CS 540 Introduction to Artificial Intelligence
Linear Models & Linear Regression

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Based on slides by Fred Sala

Outline

- Unsupervised Learning: Density Estimation
  - Kernel density estimation: high-level intro
- Supervised Learning & Linear Models
  - Parameterized model, model classes, linear models, train vs. test
- Linear Regression
  - Least squares, normal equations, residuals, logistic regression

Short Intro to Density Estimation

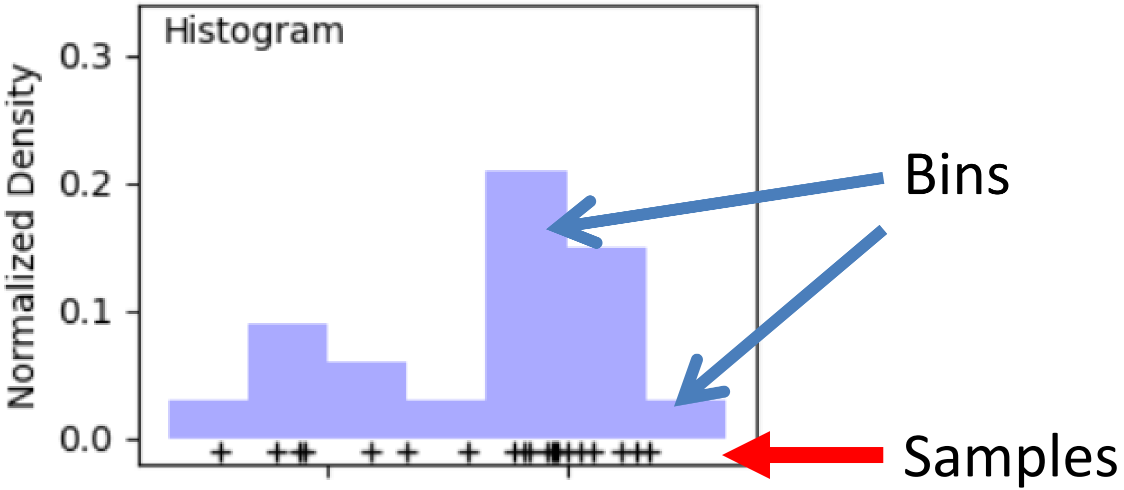
Goal: given samples $x_1, \ldots, x_n$ from some distribution P, estimate P.

- Compute statistics (mean, variance)
- Generate samples from P
- Run inference

Zach Monge

Simplest Idea: Histograms

Goal: given samples $x_1, \ldots, x_n$ from some distribution P, estimate P.



Define bins; count # of samples in each bin, normalize

Simplest Idea: Histograms

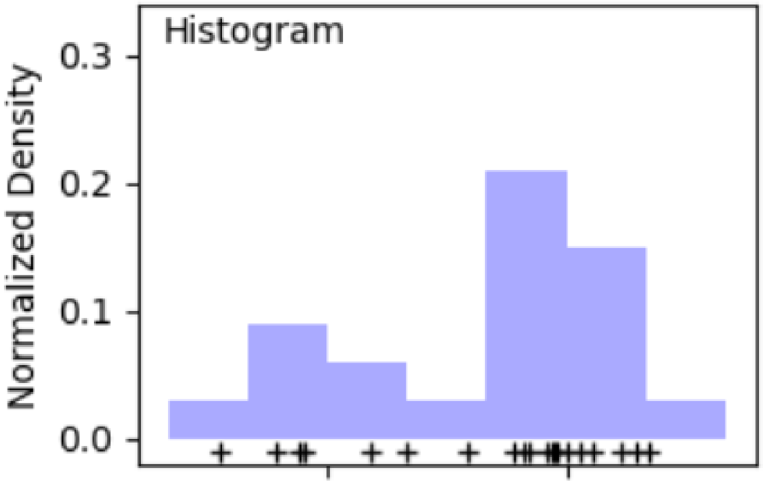
Goal: given samples $x_1, \ldots, x_n$ from some distribution P, estimate P.

Downsides:

i) High-dimensions: most bins empty

ii) Not continuous

iii) How to choose bins?



Kernel Density Estimation

Goal: given samples $x_1, \ldots, x_n$ from some distribution P, estimate P.

Idea: represent density as combination of “kernels”

$$f(x) = \frac{1}{nh}\sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right)$$

Center at each point

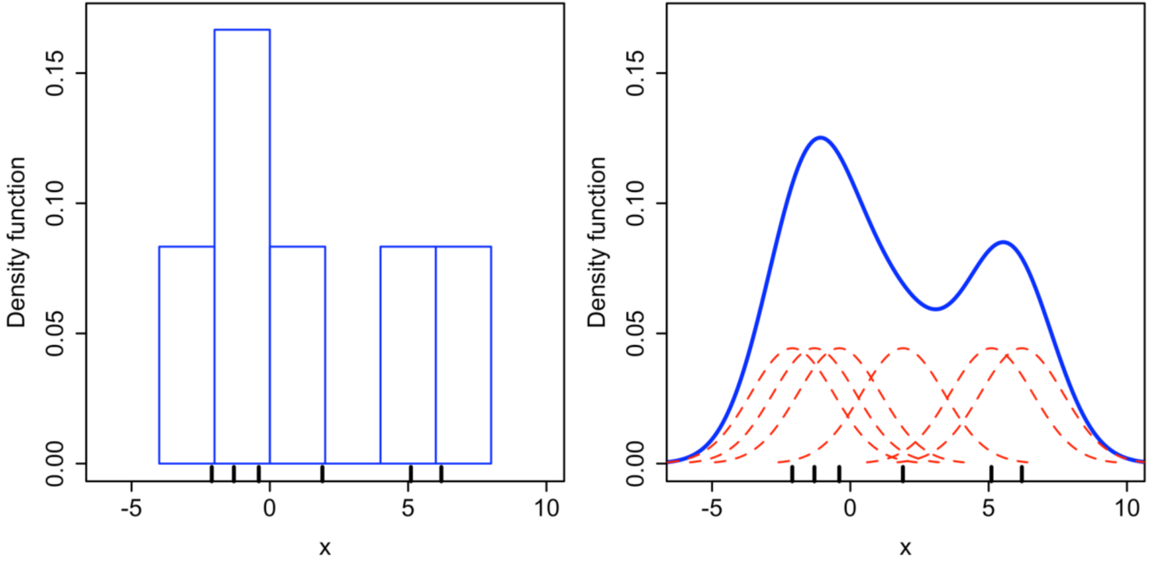
Kernel function: often Gaussian

Width parameter

Kernel Density Estimation

Idea: represent density as combination of kernels

- "Smooth" out the histogram



Break & Quiz

Q 1.1: Which of the following is not true?

- A. Using a Gaussian kernel for KDE, all possible values for x_i will have non-zero probability.
- B. The goal of KDE is to approximate the true probability distribution function of X.
- C. When using a histogram, every bucket must be represented explicitly in memory
- D. With some kernels, KDE can assign zero probability to some subset of values for x_i.

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Break & Quiz

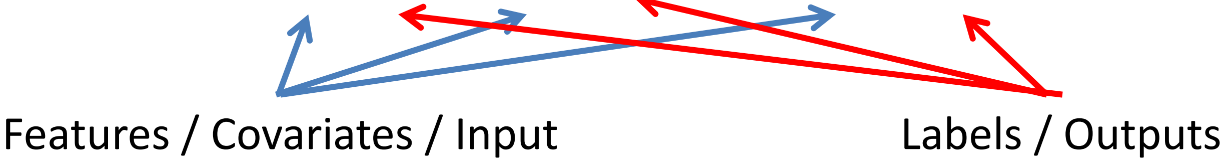
Q 1.1: Which of the following is not true?

- A. Using a Gaussian kernel for KDE, all possible values for x_i will have non-zero probability. (Gaussian PDF positive for all inputs)
- B. The goal of KDE is to approximate the true probability distribution function of X. (same goal as histograms)
- **C. When using a histogram, every bucket must be represented explicitly in memory**
- D. With some kernels, KDE can assign zero probability to some subset of values for x_i. (Consider K = uniform(0,1))

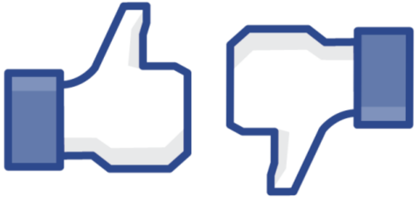
Back to Supervised Learning

Supervised learning:

- Make predictions, classify data, perform regression
- Dataset: $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)$



- Goal: find function $f : X \rightarrow Y$ to predict label on **new** data



Back to Supervised Learning

How do we know a function *f* is good?

- Intuitively: "matches" the dataset $f(x_i) \approx y_i$
- More concrete: pick a **loss function** to measure this: $\ell(f(x), y)$
- Training loss/empirical loss/empirical risk

$$\frac{1}{n}\sum_{i=1}^{n}\ell(f(x_i), y_i)$$

Loss / Cost / Objective Function

- Find a *f* that minimizes the loss on the training data (ERM)

Loss Functions

What should the loss look like?

- If $f(x_i) \approx y_i$, should be small (0 if equal!)
- For classification: 0/1 loss $\ell(f(x), y) = 1\{f(x_i) \neq y_i\}$
- For regression, square loss $\ell(f(x), y) = (f(x_i) - y_i)^2$

Others too! We'll see more.

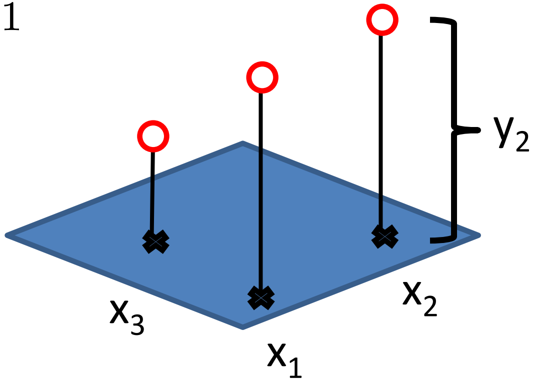
Functions/Models

The function *f* is usually called a model

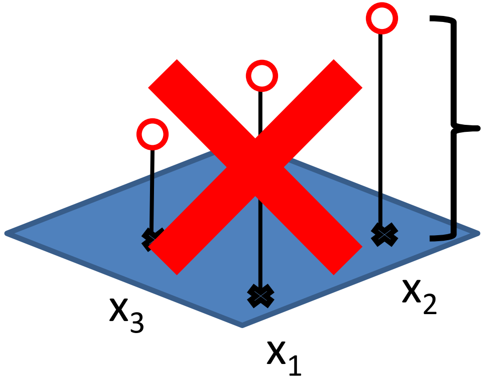
- Which possible functions should we consider?
- One option: **all functions**
  - Not a good choice. Consider

$$f(x) = \sum_{i=1}^{n} 1\{x = x_i\} y_i$$

  - Training loss: **zero.** Can't do better!
  - How will it do on *x* not in the training set?



Functions/Models



Don't want all functions

- Instead, pick a specific class
- Parametrize it by weights/parameters
- **Example:** linear models

$$f(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_d x_d = \theta_0 + x^T \theta$$

Weights/ Parameters

Training The Model

- Parametrize it by weights/parameters
- Minimize the loss

Best parameters = best function *f*

$$\min_\theta \frac{1}{n}\sum_{i=1}^{n}\ell(f(x_i), y_i)$$

Linear model class *f*

$$= \frac{1}{n}\sum_{i=1}^{n}\ell(\theta_0 + x_i^T\theta, y_i)$$

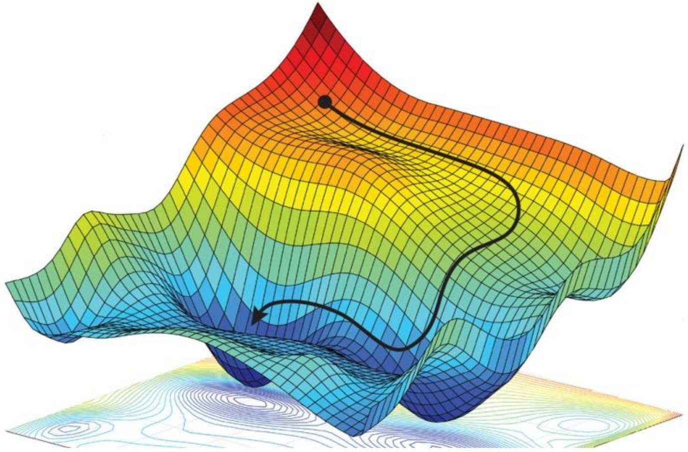
Square loss

$$= \frac{1}{n}\sum_{i=1}^{n}(\theta_0 + x_i^T\theta - y_i)^2$$

How Do We Minimize?

- Need to solve something that looks like $\min_{\theta} g(\theta)$
- Generic optimization problem; many algorithms
  - A popular choice: **stochastic gradient descent (SGD)**

- Most algorithms iterative: find some sequence of points heading towards the optimum



M. Hutson

Train vs Test

Now we've trained, have some *f* parametrized by θ

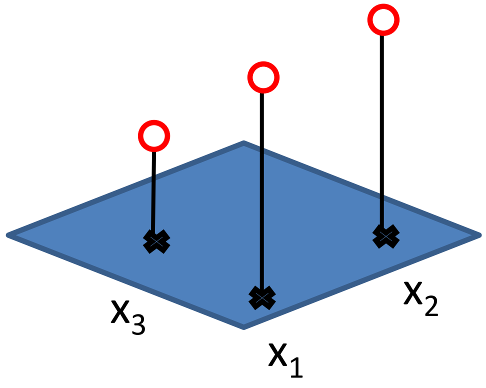
- Train loss is small → *f* predicts most x_i correctly
- How does *f* do on points not in training set? **"Generalizes!"**
- To evaluate this, create a **test** set. Do **not** train on it!

$$\underbrace{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)}_{\text{Training Data}} \quad \underbrace{(\mathbf{x}_{n+1}, y_{n+1}), \ldots, (\mathbf{x}_{n+p}, y_{n+p})}_{\text{Test Data}}$$

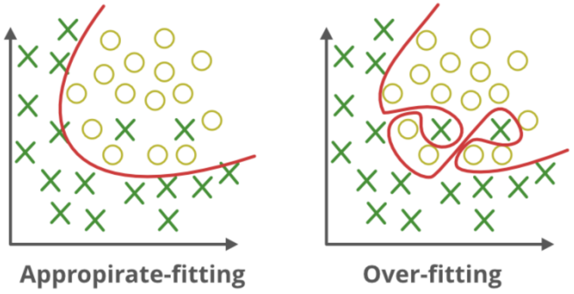
Train vs Test

Use the test set to evaluate *f*

- Why? Back to our "perfect" train function
- Training loss: 0. Every point matched perfectly
- How does it do on test set? **Fails completely**!



- Test set helps detect **overfitting**
  - Overfitting: too focused on train points
  - "Bigger" class: more prone to overfit
    - Need to consider **model capacity**



GFG

Break & Quiz

Q 2.1: When we train a model, we are

- A. Optimizing the parameters and keeping the features fixed.
- B. Optimizing the features and keeping the parameters fixed.
- C. Optimizing the parameters and the features.
- D. Keeping parameters and features fixed and changing the predictions.

Break & Quiz

Q 2.1: When we train a model, we are

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Break & Quiz

Q 2.1: When we train a model, we are

- **A. Optimizing the parameters and keeping the features fixed.**
- B. Optimizing the features and keeping the parameters fixed) (Feature vectors *x*i don't change during training).
- C. Optimizing the parameters and the features. (Same as B)
- D. Keeping parameters and features fixed and changing the predictions. (We can't train if we don't change the parameters)

Break & Quiz

- **Q 2.2**: You have trained a classifier, and you find there is significantly **higher** loss on the test set than the training set. What is likely the case?

- A. You have accidentally trained your classifier on the test set.
- B. Your classifier is generalizing well.
- C. Your classifier is generalizing poorly.
- D. Your classifier is ready for use.

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Break & Quiz

- **Q 2.2**: You have trained a classifier, and you find there is significantly **higher** loss on the test set than the training set. What is likely the case?

- A. You have accidentally trained your classifier on the test set. **(No, this would make test loss lower)**
- B. Your classifier is generalizing well. **(No, test loss is high means poor generalization)**
- **C. Your classifier is generalizing poorly.**
- D. Your classifier is ready for use. **(No, will perform poorly on new data)**

Break & Quiz

- **Q 2.3**: You have trained a classifier, and you find there is significantly **lower** loss on the test set than the training set. What is likely the case?

- A. You have accidentally trained your classifier on the test set.
- B. Your classifier is generalizing well.
- C. Your classifier is generalizing poorly.
- D. Your classifier needs further training.

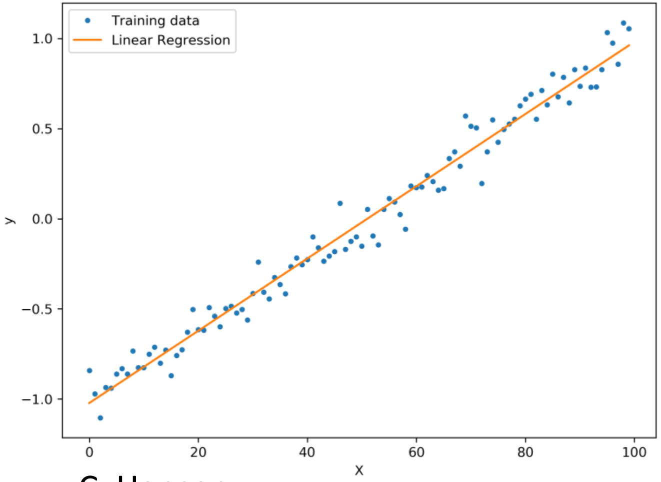
Break & Quiz

- **Q 2.3**: You have trained a classifier, and you find there is significantly **lower** loss on the test set than the training set. What is likely the case?

- **A. You have accidentally trained your classifier on the test set.** (This is very likely, loss will usually be the lowest on the data set on which a model has been trained)
- B. Your classifier is generalizing well.
- C. Your classifier is generalizing poorly.
- D. Your classifier needs further training.

Linear Regression

Simplest type of regression problem.



C. Hansen

- **Inputs**: $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)$
  - *x*'s are vectors, *y*'s are scalars.
  - "**Linear**": predict a linear combination of x components + intercept

$$f(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_d x_d = \theta_0 + x^T \theta$$

- **Want**: optimal parameters

Linear Regression Setup

Problem Setup

- Goal: figure out how to minimize square loss
- Let's organize it. Train set $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)$
  - Since $f(x) = \theta_0 + x^T\theta$, wrap intercept: $f(x) = x^T\theta$
  - Take train data and make it a matrix/vector: $X = [x_1 \; x_2 \ldots x_n]$
  - Then, square loss is

$$\frac{1}{n}\sum_{i=1}^{n}(x_i^T\theta - y_i)^2 = \frac{1}{n}\|X^T\theta - y\|^2$$

Finding The Optimal Parameters

Have our loss: $\frac{1}{n}\|X^T\theta - y\|^2$

- Could optimize it with SGD, etc…
- No need: minimum has a solution (easy with vector calculus)

$$\hat{\theta} = (X^TX)^{-1}X^Ty$$

Hat: indicates an estimate

Not always invertible…

“Normal Equations”

How Good are the Optimal Parameters?

Now we have parameters $\hat{\theta} = (X^T X)^{-1} X^T y$

- How good are they?
- Predictions are $f(x_i) = \hat{\theta}^T x_i = ((X^T X)^{-1} X^T y)^T x_i$
- Errors ("**residuals**")

$$|y_i - f(x_i)| = |y_i - \hat{\theta}^T x_i| = |y_i - ((X^T X)^{-1} X^T y)^T x_i|$$

- If data is linear, residuals are 0. Almost never the case!

Train/Test for Linear Regression?

So far, residuals measure error on **train** set

- Sometimes that's all we care about (**Fixed Design LR**)
  - Data is deterministic.
  - Goal: find best linear relationship on dataset
- Or, create a test set and check (**Random Design LR**)
  - Common: assume data is $y = \theta^T x + \varepsilon$
  - The more noise, the less linear

0-mean
Gaussian noise

Linear Regression → Classification?

What if we want the same idea, but *y* is 0 or 1?

- Need to convert the $\theta^T x$ to a probability in [0,1]

$$p(y=1|x) = \frac{1}{1+\exp(-\theta^T x)}$$

Logistic function

Why does this work?

- If $\theta^T x$ is really big, $\exp(-\theta^T x)$ is really small → *p* close to 1
- If really negative exp is huge → *p* close to 0

"Logistic Regression"