Bootcamp 2023

Regularization and Hyperparameter Tuning

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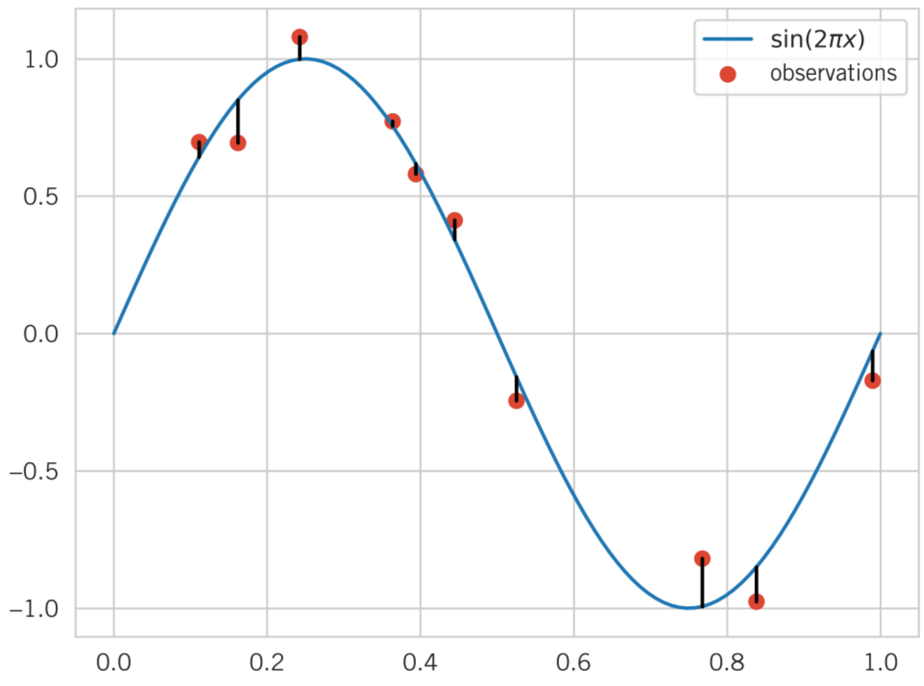
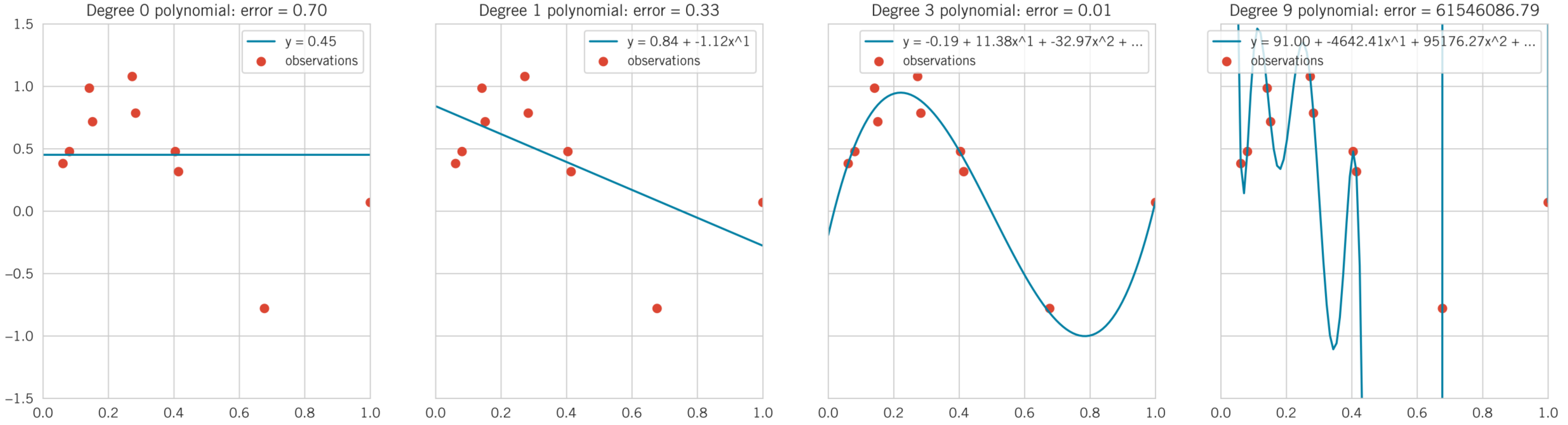
Regularization

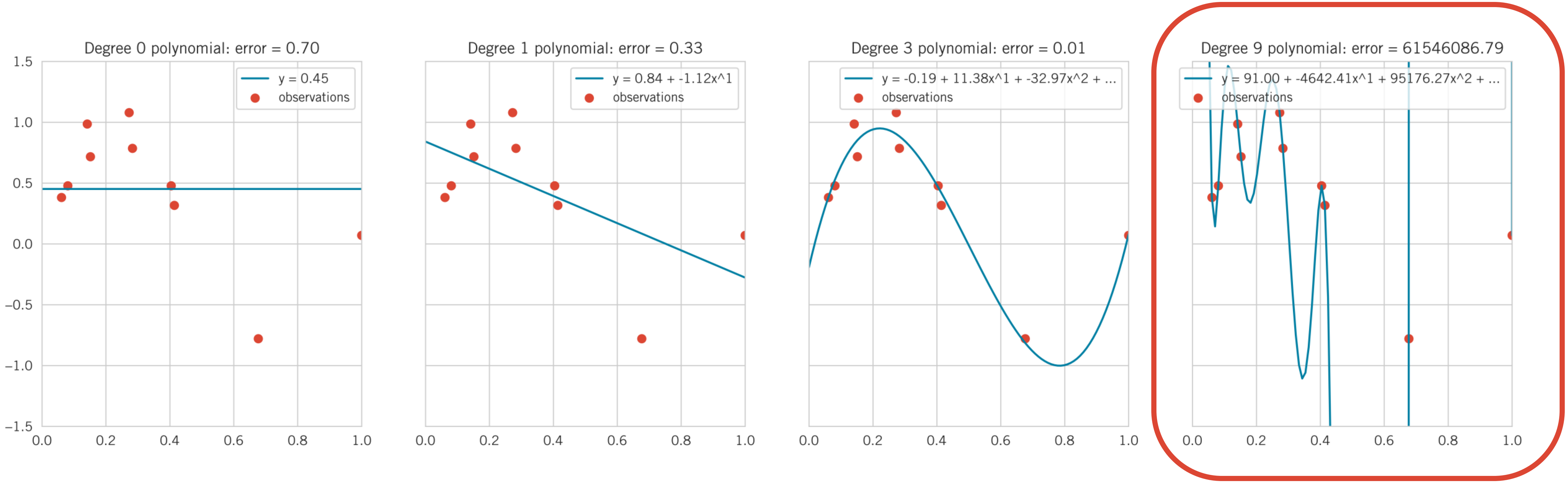
- Start with data points (x, y) generated by adding noise to $\sin(2\pi x)$
- Each noisy point has a <u>residual</u>: the difference between the point and the true value
- $E(y_{obs}) = \frac{1}{n}\sum_{n=1}^{N}(y_{obs} - y)^2$
- Mean Squared Error



Polynomial Regression



Polynomial Regression

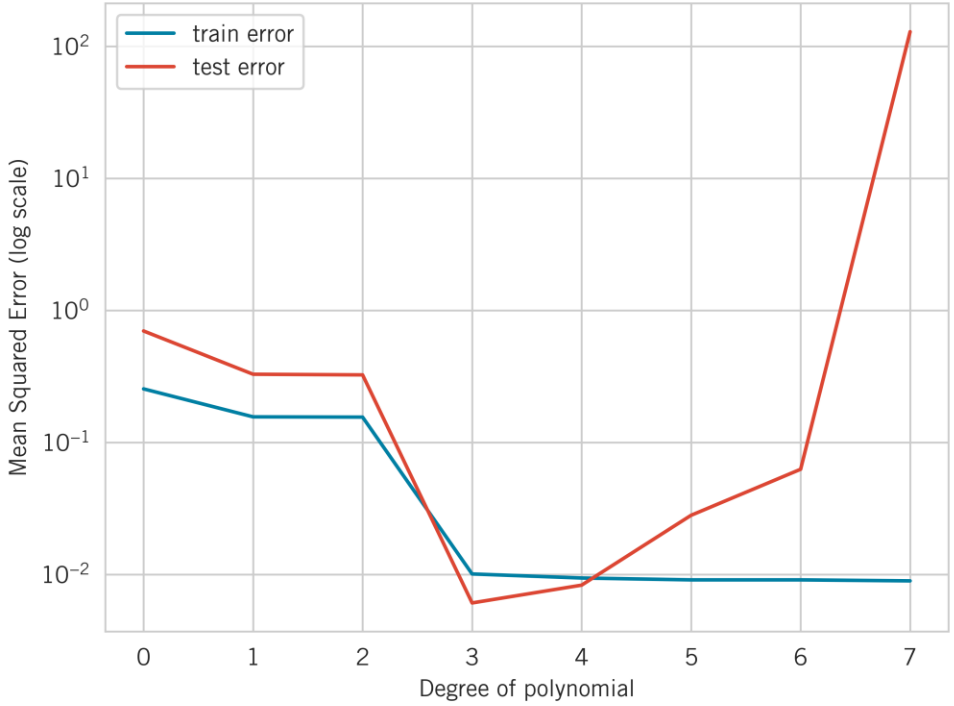


Underfitting: The model is <u>not complex enough</u> for the data

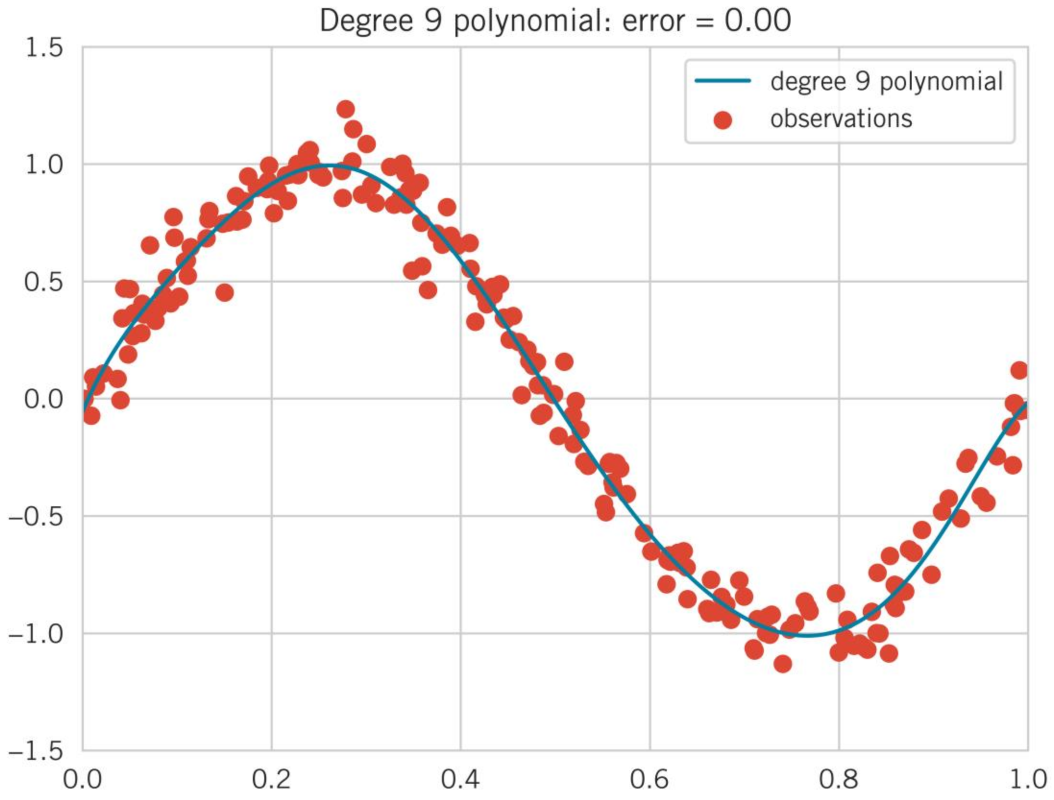
Overfitting: the model is <u>too complex</u> for the data

Error as a function of degree of polynomial

- Overfitting occurs when the test performance decouples from the train performance
- Train error will typically trend toward zero as the model gets more complex
- With a complex enough model, it can “memorize” every training sample



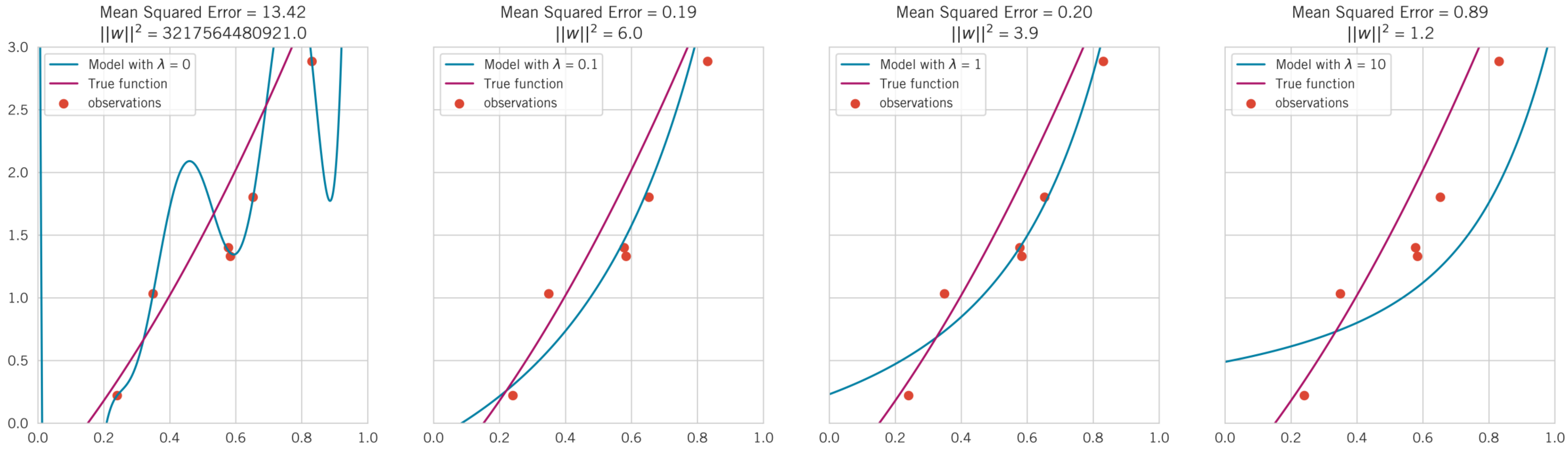
Dealing with overfitting (1): more data



Dealing with overfitting (2): regularization

- For some model $f(x, \boldsymbol{w})$ where x is the input and w are the parameters:
- $E(f) = \underbrace{\frac{1}{n}\sum_{n=1}^{N}(f(x, \boldsymbol{w}) - y)^2}_{\text{Mean Squared Error}} + \underbrace{\lambda||\boldsymbol{w}||^2}_{\text{Penalty on the size of parameters}}$

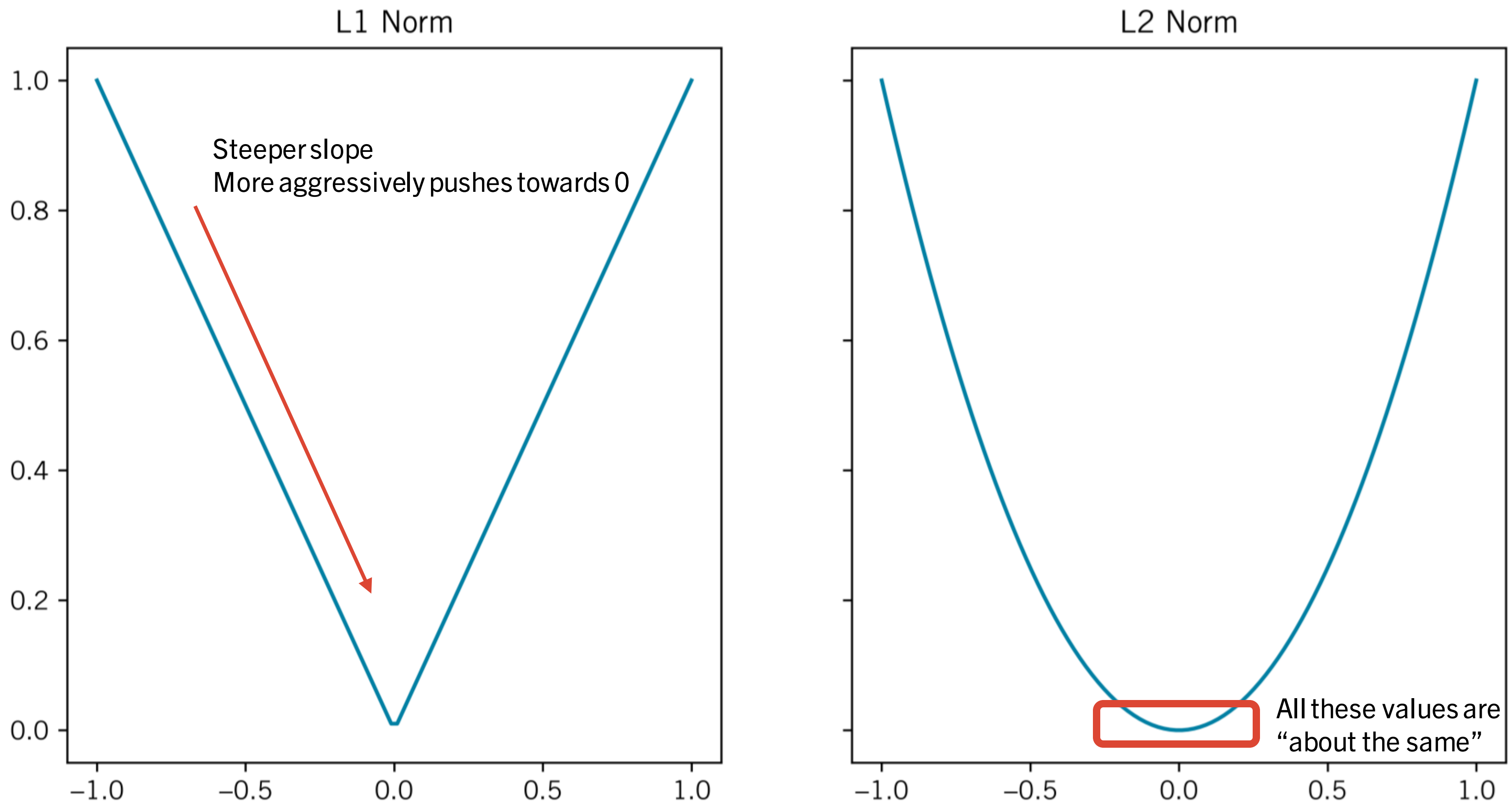
Effect of regularization



L1 and L2 regularization

- L1 Regularization (aka LASSO): $\lambda \sum ||\boldsymbol{w}||$
  - Tends to produce sparse solutions, where some coefficients are zero
  - Useful for feature selection, as unimportant features are ignored
  - Less stable when multiple correlated features exist
- L2 Regularization (aka Ridge): $\lambda \sum \boldsymbol{w}^2$
  - Tends to distribute weights evenly and doesn't push coefficients to zero.
  - More stable solution where multiple correlated predictors exist, will include all of them.
  - Tends to perform better when all features are relevant.

L1 and L2 regularization



Regularization in Neural Networks: L1 & L2

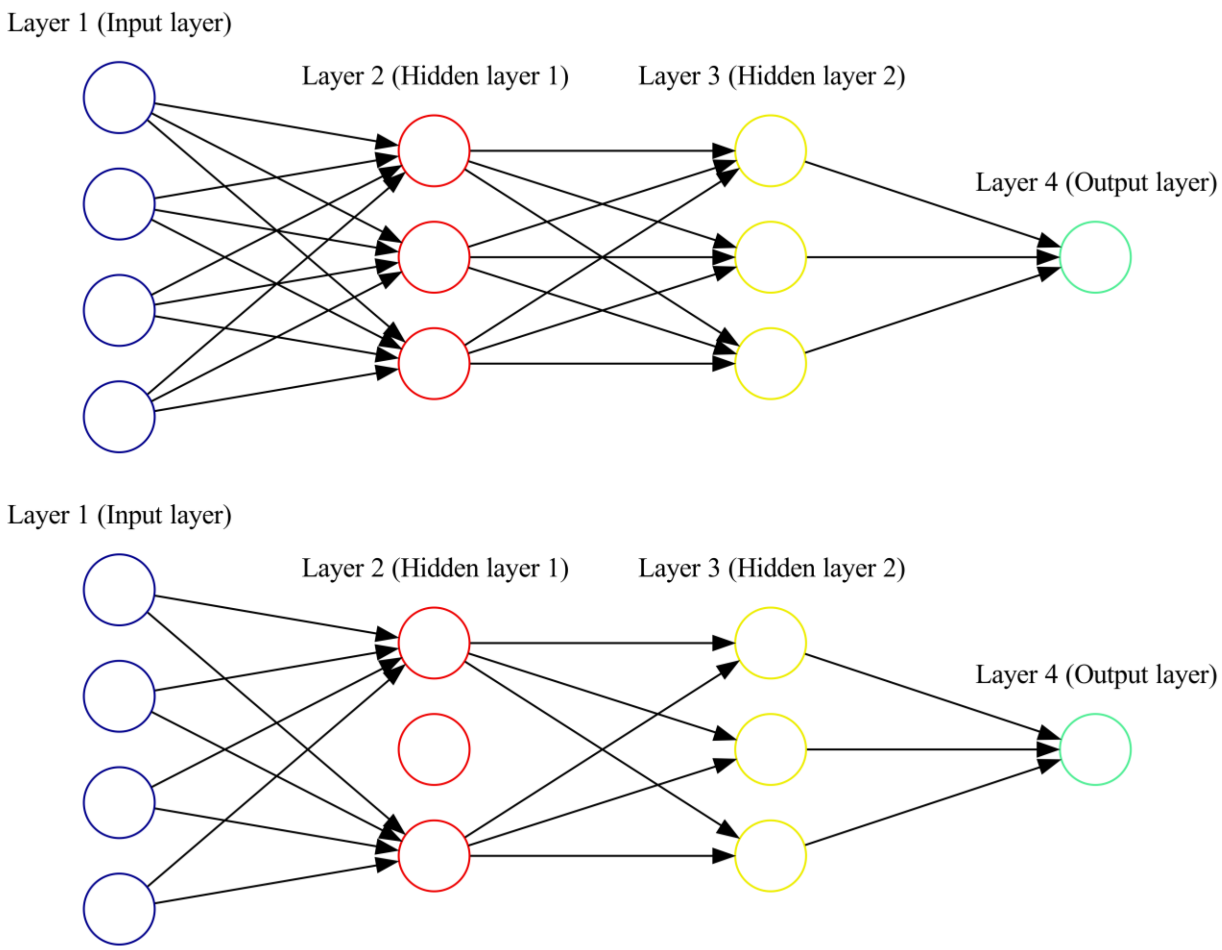
- We can directly apply L1 and L2 regularization to neural networks
- In TensorFlow, they are added when defining network architecture
- In PyTorch, they are added when defining the training loop

```
model = tf.keras.Sequential([
    layers.Dense(64, activation='relu',
                 kernel_regularizer=regularizers.l1(0.01)),
    layers.Dense(1)
])
```

```
for inputs, targets in dataloader:
    optimizer.zero_grad()

    outputs = model(inputs)
    loss = criterion(outputs, targets)

    l1_norm = sum(p.abs().sum() for p in model.parameters())
    loss = loss + lmbda * l1_norm

    loss.backward()
    optimizer.step()
```

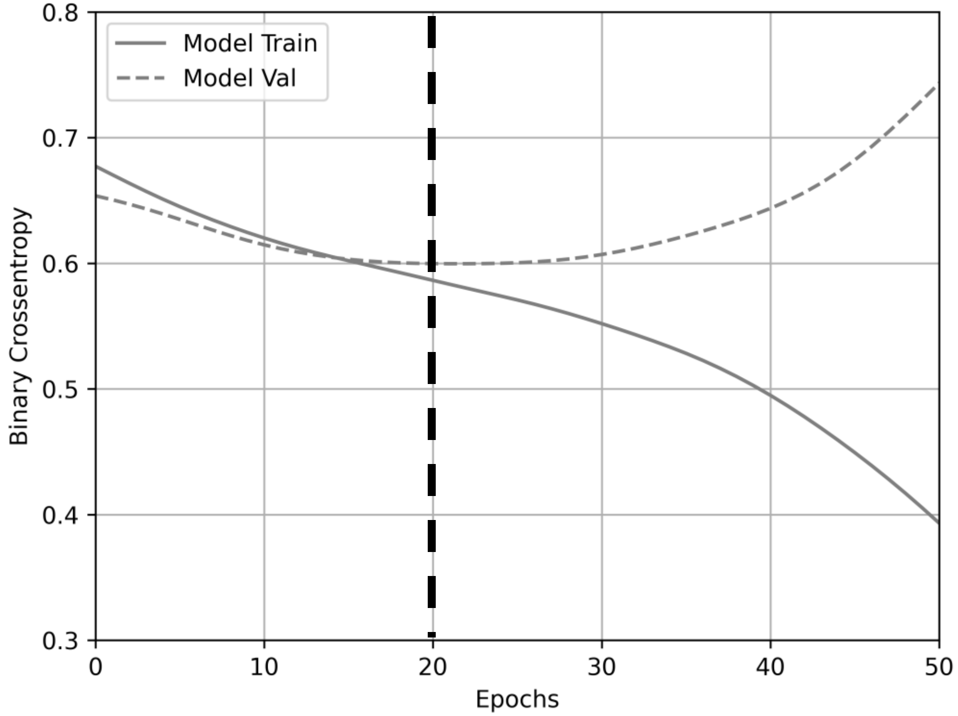
Regularization in Neural Networks: Dropout

- During training, randomly “drop” connections to individual nodes
- Reduces downstream nodes’ dependence on a single input



Regularization in Neural Networks: Early Stopping

- As model training continues, weights begin to be fit to noise in the training data
- Training loss continues to decrease, but validation loss plateaus (or even increases!)
- Every N epochs, check if validation loss is still improving



Regularization in Neural Networks: Other Methods

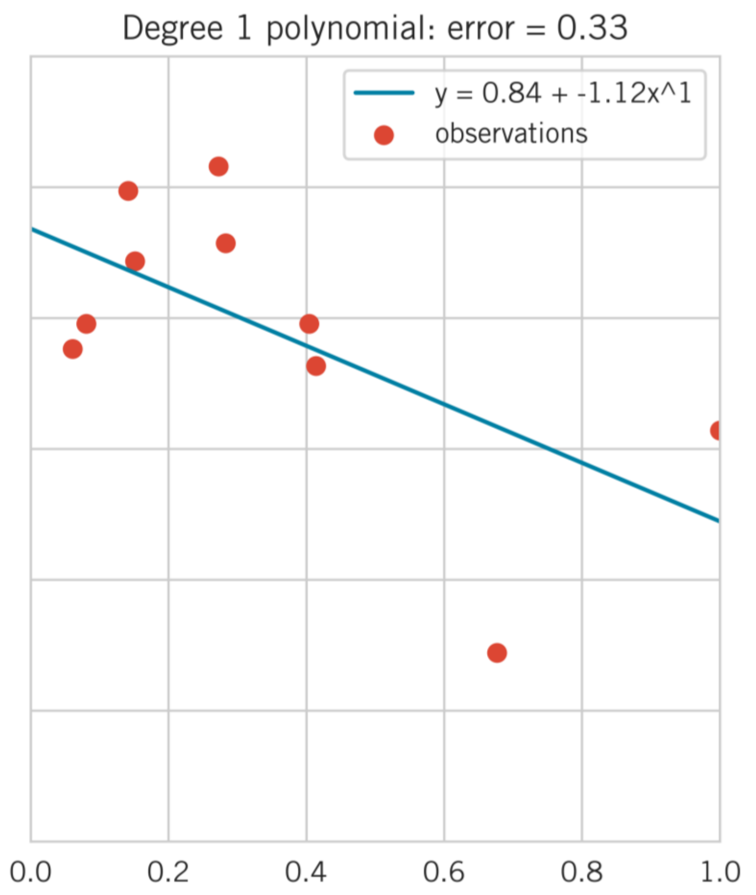
- Noise Injection
  - Involves adding a small amount of noise to input data
  - Makes the model less sensitive to specific details of the input
- Data Augmentation
  - Increase the training data size by creating alternate versions of samples
  - For images, this could be flipping, rotating, cropping…
  - For text, this could be synonym replacement or sentence shuffling

Bias / Variance Tradeoff

- Regularization handles overfitting, a high variance problem.
- Overfitting: model too sensitive to training data specifics.
- Conversely, underfitting represents high bias.
- The goal: balance <u>bias</u> (flexibility to learn) and <u>variance</u> (ability to generalize).

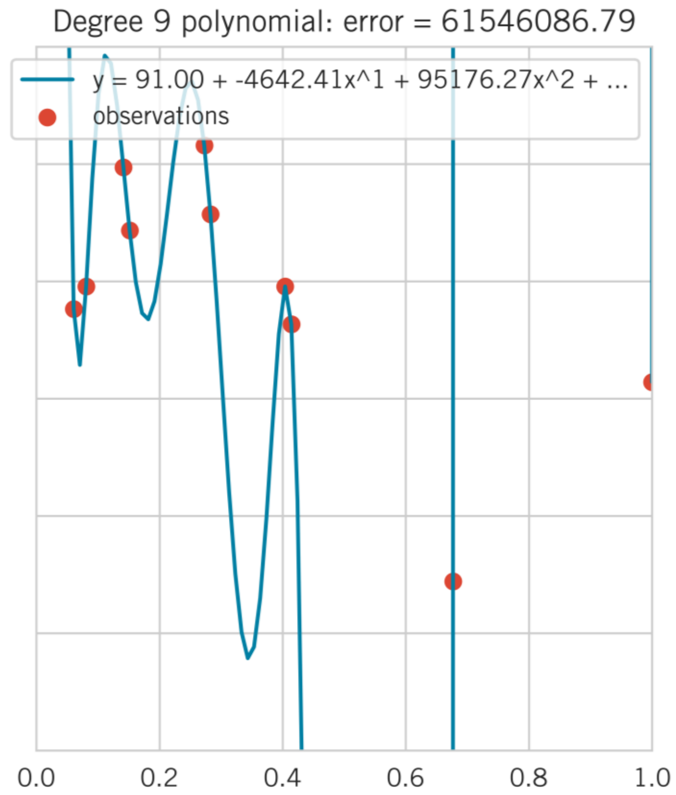
Bias / Variance Tradeoff: Bias

- Bias: Error from assumptions the model makes about the data
- Linear model assumes the data is linear
- In general, a simpler model is making more assumptions → high bias



Bias / Variance Tradeoff: Variance

- Variance: Algorithm's sensitivity to noise
- More complex models are more sensitive!
- High variance hurts generalization



Bias / Variance Tradeoff

Error = Noise + Bias + Variance

- Noise
  - Random variations in data
- Bias
  - Error from assumptions the model makes about the data
  - Less complex model → more assumptions
- Variance
  - Algorithm's sensitivity to noise
  - More complex algorithms are more sensitive

Parameters vs Hyperparameters

- Parameters:
  - Values learned from the data during training
  - In NNs, weights and biases

- Hyperparameters:
  - Settings affecting the structure or training process of the model
  - Not learned during training, but defined beforehand
  - Everything we've been discussing this afternoon

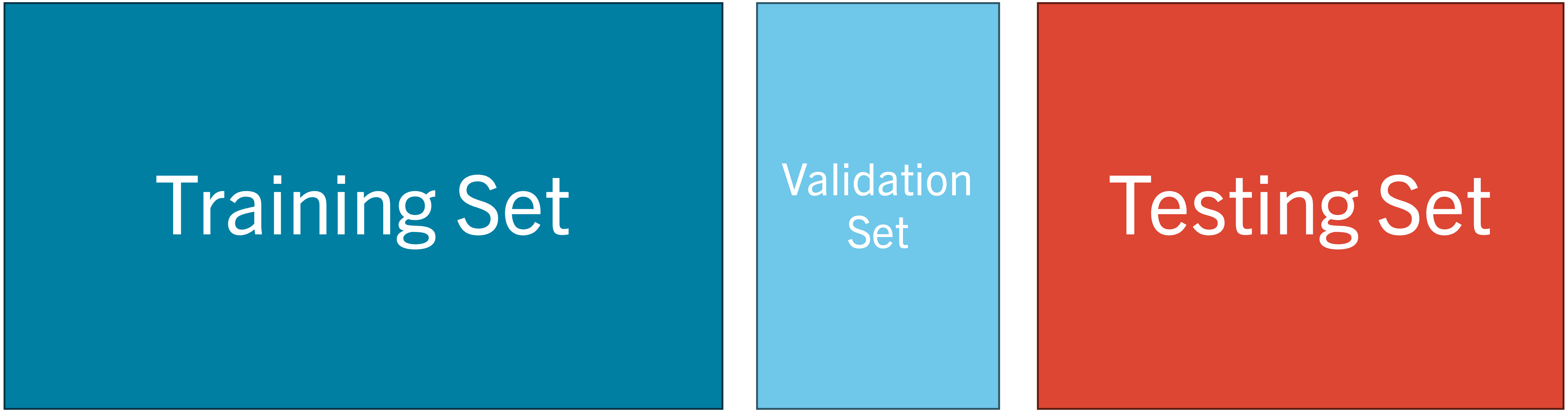
How do we choose?

- We've presented many options for improving the performance of a model
- Each one comes with its own decisions
  - L2 Norm: What value for λ?
  - Dropout: How frequently should nodes be disconnected?
- Even more things need to be configured in a neural network!
  - Learning rate
  - Network depth, width
  - Optimizer…

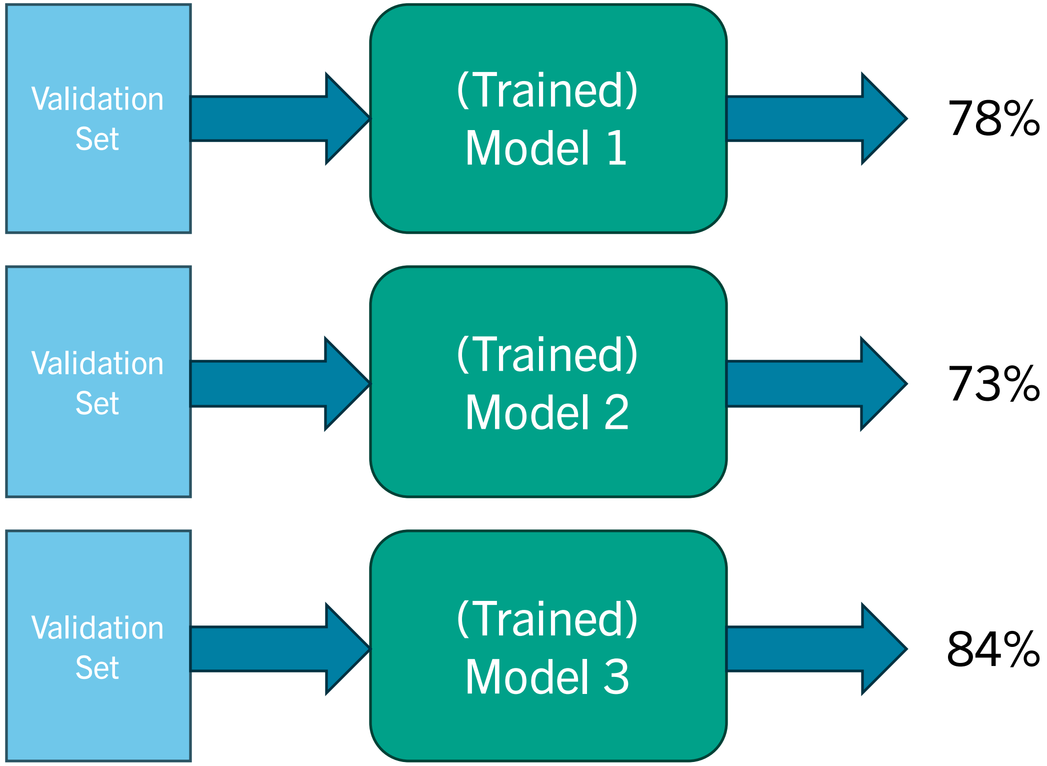
Hyperparameter Tuning

- Before selecting our final model, we explore the <u>space</u> of possible configurations
- This exploration is known as hyperparameter tuning
- Hyperparameter tuning methods aim to find the combination of hyperparameters that yields the most predictive model.
- The aim is not only to improve model accuracy but also to prevent issues like overfitting and underfitting
- Note: Hyperparameter tuning can be time-consuming and computationally intensive, but the payoff is a more effective and reliable model.

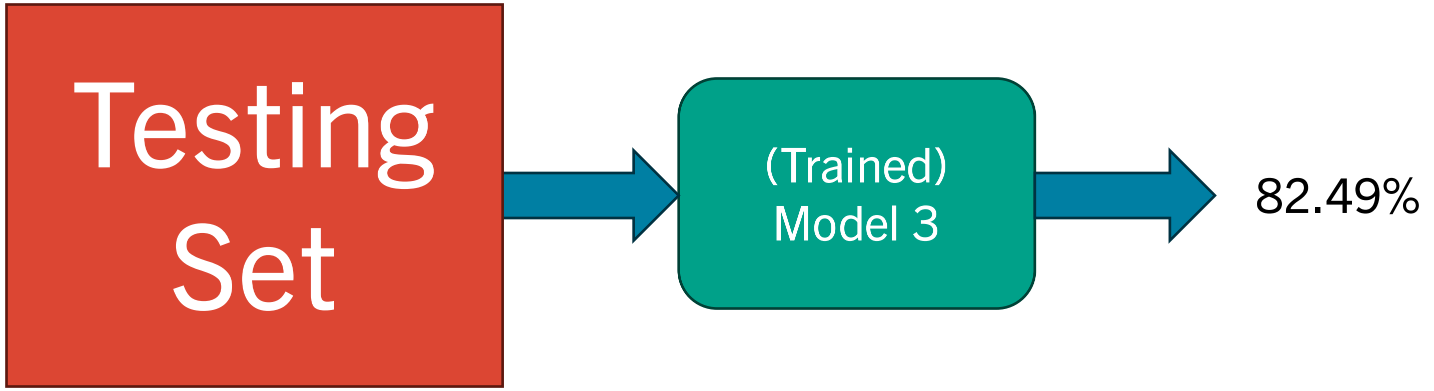
Hyperparameter Tuning: Validation Set



Hyperparameter Tuning: Validation Set



Hyperparameter Tuning: Validation Set



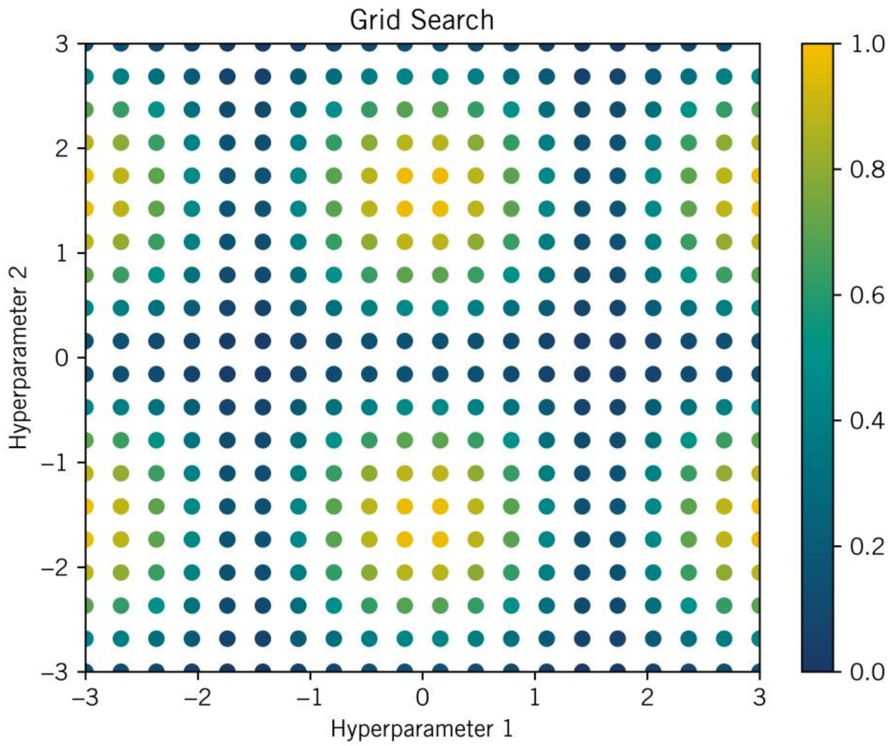
Defining the Search Space

- Instead of a model, we can build a hypermodel
- Replace concrete definitions with range of acceptable values

```
n_layers = 5

n_layers = hp.Int('layers', min_value=1, max_value=15) # Keras Tuner

n_layers = trial.suggest_int('layers', 1, 15) # Optuna
```

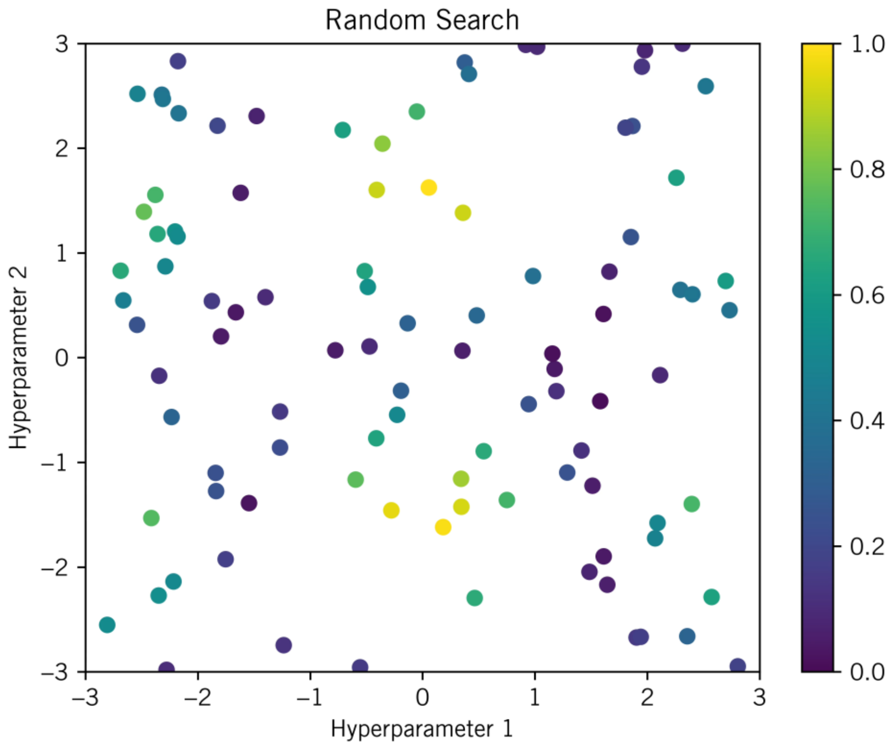
Finding Optimal Parameters: Grid Search

- Naïve approach: try every possible combination
  - This is actually an accepted method!
  - Guaranteed to find the best combination in the defined space
  - Quickly becomes intractable with more parameters



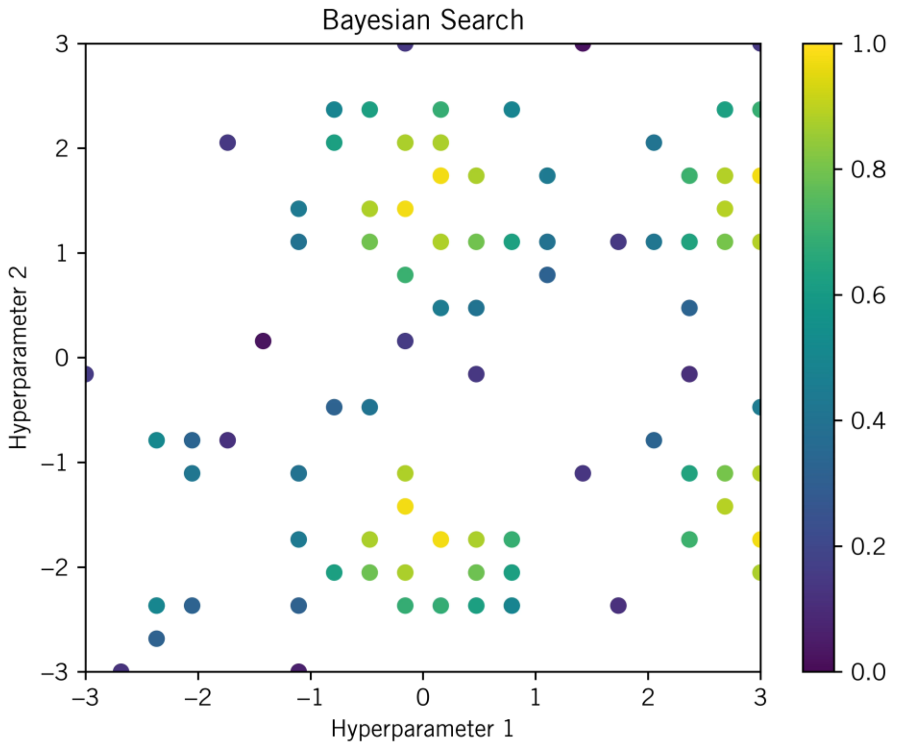
Finding Optimal Parameters: Random Search

- A more efficient alternative to Grid Search.
- Randomly samples the defined space of hyperparameters.
- Not guaranteed to find the best combination, but often finds a good combination quickly.
- Particularly useful when dealing with a larger number of parameters



Finding Optimal Parameters: Bayesian Search

- An advanced, intelligent approach to hyperparameter tuning.
- Uses information from past evaluations to choose the next parameters.
- Creates a probabilistic model mapping hyperparameters to a probability of a score on the objective function.
- Balances exploration (testing new, uncertain parameters) with exploitation (choosing parameters that look promising).
- Highly efficient, especially when evaluations are costly (e.g., tuning deep neural networks).



Preparing for Hyperparameter Tuning

- **Start with a Reasonable Baseline**: Use known good configurations from the literature as a starting point, or use heuristics to choose a good initial configuration.
- **Scale Up Gradually**: Start with a smaller network or fewer epochs while tuning, then scale up once you've narrowed the hyperparameter range.
- **Focus on the Most Impactful Parameters**: Not all hyperparameters are created equal. Often, the learning rate, batch size, and number of layers will have a big impact on performance.

Efficient Hyperparameter Tuning

- **Coarse to Fine Search**: Begin with a broad range and refine the search space as you identify promising regions.
- **Parallelize Hyperparameter Search**: If resources permit, train multiple models with different hyperparameters in parallel.
- **Use Automated Tuning if Possible**: Consider using automated tuning libraries, which can handle the tuning process more efficiently.
- **Record and Analyze Results**: Keep track of the performance for each set of hyperparameters. Visualization or analysis of these results can often yield insights and guide the search.

Neural Network Playground

https://playground.tensorflow.org