

# Implementación de Métodos de Aprendizaje Automatizado en problemas colisionales

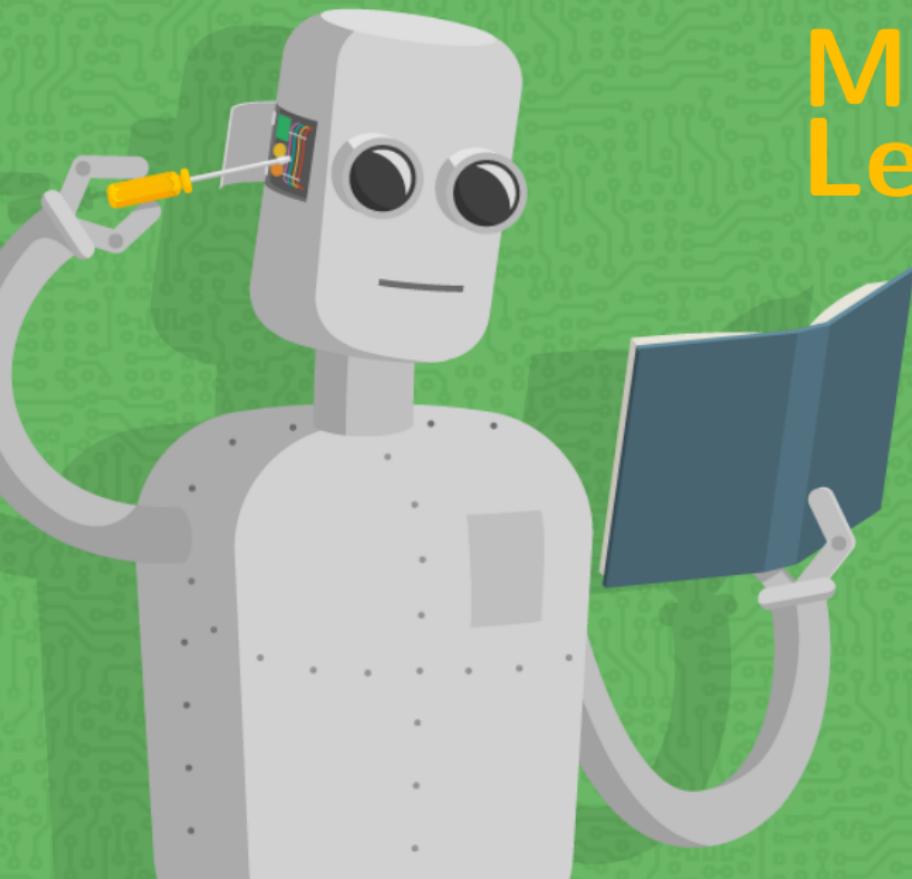
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2 de Septiembre – Buenos Aires



# Machine Learning

# Problema 1: Potenciales DIM

# Método de Inversión Depurada (DIM)

$$T_{fi} = |\langle \psi_f | V | \psi_i \rangle|^2$$

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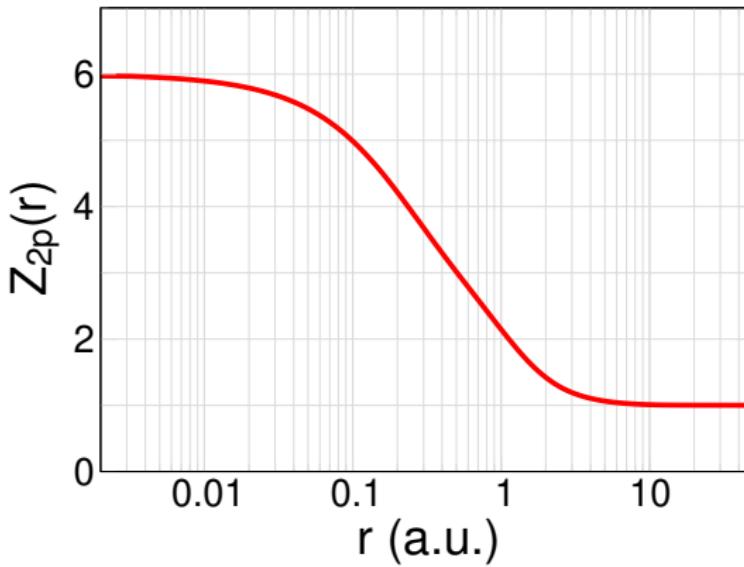
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$$V_{nl}(r) = \frac{1}{2} \frac{P''_{nl}(r)}{P_{nl}(r)} - \frac{l(l+1)}{2r^2} + E_{nl}$$

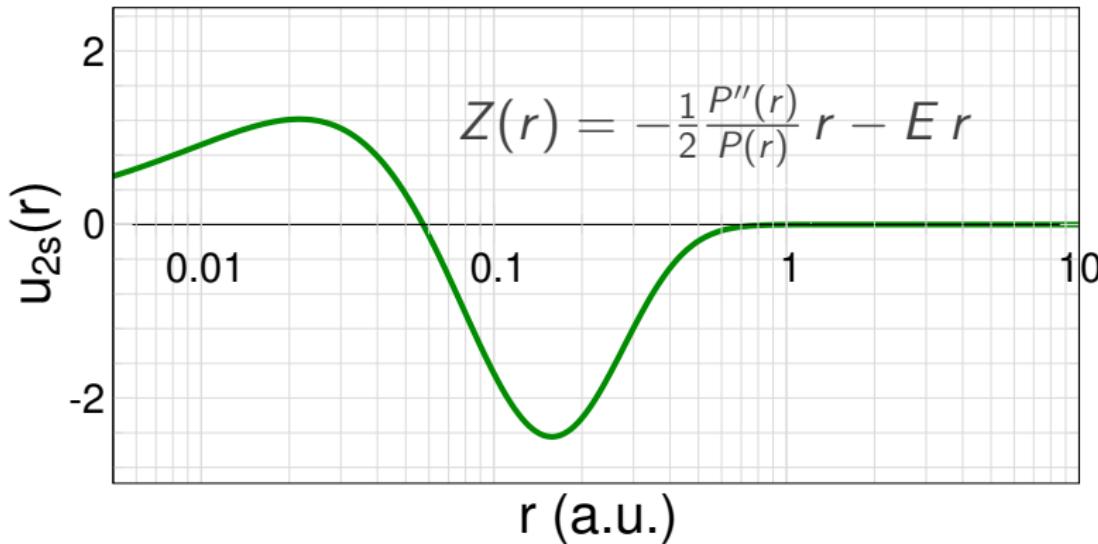
# Método de Inversión Depurada (DIM)

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



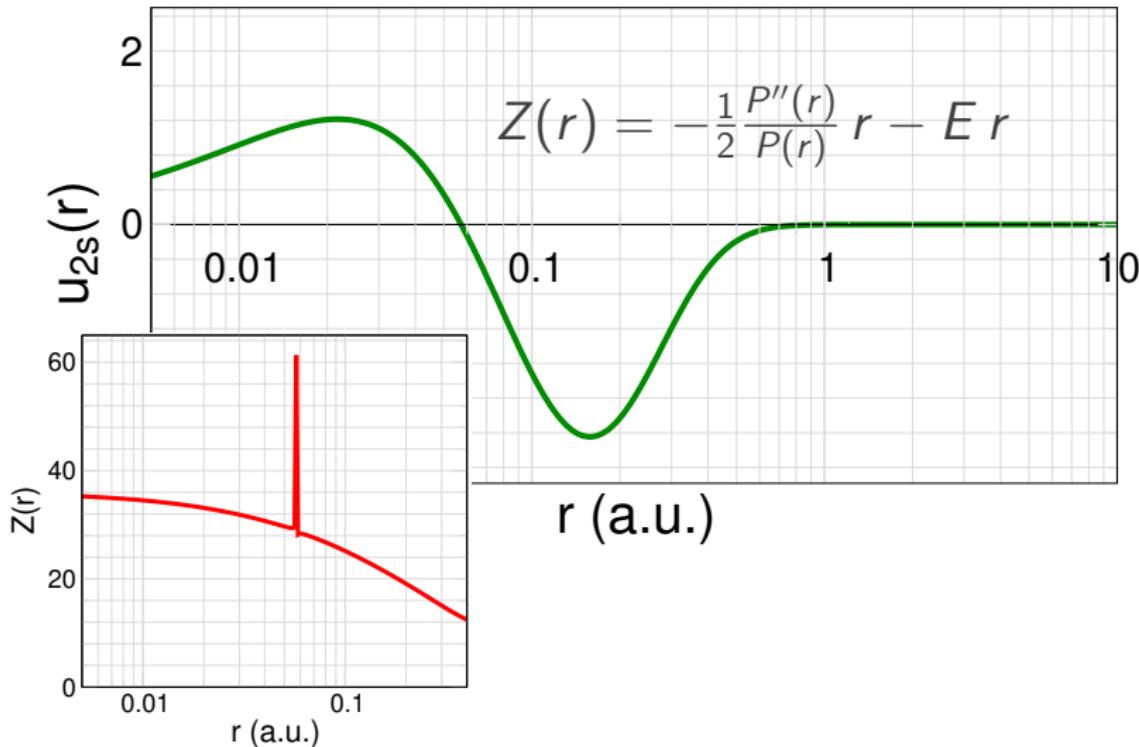
# Houston, we have a problem!

Kr



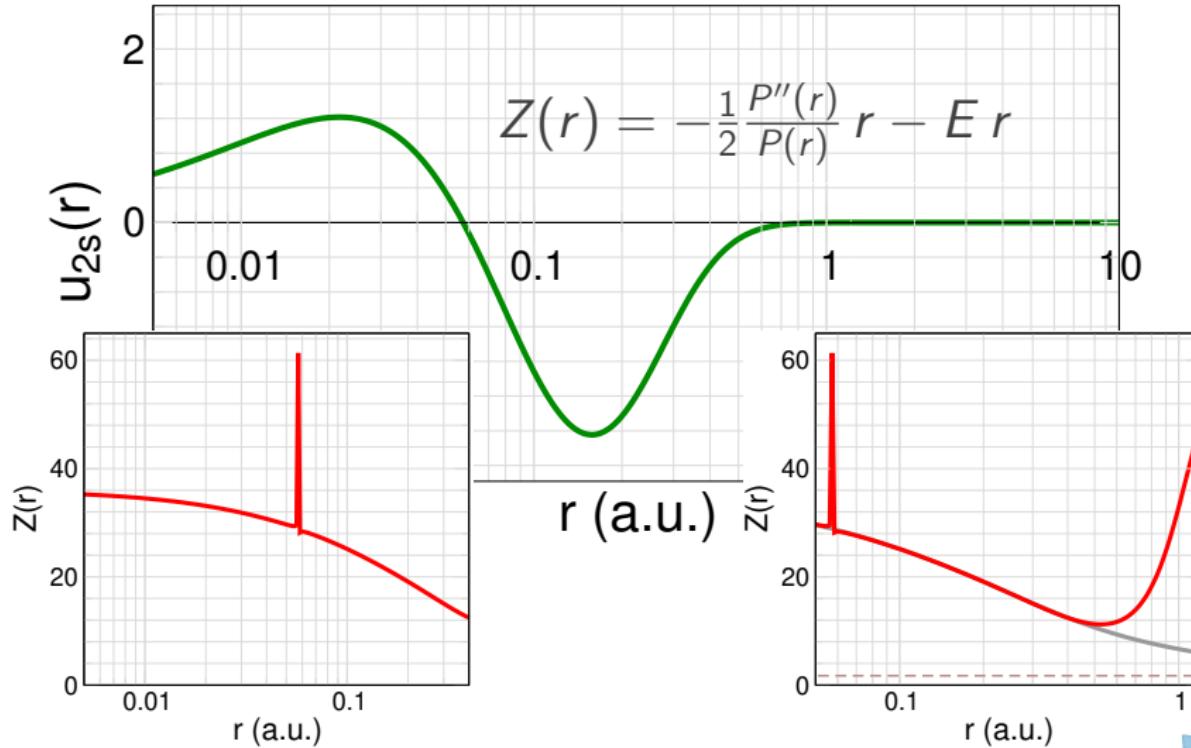
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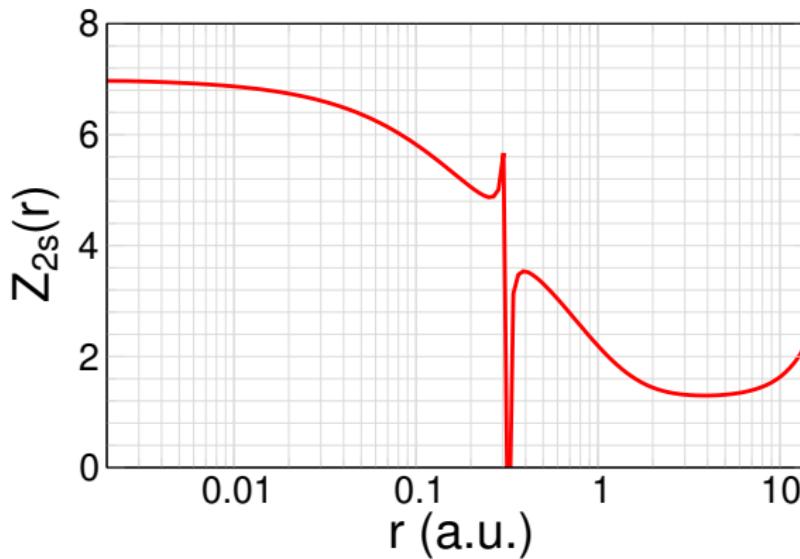
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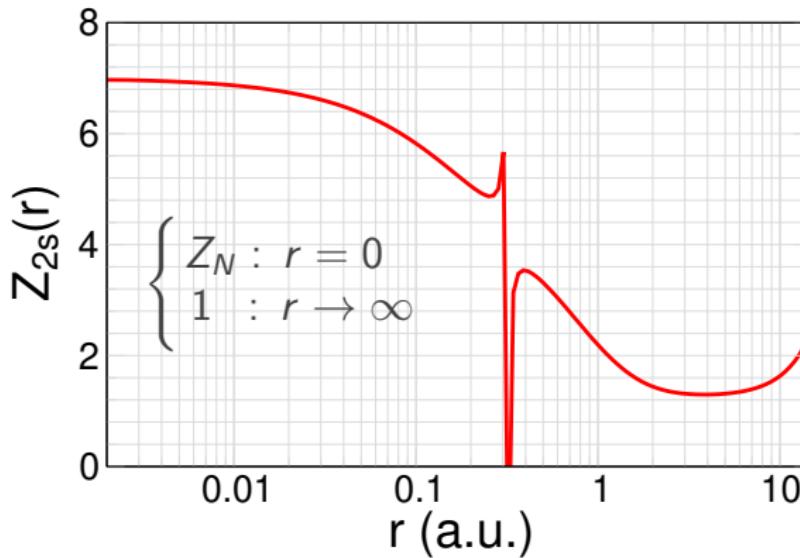
# Depuración

N



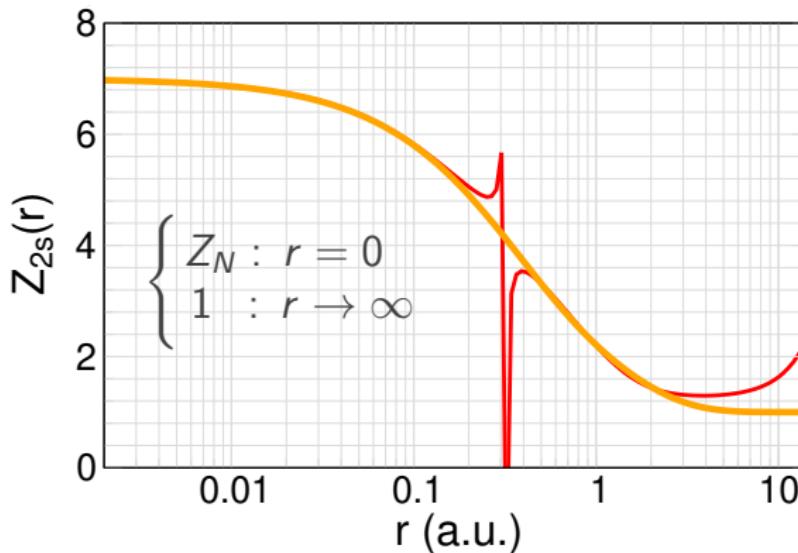
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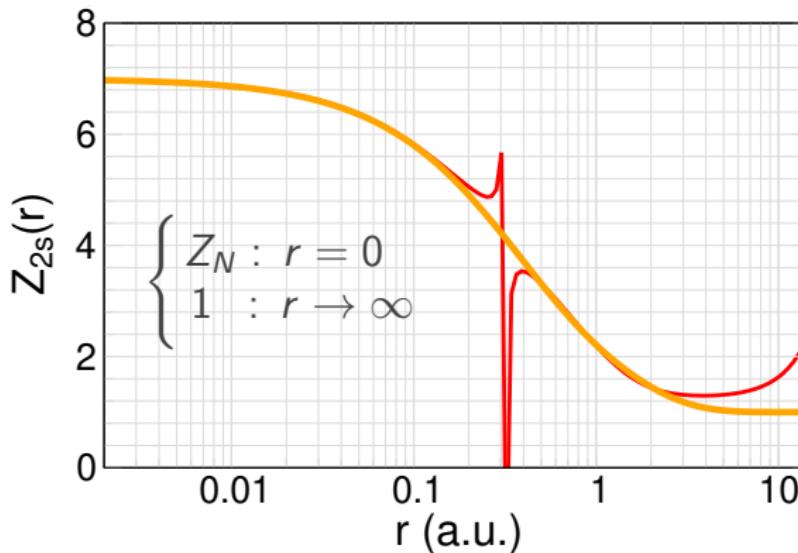
N



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

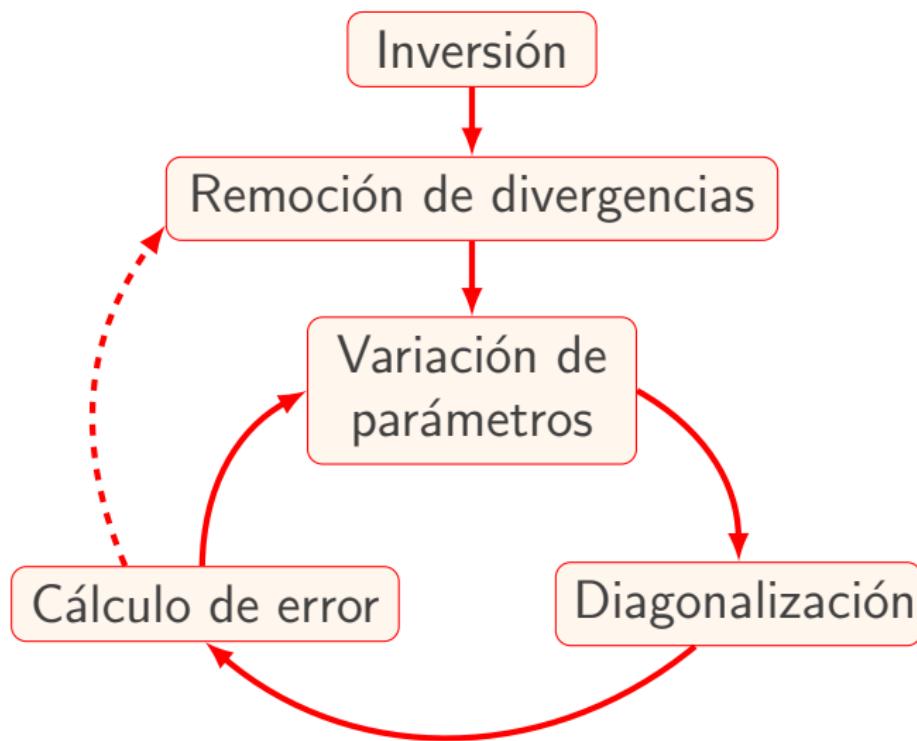
# Depuración

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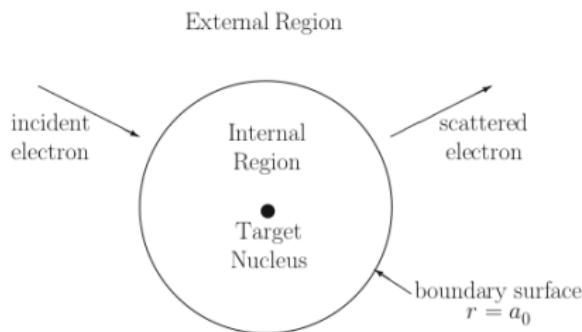
$$Z(r) = 1 + \sum_j \alpha_j e^{-\beta_j r}$$

# Procedimiento



# Problema 2: R-Matrix

# R-Matrix



Estructura del blanco

AUTOSTRUCTURE



Región interna

RMATRXI



Región externa

STGF

# Descripción del blanco

$$\Phi_i(\mathbf{r}) = \sum_j c_{ji} P_j(r) Y_j(\hat{\mathbf{r}})$$

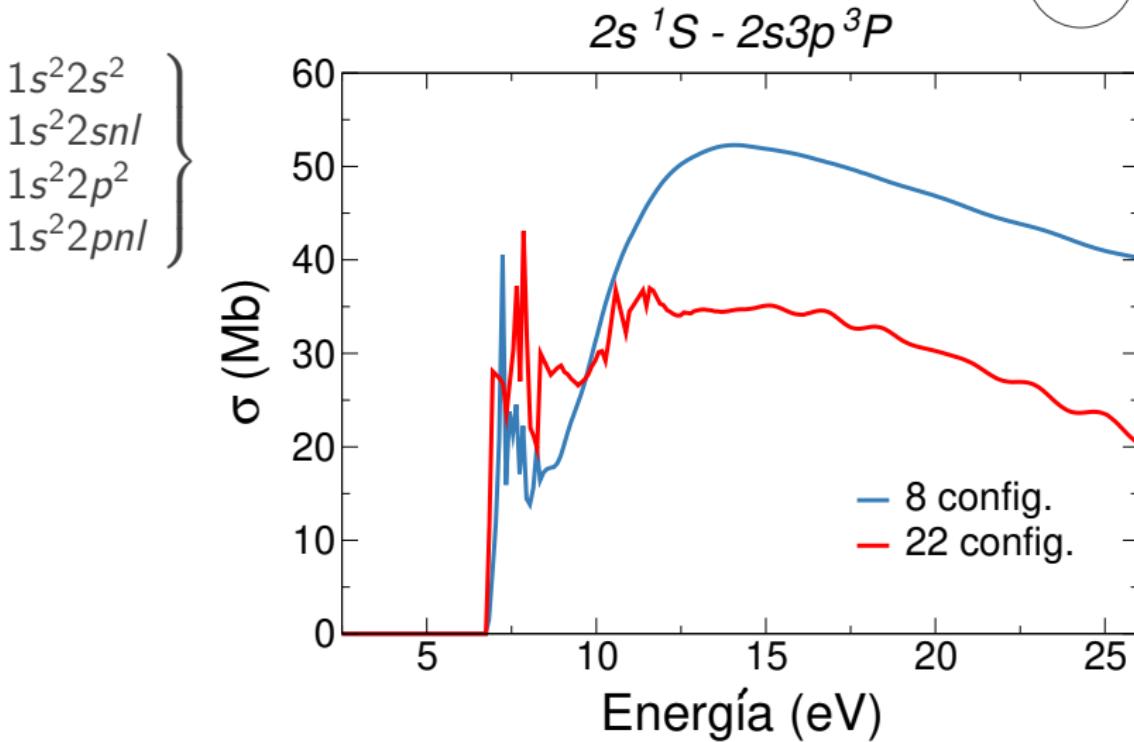
Número de configuraciones

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

Parámetro de escaleo

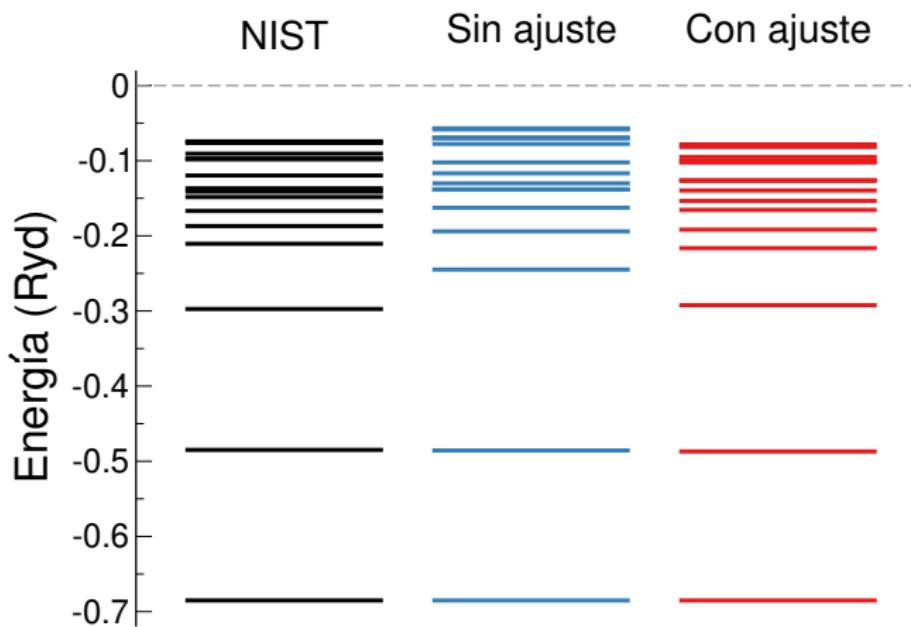
- Thomas–Fermi–Dirac–Amaldi
- Slater-Type-Orbital de Burgess

# Influencia de $N$



# Influencia de $\lambda_{nl}$

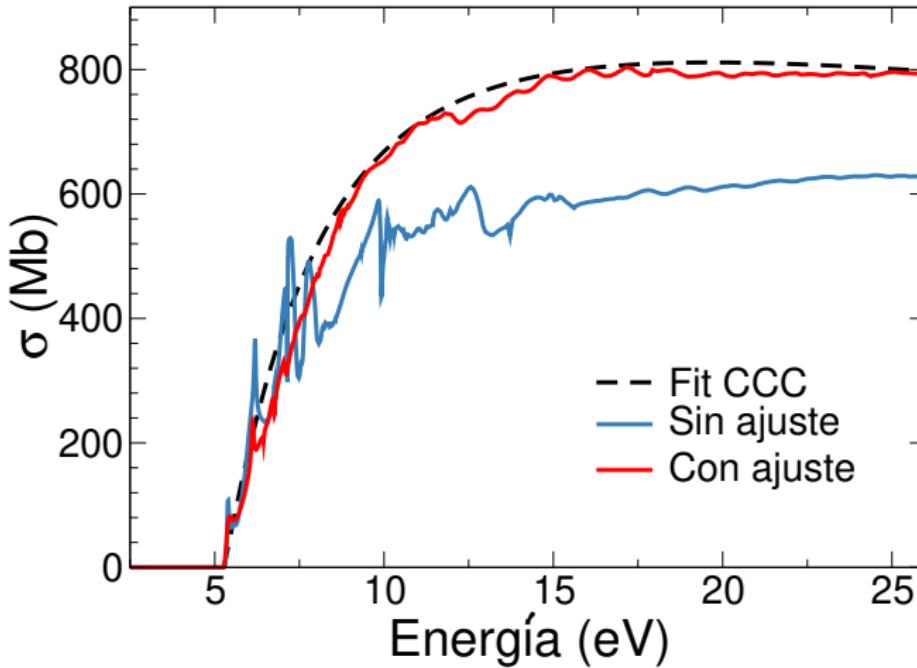
Be



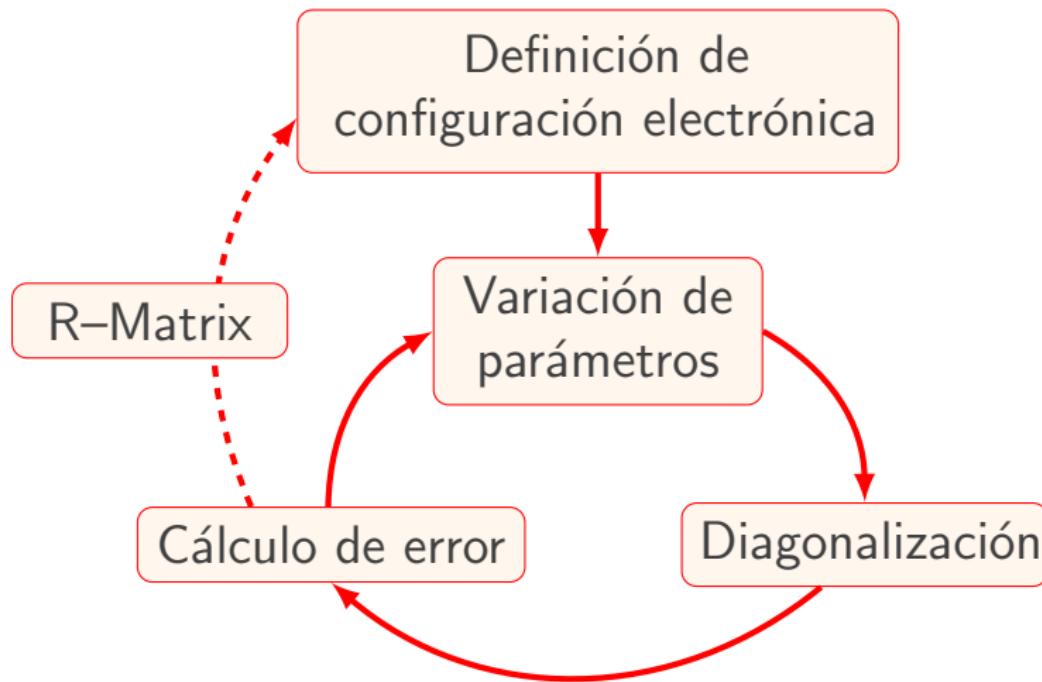
# Influencia de $\lambda_{nl}$

Be

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



# Procedimiento



# Síntesis del problema

Función de costo:

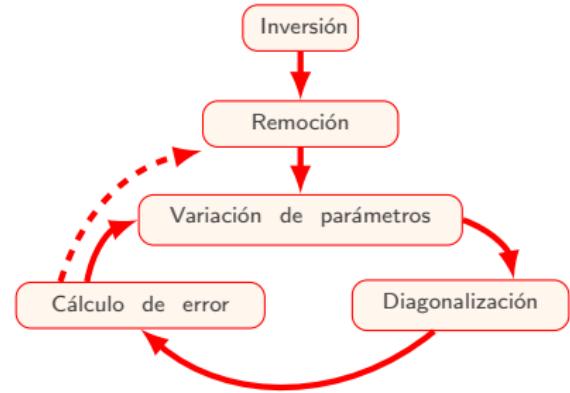
$$J = \sum_j \left| \frac{\tilde{E}_j(\xi) - E_j}{E_j} \right|$$

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

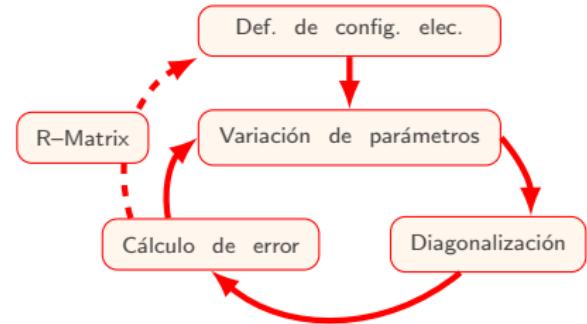
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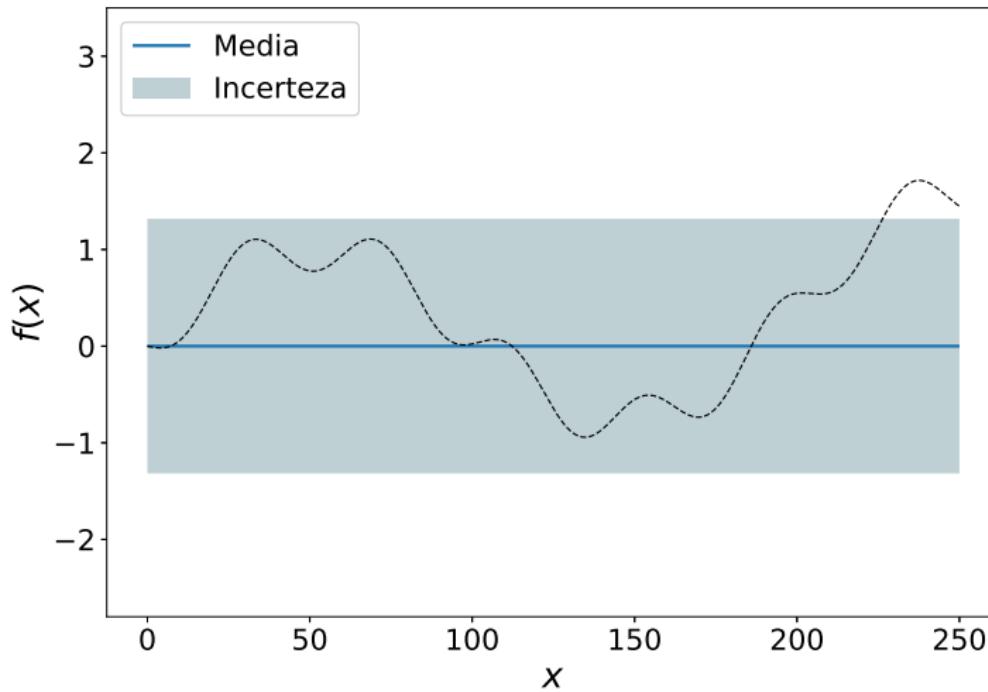


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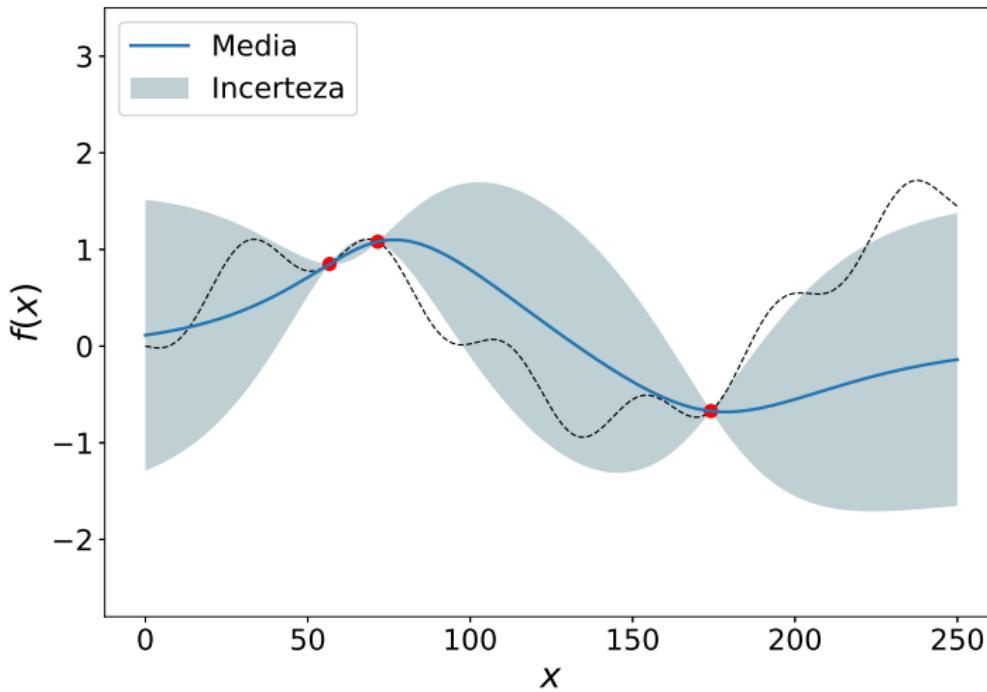


# Optimización Bayesiana con Procesos Gaussianos

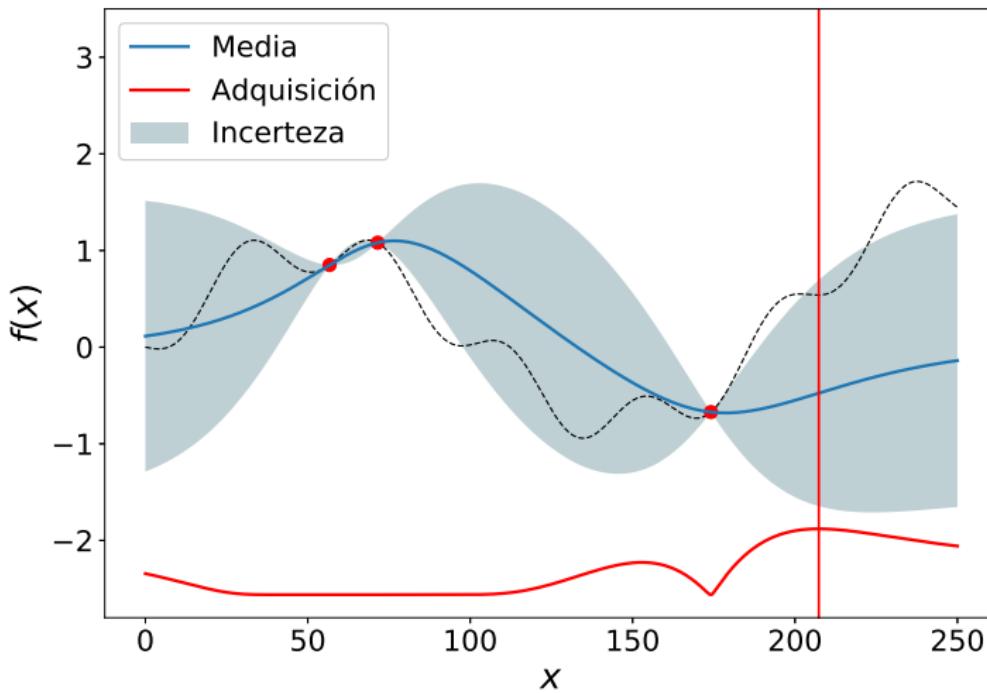
# Procesos Gaussianos



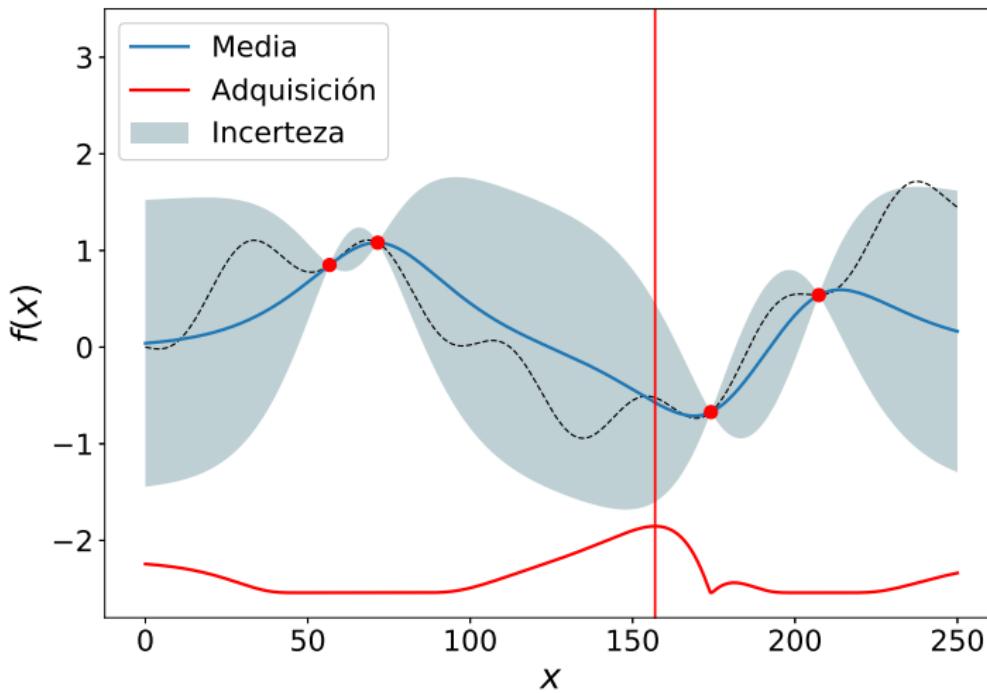
# Procesos Gaussianos



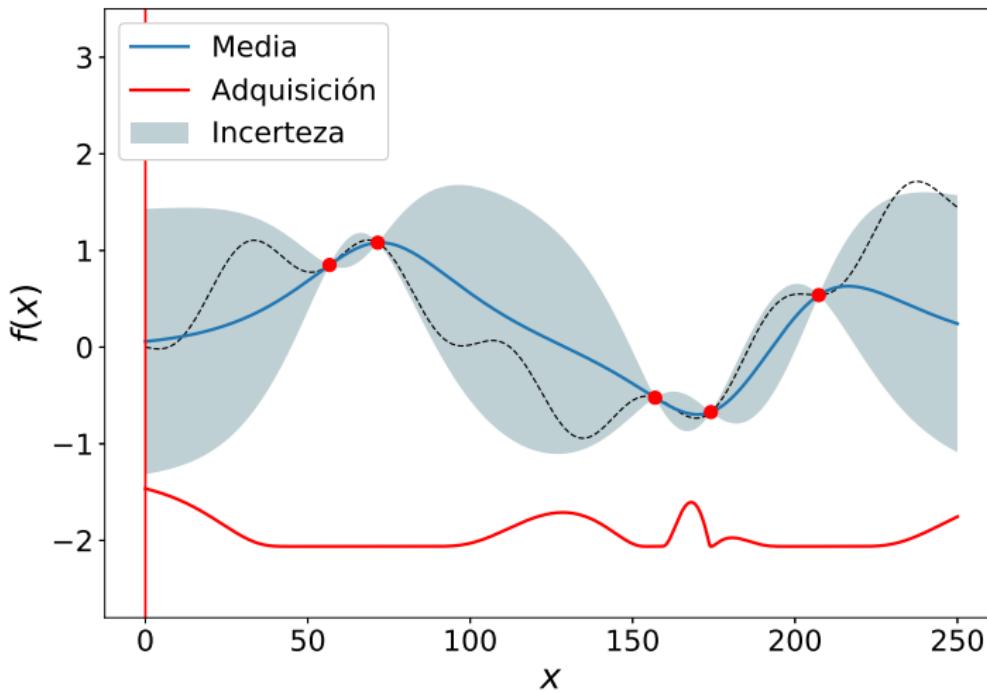
# Procesos Gaussianos



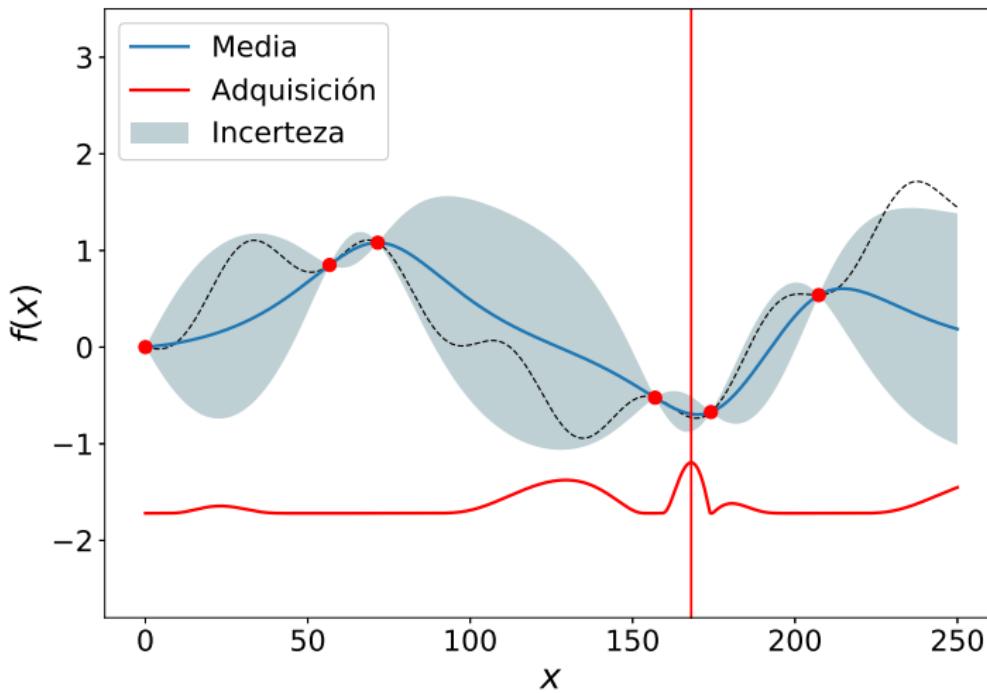
# Procesos Gaussianos



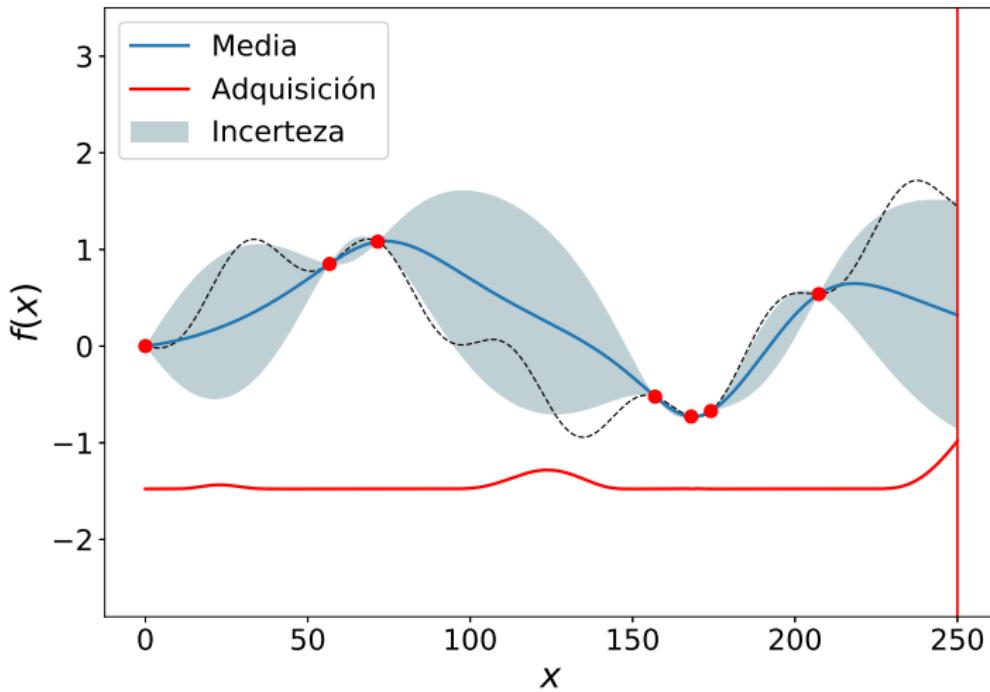
# Procesos Gaussianos



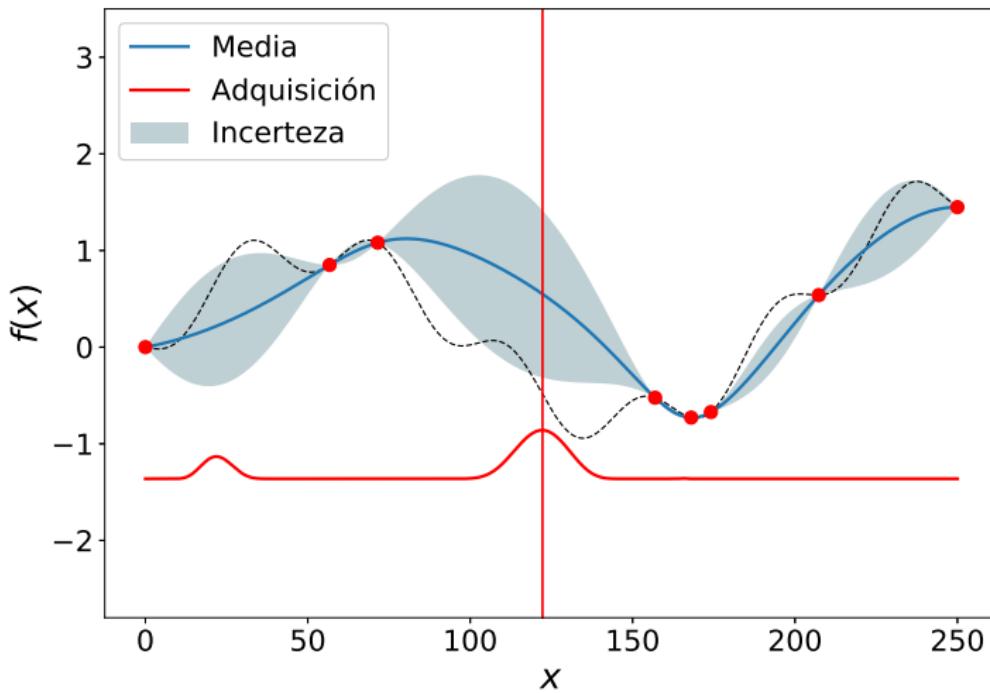
# Procesos Gaussianos



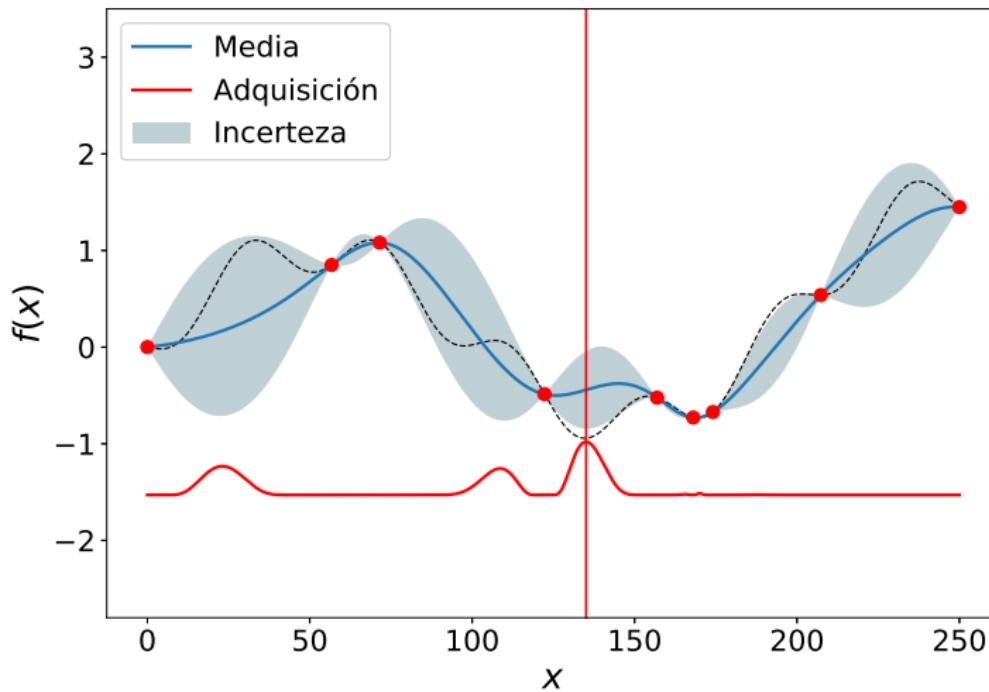
# Procesos Gaussianos



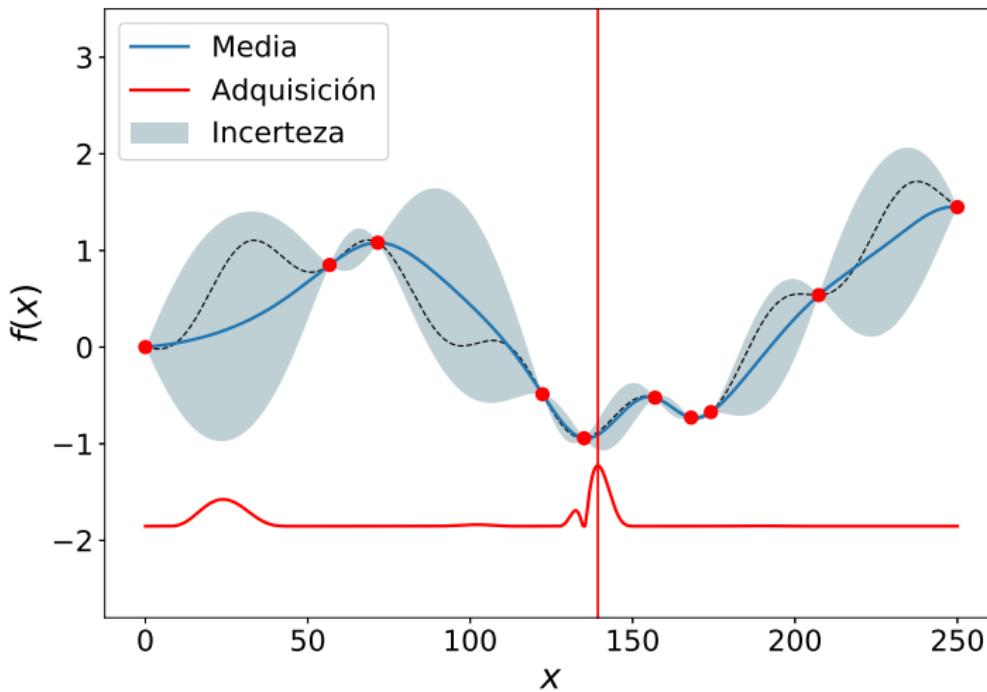
# Procesos Gaussianos



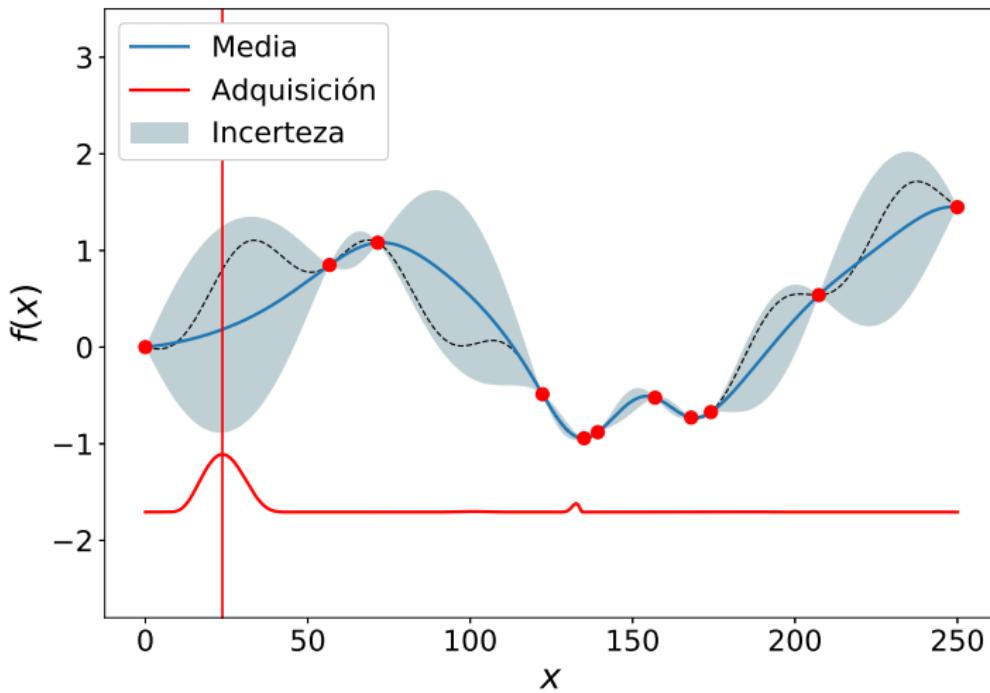
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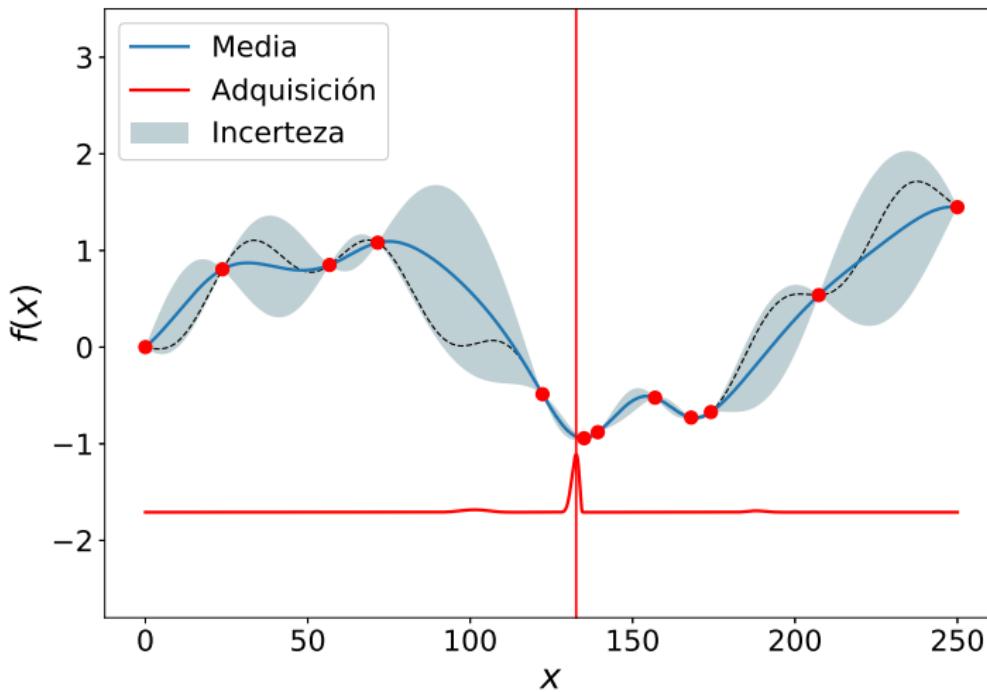
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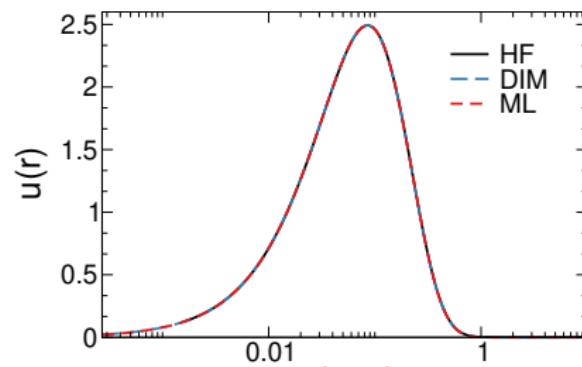
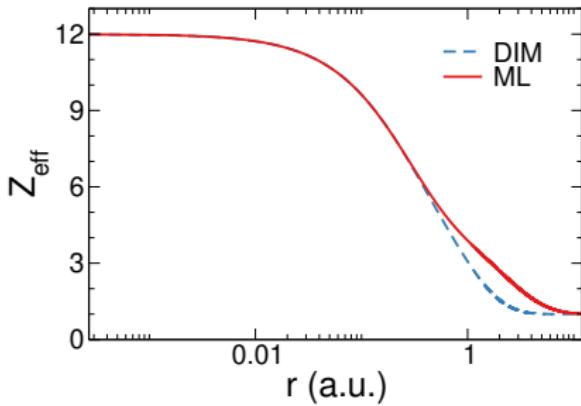


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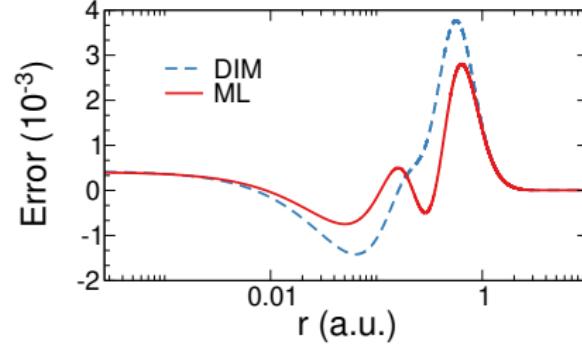


# Resultados

# DIM: Mg



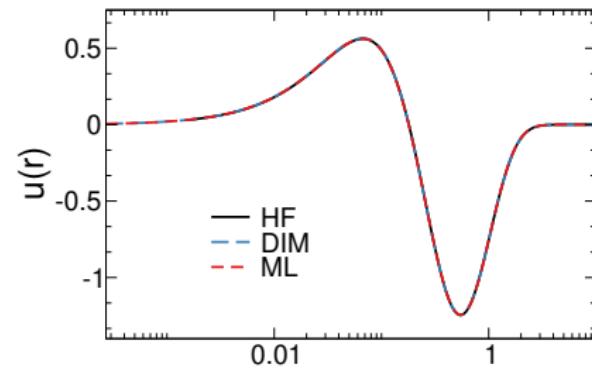
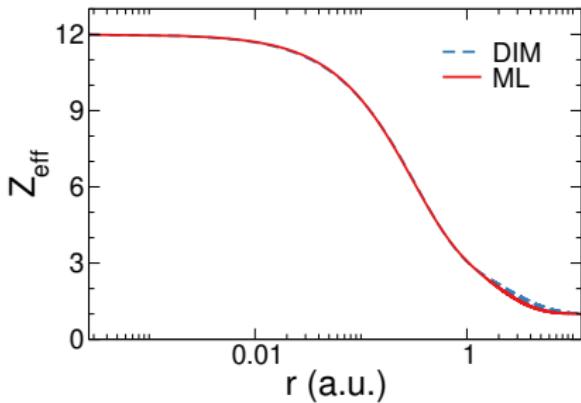
$E$  ✓  
 $\langle r \rangle$   
 $\langle 1/r \rangle$   $10^{-2}$



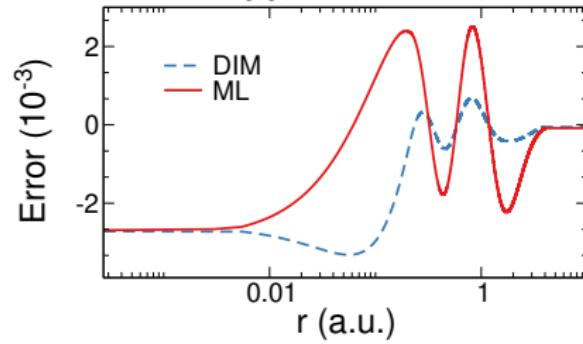
1s

# DIM: Mg

2s

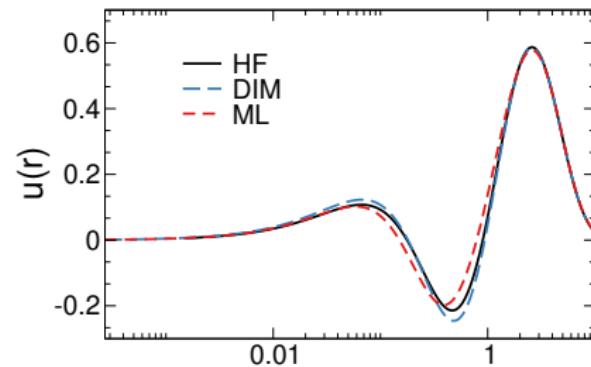
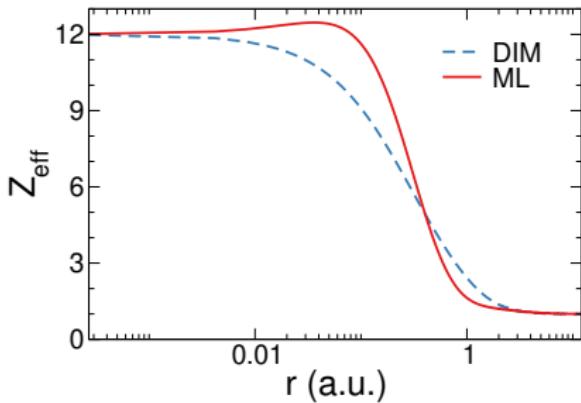


$$\begin{array}{c} E \\ \langle r \rangle \\ \langle 1/r \rangle \end{array} \quad 10^{-2}$$



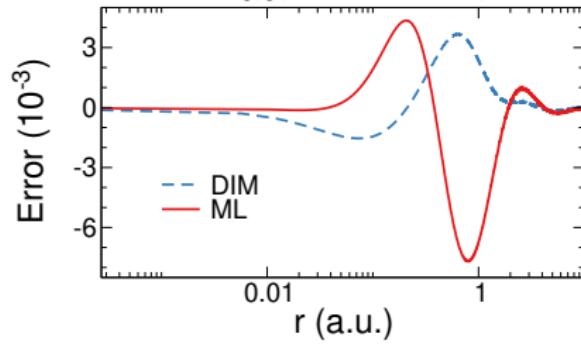


# DIM: Mg



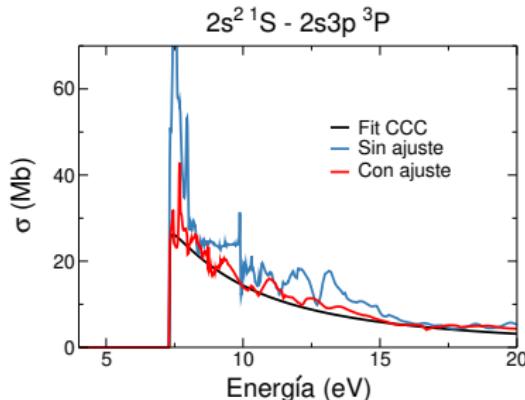
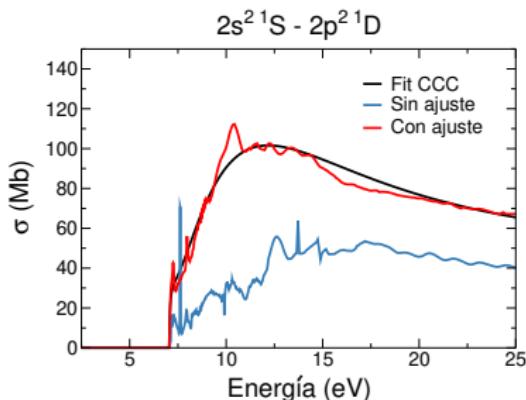
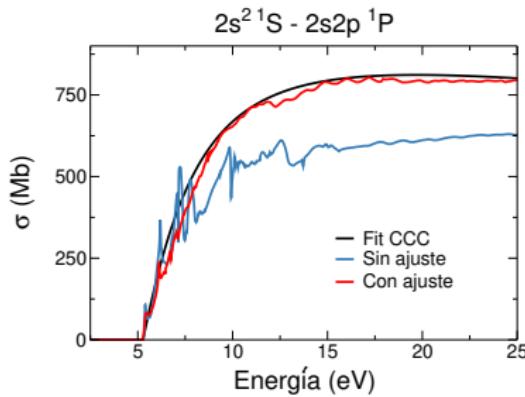
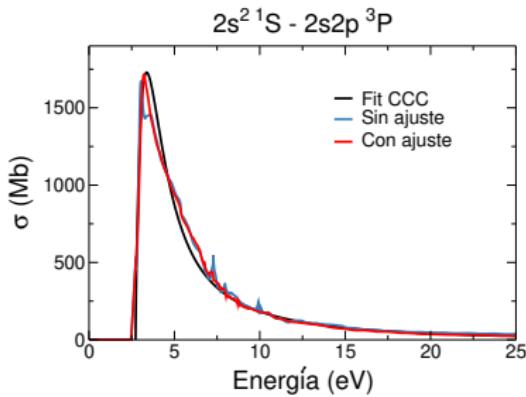
$$\begin{array}{c} E \\ \langle r \rangle \\ \langle 1/r \rangle \end{array} \quad 10^{-1}$$

A green checkmark is placed next to the  $\langle r \rangle$  term.



3s

# R-Matrix: Be



# Conclusiones

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  - Estructura del blanco en R-Matrix

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- 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 campo