

## Supplementary material

**Jujube stones based highly efficient activated carbon for methylene blue adsorption: kinetics and isotherms modeling, thermodynamics and mechanism study, optimization via Response surface methodology and machine learning approaches.**

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The following ten kernel functions ((S1 to S10) were used in this work

### Squared Exponential Kernel

$$k(x_i, x_j | \theta) = \sigma_f^2 \exp \left[ -\frac{1}{2} \frac{(x_i - x_j)^T (x_i - x_j)}{\sigma_l^2} \right] \quad (\text{S1})$$

Where  $\sigma_l$  is the characteristic length scale, and  $\sigma_f$  is the signal standard deviation.

- **Exponential Kernel**

$$k(x_i, x_j | \theta) = \sigma_f^2 \exp \left[ -\frac{r}{\sigma_l} \right] \quad (\text{S2})$$

Where  $\sigma_l$  is the characteristic length scale and  $r = \sqrt{(x_i - x_j)^T (x_i - x_j)}$

- **Matern 3/2**

$$k(x_i, x_j | \theta) = \sigma_f^2 \left( 1 + \frac{\sqrt{3}r}{\sigma_l} \right) \exp \left( -\frac{\sqrt{3}r}{\sigma_l} \right) \quad \text{where } r = \sqrt{(x_i - x_j)^T (x_i - x_j)} \quad (\text{S3})$$

- **Matern 5/2**

$$k(x_i, x_j | \theta) = \sigma_f^2 \left( 1 + \frac{\sqrt{5}r}{\sigma_l} + \frac{5r^2}{3\sigma_l^2} \right) \exp \left( -\frac{\sqrt{5}r}{\sigma_l} \right) \quad \text{where } r = \sqrt{(x_i - x_j)^T (x_i - x_j)} \quad (\text{S4})$$

- **Rational Quadratic Kernel**

$$k(x_i, x_j | \theta) = \sigma_f^2 \left( 1 + \frac{r^2}{2\alpha\sigma_l^2} \right)^{-\alpha} \quad (\text{S5})$$

Where:  $\sigma_l$  is the characteristic length scale,  $\alpha$  is a positive-valued scale mixture parameter.

$$r = \sqrt{(x_i - x_j)^T (x_i - x_j)}$$

- **ARD Squared Exponential Kernel**

$$k(x_i, x_j | \theta) = \sigma_f^2 \exp \left[ -\frac{1}{2} \sum_{m=1}^d \frac{(x_{im} - x_{jm})^2}{\sigma_m^2} \right] \quad (\text{S6})$$

- **ARD Exponential Kernel**

$$k(x_i, x_j | \theta) = \sigma_f^2 \exp(-r) \quad \text{where } r = \sqrt{\sum_{m=1}^d \frac{(x_{im} - x_{jm})^2}{\sigma_m^2}} \quad (\text{S7})$$

- **ARD Matern 3/2**

$$k(x_i, x_j | \theta) = \sigma_f^2 (1 + \sqrt{3}r) \exp(-\sqrt{3}r) \quad \text{where } r = \sqrt{\sum_{m=1}^d \frac{(x_{im} - x_{jm})^2}{\sigma_m^2}} \quad (\text{S8})$$

- **ARD Matern 5/2**

$$k(x_i, x_j | \theta) = \sigma_f^2 \left( 1 + \sqrt{5}r + \frac{5}{3}r^2 \right) \exp(-\sqrt{5}r) \quad \text{Where } r = \sqrt{\sum_{m=1}^d \frac{(x_{im} - x_{jm})^2}{\sigma_m^2}} \quad (\text{S9})$$

- **ARD Rational Quadratic Kernel**

$$k(x_i, x_j | \theta) = \sigma_f^2 \left( 1 + \frac{1}{2\alpha} \sum_{m=1}^d \frac{(x_{im} - x_{jm})^2}{\sigma_m^2} \right)^{-\alpha} \quad (\text{S10})$$

$$R = \frac{\sum_{i=1}^N (y_{\text{exp}} - \bar{y}_{\text{exp}})(y_{\text{pred}} - \bar{y}_{\text{pred}})}{\sqrt{\sum_{i=1}^N (y_{\text{exp}} - \bar{y}_{\text{exp}})^2 \sum_{i=1}^N (y_{\text{pred}} - \bar{y}_{\text{pred}})^2}} \quad (\text{S11})$$

$$R_{\text{adj}}^2 = 1 - \frac{(1 - R^2)(N - 1)}{N - K - 1} \quad (\text{S12})$$

$$RMSE = \sqrt{\left(\frac{1}{N}\right) \left(\sum_{i=1}^N [(y_{\text{exp}} - y_{\text{pred}})]^2\right)} \quad (\text{S13})$$