Session 2 - Optimisation strategies

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(Stochastic) Gradient Descent

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Momentum and related optimisers

Other strategies

Continuum gradient descent

- For now, let us consider an abstract, differentiable loss function $\mathcal{L} : \mathbb{R}^N \to \mathbb{R}$ and try to minimise it.
- As with loss functions, we will start by thinking "in the continuum", with the gradient descent: Given an initial state θ_0, we aim to find the solution to

$$\begin{aligned} \theta'(t) &= -\nabla \mathcal{L}(\theta(t)). \\ \theta(0) &= \theta_0. \end{aligned} \tag{1}$$

- The chain rule gives that

$$\frac{d}{dt}\mathcal{L}(\theta(t)) = \theta'(t) \cdot \nabla \mathcal{L}(\theta(t)) = -||\nabla \mathcal{L}(\theta(t))||^2.$$

- The loss decreases.

Continuum gradient descent

- We don't just want it to decrease, we want it to decrease *quickly*.
- Lets keep things simple - Say $\mathcal{L}(\theta) = \frac{1}{2} A\theta \cdot \theta$, A a PD symmetric matrix. Then $\theta^* = 0$ is the minimiser, and $\theta'(t) = -A\theta(t)$.
- If $\lambda_{\min}$ is the smallest eigenvalue of A, then we expect

$$||\theta(t)|| \leq C \exp(-\lambda_{\min} t).$$

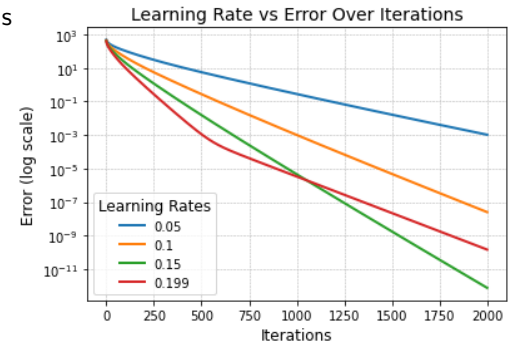
- That is, a (nearly) degenerate matrix A will lead to slow convergence.

Discrete gradient descent

- Of course, we have to discretise. Effectively, we use finite differences: We initialise at θ_0, and update via
$$\theta_{k+1} = \theta_k - \gamma \nabla \mathcal{L}(\theta_k).$$
- Again, if $\mathcal{L}$ is quadratic, we obtain
$$\theta_{k+1} = (I - \gamma A)\theta_k.$$
- The solution is $\theta_k = (I - \gamma A)^k \theta_0$, so the norm is $||\theta_k|| \sim ||I - \gamma A||^k$ (in operator norm).
- We can see two problems - if the smallest eigenvalue of $1 - \gamma \lambda_{min}(A) \approx 1$, or $1 - \gamma \lambda_{max}(A) \approx -1$, then convergence will be very slow. If $1 - \gamma \lambda_{max}(A) > 1$, the norm will explode.
- That is, γ too big means things explode, γ too small means it takes forever.

Examples with learning rates

- We consider our linear problem, where the matrix A is such that it has eigenvalues distributed log-uniformly between 10^{-1} and 10.
- If $\gamma < 0.2$, we should have exponential convergence.
- Let's see the effect of the learning rate.
- If $\gamma > 0.2$, then the error explodes exponentially.



Stochastic gradient descent

- In reality, we can't always access the full gradient $\mathcal{L}$.
- In "interpolation" problems, it may be too memory-intensive to evaluate the loss over the entire data set (and we only have a finite sample).
- In PDEs, we cannot integrate the loss exactly, we can only use a quadrature rule with error.
- This yields a *stochastic gradient descent*. We have a collection of "data" ξ, and a loss function that can be written as

$$\mathcal{L}(\theta) = \frac{1}{J}\sum_{j=1}^{J} L(\theta;\xi_j) \quad \text{or} \quad \mathcal{L}(\theta) = \mathbb{E}\left(L(\theta;\xi)\right).$$

- We then perform updates as

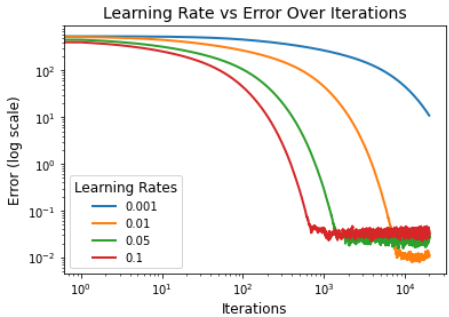
$$\theta_{k+1} = \theta_k - \gamma \underbrace{\frac{\partial L}{\partial \theta}(\theta_k,\xi_k)}_{\text{Stochastic gradient}} = \theta_k - \gamma \underbrace{\frac{\partial \mathcal{L}}{\partial \theta}(\theta_k)}_{\text{Exact gradient}} - \gamma \underbrace{\epsilon_k}_{\text{Error}}.$$

The good and the bad of SGD

- By introducing noise into the system, this can help prevent overfitting when data is finite, as it is harder for the NN to "cheat".
- It can also help the NN "jump" out of undesirable local minima.
- Noisy gradients can also impede convergence.
- The "best" we can usually hope for is to reach an equilibrium where we are oscillating around a "good" minimiser.
- If we split into batches, the parameters update per batch, not per epoch, and this adds an "overhead" cost (potentially big, potentially small).

SGD with "infinite data"

- Let's return to a toy linear problem, but now with a noisy gradient.
- We take $\theta_{k+1} = \theta_k - \gamma(A\theta_k + \epsilon_k)$, where ϵ_k is a random variable with mean zero and variance 10^{-2}.
- Recall that in the case without noise, we had exponential convergence, achieving errors of order 10^{-11} in some cases in a few thousand iterations.



SGD with noisy data

- The noise impedes the convergence significantly.
- In our toy linear model, we can explicitly compute the long term behaviour: The iterates behave as

$$x_k \sim \mathcal{N}(0, V)$$

- The covariance V solves

$$(1 - \gamma A)V(1 - \gamma A) + \gamma^2 \Sigma = V.$$

- This is a steady state, on average the exact solution, but positive variance.
- As $\gamma \to 0$, $V = O(\gamma)$ - we should reduce step sizes.

SGD with noisy data

- One method to overcome this is to reduce the learning rate during training, so $\gamma = \gamma_k$.
- Whilst exponential decrease is common in the literature, there are various works that suggest an algebraic decay is better - $\gamma_k \sim k^{-\alpha}$ with $\alpha \in \left(\frac{1}{2}, 1\right]$.[a][b]
- When algebraic, under technical hypotheses (that probably don't hold in NNs...), we have that

$$\frac{\theta_k - \theta^*}{\gamma_k} \to \mathcal{N}(0, V),$$

where V solves a Lyupanov equation,

$$VH_{\mathcal{L}}(\theta^*) + H_{\mathcal{L}}(\theta^*)V = \mathrm{Var}(\nabla \mathcal{L}(\theta^*))$$

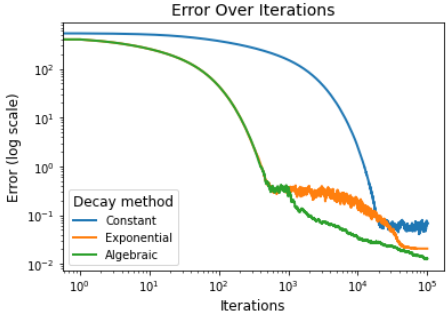
- This suggests two things: Degeneracy of the Hessian or large variances make V big (poor convergence).

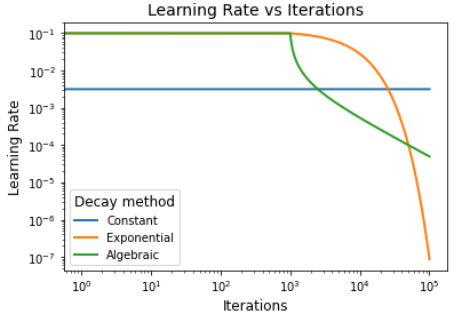
[a] Tiejun Li, Tiannan Xiao, and Guoguo Yang. Revisiting the central limit theorems for the SGD-type methods. arXiv preprint arXiv:2207.11755, 2022.

[b] Guillaume Garrigos and Robert M Gower. Handbook of convergence theorems for (stochastic) gradient methods. arXiv preprint arXiv:2301.11235, 2023.

Decaying learning rates

- We consider our toy, linear, noisy model, taking $\theta_{k+1} = \theta_k - \gamma_k(A\theta_k + \epsilon_k)$.
- We consider 3 regimes - A constant learning rate, an exponentially decaying learning rate, and an algebraically ($\sim \frac{1}{k}$) decaying learning rate.





Some concluding remarks on SGD

- Gradient descent for simple, deterministic problems has exponential convergence.
- When noise is present, this significantly impedes convergence.
- Decaying learning rates can overcome this, but convergence will be much slower - if it converges at all.

Momentum and related optimisers

(Stochastic) Gradient Descent

Momentum and related optimisers

Other strategies

Momentum

- (S)GD can be understood as a discretisation of a continuum gradient descent, $\theta' = -\nabla\mathcal{L}(\theta)$.
- Momentum methods can be understood as discretisations of a second order system,

$$\theta'' + \mu\theta' = -\nabla\mathcal{L}(\theta).$$

- The updates in the discrete system are written as

$$\begin{aligned} m_{k+1} &= \beta m_k - \gamma\nabla\mathcal{L}(\theta_k) \\ \theta_{k+1} &= \theta_k + m_{k+1}. \end{aligned} \tag{2}$$

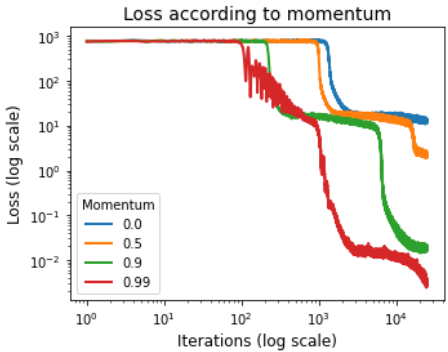
- $0 < \beta < 1$ is typically taken close to 1.

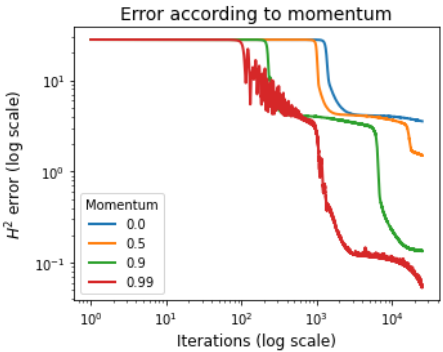
The good and bad of Momentum

- The momentum vector m acts like an "average" of recent gradients - This can smooth out noisy gradients.
- When the loss is very "flat", momentum can accelerate convergence (think of a ball rolling down a soft slope)
- Near a minimum, the use of momentum may lead to more oscillatory behaviour (think damped harmonic oscilator versus exponential decay $y' = -\omega y$).
- When the gradient is changing a lot, the momentum "remembers" previous gradients that are not as useful, this can lead to instability.

Examples SGD(+M)

- We revisit our 1D PINN problem, using SGD with a fixed learning rate (10^{-3}) and varying the momentum parameter.





The holy grail - Newton methods

- Each component of the trainable parameters θ has a different "role", and will generally perform better if a correct learning rate is defined for each one.
- The Newton method goes further, we approximate the loss locally via

$$\mathcal{L}(\theta) \approx \mathcal{L}(\theta_k) + \nabla\mathcal{L}(\theta_k) \cdot (\theta - \theta_k) + \frac{1}{2} H_{\mathcal{L}}(\theta_k) \cdot (\theta - \theta_k) \cdot (\theta - \theta_k),$$

  whose exact minimum is attained at

$$\theta = \theta_k - H_{\mathcal{L}}(\theta_k)^{-1} \nabla\mathcal{L}(\theta_k).$$

- The problem is the cost - if we have 5,000 variables, the Hessian involves evaluating $O(10^7)$ derivatives, then we have to solve the corresponding linear system. As the Hessian is usually very ill-conditioned, "small" errors in $H_{\mathcal{L}}$ lead to big errors in its inverse.
- Nonetheless, they tell us that we should be thinking of "learning rates" that act on different parameters differently and depend on the local structure of the loss.

Adam

- There are many different optimisers with varying levels of sophisitication and applicability - One of the most popular is Adam (which I have used in almost every simulation I have shown), employing adaptive moment estimates to obtain per-parameter learning rates.
- The precise algorithm has many ingredients, but the key objects are a momentum estimate m_k and a second-moment estimate v_k of $\nabla\mathcal{L}(\theta_k)^2$, then

$$\theta_{k+1} = \theta_k - \gamma \frac{1}{\sqrt{v_k} + \epsilon} m_k.$$

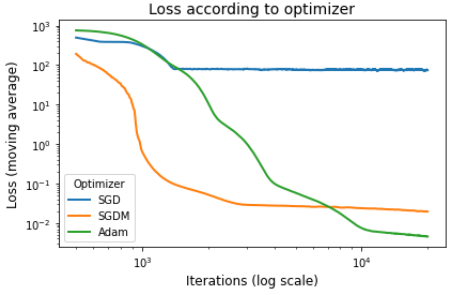
- $\gamma \frac{1}{\sqrt{v_k}+\epsilon}$ acts as an effective learning rate - hand waving arguments say that it captures both the noise and curvature (Hessian) of the loss.

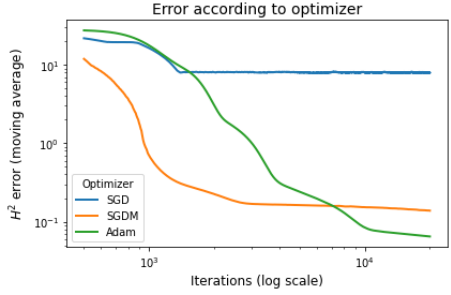
The good and the bad of Adam

- Adam is typically significantly faster to converge than SGD (in my experience, a lot).
- It is not as sensitive as SGD to the chosen learning rate - it adapts the learning rate itself. In particular, it is more "scale invariant".
- Adam can be very unstable - You may have noticed that in the previous simulations the loss occasionally "jumps" and then quickly returns to its original value.
- Adam contains many parameters that need to be tuned (learning rate, decay for first moment estimates, decay for second moment estimates, regulariser ϵ)

Comparison Adam vs SGD

- We employ SGD, SGDM and Adam on the same problem with the same initial learning rate for a 1D PINN problem.
- Note: I have shown moving averages - All three are noisy.
- SGDM required fine-tuning of the momentum parameter, Adam used the default settings.





Some concluding remarks on momentum-based methods

- Momentum and Adam can yield significant gains in convergence for the same cost.
- Adam tends to be the optimiser of choice for problems with NNs.
- Momentum/Adam methods have internal hyperparameters that need to be tuned, and this may heavily effect convergence.
- Different trainable parameters have different roles, and may need different approaches (simplest case - distinct learning rates)

Other strategies

(Stochastic) Gradient Descent

Momentum and related optimisers

Other strategies

Least-square solver

- The issue with Newton methods is the cost, the system is huge, the derivatives expensive to compute, the loss is not convex and it may be unstable.
- Take a fully-connected feedforward NN, and we will write it as

$$u_{NN}(x) = \sum_{n=1}^{N} c_n u_n(x).$$

- Each u_n corresponds to a node in the last layer, c_n are trainable.
- We can rewrite the mean-squared error loss as

$$\begin{aligned}\mathcal{L}(u_{NN}) =& \frac{1}{J}\sum_{j=1}^{J}(u_{NN}(x_j) - y_j)^2 \\ =& \sum_{n,m=1} c_n c_m \left(\frac{1}{J}\sum_{j=1}^{J} u_n(x_j)u_m(x_j)\right) - 2\sum_{n=1}^{N} c_n \left(\frac{1}{J}\sum_{j=1}^{J} u_n(x_j)y_j\right) + \text{constant}.\end{aligned}$$

Least-squares solver

- We can write the loss, defining ω to be the other trainable parameters of u_{NN} apart from c, as

$$\mathcal{L}(u_{NN}) = A(\omega)c \cdot c - 2b(\omega) \cdot c + \text{constant},$$

  whose exact minimiser over c is $A(\omega)^{-1}b(\omega)$.
- By defining $c = c(\omega) = A(\omega)^{-1}b(\omega)$, we obtain a (very non-linear) loss to be optimised over ω, which can be done via (e.g.) SGD or Adam.
- The idea is that the loss is quadratic in a certain variables, so we can find the minimum via linear algebra, whilst the remaining variables can be solved by a gradient-based method.
- This is the idea of the hybrid LS-solver of Cyr et. al. [a]

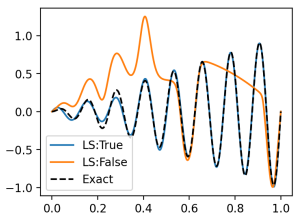
[a] Cyr, Eric C., et al. "Robust training and initialization of deep neural networks: An adaptive basis viewpoint." Mathematical and Scientific Machine Learning. PMLR, 2020.

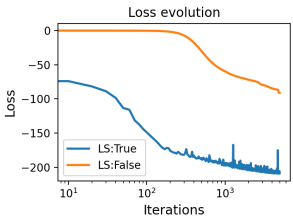
The good and the bad of LS

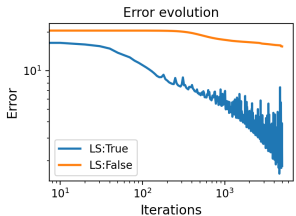
- The method can be very good at approximating oscillatory solutions, where many gradient-based methods get trapped easily in local minima.
- It can highly accelerate convergence, even improving the initial loss by orders of magnitude.
- Matrix inverses are very sensitive, errors in $A(\omega)$ can lead to large errors in $A(\omega)^{-1}$ - and this can produce erroneous results.
- It is unclear how to apply the idea to minibatches with data - Constructing the full LS system is expensive, but lacking data points may lead to significant errors.
- Key idea: Different variables play different roles in the NN, so we should think about more "structured" optimisers - SGD treats everything the same.

LS Example

- We take a Deep Ritz Method in 1D with an oscillatory solution.
- Note - there is little noise, this is because LS is very unstable with poor integration, so I used a very precise integration method (not feasible in 3D).
- We see Adam fails - this highlights the issue of *spectral bias*.

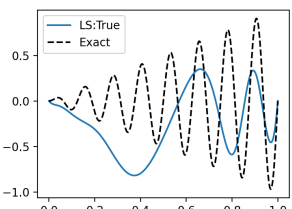


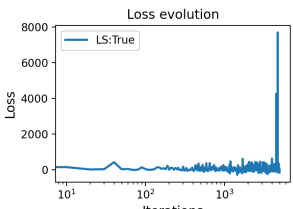


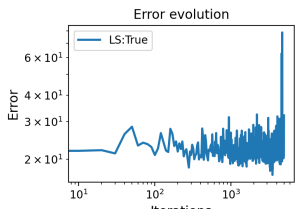


LS Example

- If we use fewer integration points, we can see how sensitive the LS method is to integration errors







Spectral bias

- Neural Networks suffer from *spectral bias*, also referred to as the *frequency principle* (F-principle).
- It states that, during training, first the low-frequency features are learned, and then the high frequency features.
- The "corollary" of this is that when solutions are naturally high frequency, it can be hard to train an NN to approximate it.
- It also means that the error at the end of training should be dominated by high-frequency components.
- We can try to take advantage of this idea to develop a new training approach.

Multilevel NNs

- Multi-level Neural Networks[a] are based on a multi-step training process.
- We will not follow their exact methodology, but instead the spirit of it here.
- Suppose we have a PINNs type-problem, $u''(x) = f(x)$, and we train a neural network u_0 to approximate the solution.
- The error, $u_1 = u - u_0$, also satisfies an ODE,

$$u_1''(x) = u''(x) - u_0''(x) = f(x) - u_0''(x).$$

- We can then view u_0 as fixed (no more training), and try to approximate the error. This is an ODE of the same type and $u_0 + u_1$ is our approximate solution.
- We train u_1 with this loss and consider $u_0 + u_1$, and repeat for the error $u_2 = u - (u_1 + u_2)$.

[a] Aldirany, Ziad, et al. "Multi-level neural networks for accurate solutions of boundary-value problems." Computer Methods in Applied Mechanics and Engineering 419 (2024): 116666.

Multilevel NNs

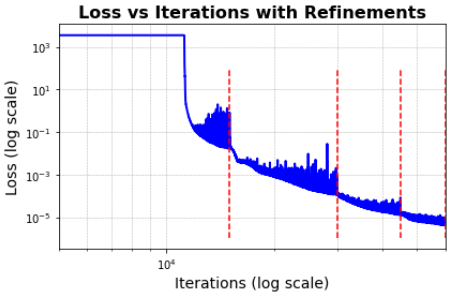
- Due to the F-principle, we expect u_1 to have high-frequency modes, u_2 to have higher-frequency modes and so on.
- As such, we use an architecture that facilitates high-frequency modes.
- We take the first layer of our NN to be

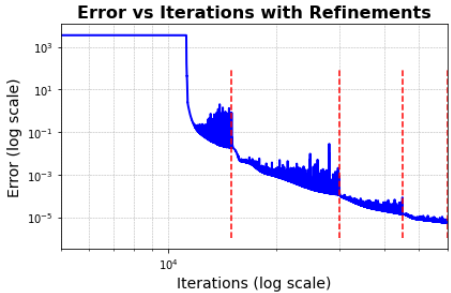
$$L_1(x) = (x, \cos(k_1 x), \sin(k_1 x), \cos(k_2 x), \sin(k_2 x), ...)$$

  for some $(k_i)_{i=1}^K$. The remaining layers are those of a fully-connected feed-forward NN. (These are known as *Fourier features* and aid with the approximation of high-frequency components)
- We take higher frequencies in the later refinements.

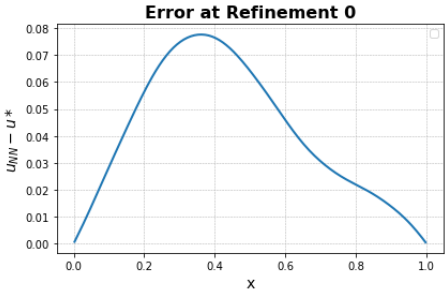
Multilevel NNs

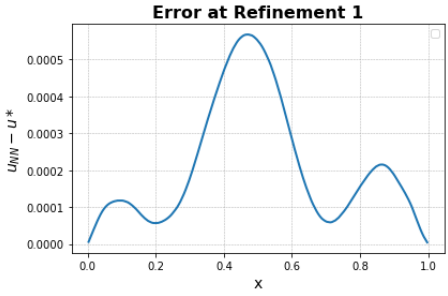
- We show the results of training below, with refinements marked in red.
- We see not only a reduction in the loss, but a reduction in the noise during training.

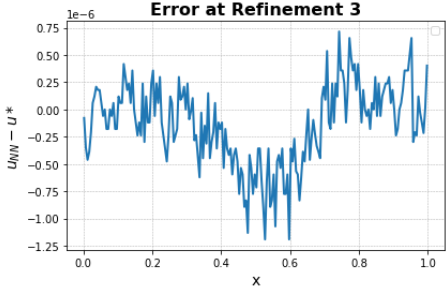




Multilevel NNs

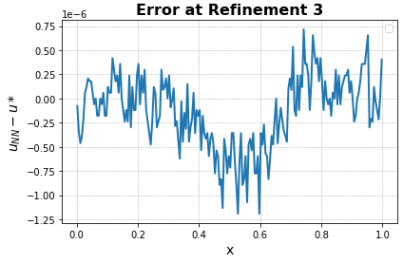


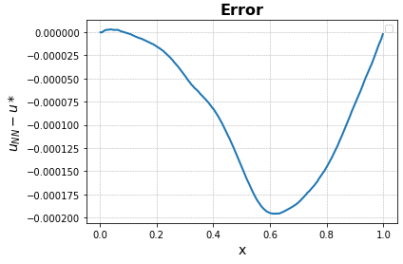


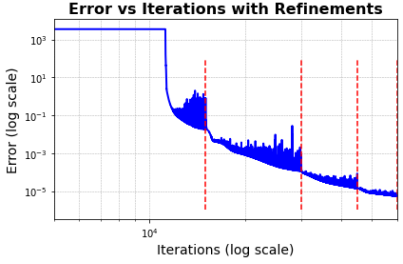


Comparison

- We can compare this with training the full neural network together.







Some concluding remarks on other strategies

- Going beyond gradient-based strategies can lead to significant gains in convergence.
- Neural networks suffer from spectral bias - low frequency features are learned easily, high frequency features are slower, if learned at all
- LS-based solvers can be a huge help, but it is unclear how they work with batches/data, are sensitive to errors, and limited to losses linear in the NN.
- Iterative strategies can train following the F-principle - this may include "forcing" high-frequency modes into your NN (Fourier Features)