Stability of loss functions for solar wind forecasting using Deep Learning

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Introduction

- Loss functions are essential for neural network training
- Lack of stability might lead to an inability to converge
- * For simplicity, we assume operation on a normalized space with values in [-1, 1]

Definitions

- Stability: resilience in the presence of frequent outliers in the distribution
- \bullet \mathcal{X} : any given dataset
- ullet ${\mathcal Y}$: labels in a dataset, such that ${\mathcal Y} \subseteq {\mathcal X}$
- $\hat{\mathcal{Y}}$: set of outputs of deep neural network model f for all $x \in \mathcal{X}$, such that $\hat{\mathcal{Y}} \subset \mathcal{X}$
- $N = \text{Size}(\mathcal{Y}) = \text{Size}(\hat{\mathcal{Y}})$. For plotting purposes, we fix N = 300
- ullet $\mathcal{G}(\mu,\sigma)$ denotes a Gaussian distribution with mean μ and standard deviation σ

MSE and MAE

- Both functions have a lower bound of zero
- Both functions are even
- Mean Squared Error:

$$\mathsf{MSE}(\mathcal{Y}, \hat{\mathcal{Y}}) = \sum_{i=1}^N \frac{(y_i - \hat{y}_i)^2}{N}, \; y_i \in \mathcal{Y}, \; \hat{y}_i \in \hat{\mathcal{Y}}$$

• Mean Absolute Error:

$$\mathsf{MAE}(\mathcal{Y}, \hat{\mathcal{Y}}) = \sum_{i=1}^{N} \frac{|y_i - \hat{y}_i|}{N}, \; y_i \in \mathcal{Y}, \; \hat{y}_i \in \hat{\mathcal{Y}})$$

Individual contribution to output

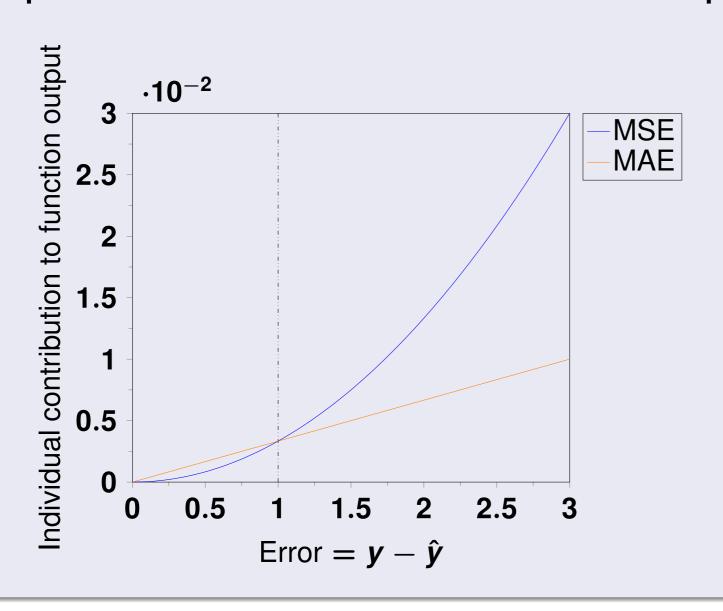
• MSE:

$$\mathsf{MSE}_i(y_i, \hat{y}_i) = \frac{(y_i - \hat{y}_i)^2}{N}, \; y_i \in \mathcal{Y}, \; \hat{y}_i \in \hat{\mathcal{Y}}$$

MAE:

$$\mathsf{MAE}_i(y_i, \hat{y}_i) = \frac{|y_i - \hat{y}_i|}{N}, \ y_i \in \mathcal{Y}, \ \hat{y}_i \in \hat{\mathcal{Y}}$$

Compared individual error contribution to function output



Derivability

- Second derivative provides information about the curvature of the loss function
- Let $E_i = y_i \hat{y}_i$:

$$\frac{d\mathsf{MSE}_i}{dE_i} = \frac{2E_i}{N} \to \frac{d^2\mathsf{MSE}_i}{dE_i} = \frac{2}{N}$$

$$\frac{d\mathsf{MAE}_i}{dE_i} = \frac{\mathsf{Sign}(E_i)}{N} \to \frac{d^2\mathsf{MAE}_i}{dE_i} = 0$$

MSE codifies a more curved space than MAE

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Considerations

- MSE weights higher errors more heavily
- MSE is less resilient to outliers than MAE \rightarrow MSE is less stable than MAE
- ullet MSE's approach can accelerate convergence in favorable scenarios ullet What conditions need to be fulfilled?

Impact of data distribution

Consider a random distribution \mathcal{D} , with mean μ and standard deviation σ . If we take a random sample \mathbf{s} , and the model currently assumes \mathcal{D} to be $\mathcal{G}(\mu, \sigma)$:

- ullet $s<\mu-\sigma$ or $s>\mu+\sigma
 ightarrow {\it E}>1.0$
- ullet $\mu \sigma \leq s \leq \mu + \sigma \rightarrow 0.0 \leq E \leq 1.0$

We consider $\mathbf{s} < \mu - \sigma$ and $> \mu + \sigma$ as outliers. Depending on \mathcal{D} :

- $\bullet \ \mathcal{D} \sim \mathcal{G}(\mu, \sigma) \rightarrow \textit{P}(\textit{\textbf{s}} < \mu \sigma) \sim \textit{P}(\textit{\textbf{s}} > \mu + \sigma) \ll \textit{P}(\mu \sigma \leq \textit{\textbf{s}} \leq \mu + \sigma)$
- $\mathcal{D} \nsim \mathcal{G}(\mu, \sigma) \to$ the distribution needs to be examined to determine probabilities

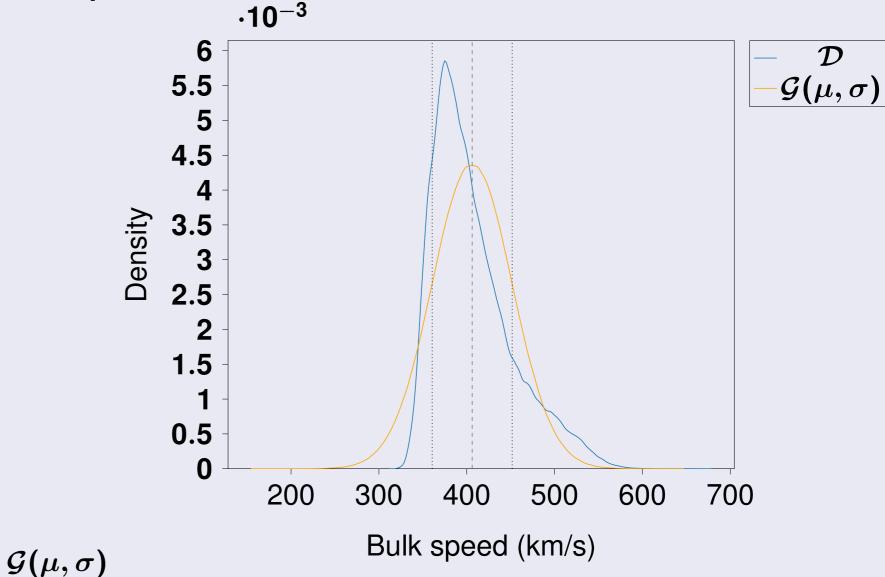
For $\mathcal{D} \sim \mathcal{G}(\mu, \sigma)$:

- $P(s < \mu \sigma) > P(s > \mu + \sigma) \rightarrow$ MSE will lead to the resulting model preferring lower values
- $P(s < \mu \sigma) < P(s > \mu + \sigma) \rightarrow$ MSE will lead to the resulting model preferring higher values
- $P(s < \mu \sigma) \sim P(s > \mu + \sigma) \sim P(\mu \sigma \le s \le \mu + \sigma) \rightarrow \text{MSE}$ might not be able to converge

Solar wind data distribution

Dataset ranges from 1 January 2011 to 1 September 2021

Comparison of observed distribution \mathcal{D} with ideal distribution



- ullet $\mathcal{D} \nsim \mathcal{G}(\mu, \sigma)$
- $P(s < \mu \sigma) \sim P(s > \mu + \sigma) \sim P(\mu \sigma \le s \le \mu + \sigma)$ observed
- MSE can lead to marked bias
 - The constant change in bias can lead to an inability to converge

Conclusions

- MAE is a more stable loss function than MSE
- MSE is applicable to most scenarios
- MSE should converge in heavy tail distributions, at the expense of biasing the resulting model
- Solar wind bulk speed data is not normally distributed
- MAE is preferred as a loss function for solar wind bulk speed regression using deep neural networks

References

- 1. Bar-Lev, S. K., Boukai, B. & Enis, P. On the mean squared error, the mean absolute error and the like. *Communications in Statistics Theory and Methods* **28**, 1813–1822 (1999).
- Willmott, C. J. & Matsuura, K. Advantages of the mean absolute error (MAE) over the root mean square error (RMSE) in assessing average model performance. *Climate Research* 30, 79–82 (2005).
- 3. Qi, J., Du, J., Siniscalchi, S. M., Ma, X. & Lee, C.-H. On Mean Absolute Error for Deep Neural Network Based Vector-to-Vector Regression. *IEEE Signal Processing Letters* **27**, 1485–1489 (2020).
- 4. Larrodera, C. & Cid, C. Bimodal distribution of the solar wind at 1 AU. *A&A* 635, A44 (2020).