Mitigating Overfitting

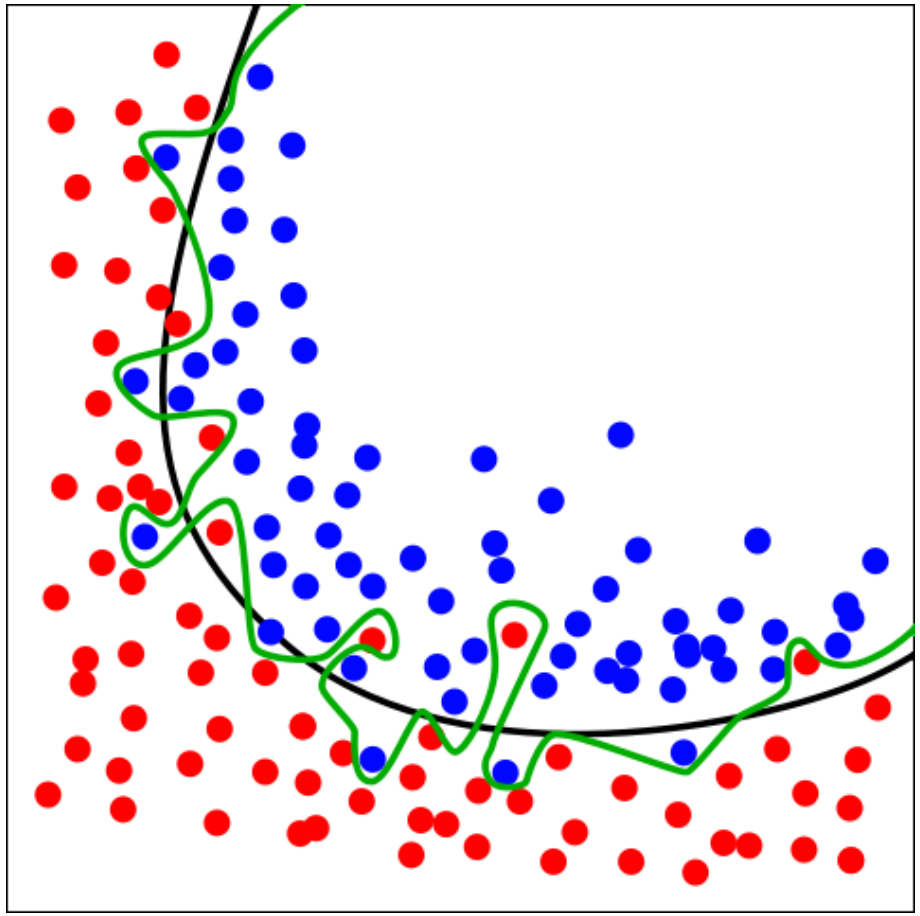
Matthew Engelhard

Recall the NDP

- Complex models are capable of dramatically overfitting the data
- We can think of this as “memorizing” the data
- It is therefore **critical** to evaluate on a held-out test set

  (supposing what you care about is out-of-sample performance)

Which boundary performs better on unseen data?



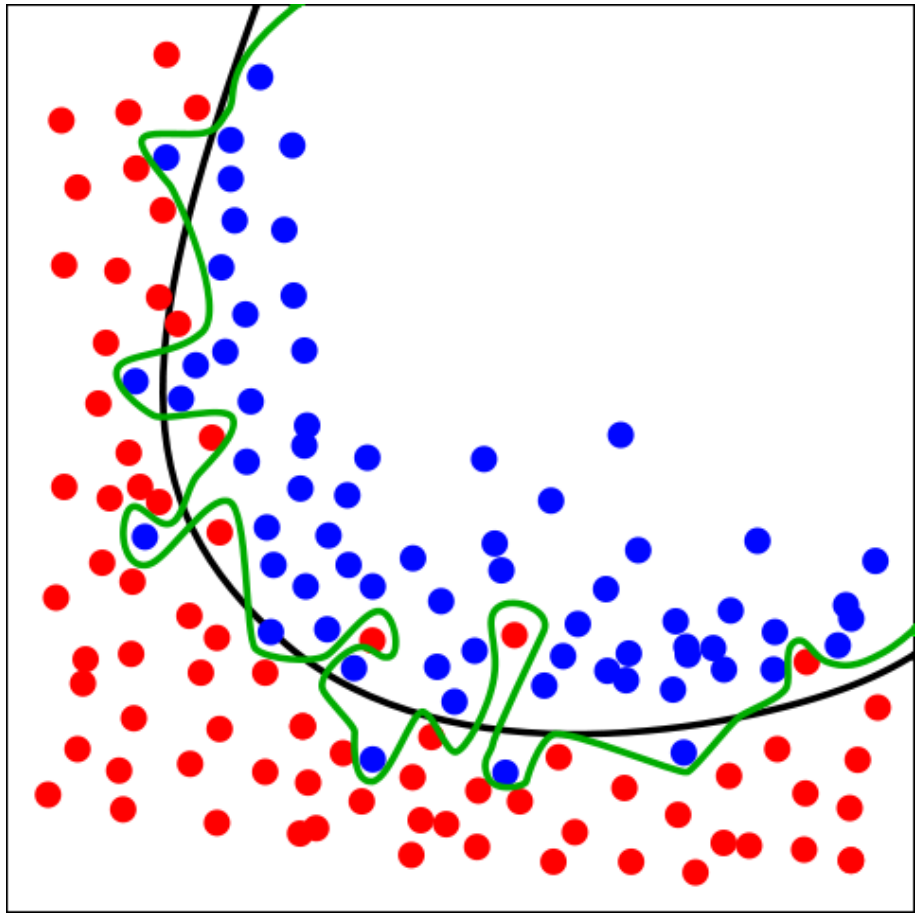
Green boundary:

- Correct predictions for *all* training data
- Very likely to be overfitting

Black boundary:

- Balance between fit and model complexity

Quantifying Overfitting



Which boundary performs better when applied to new data? And by how much?

- We can quantify overfitting as the difference in performance (usually the cross-entropy loss) between the training and validation sets
- Greater overfitting usually (but not always) means worse out-of-sample performance
- So, we almost always take steps to mitigate it

Let’s teach our robot to identify beaches.

We show it a bunch of images and ask:

What do you see?

It starts listing features from most to least obvious.

Let’s teach our robot to identify beaches.

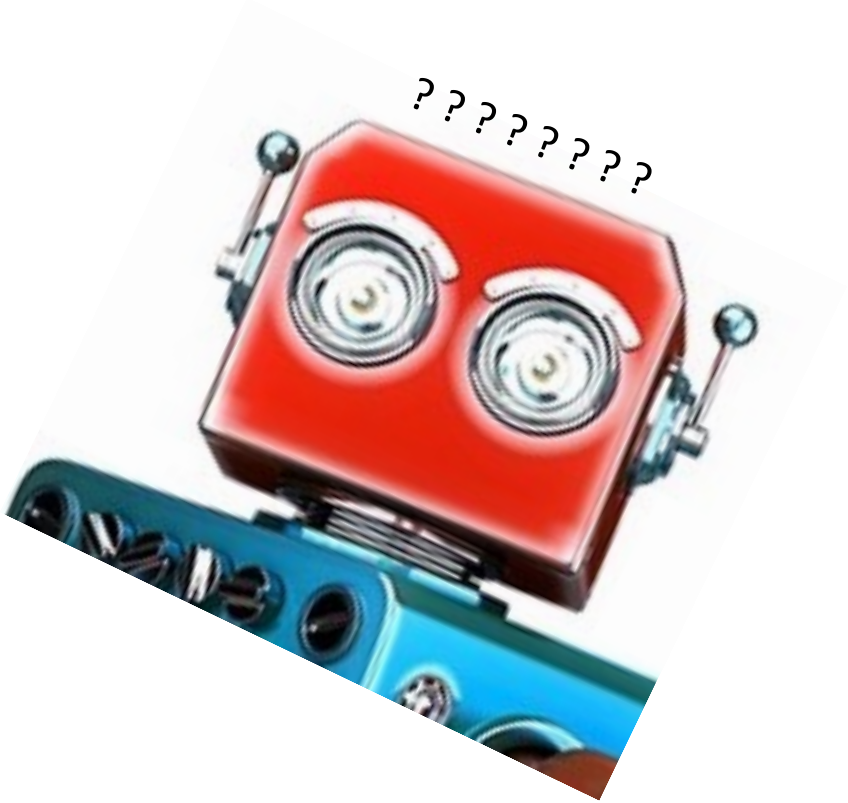
I think beaches have:

- water
- land
- sky

- sand
- palm trees
- clouds
- ripples
- foam

- white sand
- clear water
- deep blue sky
- exactly 0 or 1 seashells
- Instagram color palette

It just doesn’t know when to stop.



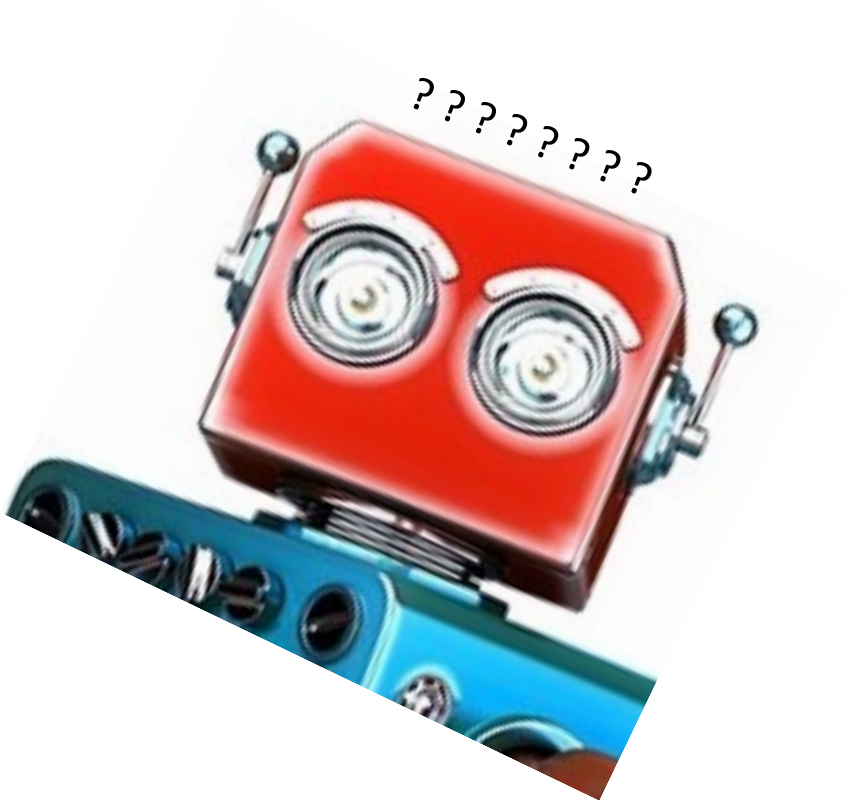
I think beaches have:

- water
- land
- sky

- sand
- palm trees
- clouds
- ripples
- foam

- white sand
- clear water
- deep blue sky
- exactly 0 or 1 seashells
- Instagram color palette

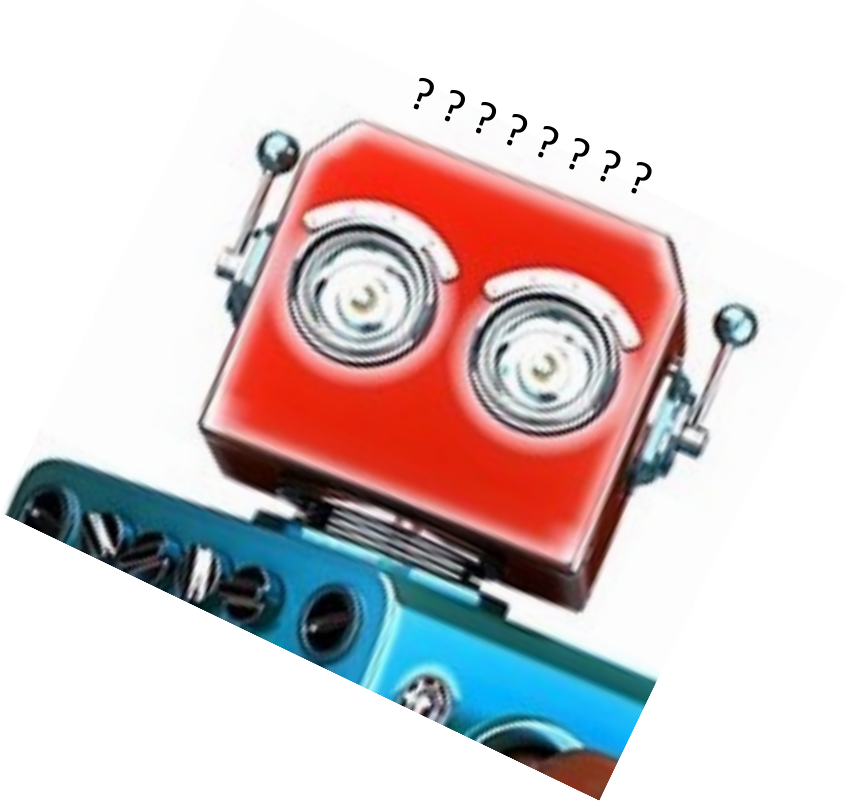
We need to give it a strategy to decide how far to go.



I think beaches have:

Sure.	• water • land • sky
Maybe?	• sand • palm trees • clouds • ripples • foam
Uh… no.	• white sand • clear water • deep blue sky • exactly 0 or 1 seashells • Instagram color palette

Strategy 1: Use as few features as you can.



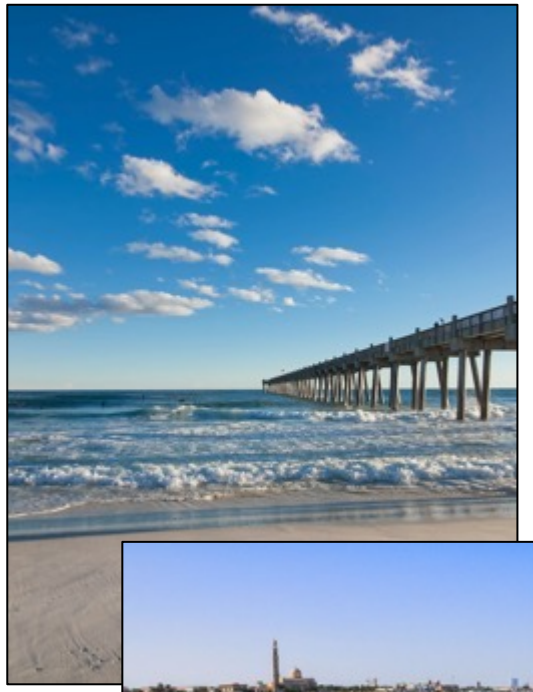
I think beaches have:

Sure.	• water • land • sky
Maybe?	• sand • palm trees • clouds • ripples • foam
Uh… no.	• white sand • clear water • deep blue sky • exactly 0 or 1 seashells • Instagram color palette

Penalize: loss, but also total parameter magnitude

Strategy 2: Keep checking other data

Training set

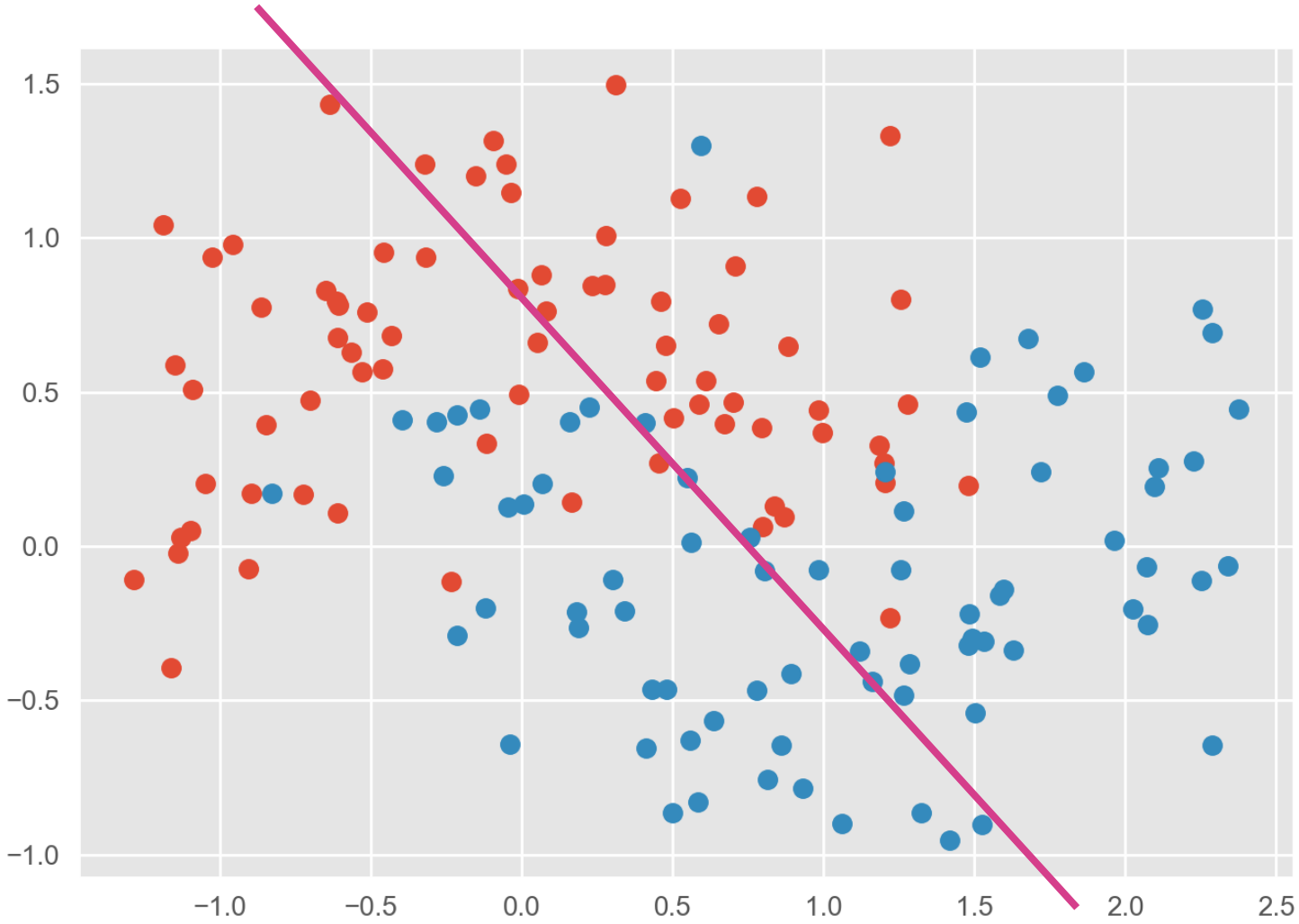


Validation set

Let’s teach a neural network to identify cancer

Initial decision boundary

(epoch 0)

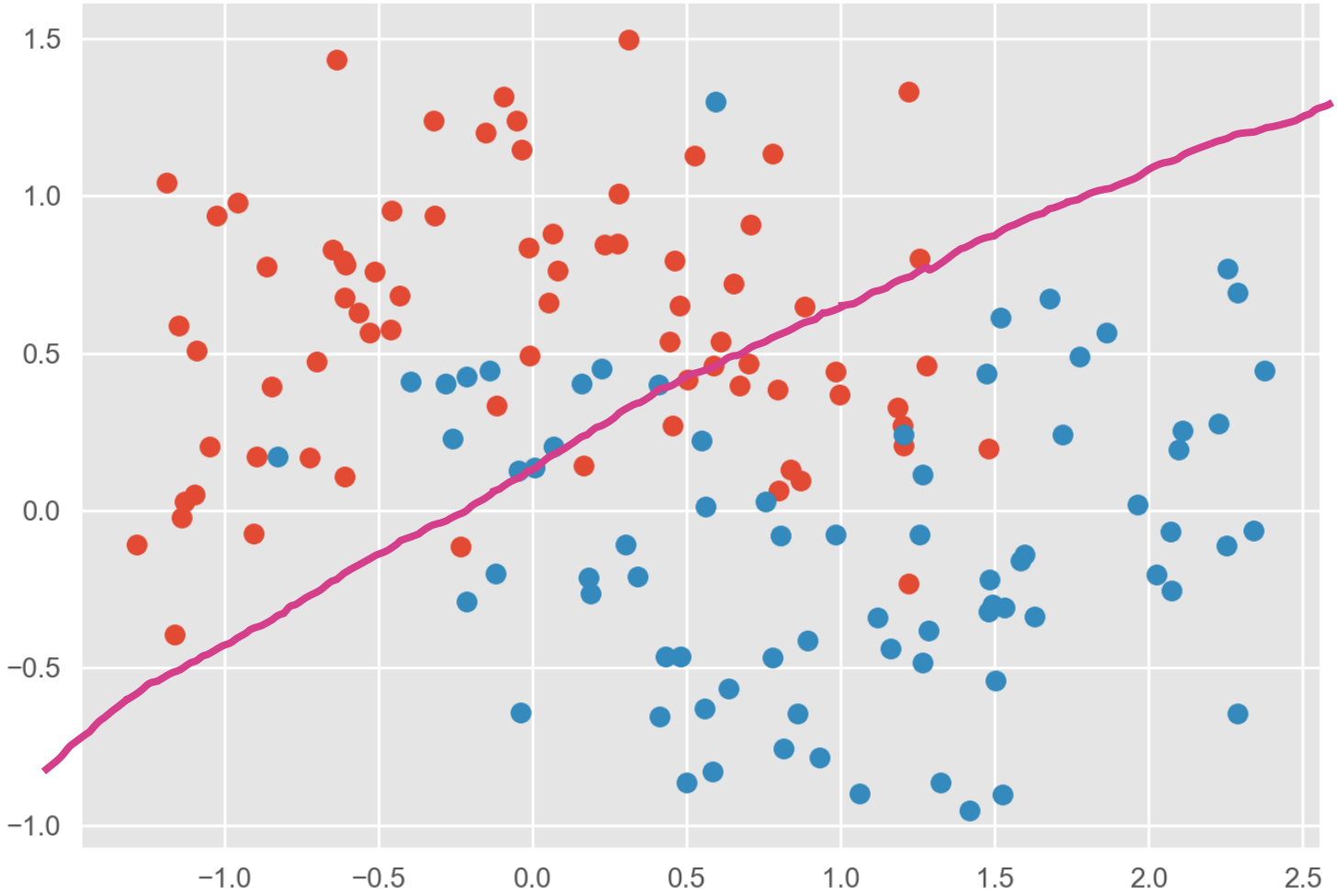


Let’s teach a neural network to identify cancer

Updated decision boundary

(epoch 1)

Sure.

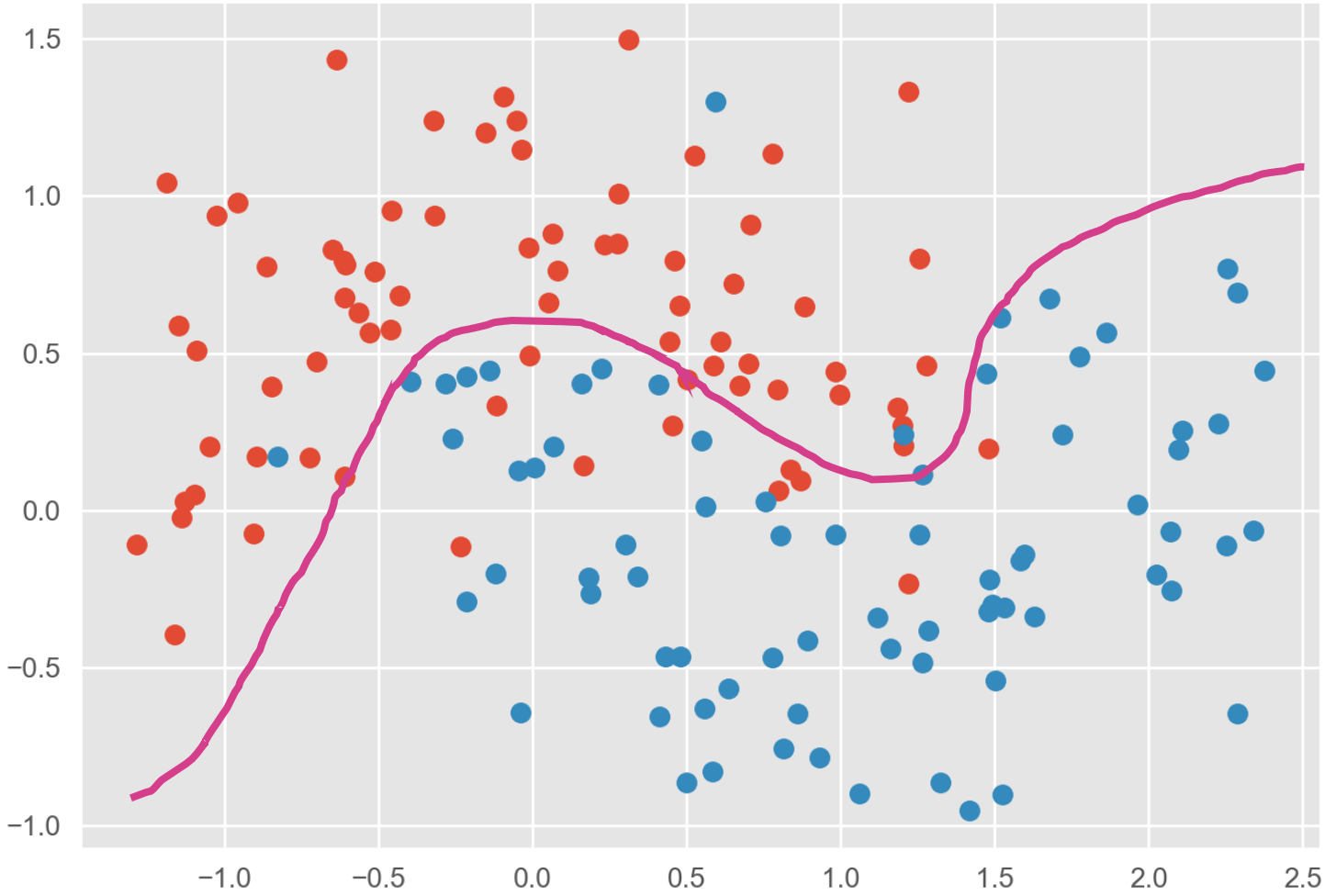


Let’s teach a neural network to identify cancer

Updated decision boundary

(epoch 4)

Wow!



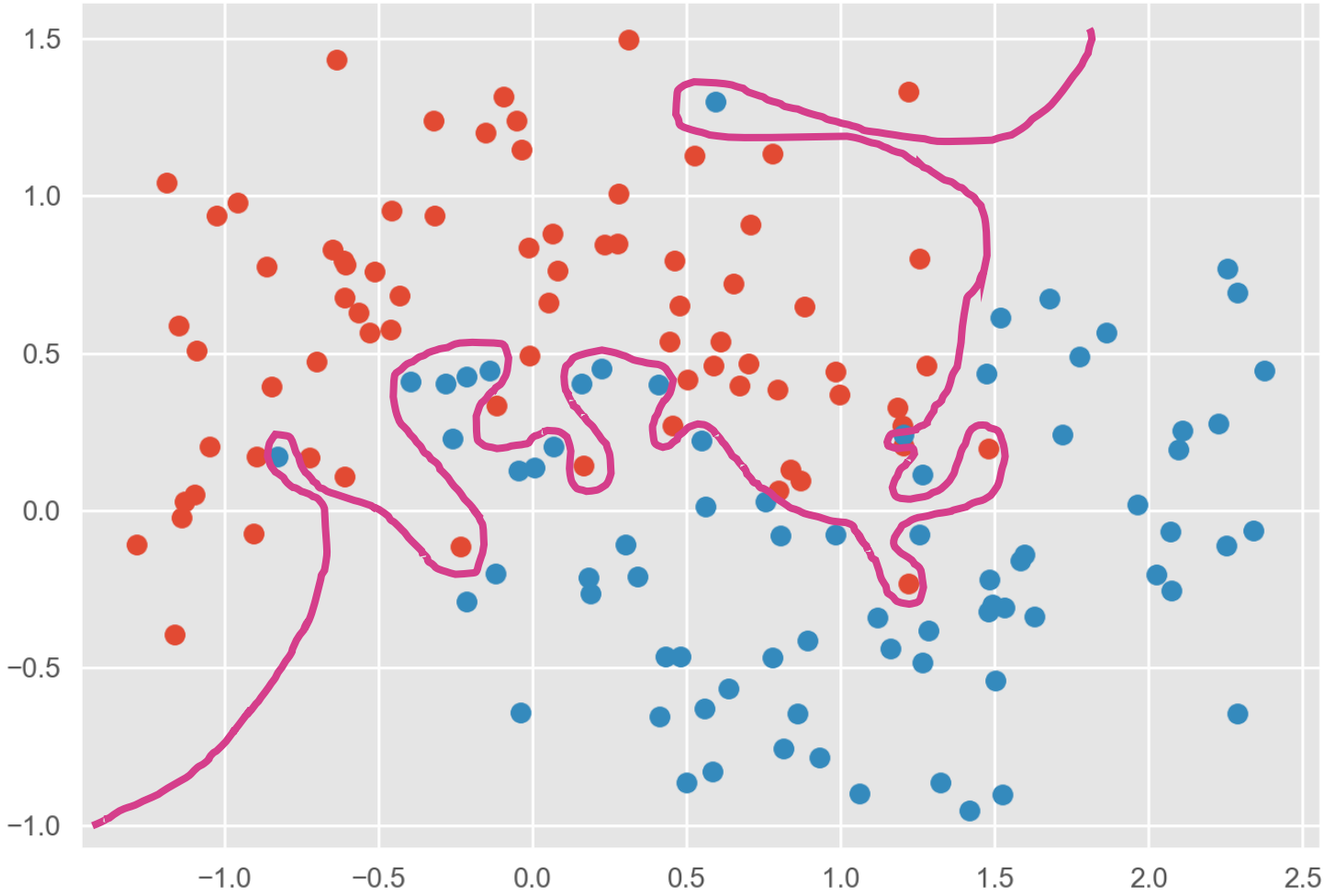
Let’s teach a neural network to identify cancer

Updated decision boundary

(epoch 23)

Uh… let’s dial it back.

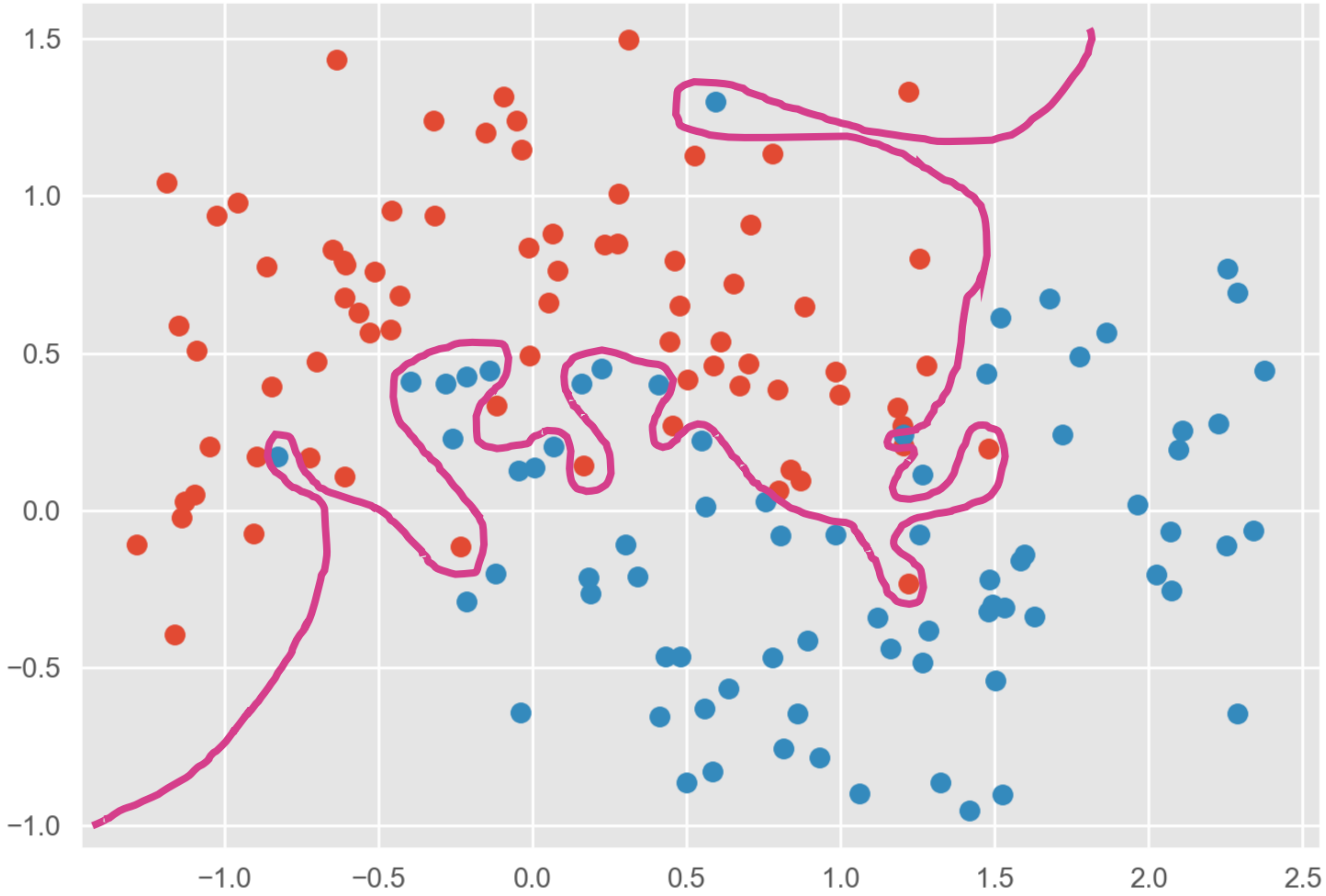
Just like our robot, it doesn’t know when to stop.



We need a strategy to decide when to stop.

Strategy 1:
Penalize complexity
(regularization)

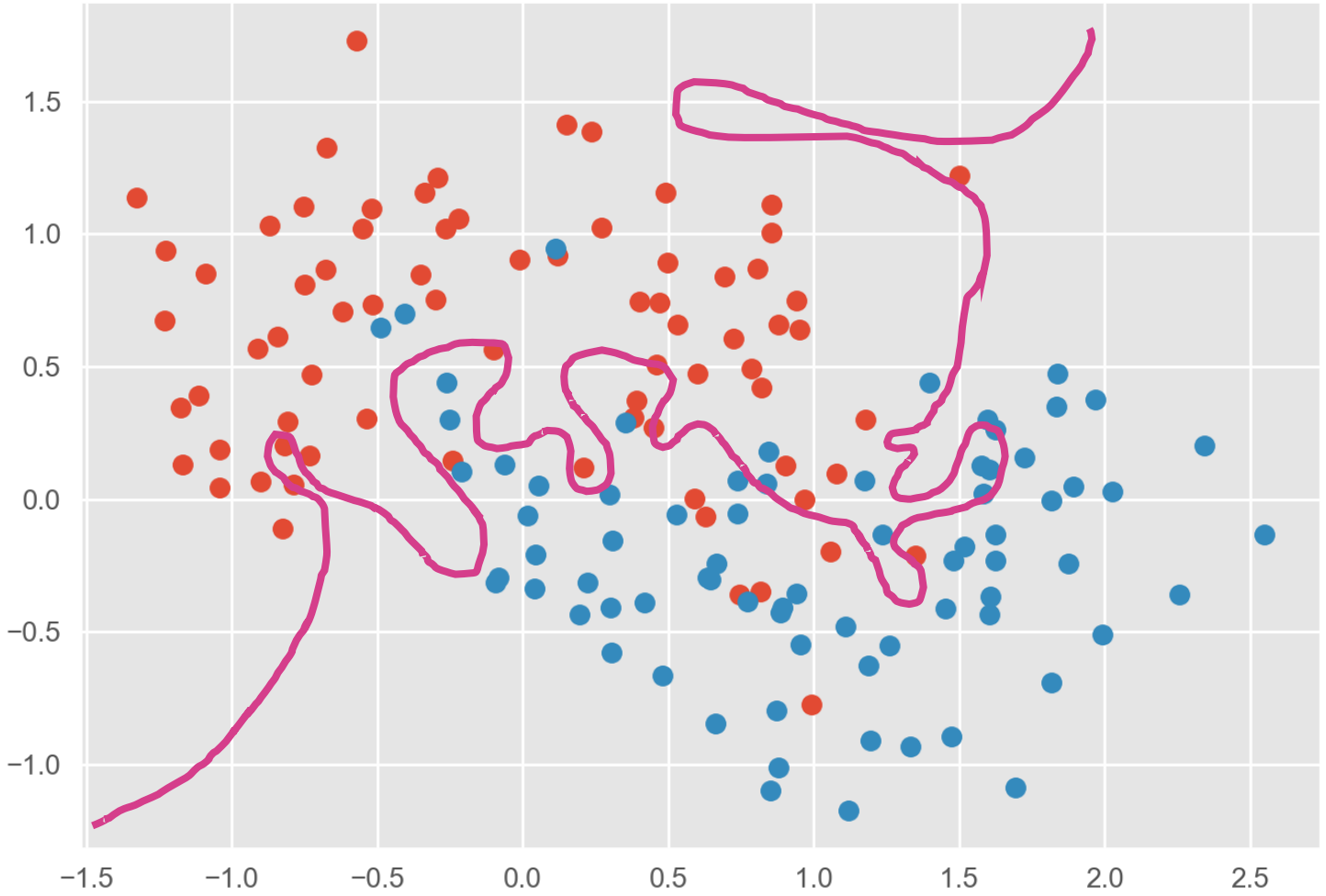
We could quantify how curvy the line is and add that value to the loss.



We need a strategy to decide when to stop.

Strategy 2:
Keep checking the validation set
(early stopping)

When our boundary no longer works well on new data, we know we've gone too far.



Strategy 1: Explicit Regularization

- We add a term to the loss (*L*) that quantifies complexity
- By minimizing the loss, we're now striking a balance between two competing objectives:
  1. Improve goodness of fit (i.e. reduce cross-entropy loss *H*)
  2. Limit complexity (i.e. reduce regularization term *R*)
- The hyperparameter λ controls how much we care about (1) vs (2)

$$L = H + \lambda R$$

Examples of Explicit Regularization

- L2 (i.e. *ridge*) regularization: $R = \sum_i \beta_i^2$
- In other words, we penalize the sum of squares of parameters
- Common in linear models and in neural networks

$$L = H + \lambda R$$

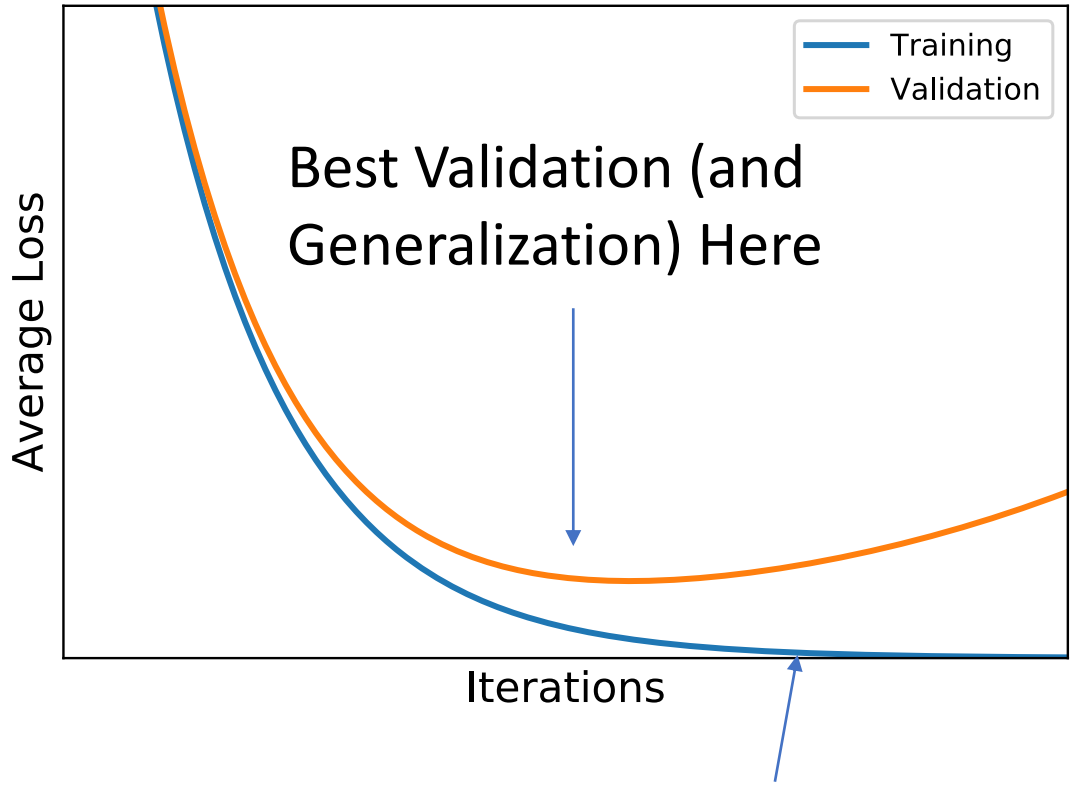
Examples of Explicit Regularization

- L1 (i.e. *LASSO*) regularization: $R = \sum_i |\beta_i|$
- In other words, we penalize the sum of absolute values of parameters
- Common in linear models; less so in neural networks
- Tends to shrink many parameters to 0
  - This may be viewed as a form of feature selection
  - This also improves interpretability

$$L = H + \lambda R$$

Strategy 2: Early Stopping

- During optimization, we can check the validation loss as we go.
- Instead of optimizing to convergence, we can optimize until the *validation* loss stops improving
  - Saves computational cost
  - Performs better on validation (and test) sets
- Widely used technique



Strategy 3: Dropout

- Exclusive to neural networks
- During training, we set some hidden features to zero at random (different features for each training step)
- This has a dual effect:
  - Parameter shrinkage (similar to L2)
  - Encourages redundancy / redundant features; in other words, the network must model the relationship between *x* and *y* in multiple ways

Mitigating Overfitting in Practice

- Machine learning almost always uses some form of regularization and/or early stopping

- Very common to use multiple forms at once
  - Dropout + early stopping in neural networks
  - Combination of L1 and L2 regularization in linear models (i.e. elastic net)

- The validation set is the key: used to choose between strategies

- You will see this when working on data science projects.

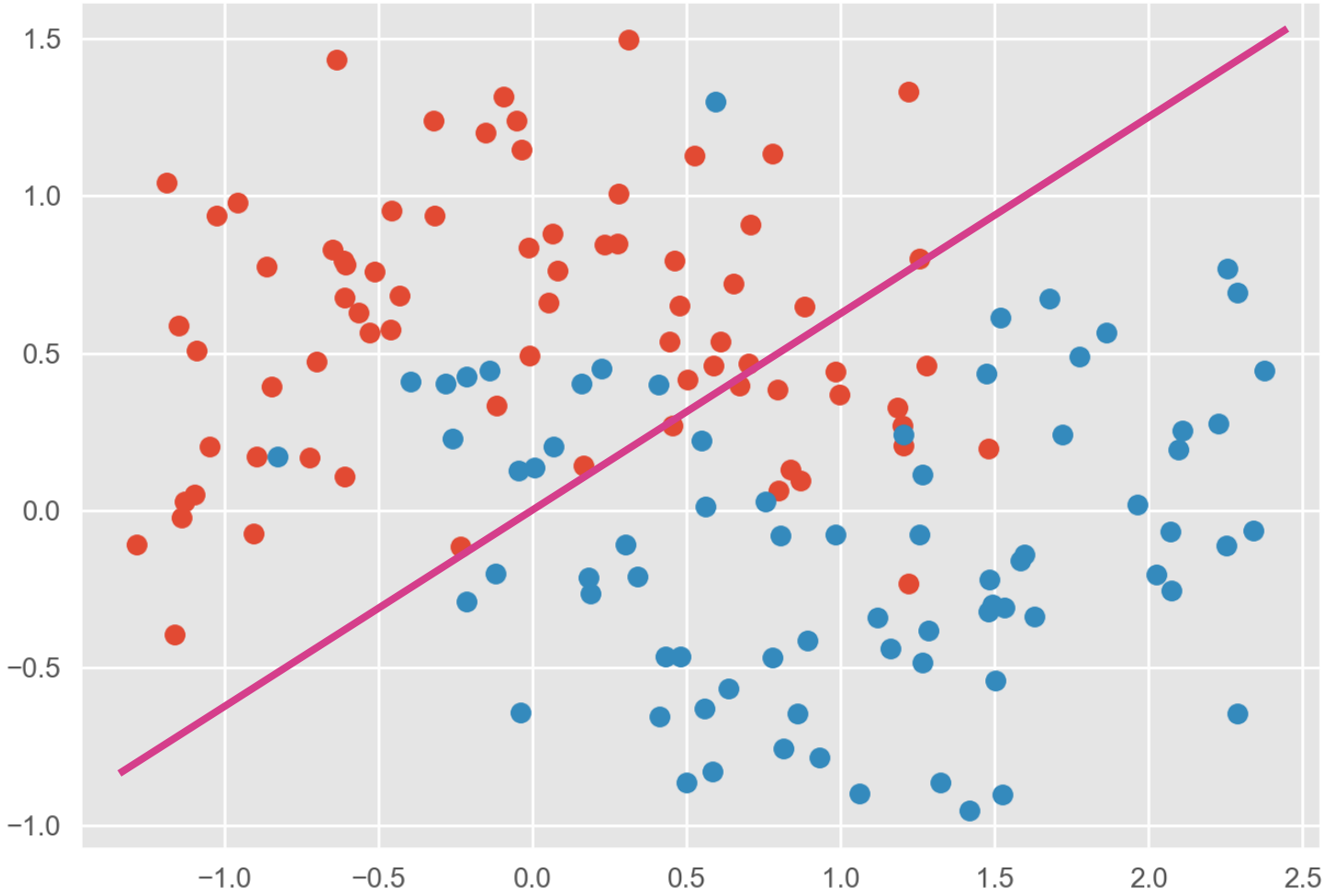
Linear models can also overfit!!! (How?)

Linear decision boundary

In this scenario ->
(# points >> # predictors)
it is not possible.

However, as # points
approaches # predictors,
we will see overfitting.

And for # points $\leq$ # predictors
(assuming linear independence),
we can memorize the dataset.



Scenarios

How to mitigate overfitting?

Scenario 1: Interpretable CDP

- You are building a clinical decision support system using variables from structured EHR fields
- You have a thousand predictors and a few thousand data points (i.e. patients) in your training set
- You want it to be easy for providers to understand how the model works, and what features are important

Scenario 2: Pure prediction

- You are building a neural network-based model that identifies nicotine withdrawal from digital health data
- Your input data is a high-dimensional time series of physiologic measurements from multiple sensors
- There is no need to interpret or explain the model: you care only about out-of-sample performance

Overfitting in linear models

(time permitting)

Suppose we have the following data

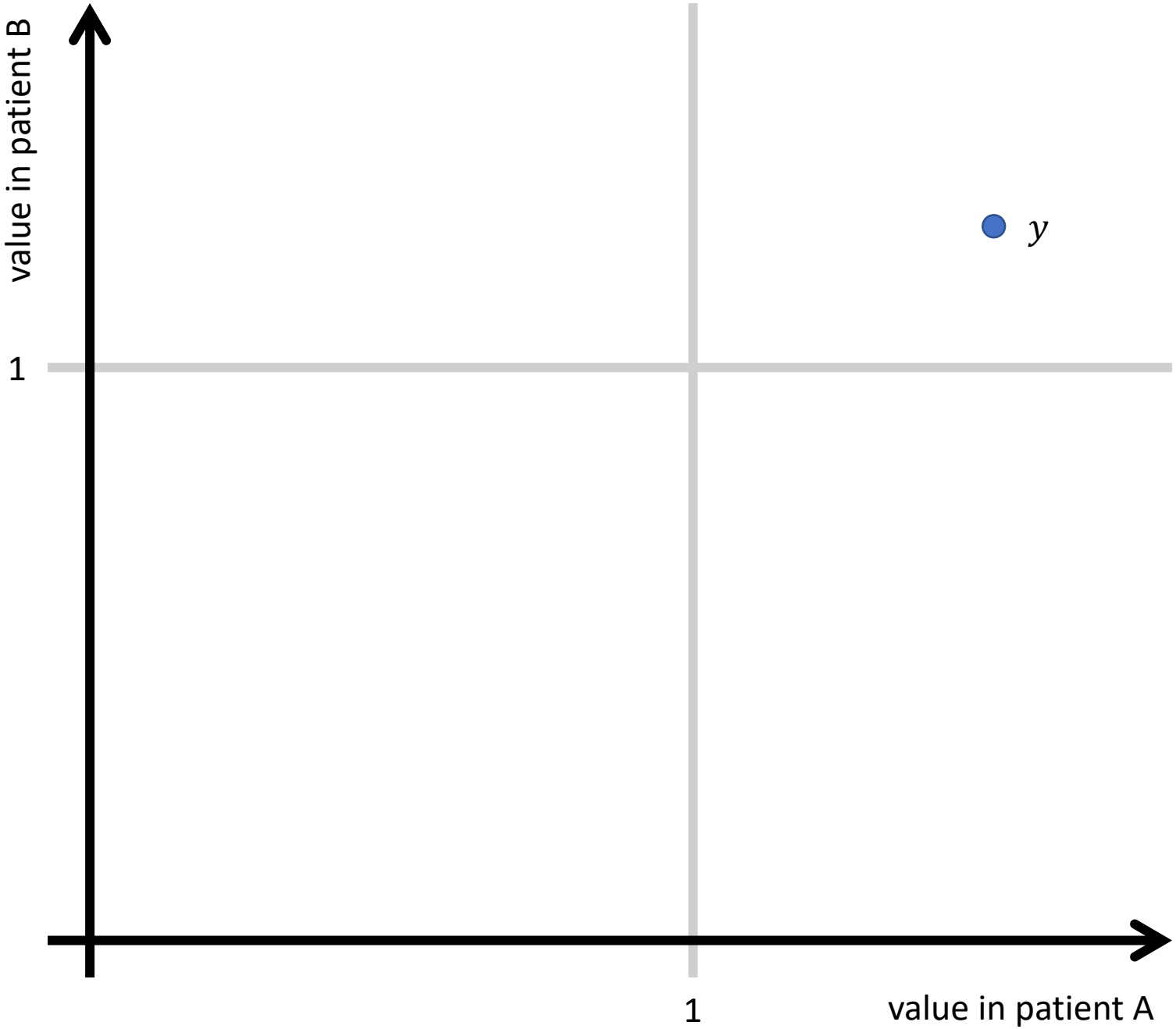
Patient	Predictor 1 (numeric)	Predictor 2 (numeric)	Outcome (numeric)
A	.5	.75	1.5
B	1	.75	1.25

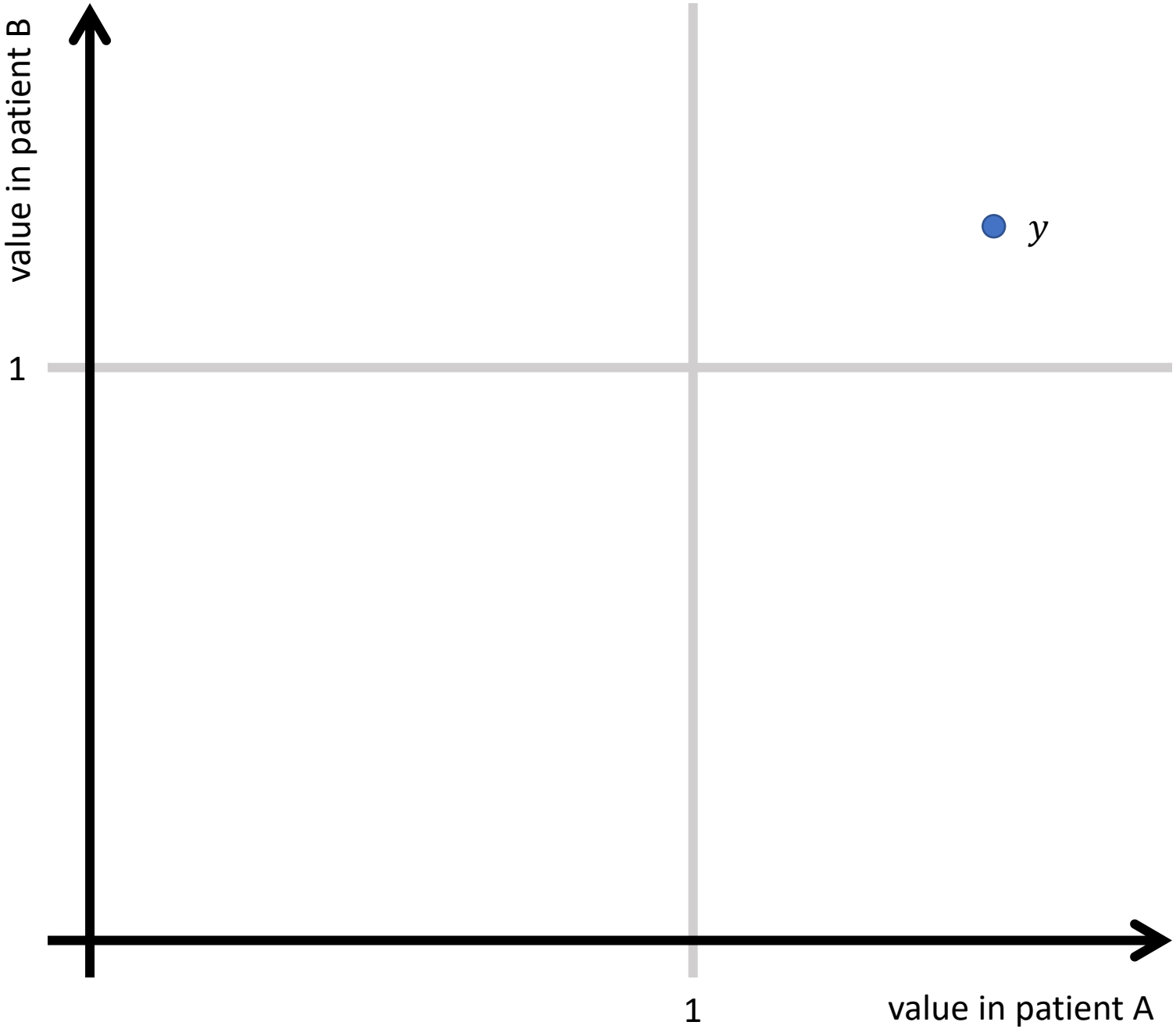
> Goal: find the linear equation that best predicts the outcome

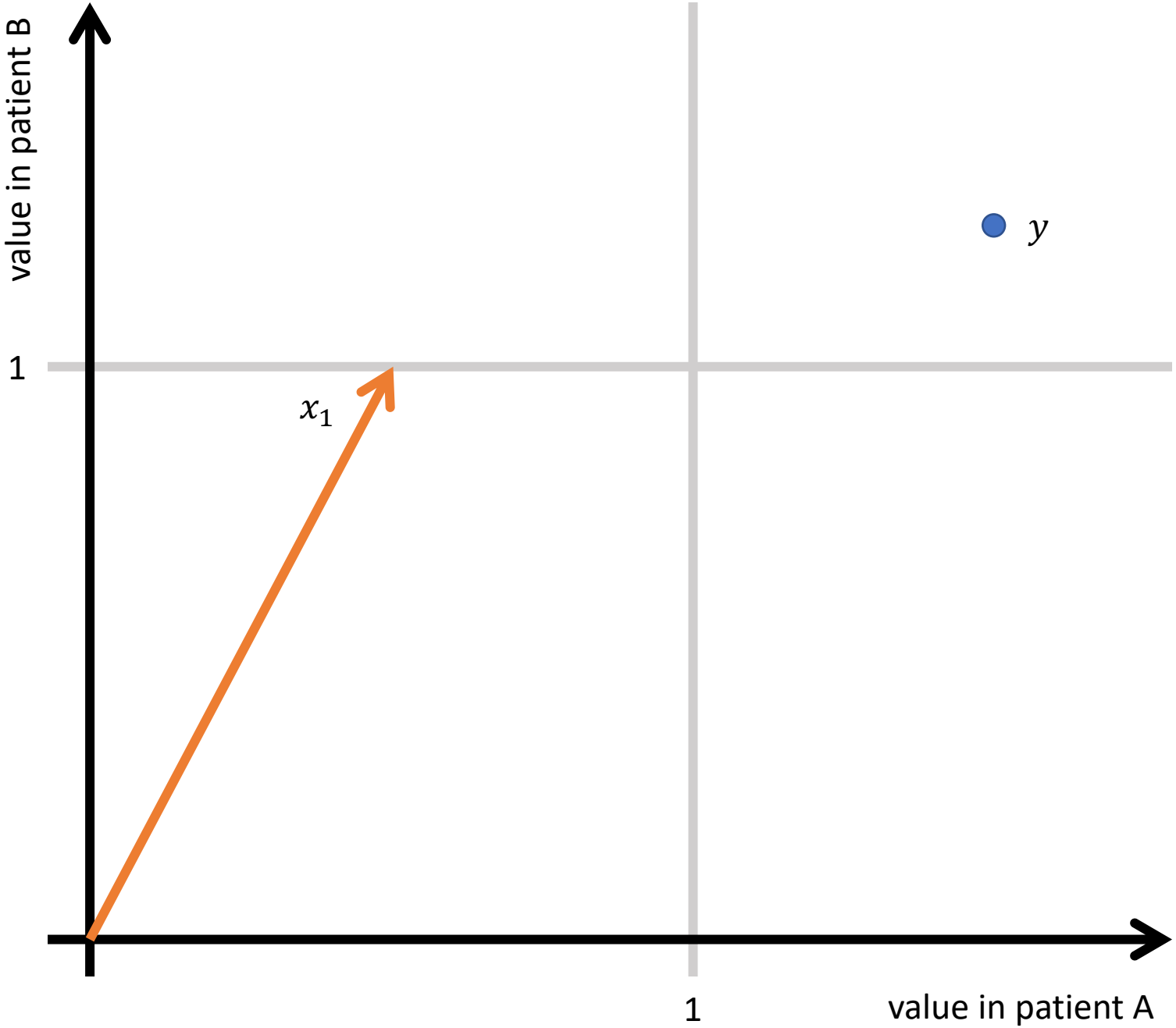
Patient	$\boldsymbol{x}_1$	$\boldsymbol{x}_2$	$\boldsymbol{y}$
A	.5	.75	1.5
B	1	.75	1.25

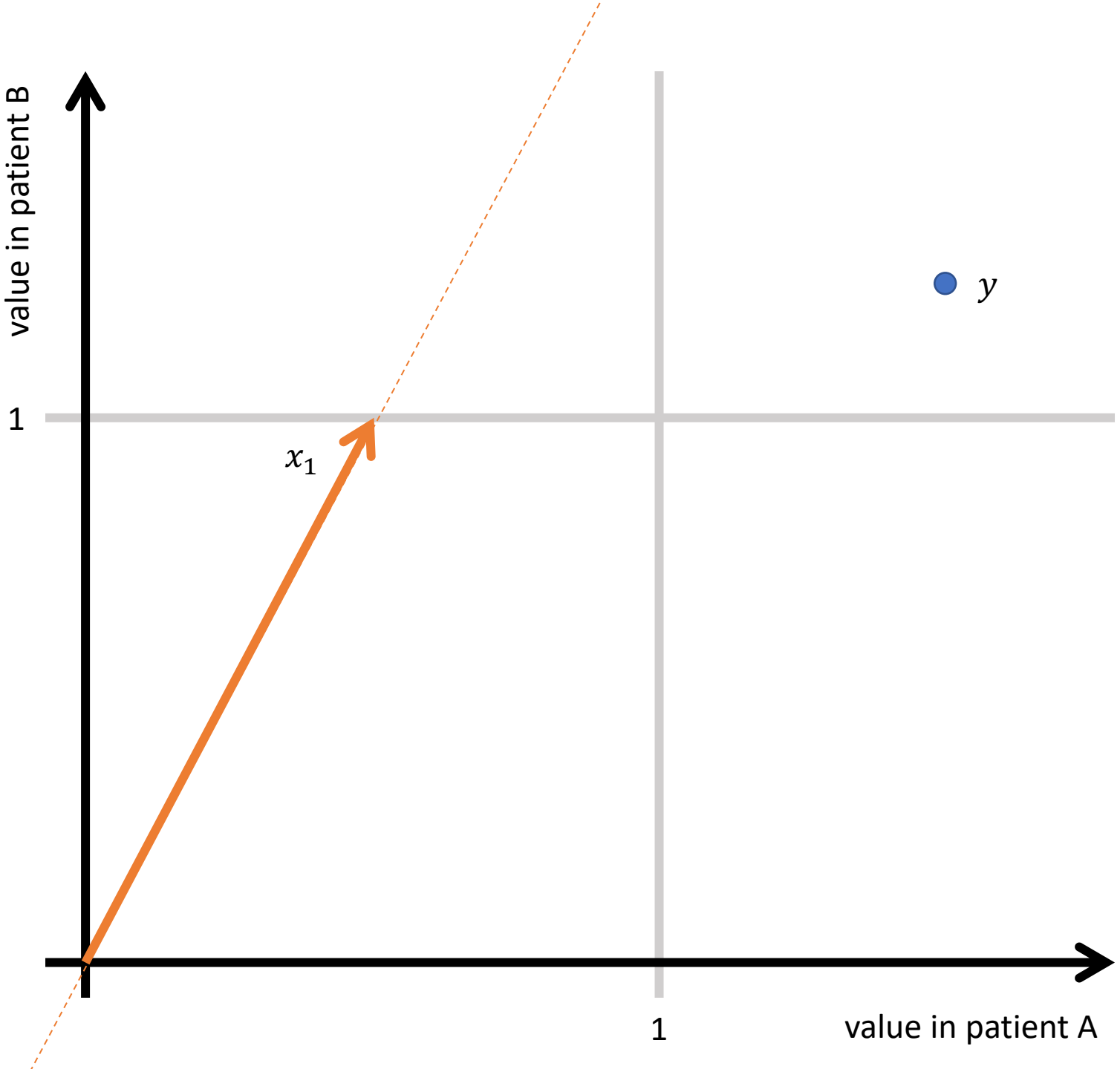
> Goal: find the linear equation that best predicts the outcome

$$b_1\boldsymbol{x}_1 + b_2\boldsymbol{x}_2 = \boldsymbol{y}$$


value in patient B
1
y
1
value in patient A


value in patient B
1
y
1
value in patient A


value in patient B
1
x_1
y
1
value in patient A



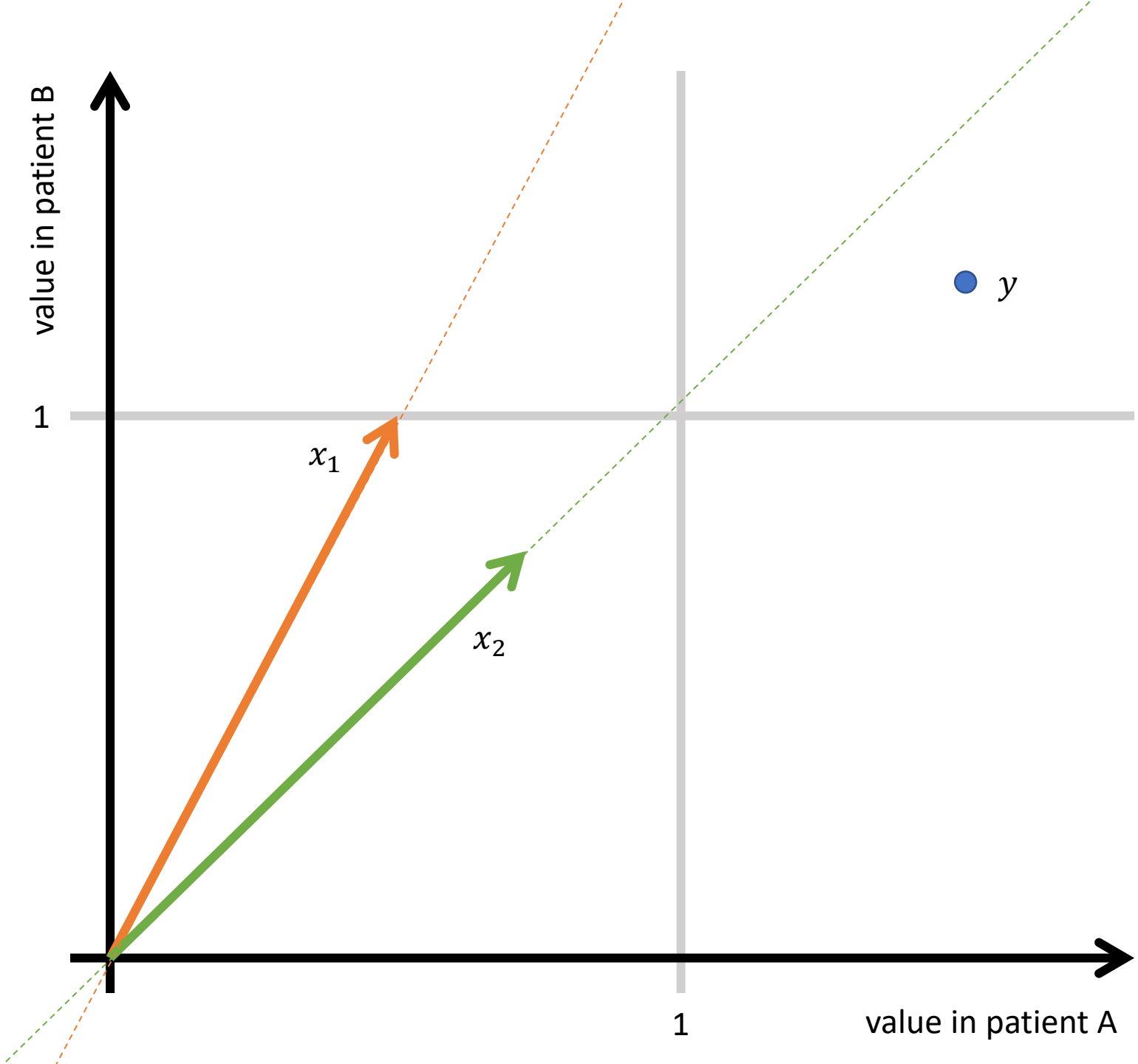
Goal: Predict y with x_1 only

From a graphical perspective, our goal is to get as close as possible to y, but we can only move in the x_1 direction

---

$p < n$

More patients than predictors.



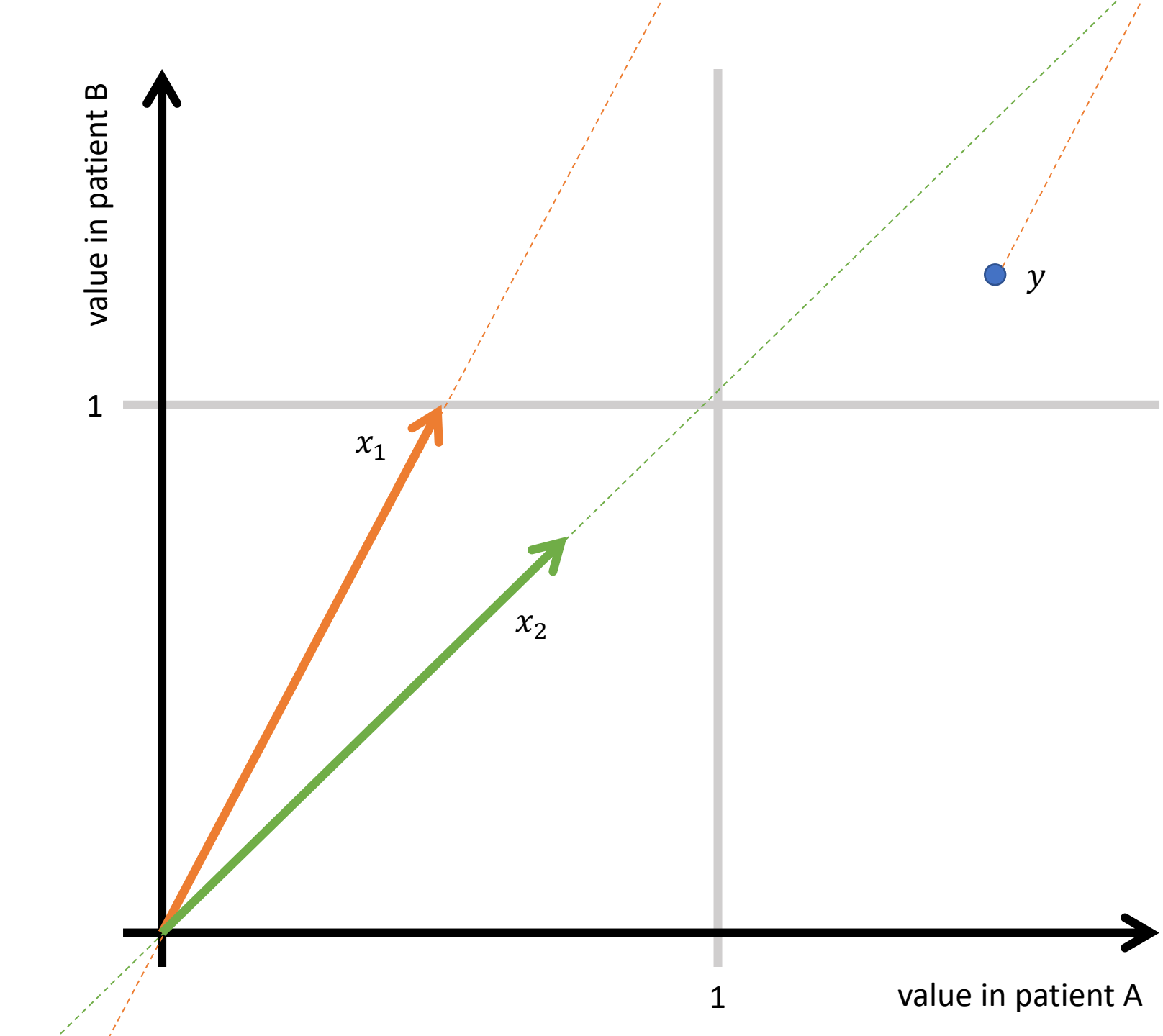
Goal: Predict y with x_1, x_2

From a graphical perspective, our goal is to get as close as possible to y. We can now move in both the x_1 direction and the x_2 direction.

$p = n$

Can always* predict perfectly on training set

*assuming linearly independent predictors



Goal: Predict y with x_1, x_2

From a graphical perspective, our goal is to get as close as possible to y. We can now move in both the x_1 direction and the x_2 direction.

$p = n$

Can always* predict perfectly on training set

*assuming linearly independent predictors

Takeaways

- When # points $\leq$ # predictors, we can get perfect predictions (i.e. memorize the dataset)
- However, this typically requires very large model coefficients
- Regularization therefore prevents this behavior, and therefore tends to give us better generalization (i.e. out of sample) performance

Cross-Validation

(time permitting)

Traditional “split” for development + eval

Cross validation: rotate the test set

Round 1: Train on 1-4, test on 5
Round 2: Train on all but 4, test on 4
Round 3: Train on all but 3, test on 3
Round 4: Train on all but 2, test on 2
Round 5: Train on 2-5, test on 1

Why would we do this?

- More data for the evaluation
- Better estimate of out-of-sample performance

What happened to the validation set?

- Use “flat” cross-validation (below) versus “nested” cross-validation
- Both give unbiased estimates and flat is easier

Round 1: Train on 1-3, validate on 4, test on 5
Round 2: Train on 2-4, validate on 5, test on 1
Round 3: Train on 3-5, validate on 1, test on 2
Round 4: Train on 4, 5, and 1; validate on 2, test on 3
Round 5: Train on 5, 1, and 2; validate on 3, test on 4