Bayesian Deep Learning and Uncertainty

Christos Louizos, Max Welling

Amsterdam Machine Learning Lab

University of Amsterdam

Overview

- Part 1:
  - Structured approximate posteriors in Bayesian neural nets
- Part 2:
  - Exploring model uncertainty

Part 1

Structured and Efficient Variational Deep Learning with Matrix Gaussian Posteriors

ICML 2016

VI for Bayesian neural networks (BNNs)

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Stochastic gradient VI for BNNs optimizes:

$$\mathbb{E}_{\prod_{i=1}^{H} q(\mathbf{W}_i)}[\log p(\mathbf{y}|\mathbf{x}, \mathbf{W}_{1:H})] - \sum_{i=1}^{H} KL(q(\mathbf{W}_i), p(\mathbf{W}_i))$$

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Usual choices for q are fully factorized Gaussians

$$q(\mathbf{W}_i) = \prod_{r=1}^{R} \prod_{c=1}^{C} \mathcal{N}(\mu_{rc}, \sigma_{rc}^2)$$

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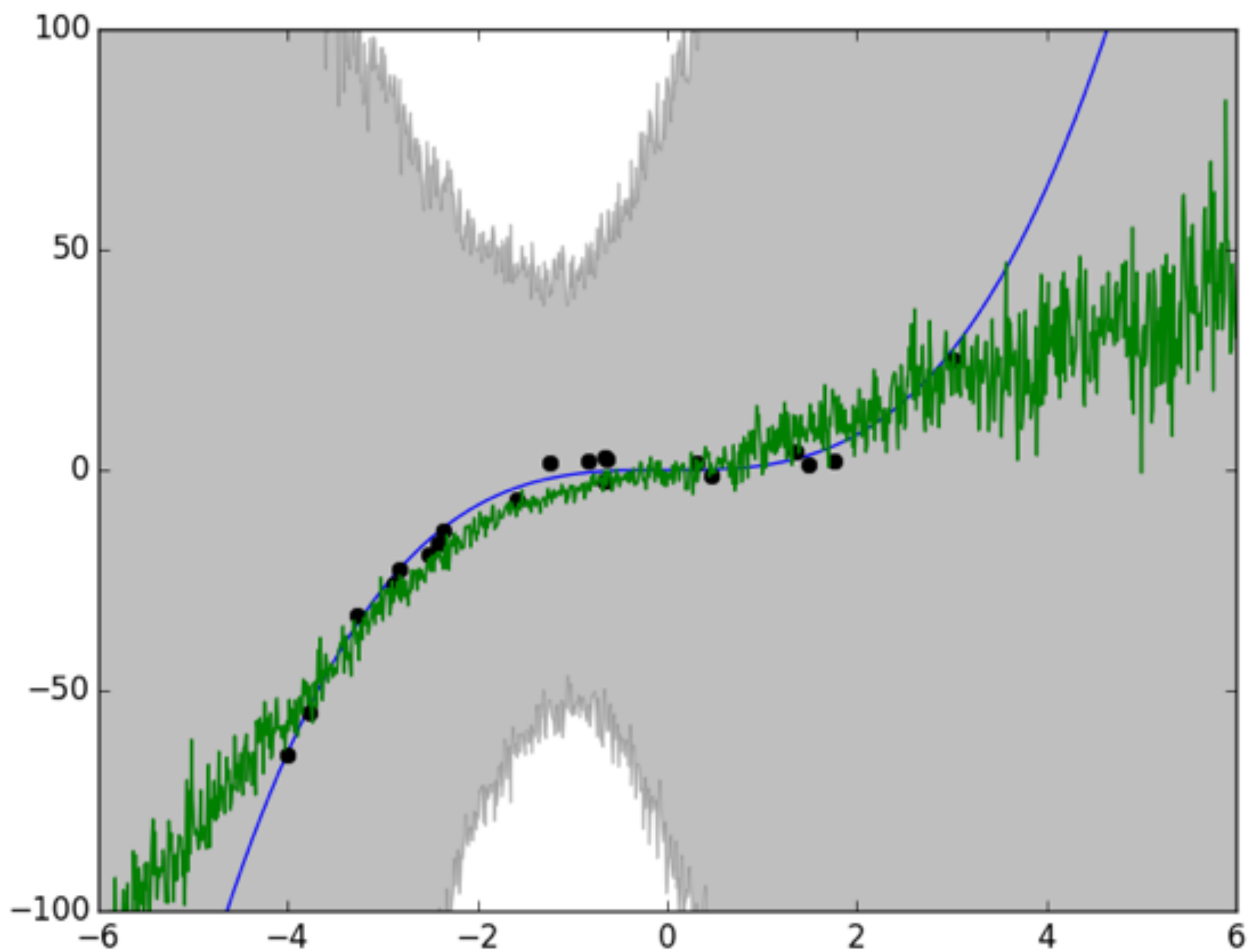

Fully factorized VI BNN

Structured VI for BNNs

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Simple idea

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Assume a matrix Gaussian posterior over each weight matrix:

$$\begin{aligned} q(\mathbf{W}_i) &= \mathcal{MN}(\mathbf{M}_{r\times c}, \mathbf{U}_{r\times r}, \mathbf{V}_{c\times c}) \\ &= \mathcal{N}(vec(\mathbf{M}), \mathbf{U}\otimes\mathbf{V}) \end{aligned}$$

M corresponds to the mean matrix

U corresponds to the row covariance

V corresponds to the column covariance

Structured VI with matrix Gaussian posteriors

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Structured VI with matrix Gaussian posteriors

- Compactly model correlations among weights
- "Full" matrix Gaussian is still expensive
- Low rank approximations for **U**, **V**
  - Diagonal approximations reduce parameters greatly
  - Still maintain some correlations among weights

Structured VI with matrix Gaussian posteriors

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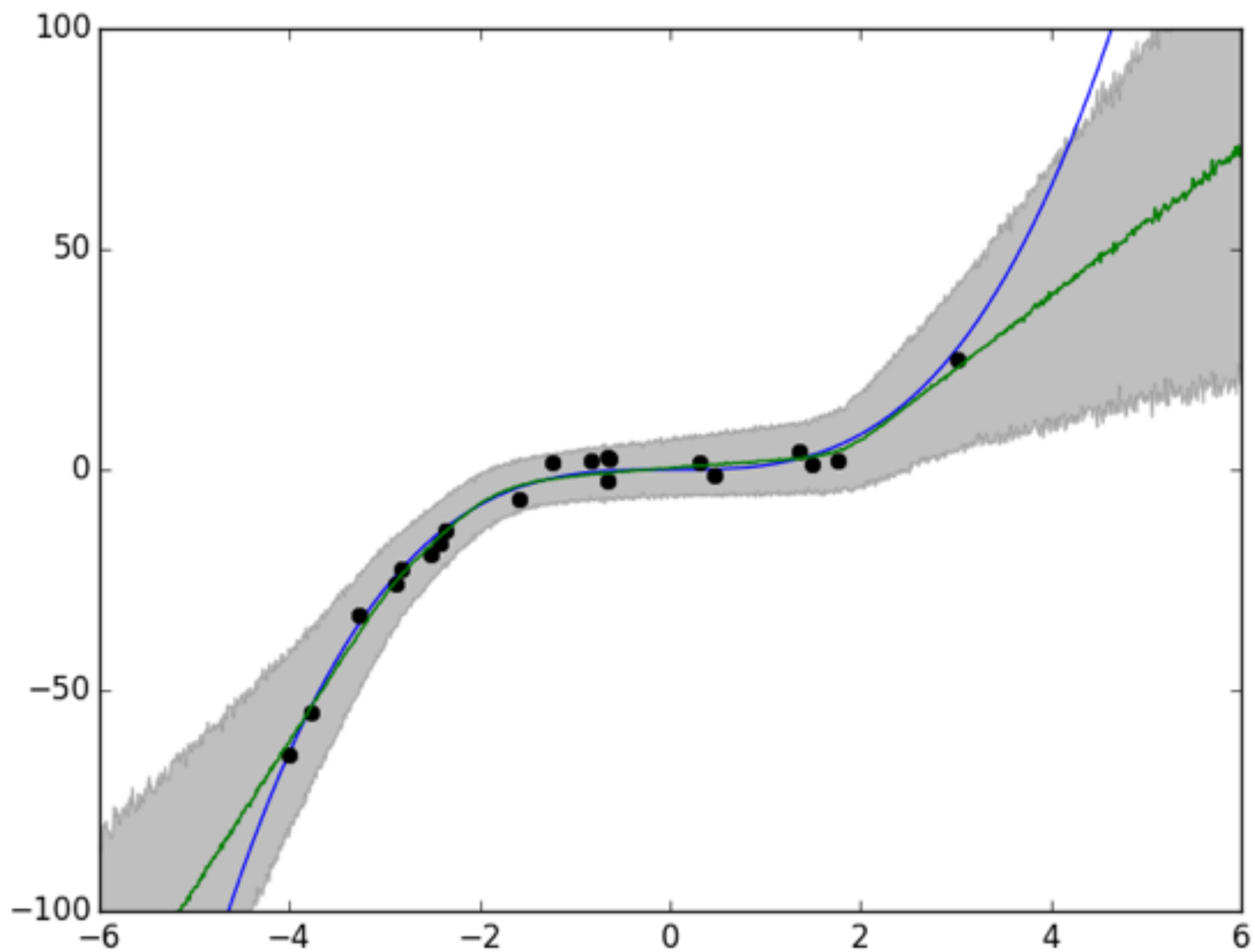
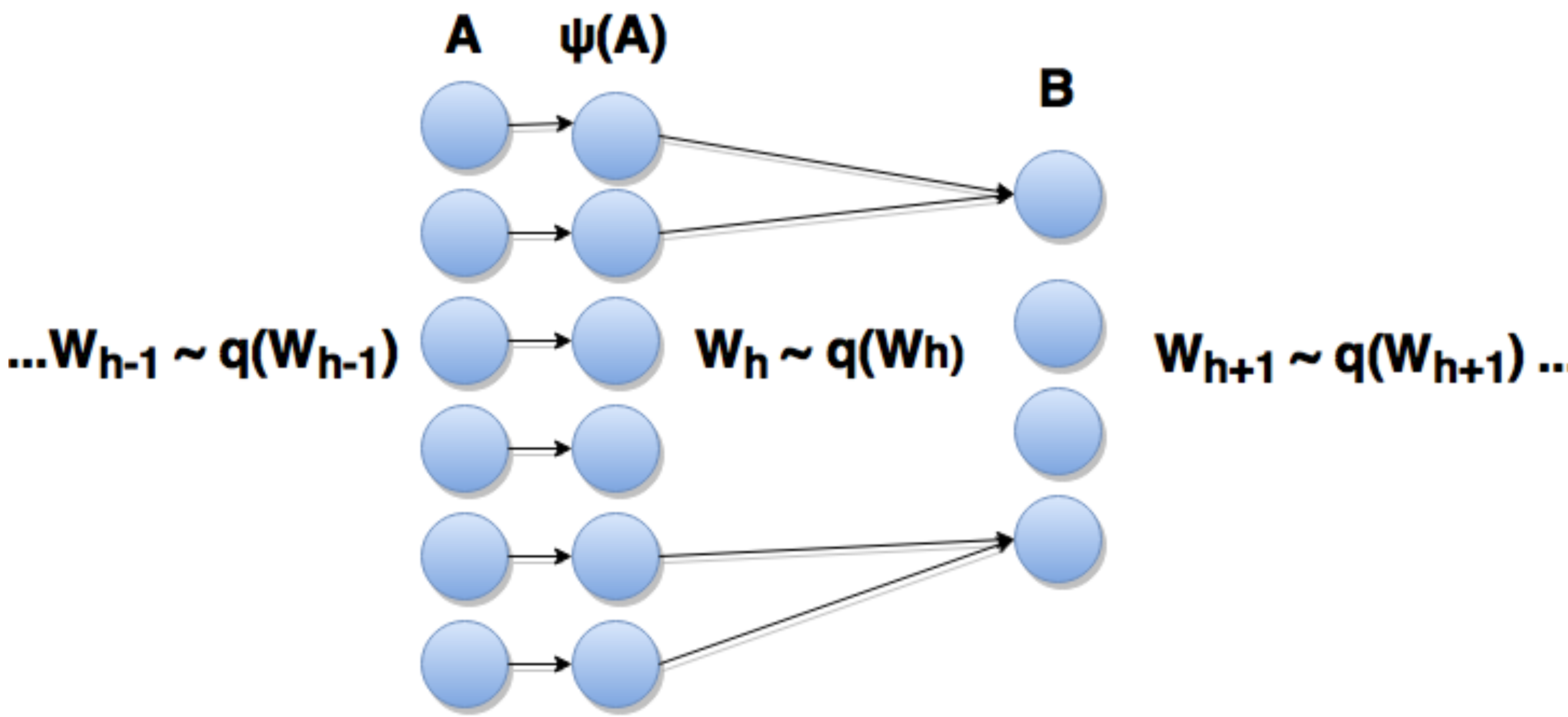


Structured VI BNN

Global posterior sampling

Global posterior sampling

In order to perform stochastic gradient VI we have to sample the approximate weight posterior at each layer:



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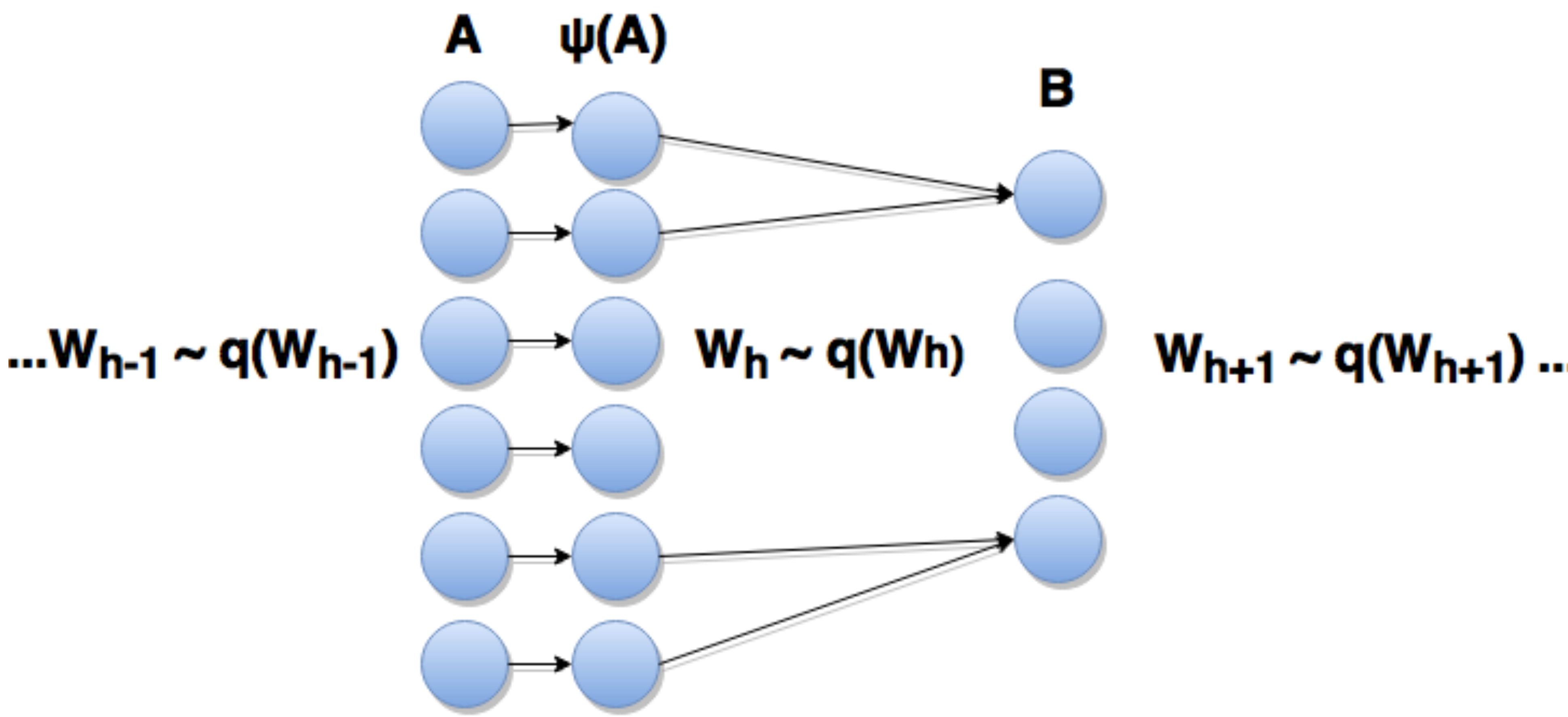

where **A** is a mini batch of the previous layer output, **ψ**(.) is an element wise nonlinearity and **B** is the layer output

Local posterior sampling

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$$\mathbf{B}[r,c] \sim \mathcal{N}\left(\sum_c \psi(\mathbf{A})[r,c]\mu_{rc}, \sum_c \psi(\mathbf{A})[r,c]^2 \sigma_{rc}^2 \right)$$

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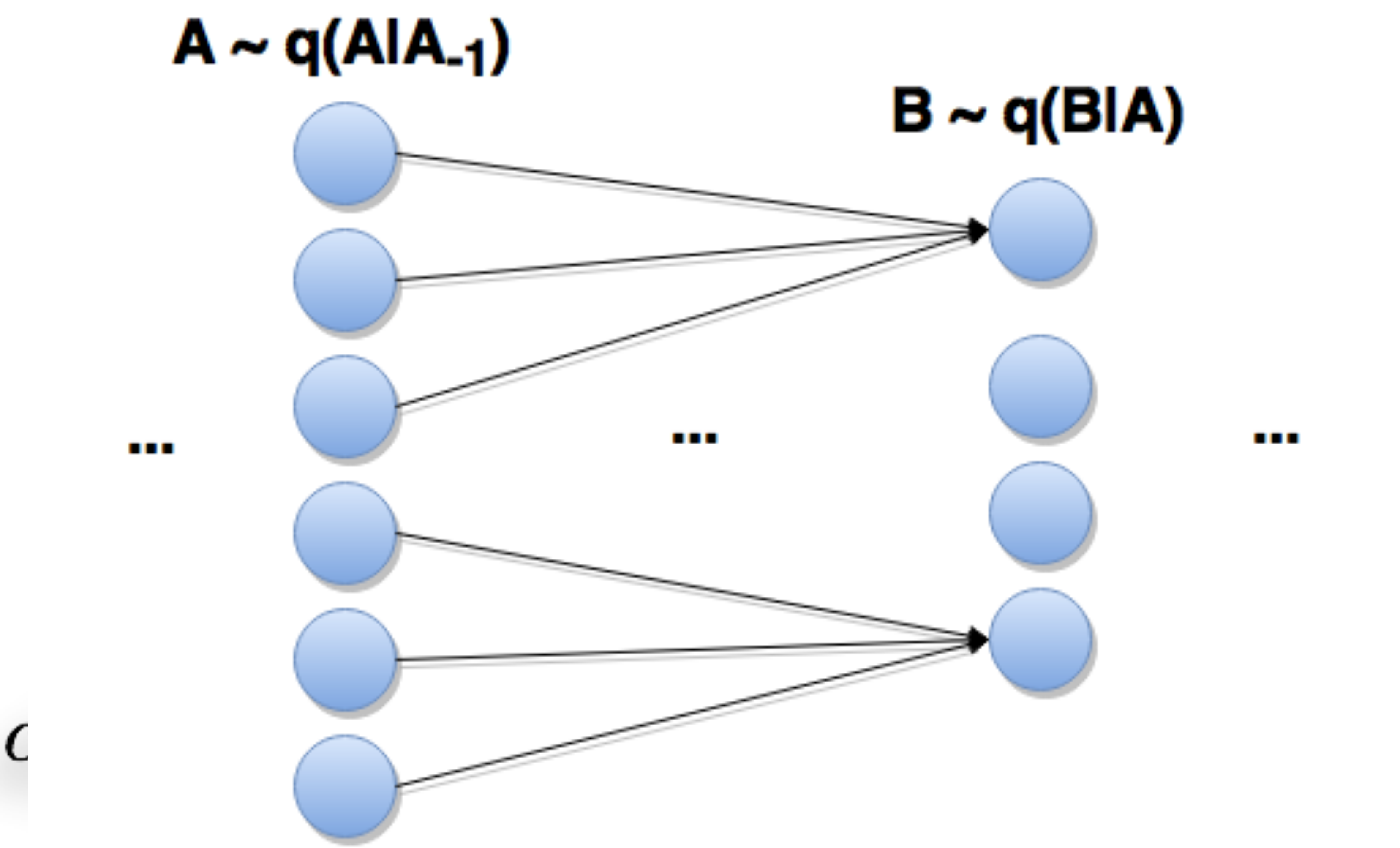

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or else:

$$\mathbf{B} \sim \mathcal{N}(vec(\psi(\mathbf{A})\mathbf{M}_h), \mathbf{K}(\mathbf{A}, \mathbf{A}))$$

$$\mathbf{K}(\mathbf{A}, \mathbf{A}) = \mathbf{K}_{out} \otimes \mathbf{K}_{in}(\mathbf{A}, \mathbf{A})$$

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Local posterior sampling with a Matrix Gaussian

Similarly we have that:

So we can view each layer as a finite rank multi-output Gaussian Process and the whole network as a deep Gaussian Process[2] with a specific kernel!

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[2] “Deep Gaussian Processes”, Andreas C. Damianou, Neil D. Lawrence, AISTATS 2013

Sampling a matrix Gaussian

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In order to sample the matrix Gaussian at each layer we have to do:

$$\mathbf{B} = \psi(\mathbf{A})\mathbf{M}_h + \mathbf{K}_{in}(\mathbf{A},\mathbf{A})^{\frac{1}{2}}\mathbf{E}\mathbf{K}_{out}^{\frac{1}{2}}$$

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Expensive since we have to compute the square root of the input kernel for each mini-batch.

Inducing points for BNNs

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To scale it up we introduce pseudo input-output pairs and assume conditional independence for the elements of **B** (FITC GP approximation):

$$
\begin{aligned}
\mathbf{b} &\sim p(\mathbf{b}|\mathbf{a}, \tilde{\mathbf{B}}, \tilde{\mathbf{A}}) \\
&\sim \mathcal{N}(\psi(\mathbf{a})\mathbf{M}_h + \mathbf{K}_{in}(\mathbf{a}, \tilde{\mathbf{A}})\mathbf{K}_{in}(\tilde{\mathbf{A}}, \tilde{\mathbf{A}})^{-1}(\tilde{\mathbf{B}} - \tilde{\mathbf{A}}\mathbf{M}_h), \\
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\end{aligned}$$

Advantages

- Sampling scales cubically with the amount of inducing points
- Variance reduction if real inputs are “similar”

Regression experiments

Regression experiments

	Avg. Test RMSE and Std. Errors				Avg. Test LL and Std. Errors			
Dataset	**VI**	**PBP**	**Dropout**	**VMG**	**VI**	**PBP**	**Dropout**	**VMG**
Boston	4.32±0.29	3.01±0.18	2.97±0.85	**2.81±0.11**	-2.90±0.07	-2.57± 0.09	**-2.46±0.25**	-2.54±0.08
Concrete	7.19±0.12	5.67±0.09	5.23± 0.53	**4.70±0.14**	-3.39±0.02	-3.16±0.02	-3.04±0.09	**-2.98±0.03**
Energy	2.65±0.08	1.80±0.05	1.66±0.19	**1.16±0.03**	-2.39±0.03	-2.04±0.02	-1.99±0.09	**-1.45±0.03**
Kin8nm	0.10±0.00	0.10±0.00	0.10±0.00	**0.08±0.00**	0.90±0.01	0.90±0.01	0.95±0.03	**1.14±0.01**
Naval	0.01±0.00	0.01±0.00	0.01±0.00	**0.00±0.00**	3.73±0.12	3.73±0.01	3.80±0.05	**5.84±0.00**
Pow. Plant	4.33±0.04	4.12±0.03	4.02±0.18	**3.88±0.03**	-2.89±0.01	-2.84±0.01	-2.80±0.05	**-2.78±0.01**
Protein	4.84±0.03	4.73±0.01	4.36±0.04	**4.14±0.01**	-2.99±0.01	-2.97±0.00	-2.89±0.01	**-2.84±0.00**
Wine	0.65±0.01	0.64±0.01	0.62±0.04	**0.61±0.01**	-0.98±0.01	-0.97±0.01	-0.93±0.06	**-0.93±0.02**
Yacht	6.89±0.67	1.02±0.05	1.11±0.38	**0.77±0.06**	-3.43±0.16	-1.63±0.02	-1.55±0.12	**-1.29±0.02**
Year	9.034±NA	8.879±NA	8.849±NA	**8.780±NA**	-3.622±NA	-3.603±NA	**-3.588±NA**	-3.589±NA

Table 1. Average test set RMSE, predictive log-likelihood and standard errors for the regression datasets. VI, PBP and Dropout correspond to the variational inference method of (Graves, 2011), probabilistic backpropagation (Hernández-Lobato & Adams, 2015) and dropout uncertainty (Gal & Ghahramani, 2015). VMG (Variational Matrix Gaussian) corresponds to the proposed model.

Classification experiments

Classification experiments

Method	# layers	Test err.
Max. Likel. (Simard et al., 2003)	2×800	1.60
Dropout (Srivastava, 2013)	-	1.25
DropConnect (Wan et al., 2013)	2×800	1.20
Bayes B. SM (Blundell et al., 2015)	2×400	1.36
	2×800	1.34
	2×1200	1.32
Var. Dropout (Kingma et al., 2015)	3×150	≈ 1.42
	3×250	≈ 1.28
	3×500	≈ 1.18
	3×750	≈ 1.09
VMG	2×400	**1.15**
	3×150	1.18
	3×250	1.11
	3×500	1.08
	3×750	**1.05**

Table 2. Test errors for the permutation invariant MNIST dataset. Bayes B. SM correspond to Bayes by Backprop with the scale mixture prior and the variational dropout results are from the Variational (A) model that doesn't downscale the KL-divergence (so as to keep the comparison fair).

Part 2

Model uncertainty from BNNs in classification

Opinion: Why are we Bayesian?

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  - Self-driving cars
  - Medical applications

How well do deep BNNs capture uncertainty?

- A simple way to measure the quality
  - Visualize class distribution on perturbed unseen inputs[3]
    - Rotations, translations, scalings
  - Ideally the model should be uncertain
- Experiment with Weight decay, Dropout, Matrix Gaussian posteriors, SGLD, Bootstrap

[3] “Dropout as a Bayesian Approximation: Representing Model Uncertainty in Deep Learning”,Yarin Gal, Zoubin Ghahramani, ICML 2016

Uncertainty testbed

- Simple LeNet network on MNIST
  - Two convolutional, two fully connected layers
- Dropout network: 0.5 dropout rate for all layers[4]
- Matrix Gaussian network
  - 20 pseudo patches/inputs for convolutional, fully connected layers respectively
- 100 samples for SGLD and 20 for Bootstrap
- All networks (except Bootstrap) had N(0, 1) priors over the parameters

[4] “Bayesian Convolutional Neural Networks with Bernoulli Approximate Variational Inference”,Yarin Gal, Zoubin Ghahramani

Weight decay rotations

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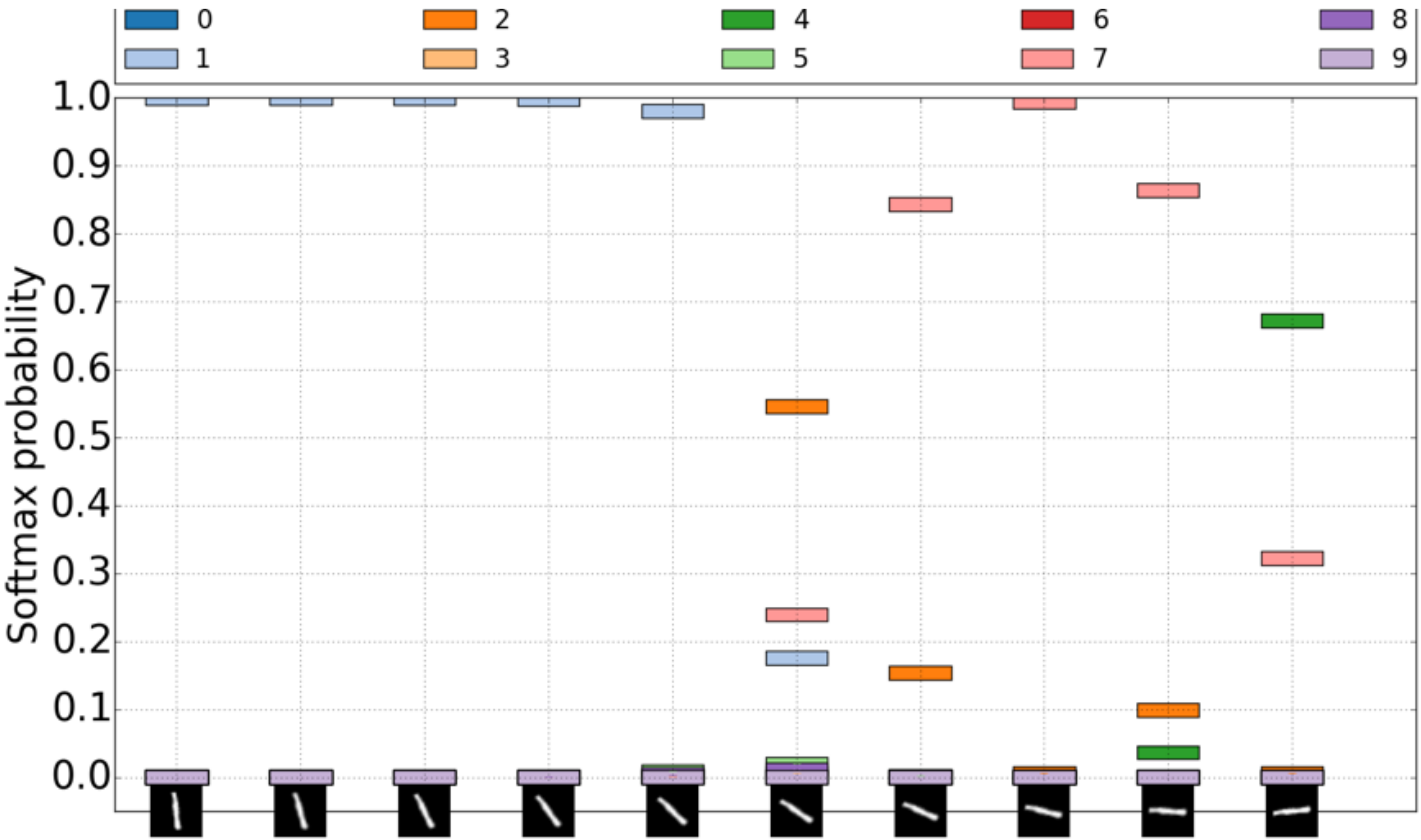

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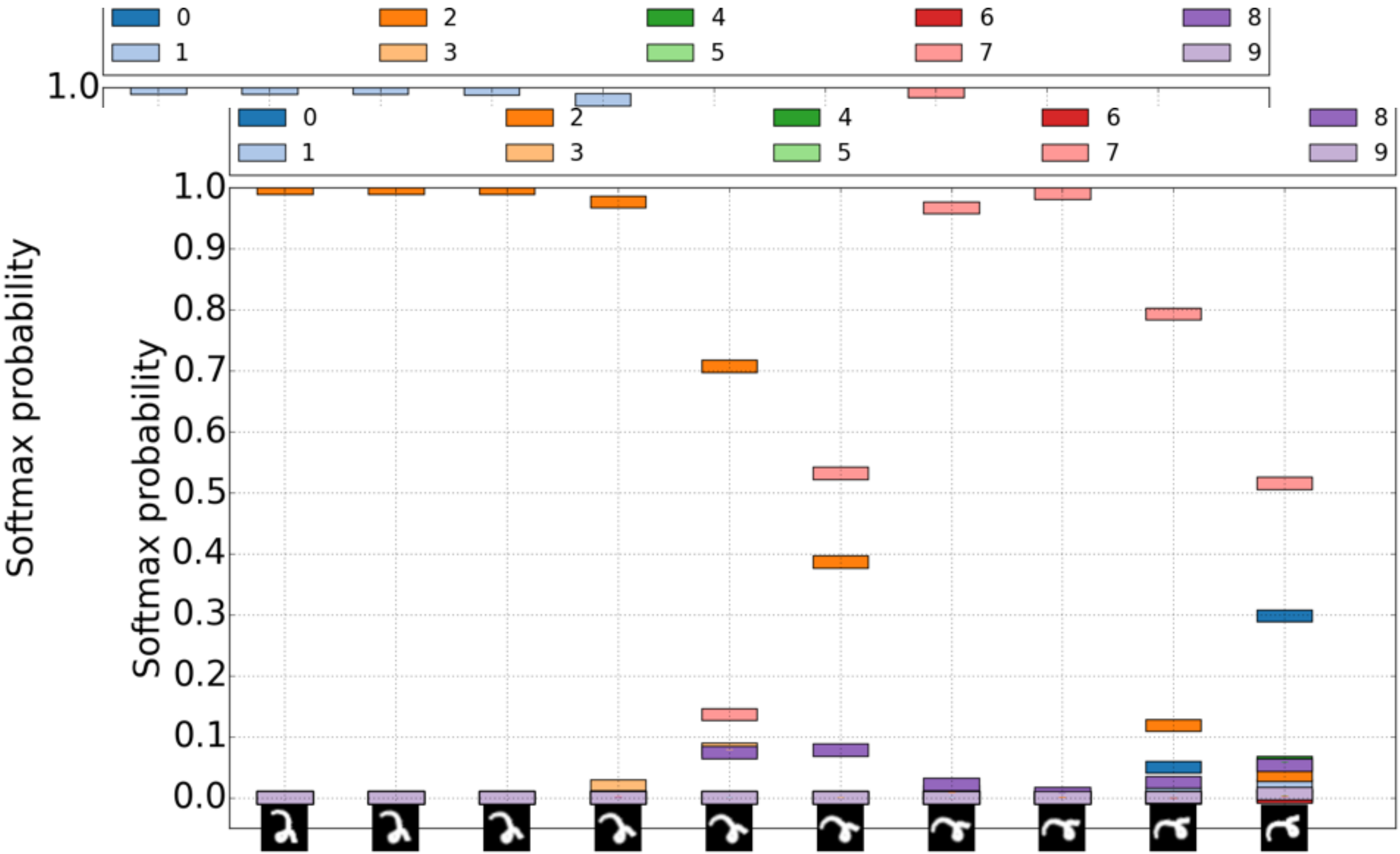

Dropout rotations

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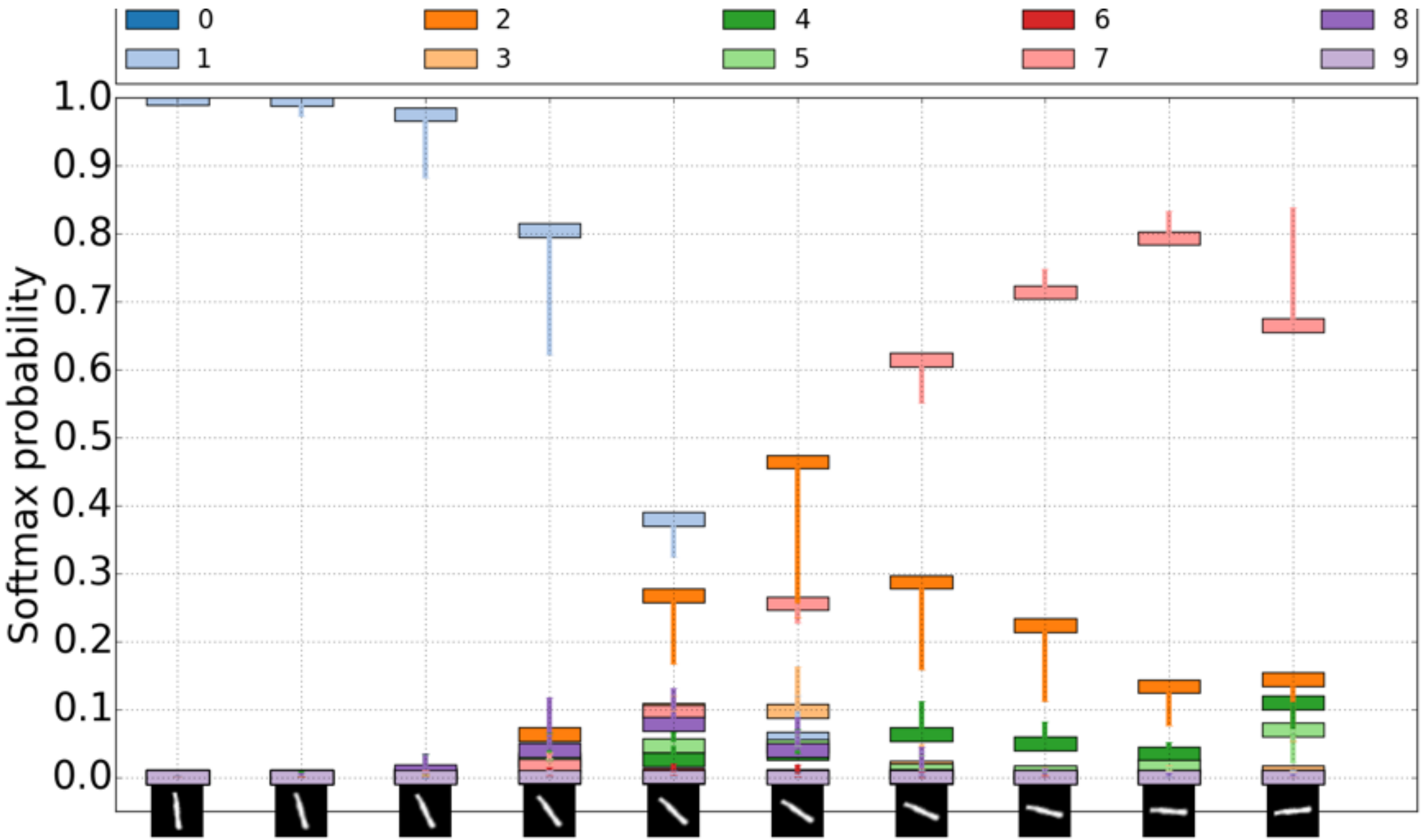

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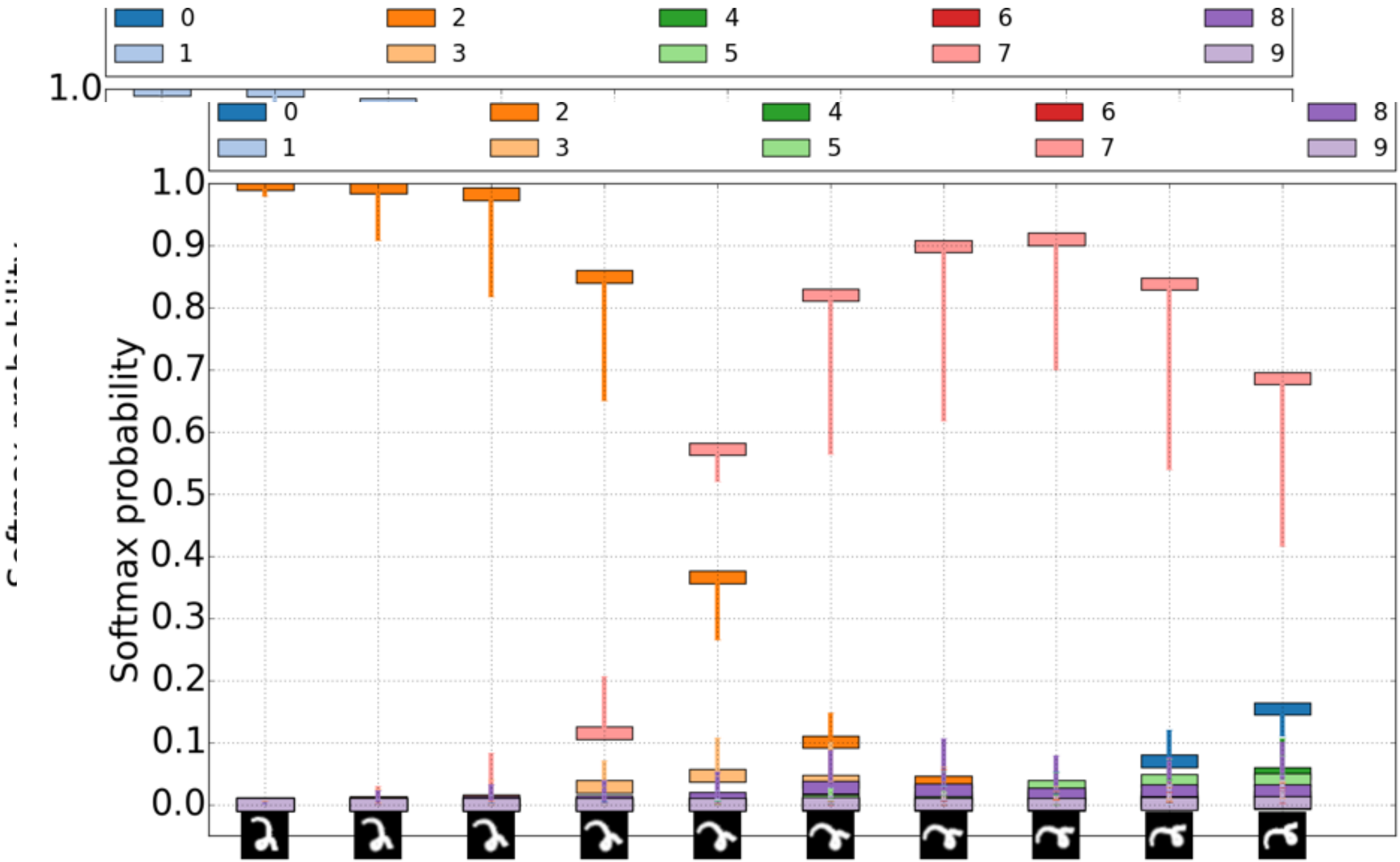

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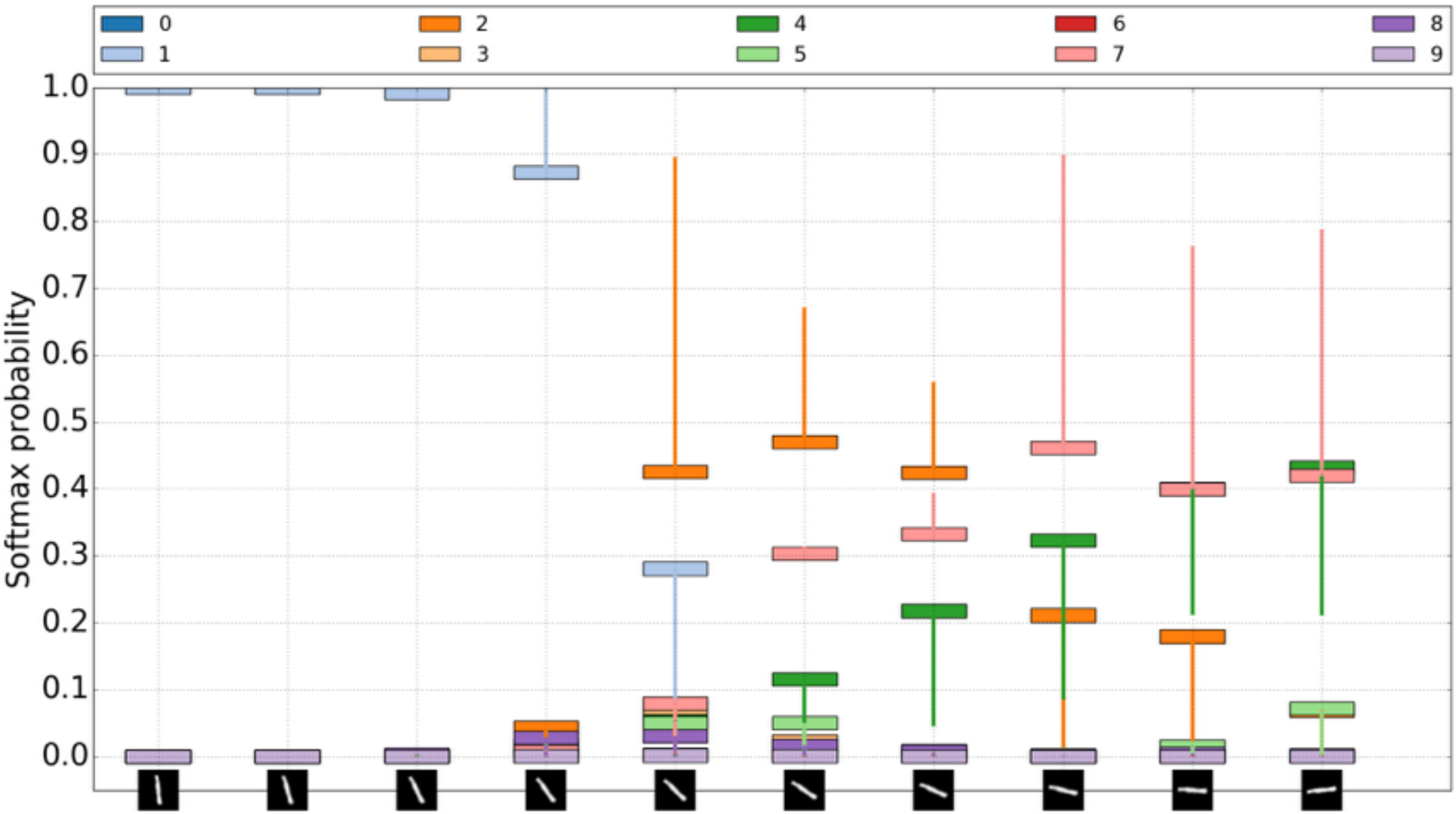

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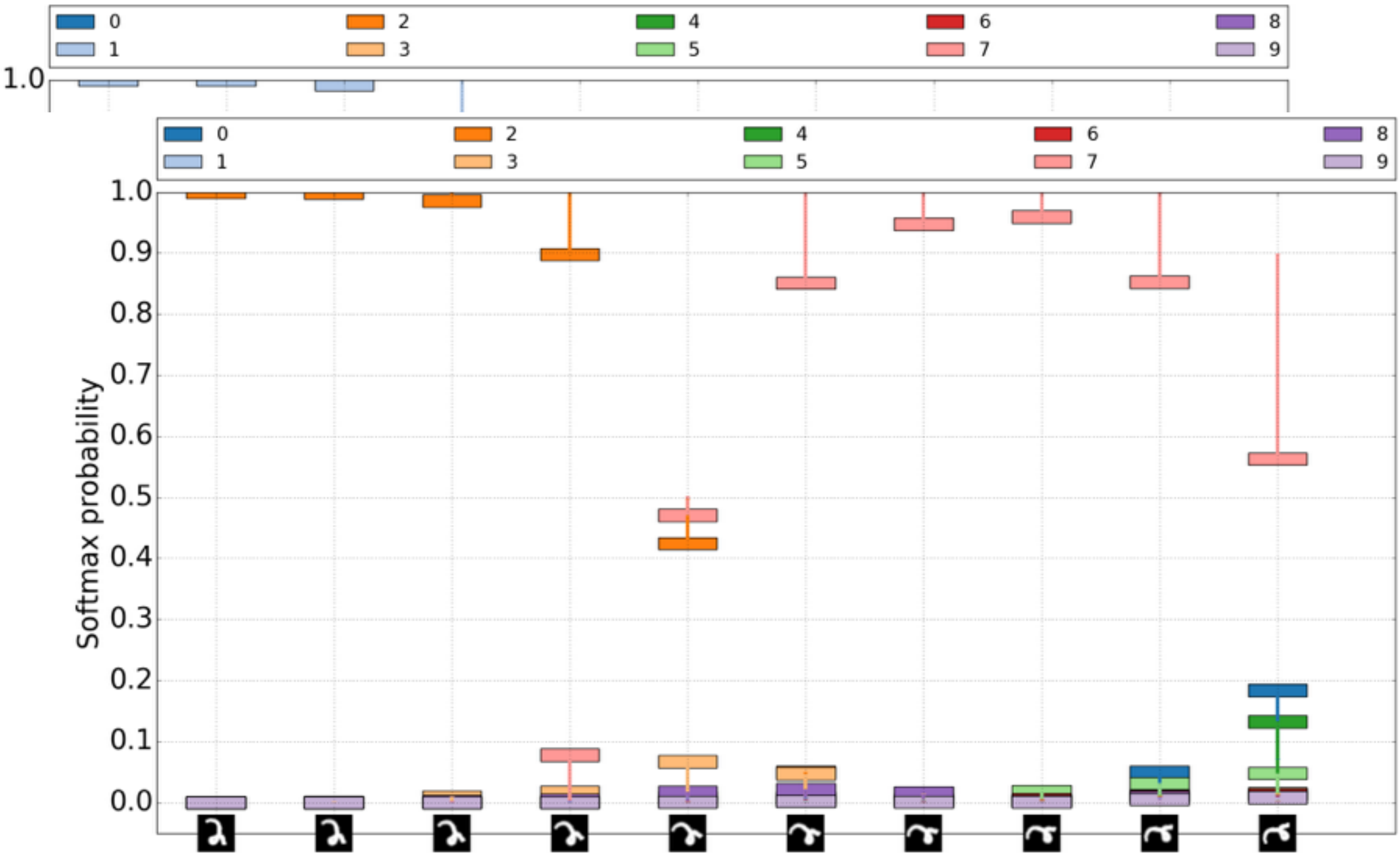

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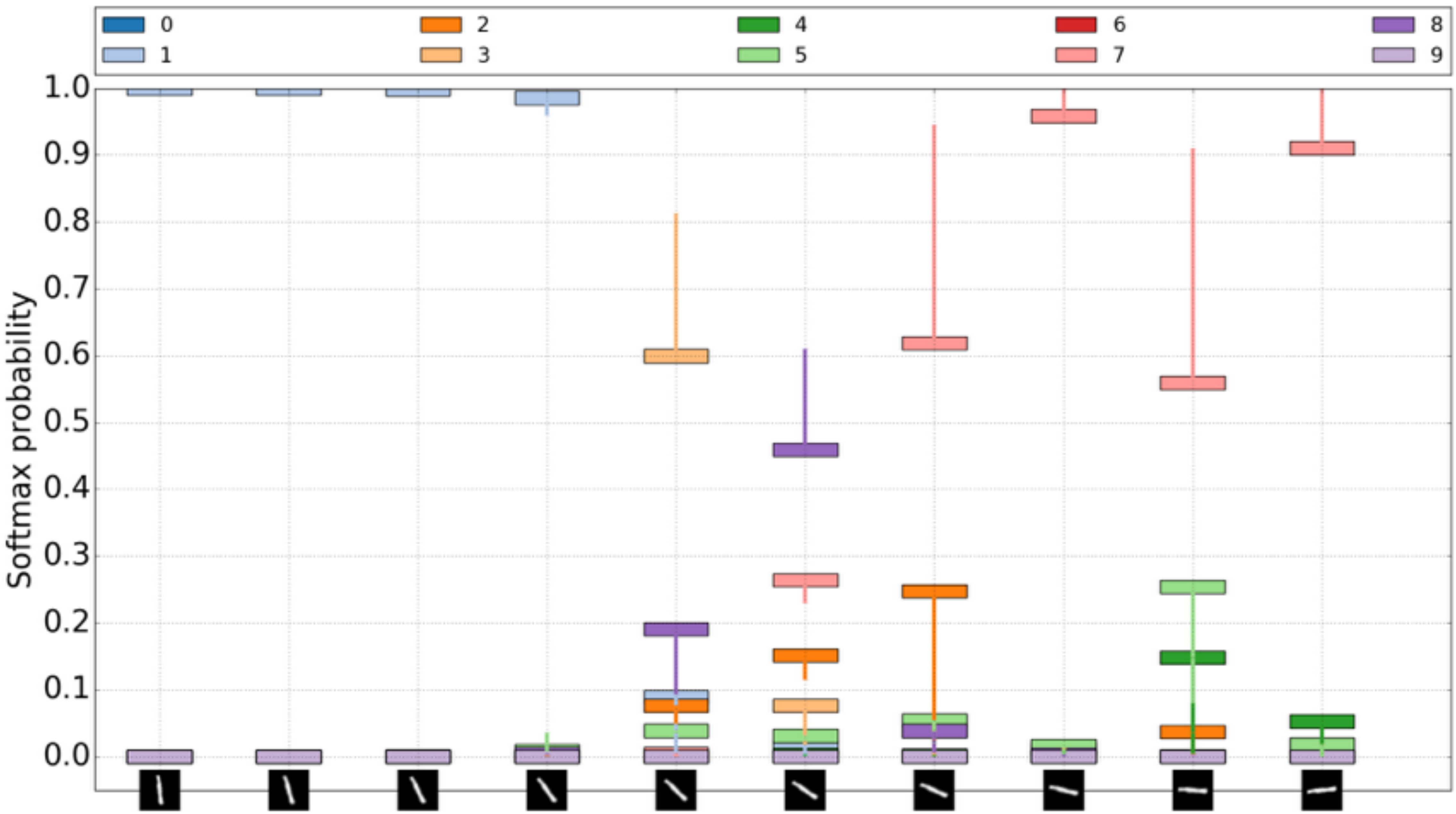

SGLD rotations

Bootstrap rotations

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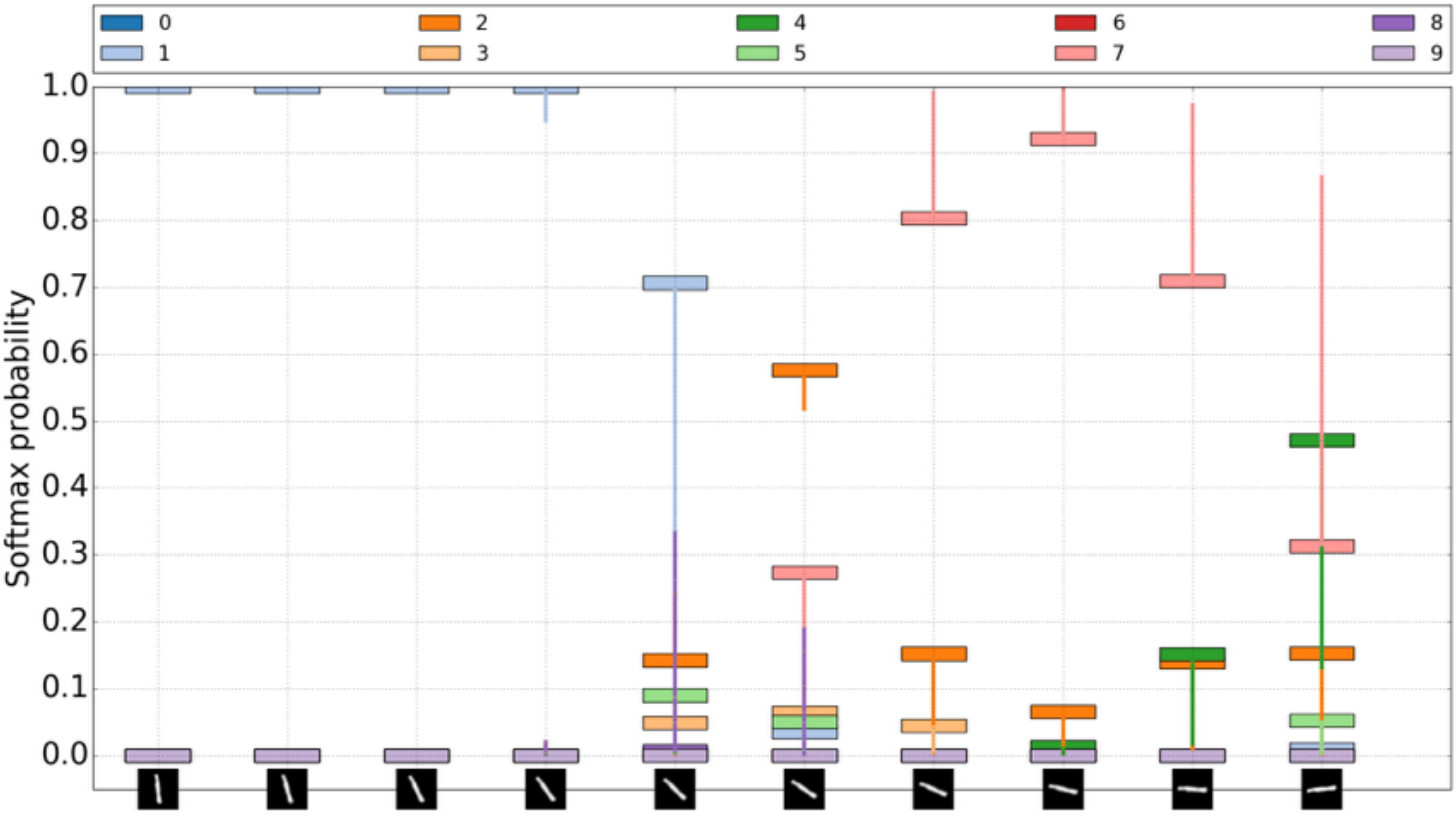

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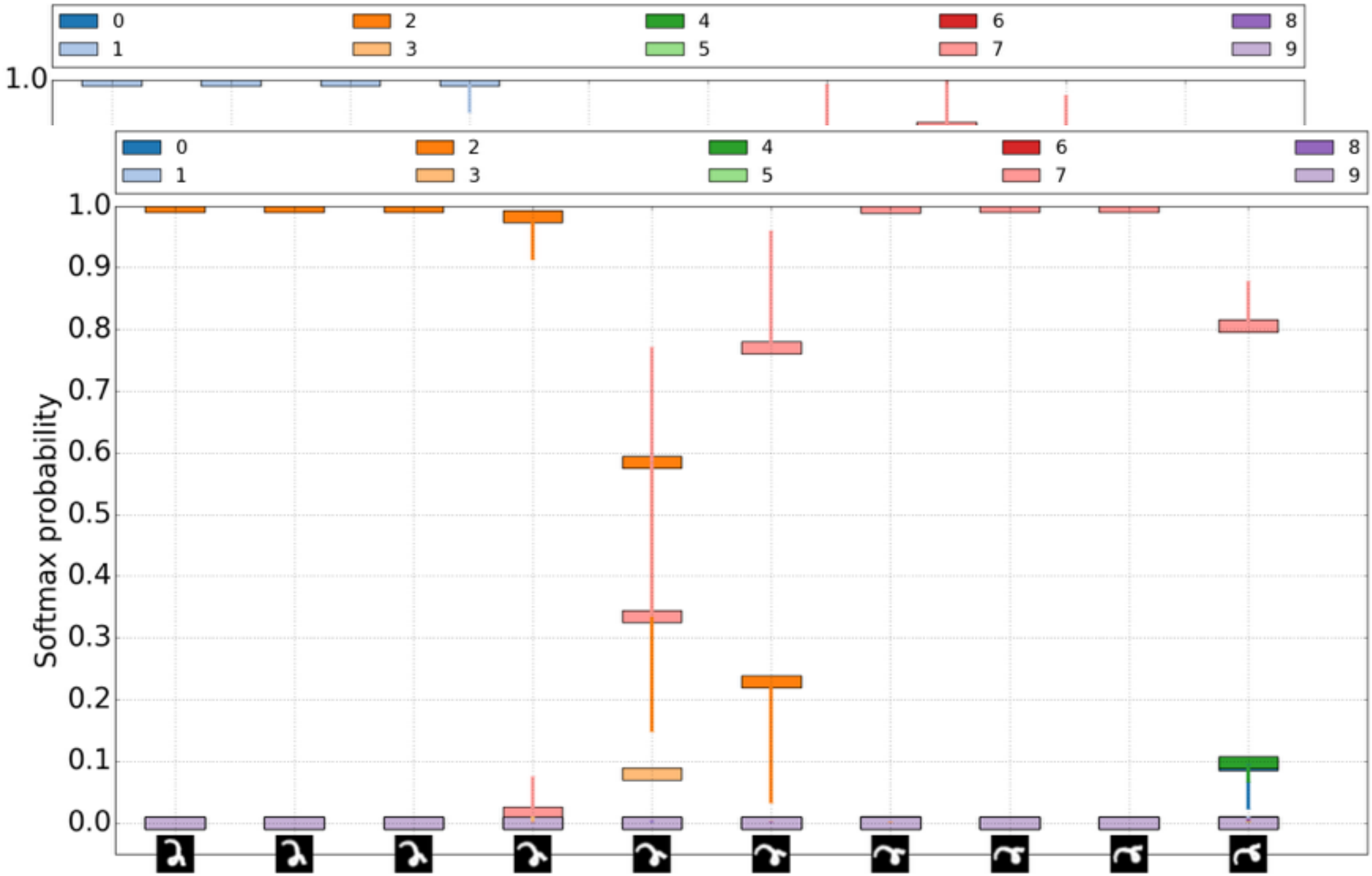

Weight decay translations

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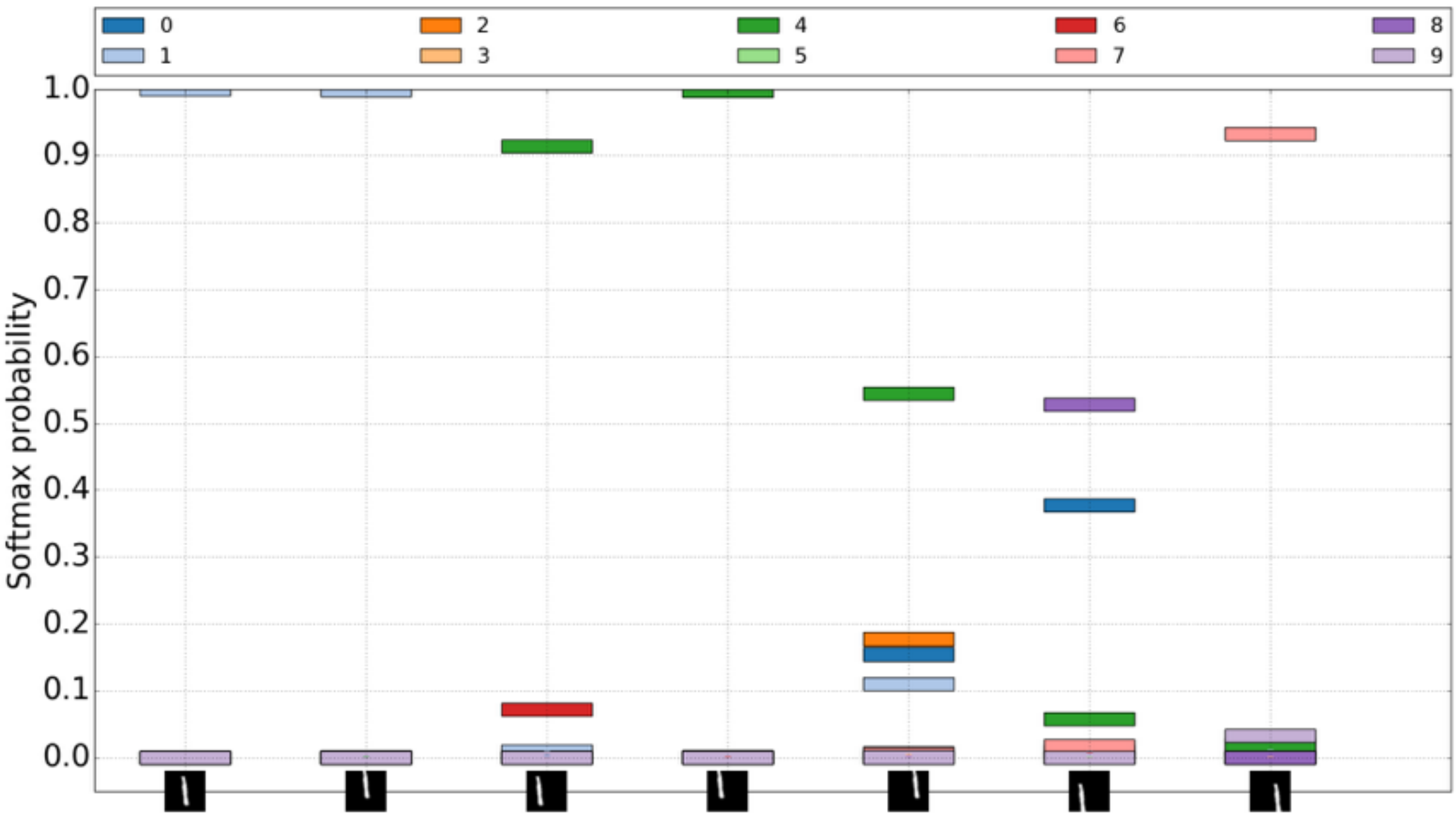

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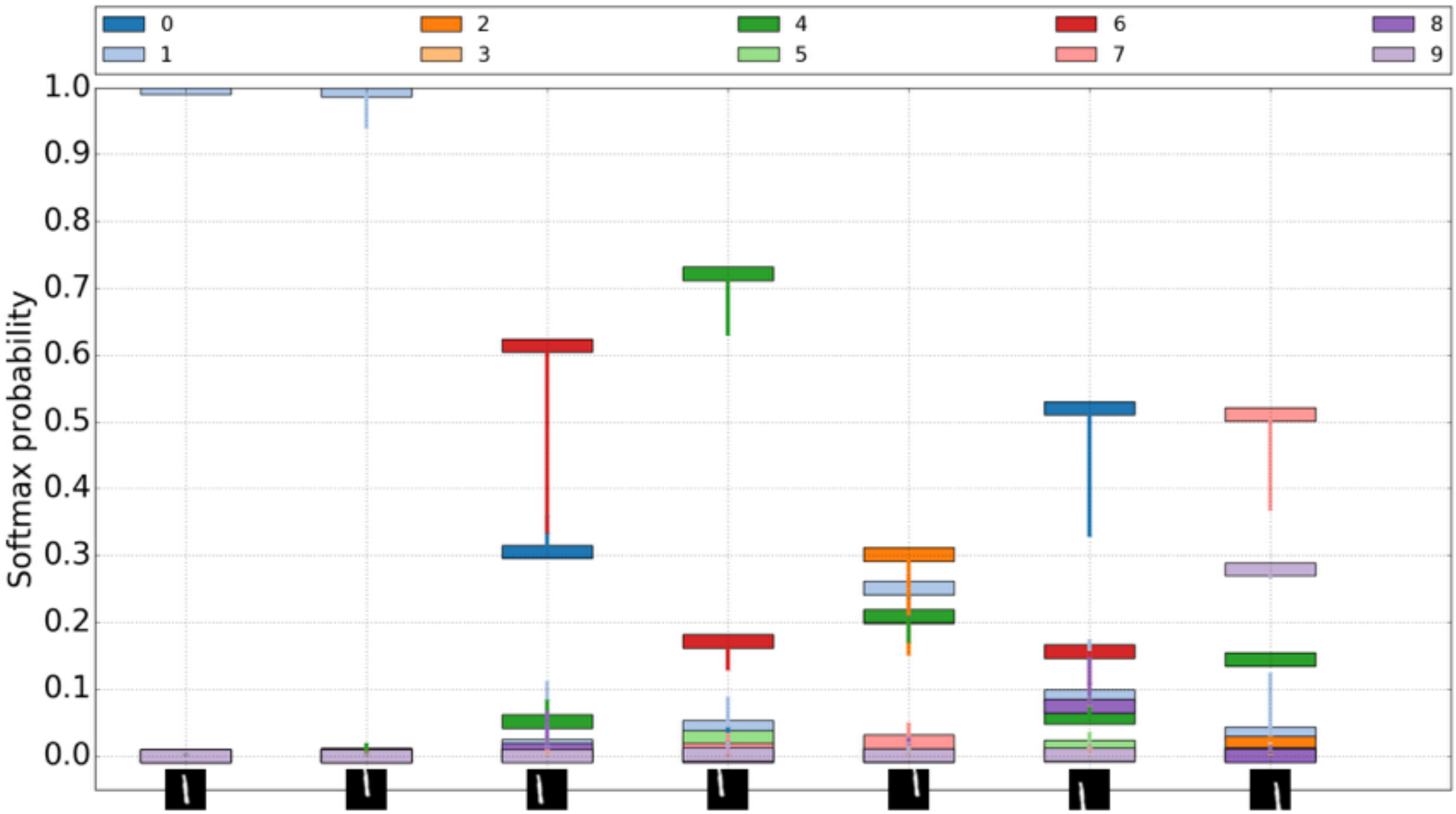

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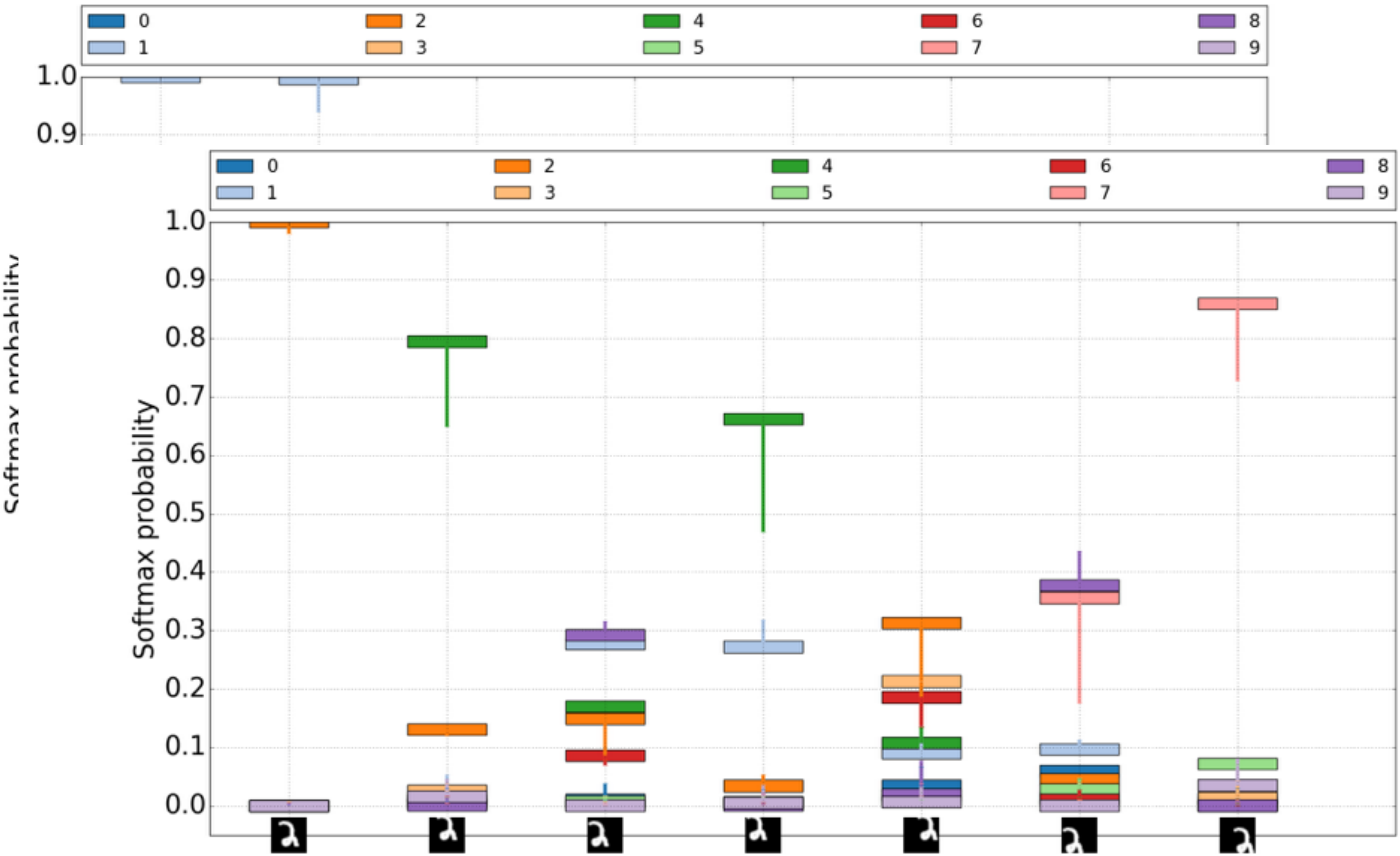

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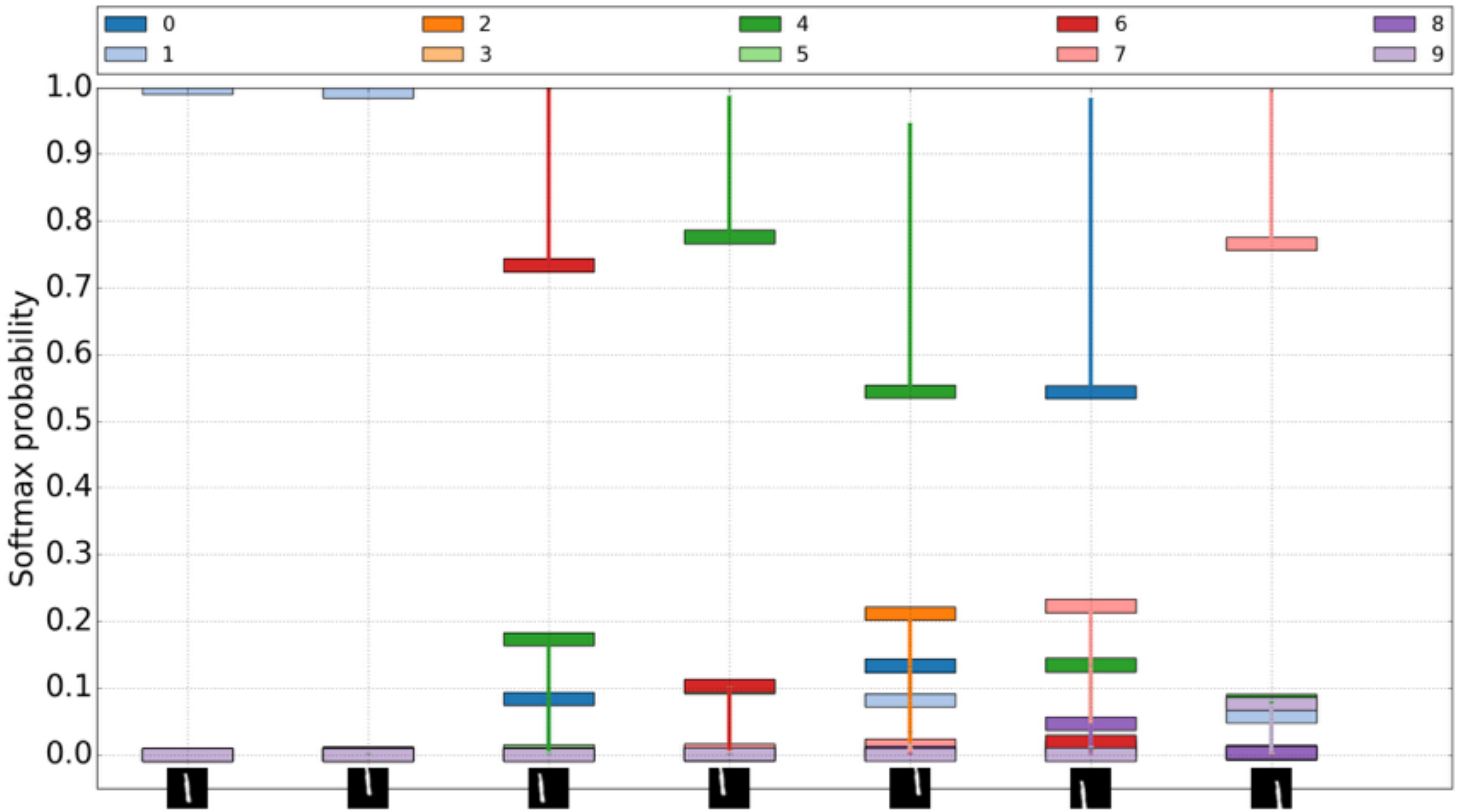

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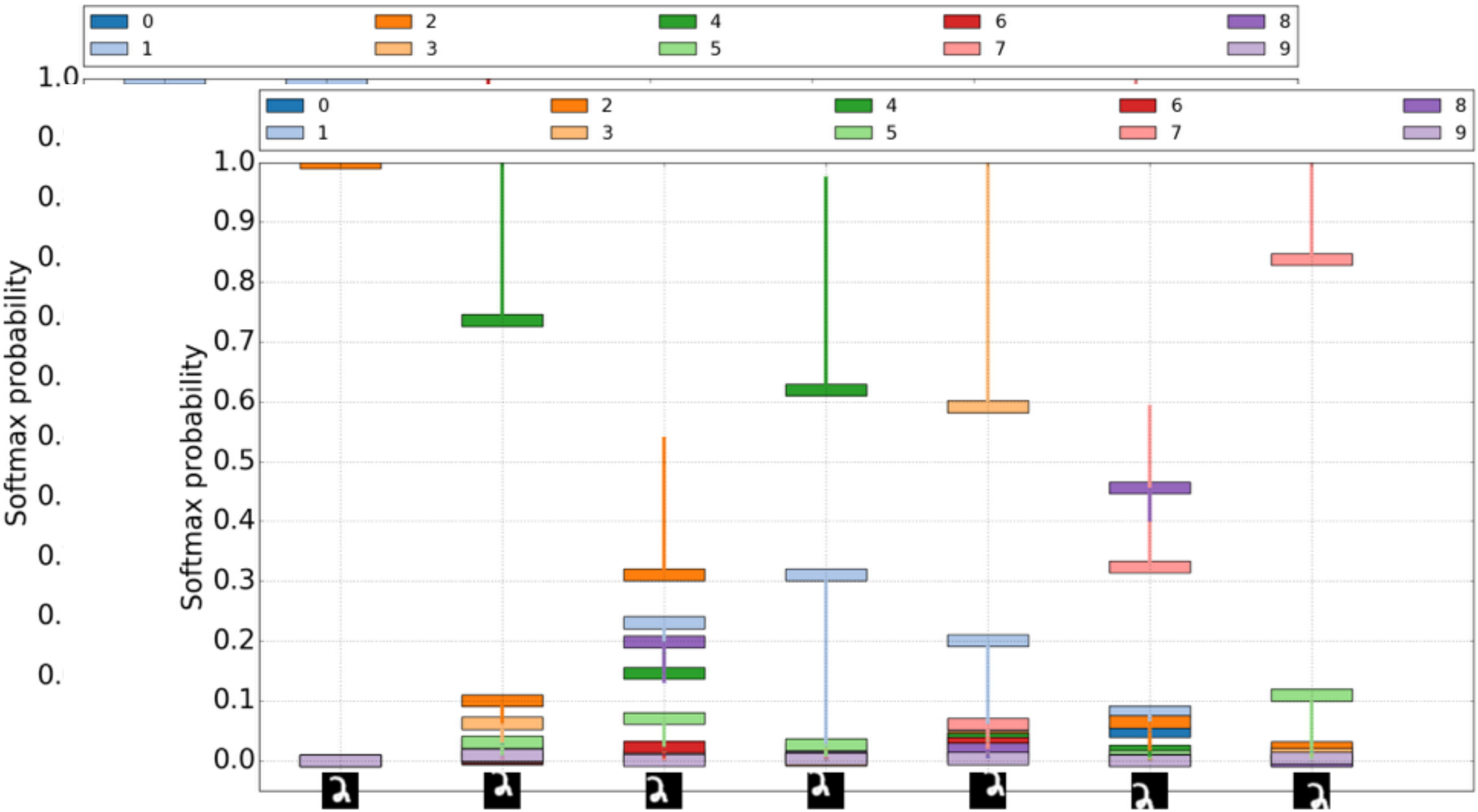

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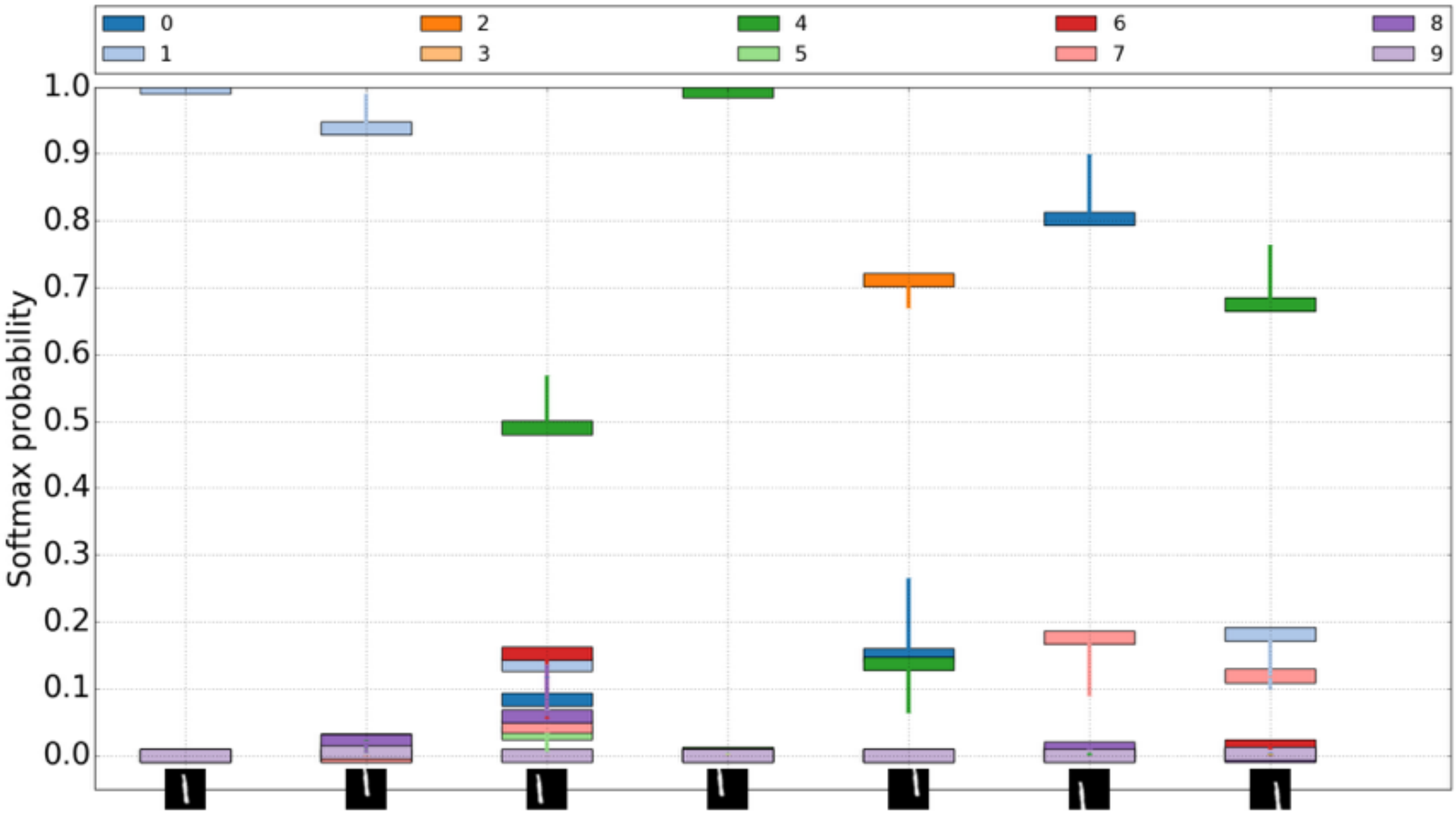

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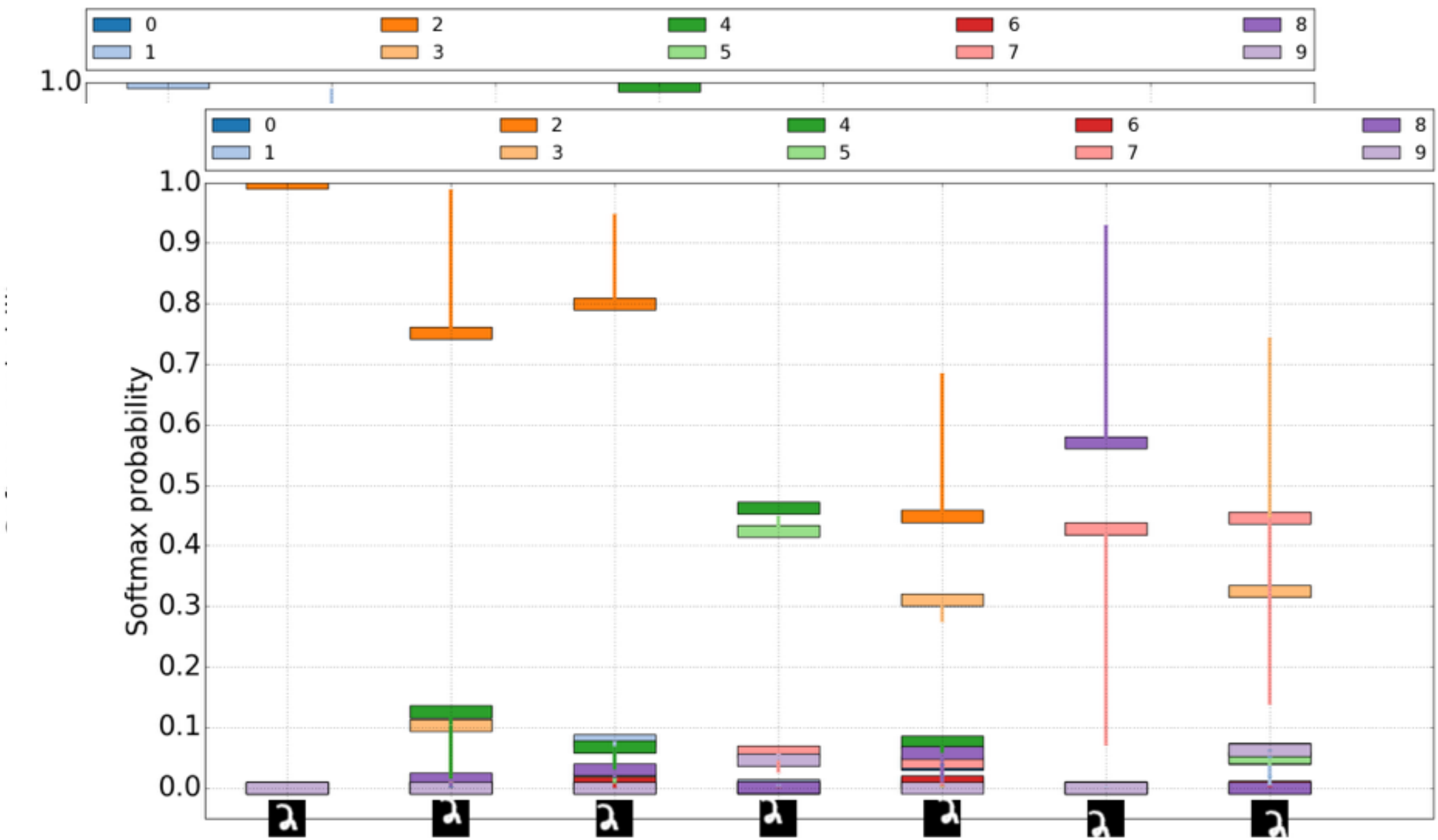

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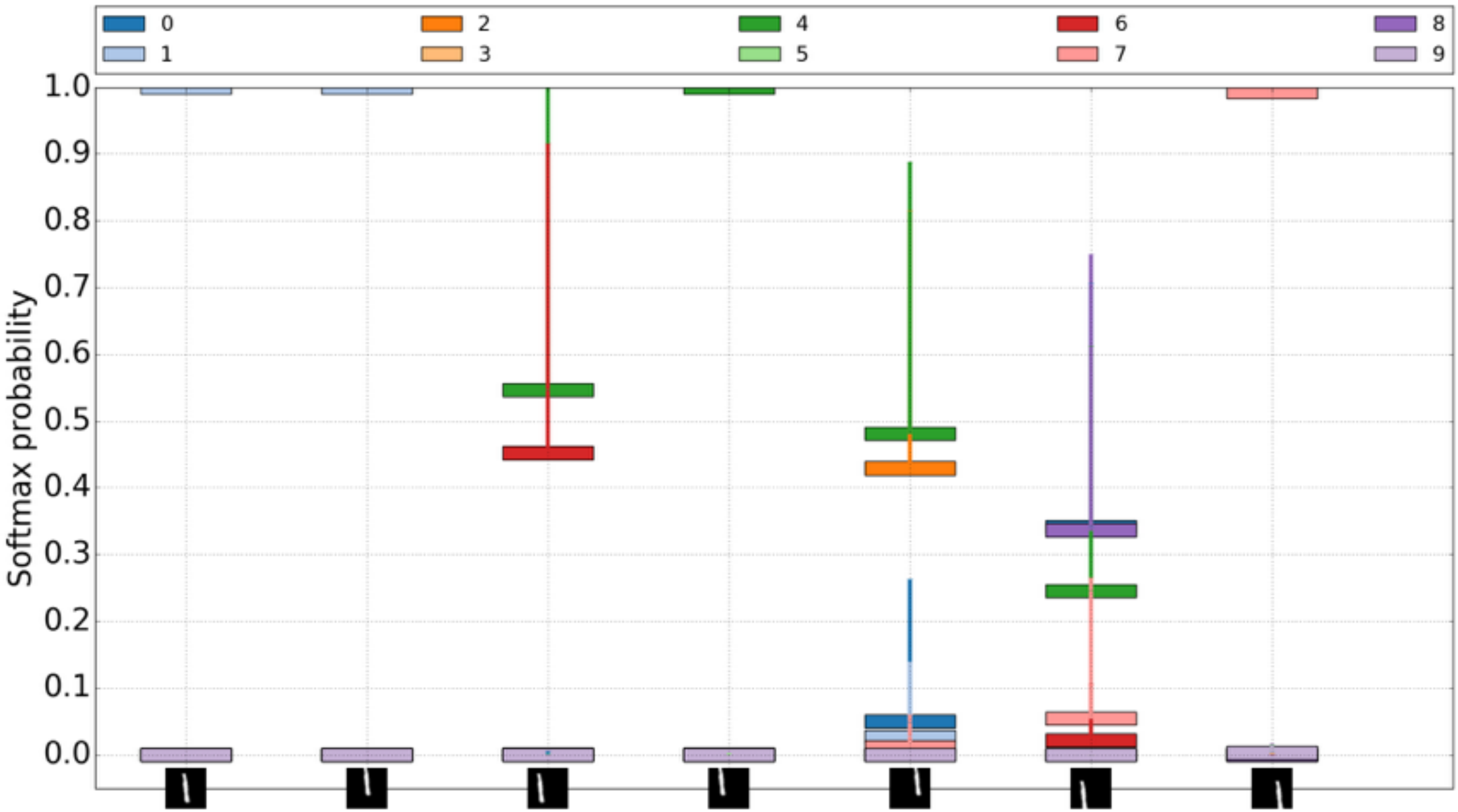

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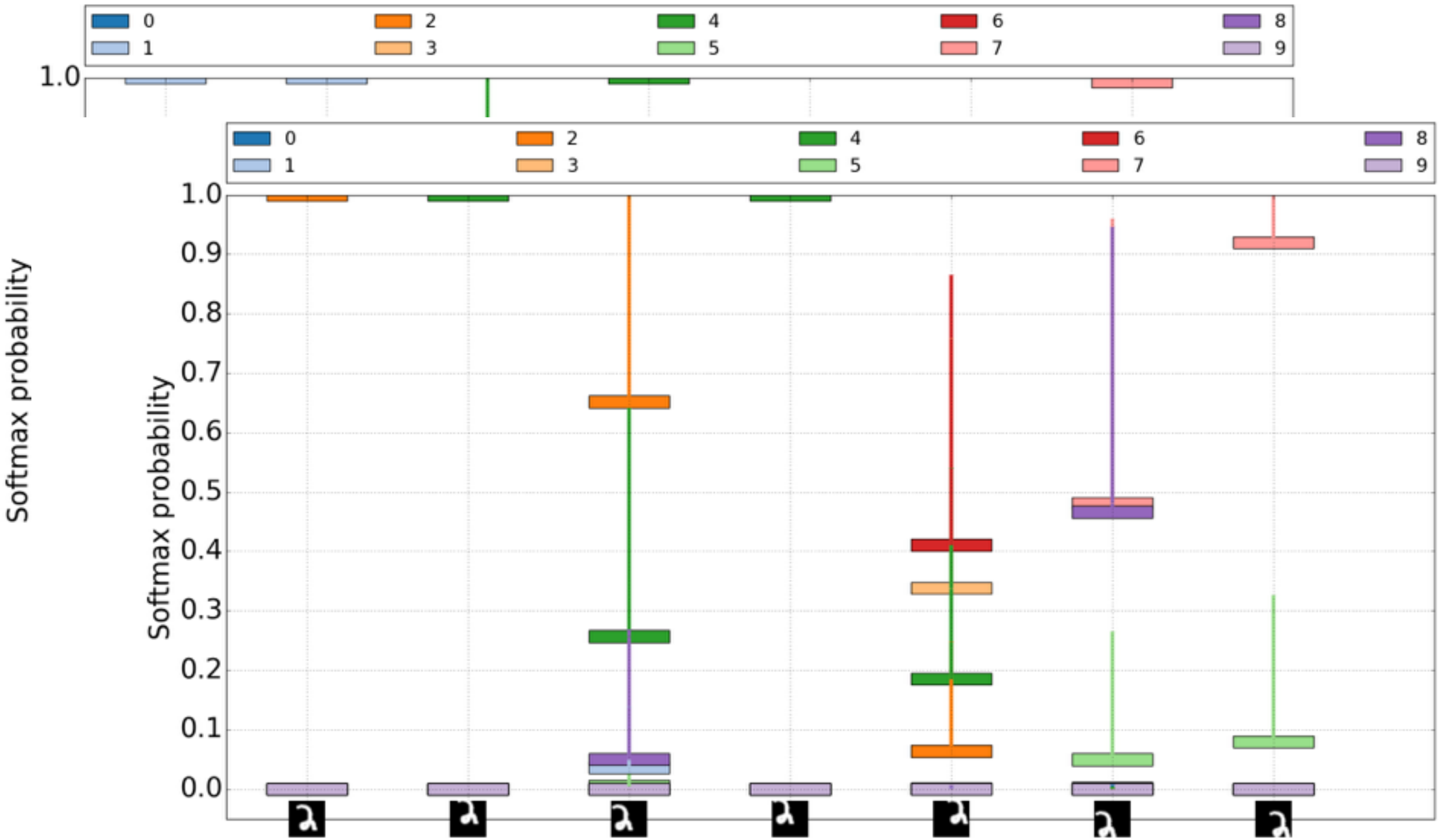

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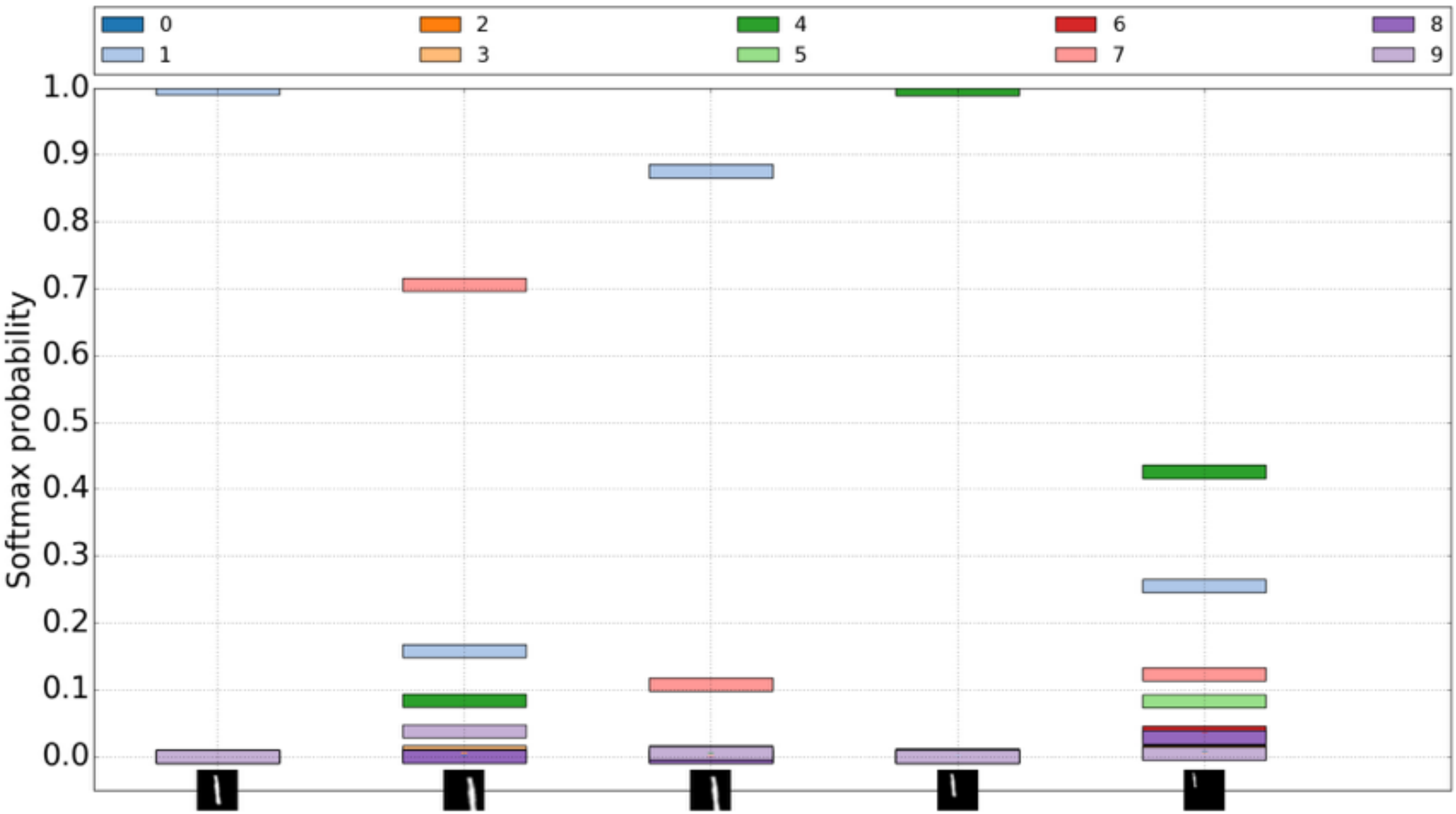

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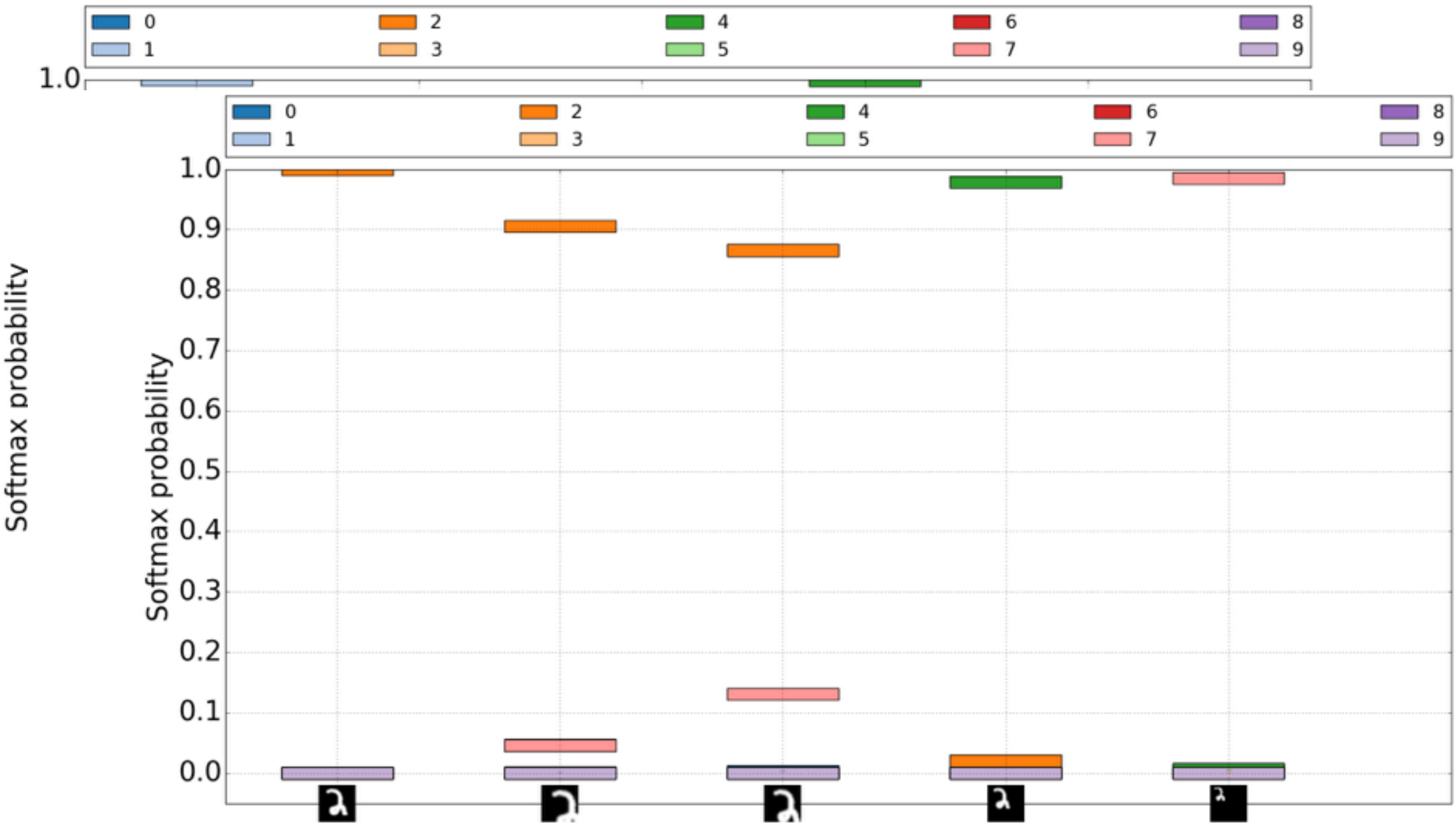

Dropout scaling

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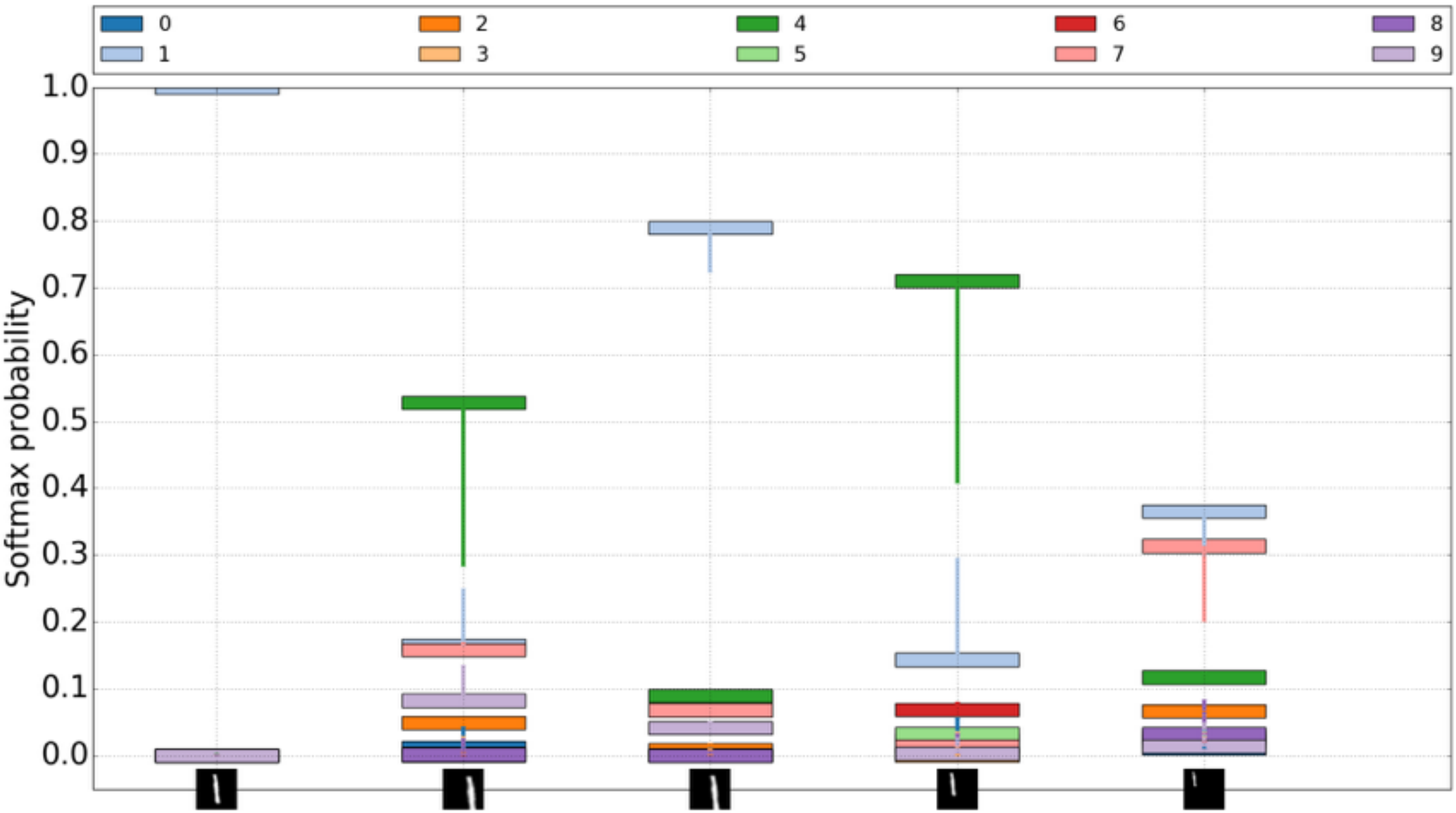

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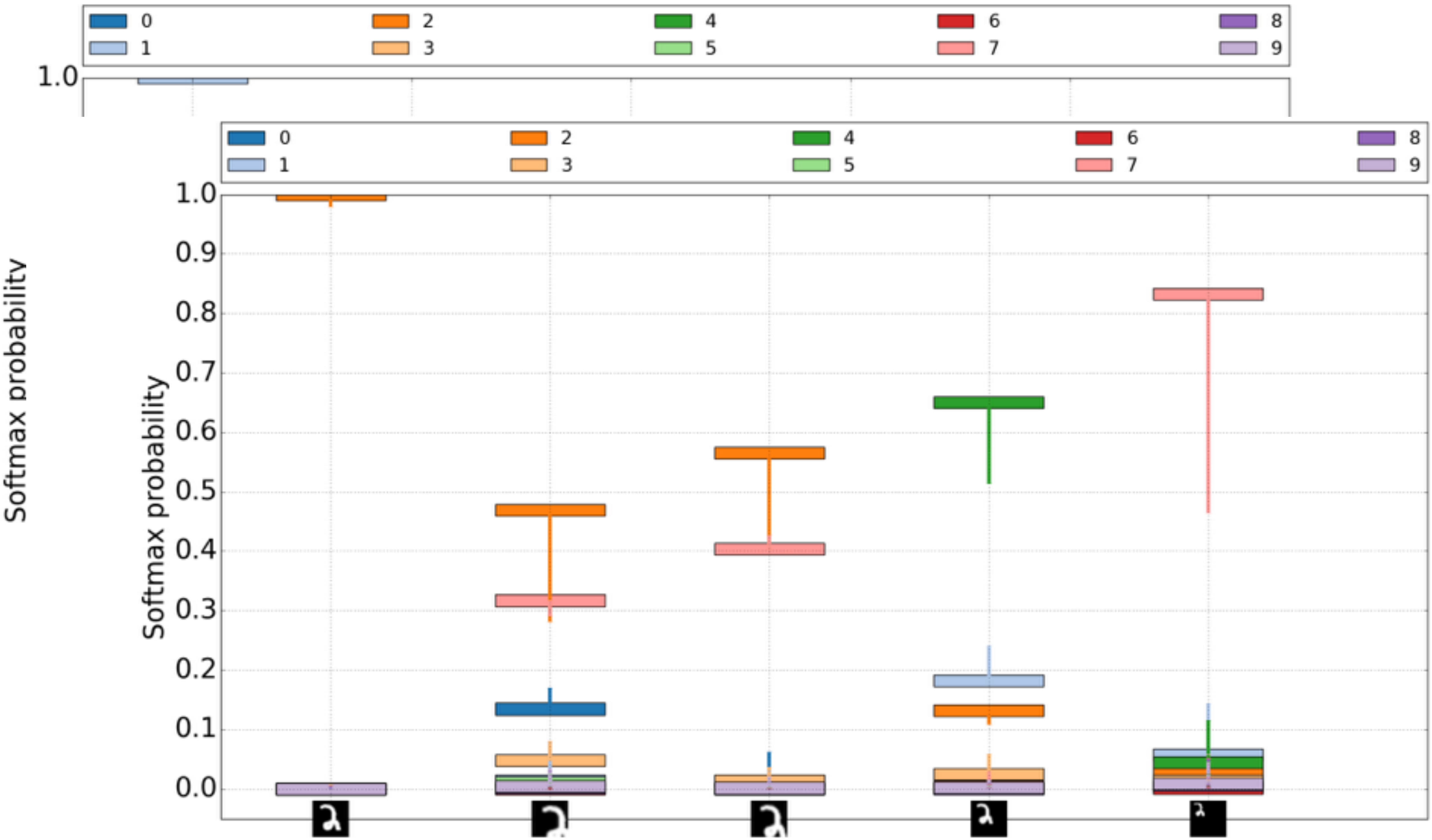

Matrix Gaussian scaling

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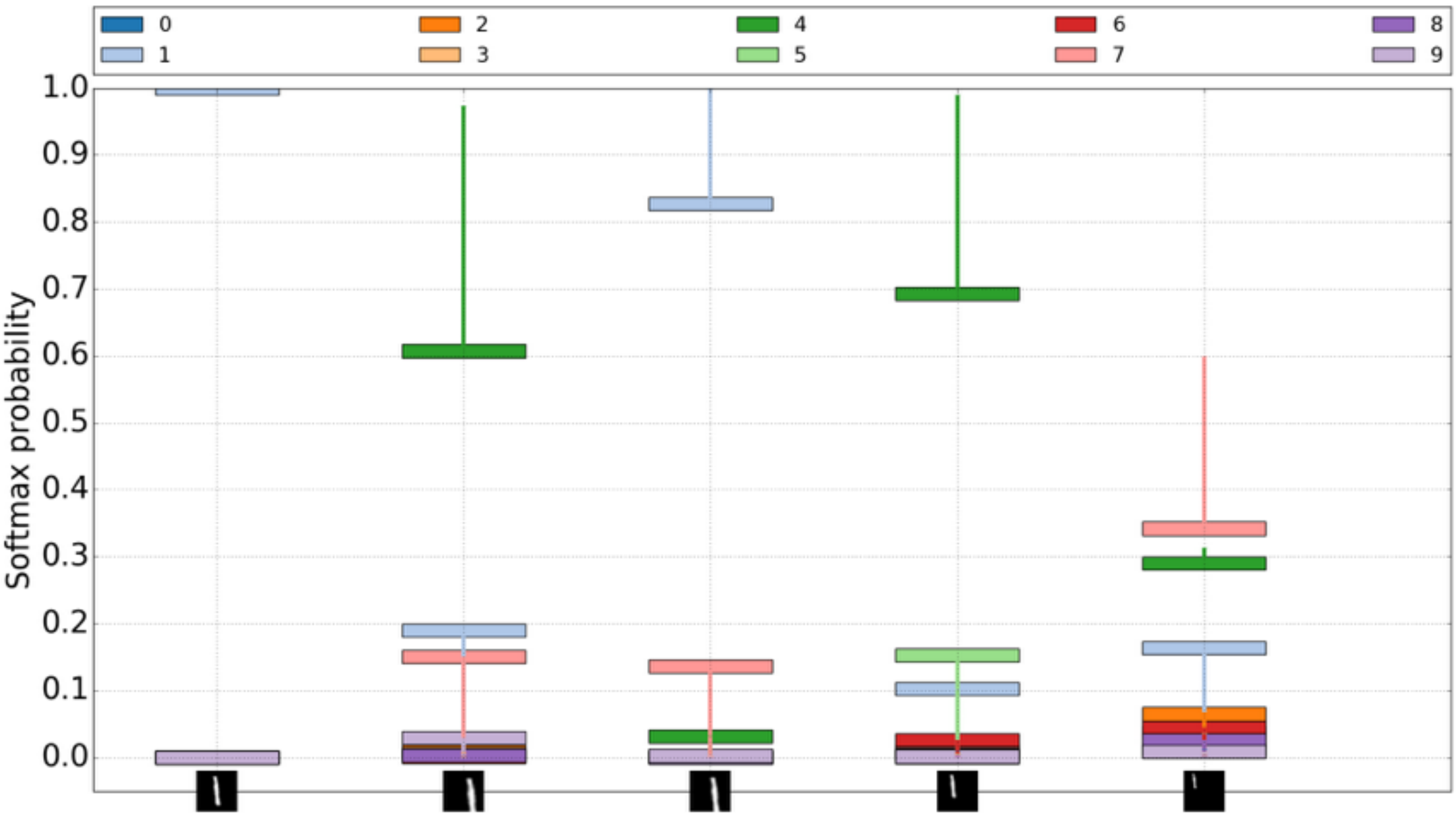
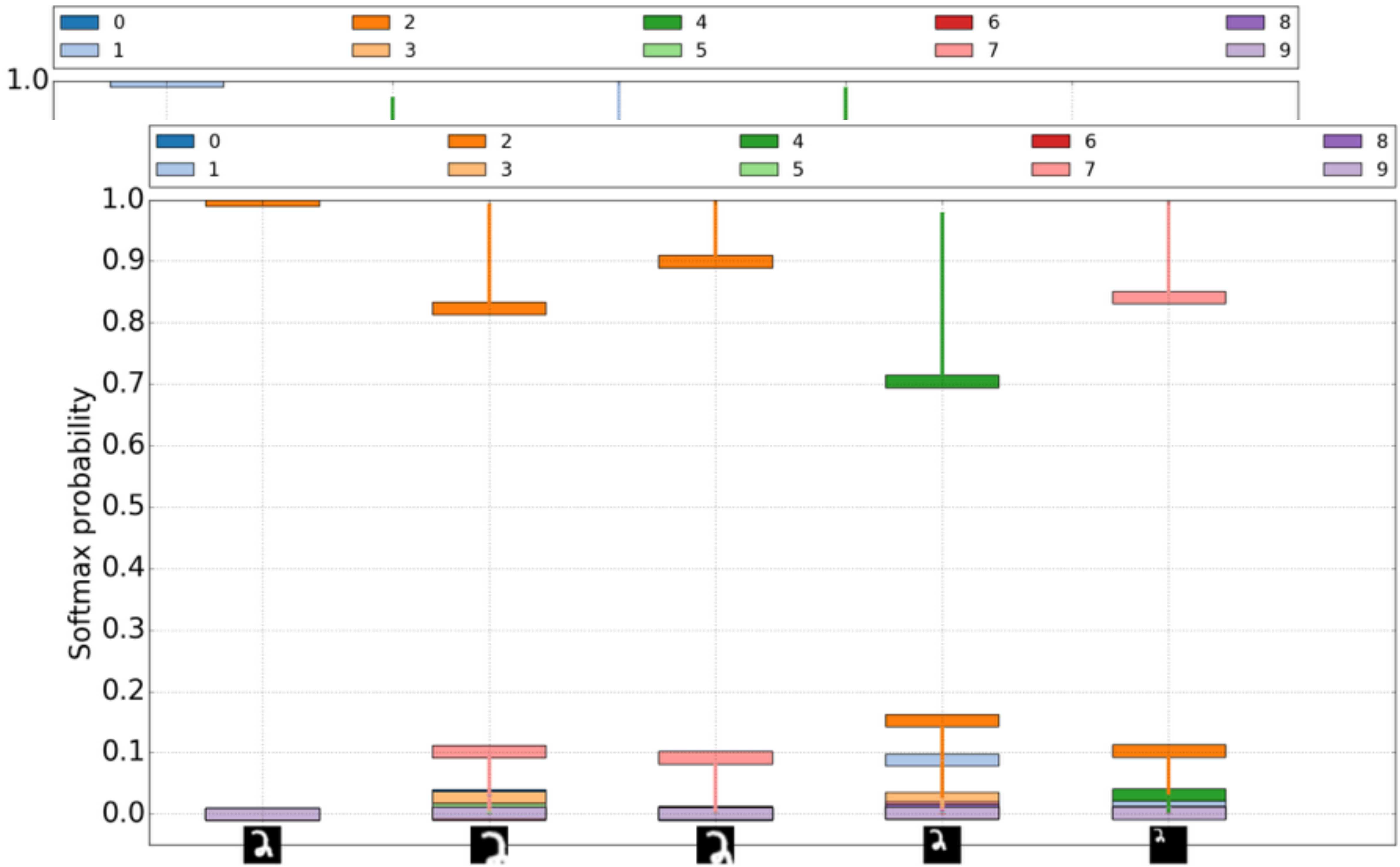


Matrix Gaussian scaling



SGLD scaling

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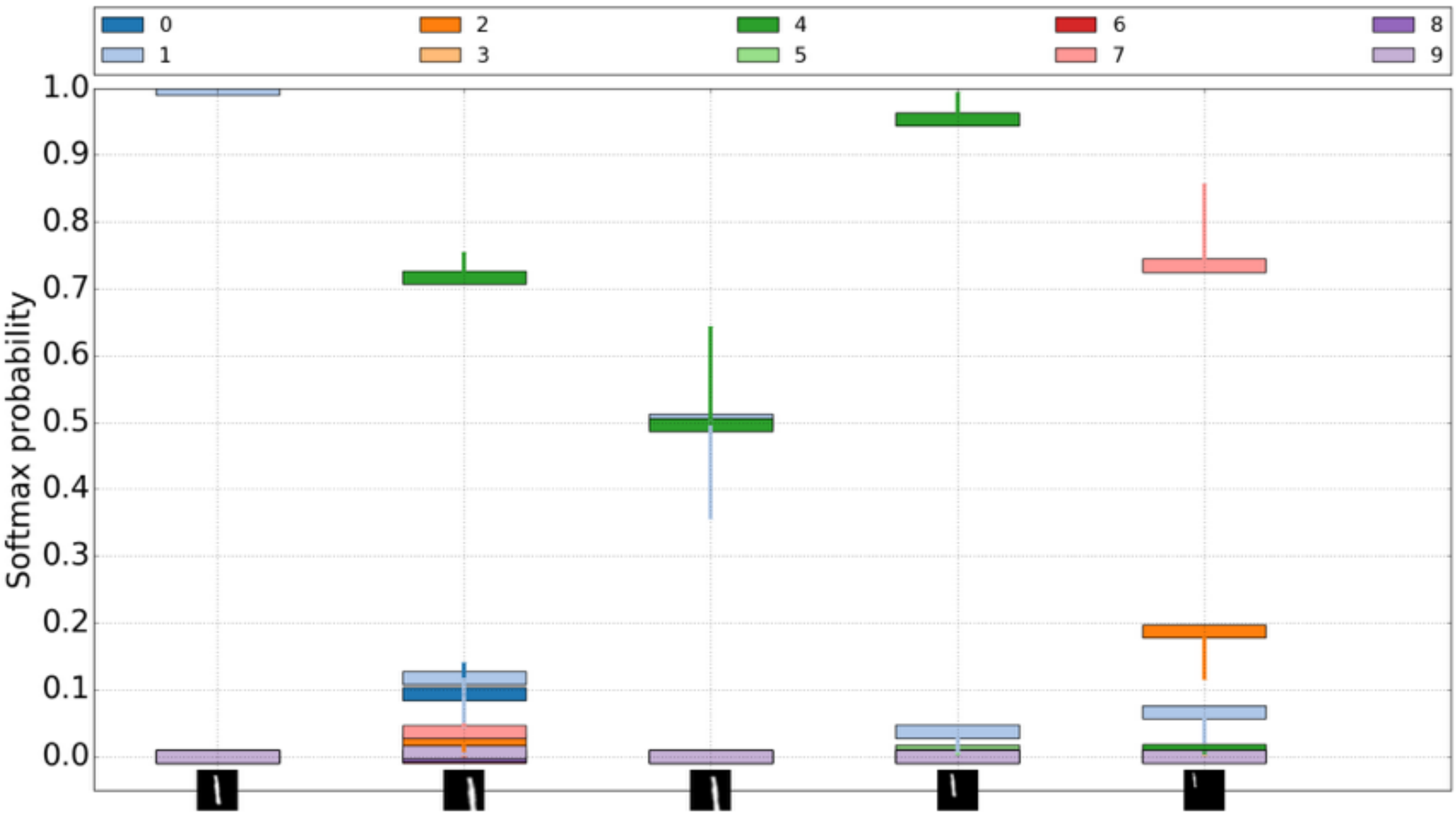
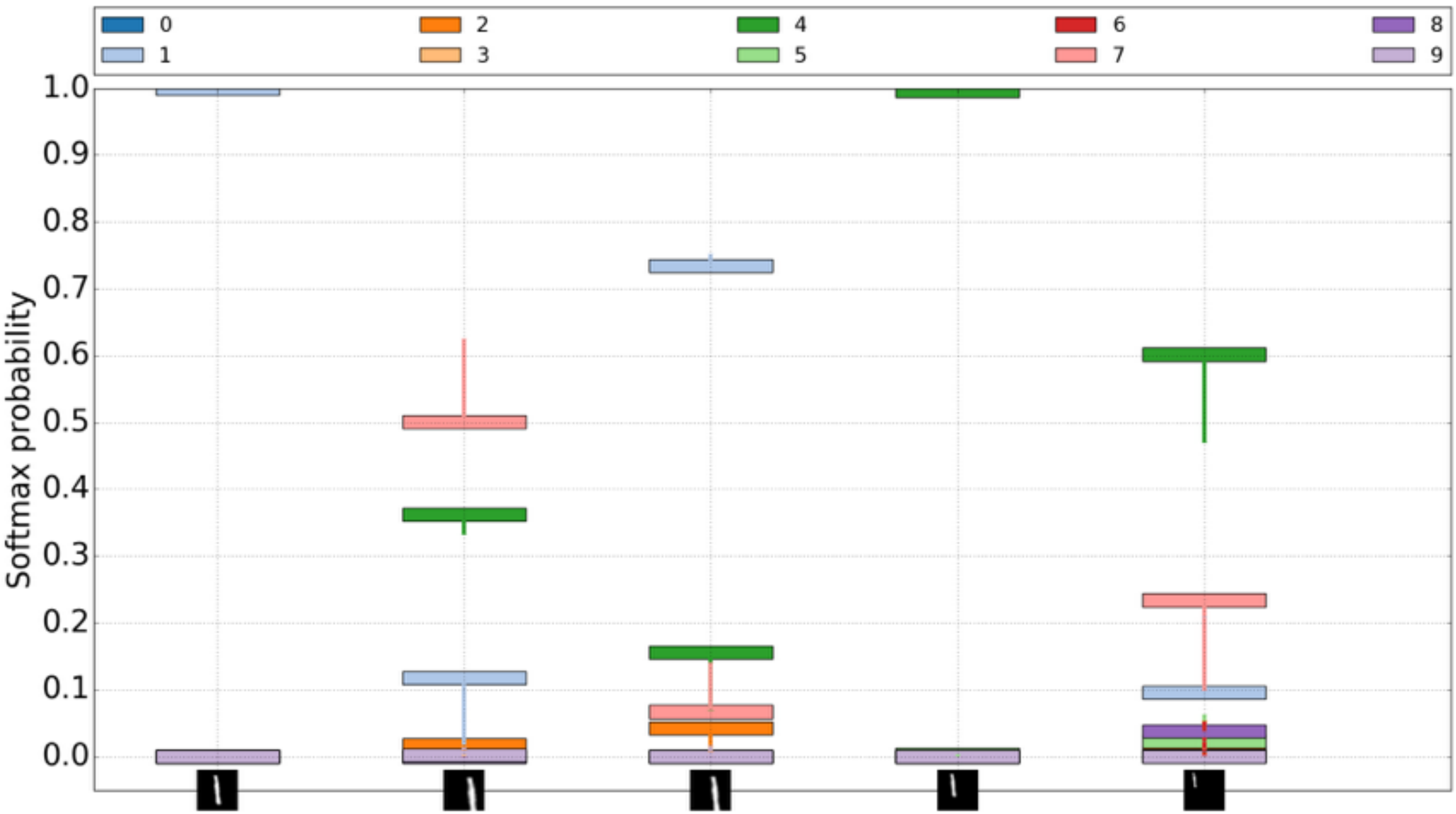


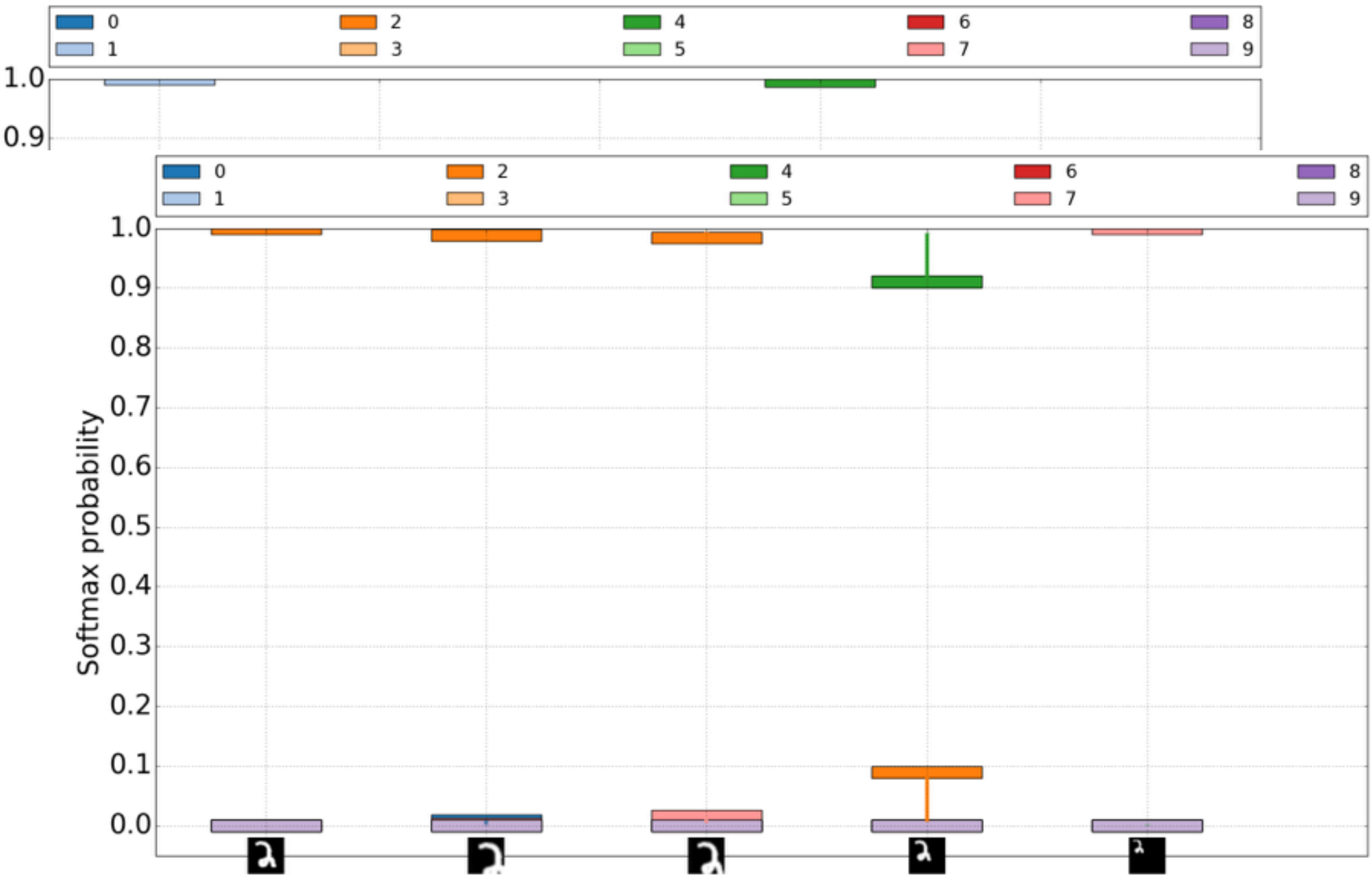
SGLD scaling

Bootstrap scaling

Bootstrap scaling



Bootstrap scaling



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    - But still in most cases we have erroneous overconfidence
- In general it appears to not be a parameter prior problem as it affects even the frequentist bootstrap
    - Although a better prior might fix it
- This suggests that the model itself (neural network) is not capable (at least as they are right now) to output reasonable probabilities

Thanks!