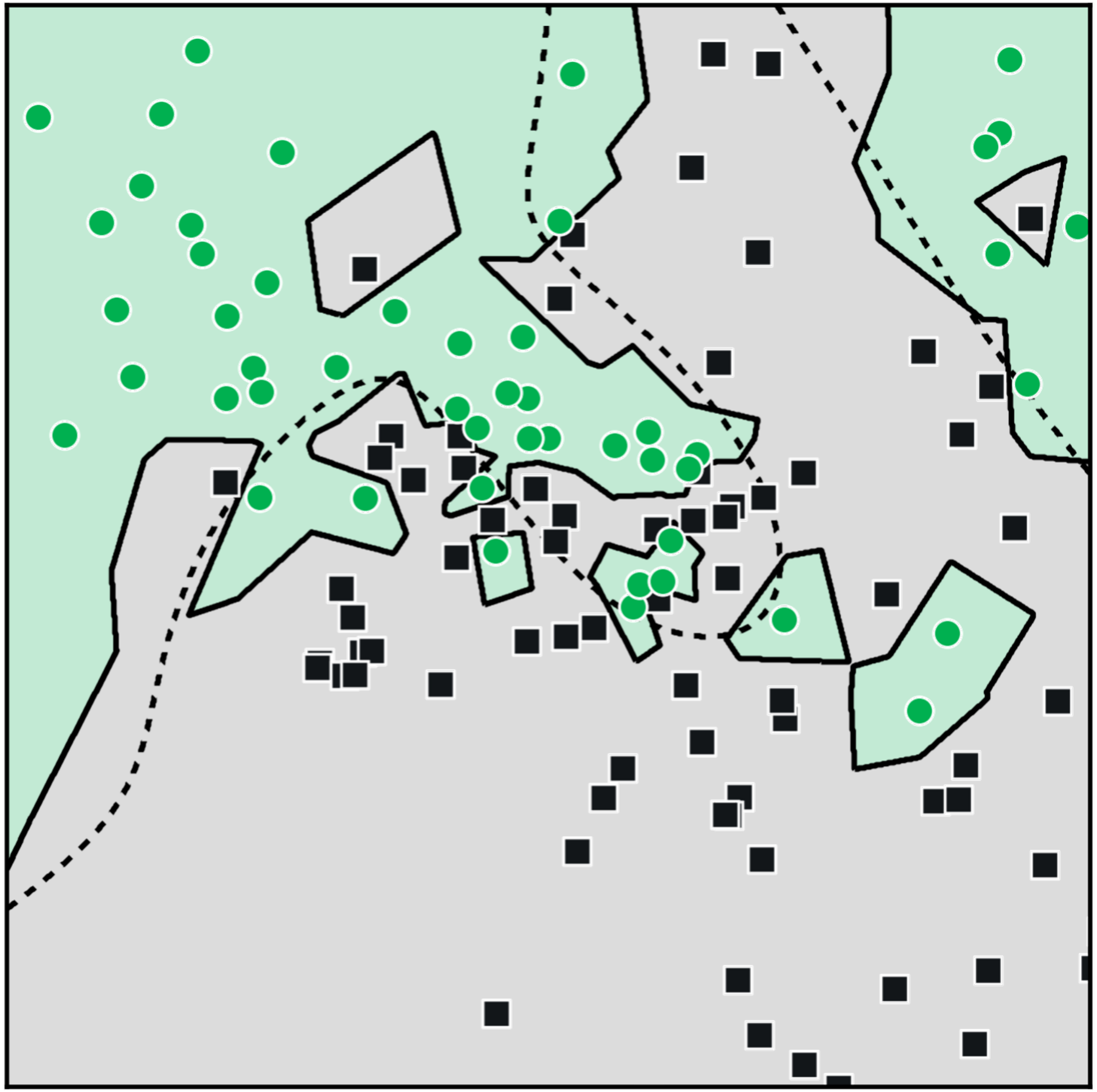
# Reducing Overfit

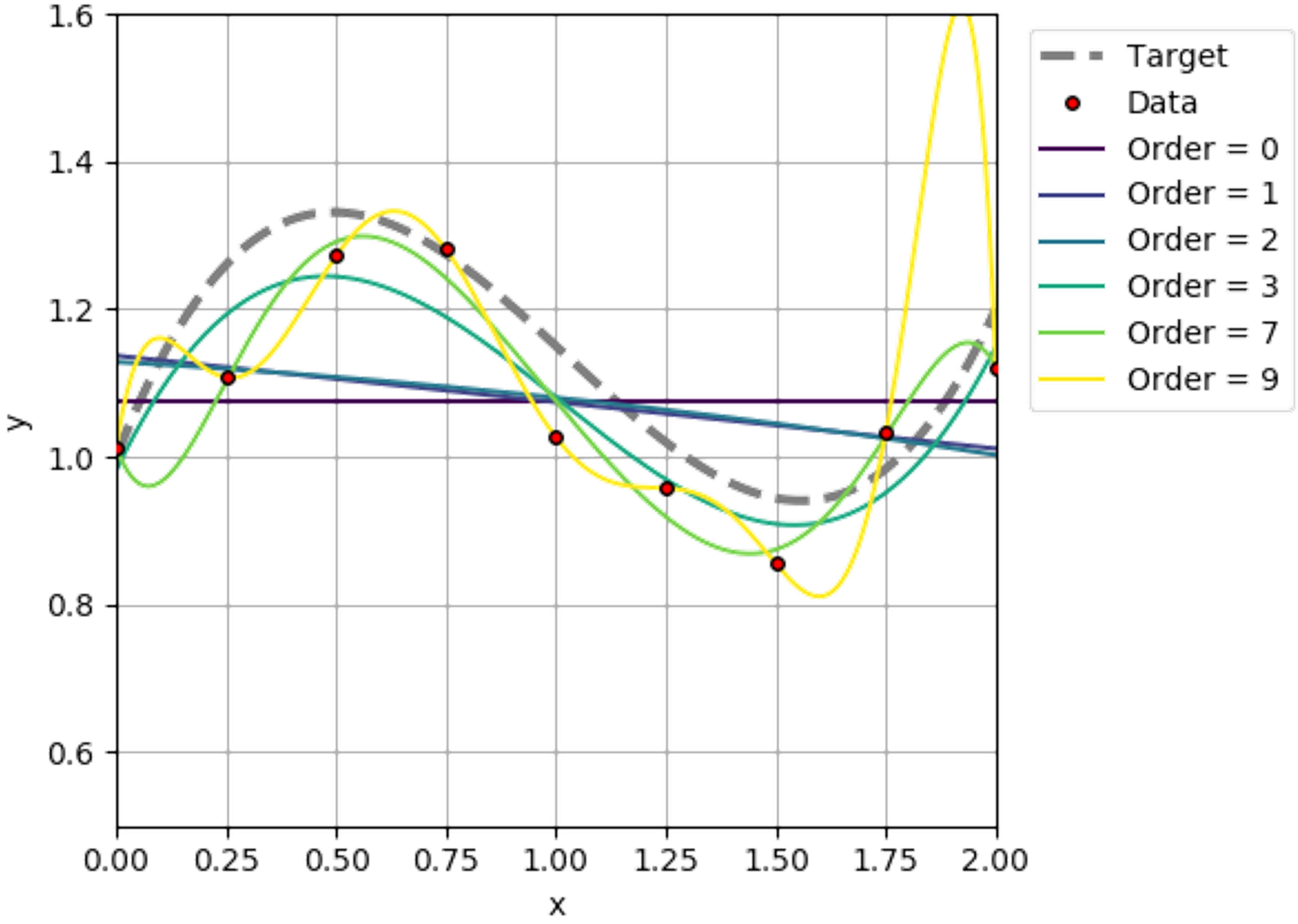
# We’ve seen overfit in classification…

**Overfitting** to the training data

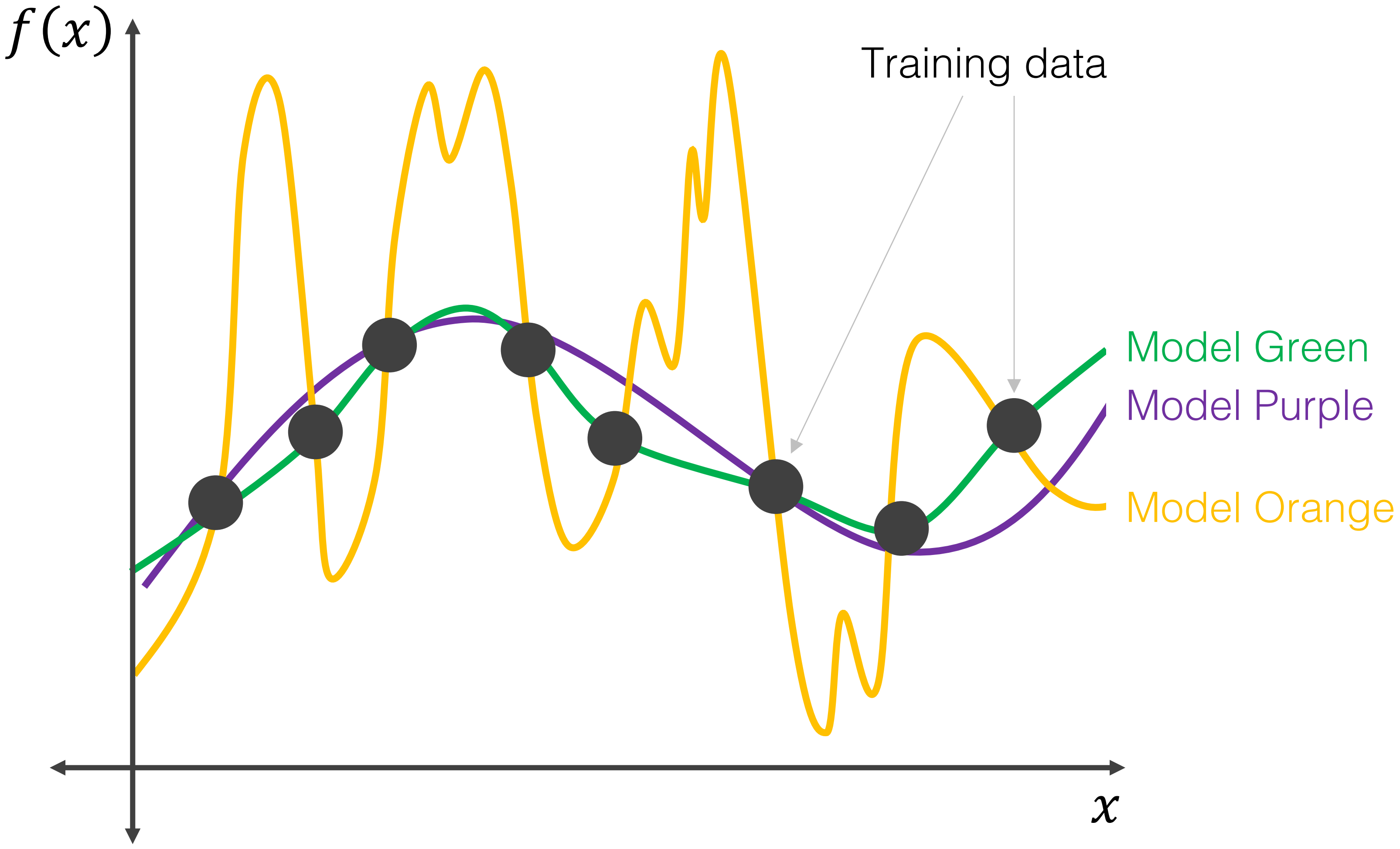
High model **variance**



# …and have seen overfit in regression…



# How do we limit overfitting?




How do we know which solution is best?

- Models orange and green both perfectly fit the training data
- Use which model **generalizes best** on held out data

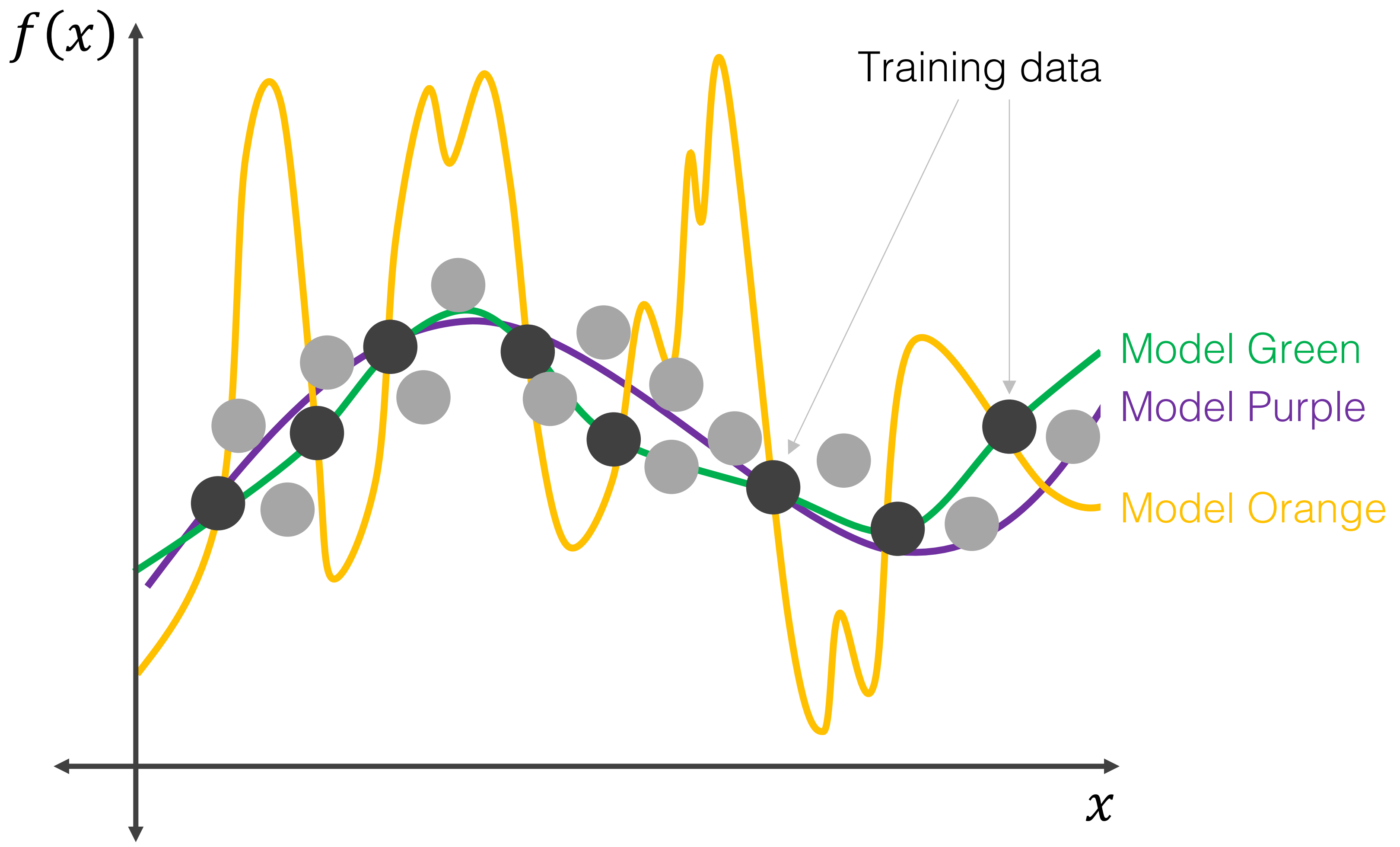
How do enable the algorithm to find solutions that generalize better?

## Option #1: Add more data!

(Not always possible)

## Option #2: Limit model flexibility to reduce overfit

# Adding representative training data typically helps




**Adding more data**…

Reduces spurious correlations

"fills in" the feature space

Constrains the model to perform well on a broader set of examples

# How do we reduce overfit?

## Option #1: Add more data!
(Not always possible)

## Option #2: Limit model flexibility to reduce overfit

# Options for limiting model flexibility

1. Variable/feature subset selection
2. Regularization/shrinkage
3. Dimensionality reduction
(in a lecture coming soon!)

**These all reduce the number of features modeled and/or model flexibility**

# Our conceptual tool…


Image from Speckyboy.com

# Occam's Razor / Law of Parsimony

All else being equal, choose the **simpler** solution

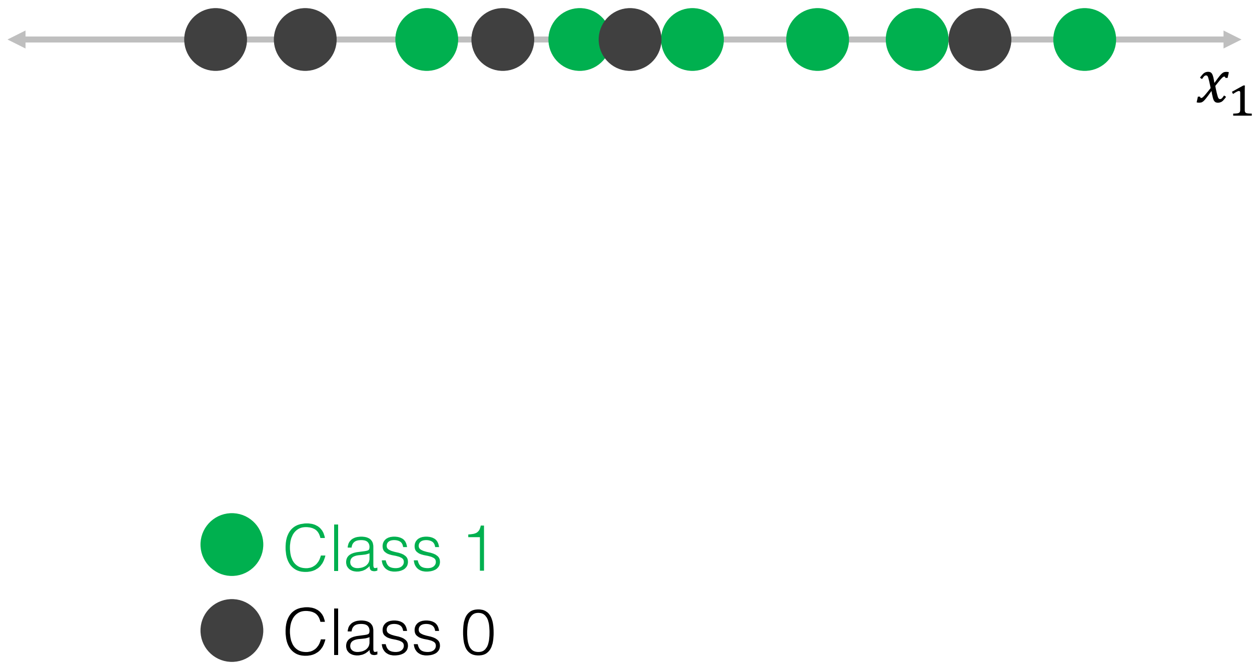
# Options for limiting model flexibility

1. **Variable/feature subset selection**

2. Regularization/shrinkage

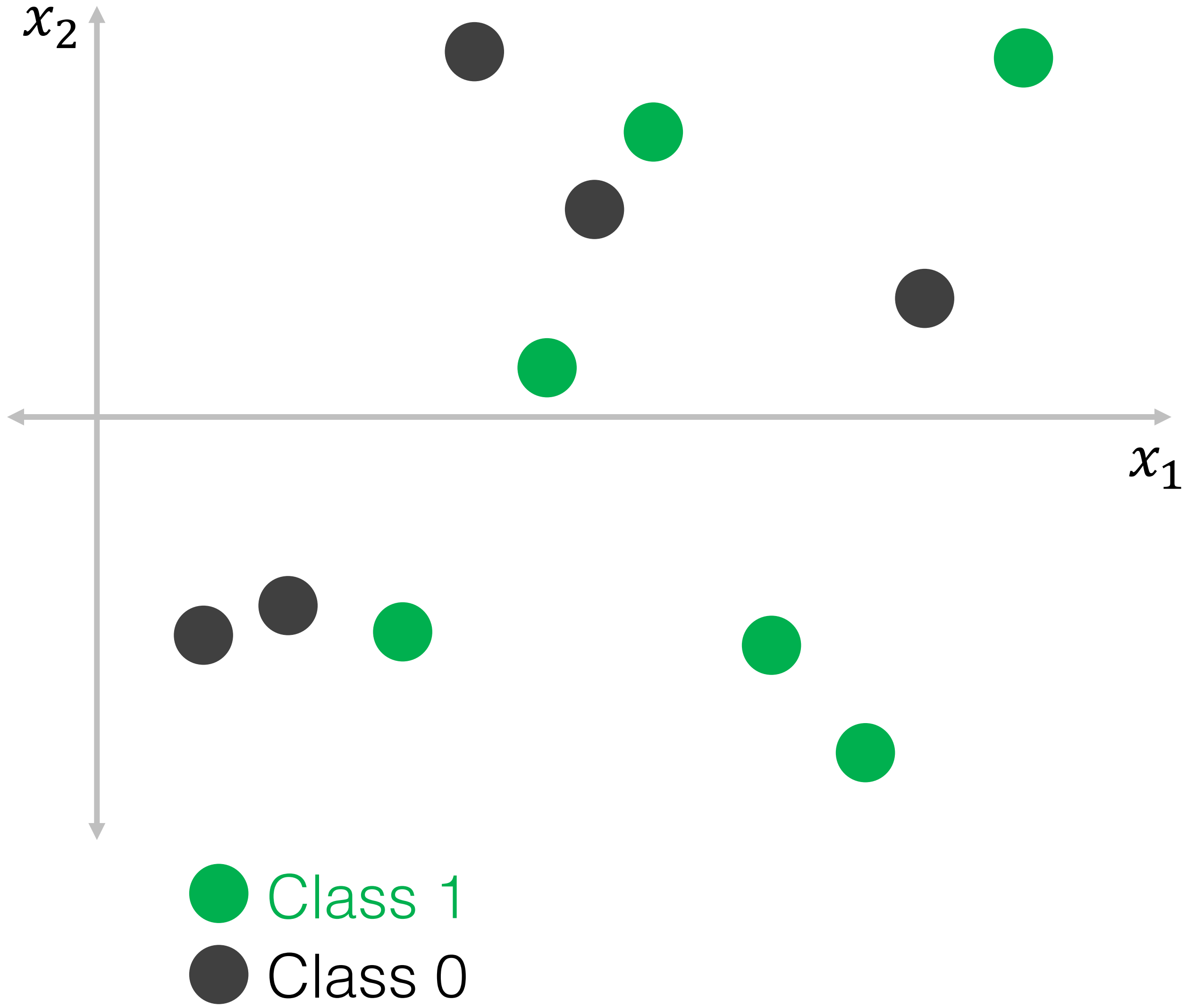
3. Dimensionality reduction

# What's the problem with adding features?




Binary classification with one feature

# What's the problem with adding features?




Features that are not meaningful make the problem harder

Additional features increase flexibility in most models
(e.g. a linear model with an extra feature will have an extra parameter)

**Example**: what if $x_2$ is random noise? The model may still use it in its predictions.

# Feature (variable) selection

Manual feature engineering

(e.g. use domain knowledge to remove less informative features)

Filter methods

(e.g. remove highly correlated features)

Wrapper methods

(e.g. subset selection)

Embedded methods

(e.g. LASSO regularization)

# Wrapper methods for variable subset selection

Search for subsets of features that perform well

Exhaustive search
Forward selection
Backwards selection
Simulated annealing
Genetic algorithms
Particle swarm optimization

**Challenge**: requires rerunning the training algorithm (computationally expensive)

# Forward selection

- Start with no features
- Greedily include the one feature that most improves performance
- Stop when a desired number of features is reached

# Backward selection

- Start with all features included
- Greedily remove the feature that decreases performance least
- Stop when a desired number of features is reached

Challenge: requires rerunning the training algorithm (computationally expensive)

# Options for limiting model flexibility

1. Variable/feature subset selection

2. **Regularization/shrinkage**

3. Dimensionality reduction

# Regularization

Constraining a model to prevent overfitting or solve an ill-posed problem
(does not have a unique solution)

# Regularization

a.k.a. shrinkage

Adjust the **cost/loss function** to penalize larger parameters

$$C(\boldsymbol{w}) = E(\boldsymbol{w}, \boldsymbol{X}, \boldsymbol{y}) \qquad + \quad \lambda R(\boldsymbol{w})$$

For example:

$$C(\boldsymbol{w}) = \sum_{i=1}^{n} (\boldsymbol{w}^T \boldsymbol{x}_i - y_i)^2 + \lambda \sum_{j=1}^{p} w_j^2$$

Square error

$L_2$ regularization penalty

This term causes the estimated parameter values to "shrink"

# Regularization

a.k.a. shrinkage

Adjust the **cost/loss function** to penalize larger parameter values

**a.k.a….**

L$_2$ regularization $$C(\boldsymbol{w}) = \sum_{i=1}^{n} (\boldsymbol{w}^T \boldsymbol{x}_i - y_i)^2 + \lambda \sum_{j=1}^{p} w_j^2$$ **ridge regression** or weight decay (Tikhonov regularization)

L$_1$ regularization $$C(\boldsymbol{w}) = \sum_{i=1}^{n} (\boldsymbol{w}^T \boldsymbol{x}_i - y_i)^2 + \lambda \sum_{j=1}^{p} |w_j|$$ least absolute shrinkage and selection operator (**LASSO**)

L$_2$ & L$_1$ regularization $$C(\boldsymbol{w}) = \sum_{i=1}^{n} (\boldsymbol{w}^T \boldsymbol{x}_i - y_i)^2 + \lambda_1 \sum_{j=1}^{p} |w_j| + \lambda_2 \sum_{j=1}^{p} w_j^2$$ **elastic net** regularization

# To explain how regularization works, we need to know our Norms

Normal Rockwell (painter)

Norm Macdonald (comedian)

# …other norms


Norman Borlaug (agronomist)

Norm Peterson (character on Cheers)

# Norm

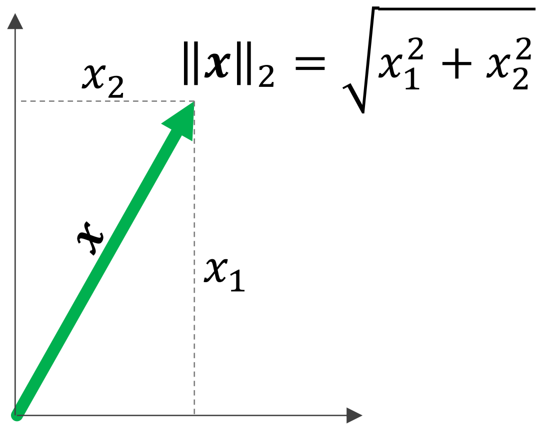
A function that assigns a positive **length or size** to a vector

The most familiar is likely the **Euclidean**, or $L_2$ norm:

$$\|\boldsymbol{x}\|_2 \triangleq \sqrt{x_1^2 + \cdots + x_n^2} = \left(\sum_{i=1}^{n} x_i^2\right)^{\frac{1}{2}} = \sqrt{\boldsymbol{x}^T\boldsymbol{x}}$$

You'll often see this in its squared form:

$$\|\boldsymbol{x}\|_2^2 \triangleq x_1^2 + \cdots + x_n^2 = \sum_{i=1}^{n} x_i^2 = \boldsymbol{x}^T\boldsymbol{x}$$

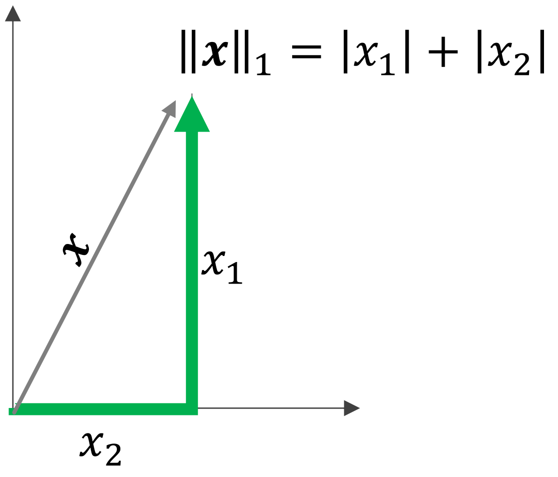


# Norms

There's also the $\boldsymbol{L_1}$ **norm**

(a.k.a taxicab or Manhattan distance)

$$\|\boldsymbol{x}\|_1 \triangleq |x_1| + \cdots + |x_n| = \sum_{i=1}^{n} |x_i|$$




The general $\boldsymbol{L_p}$ **norm**:

$$\|\boldsymbol{x}\|_p \triangleq \left(\sum_{i=1}^{n} |x_i|^p\right)^{\frac{1}{p}}$$

In the limit, the **infinity norm** is the maximum entry of the vector $\boldsymbol{x}$:

$$\|\boldsymbol{x}\|_\infty \triangleq \max_i |x_i|$$

# Norms for a vector

Assume a 2-D vector: $\boldsymbol{w} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}$

$$\|\boldsymbol{w}\|_1 = |w_1| + |w_2|$$

$$= |1| + |3|$$

$$= 4$$

$$\|\boldsymbol{w}\|_2 = \sqrt{w_1^2 + w_2^2}$$

$$= \sqrt{1^2 + 3^2}$$

$$= 10$$

$$\|\boldsymbol{w}\|_\infty = \max_i |w_i|$$

$$= 3$$

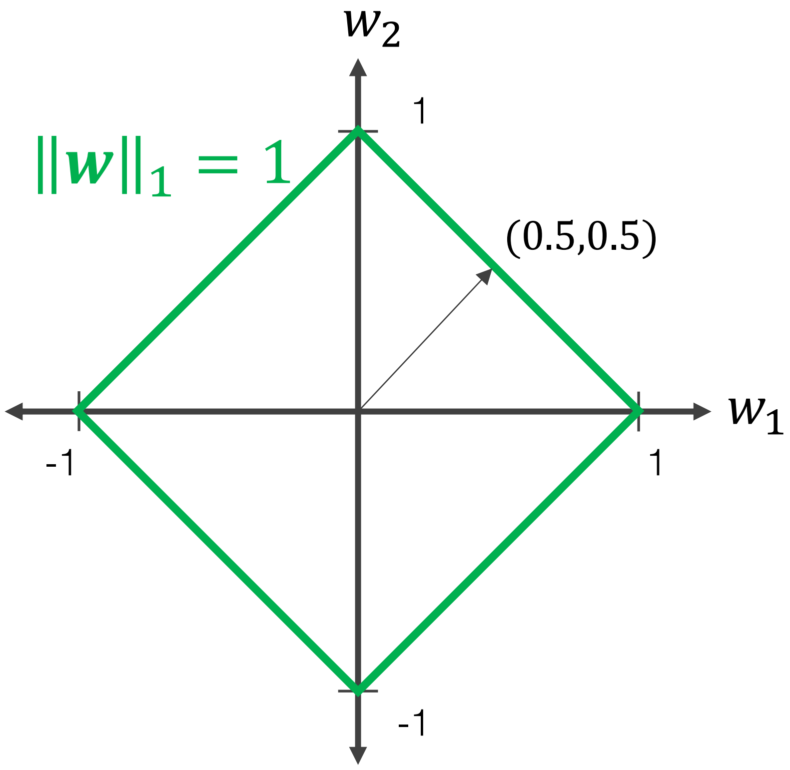
# Unit Norms

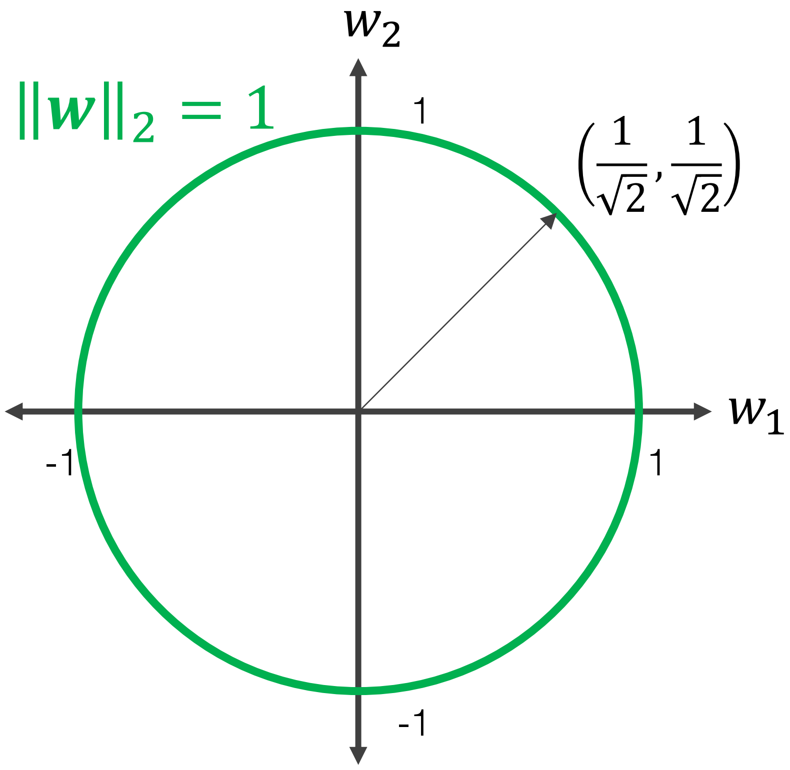
Assume a 2-D vector: $\boldsymbol{w} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$

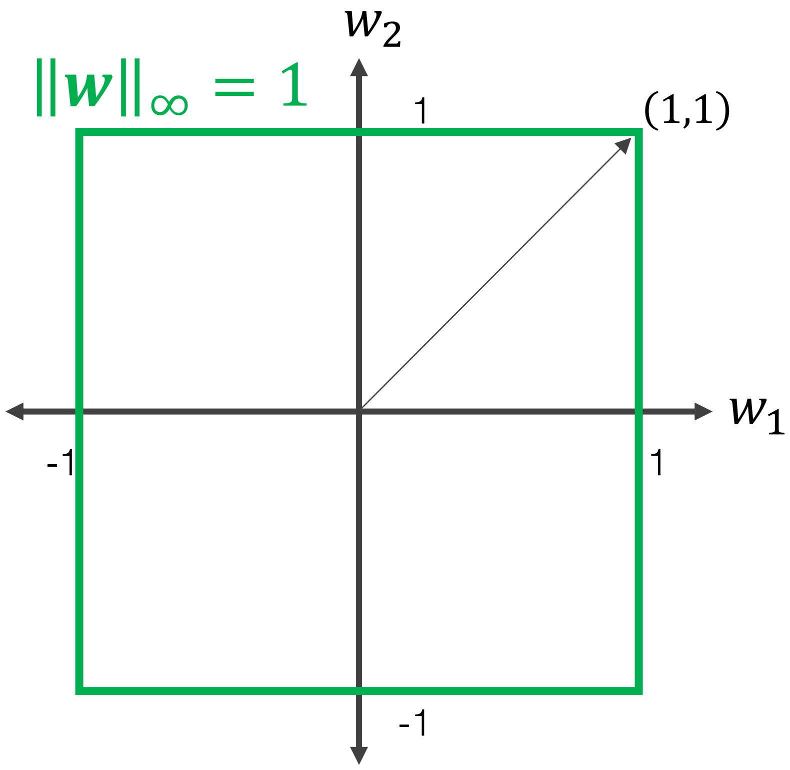
All possible values of $\boldsymbol{w}$ that have a norm of 1

(Plotted as the green lines below)

$$\|\boldsymbol{w}\|_1 = \sum_{i=1}^{n} |w_i| \qquad \|\boldsymbol{w}\|_2 = \sqrt{w_1^2 + w_2^2} \qquad \|\boldsymbol{w}\|_\infty = \max_i |w_i|$$

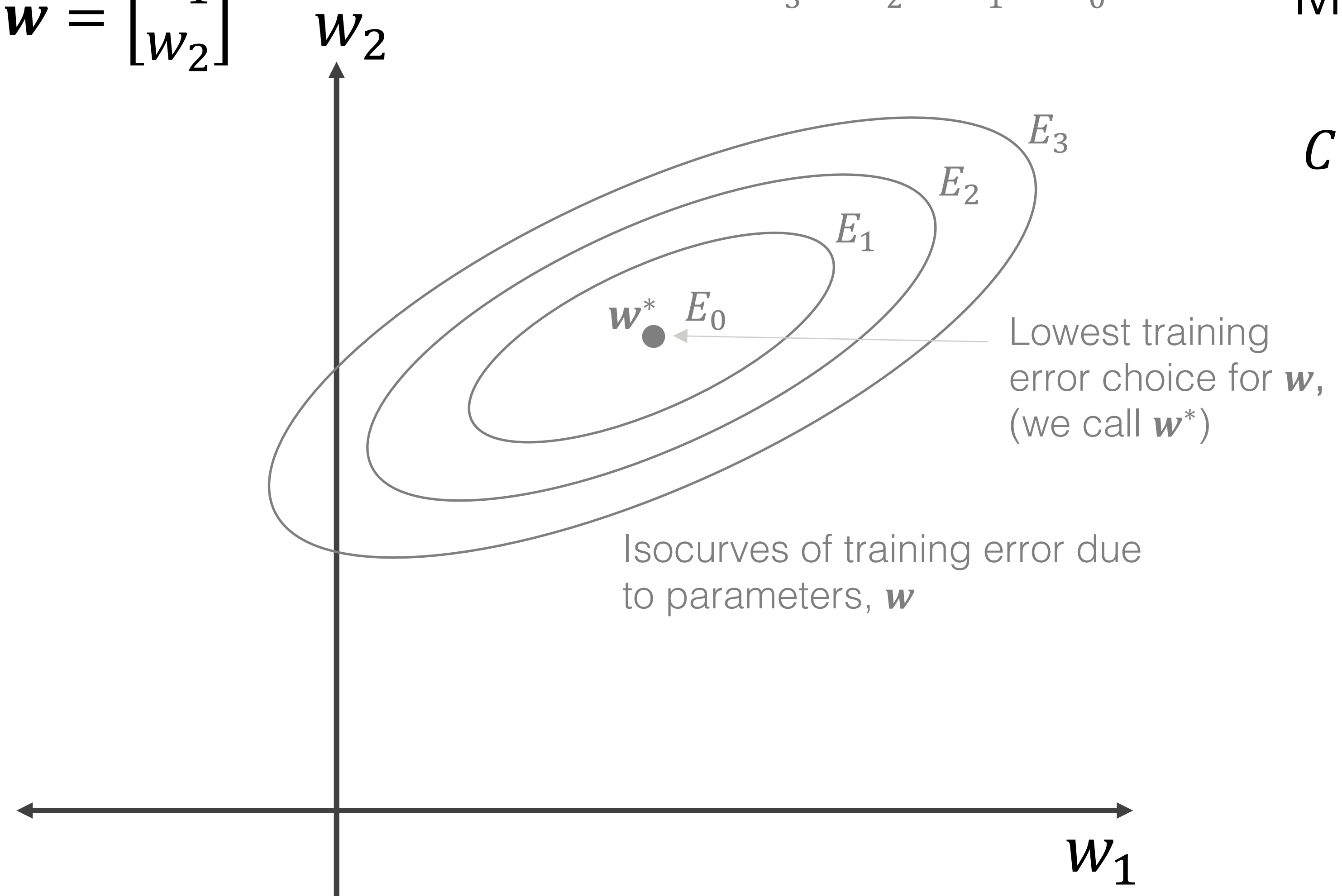


$$\boldsymbol{w} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$$

$E_3 > E_2 > E_1 > E_0$

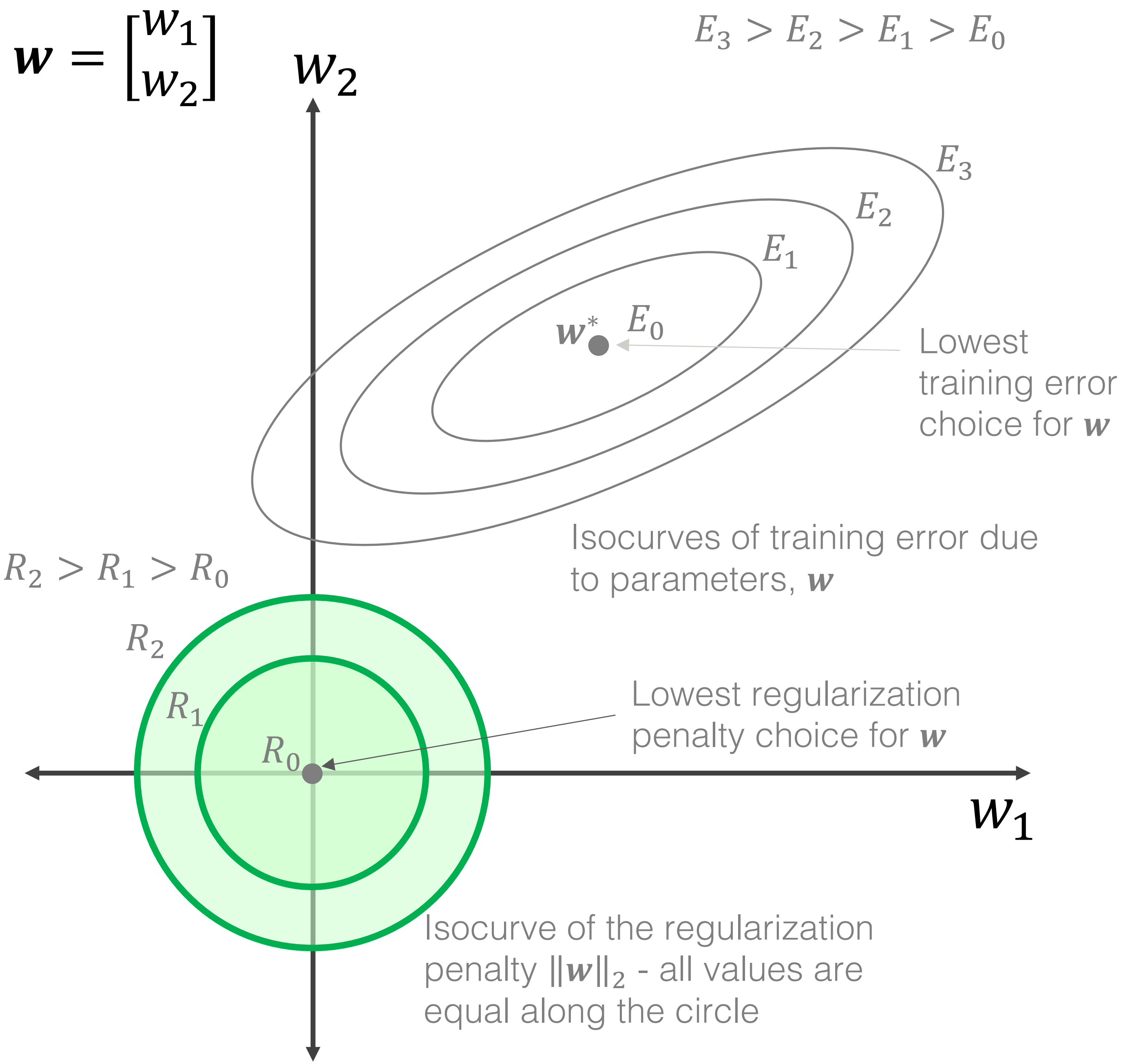



Every point in this space corresponds to a possible choice of model parameters $\boldsymbol{w}$

## Minimize cost function:

$$C(\boldsymbol{w}) = \underbrace{\sum_{i=1}^{n} (\boldsymbol{w}^T \boldsymbol{x}_i - y_i)^2}_{\text{Training error term (E)}}$$

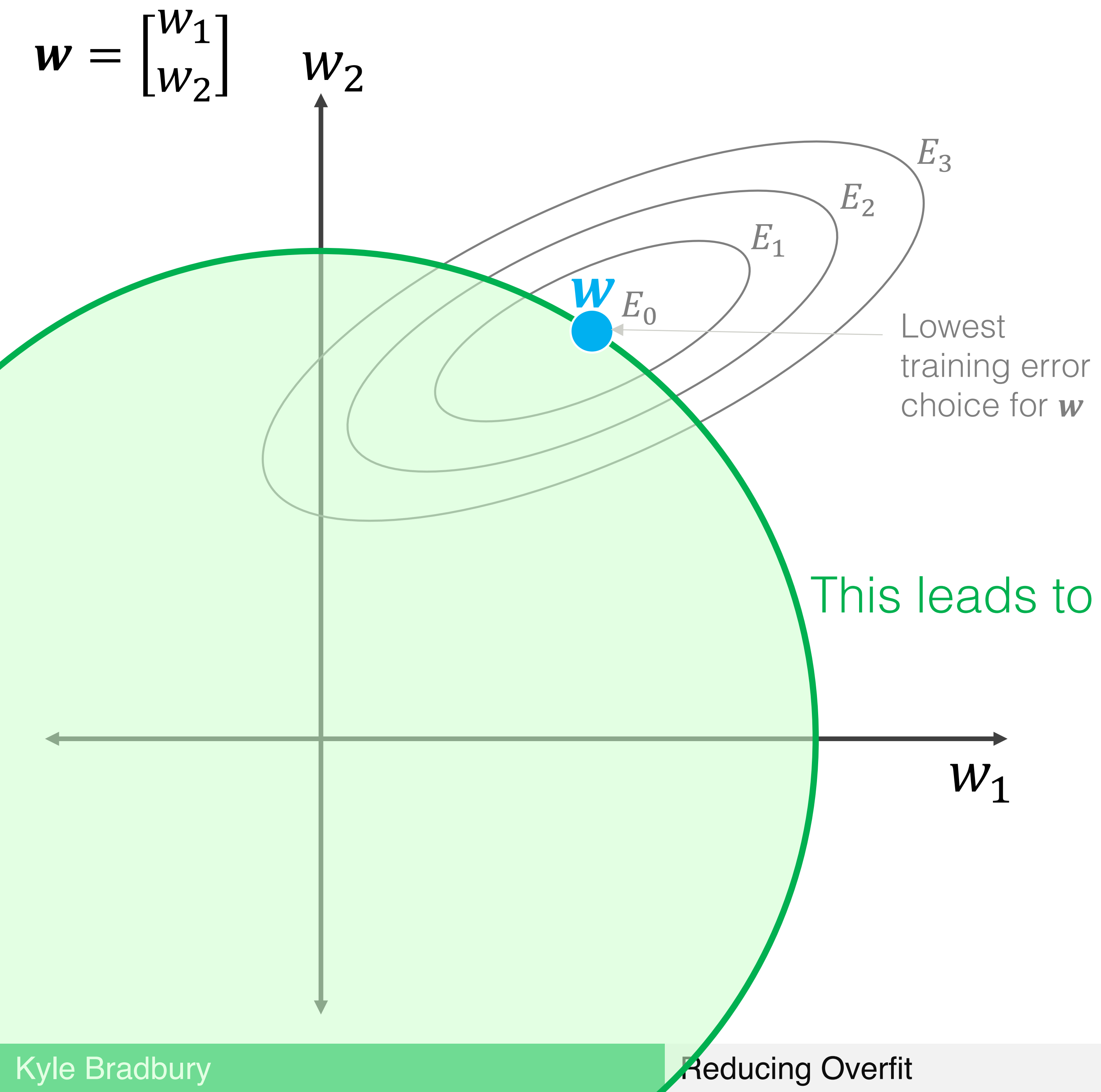
**First, let's just minimize training error**




Minimize cost function:

$$C(\boldsymbol{w}) = \underbrace{\sum_{i=1}^{n} (\boldsymbol{w}^T \boldsymbol{x}_i - y_i)^2}_{\text{Training error term (E)}} + \underbrace{\lambda \sum_{j=1}^{p} w_j^2}_{\text{Regularization penalty (R)}}$$

**Next, let's add a regularization penalty**




Minimize cost function:

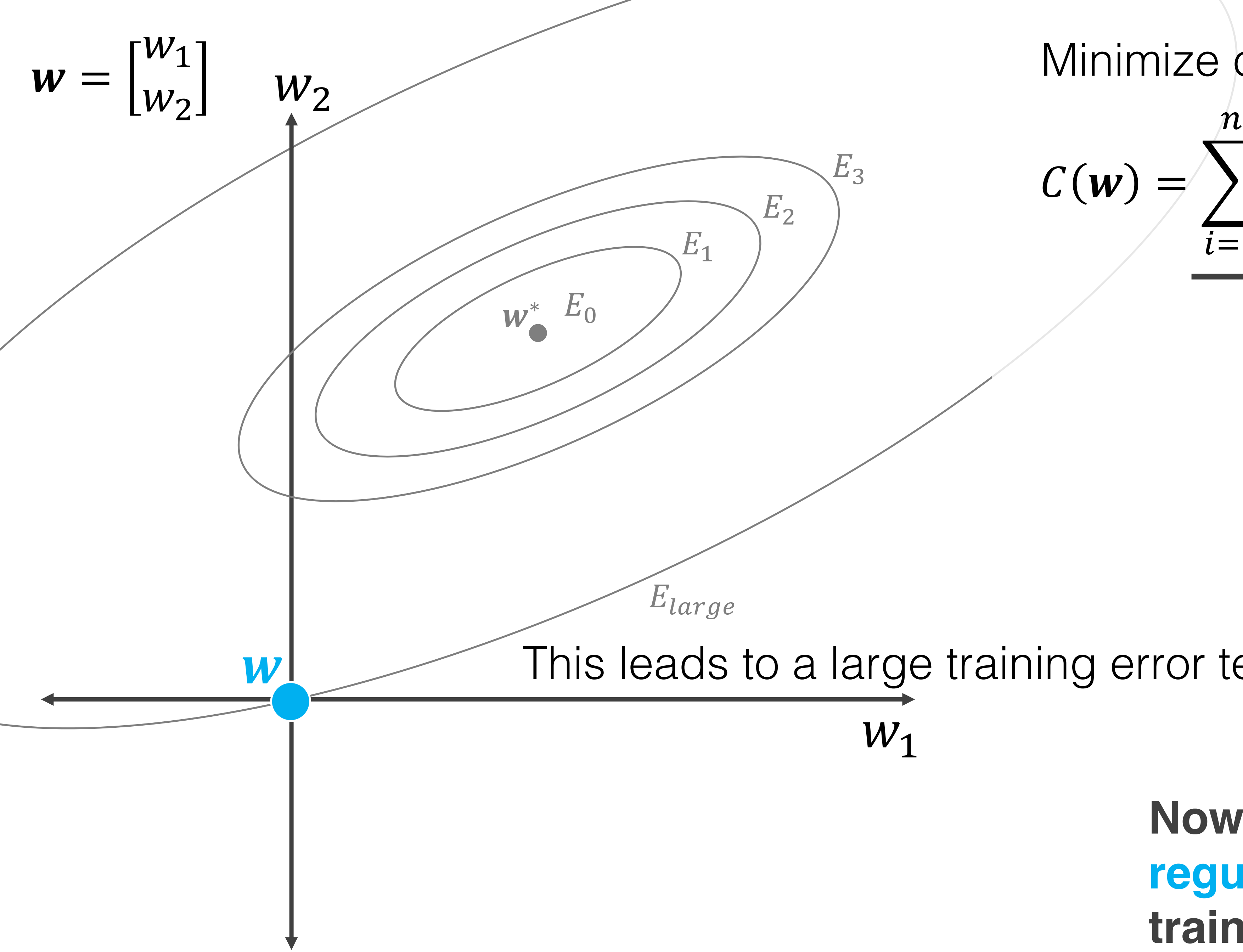
$$C(\boldsymbol{w}) = \underbrace{\sum_{i=1}^{n} (\boldsymbol{w}^T \boldsymbol{x}_i - y_i)^2}_{\text{Training error}} + \underbrace{\lambda \sum_{j=1}^{p} w_j^2}_{\text{Regularization penalty}}$$

**Small** **Large**

This leads to a large regularization penalty

**Now if we only minimize training error, the regularization penalty is large**

$$\boldsymbol{w} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$$



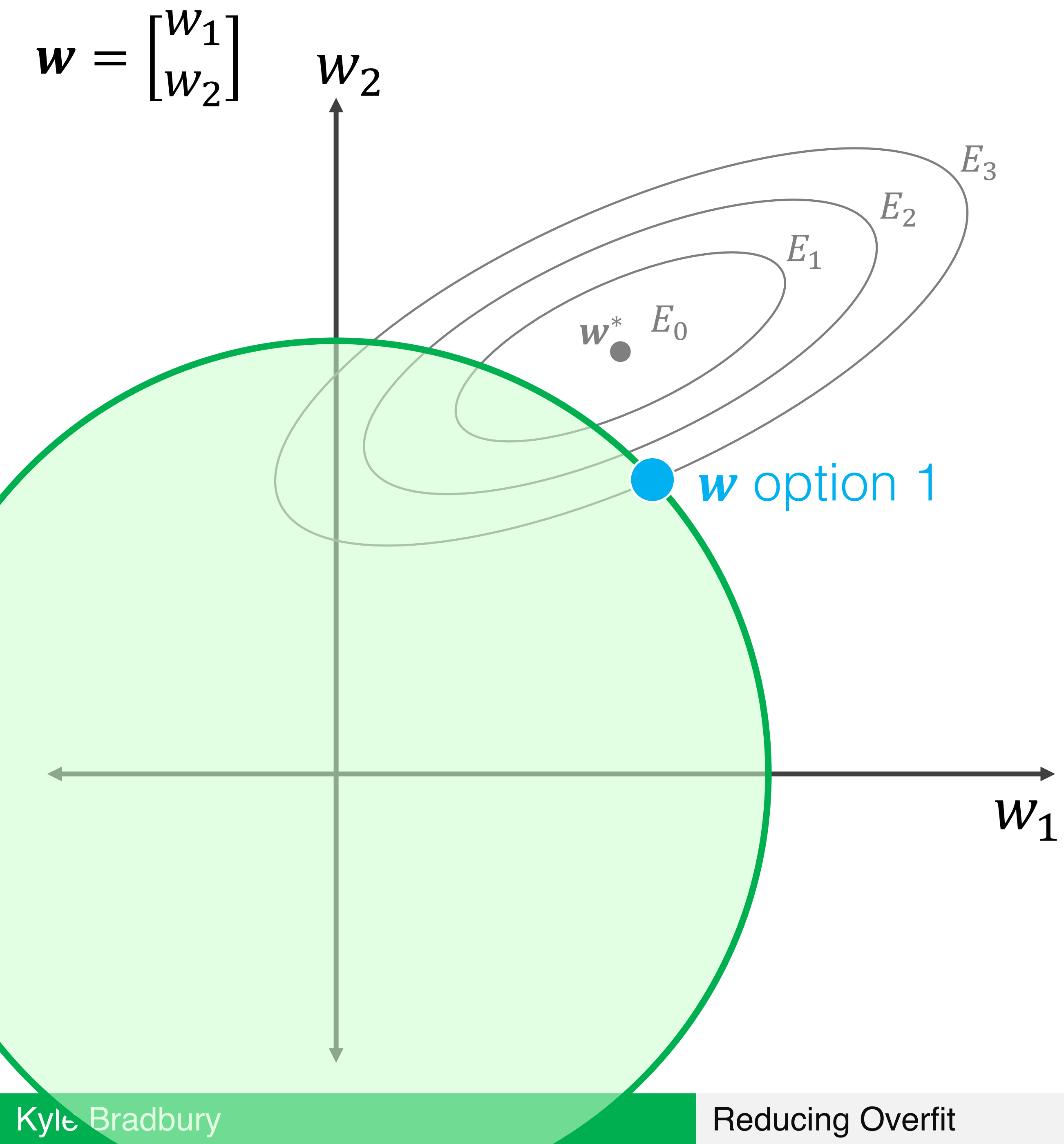

This leads to a large training error term…

Minimize cost function:

$$C(\boldsymbol{w}) = \underbrace{\sum_{i=1}^{n} (\boldsymbol{w}^T \boldsymbol{x}_i - y_i)^2}_{\text{Training error}} + \underbrace{\lambda \sum_{j=1}^{p} w_j^2}_{\text{Regularization penalty}}$$

**Large** **Small**

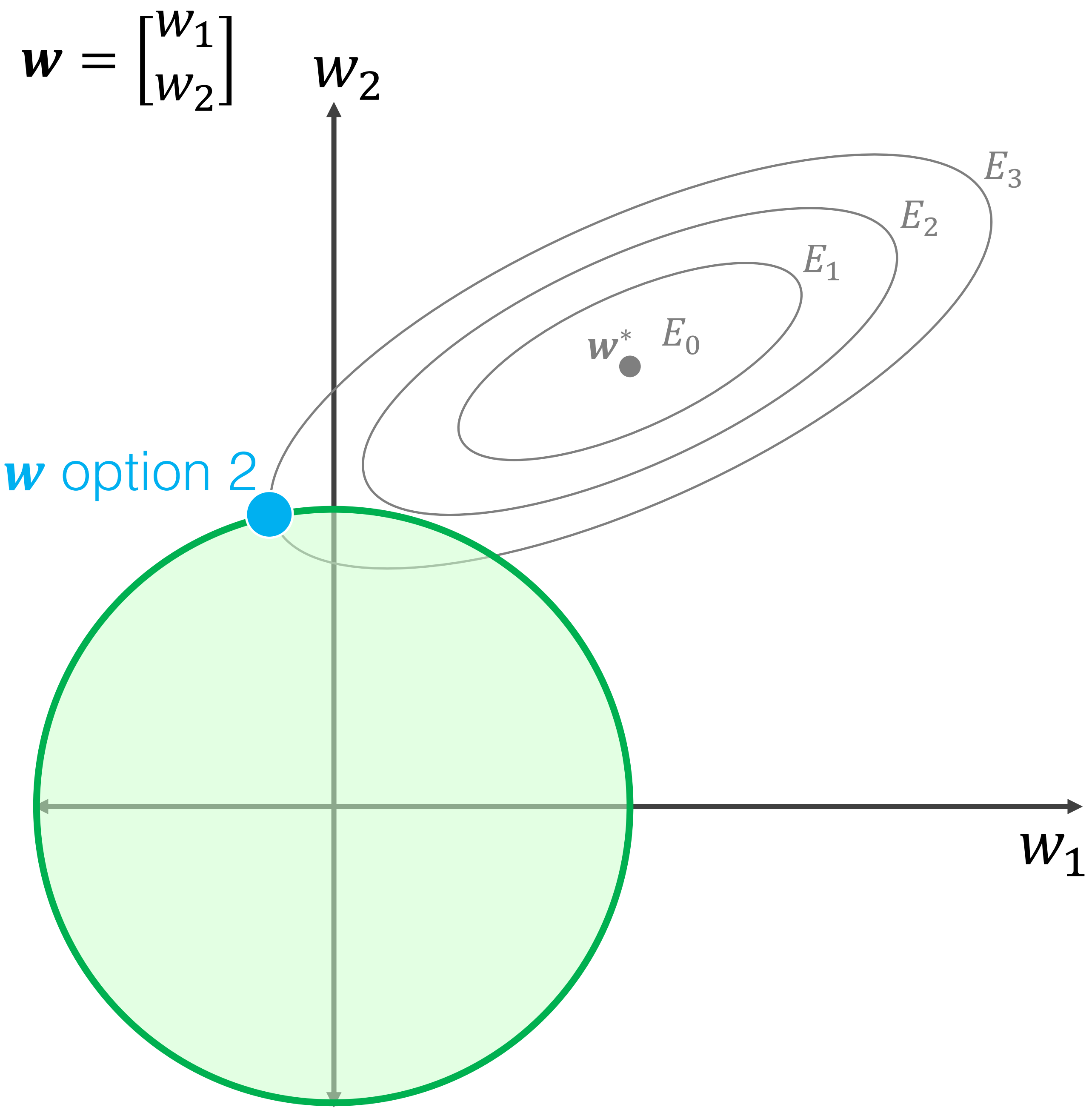
**Now if we only minimize regularization penalty, the training error is large**




Minimize cost function:

$$C(\mathbf{w}) = \underbrace{\sum_{i=1}^{n} (\mathbf{w}^T \mathbf{x}_i - y_i)^2}_{\text{Training error}} + \underbrace{\lambda \sum_{j=1}^{p} w_j^2}_{\text{Regularization penalty}}$$

For any level of training error (assume $E_3$ here), there may be many parameter values that result in an equivalent training error




Minimize cost function:

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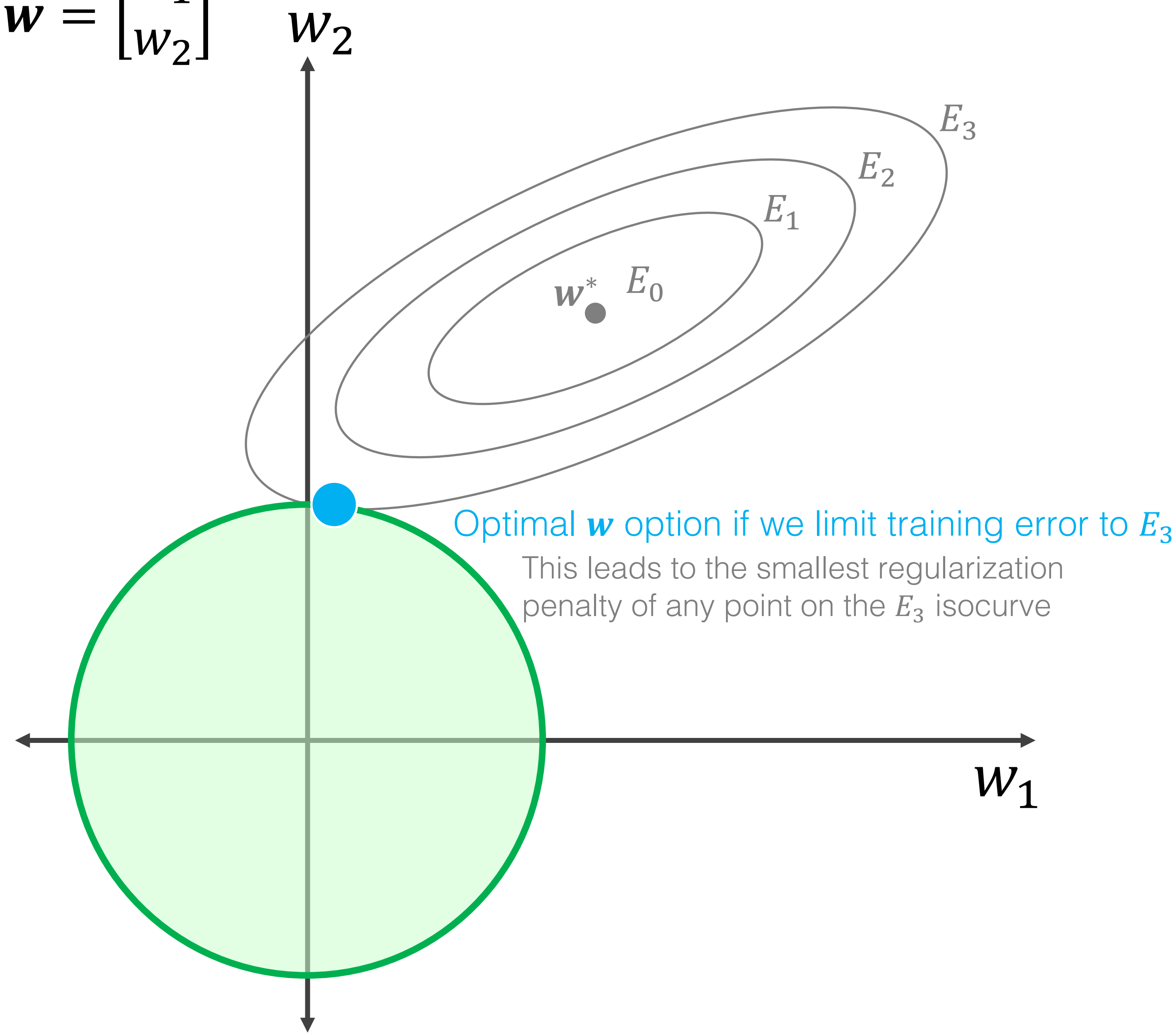
For any level of training error (assume $E_3$ here), there may be many parameter values that result in an equivalent training error

$\boldsymbol{w} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$

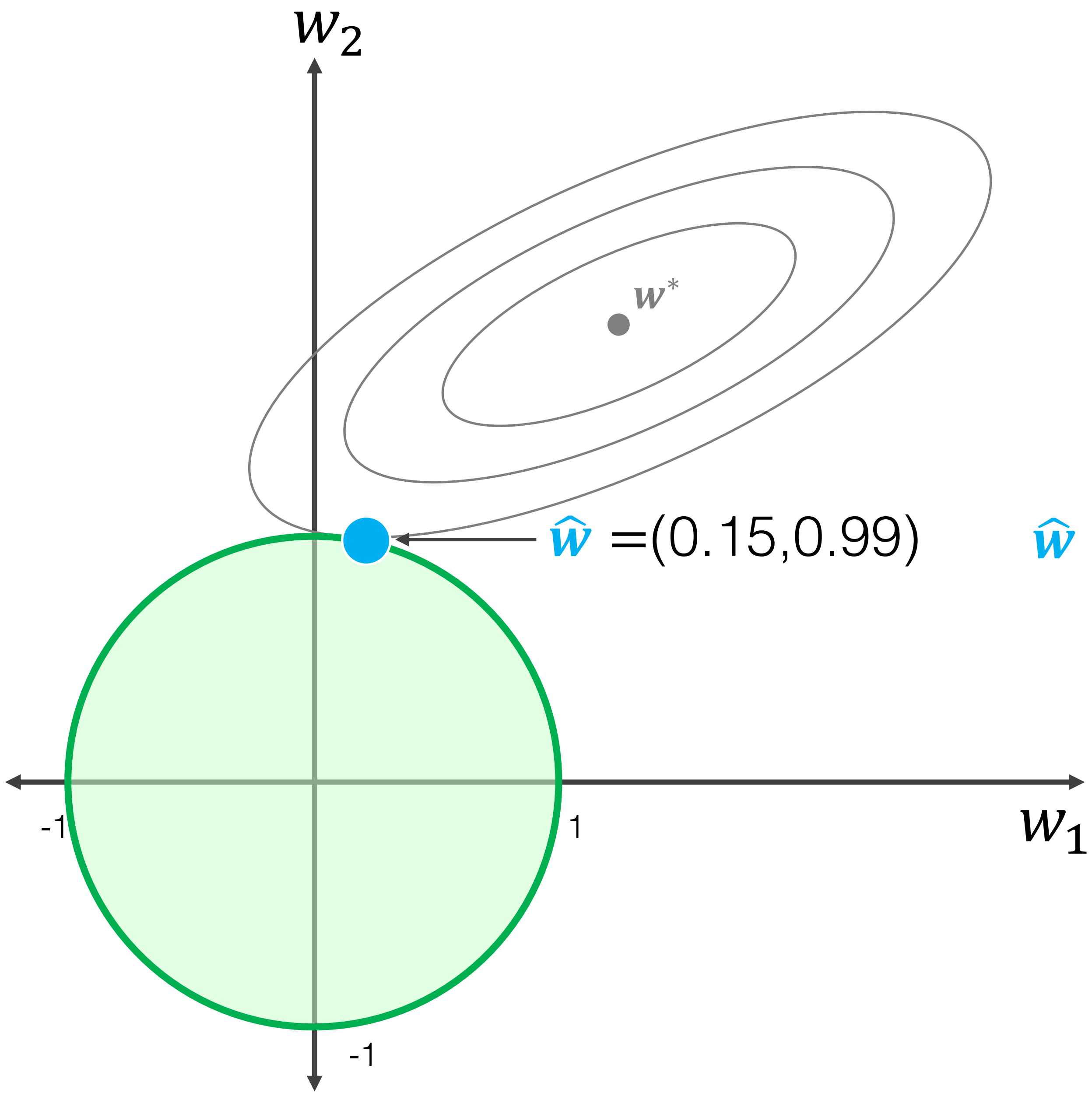



Minimize cost function:

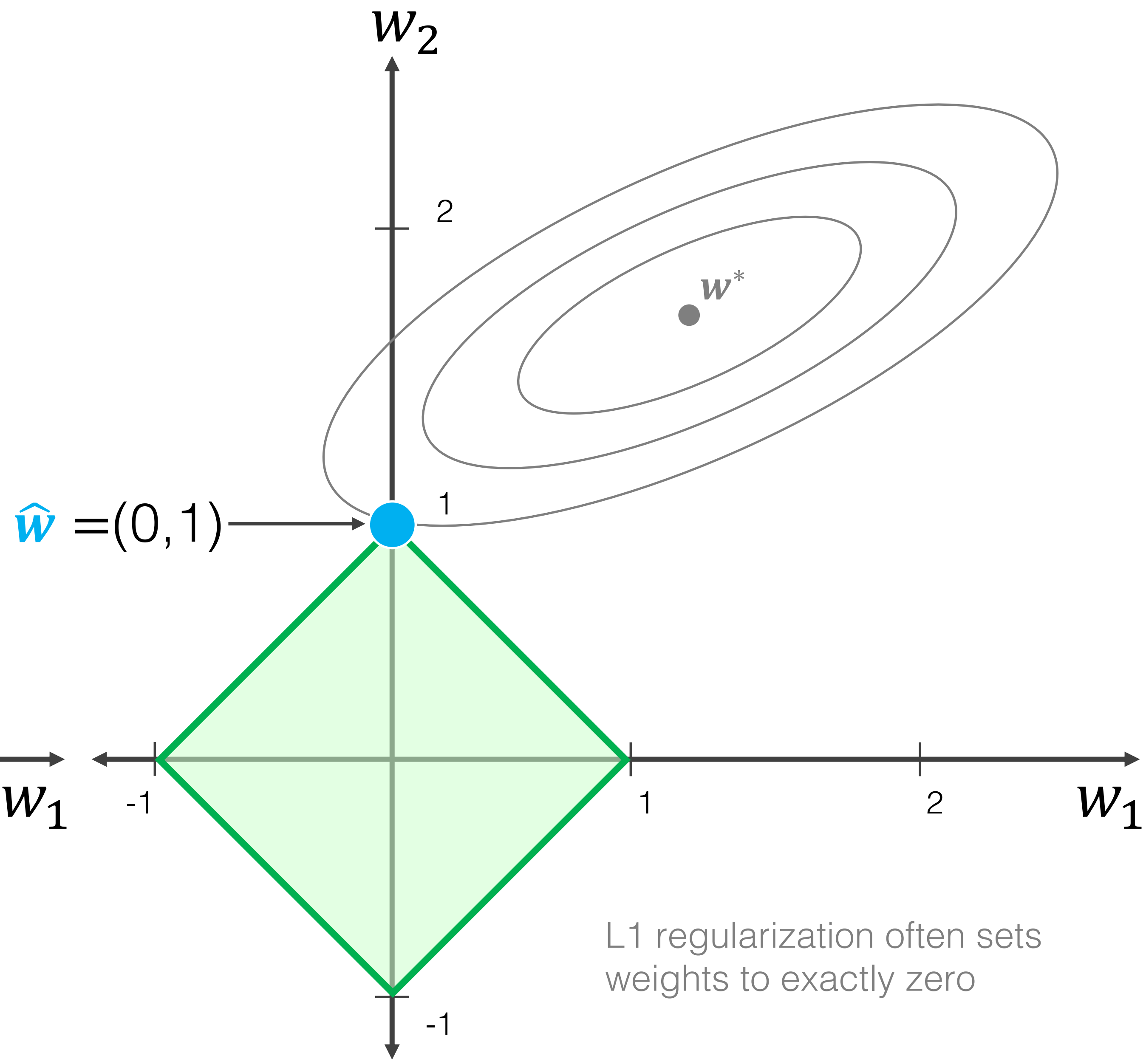
$$C(\boldsymbol{w}) = \underbrace{\sum_{i=1}^{n} (\boldsymbol{w}^T \boldsymbol{x}_i - y_i)^2}_{\text{Training error}} + \underbrace{\lambda \sum_{j=1}^{p} w_j^2}_{\text{Regularization penalty}}$$

However, we can choose between the options by minimizing the regularization penalty

## Ridge: $L_2$ regularization




## LASSO: $L_1$ regularization



# Regularization reduces variance

Leads to smaller model parameters

$L_1$ regularization also performs variable selection

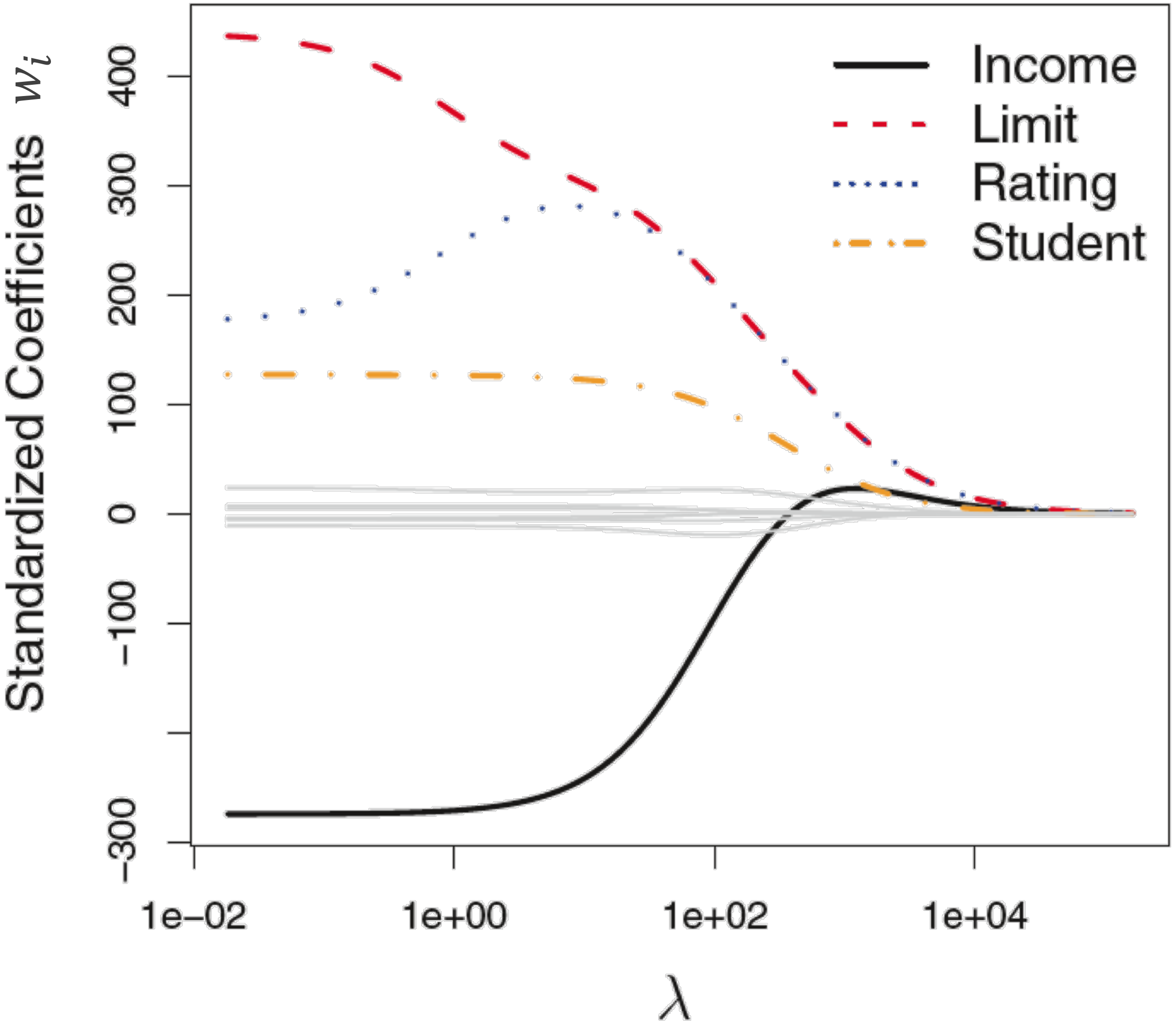
# Example: predicting credit default

11 features to use to predict default:

- Income
- Credit limit
- Credit rating
- Credit balance
- Number of credit cards
- Age
- Education
- Gender
- Student status
- Ethnicity
- Marriage status

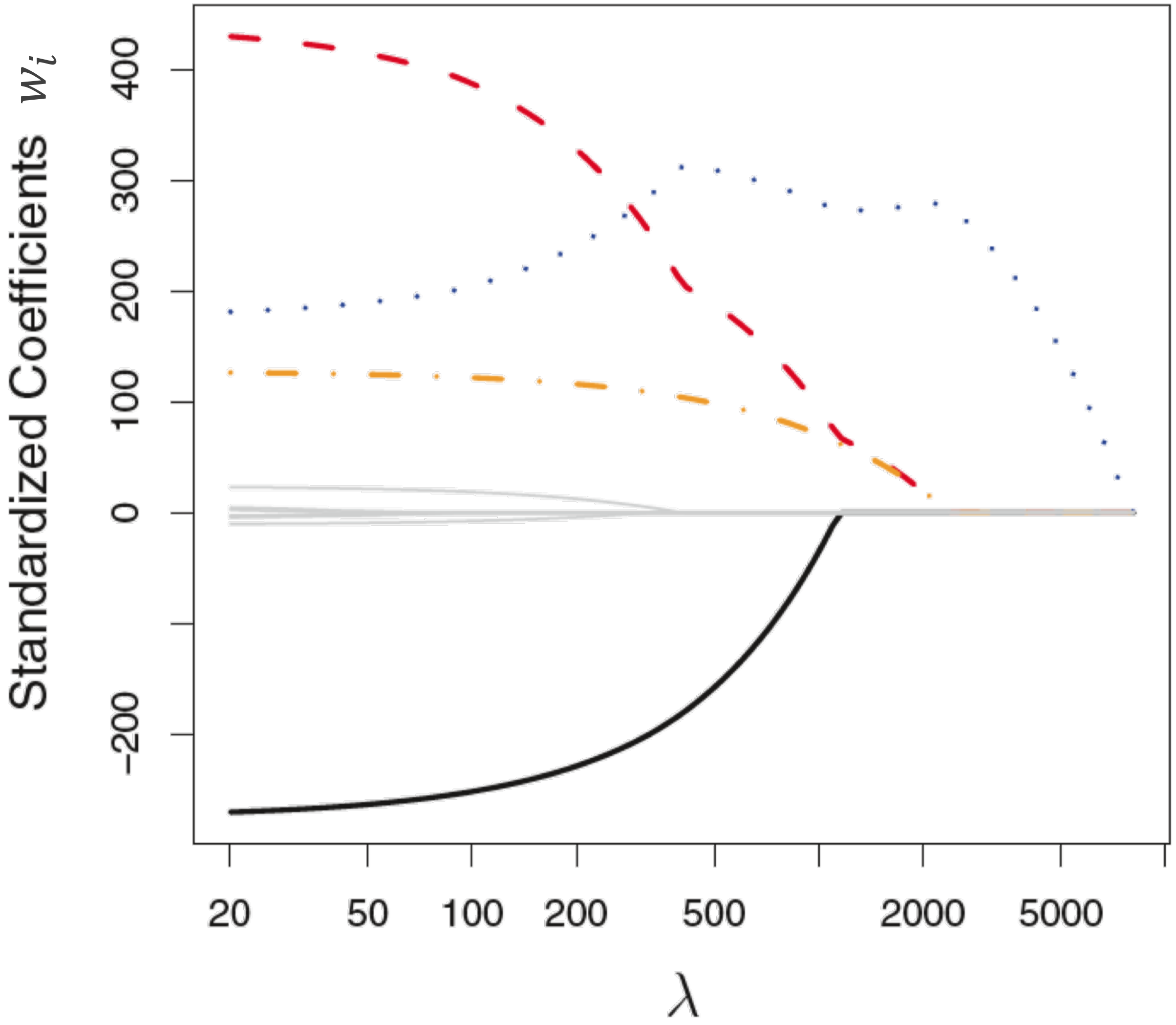
# $L_2$ regularization

Ridge regression



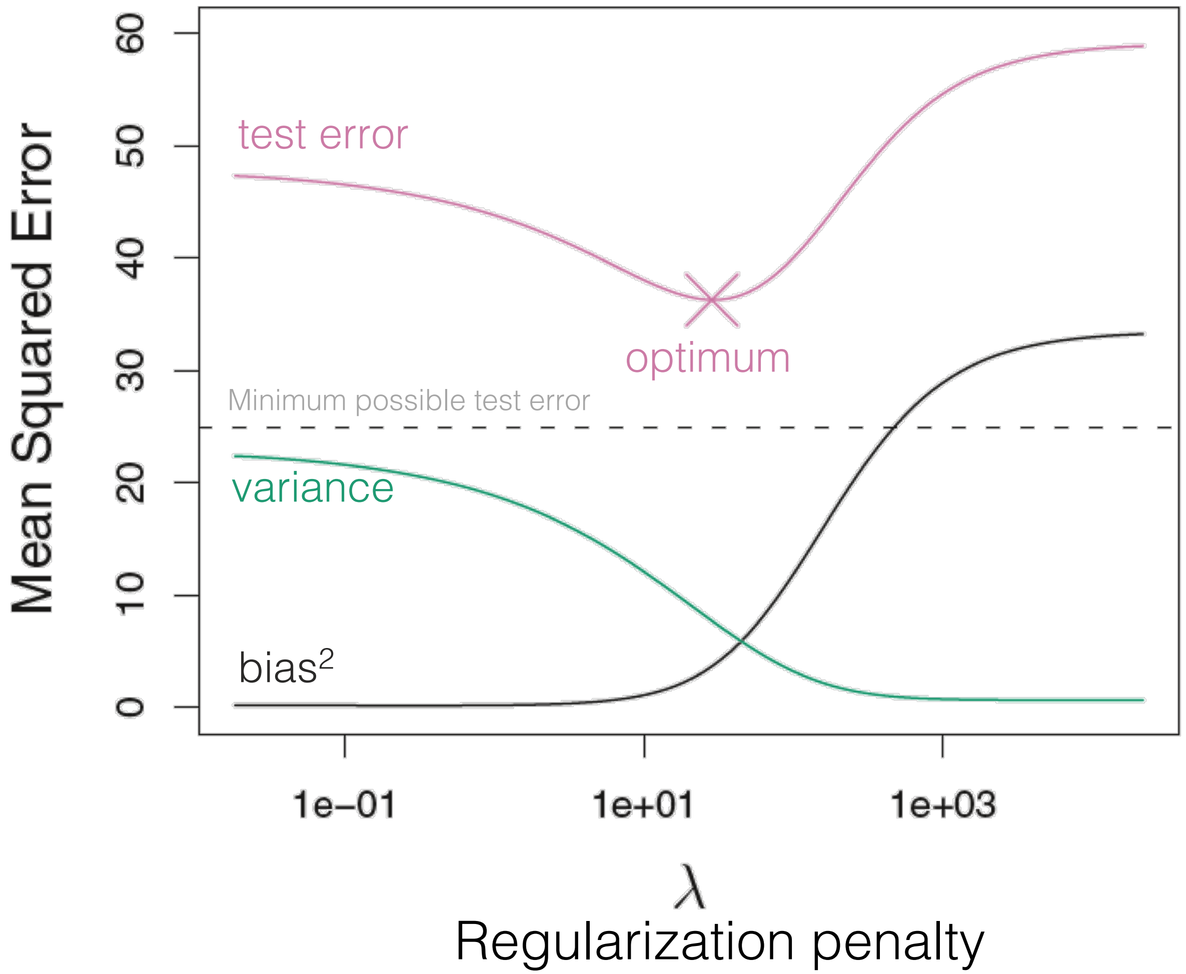

# $L_1$ regularization

LASSO regularization

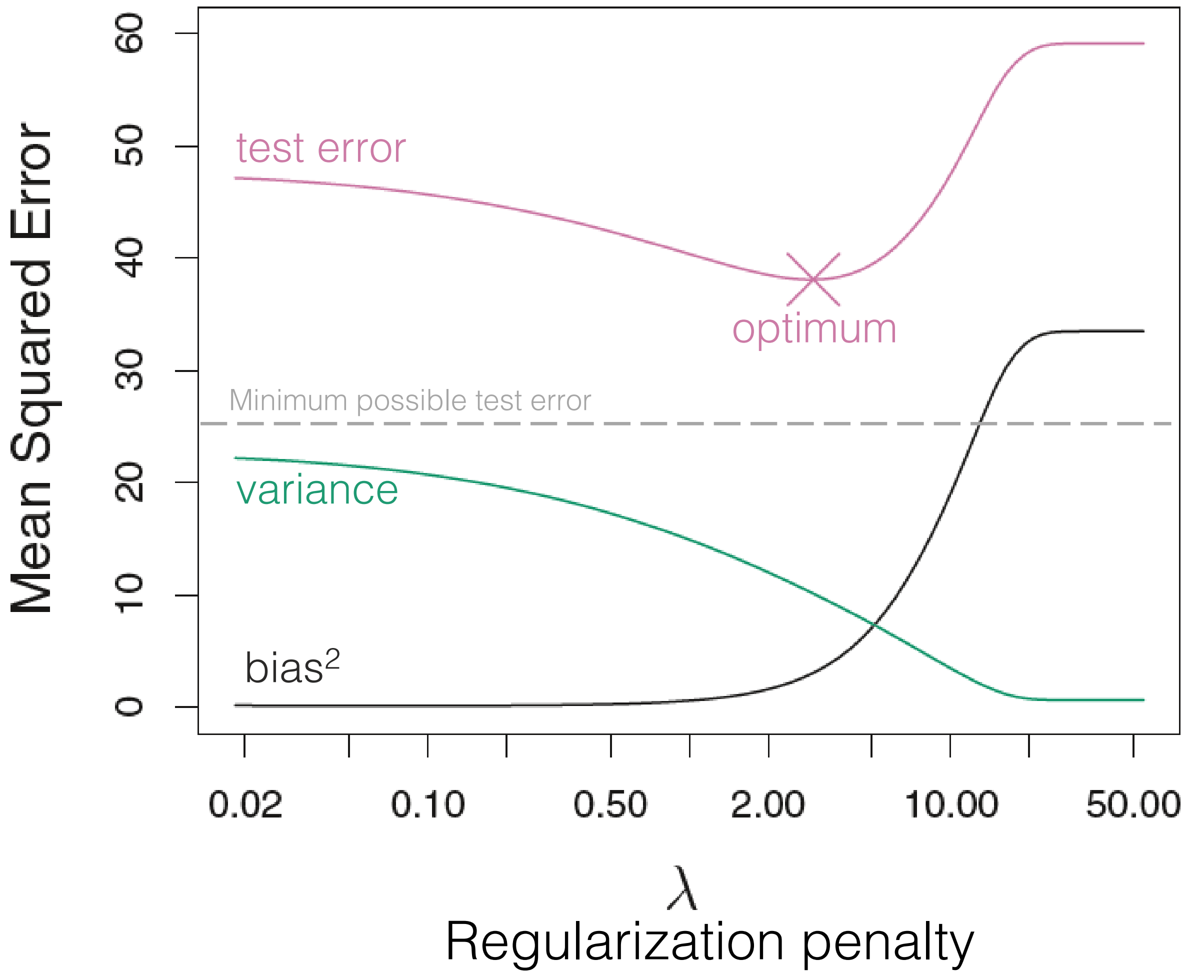



Images from James et al., An Introduction to Statistical Learning

## $L_2$ regularization




## $L_1$ regularization




Images from James et al., An Introduction to Statistical Learning

# Underdetermined systems and OLS

Number of features

$$X = \overbrace{\begin{bmatrix} \quad & & \quad \\ & & \\ & & \end{bmatrix}}^{p} \left.\vphantom{\begin{bmatrix} \\ \\ \\ \end{bmatrix}}\right\} N$$

Number of samples

If $p > N$, then the system is **underdetermined**

Often means there are infinitely many solutions

Ridge regression makes this problem solvable

# Choosing the regularization parameter $\lambda$

- $\lambda$ is a hyperparameter
- Use a training, validation, and test set
- Can also apply nested cross validation

| Train | Validation | Test |
|---|---|---|
| Used for model training / fitting | Used to optimize hyperparameters | Used to evaluate generalization performance |

# Strengths of $L_1$ and $L_2$ regularization

Ridge regression ($L_2$ regularization) handles **multicollinearity** well

LASSO regularization ($L_1$ regularization) reduces the number of predictors in a model (yields **sparse** models)

You can use a little of both via elastic net regularization

These approaches can be easily added to many cost functions

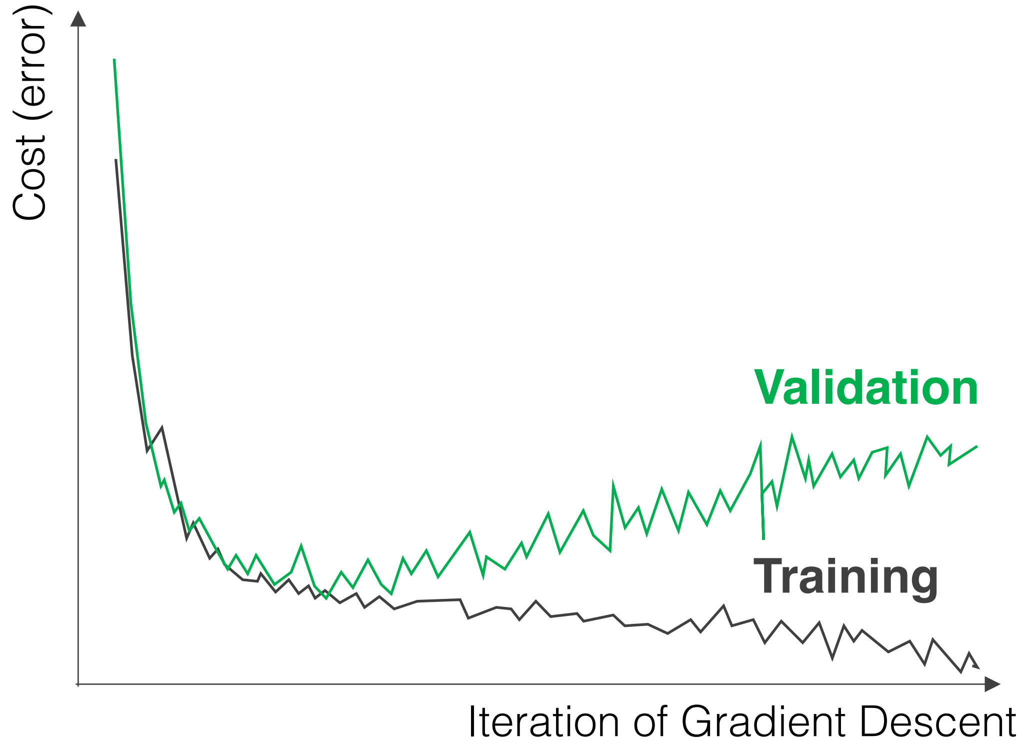
# One more approach: Early Stopping

Iterative learning (training) methods, (e.g. gradient descent) tend to learn more complex models over time

Stop the fitting process earlier, before overfit has occurred

Common in neural network training

Learning Curves



# Takeaways

Reducing the number of features in a model may improve generalization error by reducing overfit

Overly flexible models can be regularized to reduce overfit (reducing variance)

$L_1$ and $L_2$ regularization are effective tools for battling overfit