

How to Train Better: Exploiting the Separability of Deep Neural Networks

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Dynamics and Discretization: PDEs, Sampling, and Optimization
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Collaborators for This Talk

Train Like a (Var)Pro



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slimTrain

Train Like a (Var)Pro: Efficient Training of Neural Networks with Variable Projection
To appear in SIMODS. [arXiv:2007.13171](https://arxiv.org/abs/2007.13171).
Code on [Meganet.m](https://meganet.m).

slimTrain – A Stochastic Approximation Method for Training Separable Deep Neural Networks
Submitted to SISC. [arXiv:2109.14002](https://arxiv.org/abs/2109.14002).
Code on [Meganet.m](https://meganet.m) and [slimTrain](https://slimtrain.com).

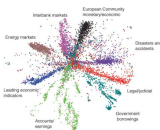
Deep Neural Networks are Great, But...

Classification



(Krizhevsky 2009)

Autoencoders



(Hinton and Salakhutdinov 2006)

GANS

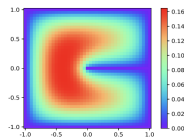
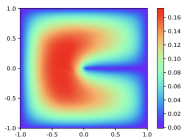


(Goodfellow et al. 2014)



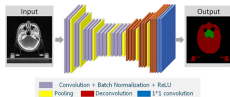
Recommender Systems
(Covington, Adams, and Sargin 2016)

Solving High-Dimensional PDEs



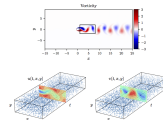
(E and Yu 2018; Han, Jentzen, and E 2018)

Segmentation



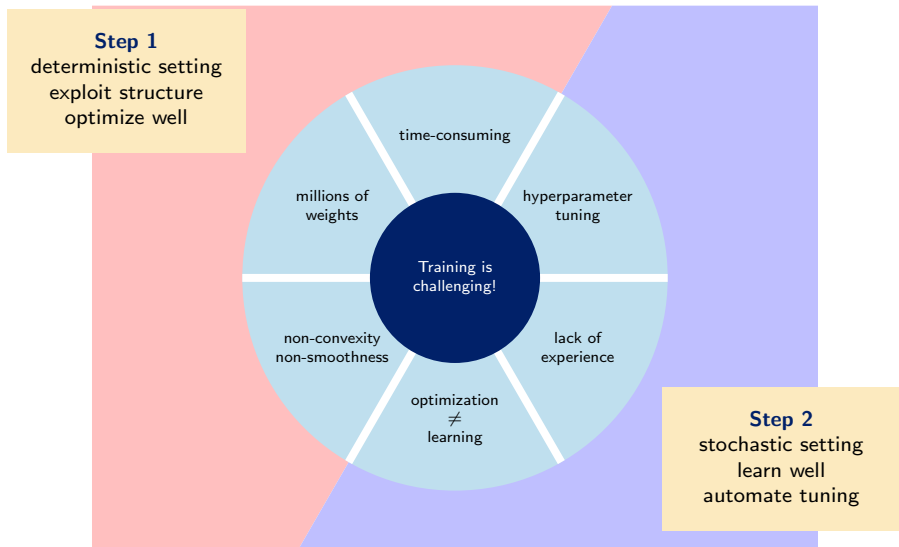
(Men et al. 2017)

PINNs

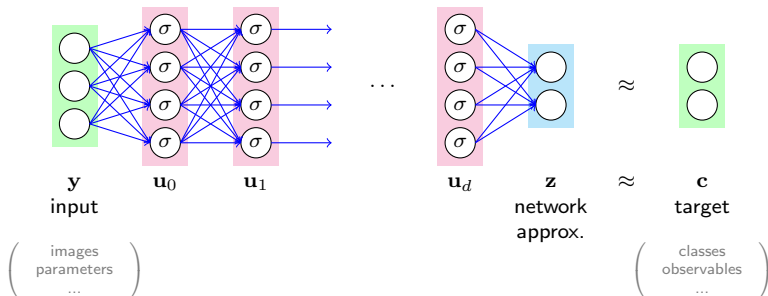


(Raissi, Perdikaris, and Karniadakis 2019)

Deep Neural Networks are Great, But...



Separable Deep Neural Networks



Goal: find weights (\mathbf{W}, θ) such that

$$\mathbf{W}F(\mathbf{y}, \theta) \approx \mathbf{c}$$

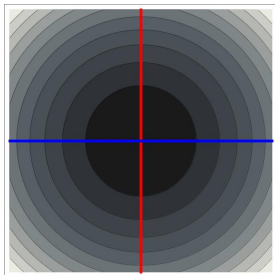
for all input-target pairs (\mathbf{y}, \mathbf{c}) by solving

$$\min_{\mathbf{W}, \theta} \Phi(\mathbf{W}, \theta) \equiv \underbrace{\mathbb{E} L(\mathbf{W}F(\mathbf{y}, \theta), \mathbf{c})}_{\text{loss}} + \underbrace{R(\theta) + S(\mathbf{W})}_{\text{regularization}}$$

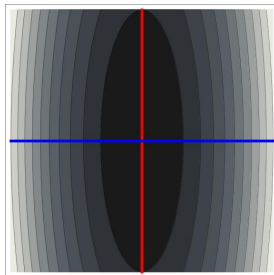
A Couple of Notes on Coupling

$$\min_{\mathbf{W}, \theta} \Phi(\mathbf{W}, \theta)$$

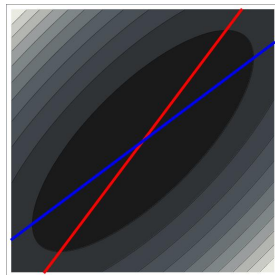
well-conditioned



ill-conditioned



coupled + ill-conditioned



— optimal \mathbf{W} for given θ
— optimal θ for given \mathbf{W}

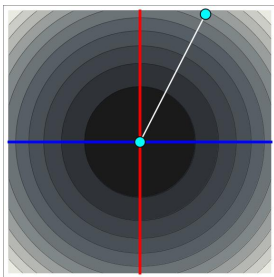
A Couple of Notes on Coupling

well-conditioned

$$\min_{\mathbf{W}, \theta} \Phi(\mathbf{W}, \theta)$$

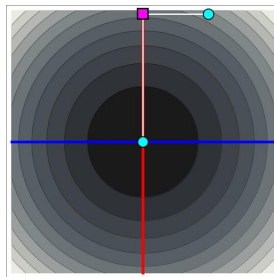
□ half step
● full step

gradient descent



$$(\mathbf{W}, \theta) \leftarrow (\mathbf{W}, \theta) - \gamma \nabla \Phi$$

alternating directions



$$\mathbf{W} \leftarrow \arg \min_{\mathbf{W}} \Phi(\mathbf{W}, \theta)$$

$$\theta \leftarrow \arg \min_{\theta} \Phi(\mathbf{W}, \theta)$$

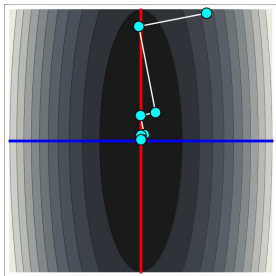
A Couple of Notes on Coupling

ill-conditioned

$$\min_{\mathbf{W}, \theta} \Phi(\mathbf{W}, \theta)$$

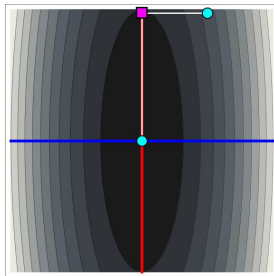
□ half step
● full step

gradient descent



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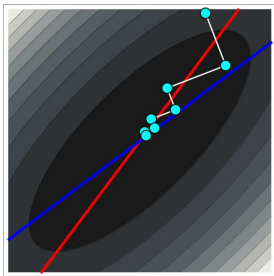
A Couple of Notes on Coupling

coupled + ill-conditioned

$$\min_{\mathbf{W}, \theta} \Phi(\mathbf{W}, \theta)$$

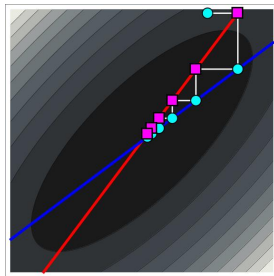
□ half step
● full step

gradient descent



$$(\mathbf{W}, \theta) \leftarrow (\mathbf{W}, \theta) - \gamma \nabla \Phi$$

alternating directions



$$\mathbf{W} \leftarrow \arg \min_{\mathbf{W}} \Phi(\mathbf{W}, \theta)$$

$$\theta \leftarrow \arg \min_{\theta} \Phi(\mathbf{W}, \theta)$$

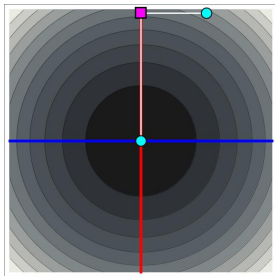
A Couple of Notes on Coupling

updating
with coupling

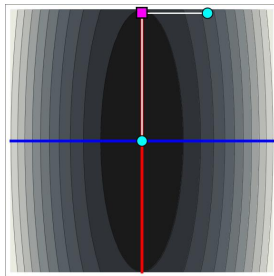
$$\min_{\mathbf{W}, \theta} \Phi(\mathbf{W}, \theta)$$

□ half step
● full step

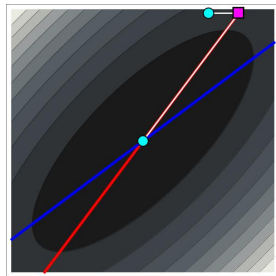
well-conditioned



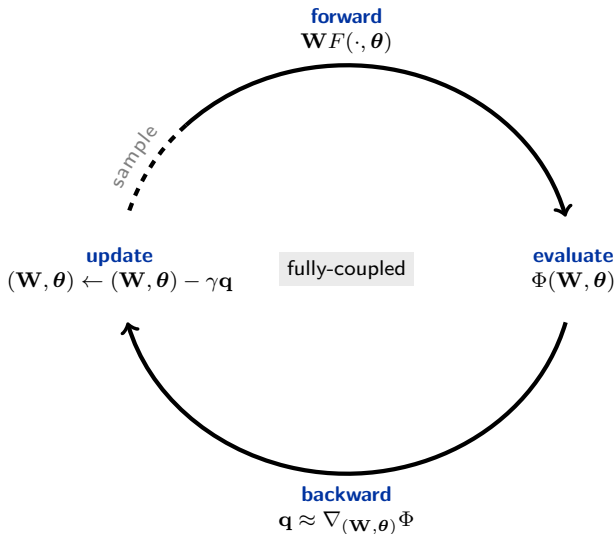
ill-conditioned



coupled + ill-conditioned



The Training Cycle



Two Schools of Training

Sample Average Approximation (SAA)

(Kleywegt, Shapiro, and Mello 2002; Linderth, Shapiro, and Wright 2006)

$$\min_{\mathbf{W}, \theta} \frac{1}{|\mathcal{T}|} \sum_{(\mathbf{y}, \mathbf{c}) \in \mathcal{T}} L(\mathbf{W}F(\mathbf{y}, \theta), \mathbf{c}) + \text{reg.}$$

- ☺ Deterministic
- ☺ Parallelizable
- ☹ Proclivity to overfit
- ☹ Expensive memory-wise

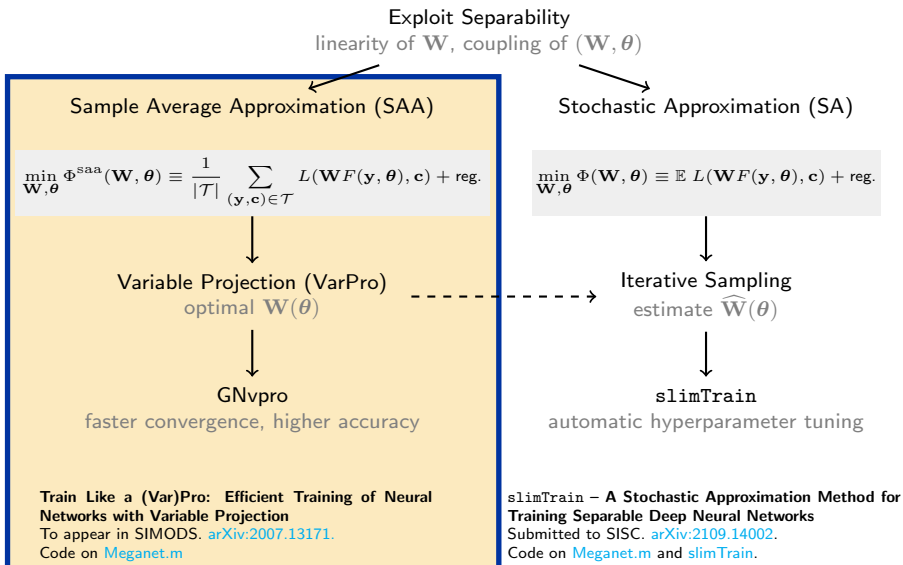
Stochastic Approximation (SA)

(Nemirovski et al. 2009; Robbins and Monro 1951)

$$\min_{\mathbf{W}, \theta} \mathbb{E} L(\mathbf{W}F(\mathbf{y}, \theta), \mathbf{c}) + \text{reg.}$$

- ☺ Memory-efficient
- ☺ Generalization
- ☹ Sensitive to hyperparameters
- ☹ Slow to converge (Agarwal et al. 2012)

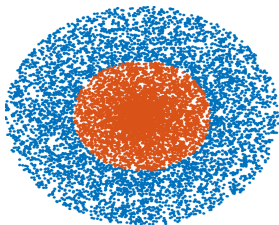
Roadmap to Better Training



Geometric Intuition for Variable Projection (VarPro)

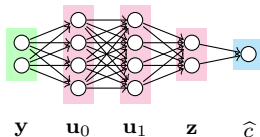
inputs

$$\{\mathbf{y}^{(1)}, \dots, \mathbf{y}^{(|\mathcal{T}|)}\} \subset \mathbb{R}^2$$



outputs

$$\{\mathbf{z}^{(1)}, \dots, \mathbf{z}^{(|\mathcal{T}|)}\} \subset \mathbb{R}^2$$



$$\mathbf{u}_0 = \sigma(\mathbf{K}_0 \mathbf{y} + \mathbf{b}_0) \quad \in \mathbb{R}^4$$

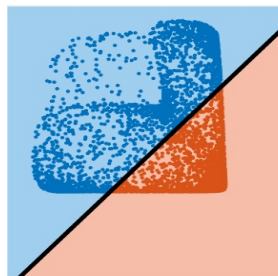
$$\mathbf{u}_1 = \sigma(\mathbf{K}_1 \mathbf{u}_0 + \mathbf{b}_1) \quad \in \mathbb{R}^4$$

$$\mathbf{z} = \sigma(\mathbf{K}_2 \mathbf{u}_1 + \mathbf{b}_2) \quad \in \mathbb{R}^2$$

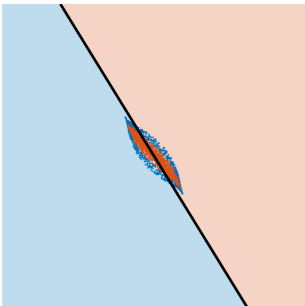
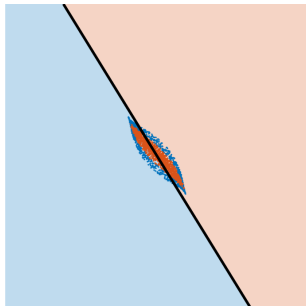
$$\hat{c} = \mathbf{W} \mathbf{z} \quad \in \mathbb{R}$$

outputs

$$\{c^{(1)}, \dots, c^{(|\mathcal{T}|)}\} \subset \{0, 1\}$$



Geometric Intuition for Variable Projection (VarPro)

network weights \mathbf{W} optimal $\mathbf{W}(\theta)$ 

Variable Projection

SAA Full Optimization Problem

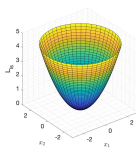
$$\min_{\mathbf{W}, \theta} \Phi^{\text{saa}}(\mathbf{W}, \theta) \equiv \frac{1}{|\mathcal{T}|} \sum_{(\mathbf{y}, \mathbf{c}) \in \mathcal{T}} L(\mathbf{W}F(\mathbf{y}, \theta), \mathbf{c}) + R(\theta) + S(\mathbf{W})$$

Reduced Optimization Problem

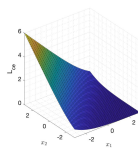
$$\min_{\theta} \Phi_{\text{red}}^{\text{saa}}(\theta) \equiv \Phi^{\text{saa}}(\mathbf{W}(\theta), \theta) \quad \text{s.t.} \quad \mathbf{W}(\theta) = \arg \min_{\mathbf{W}} \Phi^{\text{saa}}(\mathbf{W}, \theta)$$

Assume $\Phi^{\text{saa}}(\mathbf{W}, \theta)$ is smooth and strictly convex in the first argument.

Least Squares Loss



Cross Entropy Loss



Use **Newton-Krylov Trust Region Method** to solve for $\mathbf{W}(\theta)$ to high accuracy.

Optimizing θ : Gauss-Newton-Krylov VarPro (GNvpro)

Reduced Optimization Problem

$$\min_{\theta} \Phi_{\text{red}}^{\text{saa}}(\theta) \equiv \frac{1}{|\mathcal{T}|} \sum_{(\mathbf{y}, \mathbf{c}) \in \mathcal{T}} L(\mathbf{W}(\theta)F(\mathbf{y}, \theta), \mathbf{c}) + R(\theta) + S(\mathbf{W}(\theta))$$

First-Order Methods: Update $\theta \leftarrow \theta - \gamma \mathbf{p}$ where $\mathbf{p} \approx \nabla \Phi_{\text{red}}^{\text{saa}}(\theta)$

$$\nabla_{\mathbf{W}} \Phi^{\text{saa}}(\mathbf{W}(\theta), \theta) = \mathbf{0} \implies \nabla_{\theta} \Phi_{\text{red}}^{\text{saa}}(\theta) = \nabla_{\theta} \Phi^{\text{saa}}(\mathbf{W}(\theta), \theta)$$

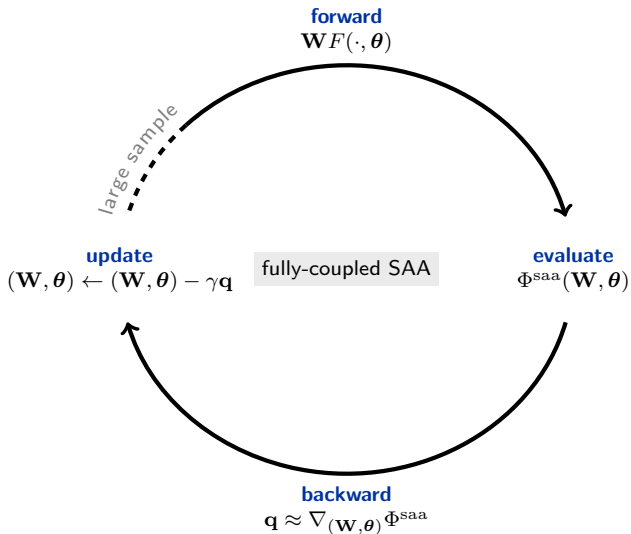
Gauss-Newton-Krylov Trust Region Method: Update $\theta_{\text{trial}} = \theta^{(k)} + \mathbf{p}$

$$\min_{\mathbf{p}} \nabla_{\theta} \Phi_{\text{red}}^{\text{saa}}(\theta^{(k)})^{\top} \mathbf{p} + \frac{1}{2} \mathbf{p}^{\top} \nabla_{\theta}^2 \Phi_{\text{red}}^{\text{saa}}(\theta^{(k)}) \mathbf{p} \quad \text{s. t.} \quad \|\mathbf{p}\| \leq \Delta^{(k)}$$

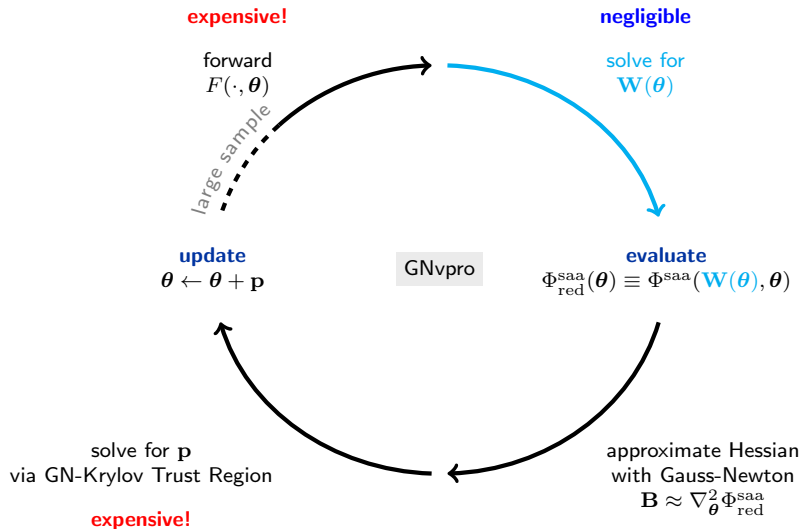
Approximate the Hessian by

$$\nabla_{\theta}^2 \Phi_{\text{red}}^{\text{saa}}(\theta) \approx J_{\theta}(\mathbf{W}(\theta)F(\mathbf{y}, \theta))^{\top} \nabla^2 L J_{\theta}(\mathbf{W}(\theta)F(\mathbf{y}, \theta)) + \nabla^2 R$$

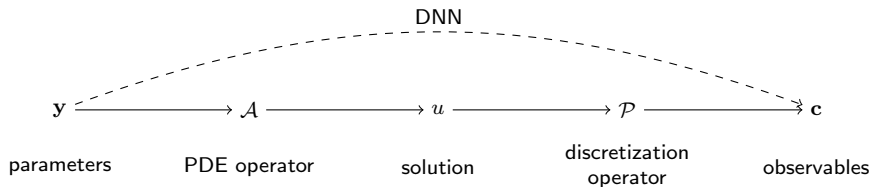
Train Like a (Var)Pro



Train Like a (Var)Pro



PDE Surrogate Modeling



$$c = \mathcal{P}u \quad \text{subject to} \quad \mathcal{A}(u; \mathbf{y}) = 0$$

PDEs and Network Architectures:

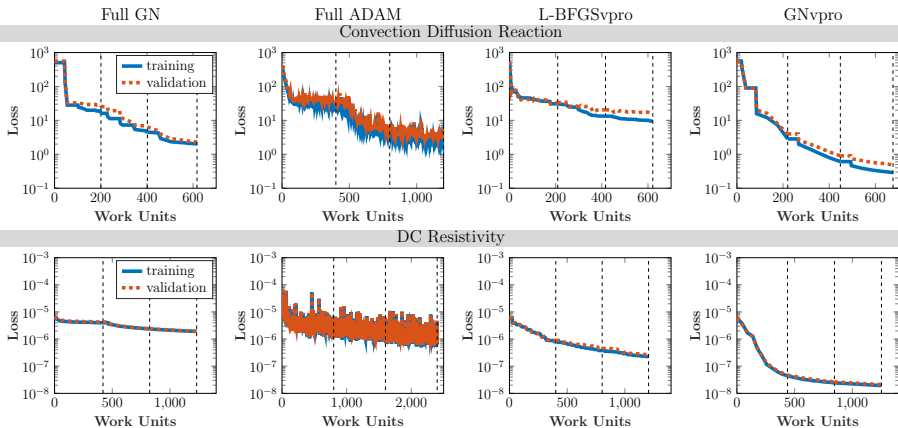
- Convection Diffusion Reaction: ([Grasso and Innocente 2018](#); [Choquet and Comte 2017](#))

$$\mathbf{y} \in \mathbb{R}^{55} \rightarrow \underbrace{\mathbb{R}^8 \rightarrow \dots \rightarrow \mathbb{R}^8}_d \rightarrow \mathbb{R}^{72} \ni \mathbf{c}$$

- Direct Current Resistivity: ([Seidel and Lange 2007](#); [Dey and Morrison 1979](#))

$$\mathbf{y} \in \mathbb{R}^3 \rightarrow \underbrace{\mathbb{R}^{16} \rightarrow \dots \rightarrow \mathbb{R}^{16}}_d \rightarrow \mathbb{R}^{882} \ni \mathbf{c}$$

PDE Surrogate Modeling

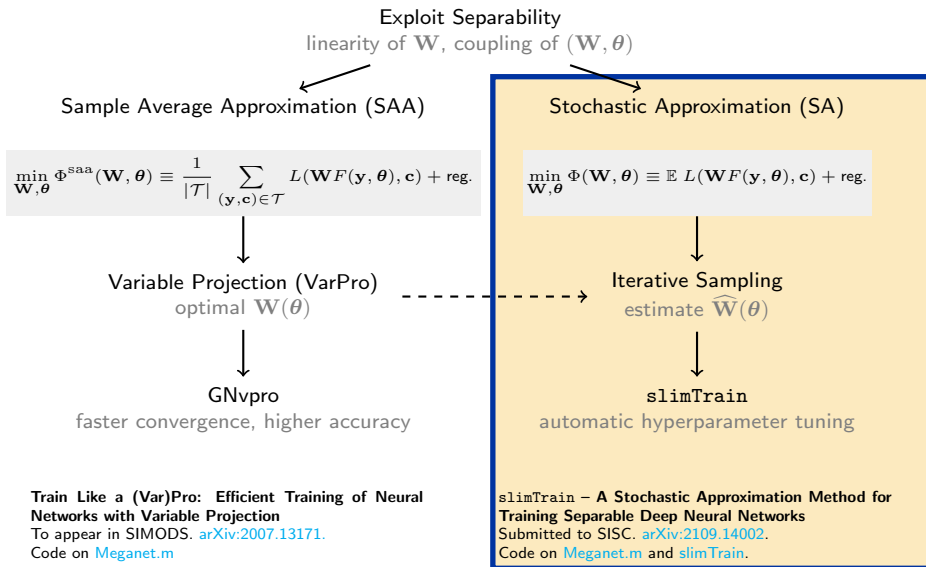


Work Units = number of forward and backward passes through network

SGD: 2 work units per epoch (1 forward pass, 1 backward pass)

GNvpro: 2 work units + $2r$ work units for rank- r approx. to $\nabla_{\theta}^2 \Phi_{\text{red}}$ per iteration

Roadmap to Better Training



Does VarPro Extend to Stochastic Approximation?

Consider the reduced *stochastic* optimization problem

$$\begin{aligned} \min_{\boldsymbol{\theta}} \Phi_{\text{red}}(\boldsymbol{\theta}) &\equiv \Phi(\widehat{\mathbf{W}}(\boldsymbol{\theta}), \boldsymbol{\theta}) \\ \text{s. t. } \widehat{\mathbf{W}}(\boldsymbol{\theta}) &= \arg \min_{\mathbf{W}} \Phi(\mathbf{W}, \boldsymbol{\theta}). \end{aligned}$$

Key Idea of SA: use minibatches $\mathcal{T}_k \subset \mathcal{T}$ to update $\boldsymbol{\theta}$

Key Ingredient: need an unbiased derivative estimate of $\boldsymbol{\theta}$

$$\mathbb{E} (D_{\boldsymbol{\theta}} \Phi_{\text{red},k}(\boldsymbol{\theta})) = D_{\boldsymbol{\theta}} \Phi_{\text{red}}(\boldsymbol{\theta}) \quad \Phi_{\text{red},k} \approx \Phi_{\text{red}} \text{ using } \mathcal{T}_k$$

Proof:

$$\mathbb{E} (D_{\boldsymbol{\theta}} \Phi_{\text{red},k}(\boldsymbol{\theta})) = \underbrace{\mathbb{E} \left([D_{\mathbf{W}} \Phi_k(\mathbf{W}, \boldsymbol{\theta})]_{\mathbf{W}=\widehat{\mathbf{W}}(\boldsymbol{\theta})} \right)}_{=0} D_{\boldsymbol{\theta}} \widehat{\mathbf{W}}(\boldsymbol{\theta}) + \underbrace{\mathbb{E} \left([D_{\tilde{\boldsymbol{\theta}}} \Phi_k(\widehat{\mathbf{W}}(\boldsymbol{\theta}), \tilde{\boldsymbol{\theta}})]_{\tilde{\boldsymbol{\theta}}=\boldsymbol{\theta}} \right)}_{D_{\boldsymbol{\theta}} \Phi_{\text{red}}(\boldsymbol{\theta})}$$

In practice, use an effective iterative scheme to estimate $\widehat{\mathbf{W}}(\boldsymbol{\theta})$ and reduce bias.

Exploiting Separability with Iterative Sampling

Consider the stochastic least-squares problem with Tikhonov regularization

$$\min_{\mathbf{w}, \boldsymbol{\theta}} \Psi(\mathbf{w}, \boldsymbol{\theta}) \equiv \mathbb{E} \frac{1}{2} \|\mathbf{A}(\mathbf{y}, \boldsymbol{\theta})\mathbf{w} - \mathbf{c}\|_2^2 + \frac{1}{2} \alpha \|\mathbf{L}\boldsymbol{\theta}\|_2^2 + \frac{1}{2} \lambda \|\mathbf{w}\|_2^2$$

Iterative Sampling for \mathbf{w}

(Chung et al. 2020; Slagel et al. 2019; Chung, Chung, and Slagel 2019)

$$\mathbf{w}_k = \mathbf{w}_{k-1} - \mathbf{s}_k(\boldsymbol{\theta}_{k-1})$$

SGD Variant for $\boldsymbol{\theta}$

(Kingma and Ba 2014; Chen et al. 2021; Yao et al. 2020; Duchi, Hazan, and Singer 2011)

$$\boldsymbol{\theta}_k = \boldsymbol{\theta}_{k-1} - \gamma \mathbf{p}_k(\mathbf{w}_k)$$

Why Iterative Sampling?

- 😊 known convergence properties
- 😊 incorporate global curvature information (challenging in SA (Bottou and Cun 2004; Gower and Richtárik 2017; Byrd et al. 2016; Wang et al. 2017; Chung et al. 2017))
- 😊 no learning rate
- 😊 adaptive choice of regularization parameter

Sampled Limited-Memory Tikhonov (slimTik)

$$\min_{\mathbf{w}} \mathbb{E} \frac{1}{2} \|\mathbf{A}(\mathbf{y}, \boldsymbol{\theta}_{k-1})\mathbf{w} - \mathbf{c}\|_2^2 + \frac{1}{2} \lambda \|\mathbf{w}\|_2^2.$$

At iteration k , update linear weights by

$$\mathbf{w}_k = \mathbf{w}_{k-1} - \underbrace{\mathbf{B}_k \mathbf{g}_k(\mathbf{w}_{k-1})}_{\mathbf{s}_k(\Lambda_k)}$$

Local Gradient Information (batch k)

$$\mathbf{g}_k(\mathbf{w}_{k-1}) = \mathbf{A}_k^\top (\mathbf{A}_k \mathbf{w}_{k-1} - \mathbf{c}_k) + \Lambda_k \mathbf{w}_{k-1}$$

Global Curvature Information (all batches)

$$\mathbf{B}_k = \left((\Lambda_k + \sum_{i=1}^{k-1} \Lambda_i) \mathbf{I} + \sum_{i=k-r}^k \mathbf{A}_i^\top \mathbf{A}_i \right)^{-1}$$

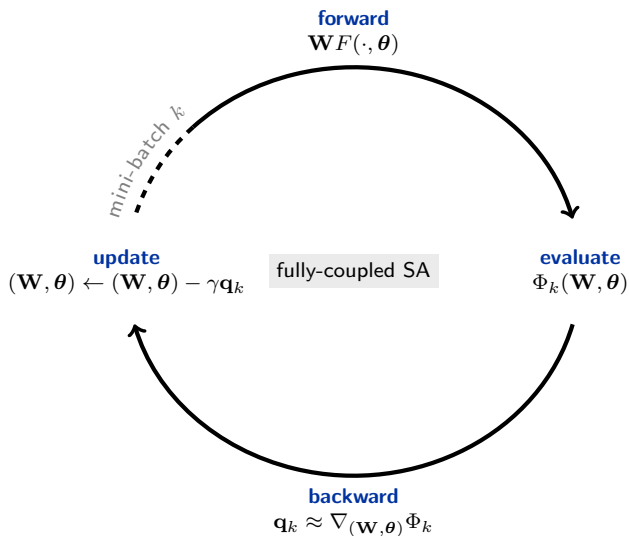
$\mathbf{A}_j(\boldsymbol{\theta}_{j-1})$: output features for batch j

\mathbf{c}_j : target features for batch j

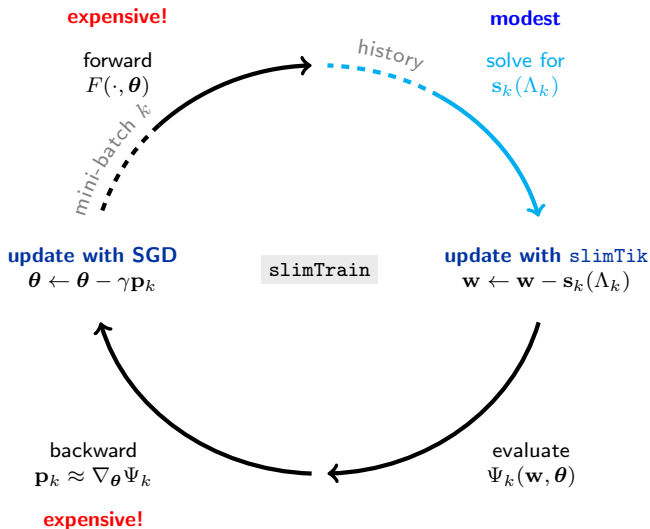
Λ_j : (optimal) reg. parameter for batch j

- ☺ Use sampled regularization parameter selection methods (e.g., sGCV) to choose Λ_k .
- ☹ Curvature information depends on older $\boldsymbol{\theta}$ iterates.
- ☺ Use **sampled limited-memory Tikhonov (slimTik)** with memory depth $r \in \mathbb{N}_0$.

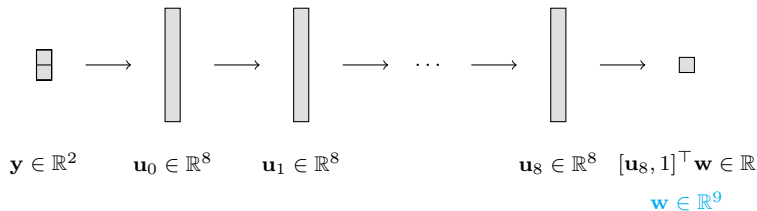
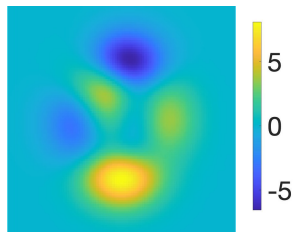
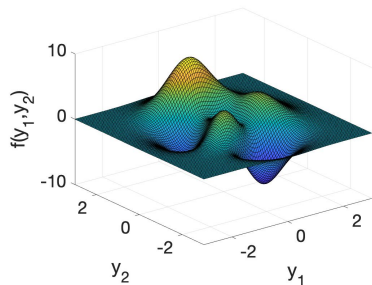
slimTrain: Sampled Limited-Memory Training



slimTrain: Sampled Limited-Memory Training

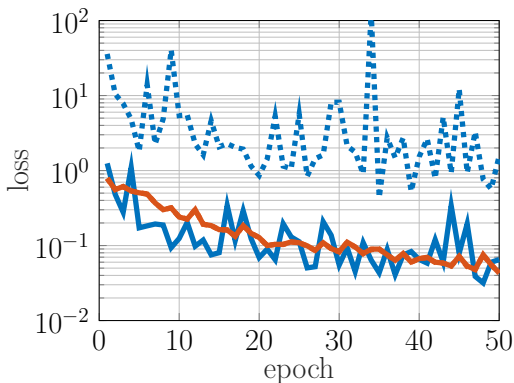


Function Approximation: Peaks

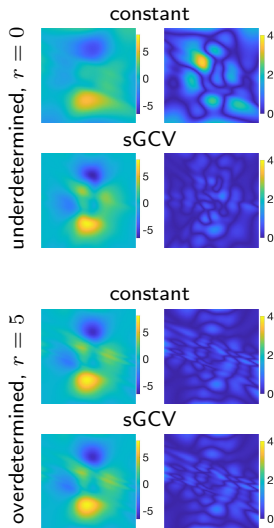


Function Approximation: Peaks

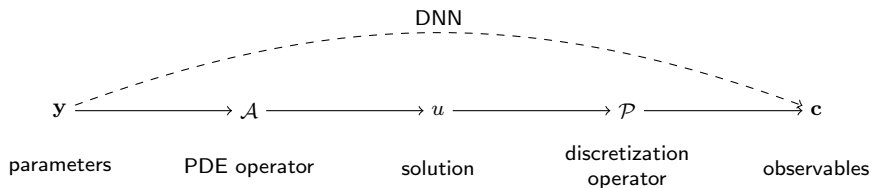
batch size = 5, $\gamma = 10^{-3}$, $\lambda = 10^{-10}$



●●● slimTrain, constant: $r = 0$	— slimTrain, sGCV: $r = 0$
●●● slimTrain, constant: $r = 5$	— slimTrain, sGCV: $r = 5$



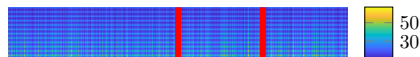
PDE Surrogate Modeling: CDR



$$c = \mathcal{P}u \quad \text{subject to} \quad \mathcal{A}(u; \mathbf{y}) = 0$$

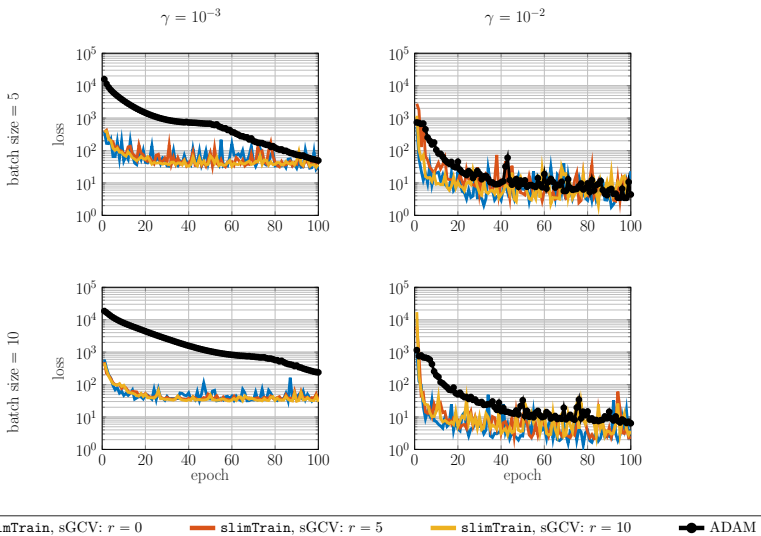
Convection Diffusion Reaction: ([Grasso and Innocente 2018](#); [Choquet and Comte 2017](#))

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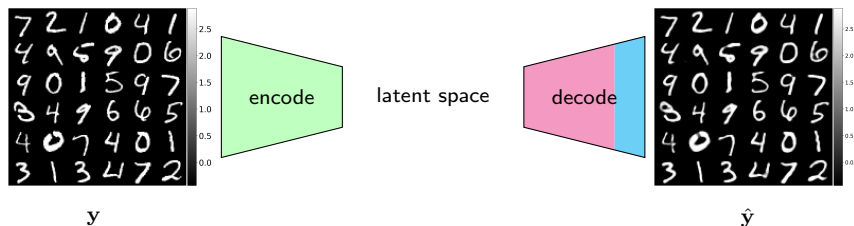


observables

PDE Surrogate Modeling: CDR



Dimensionality Reduction: Autencoder



Goal: Train two networks such that $\hat{\mathbf{y}} \approx \mathbf{y}$ for all inputs \mathbf{y} .

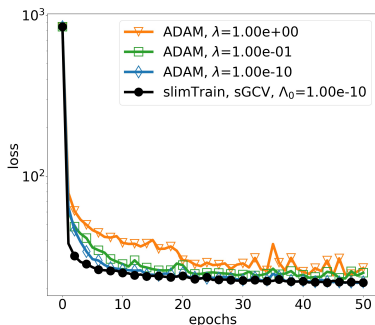
$$\min_{\mathbf{w}, \boldsymbol{\theta}_{\text{dec}}, \boldsymbol{\theta}_{\text{enc}}} \mathbb{E} \frac{1}{2} \|\mathbf{K}(\mathbf{w}) F_{\text{dec}}(F_{\text{enc}}(\mathbf{y}, \boldsymbol{\theta}_{\text{enc}}), \boldsymbol{\theta}_{\text{dec}}) - \mathbf{y}\|_2^2 + \text{reg.}$$

Final Layer: $\mathbf{K}(\mathbf{w})$ is a (transposed) convolutional operator

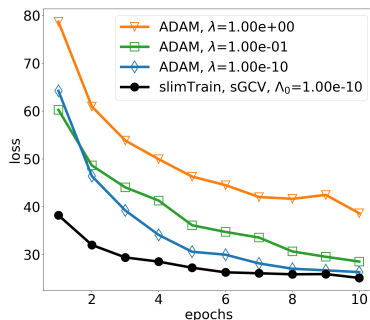
Dimensionality Reduction: Autencoder

Full Data Regime: 50,000 training images

Initial evaluation + full 50 epochs

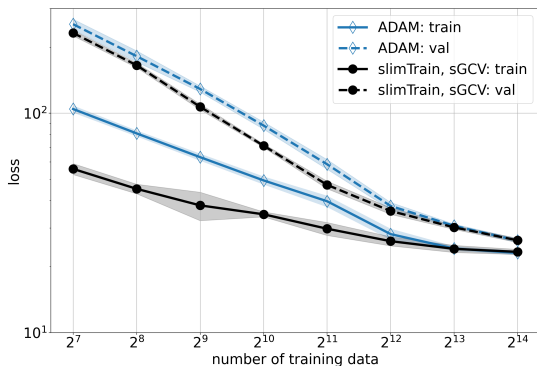


Epochs 1 to 10



Dimensionality Reduction: Autencoder

Limited Data Regime: best loss in 50 epochs



Wrapping Up

Exploiting separability makes DNN training easier!

GNvpro...

- accelerates training to high accuracy
- can be applied to non-quadratic loss functions

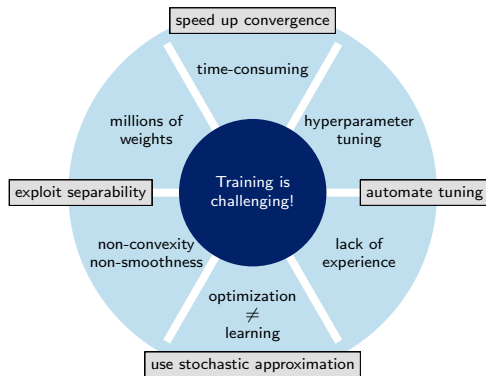
slimTrain...

- automates regularization parameter selection
- can outperform ADAM with recommended settings and with limited data

Train Like a (Var)Pro: Efficient Training of Neural Networks with Variable Projection

To appear in SIMODS. [arXiv:2007.13171](https://arxiv.org/abs/2007.13171).

Code on [Meganet.m](https://meganet.m).



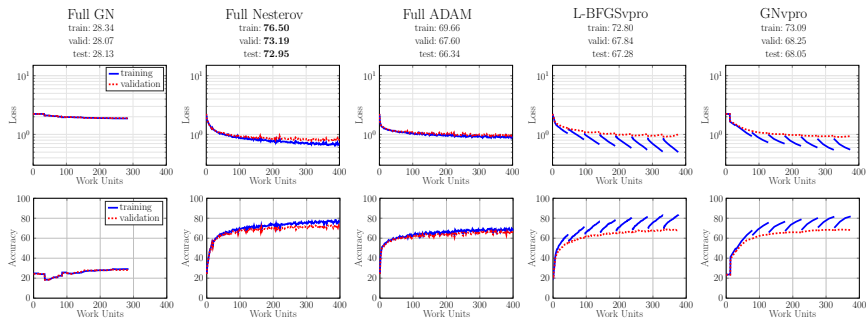
slimTrain – A Stochastic Approximation Method for Training Separable Deep Neural Networks

Submitted to SISC. [arXiv:2109.14002](https://arxiv.org/abs/2109.14002).

Code on [Meganet.m](https://meganet.m) and slimTrain.

Thanks for Listening! For more Q&A, please reach out to elizabeth.newman@emory.edu and lruthotto@emory.edu

Image Classification: CIFAR-10



$$\mathbf{y} \in \mathbb{R}^{32 \times 32 \times 3} \xrightarrow{\substack{5 \times 5 \\ \text{conv}}} \mathbb{R}^{32 \times 32 \times 32} \xrightarrow{\substack{2 \times 2 \\ \text{pool}}} \mathbb{R}^{16 \times 16 \times 32} \xrightarrow{\substack{5 \times 5 \\ \text{conv}}} \mathbb{R}^{16 \times 16 \times 64} \xrightarrow{\substack{16 \times 16 \\ \text{pool}}} \mathbb{R}^{64} \longrightarrow \mathbb{R}^{10} \ni \mathbf{c}$$

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