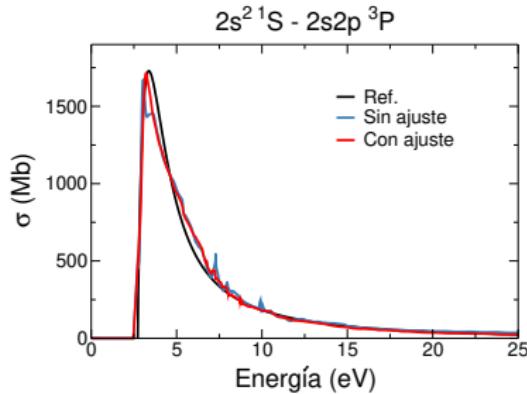


$E$  ✓  
 $\langle r \rangle$   $10^{-1} \%$   
 $\langle 1/r \rangle$



3s

# R-Matrix: Be



# Conclusiones

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  - Estructura del blanco en R-Matrix

# Conclusiones

- Estudiamos métodos y herramientas de aprendizaje automatizado
- Implementamos estos métodos en problemas de física atómica
  - Método de Inversión Depurada
  - Estructura del blanco en R-Matrix
- El éxito en estos ejemplos sugiere que estos métodos se podrían utilizar en otros problemas del área

A white humanoid robot with large, expressive eyes and a simple mouth line. It has a grey cylindrical body with a vertical row of small circular holes. The robot's right arm is extended, holding a yellow-handled screwdriver and pointing it towards its own head. Its left arm is also extended, holding a thick blue book. The background is a green surface covered with a dense pattern of light green circuit boards and connecting lines.

Gracias.