Heterogeneity, Hyperparameters, and GPUs: Towards Useful Transport Calculations Using Neural Networks

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October 5, 2021

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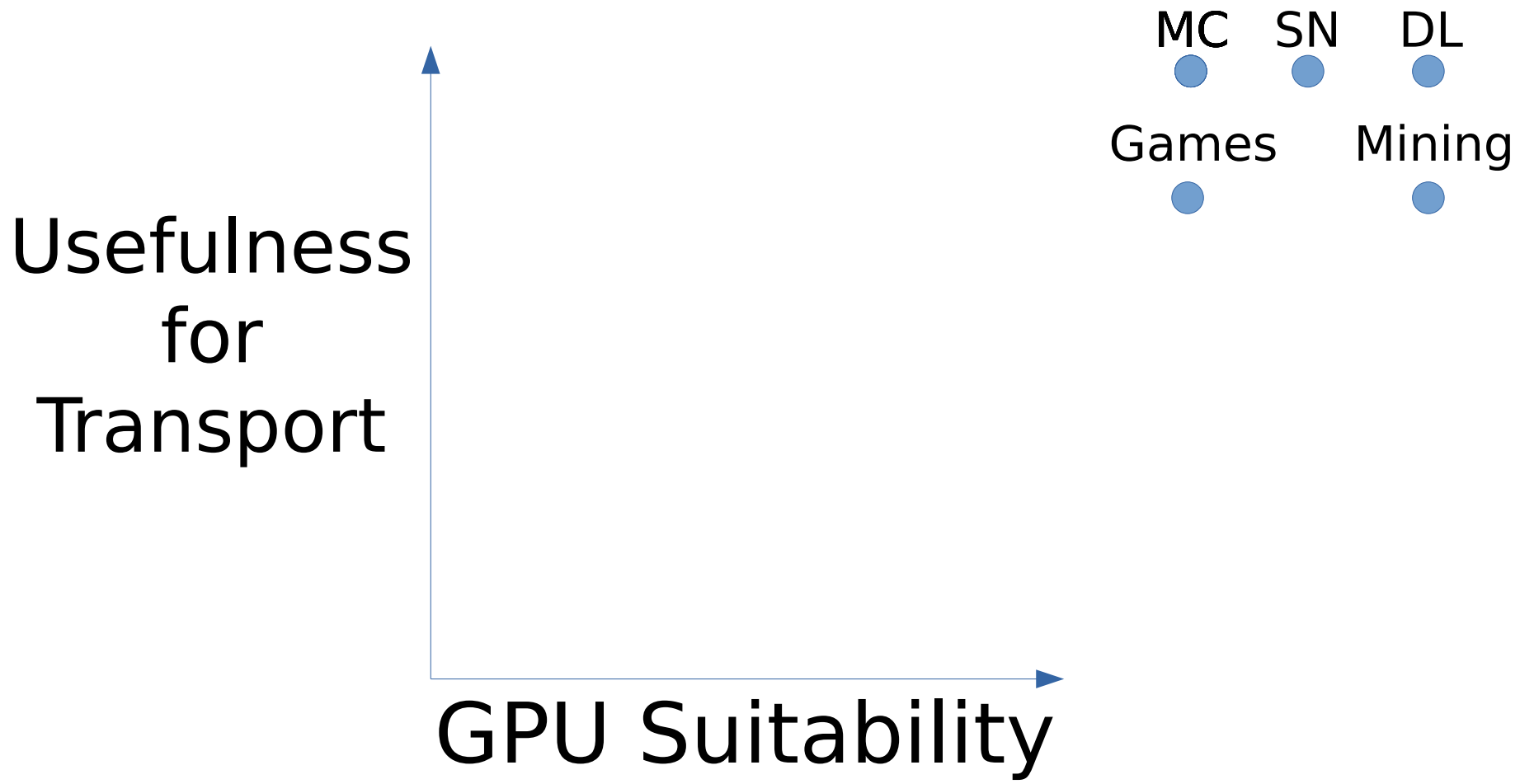
This talk has three parts

1) Motivation
2) Methods
3) Results
   - The transport equation can be solved using a neural network (NN).

Can we use what GPUs were designed for?



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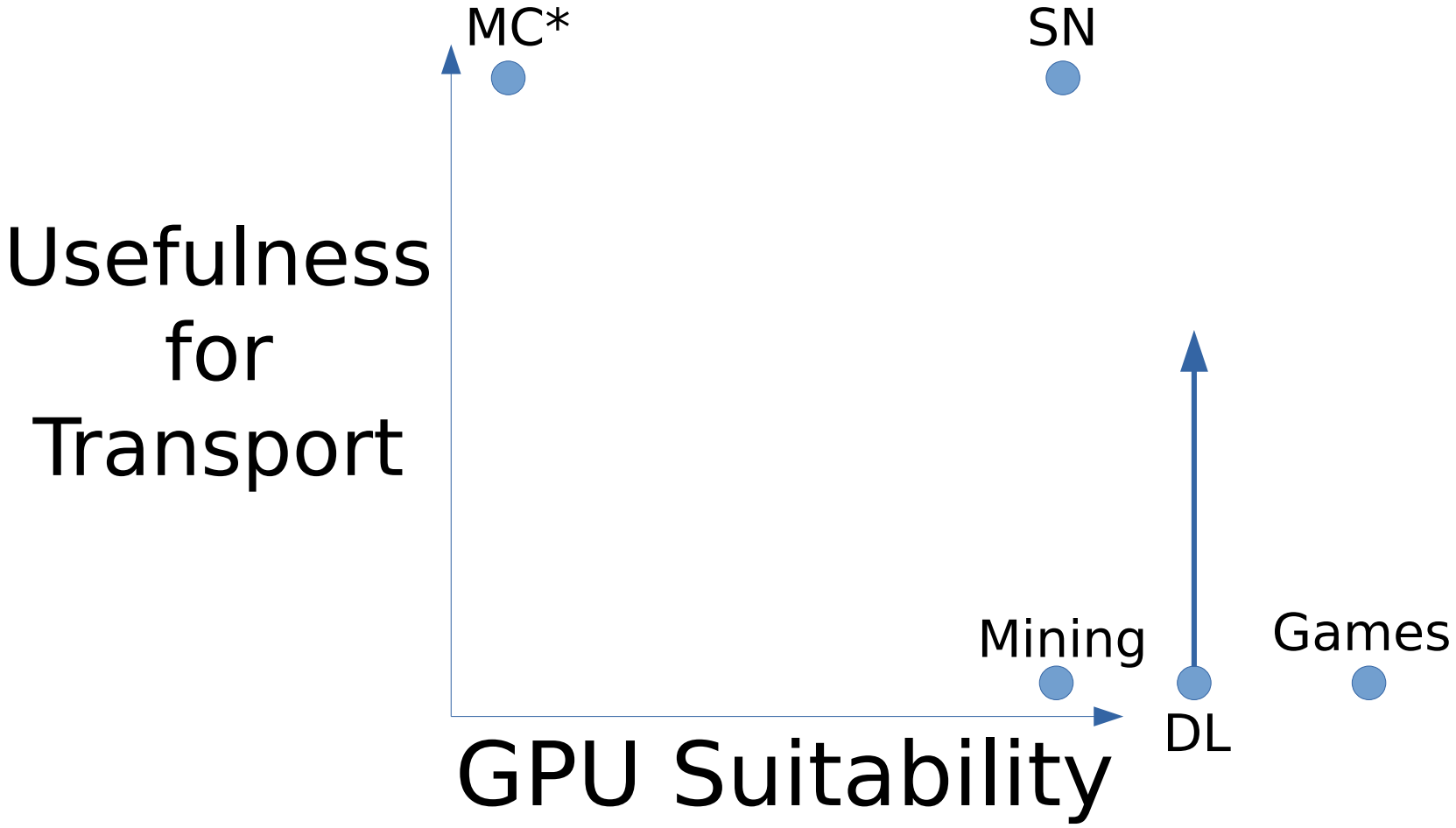
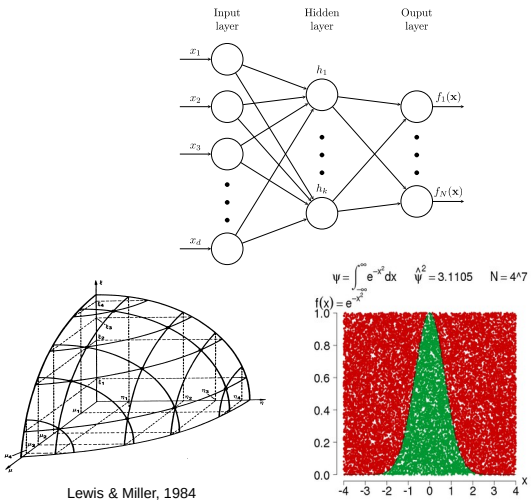


**History-based* Monte Carlo

Can we improve previous results?



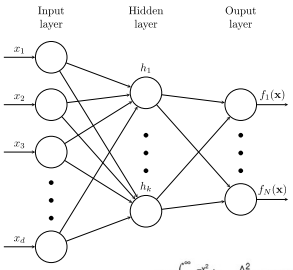
Lewis & Miller, 1984

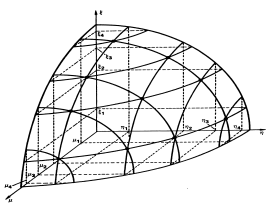
http://mike.pozulp.com/2019nnPaper.pdf

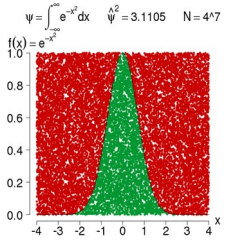
http://mike.pozulp.com/2019nnSlides.pdf

http://mike.pozulp.com/2019nnErrata.pdf

We added Het, Hyp, and GPUs







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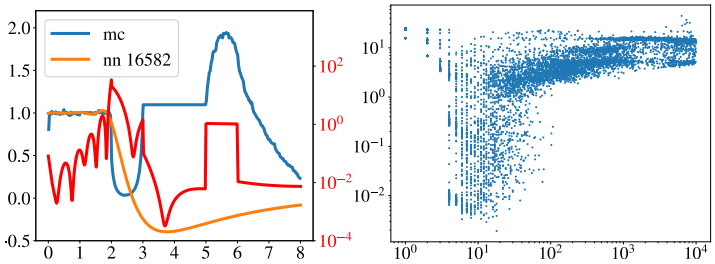

Time(%)	Time	Calls
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1.90	2.91627s	7

http://mike.pozulp.com/2021hhg.pdf

https://github.com/llnl/narrows

A neural network is a function approximation technique

- Input $\mathbf{x} \in \mathbb{R}^d$
- Output $f(\mathbf{x}) \in \mathbb{R}^N$
- Non-linear activation function

$$h_i = \sigma(\mathbf{w}_i^T \mathbf{x} + b_i)$$

- Weights $\mathbf{w}_i \in \mathbb{R}^n$
- Biases b_i

The neural network minimizes a loss function

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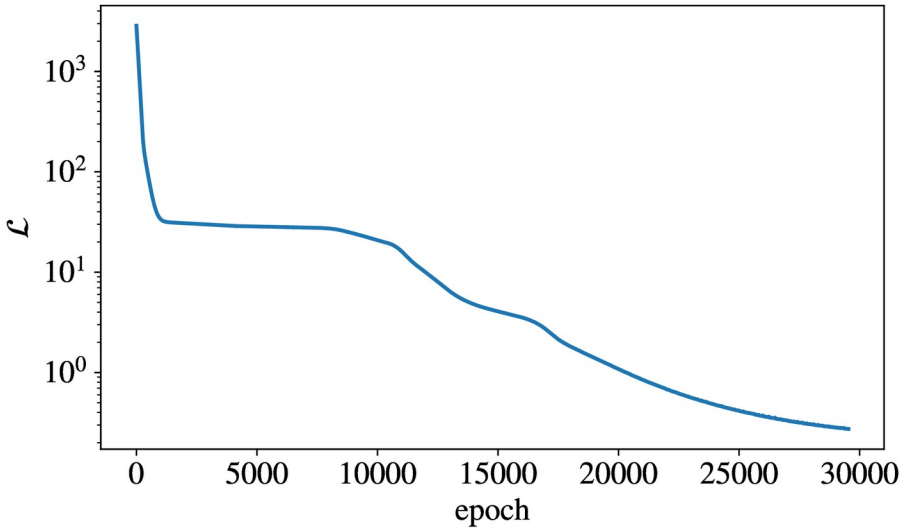
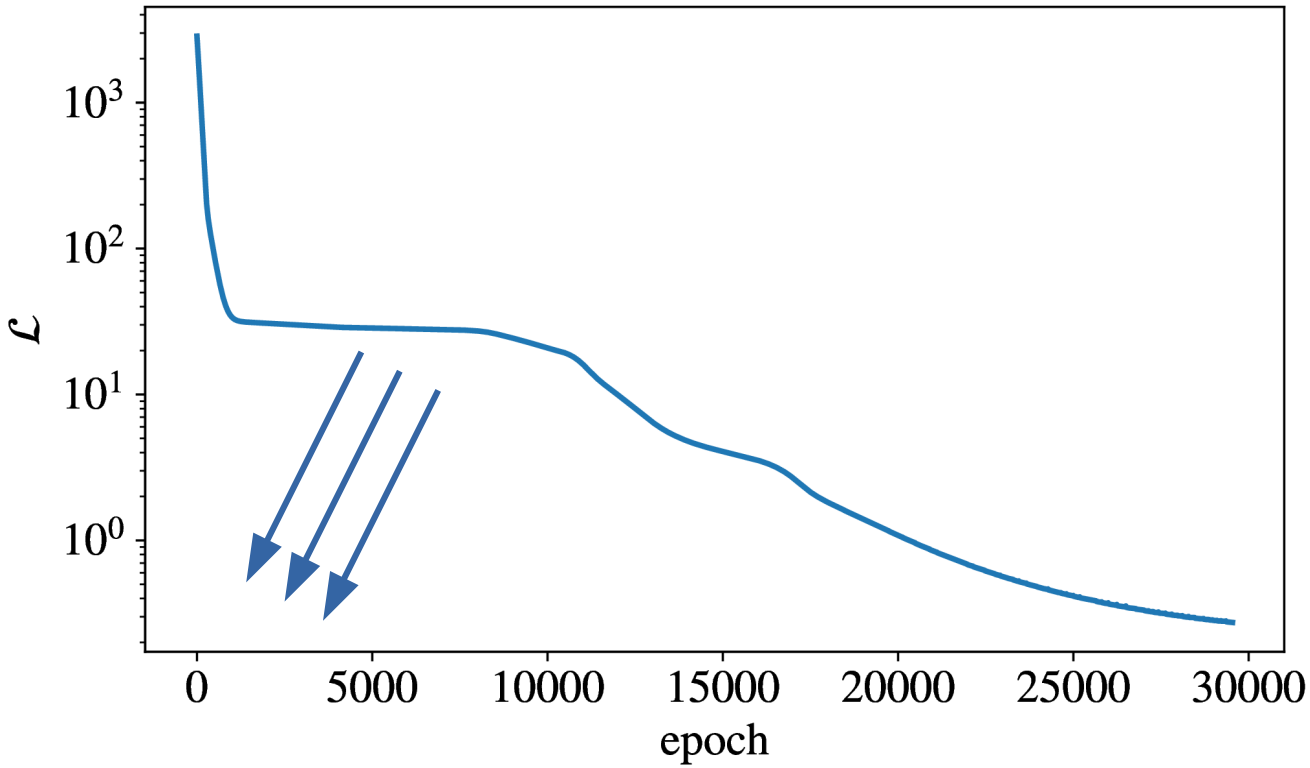


Hyperparameters affect convergence



We solved a 1D mono-energetic transport equation with linearly anisotropic scattering

$$\mu \frac{\partial \psi(z,\mu)}{\partial z} + \Sigma_t(z)\psi(z,\mu) = \frac{1}{2}\left[\Sigma_{s0}(z)\phi_0(z) + 3\Sigma_{s1}(z)\phi_1(z)\mu + Q(z)\right] \quad (1a)$$

$$\psi(z = 0, \mu > 0) = 0 \quad (1b)$$

$$\psi(z = z_{\max}, \mu < 0) = 0 \quad (1c)$$

Heterogeneity means multi-material

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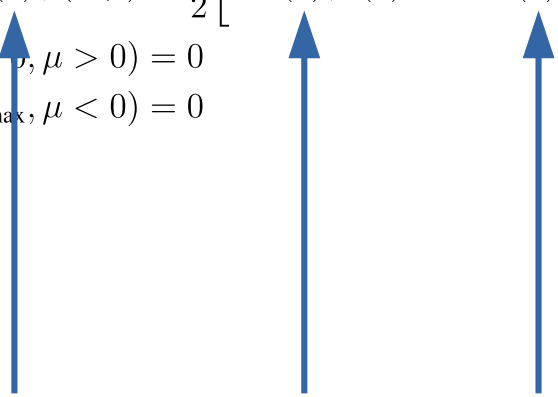

We used this loss function

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$$\begin{aligned}\mathcal{L} = &\left\| \boldsymbol{\nabla}\hat{\boldsymbol{\Psi}}\mathrm{diag}(\boldsymbol{\mu}) + \boldsymbol{\Sigma_t}\hat{\boldsymbol{\Psi}} - \frac{1}{2}\left(\boldsymbol{\Sigma_{s0}}\hat{\boldsymbol{\Phi}}_0 \mathbb{1}_N^T - 3\boldsymbol{\Sigma_{s1}}\hat{\boldsymbol{\Phi}}_1\boldsymbol{\mu}^T - \boldsymbol{Q}\right)\right\|_F^2 \\ &+ \gamma_L \|\hat{\boldsymbol{\Psi}}^{\mu>0}(z=0) - \boldsymbol{\Psi}_L\|_F^2 \\ &+ \gamma_R \|\hat{\boldsymbol{\Psi}}^{\mu<0}(z=z_{\max}) - \boldsymbol{\Psi}_R\|_F^2\end{aligned} \tag{2}$$

We solved for scalar flux, current

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We used this convergence criterion

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$$\left|\mathcal{L}^{(l+1)} - \mathcal{L}^{(l)}\right| < \epsilon \tag{5}$$

We used this NN architecture

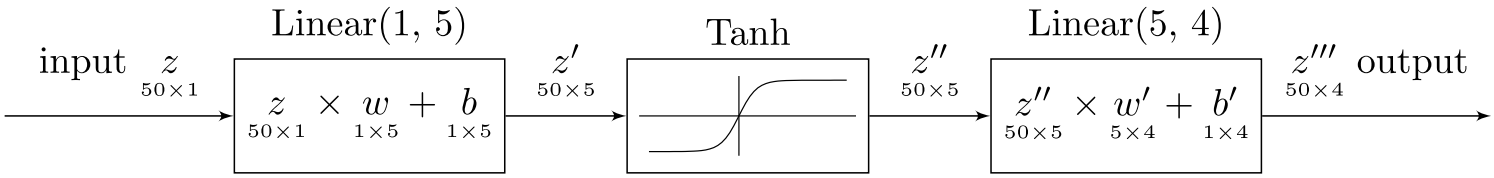

Figure 1: Default NN architecture.

$$p(h, N) = (h + h) + (hN + N)$$

p	number of parameters
h	number of hidden layer nodes
N	number of ordinates

$$p(5, 4) = 34$$

We used a 6-step procedure

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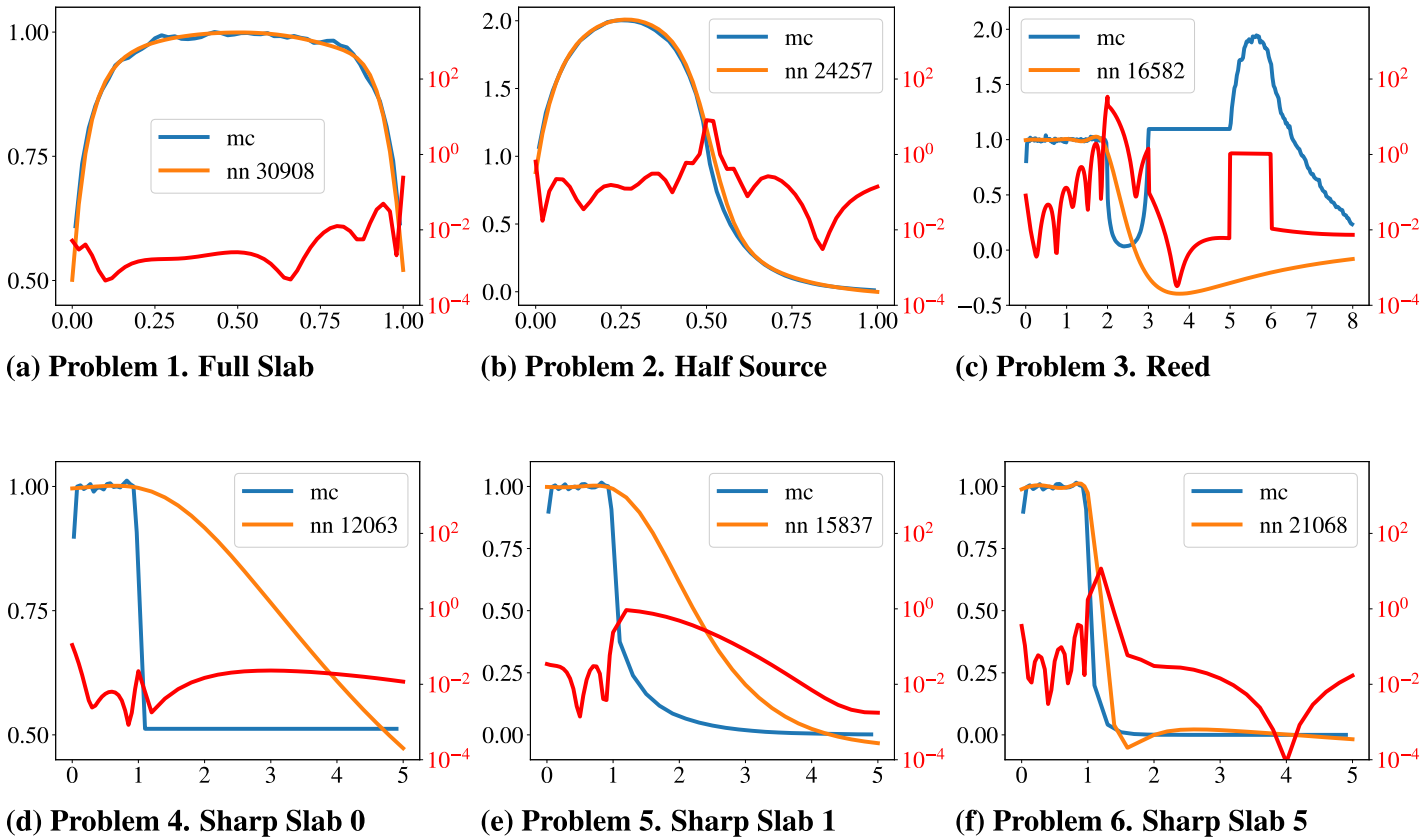
5. Use the gradients computed above to update each parameter in the network such that the parameters are updated in the direction that decreases the loss the most.
6. Repeat the forward and backwards passes until the convergence criterion in Eq. (5) is achieved.

We ran six problems



(a) Problem 1. Full Slab (b) Problem 2. Half Source (c) Problem 3. Reed

(d) Problem 4. Sharp Slab 0 (e) Problem 5. Sharp Slab 1 (f) Problem 6. Sharp Slab 5

Figure 2: Scalar flux plots for six transport problems.

We made progress in understanding NN accuracy for heterogeneous problems but failed to accurately solve the most heterogeneous problem

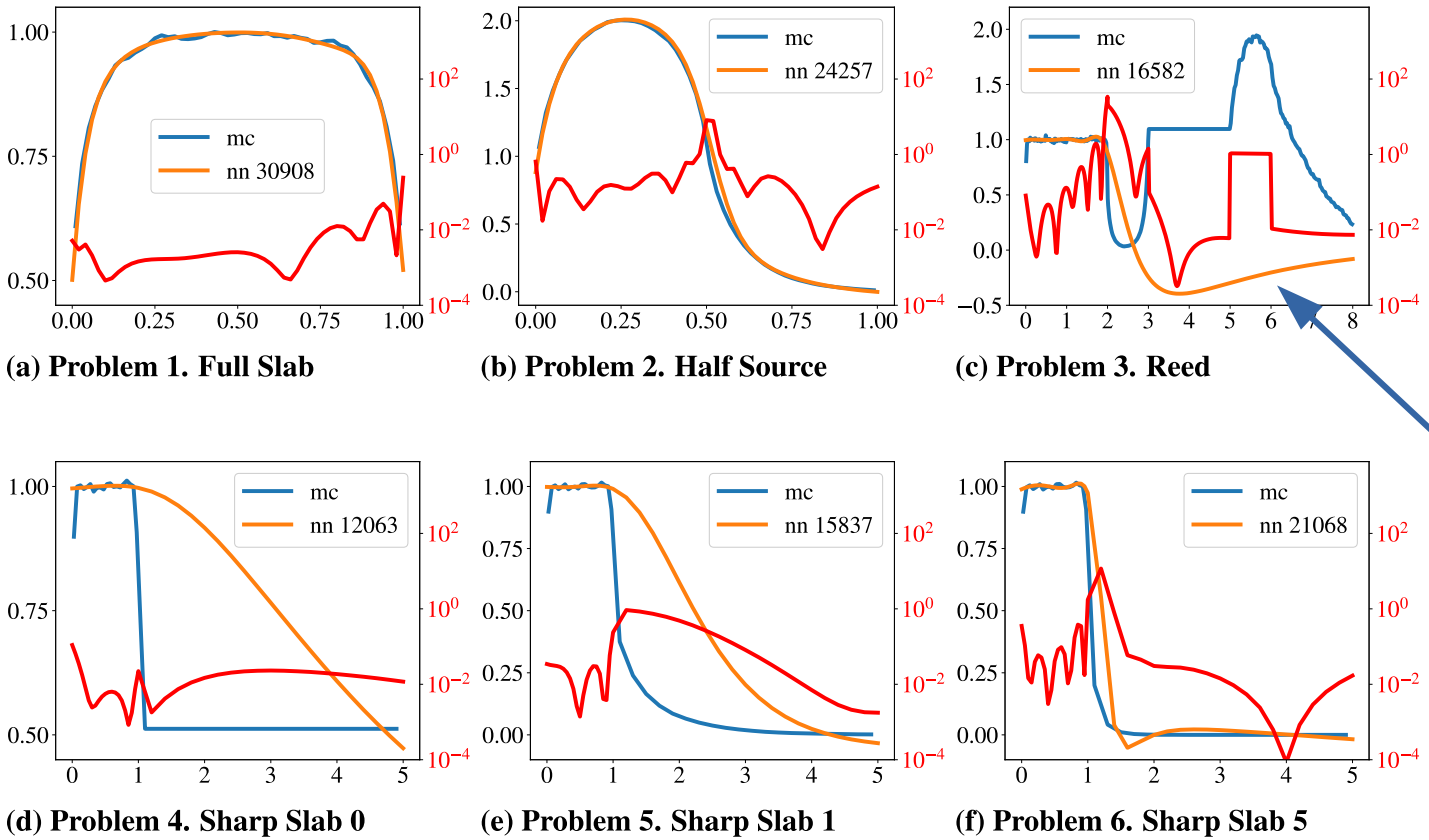


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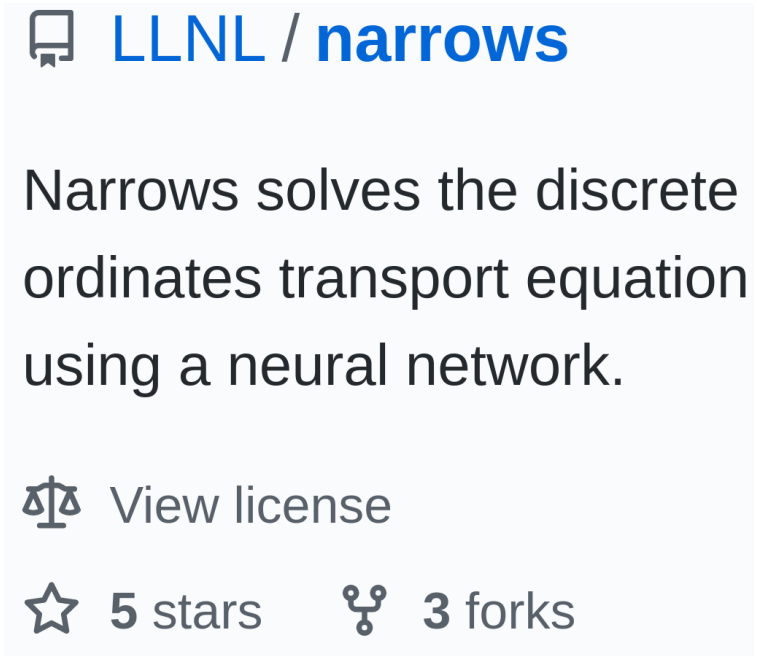
Figure 2: Scalar flux plots for six transport problems.

But we released our code...



github.com/llnl/narrows

...and Ravi Kumar solved it!

LLNL / narrows

Narrows solves the discrete ordinates transport equation using a neural network.

View license

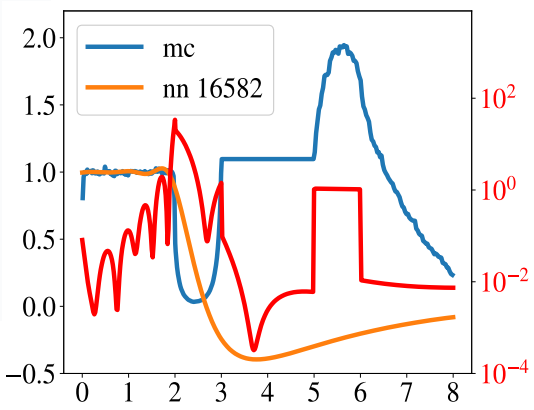
5 stars 3 forks

github.com/llnl/narrows

A Study of Artificial Neural Networks for the Solution of Multi-group Slab Geometry Discrete Ordinates Transport Problems with Material Heterogeneity

by

Ravi Kumar



(c) Problem 3. Reed

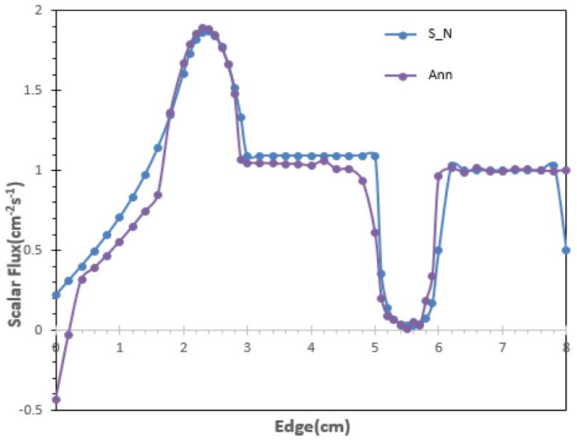


Figure 14: Scalar flux comparison for Reed's problem.

ir.library.oregonstate.edu/concern/graduate_thesis_or_dissertations/zs25xg841

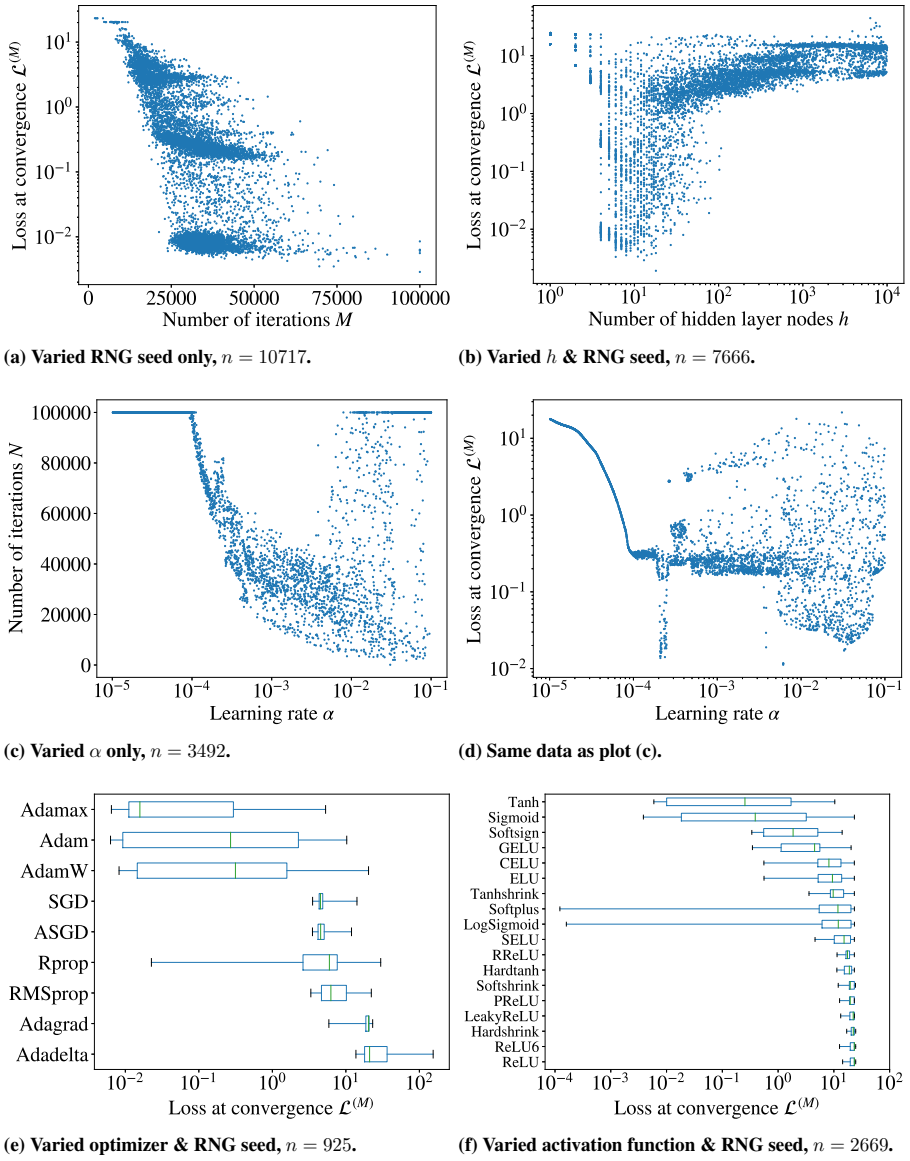
Kumar went deeper than we did

Table 1: Classification of hyperparameters.

Considered in this study	For future studies	Not applicable
RNG seed	Input vector size	Mini-batch size
Number of hidden layer nodes h	Number of hidden layers	Early stopping
Learning rate α	Optimizer-specific (eg β_1, β_2)	Dropout
Choice of optimizer	Regularization	
Choice of activation function	Initialization	
	Scaling inputs	

Hyp study found sensitivities to

- RNG seed (a-f)



(a) Varied RNG seed only, $n = 10717$.

(b) Varied h **& RNG seed,** $n = 7666$.

(c) Varied α **only,** $n = 3492$.

(d) Same data as plot (c).

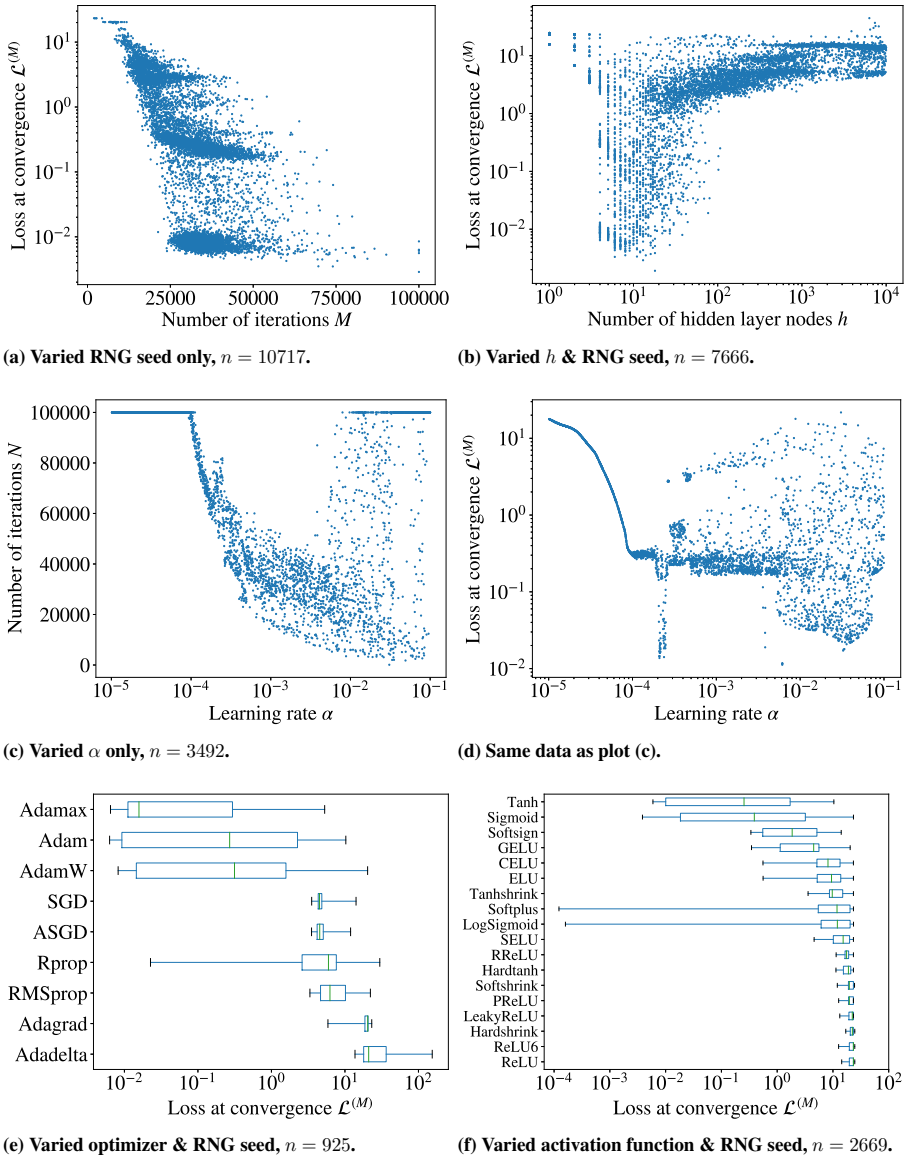
(e) Varied optimizer & RNG seed, $n = 925$.

(f) Varied activation function & RNG seed, $n = 2669$.

Figure 3: Hyperparameter study results for Problem 1.

Hyp study found sensitivities to

- RNG seed (a-f)
- Number of hidden layer nodes (b)



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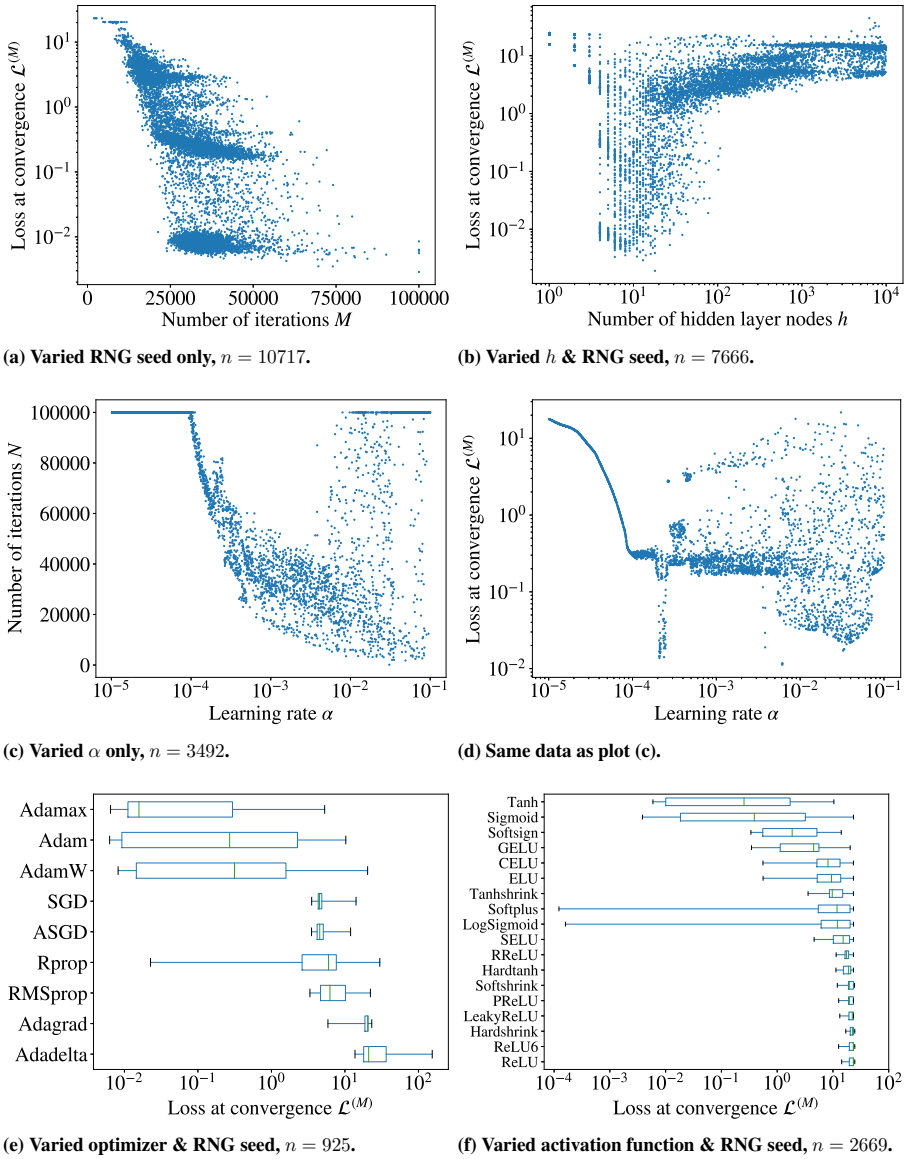

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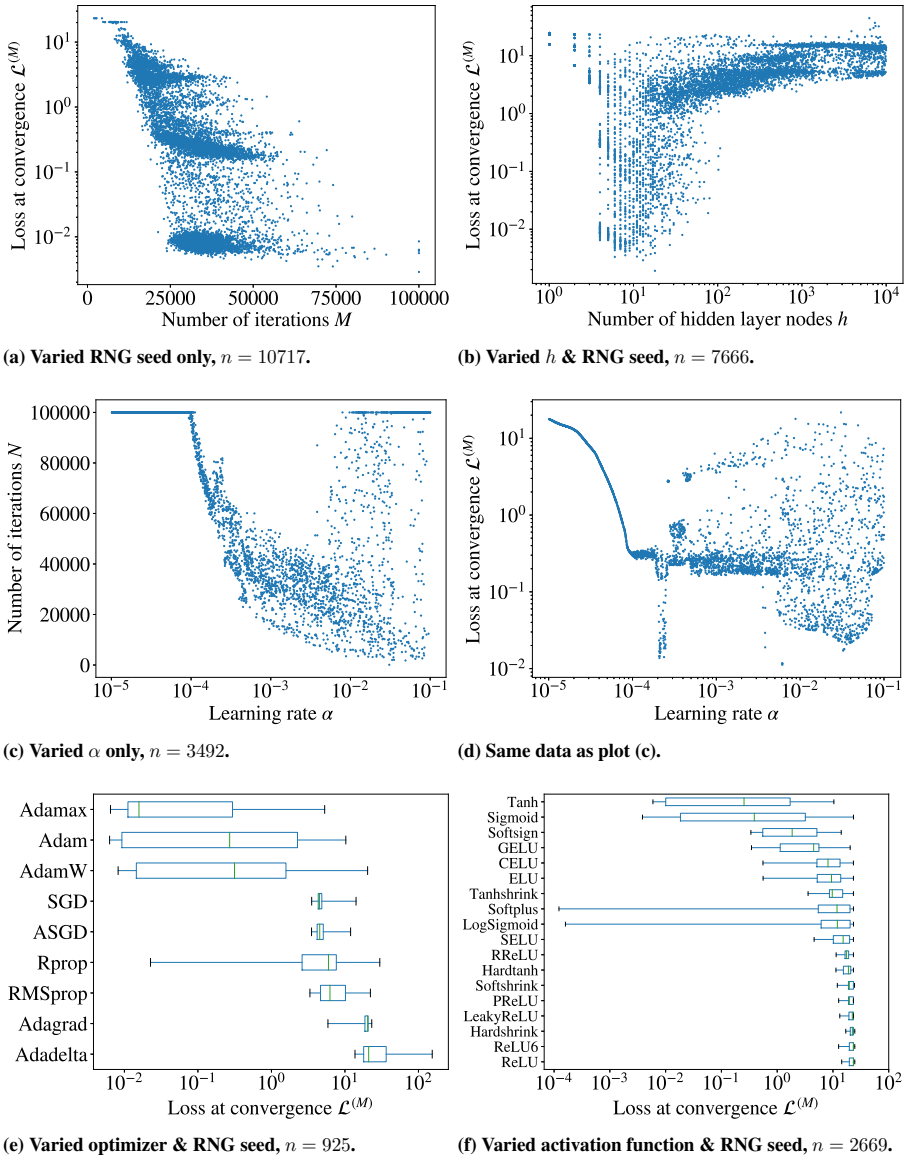

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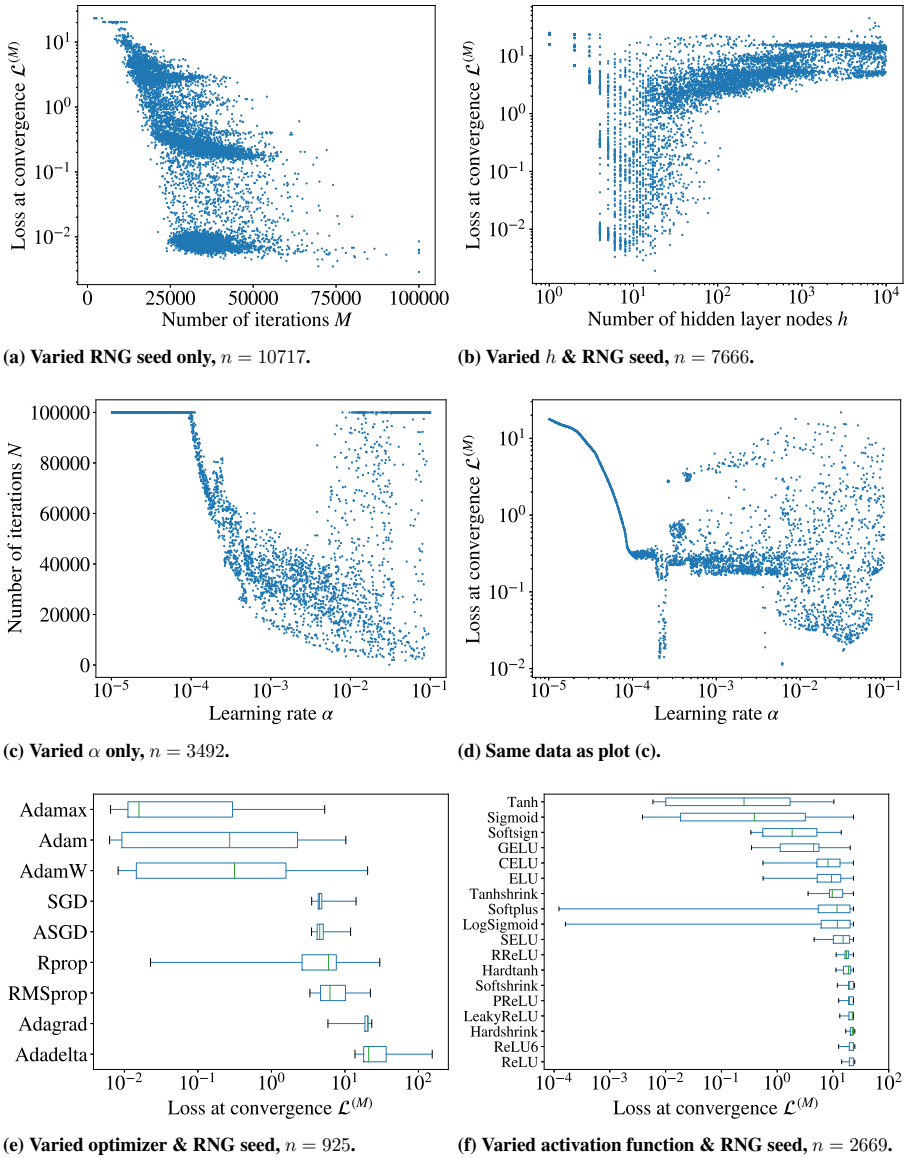

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Figure 3: Hyperparameter study results for Problem 1.

We observed a GPU slowdown

	Runtime	Slowdown
1 P9 core	2 min 3 sec	1x
V100 GPU	5 min 44 sec	2.8x

A bigger network could help

	Runtime	Slowdown
1 P9 core	2 min 3 sec	1x
V100 GPU	5 min 44 sec	2.8x

- NN is serial w.r.t. optim iters

  => available concurrency limited by:

  - Number of parameters
  - Number of training data points

AlexNet >> Narrows

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	Parameters	Training data
Narrows	34	50 scalars
AlexNet	60 million	1.2 million images

Kernel launch and runtime API overheads dominate execution

Table 2: Five most expensive GPU kernels per `nvprof`.

Time(%)	Time	Calls	Avg	Min	Max	Name
11.80	3.50177s	887996	3.9430us	3.8080us	5.1520us	_ZN2at6native6moder...
11.75	3.48571s	503200	6.9270us	4.9270us	10.272us	_ZN2at6native13redu...
8.42	2.49947s	680804	3.6710us	3.5830us	4.8640us	_ZN2at6native6moder...
7.24	2.14960s	266400	8.0690us	7.9360us	345.34us	volta_sgemm_32x32_s...
6.55	1.94456s	503200	3.8640us	3.7440us	5.0880us	_ZN2at6native6moder...

Table 3: Five most expensive CUDA runtime API calls per `nvprof`.

Time(%)	Time	Calls	Avg	Min	Max	Name
54.06	82.7777s	6127206	13.509us	10.640us	7.3316ms	cudaLaunchKernel
21.69	33.2049s	40848436	812ns	593ns	6.1128ms	cudaGetDevice
11.25	17.2308s	17997061	957ns	664ns	668.65us	cudaSetDevice
6.85	10.4897s	562472	18.649us	10.318us	49.983ms	cudaMemcpyAsync
1.90	2.91627s	7	416.61ms	10.307us	2.91571s	cudaMalloc

We have action items

Action items

- Add depth
  - Verify Kumar
- Run big (S32, 10k)
  - Reduce GPU slowdown

We have a wish list

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Wish list

- Performance
- Multigroup
- 2D
- Conservation
- Symmetry preservation

These are the paper authors

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- Symmetry preservation




References

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