

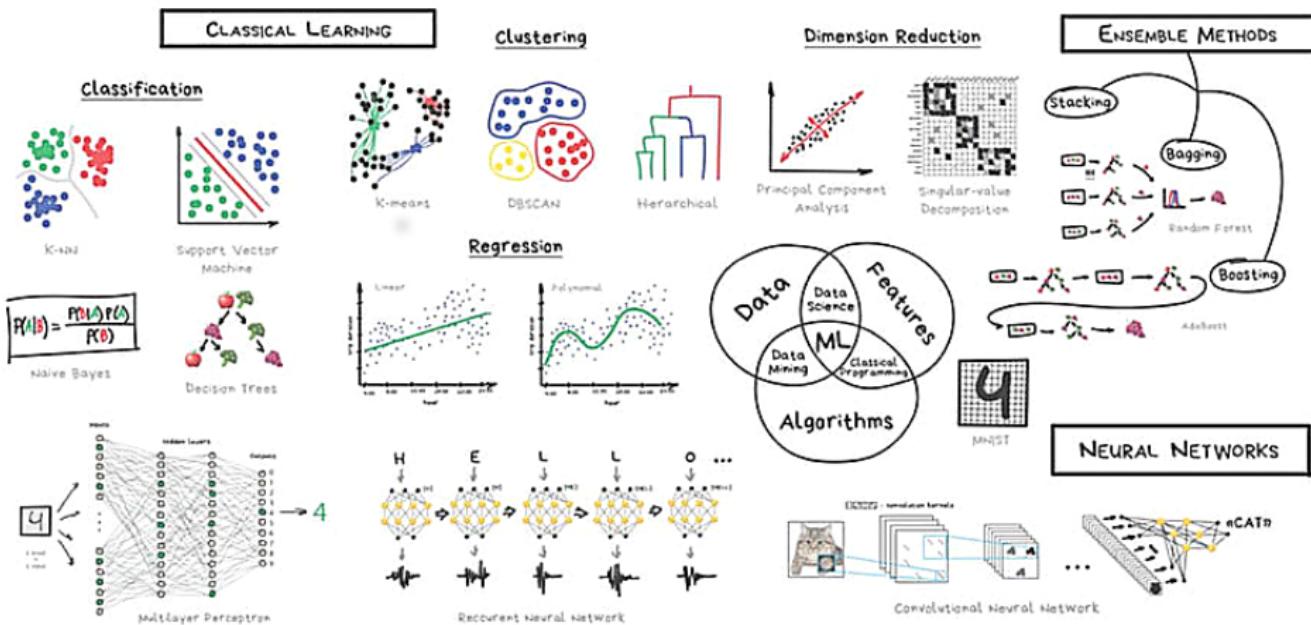
Implementación de Métodos de Aprendizaje Automatizado en problemas colisionales



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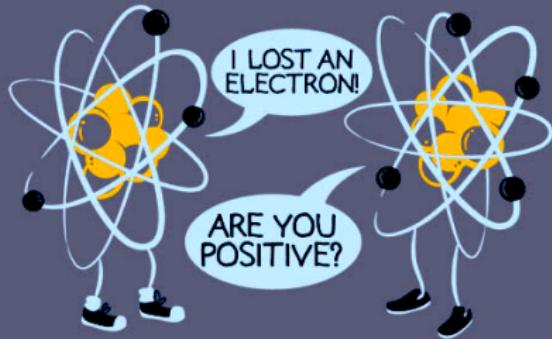
3 de Septiembre – Buenos Aires



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)

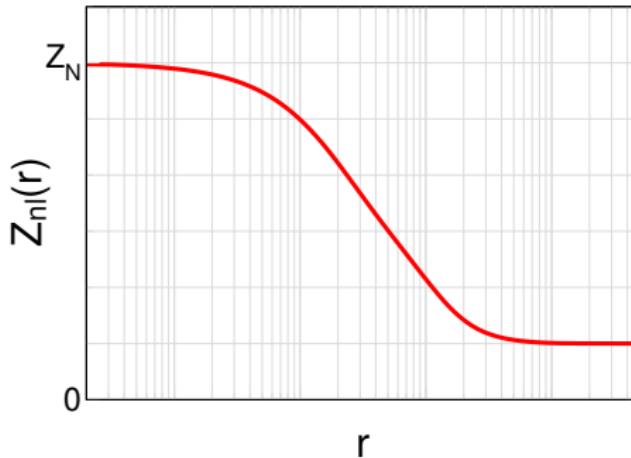
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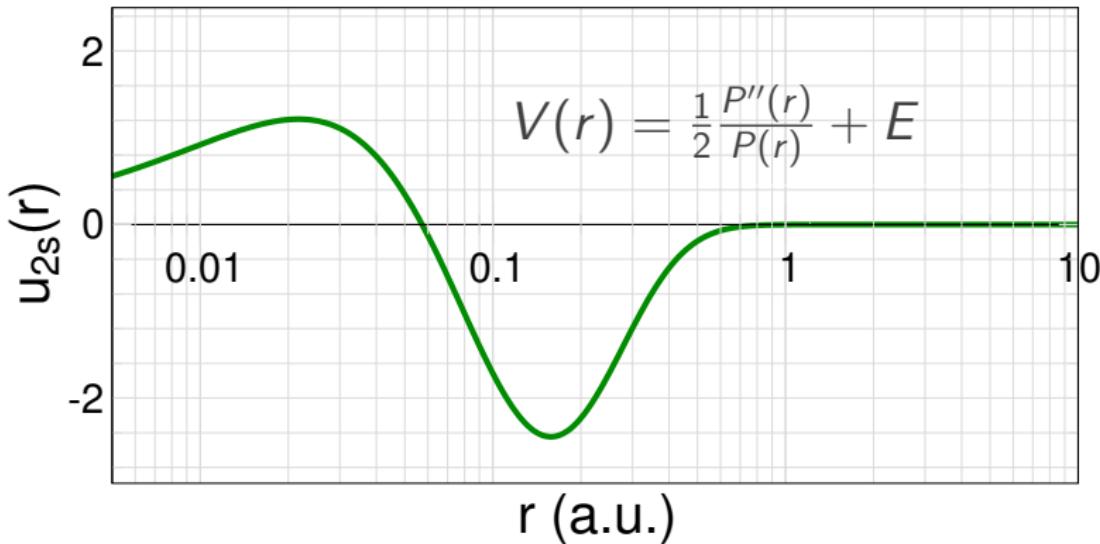
$$V_{nl}(r) = \frac{1}{2} \frac{P''_{nl}(r)}{P_{nl}(r)} - \frac{l(l+1)}{2r^2} + E_{nl}$$



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

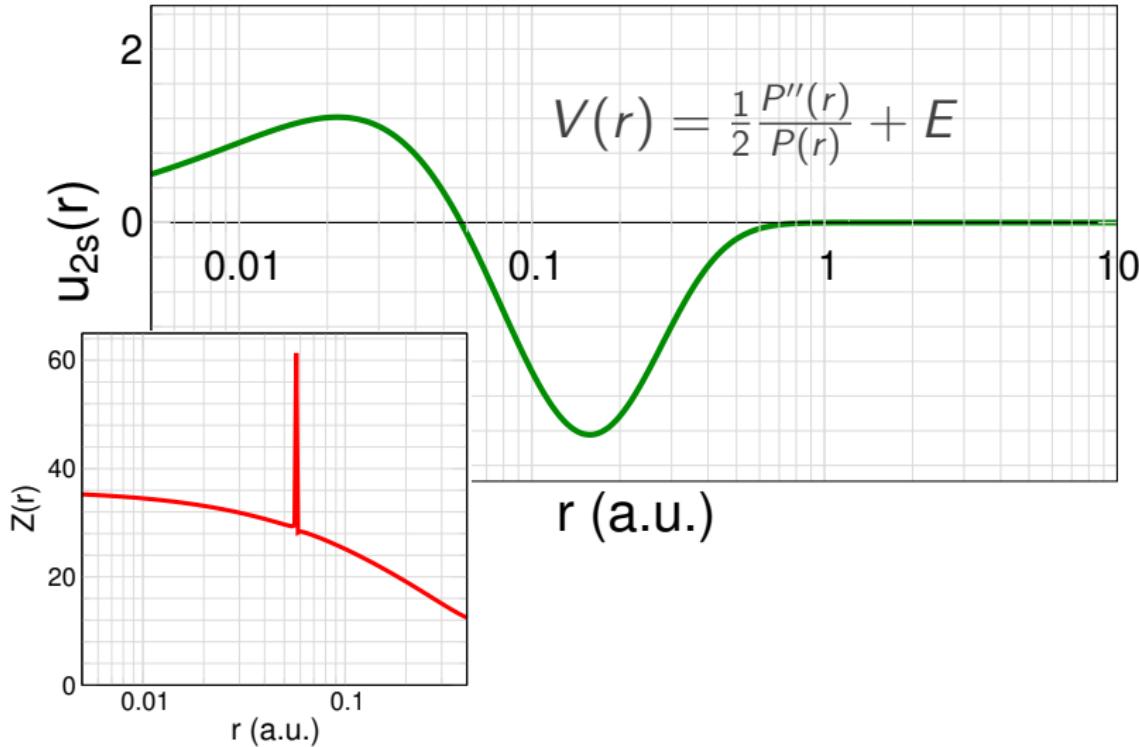
Houston, we have a problem!

Kr



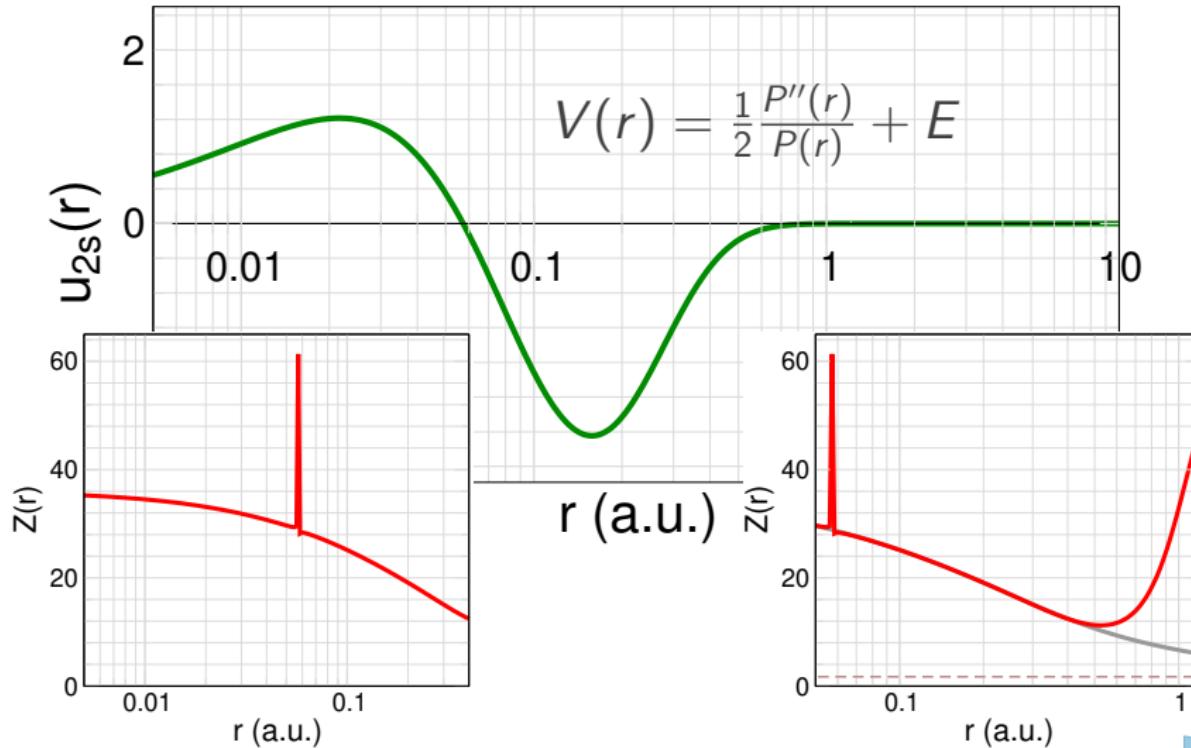
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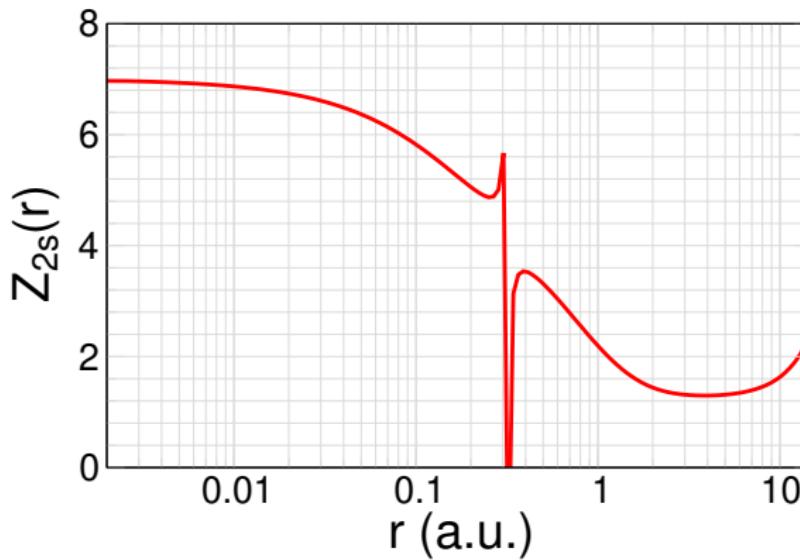
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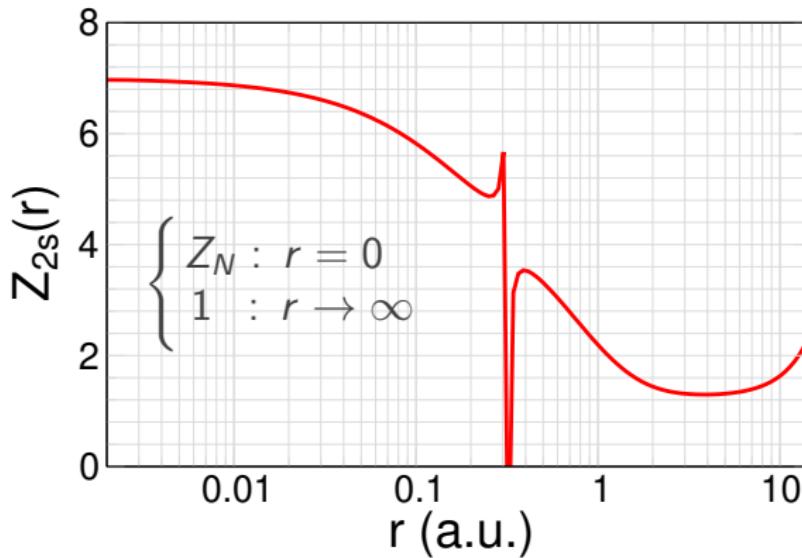
Depuración

N



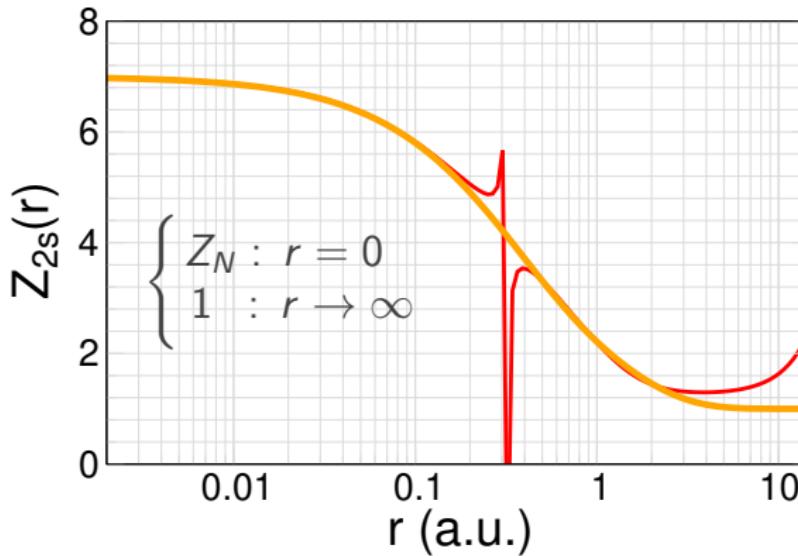
Depuración

N



Depuración

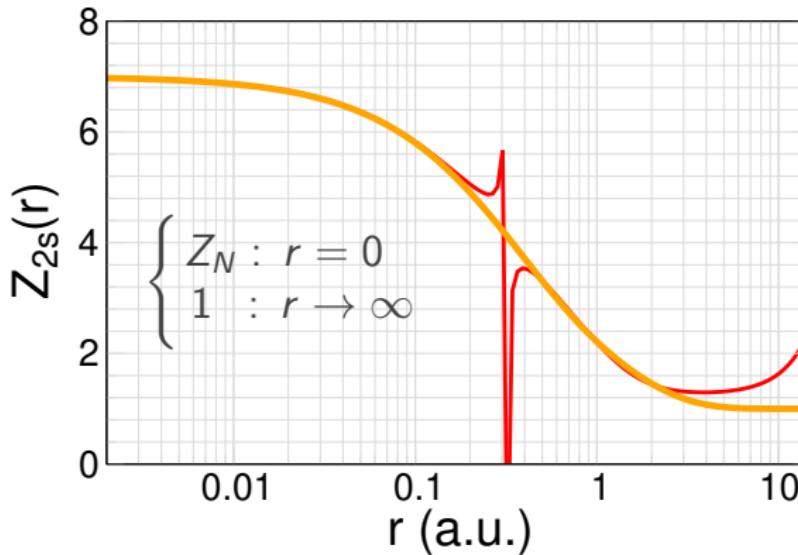
N



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

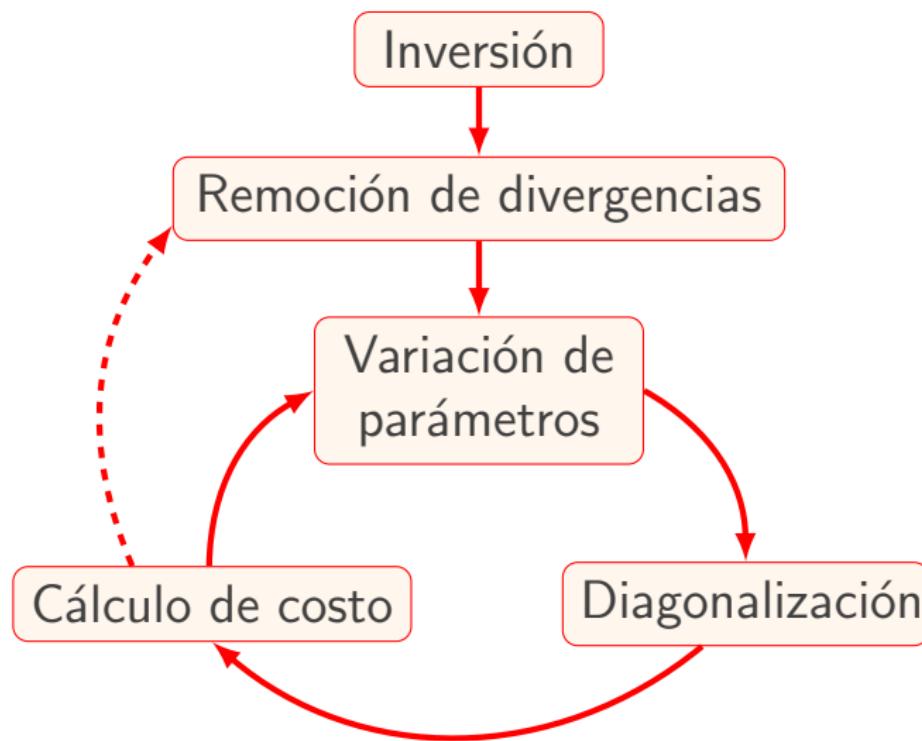
Depuración

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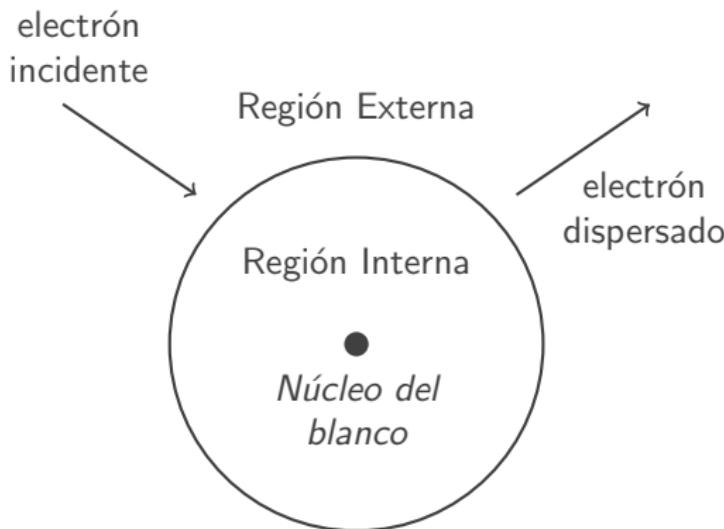
Procedimiento



Problema 2:

Cálculos colisionales (R-Matrix)

R-Matrix



Estructura del blanco

AUTOSTRUCTURE



Región Interna

RMATRXI



Región Externa

STGF

Descripción del blanco

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

Descripción del blanco

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N

Configuraciones

Descripción del blanco

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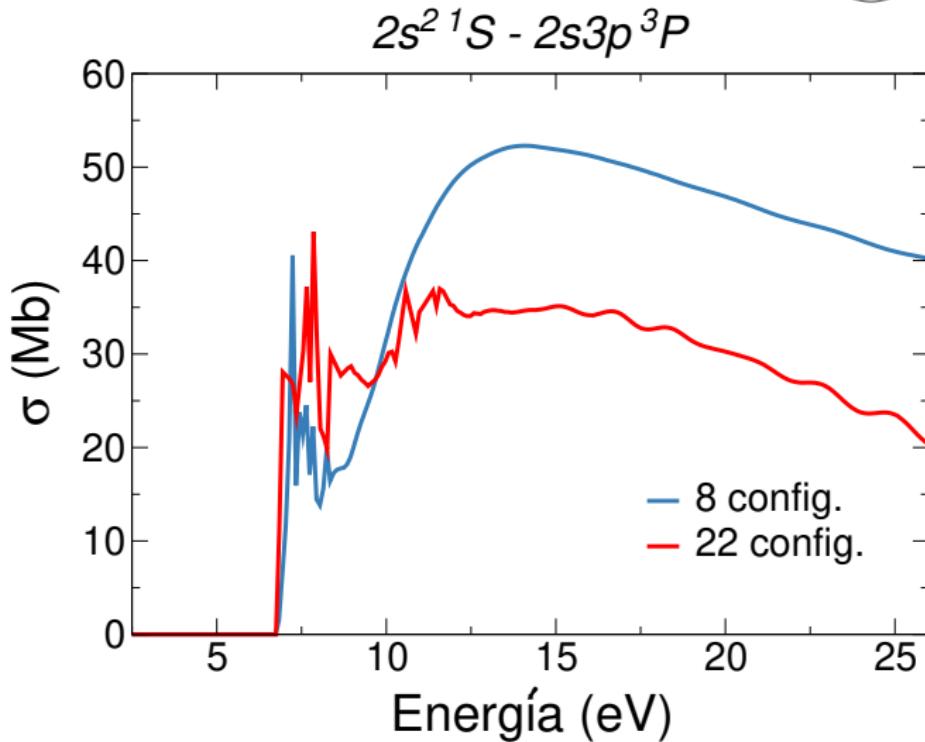
$$\left[\frac{1}{2} \frac{d^2}{dr^2} - \frac{l(l+1)}{2r^2} + V_{nl}^{\text{eff}}(\lambda_{nl}, r) + E_{nl} \right] P_{nl}(r) = 0$$

Parámetro de escaleo

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

Dependencia de CI (N)

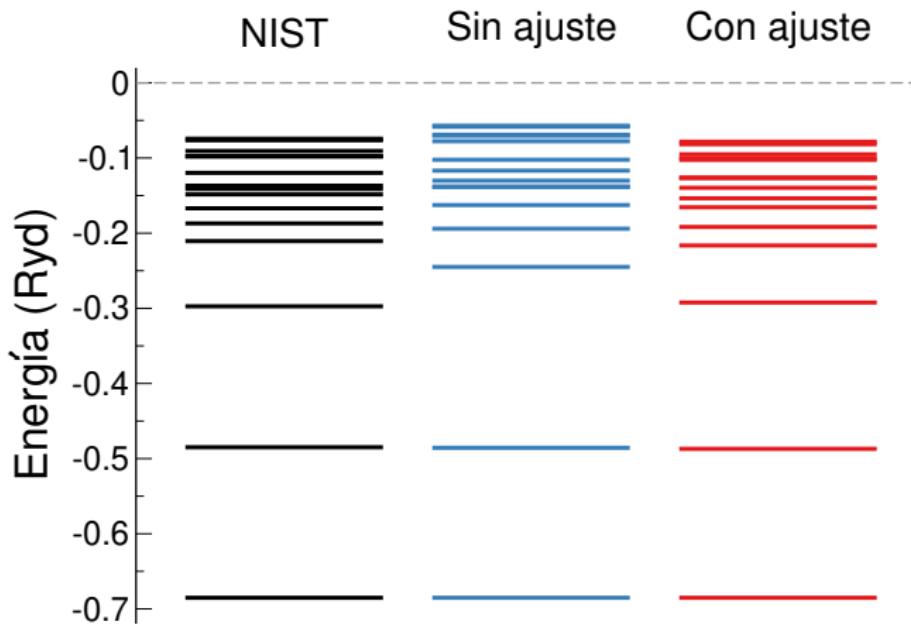
$1s^2 2s^2$
 $1s^2 2snl$
 $1s^2 2p^2$
 $1s^2 2pnl$



Be

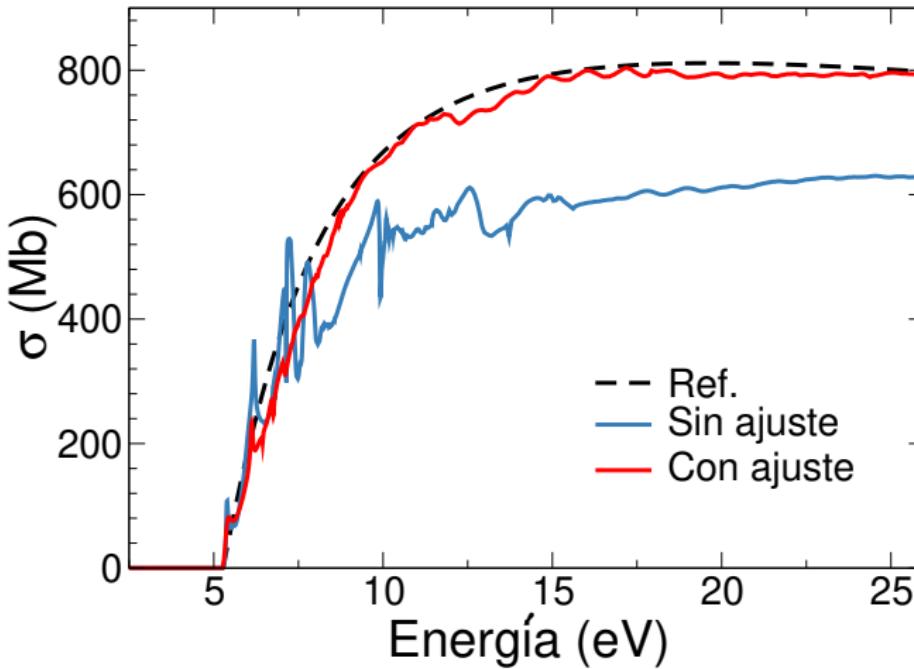
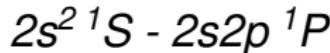
Dependencia de escaleo (λ_{nl})

Be

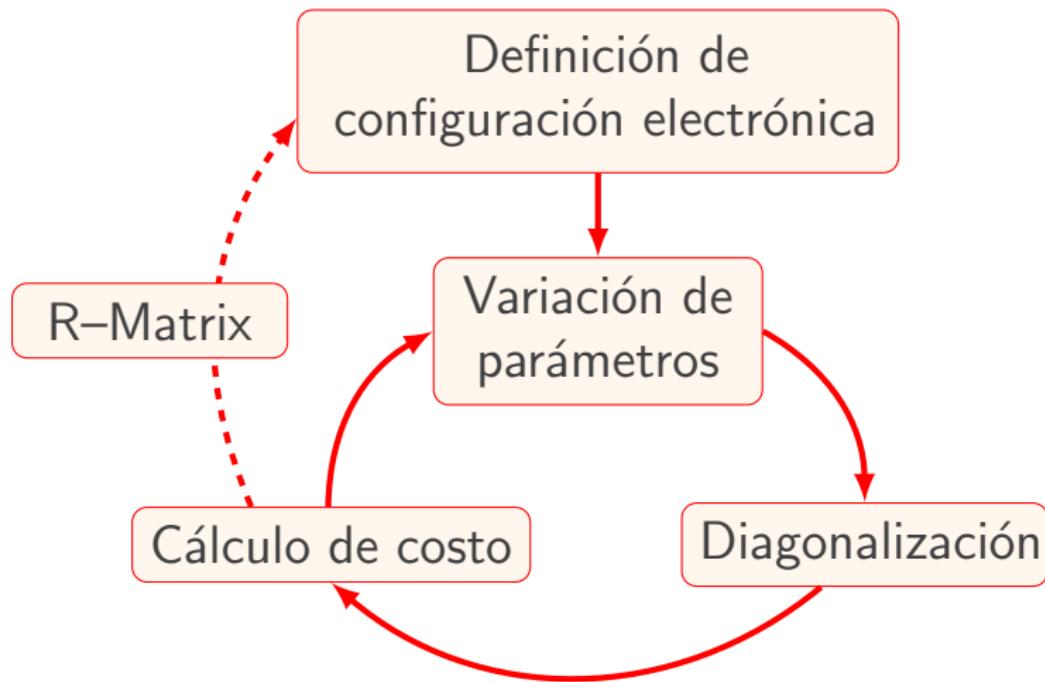


Dependencia de escaleo (λ_{nl})

Be



Procedimiento



Síntesis del problema

Función de costo:

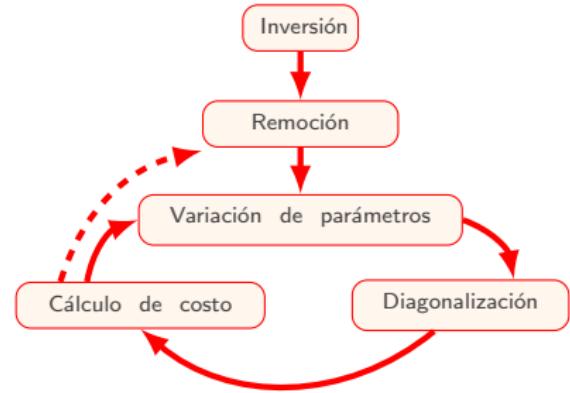
$$J = \sum_j \left| \frac{\tilde{E}_j(\xi) - E_j}{E_j} \right|$$

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

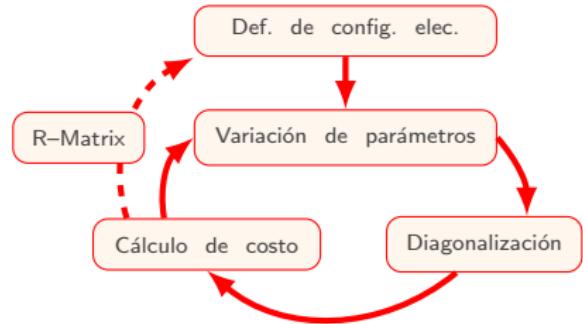
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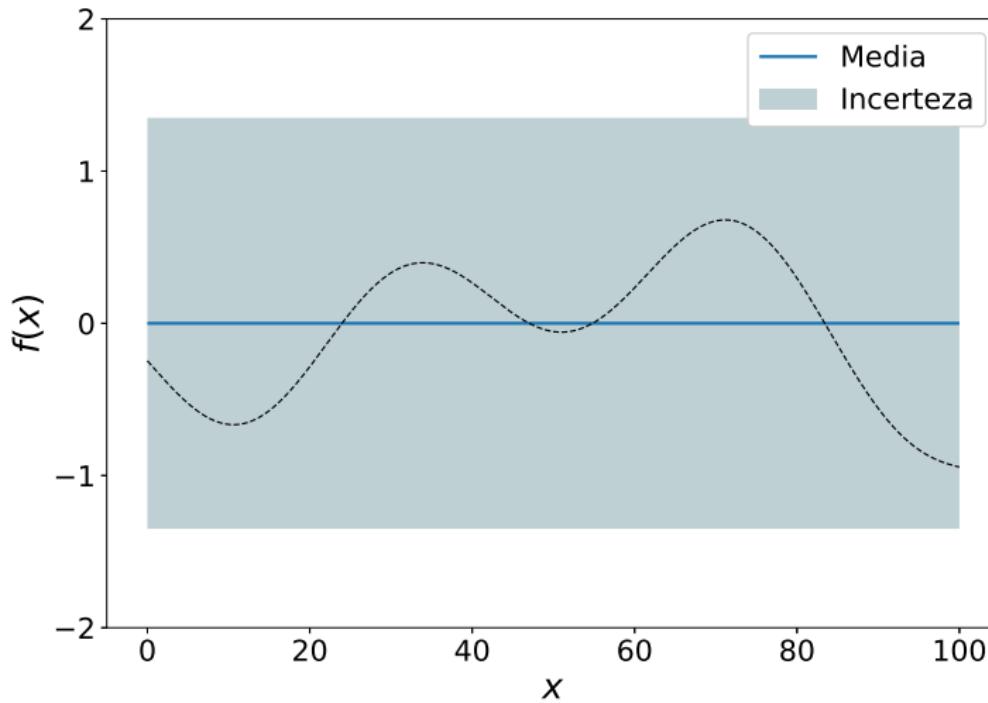


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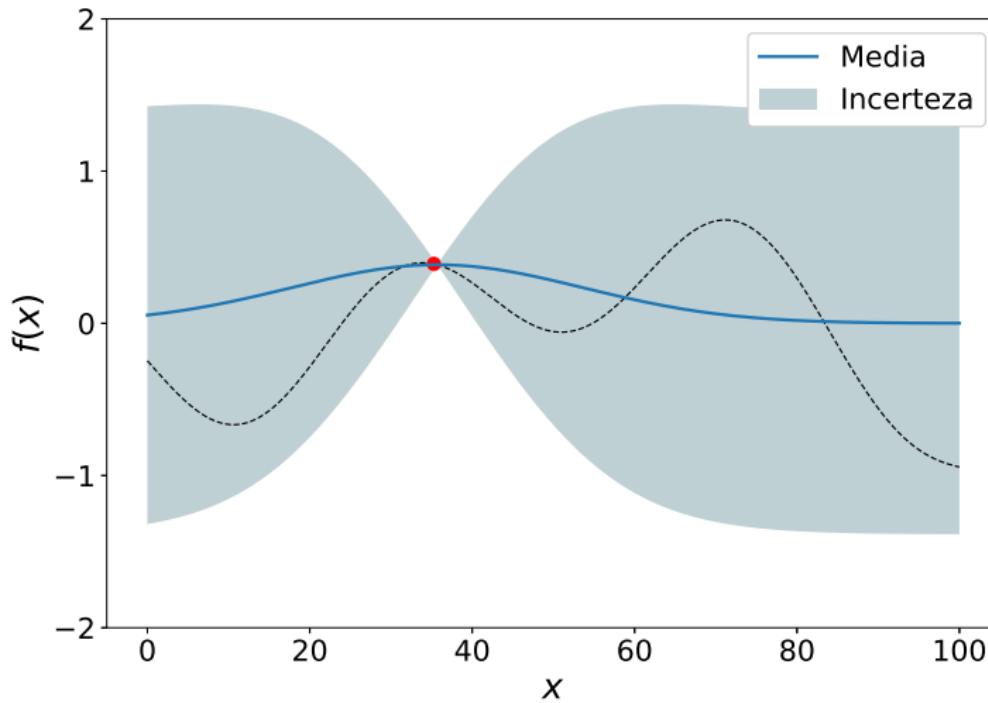


Optimización Bayesiana con Procesos Gaussianos

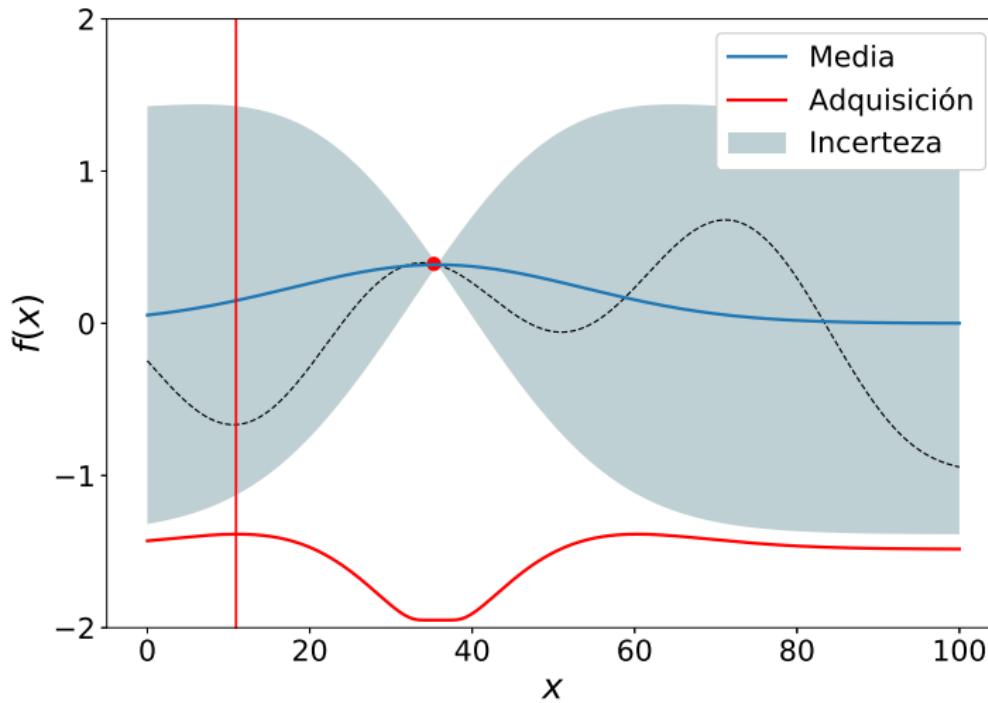
Procesos Gaussianos



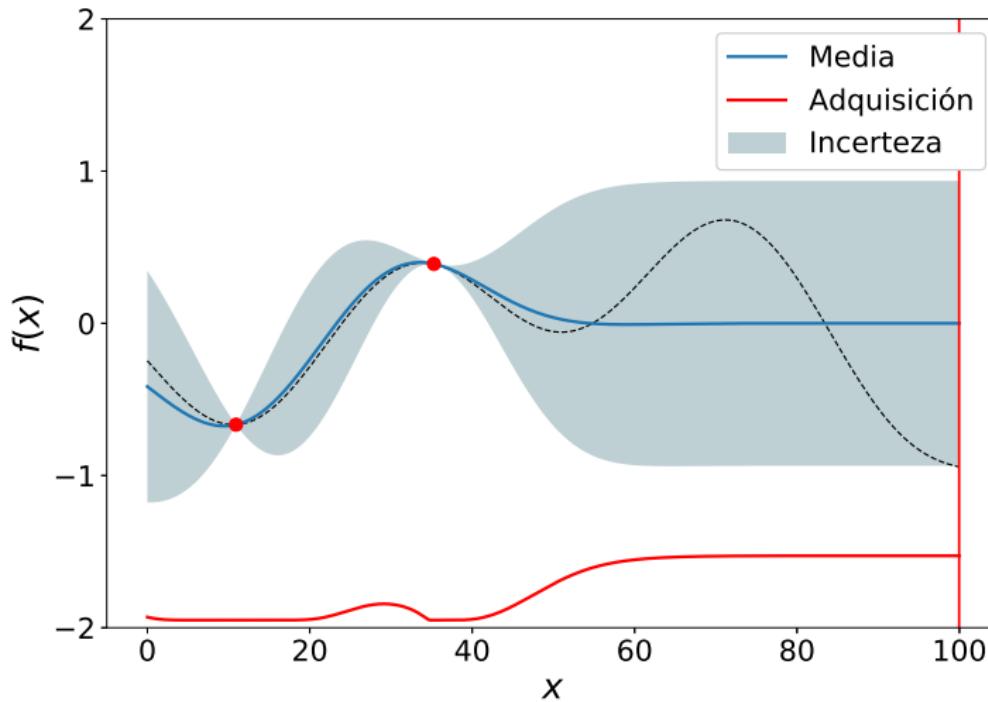
Procesos Gaussianos



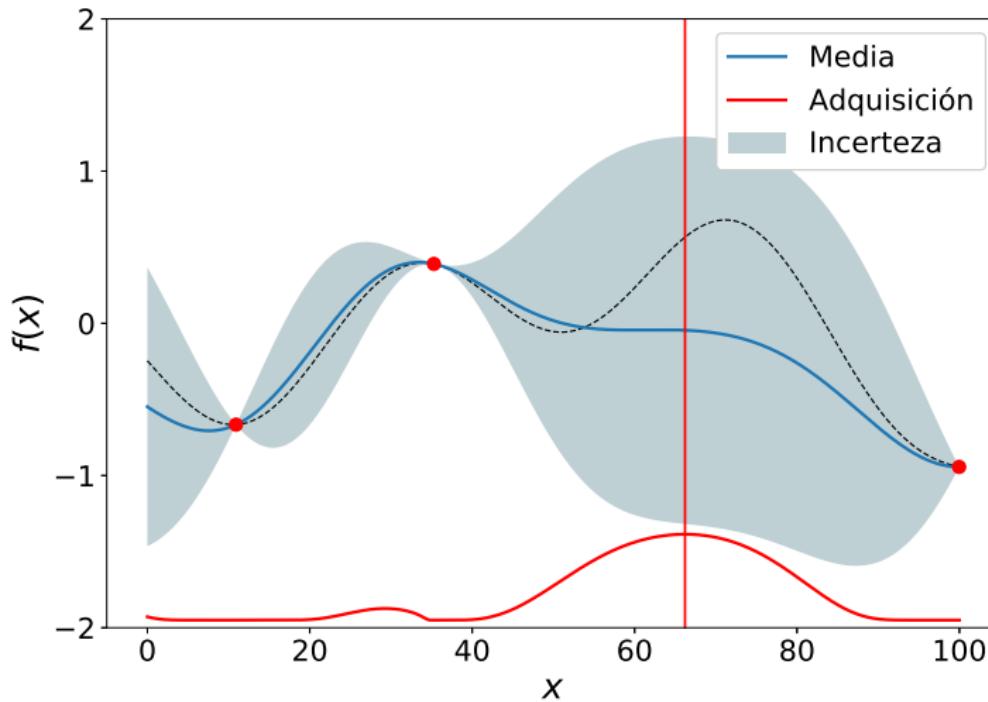
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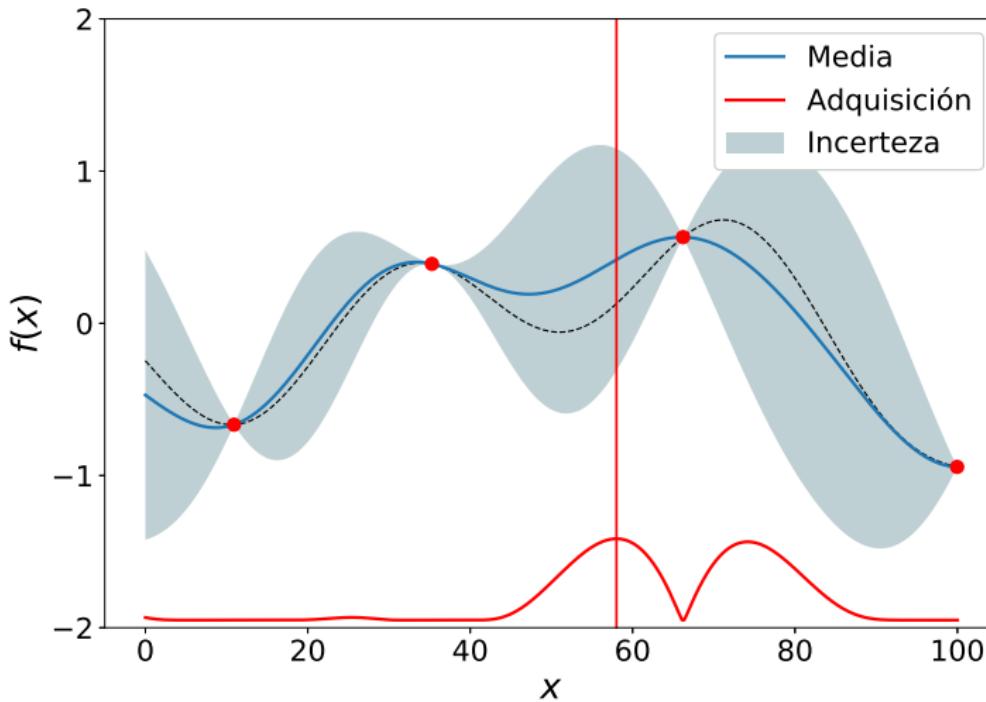
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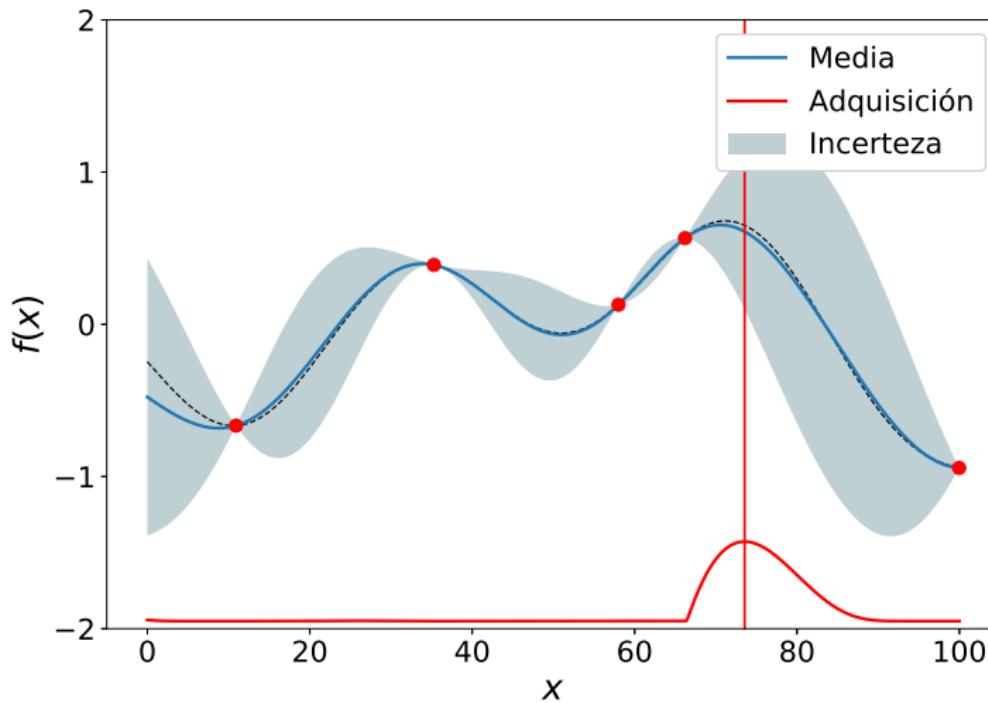
Procesos Gaussianos



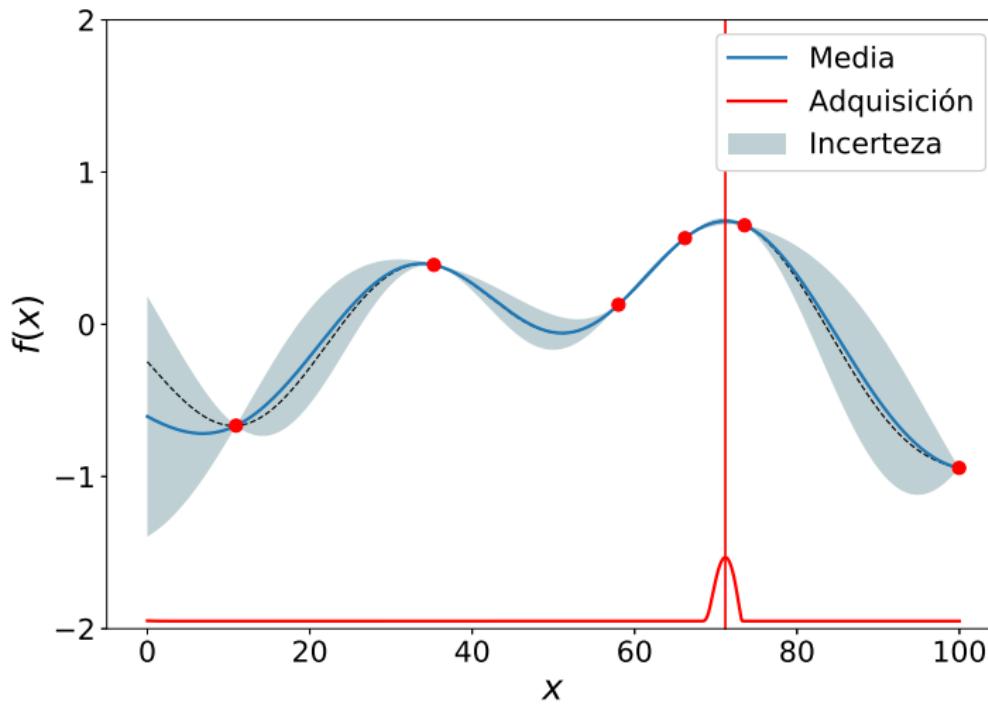
Procesos Gaussianos



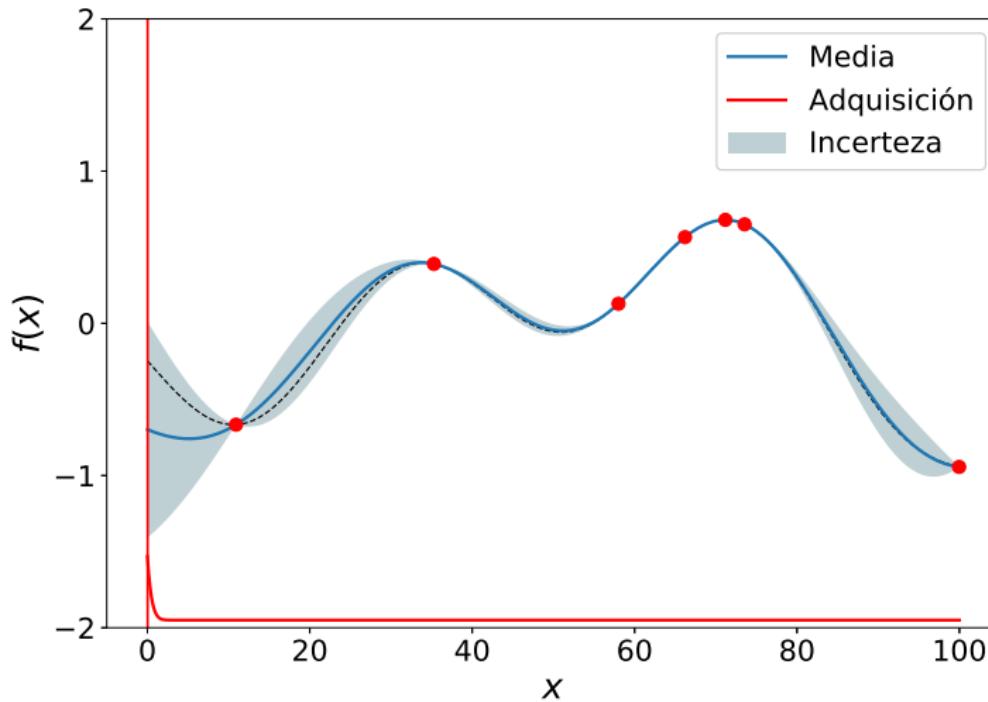
Procesos Gaussianos



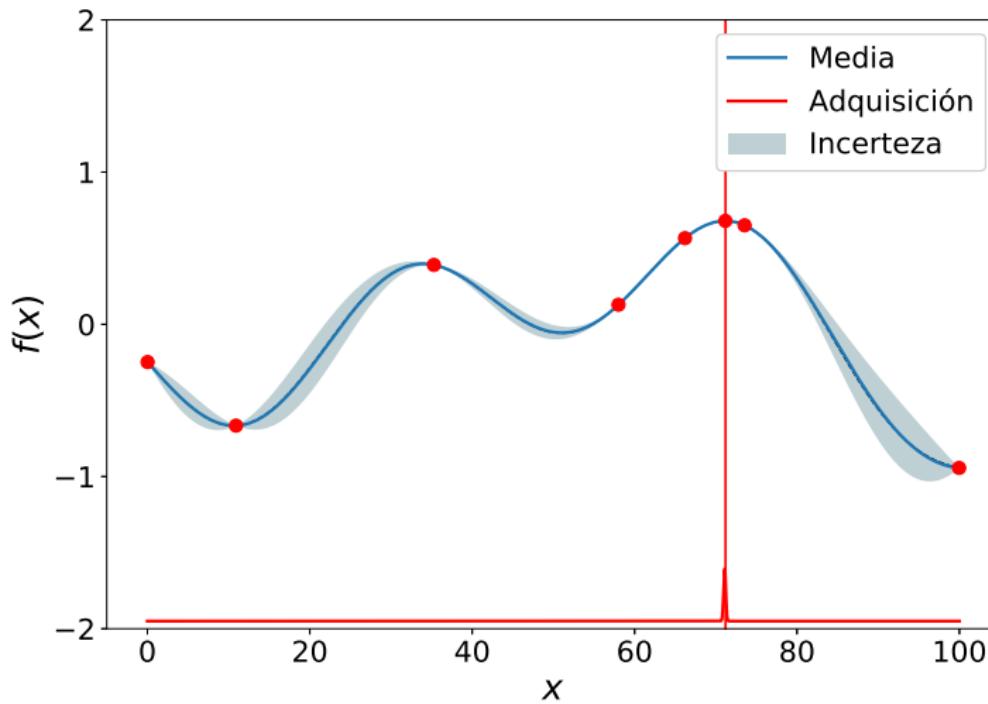
Procesos Gaussianos



Procesos Gaussianos

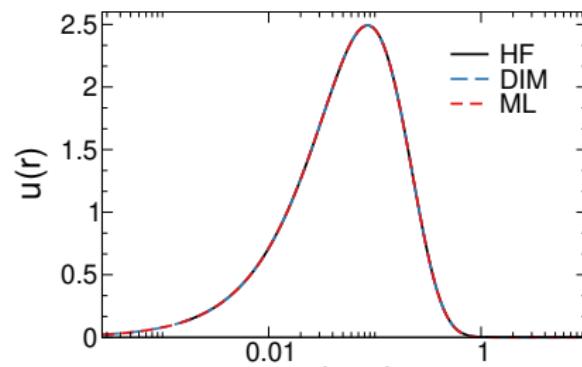
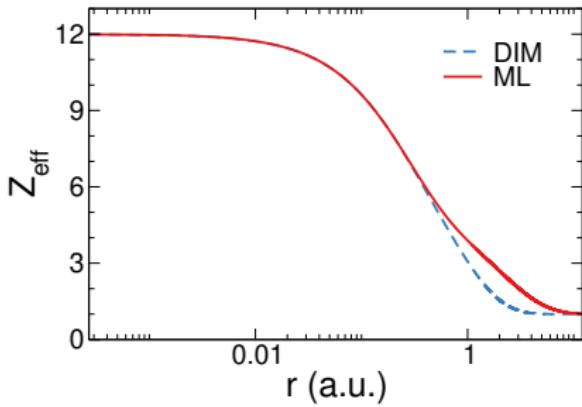


Procesos Gaussianos

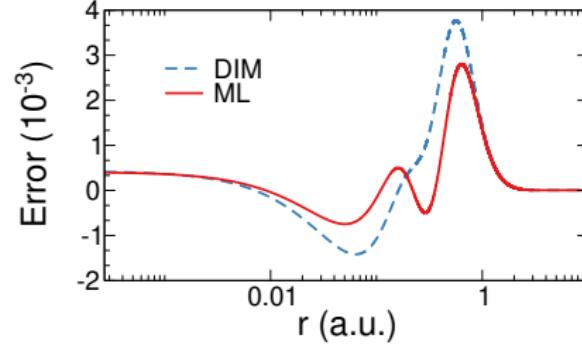


Resultados

DIM: Mg



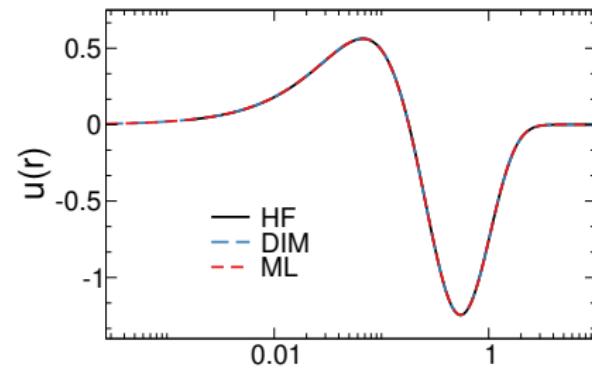
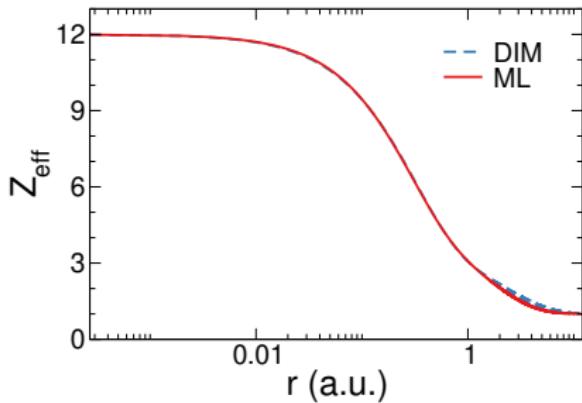
E ✓
 $\langle r \rangle$ $10^{-2} \%$
 $\langle 1/r \rangle$



1s

DIM: Mg

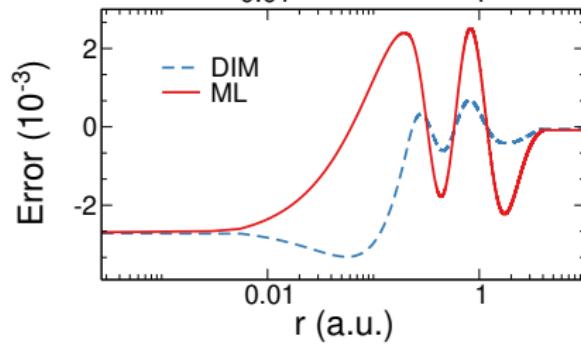
2s



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

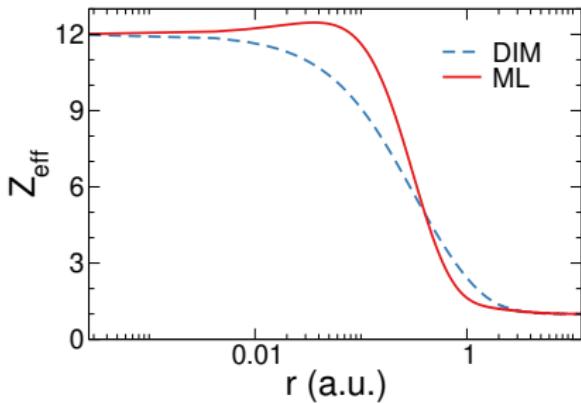
✓

$10^{-2} \%$

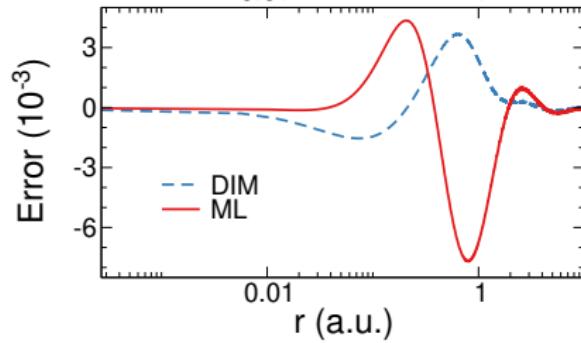
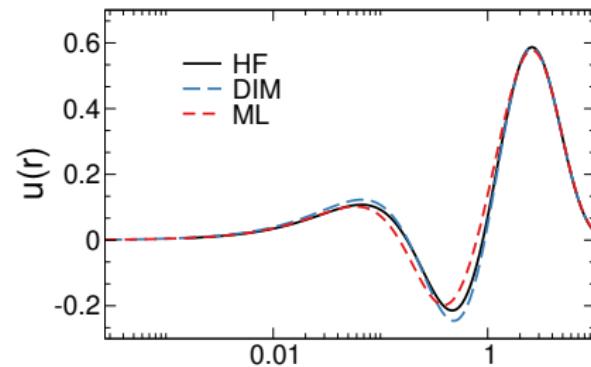




DIM: Mg

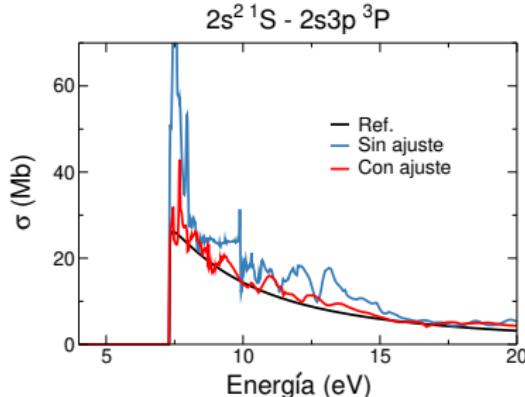
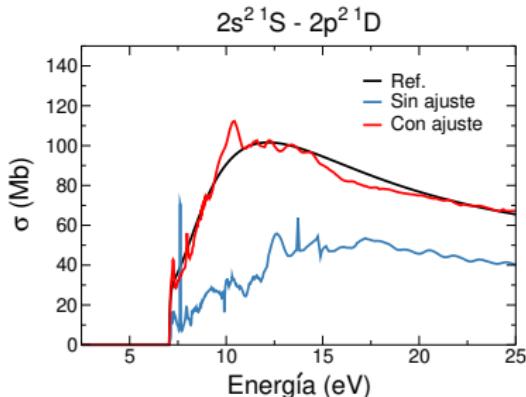
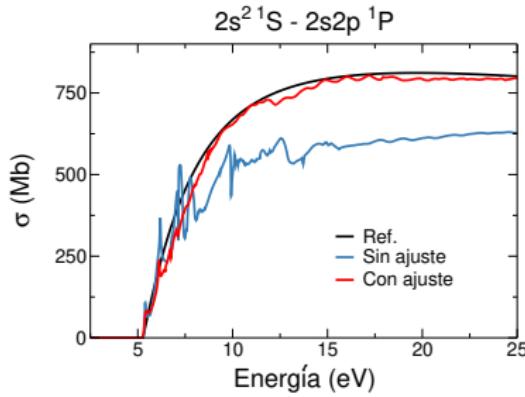
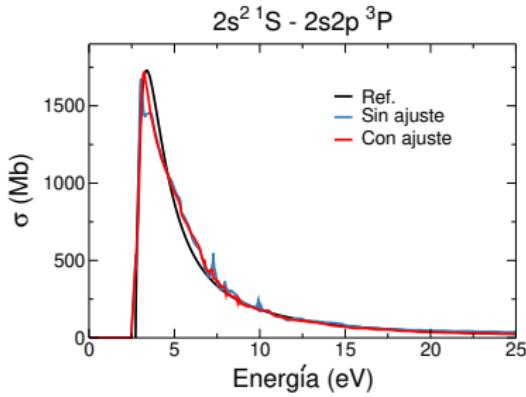


$$\begin{matrix} E \\ \langle r \rangle \\ \langle 1/r \rangle \end{matrix} \quad \checkmark \quad 10^{-1}\%$$



3s

R-Matrix: Be



Conclusiones

- Estudiamos métodos y herramientas de aprendizaje automatizado

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 - Estructura del blanco en R-Matrix

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 área

