CPSC 340: Machine Learning and Data Mining

Feature Engineering

Spring 2022 (2021W2)

Admin

- Assignment 4: due next Friday

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.

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

  - Predict by taking ‘c’ maximizing $w_c^Tx_i$.
- Multi-class SVMs:
  - Trains the w_c jointly to encourage maximum $w_c^Tx_i$ to be correct $w_{y_i}^Tx_i$.

$$f(w_1, w_2, \dots, w_k) = \sum_{i=1}^{n} \sum_{c \neq y_i} \max\{0, 1 - w_{y_i}^T x_i + w_c^T x_i\} + \frac{\lambda}{2} \sum_{c=1}^{k} \|w_c\|^2$$

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:

Note: W is a matrix (first time in this class)

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

- 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 $z = w^Tx_i$ into $p(y_i \mid w, x_i)$ using sigmoid(z).
- Now consider the multi-class case:
  - We have ‘k’ real numbers $z_i = w_c^Tx_i$, 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’.
  - This is the multi-class equivalent of sigmoid (transform stuff to [0,1])

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 $w_c^Tx_i$.
  - Or in matrix notation:

$$\underbrace{\begin{bmatrix} w_1^Tx_1 & w_2^Tx_1 & \cdots & w_k^Tx_1 \\ w_1^Tx_2 & w_2^Tx_2 & \cdots & w_k^Tx_2 \\ & \vdots & & \\ w_1^Tx_n & w_2^Tx_2 & \cdots & w_k^Tx_n \end{bmatrix}}_{XW^T} = \underbrace{\begin{bmatrix} \text{---} & x_1^T & \text{---} \\ \text{---} & x_2^T & \text{---} \\ & \vdots & \\ \text{---} & x_n^T & \text{---} \end{bmatrix}}_{X} \underbrace{\begin{bmatrix} | & | & & | \\ w_1 & w_2 & \cdots & w_k \\ | & | & & | \end{bmatrix}}_{W^T}$$

  - 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")

(pause)

Feature Engineering

- “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

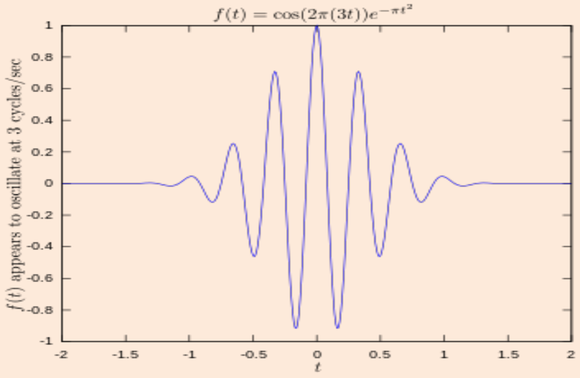
- Non-linear feature/label transforms can make things more linear:
  - Polynomial, exponential/logarithm, sines/cosines, RBFs.

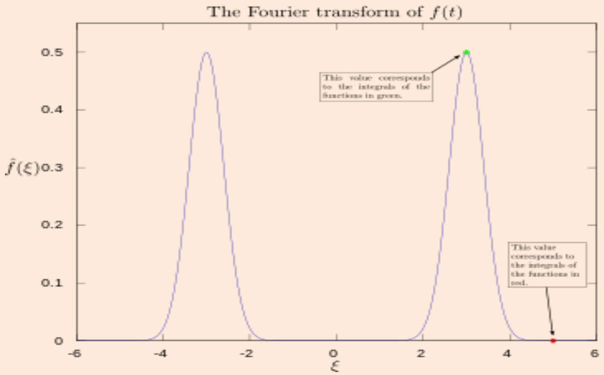
www.google.com/finance

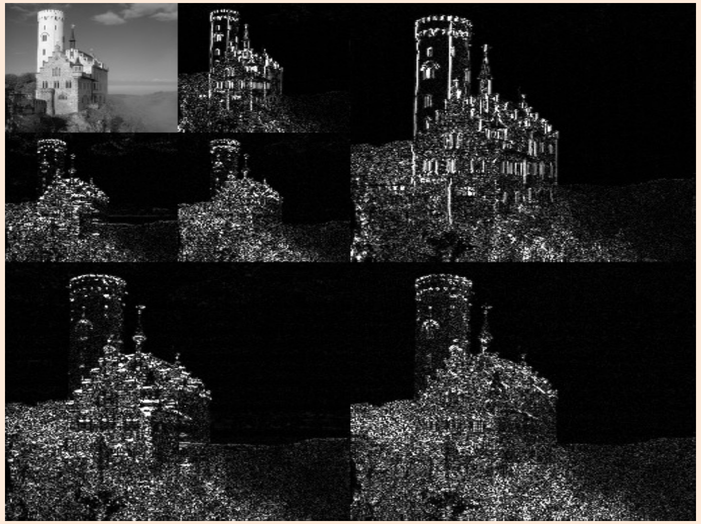
bonus!

Domain-Specific Transformations

- In some domains there are natural transformations to do:
  - Fourier coefficients and spectrograms (sound data).
  - Wavelets (image data).
  - Convolutions (coming later in the course!).







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.

(pause)

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

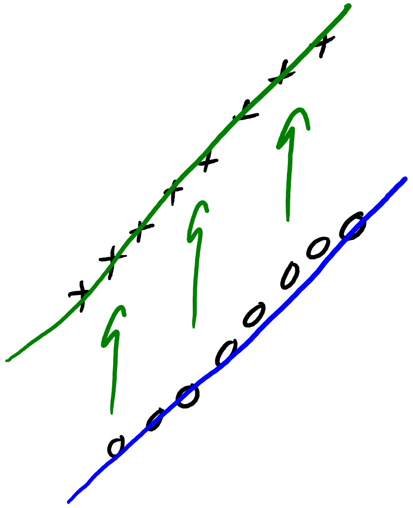
- What is the effect of a binary features on linear regression?

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

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

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

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



- 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?

bonus!

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.

bonus!

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:

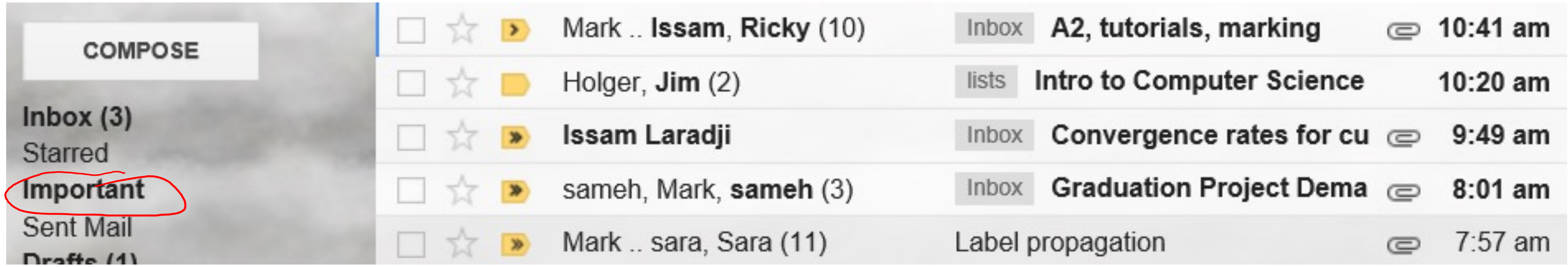
Rating
Bad
Very Good
Good
Good
Very Bad
Good
Medium

≥ 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”.

(pause)

Motivation: “Personalized” Important E-mails



Mark .. Issam, Ricky (10)	Inbox	A2, tutorials, marking	10:41 am
Holger, Jim (2)	lists	Intro to Computer Science	10:20 am
Issam Laradji	Inbox	Convergence rates for cu	9:49 am
sameh, Mark, sameh (3)	Inbox	Graduation Project Dema	8:01 am
Mark .. sara, Sara (11)		Label propagation	7:57 am

- 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

⇒

“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

⇒

“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.

“Global” and “Local” Features

- Consider the following weird feature transformation for identifying important e-mails:

“CPSS”	“340”
1	0
1	0
1	1
0	0
1	1

⇒

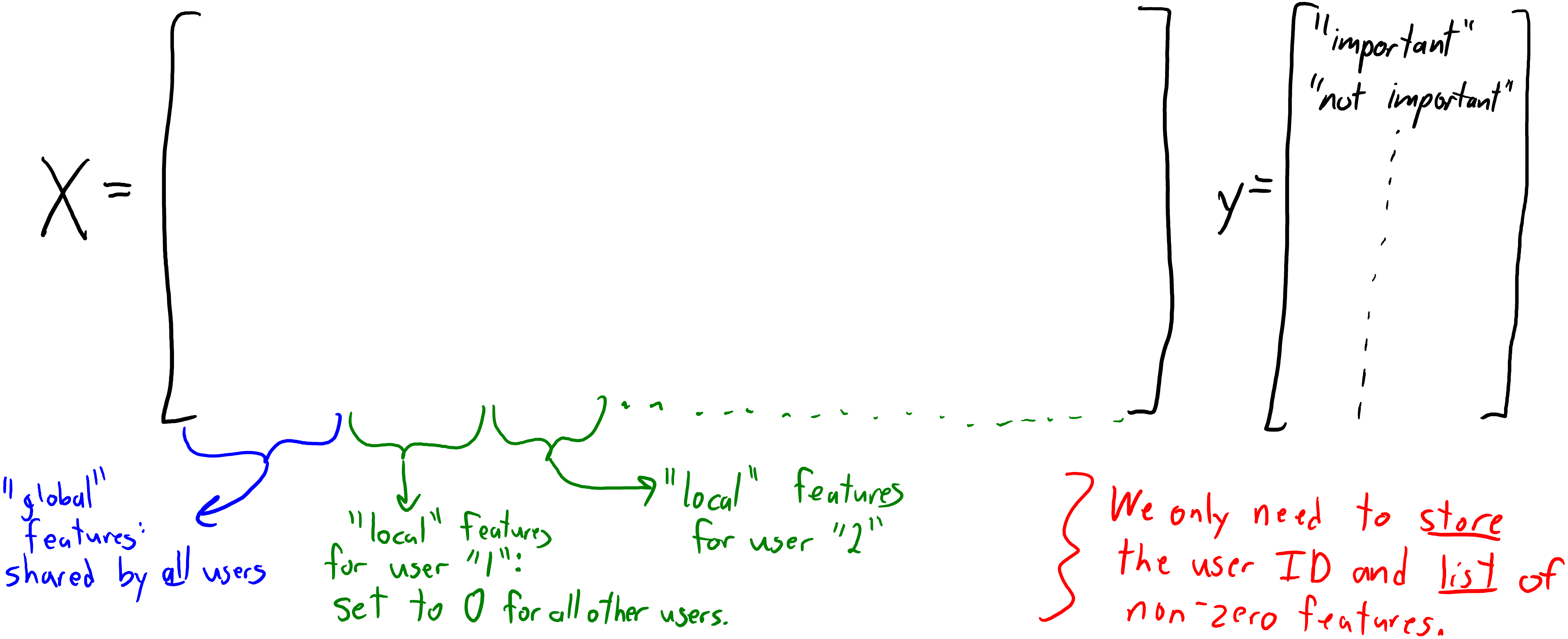
“CPSC” (any user)	“340” (any user)	“CPSC” (user?)	“340” (user?)
1	0	User 1	<no “340”>
1	0	User 1	<no “340”>
1	1	User 2	User 2
0	0	<no “CPSC”>	<no “340”>
1	1	User 3	User 3

- The categorical (user?) features get expanded out into ‘k’ binary features.
  - Where ‘k’ is the number of users.
  - All those features are set to 0 if the word was not used.

- “Any user” (“global”) features increase/decrease importance of word for every user.
- “User” (“local”) features increase/decrease importance of word for specific users.
  - Lets us learn more about users where we have a lot of data

The Big Global/Local Feature Table for E-mails

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



X =
y =
"important"
"not important"
"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.

Predicting Importance of E-mail For New User

- Consider a new user:
  - We start out with no information about them.
  - So we use global features to predict what is important to a generic user.

$$\hat{y}_i = \text{sign}(\underbrace{w_g^T x_{ig}})$$

features/weights shared across users.

  - Local features are initialized to zero.
- With more data, update global features and user's local features:
  - Local features make prediction *personalized*.

$$\hat{y}_i = \text{sign}(w_g^T x_{ig} + \underbrace{w_u^T x_{iu}})$$

features/weights specific to user.

  - What is important to *this* user?
- G-mail system: classification with logistic regression.
  - Trained with a variant of stochastic gradient (later).

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: back to SVMs and the “kernel trick”

bonus!

Cyclic Features

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

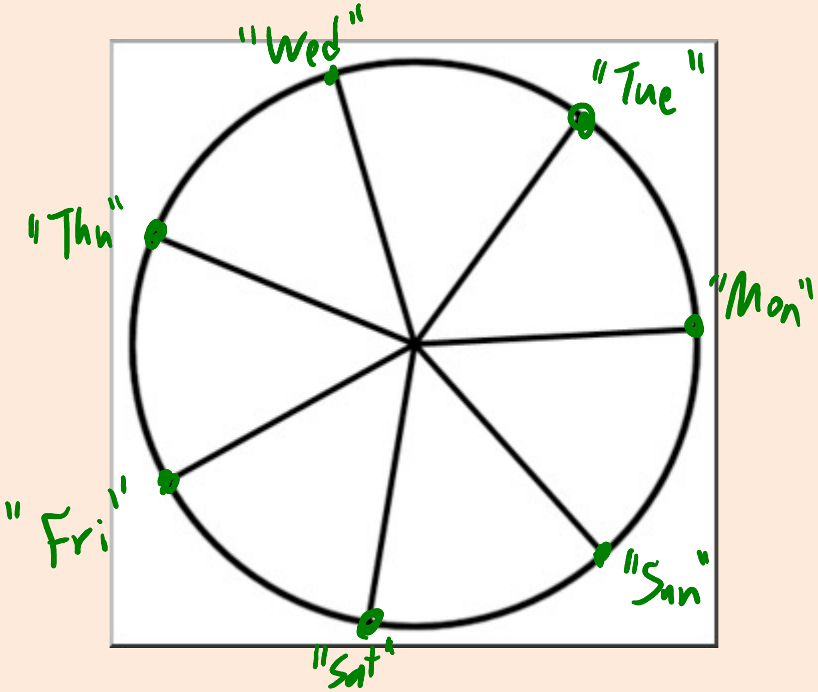
Time	Day	Date	Month	Year
12:05pm	Wed	29	Jul	15
10:20am	Sun	24	Apr	16
9:10am	Tue	3	May	16
11:20am	Sun	15	Jun	18
10:15pm	Thu	8	Aug	19

- 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”.

bonus!

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”.

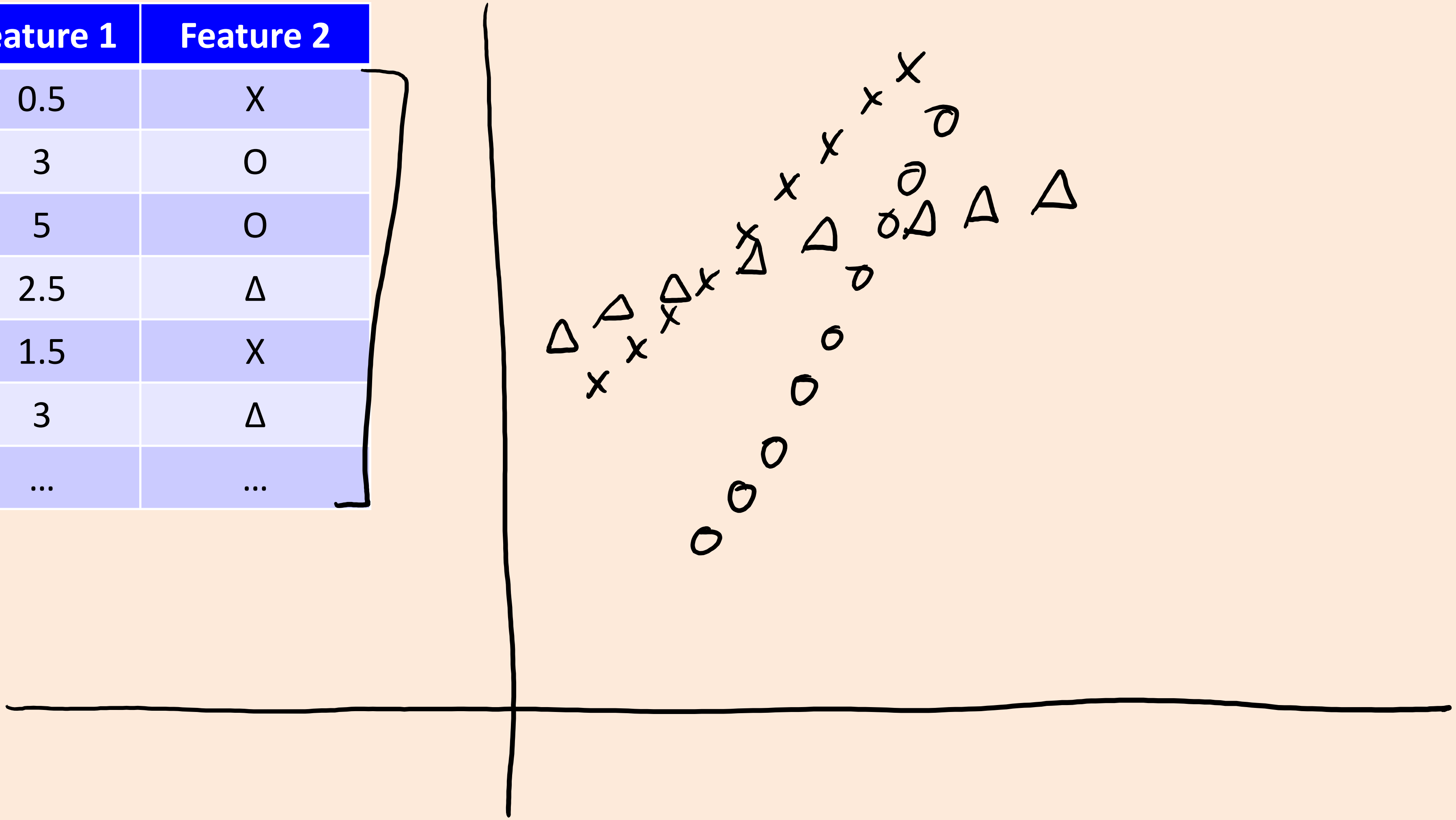
https://www.abcteach.com/documents/clip-art-circle07-77-bw-i-abcteachcom-17022

bonus!

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
…	…

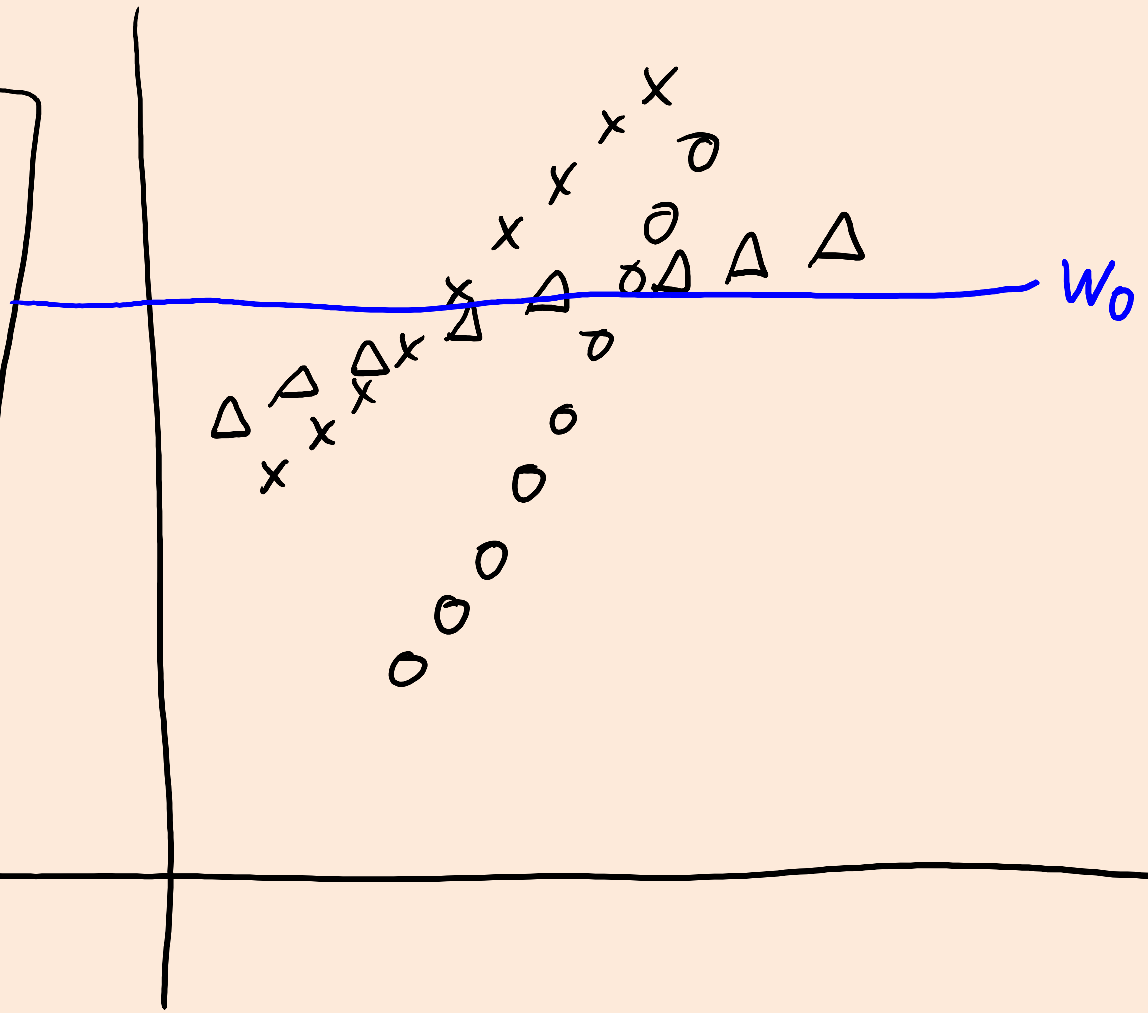


bonus!

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 <u>bias</u>

$y_i = w_0$

bonus!

Linear Models with Binary Features

$X =$

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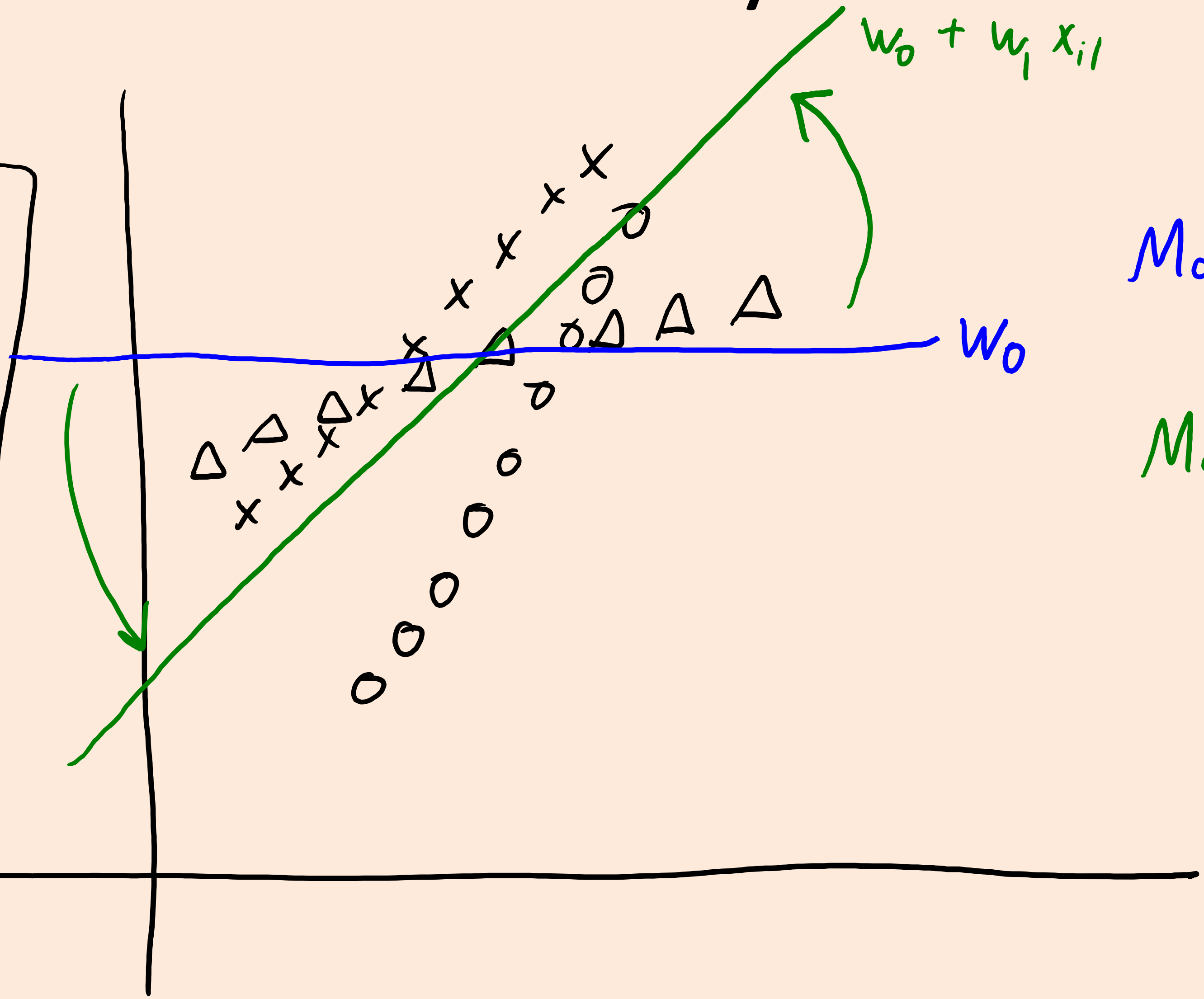
3	Δ
…	…



Model 1: only bias

$y_i = w_0$

Model 2: bias + feature 1

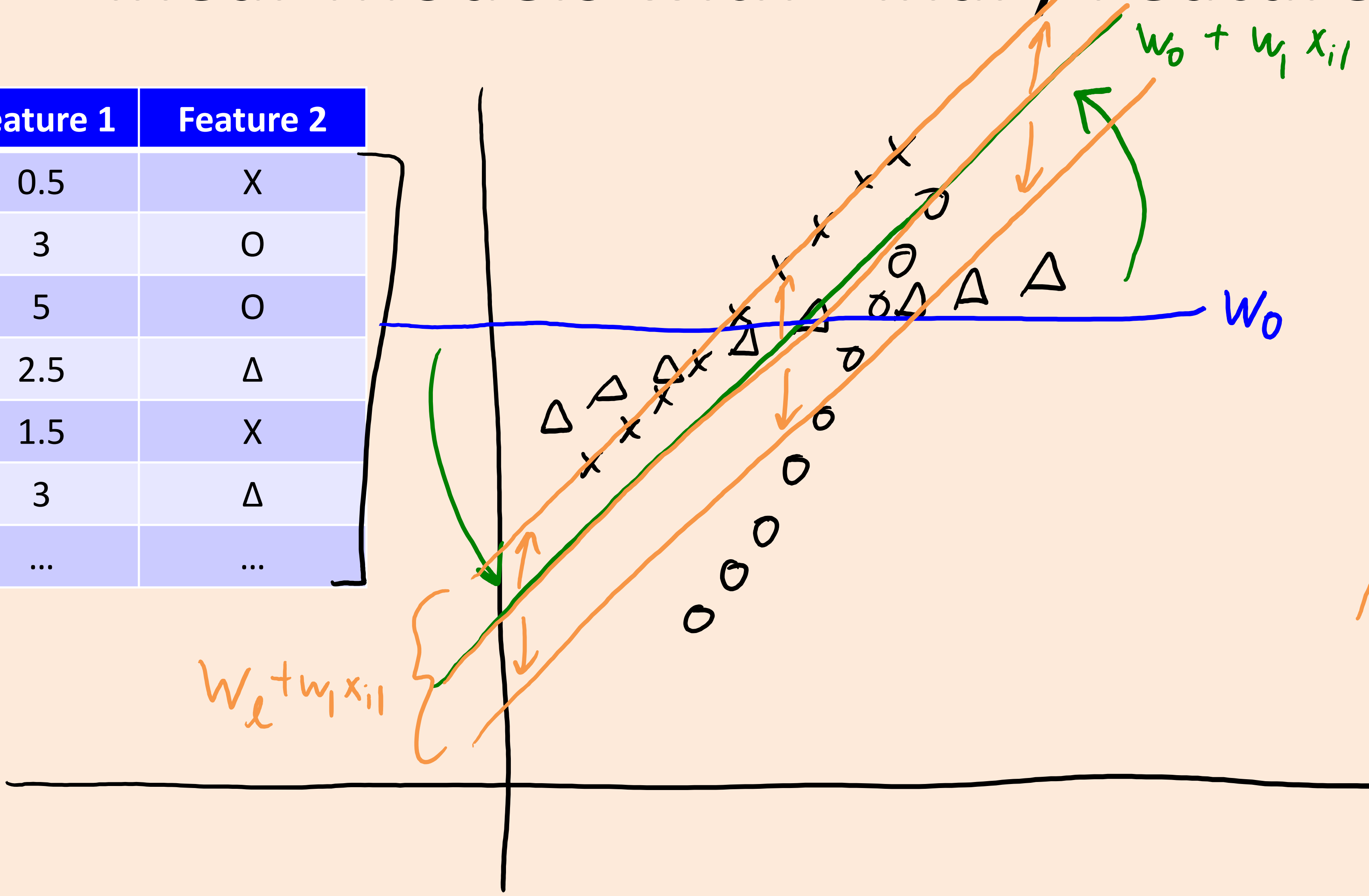
$y_i = w_0 + w_1 x_{i1}$

bonus!

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

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

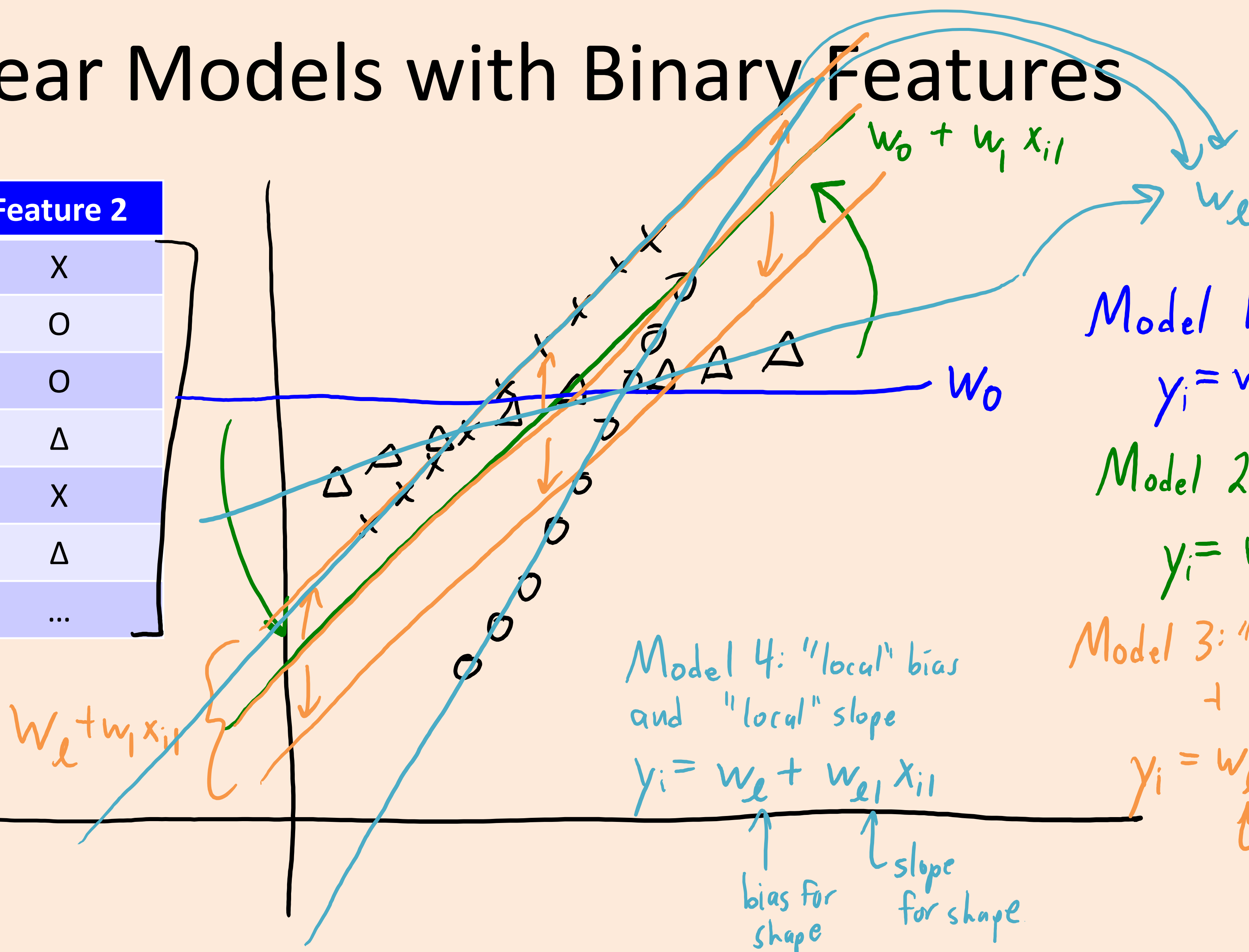
$\uparrow$ shape

bonus!

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

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

shape

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

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

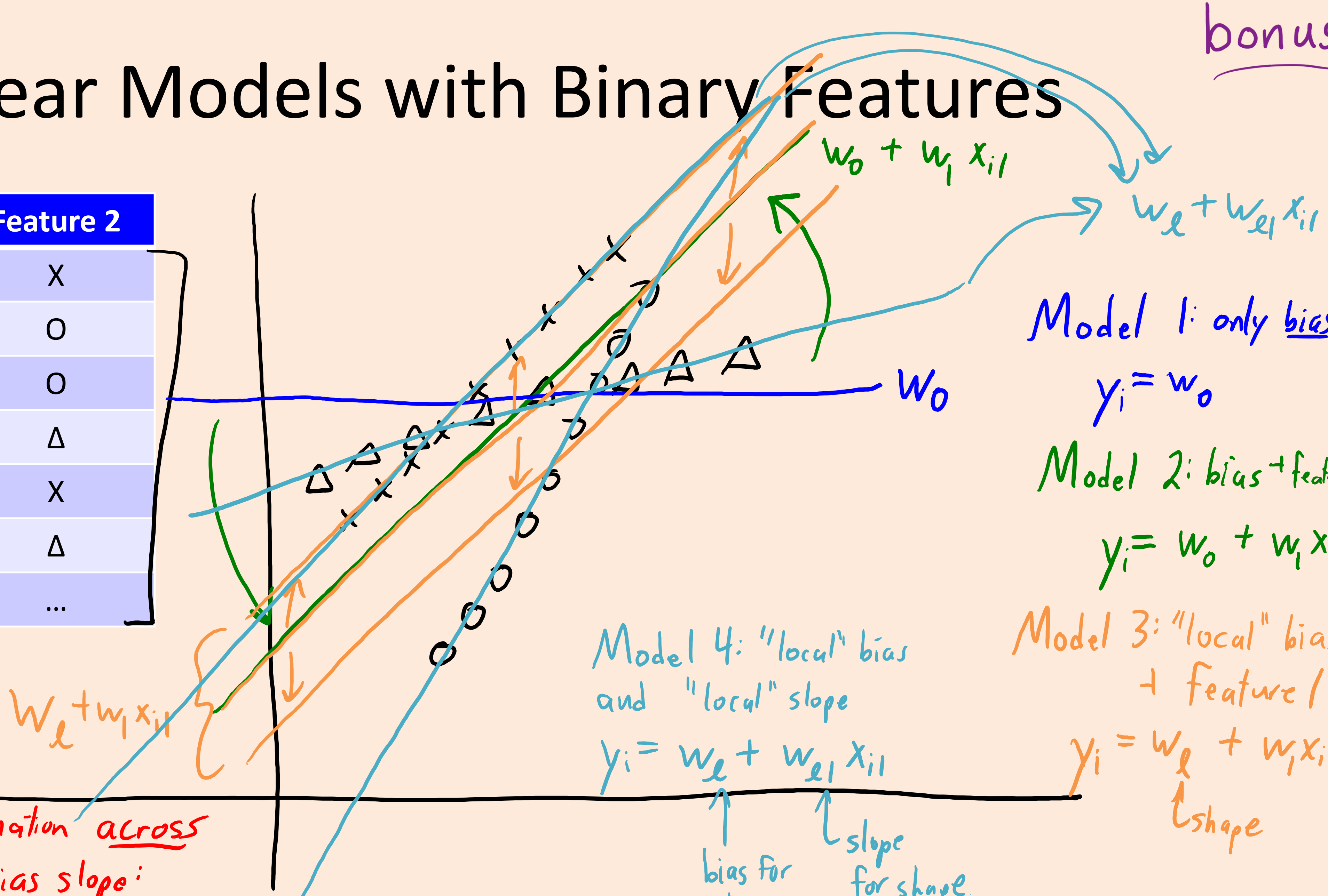
bias for shape

slope for shape

bonus!

Linear Models with Binary Features

$$X = \begin{array}{cc} \text{Feature 1} & \text{Feature 2} \\ \hline 0.5 & X \\ 3 & O \\ 5 & O \\ 2.5 & \Delta \\ 1.5 & X \\ 3 & \Delta \\ \dots & \dots \end{array}$$



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

$y_i = \underset{\uparrow\ \text{shape}}{w_e} + w_1 x_{i1}$

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

$y_i = \underset{\substack{\uparrow \\ \text{bias for shape}}}{w_e} + \underset{\substack{\uparrow \\ \text{slope for shape}}}{w_{e1}} x_{i1}$

Could also share information across categories with global bias slope:

$y_i = w_0 + w_1 x_{i1} + w_e + w_{e1} x_{i\ell}$