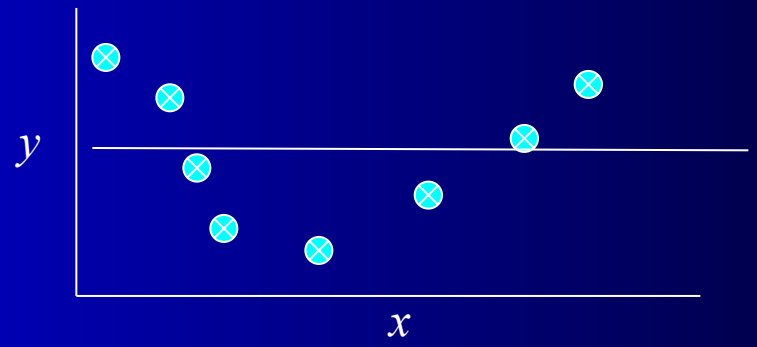
Overfit and Inductive Bias: How to generalize on novel data

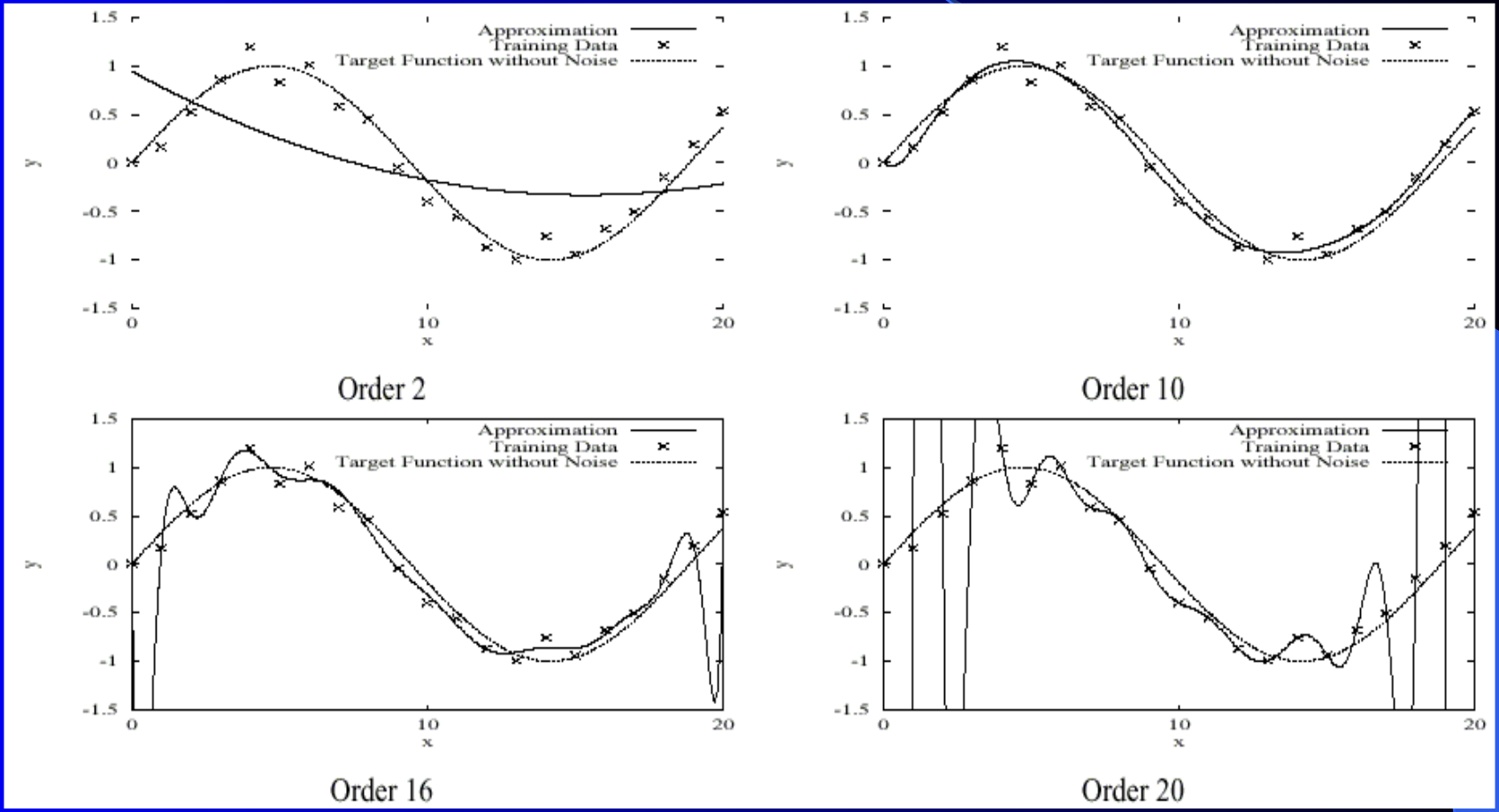
Non-Linear Tasks

- Linear Regression will not generalize well to the task below
- Needs a non-linear surface – Could use one of our future models
- Could also do a feature pre-process like with the quadric machine
  - For example, we could use an arbitrary polynomial in x
  - Thus, it is $Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \ldots + \beta_n X^n$ solved with delta rule
  - What order polynomial should we use? – Overfit issues can occur



Overfitting

Typically try to learn a model just complex enough to do well and no more complex than that



Avoiding Overfit

- Regularization: *any modification we make to learning algorithm that is intended to reduce its generalization error but not its training error*
- Occam's Razor – William of Ockham (c. 1287-1347)
  - Favor simplest explanation which fits the data
- General Key: Focus on patterns/rules that really matter and ignore others
- More Training Data (vs. overtraining on same data)
  - Data set augmentation – Fake data, Can be very effective, Jitter, but take care…
  - Denoising – add random noise to inputs during training – can act as a regularizer
  - Adding noise to models. e.g. (Random Forests, Dropout , discuss with ensembles)
- *Early Stopping* – Very common regularization approach: Start with simple model (small parameters/weights) and stop training as soon as we attain good generalization accuracy (and before parameters get large)
  - Common early stopping approach is to use a validation set (next slide)
- We will discuss other model specific approaches with specific models

Regularization

- Way to avoid overfitting – Keep the model simple
  - E.g., keep decision surfaces smooth
- Make complexity an explicit part of the loss function
- Regularization approach: Model (h) selection
  - Minimize $F(h) = Error(h) + \lambda \cdot Complexity(h)$
  - Tradeoff error/accuracy vs complexity
- Two common approaches
  - Lasso (L1 regularization)
  - Ridge (L2 regularization)

Note: often used with regression; applicable to many techniques

L1 (Lasso) Regularization

- We add a model complexity term to the loss function:

$$L\left(\vec{w}\right) = E\left(\vec{w}\right) + \lambda \sum \left| w_i \right|$$

- The gradient descent is given by:

$$-\nabla L\left(\vec{w}\right) = -\nabla E\left(\vec{w}\right) - \lambda$$

  - This is also called weight decay
  - Decay magnitude towards 0

- Common values for lambda are 0, .01, .03, etc.

- Weights that should be significant stay large enough, but weights just being nudged by a few data instances go to 0

L2 (Ridge) Regularization

- We add a model complexity term to the loss function:

$$L\left(\vec{w}\right) = E\left(\vec{w}\right) + \lambda \sum w_i^2$$

- The gradient descent is given by:

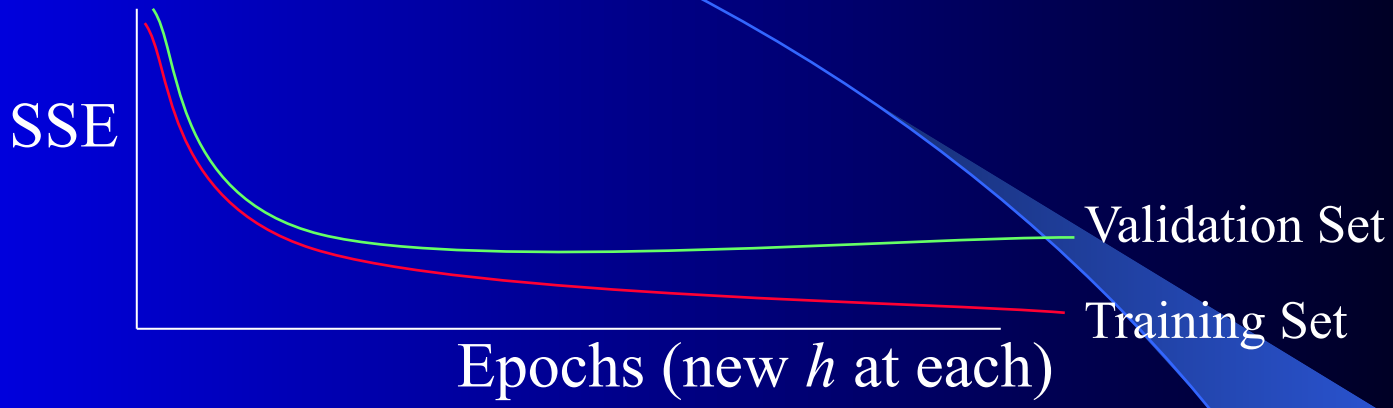
$$-\nabla L\left(\vec{w}\right) = -\nabla E\left(\vec{w}\right) - 2\lambda w_i$$

- Regularization portion of weight update is scaled by weight value (fold 2 into λ)
  - Decreases change when weight small (<0), otherwise increases
  - λ is % of weight change, .03 means 3% of the weight is decayed each time

L1 vs. L2 Regularization

- L1 drives many weights all the way to 0 (sparse representation and feature reduction)
- L1 more robust to large weights (outliers), while L2 acts more dramatically with large weights
- L1 leads to simpler models, but L2 often more accurate with more complex problems which require a bit more complexity

Early Stopping/Model Selection with a Validation Set



- There is a different model *h* after each epoch
- Select a model in the area where the validation set accuracy flattens
- Keep *bssf* (Best Solution So Far). Once you go *w* epochs with no improvement stop and use the parameters at the *bssf w* epochs ago.
- The validation set comes out of training set data
- Still need a separate test set to use after selecting model *h* to predict future accuracy
- Simple and unobtrusive, does not change objective function, etc
  - Can be done in parallel on a separate processor
  - Can be used alone or in conjunction with other regularization approaches

BIAS & VARIANCE

Bias & Variance

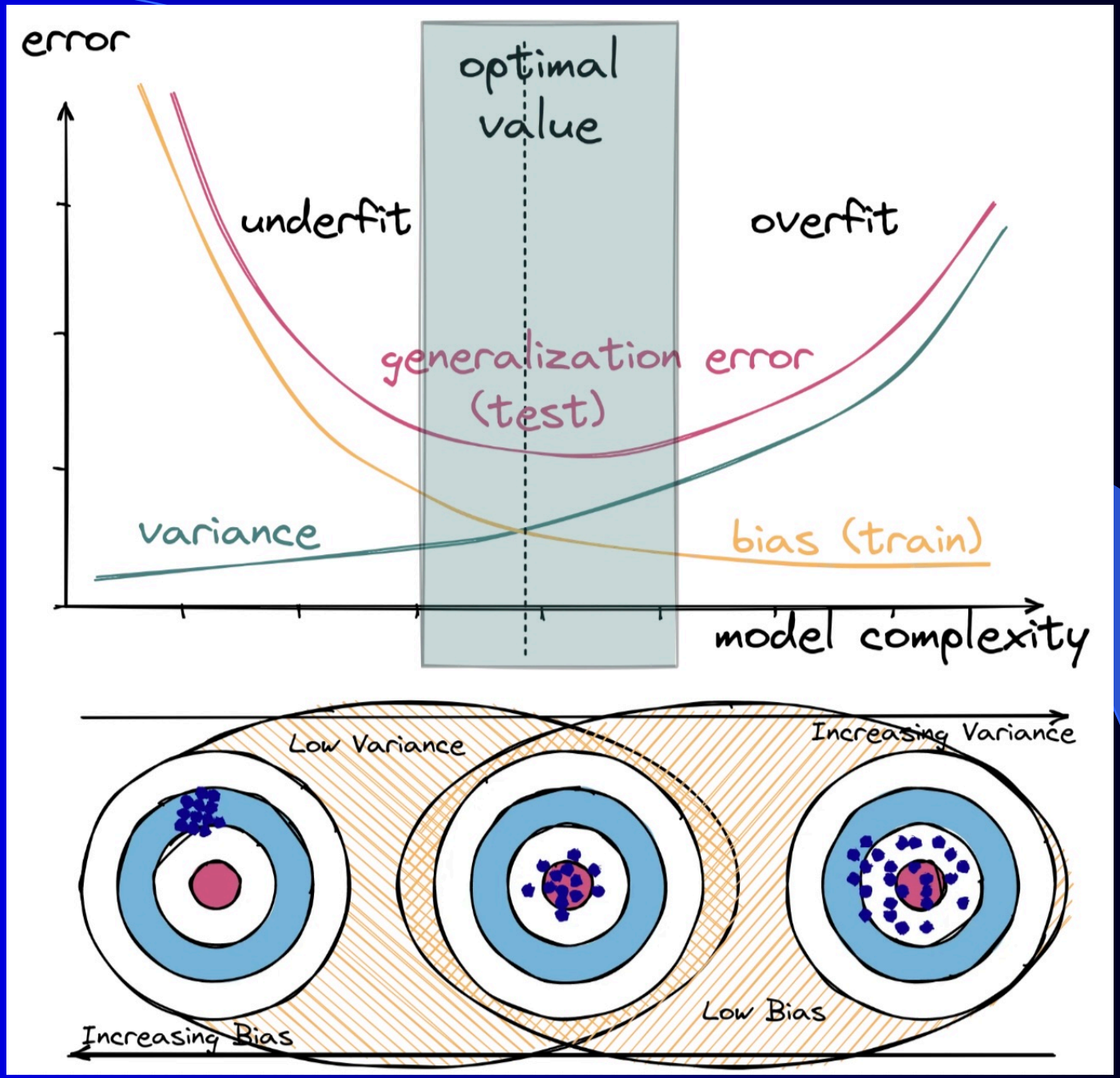
- Learning involves the ability to generalize from past experience to deal with new situations
- If we are only consistent with what we have seen, we can't generalize beyond our experience
  - All the cats I have seen are yellow.
  - What happens when I see a black cat?
- Bias is choosing one generalization over another
- Variance is how varied my choices are

Bias vs. Variance

- If there is **no bias**, the outcome of the learner is highly dependent on the training data, and thus there is **much variance** among the models induced from different sets of observations
  - Learner memorizes (overfits)
- If there is a **strong bias**, the outcome of the learner is much less dependent on the training data, and thus there is **little variance** among induced models
  - Learner ignores observations
- Formalized as:
  - **Bias-variance trade-off**

Bias-Variance Trade-off

- Weak/no bias
  - Observed instances are memorized
  - Learner **overfits**
- Strong/extreme bias
  - Observed instances are mostly ignored
  - Learner **underfits**
- Example: fitting arbitrary polynomial vs straight line to sine wave-like observations
- Bias-Variance Error Decomposition
  - All learning algorithms have a bias
    - Decision trees (simplicity), k-NN (similarity), etc.
  - All learning algorithms may be subject to variance in the data
  - Two sources of error
- How can we estimate the bias and variance of an algorithm?
  - Run the algorithm on different random variations of several datasets
  - Examine the errors made for each variation
    - If the algorithm tends to make the **same errors**, then it must have a **strong(er) bias** [one may need a more flexible algorithm]
    - If the algorithm tends to make **random errors**, then it must have a **strong(er) variance** [one may need a less flexible algorithm or more data]


error
optimal value
underfit
overfit
generalization error (test)
variance
bias (train)
model complexity
Low Variance
Increasing Variance
Increasing Bias
Low Bias

Example Code

- BiasVariance.ipynb – on Learning Suite

Your Projects

- Your goal in the group project is to get the highest possible generalization accuracy on a real-world application. You will come up with some task which you believe could be generalized with machine learning and as a group you will go through all the steps from beginning to end to get a good result.
- After you have come up with basic features and data, you will choose machine learning model(s), and format the data to fit the model(s).
- You will then try your model on novel data and report on your performance.

Your Project Proposals

- Examples – Look at UC Irvine Data Set or Kaggle to get a feel of what data sets look like
- Stick with supervised classification problems for the most part for the project proposals
- Choose tasks which interest you
- Too hard vs Too Easy
  - Data should be able to be gathered in a relatively short time
  - And, want you to have to battle with the data/features a bit
- See description in Learning Suite
  - Remember your example instance!
  - Give one fully specified example of a data set instance based on your proposed features, including a reasonable representation (continuous, nominal, etc.) and value for each feature. Make sure you include the target output value as part of the instance.

Feature Selection, Preparation, and Reduction

- Learning accuracy depends on the data!
  - *Is the data representative of future novel cases* - critical
  - Relevance
  - Amount
  - Quality
    - Noise
    - Missing Data
    - Skew
  - Proper Representation
  - How much of the data is labeled (output target) vs. unlabeled
  - Is the number of features/dimensions reasonable?
    - Reduction

Gathering Data

- Consider the task – What kinds of features could help
- Data availability
  - Significant diversity in cost of gathering different features
  - More the better (in terms of number of instances, not necessarily in terms of number of dimensions/features)
    - The more features you have the more data you need
  - Data augmentation, Jitter – Increased data can help with overfit – handle with care!
- Labeled data is best
- If not labeled
  - Could set up studies/experts to obtain labeled data
  - Use unsupervised and semi-supervised techniques
    - Clustering
    - Active Learning, Bootstrapping, Oracle Learning, etc.

Feature Selection - Examples

- Invariant Data
  - For character recognition: Size, Rotation, Translation Invariance
    - Especially important for visual tasks
- Character Recognition Class Assignment Example
  - Assume we want to write a character with a pen and have the system output which character it is
  - What features should we use and how would we train/test the system?

When to Gather More Data

- When trying to improve performance, you may need
  - More Data
  - Better Input Features
  - Different Machine learning models or hyperparameters
  - Etc.

- One way to decide if you need more/better data
  - Compare your accuracy on training and test set
  - If bad training set accuracy then you probably need better data, features, noise handling, etc., or you might need a different learning model/hyperparameters
  - If test set accuracy is much worse than training set accuracy then gathering more data is usually a good direction, though overfit or learning model/hyperparameters could still be a major issue