Implicit Jacobian Regularization Weighted with Impurity of Probability Output

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Well-Generalized Models

 $\leftarrow \mathsf{SGD} \rightarrow$

Other Algorithms e.g. Full-batch GD

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- Natural Selection = Selection by Practitioners
- Leaves = Well-Generalized Models (goal)
- Giraffes = Learning Algorithms
- Giraffes w/ long necks = SGD (and its variants)
- Long neck = ?

Q. What are the advantageous features of SGD to find well-generalized models?

- Natural Selection = Selection by Practitioners
- Leaves = Well-Generalized Models (goal)
- Giraffes = Learning Algorithms
- Giraffes w/ long necks = SGD (and its variants)
- Long neck = Implicit Regularization in SGD!

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A. Implicit Regularization in SGD!

Implicit Jacobian Regularization Weighted with Impurity of Probability Output

$$\frac{2}{\eta} \approx \|H\|$$



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$$\begin{aligned} \frac{2}{\eta} &\approx \|H\| \approx \|G\| \\ &\uparrow \\ \text{Gauss-Newton Approximation} \\ H &:= \langle \nabla_{\theta}^2 \ell \rangle \\ G &:= \langle \nabla_{\theta} z \nabla_z^2 \ell \nabla_{\theta} z^\top \rangle = \langle JMJ^\top \rangle \\ J &:= \nabla_{\theta} z \\ M &:= \nabla_z^2 \ell \\ \text{where } \langle \cdot \rangle = \mathbb{E}_{\mathcal{D}}[\cdot] \end{aligned}$$

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At the Edge of Stability [CKL+21], $J := \nabla_{\theta} z$ \downarrow $\frac{2}{\eta} \approx \|H\| \approx \|G\| = \langle \lambda^* \|J\|^2 \rangle$ \uparrow Our Main Theorem

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$$\frac{2}{\eta} \approx \|H\| \approx \|G\| = \langle \lambda^* \|J\|^2 \rangle$$

• λ^* controls the effectiveness of IJR (high $\lambda^* \Rightarrow \text{low } \|J\|^2$). \uparrow Implicit Jacobian Regularization

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- λ^* controls the effectiveness of IJR (high $\lambda^* \Rightarrow \text{low } ||J||^2$).
- λ^* is bounded above by the norm ||M||.

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- The lower the norm $||M|| \downarrow$, the weaker the regularization effect \downarrow .
- The norm ||*M*|| acts as an adaptive regularization weight.

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- The lower the norm $||M|| \downarrow$, the weaker the regularization effect \downarrow .
- The norm ||M|| acts as an adaptive regularization weight.
- How does ||*M*|| evolve during training?

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$$M := \nabla_z^2 \ell = \operatorname{diag}(p) - pp^\top$$

 $p_{(1)}$ is the proability of the most probable class.





Figure: Inverted U-shaped curve of evolution of ||M||

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Active Regularization Period (ARP)

 $\begin{array}{lll} & \mbox{beginning} & \rightarrow \mbox{ not at the Edge of Stability yet.} \\ & \mbox{II early (ARP)} \rightarrow \mbox{high impurity} \rightarrow \mbox{strong regularization (IJR)} \\ & \mbox{III} & \mbox{later} & \rightarrow \mbox{ low impurity} \rightarrow \mbox{weak regularization (IJR)} \end{array}$



Figure: Dark orange color indicates a high impurity $\langle \lambda^{(1)} \rangle$.

• Explicit Jacobian Regularization (two-step update like SAM [FKM+21])

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