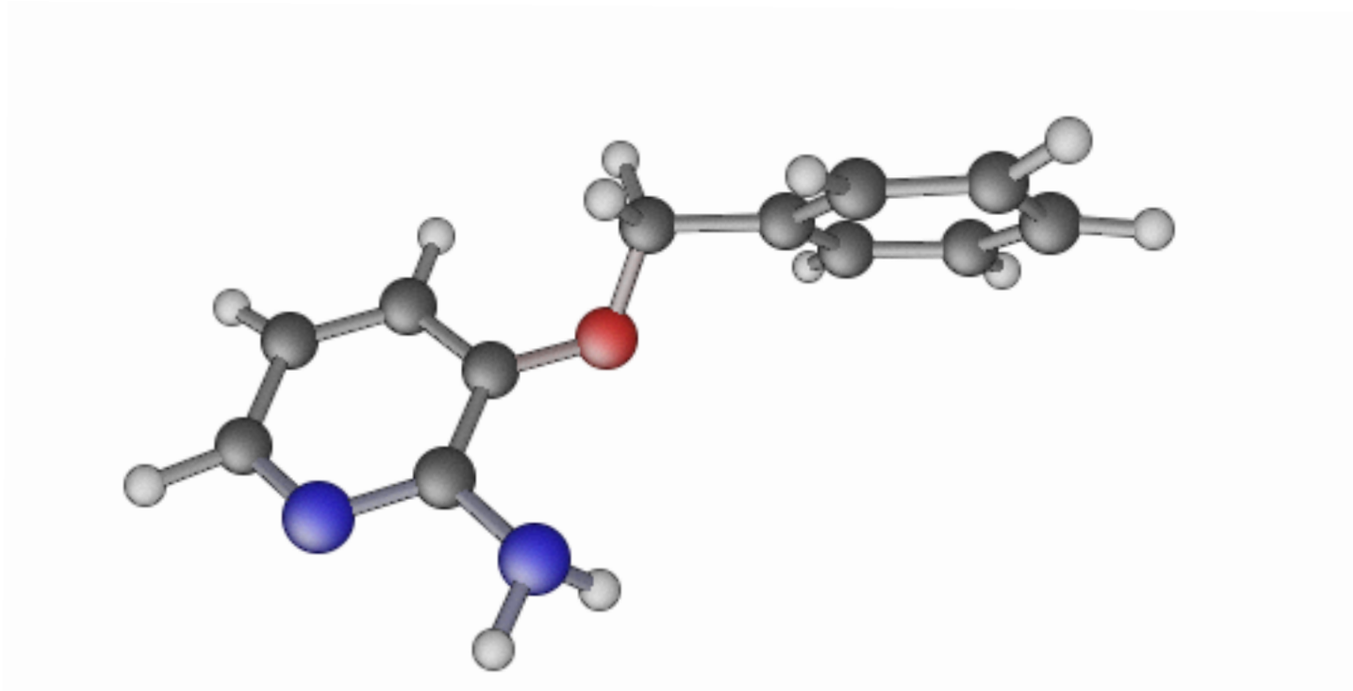
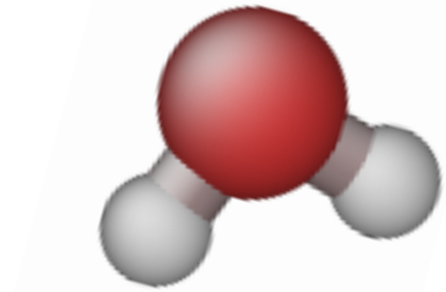
Learning Quantum Mechanics, machines vs. humans.

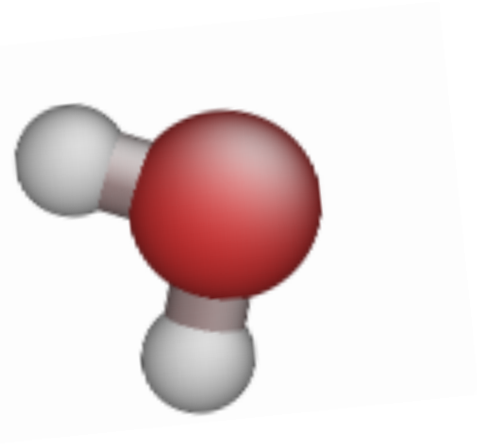
Alan Nichol
@alanmnichol

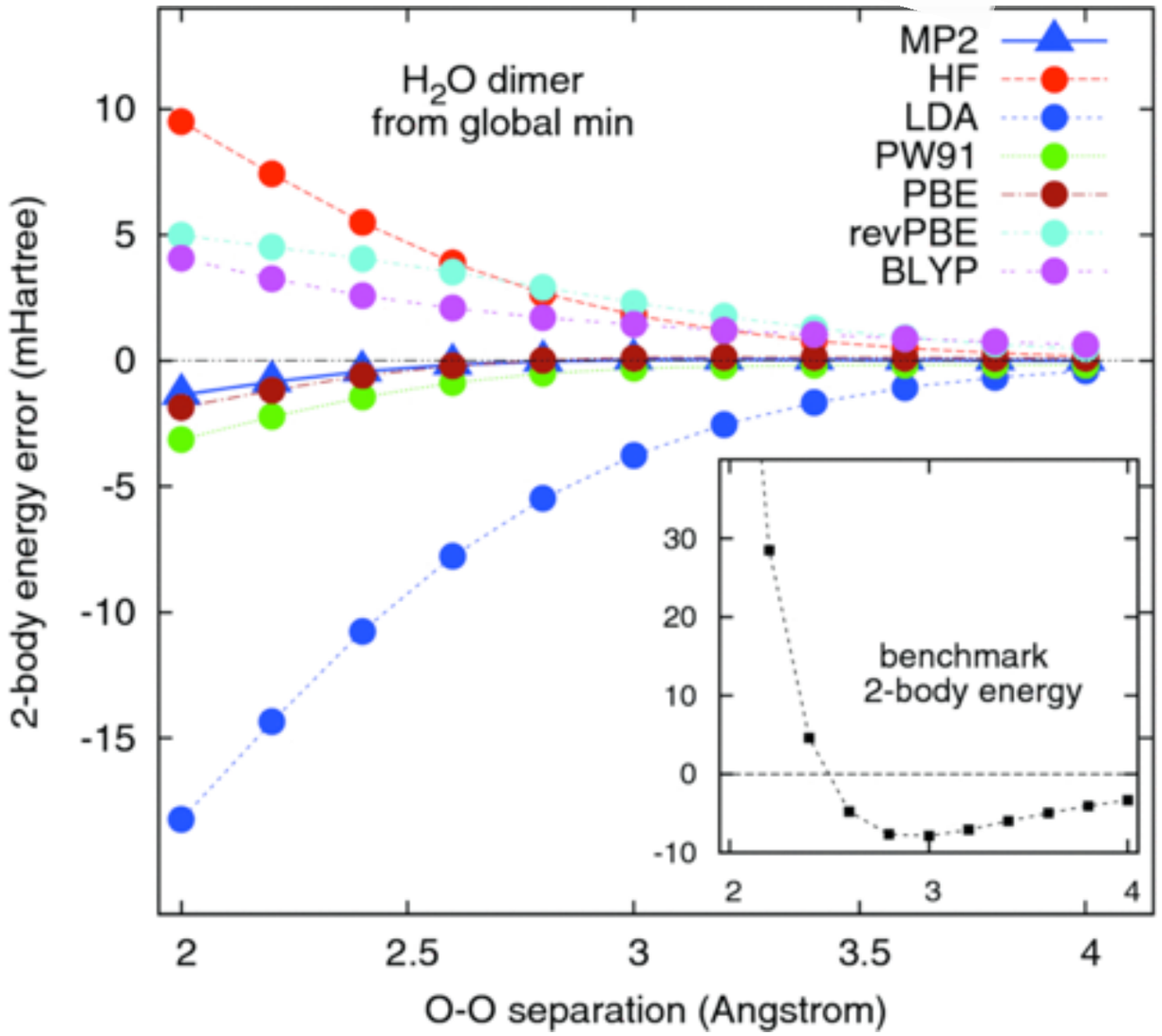
$$\mathcal{H}\Psi \quad = \quad E\Psi$$

$$\Psi(x_i, X_j) = \psi(x_i; X_j)\chi(X_j)$$



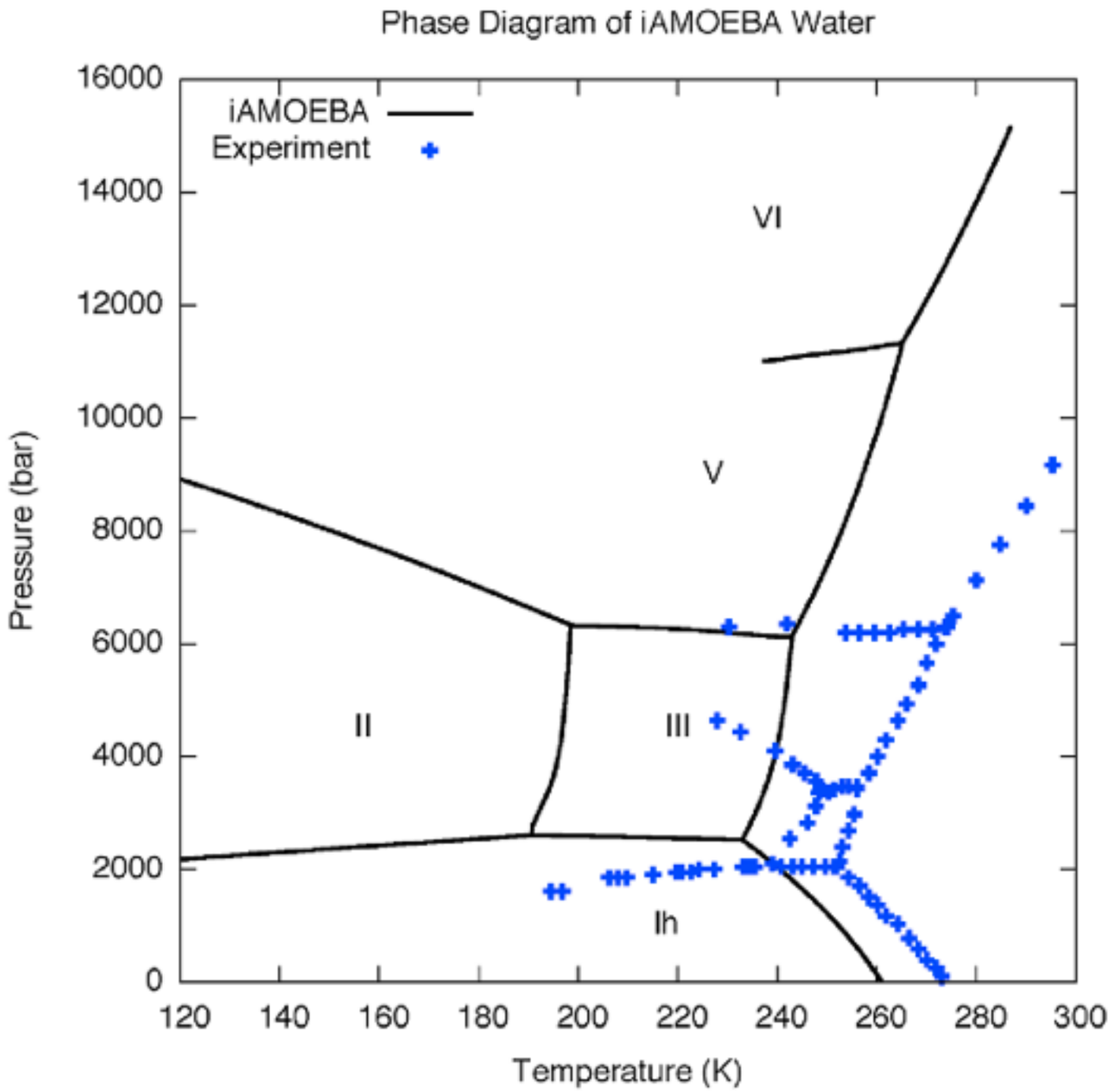






benchmark	3 hours	O(N^7)
MP2	20 mins	O(N^3)
HF	1 min	O(N^3)

[1] Many-body exchange-overlap interactions in rare gases and water



Systematic Improvement of a Classical Molecular Model for Water, LPW

Jargon-free Gaussian Processes 1

$$\mathcal{D} = \{x_i, y_i\} \qquad y_i = f(x_i; \mathbf{w}) + \varepsilon_i$$

$$f(x, \mathbf{w}) = \sum w_i \phi_i(x) \qquad \mathbf{R}_{ih} \equiv \phi_i(x_n)$$

$$|\mathbf{y} - \mathbf{f}|^2 = |\mathbf{y} - \mathbf{R}\mathbf{w}|^2 = (\mathbf{y} - \mathbf{R}\mathbf{w})^T (\mathbf{y} - \mathbf{R}\mathbf{w})$$

$$\mathbf{w} = (\mathbf{R}^T\mathbf{R})^{-1}\mathbf{R}^T\mathbf{y}$$

$$y_* \approx f_* = \sum \phi_i(x_*) w_i$$

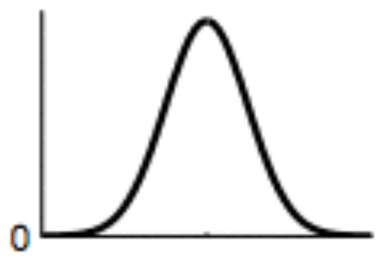
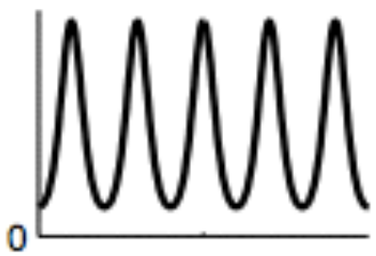
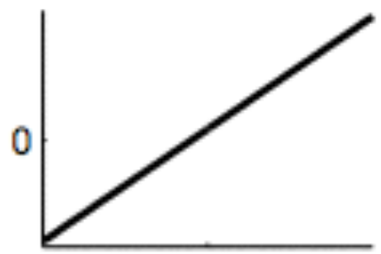
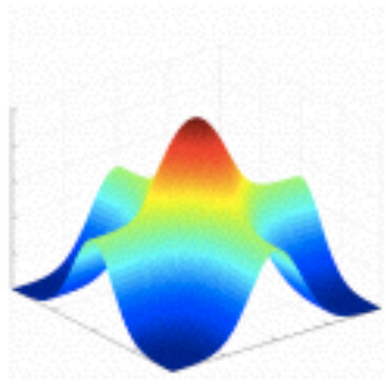
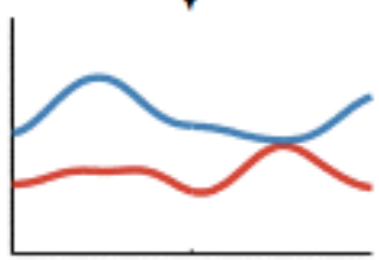
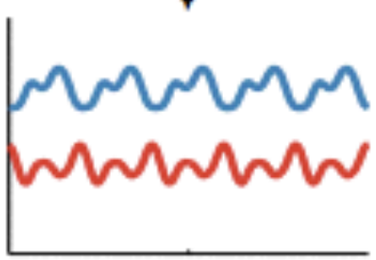
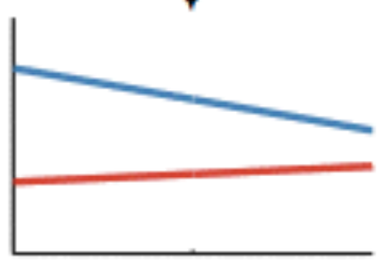
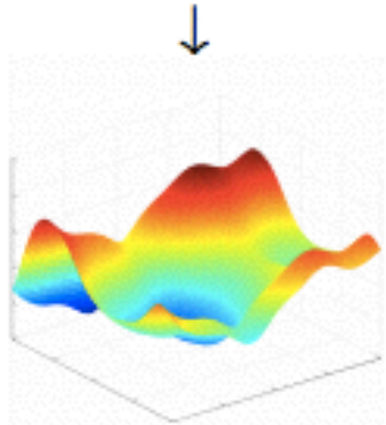
$$f_* = \delta_{*n}\mathbf{R}_{ni} \cdot (\mathbf{R}^T\mathbf{R})^{-1}\mathbf{R}^T\mathbf{y}$$

$$\mathbf{Q} \equiv \mathbf{R}^T\mathbf{R}$$

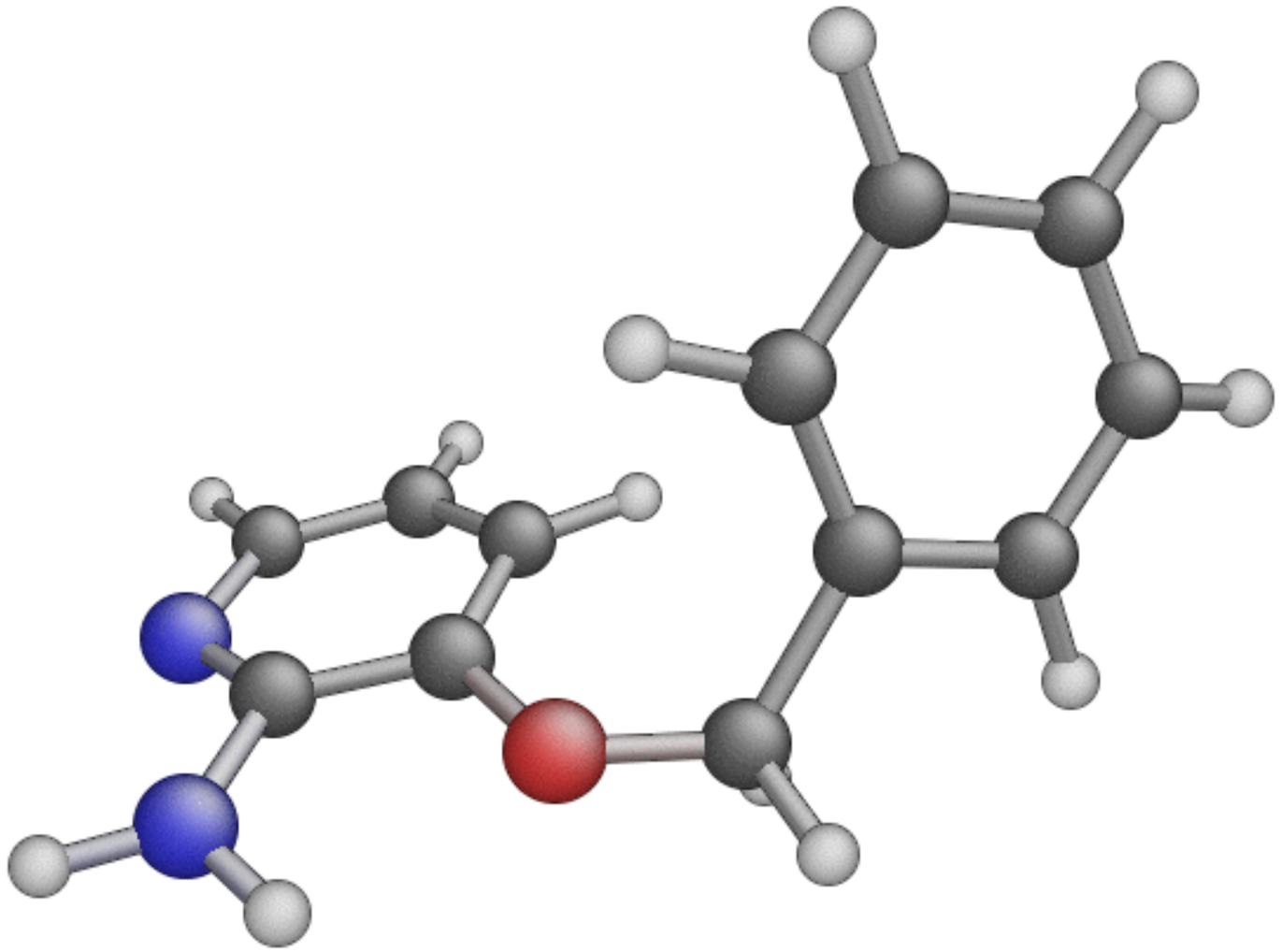
further reading :
http://www.gaussianprocess.org/gpml/

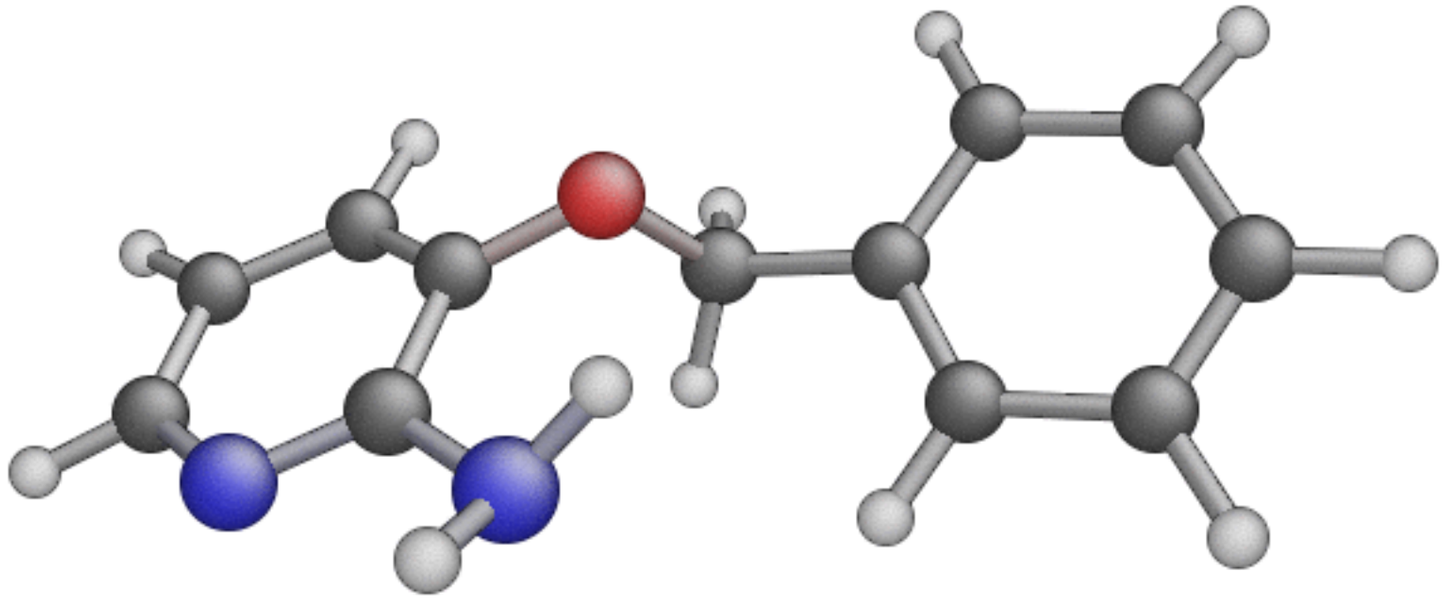
Jargon-free Gaussian Processes 2

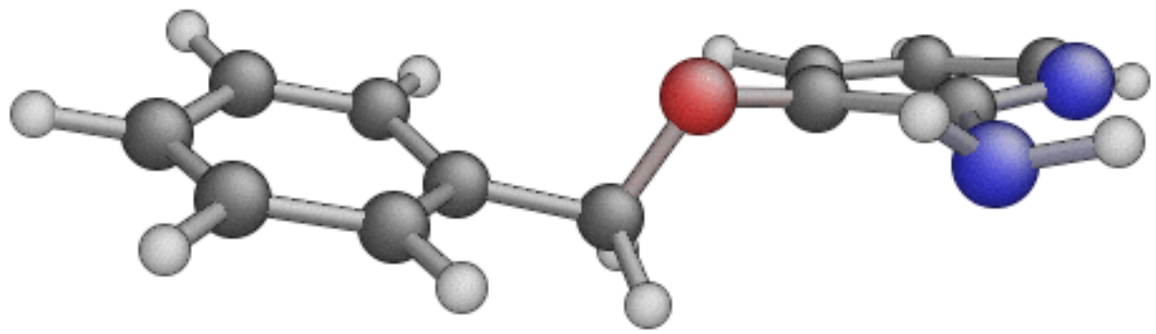
$$\mathbf{Q}_{n,n'} = \langle f_n, f_{n'} \rangle = k(x_n, x_{n'})$$

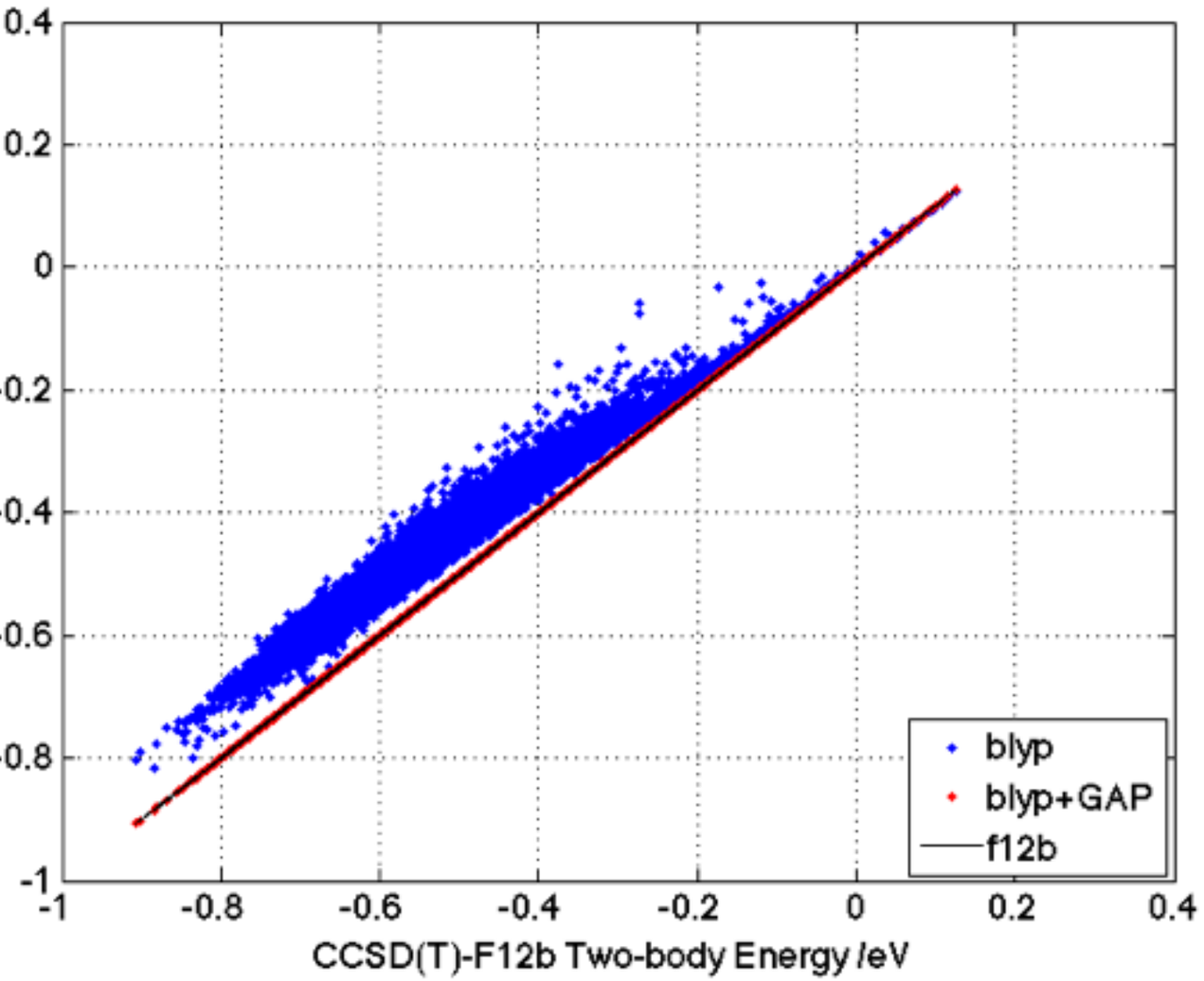
$k(x,x') =$	$\sigma_f^2 \exp\left(-\frac{(x-x')^2}{2\ell^2}\right)$	$\sigma_f^2 \exp\left(-\frac{2}{\ell^2}\sin^2\left(\pi\frac{x-x'}{p}\right)\right)$	$\sigma_f^2(x-c)(x'-c)$	$k_1(x_1,x_1') + k_2(x_2,x_2')$
Plot of $k(x,x')$:				
	$x - x'$	$x - x'$	x (with $x' = 1$)	$f_1(x_1) + f_2(x_2)$
Functions $f(x)$ sampled from GP prior:				
	x	x	x	
Type of structure:	local variation	repeating structure	linear functions	

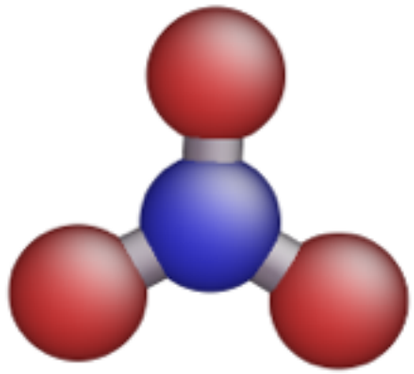
David Duvenaud, PhD Thesis, University of Cambridge

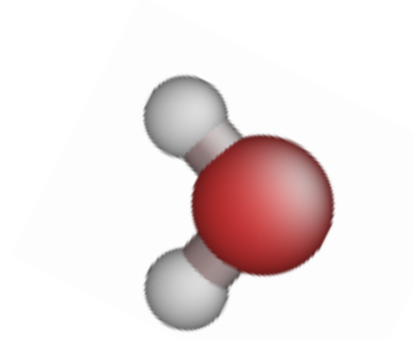




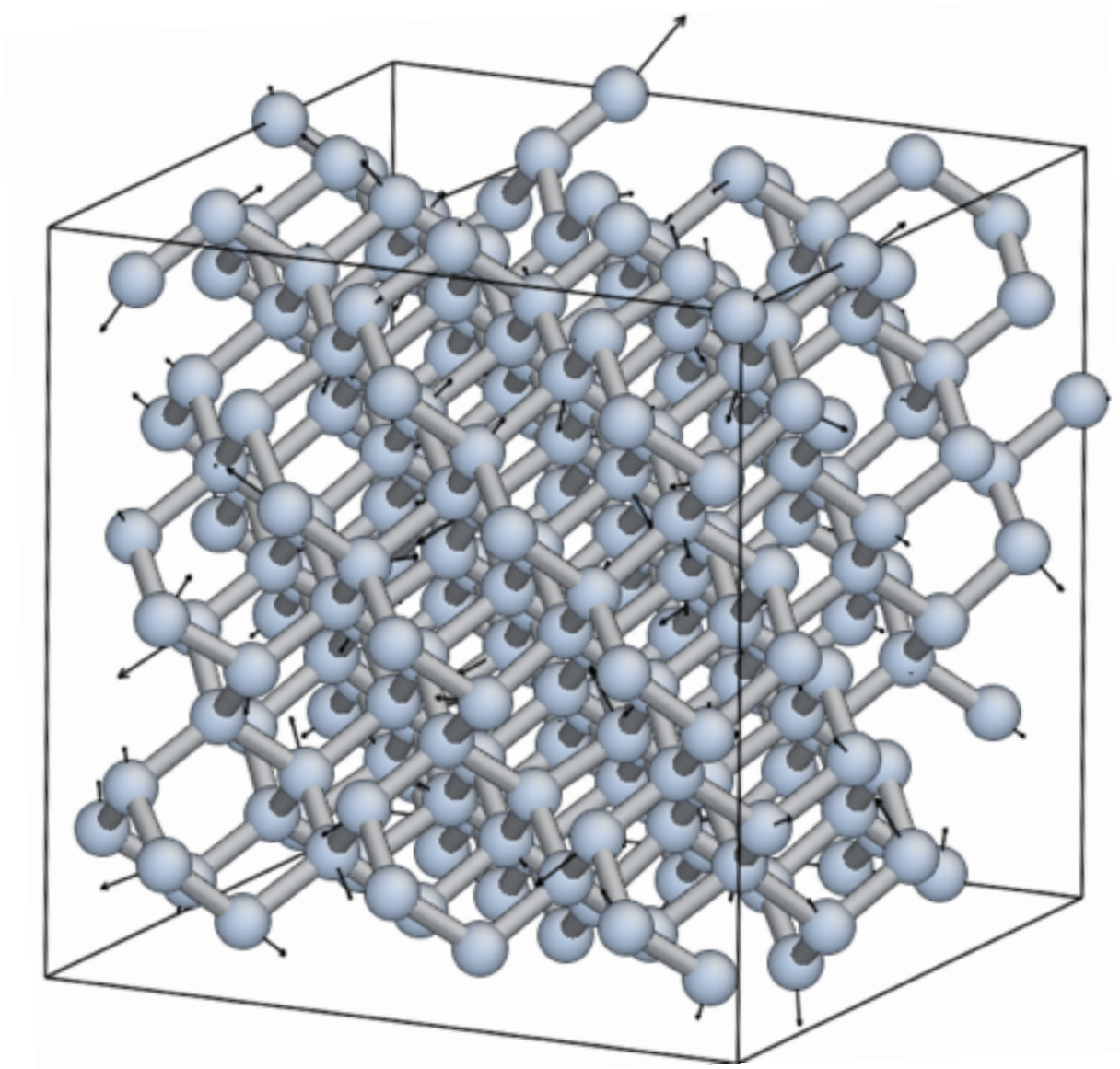








benchmark	3 hours	O(N^7)
MP2	20 mins	O(N^5)
GAP	10 ms	O(N)

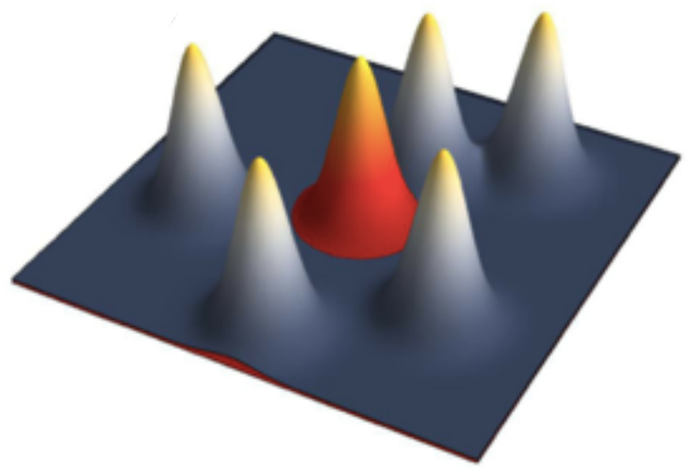


$$\tilde{\mathbf{Q}} = \mathbf{L}\mathbf{Q}\mathbf{L}^T$$

$$\rho_i(\mathbf{r}) = \sum_j \exp\left(-|\mathbf{r} - \mathbf{r}_{ij}|^2/2\sigma^2\right) = \sum_j \sum_{lm} c_{nlm}^{(i)j} g_n(r) Y_{lm}(\hat{\mathbf{r}})$$

- Overlap integral

$$S(\rho_i, \rho_{i'}) = \int \rho_i(\mathbf{r}) \rho_{i'}(\mathbf{r}) d\mathbf{r},$$



- Integrate over all 3D rotations:

$$k(\rho_i, \rho_{i'}) = \int \left|S(\rho_i, \hat{R}\rho_{i'})\right|^2 d\hat{R} = \int d\hat{R} \left| \int \rho_i(\mathbf{r}) \rho_{i'}(\hat{R}\mathbf{r}) d\mathbf{r} \right|^2$$

- After LOTS of algebra: SOAP kernel

$$k(\rho_i, \rho_{i'}) = \sum_{n,n',l} p_{nn'l}^{(i)} p_{nn'l}^{(i')}$$

$$K(\mathbf{q}, \mathbf{q}') \propto |k(\rho, \rho')|^{\xi}$$

One grad student/system

my deep NN can do anything

Acknowledgements

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