CPSC 330 Lecture 8: Hyperparameter Optimization

Firas Moosvi (Slides adapted from Varada Kolhatkar)

Announcements

- Important information about midterm 1
  - https://piazza.com/class/m01ukubppof625/post/249
- Reminder of my office hours
  - Wednesdays from 12:30 to 1:30 PM in my office ICCS 253
- HW3 is due today 11:59 pm.
- HW4 has been released

Recap: Logistic regression

- A **linear model used for binary classification** tasks.
  - There is a variant of logistic regression called multinomial logistic regression for multiclass classification.
- Parameters:
  - Coefficients (Weights): The model learns a coefficient or a weight associated with each feature that represents its importance.
  - Bias (Intercept): A constant term added to the linear combination of features and their coefficients.

Recap: Logistic regression

- The model computes a weighted sum of the input features' values, adjusted by their respective coefficients and the bias term.
- This weighted sum is passed through a sigmoid function to transform it into a probability score, indicating the likelihood of the input belonging to the "positive" class.

$$P_{hat} = \sigma\left(\sum_{i=1}^{d} w_i x_i + b\right)$$

- P_{hat} is the predicted probability of the example belonging to the positive class.
- w_i is the learned weight associated with feature i
- x_i is the value of the input feature i
- b is the bias term

Recap: Logistic regression

- For a dataset with d features, the decision boundary that separates the classes is a $d - 1$ dimensional hyperplane.
- Complexity hyperparameter: `C` in `sklearn`.
  - Higher `C` $\longrightarrow$ more complex model meaning larger coefficients
  - Lower `C` $\longrightarrow$ less complex model meaning smaller coefficients

Recap: `CountVectorizer` input

- Primarily designed to accept either a `pandas.Series` of text data or a 1D `numpy` array. It can also process a list of string data directly.
- Unlike many transformers that handle multiple features (`DataFrame` or 2D `numpy` array), `CountVectorizer` a single text column at a time.
- If your dataset contains multiple text columns, you will need to instantiate separate `CountVectorizer` objects for each text feature.
- This approach ensures that the unique vocabulary and tokenization processes are correctly applied to each specific text column without interference.

Hyperparameter optimization motivation

Data

```
sms_df = pd.read_csv(DATA_DIR + "spam.csv", encoding="latin-1")
sms_df = sms_df.drop(columns = ["Unnamed: 2", "Unnamed: 3", "Unnamed: 4"])
sms_df = sms_df.rename(columns={"v1": "target", "v2": "sms"})
train_df, test_df = train_test_split(sms_df, test_size=0.10, random_state=42)
X_train, y_train = train_df["sms"], train_df["target"]
X_test, y_test = test_df["sms"], test_df["target"]
train_df.head(4)
```

	target	sms
3130	spam	LookAtMe!: Thanks for your purchase of a video...
106	ham	Aight, I'll hit you up when I get some cash
4697	ham	Don no da:)whats you plan?
856	ham	Going to take your babe out ?

Model building

- Let's define a pipeline

```
pipe_svm = make_pipeline(CountVectorizer(), SVC())
```

- Suppose we want to try out different hyperparameter values.

```
parameters = {
    "max_features": [100, 200, 400],
    "gamma": [0.01, 0.1, 1.0],
    "C": [0.01, 0.1, 1.0],
}
```

Hyperparameter optimization with loops

- Define a parameter space.
- Iterate through possible combinations.
- Evaluate model performance.
- What are some limitations of this approach?

`sklearn` methods

- `sklearn` provides two main methods for hyperparameter optimization
  - Grid Search
  - Random Search

Grid Search

- Covers all possible combinations from the provided grid.
- Can be parallelized easily.
- Integrates cross-validation.

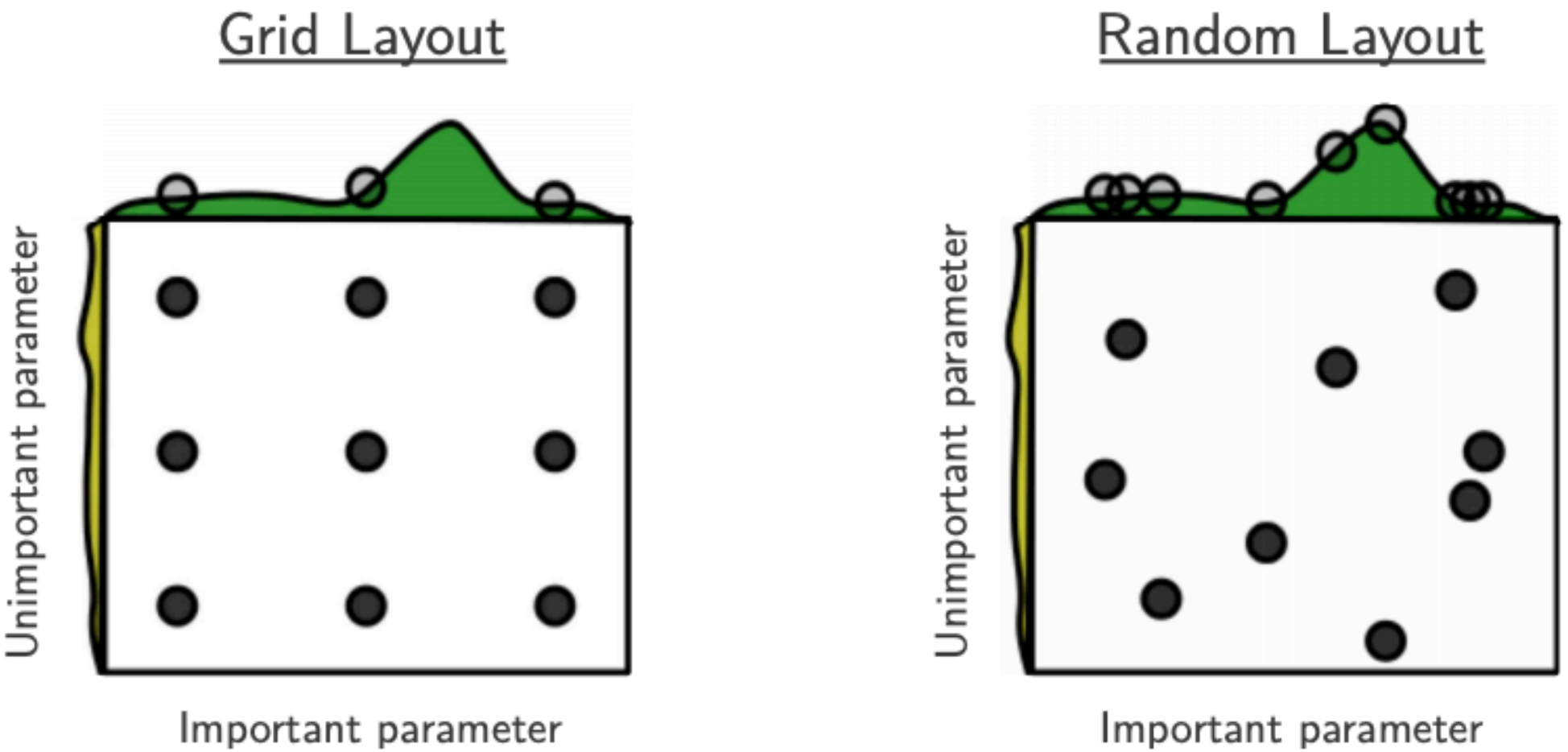
Grid search example

```
from sklearn.model_selection import GridSearchCV

pipe_svm = make_pipeline(CountVectorizer(), SVC())

param_grid = {
    "countvectorizer__max_features": [100, 200, 400],
    "svc__gamma": [0.01, 0.1, 1.0],
    "svc__C": [0.01, 0.1, 1.0],
}
grid_search = GridSearchCV(pipe_svm,
                  param_grid = param_grid,
                  n_jobs=-1,
                  return_train_score=True
                 )
grid_search.fit(X_train, y_train)
grid_search.best_score_
```

```
0.9782606272997375
```

Random Search

- More efficient than grid search when dealing with large hyperparameter spaces.
- Samples a given number of parameter settings from distributions.



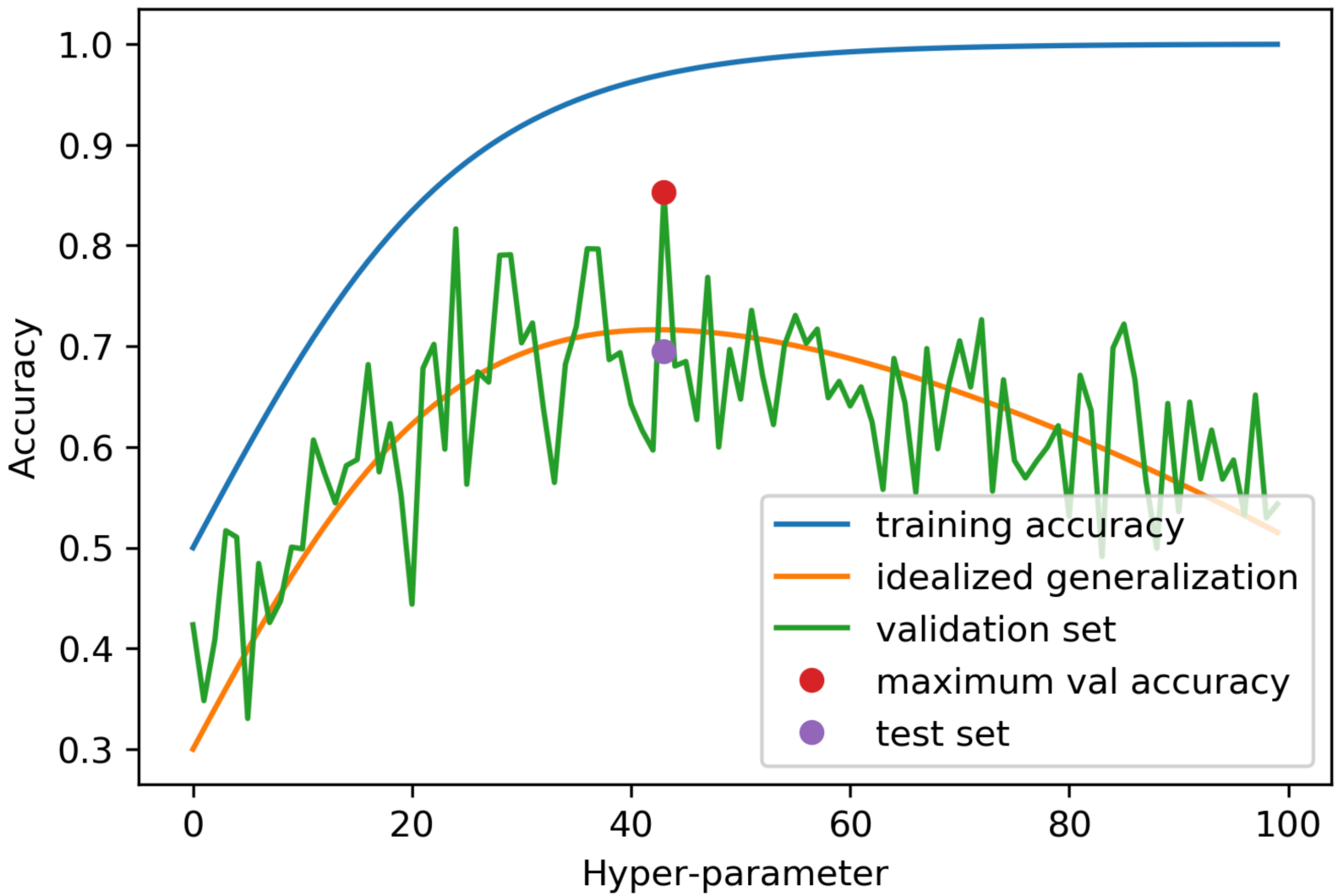
Random search example

```
from sklearn.model_selection import RandomizedSearchCV
from scipy.stats import randint

pipe_svc = make_pipeline(CountVectorizer(), SVC())

param_dist = {
    "countvectorizer__max_features": randint(100, 2000),
    "svc__C": uniform(0.1, 1e4),  # loguniform(1e-3, 1e3),
    "svc__gamma": loguniform(1e-5, 1e3),
}
random_search = RandomizedSearchCV(pipe_svm,
                   param_distributions = param_dist,
                   n_iter=10,
                   n_jobs=-1,
                   return_train_score=True)

# Carry out the search
random_search.fit(X_train, y_train)
random_search.best_score_
```

```
0.9812518532227668
```

Optimization bias

- Why do we need separate validation and test datasets?



Mitigating optimization bias.

- Cross-validation
- Ensembles
- Regularization and choosing a simpler model

(iClicker) Exercise 8.1

iClicker cloud join link: https://join.iclicker.com/VYFJ

Select all of the following statements which are TRUE.

- a. If you get best results at the edges of your parameter grid, it might be a good idea to adjust the range of values in your parameter grid.
- b. Grid search is guaranteed to find the best hyperparameter values.
- c. It is possible to get different hyperparameters in different runs of RandomizedSearchCV.

Questions for you

- You have a dataset and you give me 1/10th of it. The dataset given to me is rather small and so I split it into 96% train and 4% validation split. I carry out hyperparameter optimization using a single 4% validation split and report validation accuracy of 0.97. Would it classify the rest of the data with similar accuracy?
  - Probably
  - Probably not

Questions for class discussion

- Suppose you have 10 hyperparameters, each with 4 possible values. If you run `GridSearchCV` with this parameter grid, how many experiments will be carried out?
- Suppose you have 10 hyperparameters and each takes 4 values. If you run `RandomizedSearchCV` with this parameter grid with `n_iter=20`, how many cross-validation experiments will be carried out?

Looking Ahead

Group Work: Invention Activity

So far we have looked only at `score` as a metric for evaluating our metrics.

What else could be used as a possible metric? Think of what else might be important for machine learning practioners and stakeholders?

In your group, brainstorm 4 alternative options:

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-
-
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