SUPPORTING INFORMATION

ZeoNet: 3D convolutional neural networks for predicting adsorption in nanoporous zeolites

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Additional Tables

Table S1: r^2 and MSE for 10 subsets each of 2,000 samples

Subset	1	2	3	4	5	6	7	8	9	10
r^2	0.679	0.657	0.660	0.639	0.682	0.674	0.667	0.668	0.655	0.673
MSE	51.931	58.803	54.997	60.362	50.913	55.191	54.816	57.115	57.634	55.002

Table S2: r^2 and MSE for 4 subsets each of 5,000 samples

Subset	1	2	3	4
r^2	0.664	0.662	0.667	0.667
MSE	55.290	55.512	56.393	55.510

Table S3: r^2 and MSE for 2 subsets each of 10,000 samples

Subset	1	2
r^2	0.663	0.667
MSE	55.401	55.952

Table S4: r^2 and MSE for the full set of 20,104 samples

Fullset	1
r^2	0.665
MSE	55.767

Table S5: Comparing r^2 and MSE for distance grids of different resolutions while keeping an input tensor size of 100^3. The grid resolution with the highest performance for each model is shown in bold.

$\Delta d/[\text{Å}]$	0.15		0.3		0.45		0.6		0.75		0.9		1	
AlexNet	0.676	54.0	0.882	19.7	0.936	10.6	0.942	9.7	0.945	9.2	0.944	9.4	**0.946**	**9.0**
VGG16	0.851	24.9	0.896	17.3	**0.962**	**6.4**	0.945	9.1	0.952	8.0	0.924	12.7	0.919	13.5
ResNet18	0.879	20.1	**0.973**	**4.6**	0.972	4.6	0.968	5.3	0.969	5.2	0.963	6.2	0.961	6.5
DenseNet121	0.881	19.9	0.975	4.2	**0.976**	**4.0**	0.974	4.3	0.971	4.8	0.970	5.0	0.968	5.3

Table S6: Comparing r^2 and MSE of ResNet18 for distance grids of different input dimensions and a fixed grid resolution of 0.45 Å.

Input Dim.	32		48		64		82		100	
$L/[\text{Å}]$	14.4		21.6		28.8		36.9		45	
ResNet18	0.845	25.8	0.953	7.9	0.967	5.6	0.973	4.5	0.972	4.6

Table S7: Comparing r^2 and MSE of ResNet18 for distance grids of a fixed input volume, $L = 15$ Å, achieved by different combinations of input dimensions and grid resolutions.

$\Delta d/[\text{Å}]$	0.15		0.3		0.6	
Input Dim.	100		50		25	
ResNet18	0.879	20.1	0.878	20.3	0.865	22.5

Additional Figures

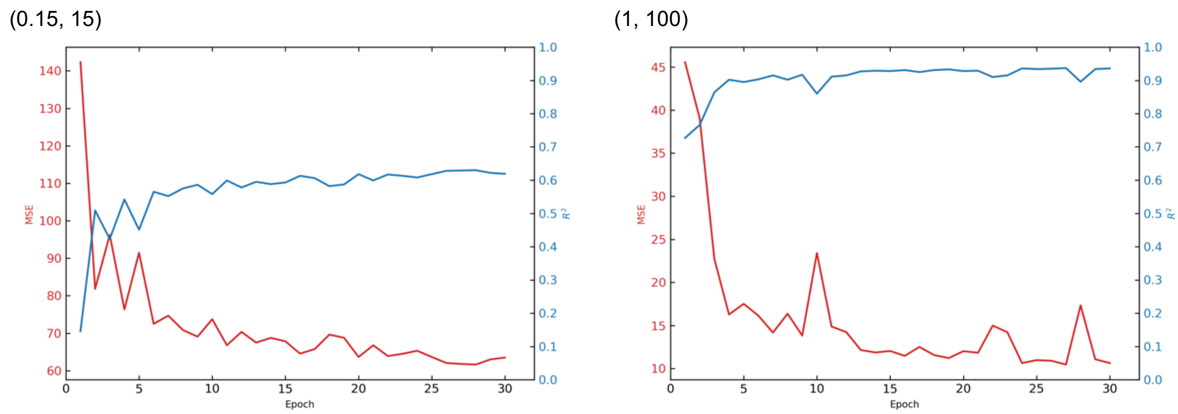

Figure S1: r^2 and MSE as a function of epoch during training of AlexNet for binary occupancy grids with a fixed input tensor shape of 100^3, achieved by different combinations of input dimensions and grid resolutions. The input representations are given in parentheses, $(\Delta d, L)$ in Å

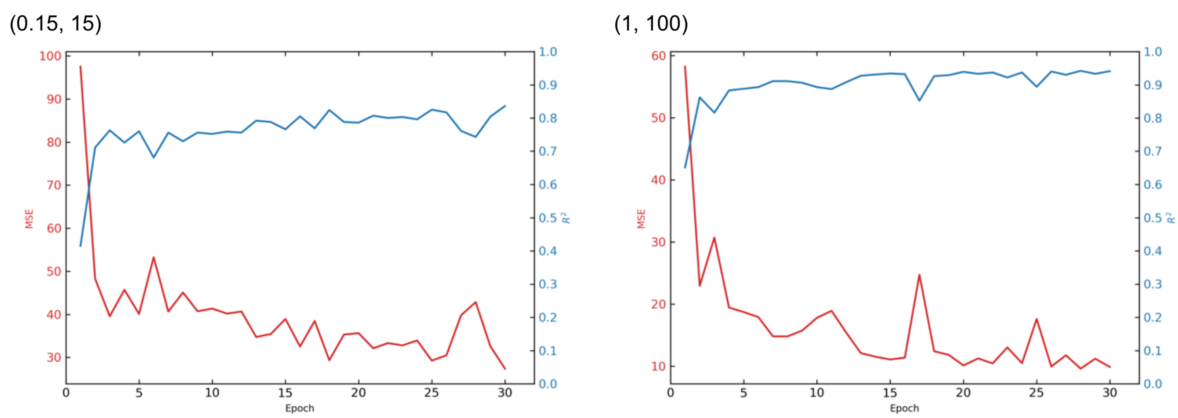

Figure S2: r^2 and MSE as a function of epoch during training of VGG16 for binary occupancy grids with a fixed input tensor shape of 100^3, achieved by different combinations of input dimensions and grid resolutions. The input representations are given in parentheses, $(\Delta d, L)$ in Å.

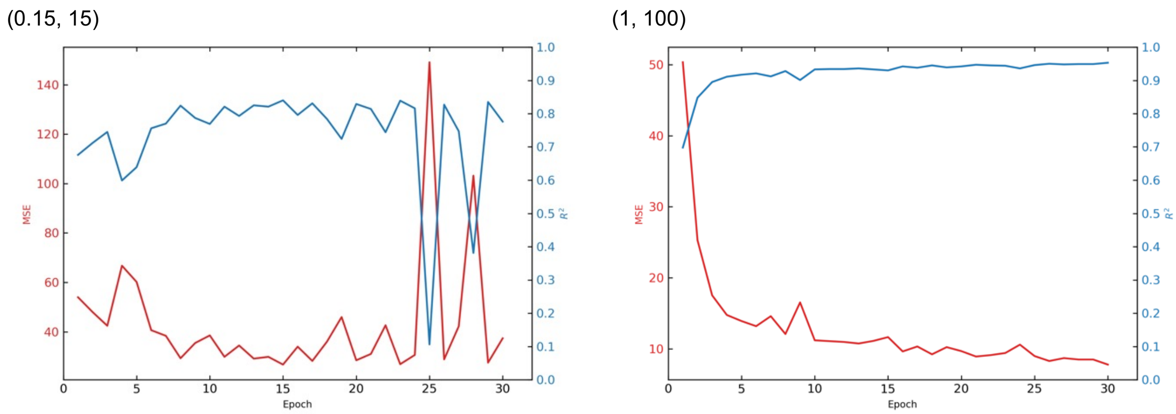

Figure S3: r^2 and MSE as a function of epoch during training of ResNet18 for binary occupancy grids with a fixed input tensor shape of 100^3, achieved by different combinations of input dimensions and grid resolutions. The input representations are given in parentheses, $(\Delta d, L)$ in Å.

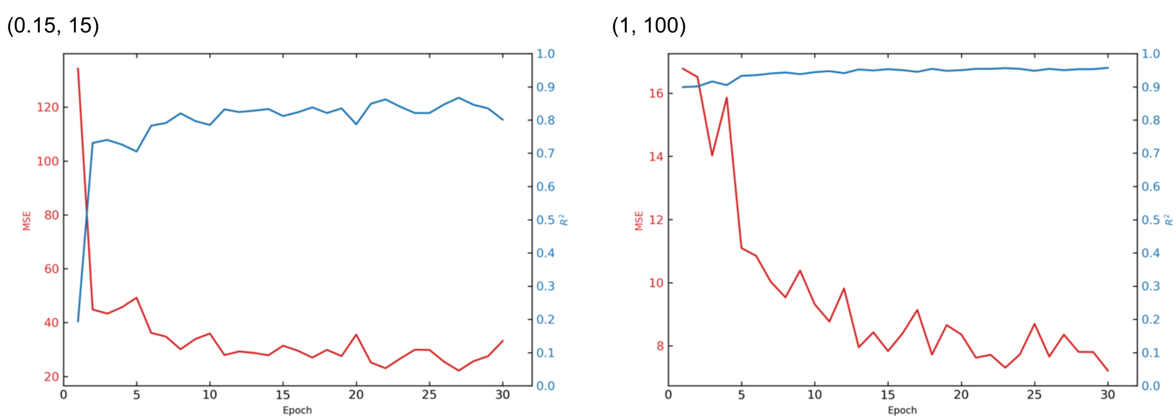

Figure S4: r^2 and MSE as a function of epoch during training of DenseNet121 for binary occupancy grids with a fixed input tensor shape of 100^3, achieved by different combinations of input dimensions and grid resolutions. The input representations are given in parentheses, $(\Delta d, L)$ in Å.

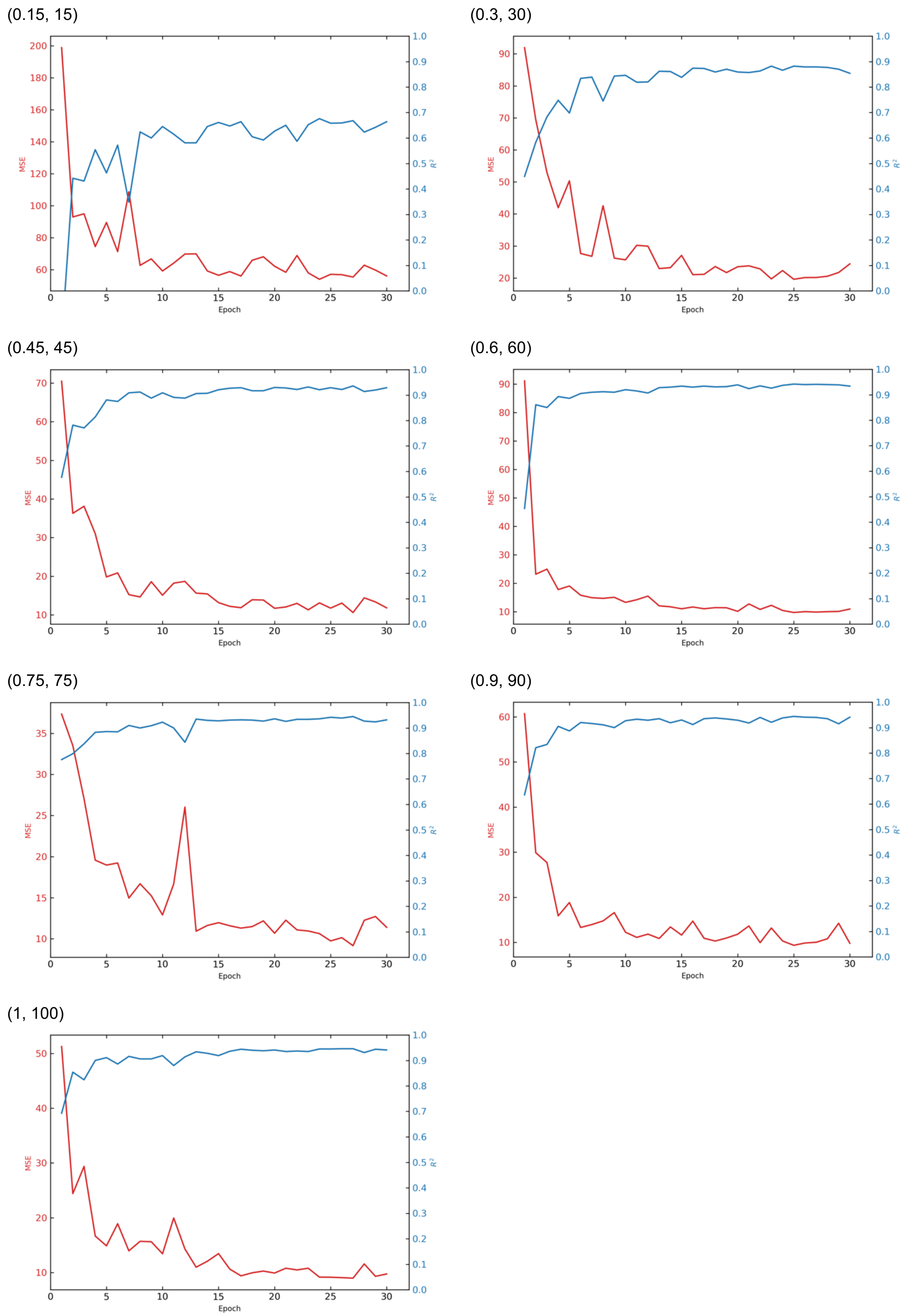

Figure S5: r^2 and MSE as a function of epoch during training of AlexNet for distance grids with a fixed input tensor shape of 100^3, achieved by different combinations of input dimensions and grid resolutions. The input representations are given in parentheses, $(\Delta d, L)$ in Å.

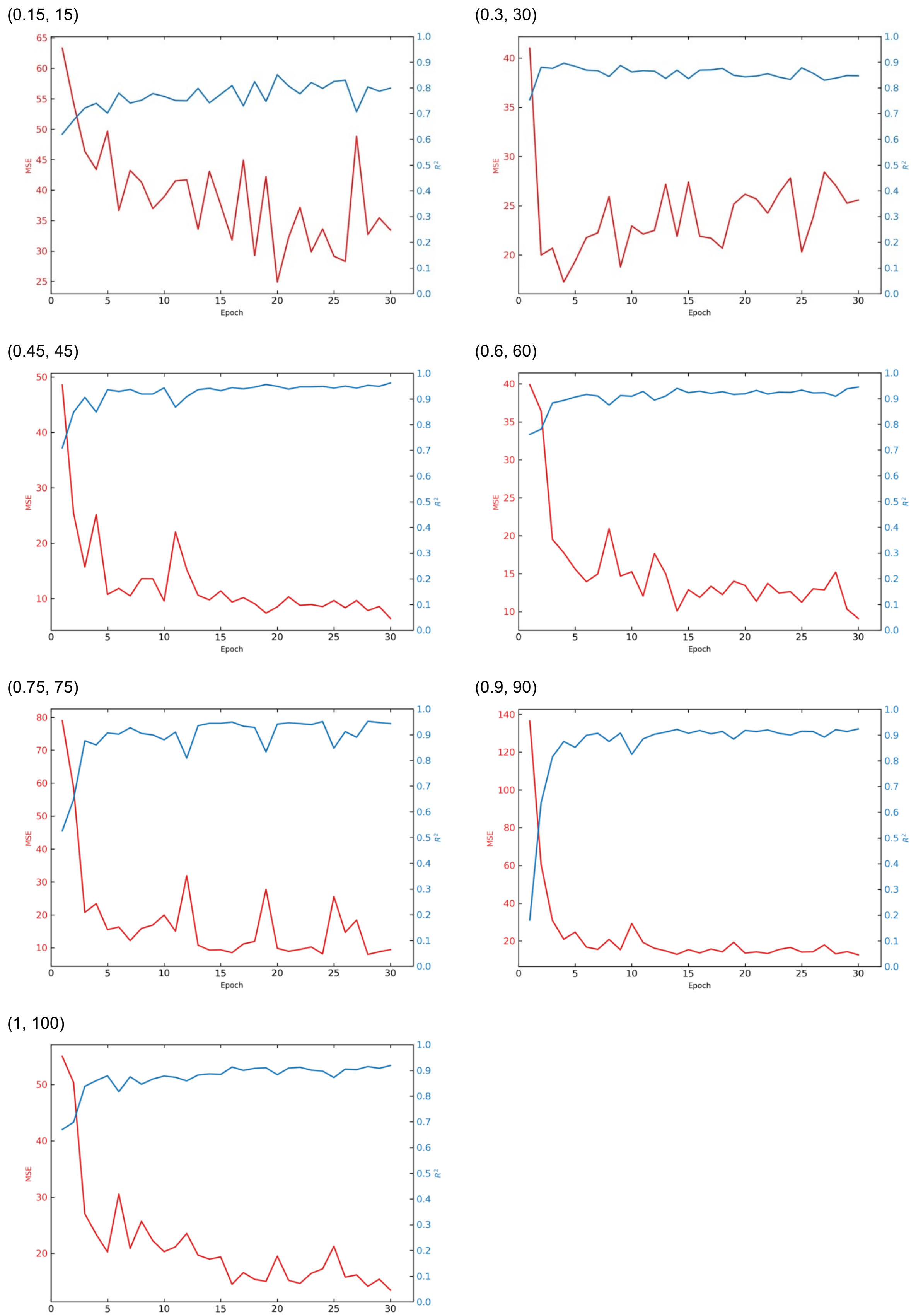

Figure S6: r^2 and MSE as a function of epoch during training of VGG16 for distance grids with a fixed input tensor shape of 100^3, achieved by different combinations of input dimensions and grid resolutions. The input representations are given in parentheses, $(\Delta d, L)$ in Å.

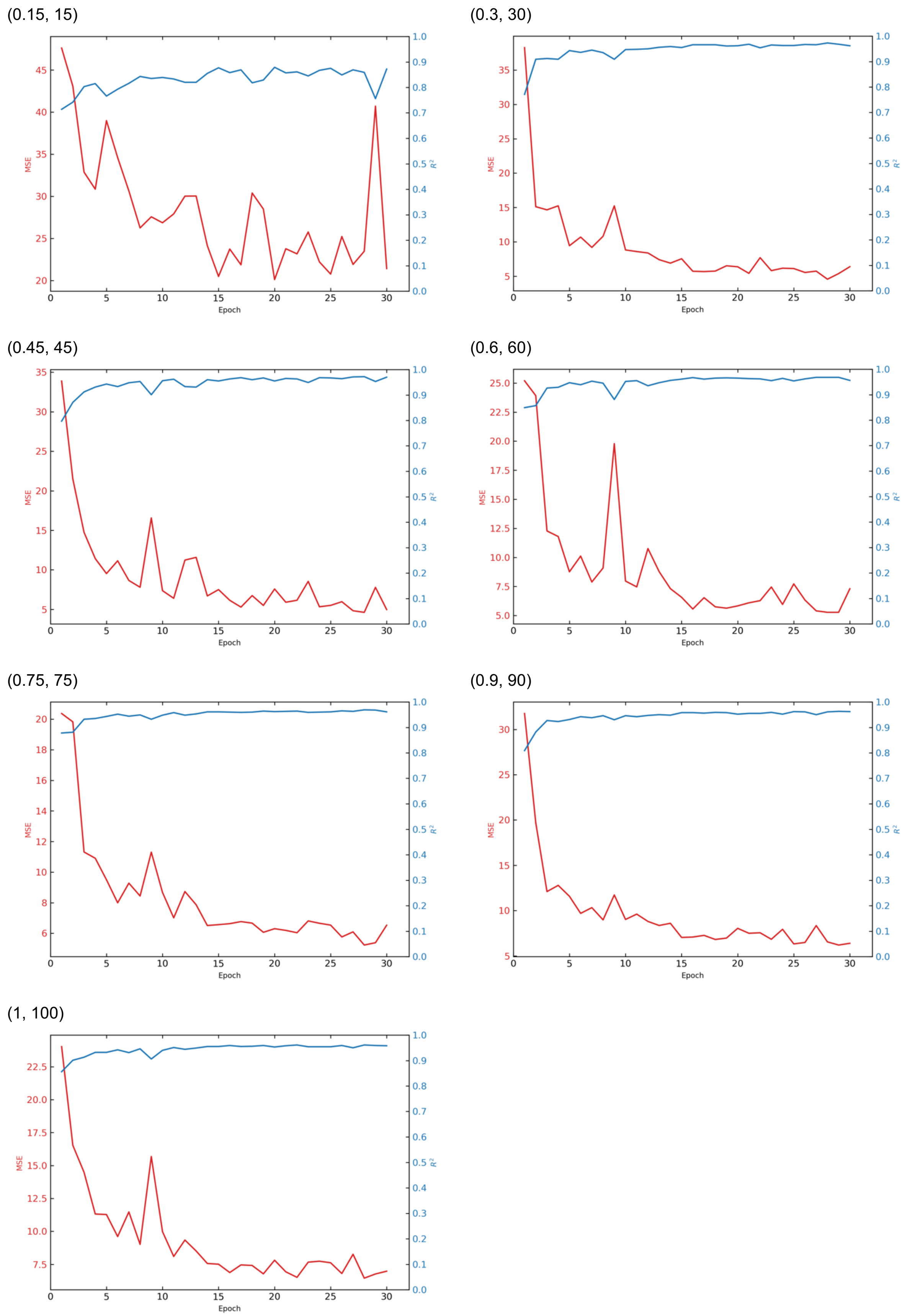

Figure S7: r^2 and MSE as a function of epoch during training of ResNet18 for distance grids with a fixed input tensor shape of 100^3, achieved by different combinations of input dimensions and grid resolutions. The input representations are given in parentheses, $(\Delta d, L)$ in Å.

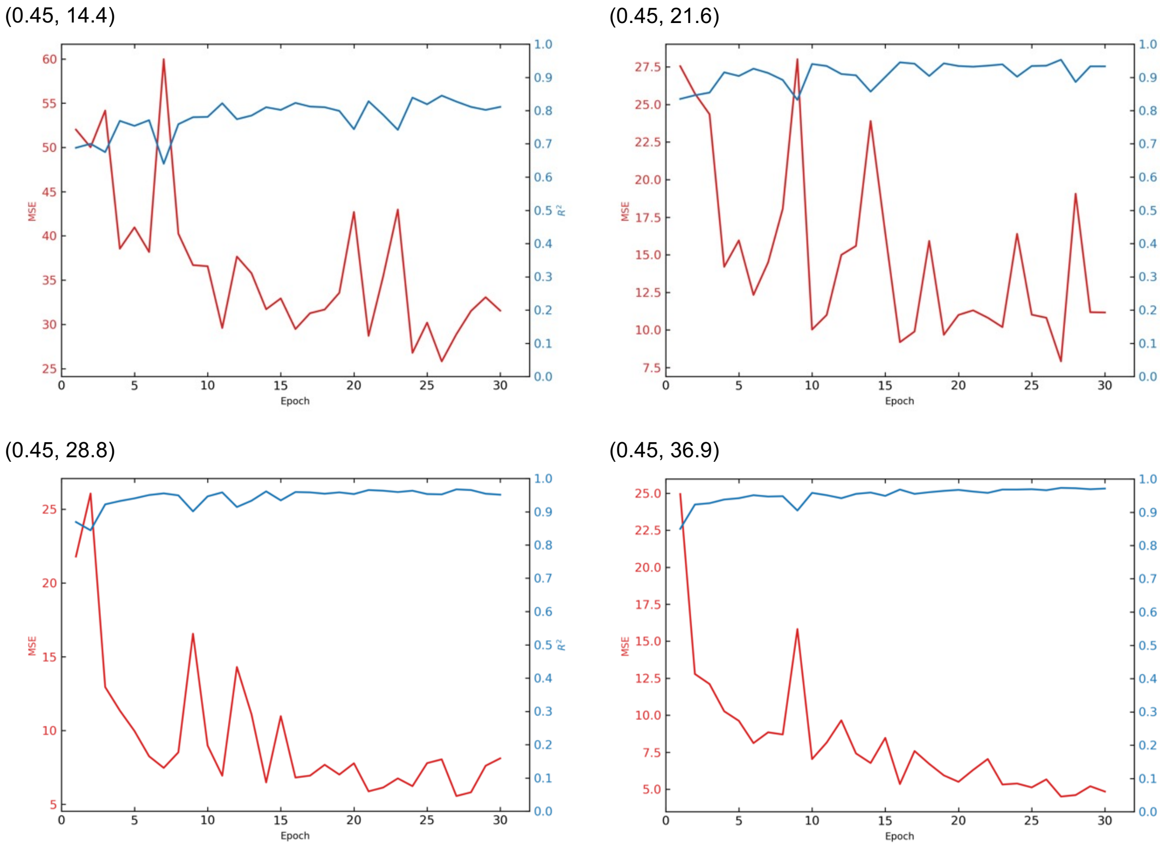

Figure S8: r^2 and MSE as a function of epoch during training of ResNet18 for distance grids with a fixed grid resolution of 0.45 Å, achieved by different combinations of input dimensions and shapes. The input representations are given in parentheses, $(\Delta d, L)$ in Å.

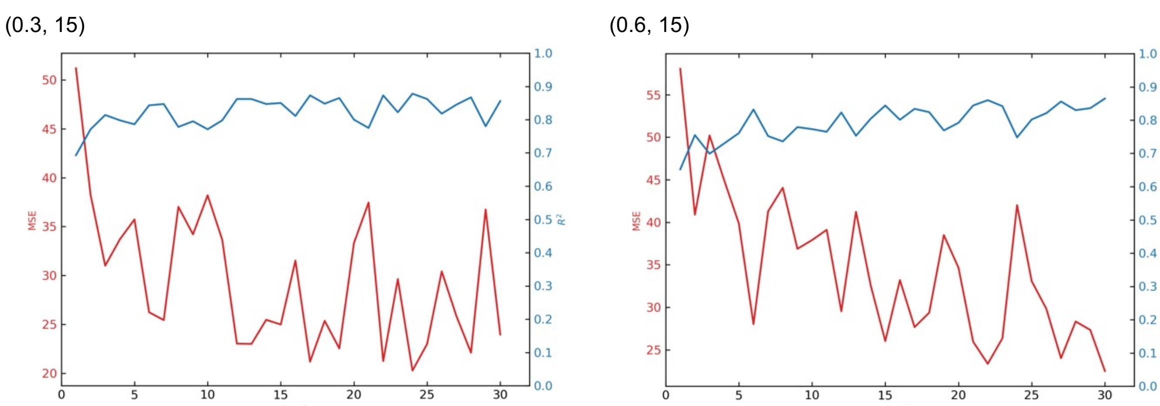

Figure S9: r^2 and MSE as a function of epoch during training of ResNet18 for distance grids with a fixed linear dimension of 15 Å, achieved by different combinations of input shapes and grid resolutions. The input representations are given in parentheses, $(\Delta d, L)$ in Å.

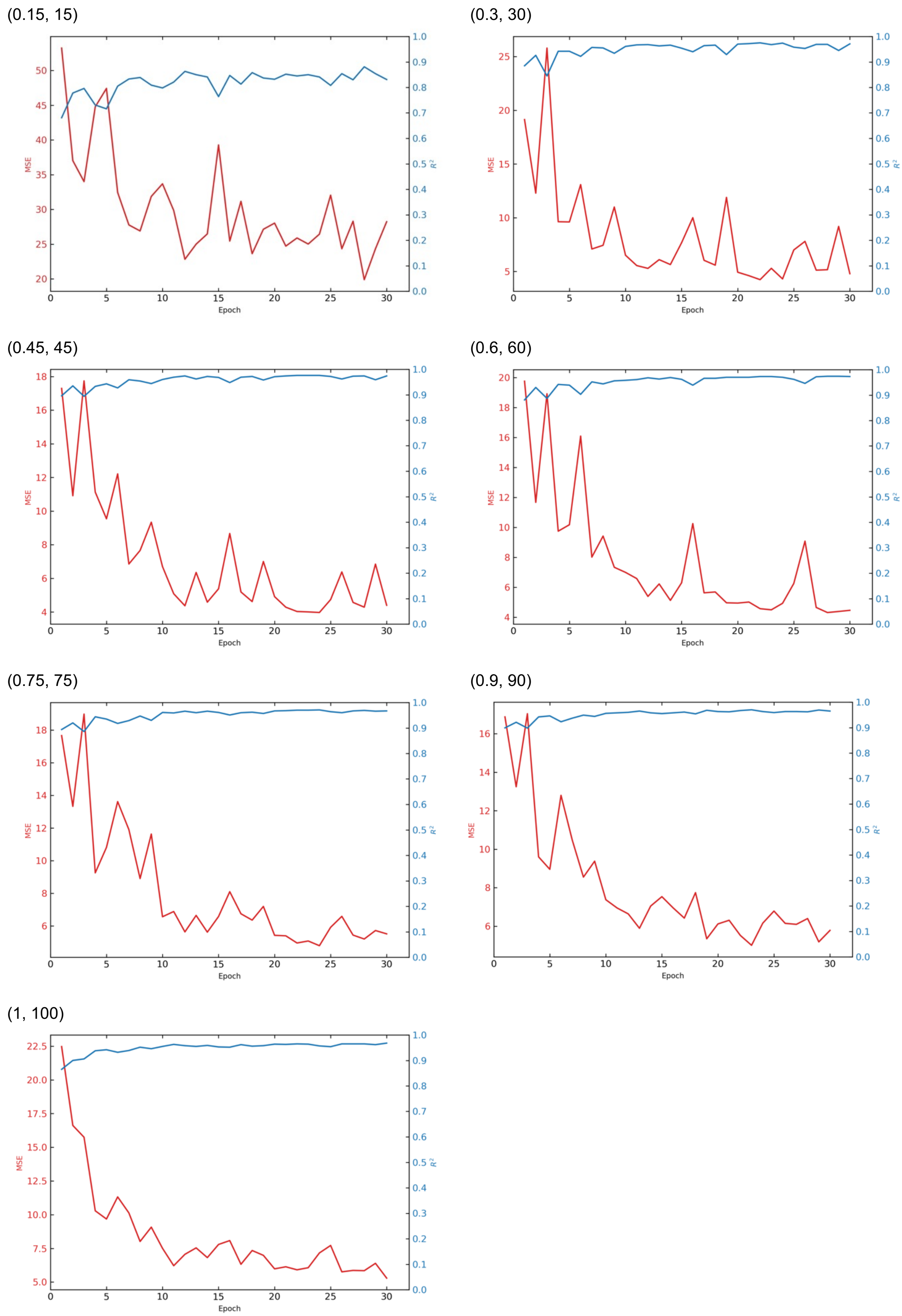

Figure S10: r^2 and MSE as a function of epoch during training of DenseNet121 for distance grids with a fixed input tensor shape of 100^3, achieved by different combinations of input dimensions and grid resolutions. The input representations are given in parentheses, $(\Delta d, L)$ in Å.

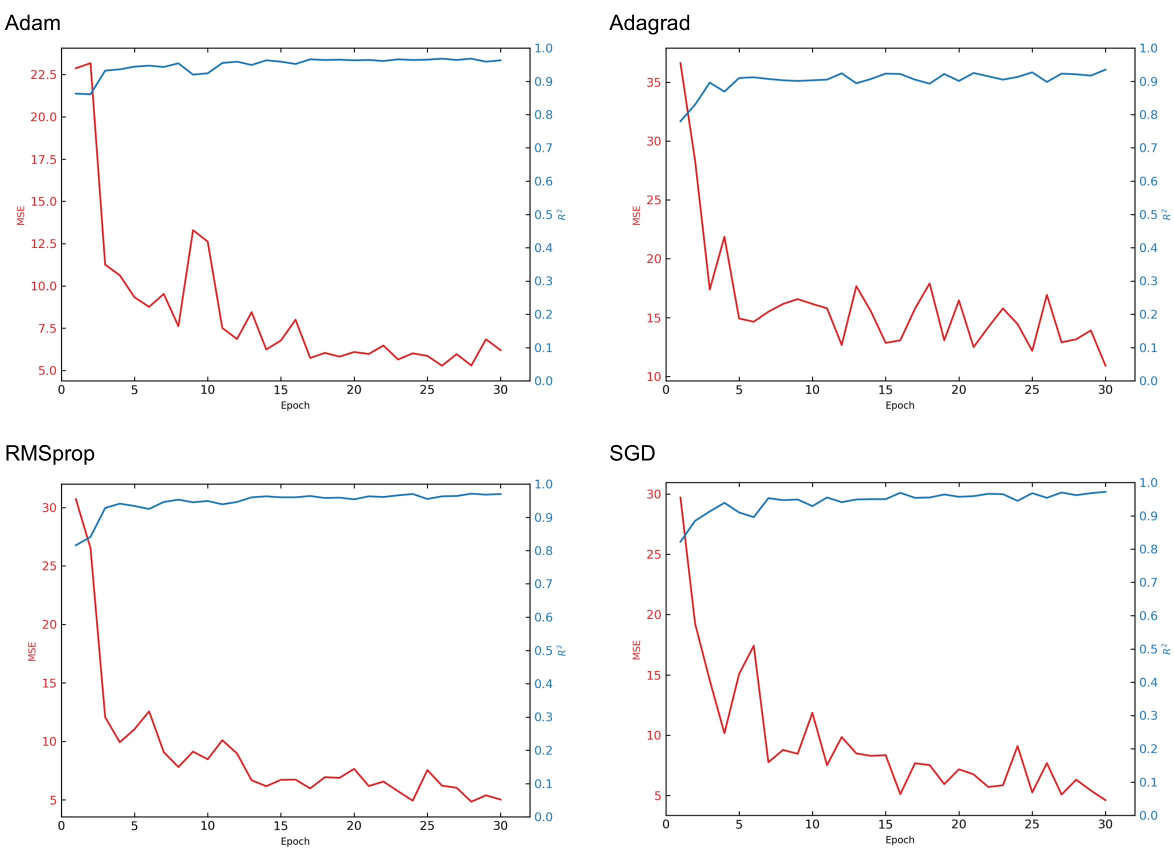

Figure S11: r^2 and MSE as a function of epoch during training of ResNet18 for distance grids with batch sizes of 4, learning rates of 0.00025, and different optimizers.

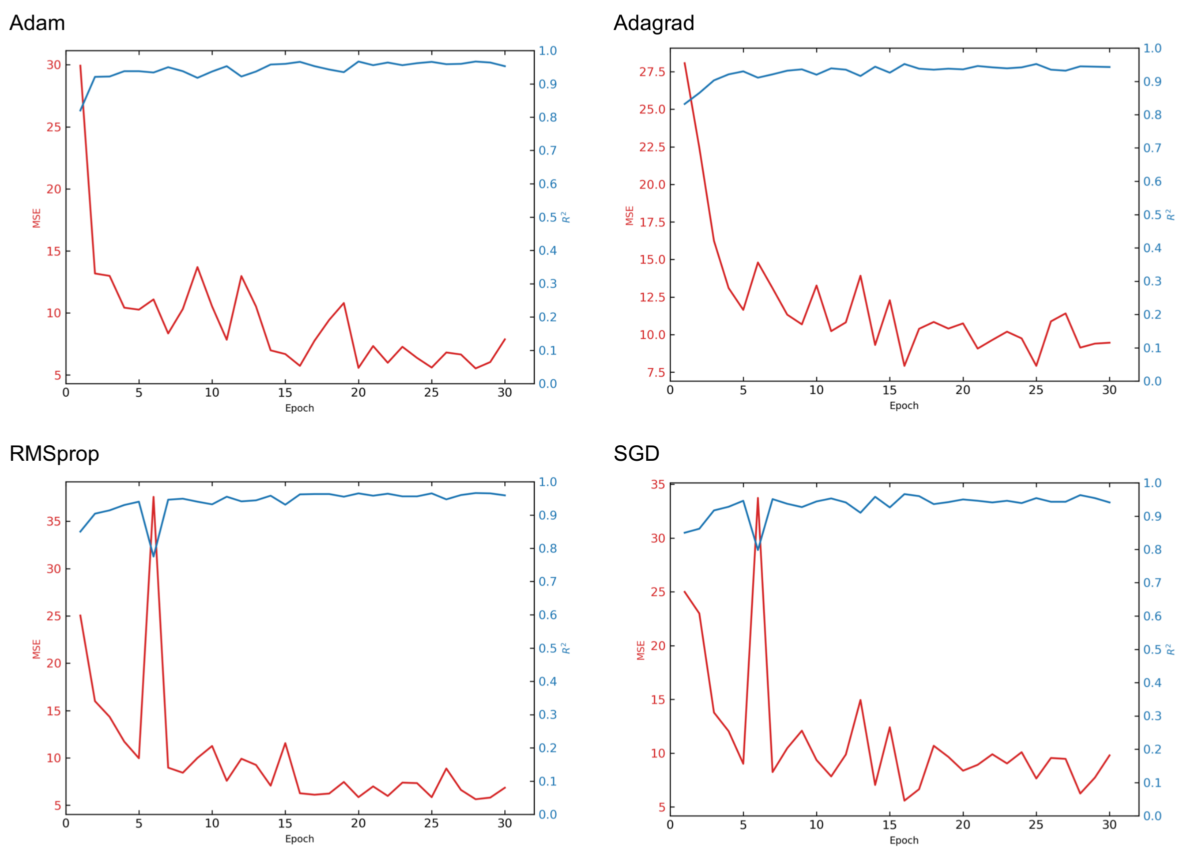

Figure S12: r^2 and MSE as a function of epoch during training of ResNet18 for distance grids with batch sizes of 8, learning rates of 0.0005, and different optimizers.

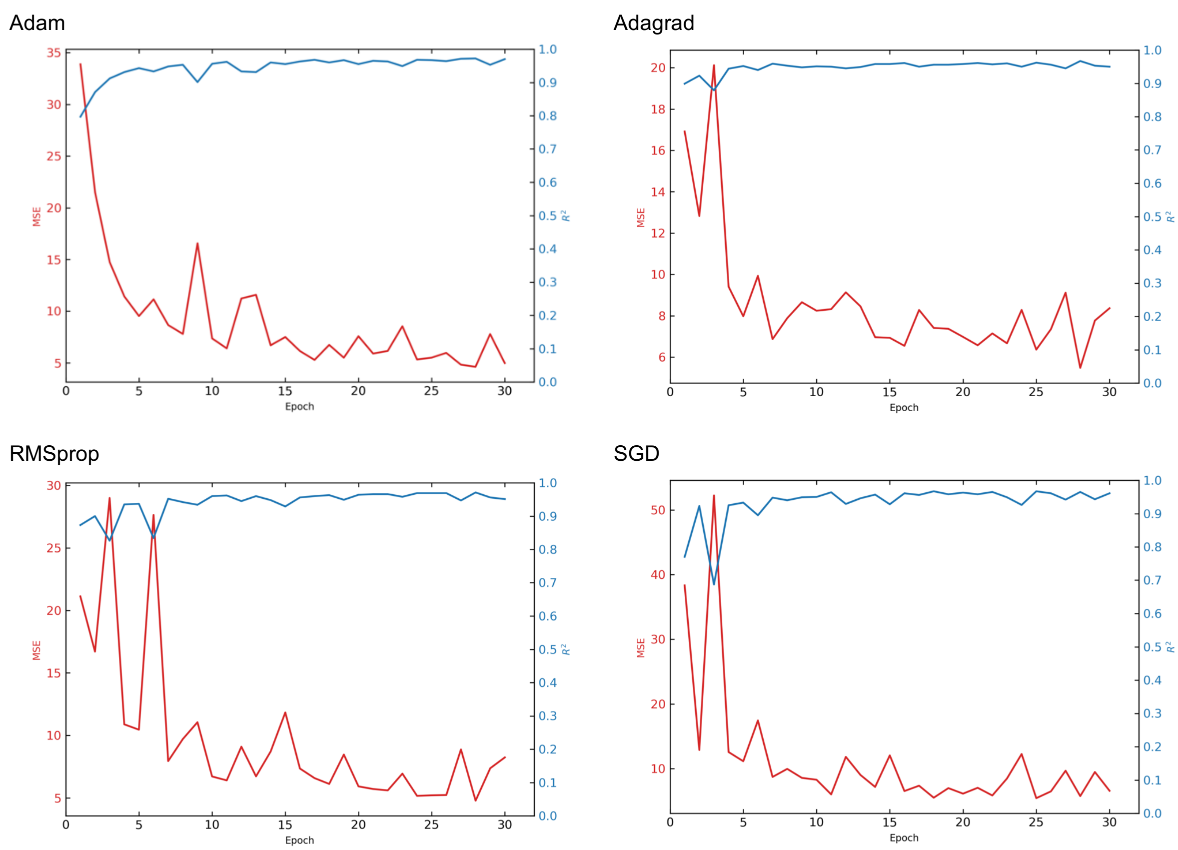

Figure S13: r^2 and MSE as a function of epoch during training of ResNet18 for distance grids with batch sizes of 16, learning rates of 0.001, and different optimizers.

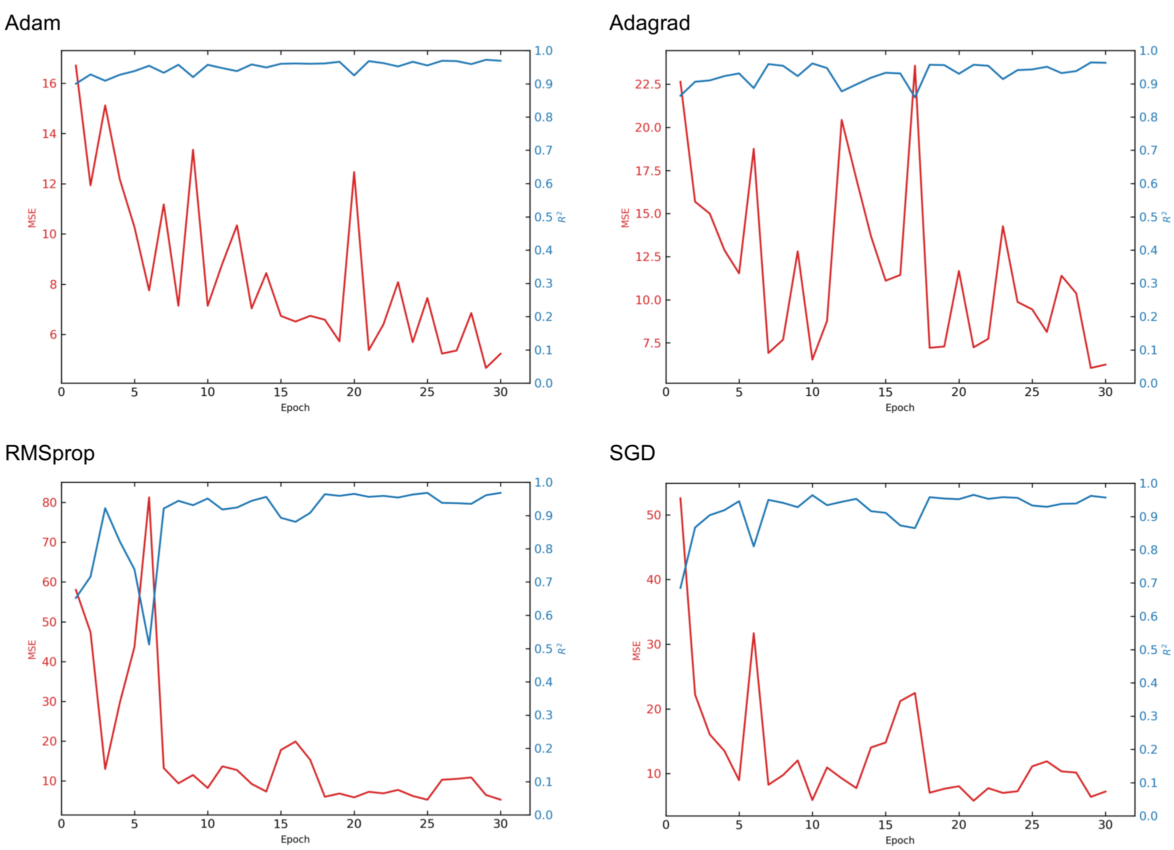

Figure S14: r^2 and MSE as a function of epoch during training of ResNet18 for distance grids with batch sizes of 64, learning rates of 0.001, and different optimizers.

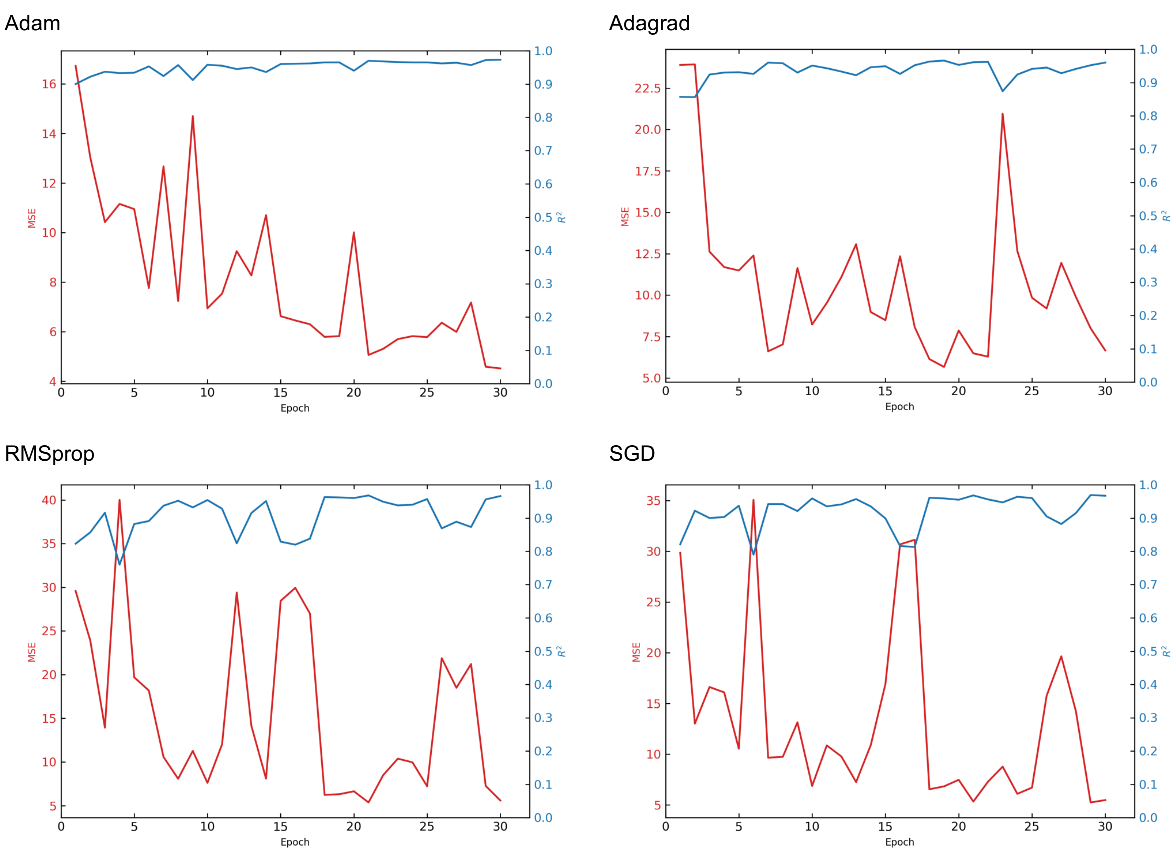

Figure S15: r^2 and MSE as a function of epoch during training of ResNet18 for distance grids with batch sizes of 64, learning rates of 0.002, and different optimizers.

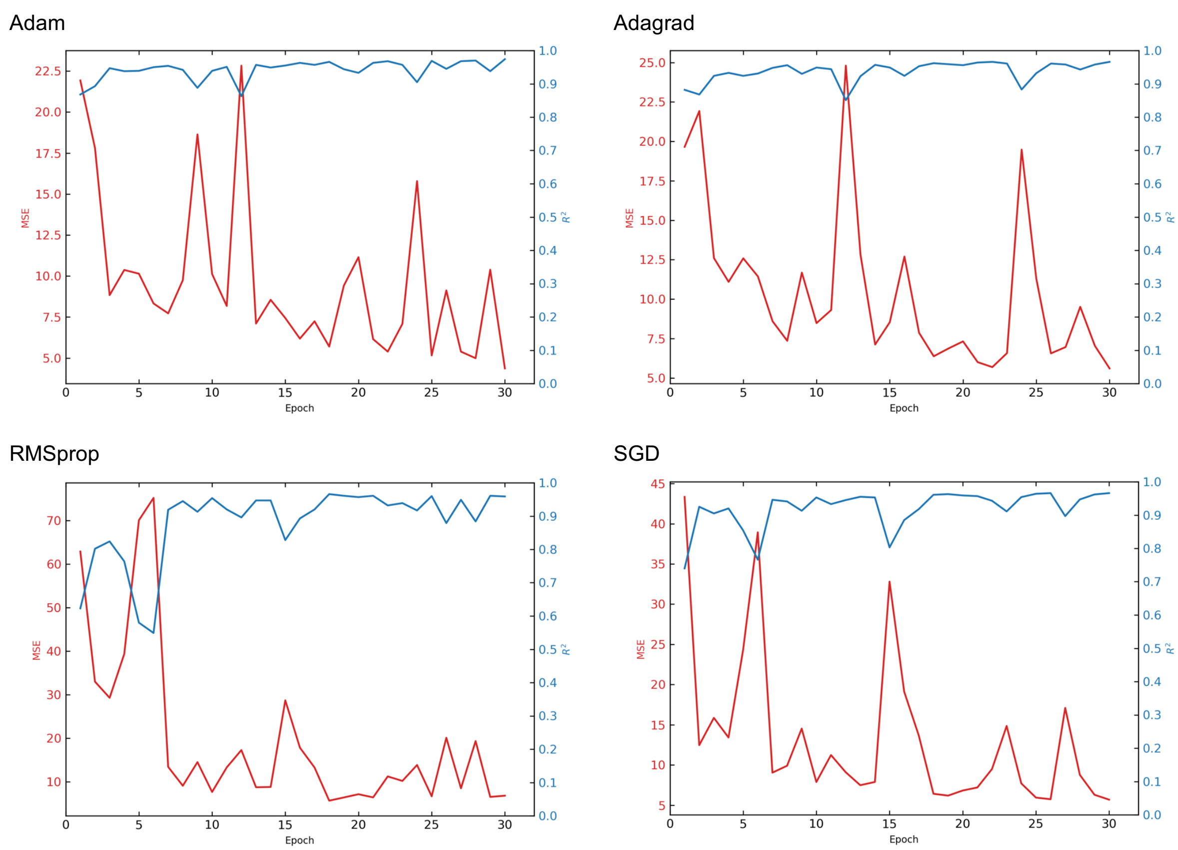

Figure S16: r^2 and MSE as a function of epoch during training of ResNet18 for distance grids with batch sizes of 64, learning rates of 0.004, and different optimizers.