Lecture 20
Linear Model Case Study

Lennard-Jones potential modeling using Gaussians

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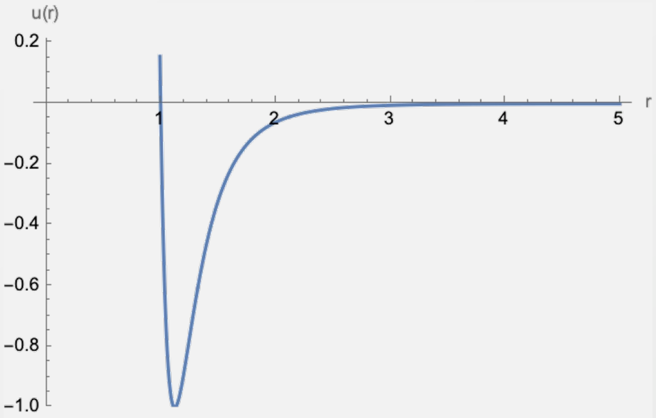
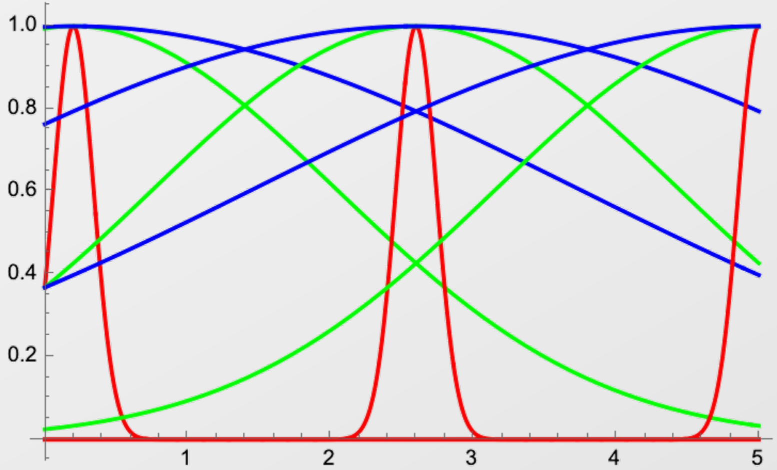
Case study: model the LJ potential with sum of many Gaussians





$n_{\mathrm{G}} = 3$

$$\mathbf{X} = \begin{pmatrix} x_1^{(1)} & x_2^{(1)} & \cdots & x_p^{(1)} \\ x_1^{(2)} & x_2^{(2)} & \cdots & x_p^{(2)} \\ \vdots & \vdots & \ddots & \vdots \\ x_1^{(n)} & x_2^{(n)} & \cdots & x_p^{(n)} \end{pmatrix}$$

n {*r*,*u*} pairs

p Gaussians (features)

OLS: $\hat{\mathbf{w}} = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{y}$

Ridge: $\hat{\mathbf{w}} = (\mathbf{X}^{\mathrm{T}}\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{y}$

Case study: model the LJ potential with sum of many Gaussians. Some activities to do

- Implement OLS directly, and using Mma's `Fit` function
  - Compute test-set MSE and compare PES $\hat{\mathbf{w}} = (\mathbf{X}^{\mathrm{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{y}$
  - Examine effect of precision on results (wp=50 vs 100 for nG = 5)
- Implement Ridge regression using Mma's `Fit` function
  - Examine effect of λ on validation MSE $\hat{\mathbf{w}} = (\mathbf{X}^{\mathrm{T}}\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^{\mathrm{T}}\mathbf{y}$