Table 1 Test functions

No	Functions	Input distribution
1	$y^3 = \sin(x) + 0.2x + (x-0.5)^2/16 + 0.5$ $y^2 = \sin(x) + 0.8x + (x-0.5)^2/45 + 0.5$ $y^1 = \sin(x) + 0.2x + 0.5$	$x \sim N(1.5, 1.33^2)$
2	$y^3 = -\sin(x) - \exp\left(\frac{x}{100}\right) + 10,$ $y^2 = y^3 + 0.3 - 0.03(x-3)^2,$ $y^1 = y^3 + 0.3 - 0.03(x-7)^2$	$x \sim N(5, 0.83^2)$
3	$y^2 = \left(x - \sqrt{2}\right)\sin^2(8\pi x)$ $y^1 = \sin(8\pi x)$	$x \sim U(0,1)$
4	$y^3 = \left(1 - e^{\frac{-1}{2x_2}}\right)\left(\frac{1000t_f x_1^3 + 1900x_1^2 + 2092x_1 + 60}{1000t_l x_1^3 + 500x_1^2 + 4x_1 + 20}\right)$ $y^2 = \left(1 - e^{\frac{-1}{2x_2}}\right)\left(\frac{1000t_f x_1^3 + 1900x_1^2 + 2092x_1 + 60}{1000t_l x_1^3 + 500x_1^2 + 4x_1 + 20}\right) + \frac{5e^{-t_f}x_1^{t_h/2}}{x_2^{2+t_h}+1}$ $y^1 = \left(1 - e^{\frac{-1}{2x_2}}\right)\left(\frac{1000t_f x_1^3 + 1900x_1^2 + 2092x_1 + 60}{1000t_l x_1^3 + 500x_1^2 + 4x_1 + 20}\right) + \frac{5e^{-t_f}x_1^{t_h/2}}{x_2^{2+t_h}+1} + \frac{10x_1^2 + 4x_2^2}{50x_1x_2 + 10}$ $t_f = 0.2; t_h = 0.3; t_l = 0.1;$	$x_{1,2} \sim N(0.5, 0.1^2)$
5	$y^3 = 25(x_1-2)^2 + (x_2-2)^2 + (x_3-1)^2 + (x_4-4)^2 + (x_5-1)^2 + (x_6-4)^2$ $y^2 = 20(x_1-2)^2 + 0.95(x_2-2)^2 + 0.8(x_3-1)^2 + 1.05(x_4-4)^2 + 0.8(x_5-1)^2 + 0.7(x_6-4)^2$ $y^1 = 15(x_1-2)^2 + 0.85(x_2-2)^2 + 0.6(x_3-1)^2 + 1.35(x-4)^2 + 0.6(x_5-1)^2 + 0.6(x_6-4)^2$	$x_{1,\ldots,6} \sim N(5, 0.5^2)$
6	$y^3 = x_1^2 + x_2^2 + x_1x_2 - 4x_1 - 6x_2 + (x_3-2)^2 + 4(x_4-5)^2 + (x_5-3)^2$ $+2(x_6-1)^2 + 5x_7^2 + 7(x_8-3)^2 + 2(x_9-2)^2 + (x_{10}-1)^2 + 11$ $y^2 = 0.8x_1^2 + 0.7x_2^2 + 0.5x_1x_2 - 4x_1 - 6x_2 + (x_3-2)^2 + 4(x_4-5)^2 + 1.1(x_5-3)^2$ $+2(x_6-1)^2 + 4.5x_7^2 + 7(x_8-3)^2 + 2(x_9-2)^2 + (x_{10}-1)^2 + 10$ $y^1 = 0.5x_1^2 + 0.6x_2^2 + 0.3x_1x_2 - 3x_1 - 5x_2 + (x_3-2)^2 + 4.5(x_4-5)^2 + 1.2(x_5-3)^2$ $+2(x_6-1)^2 + 3x_7^2 + 7(x_8-3)^2 + 2(x_9-2)^2 + (x_{10}-1)^2 + 10$	$x_{1,\ldots,10} \sim N(2.5, 0.2^2)$
7	$y^3 = (x_1-1)^2 + \sum_{i=2}^{15} i(2x_i^2 - x_{i-1})^2$ $y^2 = 0.9(x_1-1)^2 + 0.9\sum_{i=2}^{15} i(2x_i^2 - x_{i-1})^2 - \sum_{i=1}^{15} 0.1x_ix_{i+1}$ $y^1 = 0.8(x_1-1)^2 + 0.7\sum_{i=2}^{15} i(2x_i^2 - x_{i-1})^2 - \sum_{i=1}^{15} 0.2x_ix_{i+1}$	$x_{1,\ldots,15} \sim N(1, 0.15^2)$
8	$y^3 = (x_1-1)^2 + \sum_{i=2}^{20} (x_i - x_{i-1})^2$ $y^2 = 0.8(x_1-1)^2 + 0.8\sum_{i=2}^{20} (x_i - x_{i-1})^2 - \sum_{i=1}^{20} 0.2x_ix_{i+1}$ $y^1 = 0.5(x_1-1)^2 + 0.6\sum_{i=2}^{20} (x_i - x_{i-1})^2 - \sum_{i=1}^{20} 0.5x_ix_{i+1}$	$x_{1,\ldots,20} \sim N(1, 0.15^2)$

per layer of the BNN is used; the dropout is set to 0.5, and a batch normal layer is added after each layer of neural network to suppress overfitting.

Table 3 presents the RMSEs of the metamodel constructed using the proposed ML-MFBNN method, Co-Kriging, and H-BNN, and the relative errors of the mean