Unsupervised Neural Network Methods for Solving Differential Equations

Learning the Loss Function & Sampling Strategies

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Table of Contents

Table of Contents

Differential Equations

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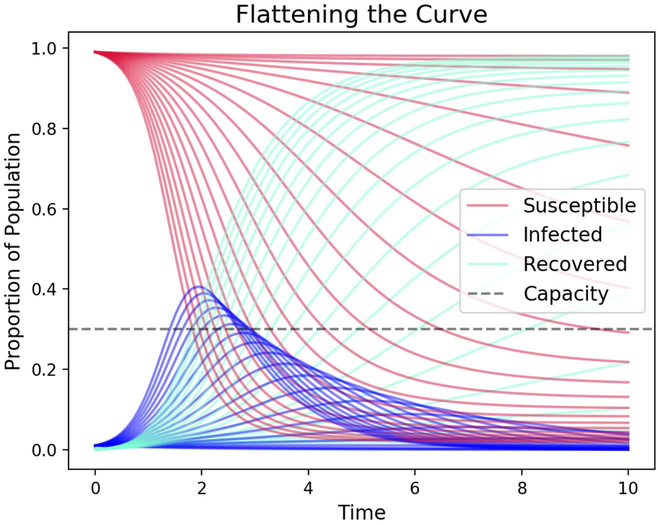
- They relate quantities to rates of change (i.e. derivatives)
- Applied to physics, chemistry, biology, engineering, economics
- However, equations of practical interest are generally not analytically solvable
- Instead, numerical methods compute approximate solutions over a discrete mesh or grid

Example: Fluid Flow

Credit: Pavel Dobryakov

https://paveldogreat.github.io/WebGL-Fluid-Simulation/

Example: Infectious Disease



Why Neural Networks?

Traditional numerical methods perform well and the theory for stability and convergence is well-established. Why use neural networks? Some potential advantages:

- Remove reliance on finely-crafted grids which suffer the "curse of dimensionality"; can be more tractable in high-dimensional settings (Sirignano & Spiliopoulos, 2018; Raissi, 2018; Han et al., 2017)

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- Can more precisely obey certain constraints, such as conservation of energy (Mattheakis et al., 2020)
- Embarassingly data-parallel, even in temporal dimensions; more readily parallelizable for computational speedup

Table of Contents

Artificial Neural Networks

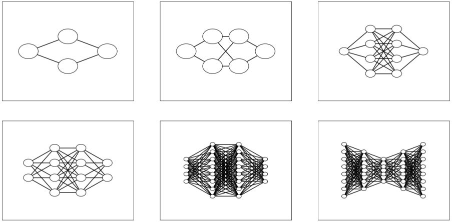
Parametric models loosely based on the human brain. Sequence of affine transformations followed by activation functions:

$$y = f_{\text{layer}_n}\left(f_{\text{layer}_{n-1}}\left(\ldots\left(f_{\text{layer}_1}(x)\right)\ldots\right)\right)$$

where

$$f_{\text{layer}_i}(x) = \sigma\left(W_i^T x + b_i\right) \forall i \in [1, \ldots n]$$

with $\sigma(\cdot) = \tanh(\cdot)$, for example.



Unsupervised Neural Networks for Differential Equations

Lagaris et al. (1998) proposed solving differential equations in an unsupervised manner with neural networks. Consider differential equations of the form

$$F(x, \Psi(x), \Delta\Psi(x), \Delta^2\Psi(x)) = 0. \tag{1}$$

The learning problem is formulated as minimizing the sum of squared errors (i.e. residuals) of the above equation

$$\min_{\theta} \sum_{x \in D} F(x, \Psi_\theta(x), \Delta\Psi_\theta(x), \Delta^2\Psi_\theta(x))^2 \tag{2}$$

where Ψ_θ is a neural network parameterized by θ, and $\Psi_\theta(x)$ yields predicted solutions.

Adjusting for Constraints

Mattheakis et al. (2019) consider adjusting the neural network solution $N(t)$ to satisfy the initial condition $N(t_0) = x_0$. This is achieved by applying the transformation

$$\tilde{N}(t) = x_0 + \left(1 - e^{-(t - t_0)}\right) N(t) \tag{3}$$

Intuitively, this adjusts the output of the neural network $N(t)$ to be exactly x_0 when $t = t_0$, and decays this constraint exponentially in t. We apply this adjustment throughout to satisfy initial and boundary conditions.

Example: Simple Harmonic Oscillator

Consider the motion $x(t)$ of an oscillating body (e.g. a mass on a frictionless spring) given by

$$\ddot{x}(t) + x(t) = 0 \tag{4}$$

with initial conditions $x_0 = 0$ and $\dot{x}_0 = 1$.[1] We optimize

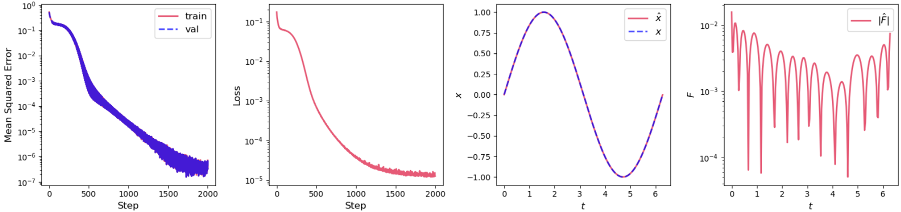
$$\min_{\theta} \sum_{t \in T} \left(\hat{\ddot{x}}_\theta(t) + \hat{x}_\theta(t) \right)^2 \tag{5}$$

to train the model, where $\hat{x}_\theta(t)$ is the output of the neural network.

[1] Exact analytical solution $x(t) = sin(t)$

Example: Simple Harmonic Oscillator

A two hidden layer network composed of 30 units per layer solves this problem to a high degree of accuracy (low mean squared error).



For more detail on this classical unsupervised neural network approach, see e.g. Lagaris et al. (1998); Mattheakis et al. (2019).

Table of Contents

Motivation

- Classical setting of data following a Gaussian noise model

$$y = x + \epsilon, \quad \epsilon \sim N(0, \sigma^2) \tag{6}$$

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- Deterministic differential equations, with no noise model, have no such justification. To circumvent this we propose *learning the loss function* with Generative Adversarial Networks (GANs)
- Moreover, GANs have been shown to excel in scenarios where classic loss functions struggle (Larsen et al., 2015; Ledig et al., 2016; Karras et al., 2018)

Generative Adversarial Networks (GANs)

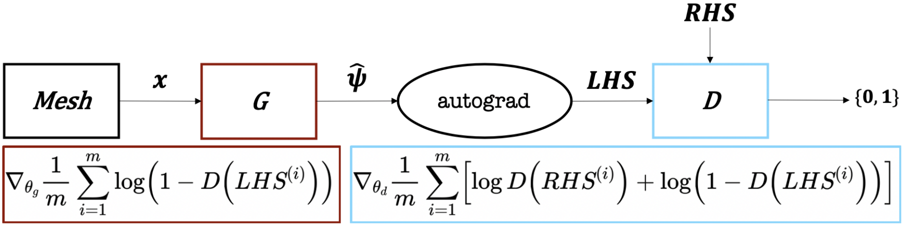
Goodfellow et al. (2014) introduced GANs as a two player game between a generator G and discriminator D such that the generator attempts to trick the discriminator to classify "fake" samples as "real". Formally, one optimizes the minimax objective

$$\min_G \max_D V(D, G) = \mathbb{E}_{x \sim p_{\text{data}}(x)}[\log D(x)] + \mathbb{E}_{z \sim p_z(z)}[1 - \log D(G(z))] \quad (7)$$

where $x \sim p_{\text{data}}(x)$ denotes samples from the empirical data distribution and $p_z \sim \mathcal{N}(0, 1)$ samples in latent space. In practice, the optimization alternates between gradient ascent and descent steps for D and G respectively.

Differential Equation GAN (DEQGAN)

Separate equation into left-hand side *LHS* and right-hand side *RHS*, and set *LHS* as the “fake” component and *RHS* as “real”. DEQGAN learns to approximately solve the equation by setting $LHS = RHS$.



DEQGAN Algorithm

Algorithm 1 DEQGAN

Input: Differential equation F, generator $G(\cdot;\theta_g)$, discriminator $D(\cdot;\theta_d)$, mesh x of m elements with spacing d, initial/boundary condition adjustment ϕ, learning rates α_G, α_D, Adam moment coefficients $\beta_{G1}, \beta_{G2}, \beta_{D1}, \beta_{D2}$

for $i = 1$ **to** N **do**

    Sample m points $x_s \sim x + \mathcal{N}(0, \frac{d}{3})$

    Forward pass $\hat{\psi} = G(x_s)$

    Adjust for conditions $\hat{\psi}' = \phi(\hat{\psi})$

    Set $LHS = F(x, \hat{\psi}', \nabla\hat{\psi}', \nabla^2\hat{\psi}')$, $RHS = \mathbf{0}$

    Update generator $\theta_g \leftarrow Adam(\theta_g, \alpha_G, -\eta_G, \beta_{G1}, \beta_{G2})$

    Update discriminator $\theta_d \leftarrow Adam(\theta_d, \alpha_D, \eta_D, \beta_{D1}, \beta_{D2})$

end for

Return G

Extensions to Traditional GANs

- Two Time-Scale Update Rule (TTUR): discriminator and generator trained with separate learning rates; in some cases, TTUR ensures convergence to a stable local Nash equilibrium (Heusel et al., 2017)

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- Two Time-Scale Update Rule (TTUR): discriminator and generator trained with separate learning rates; in some cases, TTUR ensures convergence to a stable local Nash equilibrium (Heusel et al., 2017)
- Spectral Normalization (Miyato et al., 2018):

$$W_{SN} = \frac{W}{\sigma(W)}, \tag{8}$$

where

$$\sigma(W) = \max_{\|h\|_2 \leq 1} \|Wh\|_2, \tag{9}$$

which bounds the Lipschitz constant of the discriminator ≤ 1.

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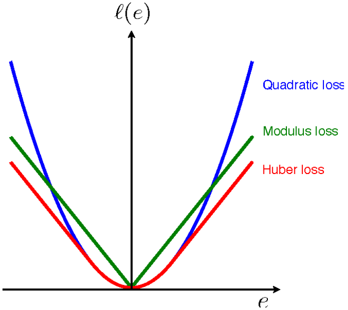

Credit: Pediredla & Seelamantula (2011)

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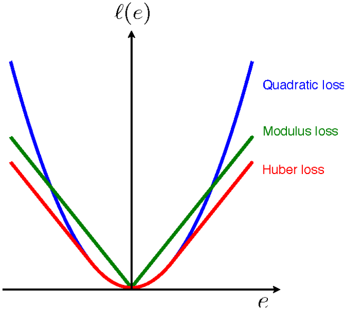


Credit: Pediredla & Seelamantula (2011)

- Show that DEQGAN obtains multiple orders of magnitude lower mean squared errors than classical neural network methods

Experiment: Exponential Decay

Consider a model for population decay $x(t)$ given by the exponential differential equation

$$\dot{x}(t) + x(t) = 0, \tag{10}$$

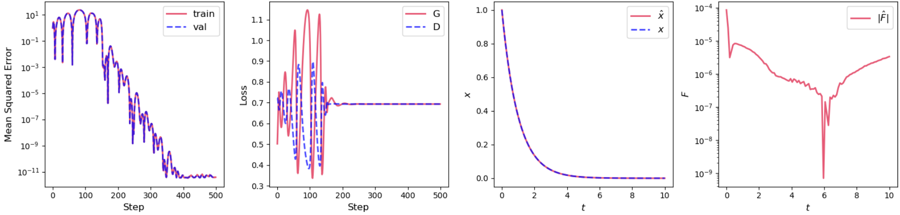
with initial condition $x(0) = 1$.[2] We set

$$LHS = \dot{x}(t) + x(t),$$

$$RHS = 0.$$

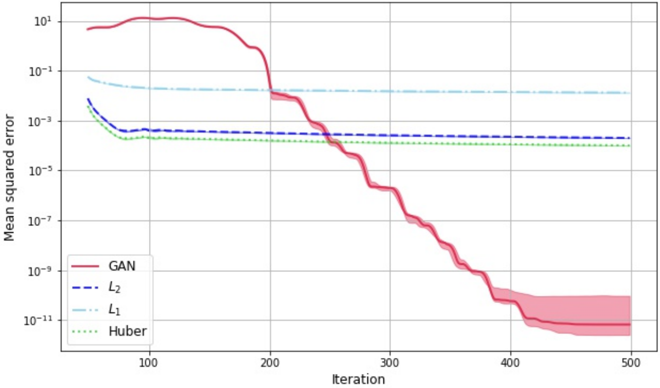
[2] The ground truth solution $x(t) = e^{-t}$ can be obtained analytically.

Experiment: Exponential Decay



- G and D losses initially exhibit high variability but reach equilibrium
- Mean squared error decreases to 10^{-11} by step $\sim$400

Experiment: Exponential Decay



- DEQGAN achieves $\sim 10^{-6}$ times lower mean squared error than classic loss functions (see video)

Experiment: Simple Oscillator

Consider the motion of an idealized oscillating body $x(t)$, which can be modeled by the simple harmonic oscillator differential equation

$$\ddot{x}(t) + x(t) = 0, \tag{11}$$

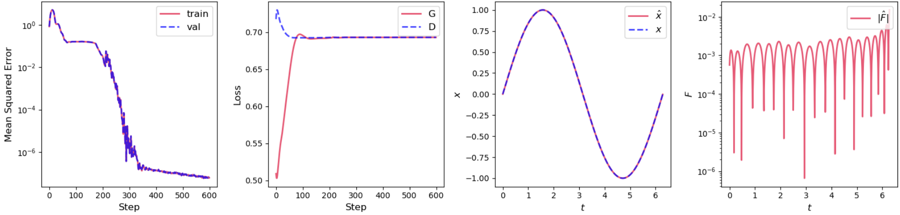
with initial conditions $x(0) = 0$, and $\dot{x}(0) = 1$.[3] We set

$$LHS = \ddot{x}(t) + x(t),$$

$$RHS = 0.$$

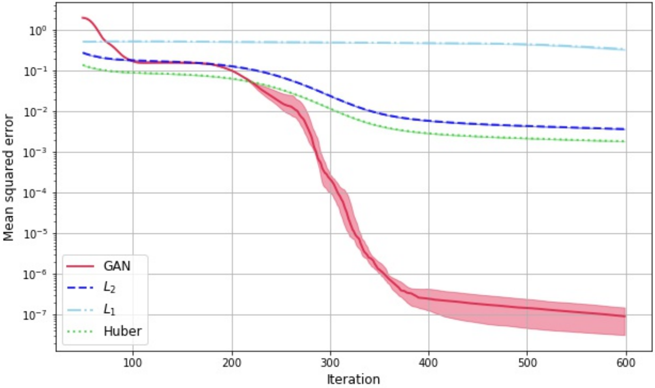
[3] This differential equation has an exact solution $x(t) = \sin t$.

Experiment: Simple Oscillator



- G and D losses reach equilibrium almost monotonically
- Mean squared error decreases to $\sim 10^{-7}$

Experiment: Simple Oscillator



- DEQGAN achieves $\sim 10^{-4}$ times lower mean squared error than classical loss functions (see video)

Experiment: Nonlinear Oscillator

Consider the less idealized motion $x(t)$ of an oscillating body subject to additional forces, given by the nonlinear oscillator differential equation

$$\ddot{x}(t) + 2\beta\dot{x}(t) + \omega^2 x(t) + \phi x(t)^2 + \epsilon x(t)^3 = 0, \tag{12}$$

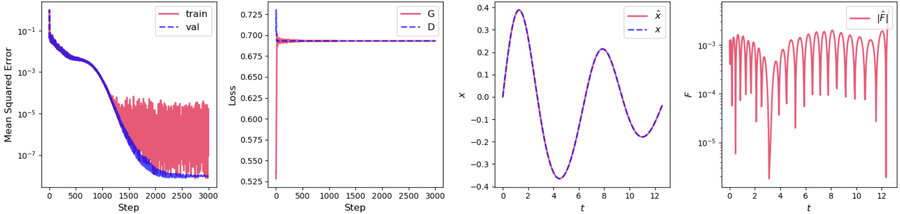
with $\beta = 0.1, \omega = 1, \phi = 1, \epsilon = 0.1$ and initial conditions $x(0) = 0$ and $\dot{x}(0) = 0.5$.[4] We set

$$LHS = \ddot{x} + 2\beta\dot{x} + \omega^2 x + \phi x^2 + \epsilon x^3,$$

$$RHS = 0.$$

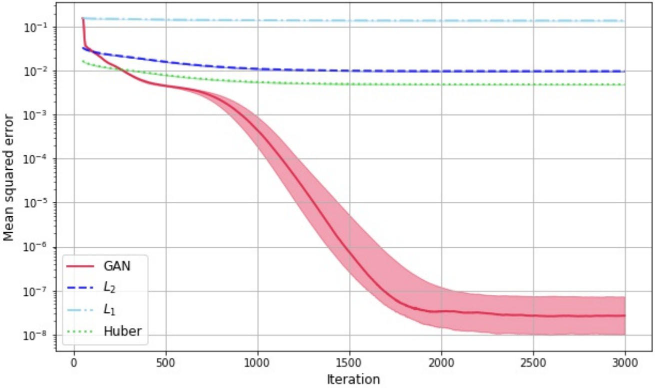
[4] The equation does not have an analytical solution. We use the fourth-order Runge-Kutta method to obtain "ground truth" solutions.

Experiment: Nonlinear Oscillator



- Fast convergence of G and D losses
- Validation mean squared error reaches $\sim 10^{-7}$

Experiment: Nonlinear Oscillator



- DEQGAN reaches $\sim 10^{-5}$ times lower error than classical loss functions (see video)

Experiment: SIR System of Equations

Consider the Susceptible $S(t)$, Infected $I(t)$, Recovered $R(t)$ model for the spread of an infectious disease over time t:

$$\frac{dS}{dt} = -\beta \frac{IS}{N} \tag{13}$$

$$\frac{dI}{dt} = \beta \frac{IS}{N} - \gamma I \tag{14}$$

$$\frac{dR}{dt} = \gamma I \tag{15}$$

with $\beta = 3, \gamma = 1$, constant population $N = S + I + R$, and initial conditions $S_0 = 0.99, I_0 = 0.01, R_0 = 0$.[5]

[5] We obtain ground truth solutions through numerical integration.

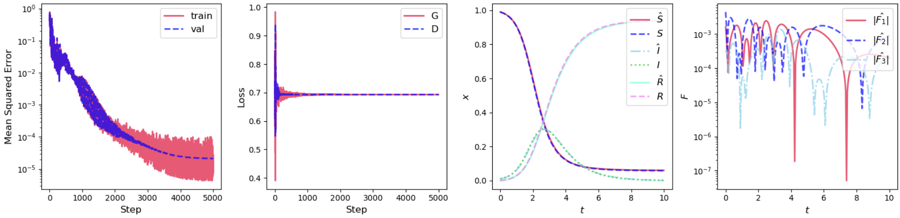
Experiment: SIR System of Equations

We set

$$LHS = \left[\frac{dS}{dt} + \beta\frac{IS}{N}, \frac{dI}{dt} - \beta\frac{IS}{N} + \gamma I, \frac{dR}{dt} - \gamma I\right]^T,$$

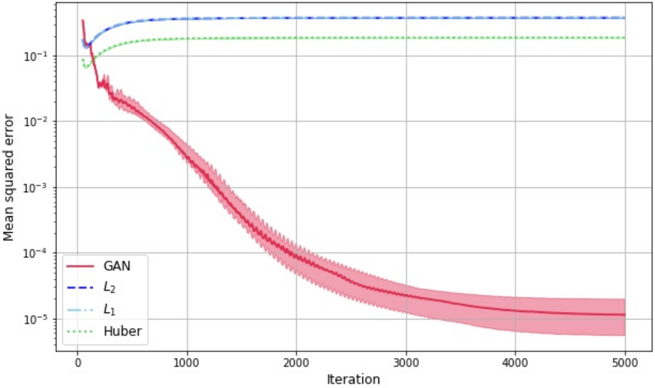
$$RHS = [0, 0, 0]^T.$$

Experiment: SIR System of Equations



- Fast convergence of G and D losses to equilibrium
- Validation mean squared error reaches $\sim 10^{-5}$
- Residuals are small for each equation

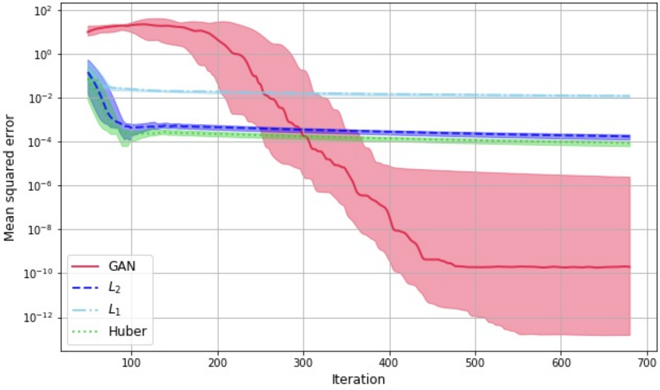
Experiment: SIR System of Equations



- DEQGAN obtains $\sim 10^{-4}$ times lower mean squared error; classic methods collapse to trivial solution (see video)

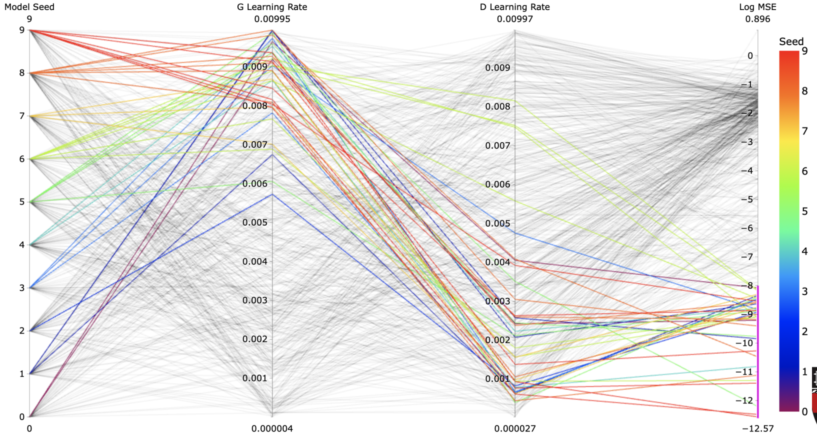
Discussion: Instability to Model Initialization

- High variability in solution accuracy when model weight initialization (either D or G, or both) not fixed (via random seed)



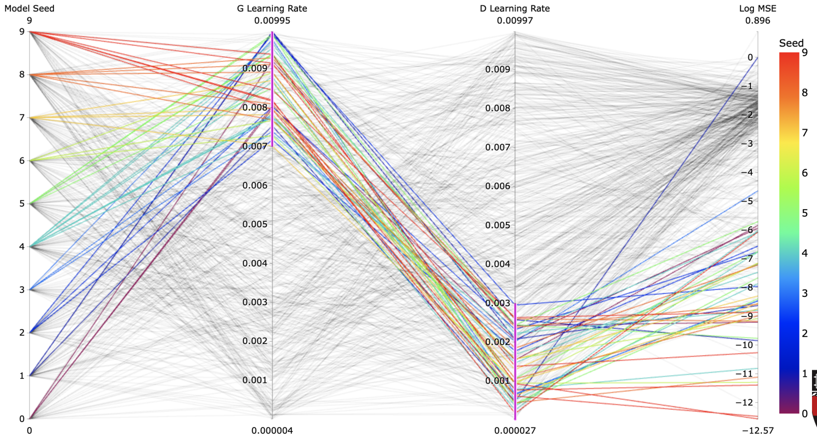
Instability: Varying Model Initialization

- Random search shows settings exist for each model weight initialization seed that perform well (filtering on MSE $\leq 10^{-8}$)



Instability: Pattern of Hyperparameters

- High generator and low discriminator learning rates mostly lead to best performance; still requires hyperparameter search



Instability: Solution

- Perform hyperparameter tuning (e.g. random search) with fixed model initialization

[6] Ray-Tune: `https://docs.ray.io/en/latest/tune.html`

Instability: Solution

- Perform hyperparameter tuning (e.g. random search) with fixed model initialization
- Leverage hyperparameter tuning schedulers (e.g. asynchronous Hyperband) to quickly and reliably find good hyperparameter settings[6]

[6] Ray-Tune: `https://docs.ray.io/en/latest/tune.html`

Discussion: Prior Formulations

For completeness, briefly mention negative results:

- Balancing: e.g. setting $LHS = \dot{x}$ and $RHS = -x$ for exponential. Fails possibly because "real" data distribution $p_{\text{data}}(x)$ changing as generator updated

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- Balancing: e.g. setting $LHS = \dot{x}$ and $RHS = -x$ for exponential. Fails possibly because "real" data distribution $p_{\text{data}}(x)$ changing as generator updated
- Semi-Supervised: worse than fully unsupervised; perhaps because unsupervised solutions require adhering to equation, while supervised do not
- Other GAN Extensions: conditional GAN & Wasserstein GAN with gradient penalty (WGAN-GP); both sub-optimal upon reformulation and implementation of spectral normalization

Table of Contents

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- Unsupervised neural network method for differential equations is not constrained to a fixed grid of points
- Non-convex optimization procedures often benefit from introducing stochasticity (e.g. *stochastic* gradient descent); sampling can induce useful stochasticity
- Our empirical results show that the choice of sampling procedure has significant impact on convergence and accuracy

Methods

- Fixed grid: no sampling, use the same fixed set of points at each gradient step

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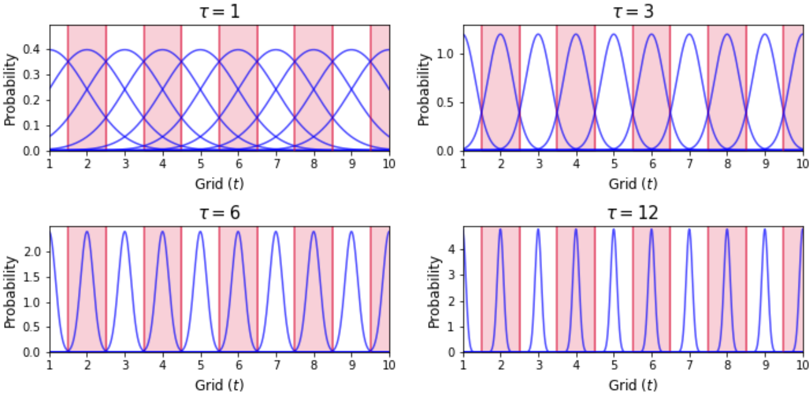
- Fixed grid: no sampling, use the same fixed set of points at each gradient step
- Uniformly sampling: each point is sampled i.i.d. uniform with support over the domain of the problem $x \sim U(D)$
- "Perturbed" sampling: "jitter" points from a fixed grid with i.i.d. Gaussian noise. For each point in the mesh, add

$$\epsilon \sim \mathcal{N}\left(\mu = 0, \sigma = \frac{\Delta x}{\tau}\right) \tag{16}$$

where Δx is the inter-point spacing, and τ is a hyperparameter that controls sample variance

Effect of Tau



Example: Reynolds-Averaged Navier Stokes

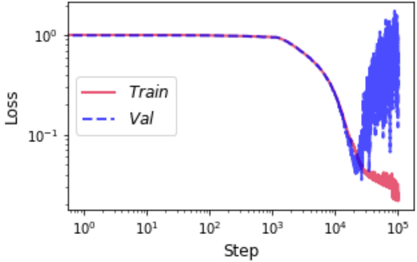
Consider the Reynolds-Averaged Navier Stokes (RANS) equation for the average velocity profile u of an incompressible fluid at position y in a one-dimensional channel given by

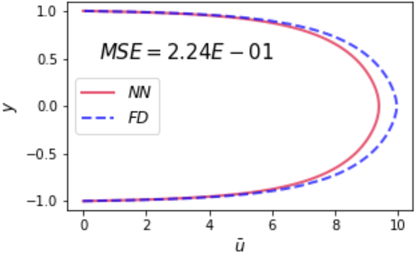
$$\nu \frac{d^2 u}{dy^2} - \frac{d}{dy}\left((\kappa y)^2 \left|\frac{du}{dy}\right| \frac{du}{dy}\right) - \frac{1}{\rho}\frac{dp}{dx} = 0 \tag{17}$$

where $\nu = 0.0055, \kappa = 0.41, \rho = 1$ are given constants and $\frac{dp}{dx} = -1$ is a given pressure gradient.

Example: RANS with Fixed Grid

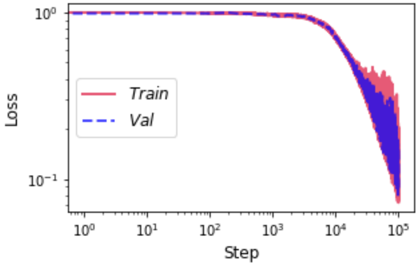
- Overfitting: validation loss diverges by step $\sim 10^4$

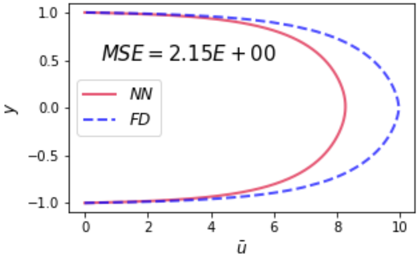




Example: RANS with Uniform Sampling

- Overfitting reduced but loss exhibits higher variance; mean squared error is higher (solution is worse)





Example: RANS with Perturbed Sampling

- Overfitting eliminated, loss variance reduced, and lowest mean squared error (best solution)

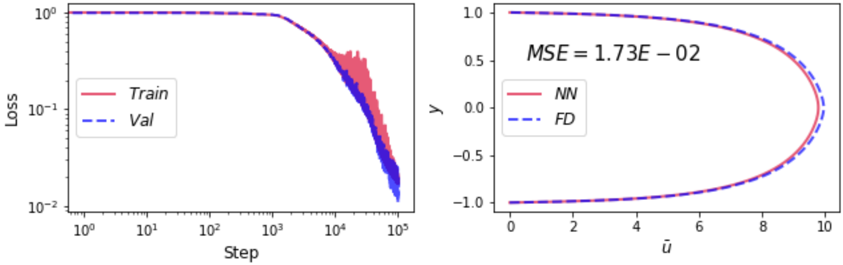


Table of Contents

Conclusion

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- Showed that DEQGAN obtains orders of magnitude lower mean squared errors than classical unsupervised neural network methods with L_1, L_2, and Huber loss functions
- Provided a foundation for future work on learning the loss function for differential equations with unsupervised neural networks
- Introduced a sampling technique that yields robustness to overfitting while improving solution quality

Future Work

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- Investigate more sophisticated sampling techniques, e.g. active learning

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- Family and friends for unconditional love and support

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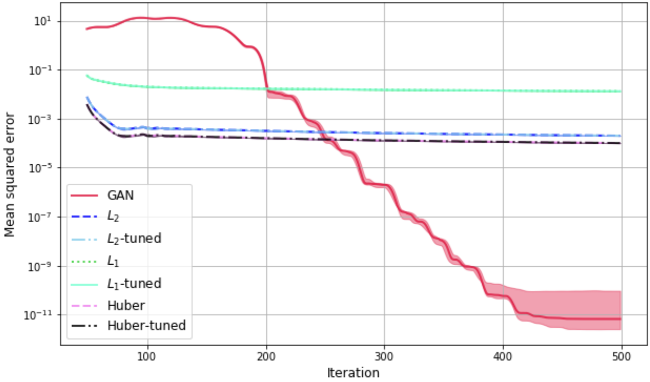
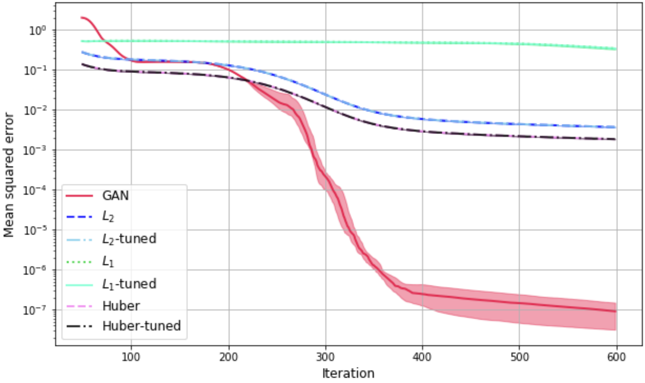
Questions?

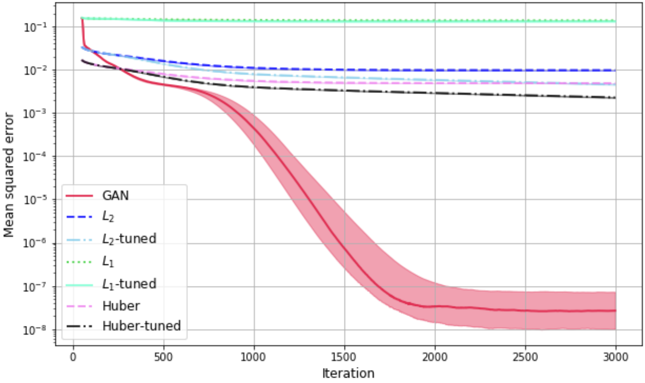
Additional Material: Exponential with Classical Tuning



Additional Material: Simple Oscillator with Classical Tuning



Additional Material: Nonlinear Oscillator with Classical Tuning



Additional Material: SIR System with Classical Tuning