

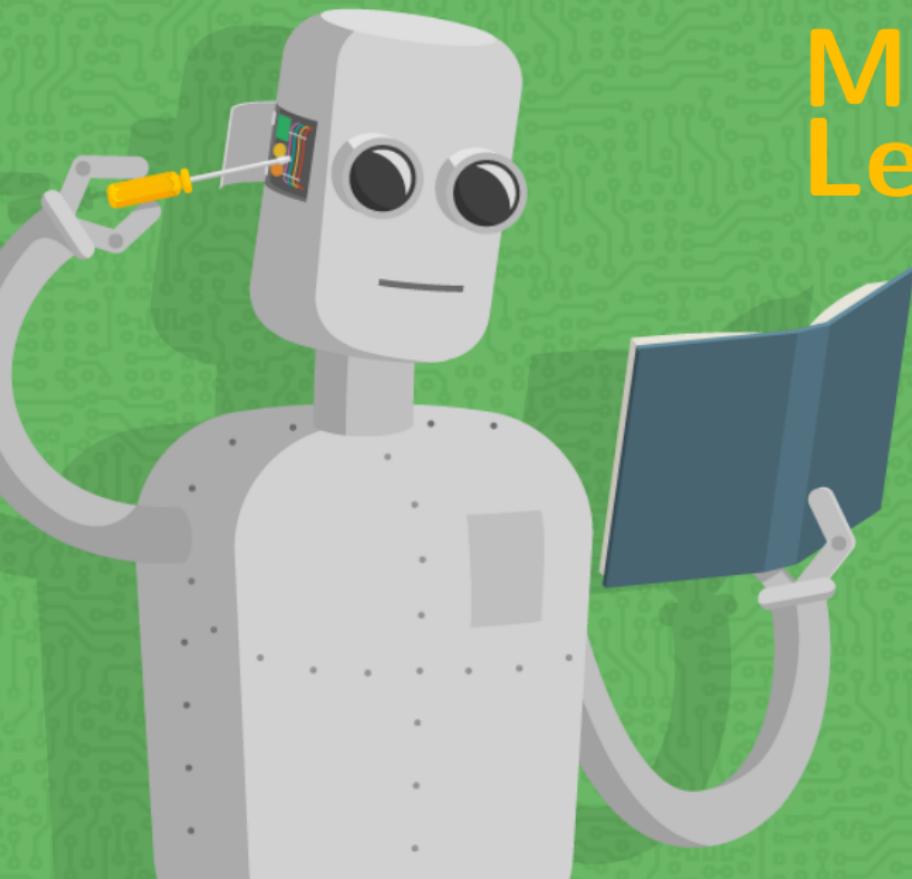
Implementación de Métodos de Aprendizaje Automatizado en problemas colisionales



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

alemendez@iafe.uba.ar

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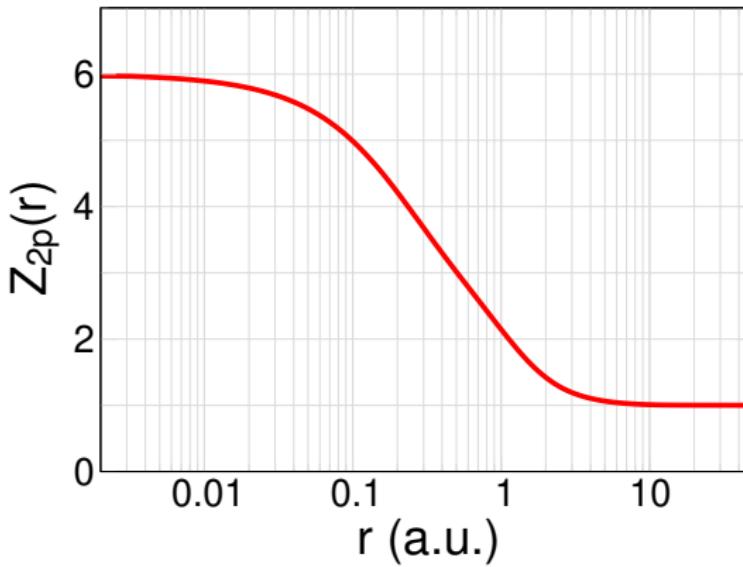
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$$V_{nl}(r) = \frac{1}{2} \frac{P''_{nl}(r)}{P_{nl}(r)} - \frac{l(l+1)}{2r^2} + E_{nl}$$

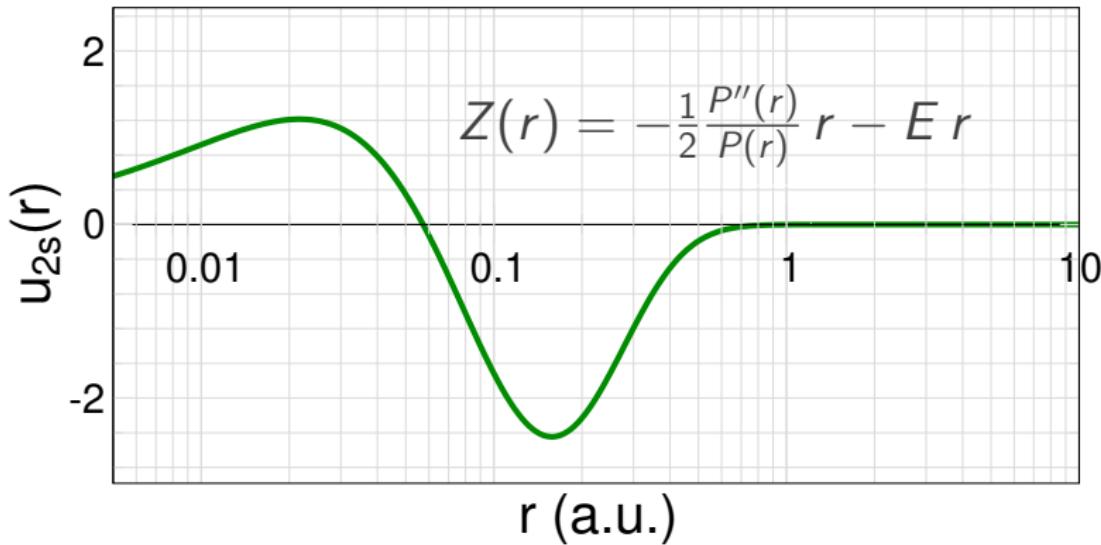
Método de Inversión Depurada (DIM)

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



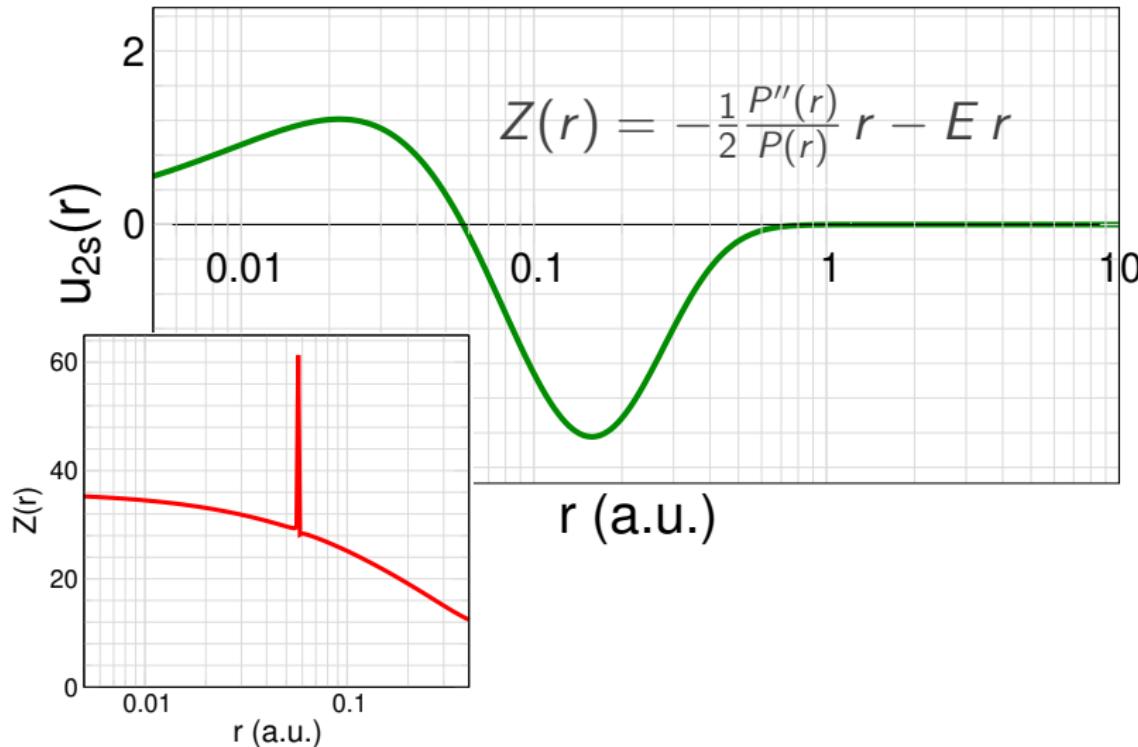
Houston, we have a problem!

Kr



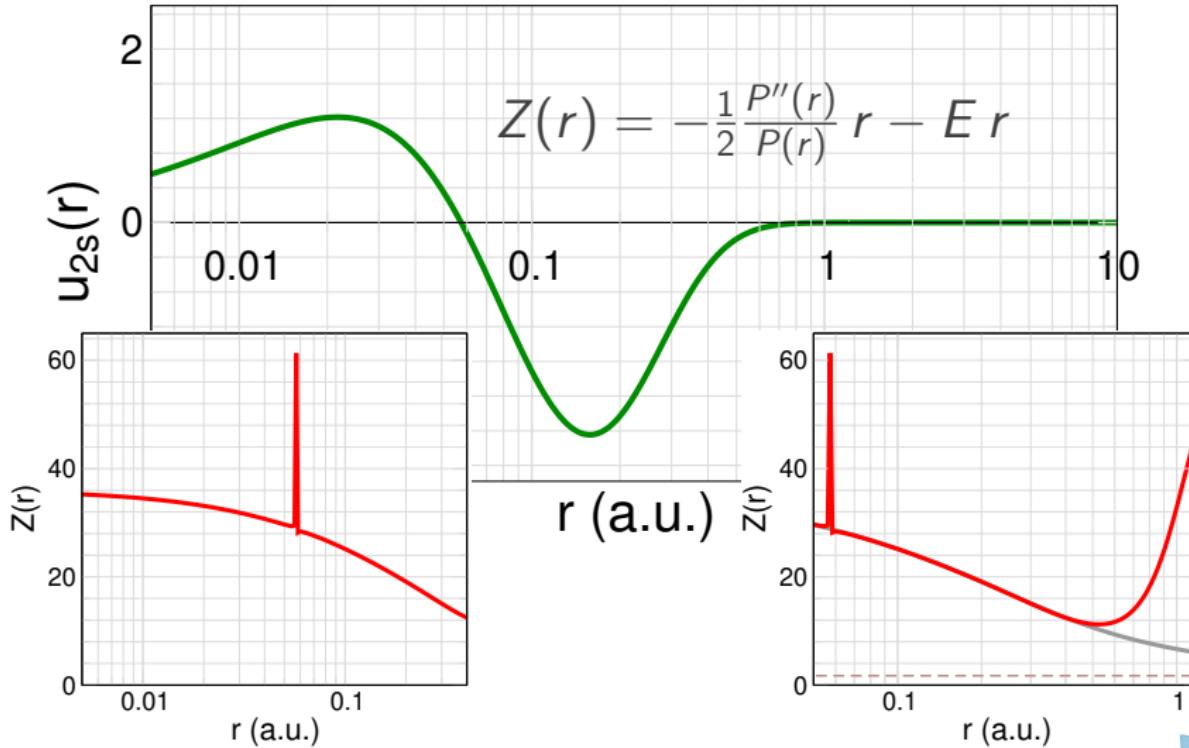
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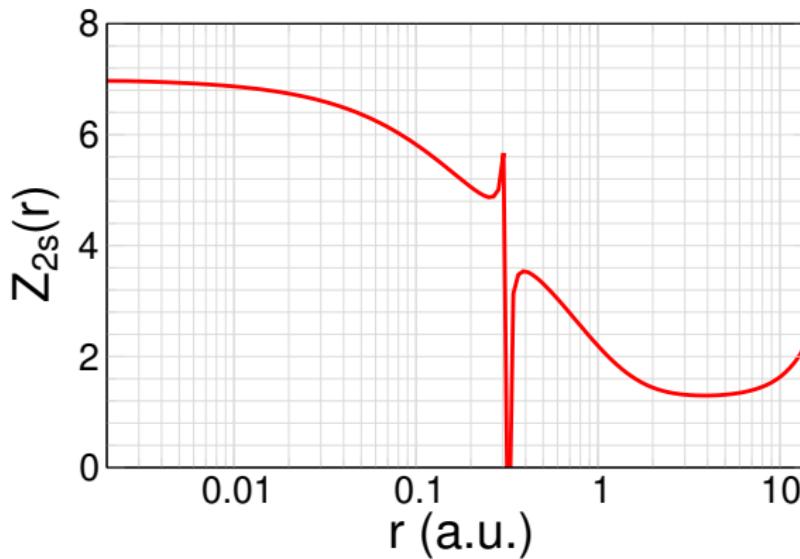
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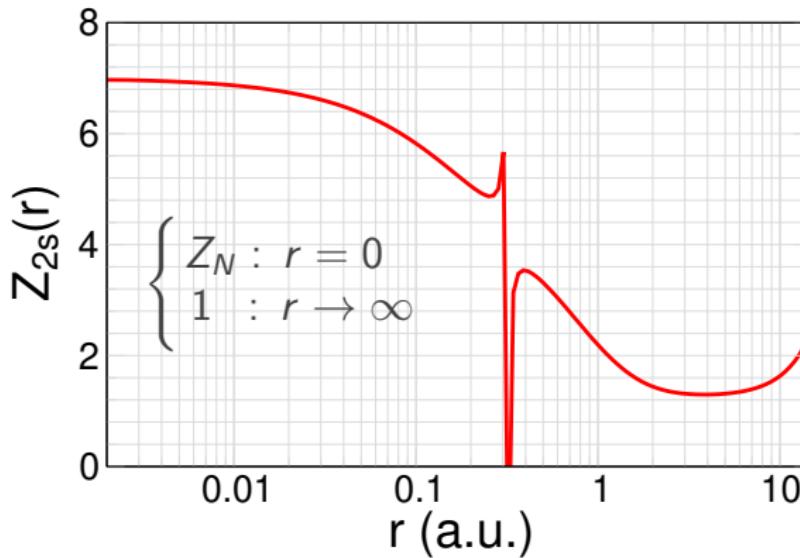
Depuración

N



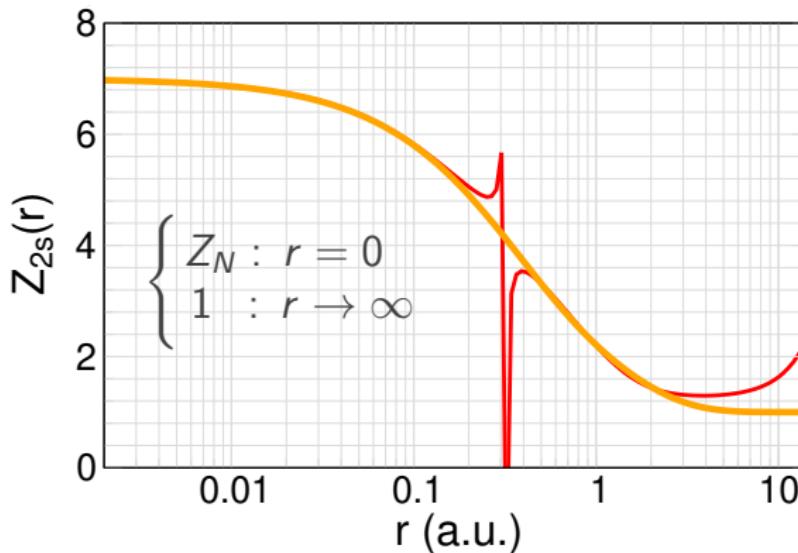
Depuración

N



Depuración

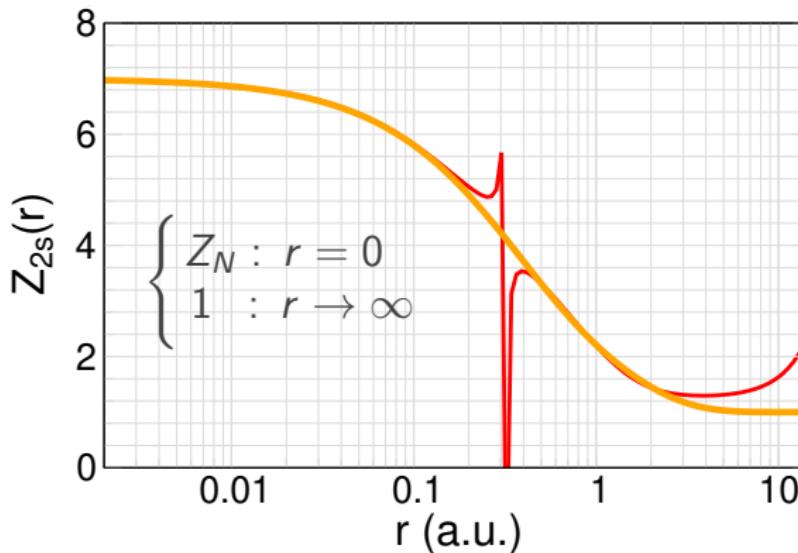
N



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

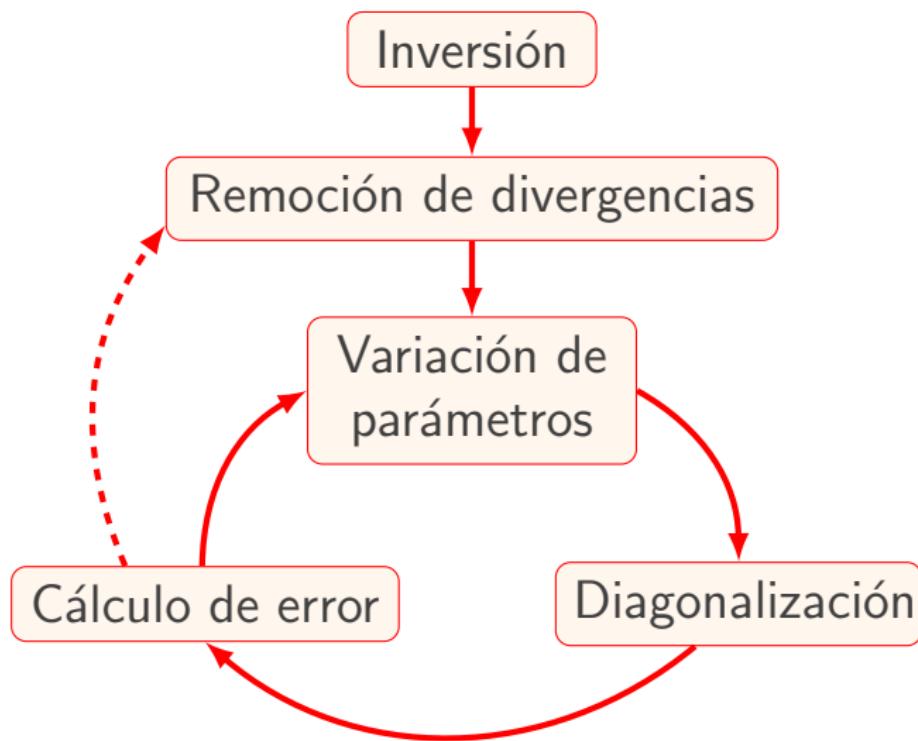
Depuración

N



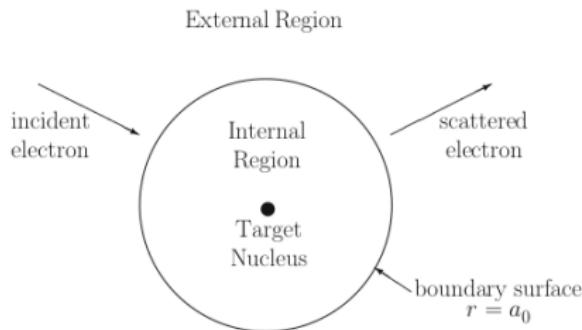
$$Z(r) = 1 + \sum_j \alpha_j e^{-\beta_j r}$$

Procedimiento



Problema 2: R-Matrix

R-Matrix



Estructura del blanco

AUTOSTRUCTURE



Región interna

RMATRXI



Región externa

STGF

Descripción del blanco

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

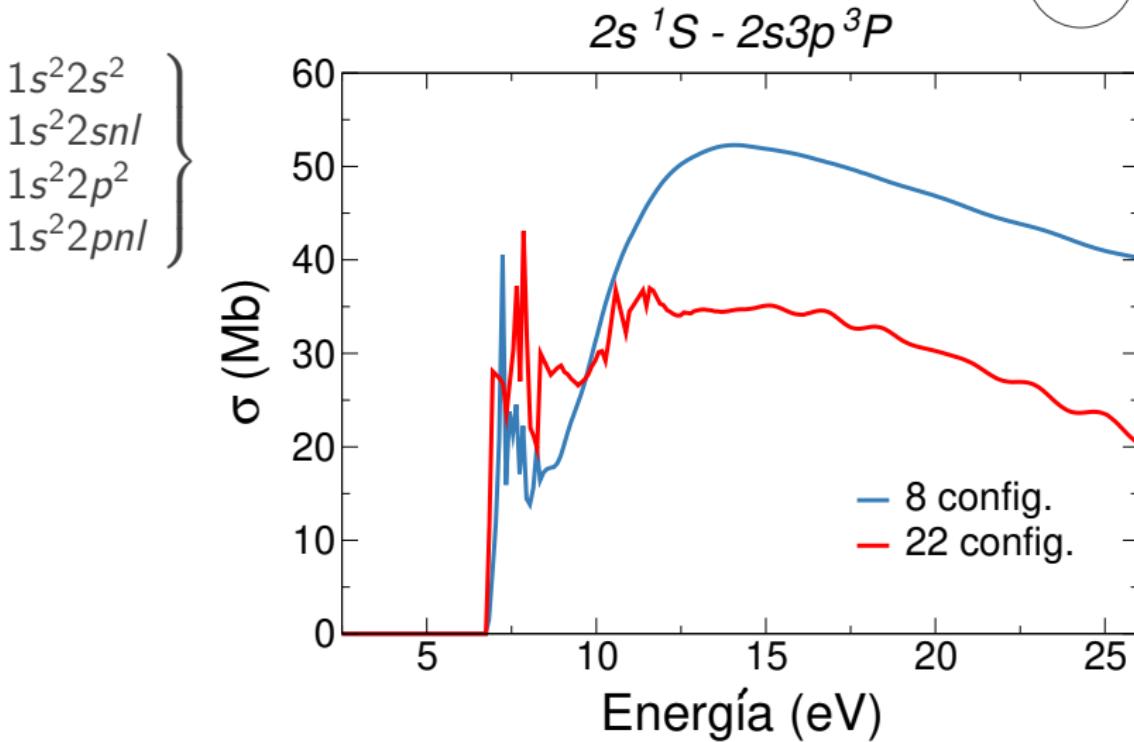
Número de configuraciones

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

Parámetro de escaleo

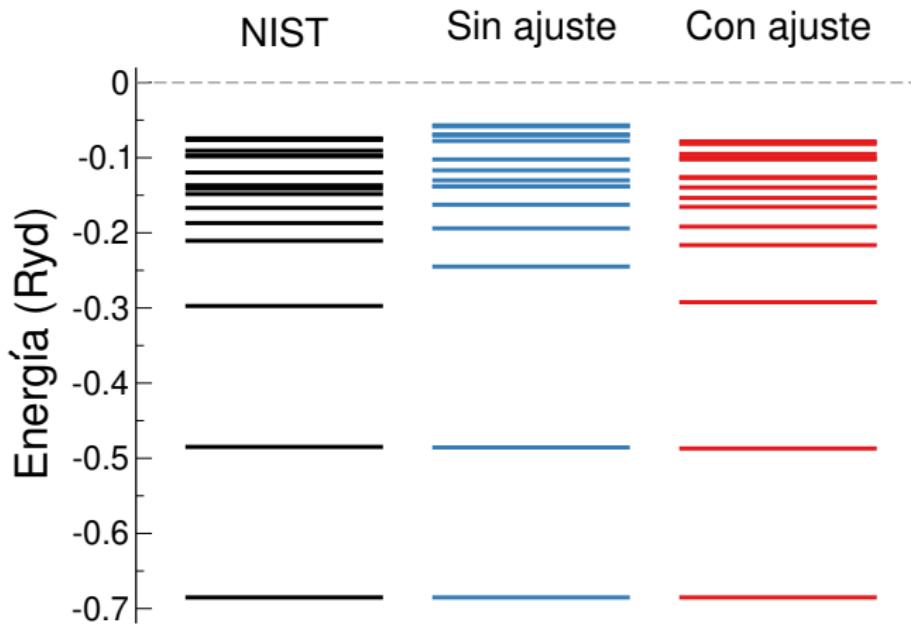
- Thomas–Fermi–Dirac–Amaldi
- Slater-Type-Orbital de Burgess

Influencia de N



Influencia de λ_{nl}

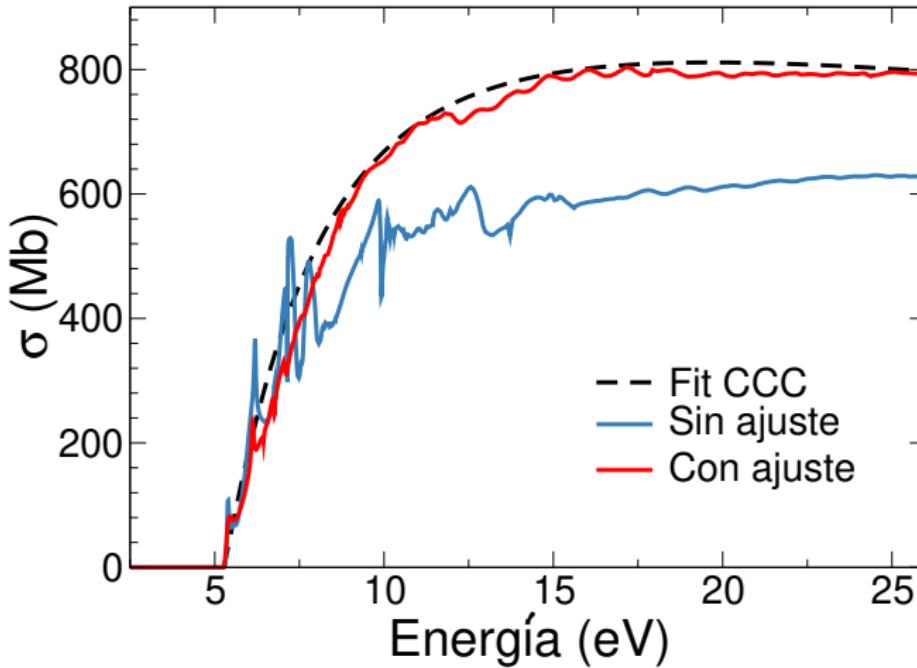
Be



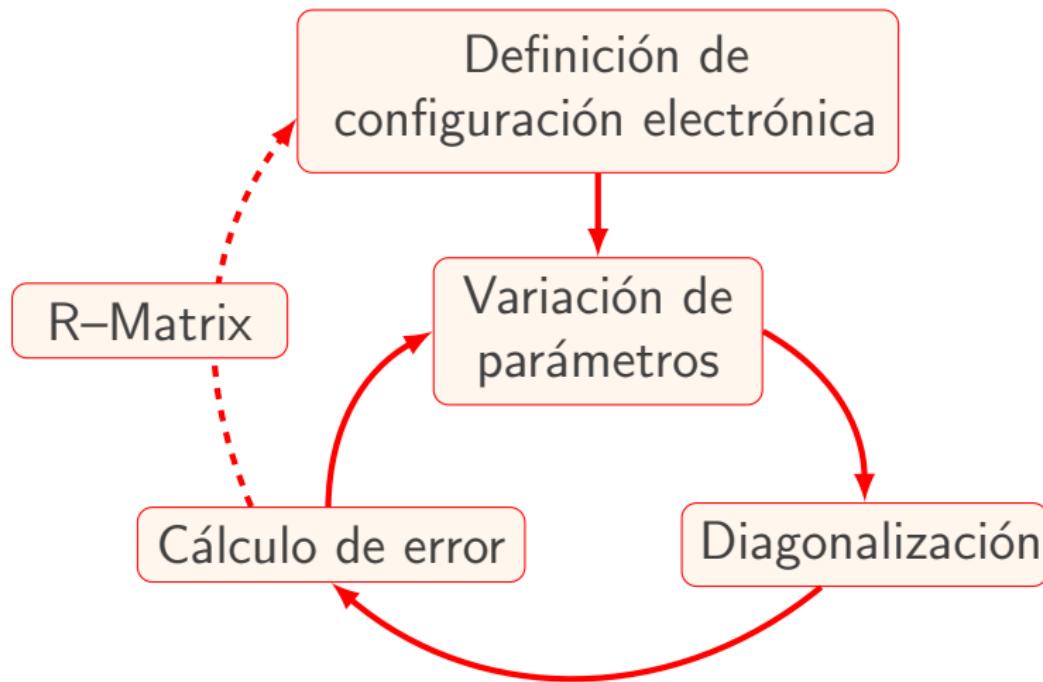
Influencia de λ_{nl}

Be

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



Procedimiento



Síntesis del problema

Función de costo:

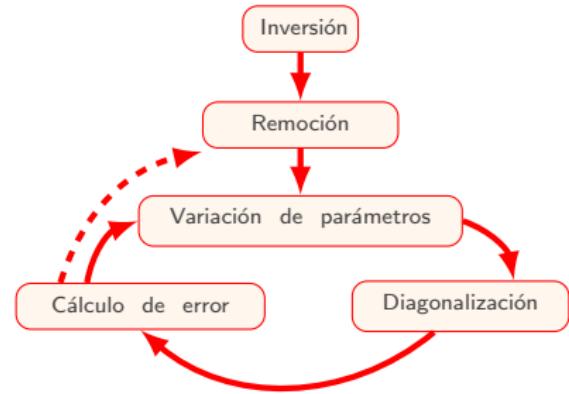
$$J = \sum_j \left| \frac{\tilde{E}_j(\xi) - E_j}{E_j} \right|$$

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

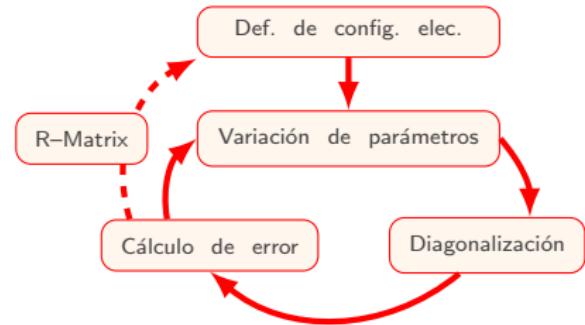
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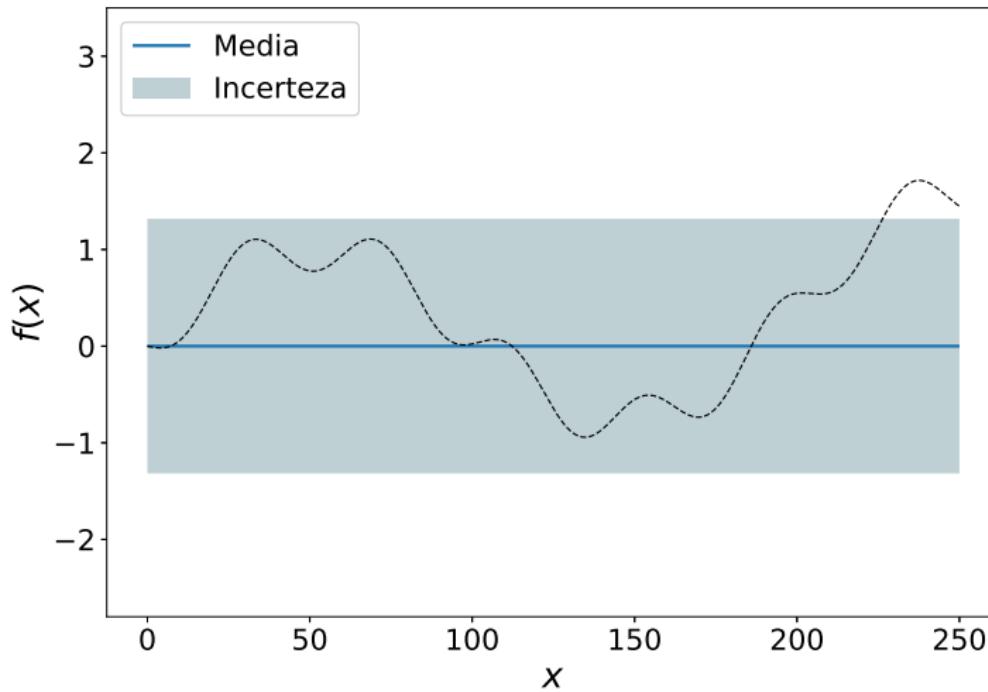


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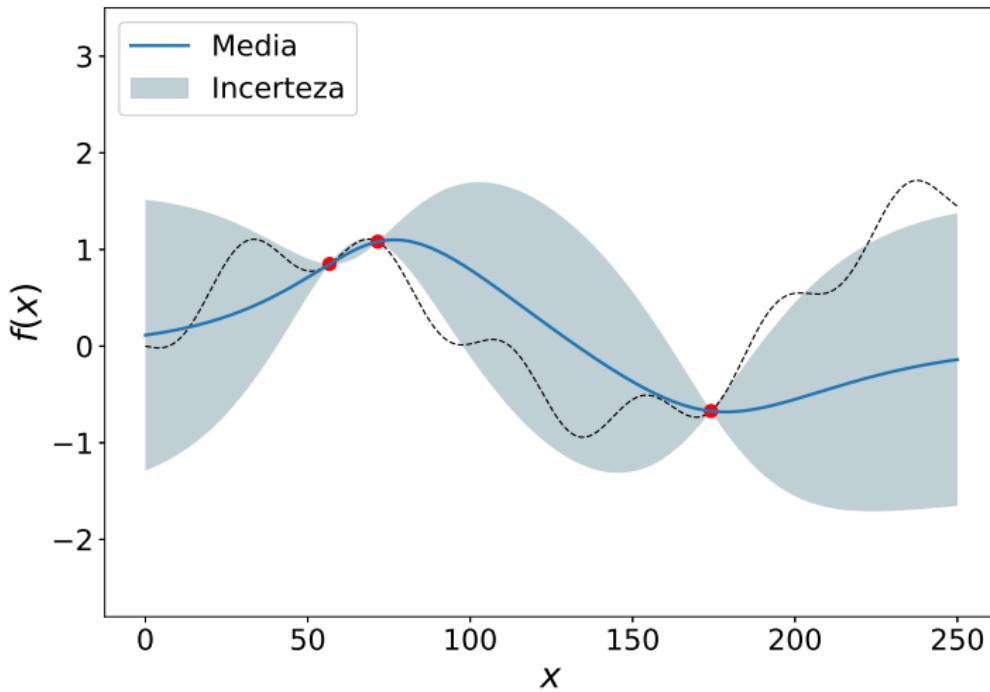


Optimización Bayesiana con Procesos Gaussianos

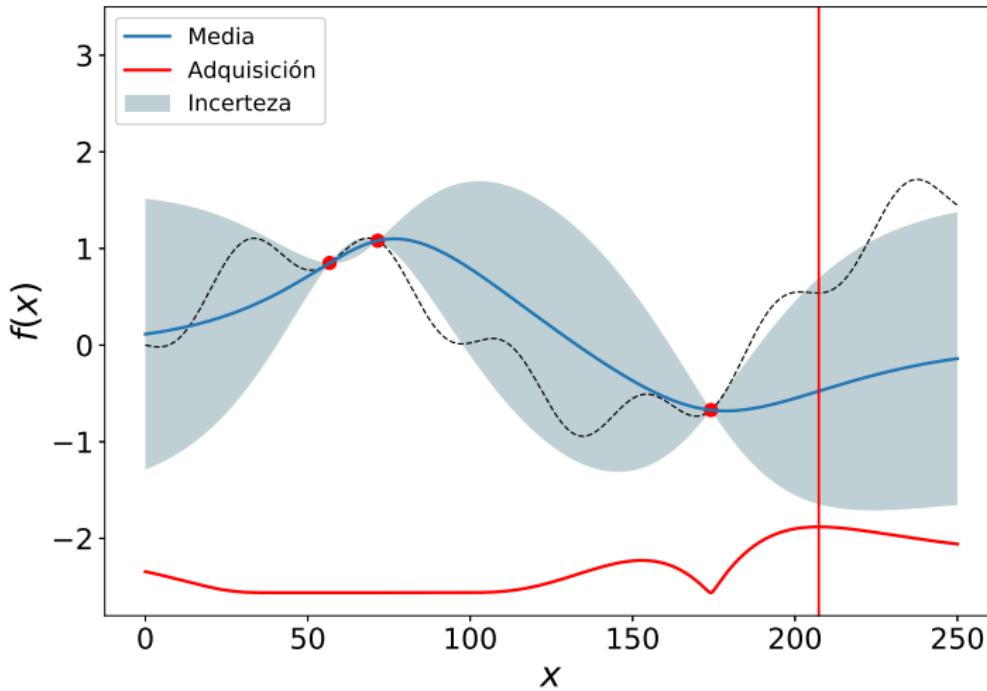
Procesos Gaussianos



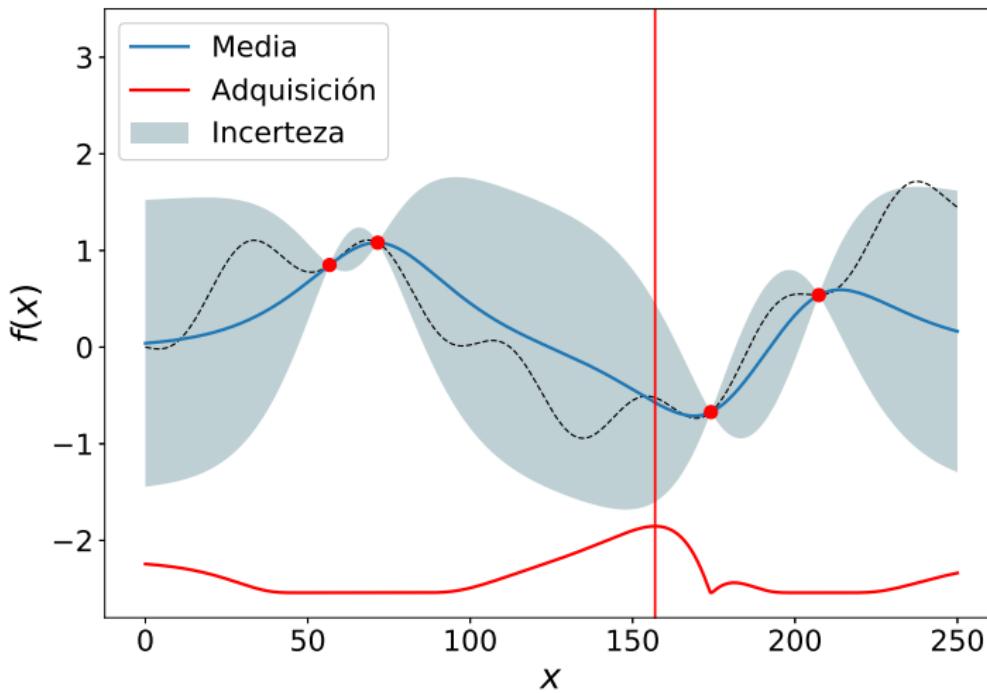
Procesos Gaussianos



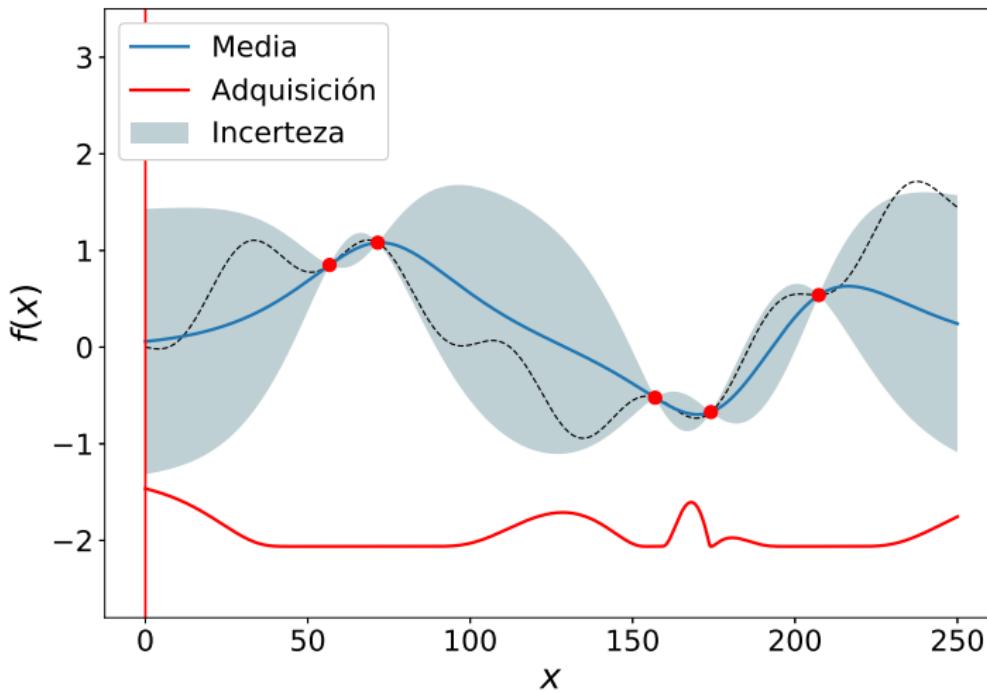
Procesos Gaussianos



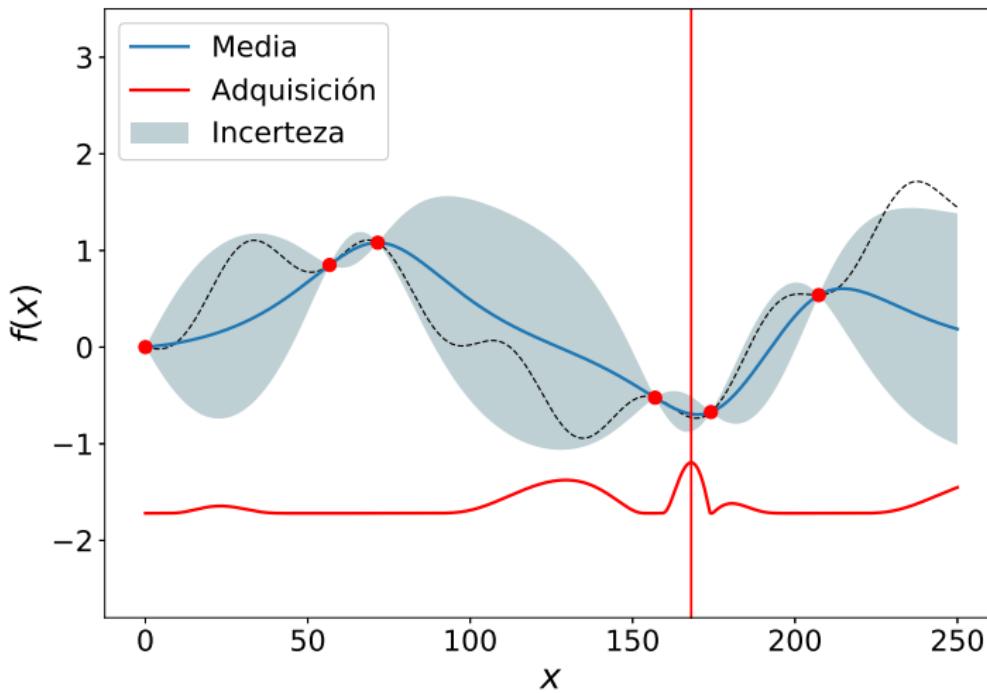
Procesos Gaussianos



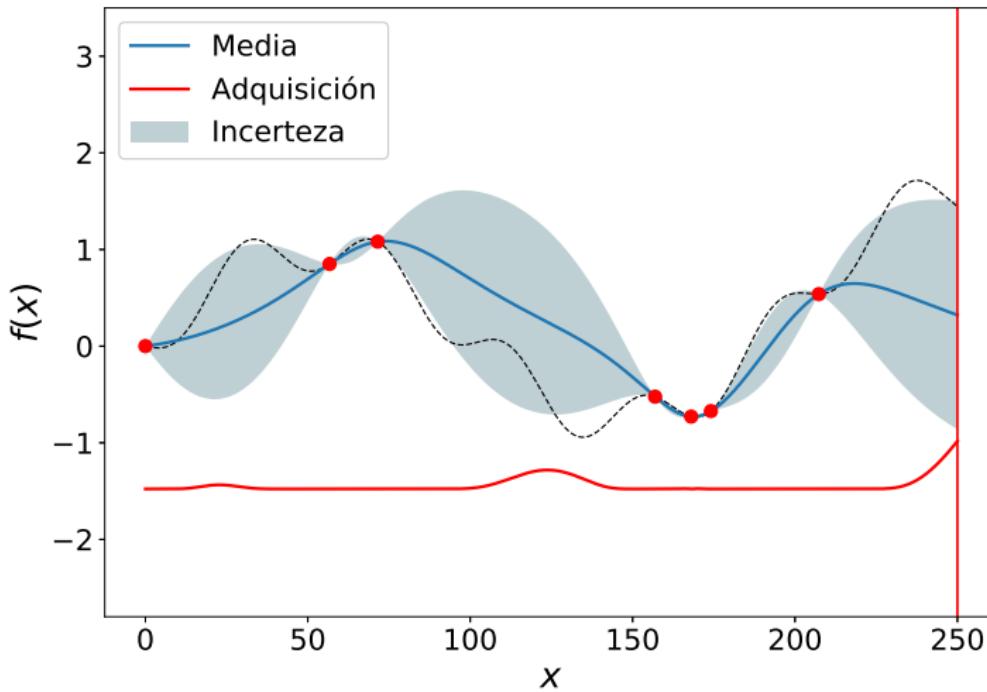
Procesos Gaussianos



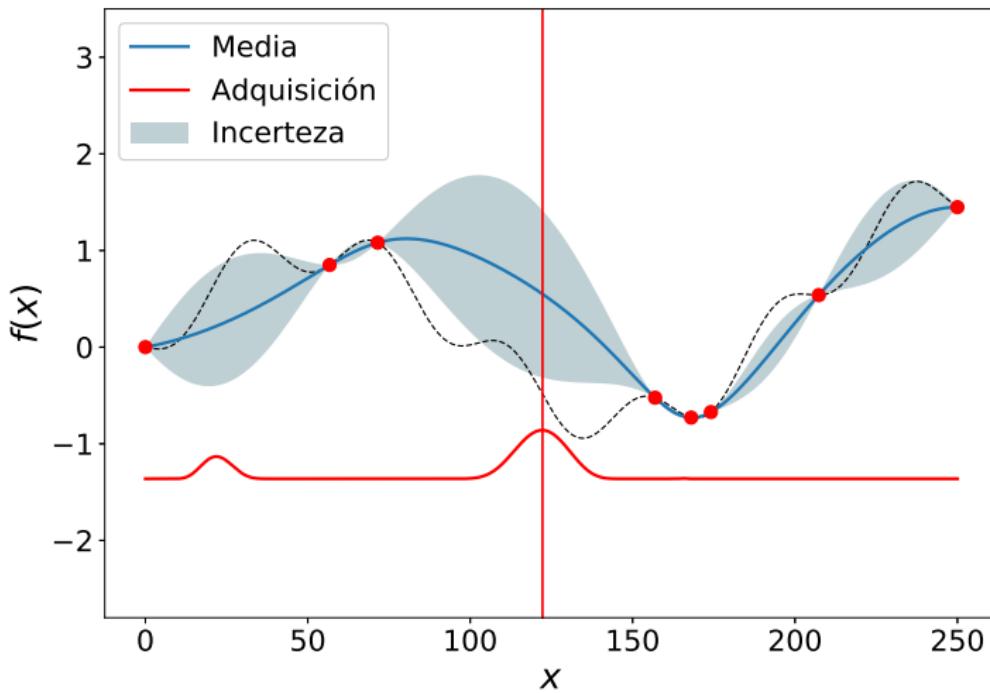
Procesos Gaussianos



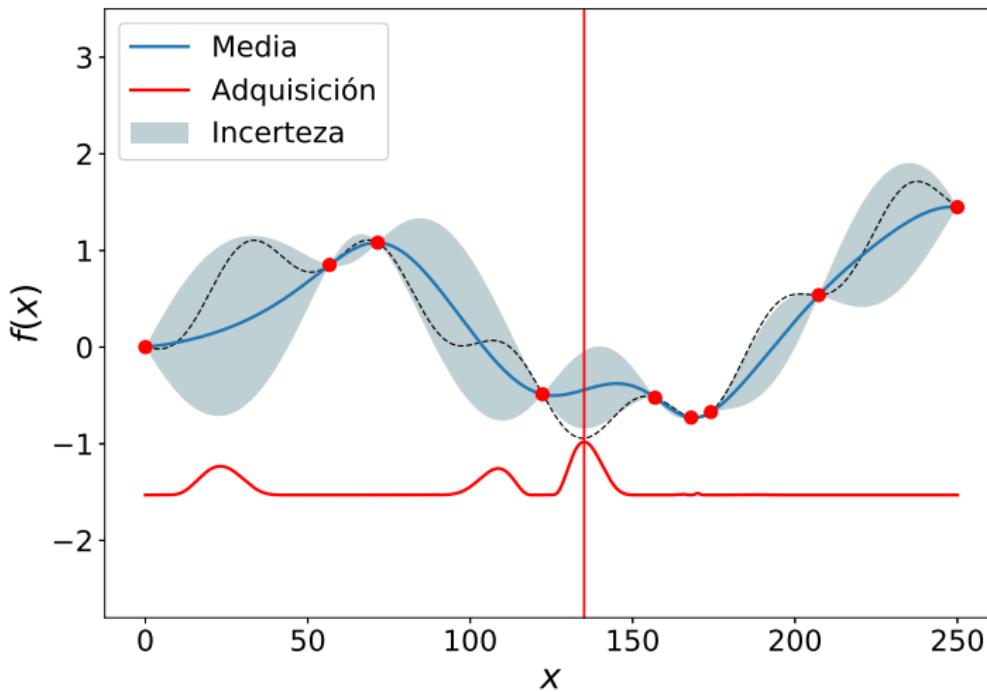
Procesos Gaussianos



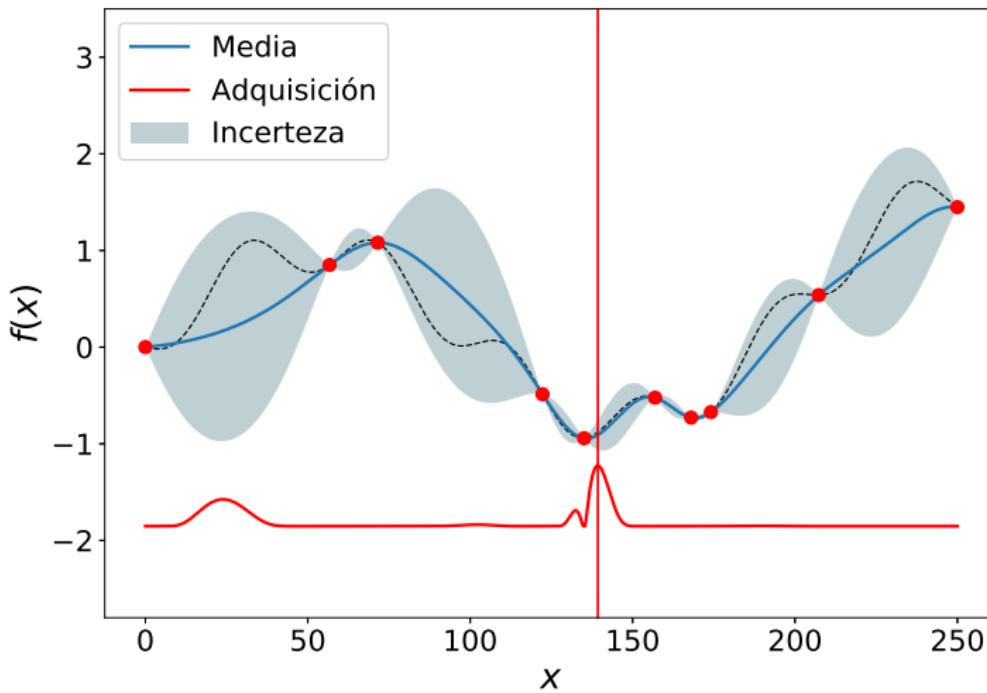
Procesos Gaussianos



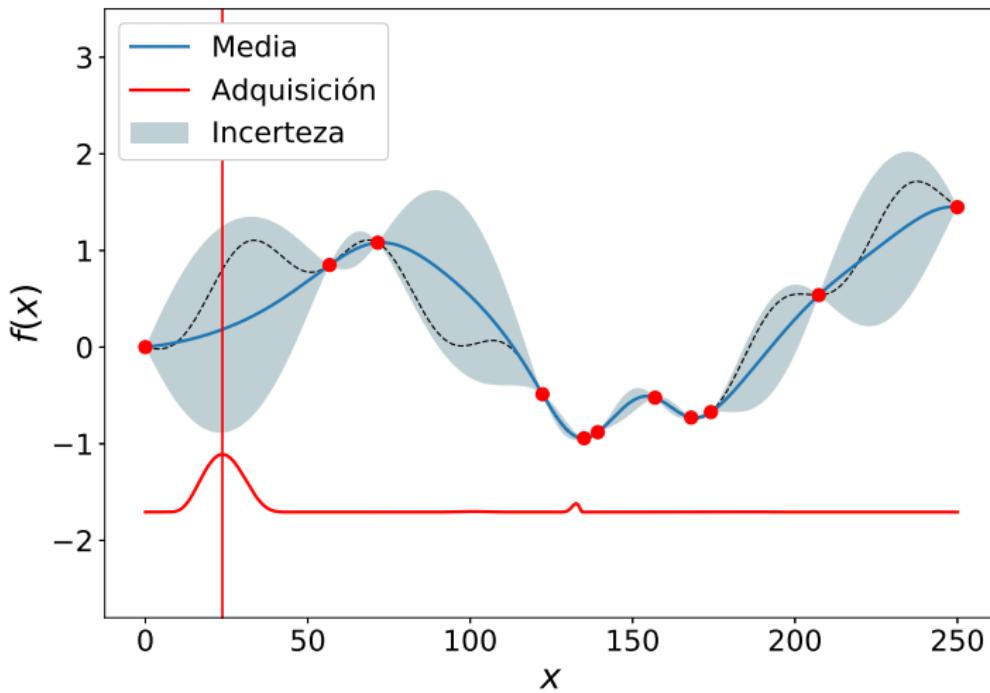
Procesos Gaussianos



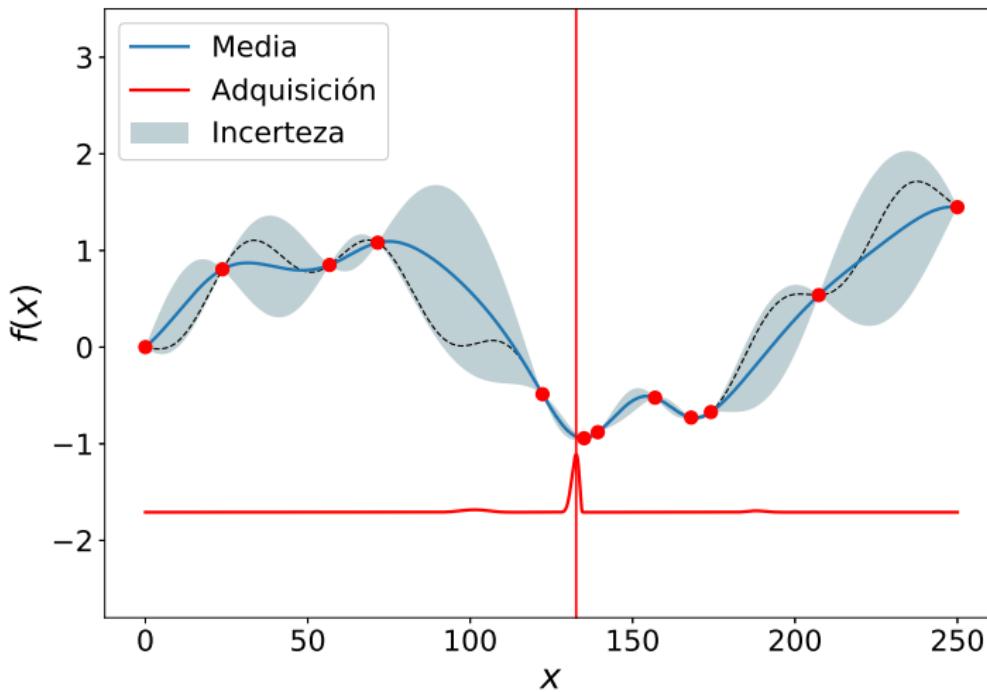
Procesos Gaussianos



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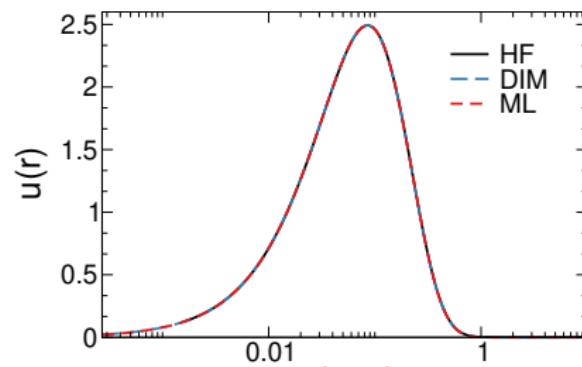
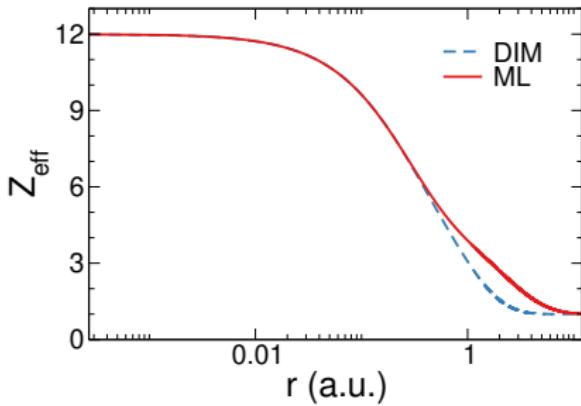


Procesos Gaussianos

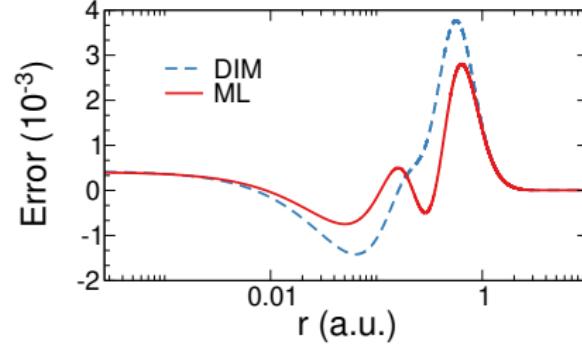


Resultados

DIM: Mg



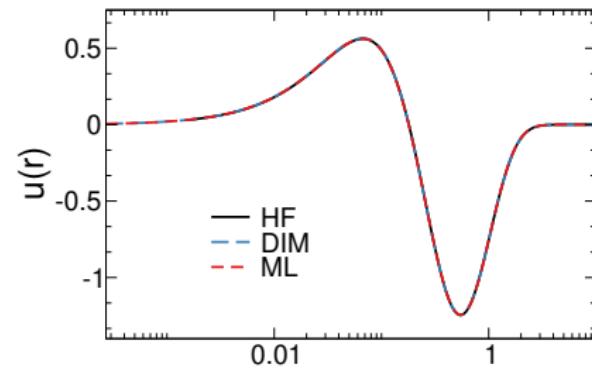
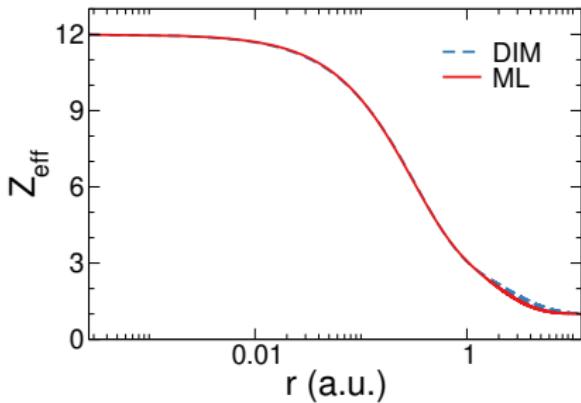
E ✓
 $\langle r \rangle$
 $\langle 1/r \rangle$ 10^{-2}



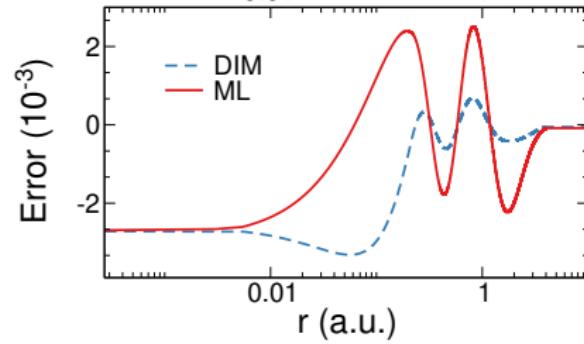
1s

DIM: Mg

2s

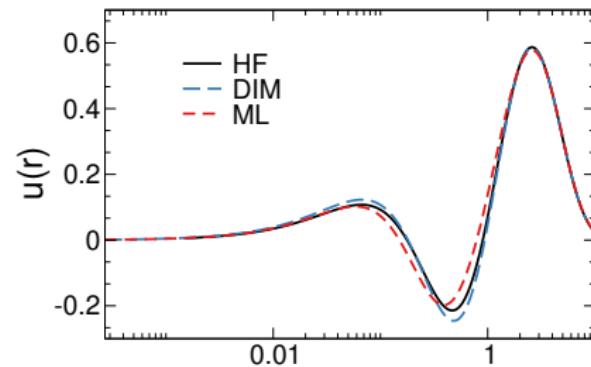
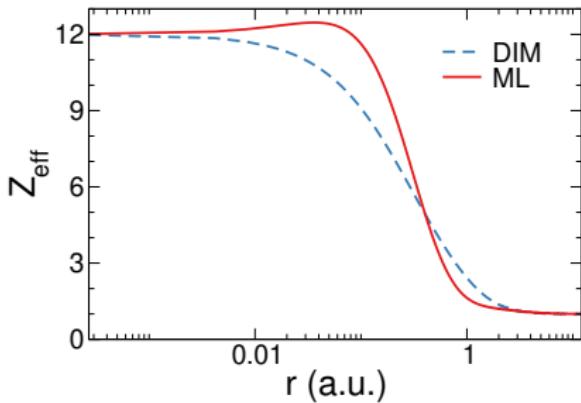


$$\begin{array}{c} E \\ \langle r \rangle \\ \langle 1/r \rangle \end{array} \quad 10^{-2}$$

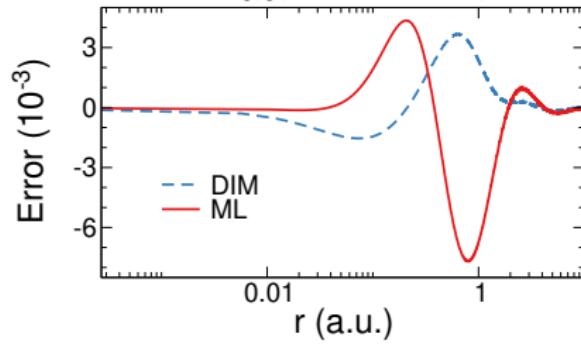




DIM: Mg

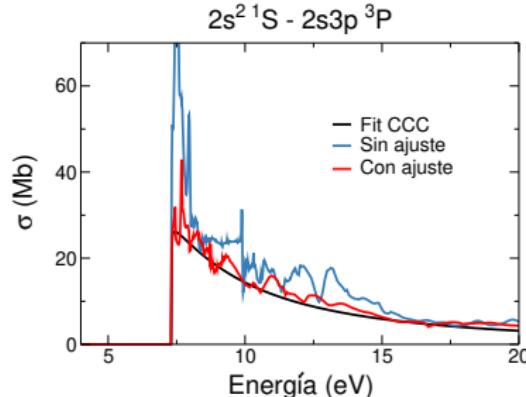
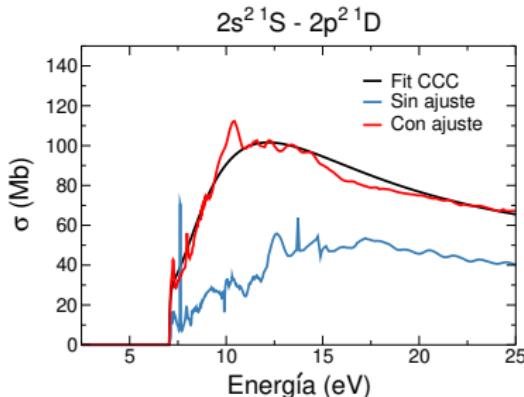
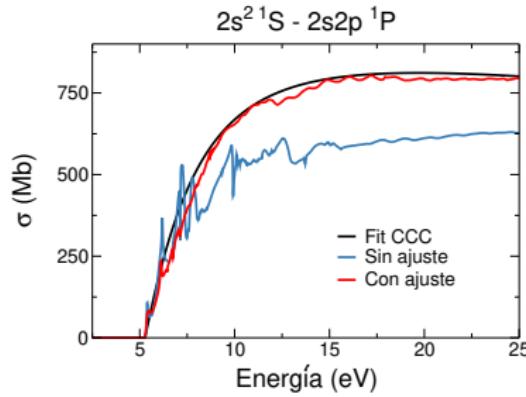
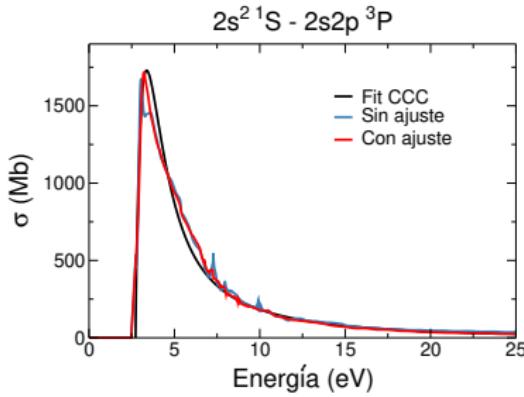


$$\begin{array}{c} E \\ \langle r \rangle \\ \langle 1/r \rangle \end{array} \quad 10^{-1}$$



3s

R-Matrix: Be



Conclusiones

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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