Deep Learning for Bacteria Identification using Raman Spectroscopy

Advanced Machine Learning

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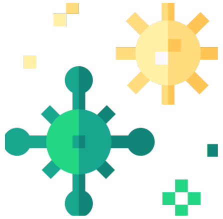
Introduction

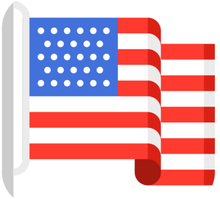
- *Raman spectroscopy* has the potential to identify the species of bacteria and its antibiotic susceptibility

- Classical ML techniques have been widely applied, while relatively little work was done in adapting DL models

Bacterial infections



6.7 million deaths every year



$33 billion for annual healthcare spending in the USA

Project Goals

30-class task

- *Develop* an efficient CNN architecture
- *Compare* it with a state-of-the-art CNN

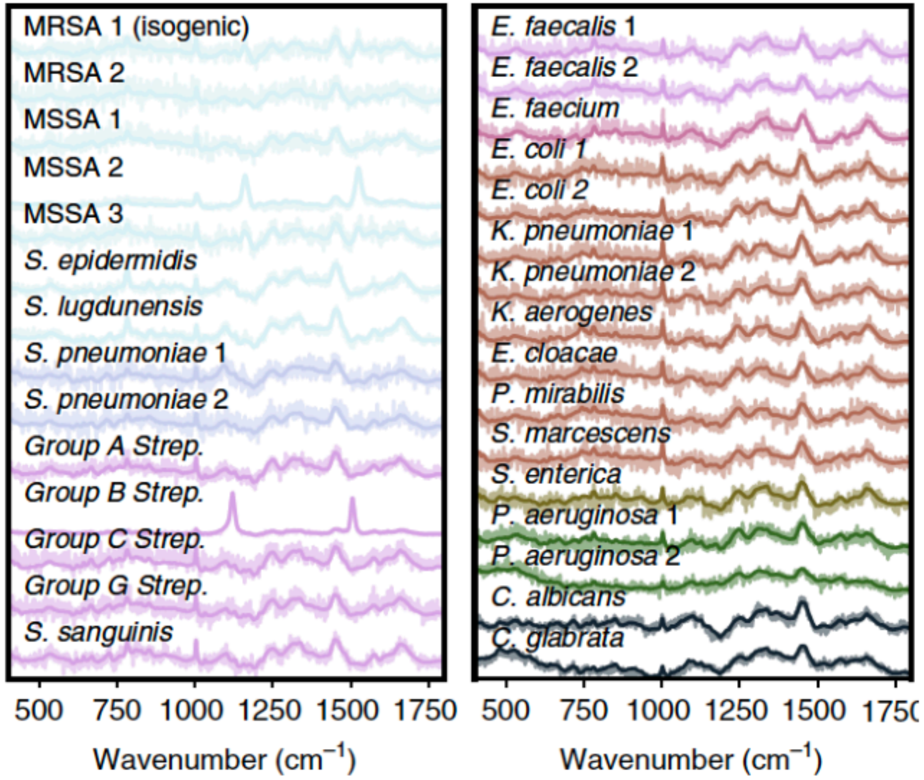
15-class task

- *Fine-tuning* process on our CNN model
- *Compare* it against two ML algorithms

Dataset

- *Training* dataset of 60 000 spectra (2 000 per class)
- *Fine-tuning* and (<u>independent</u>) *test* datasets each of 3 000 spectra (100 per class)
- 30 bacterial isolate classes

94% of all bacterial infections treated at Stanford Hospital in the years 2016–2017



30-Class Task – Challenge

- Is the reference CNN architecture *overkill*?

Reference CNN

- 26 layers
- 1 340 000 parameters

30-Class Task – CNN

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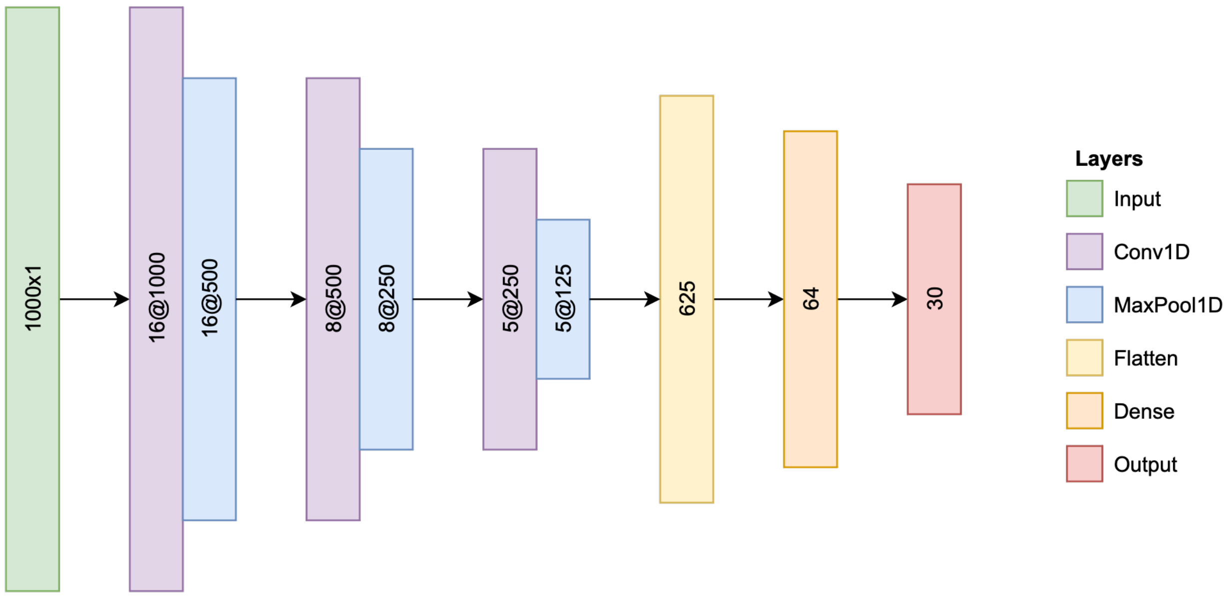


Reference CNN

- 26 layers
- 1 340 000 parameters

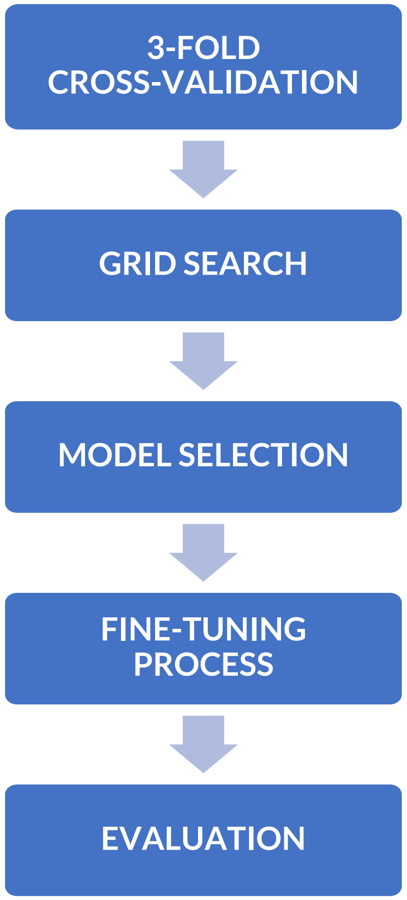
Proposed CNN

- 6 layers
- 42 000 parameters (*96.8% less*)

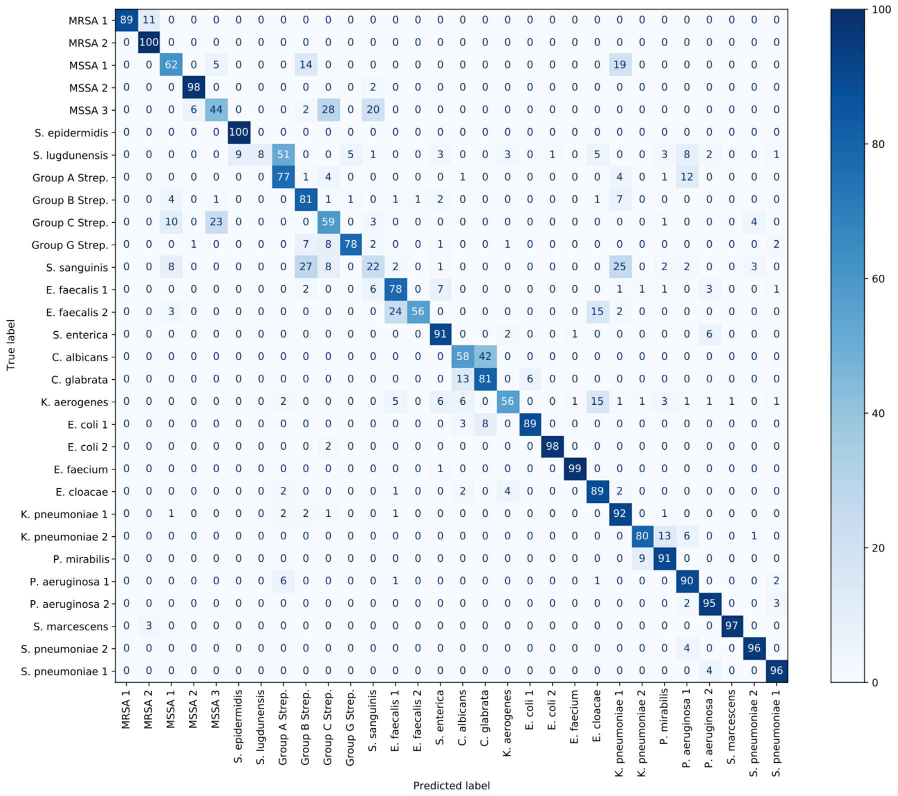
30-Class Task – Experimental Plan

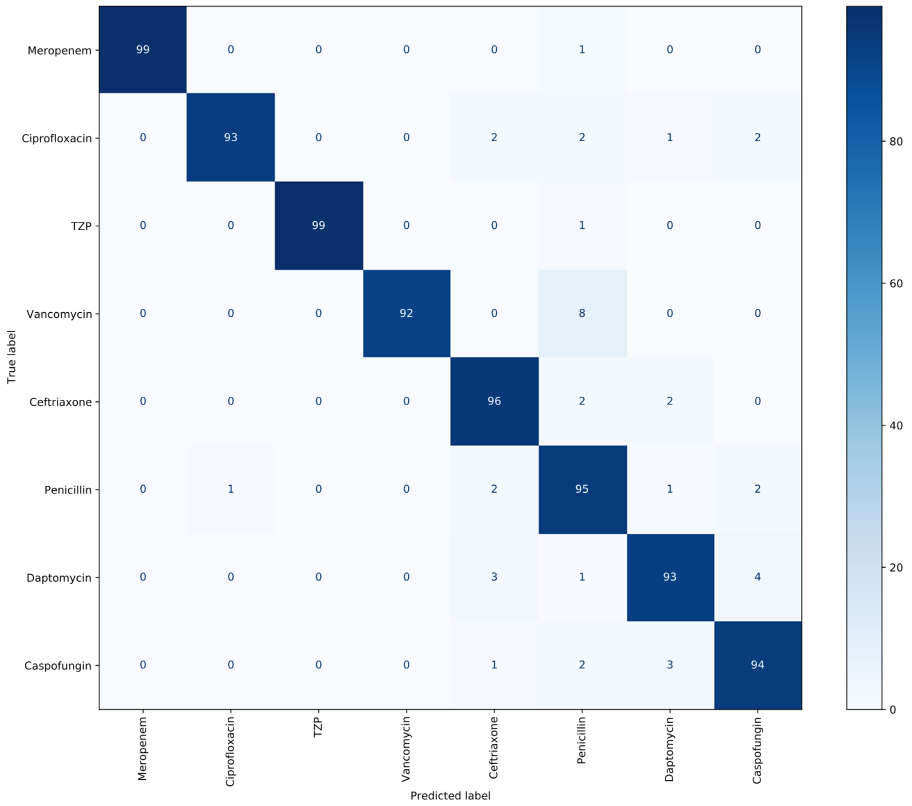
- *3-fold cross-validation* on the training data via *grid search* (144 experiments in total)
- Average test accuracy to perform *model selection*
- Split *fine-tuning* data into 80% train and 20% validation to further train and detect <u>overfitting</u>
- *Evaluation* on test data

Hyperparameter	Values
batch_size	16, 32, *64*
conv_layer	2, *3*
filters	*16*, 32
kernel_size	*3*, 5
units	*256*, 512, 1024
dropout_rate	.3, *.5*



30-Class Task – Results





REFERENCE:
82.2±0.3%

PROPOSED:
78.3%

REFERENCE:
97.0±0.3%

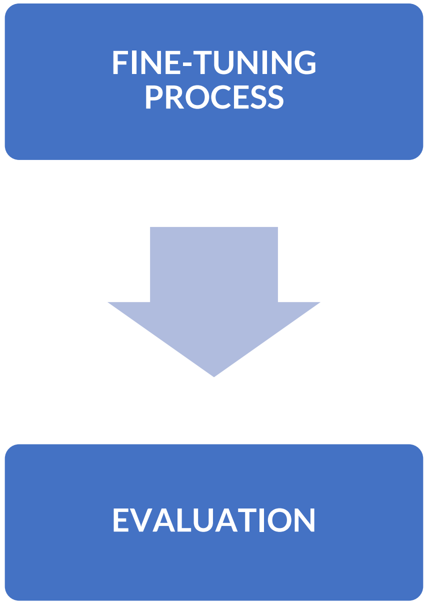
PROPOSED:
94.9%

15-Class Task – Challenge

- Can SVM and MLP be used on a smaller 15-class classification task?
- Are the *performances comparable* to those achieved by our CNN model?

15-Class Task – CNN

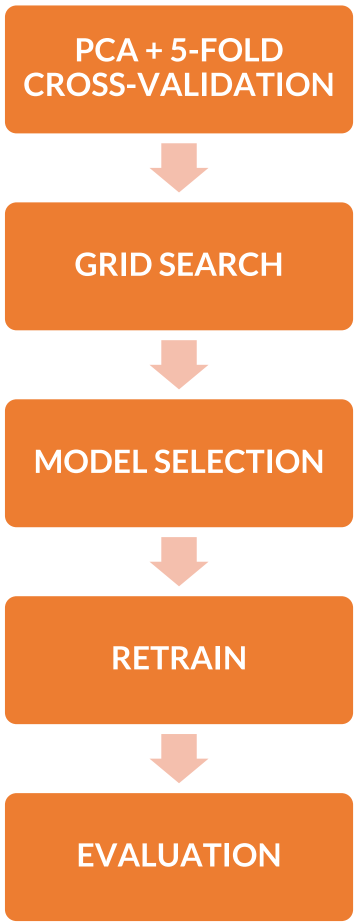
- Can SVM and MLP be used on a smaller 15-class classification task?
- Are the *performances comparable* to those achieved by our CNN model?
- For the CNN model we exploit the *fine-tuning process* on the 15-class



15-Class Task – SVM

- *PCA* to reduce input dimension from 1000 to 20
- *5-fold cross-validation* on fine-tuning dataset via *grid search* (32 experiments in total)
- Average test accuracy to perform *model selection*
- *Retraining* on the entire fine-tuning dataset
- *Evaluation* on test data

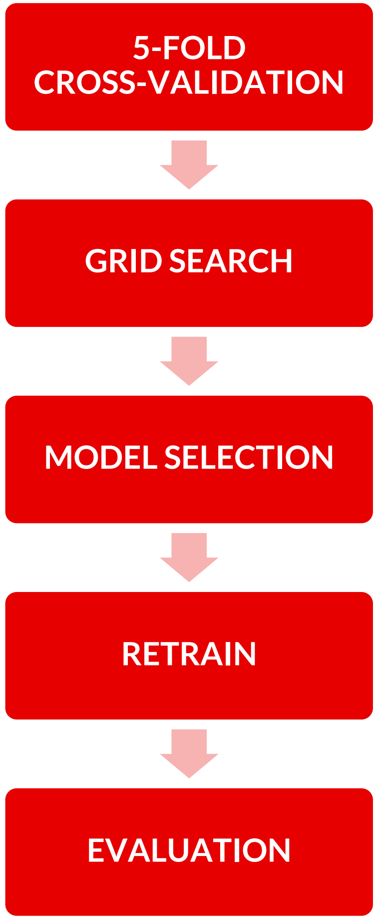
Hyperparameter	Values
kernel	rbf, *linear*
gamma	*0*, .001, .0001
C	*1*, 10, 100, 1000



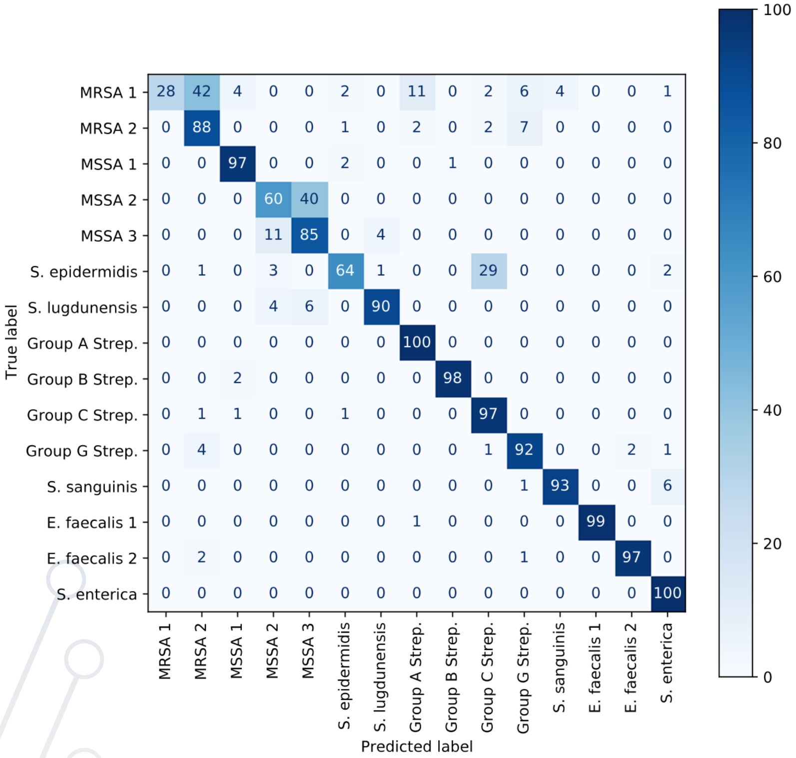
15-Class Task – MLP

- *5-fold cross-validation* on fine-tuning dataset via *grid search* (36 experiments in total)
- Average test accuracy to perform *model selection*
- Split fine-tuning data into 80% train and 20% validation to *retrain* the selected model and detect <u>overfitting</u>
- *Evaluation* on test data

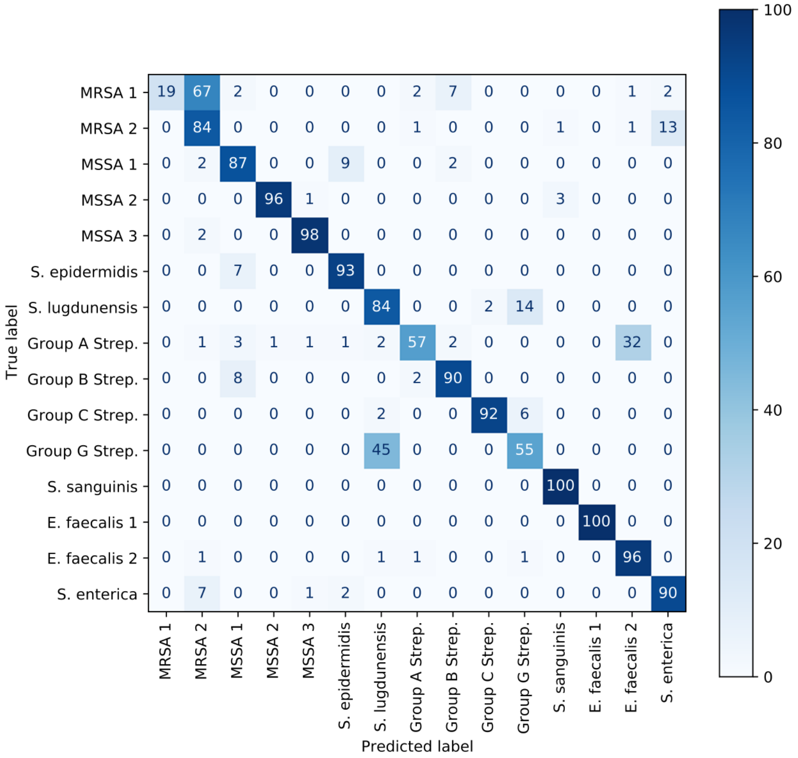
Hyperparameter	Values
batch_size	16, 32, *64*
units	*256*, 512
hidden_layers	*1*, 2, 3
dropout_rate	.3, *.5*



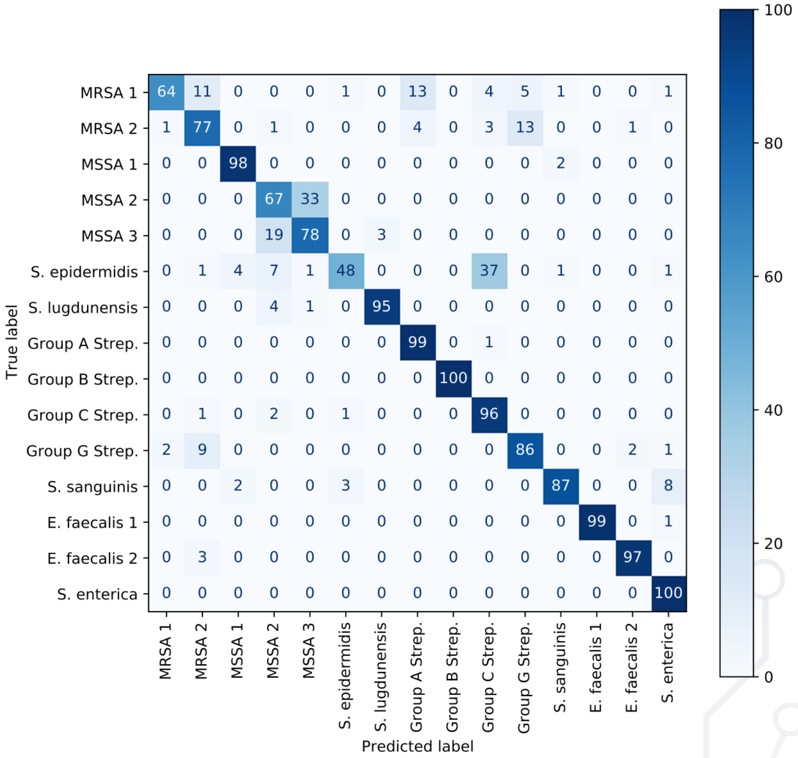
15-Class Task – Bacterial Results



CNN:
85.1%

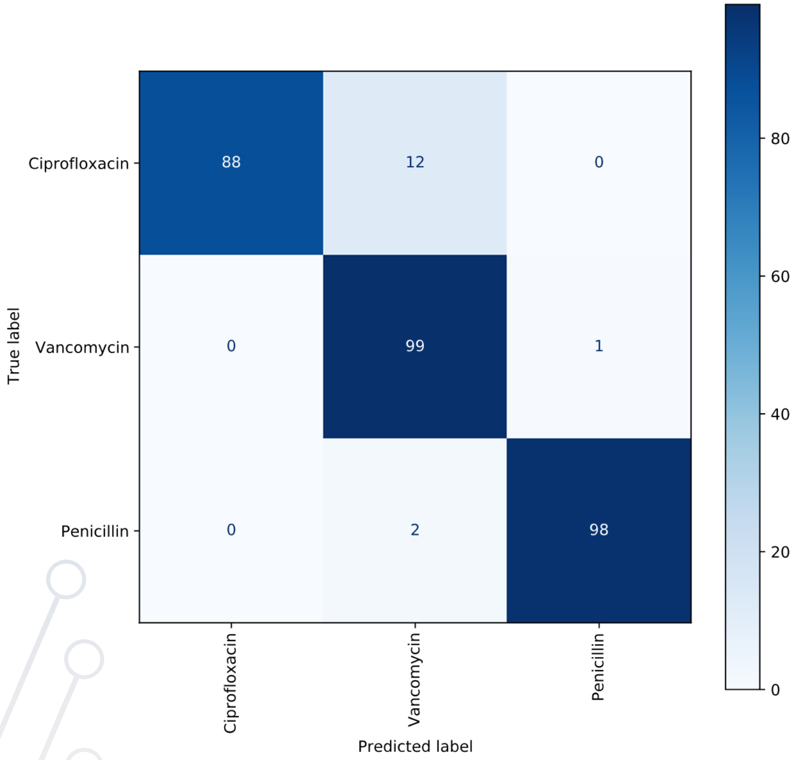


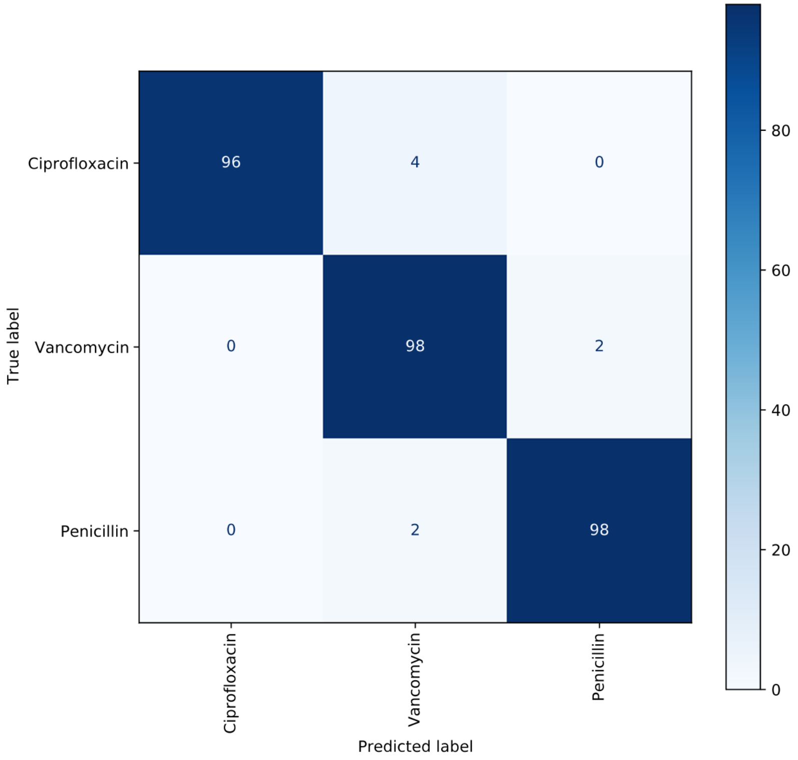
SVM:
82.7%

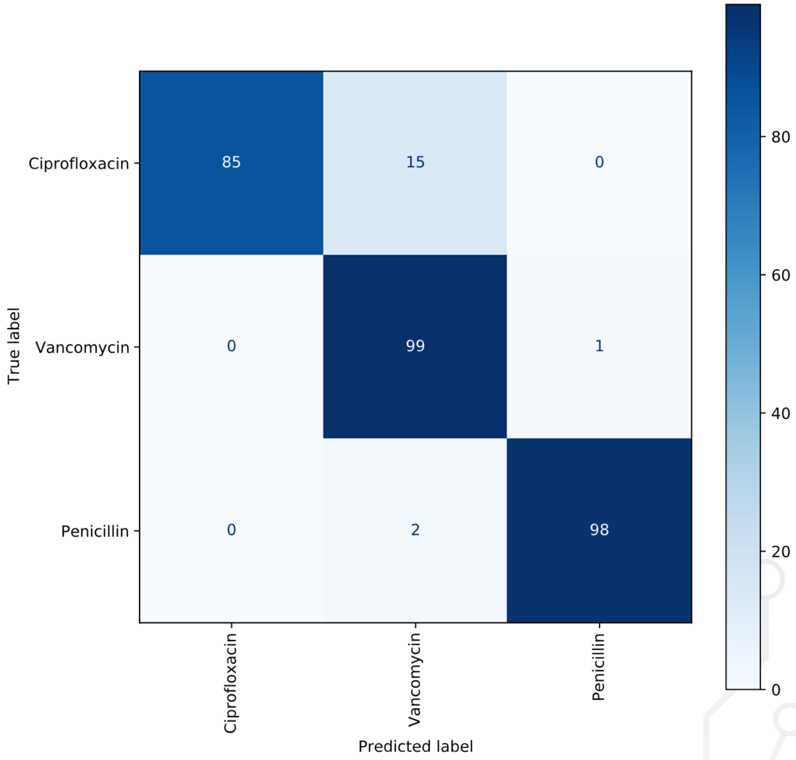


MLP:
85.0%

15-Class Task – Antibiotics Results







CNN: **98%**

SVM: **97.7%**

MLP: **97.5%**

Conclusions

- On the 30-class task, the presented CNN architecture achieves *comparable performance* with a state-of-the-art CNN, although with *less parameters*
- On the 15-class task, classical ML techniques reported *good results*
- In general, *misclassifications* are mostly within antibiotic groupings, and thus do not affect the treatment outcome

DL techniques applied to Raman spectra would allow for accurate and targeted treatment of bacterial infections within hours, reducing healthcare costs, antibiotics misuse and improving patient outcomes

References

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