CSC510 SOFTWARE ENGINEERING

AI + SE

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WHAT YOU WILL LEARN TODAY

→ Slightly fast-paced: we have a lot of ground to cover!
→ The importance of theory in applied ML, such as in SE
→ The temporal delay between AI venues (NeurIPS, ICLR, ICML, JMLR, etc.) and SE venues (ICSE, TSE, JSS, etc.)
→ The ML4SE process
→ A gentle introduction to SE4ML

OVERVIEW

1. The varying perspectives

2. Examples

3. The AI4SE process

4. SE4ML

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- Applied ML focuses on results, with lesser focus on why something works.
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  - However, some papers use intuitions (not backed by theory) to understand certain behaviors of algorithms, and devise ways to circumvent or prevent it [18].

AI FOR SE VS. AI FOR SE

- → A slightly philosophical approach: which do you treat as a first-class citizen?
- → More precisely, how much domain knowledge do you use in your learning?

THEORETICAL AI IN SE

→ Monolithic architecture to microservices: Desai et al. [6]

$$\min_{W,O,M,C} \mathcal{L}_{total} = \alpha_1 \mathcal{L}_{str} + \alpha_2 \mathcal{L}_{attr} + \alpha_3 \mathcal{L}_{clus}$$

$$\text{such that } \sum_{i \in V} O_{si} = \sum_{i \in V} O_{ai} = 1$$

$$M \in \{0, 1\}^{|V| n \times K}, O_{si}, O_{ai} > 0$$

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- Feedforward networks work very well: Yedida and Menzies [18]:
  - From Hornik [10]: If ψ is unbounded and nonconstant, then $\mathfrak{R}(\psi)$ is dense in $L^p(\mu)$ for all finite measures μ on $\mathbb{R}^k$.
  - From Montufar et al. [14] The maximal number of linear regions of the functions computed by a neural network with n_0 input units and L hidden layers, with $n_i \geq n_0$ rectifiers at the i-th layer, is lower bounded by

$$\left(\prod_{i=1}^{L-1} \left\lfloor \frac{n_i}{n_0} \right\rfloor^{n_0} \right) \sum_{j=0}^{n_0} \binom{n_L}{j}$$

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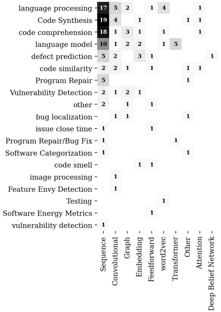
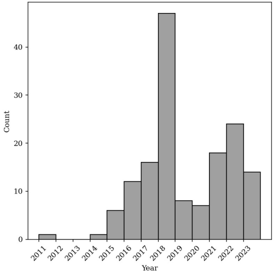
- Our current work: hyper-parameter optimization using smoothness of the loss function.

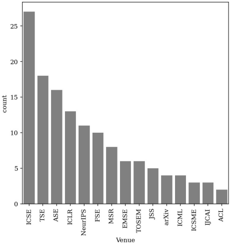
APPLIED AI IN SE

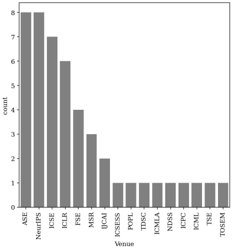
- → 95% of papers in AI for SE
- → Xu et al. [17]: Stack Overflow posts to vectors
- → Prenner and Robbes [16]: Transformer models are competitive when used for small SE datasets, especially for natural language.
- → Agrawal et al. [1]: A novel hyper-parameter optimization that relies on the $\epsilon-$domination principle.

DL FOR SE: A BROAD VIEW









DATA COLLECTION

- Two main ways: static attributes and automated methods
- Static methods:
  - Example: the PROMISE repository [13]
  - Rather out of fashion lately
- Automated methods:
  - Source-code based, using Transformer architectures [7, 8, 12]
  - Graph neural networks: [15, 19]

LEARNING ALGORITHMS I

- Gaussian Discriminant Analysis: when your data comes from Gaussian distributions.
  - A fun example from computational neuroscience: decision making in the visual cortex uses a likelihood ratio to discriminate between signals and noise (why? see Neyman-Pearson lemma) [3, 5]
  -

$$
\begin{aligned}
y &\sim \text{Bernoulli}(\phi) \\
\mathrm{x}|y = 0 &\sim \mathcal{N}(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}) \\
\mathrm{x}|y = 1 &\sim \mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma})
\end{aligned}
$$

LEARNING ALGORITHMS II

- Support Vector Machines: when you can take advantage of kernel learning and want a maximum-margin classifier.

$$\max_{\boldsymbol{\lambda}} \sum_{i=1}^{m} \lambda_i - \frac{1}{2} \sum_{i=1}^{m} \sum_{j=1}^{m} \lambda_i \lambda_j y^{(i)} y^{(j)} \left\langle x^{(i)}, x^{(j)} \right\rangle$$

$$\text{s.t. } \lambda_i \geq 0$$

$$\sum_{i=1}^{m} \lambda_i y^{(i)} = 0$$

- Decision trees: When you need interpretable decision-making
  - Very useful in the context of knowledge distillation: Liu et al. [11]
- Neural networks: when you want automated feature extraction, want to make use of pre-trained models, or want a higher VC-dimension.

LEARNING ALGORITHMS III

- → Deep ReLU networks have a much higher VC-dimension than classical models: Bartlett et al. [2], Harvey et al. [9]: VC-dimension is $\mathcal{O}(WL \log W)$ or $\Theta(WU)$
- → They can require much more computational power, however.

ANALYSIS

- Statistics!
  - Your results mean nothing without stats to back them up.
  - Examples: t-test (parametric, assumes t-distributed), Kruskal-Wallis (non-parametric, independence), ANOVA (parametric, homogeneity of variance), Mann-Whitney (non-parametric, independence),
  - Mantel-Haenszel: for testing the association between two categorical variables (example: smoking/not smoking vs. lung cancer/cancer-free), when controlling for a confounding variable (example: age)
- Pretty graphs
  - Even peer-reviewers want something pretty to look at.
  - Common tools: Matplotlib, Seaborn, plot.ly

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  - As discussed previously, we can exploit theoretical results (Hornik [10], Montufar et al. [14])
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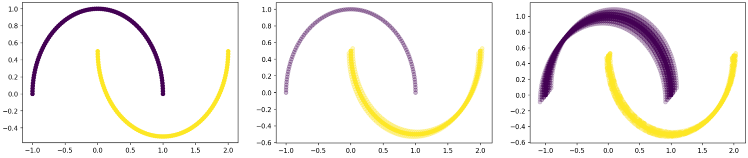
- Compute: Slurm cluster

FUZZY SAMPLING



(a) Original data (b) Fuzzy sampling (c) Ultrasampling

HYPER-PARAMETER OPTIMIZATION —

Theorem (Smoothness for feedforward networks)

For a feedforward network with ReLU activations in the hidden layers and a softmax activation at the last layer, the $\beta-$smoothness of the cross-entropy loss is given by

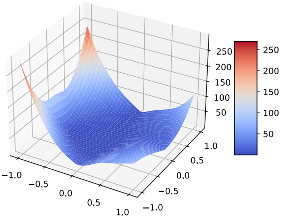
$$\|\nabla_W^2 E\| \leq \frac{k-1}{km} \max \frac{\|a_j^{L-1}\|}{\|W^{[L]}\|} \tag{2}$$

There is, of course, some theoretical backing for using the maximum smoothness: Let $f(X,h) = \|\nabla^2 \mathcal{L}(\cdot)\|$

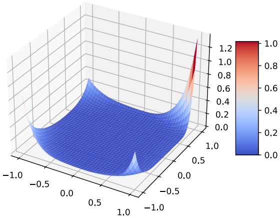
$$\max_h \min_X f(X,h) \leq \min_h \max_X f(X,h) \leq \max_h \max_X f(X,h) \tag{1}$$

where the left part is the $\mu-$strong convexity (exercise: prove this).

MAXIMIZING SMOOTHNESS



(a) Before HPO



(b) After HPO

STATISTICS

- → We will compare with the state-of-the-art, along with other SOTA HPO methods
- → Kruskal-Wallis test (group medians), followed by pairwise Mann-Whitney (Wilcoxon rank-sum) tests, and adjust p-values using Benjamini-Hochberg correction to adjust for Type-I errors

INTRODUCING: MLOPS

- → Software processes have evolved longer than ML coding practices
- → As such, a lot of ML code is...subpar (ironically, this seems especially true in SE venues)
- → MLOps abstracts model and data versioning, experiment tracking, dashboarding, and more
- → We will look at a small example using MLFlow: **https://github.com/yrahul3910/mlflow-demo**

USING MLFLOW

→ Set up an experiment:

```
# Create an experiment
experiment_id = mlflow.create_experiment('mnist')
experiment = mlflow.get_experiment(experiment_id)
print('Artifact location:', experiment.artifact_location)
```

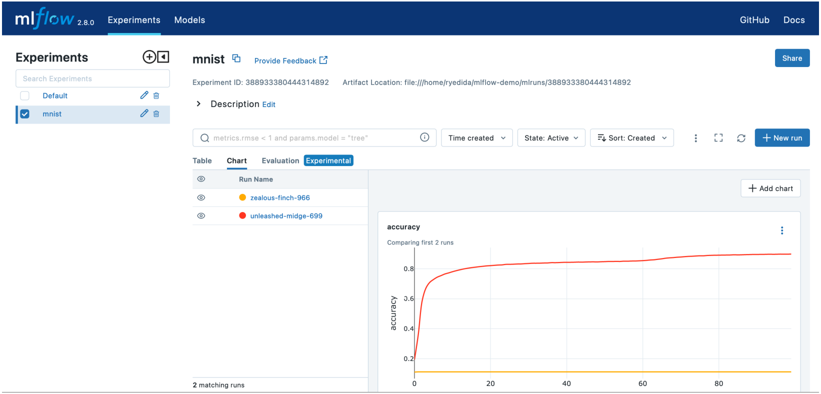
→ Your main loop:

```
with mlflow.start_run(experiment_id=experiment_id):
    # Get the config
    config = get_hyperparams(choices)

    # Log parameters
    for param, val in config.items():
        mlflow.log_param(param, val)

    val_acc = run_experiment(X_train, X_test, y_train, y_test, config)
    mlflow.log_metric('val_acc', val_acc)
```

→ Start the UI server

```
mlflow ui --host 0.0.0.0 --port 5000
```

MLFLOW UI


mlflow 2.8.0
Experiments
Models
GitHub
Docs
Experiments
Search Experiments
Default
mnist
mnist
Provide Feedback
Share
Experiment ID: 388933380444314892
Artifact Location: file:///home/ryedida/mlflow-demo/mlruns/388933380444314892
Description Edit
metrics.rmse < 1 and params.model = "tree"
Time created
State: Active
Sort: Created
New run
Table
Chart
Evaluation
Experimental
Run Name
zealous-finch-966
unleashed-midge-699
2 matching runs
Add chart
accuracy
Comparing first 2 runs
accuracy
0.8
0.6
0.4
0.2
0
20
40
60
80

CLOUD COMPUTING

- Model training: With deeper models, cloud computing may be more cost-effective.
  - Example: on Google Cloud, an A100 with 85GB RAM and 12 vCPUs costs about $89/day.
  - Niceties such as multi-GPU training and flexible instance scaling makes training very convenient.
  - Notebooks can be used too: AWS SageMaker
- Data sharing:
  - When your data size gets excessive, it might be better to store it on the cloud.
  - Example: AWS S3, Google Cloud Storage

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