Neural Networks as Model Selection with Incremental MDL Normalization

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Neuroscience inspirations

- Regularity collection in a hierarchical encoding process
  - In biological brains of primates, high-level brain areas are known to send top-down feedback connections to lower-level areas to encourage the selection of the most relevant information in the current input given the current task.

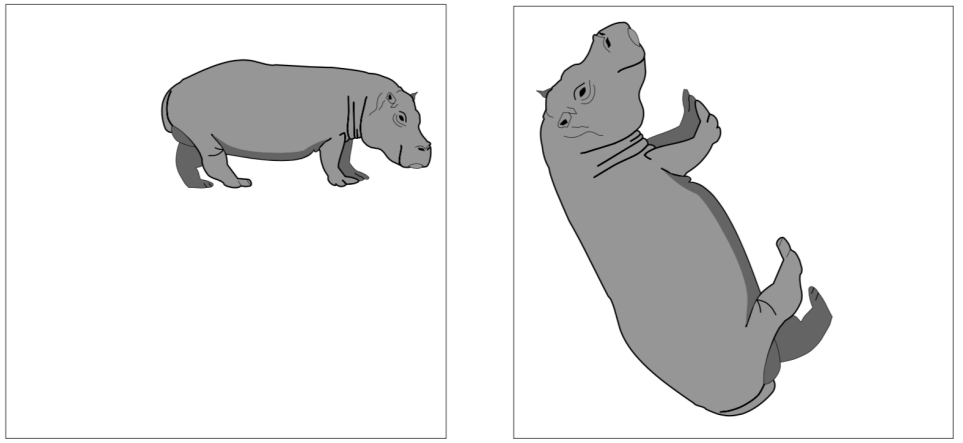
- Hierarchical neural coding in visual adaptation
  - Vertical orientation reduce their firing rates to that orientation after the adaptation.
  - While the cell responses to other orientations may increase.

- Contradicts to Bayesian assumptions (more probable, the larger firing rate)
  - However, well match the information theoretical point-of-view that the most relevant information (saliency), which depends on the statistical regularity, have higher “information”, just as the firing of the neurons.

Implicit space of neural networks

- If we consider the neural networks as population codes, the constraint space can be subdivided into the ***input-vector space***, the ***hidden-vector space***, and the ***implicit space***, which represents the underlying dimensions of variability in the other two spaces, i.e., a reduced representation of the constraint space.

- Implicit space: scale + rotation



- The relevant information about the implicit space can be constrained to ensure a minimized description length of the neural networks.

Minimum Description Length (MDL)

- Given a model class Θ consisting of a finite number of models parameterized by the parameter set θ.
- Given a data sample x, each model in the model class describes a probability P (x|θ) with the code length computed as − log P (x|θ). The minimum code length given any arbitrary θ would be given by

$$L(x|\hat{\theta}(x)) = -\log P(x|\hat{\theta}(x))$$

Compress most efficiently, yield maximum likelihood.

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optimal models vary from sample to sample~

Universal Codes

Solution:

We can define a universal code $\bar{P}(x)$ for a model class Θ, such that for any data sample x, the shortest code for x is always $\mathrm{L}\left(x\middle|\hat{\theta}(x)\right)$.

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Normalized Maximum Likelihood (NML)

- To select for a proper optimal universal code, a cautious approach would be to assume a worst-case scenario in order to make “safe” inferences about the unknown world.

$$R(p\|\Theta) = \max_q E_q[\ln \frac{f(x|\hat{\theta}_x)}{p(x)}]$$

- where the “worst” distribution q(·) is allowed to be any p(x) probability distribution.

- Among the optimal universal code, the normalized maximum likelihood (NML) probability minimizes the worst-case regret and avoids assigning an arbitrary distribution to Θ.

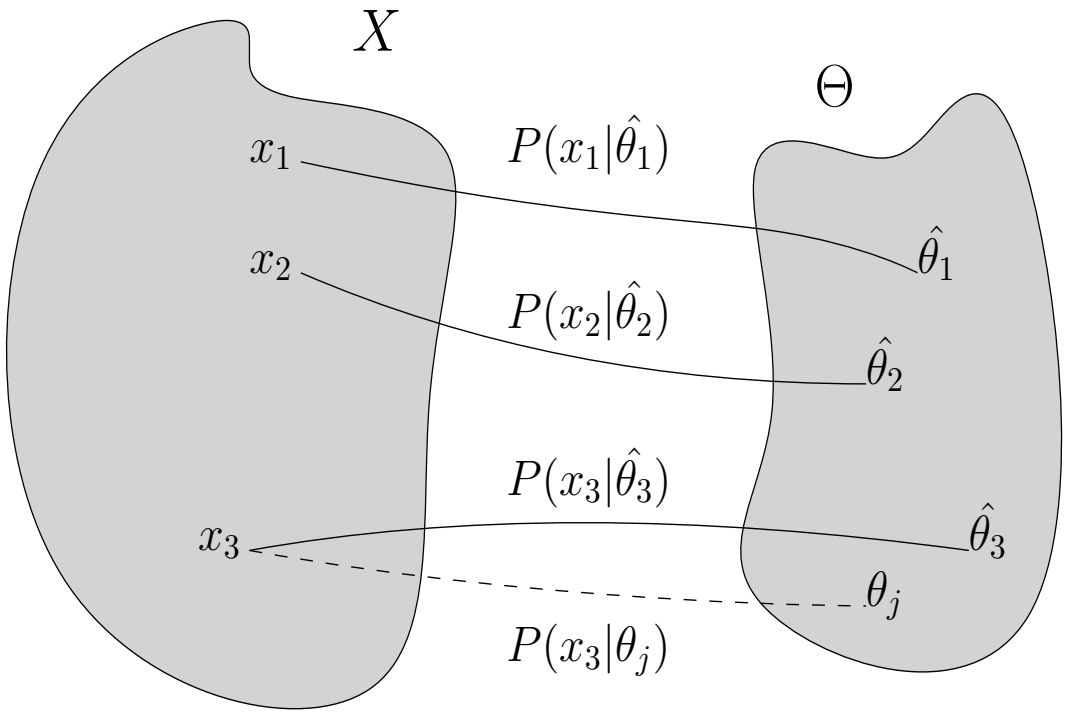
Normalized Maximum Likelihood (NML)

$$P_{NML}(x) = \frac{P(x|\hat{\theta}(x))}{\sum_{x'} P(x'|\hat{\theta}(x'))}$$

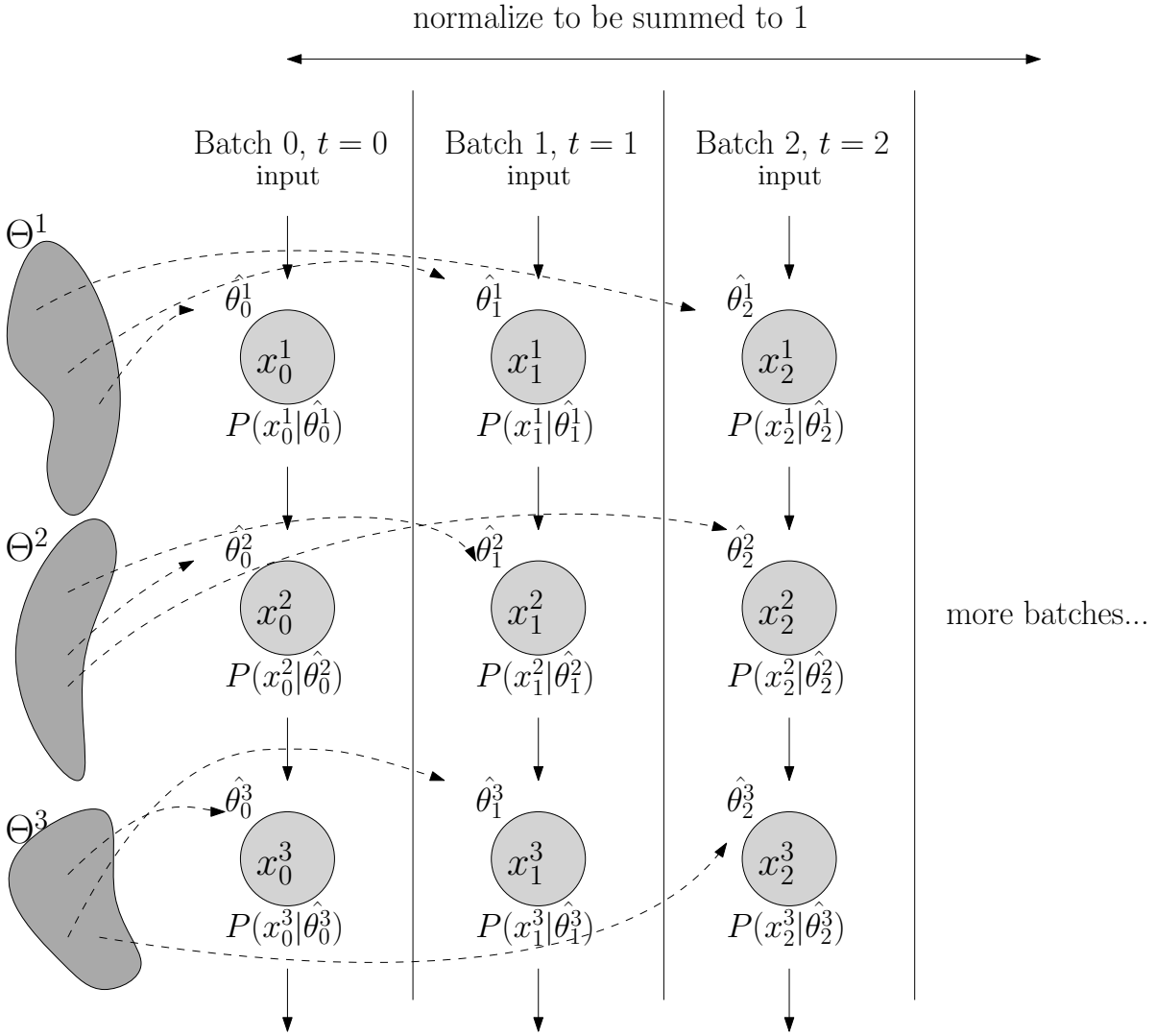
Then, the regret is the same for all data sample x is given by:

$$\begin{aligned} COMP(\Theta) &\equiv regret_{NML} \\ &\equiv -\log P_{NML}(x) + \log P(x|\hat{\theta}(x)) \\ &= \log \sum_{x'} P(x'|\hat{\theta}(x')) \end{aligned}$$

which defines the model class complexity as it indicates how many different data samples can be well explained by the model class Θ.



Neural Networks as Model Selection



$$P_{NML}(x_i) = \frac{P(x_i|\hat{\theta}_i(x_i))}{\sum_{j=0}^{i} P(x_j|\hat{\theta}_j(x_j))}$$

- where $\widehat{\theta_1}\ (x_1)$ refers to the model parameter already optimized for i − 1 steps, and have seen sequential data sample x_0 through x_{i-1}.
- This distribution is updated every time a new data sample is given, and can therefore be computed incrementally, as in batch-based training.

Regularity Normalization (RN)

Algorithm 1 Regularity Normalization (RN)

Input: Values of x over a mini-batch: $\mathcal{B} = \{x_{1,\dots,m}\}$;
Parameter: $COMP_t$, $\hat{\theta}_t$
Output: $y_i = RN(x_i)$

$$COMP_{t+1} = \text{increment}(COMP_t,\ P(x_i|\hat{\theta}_t(x_i)))$$
$$L_{x_i} = COMP_{t+1} - \log P(x_i|\hat{\theta}_t(x_i))$$
$$y_i = L_{x_i} * x_i$$

Normalization factor – optimal universal code length for the given input

Variants: SN, RLN, RBN

- Saliency Normalization (SN)
  - NML distribution can be modified to also include a data prior function, s(x)

$$P_{NML}(x) = \frac{s(x)P(x|\hat{\theta}(x))}{\sum_{x'} s(x')P(x'|\hat{\theta}(x'))}$$

  - S(x) can be the emphasis of certain inputs, to the cost of certain data, or even top-down attention etc.

- Regularity Batch Normalization (RBN)
- Regularity Layer Normalization (RLN)

Contenders for empirical evaluations

- Regularity Normalization
- Regularity Batch Normalization
- Regularity Layer Normalization
- Saliency Normalization

vs.

- Batch Normalization
- Layer Normalization
- Weight Normalization

Imbalanced MNIST problem with FFNN

- Hypothesis:
  - RN should better adapt to the regularity of the data distribution than other methods, tackling the imbalanced data issue by up-weighting the activation of the rare sample features and down-weighting those of the dominant sample features.

- To simulate changes in the context (input) distribution, in each epoch we randomly choose n classes out of the ten, and set their sampling probability to be 0.01 (only 1% of those n classes are used in the training).

- 784-1000-1000-10 FFNN with ReLU

Imbalanced MNIST problem with FFNN

Table 1. Heavy-Tailed Scenario 1: Under-represented Minorities
Test errors of the imbalanced permutation-invariant MNIST 784-1000-1000-10 task

	"Balanced"	"Rare minority"		
	$n = 0$	$n = 1$	$n = 2$	$n = 3$
baseline	4.80 ± 0.15	14.48 ± 0.28	23.74 ± 0.28	32.80 ± 0.22
BN	$\mathbf{2.77 \pm 0.05}$	12.54 ± 0.30	21.77 ± 0.25	30.75 ± 0.30
LN	3.09 ± 0.11	8.78 ± 0.84	14.22 ± 0.65	20.62 ± 1.46
WN	4.96 ± 0.11	14.51 ± 0.44	23.72 ± 0.39	32.99 ± 0.28
RN	4.91 ± 0.39	8.61 ± 0.86	14.61 ± 0.58	19.49 ± 0.45
RLN	5.01 ± 0.29	9.47 ± 1.21	$\mathbf{12.32 \pm 0.56}$	22.17 ± 0.94
LN+RN	4.59 ± 0.29	$\mathbf{8.41 \pm 1.16}$	12.46 ± 0.87	$\mathbf{17.25 \pm 1.47}$
SN	7.00 ± 0.18	12.27 ± 1.30	16.12 ± 1.39	24.91 ± 1.61

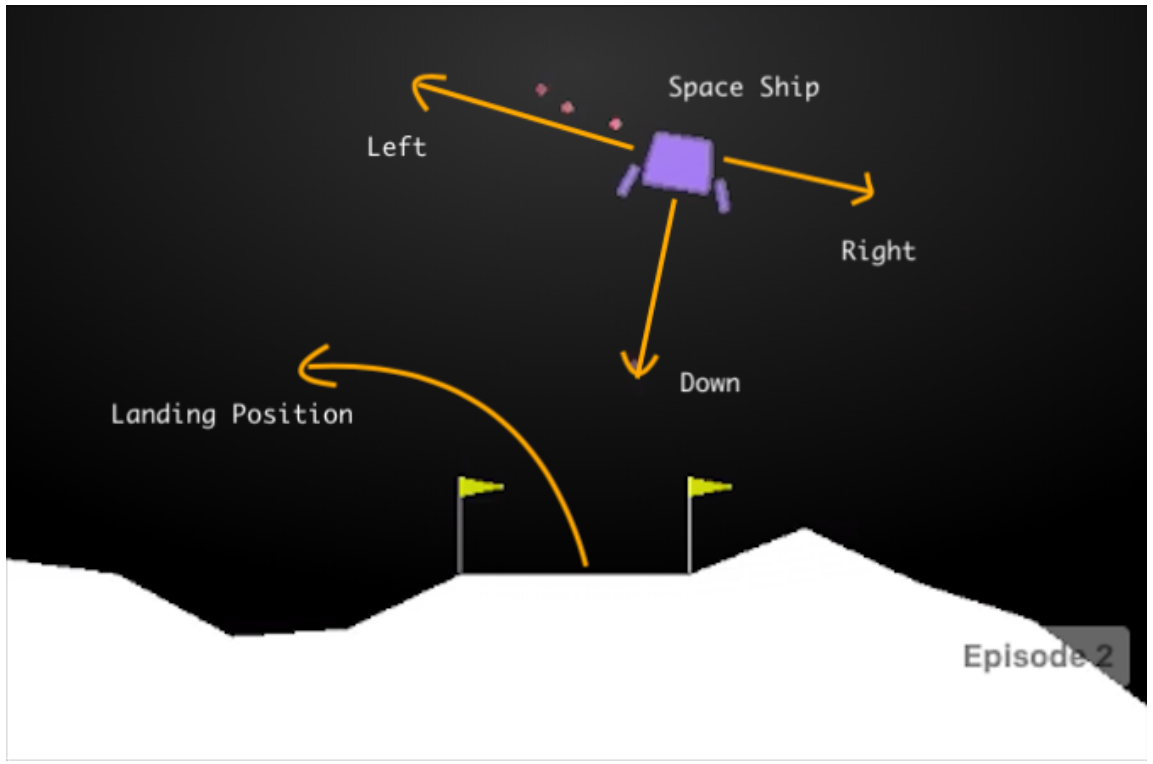
Imbalanced MNIST problem with FFNN

Table 2. Heavy-Tailed Scenario 2: Over-represented Minorities
Test errors of the imbalanced permutation-invariant MNIST 784-1000-1000-10 task

	"Highly imbalanced"				"Dominant oligarchy"	
	$n = 4$	$n = 5$	$n = 6$	$n = 7$	$n = 8$	$n = 9$
baseline	42.01 ± 0.45	51.99 ± 0.32	60.86 ± 0.19	70.81 ± 0.40	80.67 ± 0.36	90.12 ± 0.25
BN	40.67 ± 0.45	49.96 ± 0.46	59.08 ± 0.70	67.25 ± 0.54	76.55 ± 1.41	80.54 ± 2.38
LN	26.87 ± 0.97	34.23 ± 2.08	36.87 ± 0.64	41.73 ± 2.74	$\mathbf{41.20 \pm 1.13}$	$\mathbf{41.26 \pm 1.30}$
WN	41.95 ± 0.46	52.10 ± 0.30	60.97 ± 0.18	70.87 ± 0.39	80.76 ± 0.36	90.12 ± 0.25
RN	$\mathbf{23.35 \pm 1.22}$	33.84 ± 1.69	41.47 ± 1.91	60.46 ± 2.88	81.96 ± 0.59	90.11 ± 0.24
RLN	23.76 ± 1.56	32.23 ± 1.66	43.06 ± 3.56	57.30 ± 6.33	88.36 ± 1.77	89.55 ± 0.32
LN+RN	25.65 ± 1.91	$\mathbf{28.71 \pm 1.97}$	$\mathbf{33.14 \pm 2.49}$	$\mathbf{36.08 \pm 2.09}$	44.54 ± 1.74	82.29 ± 4.44
SN	31.07 ± 1.41	41.87 ± 1.78	52.88 ± 2.09	68.44 ± 1.42	83.34 ± 1.85	82.41 ± 2.30

RL problem with DQN

- OpenAI Lunarlander-V2 environment



- DQN with two hidden units of 64 neurons
- Experience replay
- Adam optimizer

RL problem with DQN

Algorithm 1 Deep Q-learning with Experience Replay

Initialize replay memory $\mathcal{D}$ to capacity N
Initialize action-value function Q with random weights
for episode $= 1, M$ **do**
  Initialise sequence $s_1 = \{x_1\}$ and preprocessed sequenced $\phi_1 = \phi(s_1)$
  for $t = 1, T$ **do**
    With probability ϵ select a random action a_t
    otherwise select $a_t = \max_a Q^*(\phi(s_t), a; \theta)$
    Execute action a_t in emulator and observe reward r_t and image x_{t+1}
    Set $s_{t+1} = s_t, a_t, x_{t+1}$ and preprocess $\phi_{t+1} = \phi(s_{t+1})$
    Store transition $(\phi_t, a_t, r_t, \phi_{t+1})$ in $\mathcal{D}$
    Sample random minibatch of transitions $(\phi_j, a_j, r_j, \phi_{j+1})$ from $\mathcal{D}$
    Set $y_j = \begin{cases} r_j & \text{for terminal } \phi_{j+1} \\ r_j + \gamma \max_{a'} Q(\phi_{j+1}, a'; \theta) & \text{for non-terminal } \phi_{j+1} \end{cases}$
    Perform a gradient descent step on $(y_j - Q(\phi_j, a_j; \theta))^2$ according to equation 3
  end for
end for

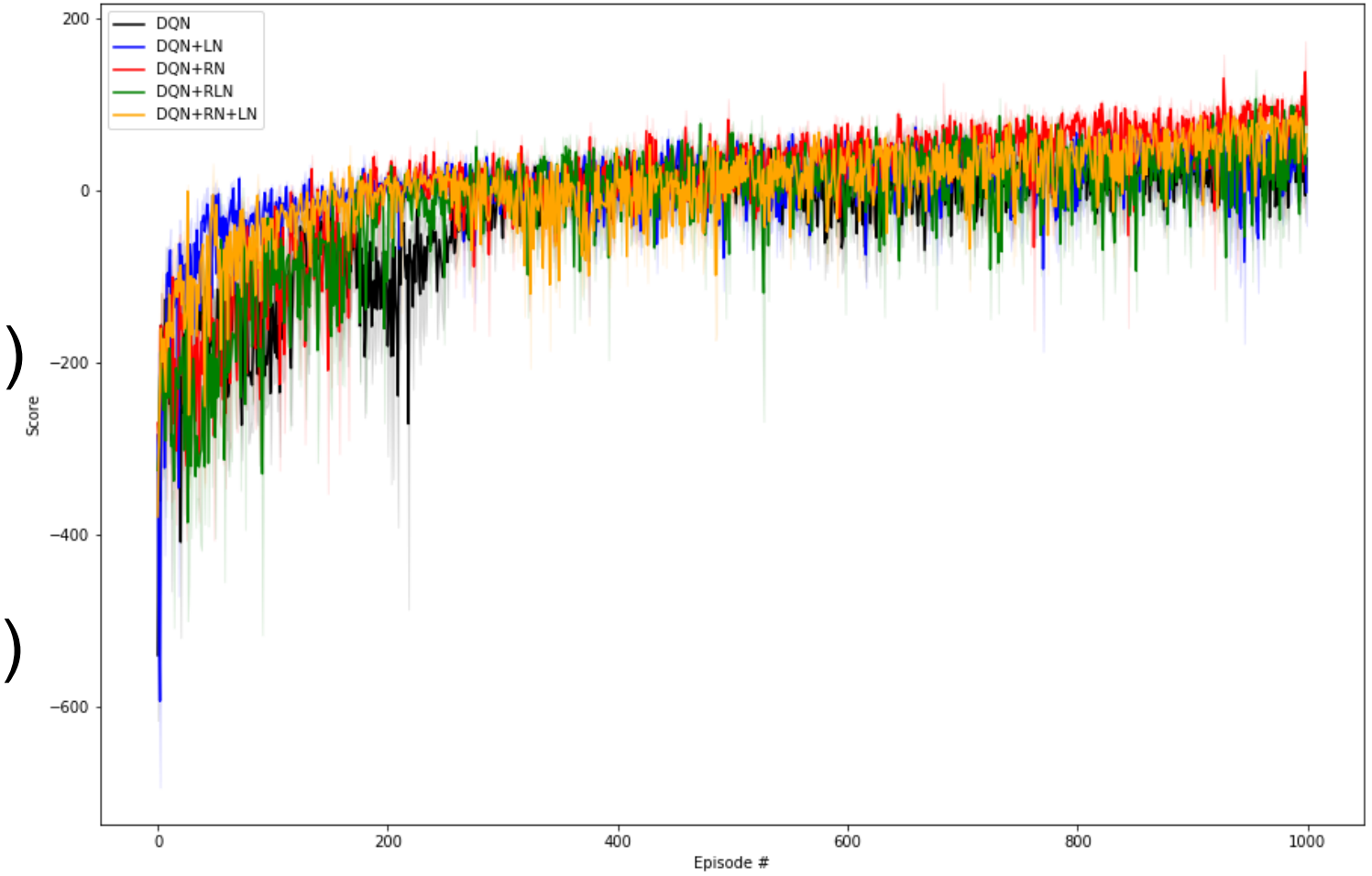
Apply RN, RLN, LN, BN, SN.
Update regularity statstics.

RL problem with DQN

- Average final scores:

- RN (76.95 ± 4.44)
- RN+LN (65.82 ± 10.91)
- RLN (49.27 ± 40.35)

- Baseline (37.17 ± 8.82)
- LN (-1.54 ± 39.14)



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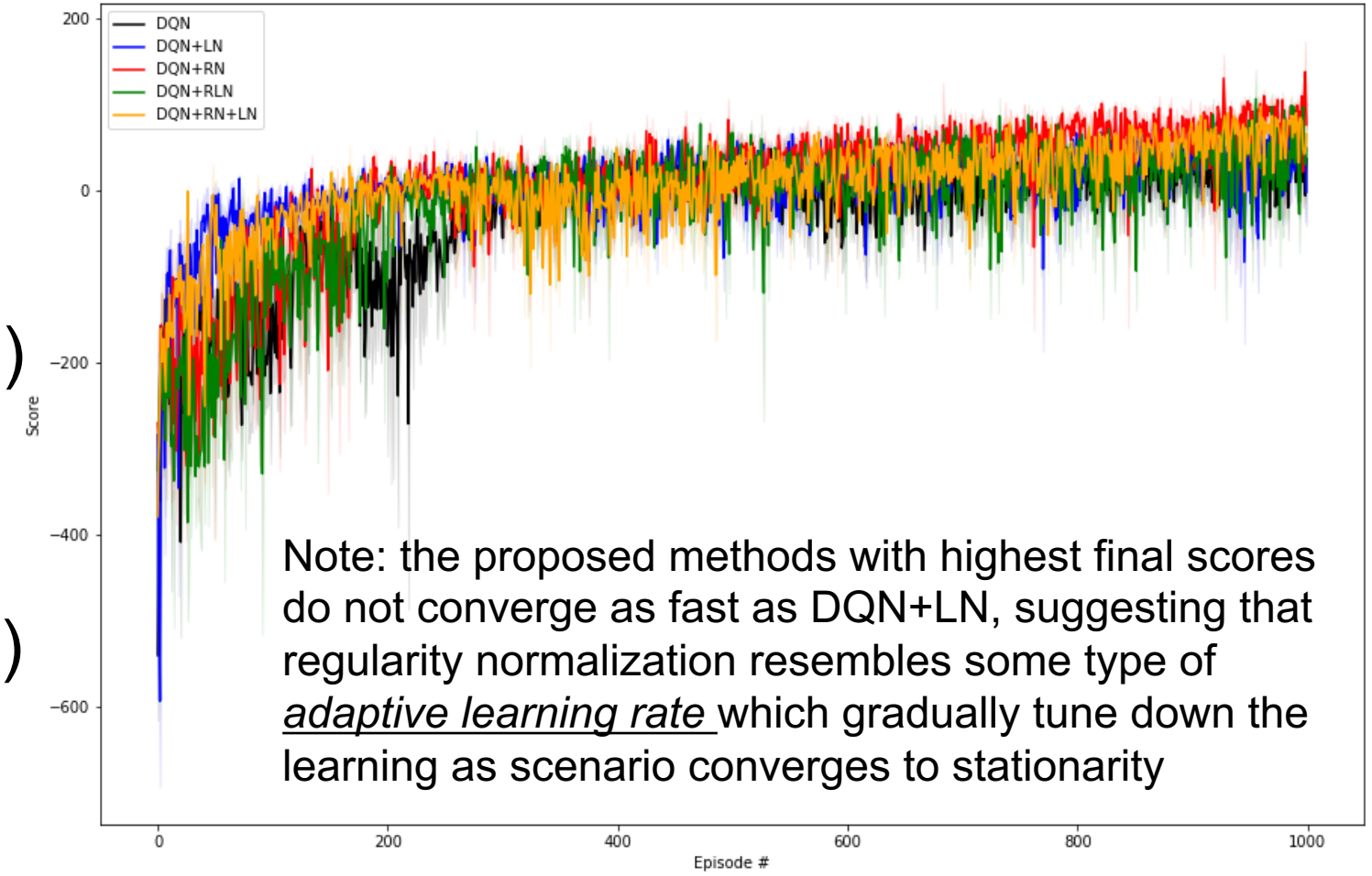

Note: the proposed methods with highest final scores do not converge as fast as DQN+LN, suggesting that regularity normalization resembles some type of *adaptive learning rate* which gradually tune down the learning as scenario converges to stationarity

Discussion and ongoing directions

- Extend to fully Bayesian variational approach to include the regularity estimation as part of the optimization process.

- Investigate the changes in overall loss or probability as the computation of NML makes selection on the model.

- MDL → ensemble modeling process and usually involves multiple models.
- Assumption
  - that the only model trained at each step is the local “best” model learned so far, but local maximal likelihood may not be a global best approach for model combinations.
- Can we theoretically support the assumption above for our greedy approach for “optimal parameters”?

Future work and next steps

- Top-down attention given by data prior (such as feature extracted from signal processing, or task-dependent information) → Top-down meta learning:
  - How different functions of s(x) behave in different task settings.

- RN as Unsupervised attention mechanism
  - Unsupverised + Supervised Attention with top-down attention from either oracle supervision or other meta information.

- Convolutional and recurrent cases.
- Non-stationary rewards in a changing environments.

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Thanks! Questions?

- Feel free to also check out my other project in IJCAI poster session:

Split Q Learning: Reinforcement Learning with Two-Stream Rewards

Poster #908 in **Hall A** August 15th
Talk in area **2605** August 12th at **13:35**