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# NADS: Neural Architecture Distribution Search for Uncertainty Awareness

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## 1. Fixed Model Ablation Study

Table 1. OoD detection results on various training and testing experiments comparing our method with a baseline ensembling method that uses a fixed architecture trained multiple times with different random initializations.

| $D_{in}$ | $D_{out}$  | FPR% at TPR 95% |              | AUROC%        |              | AUPR%         |              |
|----------|------------|-----------------|--------------|---------------|--------------|---------------|--------------|
|          |            | Base Ensemble   | Ours         | Base Ensemble | Ours         | Base Ensemble | Ours         |
| CIFAR10  | SVHN       | 50.07           | <b>17.05</b> | 93.48         | <b>97.65</b> | 95.98         | <b>99.07</b> |
|          | Texture    | 6.22            | <b>0.25</b>  | 97.68         | <b>99.81</b> | 97.44         | <b>99.86</b> |
|          | Places365  | 1.03            | <b>0.00</b>  | 99.59         | <b>100</b>   | 99.97         | <b>100</b>   |
|          | LSUN       | 34.35           | <b>0.44</b>  | 91.55         | <b>99.83</b> | 92.15         | <b>99.89</b> |
|          | CIFAR100   | 65.13           | <b>36.36</b> | 78.44         | <b>91.23</b> | 79.44         | <b>91.60</b> |
|          | Gaussian   | <b>0.00</b>     | <b>0.00</b>  | <b>100</b>    | <b>100</b>   | <b>100</b>    | <b>100</b>   |
|          | Rademacher | <b>0.00</b>     | <b>0.00</b>  | <b>100</b>    | <b>100</b>   | <b>100</b>    | <b>100</b>   |

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## 2. OoD Detection Performance Comparison with ODIN

Table 2. OoD detection results on various training and testing experiments comparing our method with ODIN (Liang et al., 2017).

| $D_{in}$ | $D_{out}$  | FPR% at TPR 95% |              | AUROC%      |              | AUPR%       |              |
|----------|------------|-----------------|--------------|-------------|--------------|-------------|--------------|
|          |            | ODIN            | Ours         | ODIN        | Ours         | ODIN        | Ours         |
| MNIST    | not-MNIST  | 8.7             | <b>0.00</b>  | 98.2        | <b>100</b>   | 98.0        | <b>100</b>   |
|          | F-MNIST    | 65              | <b>0.00</b>  | 88.6        | <b>100</b>   | 90.5        | <b>100</b>   |
|          | K-MNIST    | 36.5            | <b>0.76</b>  | 94.0        | <b>99.80</b> | 94.6        | <b>99.84</b> |
| SVHN     | Texture    | 33.9            | <b>0.07</b>  | 92.4        | <b>99.26</b> | 88.2        | <b>97.75</b> |
|          | Places365  | 22.2            | <b>0.00</b>  | 94.9        | <b>99.99</b> | 99.8        | <b>99.99</b> |
|          | LSUN       | 26.8            | <b>0.02</b>  | 93.5        | <b>99.99</b> | 93.1        | <b>99.99</b> |
|          | CIFAR10    | 21.6            | <b>0.37</b>  | 94.8        | <b>99.92</b> | 94.4        | <b>99.83</b> |
| CIFAR10  | SVHN       | 36.5            | <b>17.05</b> | 89.7        | <b>97.65</b> | 95.6        | <b>99.07</b> |
|          | Texture    | 76.2            | <b>0.25</b>  | 81.4        | <b>99.81</b> | 76.7        | <b>99.86</b> |
|          | Places365  | 44.0            | <b>0.00</b>  | 89.0        | <b>100</b>   | 99.6        | <b>100</b>   |
|          | LSUN       | 3.9             | <b>0.44</b>  | 99.2        | <b>99.83</b> | 99.2        | <b>99.89</b> |
|          | CIFAR100   | 45.4            | <b>36.36</b> | 88.3        | <b>91.23</b> | 88.5        | <b>91.60</b> |
|          | Gaussian   | 0.1             | <b>0.00</b>  | <b>100</b>  | <b>100</b>   | 99.9        | <b>100</b>   |
|          | Rademacher | 0.3             | <b>0.00</b>  | 99.9        | <b>100</b>   | 99.8        | <b>100</b>   |
| CIFAR100 | SVHN       | <b>32.8</b>     | 45.92        | 90.3        | <b>94.35</b> | 95.3        | <b>96.01</b> |
|          | Texture    | 78.9            | <b>0.42</b>  | 75.7        | <b>99.76</b> | 64.5        | <b>99.81</b> |
|          | Places365  | 63.3            | <b>0.012</b> | 79.0        | <b>99.99</b> | 99.1        | <b>99.99</b> |
|          | LSUN       | <b>17.6</b>     | 38.85        | <b>96.8</b> | 90.65        | <b>96.5</b> | 90.61        |
|          | CIFAR10    | 78.2            | <b>45.62</b> | 70.6        | <b>83.27</b> | 69.7        | <b>81.48</b> |
|          | Gaussian   | 1.3             | <b>0.00</b>  | 99.5        | <b>100</b>   | 97.8        | <b>100</b>   |
|          | Rademacher | 13.8            | <b>0.00</b>  | 92.7        | <b>100</b>   | 75.0        | <b>100</b>   |

### 3. Additional Sample Architectures

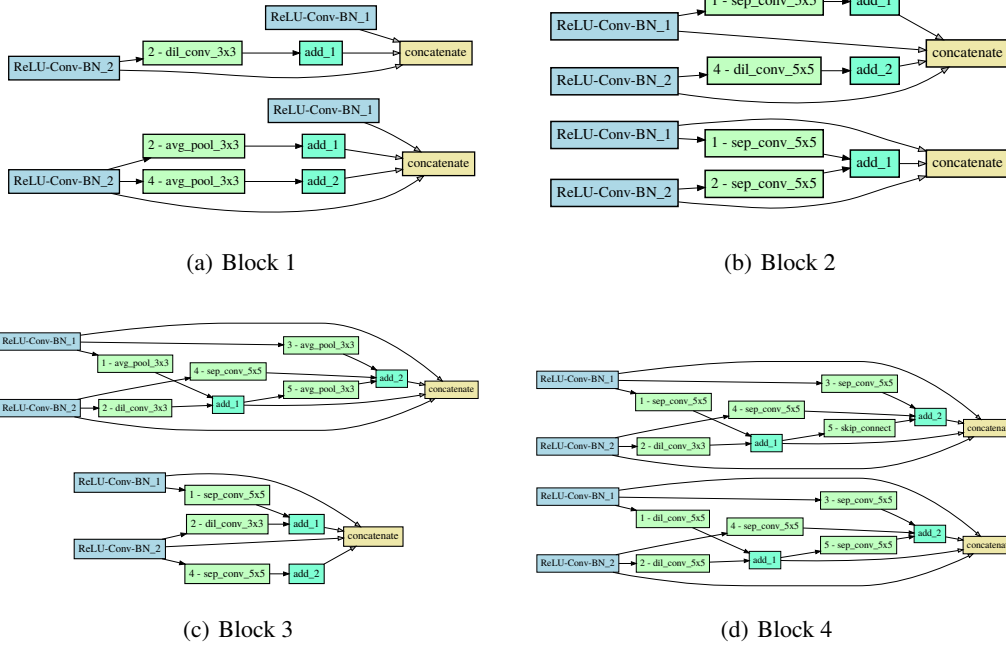


Figure 1. Maximum likelihood architectures inferred by our search algorithm on CelebA. Shown are two samples taken from each block.

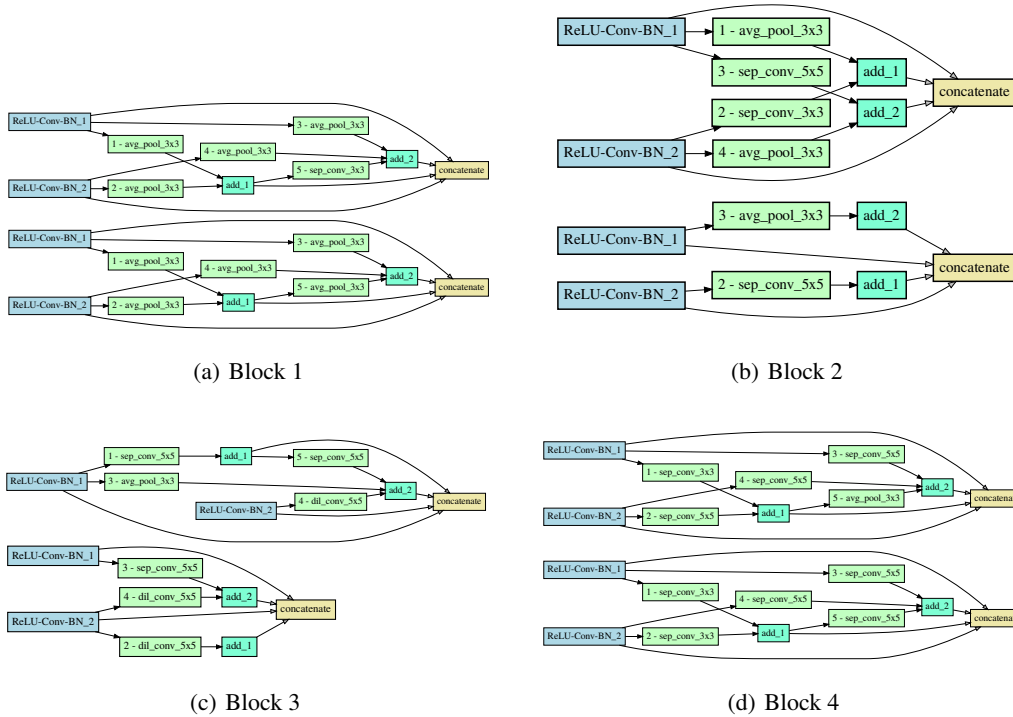


Figure 2. Maximum likelihood architectures inferred by our search algorithm on MNIST. Shown are two samples taken from each block.

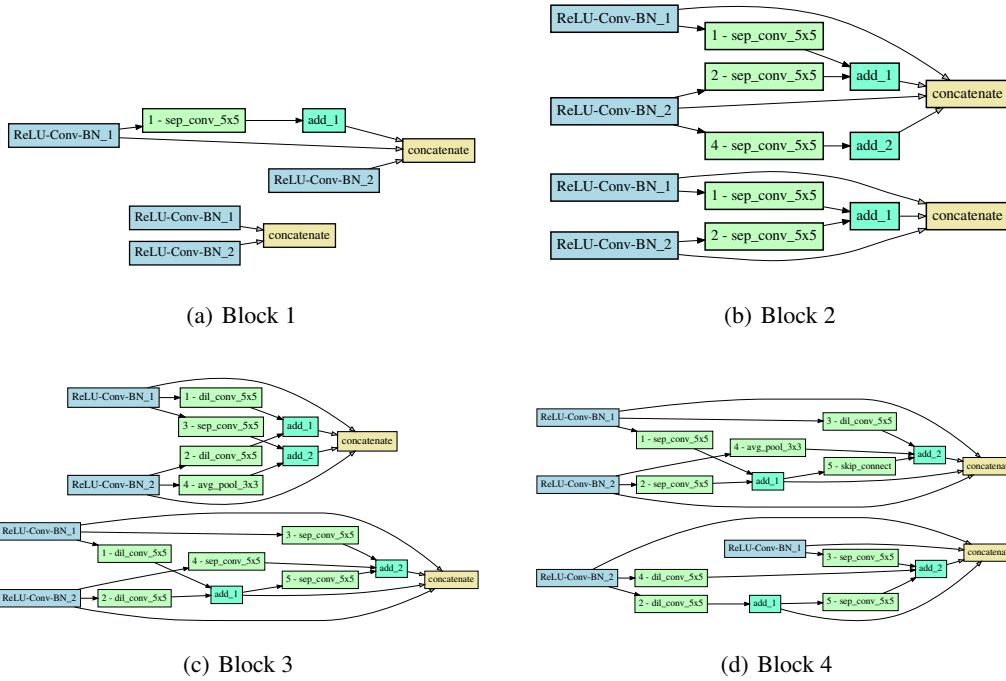


Figure 3. Maximum likelihood architectures inferred by our search algorithm on SVHN. Shown are two samples taken from each block.

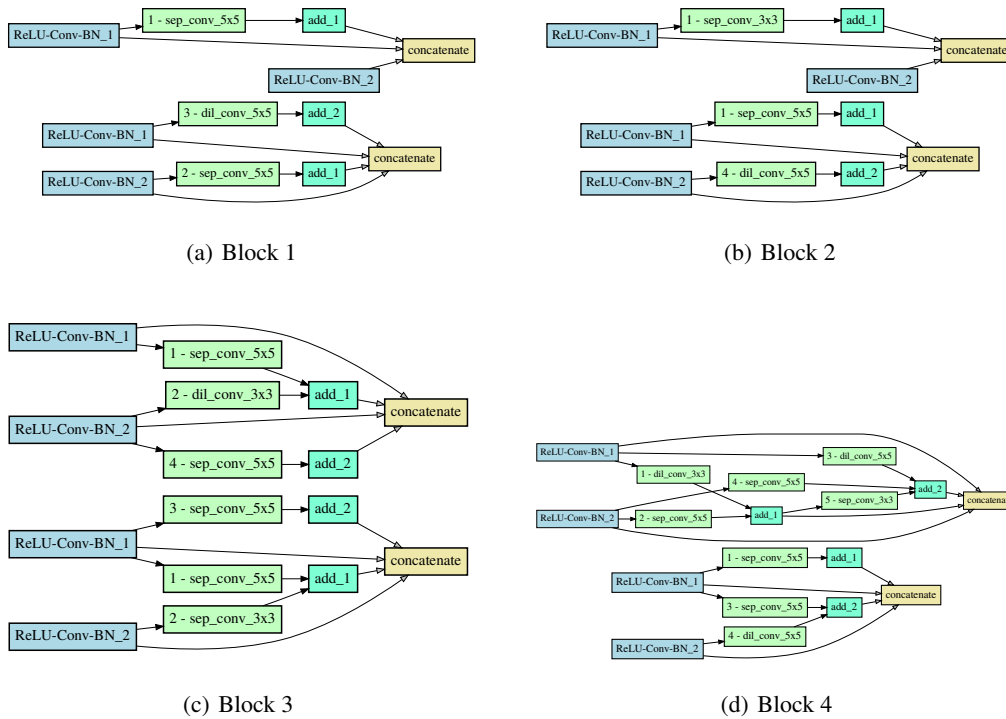


Figure 4. Maximum likelihood architectures inferred by our search algorithm on CIFAR-10. Shown are two samples taken from each block.

#### 4. Image Generation Samples



Figure 5. Samples taken from randomly sampled NADS architectures searched on CelebA. Images were not cherry-picked and the architectures were sampled without further retraining.



Figure 6. Samples taken from randomly sampled NADS architectures searched on MNIST. Images were not cherry-picked and the architectures were sampled without further retraining.



Figure 7. Samples taken from randomly sampled NADS architectures searched on SVHN. Images were not cherry-picked and the architectures were sampled without further retraining.



Figure 8. Samples taken from randomly sampled NADS architectures searched on CIFAR-10. Images were not cherry-picked and the architectures were sampled without further retraining.

### 5. Likelihood Estimation Models Assign Higher Likelihood to OoD Data

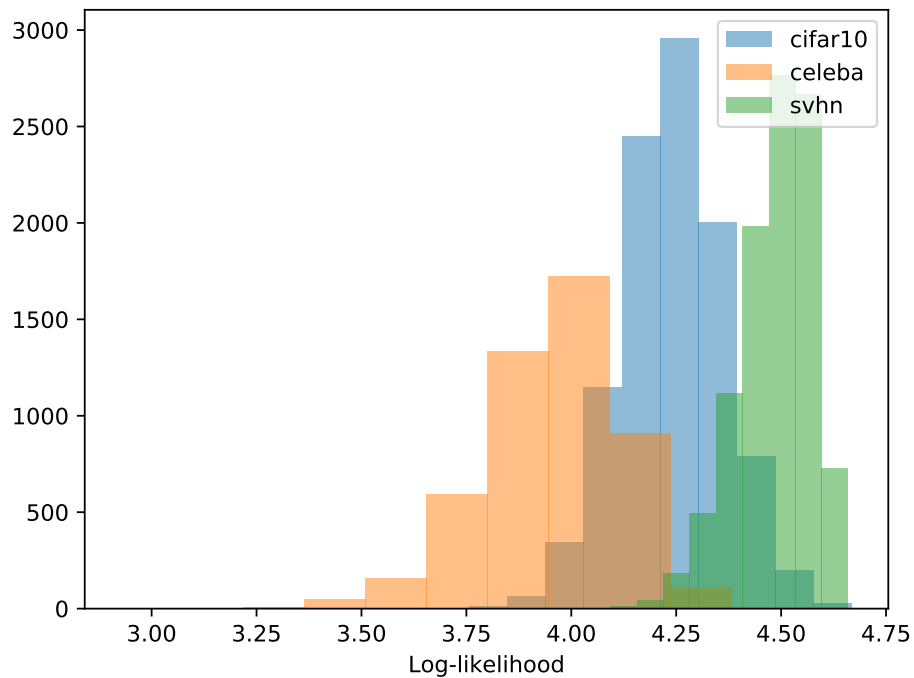


Figure 9. Likelihood distributions of different datasets evaluated on a Glow model trained on CelebA. The model assigns higher likelihood to OoD samples from CIFAR-10 and SVHN.

## 6. Effect of Ensemble Size

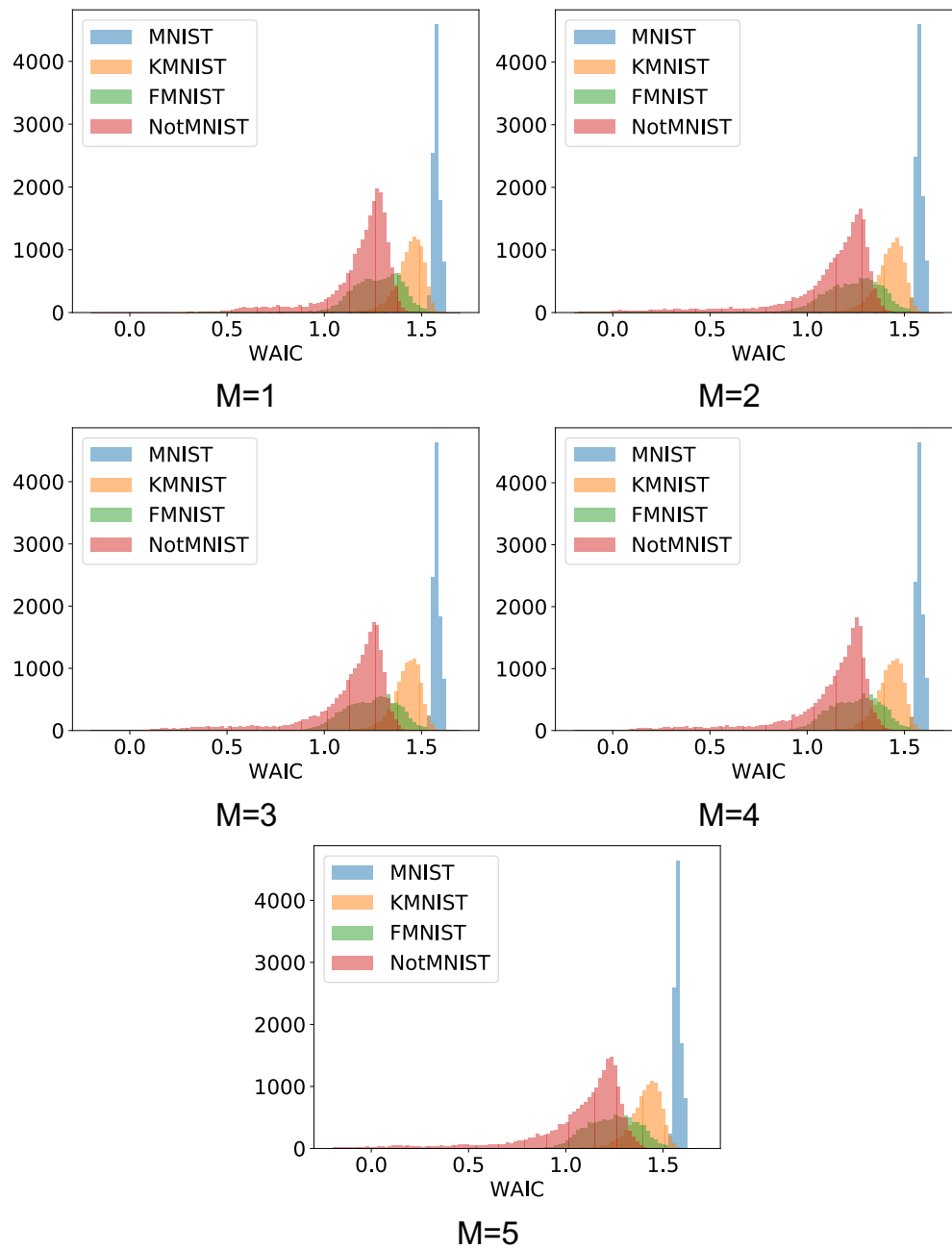


Figure 10. Effect of ensemble size to the distribution of WAIC scores estimated by model ensembles trained on MNIST.

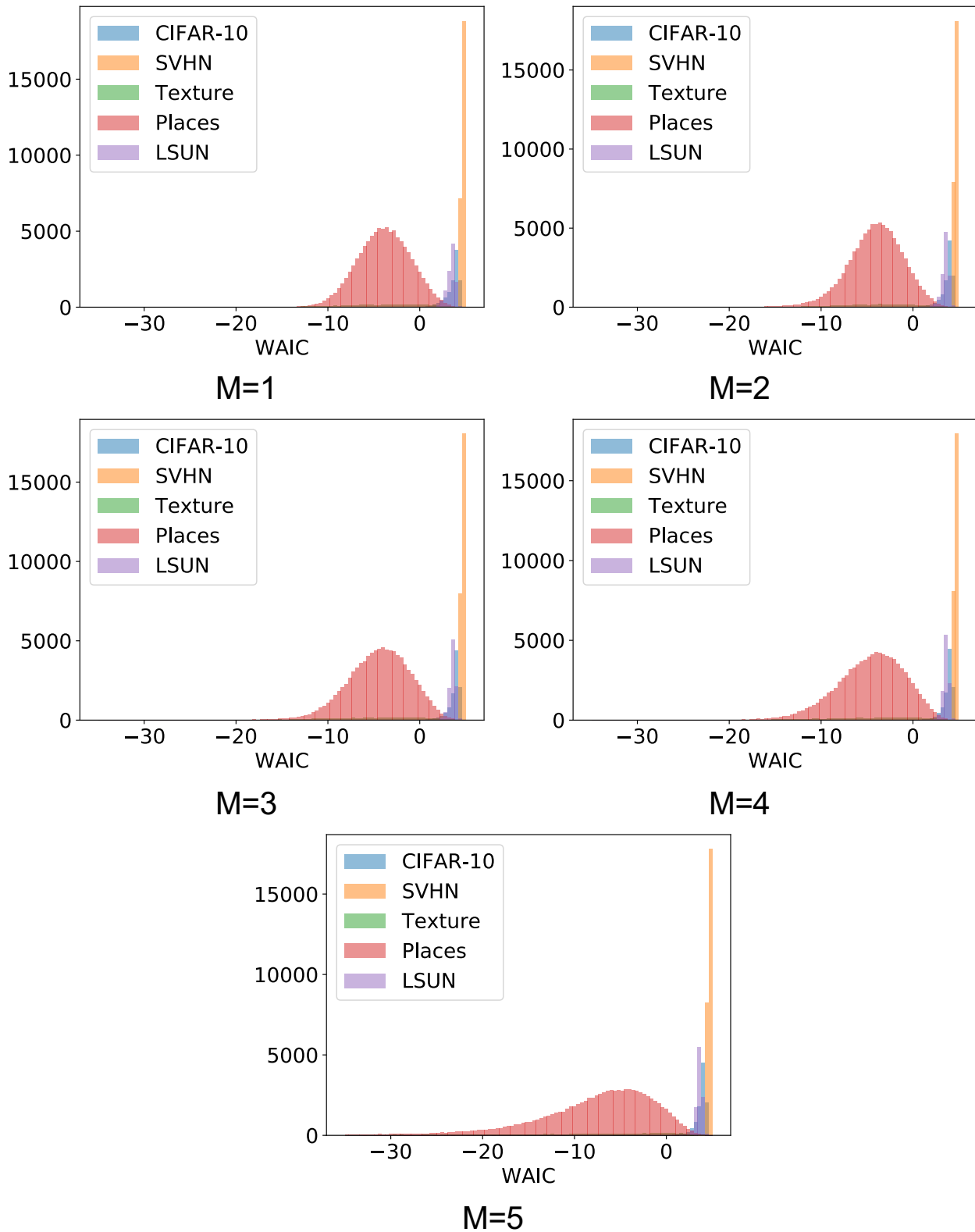


Figure 11. Effect of ensemble size to the distribution of WAIC scores estimated by model ensembles trained on SVHN.



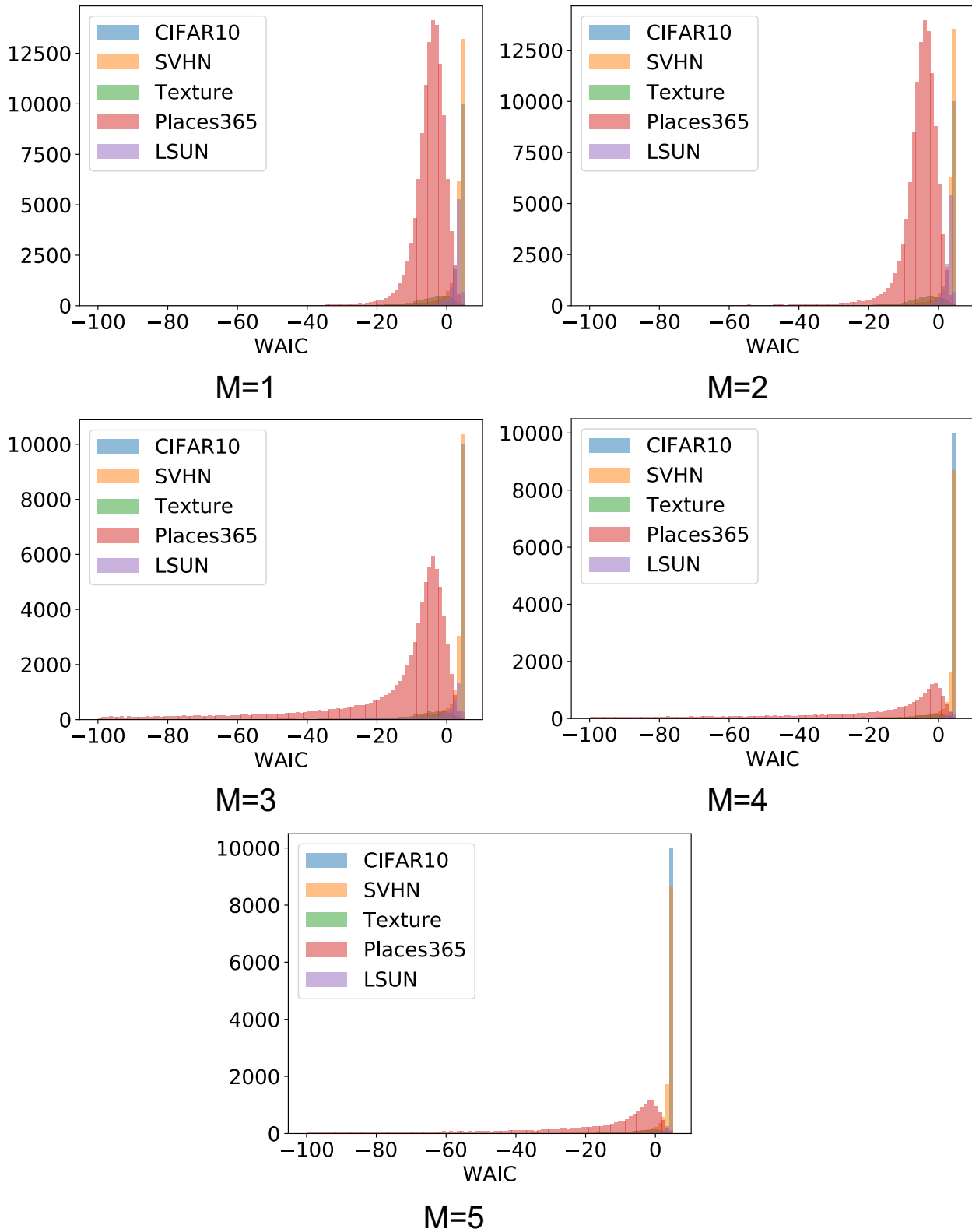


Figure 12. Effect of ensemble size to the distribution of WAIC scores estimated by model ensembles trained on CIFAR-10.

## 7. Additional ROC and Precision-Recall Curves

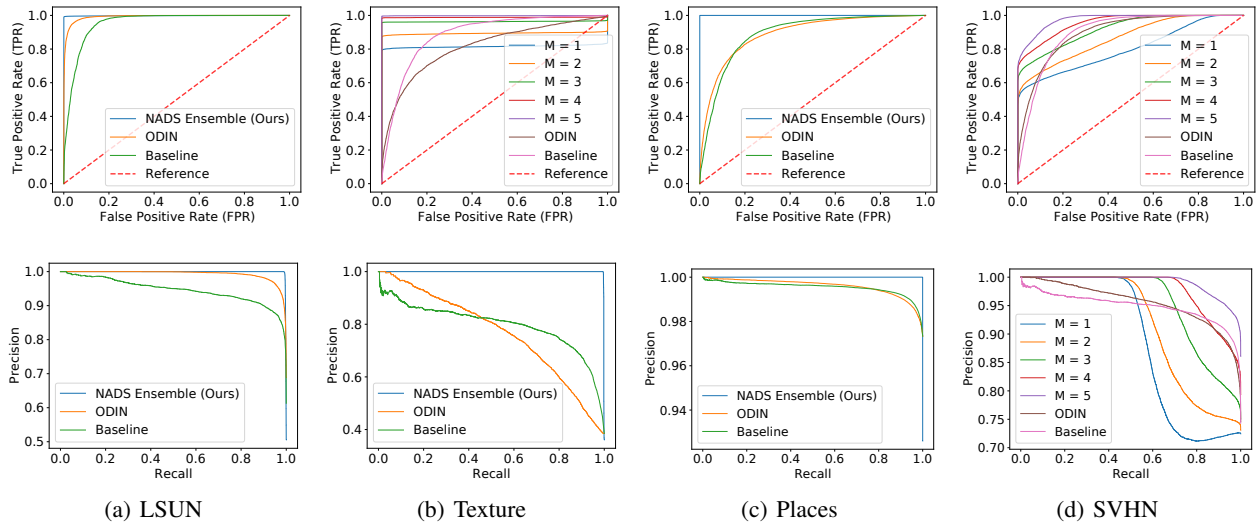


Figure 13. ROC and PR curve comparison of methods trained on CIFAR-10

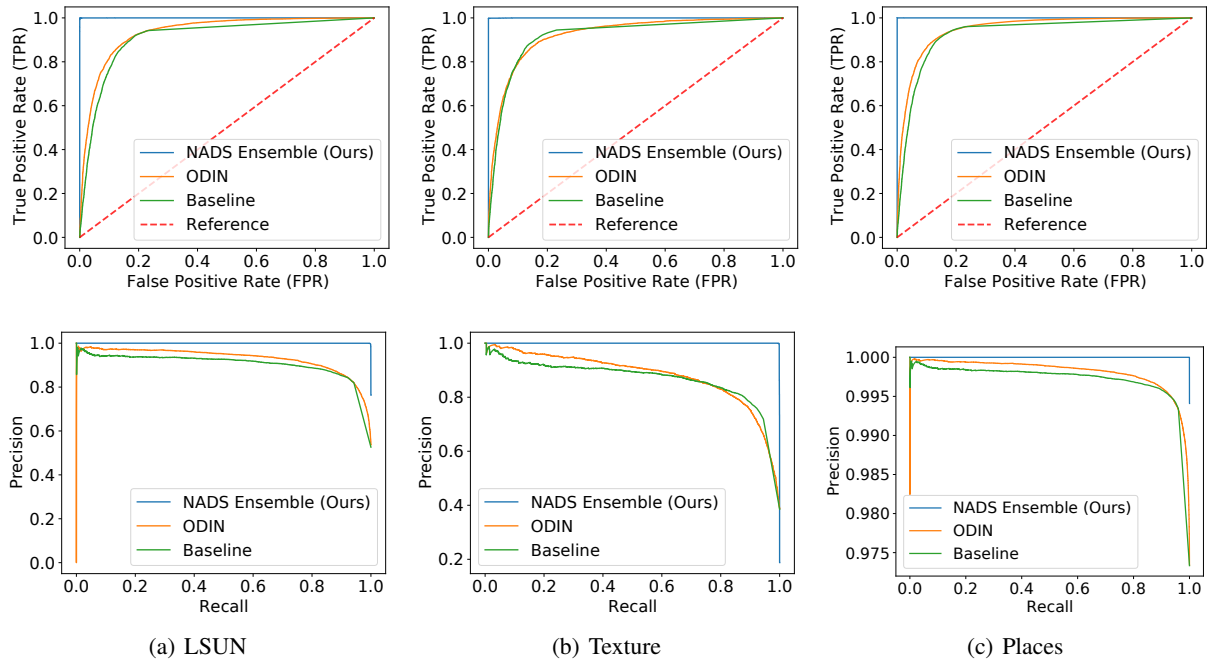


Figure 14. ROC and PR curve comparison of methods trained on SVHN

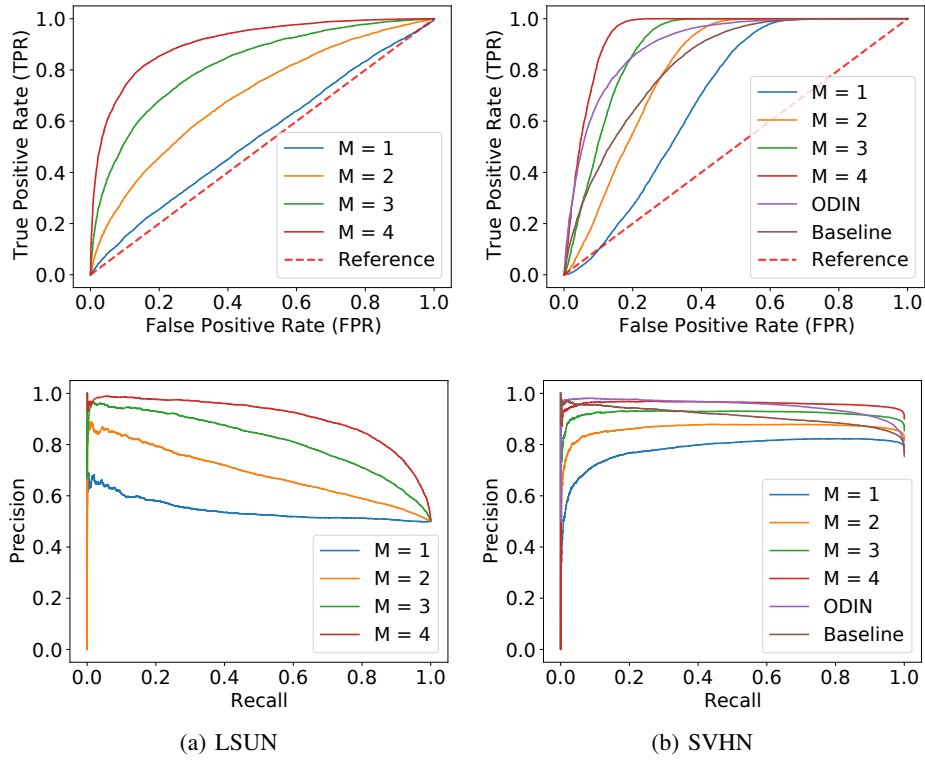


Figure 15. ROC and PR curve comparison of methods trained on CIFAR-100

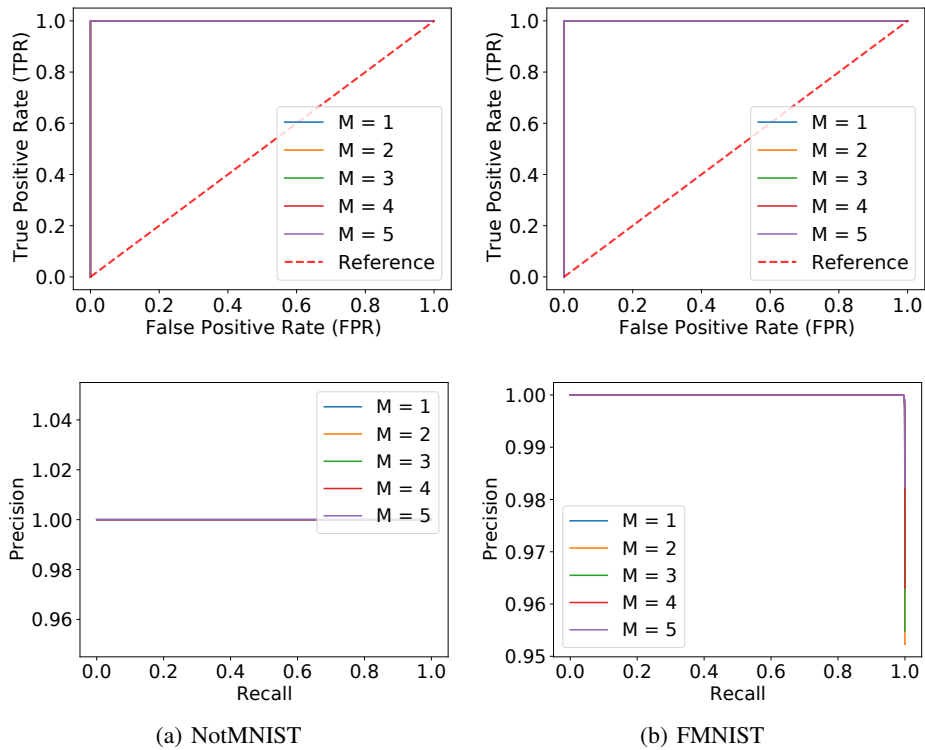


Figure 16. ROC and PR curve comparison of methods trained on MNIST

## References

Liang, S., Li, Y., and Srikant, R. Enhancing the reliability of out-of-distribution image detection in neural networks. *arXiv preprint arXiv:1706.02690*, 2017.