

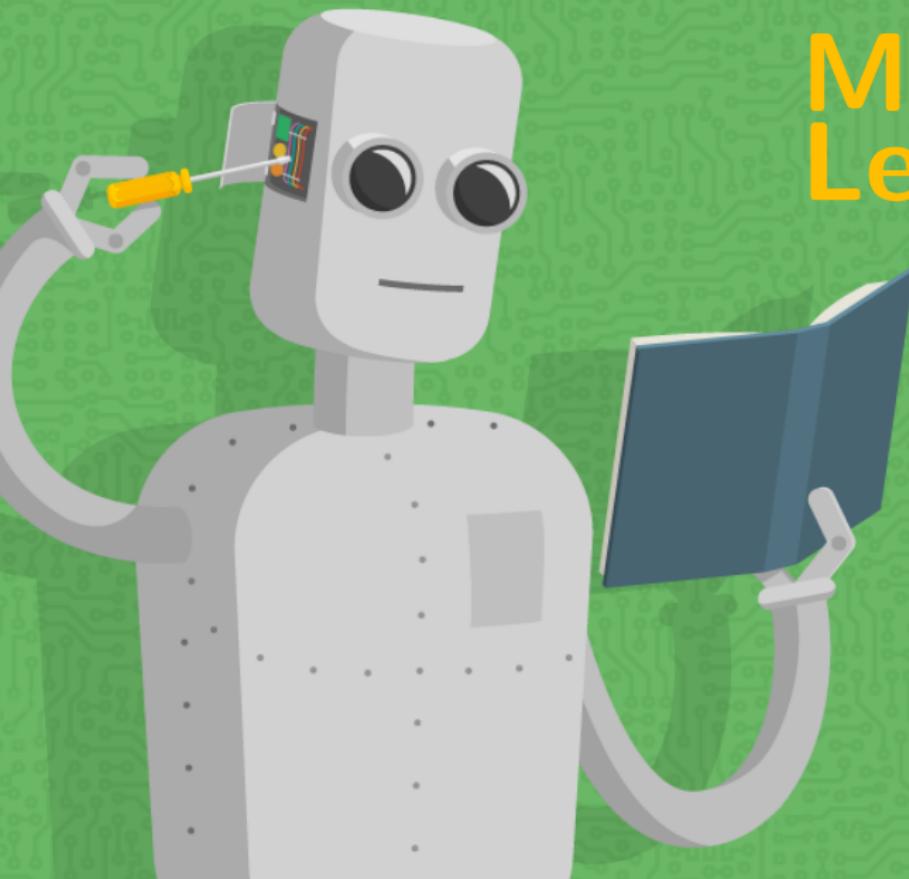
Implementación de Métodos de Aprendizaje Automatizado en problemas colisionales



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

alemendez@iafe.uba.ar

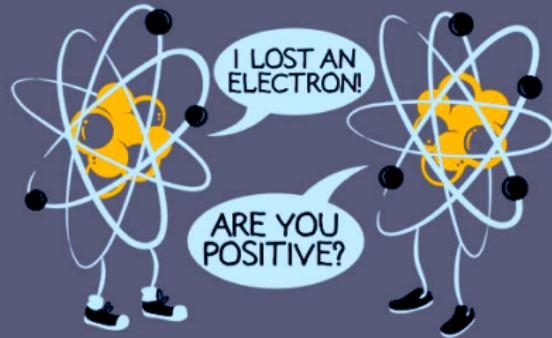
3 de Septiembre – Buenos Aires



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)

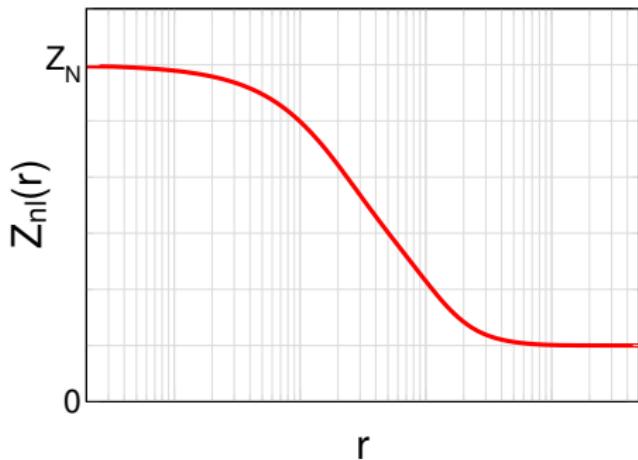
$$\left[-\frac{1}{2} \frac{d^2}{dr^2} + \frac{l(l+1)}{2r^2} + V_{nl}(r) \right] P_{nl}(r) = E_{nl} P_{nl}(r)$$

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

Método de Inversión Depurada (DIM)

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

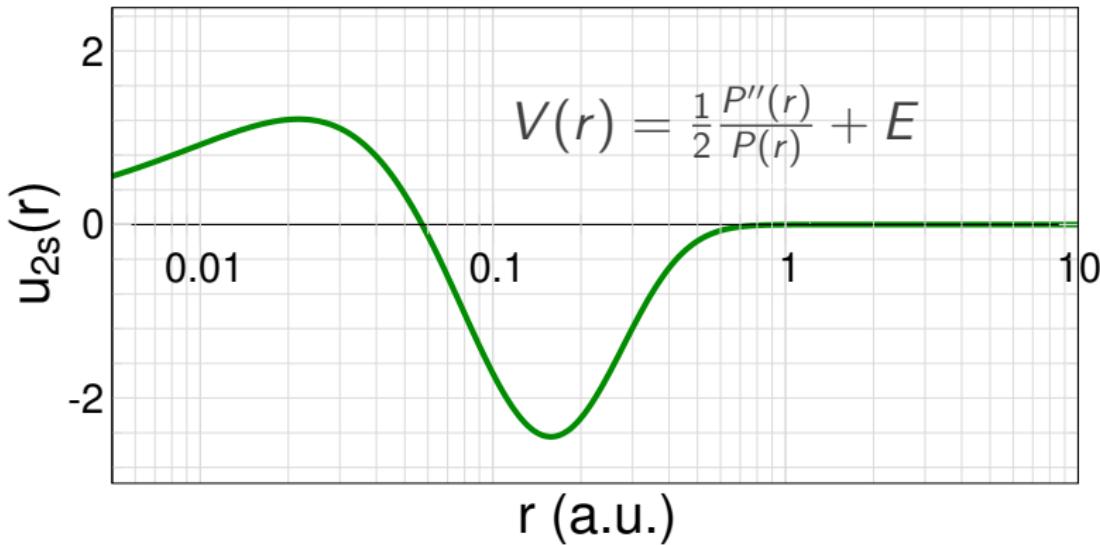
$$V_{nl}(r) = \frac{1}{2} \frac{P''_{nl}(r)}{P_{nl}(r)} - \frac{l(l+1)}{2r^2} + E_{nl}$$



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

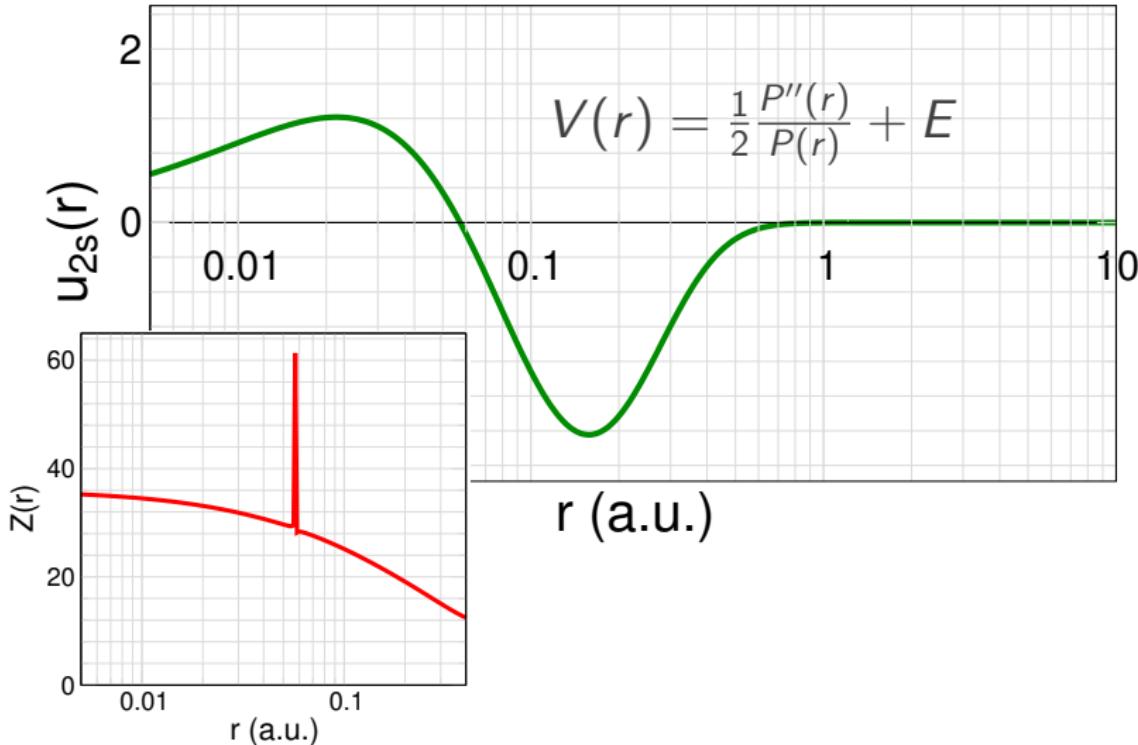
Houston, we have a problem!

Kr



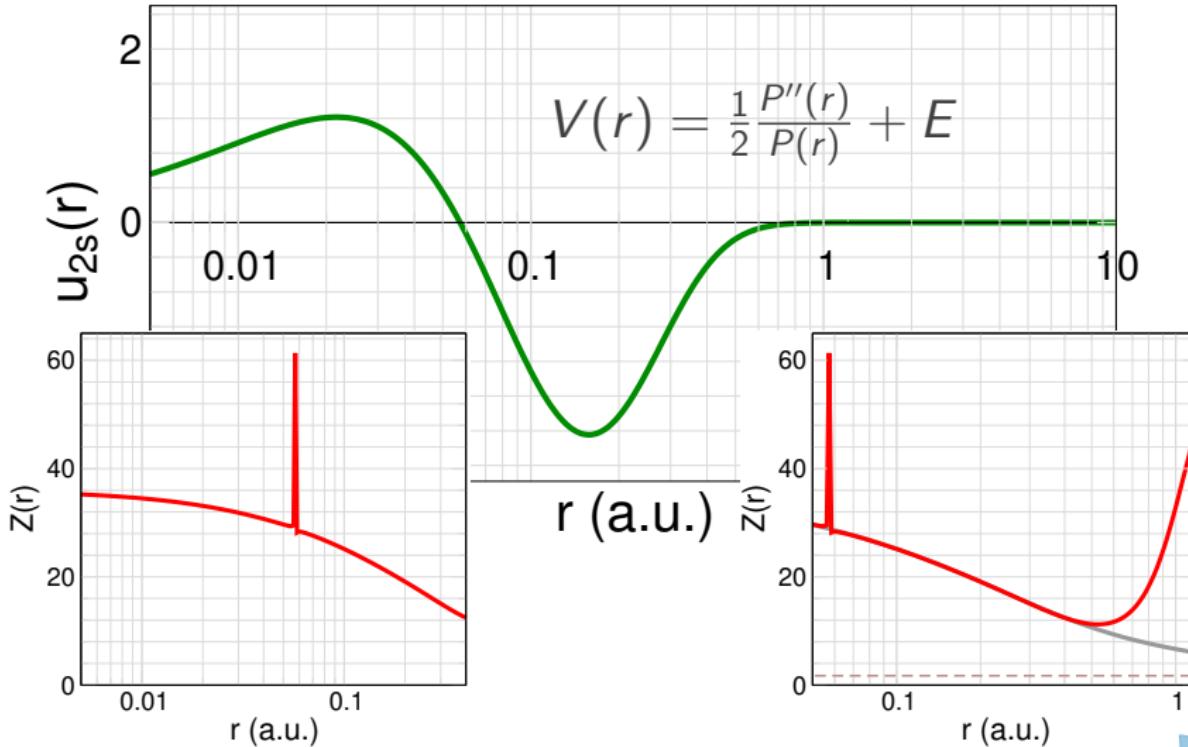
Houston, we have a problem!

Kr



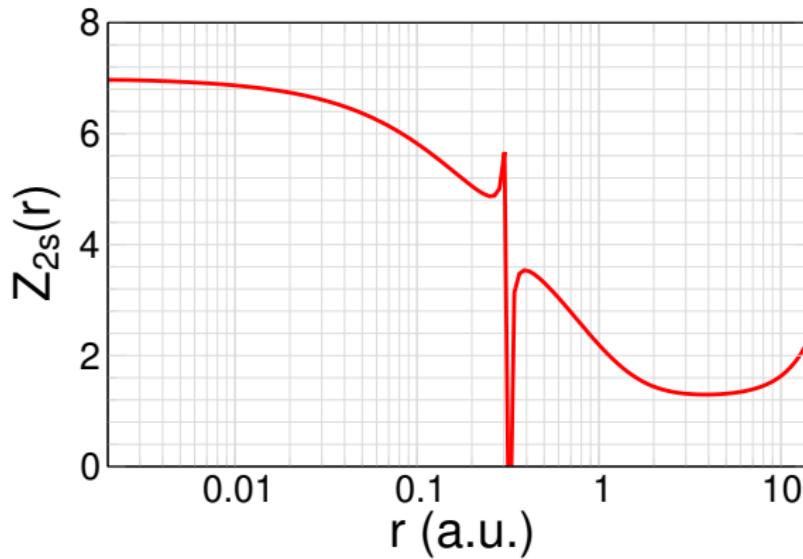
Houston, we have a problem!

Kr



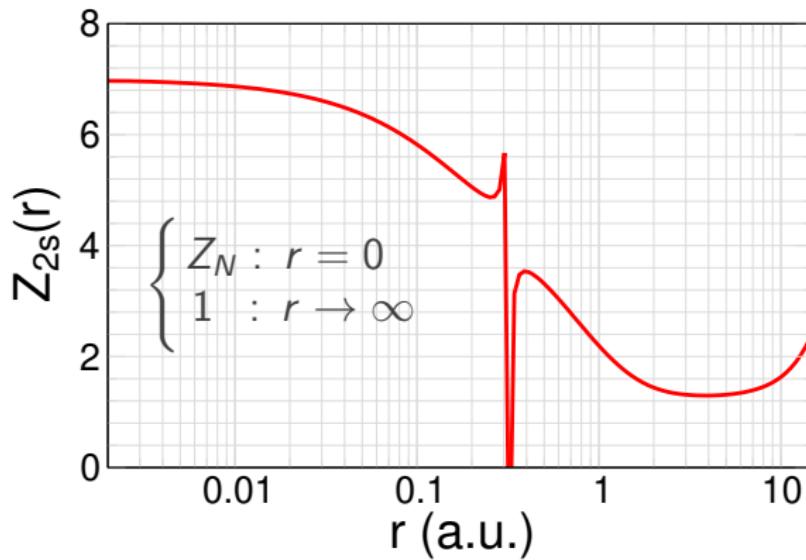
Depuración

N



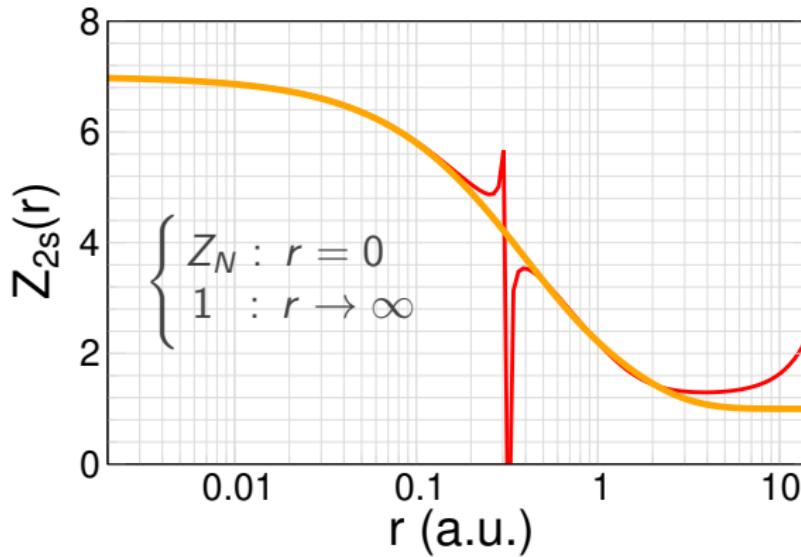
Depuración

N



Depuración

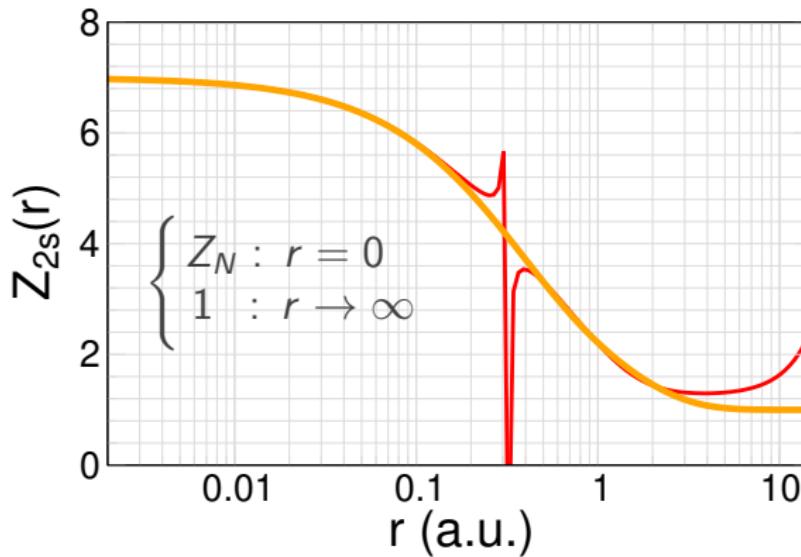
N



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

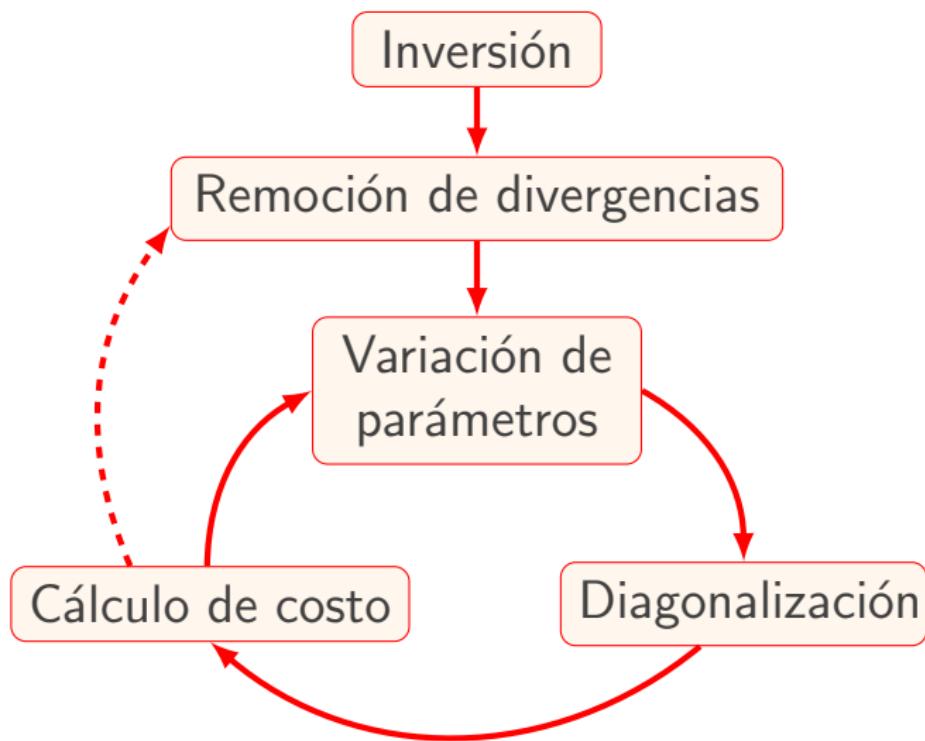
Depuración

N



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

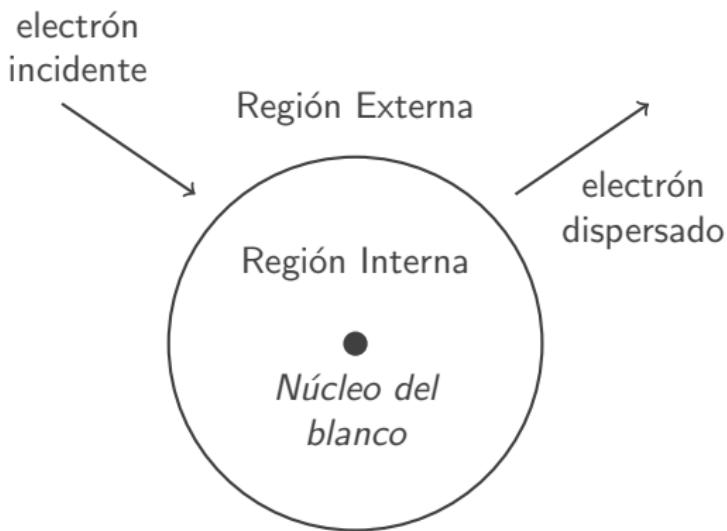
Procedimiento



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

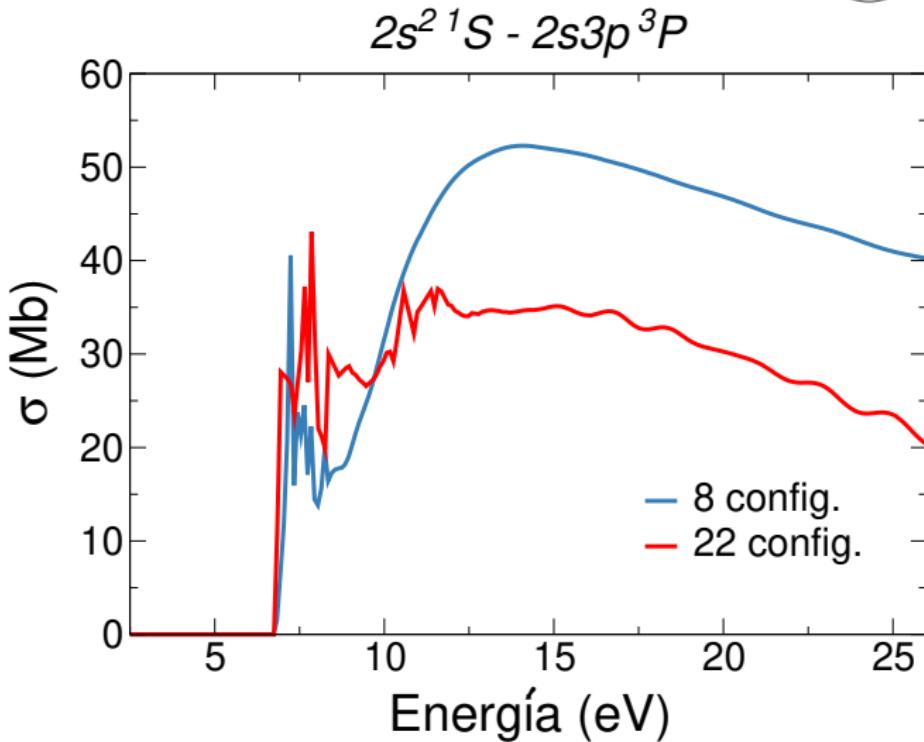
$$\left[\frac{1}{2} \frac{d^2}{dr^2} - \frac{l(l+1)}{2r^2} + V_{nl}^{\text{eff}}(\lambda_{nl}, r) + E_{nl} \right] P_{nl}(r) = 0$$

Parámetro de escaleo

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

Dependencia de CI (N)

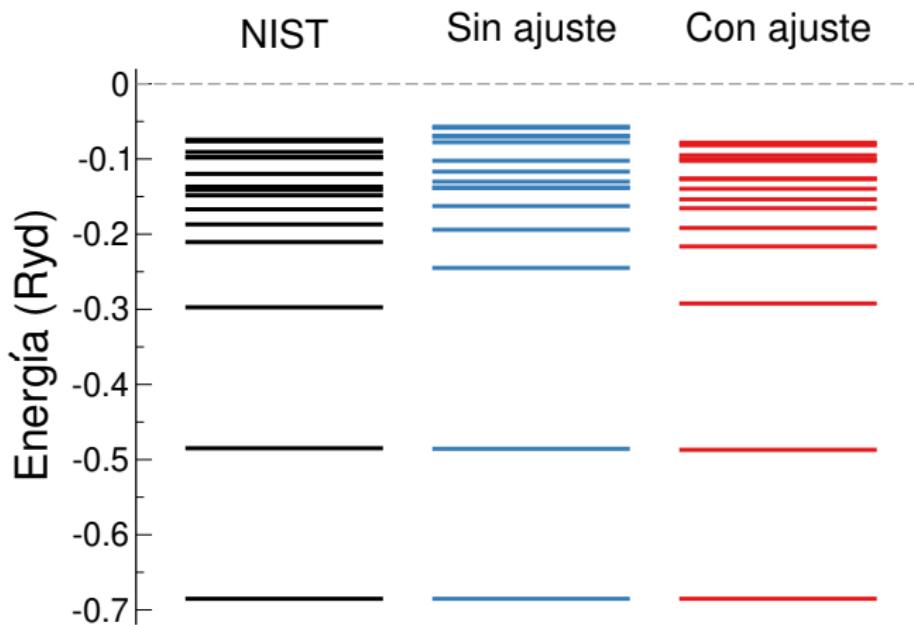
$1s^2 2s^2$
 $1s^2 2snl$
 $1s^2 2p^2$
 $1s^2 2pnl$



Be

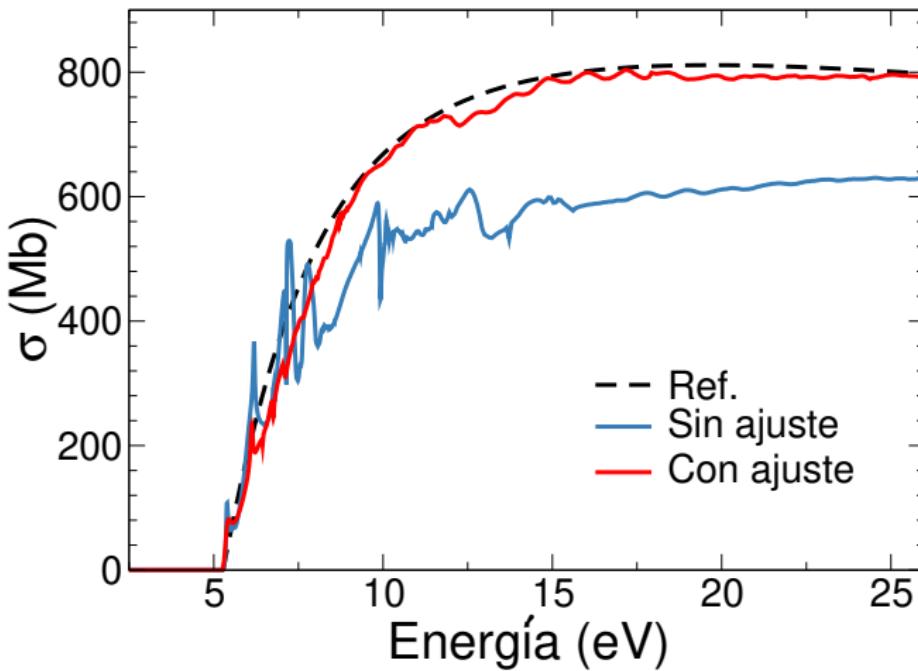
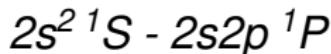
Dependencia de escaleo (λ_{nl})

Be

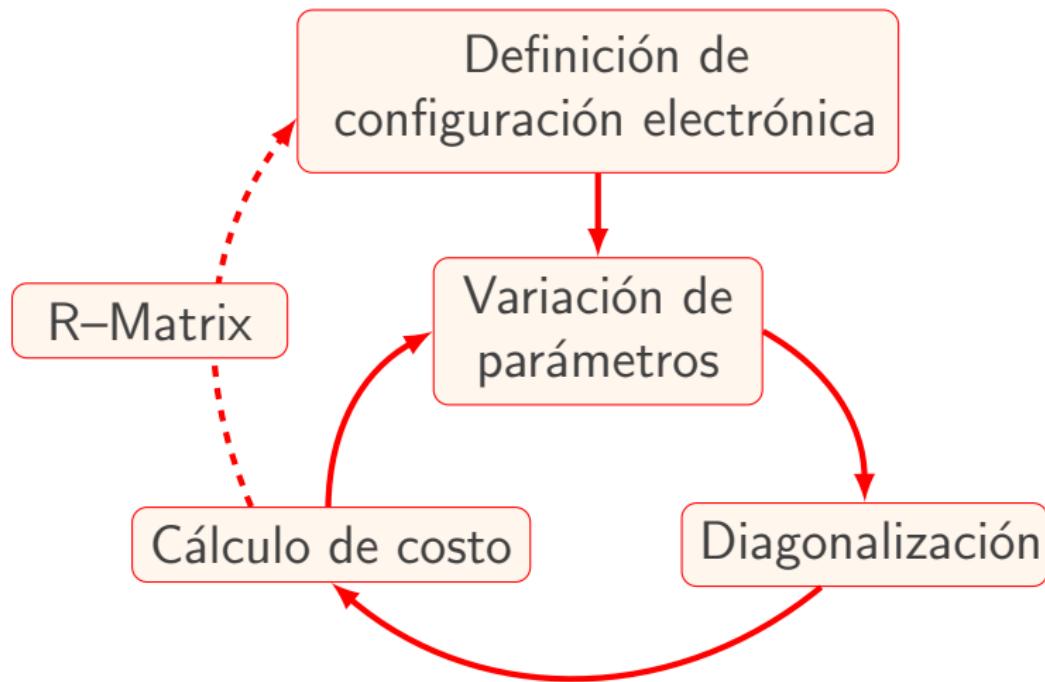


Dependencia de escaleo (λ_{nl})

Be



Procedimiento



Síntesis del problema

Función de costo:

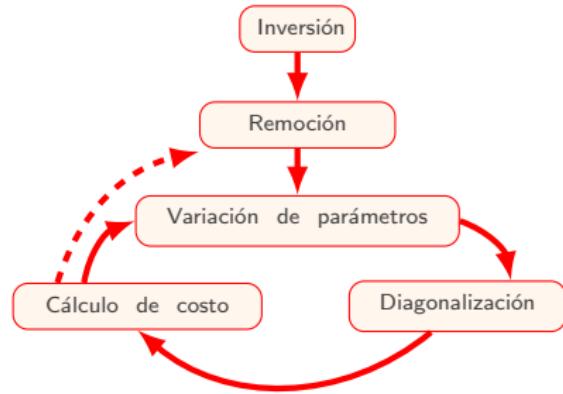
$$J = \sum_j \left| \frac{\tilde{E}_j(\xi) - E_j}{E_j} \right|$$

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

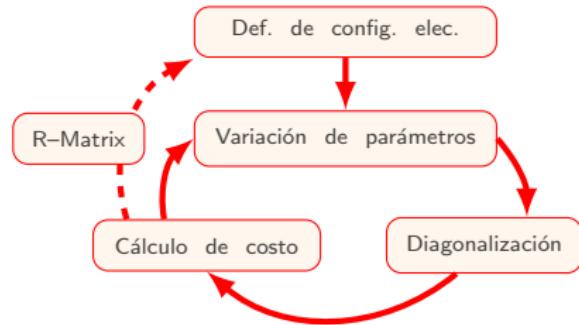
Síntesis del problema

Función de costo:

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

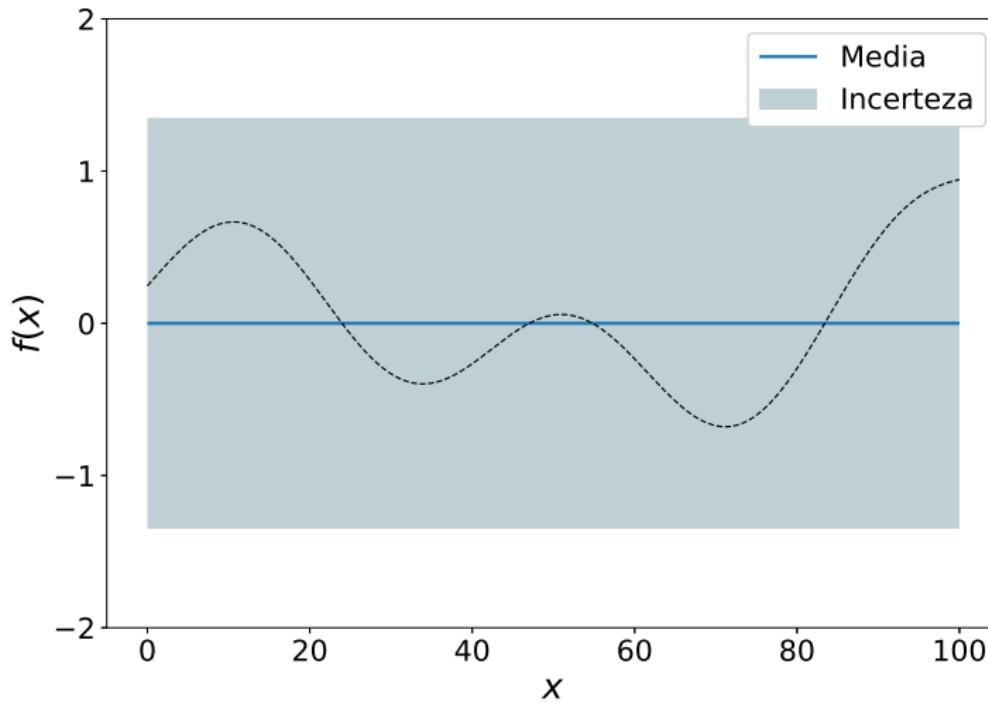


- DIM: $\xi = \{\alpha, \beta\}$
- R-Matrix: $\xi = \{N, \lambda\}$

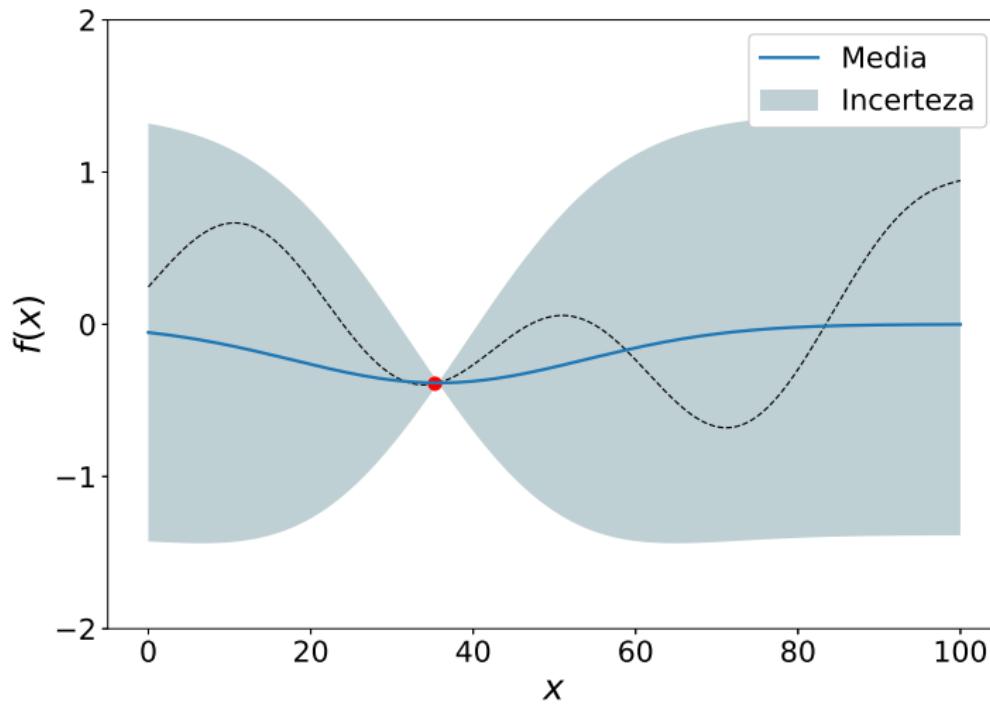


Optimización Bayesiana con Procesos Gaussianos

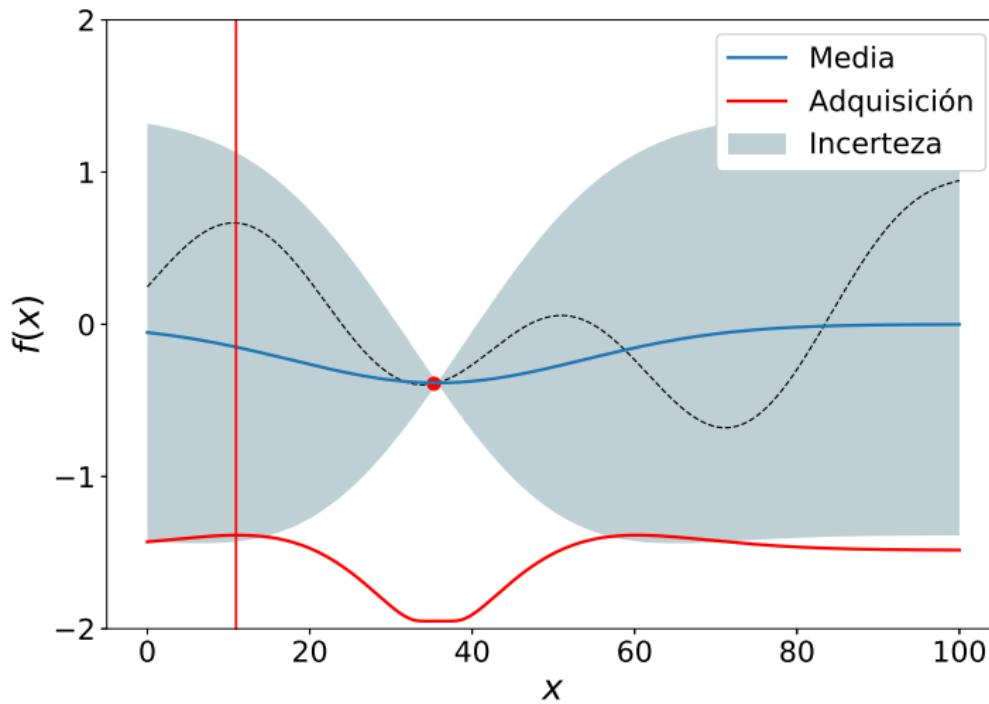
Procesos Gaussianos



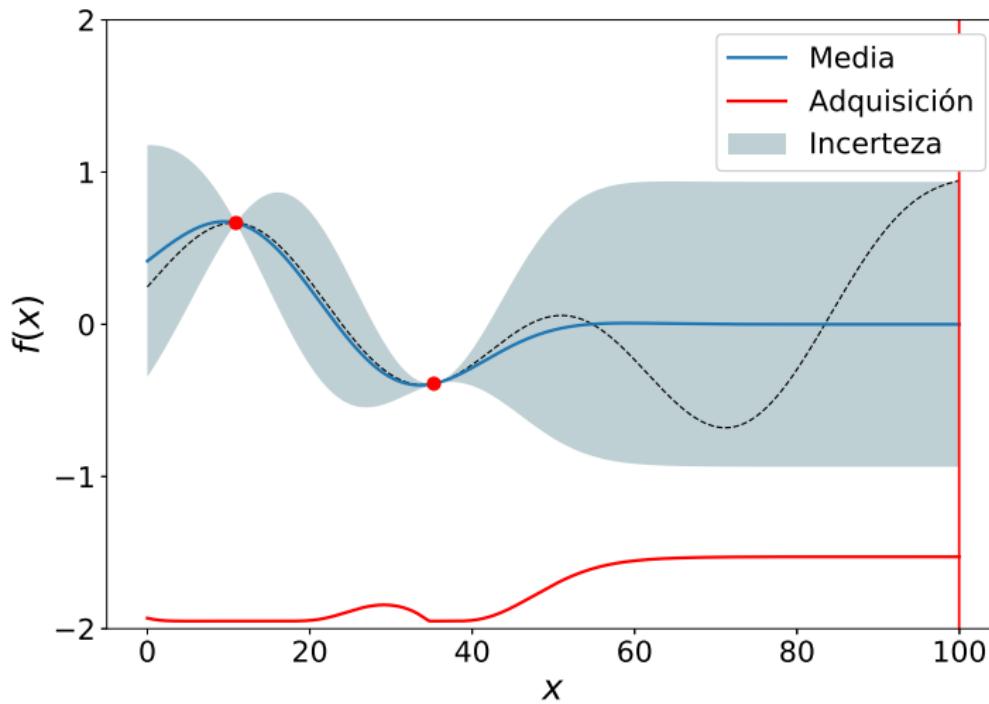
Procesos Gaussianos



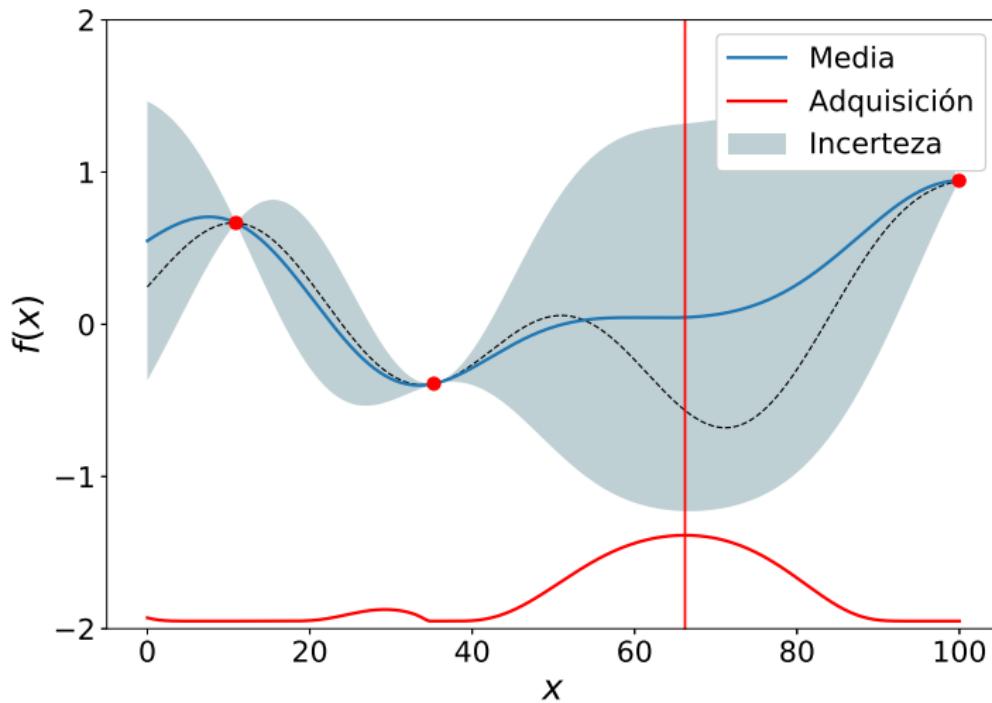
Procesos Gaussianos



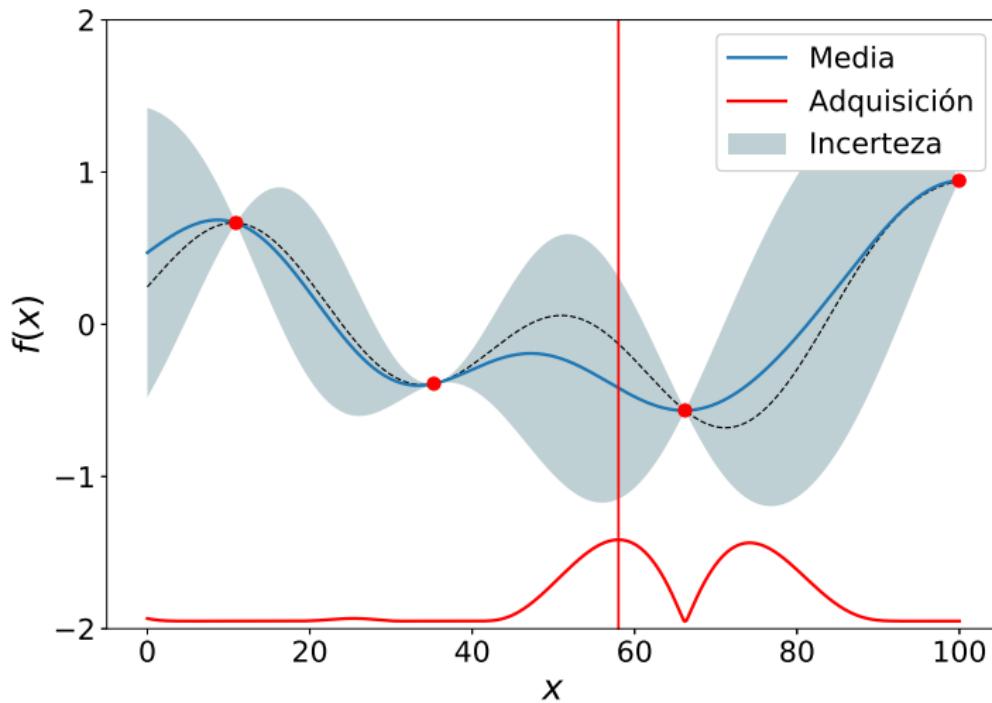
Procesos Gaussianos



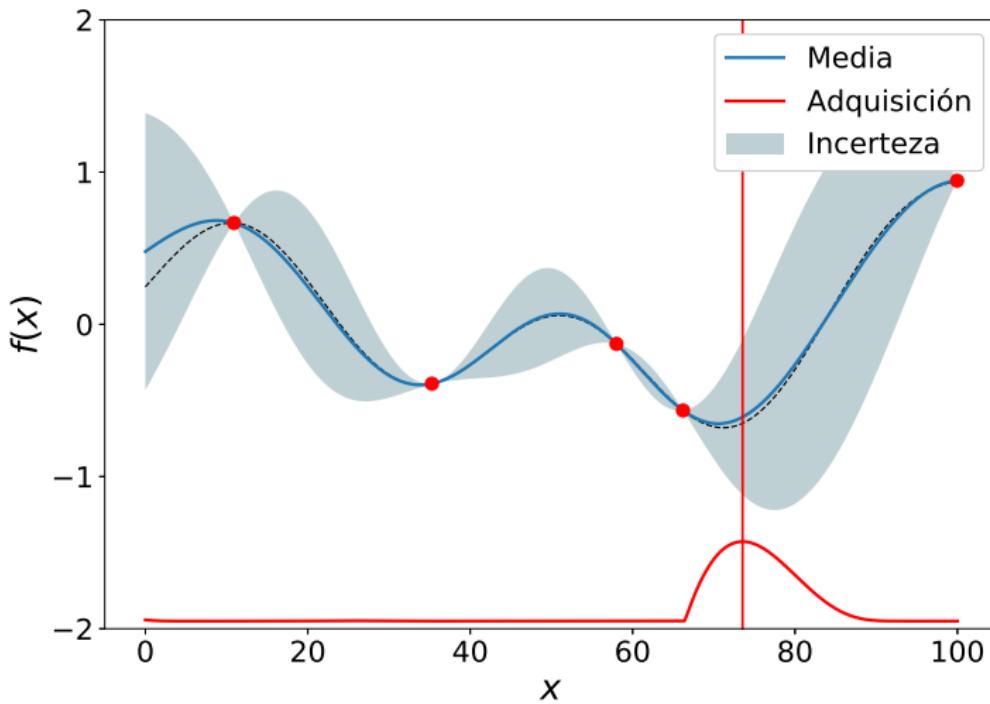
Procesos Gaussianos



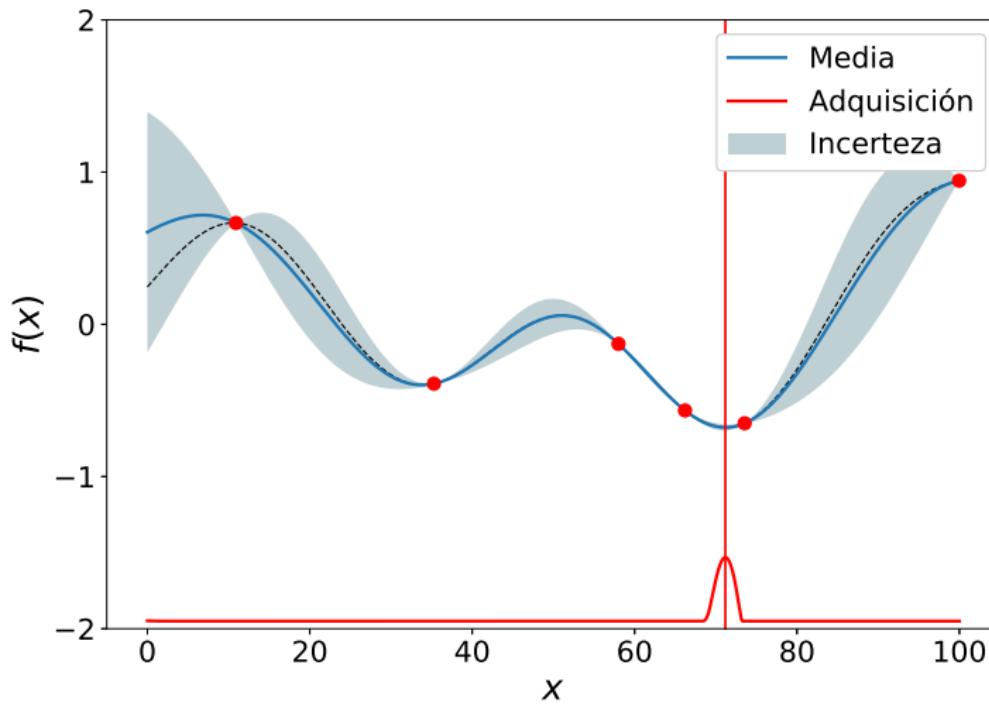
Procesos Gaussianos



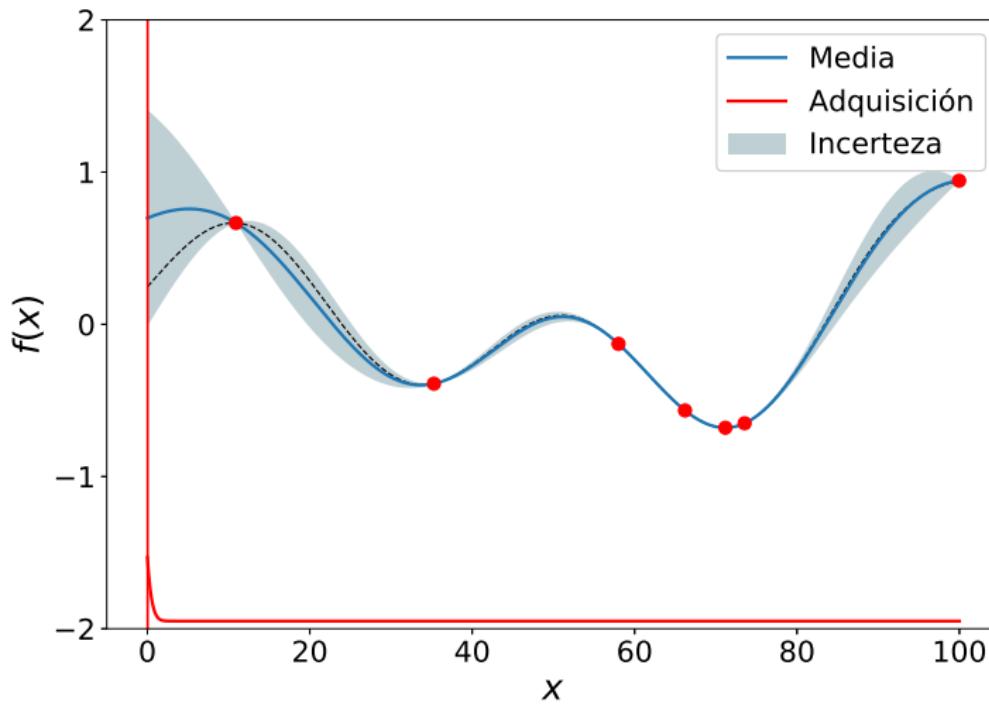
Procesos Gaussianos



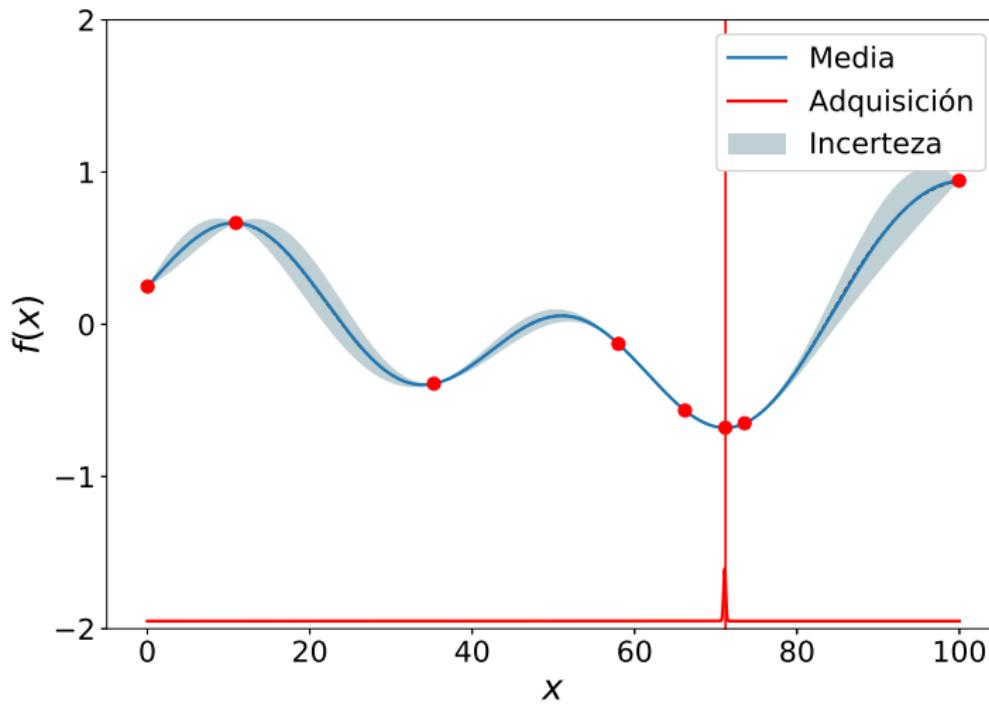
Procesos Gaussianos



Procesos Gaussianos

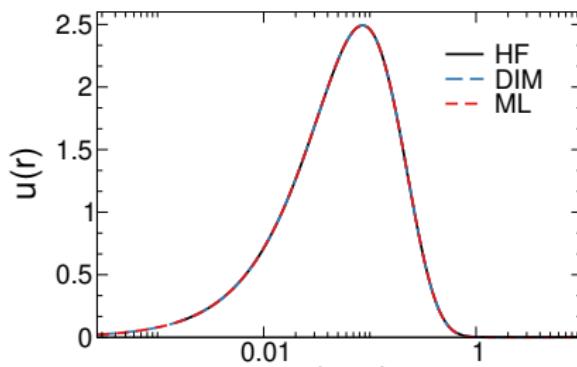
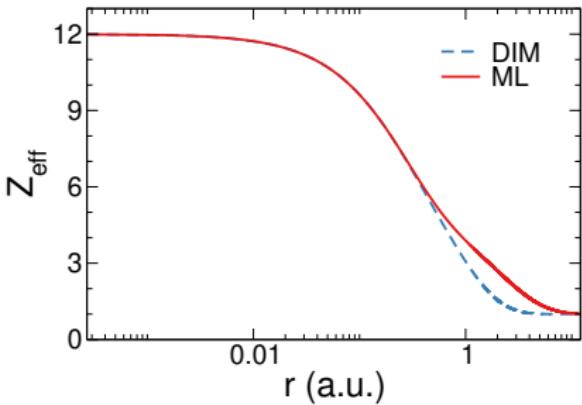


Procesos Gaussianos

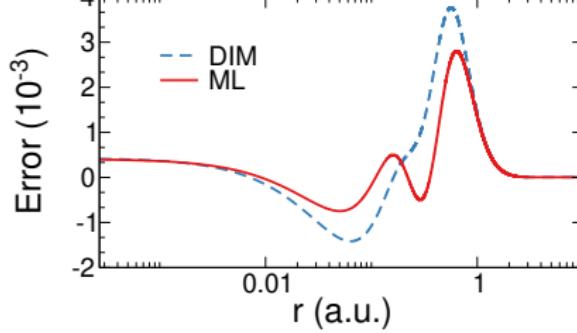


Resultados

DIM: Mg

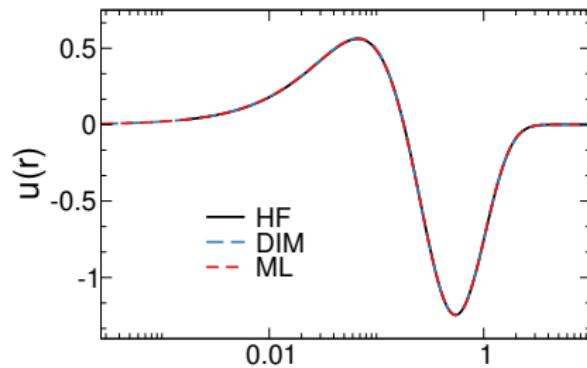
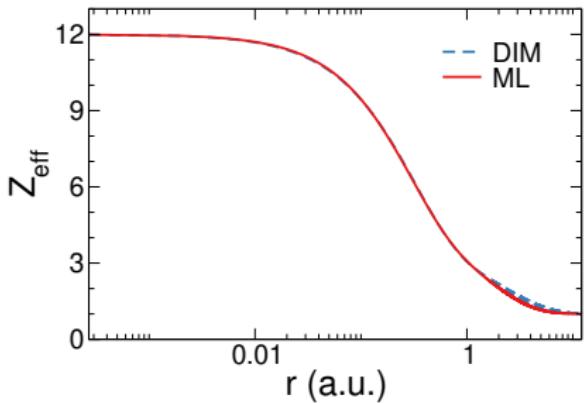


E ✓
 $\langle r \rangle$ $10^{-2} \%$
 $\langle 1/r \rangle$

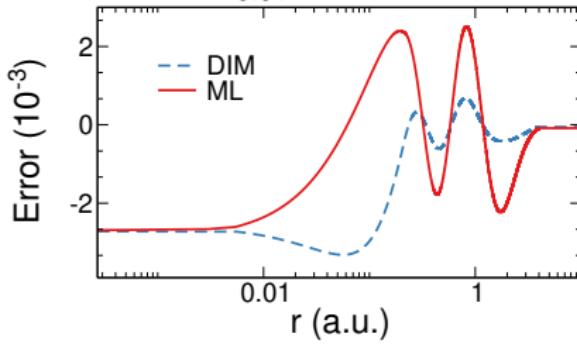


1s

DIM: Mg

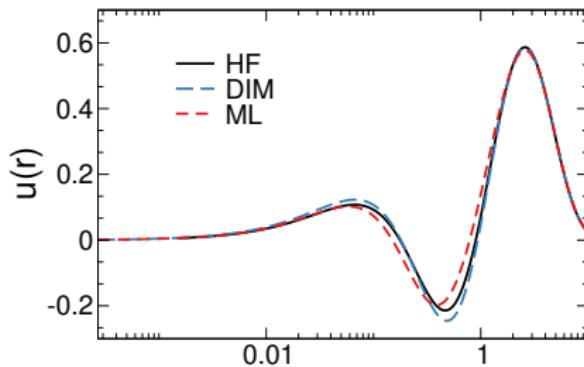
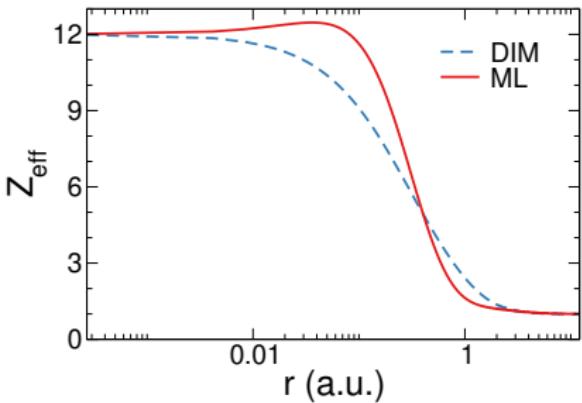


E ✓
 $\langle r \rangle$ $10^{-2} \%$
 $\langle 1/r \rangle$

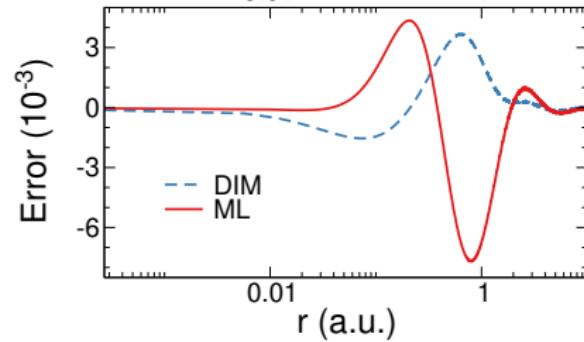


2s

DIM: Mg

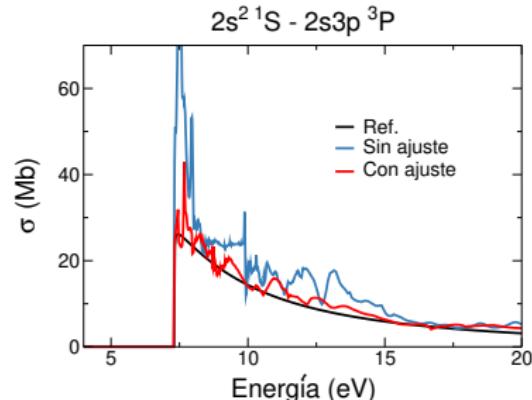
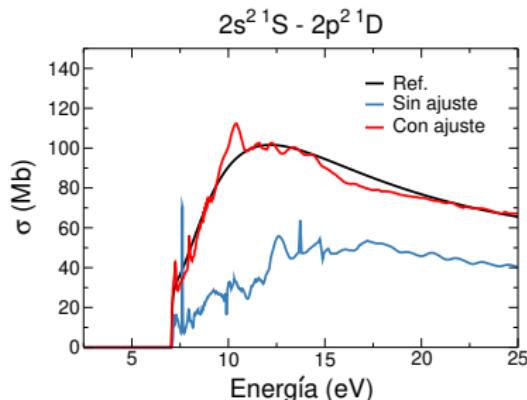
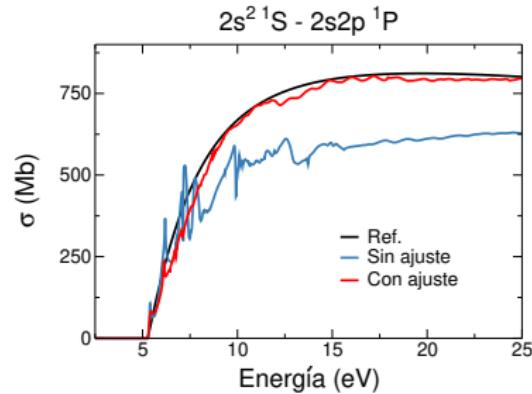
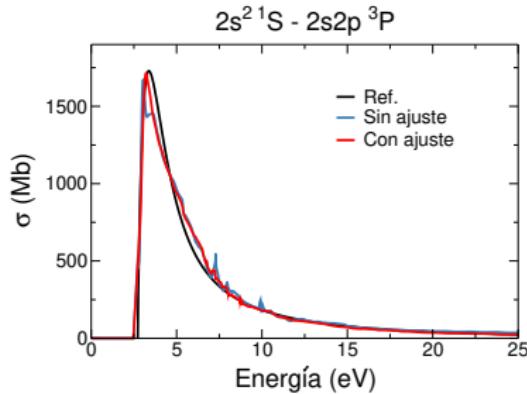


E ✓
 $\langle r \rangle$ $10^{-1} \%$
 $\langle 1/r \rangle$



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