How can we quantify, explain and apply the uncertainty of complex soil maps predicted with neural networks?

Kerstin Rau

Thomas Gläßle, Philipp Hennig, and Thomas Scholten

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machine learning new perspectives for science

Soil Science and Geomorphology
University of Tübingen

EGU

Measuring uncertainty of Neural Networks: present vs. future

what we should change

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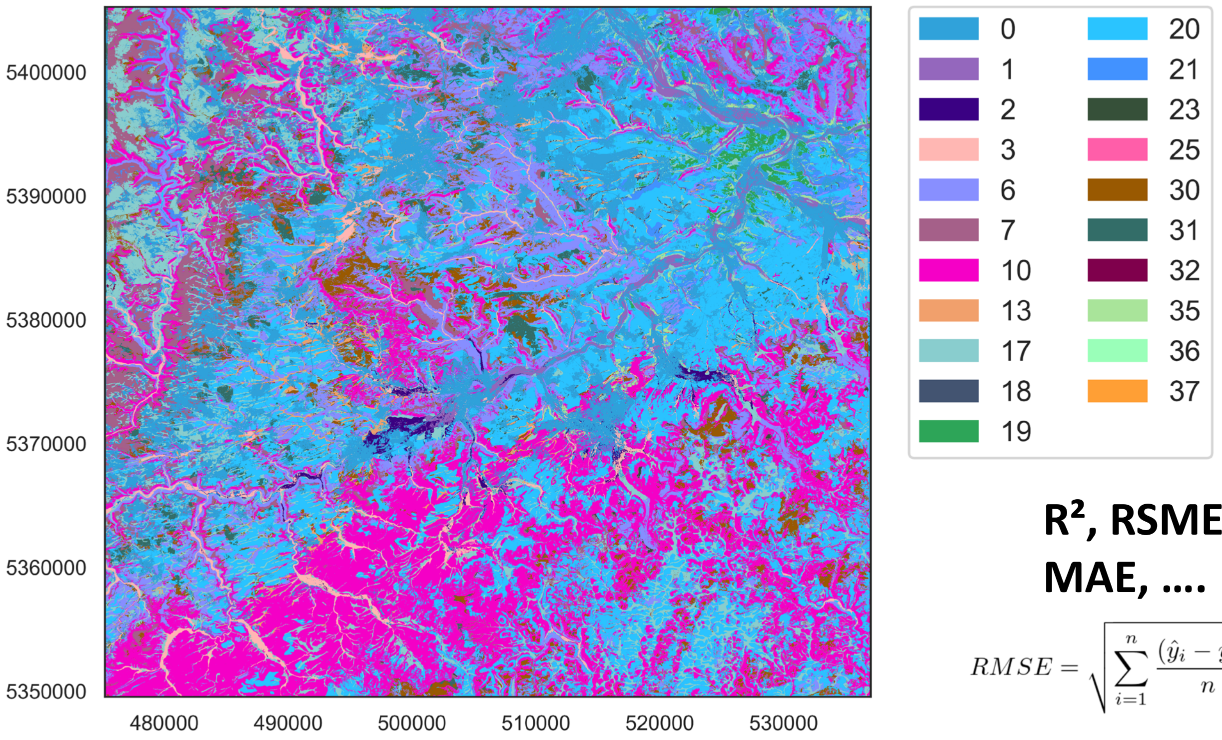
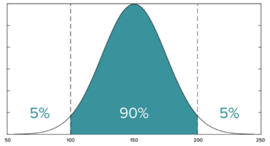


How do we now analyse the uncertainty of the map?

R², RSME, MAE, ….

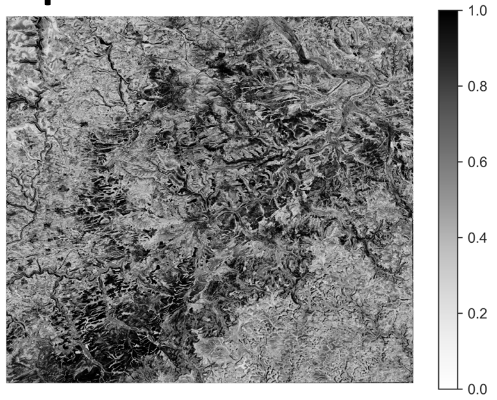
$$RMSE = \sqrt{\sum_{i=1}^{n} \frac{(\hat{y}_i - y_i)^2}{n}}$$

confidence intervals



other statistical calculation methods

looking at the probability of the predicted class



new way?

Last-Layer Laplace Approximation

PICO3b.8

Kerstin Rau, Thomas Gläßle, Philipp Hennig, and Thomas Scholten, Cluster of Excellence Machine Learning University of Tübingen

What was the inspiration and how do we want to achieve it?

a quick overview of our motivation

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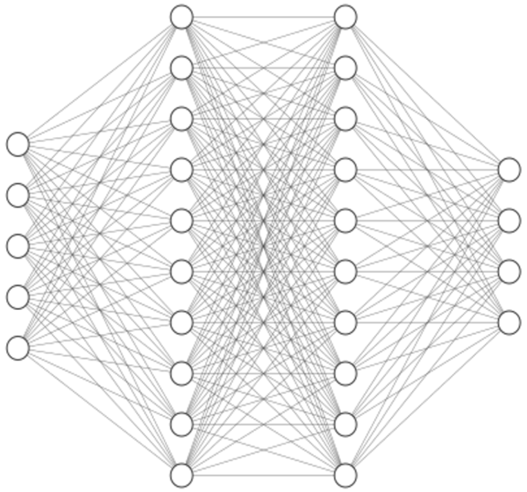
Use of Articfical Neural Networks in Geoscience increased

because

... they are able to process **large amounts** of data and compute accordingly fast, even for high-resolution maps (McBratney et al., 2003)
... with prepared build-in functions **easy to access**, programm and not difficult to customise
... were **more accurate** in predicting soil taxonomy classes and obtain high- resolution maps (Brungard et al. 2015)

but

... they are difficult to interpret
... **black box** model
... **overconfident** in areas with low data or far away (Nguyen et al., 2014; Hein et al., 2019)



and still

... often just used a **single statistical number** to evaluate their whole prediction (Meyer and Pebesma (2022))
... they do not go beyond looking at the **probability of the predicted class** or related statistical calculation methods (Wadoux et al. (2020))

idea

... using **Last-Layer Laplace Approximation** to estimate the posterior uncertainty of the model, created by Kristiadi et al., 2020, which works well with MINST or CIFAR10

why?

... help in the **interpretation** of the results
... analysis of the prediction of the artificial network for a possible **transferability**
... provide **new insights** into soil processes and the structure of the different domains.

Study area
and its special features

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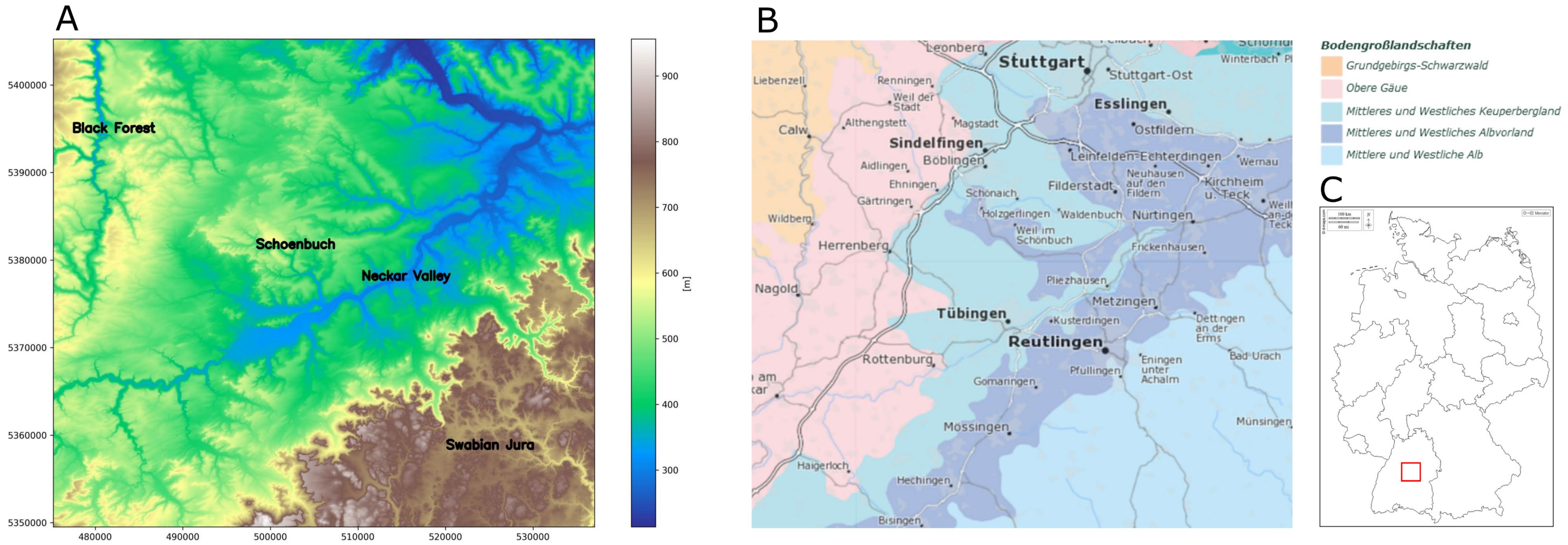

(A) Digital elevation model of the study area with its important landscapes: outstanding areas Swabian Jura (SJ) and Black Forest (BF) with their unique soil types, **(B)** Distribution of the five major soil landscapes with different characterisation: the lightest blue was formed under maritime conditions, the others under terrain, **(C)** location of the study area in Germany

Examples from our collected input data

topographic, hydrological, spectral, geological

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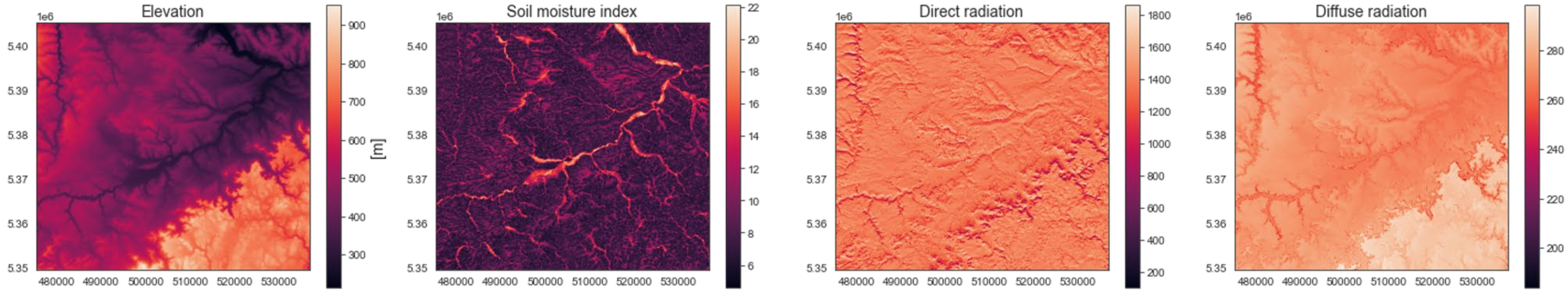
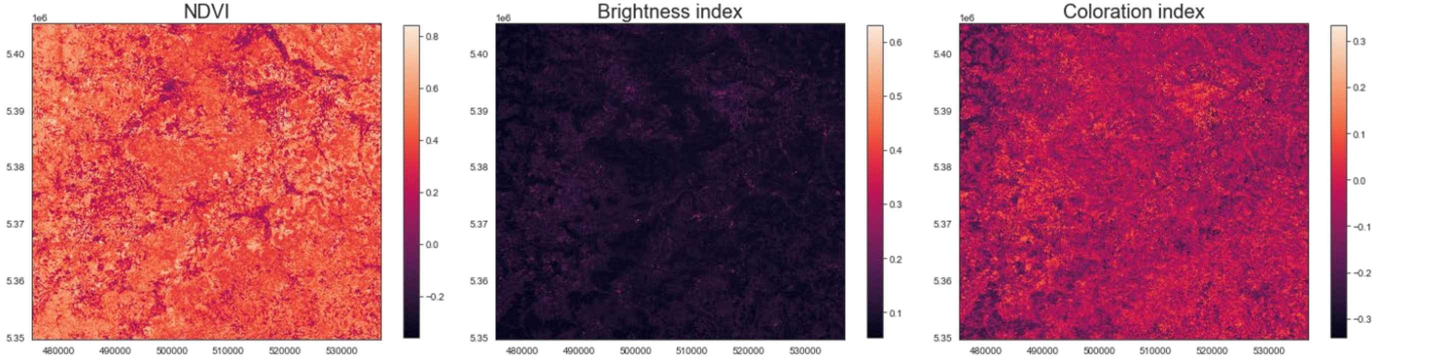
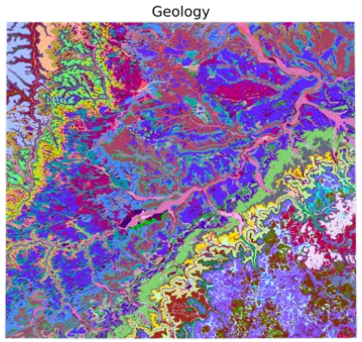
DEM and its derivates



Sentinel-2



Geology map

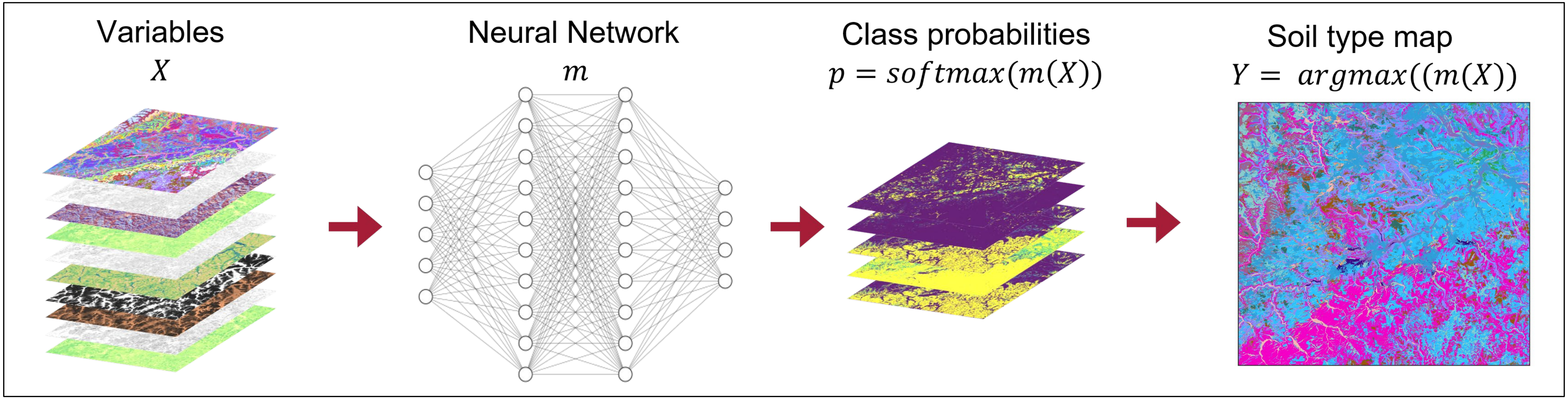


- Topographic and hydrologic indices derived from the DEM
- Spectral indices calculated with Sentinel-2 satellite bands
- Geological map

➢ In total:
33 variables with a resolution of 10 m

General setup
overview of our approach

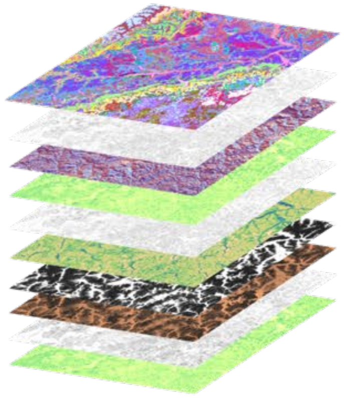
General structure of a soil type map processed with a multilayer perception with four linear layers, first three followed by a ReLU activation function. The class with the highest probability at the pixel was chosen for the map.



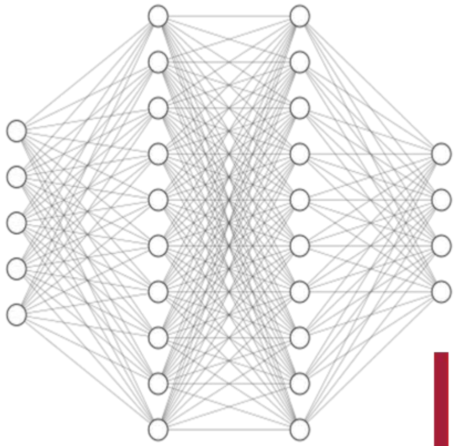
Last-layer Laplace Approximation (LA)

a Bayesian approach

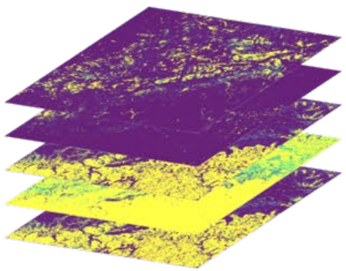
Variables
X



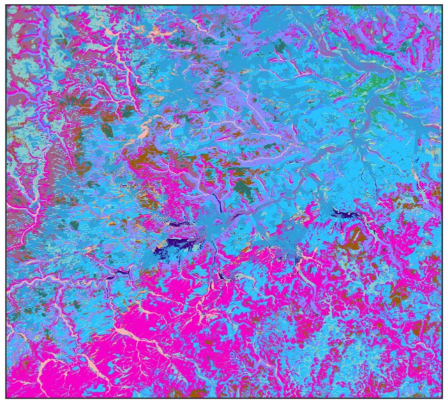
Neural Network
m



Class probabilities
$p = softmax(m(X))$



Soil type map
$Y = argmax((m(X))$



On the weights of the last linear layer!

Approximation of the posterior:

$$p(\Theta|D) \approx \mathcal{N}(\Theta; \Theta_{MAP}, \Sigma) \qquad \textit{with} \qquad \Sigma := (\nabla^2_{\Theta}\mathcal{L}(\mathcal{D};\Theta)|_{\Theta_{MAP}})^{-1}$$

where Θ_{MAP} is the maximum a posteriori estimate of the parameters, obtained by minimizing the negative log posterior $\mathcal{L}(\mathcal{D};\Theta)$.

Prediction of the soil type map

finish product?

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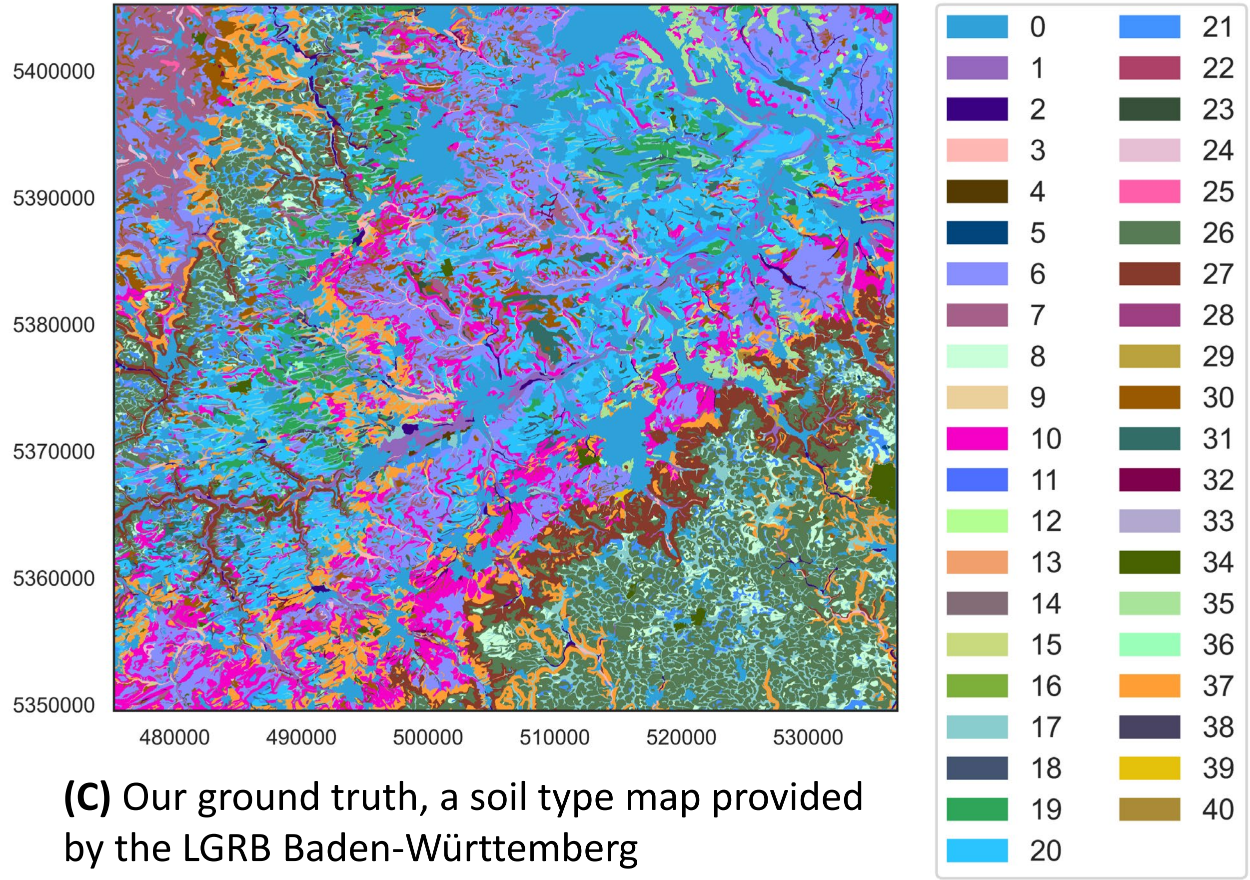
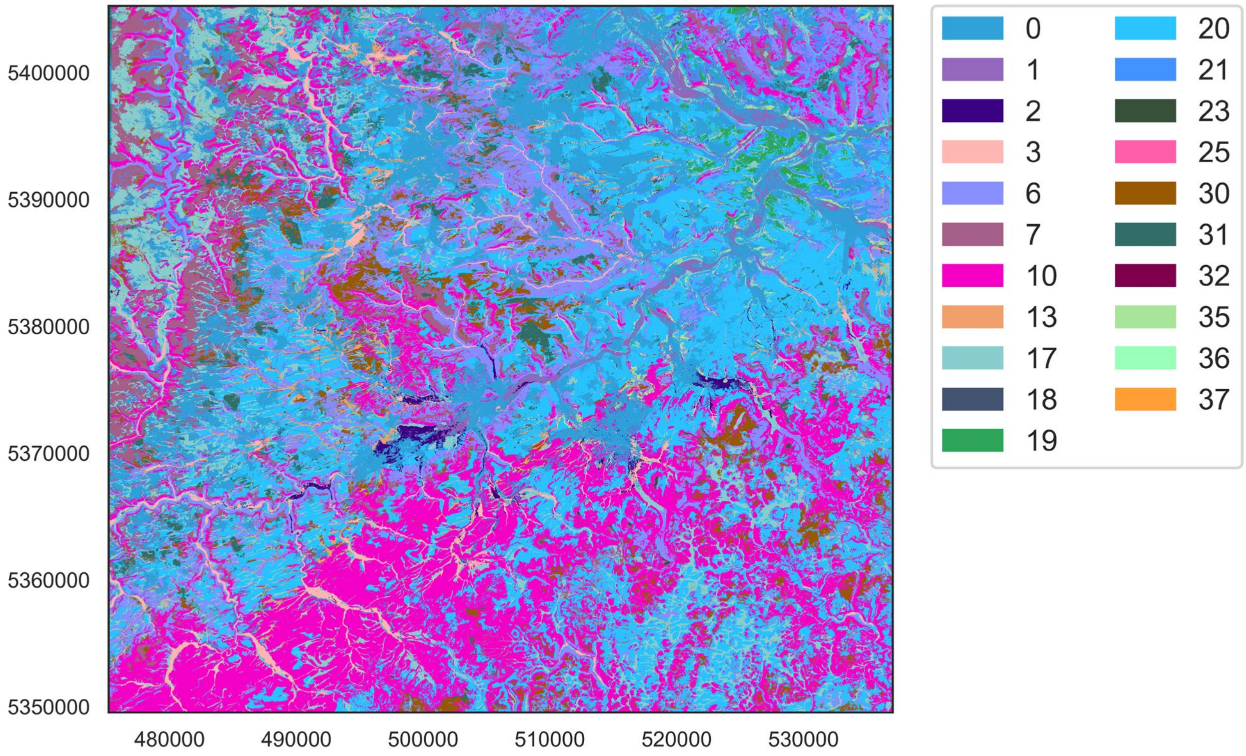
C



(C) Our ground truth, a soil type map provided by the LGRB Baden-Württemberg

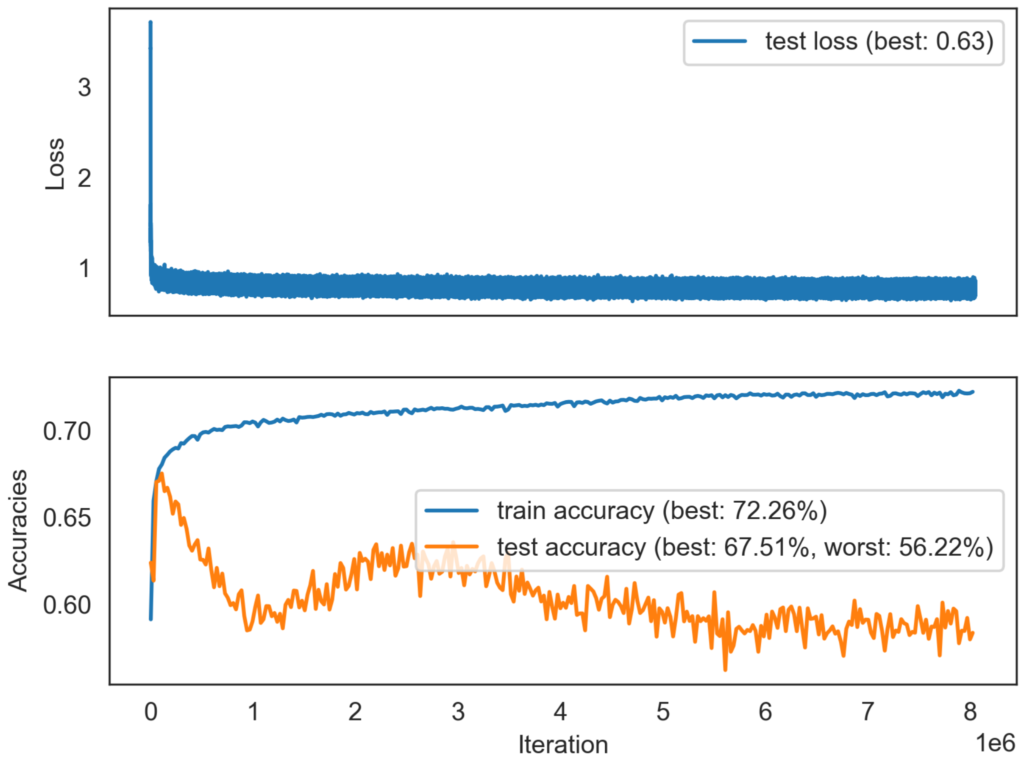
E



(E) Certain soil types (0, 10, and 17) that are generally less related to site conditions (e.g., Cambisol) are overestimated, especially in areas BF and SJ. These two areas are logically poorly represented by the MLP's choice of training areas.

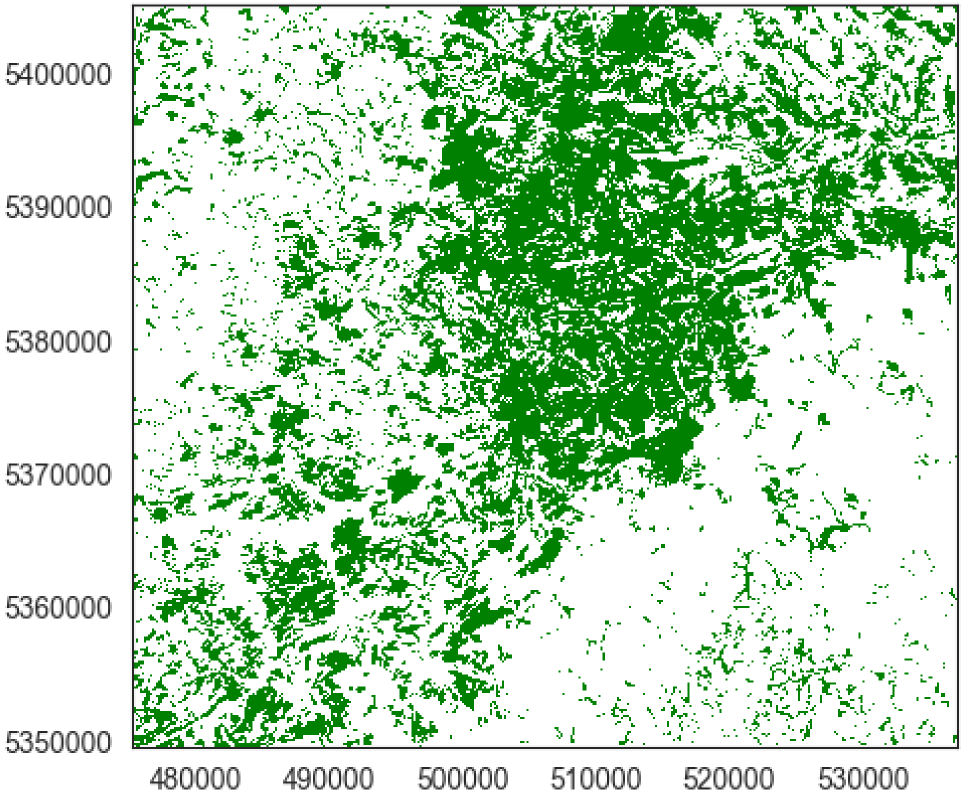
Prediction of the soil type map
performance

F



(F) Loss and accuracy of the MLP, variations in test accuracy occur, due to the uneven distribution of soil types in training and test area

G



(G) Comparison of prediction with ground truth: green means correct prediction of soil type. It **confirms that the areas BF and SJ are not well predicted.**

Uncertainty of the model

can we trust our results?

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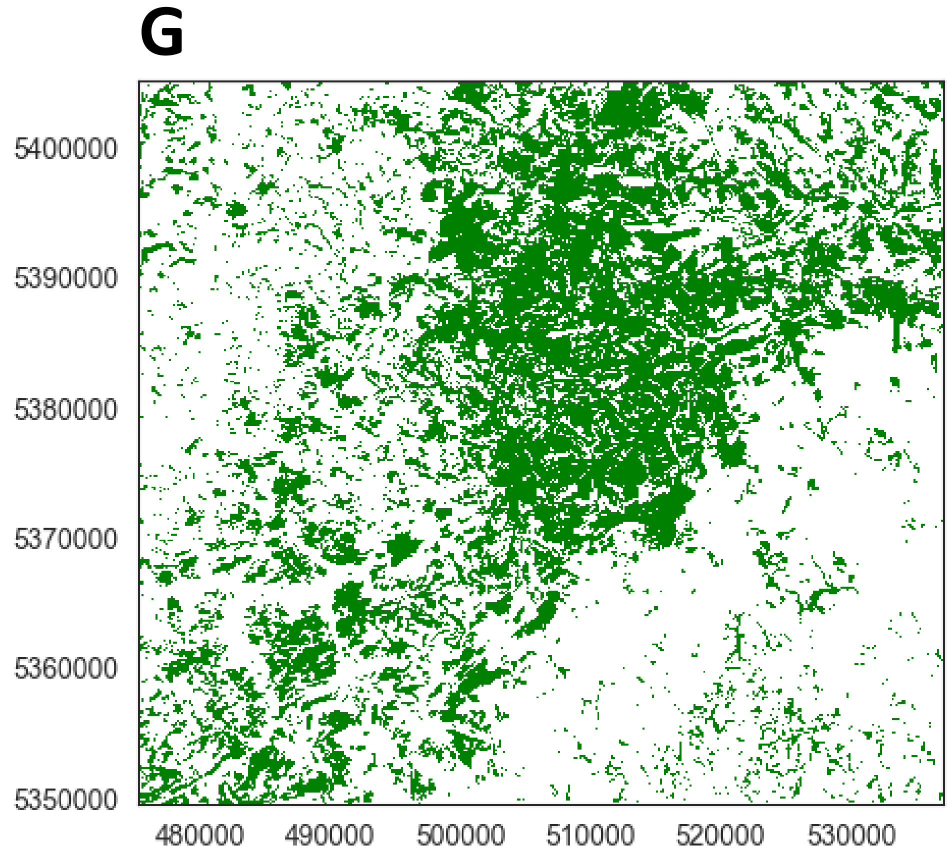
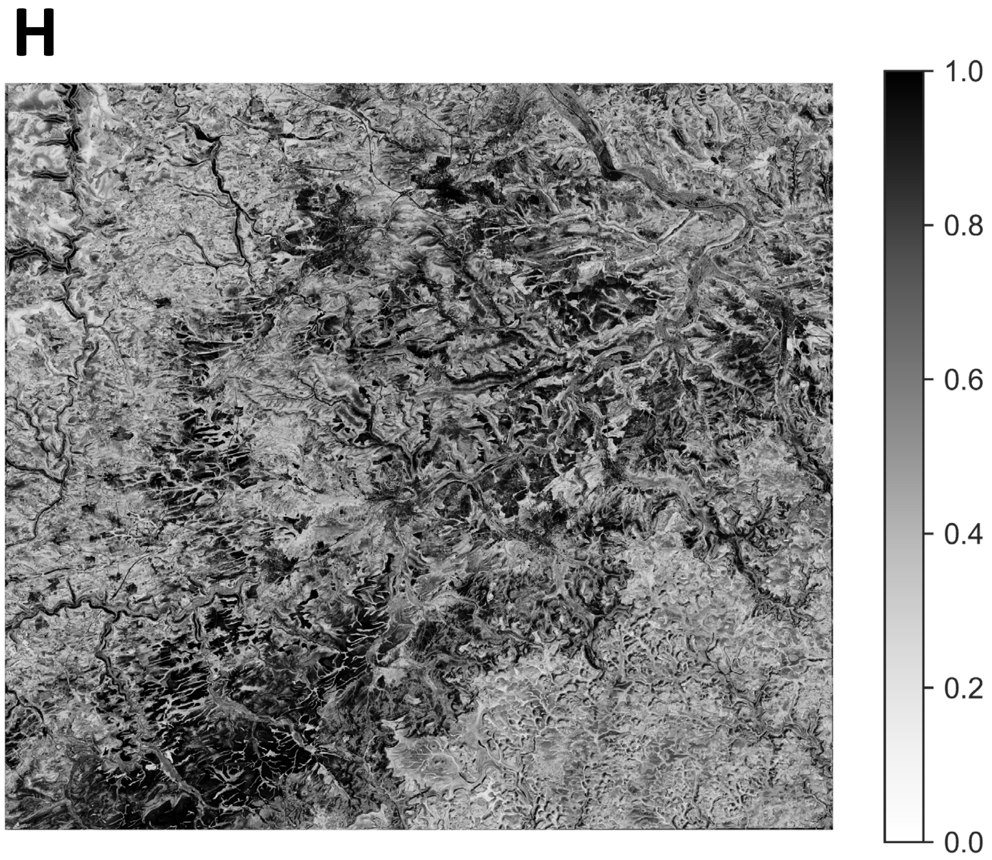




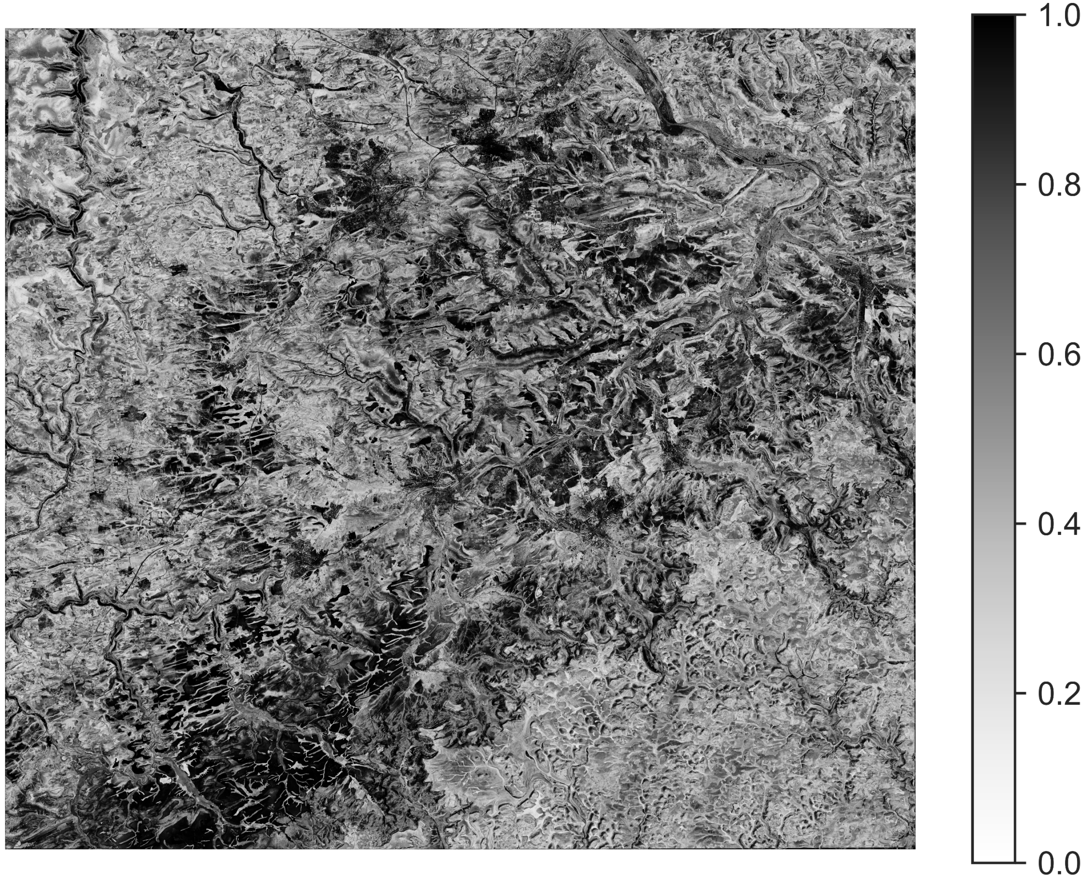
(G) Comparison of prediction with ground truth: green means correct prediction of soil type,
(H) probability of the class predicted by the MLP calculated with the SoftMax function

Results: SJ and BF were detected with high and low certainty, in the southwest of the area with high certainty up to 1 in some areas, although everywhere the prediction of soil types is wrong

Uncertainty before vs. after LA

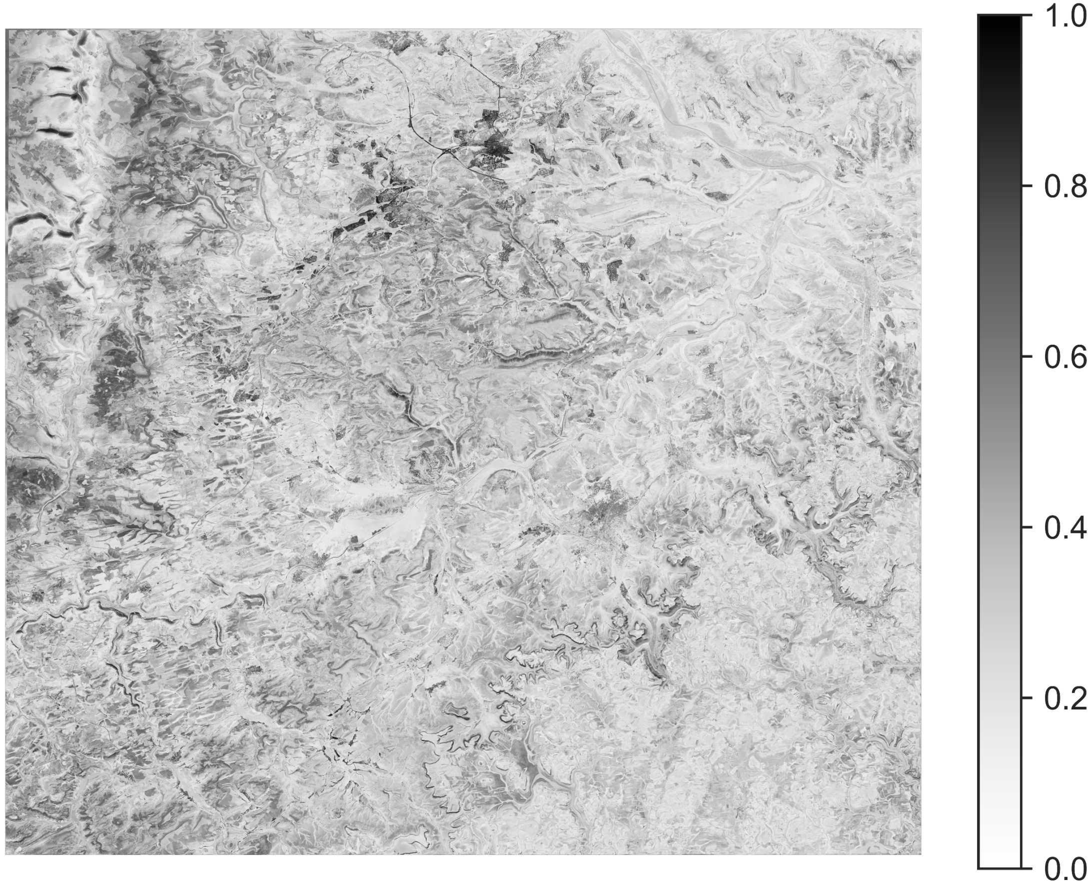
detect the overconfidence

H



applying LA

I



(H) probability of the class predicted by the MLP calculated with the SoftMax function, **(I)** probability after applying the last-layer Laplace approximation.

Result: The probability is now lower overall, but we get a more heterogeneous picture of the probability of the different classes at each point, especially around BF and SJ.

Conclusion

what we can draw from it and what we need to look at further

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- Investigate why the confidence in the training and test area also decreases.
- Look at the data pixel by pixel, what is changing for each soil class.
- Leave the test case and apply it to a real area where cartographers will also create a map.
- Comparison of pixel-based multilayer perception with multilayer perception with context-dependent input data and convolutional neural networks.
- Potential transferability to regions similar to, but spatially independent of, the training area.
- Obtain new knowledge about the relationship and similarity of soil types and their geography in different areas.

References

for the main ideas

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Thank you for your attention!
Any questions?

kerstin.rau@uni-tuebingen.de

@kerstin_rau

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