CPSC 340: Machine Learning and Data Mining

Feature Engineering

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Admin

- Final version of Assignment 4 will be online soon; due Nov 14th.
- Midterm grades will be released early next week.

Last Time: Multi-Class Linear Classifiers

- We discussed multi-class linear classification: y_i in {1,2,…,k}.
- One vs. All with +1/-1 binary classifier:
  - Train weights w_c to predict +1 for class 'c', -1 otherwise.

$$W = \underbrace{\begin{bmatrix} \text{---} \; w_1^T \; \text{---} \\ \text{---} \; w_2^T \; \text{---} \\ \vdots \\ \text{---} \; w_k^T \; \text{---} \end{bmatrix}}_{d} \Big\} k$$

  - Predict by taking 'c' maximizing $w_c^T x_i$.

- Today:
  - Multi-class extensions of the hinge loss and logistic loss.
  - Second part: how to construct good features.

Multi-Class Linear Classification (MEMORIZE)

- Back to multi-class classification where we have 1 "correct" label:

$$X = \begin{bmatrix} & & \\ & & \\ & & \end{bmatrix} \quad y = \begin{bmatrix} 27 \\ 16 \\ 8 \\ 7 \\ 21 \\ 5 \end{bmatrix}$$

train 'k' classifiers

$$\underbrace{W = \begin{bmatrix} \text{---} & w_1^T & \text{---} \\ \text{---} & w_2^T & \text{---} \\ & \vdots & \\ \text{---} & w_k^T & \text{---} \end{bmatrix}}_{\text{Predict by maximizing } w_c^T x_i}$$

- We'll use 'w_{y_i}' as classifier where $c=y_i$ (row of correct class label).
  - So if $y_i=2$ then $w_{y_i} = w_2$.

"One vs All" Multi-Class Linear Classification

- Problem: We didn't train the w_c so that the largest $w_c^T x_i$ would be $w_{y_i}^T x_i$.
  - Each classifier is just trying to get the sign right.

features x_i

$w_1^T x_i = -5$ ("cat" score)

$w_2^T x_i = -0.1$ ("dog" score)

$w_3^T x_i = -0.2$ ("human" score)

  - Here the classifier incorrectly predicts "dog".
    - "One vs All" doesn't try to put $w_2^T x_i$ and $w_3^T x_i$ on same scale for decisions like this.
    - We should try to make $w_3^T x_i$ positive and $w_2^T x_i$ negative relative to each other.
    - The multi-class hinge loss and the multi-class logistic loss do this.

https://laughingsquid.com/pug-mask-a-latex-mask-so-you-can-look-like-a-dog/

Multi-Class SVMs

- Can we define a loss that encourages largest $w_c^T x_i$ to be $w_{y_i}^T x_i$?
  - So when we maximizing over $w_c^T x_i$, we choose correct label y_i.

- Recall our derivation of the hinge loss (SVMs):
  - We wanted $y_i w^T x_i > 0$ for all 'i' to classify correctly.
  - We avoided non-degeneracy by aiming for $y_i w^T x_i \geq 1$.
  - We used the constraint violation as our loss: $\max\{0, 1 - y_i w^T x_i\}$.

- We can derive multi-class SVMs using the same steps…

Multi-Class SVMs

- Can we define a loss that encourages largest $w_c^T x_i$ to be $w_{y_i}^T x_i$?

We want $w_{y_i}^T x_i > w_c^T x_i$ for all 'c' that are not correct label y_i

If we penalize violation of this constraint it's degenerate.

We use $w_{y_i}^T x_i \geq w_c^T x_i + 1$ for all $c \neq y_i$ to avoid strict inequality

Equivalently: $0 \geq 1 - w_{y_i}^T x_i + w_c^T x_i$

- For here, there are two ways to measure constraint violation:

"Sum"

$$\sum_{c \neq y_i} \max\{0, 1 - w_{y_i}^T x_i + w_c^T x_i\}$$

"Max"

$$\max_{c \neq y_i} \{ \max\{0, 1 - w_{y_i}^T x_i + w_c^T x_i\} \}$$

Multi-Class SVMs

- Can we define a loss that encourages largest $w_c^T x_i$ to be $w_{y_i}^T x_i$?

"Sum"

$$\sum_{c \neq y_i} \max\{0, 1 - w_{y_i}^T x_i + w_c^T x_i\}$$

"Max"

$$\max_{c \neq y_i} \{\max\{0, 1 - w_{y_i}^T x_i + w_c^T x_i\}\}$$

- For each training example 'i':
  - "Sum" rule penalizes for each 'c' that violates the constraint.
  - "Max" rule penalizes for one 'c' that violates the constraint the most.
    - "Sum" gives a penalty of 'k-1' for W=0, "max" gives a penalty of '1'.
- If we add L2-regularization, both are called multi-class SVMs:
  - "Max" rule is more popular, "sum" rule usually works better.
  - Both are convex upper bounds on the 0-1 loss.

Multi-Class Logistic Regression

- We derived binary logistic loss by smoothing a degenerate 'max'.
  - A degenerate constraint in the multi-class case can be written as:

$$w_{y_i}^T x_i \geq \max_c \{w_c^T x_i\}$$

$$\text{or} \quad 0 \geq -w_{y_i}^T x_i + \max_c \{w_c^T x_i\}$$

- We want the right side to be as small as possible.
- Let's smooth the max with the log-sum-exp:

$$-w_{y_i}^T x_i + \log\left(\sum_{c=1}^{k} \exp(w_c^T x_i)\right)$$

  - This is no longer degenerate: with W=0 this gives a loss of log(k).
- Called the softmax loss, the loss for multi-class logistic regression.

Multi-Class Logistic Regression

- We sum the loss over examples and add regularization:

$$f(W) = \sum_{i=1}^{n}\Big[\underbrace{-w_{y_i}^T x_i}_{\text{Tries to make } w_c^T x_i \text{ big for the correct label}} + \underbrace{\log\Big(\sum_{c=1}^{k} \exp(w_c^T x_i)\Big)}_{\text{Approximates } \max_c\{w_c^T x_i\} \text{ so tries to make } w_c^T x_i \text{ small for all labels.}}\Big] + \underbrace{\frac{\lambda}{2}\sum_{c=1}^{k}\sum_{j=1}^{d} w_{cj}^2}_{\text{Usual } L_2\text{-regularizer on elements of 'W'}}$$

- This objective is convex (should be clear for 1st and 3rd terms).
  – It's differentiable so you can use gradient descent.
- When k=2, equivalent to using binary logistic loss.
  – Not obvious at the moment.

Softmax Function: Multi-Class Probabilities

- Previously we talked about converting to probabilities.
  - In binary case, we convert from $z = w^T x_i$ into $p(y_i \mid w, x_i)$ using sigmoid(z).
- Now consider the multi-class case:
  - We have 'k' real numbers $z_i = w_c^T x_i$, want to map the z_i to probabilities.
- Most common way to do this is with softmax function:

$$p(y \mid z_1, z_2, \dots, z_k) = \frac{\exp(z_y)}{\sum_{c=1}^{k} \exp(z_c)}$$

  - Taking $\exp(z_c)$ makes it non-negative.
  - Denominator makes it sum to 1 over the 'k' values of 'c'.
  - So this gives a probability for each of the 'k' possible values of 'c'.
    - And the softmax loss is the negative of the logarithm of these probabilities.

Multi-Class Linear Prediction in Matrix Notation

- In multi-class linear classifiers our weights are:

$$W = \left.\underbrace{\begin{bmatrix} \text{---} & w_1^T & \text{---} \\ \text{---} & w_2^T & \text{---} \\ & \vdots & \\ \text{---} & w_k^T & \text{---} \end{bmatrix}}_{d}\right\} k$$

- To predict on all training examples, we first compute all $w_c^T x_i$.
  - Or in matrix notation:

$$\underbrace{\begin{bmatrix} w_1^T x_1 & w_2^T x_1 & \cdots & w_k^T x_1 \\ w_1^T x_2 & w_2^T x_2 & \cdots & w_k^T x_2 \\ & \vdots & & \\ w_1^T x_n & w_2^T x_n & \cdots & w_k^T x_n \end{bmatrix}}_{XW^T} = \underbrace{\begin{bmatrix} \text{---} & x_1^T & \text{---} \\ \text{---} & x_2^T & \text{---} \\ & \vdots & \\ \text{---} & x_n^T & \text{---} \end{bmatrix}}_{X} \underbrace{\begin{bmatrix} | & | & & | \\ w_1 & w_2 & \cdots & w_k \\ | & | & & | \end{bmatrix}}_{W^T}$$

  - So predictions are maximum column indices of XW^T (which is 'n' by 'k').

Digression: Frobenius Norm

- The Frobenius norm of a ('k' by 'd') matrix 'W' is defined by:

$$\|W\|_F = \sqrt{\sum_{c=1}^{k}\sum_{j=1}^{d} w_{jc}^2}$$

(L2-norm if you "stack" elements into one big vector)

- We can use this to write regularizer in matrix notation:

$$\frac{\lambda}{2}\sum_{c=1}^{k}\sum_{j=1}^{d} w_{cj}^2 = \frac{\lambda}{2}\sum_{c=1}^{k}\|w_c\|^2$$ ("L2-regularizer on each vector")

$$= \frac{\lambda}{2}\|W\|_F^2$$ ("Frobenius-regularizer on matrix")

Next Topic: Feature Engineering

Feature Engineering

- “…some machine learning projects succeed and some fail. What makes the difference? Easily the most important factor is the features used.”
  - Pedro Domingos

- “Coming up with features is difficult, time-consuming, requires expert knowledge. "Applied machine learning" is basically feature engineering.”
  - Andrew Ng

Feature Engineering

- Better features usually help more than a better model.

- Good features would ideally:
  - Allow learning with few examples, be hard to overfit with many examples.
  - Capture most important aspects of problem.
  - Reflects invariances (generalize to new scenarios).

- There is a trade-off between simple and expressive features:
  - With simple features overfitting risk is low, but accuracy might be low.
  - With complicated features accuracy can be high, but so is overfitting risk.

Feature Engineering

- The best features may be dependent on the model you use.

- For counting-based methods like naïve Bayes and decision trees:
  – Need to address coupon collecting, but separate relevant "groups".

- For distance-based methods like KNN:
  – Want different class labels to be "far".

- For regression-based methods like linear regression:
  – Want labels to have a linear dependency on features.

Discretization for Counting-Based Methods

- For counting-based methods:
  - Discretization: turn continuous into discrete.

Age
23
23
22
25
19
22

< 20	>= 20, < 25	>= 25
0	1	0
0	1	0
0	1	0
0	0	1
1	0	0
0	1	0

  - Counting age "groups" could let us learn more quickly than exact ages.
    - But we wouldn't do this for a distance-based method.

Standardization for Distance-Based Methods

- Consider features with different scales:

Egg (#)	Milk (mL)	Fish (g)	Pasta (cups)
0	250	0	1
1	250	200	1
0	0	0	0.5
2	250	150	0

- Should we convert to some standard 'unit'?
  - It doesn't matter for counting-based methods.
- It matters for distance-based methods:
  - KNN will focus on large values more than small values.
  - Often we "standardize" scales of different variables (e.g., convert everything to grams).
  - Also need to worry about correlated features.

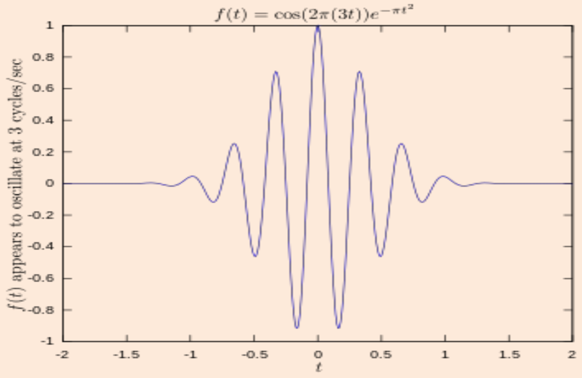
Non-Linear Transformations for Regression-Based

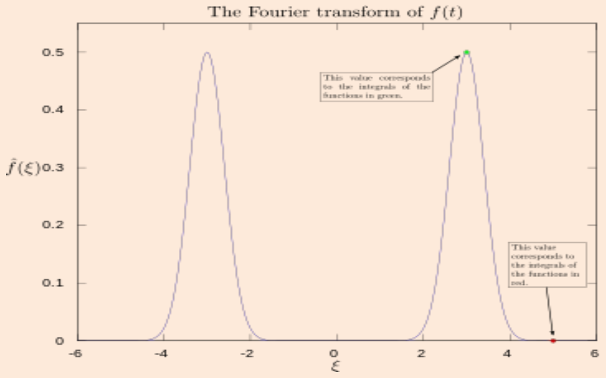
- Non-linear feature/label transforms can make things more linear:
  - Polynomial, exponential/logarithm, sines/cosines, RBFs.

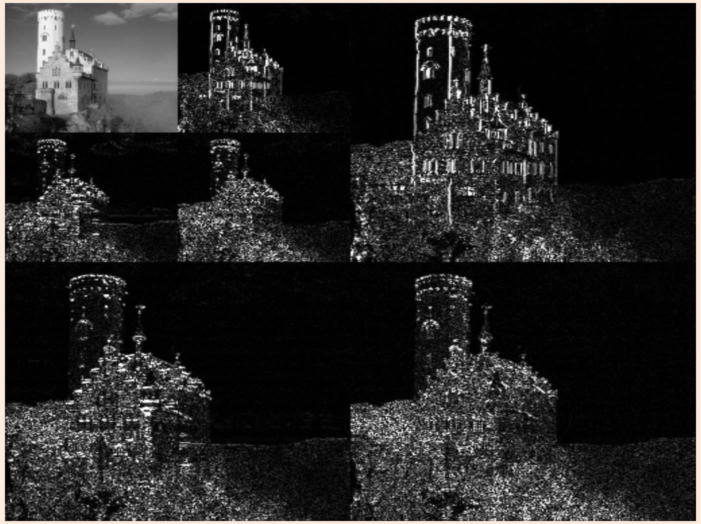
www.google.com/finance

Domain-Specific Transformations

- In some domains there are natural transformations to do:
  - Fourier coefficients and spectrograms (sound data).
  - Wavelets (image data).
  - Convolutions (we'll talk about these soon).







https://en.wikipedia.org/wiki/Fourier_transform
https://en.wikipedia.org/wiki/Spectrogram
https://en.wikipedia.org/wiki/Discrete_wavelet_transform

Discussion of Feature Engineering

- The best feature transformations are application-dependent.
  - It's hard to give general advice.

- My advice: ask the domain experts.
  - Often have idea of right discretization/standardization/transformation.

- If no domain expert, cross-validation will help.
  - Or if you have lots of data, use deep learning methods from Part 5.

- Next: I'll give some features used for text/image applications.

Next Topic: Features for Text Data

But first…

- How do we use categorical features in regression?
- Standard approach is to convert to a set of binary features:
  - "1 of k" or "one hot" encoding.

Age	City	Income
23	Van	22,000.00
23	Bur	21,000.00
22	Van	0.00
25	Sur	57,000.00
19	Bur	13,500.00
22	Van	20,000.00

Age	Van	Bur	Sur	Income
23	1	0	0	22,000.00
23	0	1	0	21,000.00
22	1	0	0	0.00
25	0	0	1	57,000.00
19	0	1	0	13,500.00
22	1	0	0	20,000.00

  - What if you get a new city in the test data?
    - Common approach: set all three variables to 0.

Digression: Linear Models with Binary Features

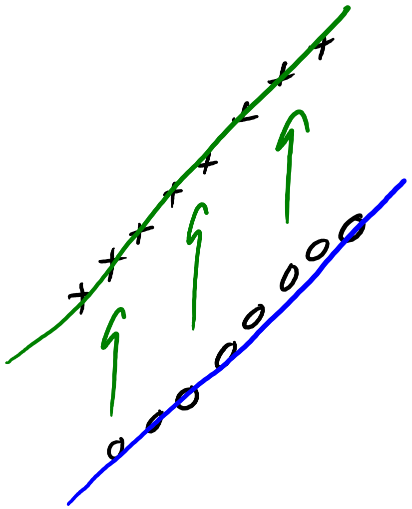
- What is the effect of a binary features on linear regression?

- Suppose we use a bag of words:
  - With 3 words {“hello”, “Vicodin”, “340“} our model would be:

$$\hat{y}_i = \underset{\text{whether "hello" appears}}{w_1 x_{i1}} + w_2 x_{i2} + \underset{\text{whether "340" appears}}{w_3 x_{i3}}$$

  - If e-mail only has “hello” and “340” our prediction is:

$$\hat{y}_i = \underset{\text{"hello" weight}}{w_1} + \underset{\text{"340" weight}}{w_3}$$



- So having the binary feature ‘j’ increases $\hat{y}_i$ by the fixed amount w_j.
  - Predictions are a bit like naïve Bayes where we combine features independently.
  - But now we’re learning all w_j together so this tends to work better.

Text Example 1: Language Identification

- Consider data that doesn't look like this:

$$X = \begin{bmatrix} 0.5377 & 0.3188 & 3.5784 \\ 1.8339 & -1.3077 & 2.7694 \\ -2.2588 & -0.4336 & -1.3499 \\ 0.8622 & 0.3426 & 3.0349 \end{bmatrix}, \quad y = \begin{bmatrix} +1 \\ -1 \\ -1 \\ +1 \end{bmatrix},$$

- But instead looks like this:

$$X = \begin{bmatrix} \text{Do you want to go for a drink sometime?} \\ \text{J'achète du pain tous les jours.} \\ \text{Fais ce que tu veux.} \\ \text{There are inner products between sentences?} \end{bmatrix}, y = \begin{bmatrix} +1 \\ -1 \\ -1 \\ +1 \end{bmatrix}.$$

- How should we represent sentences using features?

A (Bad) Universal Representation

- Treat character in position ‘j’ of the sentence as a categorical feature.
    - “fais ce que tu veux” => x_i = [f a i s ‘’ c e ‘’ q u e ‘’ t u ‘’ v e u x .]

- “Pad” end of the sentence up to maximum #characters:
    - “fais ce que tu veux” => x_i = [f a i s ‘’ c e ‘’ q u e ‘’ t u ‘’ v e u x . γ γ γ γ γ γ γ γ …]

- Advantage:
    – No information is lost, KNN can eventually solve the problem.
- Disadvantage: throws out everything we know about language.
    – Needs to learn that “veux” starting from any position indicates “French”.
        - Doesn’t even use that sentences are made of words (this must be learned).
    – High overfitting risk, you will need a lot of examples for this easy task.

Bag of Words Representation

- Bag of words represents sentences/documents by word counts:

> The **International Conference on Machine Learning** (ICML) is the leading international academic conference in machine learning

ICML	International	Conference	Machine	Learning	Leading	Academic
1	2	2	2	2	1	1

- Bag of words loses a ton of information/meaning:
  - But it easily solves language identification problem

Universal Representation vs. Bag of Words

- Why is bag of words better than "string of characters" here?
  - It needs less data because it captures invariances for the task:
    - Most features give strong indication of one language or the other.
    - It doesn't matter *where* the French words appear.
  - It overfits less because it throws away irrelevant information.
    - Exact sequence of words isn't particularly relevant here.

Text Example 2: Word Sense Disambiguation

- Consider the following two sentences:
  - "The cat ran after the mouse."
  - "Move the mouse cursor to the File menu."

- Word sense disambiguation (WSD): classify "meaning" of a word:
  - A surprisingly difficult task.

- You can do ok with bag of words, but it will have problems:
  - "Her mouse clicked on one cat video after another."
  - "We saw the mouse run out from behind the computer."
  - "The mouse was gray." (ambiguous without more context)

Bigrams and Trigrams

- A bigram is an ordered set of two words:
  - Like “computer mouse” or “mouse ran”.
- A trigram is an ordered set of three words:
  - Like “cat and mouse” or “clicked mouse on”.

- These give more context/meaning than bag of words:
  - Includes neighbouring words as well as order of words.
  - Trigrams are widely-used for various language tasks.

- General case is called n-gram.
  - Unfortunately, coupon collecting becomes a problem with larger ‘n’.

Text Example 3: Part of Speech (POS) Tagging

- Consider problem of finding the verb in a sentence:
  - “The 340 students jumped at the chance to hear about POS features.”

- Part of speech (POS) tagging is the problem of labeling all words.
  - >40 common syntactic POS tags.
  - Current systems have ~97% accuracy on standard (“clean”) test sets.
  - You can achieve this by applying a “word-level” classifier to each word.
    - That independently classifies each word with one of the 40 tags.

- What features of a word should we use for POS tagging?

POS Features

- Regularized multi-class logistic regression with these features gives ~97% accuracy:
  - Categorical features whose domain is all words ("lexical" features):
    - The word (e.g., "jumped" is usually a verb).
    - The previous word (e.g., "he" hit vs. "a" hit).
    - The previous previous word.
    - The next word.
    - The next next word.
  - Categorical features whose domain is combinations of letters ("stem" features):
    - Prefix of length 1 ("what letter does the word start with?")
    - Prefix of length 2.
    - Prefix of length 3.
    - Prefix of length 4 ("does it start with JUMP?")
    - Suffix of length 1.
    - Suffix of length 2.
    - Suffix of length 3 ("does it end in ING?")
    - Suffix of length 4.
  - Binary features ("shape" features):
    - Does word contain a number?
    - Does word contain a capital?
    - Does word contain a hyphen?

Ordinal Features

- Categorical features with an ordering are called ordinal features.

Rating
Bad
Very Good
Good
Good
Very Bad
Good
Medium

→

Rating
2
5
4
4
1
4
3

- If using decision trees, makes sense to replace with numbers.
  - Captures ordering between the ratings.
  - A rule like (rating ≥ 3) means (rating ≥ Good), which make sense.

Ordinal Features

- With linear models, "convert to number" assumes ratings are equally spaced.
  - "Bad" and "Medium" distance is similar to "Good" and "Very Good" distance.
- One alternative that preserves ordering with binary features:

Rating
Bad
Very Good
Good
Good
Very Bad
Good
Medium

→

≥ Bad	≥ Medium	≥ Good	Very Good
1	0	0	0
1	1	1	1
1	1	1	0
1	1	1	0
0	0	0	0
1	1	1	0
1	1	0	0

- Regression weight w_{medium} represents:
  - "How much medium changes prediction over bad".
- Bonus slides discuss "cyclic" features like "time of day".

Next Topic: Personalized Features

Motivation: “Personalized” Important E-mails

- Features: bad of words, trigrams, regular expressions, and so on.

- There might be some “globally” important messages:
  - “This is your mother, something terrible happened, give me a call ASAP.”

- But your “important” message may be unimportant to others.
  - Similar for spam: “spam” for one user could be “not spam” for another.

“Global” and “Local” Features

- Consider the following weird feature transformation:

“340”
1
1
1
0
1

$\Rightarrow$

“340” (any user)	“340” (user?)
1	User 1
1	User 1
1	User 2
0	<no “340”>
1	User 3

- First feature: did “340” appear in this e-mail?
- Second feature: if “340” appeared in this e-mail, who was it addressed to?

- First feature will increase/decrease importance of “340” for every user (including new users).
- Second (categorical feature) increases/decreases important of “340” for specific users.
  – Lets us learn more about specific users where we have a lot of data

“Global” and “Local” Features

- Recall we usually represent categorical features using “1 of k” binaries:

“340”
1
1
1
0
1

$\Rightarrow$

“340” (any user)	“340” (user = 1)	“340” (user = 2)
1	1	0
1	1	0
1	0	1
0	0	0
1	0	0

- First feature “moves the line up” for all users.
- Second feature “moves the line up” when the e-mail is to user 1.
- Third feature “moves the line up” when the e-mail is to user 2.

The Big Global/Local Feature Table for E-mails

- Each row is one e-mail (there are lots of rows):

$$X = \begin{bmatrix} \\ \\ \\ \end{bmatrix} \qquad y = \begin{bmatrix} \text{"important"} \\ \text{"not important"} \\ \vdots \end{bmatrix}$$

"global" features: shared by all users

"local" features for user "1": set to 0 for all other users.

"local" features for user "2"

We only need to store the user ID and list of non-zero features.

Summary

- Softmax loss is a multi-class version of logistic loss.
- Feature engineering can be a key factor affecting performance.
  - Good features depend on the task and the model.
- Bag of words: not a good representation in general.
  - But good features if word order isn't needed to solve problem.
- Text features (beyond bag of words): trigrams, lexical, stem, shape.
  - Try to capture important invariances in text data.
- Global vs. local features allow "personalized" predictions.

- Next time: feature engineering for image and sound data.

Cyclic Features

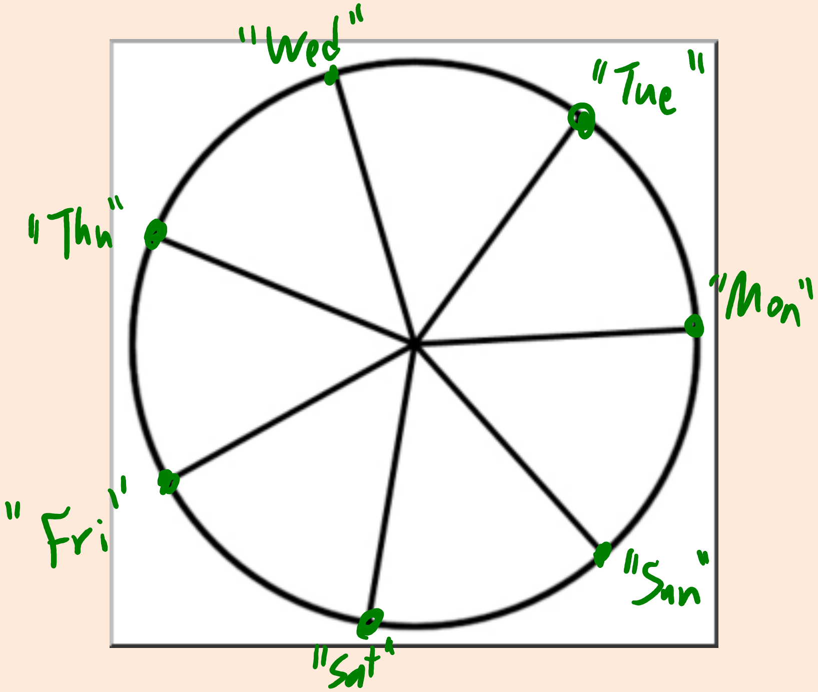
- Cyclic features arise in many settings, especially with times:

Time	Day	Date	Month	Year
12:05pm	Wed	29	Jul	15
10:20am	Sun	24	Apr	16
9:10am	Tue	3	May	16
11:20am	Sun	15	Jun	18
10:15pm	Thu	8	Aug	19

- Could use ordinal: “Jan”->1, “Feb”->2, “Mar”->3, and so on.
  - Reflects ordering of months
  - But this says that “Jan” and “Dec” are far.
  - We might want to incorporate the “cycle” that “1” comes after “12”.

Cyclic Features

- One way to model cyclic features is as coordinates on unit circle.
  - Dividing circumference evenly across the cyclic values.



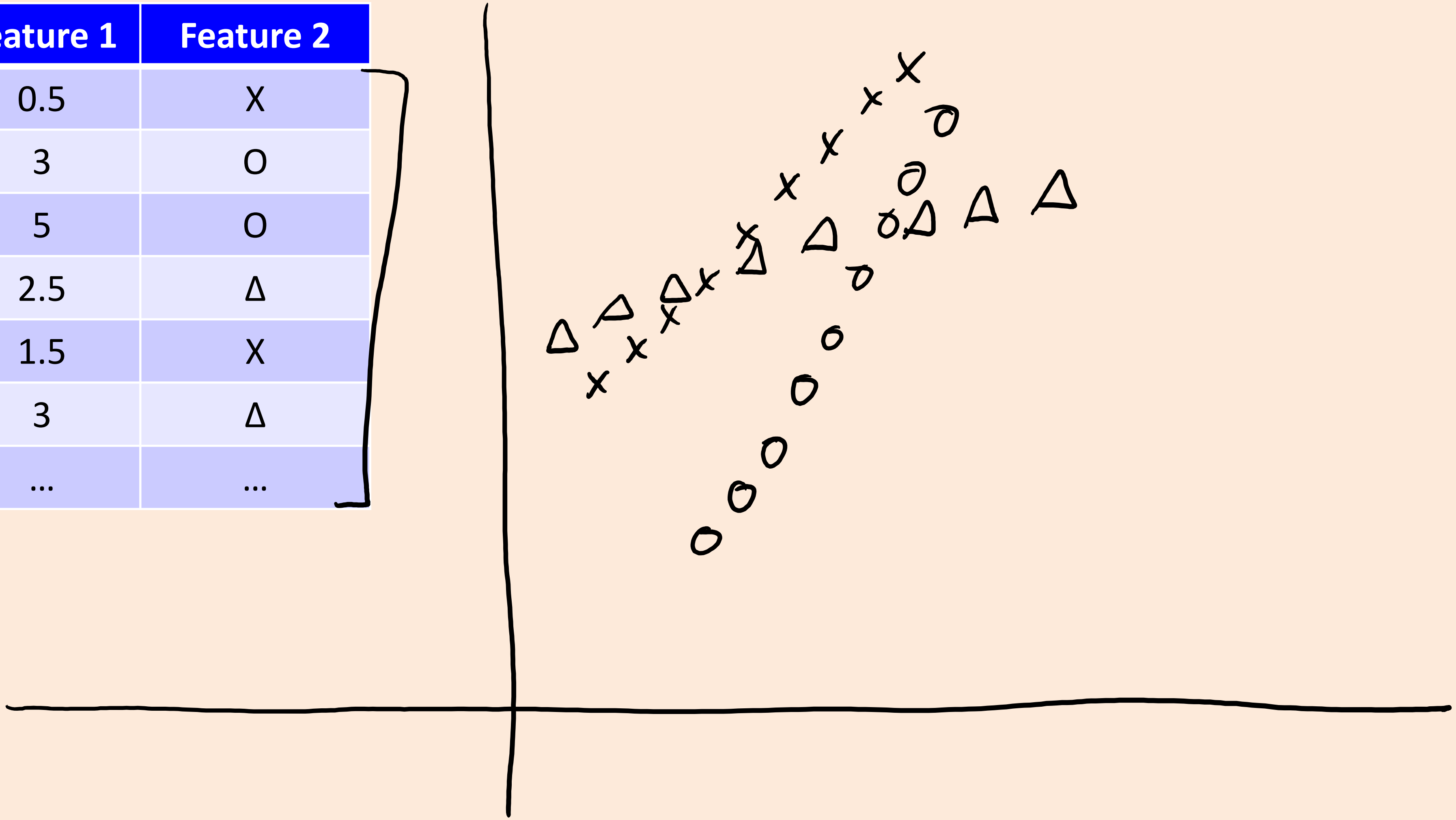
- Replace "Day" with the x-coordinate and y-coordinate (2 features).
  - Reflects that "Mon" is same distance from "Tue" as it is from "Sun".

https://www.abcteach.com/documents/clip-art-circle07-77-bw-i-abcteachcom-17022

Linear Models with Binary Features

$X =$

Feature 1	Feature 2
0.5	X
3	O
5	O
2.5	Δ
1.5	X
3	Δ
…	…



Linear Models with Binary Features

$X =$

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0.5	X
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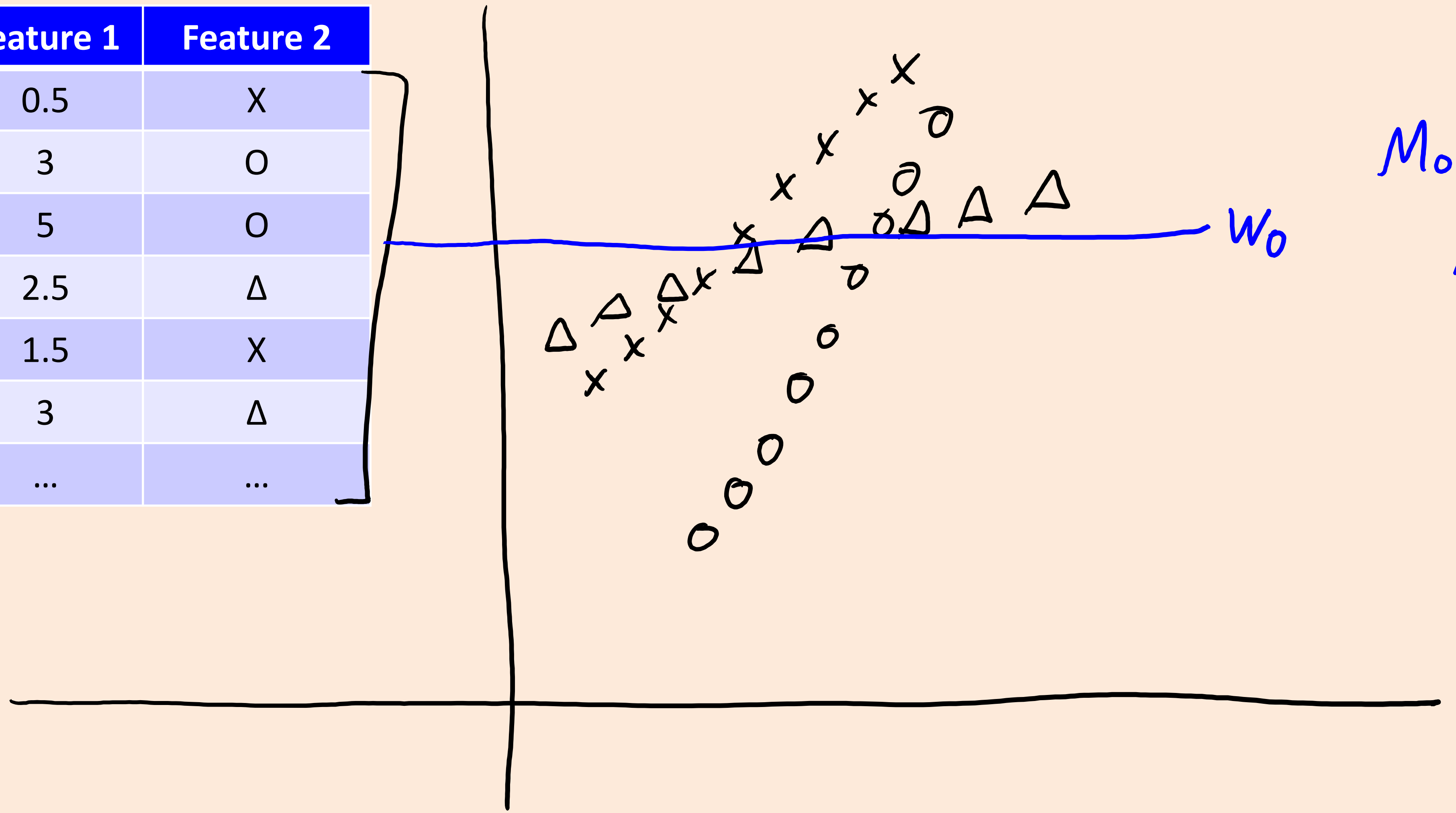
2.5	Δ
1.5	X
3	Δ
…	…



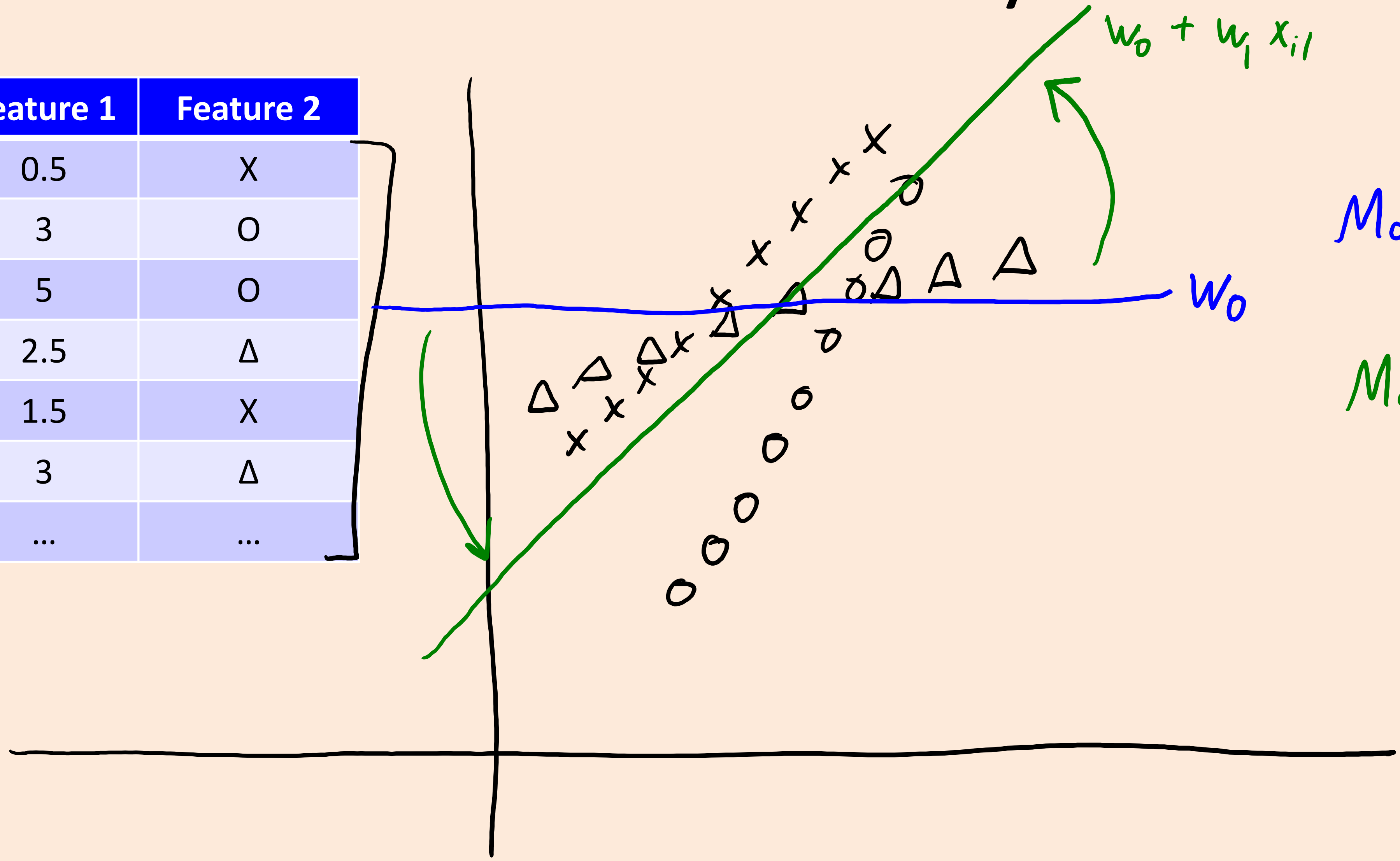
Model 1: only bias

$y_i = w_0$

Linear Models with Binary Features

$X =$

Feature 1	Feature 2
0.5	X
3	O
5	O
2.5	Δ
1.5	X
3	Δ
…	…



Model 1: only bias

$y_i = w_0$

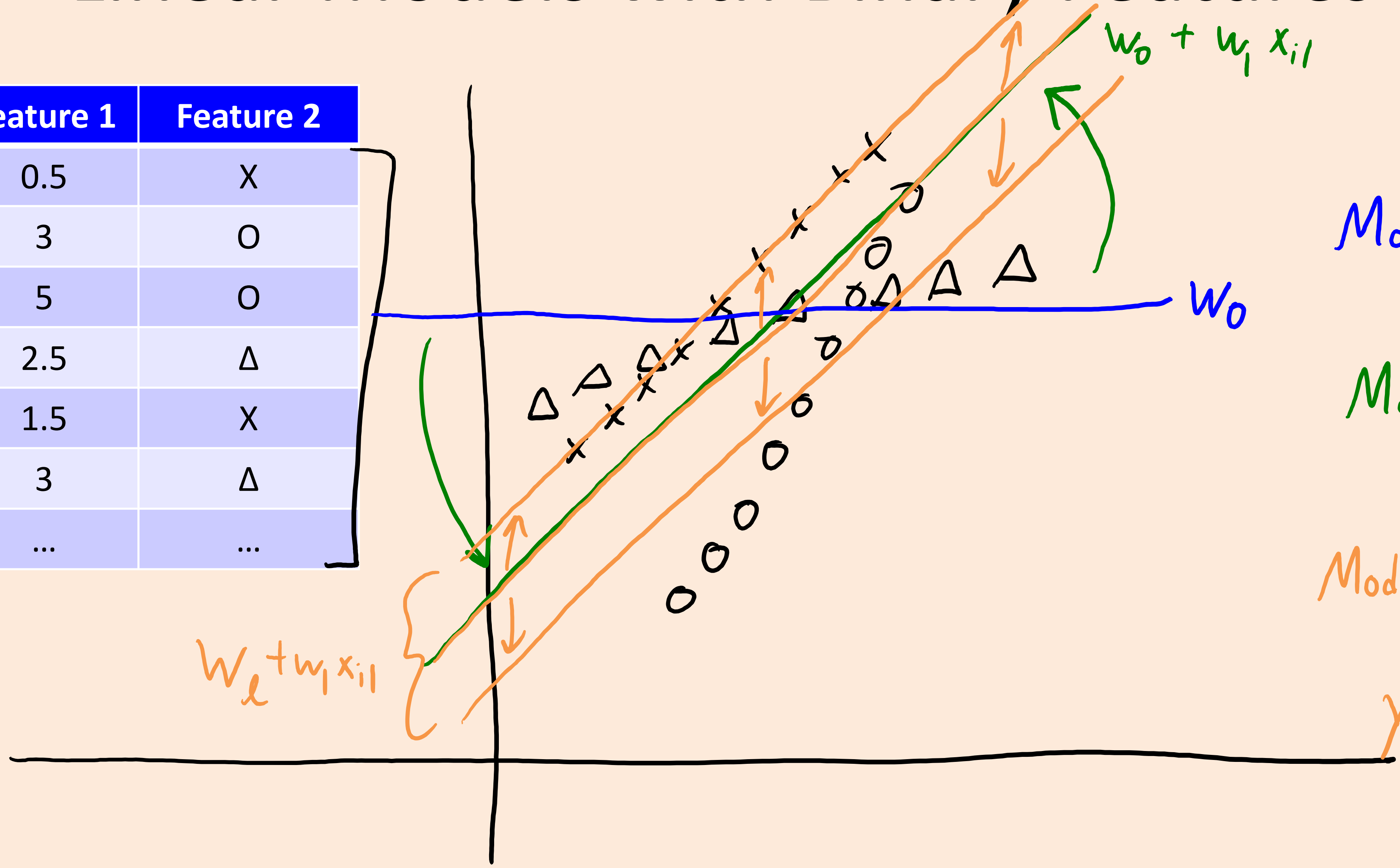
Model 2: bias + feature 1

$y_i = w_0 + w_1 x_{i1}$

Linear Models with Binary Features

$X =$

Feature 1	Feature 2
0.5	X
3	O
5	O
2.5	Δ
1.5	X
3	Δ
…	…



Model 1: only bias

$y_i = w_0$

Model 2: bias + feature 1

$y_i = w_0 + w_1 x_{i1}$

Model 3: "local" bias + feature 1

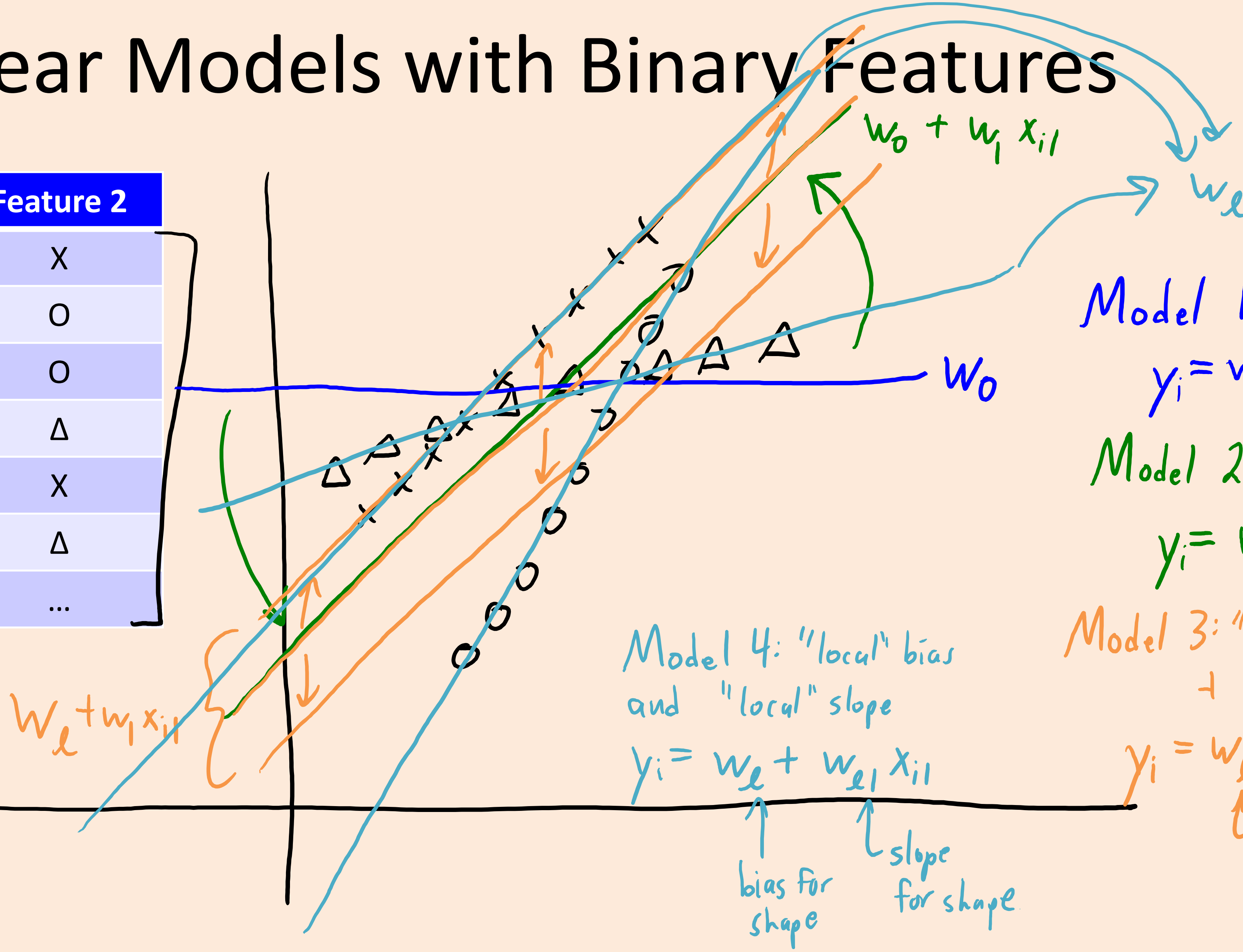
$y_i = w_\ell + w_1 x_{i1}$

ℓ shape

Linear Models with Binary Features

$X =$

Feature 1	Feature 2
0.5	X
3	O
5	O
2.5	Δ
1.5	X
3	Δ
…	…



Model 1: only bias

$y_i = w_0$

Model 2: bias + feature 1

$y_i = w_0 + w_1 x_{i1}$

Model 3: "local" bias + feature 1

$y_i = w_\ell + w_1 x_{i1}$

w_ℓ: shape

Model 4: "local" bias and "local" slope

$y_i = w_\ell + w_{\ell 1} x_{i1}$

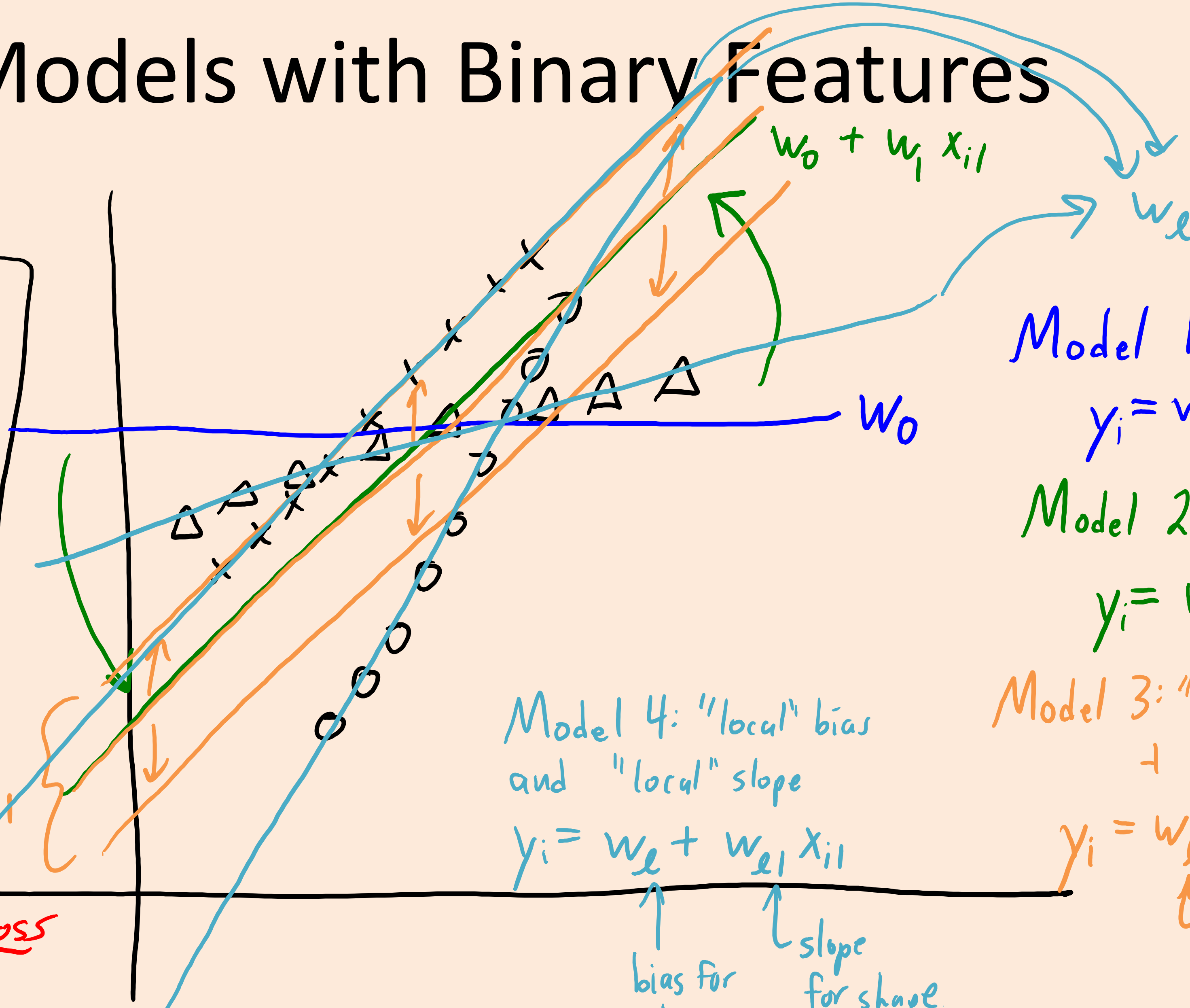
w_ℓ: bias for shape

$w_{\ell 1}$: slope for shape

Linear Models with Binary Features

$X =$

Feature 1	Feature 2
0.5	X
3	O
5	O
2.5	Δ
1.5	X
3	Δ
…	…



Model 1: only bias

$y_i = w_0$

Model 2: bias + feature 1

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Model 3: "local" bias + feature 1

$y_i = w_\ell + w_1 x_{i1}$

shape

Model 4: "local" bias and "local" slope

$y_i = w_\ell + w_{\ell 1} x_{i1}$

bias for shape

slope for shape

Could also share information across categories with global bias slope:

$y_i = w_0 + w_1 x_{i1} + w_\ell + w_{\ell 1} x_{i\ell}$