CPSC 340:
Machine Learning and Data Mining

Non-Parametric Feature Transforms
Summer 2021

Admin

- Midterm is tomorrow.
  - Manually-graded portion on Gradescope
    - 55 minutes
    - Handwritten or typeset
  - Auto-graded potion on Canvas
    - 45 minutes
    - Multiple choice
  - The two portions are equally weighted
- Please don't ask broad questions on Piazza tomorrow
  - If you have issues with exams, etc., make a private post
- Assignment 4 is due Monday, June 7, 2021

In This Lecture

1. Standardization (5 minutes)
2. Gaussian RBF (20 minutes)
3. Linear Classifiers Intro (20 minutes)

Last Time: Regularization

- L0-regularization (AIC, BIC, Mallow's Cp, Adjusted R^2, ANOVA):
  - Adds penalty on the number of non-zeros to select features.

$$f(w) = \|Xw - y\|^2 + \lambda \|w\|_0$$

- L2-regularization (ridge regression):
  - Adding penalty on the L2-norm of 'w' to decrease overfitting:

$$f(w) = \|Xw - y\|^2 + \frac{\lambda}{2} \|w\|^2$$

- L1-regularization (LASSO):
  - Adding penalty on the L1-norm decreases overfitting and selects features:

$$f(w) = \|Xw - y\|^2 + \lambda \|w\|_1$$

Coming Up Next

STANDARDIZATION

Features with Different Scales

- Consider continuous 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 decision trees or naïve Bayes.
    - They only look at one feature at a time.
  - It doesn't matter for least squares:
    - w_j*(100 mL) gives the same model as w_j*(0.1 L) with a different w_j.

Features with Different Scales

- Consider continuous 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 matters for k-nearest neighbours:
    - "Distance" will be affected more by large features than small features.
  - It matters for regularized least squares:
    - Penalizing $(w_j)^2$ means different things if features 'j' are on different scales.

Standardizing Features

- It is common to standardize continuous features:
  - For each feature:
    1. Compute mean and standard deviation:

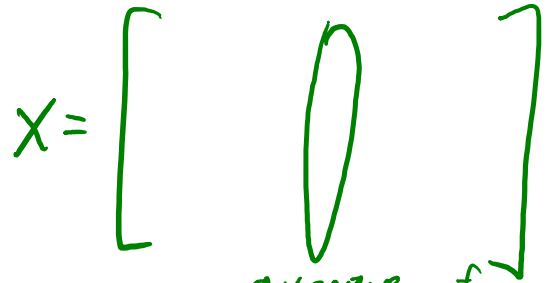
$$\mu_j = \frac{1}{n}\sum_{i=1}^{n} x_{ij} \qquad \sigma_j = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(x_{ij}-\mu_j)^2}$$

    2. Subtract mean and divide by standard deviation ("z-score")

Replace x_{ij} with $\frac{x_{ij}-\mu_j}{\sigma_j}$

  - Now changes in 'w_j' have similar effect for any feature 'j'.
- How should we standardize test data?
  - Wrong approach: use mean and standard deviation of test data.
  - Training and test mean and standard deviation might be very different.
  - Right approach: use mean and standard deviation of training data.

Standardizing Features



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    2. Subtract mean and divide by standard deviation ("z-score")

Replace x_{ij} with $\frac{x_{ij}-\mu_j}{\sigma_j}$

  - Now changes in 'w_j' have similar effect for any feature 'j'.
- If we're doing 10-fold cross-validation:
  - Compute μ_j and σ_j based on the 9 training folds (e.g., average over 9/10s of data).
  - Standardize the remaining ("validation") fold with this "training" μ_j and σ_j.
  - Re-standardize for different folds.

Standardizing Target

- In regression, we sometimes standardize the targets y_i.
  - Puts targets on the same standard scale as standardized features:

Replace y_i with $\frac{y_i - \mu_y}{\sigma_y}$

- With standardized target, setting $w = 0$ predicts mean y:
  - High regularization makes us predict closer to the average value.
- Again, make sure you standardize test data with the training stats.
- Other common transformations of y_i are logarithm/exponent:

Use $\log(y_i)$ or $\exp(\gamma y_i)$

  - Makes sense for geometric/exponential processes.

Coming Up Next

GAUSSIAN RADIAL BASIS FUNCTION

Weighted Sum of "Basis Functions"

- Features for linear models with "change of basis" are functions

"basis function" $f_j : \mathbb{R} \to \mathbb{R}$

$$y_i = w_0 f_0(x_i) + w_1 f_1(x_i) + w_2 f_2(x_i) + \cdots + w_p f_p(x_i)$$ "on-the-fly" transformation

$$y_i = v_1 z^1 + v_2 z^2 + v_3 z^3 + \cdots + v_{p+1} z^{p+1}$$ "offline" transformation

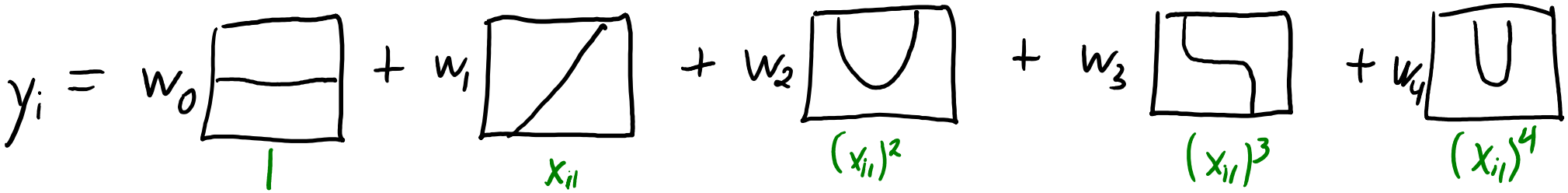
- We've been using linear models with polynomial bases:

$$y_i = w_0 \cdot 1 + w_1 x_{i1} + w_2 (x_{i1})^2 + w_3 (x_{i1})^3 + w_4 (x_{i1})^4$$

Weighted sum of basis functions

Parametric vs. Non-Parametric Transforms

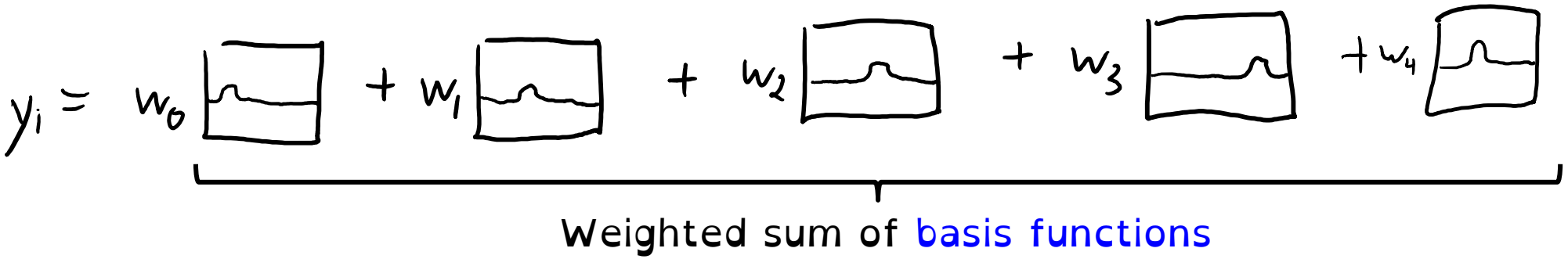
- We've been using linear models with polynomial bases:



- But polynomials are not the only possible bases:
  - Exponentials, logarithms, trigonometric functions, etc.
  - The right basis will vastly improve performance.
  - If we use the wrong basis, our accuracy is limited even with lots of data.
  - But the right basis may not be obvious.

Parametric vs. Non-Parametric Transforms

- Alternative: non-parametric bases:
  - Size of basis (number of features) grows with 'n'.
  - Model gets more complicated as you get more data.
  - Can model complicated functions where you don't know the right basis.
    - With enough data.
  - Classic example is "Gaussian RBFs" ("Gaussian" == "normal distribution").



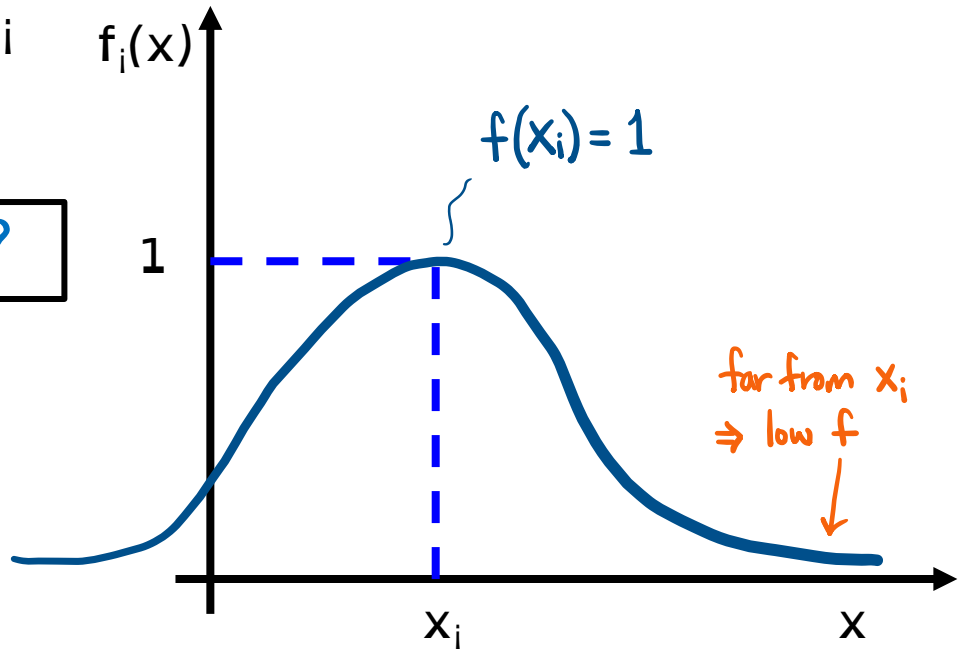
"Local Bumps"

"basis function" $f_i : \mathbb{R} \to \mathbb{R}, \quad i = 1, 2, \cdots, n$

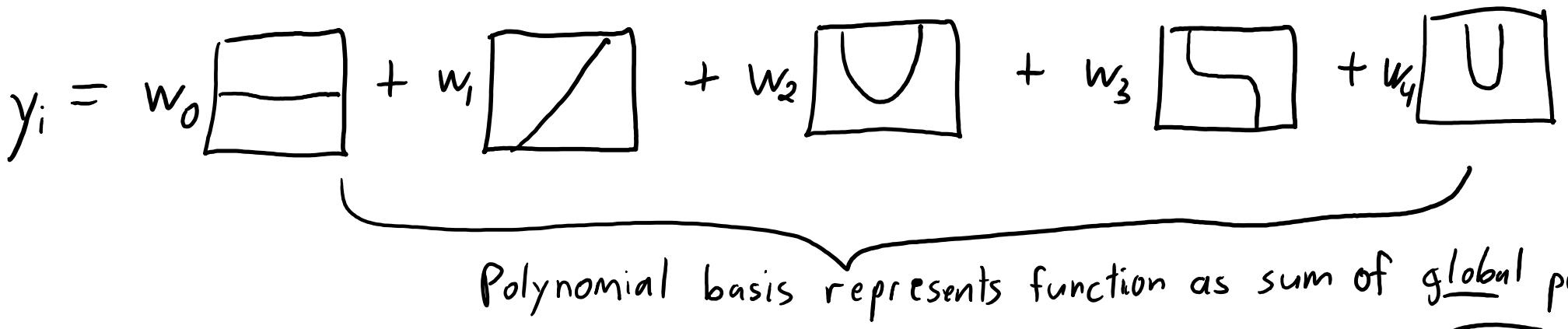
- Gaussian RBF's basis functions are "local bumps"
  - Each training example xi defines its own local bump
  - d=1: bell-curve centered at x_i

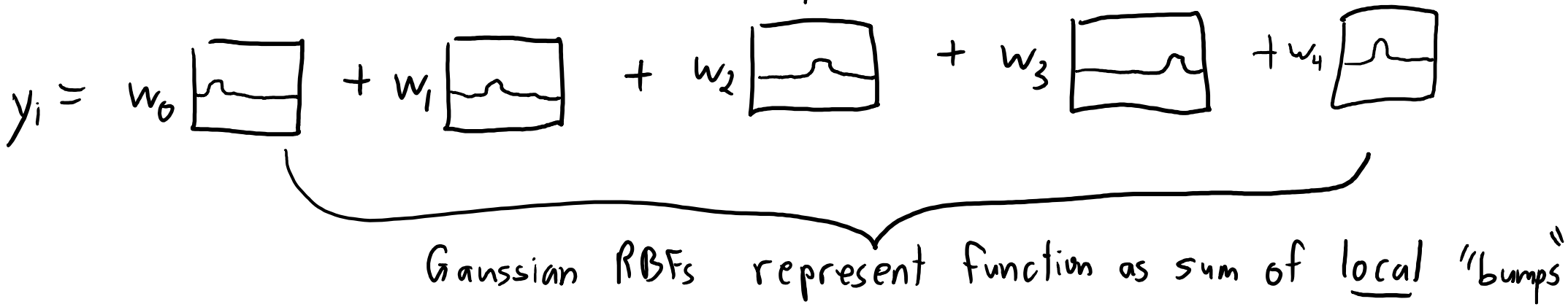
Q: How many local bumps are there?

n local bumps!



Gaussian RBFs: A Sum of "Bumps"





Q: How do we predict $\hat{y}_i$ for a test example $\tilde{x}_i$?

Prediction with Gaussian RBF Regression

$$y_i \simeq w_0 f_0(x_i) + w_1 f_1(x_i) + w_2 f_2(x_i) + w_3 f_3(x_i) + w_4 f_4(x_i)$$

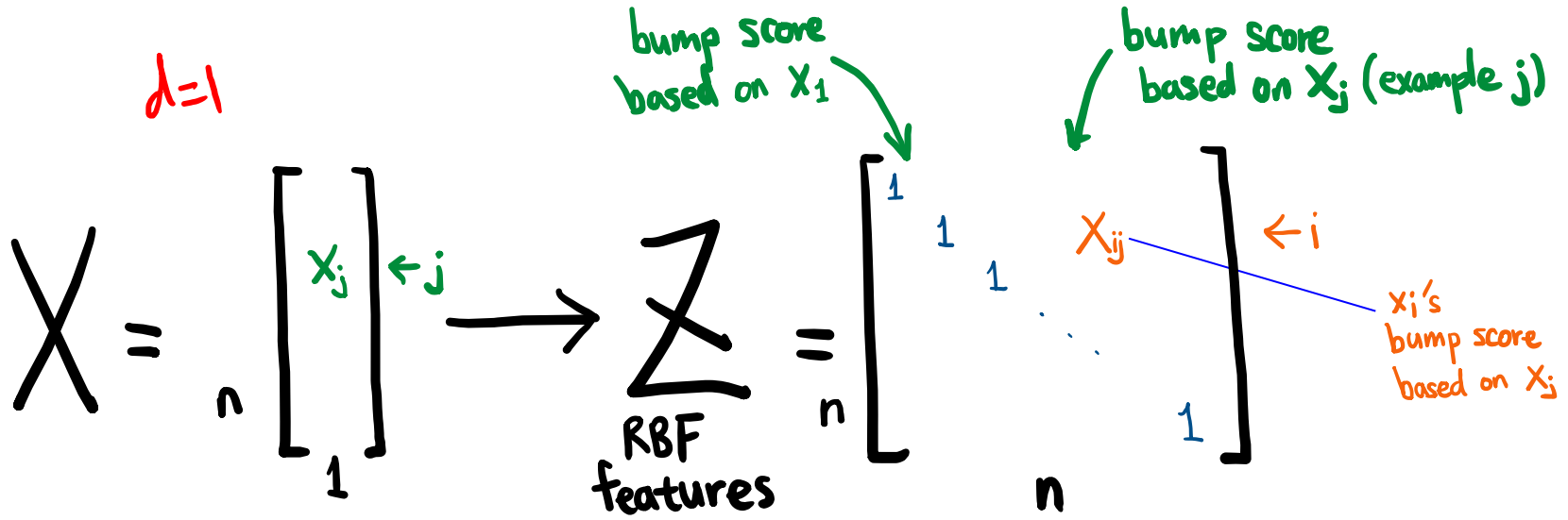
$$\tilde{x}_i = 1.4$$

$$\hat{y}_i = w_0 f_0(1.4) + w_1 f_1(1.4) + w_2 f_2(1.4) + w_3 f_3(1.4) + w_4 f_4(1.4)$$

bump 0 "score" | bump 1 "score" | bump 2 "score" | bump 3 "score" | bump 4 "score"

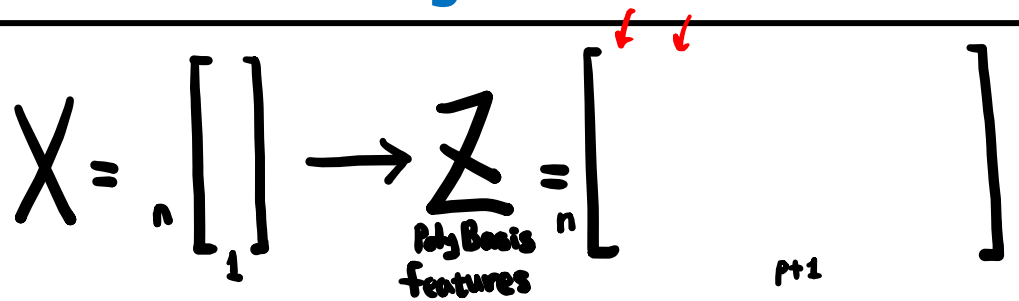
- Prediction is weighted combination of "bump scores"
- These "bump scores" are defined by training examples
  - an instance of "learned features"

"Change of Basis" for Gaussian RBFs



Q: Why are there 1s on the diagonal?

Q: Does polynomial basis give us "learned features" too?

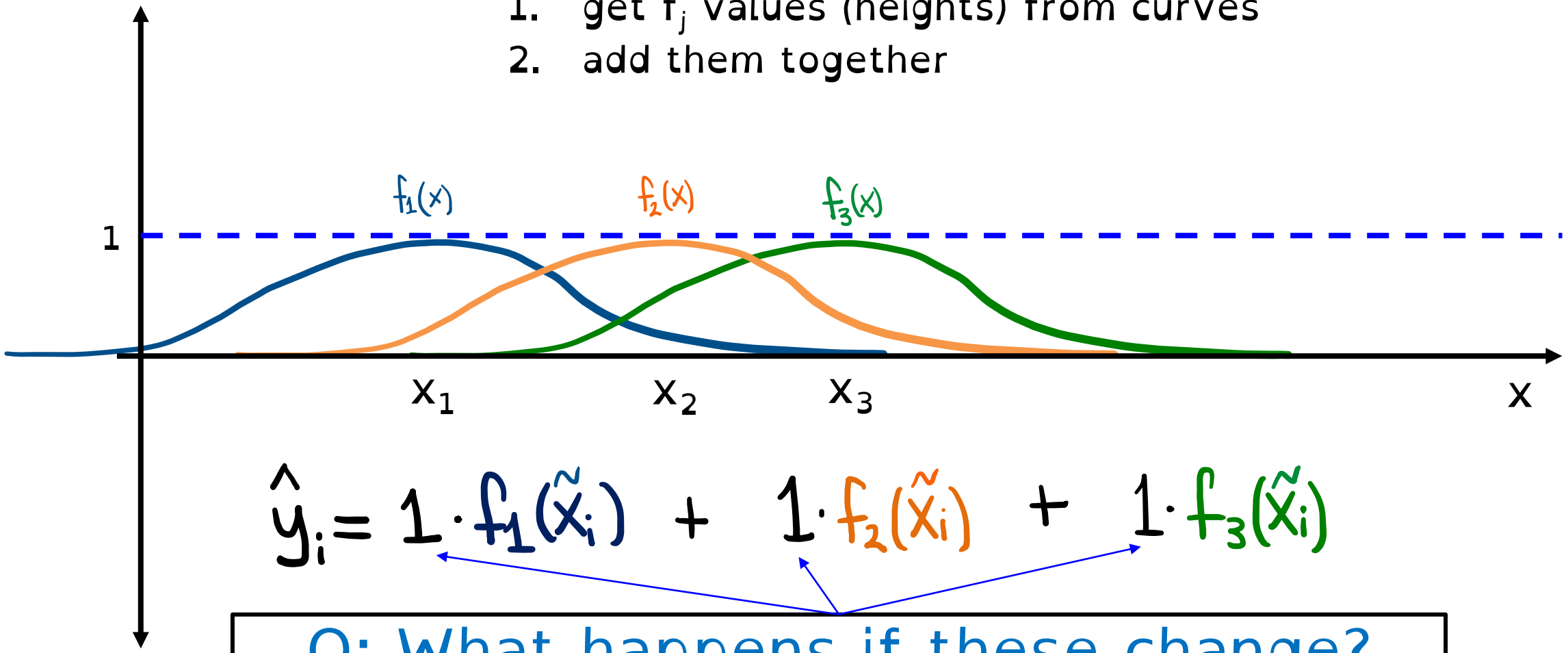


Gaussian RBFs: Universal Approximator

- Gaussian RBFs are universal approximators (compact subets of $\mathbb{R}^d$)
  - Enough bumps can approximate any continuous function to arbitrary precision.
  - Achieve optimal test error as ‘n’ goes to infinity.

Visualizing RBF Regression

- To predict $\hat{y}_i$ from $\tilde{x}_i$,
  1. get f_j values (heights) from curves
  2. add them together

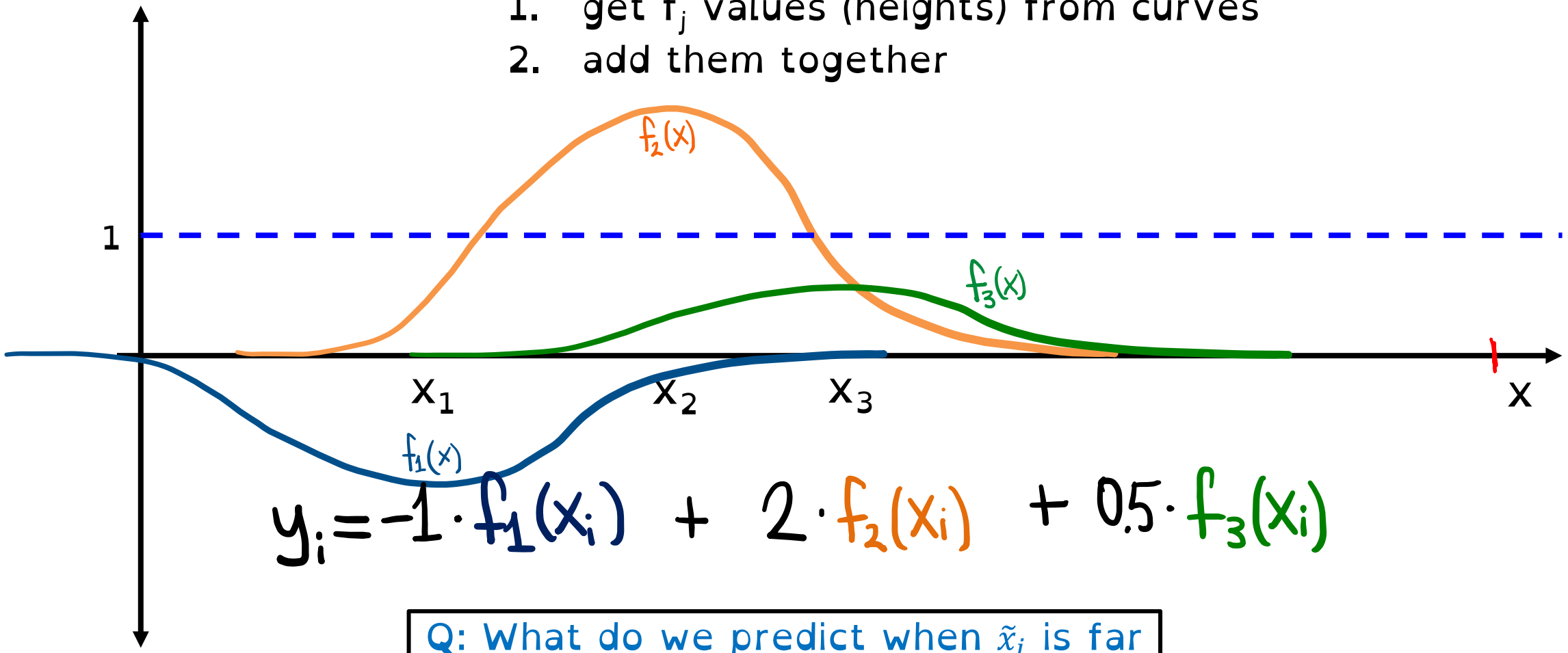


$$\hat{y}_i = 1 \cdot f_1(\tilde{x}_i) + 1 \cdot f_2(\tilde{x}_i) + 1 \cdot f_3(\tilde{x}_i)$$

Q: What happens if these change?

Visualizing RBF Regression

- To predict $\hat{y}_i$ from $\tilde{x}_i$,
  1. get f_j values (heights) from curves
  2. add them together



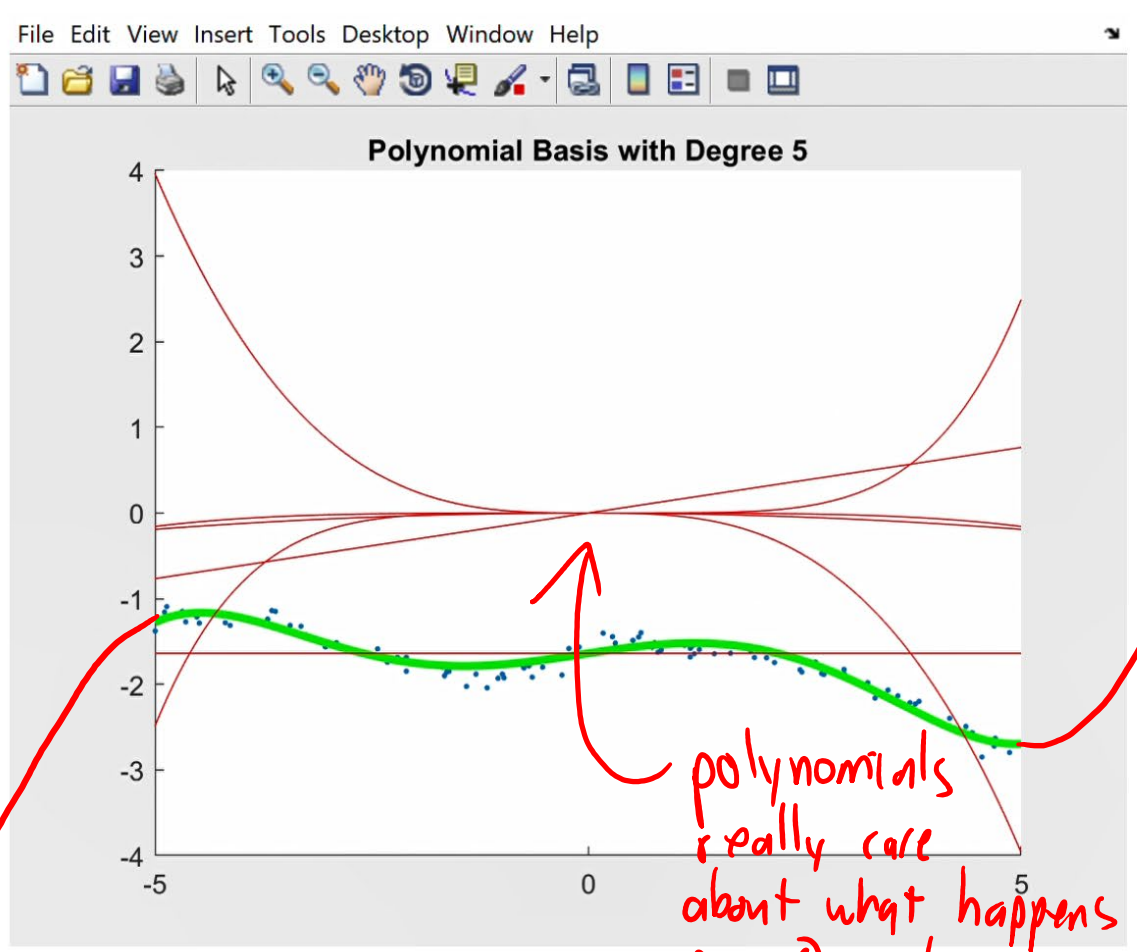
$$y_i = -1 \cdot f_1(x_i) + 2 \cdot f_2(x_i) + 0.5 \cdot f_3(x_i)$$

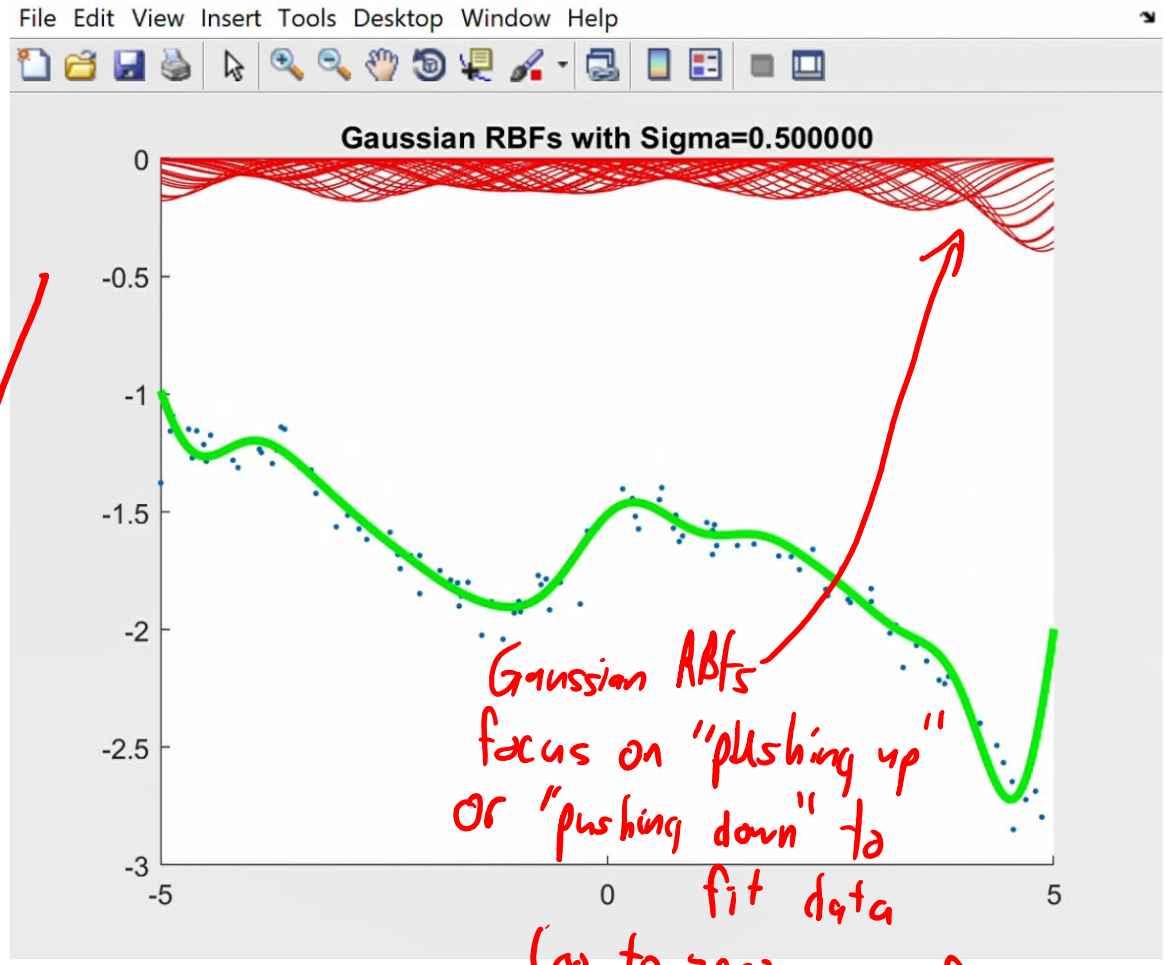
Q: What do we predict when $\tilde{x}_i$ is far away from other examples?

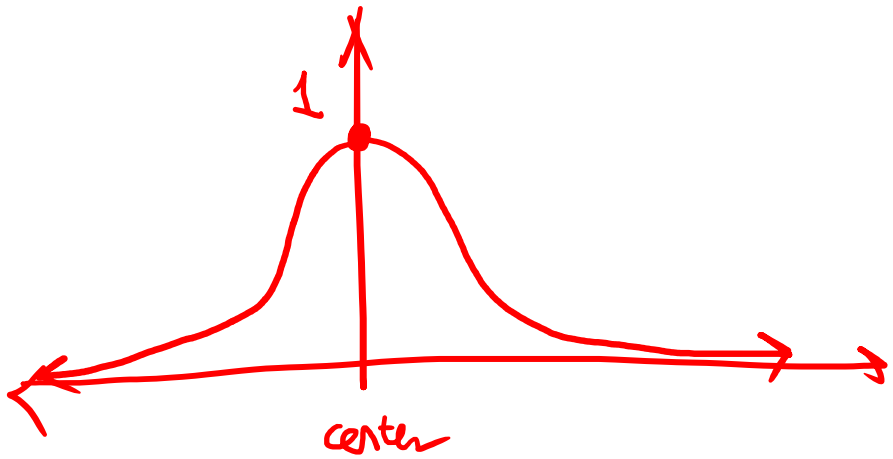
≈ 0

Gaussian RBFs: A Sum of "Bumps"

- More-realistic version (green is regression line, red is each basis):



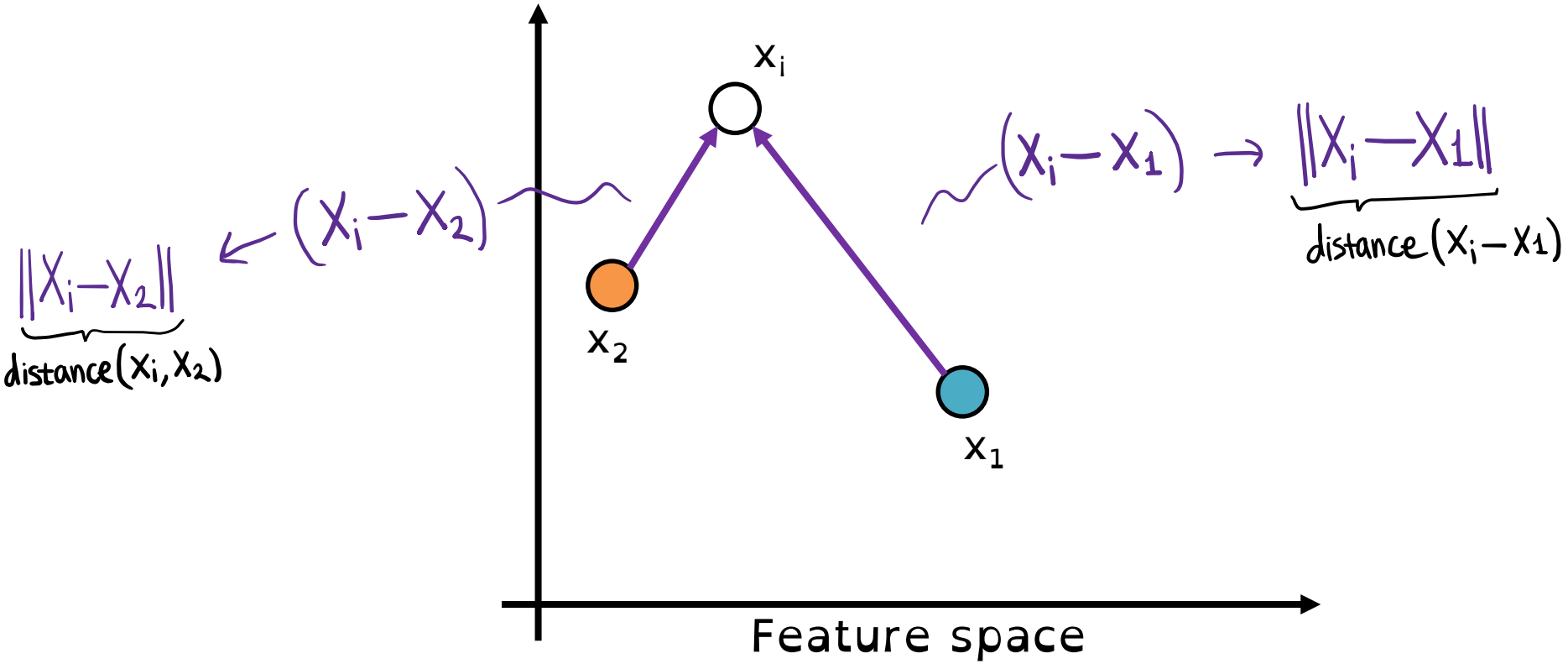




Coming Up Next

GAUSSIAN RBF IN HIGHER DIMENSIONS

Recall: Distance



Gaussian RBFs: Formal Details

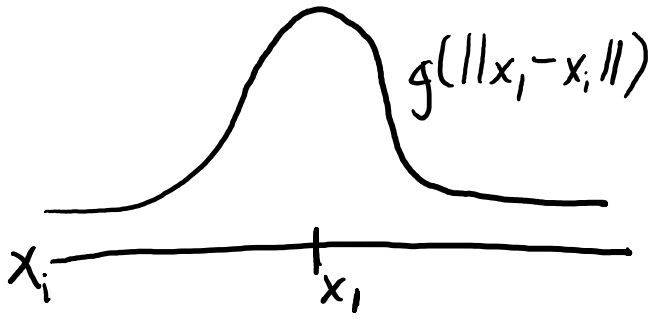
- What is a radial basis functions (RBFs)?
  - A set of non-parametric bases that depend on distances to training points.

Replace $x_i = (x_{i1}, x_{i2}, \dots, x_{in})$ with $z_i = (g(\|x_i - x_1\|), g(\|x_i - x_2\|), \dots, g(\|x_i - x_n\|))$

'd' features

'n' features

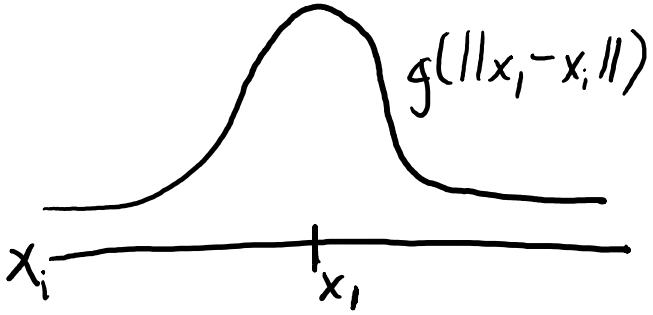
  - Have 'n' features, with feature 'j' depending on distance to example 'i'.
    - Typically the feature will decrease as the distance increases:



Gaussian RBFs: Formal Details

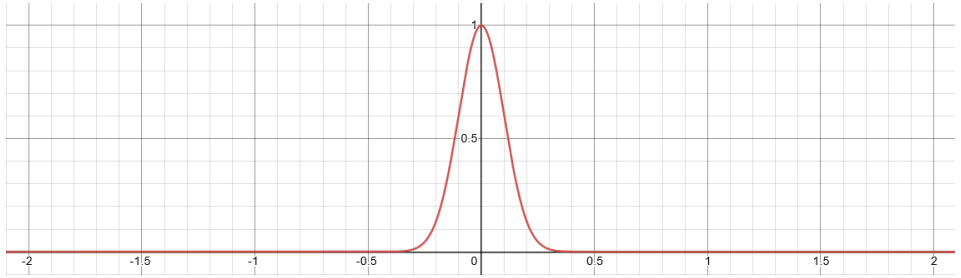
- What is a radial basis functions (RBFs)?
  - Most common choice of 'g' is Gaussian RBF:

$$g: \mathbb{R} \to \mathbb{R} \qquad g(\varepsilon) = \exp\left(-\frac{\varepsilon^2}{2\sigma^2}\right)$$

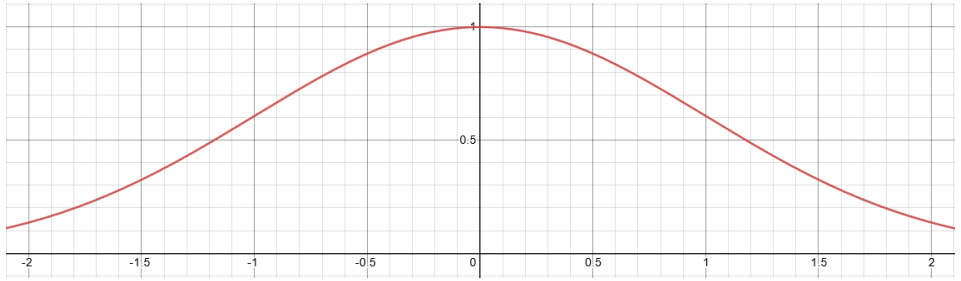


Q: What does g(ϵ) look like if σ is small?
What does it look like if σ is large?

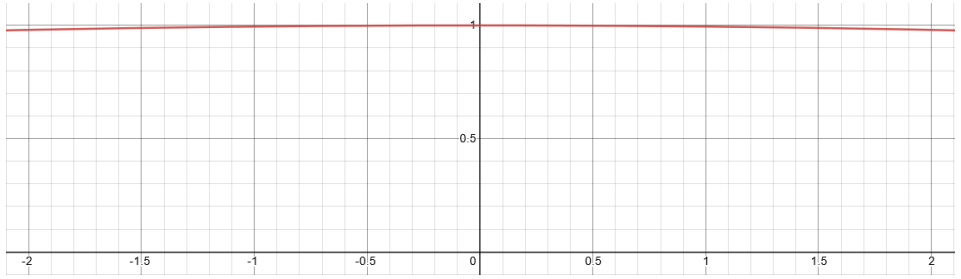
σ and Curve Width



$\sigma = 0.1$



$\sigma = 1.0$

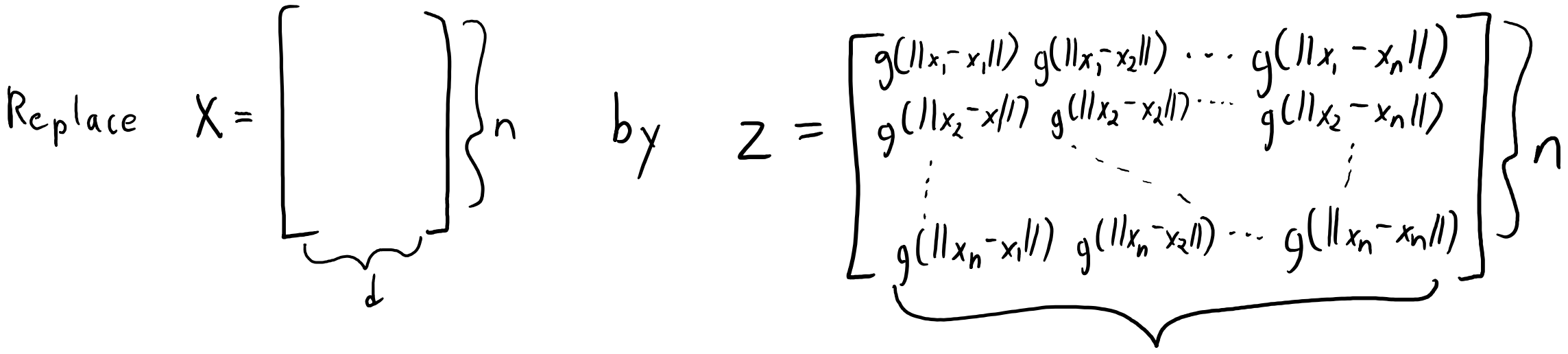


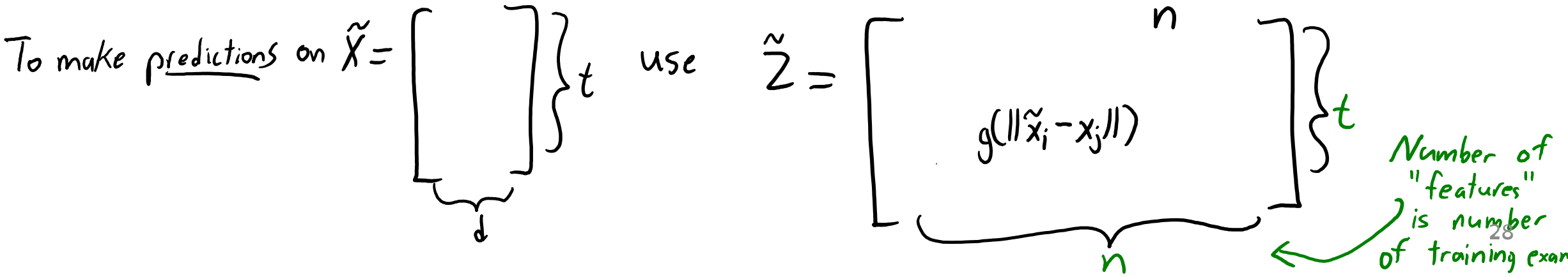
$\sigma = 10.0$

- How does σ affect the model complexity?
  - As σ increases, the model complexity (increases/decreases)
- Low sensitivity to change in feature values => low complexity of model

Gaussian RBFs: Formal Details

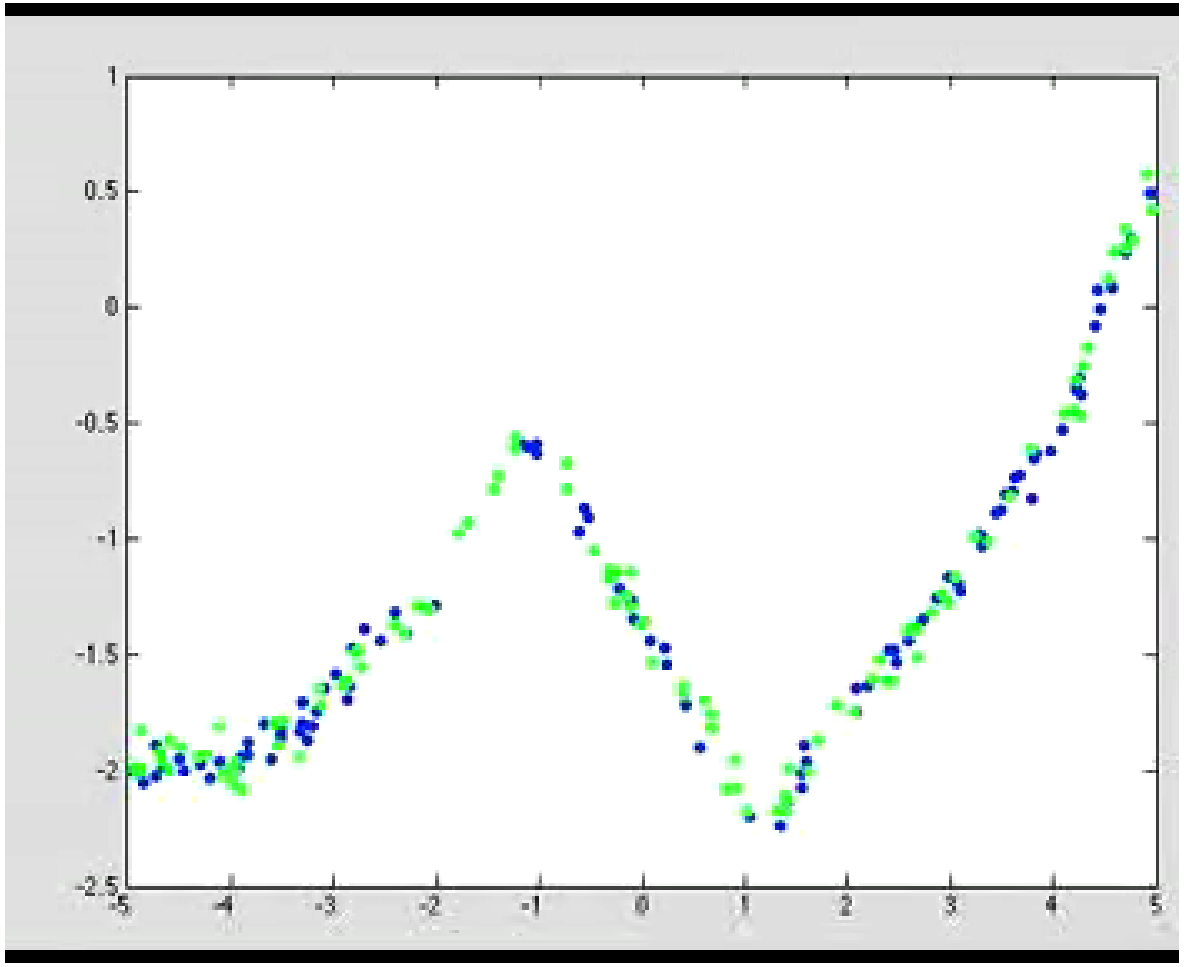
- What is a radial basis functions (RBFs)?
  - The training and testing matrices when using RBFs:





Non-Parametric Basis: RBFs

- Least squares with Gaussian RBFs for different σ values:



Could add bias and linear basis:

$$Z = \begin{bmatrix} 1 & x_1 & g(\|x_1 - x_1\|) & \cdots & g(\|x_1 - x_n\|) \\ 1 & x_2 & & & \\ 1 & x_3 & & & \\ & \vdots & & & \\ 1 & x_n & g(\|x_1 - x_n\|) & \cdots & g(\|x_n - x_n\|) \end{bmatrix}$$

1 d n

$[\quad]$ 0 0 0 0 0

Q: What do we predict when $\tilde{x}_i$ is far away from other examples?

Not zero.

RBFs and Regularization

- Gaussian Radial basis functions (RBFs) predictions:

$$\hat{y}_i = w_1 \exp\left(-\frac{\|x_i - x_1\|^2}{2\sigma^2}\right) + w_2 \exp\left(-\frac{\|x_i - x_2\|^2}{2\sigma^2}\right) + \cdots + w_n \exp\left(-\frac{\|x_i - x_n\|^2}{2\sigma^2}\right)$$

$$= \sum_{j=1}^{n} w_j \exp\left(-\frac{\|x_i - x_j\|^2}{2\sigma^2}\right)$$

  - Flexible bases that can model any continuous function.
  - But with 'n' data points RBFs have 'n' basis functions.

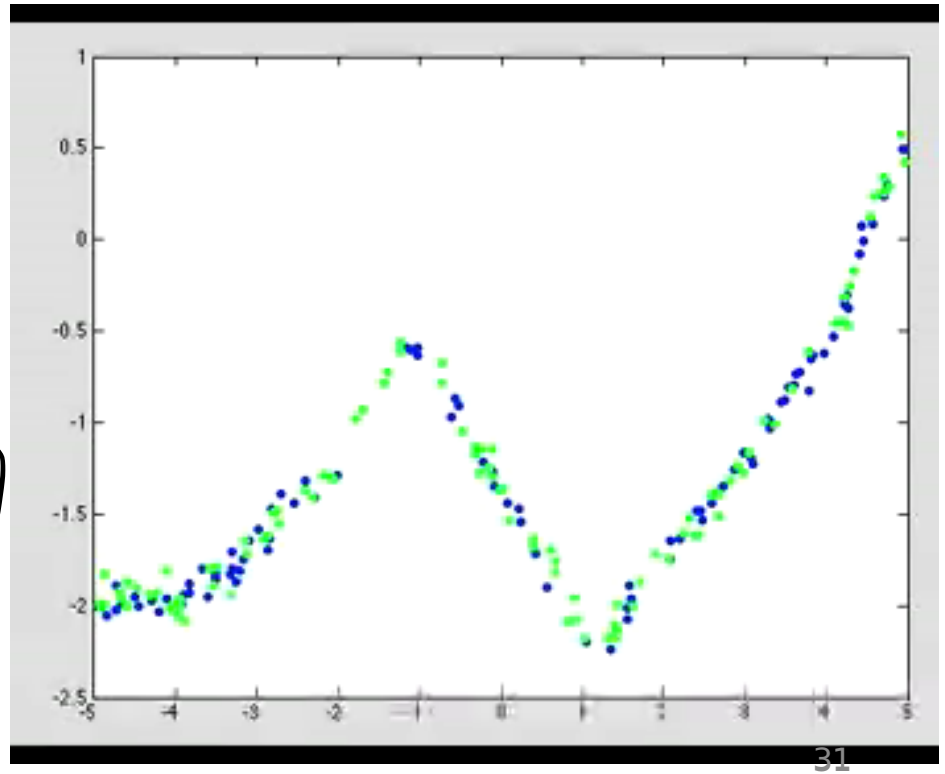
- How do we avoid overfitting with this huge number of features?
  - We regularize 'w' and use validation error to choose σ and λ.

RBFs, Regularization, and Validation

- A model that is hard to beat:
  - RBF basis with L2-regularization and cross-validation to choose σ and λ.
  - Flexible non-parametric basis, magic of regularization, and tuning for test error.

for each value of λ and σ:

- Compute Z ($n \times n$) on training data (and σ)
- Compute best v ($n \times 1$): $v = (Z^T Z + \lambda I)^{-1} Z^T y$
- Compute $\tilde{Z}$ ($t \times n$) on validation data (using train data distances)
- Make predictions $\hat{y} = \tilde{Z} v$ ($t \times 1$ = $t \times n$ $n \times 1$)
- Compute validation error $\|\hat{y} - \tilde{y}\|^2$



RBFs, Regularization, and Validation

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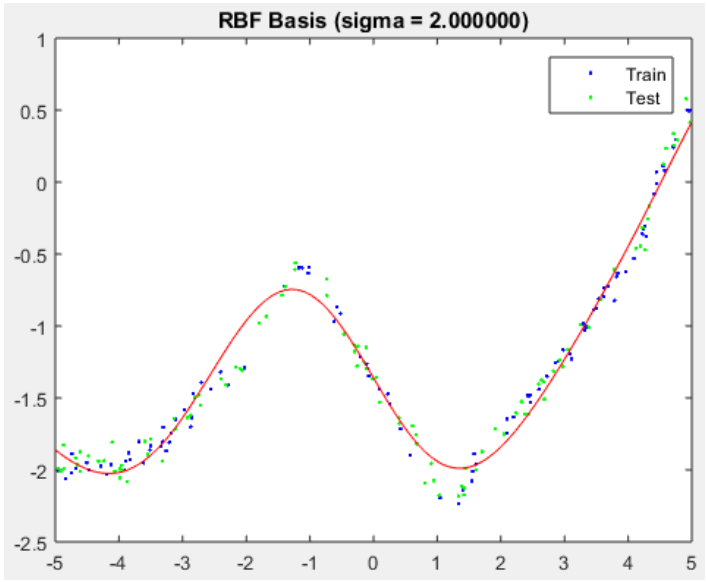
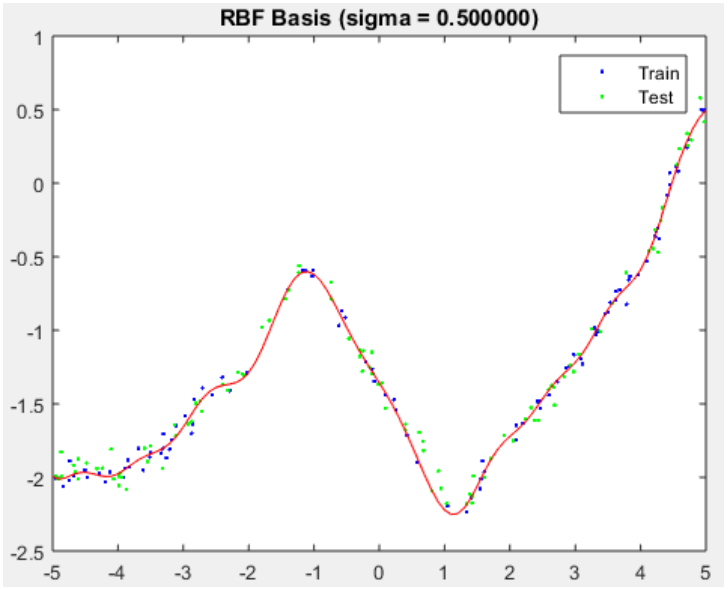
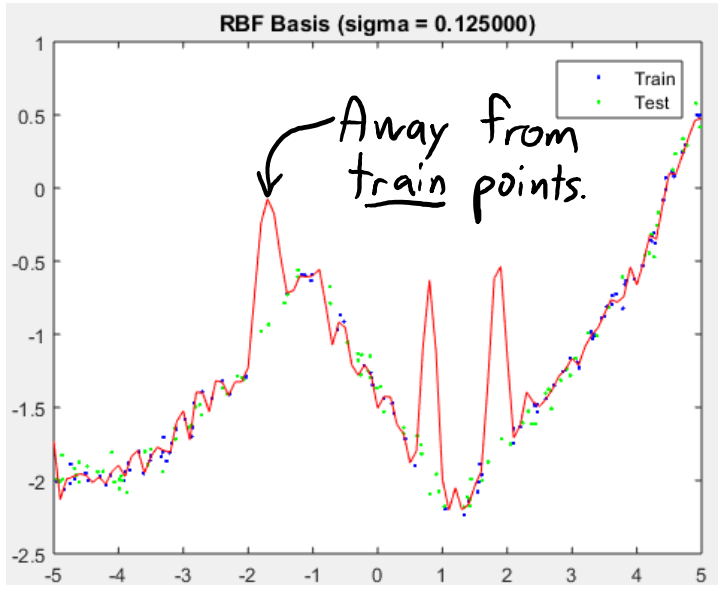
  - Flexible non-parametric basis, magic of regularization, and tuning for test error!







  - Expensive at test time: needs distance vs. all training examples.

Hyper-Parameters of Gaussian RBFs

- In this setting we have 2 hyper-parameters (σ and λ).
- More complicated models have even more hyper-parameters.
  - Searching all values is unviable (increases overfitting risk).

- Simplest approaches:
  - Exhaustive search: discretize and try all combinations
  - Random search: try random values.

Hyper-Parameter Optimization

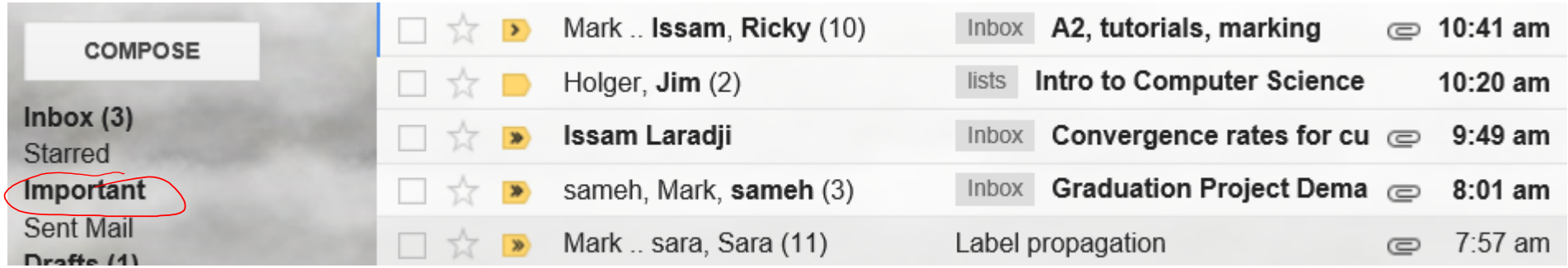
- Other common hyper-parameter optimization methods:
  - Exhaustive search with pruning:
    - If it "looks" like test error is getting worse as you decrease λ, stop decreasing it.
  - Coordinate search:
    - Optimize one hyper-parameter at a time, keeping the others fixed.
    - Repeatedly go through the hyper-parameters
  - Stochastic local search:
    - Generic global optimization methods (simulated annealing, genetic algorithms, etc.).
  - Bayesian optimization (Mike's PhD research topic):
    - Use RBF regression to build model of how hyper-parameters affect validation error.
    - Try the best guess based on the model.

Coming Up Next

LINEAR CLASSIFIERS INTRO

Motivation: Identifying Important Emails

- How can we automatically identify 'important' emails?



- A binary classification problem ("important" vs. "not important").
  - Labels are approximated by whether you took an "action" based on mail.
  - High-dimensional feature set (that we'll discuss later).

- Gmail uses regression for this binary classification problem.

Binary Classification Using Regression?

- Recall: we had classification problems in Part 1:
  - Food allergies, spam filtering, character recognition, Netflix recommendation, etc.

- Binary classification: 2 classes in label y

- Usually, we encode $y_i = \{0, 1\}$
- For linear classifiers, we encode $y_i = \{-1, +1\}$
  - e.g. +1 means "important", -1 means otherwise.

Visualizing Binary Classification

- Assumption: somewhere along the feature space, there's a boundary that (roughly) splits +1s and -1s.

- If a perfect boundary exists, the data is called "linearly separable"

Visualizing Binary Classification

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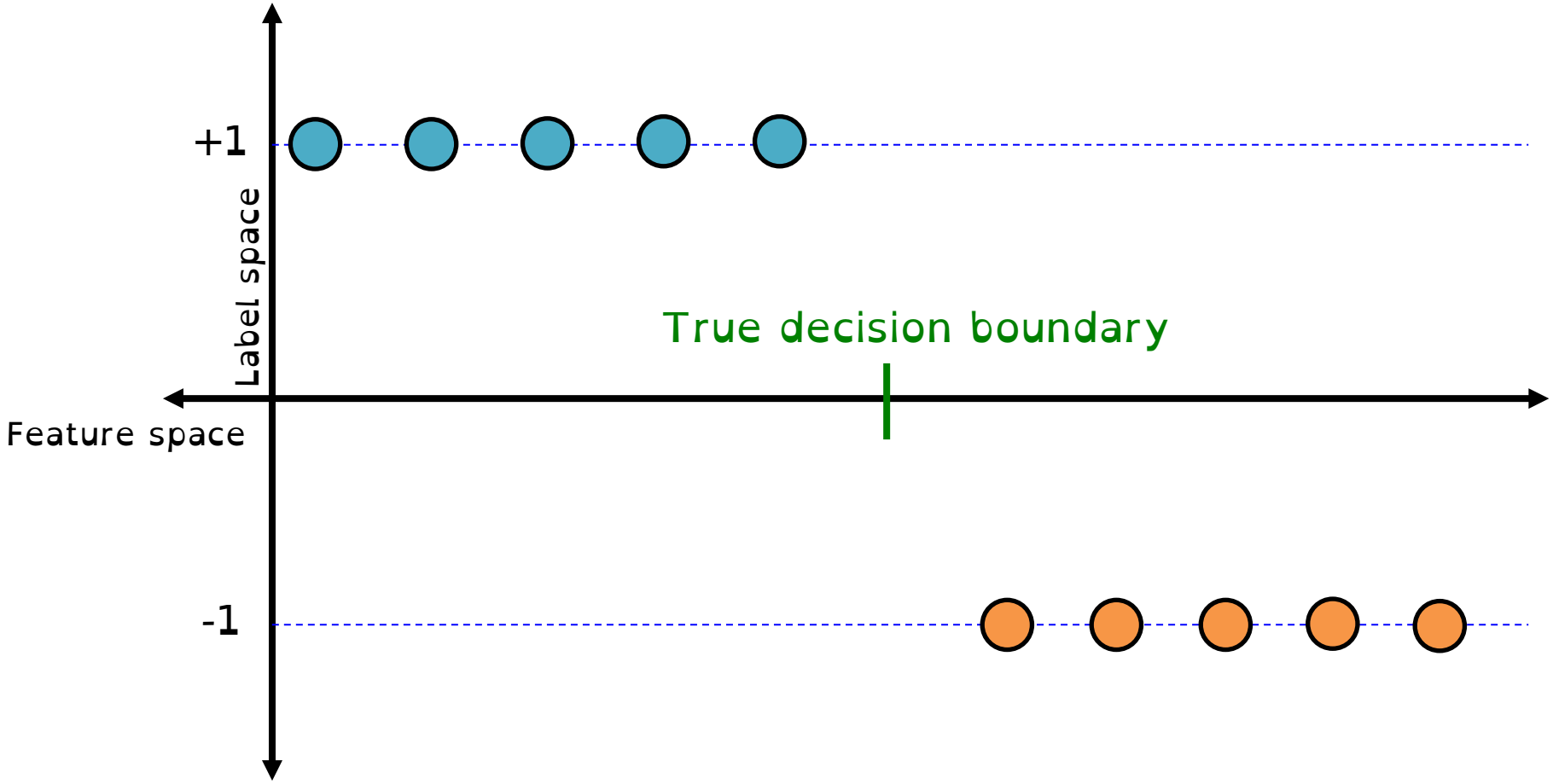

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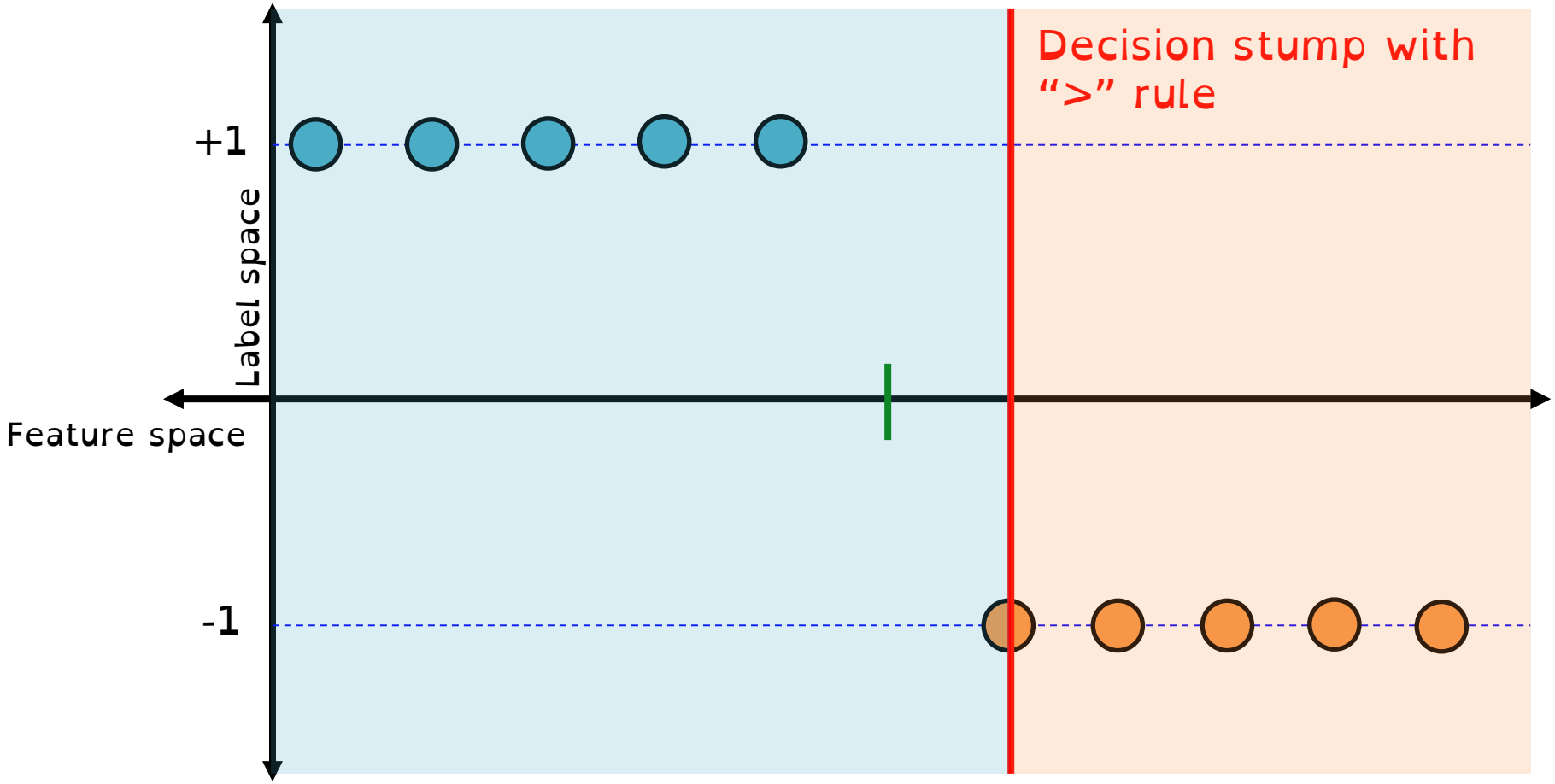

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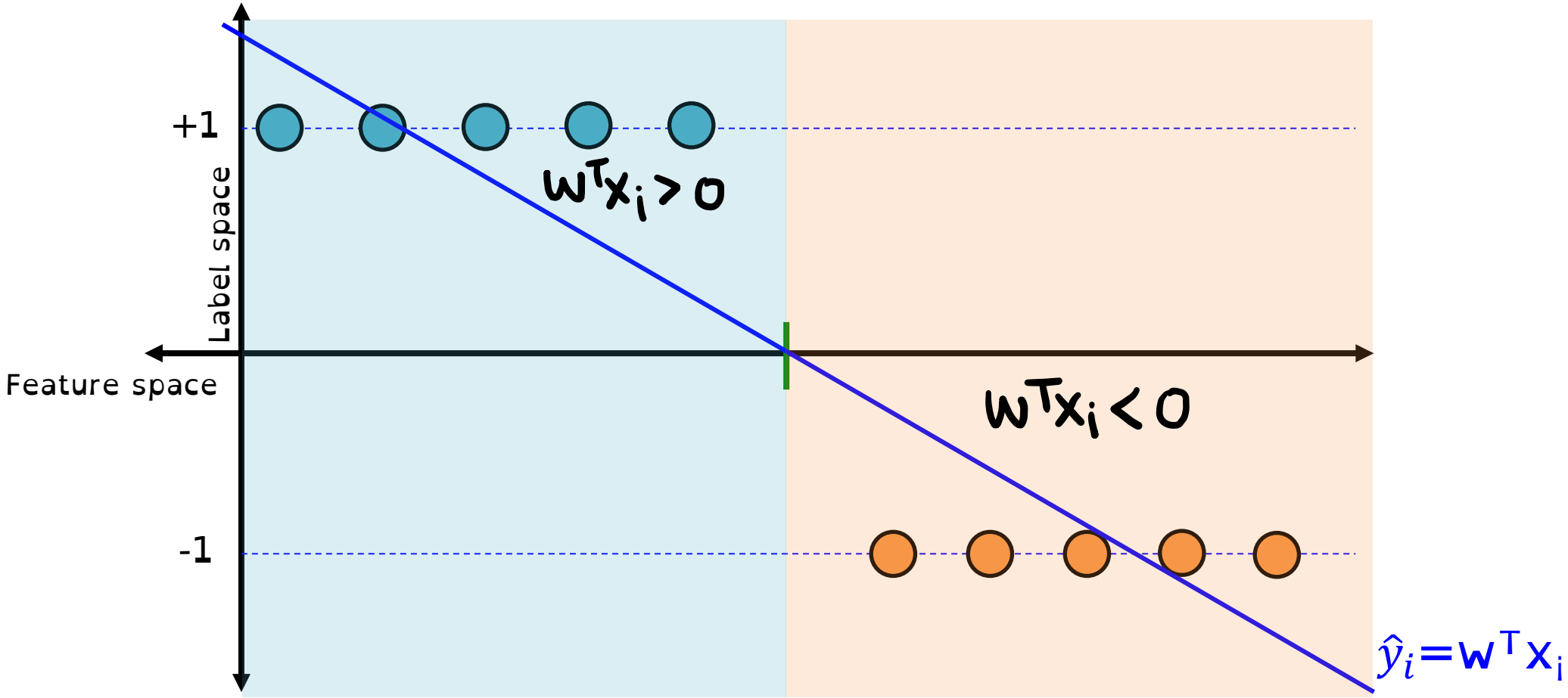
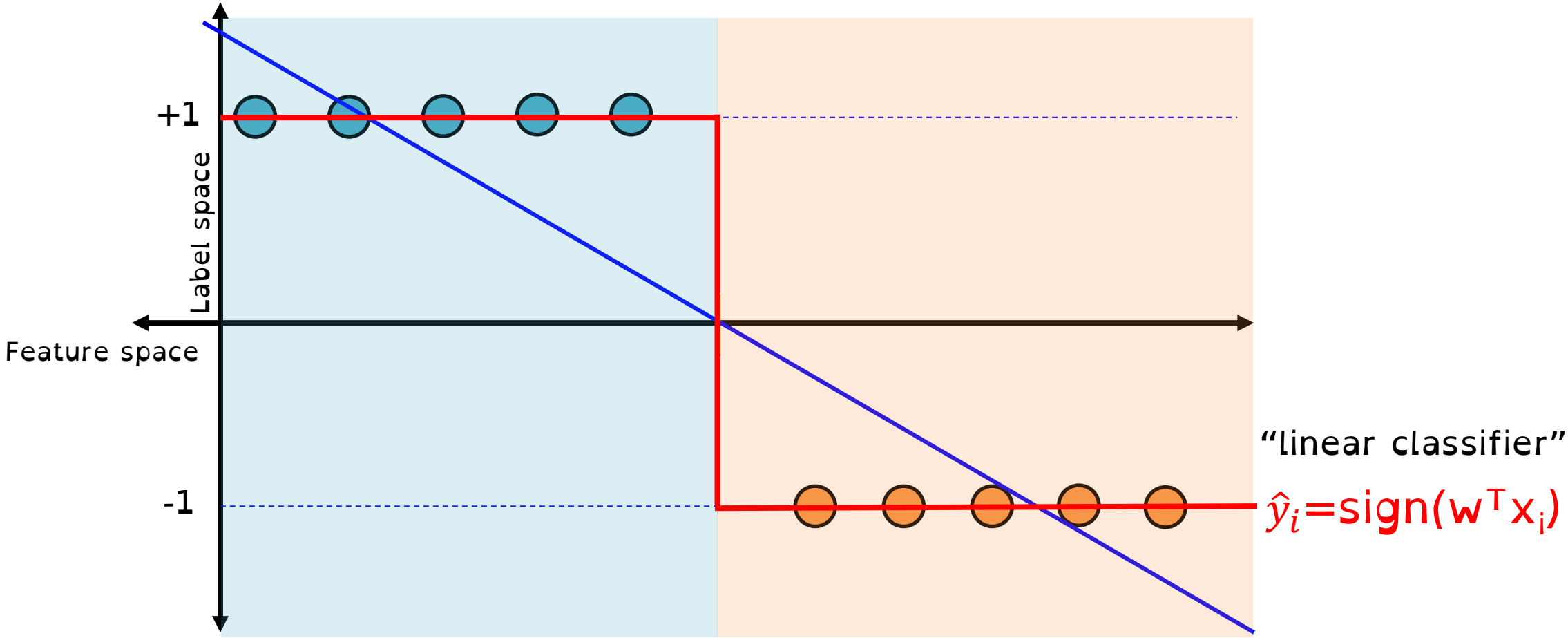


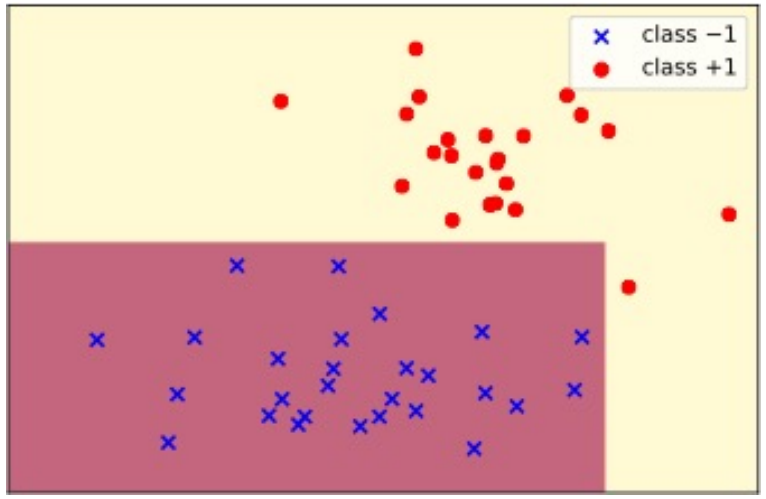
Visualizing Binary Classification

- Assumption: somewhere along the feature space, there's a boundary that (roughly) splits +1s and -1s.



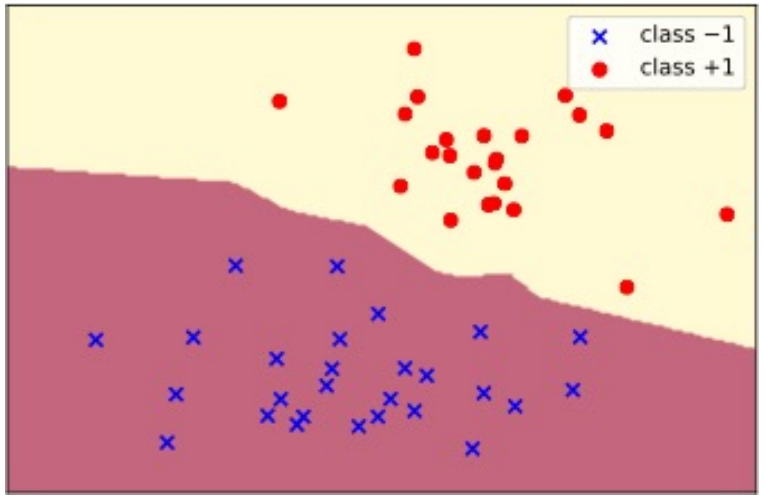
Decision Boundaries in 2D

decision tree



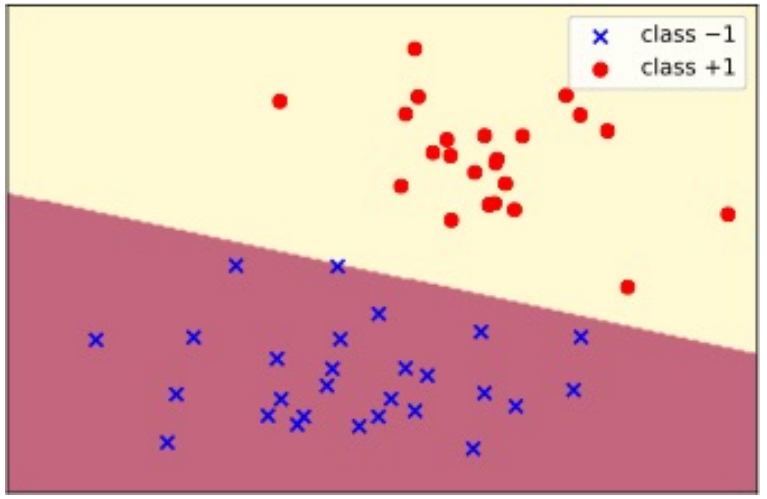
Feature space

KNN



Feature space

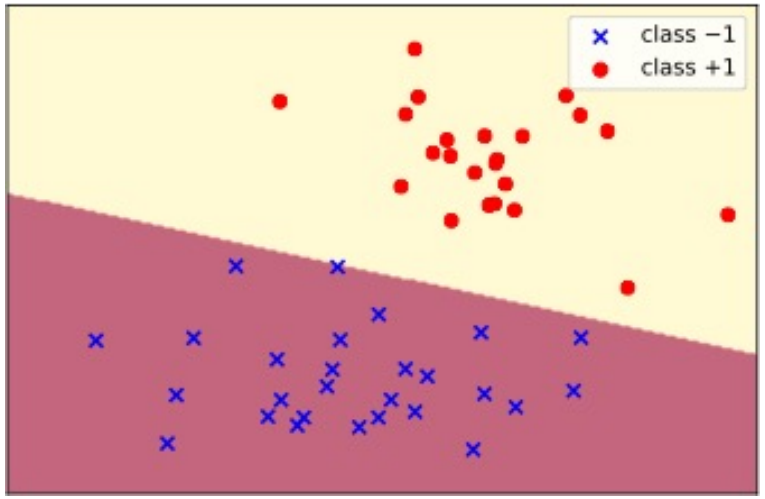
linear classifier



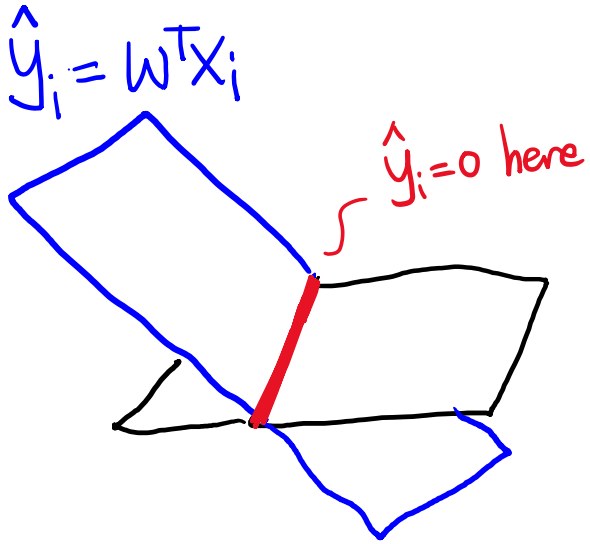
Feature space

Decision Boundaries in 2D

linear classifier



Feature space

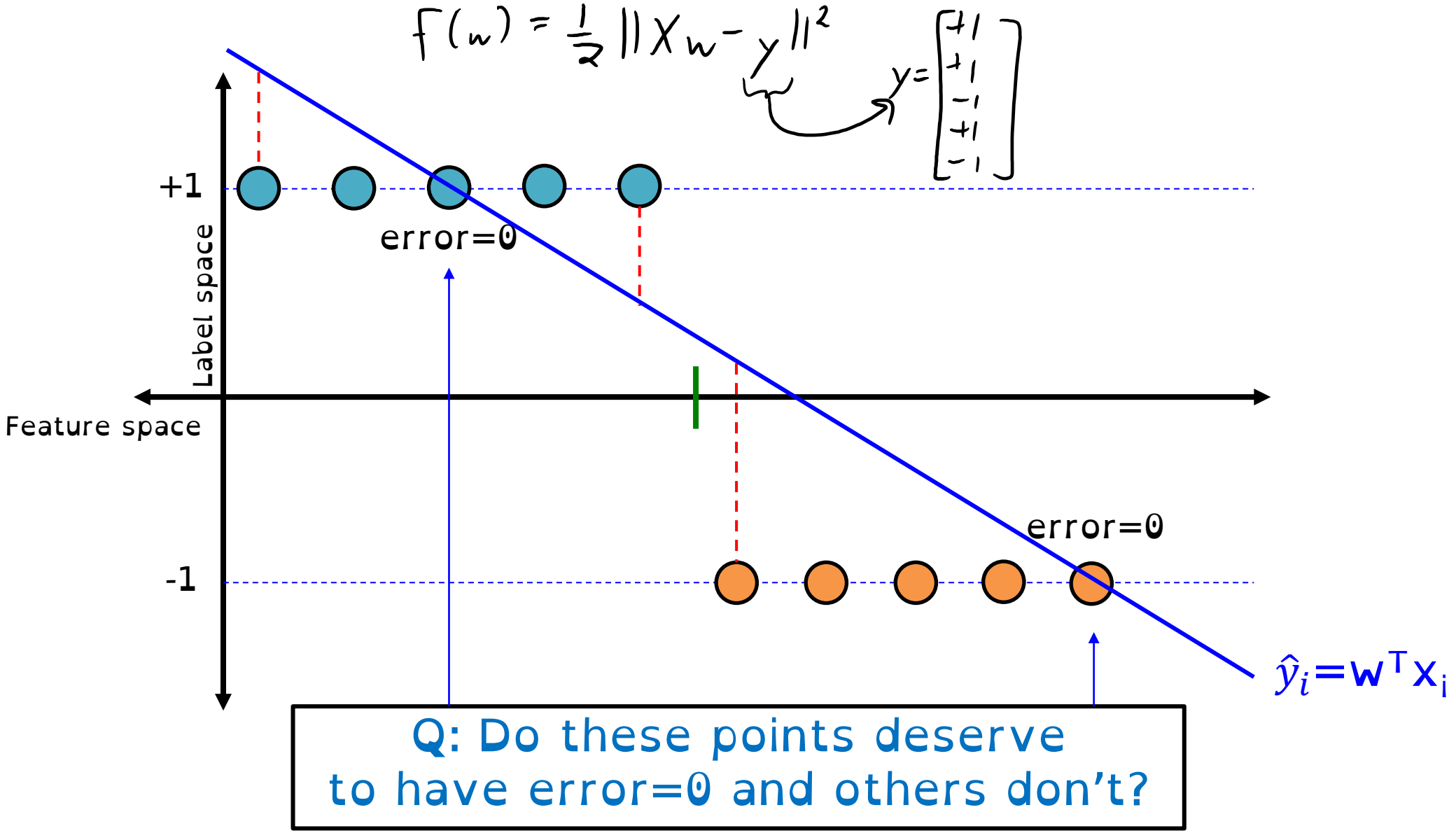


- Linear classifier would be a $\hat{y}_i = w^T x_i$ function coming out of screen:
  - The boundary is at $\hat{y}_i = 0$.

Coming Up Next

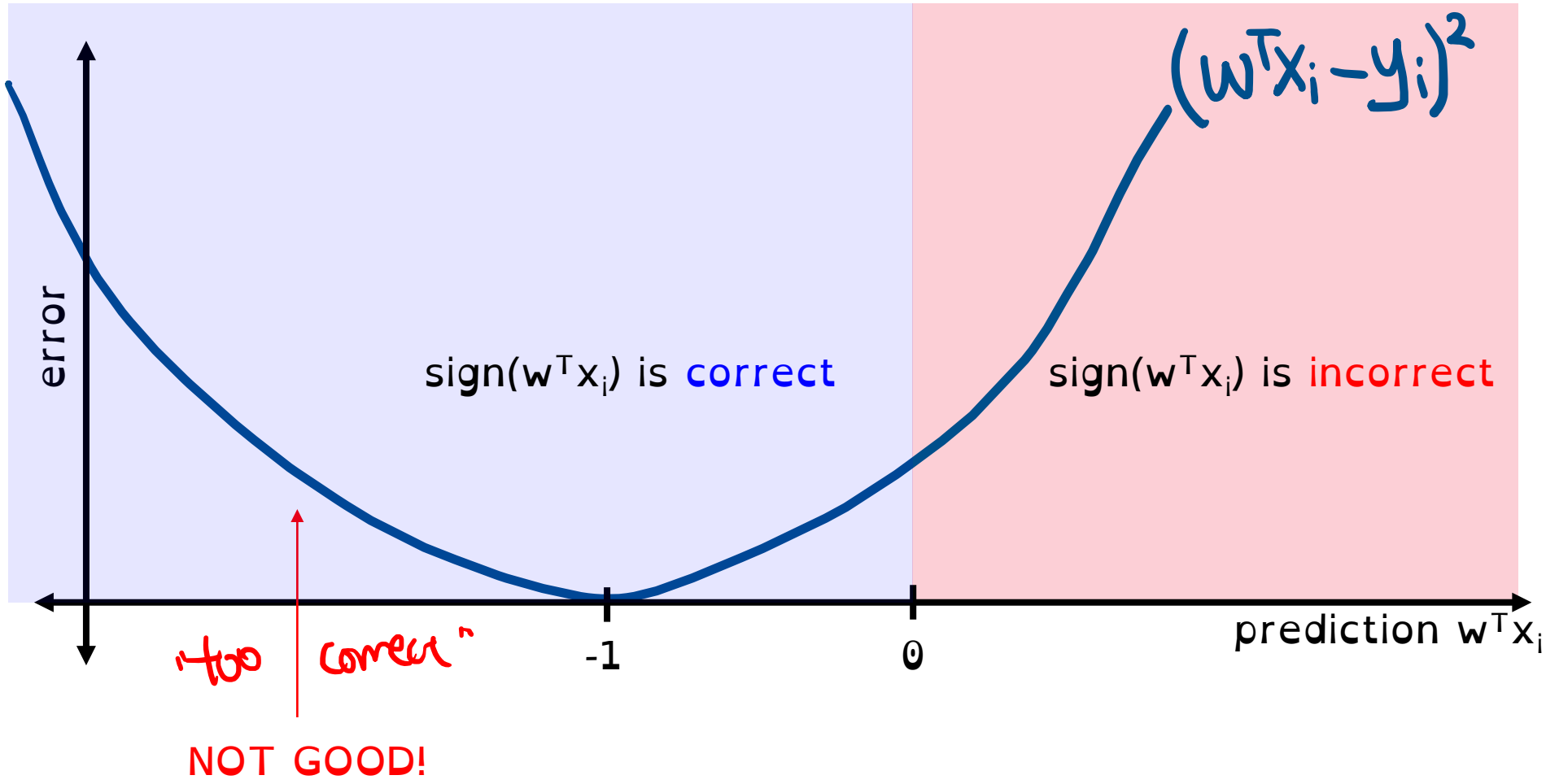
LOSSES FOR BINARY CLASSIFIERS

Should we use least squares for classification?



Should we use least squares for classification?

Given example $(x_i, -1)$



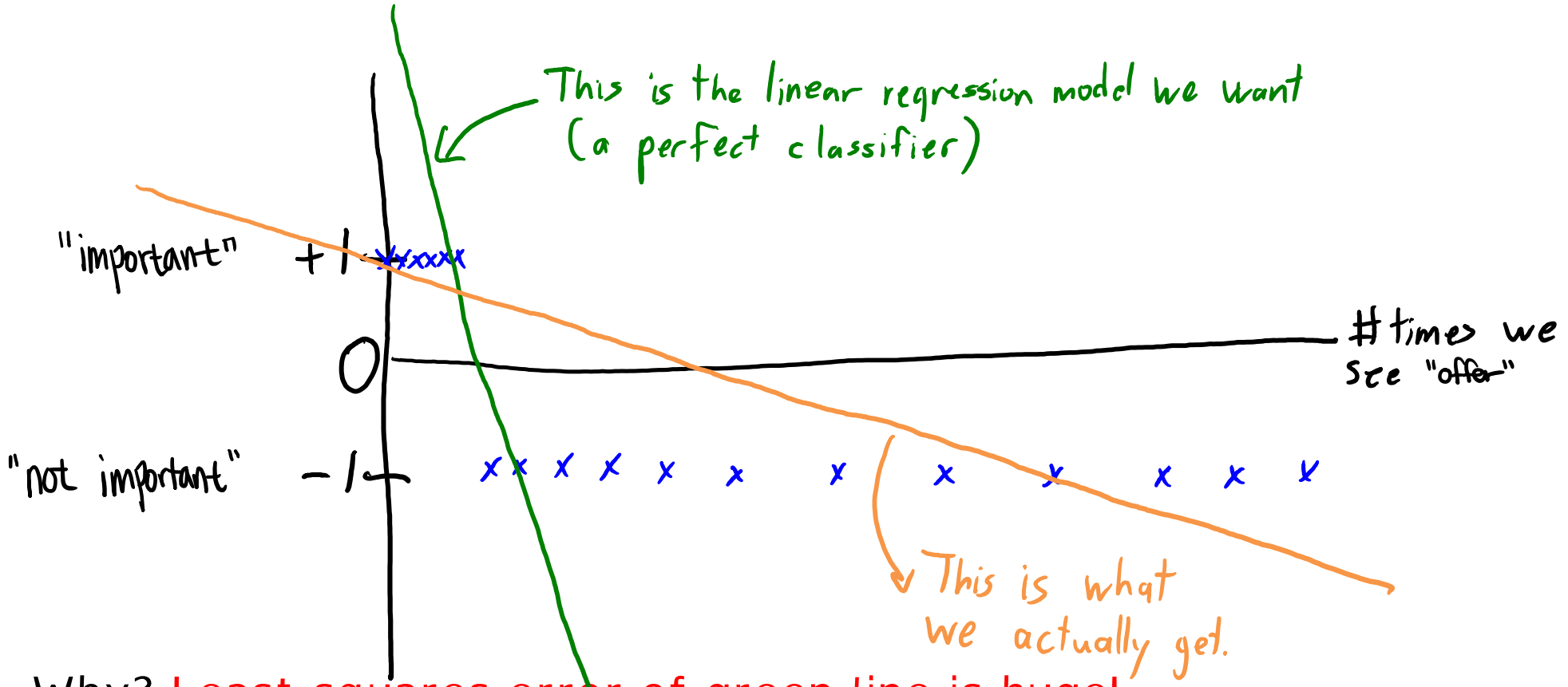
Issues with Least Squares Error

When least squares penalizes my example far from 0

- x_i far from 0 means $w^T x_i$ will be far from 0.
- sign($w^T x_i$) is correct but $(w^T x_i - y_i)^2$ is huge
  - Penalizes for examples that are "too correct"
- Also, which examples get 0 error is arbitrary

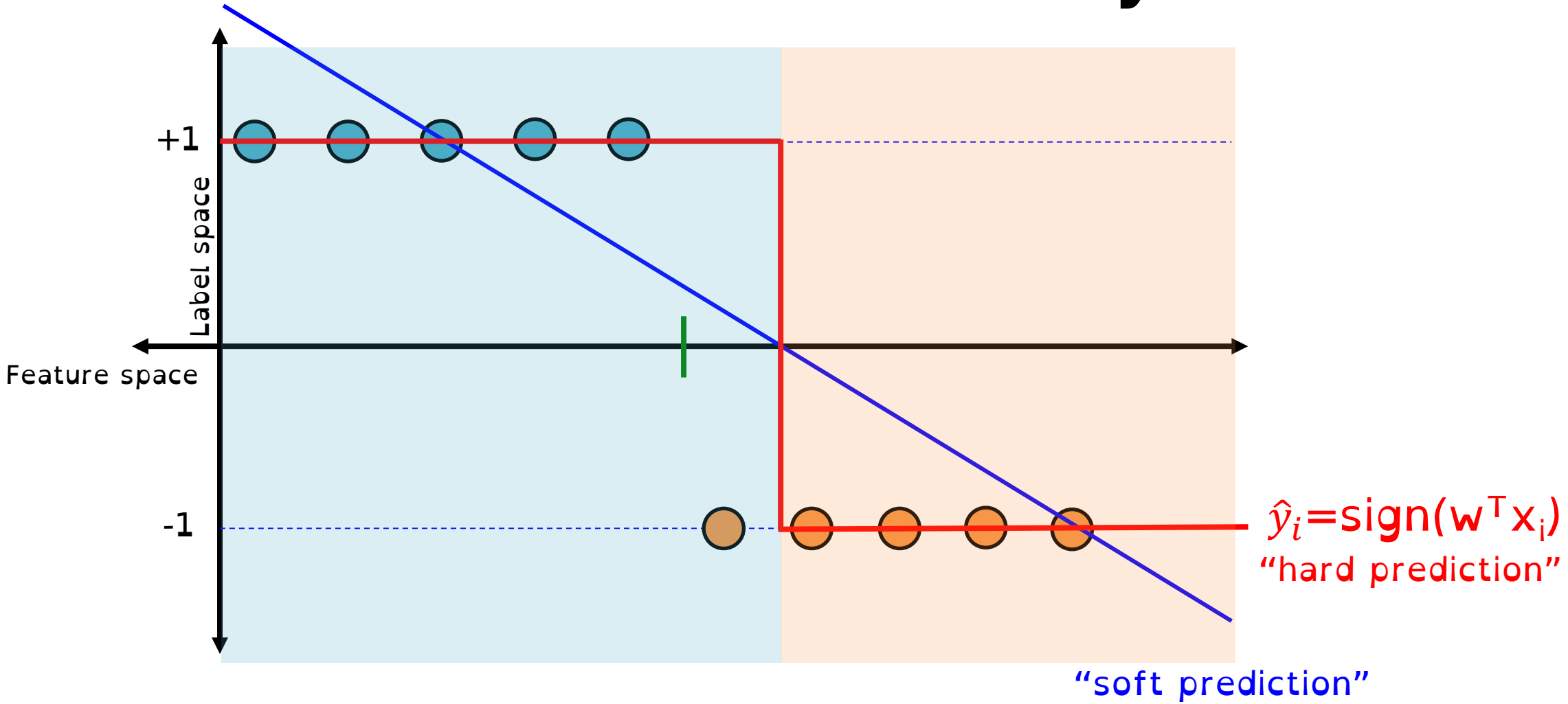
Should we use least squares for classification?

- Least squares can behave weirdly when applied to classification:



- Why? Least squares error of green line is huge!
  - The green line achieves 0 training classification error.

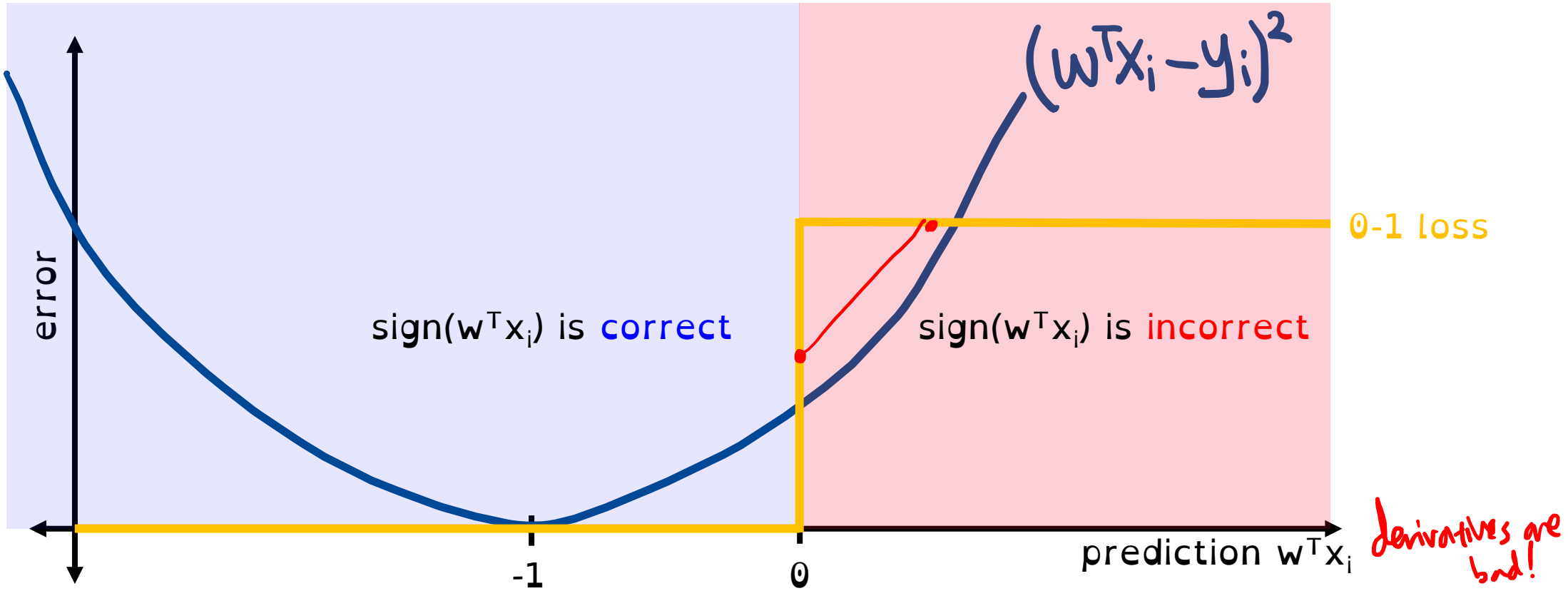
0-1 Loss: What We Really Want



- We want to minimize classification error based on "hard predictions"!

0-1 Loss: What We Really Want

Given example (x_i, -1)



Q: What's wrong with the 0-1 loss?

non-convex.
non-diff.

0-1 Loss Function

- We can write using the L0-norm as $\|\hat{y} - y\|_0$.
  - In classification it's reasonable that $\hat{y}_i = y_i$ (it's either +1 or -1).

- 0-1 loss is non-convex in 'w'.
  - It's easy to minimize if a perfect classifier exists ("perceptron").
  - Otherwise, finding the 'w' minimizing 0-1 loss is a hard problem.

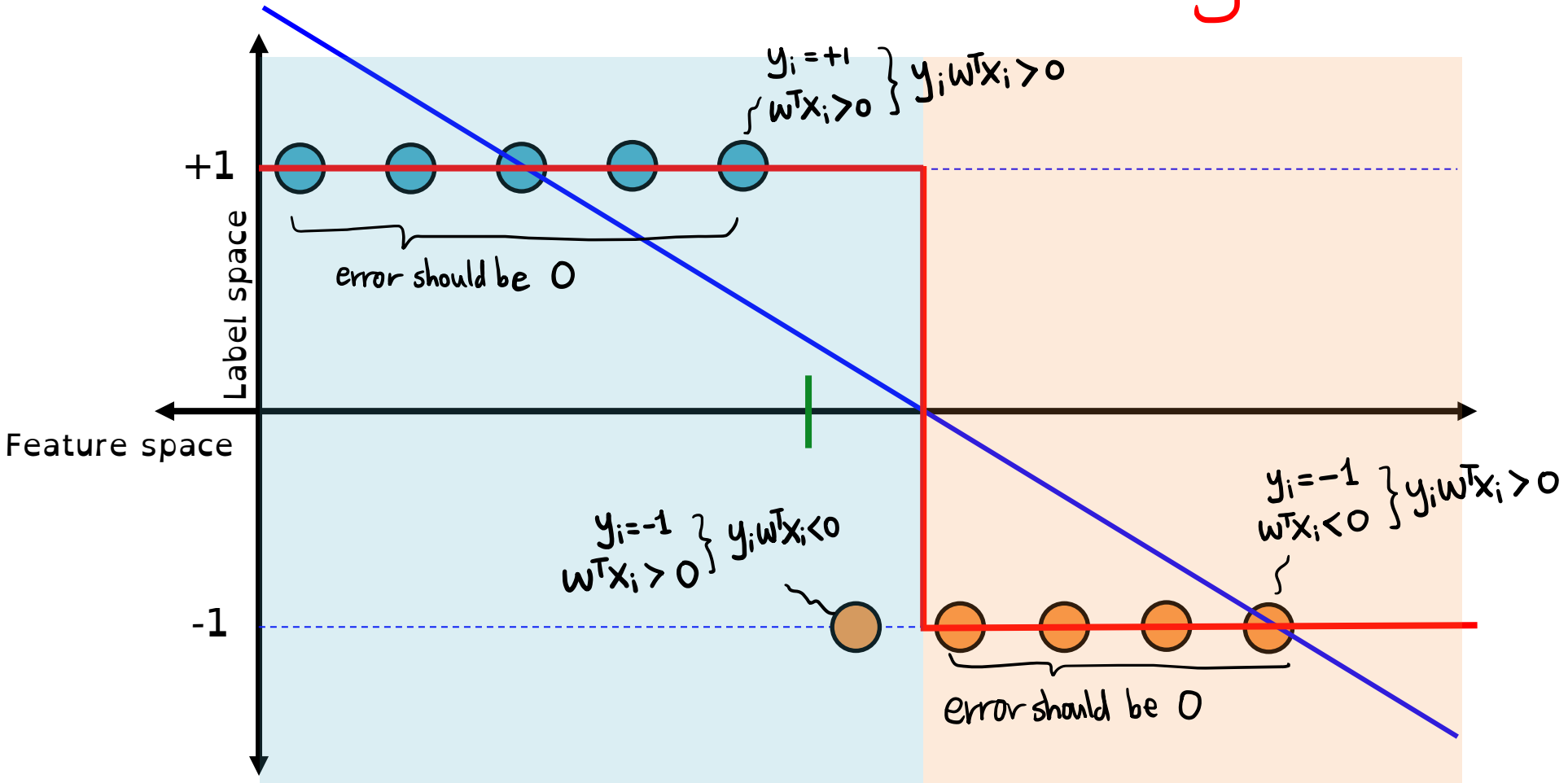
  - Gradient is zero everywhere: don't even know "which way to go".

  - NOT the same type of problem we had with using the squared loss.
    - We can minimize the squared error,
      but it might give a bad model for classification.

- Motivates convex approximations to 0-1 loss...

Degenerate Convex Approximation to 0-1 Loss

- If $y_i = +1$, we get the label right if $w^T x_i > 0$.
- If $y_i = -1$, we get the label right if $w^T x_i < 0$, or equivalently $-w^T x_i > 0$.
- So "classifying 'i' correctly" is equivalent to having $y_i \cdot w^T x_i > 0$.



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- If $y_i = -1$, we get the label right if $w^T x_i < 0$, or equivalently $-w^T x_i > 0$.
- So "classifying 'i' correctly" is equivalent to having $y_i w^T x_i > 0$.

- One possible convex approximation to 0-1 loss:
  - Minimize how much this constraint is violated.

Let's count # times $y_i w^T x_i < 0$

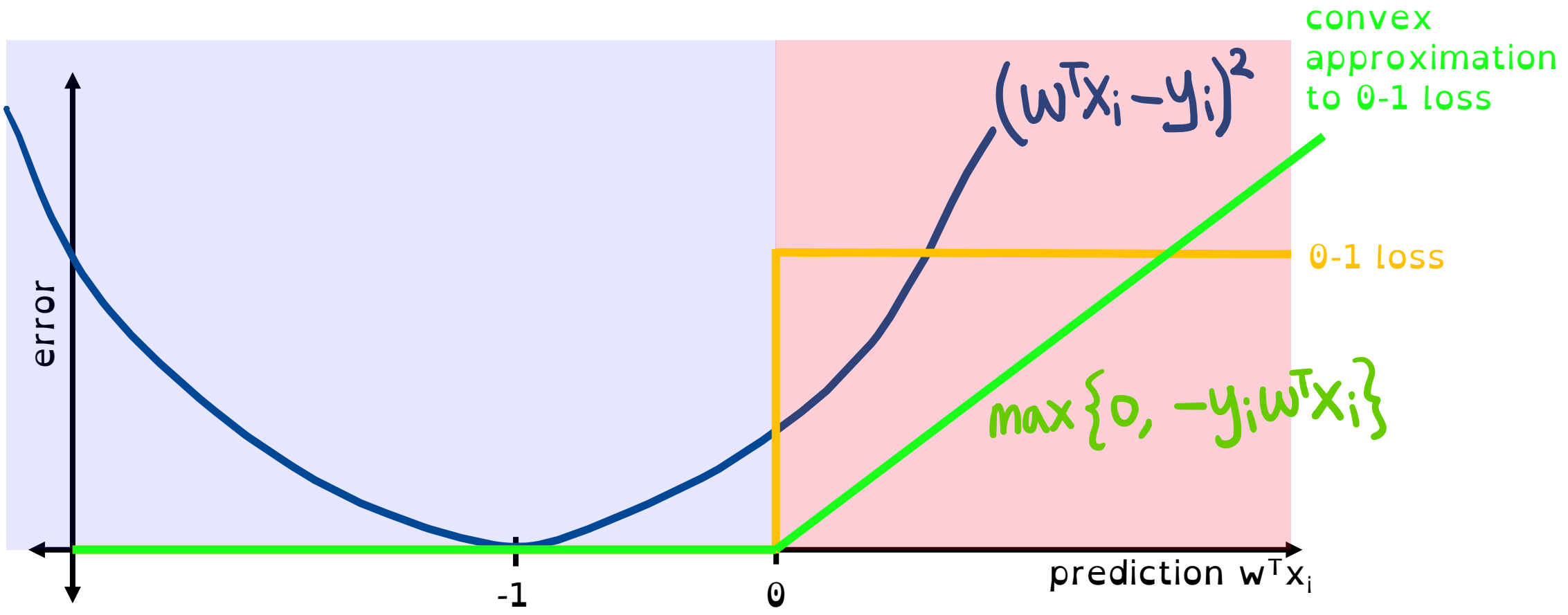
"indicator" $I(\text{stmt}) = \begin{cases} 1 \text{ if stmt is true} \\ 0 \text{ otherwise} \end{cases}$

[1] $f(w) = \sum_{i=1}^{n} I(y_i w^T x_i < 0) = \sum_{i=1}^{n} I(0 < -y_i w^T x_i)$ (0-1 loss)

[2] $\approx \sum_{i=1}^{n} \max\{0, -y_i w^T x_i\}$ (Convex approximation)

0-1 Loss: What We Really Want

Given example (x_i, -1)



Degenerate Convex Approximation to 0-1 Loss

- Our convex approximation of the error for one example is:

$$\max\{0, -y_i w^T x_i\}$$

- We could train by minimizing sum over all examples:

$$f(w) = \sum_{i=1}^{n} \max\{0, -y_i w^T x_i\}$$

- But this has a degenerate solution:

Q: When is f(w) = 0?

- There are two standard fixes: hinge loss and logistic loss.

Summary

- Feature standardization:
  - Change the unit of every feature into "z-score"
- Radial basis functions:
  - Non-parametric bases that can model any function.
- Binary classification using regression:
  - Encode using y_i in {-1,1}.
  - Use $\text{sign}(w^T x_i)$ as prediction.
  - "Linear classifier" (a hyperplane splitting the space in half).
- Least squares is a weird error for classification.
- 0-1 loss is the ideal loss, but is non-smooth and non-convex.

- Next time: logistic regression and support vector machine

Review Questions

- Q1: In what ways can standardizing the features help reduce a linear model's complexity?
- Q2: What parameters are we "learning" for standardization?
- Q3: How does the shape of the local bumps change with their coefficients in the learned linear model with Gaussian RBF basis?
- Q4: How does σ affect the prediction of the linear model with Gaussian RBF basis when the test example $\tilde{x}_i$ is far from 0?
- Q5: Why is discretization of λ and σ important for hyper-parameter optimization for the linear model with Gaussian RBF basis?

Gaussian RBFs: Pseudo-Code

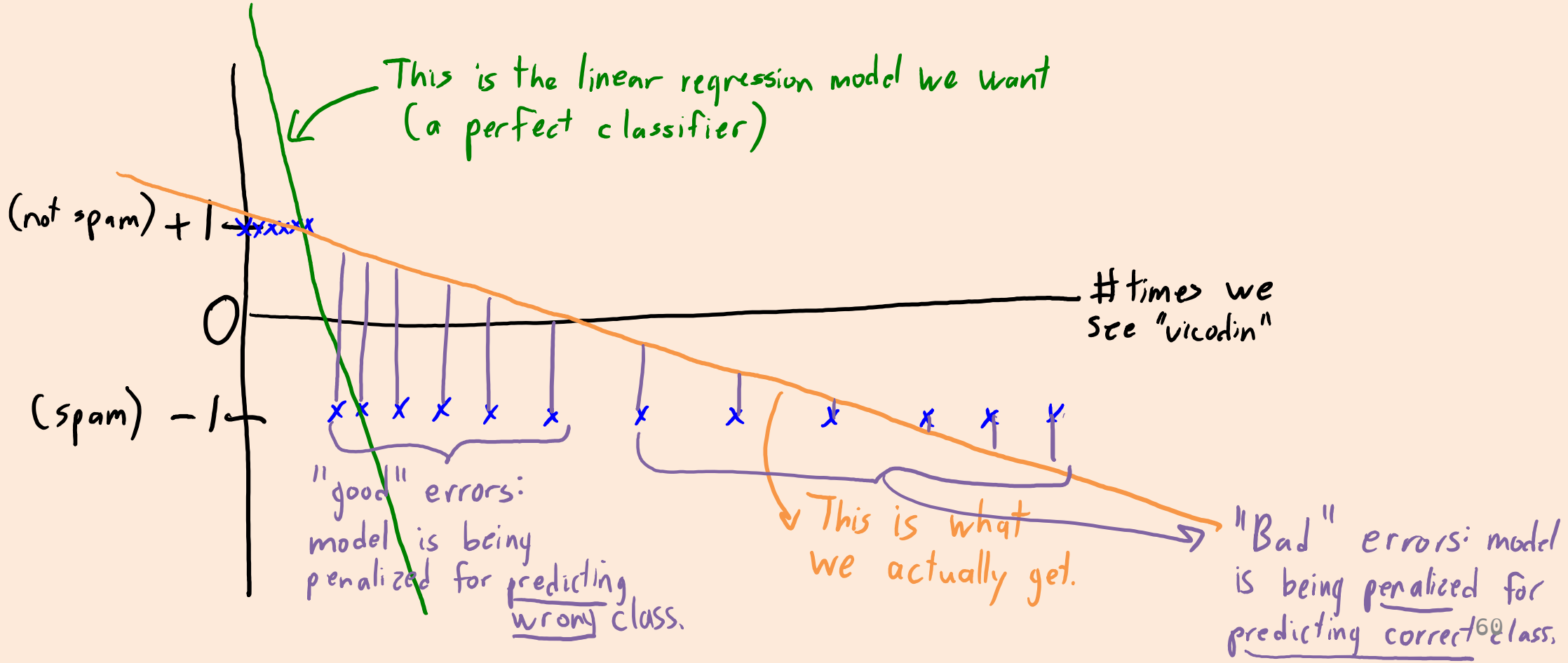
Constructing Gaussian RBFs given data 'X' and hyper-parameter σ:

```
Z = zeros(n, n)
for i1 in 1:n
    for i2 in 1:n
        Z[i1, i2] = exp(-norm(X[i1, :] - X[i2, :])^2 / 2σ^2)
```

With test data $\tilde{X}$: form $\tilde{Z}$ based on distances to training examples.

Can we just use least squares??

- What went wrong?
  - "Good" errors vs. "bad" errors.



Can we just use least squares??

- What went wrong?
  - "Good" errors vs. "bad" errors.

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

What happens if $y_i = -1$ and $w^T x_i = -1000$?