Machine Learning

CMPUT 446 and 551

Fall 2017

Martha White

What is this course about?

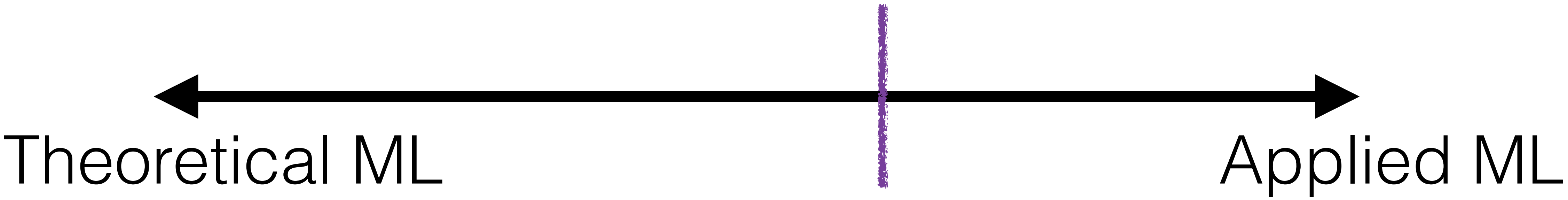
- The world is full of information and data
- Much of that data is noisy and has an element of uncertainty
  - We have incomplete knowledge of the environment (partial observability)
  - Actions of other actors not provided
- Machine learning algorithms help us analyze that data
- **Goal**: understand machine learning algorithms by deriving them from the beginning
  - our focus will be on **prediction** (on new data)

What is this course about?

- The focus is on fundamental data analysis/statistics concepts, and not necessarily on application of these algorithms
    - though you will get to do that too

- Application of algorithms is simpler when you understand their development and underlying assumptions

- Overall goal: understand how to use (heaps of) data to make predictions about novel events, including
    - what assumptions to make and how to formalize the problem
    - how to derive algorithms for your problem
    - ascertain your confidence in the predictions (i.e., evaluate your approach)



Theoretical ML

Applied ML

What is machine learning?

- We could label it in many different ways including
  - Data-driven approach to artificial intelligence
  - Applied statistics
- Some keywords associated with machine learning
  - Prediction, probability, samples, data, function, optimization, stochastic, …

ICML 2015 word cloud

What is machine learning?

- “The field of machine learning is concerned with the question of how to construct computer programs that automatically improve with experience.” -Mitchell

- “…the subfield of AI concerned with programs that learn from experience.” -Russell & Norvig

- “The goal of machine learning is to develop methods that can automatically detect patterns in data, and then to use the uncovered patterns to predict future data or other outcomes of interest.” -Murphy

Where did machine learning come from?

- Let’s first step back to the goals of artificial intelligence

- Traditional AI approaches were expert-based
    - logic approaches for theorem proving
    - expert systems

- Machine learning arose as a data-driven approach to solve artificial intelligence problems
    - why the shift? increased computation, availability of data and efficacy of data driven approaches (largely driven by availability of data)

- Many techniques from statistics, which did not arise from AI goals

What are the ultimate goals?

- The focus for many ML researchers has shifted from AI towards generally solving important (practical) problems
  - computer vision, speech recognition, clustering, modeling temporal data, …
- This includes a focus on understanding intrinsic properties of a learning problem
  - is it difficult to learn (e.g., NP-hard)?
  - how can it be formulated in a precise way? (e.g., explicit probabilistic assumptions, preference for “simpler” hypotheses)
  - how many samples are needed to learn the model (epsilon) accurately?
  - how well does the learned model generalize to new samples?

Uses of machine learning in the real world

- Character recognition for mail addresses (as early as mid 90s)
  - 30% accuracy in 1997 to 88% accuracy in 2004, 98% now

- Spam filtering p(email = spam | information about email)

- Netflix challenge (matrix completion)

- Speech recognition (matrix factorization and deep learning)

Why is ML so popular now?

- Huge increases in available data and computation
- Statistical techniques do well with lots of (representative) data
- More complex models can be learned (and engineered) with more computation
- Are we done?
  - …not at all! Much more to understand when algorithms work and why, develop algorithms that are robust in new situations, etc.

Why is ML so popular now?

- Huge increases n
- Statistical techn ntative) data
- More complex r eered) with more computation
- Are we done?
  - …not at all! Mu s work and why, develop algorit c.

THIS IS YOUR MACHINE LEARNING SYSTEM?
YUP! YOU POUR THE DATA INTO THIS BIG PILE OF LINEAR ALGEBRA, THEN COLLECT THE ANSWERS ON THE OTHER SIDE.
WHAT IF THE ANSWERS ARE WRONG?
JUST STIR THE PILE UNTIL THEY START LOOKING RIGHT.
DATA
ANSWERS

…its not this bad, but let's understand the pile!

A starting example

- Our goal: obtain a function to predict house prices, given age
  - f(age) = price of house
- Imagine you have a dataset of previous house sales this year, with attribute information Age and target Price
  - (age_1, price_1), (age_2, price_2), …, (age_9, price_9)
- Presumably these previous houses give us some information about the function between age and price
- Idea: if we can learn a function to accurately recreate these (age, price) pairs, then it could provide good predictions

Formalizing the optimization

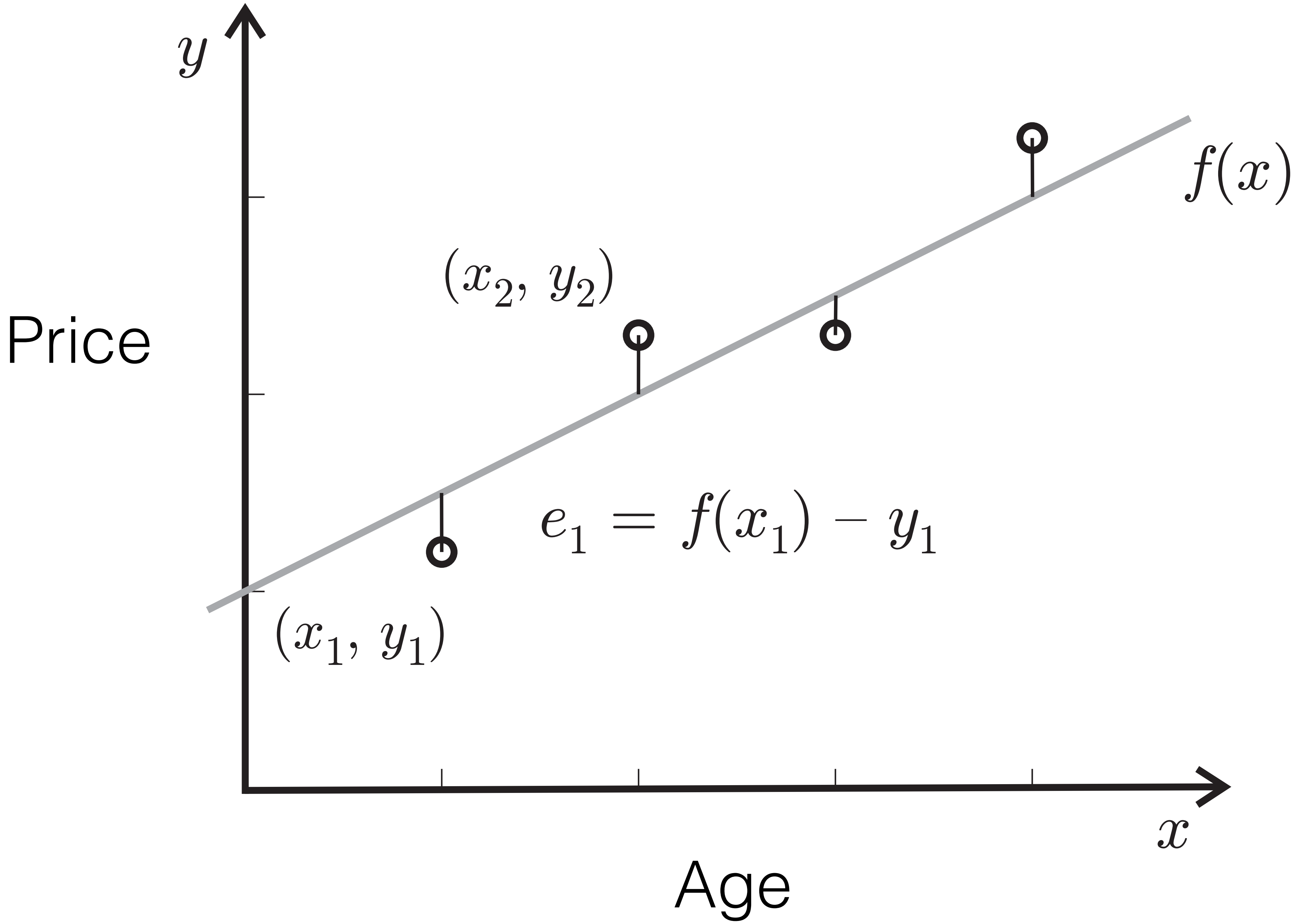
Let $x =$ age and $y =$ price

Make difference between $f(x_i)$ and y_i small

$$\text{Minimize} \sum_{i=1}^{9} (f(x_i) - y_i)^2$$

Need to pick a form for f

Linear function f



$$f(x) = w_0 + w_1 x$$

Solving for the optimal function

$$\min_{f \text{ in function space}} \sum_{i=1}^{9} (f(x_i) - y_i)^2$$

$$= \min_{w_0, w_1} \sum_{i=1}^{9} (w_0 + w_1 x_i - y_i)^2$$

- We will see later how to solve this

- Questions:
  - Would you use this to predict the price of a house? Why or why not?
  - Will this predict well? How do we know?
  - If not, what is missing to make these assessments?

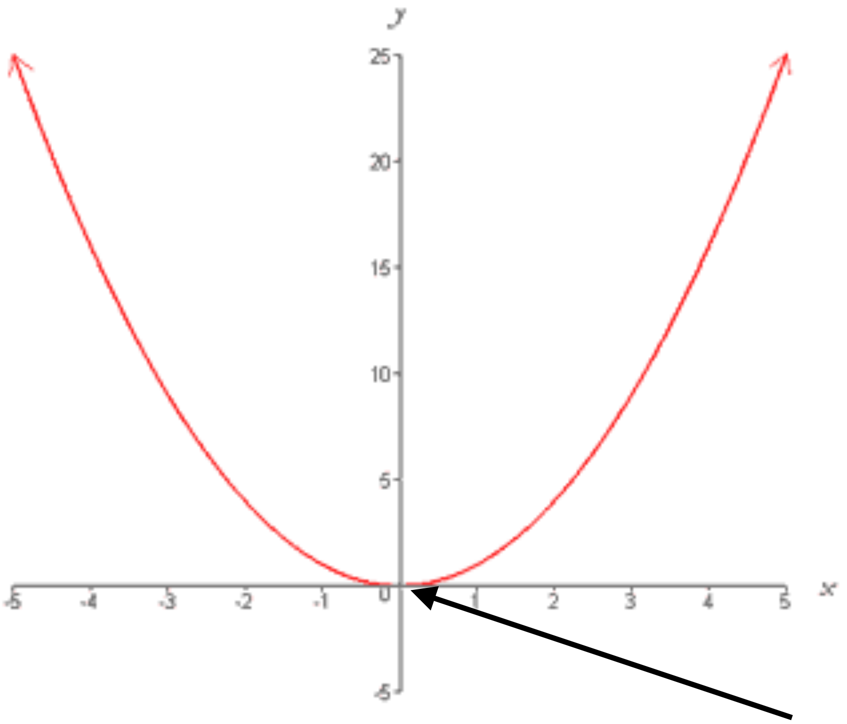
General approach

- Specify the problem and analyze the solution using a probabilistic approach
    - e.g., unlikely that we can learn a deterministic function from f(age) to price, many houses will have the same age but different prices
    - need to specify the problem so there is a distribution over targets (price), given attributes about the item (age)
    - stochasticity largely comes from partial observability
- Generalize beyond simple linear functions
    - polynomial regression
    - radial basis function network
    - neural networks

Exercise

- Solve for optimal w for function f(x) = xw

$$\min_{w} \sum_{i=1}^{n} (x_i w - y_i)^2$$

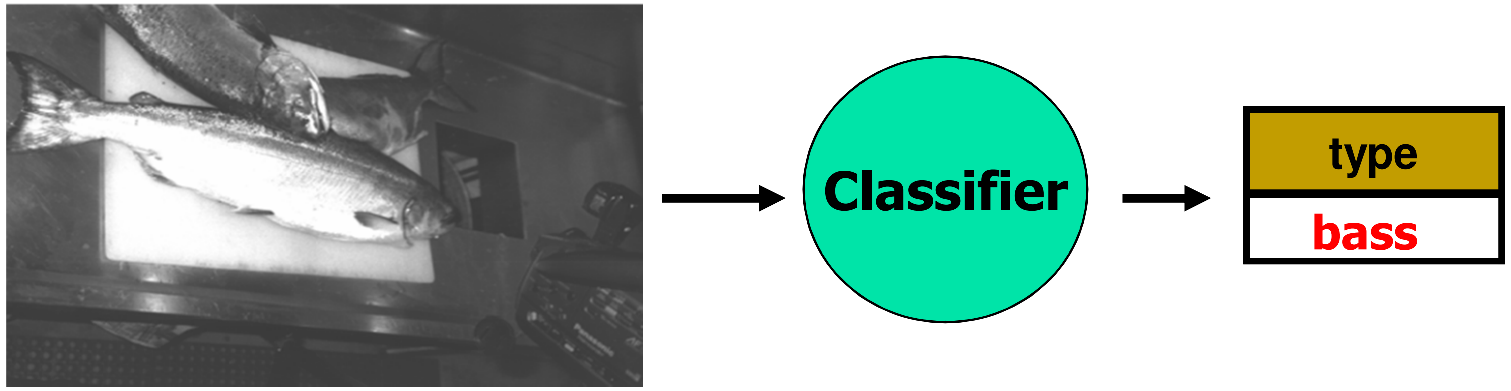


Optimal point, derivative is zero

Another example: classify fish

- What if want to predict whether a fish is a sea bass or a salmon?

- You can extract features from the image, like
  - Length
  - Width
  - Ave. pixel brightness
  - …



Classifier

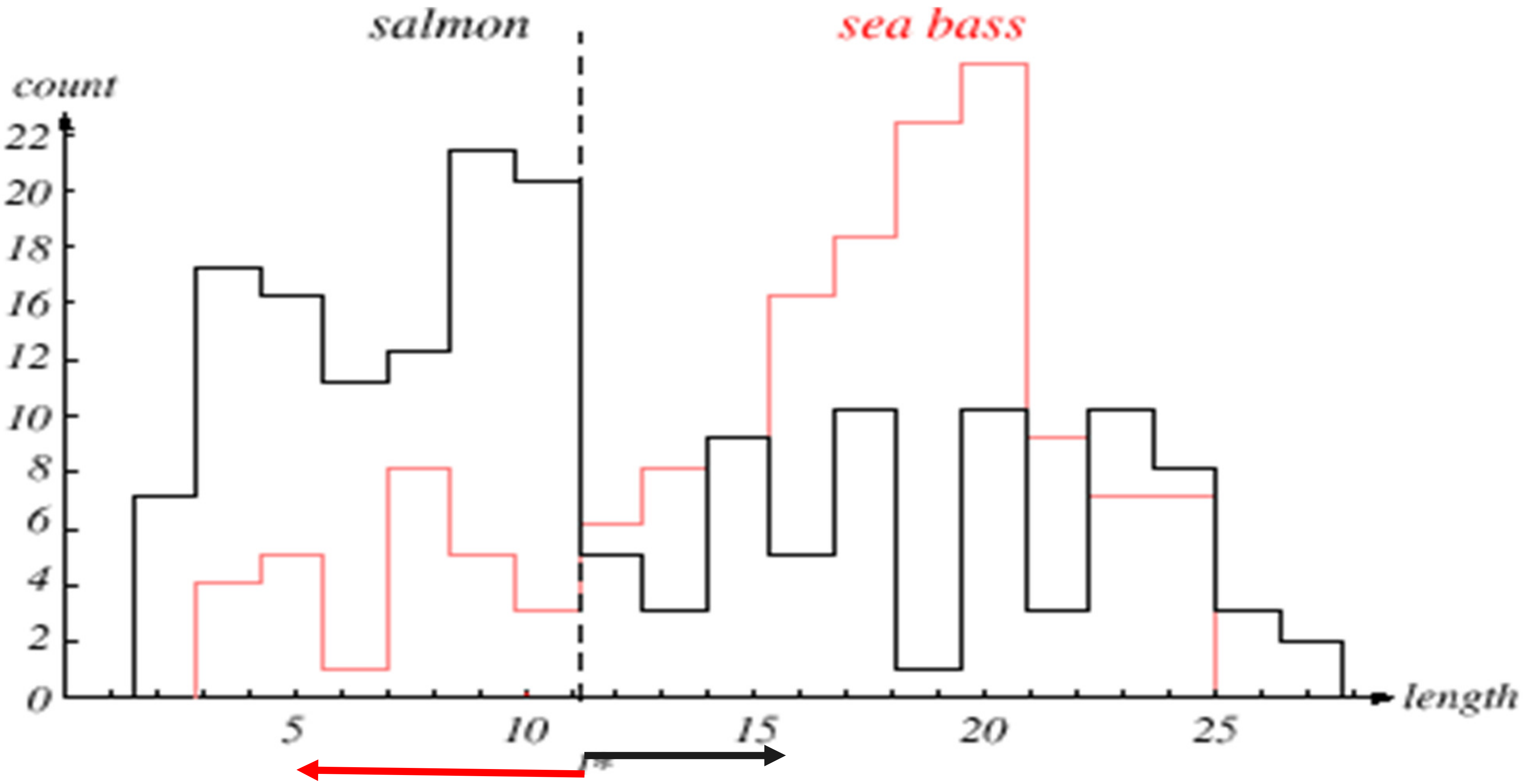
type

bass

- Is the linear function f(x) = wx a good predictor? Any issues?

- Alternative: Now want a function that either
  - returns -1 or 1
  - or return f(x) < 0 for class 1 and f(x) > 0 for class 2

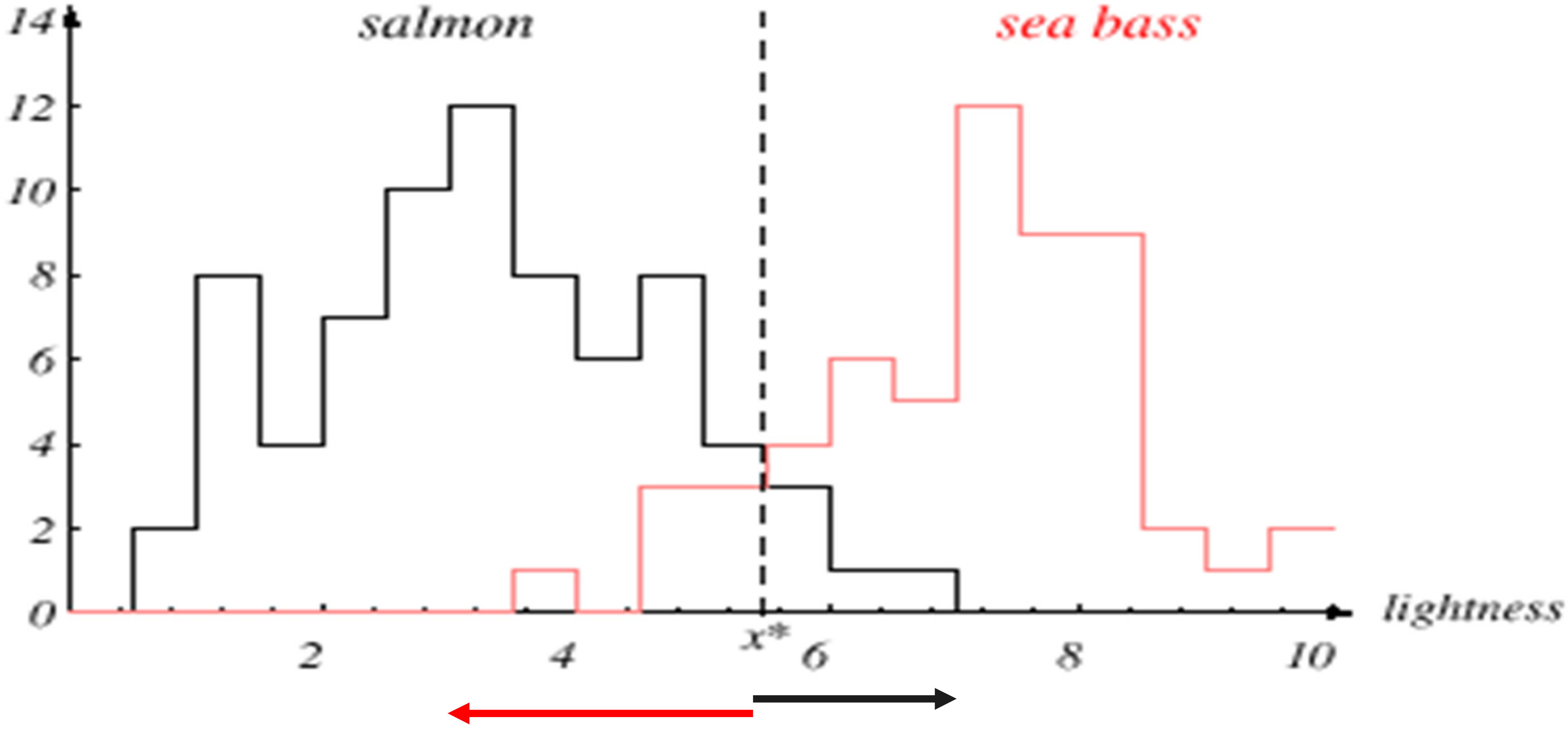
Use “length”



- f(length) = salmon, if length < 11, otherwise sea bass

- Problematic…many incorrect classifications

Use “lightness”

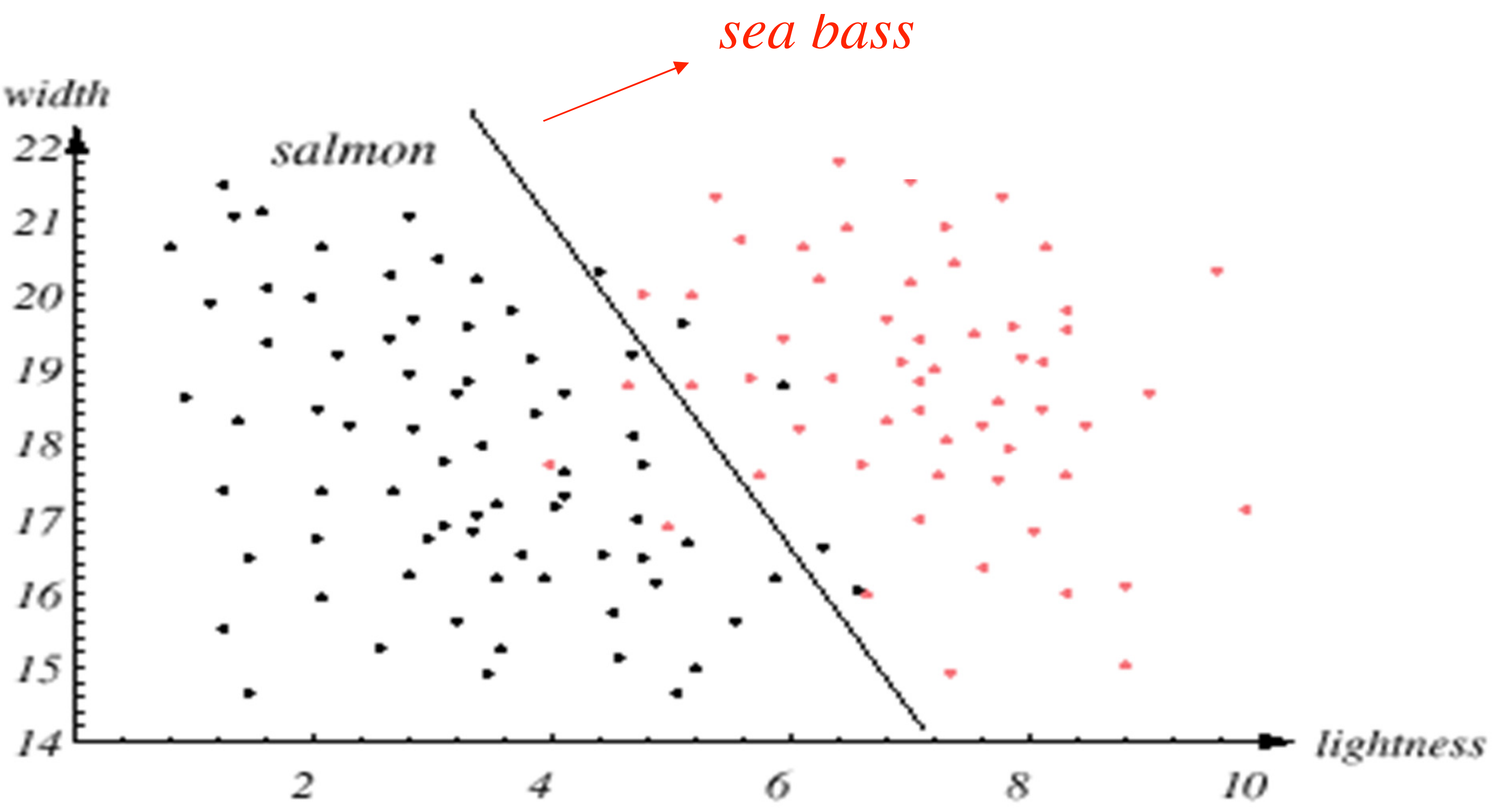


- Better…but still some incorrect classifications

We should use all the distinguishing information (features)

- Use both **lightness** and **width**
- Fish described by vector **x** = [lightness, width] = [$x_1 \quad x_2$]
- Now separate instances with a line, not just a point on an interval

Both features



- Much more accurate; less partially observable

Demo: classification

- Let’s look at a line learned by logistic regression (a simple ML algorithm) for separating two groups
- The line corresponds to a linear function
- The classifier thresholds
  - $f(x) > 0$ to get +1 (positive class, or class 1)
  - $f(x) < 0$ to give -1 (negative class, or class two)

How do learning problems differ?

- They can be categorized across several dimensions
  - **Control versus prediction:** though a control algorithm will likely use predictions to improve decision-making (e.g., reinforcement learning)
  - **Supervised and unsupervised:** supervised learning is for prediction, unsupervised learning is usually for visualization or extracting structure (e.g., clustering); some algorithms combine these two components
  - **How they are used:** empower decision-making of end user OR autonomously control system
  - … there are more, but these are some main ones

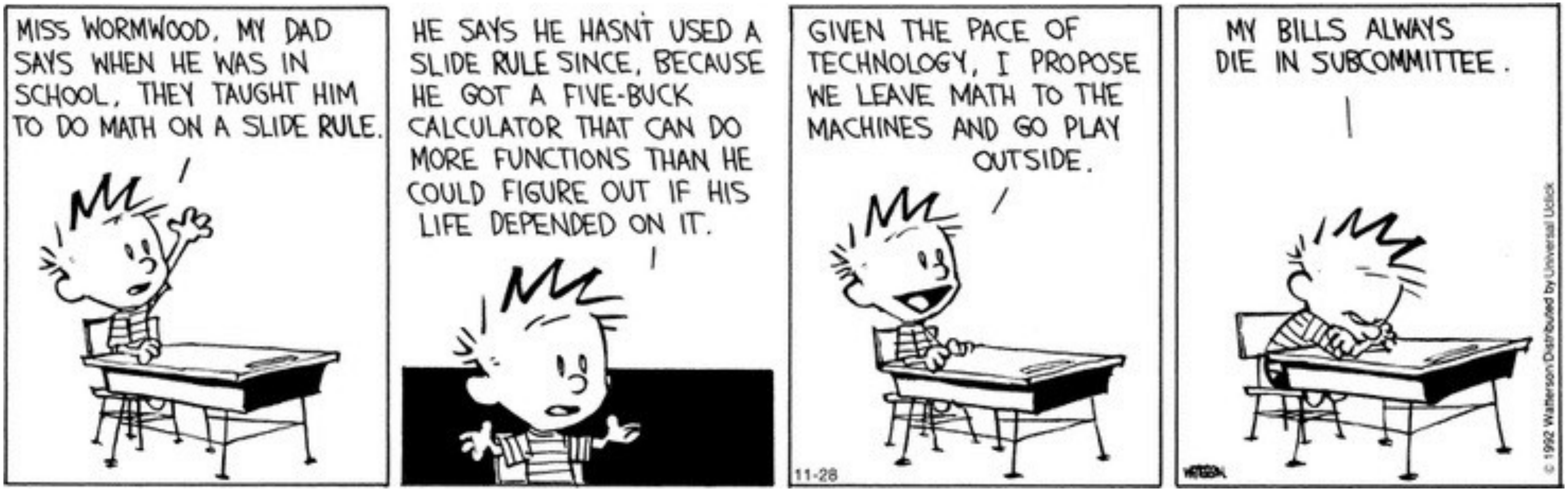
How do the algorithms differ?

- **Algorithms** also differ in many ways, even for similar problems
  - Process data incrementally (as stream) or in batch
  - Low computation (or memory) versus heavy computation (or memory)
  - Sample efficient or Data efficient (needs only a few samples to learn a good model)
  - Consistency: with more samples, model approaches “true” model
  - … other common algorithmic distinctions, such as approximate vs. exact, or randomized vs deterministic

Topic overview

- Background in probability and optimization (Chapters 1 and 2)
  - And then more advanced optimization in Chapter 6
- Parameter estimation and prediction problems (Chapters 3 and 4)
  - the core background for modeling in machine learning
- Linear regression (Chapter 5) and Generalized Linear Models (Chapter 7)
- Linear classifiers (Chapter 6)
- Representations (Chapter 9), to get nonlinear predictors (e.g., neural networks)
- Statistical learning theory and empirical evaluation (Chapter 10)
- … and any other topics listed on the syllabus if we have time (e.g., boosting)

Next class: crash course in probability


MISS WORMWOOD, MY DAD SAYS WHEN HE WAS IN SCHOOL, THEY TAUGHT HIM TO DO MATH ON A SLIDE RULE.
HE SAYS HE HASN'T USED A SLIDE RULE SINCE, BECAUSE HE GOT A FIVE-BUCK CALCULATOR THAT CAN DO MORE FUNCTIONS THAN HE COULD FIGURE OUT IF HIS LIFE DEPENDED ON IT.
GIVEN THE PACE OF TECHNOLOGY, I PROPOSE WE LEAVE MATH TO THE MACHINES AND GO PLAY OUTSIDE.
11-28
MY BILLS ALWAYS DIE IN SUBCOMMITTEE.
WATTERSON
© 1992 Watterson/Distributed by Universal Uclick

- Probabilities underly much of machine learning
  - enable precise modeling of uncertainty

- Understanding assumptions and how to build extensions is key for effectively using machine learning algorithms

Basic information

Class meets:

Time: TR 12:30pm – 1:50 pm
Place: SAB 336

Instructor:

Martha White
Office: ATH 3-05
Email: whitem@ualberta.ca
Web: marthawhite.ca

Office Hours:

Time: T 3:00pm-5:00pm (is this a good time?)
or by appointment
Place: ATH 3-05

Class Web Site:

GitHub pages: https://marthawhite.github.io/mlcourse/

Teaching Assistants

Kris De Asis
Touqir Sajed
Roberto Vega Romero
Peng Xu

Lab/Office Hours:

- Labs will typically be question and answer sessions
- Might have some labs have tutorials, if needed/requested

Come to labs and ask questions!

Textbook information

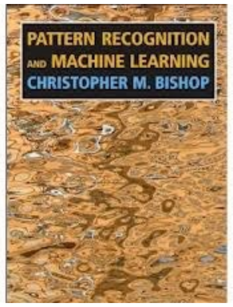
- **Main notes** provided on github course site
  - written by Predrag Radivojac and myself (about 130 pages)

- **[Optional] reference material/recommended readings:**
  - An Introduction to Statistical Learning, 2013 (accessible and concise)
  - Bayesian Reasoning and Machine Learning by D. Barber, Cambridge Press 2012.

BAYESIAN REASONING and MACHINE LEARNING

David Barber

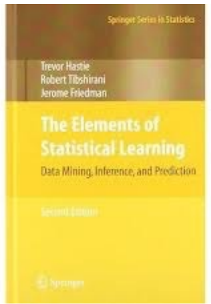
  - Pattern Recognition and Machine Learning by C. M. Bishop, Springer 2006.



PATTERN RECOGNITION AND MACHINE LEARNING

CHRISTOPHER M. BISHOP

  - The Elements of Statistical Learning by T. Hastie, R. Tibshirani, and J. Friedman, 2009



Springer Series in Statistics

Trevor Hastie
Robert Tibshirani
Jerome Friedman

The Elements of Statistical Learning

Data Mining, Inference, and Prediction

Second Edition

Springer

Marks

- 30%: Assignments (3), a mixture of mathematical and programming exercises (code provided in python)
    - Must complete assignments independently
- 15%: Mini-project: provides an opportunity to work on a more open-ended problem, using your choice of dataset and algorithms
    - Perform a principled empirical evaluation of the algorithms
    - 15% (5%) for initial draft of mini-project for UG (Grad)
    - Grads additionally have to provide feedback on mini-projects, for 10%
- 35%: Final exam, December 15, 12:30 p.m. - 2 p.m.
- 10%: Thought questions (3), show that you're reading and thinking about the material

More on grading

- E-class should show you a ranking
- This course is not curved; I decide the letter thresholds
  - Note that I don’t enjoy having to assign you a grade, but it helps you learn
- Assignments systematically tested for plagiarism and cheating
- No arguing for marks with TAs
  - should only ask: “Can you help me understand this question?
  - Even if you get 10% improvement on an assignment, at best this translates into 1% for the final grade. It is a waste of your (and everyone’s) time.

More about assignments

- **All assignments are individual:**
  - The assignments are feasible on your own; you will learn much more and get more out of the course when you accomplish this
  - In-your-head-rule: you can discuss with classmates to some extent, but no writing down solutions on a piece of paper, or copying code
- Acknowledge sources (websites, books) in your documents
  - can be typed up in LaTex; I have given you latex files on Canvas, for each assignment
  - or write legibly and upload scanned document
- We are very serious about academic honesty

My expectations

- Basic mathematical skills
  - some calculus
  - some probabilities
  - some linear algebra
  - I will give crash courses in these along the way, so if you do not have this background, a willingness to learn these topics is a prerequisite
- You are hardworking and motivated to learn (machine learning)
- You are motivated to think beyond the material and ask open-ended questions

What to expect from this course

- I know you have expectations of me too
  - I will try to be transparent in marking and course choices
  - I am here to help you learn; I will treat you with respect and listen thoughtfully to your questions (I love to answer questions and give advice!)
  - Feel free to give me feedback (e.g., Miss Martha, you are talking too fast)
  - I will provide a mechanism for anonymous feedback
- This course will be quite mathematical, with derivations of details
  - this is absolutely necessary, and will make you much more skilled in ML
- By the end of the course, you should have a good grasp of fundamental concepts in ML and algorithm derivation for ML

Thought questions

- University is about thinking and asking questions
  - e.g., research is actually about asking good questions
  - a question does not have to have an answer, but it can be thought-provoking or make you think about a topic differently
- “Thought questions” correspond to (short) readings in the notes, and should demonstrate you’ve read and thought about the topics
- There are no stupid questions (so ask any questions in class/office hours/email), but “thought questions” are to demonstrate insight and so I have some requirements

General format for thought questions

- (1) First show/explain how you understand a concept
- (2) Given this context, propose a follow-up question
- (3) [Optional] Propose an answer to the question, or how you might find it
- Additional note: framing a coherent, concise thought is a skill. When writing your thought question, ask yourself: is this clear?

Examples of “good” thought questions

- After reading about independence, I wonder how one could check in practice if two variables are independent, given a database of samples? Is this even possible? One possible strategy could be to approximate their conditional distributions, and examine the effects of changing a variable. But it seems like there could be other more direct or efficient strategies.

- PCA encodes a simple linear relationship between the data and underlying subspace. Why is PCA so widely used? It seems simple and I would not expect it to be able to encode complex properties. Potentially its simplicity is an answer.

Examples of “bad” thought questions

- I don’t understand linear regression. Could you explain it again? (i.e. a request for me to explain something, without any insight)

- Derive the maximum likelihood approach for a Gaussian. (i.e., an exercise question from a textbook)

- What is the difference between a probability mass function and a probability density function? (i.e., a question that could easily be answered from reading the definitions in the notes)

- How are Boltzmann machines and feedforward neural networks different? (i.e., again a definition)
    - But the following modification would be good: “I can see that Boltzmann machines and feedforward neural networks are different, in that the first is undirected and the second directed. How does this difference impact modeling properties and accuracy of estimation in practice?”

Anticipated questions

- Where can I find background exercises/questions?
  - Try machine learning books (e.g., Barber’s book)
  - Try applied statistics textbooks (e.g., All of Statistics)
- The course is too slow / too fast
  - If too slow, come talk to me and I’ll show you how to get more from it
  - If too fast, don’t be too frustrated; slowly the information and way of thinking start to make sense.

Anticipated questions

- Why are we learning such simple models? Isn't the modern approach neural nets and we should start there?
    - The foundational material is key for properly understanding more complex models. As you will see, building up from the foundation is critical to understanding neural nets. e.g., some do not understand that backpropagation is gradient descent, the choice of activation functions, how to choose the loss, etc.
    - Without an in-depth understanding, you will not be able to use machine learning effectively for your novel setting, and may even make terrible modeling decisions

Anticipated questions

- Why aren't we programming more? I don't need to learn about linear regression, I can just use packages.

- Quote from previous student: "One thing I would like to strengthen is the importance of knowing the mathematical details of how to deduct each model. Some people might think it is too tedious to know, but I have done projects on modifying training algorithms, like adding priors or changing the lose functions, and it requires me to know those details so that I know what I am supposed to do. Projects related to basic models, like linear regression, logistic regression, naive bayes, decision tree and support vector machine, require me to truly understand the models. Although there are various packages to choose and one don't need to implement a model from scratch, knowing the details helps in parameter tuning and feature engineering and it also makes me creative in finding new ideas."

Anticipated questions

- My math skills are poor. What should I do?
  - Math is just a tool/language. Practice and become more comfortable with this language. A common pitfall is to try to intuit all the math; I recommend against this. For example, try to learn the notation behind probability first, before getting a strong intuitive grasp, and once you are more comfortable with the notation, then start searching for intuition

- I'm rusty at programming. Am I going to fail?
  - The amount you program is limited. I provide python code to read in data and do basic learning on that data. You will simply have to modify this code, likely amounting to at most 500 lines of code.

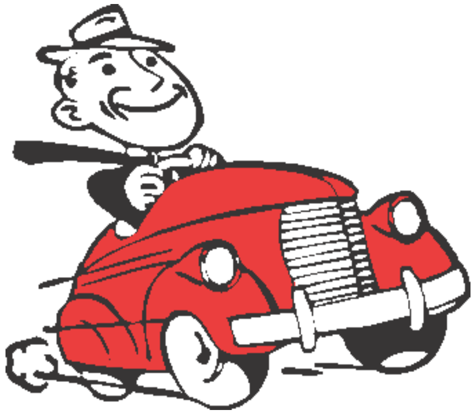
Anticipated questions

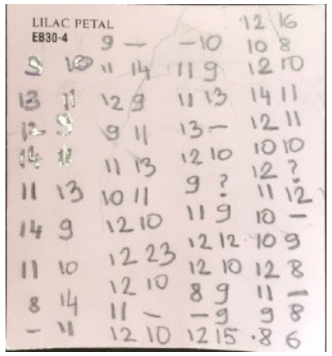
- I was hoping we would learn about topic x, but it looks like it is not listed. Can we learn about topic x?
  - With the foundations from this course, you will much more easily be able to go learn about more advanced topic x
  - Otherwise, particularly later in the course, come chat with me and we can discuss topic x

Let’s look at some fun examples!

- Commute times (independent identically distributed (iid) data)
- Weather prediction (temporally connected data)
  - machine learning is often used for time series, but in the specific case of weather, mostly expert models appear to be used (for now…)
- Octopus arm simulator (machine learning for control)
  - we will not look at control algorithms; however, their development uses the fundamental concepts in this course

Commute times

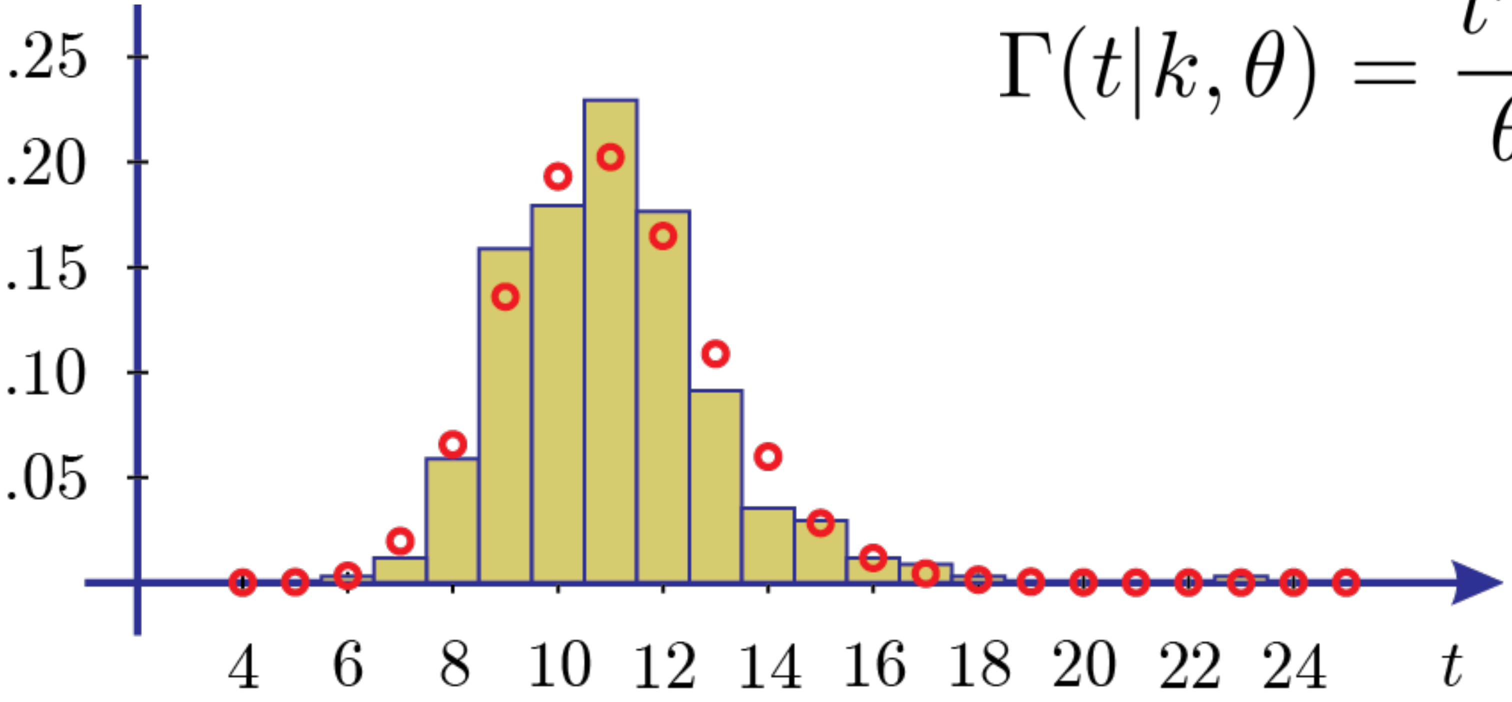


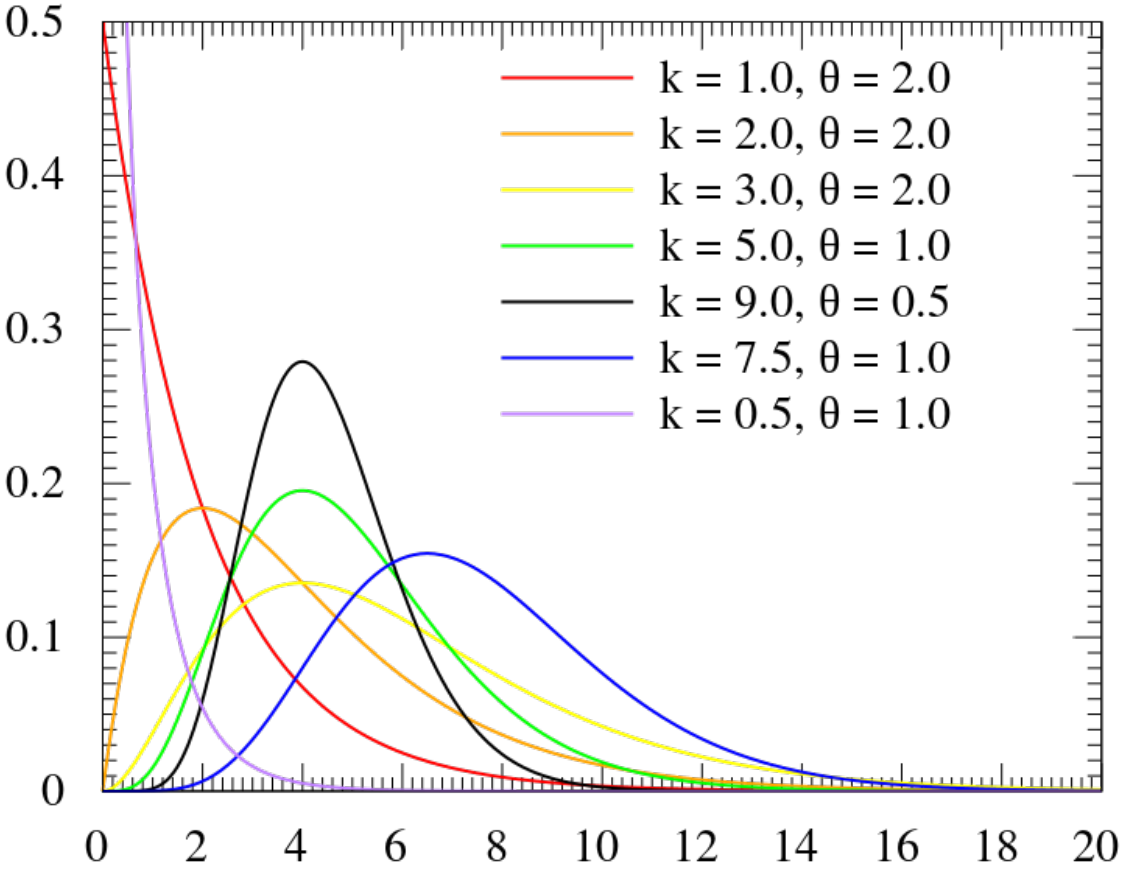


How might you try to predict your commute time for today?

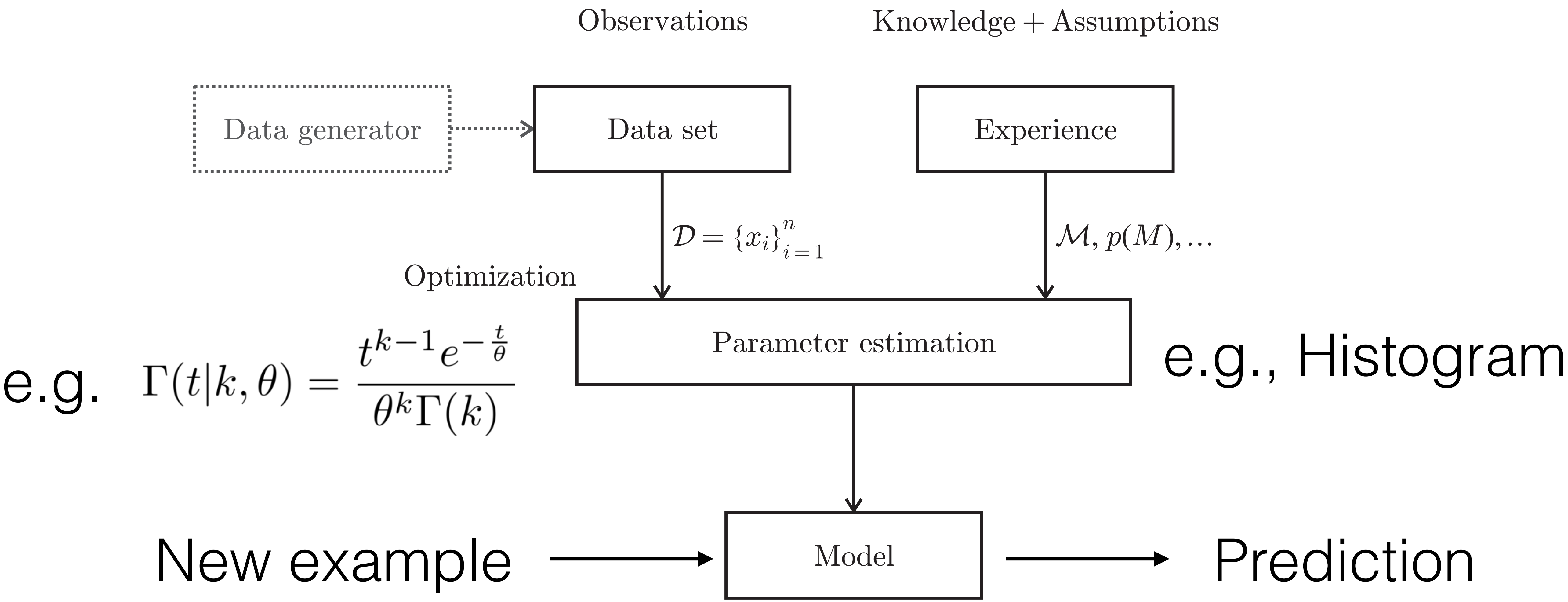
Commute times (2)

$$\Gamma(t|k,\theta) = \frac{t^{k-1}e^{-\frac{t}{\theta}}}{\theta^k\Gamma(k)}$$





Summarized flow



Observations

Knowledge + Assumptions

Data generator

Data set

Experience

$\mathcal{D} = \{x_i\}_{i=1}^{n}$

$\mathcal{M}, p(M), \ldots$

Optimization

Parameter estimation

e.g. $\Gamma(t|k,\theta) = \frac{t^{k-1}e^{-\frac{t}{\theta}}}{\theta^k \Gamma(k)}$

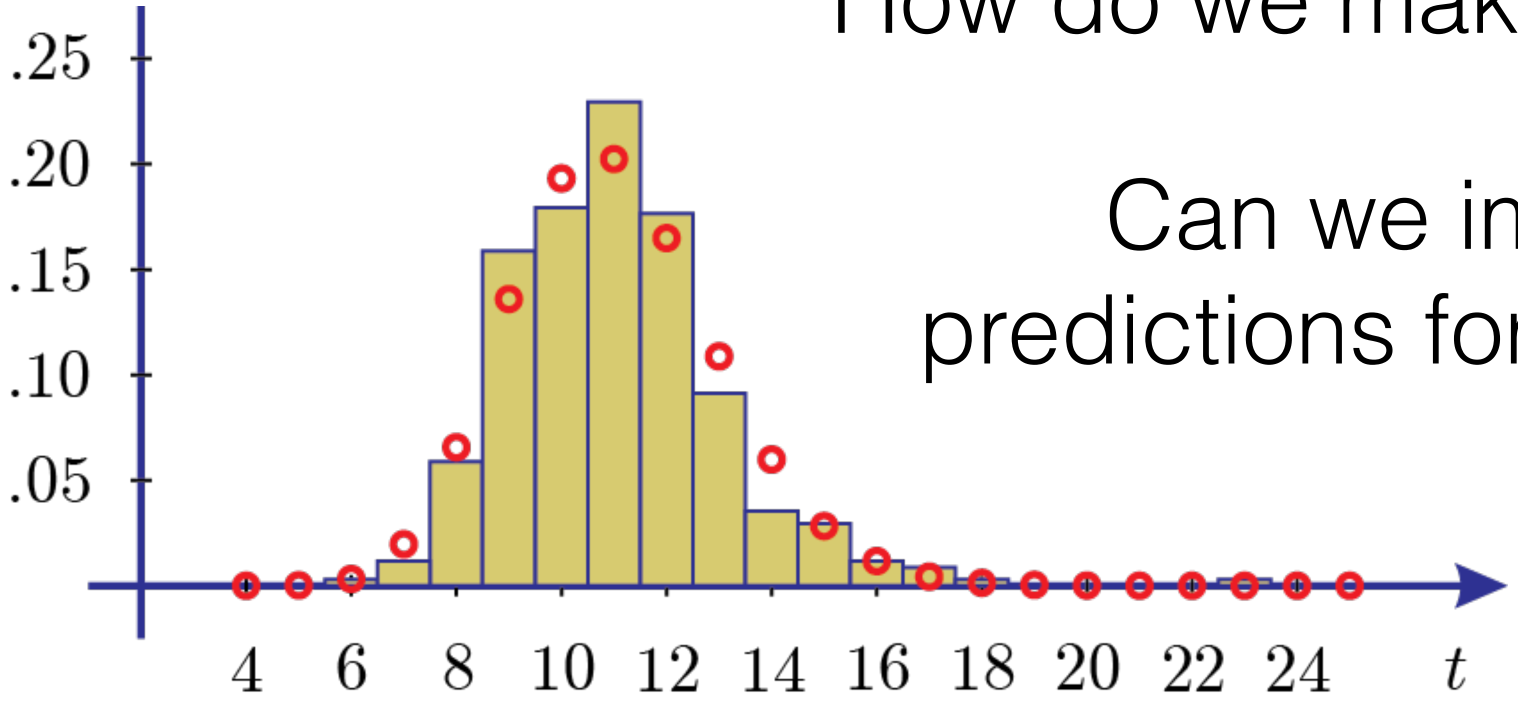
e.g., Histogram

New example

Model

Prediction

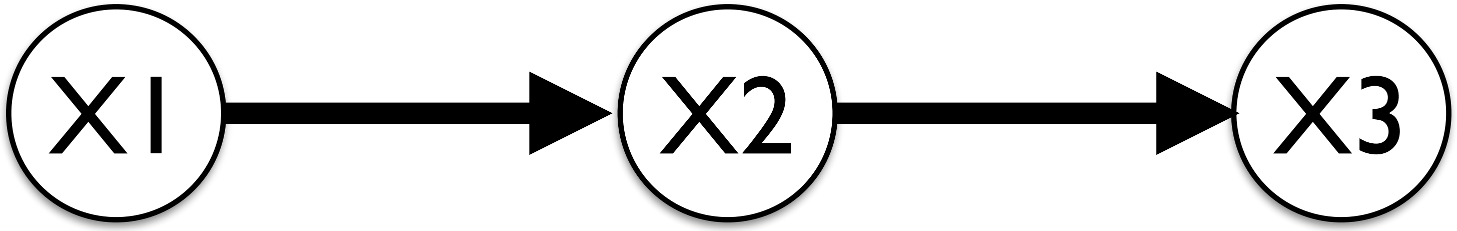
Commute times (3)



How do we make a prediction?

Can we improve our predictions for this question?

Weather prediction (time series)



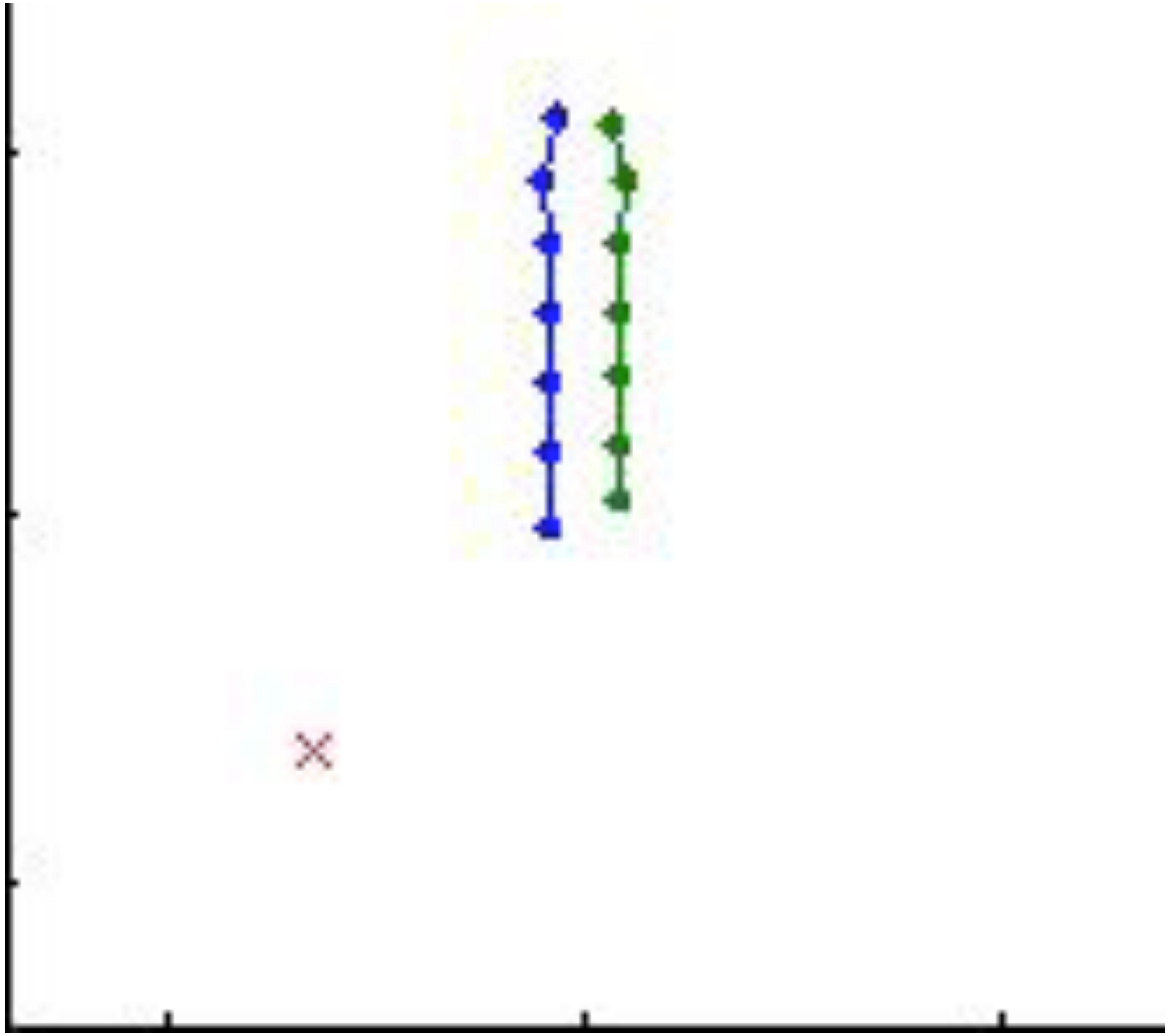
- Imagine we want to predict the probability of rain tomorrow, 2 days from now, 3 days, …

- One common strategy for time series is to use the last p points as features to predict the next point, 2 points into future, etc.

- What other strategies can you imagine?

- How do you predict a probability value, rather than say a binary value (0 or 1) or a real value?
  - Hint: these are things we will learn

Octopus arm (control)



Predict (long-term) value of action given current observations about position of arm points