

# Implementación de Métodos de Aprendizaje Automatizado en problemas colisionales

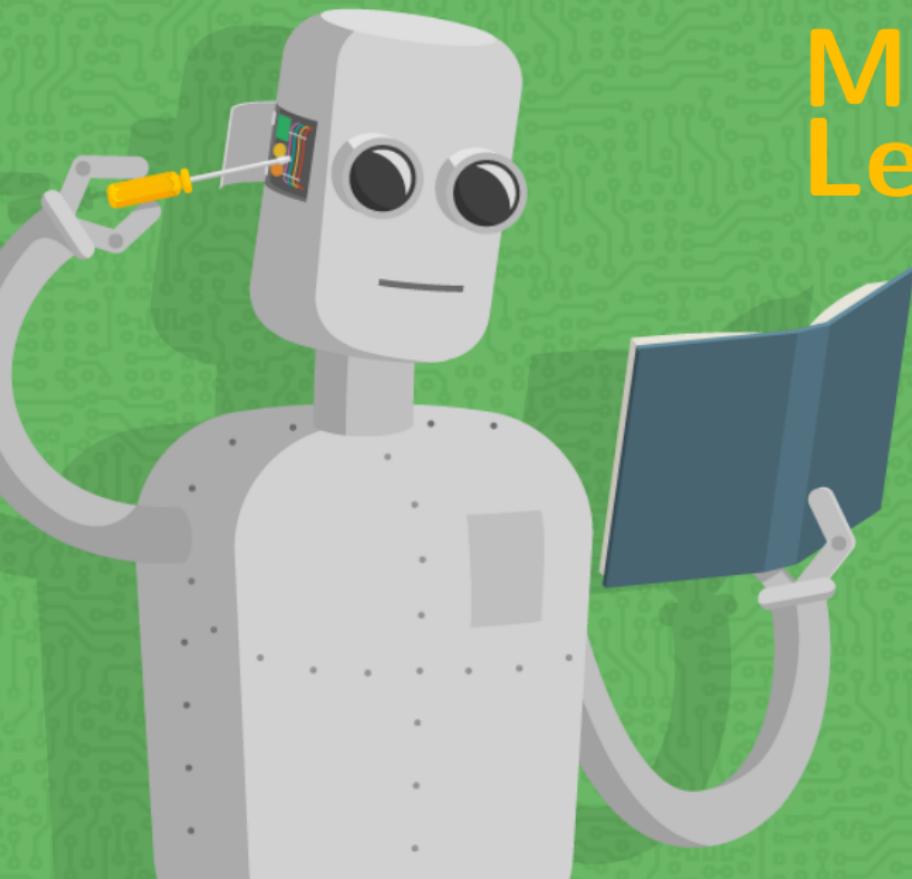
---



Alejandra Mendez,  
Juan Di Filippo,  
Sebastián López,  
Darío Mitnik,

[alemendez@iafe.uba.ar](mailto:alemendez@iafe.uba.ar)

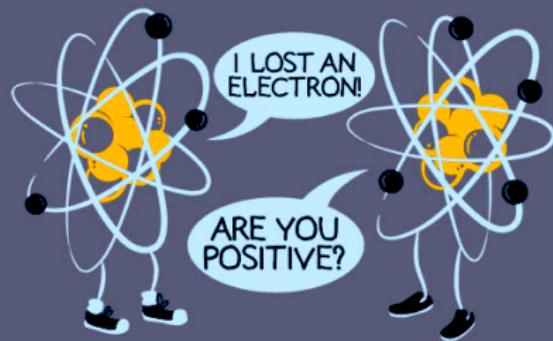
3 de Septiembre – Buenos Aires



# 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)

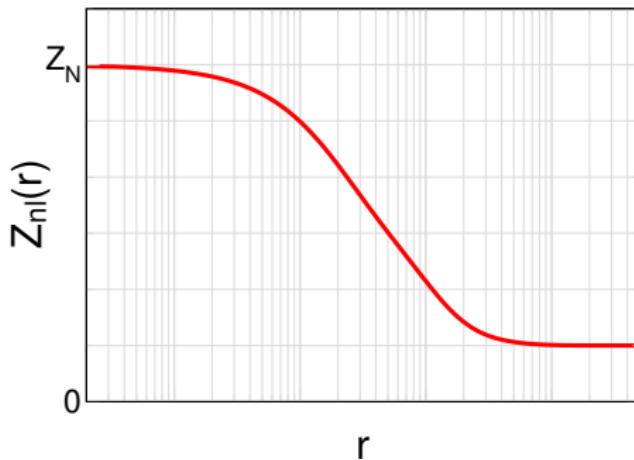
$$\left[ -\frac{1}{2} \frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + V_{nl}(r) \right] P_{nl}(r) = E_{nl} P_{nl}(r)$$

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

# Método de Inversión Depurada (DIM)

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

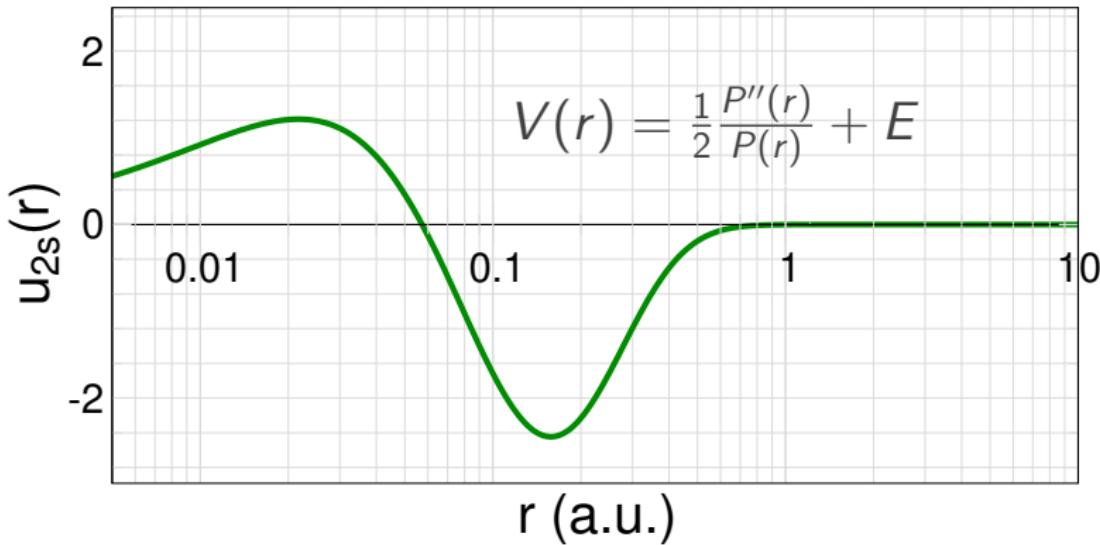
$$V_{nl}(r) = \frac{1}{2} \frac{P''_{nl}(r)}{P_{nl}(r)} - \frac{l(l+1)}{2r^2} + E_{nl}$$



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

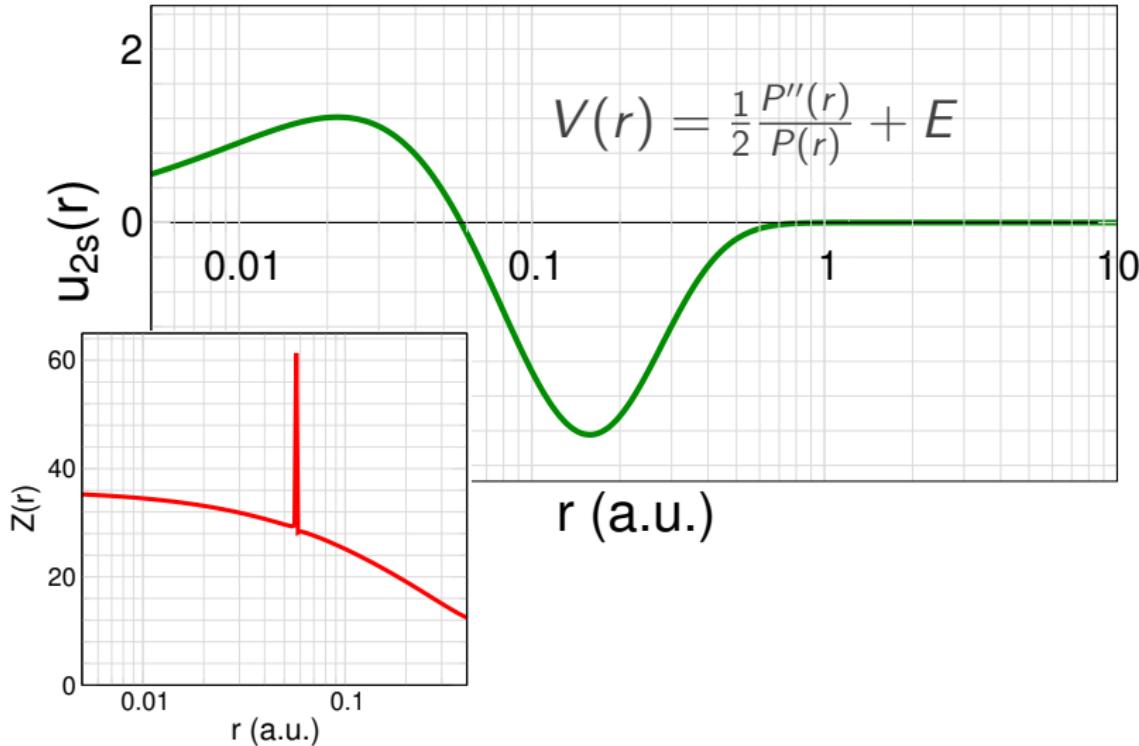
# Houston, we have a problem!

Kr



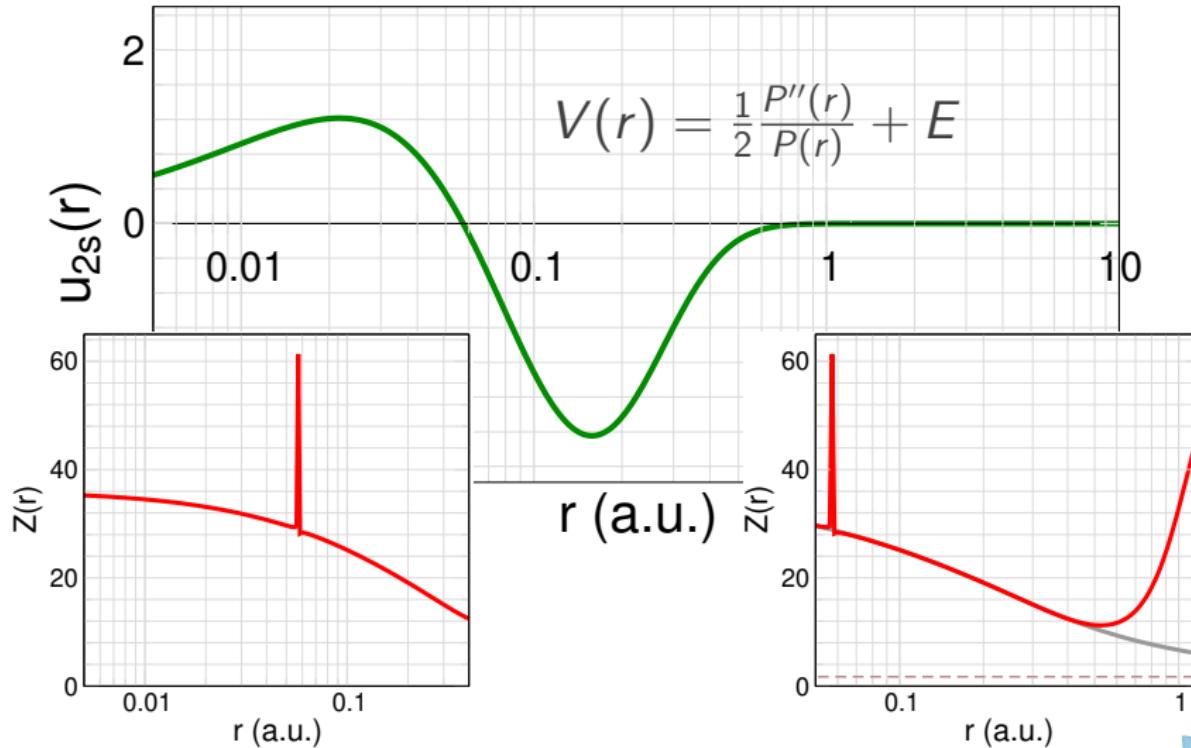
# Houston, we have a problem!

Kr



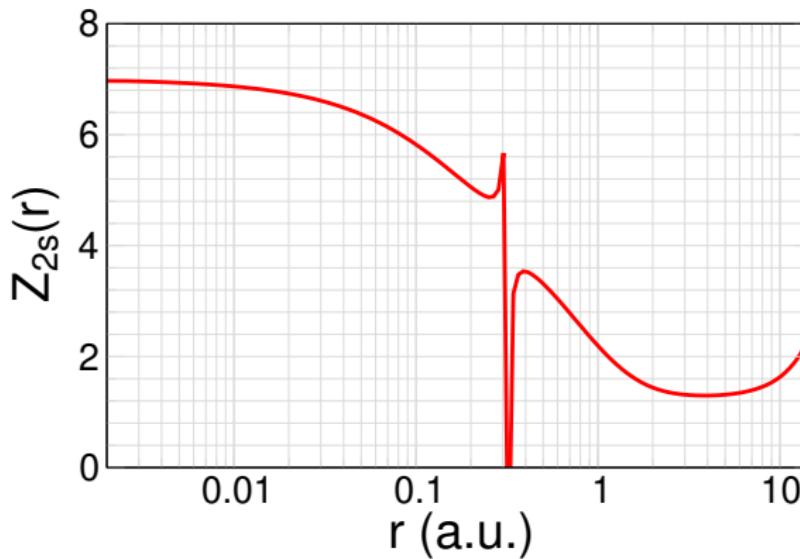
# Houston, we have a problem!

Kr



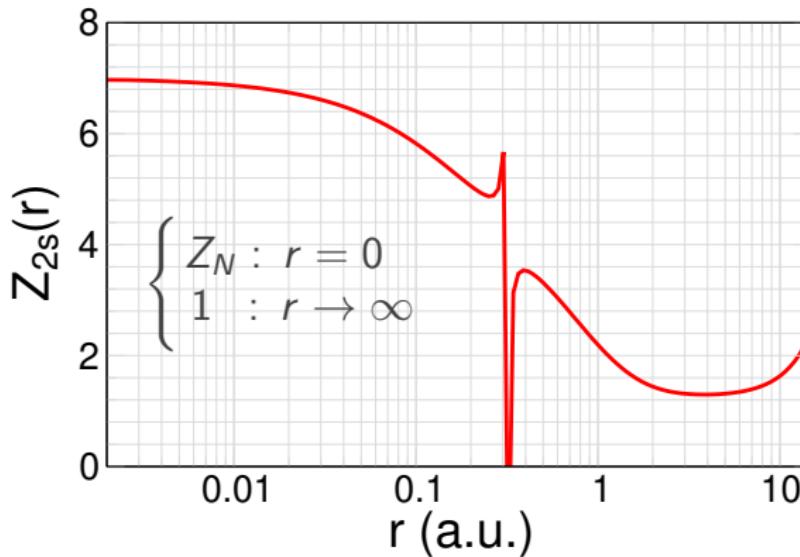
# Depuración

N



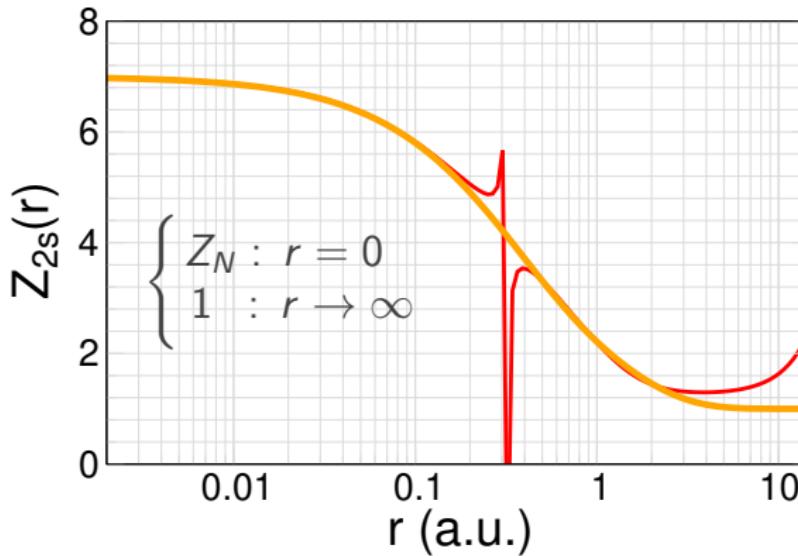
# Depuración

N



# Depuración

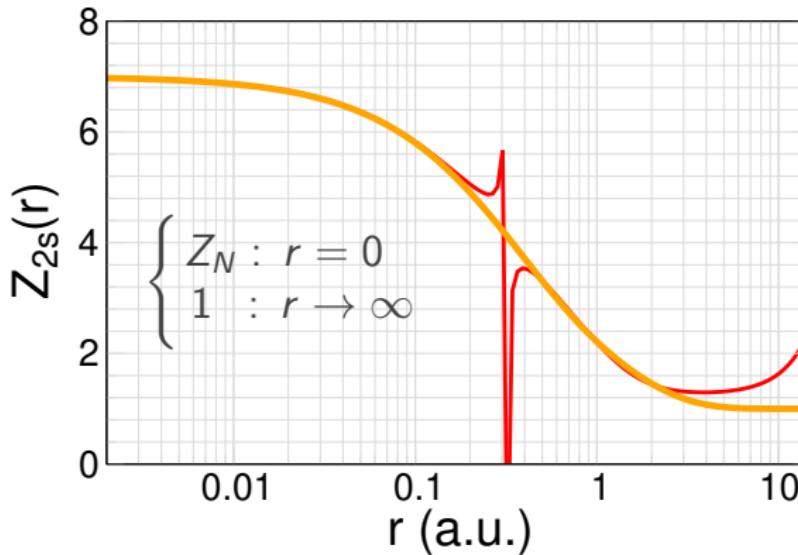
N



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

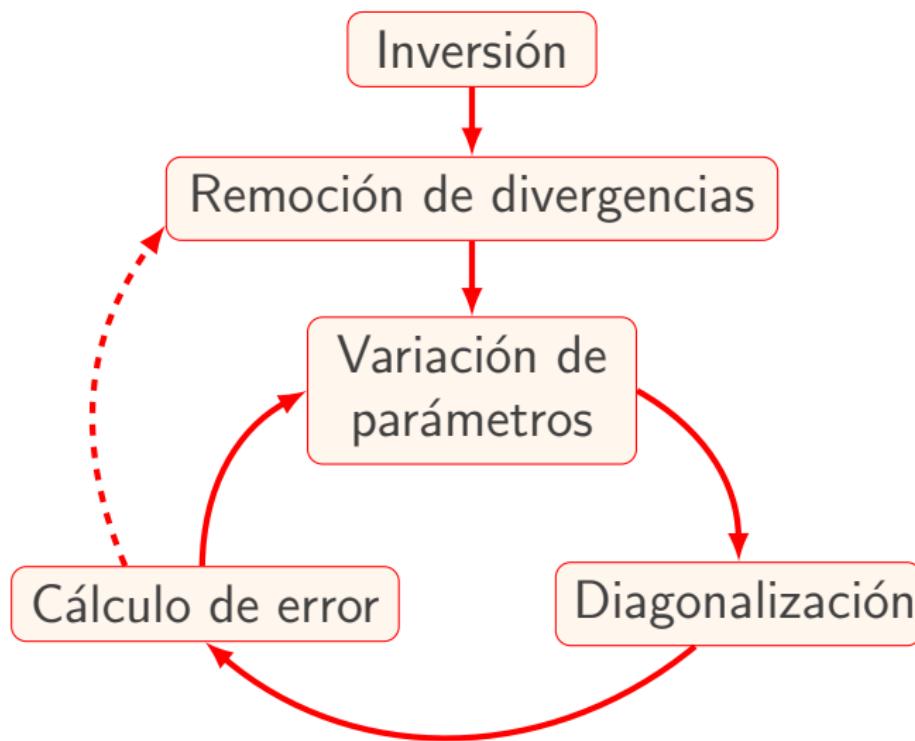
# Depuración

N



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

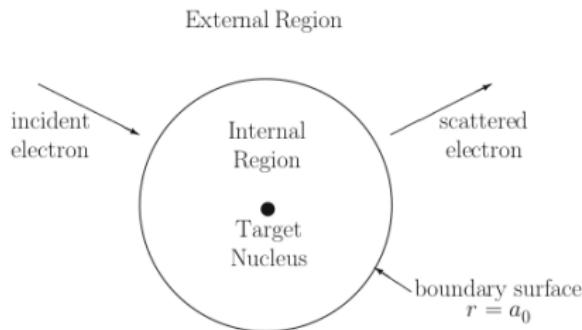
# Procedimiento



# Problema 2:

## Cálculos colisionales (R-Matrix)

# R-Matrix



Estructura del blanco

AUTOSTRUCTURE



Región interna

RMATRXI



Región externa

STGF

# Descripción del blanco

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

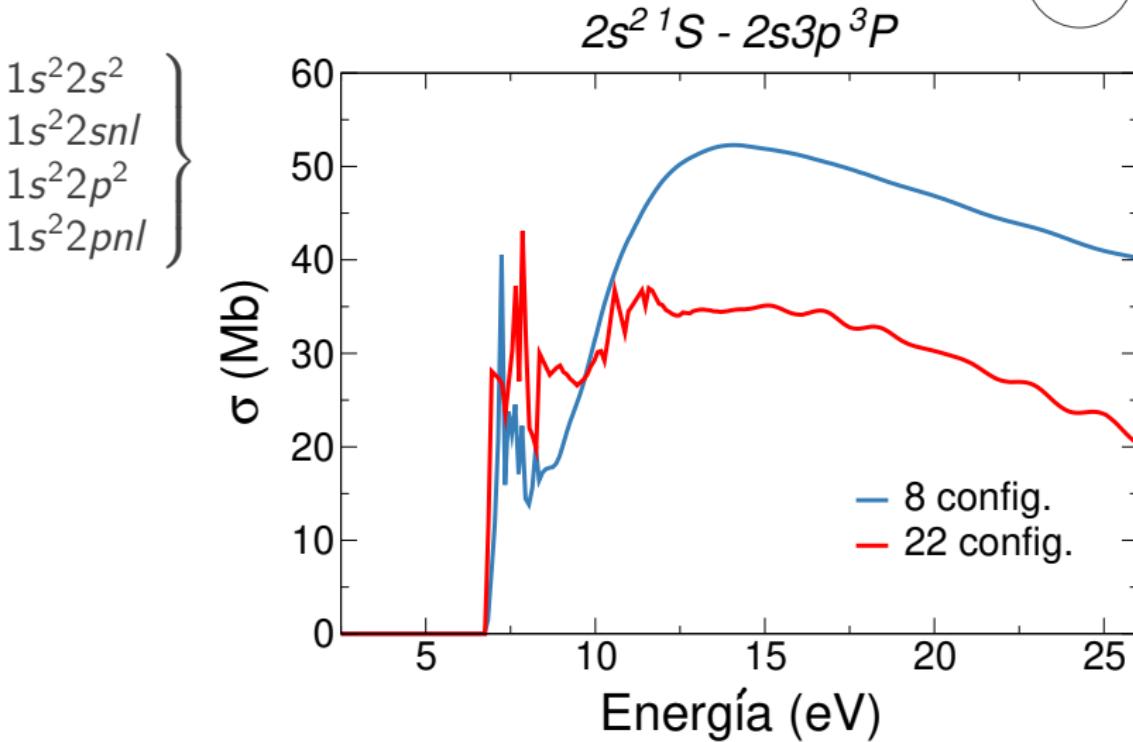
*Configuraciones*

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

*Parámetro de escaleo*

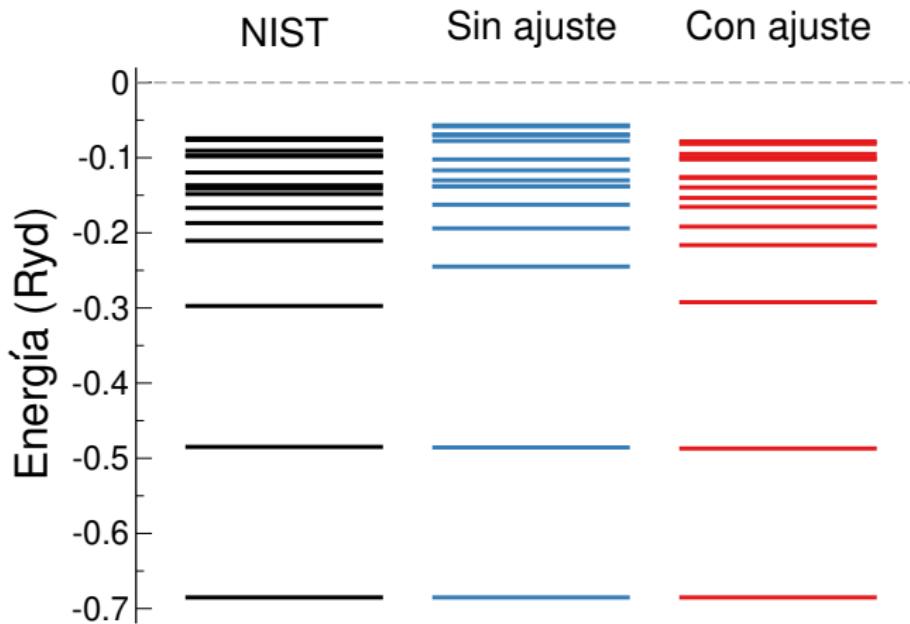
- Thomas–Fermi–Dirac–Amaldi
- Slater-Type-Orbital de Burgess

# Dependencia de CI ( $N$ )



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

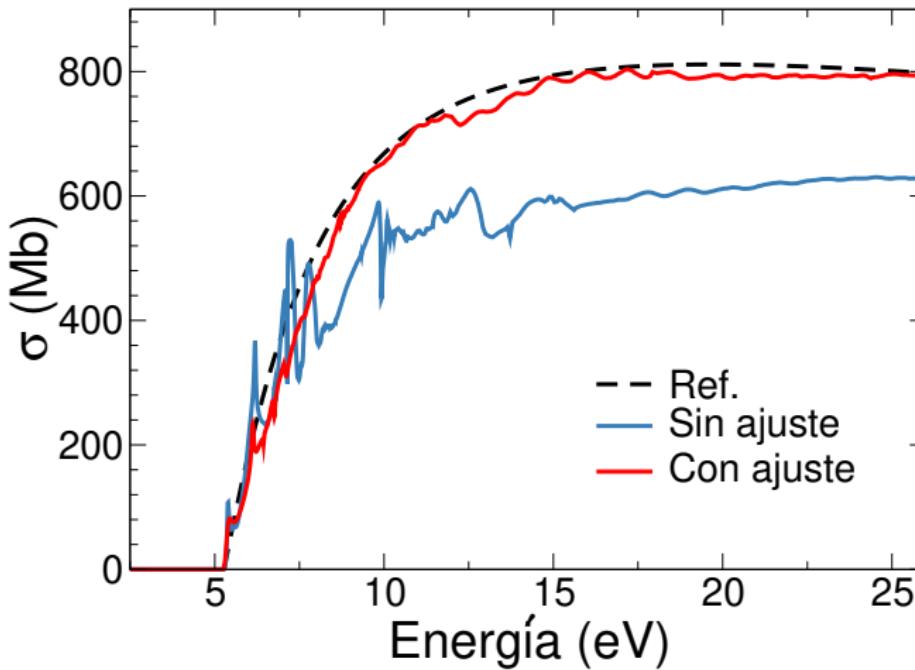
Be



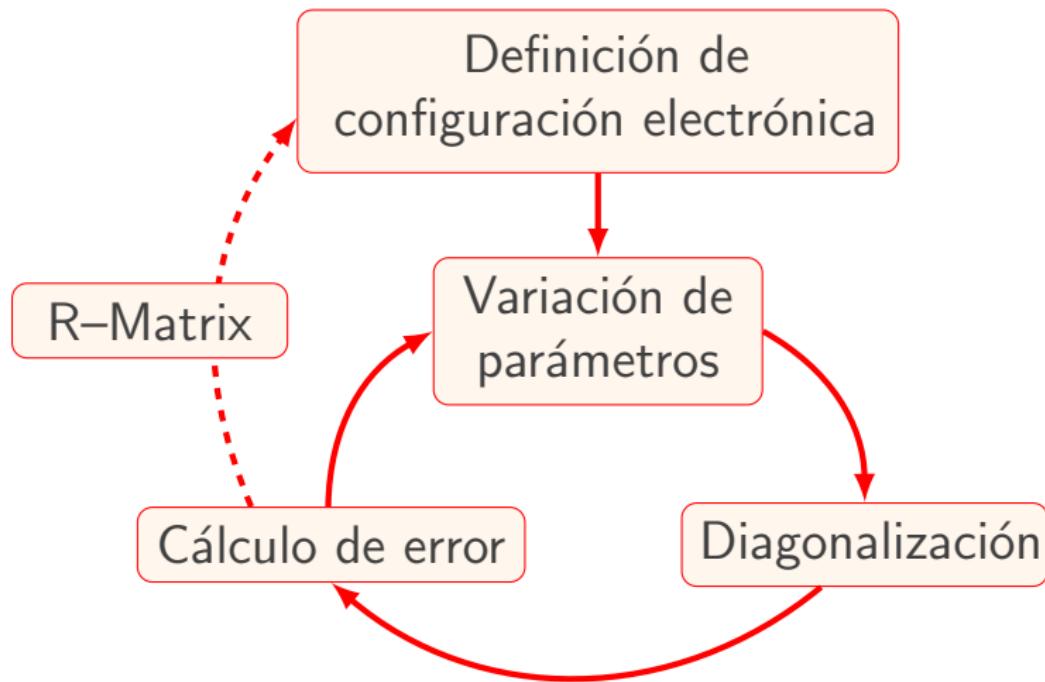
# Dependencia de orbitales ( $\lambda_{nl}$ )

Be

$2s^2 \ ^1S - 2s2p \ ^1P$



# Procedimiento



# Síntesis del problema

Función de costo:

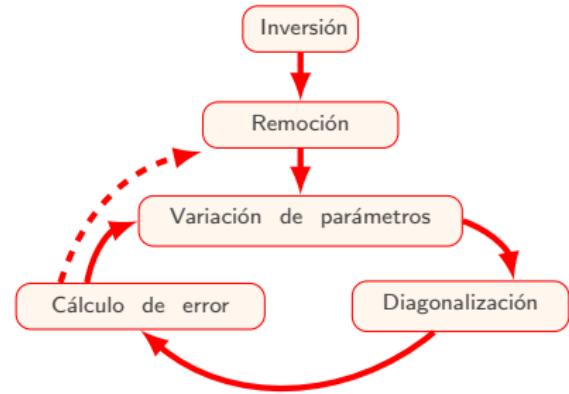
$$J = \sum_j \left| \frac{\tilde{E}_j(\xi) - E_j}{E_j} \right|$$

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

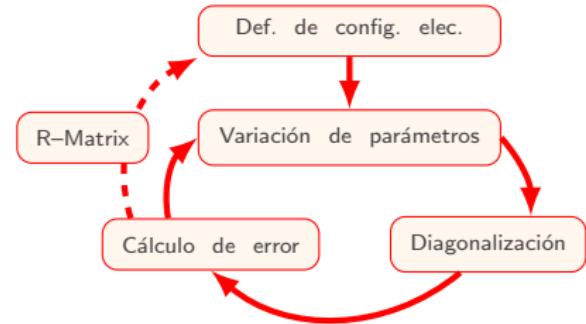
# Síntesis del problema

Función de costo:

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

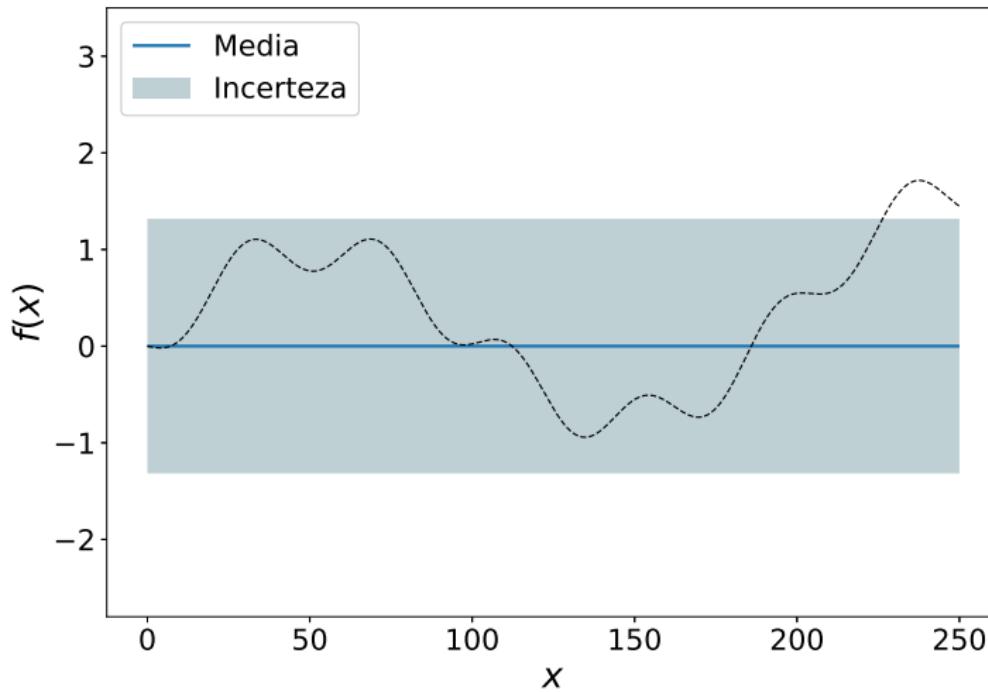


- DIM:  $\xi = \{\alpha, \beta\}$
- R-Matrix:  $\xi = \{N, \lambda\}$

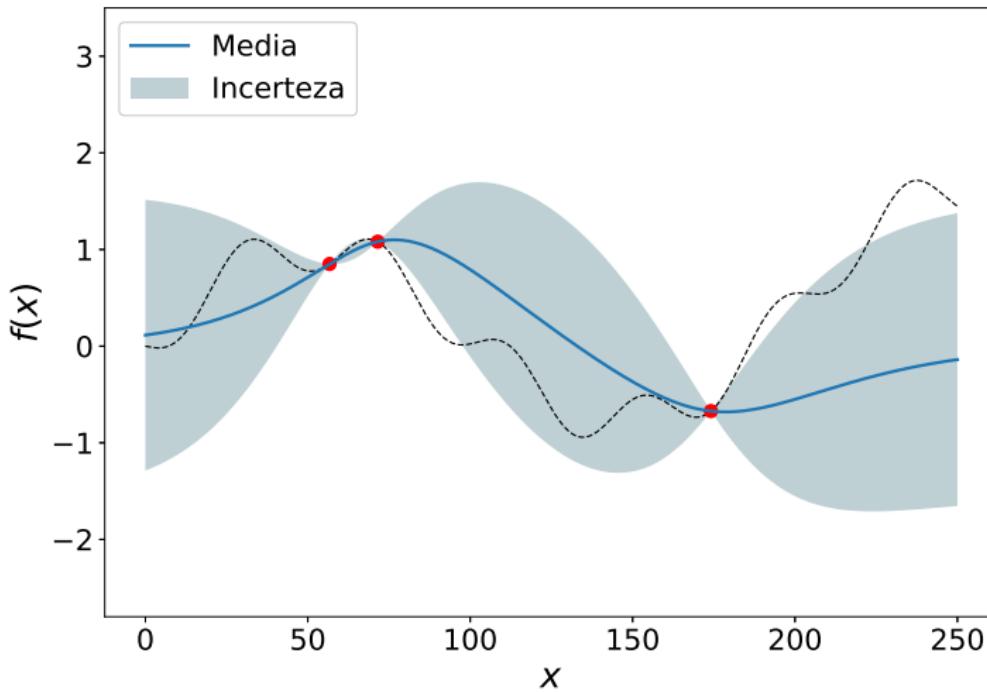


# Optimización Bayesiana con Procesos Gaussianos

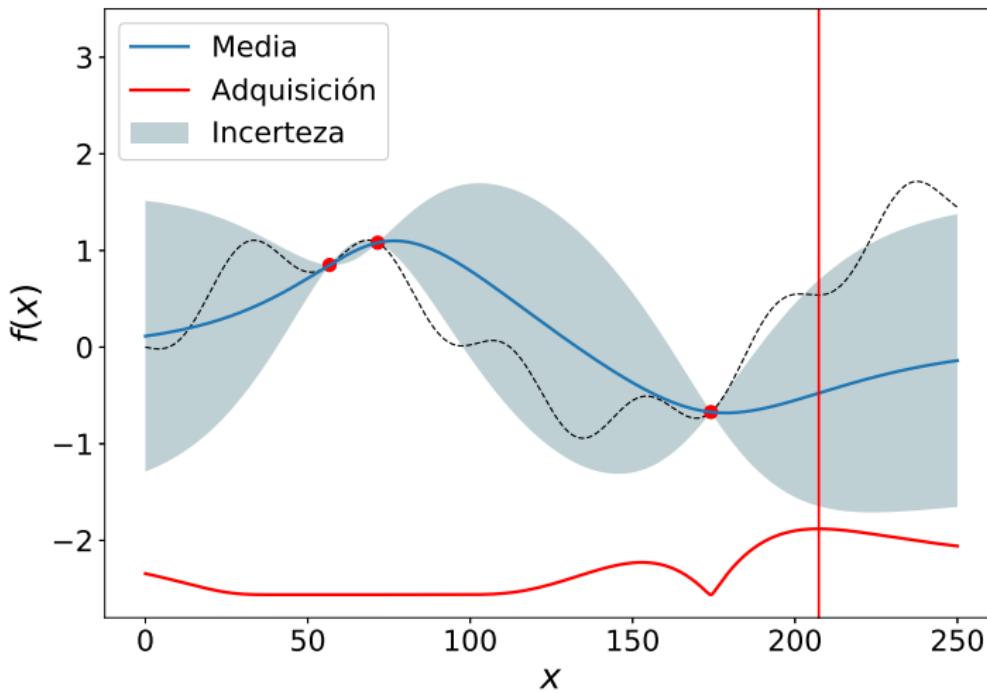
# Procesos Gaussianos



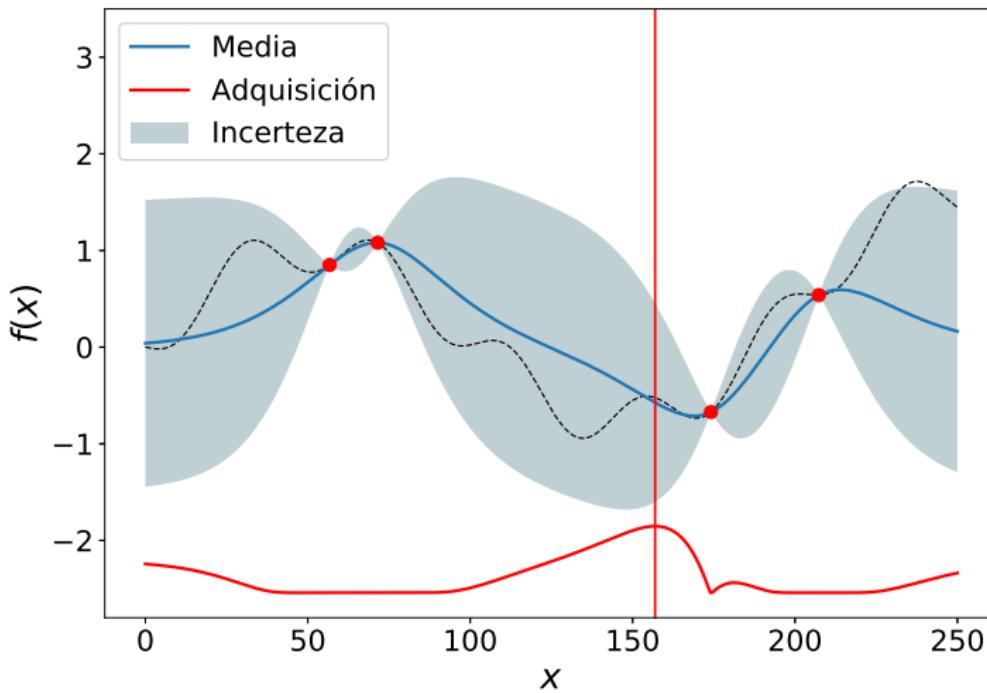
# Procesos Gaussianos



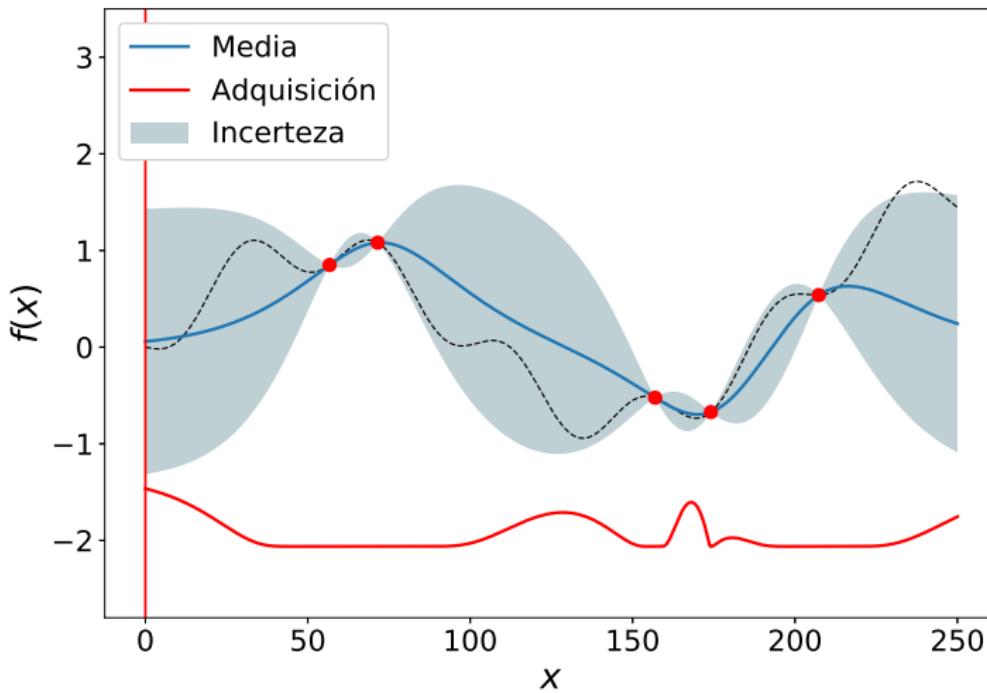
# Procesos Gaussianos



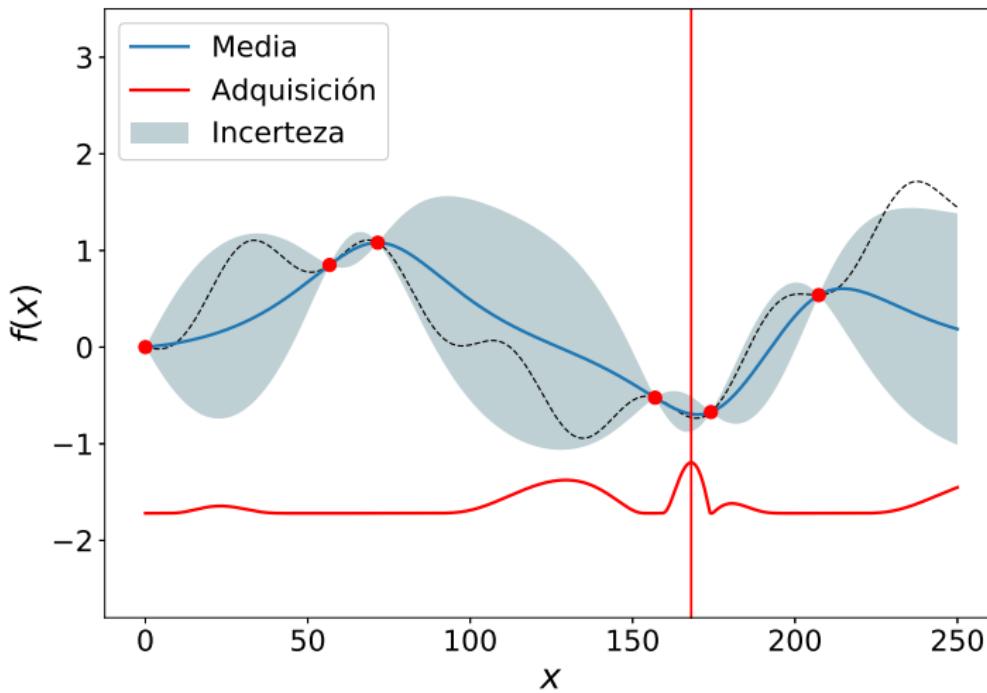
# Procesos Gaussianos



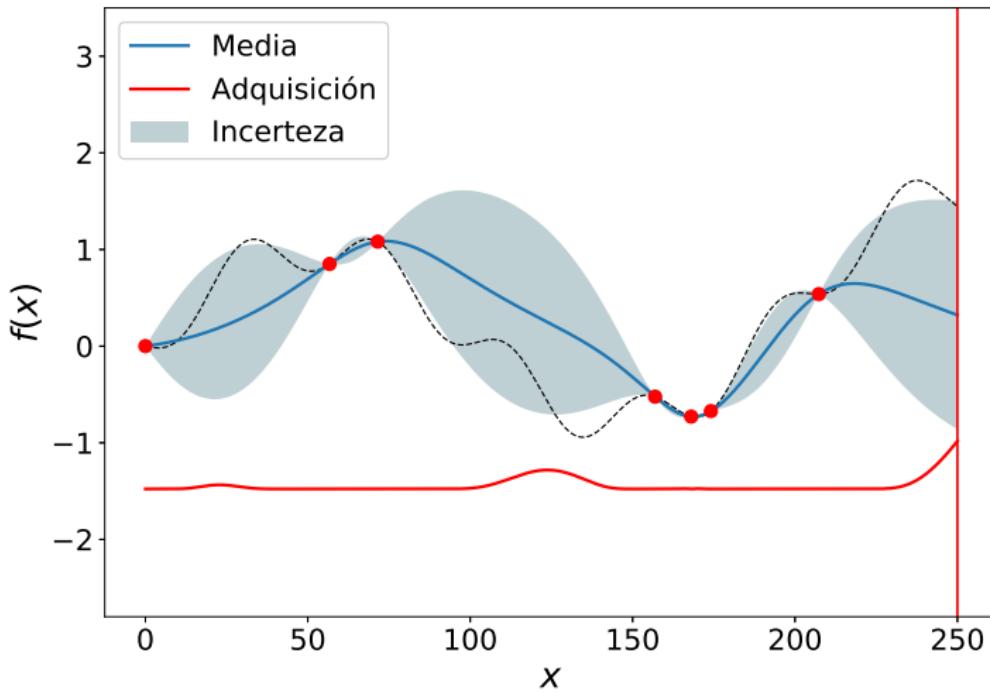
# Procesos Gaussianos



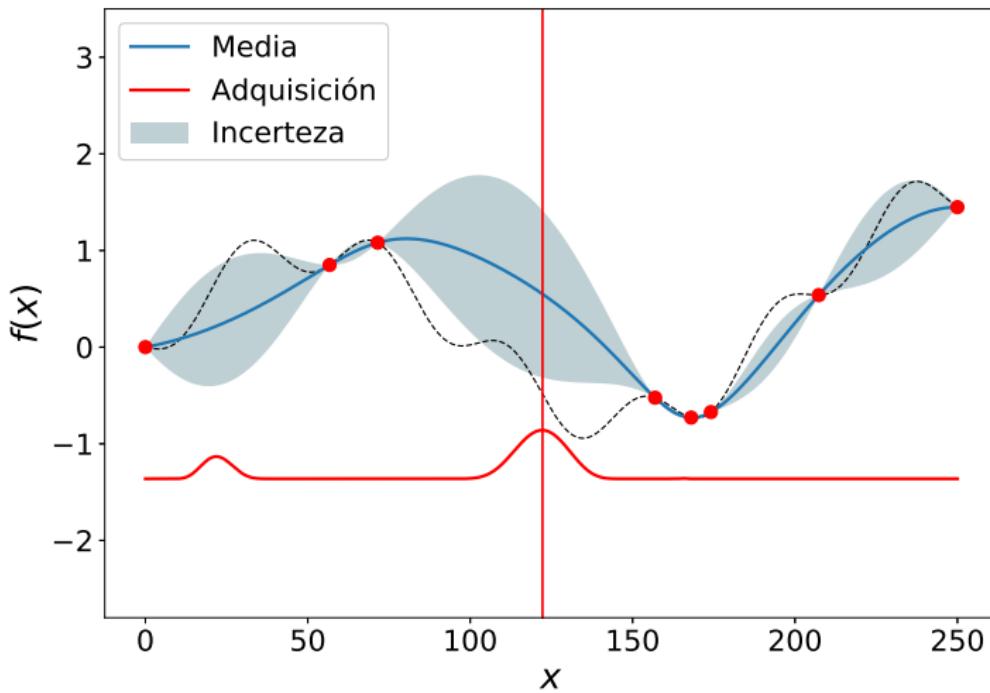
# Procesos Gaussianos



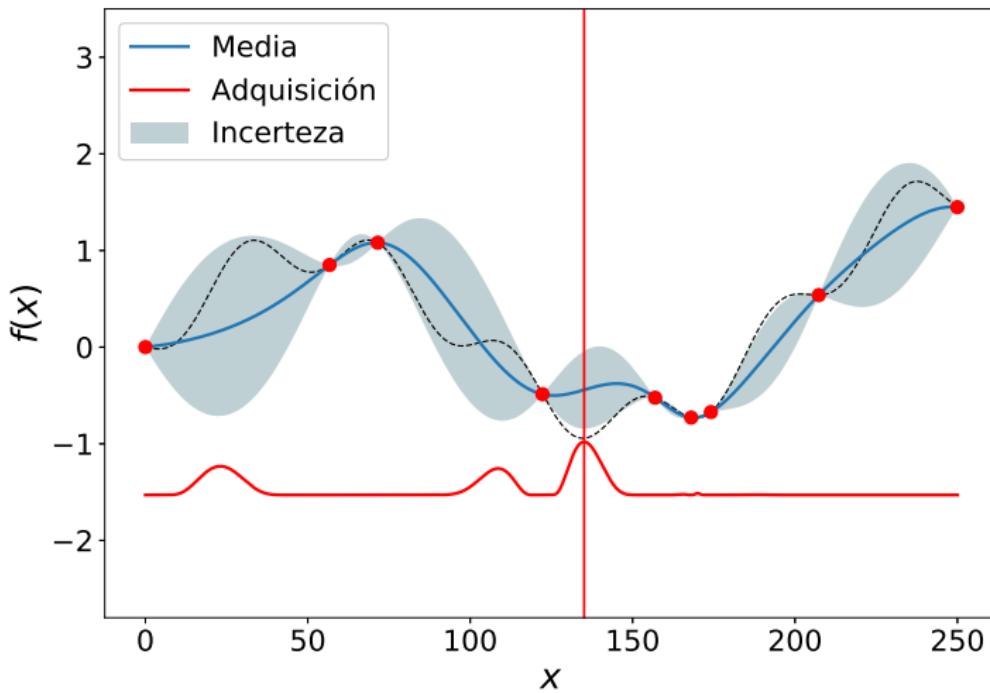
# Procesos Gaussianos



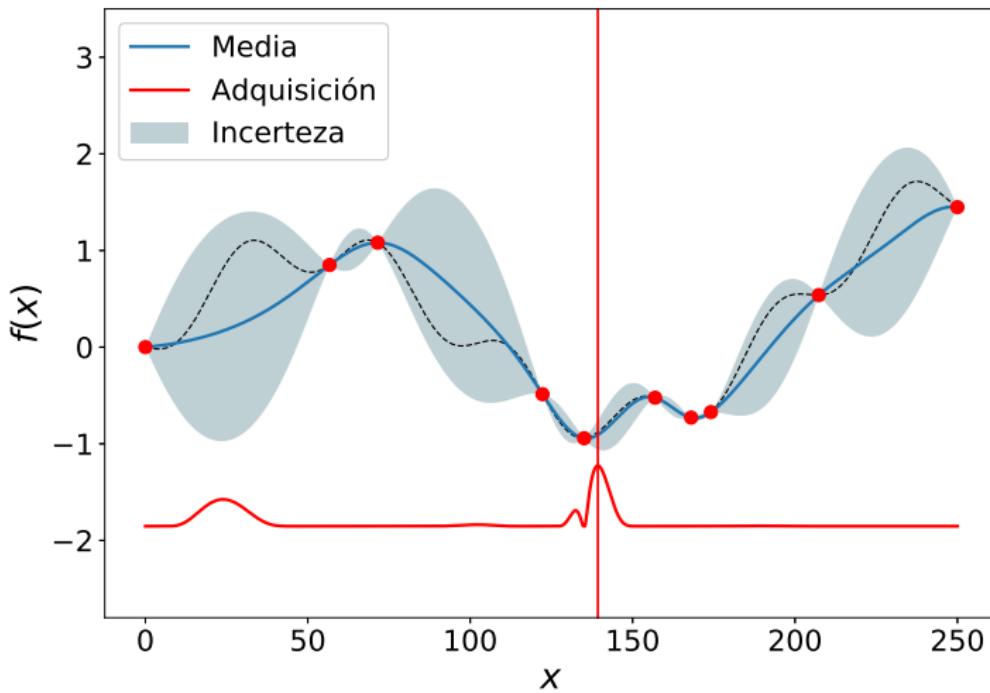
# Procesos Gaussianos



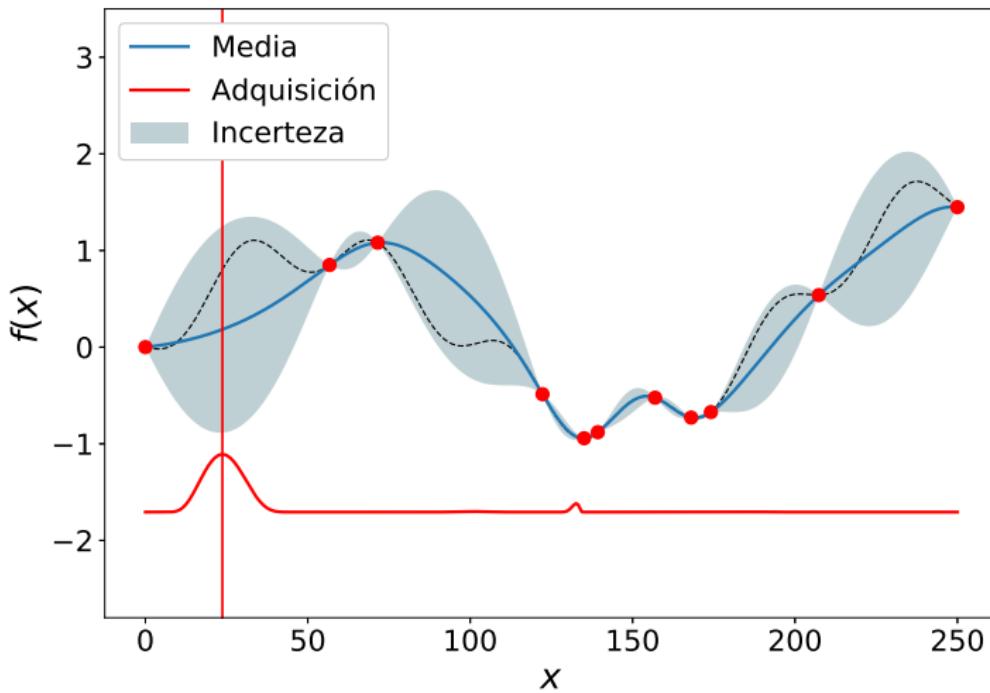
# Procesos Gaussianos



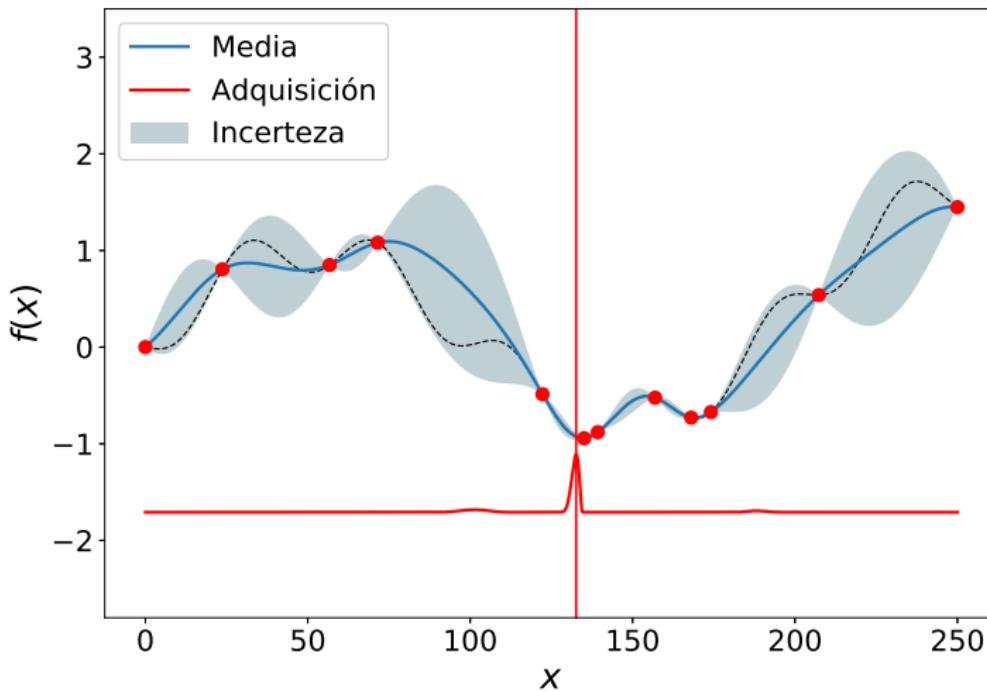
# Procesos Gaussianos



# Procesos Gaussianos

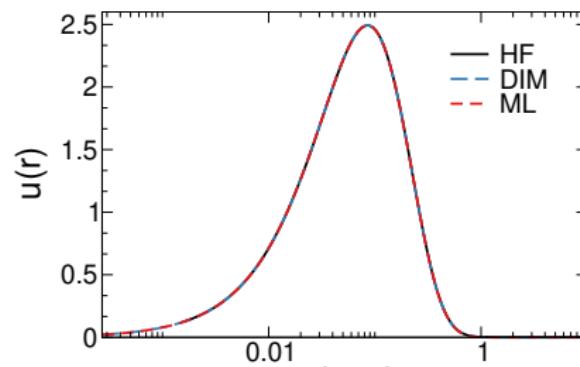
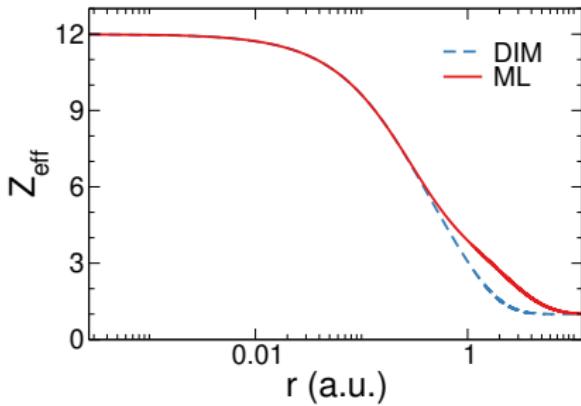


# Procesos Gaussianos

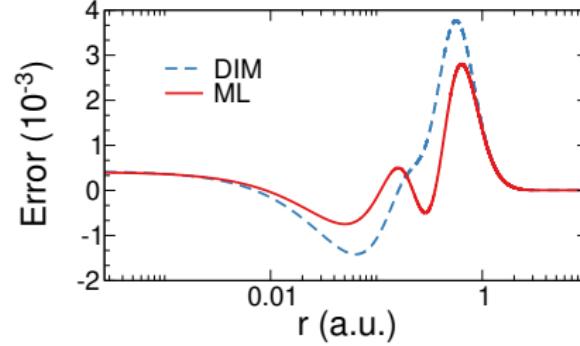


# Resultados

# DIM: Mg



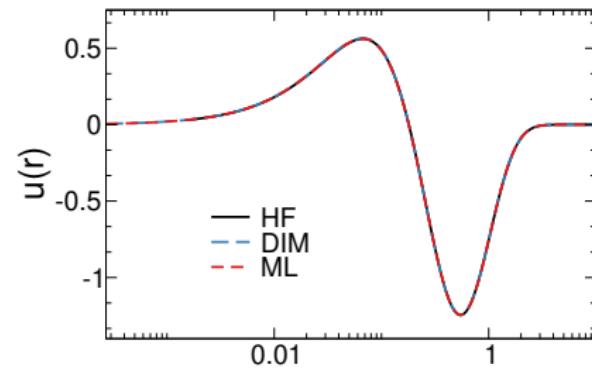
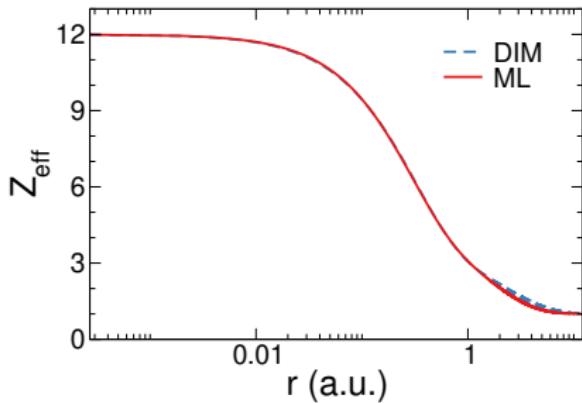
$E$  ✓  
 $\langle r \rangle$   $10^{-2} \%$   
 $\langle 1/r \rangle$



1s

# DIM: Mg

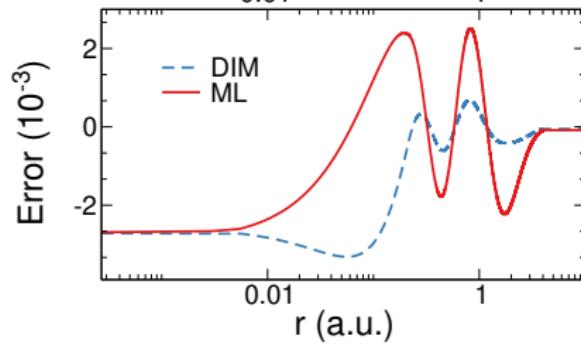
2s



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

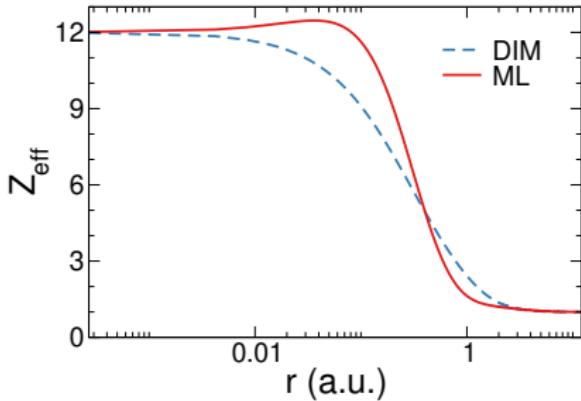
✓

$10^{-2} \%$

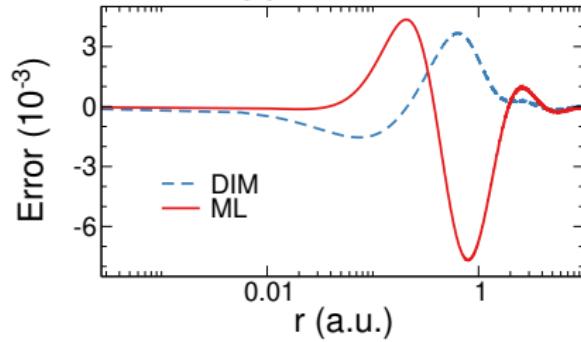
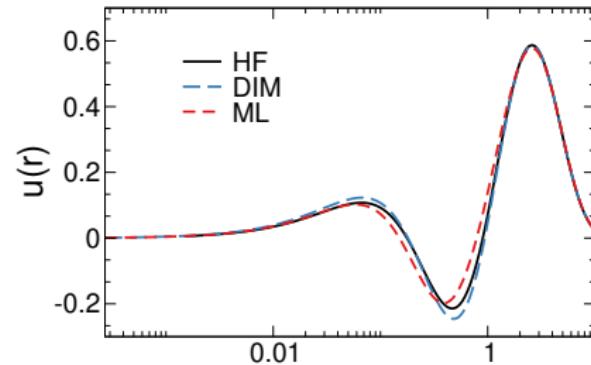




# DIM: Mg

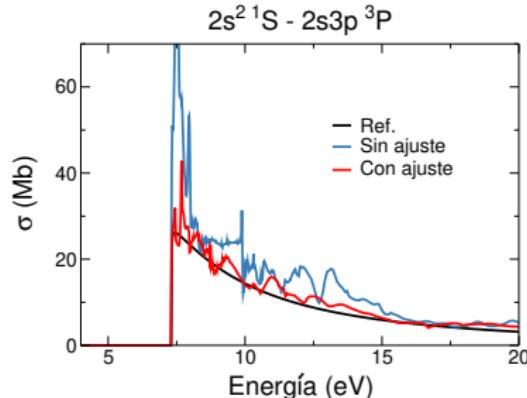
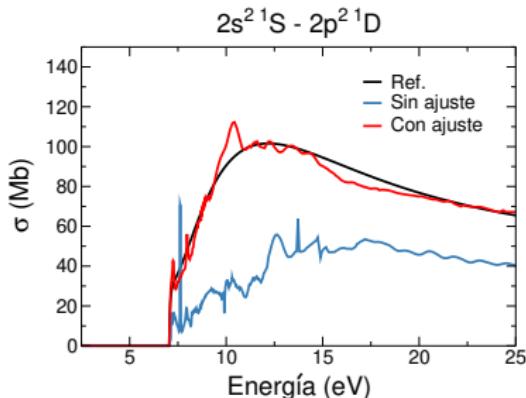
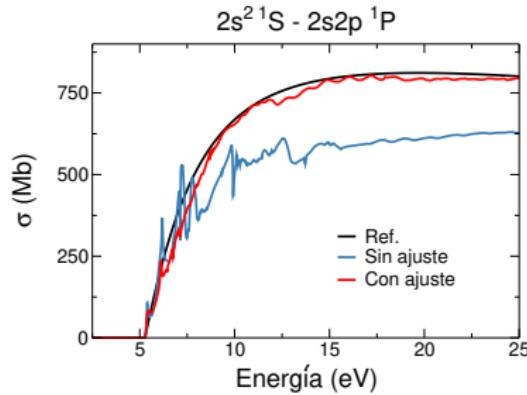
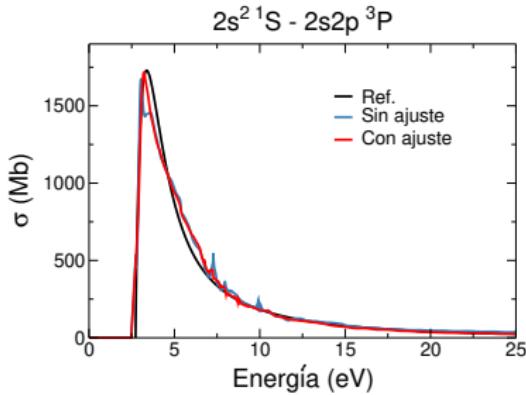


$$\begin{matrix} E \\ \langle r \rangle \\ \langle 1/r \rangle \end{matrix} \quad \checkmark \quad 10^{-1}\%$$



3s

# R-Matrix: Be



# Conclusiones

- Estudiamos métodos y herramientas de aprendizaje automatizado

# Conclusiones

- Estudiamos métodos y herramientas de aprendizaje automatizado
- Implementamos estos métodos en problemas de física atómica

# Conclusiones

- Estudiamos métodos y herramientas de aprendizaje automatizado
- Implementamos estos métodos en problemas de física atómica
  - Método de Inversión Depurada

# 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

# 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