DeepMind

The importance of discretisation drift in deep learning

Mihaela Rosca 30/05/2024



Discussed works

- Implicit Gradient Regularisation Barrett and Dherin, ICLR 2021
- Discretization drift in two player games Rosca et al, ICML 2021
- On a continuous time model of gradient descent dynamics and instability in deep learning <u>Rosca et al, TMLR 2023</u>
- On the Origin of Implicit Regularization in Stochastic Gradient Descent Smith et al, ICLR 2021
- Implicit regularisation in stochastic gradient descent: from single-objective to two-player games, <u>Rosca et al, 2023, ICML workshop</u>

There is a lot of interesting related work, check out the related work section in these papers!

You can also find an overview in <u>my thesis</u>, "On discretisation drift and smoothness regularisation in deep learning".

Aim: analyse gradient descent updates aiming to minimise function E.

$$\boldsymbol{\theta}_t = \boldsymbol{\theta}_{t-1} - h \nabla_{\boldsymbol{\theta}} E(\boldsymbol{\theta}_{t-1})$$

parameter dimension: *D h* denotes the learning rate throughout this talk.



Approaches of analysing optimisation

Discrete time

- analyse updates as used in practice
- directly accounts for the learning rate



Continuous time

- analyse the underlying continuous system
- tends to be easier analytically
- the gradient flow does not account for learning rates (there can be a gap between continuous analysis results and what happens in practice)





Appeal and challenges of continuous time

Negative gradient flow (NGF):

$$\dot{\boldsymbol{\theta}} = -\nabla_{\boldsymbol{\theta}} E$$

$$\frac{dE}{dt} = \frac{dE}{d\theta}^T \frac{d\theta}{dt} = -\left(\nabla_{\theta} E\right)^T \nabla_{\theta} E = -||\nabla_{\theta} E||^2 \le 0$$

following the NGF decreases E and that's easy to prove, but that is not true of gradient descent!



Discretization drift for Euler updates



Discretization drift for Euler updates



Modified loss functions





Implicit gradient regularisation

Barrett et Dherin, ICLR 2021

Mihaela Rosca, 2024

Backward error analysis



$$\begin{split} \tilde{\theta}(h) &= \theta_{t-1} - h \nabla_{\theta} E(\theta_{t-1}) + h^2 \left[f_1(\theta_{t-1}) + \frac{1}{2} \nabla_{\theta}^2 E(\theta_{t-1}) \nabla_{\theta} E(\theta_{t-1}) \right] + \mathcal{O}(h^3) \\ & \vdots \\ \theta_{t-1} \end{split}$$

$$\begin{split} \tilde{\theta}(h) &= \theta_{t-1} - h \nabla_{\theta} E(\theta_{t-1}) + h^2 \left[f_1(\theta_{t-1}) + \frac{1}{2} \nabla_{\theta}^2 E(\theta_{t-1}) \nabla_{\theta} E(\theta_{t-1}) \right] + \mathcal{O}(h^3) \\ \theta_{t-1} & \tilde{\theta}_{t-1} \\ \theta_t &= \theta_{t-1} - h \nabla_{\theta} E(\theta_{t-1}) \end{split}$$

$$\begin{split} \tilde{\theta}(h) = & \theta_{t-1} - h \nabla_{\theta} E(\theta_{t-1}) + h^2 \left[f_1(\theta_{t-1}) + \frac{1}{2} \nabla_{\theta}^2 E(\theta_{t-1}) \nabla_{\theta} E(\theta_{t-1}) \right] + \mathcal{O}(h^3) \\ & \theta_{t-1} & \theta_{t-1} \\ & \theta_t = \theta_{t-1} - h \nabla_{\theta} E(\theta_{t-1}) \end{split}$$

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$$\begin{split} \tilde{\theta}(h) = \theta_{t-1} - h\nabla_{\theta} E(\theta_{t-1}) + h^{2} \left[f_{1}(\theta_{t-1}) + \frac{1}{2} \nabla_{\theta}^{2} E(\theta_{t-1}) \nabla_{\theta} E(\theta_{t-1}) \right] + \mathcal{O}(h^{3}) \\ \theta_{t-1} & \tilde{\theta}_{t} \\ \theta_{t-1} & \tilde{\theta}_{t-1} \\ \theta_{t} = \theta_{t-1} - h\nabla_{\theta} E(\theta_{t-1}) \end{split}$$

IGR flow



From modified ODEs to modified losses: vector fields as negative gradients



Modified loss functions





Implicit gradient regularization

Implicit gradient regularization aids generalization.



Summary

- Backward error analysis is a technique that can be used to find modified ODEs, which have a lower order of error in learning rate to gradient descent.
- With this approach, we can find implicit regularisers.

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How about instability?

On a continuous time model of gradient descent dynamics and instability in deep learning

Rosca et al, TMLR 2023

Our goal: use a continuous time perspective to analyse gradient descent, including its observed instabilities.



Existing continuous time flows

Negative gradient flow (NGF):

$$\dot{\boldsymbol{\theta}} = -\nabla_{\boldsymbol{\theta}} E$$

Implicit Gradient Regularization flow (IGR flow):

$$\dot{\boldsymbol{\theta}} = -\nabla_{\boldsymbol{\theta}} E - \frac{h}{2} \nabla_{\boldsymbol{\theta}}^2 E \nabla_{\boldsymbol{\theta}} E$$



The IGR flow was introduced by Barrett and Dherin, 2021.

Limitations of existing continuous time flows



Existing continuous time flows do not handle instabilities observed using gradient descent.

Plenty of space to improve: deep learning



CIFAR-10, VGG



Our approach: Backward Error Analysis

Find
$$\boldsymbol{\dot{\theta}} = -\nabla_{\boldsymbol{\theta}} E + h f_1(\boldsymbol{\theta}) + \dots + h^n f_n(\boldsymbol{\theta})$$

such that the difference between gradient descent and the continuous time flow after 1 discrete update is $\mathcal{O}(h^{n+2})$.

The correction terms f_i will depend on E and its derivatives.



Our approach: Backward Error Analysis

$$\dot{\tilde{\boldsymbol{\theta}}} = -\nabla_{\boldsymbol{\theta}} E + h f_1(\boldsymbol{\theta}) + \dots + h^n f_n(\boldsymbol{\theta})$$

Our approach: look at all correction terms (in all n) which only contain first and second order derivatives of E.

Third order flow





The Principal Flow

$$\dot{\boldsymbol{\theta}} = \sum_{i=0}^{D-1} \frac{\log(1-h\lambda_i)}{h\lambda_i} (\nabla_{\boldsymbol{\theta}} E^T \mathbf{u}_i) \mathbf{u}_i$$

Properties of the Principal Flow (PF):

- is exact for quadratic losses
- generalisation of the NGF
- stability analysis correctly predicts that gradient descent is not always attracted to local minima



The Principal Flow

PF

NGF

$$\dot{\boldsymbol{\theta}} = \sum_{i=0}^{D-1} \underbrace{\frac{\log(1-h\lambda_i)}{h\lambda_i} (\nabla_{\boldsymbol{\theta}} E^T \mathbf{u}_i)}_{i} \mathbf{u}_i$$

stability coefficient in eigendirection with index i

$$\dot{ heta} = \sum_{i=0}^{D-1} igl(- (
abla_{ heta} E^T \mathbf{u}_i) igl) \mathbf{u}_i$$



The Principal Flow: exact for quadratic case





0.4

Stability coefficient is complex, with positive real part.

The Principal Flow and neural networks: small neural nets



The Principal Flow captures gradient descent better than existing flows in neural network training locally (when the number of iterations is small) both in the stable and unstable cases.



The Principal Flow and neural networks



The Principal Flow captures the dynamics of the dot product between the gradient and the leading Hessian eigenvector better than existing flows.



The edge of stability in deep learning



The edge of stability phenomenon in deep learning has been coined by Cohen et al, 2021.

The Principal Flow and edge of stability: more than just eigenvalues



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The Principal Flow and edge of stability



The stability coefficients show the strength of instabilities according to the local behaviour of other flows.



Is the Principal Flow enough to understand GD?

The PF can help explain instabilities in GD, but there are cases where higher order terms help stabilise the trajectory.

Regarding NNs, there have also been studies showing the non-quadratic form of NNs.





Is the Principal Flow enough to understand GD?

$$\nabla_{\boldsymbol{\theta}} E^T \nabla_{\boldsymbol{\theta}}^3 E \nabla_{\boldsymbol{\theta}} E = \sum_{i=0}^{D-1} \left(\mathbf{u}_i^T \nabla_{\boldsymbol{\theta}}^3 E \mathbf{u}_i \right) (\nabla_{\boldsymbol{\theta}} E^T \mathbf{u}_i)^2 \approx \sum_{i=0}^{D-1} \nabla_{\boldsymbol{\theta}} \lambda_i (\nabla_{\boldsymbol{\theta}} E^T \mathbf{u}_i)^2$$

$$\sum_{i=0}^{D-1} \nabla_{\boldsymbol{\theta}} \lambda_i (\nabla_{\boldsymbol{\theta}} E^T \mathbf{u}_i)^2 = \sum_{i=0}^{D-1} \nabla_{\boldsymbol{\theta}} \left(\lambda_i (\nabla_{\boldsymbol{\theta}} E^T \mathbf{u}_i)^2 \right) - \sum_{i=0}^{D-1} 2\lambda_i^2 (\nabla_{\boldsymbol{\theta}} E^T \mathbf{u}_i) \mathbf{u}_i.$$

when this term is close to 0, we are minimising $\lambda_i (\nabla_{\theta} E^T \mathbf{u}_i)^2$ in that direction, which can have a stabilising effect.

Stabilising training



Understanding total drift

The PF reveals an important quantity

$$\nabla_{\boldsymbol{\theta}}^2 E \nabla_{\boldsymbol{\theta}} E = \sum_{i=1}^D \lambda_i \nabla_{\boldsymbol{\theta}} E^T \mathbf{u}_i \mathbf{u}_i.$$



Understanding total drift

Investigating further reveals:

$\nabla_{\theta}^2 E \nabla_{\theta} E = 0 \qquad \text{PF} = \text{NGF}$



Understanding total drift

Investigating further reveals:

$\nabla_{\theta}^2 E \nabla_{\theta} E = 0 \qquad \text{GD= NGF}$



Bonus: Corridor Geometry in Gradient-Based Optimization

- The GD = GF condition can be proven as an iff
- With this insight, can develop a learning rate on corridors that recovers the Polyak learning rate

$\nabla_{\theta}^2 E \nabla_{\theta} E = 0 \quad \clubsuit \quad \mathsf{GD} = \mathsf{NGF}$

Corridor Geometry in Gradient-Based Optimization: Dherin and Rosca, 2024



Understanding total discretisation drift



Understanding discretisation drift



Stabilising training with Drift Adjusted Learning (DAL)

$$h(\boldsymbol{\theta}) = \frac{2}{\|\nabla_{\boldsymbol{\theta}}^2 E \nabla_{\boldsymbol{\theta}} E\| / \|\nabla_{\boldsymbol{\theta}} E\|} = \frac{2}{\|\nabla_{\boldsymbol{\theta}}^2 E \hat{\mathbf{g}}(\boldsymbol{\theta})\|}$$



DAL-p: controlling generalisation versus stability

$$h_p(oldsymbol{ heta}) = rac{2}{\left(\|
abla_{oldsymbol{ heta}}^2 E \hat{f g}(oldsymbol{ heta}) \|
ight)^p}$$



DAL-p: also leads to flat minima



At convergence, DAL leads to flatter minima than SGD.



Summary

- We need to operate in complex space to handle instabilities observed with gradient descent.
- Model continuous-time models of gradient descent can be a useful tool to understand and improve optimisation.



How about stochasticity?

How about stochasticity?

$$\boldsymbol{\theta}_{t+\mu} = \boldsymbol{\theta}_{t+\mu-1} - \nabla_{\boldsymbol{\theta}} E(\boldsymbol{\theta}_{t+\mu-1}; \mathbf{X}^{t+\mu}), \qquad \mu \in \{0, \dots, n-1\},$$

Implicit regularisation in stochastic gradient descent: from single-objective to two-player games

Rosca et Deisenroth, ICML workshop 2023

Stochasticity so far

All we have said thus far also applies to SGD, but only to 1 step of SGD.

How can we model what happens when we take multiple SGD steps?

Are there implicit regularisation effects specific to SGD?

Stochasticity: expectation over one epoch (Smith et al)

If one takes expectations over the shufflings in one epoch, Smith et al find the implicit regulariser:

$$\mathbb{E}_{\sigma} \left[E_{sgd}(\boldsymbol{\theta}) \right] = E(\boldsymbol{\theta}; \{ \mathbf{X}^{t}, \dots, \mathbf{X}^{t+n-1} \}) + \frac{h}{4n} \sum_{k=0}^{n-1} \left\| \nabla_{\boldsymbol{\theta}} E(\boldsymbol{\theta}; \mathbf{X}^{t+k}) \right\|^{2}.$$

The effect of implicit regularization is

The effect of implicit regularization is stronger for smaller batch sizes.

On the Origin of Implicit Regularization in Stochastic Gradient Descent, Smith et al, ICLR 2021

Recent work: no need to work in expectation

If we allow for a dependence on initial parameters, we can write (for any n):

$$\begin{split} \tilde{E}(\boldsymbol{\theta}) &= E(\boldsymbol{\theta}; \{\mathbf{X}^{t}, \dots, \mathbf{X}^{t+n-1}\}) + \frac{nh}{4} \underbrace{\left\| \nabla_{\boldsymbol{\theta}} E(\boldsymbol{\theta}; \{\mathbf{X}^{t}, \dots, \mathbf{X}^{t+n-1}\}) \right\|^{2}}_{full \ batch \ norm \ regularisation} \\ &- \frac{h}{n} \sum_{\mu=1}^{n-1} \underbrace{\left[\nabla_{\boldsymbol{\theta}} E(\boldsymbol{\theta}; \mathbf{X}^{t+\mu})^{T} \left(\sum_{\tau=0}^{\mu-1} \nabla_{\boldsymbol{\theta}} E(\boldsymbol{\theta}_{t-1}; \mathbf{X}^{t+\tau}) \right) \right]}_{mini-batch \ gradient \ alignment} \end{split}$$

Recent work: no need to work in expectation

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$$\tilde{E}(\boldsymbol{\theta}) = E(\boldsymbol{\theta}; \{\mathbf{X}^{t}, \mathbf{X}^{t+1}\}) + \frac{h}{2} \underbrace{\left\| \nabla_{\boldsymbol{\theta}} E(\boldsymbol{\theta}; \{\mathbf{X}^{t}, \mathbf{X}^{t+1}\}) \right\|^{2}}_{full \ batch \ norm \ regularisation} - \frac{h}{2} \underbrace{\nabla_{\boldsymbol{\theta}} E(\boldsymbol{\theta}; \mathbf{X}^{t+1})^{T} \left(\nabla_{\boldsymbol{\theta}} E(\boldsymbol{\theta}_{t-1}; \mathbf{X}^{t}) \right)}_{mini-batch \ gradient \ alignment}.$$

Recent work: no need to work in expectation

In a second step of SGD, there is an implicit regularisation effect of minimising the dot product between the current gradient and the gradient at the previous iteration!

Summary

- We can model the implicit regularisation effects of more than 1 SGD step
- There is an alignment pressure between gradients at consecutive iterations
 - empirical work needed to show its effects



Beyond single objective

How about two-player games?

Generative adversarial networks





Generative adversarial networks



 $\min_{G} \max_{D} V(D,G) = \mathbb{E}_{\boldsymbol{x} \sim p_{\text{data}}(\boldsymbol{x})} [\log D(\boldsymbol{x})] + \mathbb{E}_{\boldsymbol{z} \sim p_{\boldsymbol{z}}(\boldsymbol{z})} [\log(1 - D(G(\boldsymbol{z})))]$

Discretization Drift in Two-Player Games

Rosca et al, ICML 2021

Two-player games continuous dynamics

$$\dot{\phi} = f(\phi, \theta)$$
$$\dot{\theta} = g(\phi, \theta)$$

Two-player games



Differentiable two-player games

$$f = -\nabla_{\phi} L_f$$
$$g = -\nabla_{\theta} L_g$$

Gradient descent!

Modified ODEs for two-player games



Modified ODEs for two-player games



Goal: find f₁ and g₁

Building intuition



Building intuition



Modified ODEs as tools for stability analysis

$$\begin{split} \widetilde{J} &= \begin{bmatrix} \nabla_{\phi} \widetilde{f} & \nabla_{\theta} \widetilde{g} \\ \nabla_{\phi} \widetilde{g} & \nabla_{\theta} \widetilde{g} \end{bmatrix} = J - \frac{h}{2} \Delta \\ \text{Jacobian of the original game} \\ \Delta &= \begin{bmatrix} \alpha (\nabla_{\phi} f)^2 + \alpha \nabla_{\phi} g \nabla_{\theta} f & \alpha \nabla_{\theta} f \nabla_{\phi} f + \alpha \nabla_{\theta} g \nabla_{\theta} f \\ \lambda \nabla_{\phi} g \nabla_{\theta} g + \lambda \nabla_{\phi} f \nabla_{\phi} g & \lambda (\nabla_{\theta} g)^2 + \lambda \nabla_{\theta} f \nabla_{\phi} g \end{bmatrix} \end{split}$$
Having access different ODEs for simultaneous and alternating updates, we can now analyse the stability of simultaneous and alternating gradient descent separately.





 $L_f = -E$



 $f = \nabla_{\phi} E$



Zero-sum games: simultaneous and alternating updates

Simultaneous updates

$$\tilde{L}_{\phi} = -E + \frac{\alpha h}{4} \|\nabla_{\phi} E\|^{2} - \frac{\alpha h}{4} \|\nabla_{\theta} E\|^{2}$$
$$\tilde{L}_{\theta} = E + \frac{\lambda h}{4} \|\nabla_{\theta} E\|^{2} - \frac{\lambda h}{4} \|\nabla_{\phi} E\|^{2}$$



Alternating updates





Summary

- Discretisation drift has two terms in games: the self term and interaction term
- The interaction term can destabilise the game, and using explicit regularisation to cancel it can improve stability and performance



Going beyond SGD: momentum and Adam

Beyond SGD:

- Backward error analysis for SGD with momentum
 - Implicit regularization in Heavy-ball momentum accelerated stochastic gradient descent, Avrajit Ghosh, He Lyu, Xitong Zhang, Rongrong Wang
- Backward error analysis for Adam
 - On the Implicit Bias of Adam, Matias D. Cattaneo, Jason M. Klusowski, Boris Shigida

Edge of stability results:

- on Adam
 - Adaptive Gradient Methods at the Edge of Stability, Cohen et al
- with a student at UCL, we showed that offline RL can exhibit edge of stability
 - Investigating the edge of stability phenomenon in reinforcement learning,
 - Rares Iordan, Marc Peter Deisenroth, Mihaela Rosca



Talk summary

- Continuous time approaches are a useful tool to understand optimisation
- We can use them to find implicit regularisers as well as stabilising training
- Different dynamics between one objective and two-player games
- Discretisation drift affects all our training runs!

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