Diagnostics for Choosing a Model

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Outline

Making choices about your model

High Bias vs. High Variance

Cross-Validation

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  4. For clustering: for K-means clustering, the number `K`; for `DBSCAN` clustering, the radius `epsilon`.

Choosing Hyperparameters

How do you choose the hyperparameters?

[1] Don't touch the test data until the model, with parameters, is trained and ready to perform on data.

[2] In particular, if the hyperparameter is real-valued, then you have picked a partition (or step-size) in the interval. For example, $0.0, 0.05, 0.1, \ldots, 0.95, 1.0$ in interval $[0, 1]$.

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Let $\mathcal{L}_{test}$ be the loss value on the test data. The set of all possible M-tuples of hyperparameters has size $\prod_{j=1}^{M} N_j$. A grid search method is to train a model for each of the possible M-tuples and then compute $\mathcal{L}_{test}$. Then, you choose the model with the smallest $\mathcal{L}_{test}$ value.

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Downsides: most notably, as described it *uses the test data* to make a decision about the parameters. Can potentially cause overfitting.
It is also typically computationally expensive.

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For example, a grid search method might be applied, but choosing the model with smallest $\mathcal{L}_{valid}$, rather than $\mathcal{L}_{test}$, and this will help the $\mathcal{L}_{test}$ of the final model be a better estimate of the expected population loss.

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- In training/validation/test split of data, say that n is the number of points in training subset. For a series of values of m with $m \leq n$, train a model with your choice of hyperparameters, with just m of points from training data. Then, compute the value of $\mathcal{L}_{train}$ and $\mathcal{L}_{valid}$ on each of the resulting models.

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- Plot the curves for $\mathcal{L}_{train}$ and $\mathcal{L}_{valid}$, as functions of m. In a scenario with high Bias, they appear as depicted below. Note that the $\mathcal{L}_{train}$ and $\mathcal{L}_{valid}$ curves approach each other as m increases; however, the loss (even on training data) is too high.

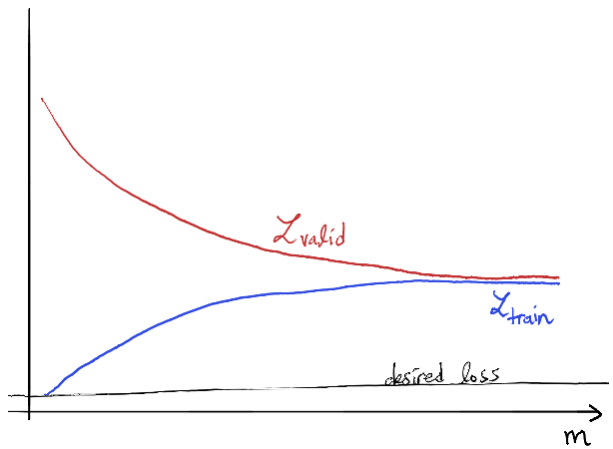
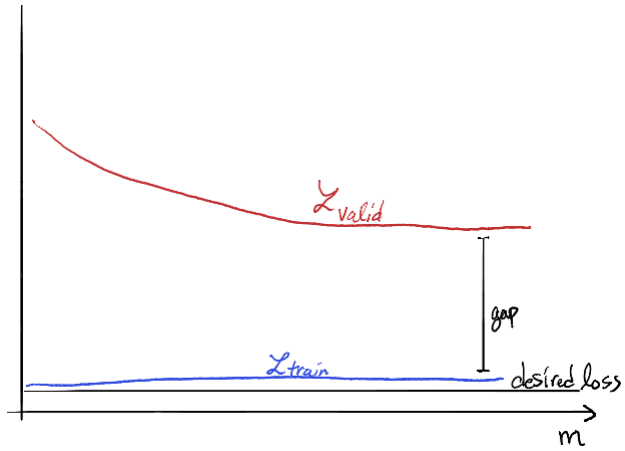


Figure: High Bias Scenario; m is the # of data points used in training.

Diagnostic to Test for High Variance

- However, if $\mathcal{L}_{train}$ and $\mathcal{L}_{valid}$ are computed as before, and their curves plotted as functions of m, then in a scenario with high Variance, they will appear as depicted below. Here, between the $\mathcal{L}_{train}$ and $\mathcal{L}_{valid}$ curves there is a gap, that remains as m increases.



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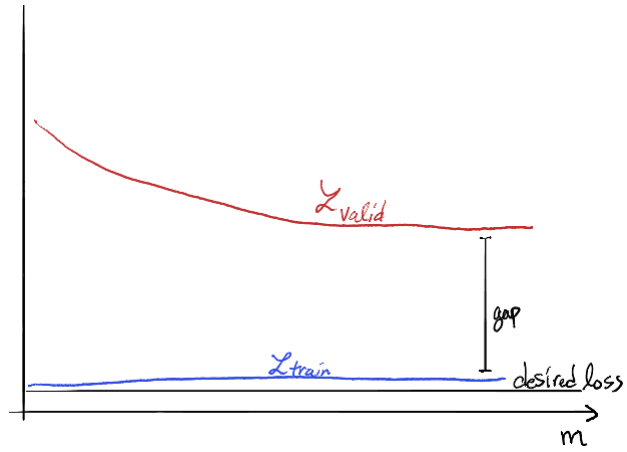

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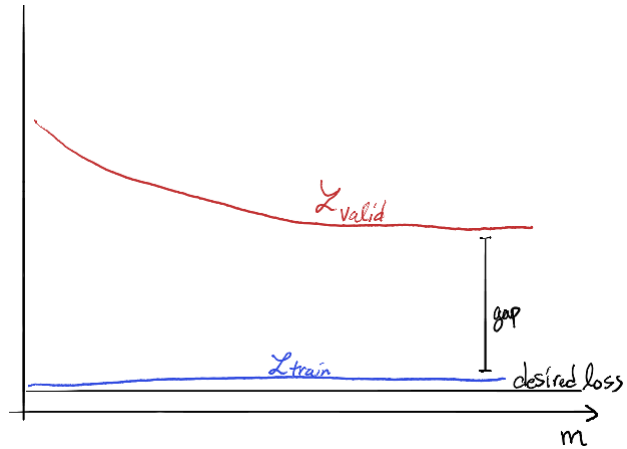

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- To see the above shape, may need to randomly re-order the training data multiple times, redo the computations, and plot the averages as the curve.

Diagnostic for high Bias versus high Variance

Recall from last lecture, the decision tree (with no maximum depth) which was fit to classify the digit in a handwritten image.
Below, the diagnostic was run when setting the maximum depth of the tree equal to 2. The curve is indicative of the Bias being high. The number of points in the training set is along the horizontal axis. [3]

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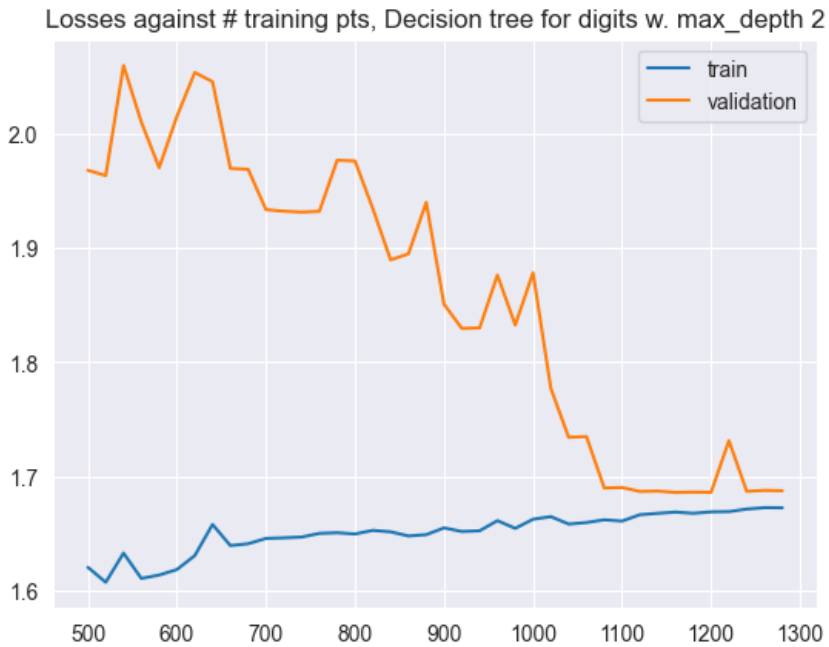

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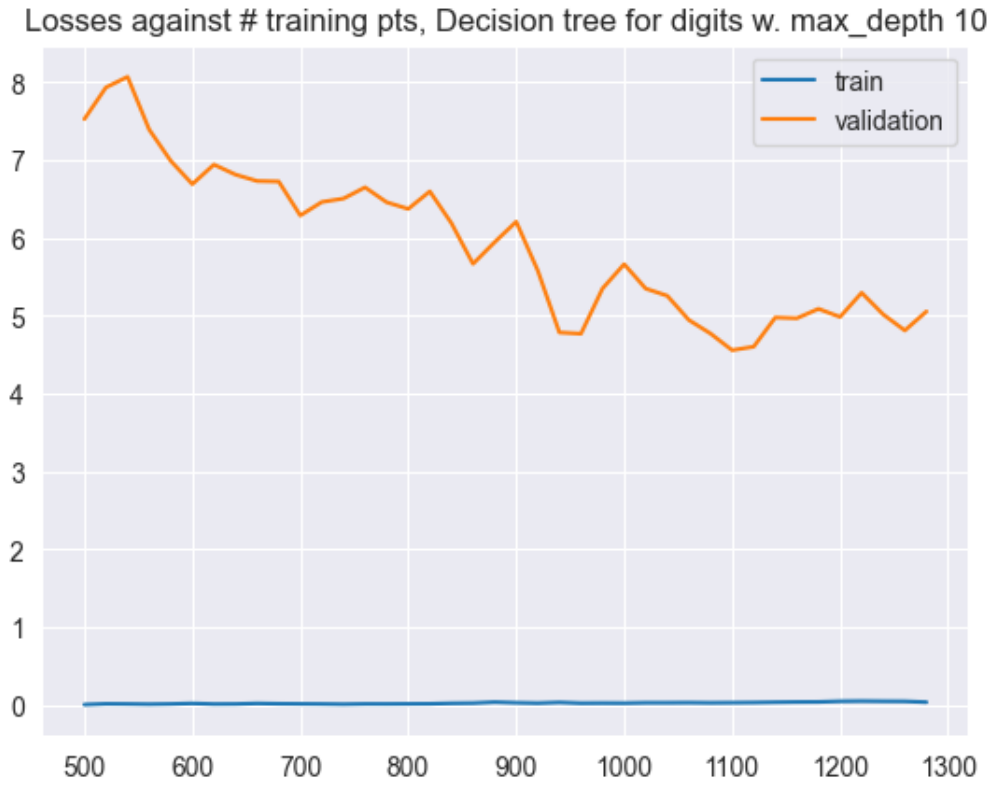
Diagnostic for high Bias versus high Variance

The same diagnostic was run, but setting the maximum depth of the tree equal to 10. The curve is shown below and is indicative of a scenario when Variance is high.



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Cross-Validation

If you are not in a "data rich" setting – that is, you do not have a large amount of data – then setting aside 10-20% of it as validation data might make it difficult to train a model that performs well. Additionally, *which* data goes into the validation subset might affect the resulting prediction function, and its performance, significantly.

A remedy is to use k-fold **cross-validation**. Commonly, practitioners use 5-fold or 10-fold cross-validation. Here, we describe the 5-fold version.

After having separated out the test data, randomly sort your remaining data into 5 subsets. For example, if `x` is the array to be separated into 5 arrays, the following would do the job.

```
indices = np.arange(len(x))
np.random.shuffle(indices)
n_subset = int(len(x)/5)
for i in range(5):
    subsets[i] = x[i*n_subset:(i+1)*n_subset]
```

Next, you train and do validation on 5 models, with training sets determined from the subsets:

train	train	train	train	valid
train	train	train	valid	train
train	train	valid	train	train
train	valid	train	train	train
valid	train	train	train	train