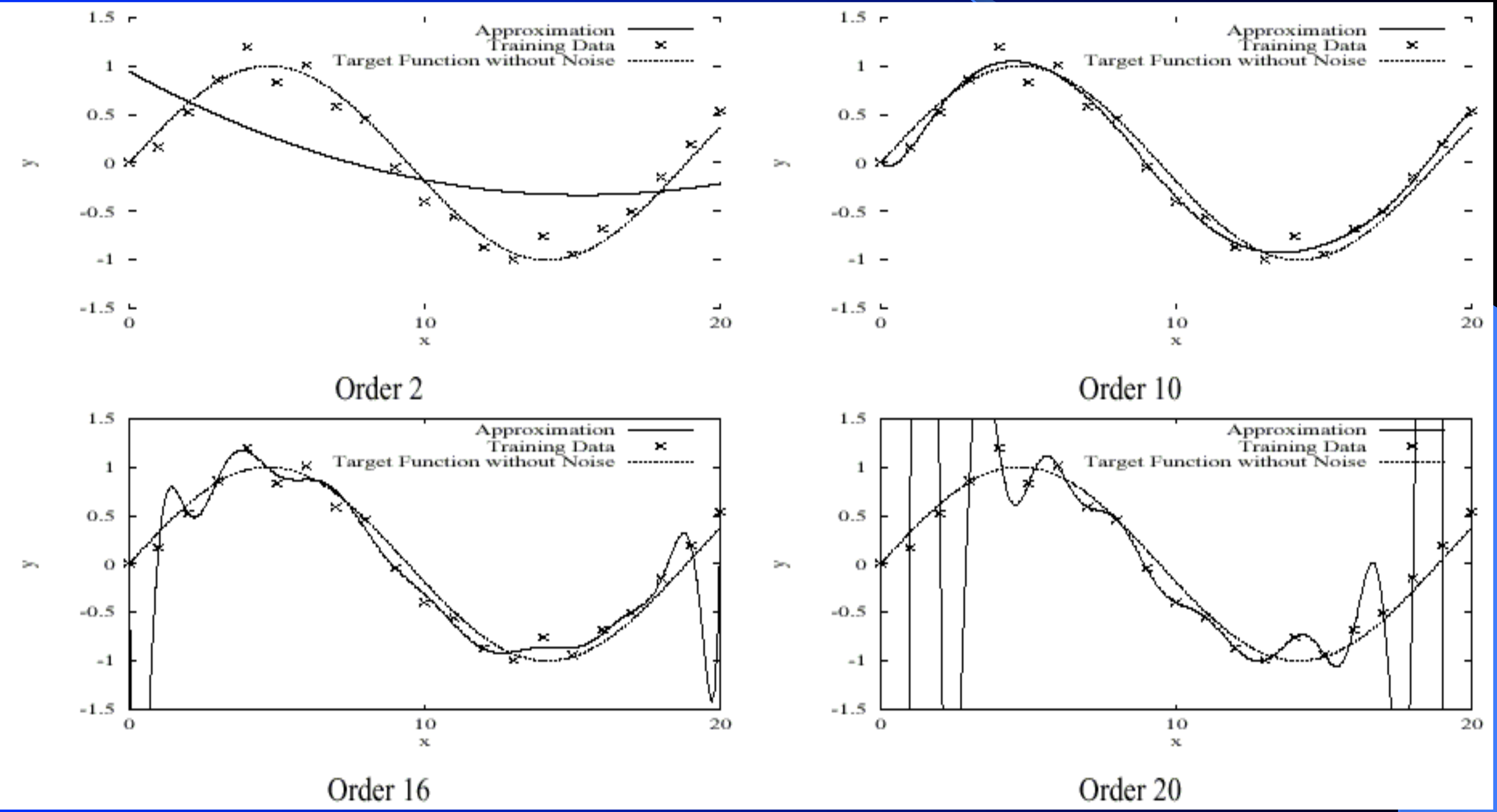
# Inductive Bias:
# How to generalize on novel data

# Overfitting

## Noise vs. Exceptions

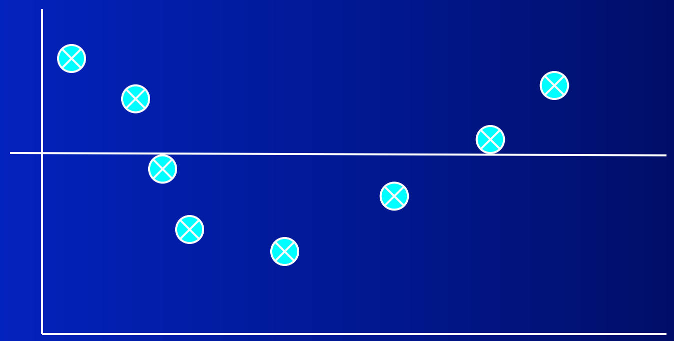


# Non-Linear Tasks

- Linear Regression will not generalize well to the task below
- Needs a non-linear surface
- Could do a feature pre-process as with the quadric machine
  - For example, we could use an arbitrary polynomial in *x*
  - Thus it is still linear in the coefficients, and can be solved with delta rule, etc.

$$Y = \beta_0 + \beta_1 X + \beta_2 X^2 + \ldots + \beta_n X^n$$

  - What order polynomial should we use? – Overfit issues can occur



# Regression Regularization

- How to avoid overfit – Keep the model simple
  - For regression, keep the function smooth
    - Inductive bias is that $f(x) \approx f(x \pm \varepsilon)$
- Regularization approach: $F(h) = Error(h) + \lambda \cdot Complexity(h)$
  - Tradeoff accuracy vs complexity
- Ridge Regression – Minimize:
  - $F(\mathbf{w}) = TSS(\mathbf{w}) + \lambda||\mathbf{w}||^2 = \Sigma\,(predicted_i - actual_i)^2 + \lambda\Sigma w_i^2$
  - Gradient of $F(\mathbf{w})$: $\boxed{\Delta w_i = c(t - net)x_i - \lambda w_i}$ (Weight decay)
  - Especially useful when the features are a non-linear transform from the initial features (e.g. polynomials in $x$)
  - Also when the number of initial features is greater than the number of examples
  - Lasso regression uses an L1 vs an L2 weight penalty: $TSS(\mathbf{w}) + \lambda\Sigma|w_i|$

# Hypothesis Space

- The Hypothesis space *H* is the set all the possible models *h* which can be learned by the current learning algorithm
  - e.g. Set of possible weight settings for a perceptron
- Restricted hypothesis space
  - Can be easier to search
  - May avoid overfit since they are usually simpler (e.g. linear or low order decision surface)
  - Often will underfit
- Unrestricted Hypothesis Space
  - Can represent any possible function and thus can fit the training set well
  - Mechanisms must be used to avoid overfit

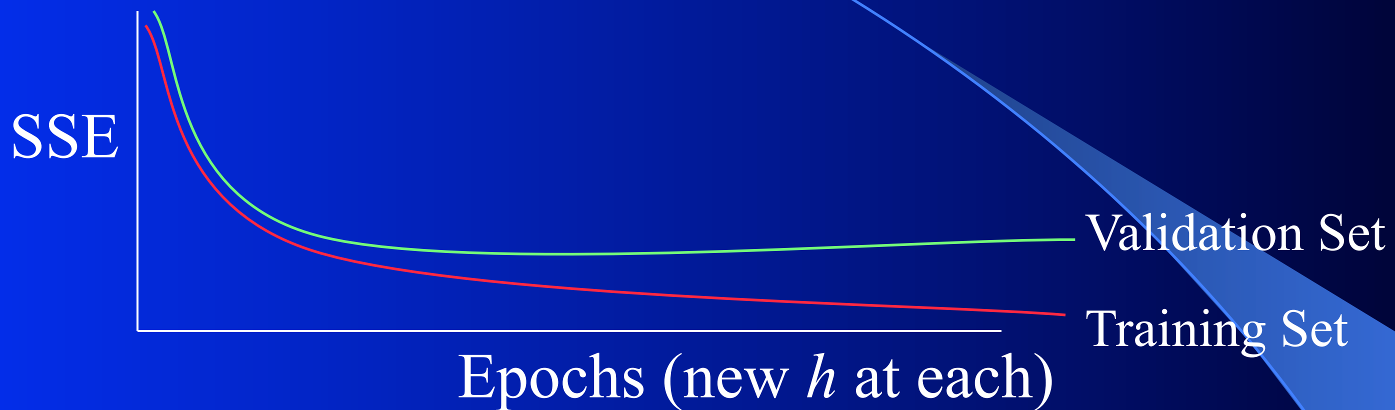
# Avoiding Overfit - Regularization

- Regularization: *any modification we make to a learning algorithm that is intended to reduce its generalization error but not its training error*
- Occam's Razor – William of Ockham (c. 1287-1347)
- Simplest accurate model: accuracy vs. complexity trade-off. Find $h \in H$ which minimizes an objective function of the form:

$$F(h) = Error(h) + \lambda \cdot Complexity(h)$$

  – Complexity could be number of nodes, size of tree, magnitude of weights, order of decision surface, etc. L2 and L1 common.
- More Training Data (vs. overtraining on same data)
  – Also 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 nodes, weights, outputs, etc. E.g. Dropout (discuss with ensembles)
- Most common regularization approach: *Early Stopping* – Start with simple model (small parameters/weights) and stop training as soon as we attain good generalization accuracy (before parameters get large)
  – Use a validation Set (next slide: requires separate test set)
- Will discuss other approaches with specific models

# Stopping/Model Selection with Validation Set




- There is a different model *h* after each epoch
- Select a model in the area where the validation set accuracy flattens
  - When no improvement occurs over *m* epochs
- 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 regularizers

# Inductive Bias

- The approach used to decide how to generalize novel cases
- One common approach is Occam's Razor – The *simplest* hypothesis which *explains/fits* the data is usually the best
- Many other rationale biases and variations

$$ABC \Rightarrow Z$$
$$A\bar{B}C \Rightarrow Z$$
$$AB\bar{C} \Rightarrow Z$$
$$A\bar{B}\bar{C} \Rightarrow Z$$
$$\bar{A}\bar{B}\bar{C} \Rightarrow \bar{Z}$$

$$\bar{A}BC \Rightarrow ?$$

- When you get the new input $\bar{A}\ B\ C$. What is your output?

# One Definition for Inductive Bias

Inductive Bias: Any basis for choosing one generalization over another, other than strict consistency with the observed training instances

Sometimes just called the *Bias* of the algorithm (don't confuse with the bias weight in a neural network).

Bias-Variance Trade-off – Will discuss in more detail when we discuss ensembles

# Some Inductive Bias Approaches

- Restricted Hypothesis Space - Can just try to minimize error since hypotheses are already simple
  - Linear or low order threshold function
  - k-DNF, k-CNF, etc.
  - Low order polynomial
- Preference Bias – Prefer one hypothesis over another even though they have similar training accuracy
  - Occam’s Razor
  - “Smallest” DNF representation which matches well
  - Shallow decision tree with high information gain
  - Neural Network with low validation error and small magnitude weights

# Need for Bias

$2^{2^n}$ Boolean functions of $n$ inputs

| x1 | x2 | x3 | Class | Possible Consistent Function Hypotheses |
|---|---|---|---|---|
| 0 | 0 | 0 | 1 | |
| 0 | 0 | 1 | 1 | |
| 0 | 1 | 0 | 1 | |
| 0 | 1 | 1 | 1 | |
| 1 | 0 | 0 | | |
| 1 | 0 | 1 | | |
| 1 | 1 | 0 | | |
| 1 | 1 | 1 | ? | |

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| 0 | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 0 | 1 | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 0 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
| 1 | 0 | 0 | | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 1 | 1 | 1 | 1 | 1 | 1 | 1 |
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Without an Inductive Bias we have no rationale to choose one hypothesis over another and thus a random guess would be as good as any other option.

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
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Inductive Bias guides which hypothesis we should prefer?
What happens in this case if we use simplicity (Occam's Razor) as our inductive Bias?

# Learnable Problems

- "Raster Screen" Problem
- Pattern Theory
  - Regularity in a task
  - Compressibility
- Don't care features and Impossible states
- Interesting/Learnable Problems
  - What we actually deal with
  - Can we formally characterize them?
- Learning a training set vs. generalizing
  - A function where each output is set randomly (coin-flip)
  - Output class is independent of all other instances in the data set
- Computability vs. Learnability (Optional)

# Computability and Learnability – Finite Problems

- Finite problems assume finite number of mappings (Finite Table)
  - Fixed input size arithmetic
  - Random memory in a RAM
- Learnable: Can do better than random on novel examples

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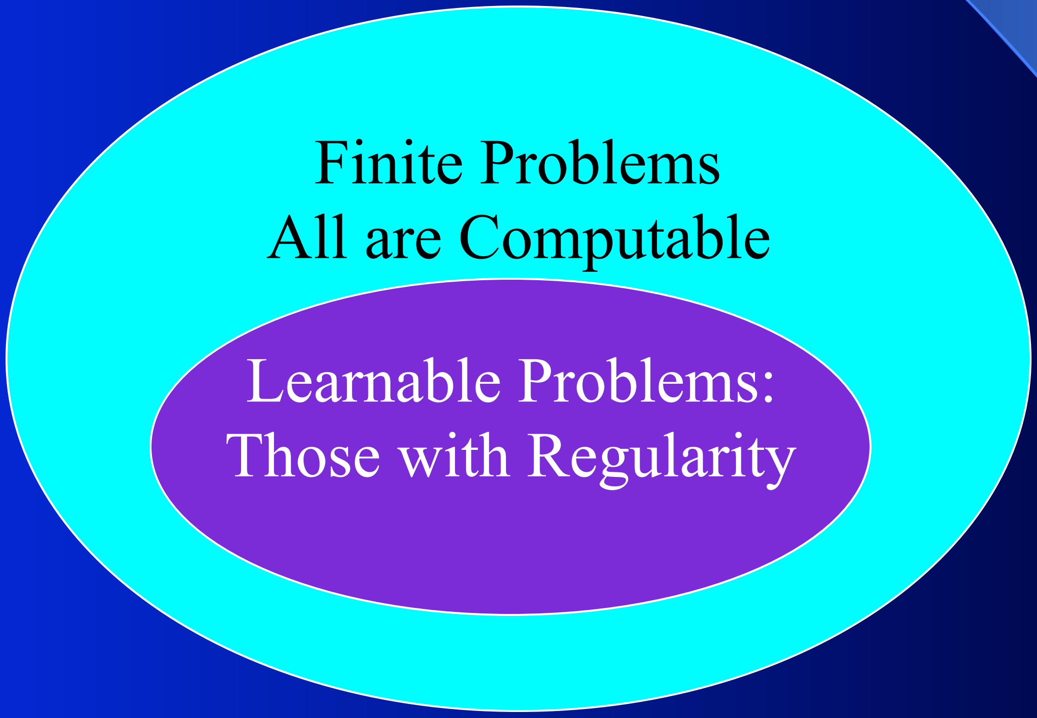

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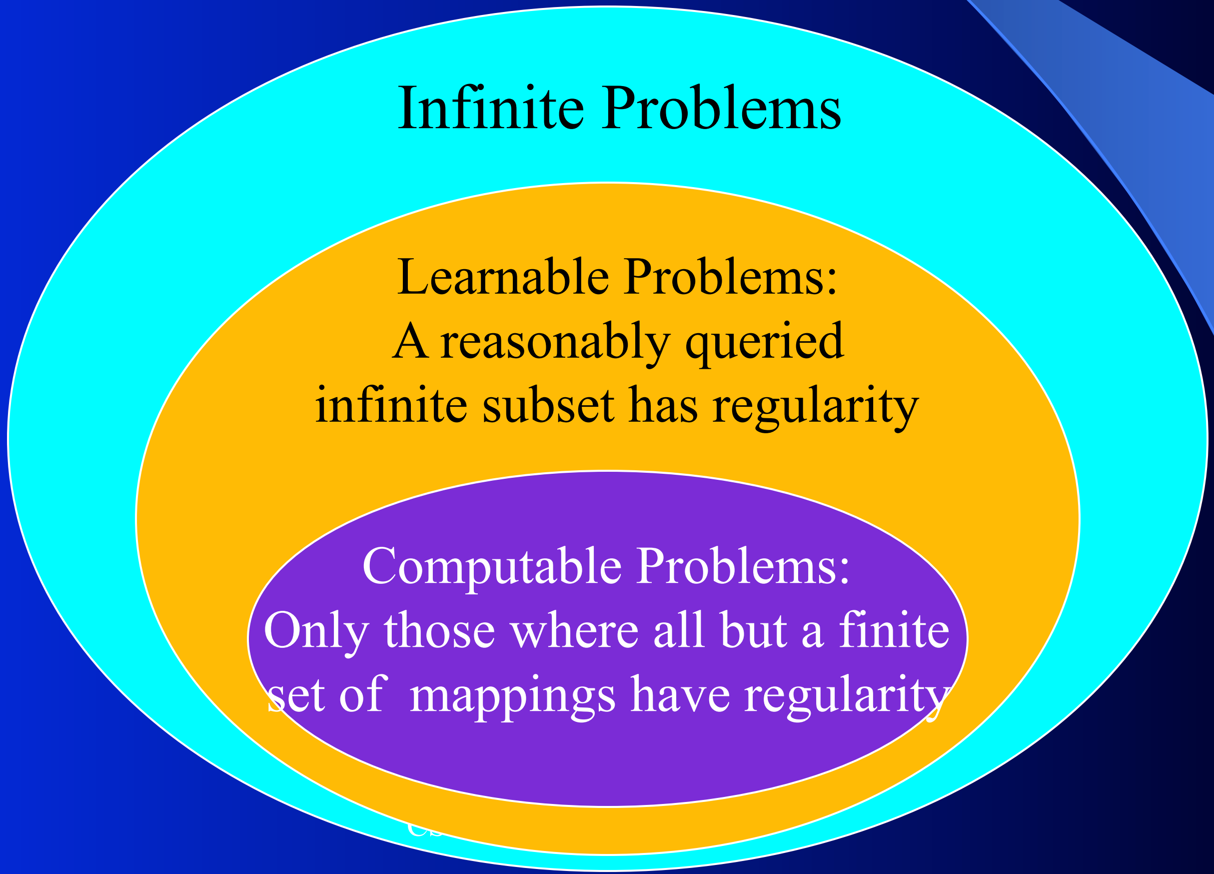
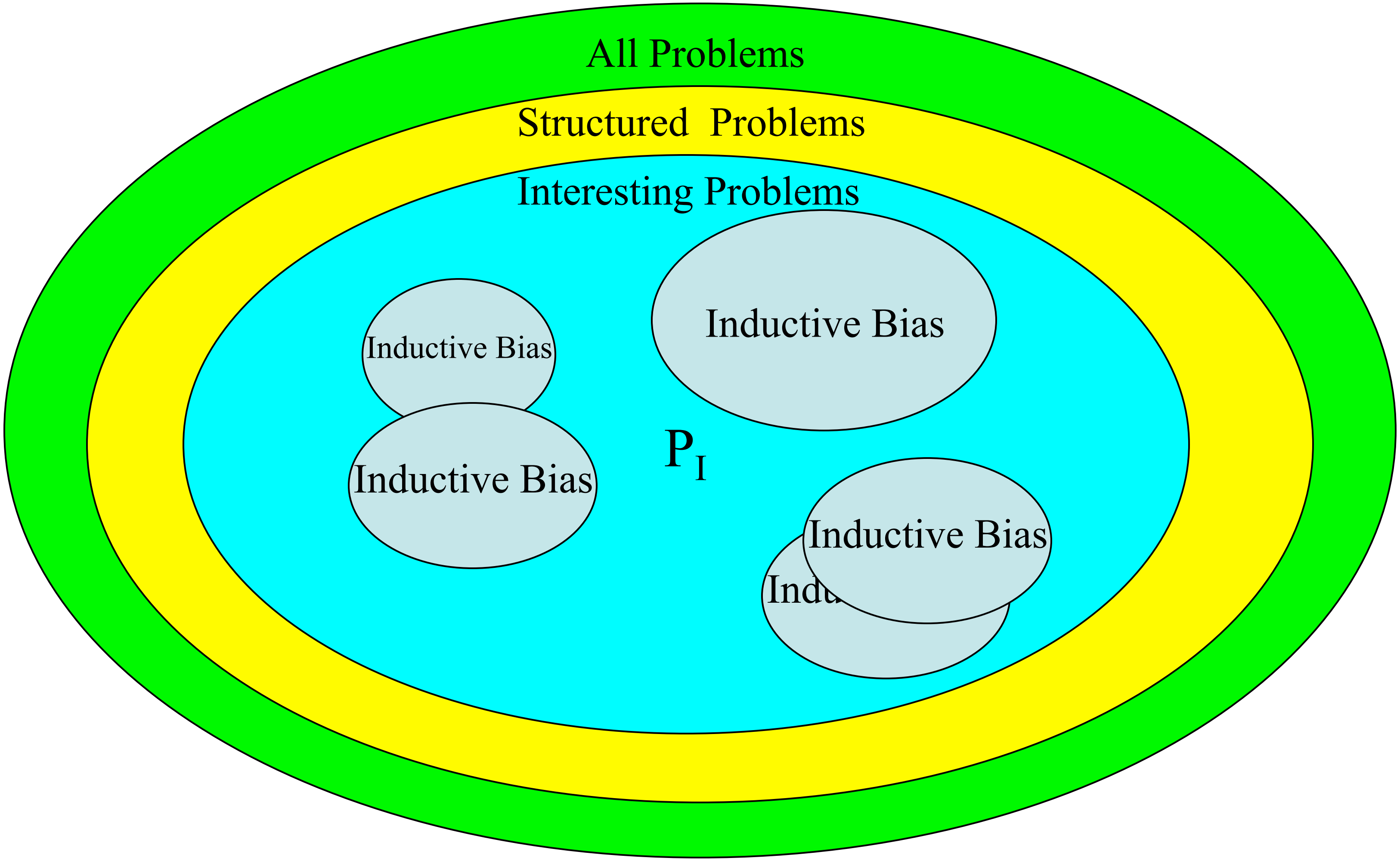


# No Free Lunch

- Any inductive bias chosen will have equal accuracy compared to any other bias over *all* possible functions/tasks, assuming all functions are equally likely. If a bias is correct on some cases, it must be incorrect on equally many cases.
- Is this a problem?
  - Random vs. Regular
  - Anti-Bias? (even though regular)
  - The "Interesting" Problems – subset of learnable?
- Are all functions equally likely in the real world?

# Interesting Problems and Biases



# More on Inductive Bias

- Inductive Bias requires some set of prior assumptions about the tasks being considered and the learning approaches available
- Tom Mitchell’s definition:  Inductive Bias of a learner is the set of additional assumptions sufficient to justify its inductive inferences as deductive inferences
- We consider standard ML algorithms/hypothesis spaces to be different inductive biases:  C4.5 (Greedy best attributes), Backpropagation (simple to complex), etc.

# Which Bias is Best?

- Not one Bias that is best on all problems
- Our experiments
  - Over 50 real world problems
  - Over 400 inductive biases – mostly variations on critical variable biases vs. similarity biases
- Different biases were a better fit for different problems
- Given a data set, which Learning model (Inductive Bias) should be chosen?

# Automatic Discovery of Inductive Bias

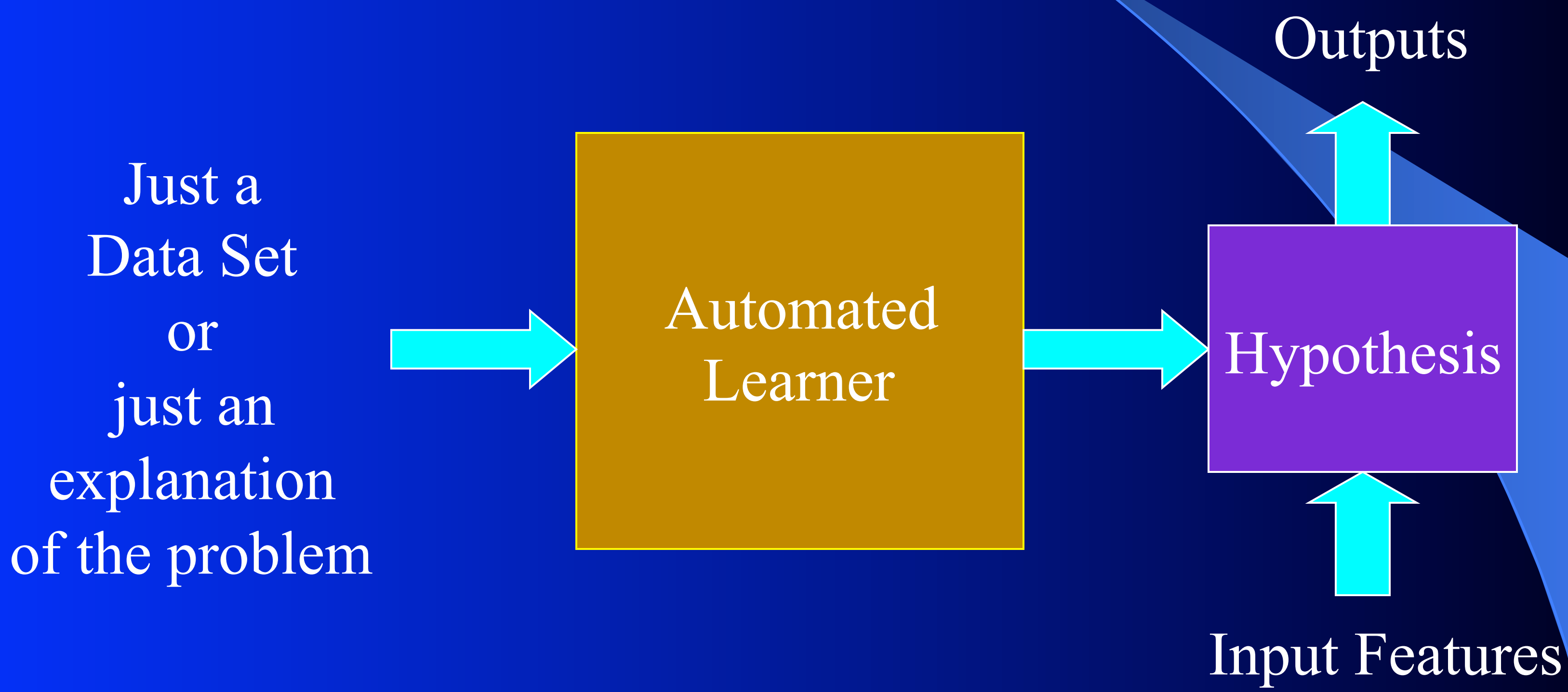
- Defining and characterizing the set of Interesting/Learnable problems
- To what extent do current biases cover the set of interesting problems
- Automatic feature selection
- Automatic selection of Bias (before and/or during learning), including all learning parameters
- Dynamic Inductive Biases (in time and space)
- Combinations of Biases – Ensembles, Oracle Learning

# Dynamic Inductive Bias in Time

- Can be discovered as you learn
- May want to learn general rules first followed by true exceptions
- Can be based on ease of learning the problem
- Example: SoftProp – From Lazy Learning to Backprop

# Dynamic Inductive Bias in Space

# ML Holy Grail: We want all aspects of the learning mechanism automated, including the Inductive Bias



# BYU Neural Network and Machine Learning Laboratory Work on Automatic Discover of Inductive Bias

- Proposing New Learning Algorithms (Inductive Biases)
- Theoretical issues
  - Defining the set of Interesting/Learnable problems
  - Analytical/empirical studies of differences between biases
- Ensembles – Wagging, Mimicking, Oracle Learning, etc.
- Meta-Learning – A priori decision regarding which learning model to use
  - Features of the data set/application
  - Learning from model experience
- Automatic selection of Parameters
  - Constructive Algorithms – ASOCS, DMPx, etc.
  - Learning Parameters – Windowed momentum, Automatic improved distance functions (IVDM)
- Automatic Bias in time – SoftProp
- Automatic Bias in space – Overfitting, sensitivity to complex portions of the space: DMP, higher order features