Reducing Overfit

Lecture 9

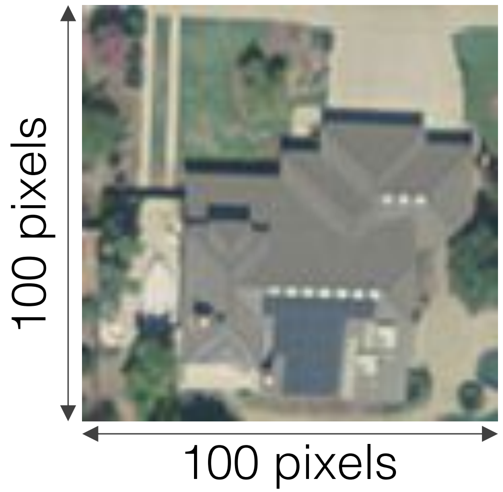
Challenge

You have a dataset with n = 1,000 samples (observations)

Each observation has p = 10,000 predictors (features)

You're asked to develop a classifier for the data

p >> n ….what do you do?

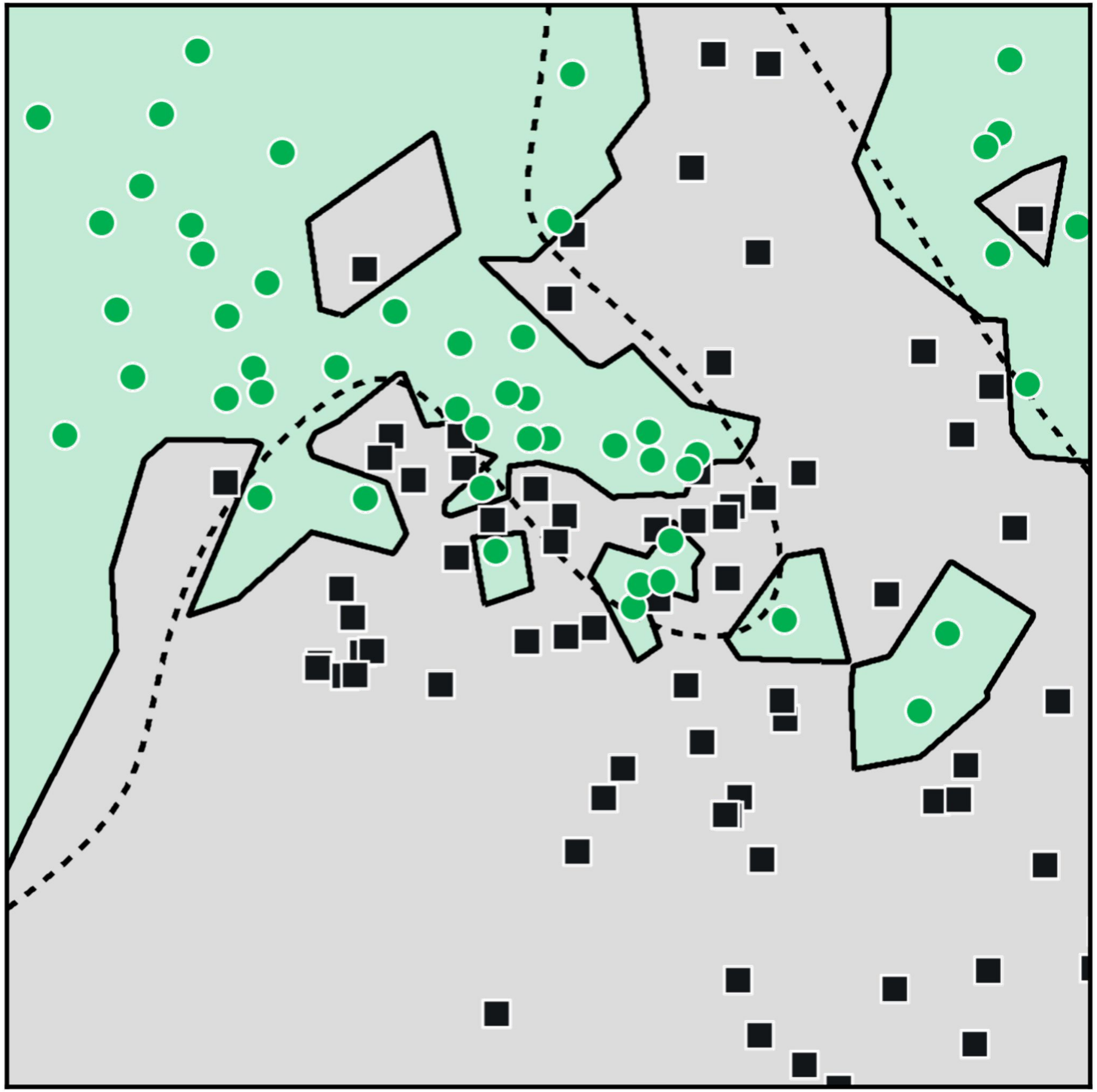


This is the case for most image classification tasks

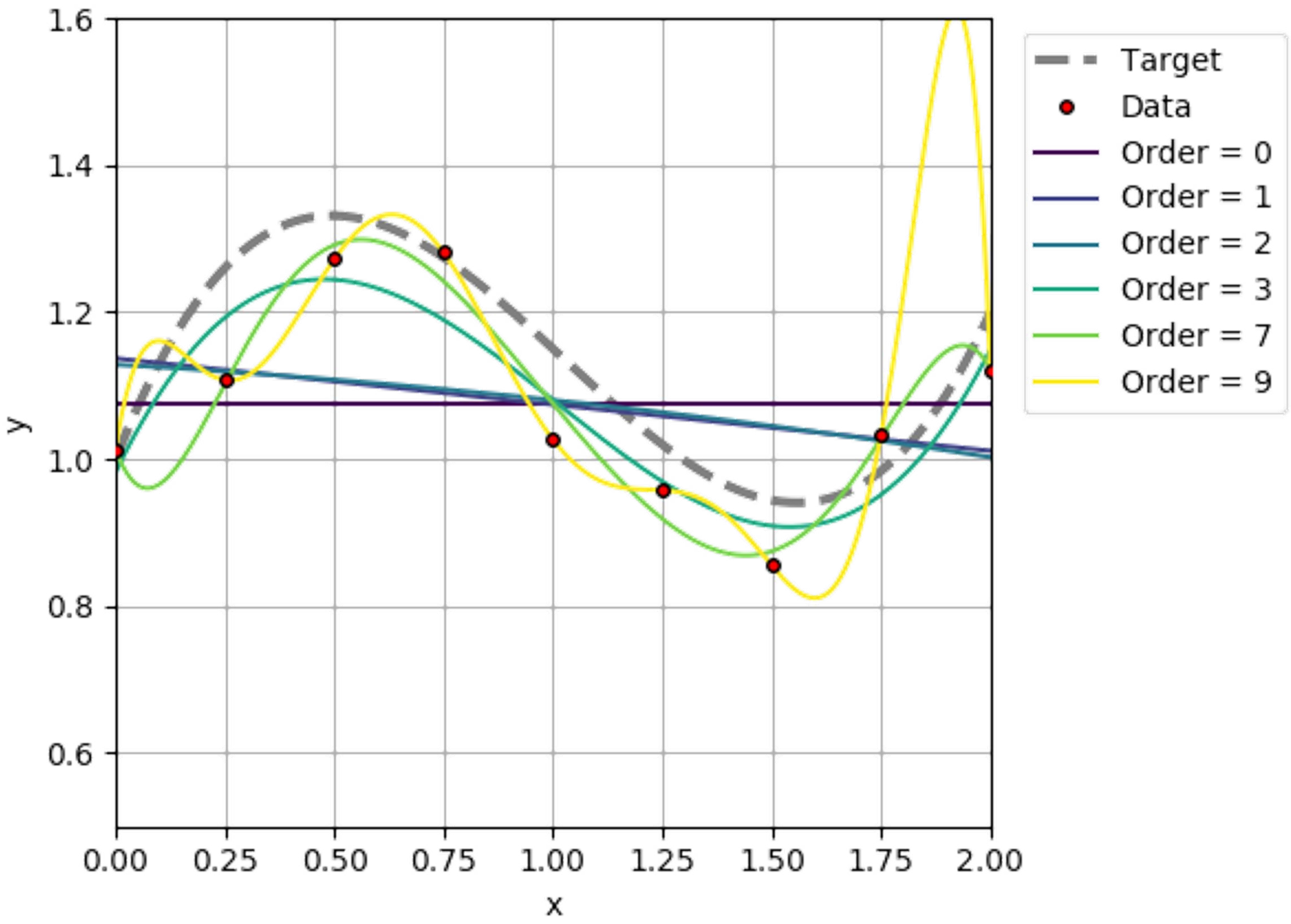
A problem…

Overfitting to the training data

High model **variance**



Overfitting to the training data



How do we reduce model variance?

Option #1: Add more data!

Option #2: Reduce model flexibility to reduce variance

Our conceptual tool…

Image from Speckyboy.com

Occam's Razor / Law of Parsimony

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

Options for reducing variance

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

Benefits of reducing the number of predictors/features

Some algorithms scale poorly with increased dimensions (computationally)

Irrelevant and redundant features can confuse algorithms - removal of these features can increase generalization performance

Often reduces training data needs

Feature (variable) selection

Filter methods
(e.g. remove correlated features)

Wrapper methods
(e.g. subset selection)

Embedded methods
(e.g. LASSO regularization)

Variable subset selection:
wrapper methods for feature 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)

Regularization

methods for variance reduction

Reduce the variance by simplifying the model during training

Techniques that reduce generalization error, but NOT training error

Recall the model fitting process

1. Choose a **hypothesis set of models** to train
   (e.g. linear regression with p predictor variables)

2. Identify a **cost function** to measure the model fit to the training data
   (e.g. mean square error)

3. **Optimize** model **parameters** to minimize cost
   (e.g. ordinary least squares or gradient descent)

Regularization

a.k.a. shrinkage

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

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

Square error

L_2 regularization penalty

This term causes the estimated parameter values to "shrink"

More generally: $L(\boldsymbol{w}) = C(\boldsymbol{w}, \boldsymbol{X}, \boldsymbol{y}) \;+\; \lambda R(\boldsymbol{w})$

Norms

Norms

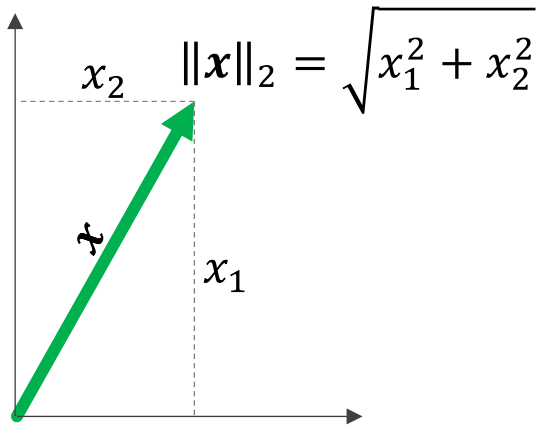
A function that assigns a positive **length or size** to a vector

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:

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

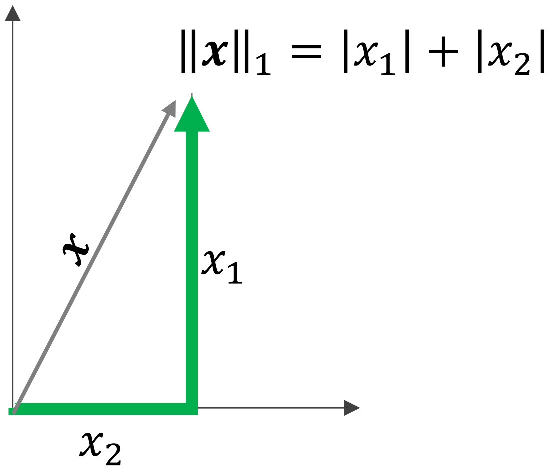


Norms

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**:

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

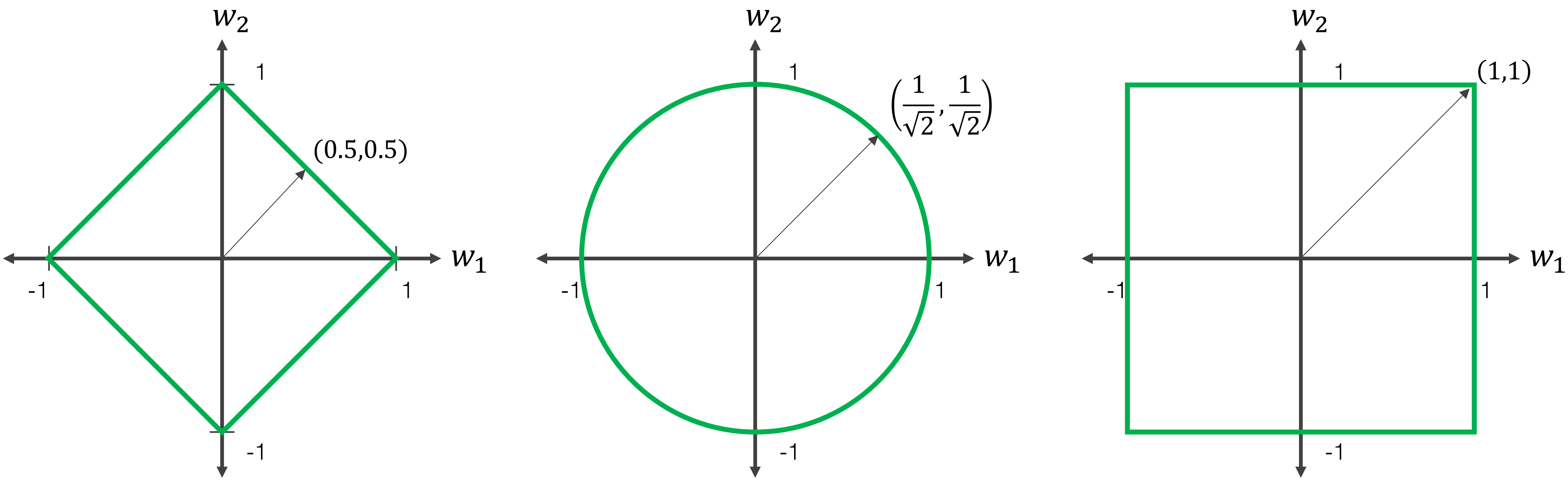
In the limit, the **infinity norm** is the maximum entry of the vector $\boldsymbol{x}$:

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

Norms of length 1

Assume a 2-D vector whose origin is (0,0): $\boldsymbol{w} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$

$\|\boldsymbol{w}\|_1 = 1$ $\|\boldsymbol{w}\|_2 = 1$ $\|\boldsymbol{w}\|_\infty = 1$



Regularization

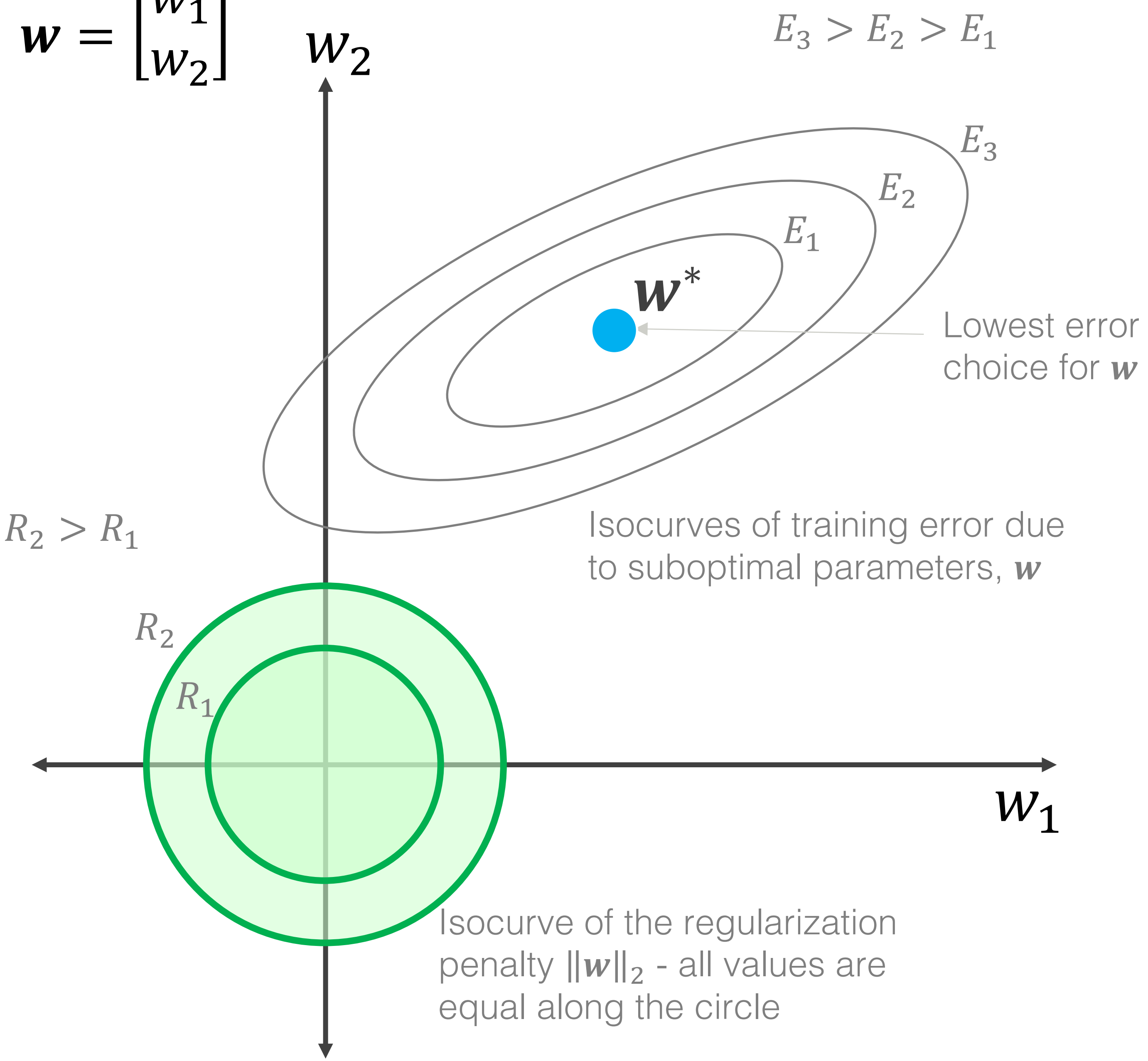
a.k.a. shrinkage

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

a.k.a….

L_2 regularization	$L(\boldsymbol{w}) = \sum_{i=1}^{n} (\boldsymbol{w}^T \boldsymbol{x}_i - y_i)^2 + \lambda \sum_{j=1}^{p} w_j^2$	**ridge regression** or weight decay (Tikhonov regularization)
L_1 regularization	$L(\boldsymbol{w}) = \sum_{i=1}^{n} (\boldsymbol{w}^T \boldsymbol{x}_i - y_i)^2 + \lambda \sum_{j=1}^{p} \lvert w_j \rvert$	least absolute shrinkage and selection operator (**LASSO**)
L_2 & L_1 regularization	$L(\boldsymbol{w}) = \sum_{i=1}^{n} (\boldsymbol{w}^T \boldsymbol{x}_i - y_i)^2 + \lambda_1 \sum_{j=1}^{p} \lvert w_j \rvert + \lambda_2 \sum_{j=1}^{p} w_j^2$	**elastic net** regularization

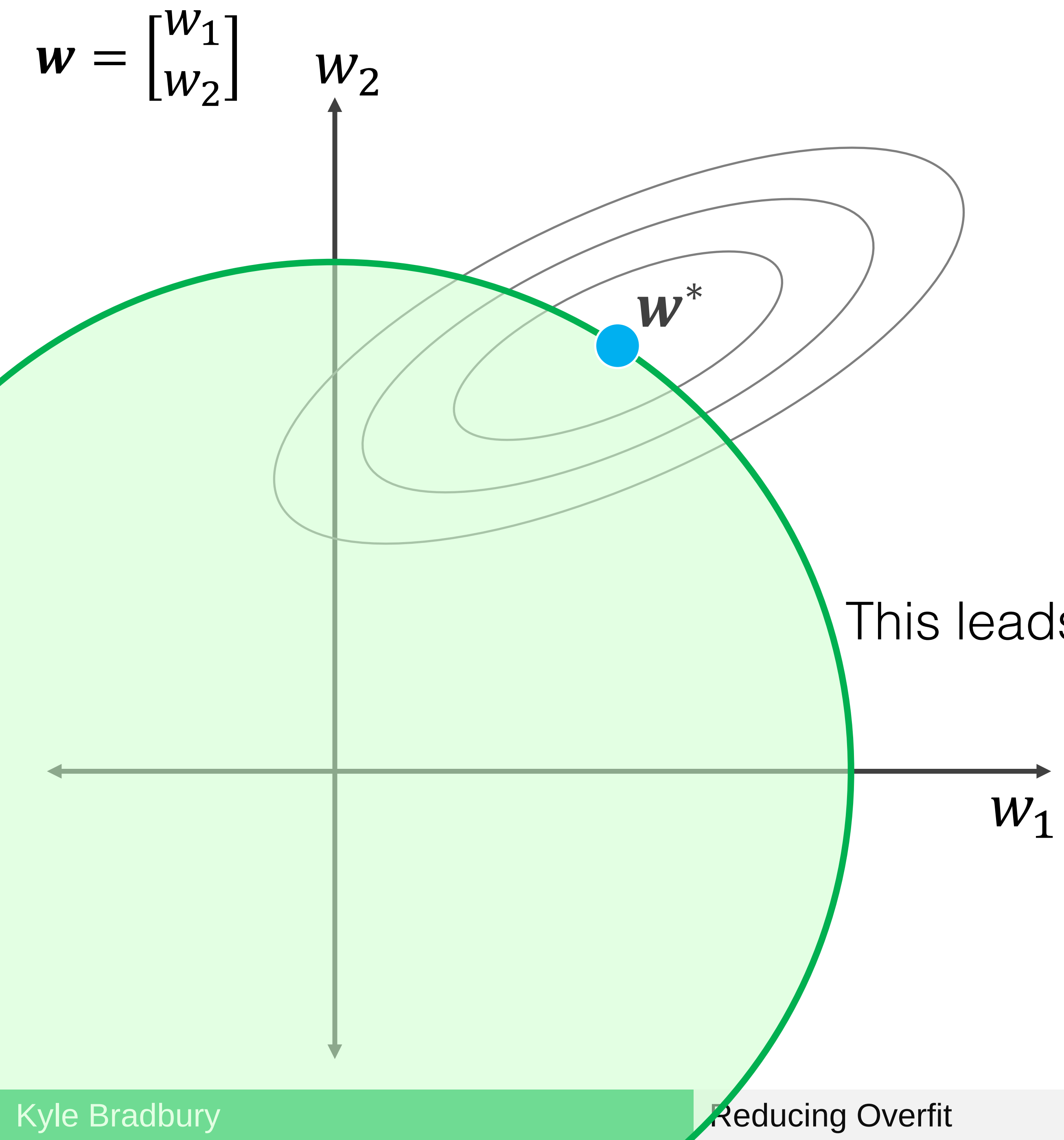
$$\boldsymbol{w} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$$



Trying to minimize my loss function:

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

First attempt let's just minimize error



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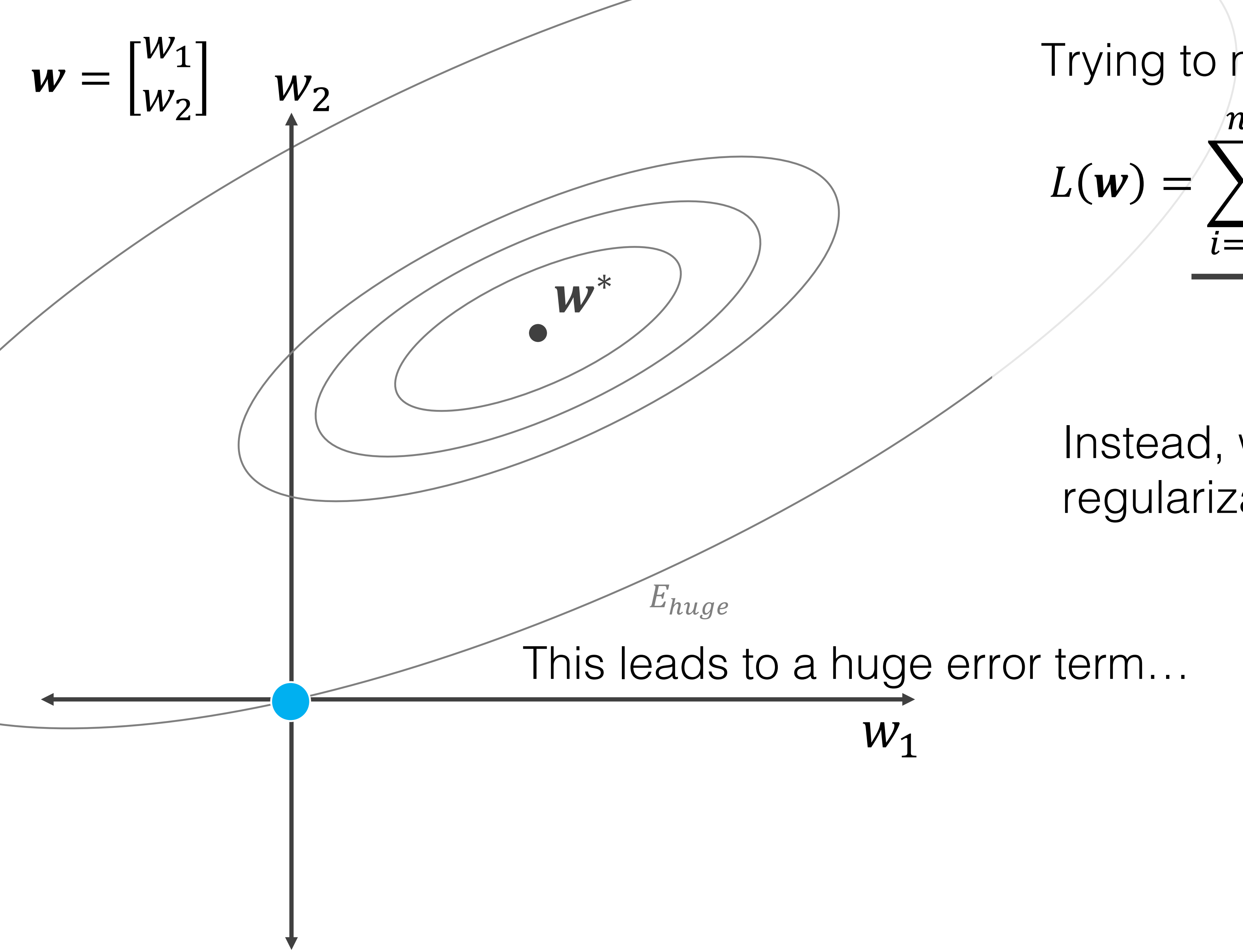
First attempt let's just minimize error

This leads to a huge regularization penalty



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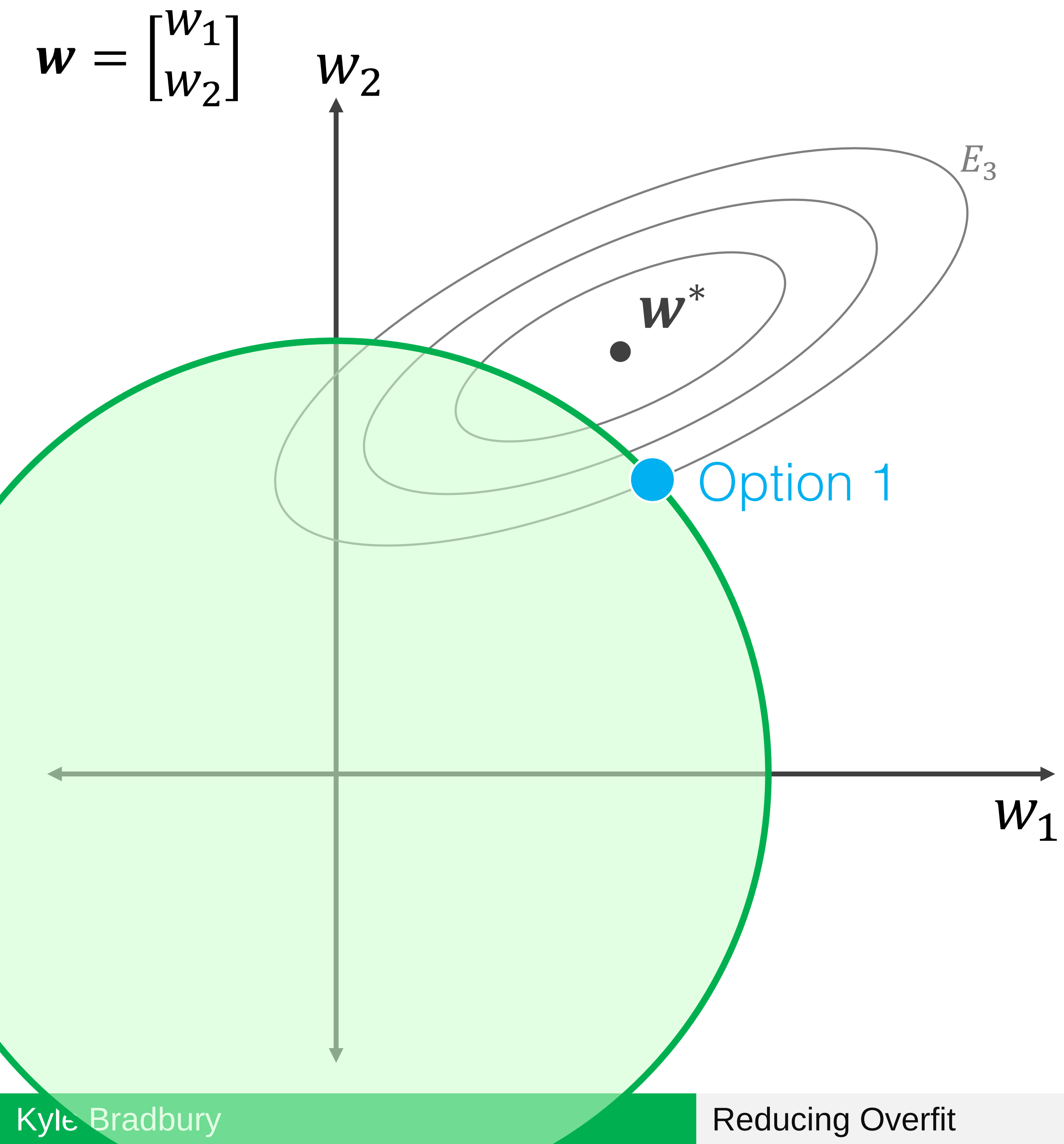
Instead, we could just minimize the regularization penalty



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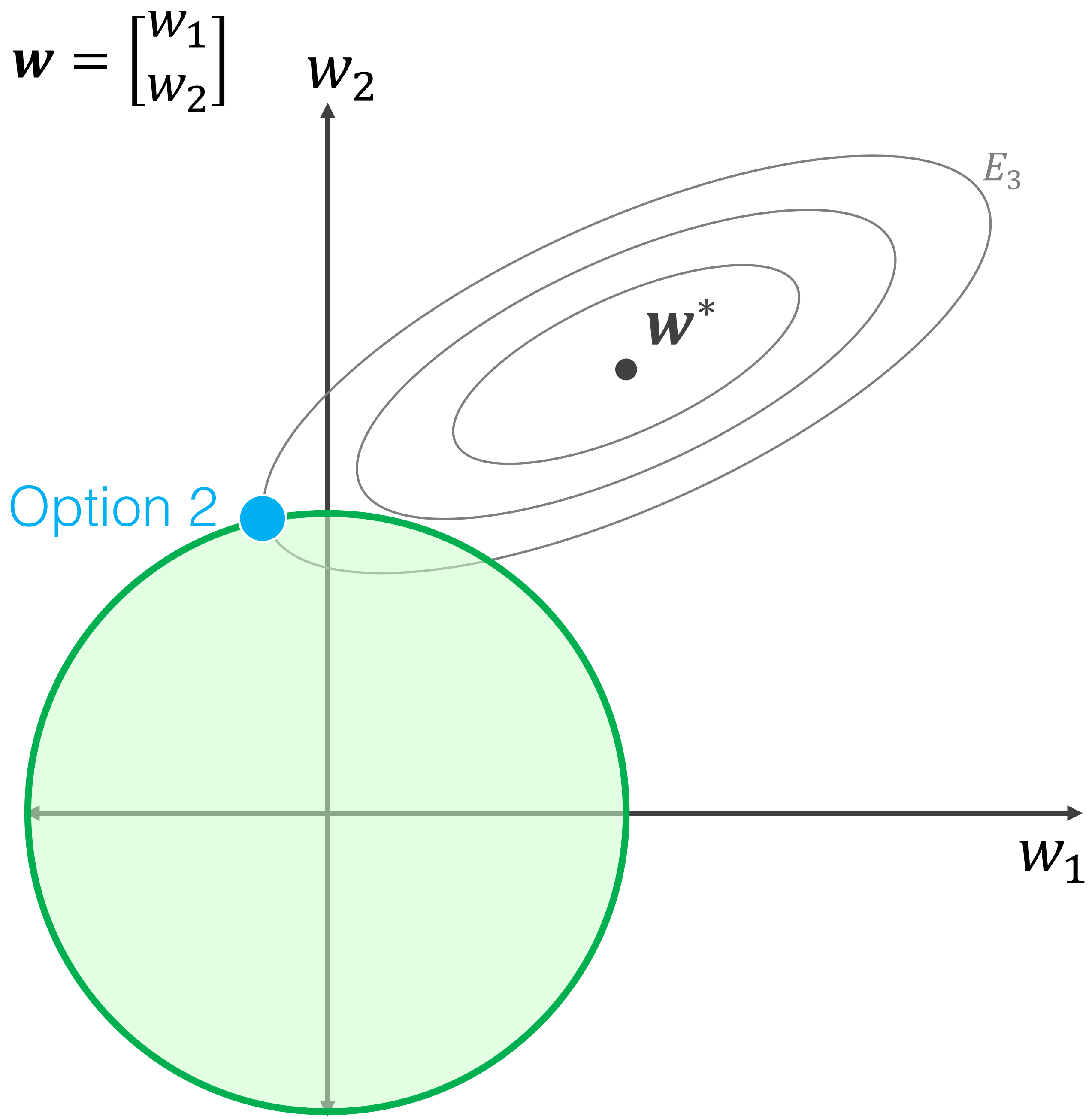
For any level of error (assume E_3 here), there may be a number of parameter values that result in an equal error term



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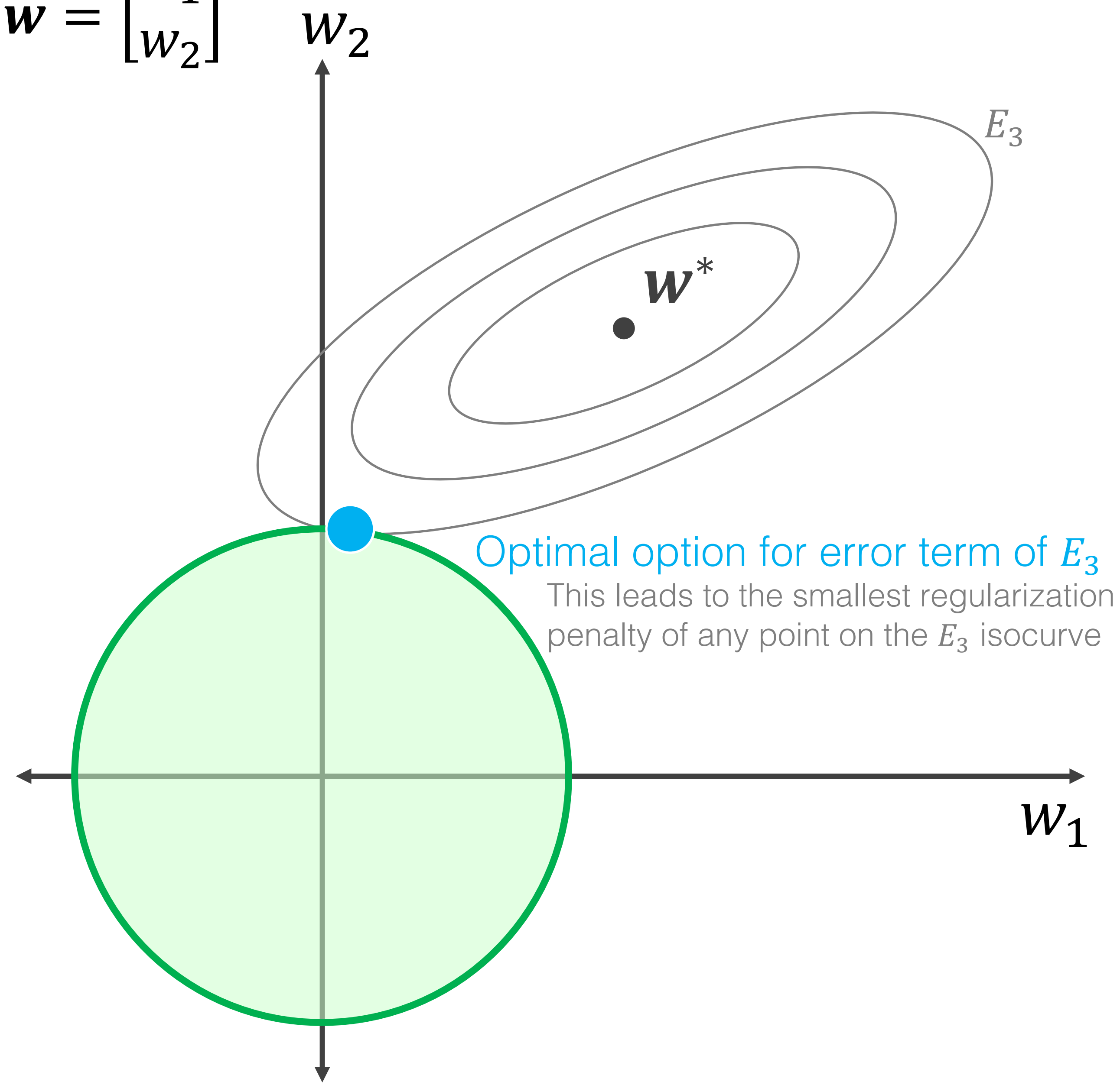
$$\mathbf{w} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$$



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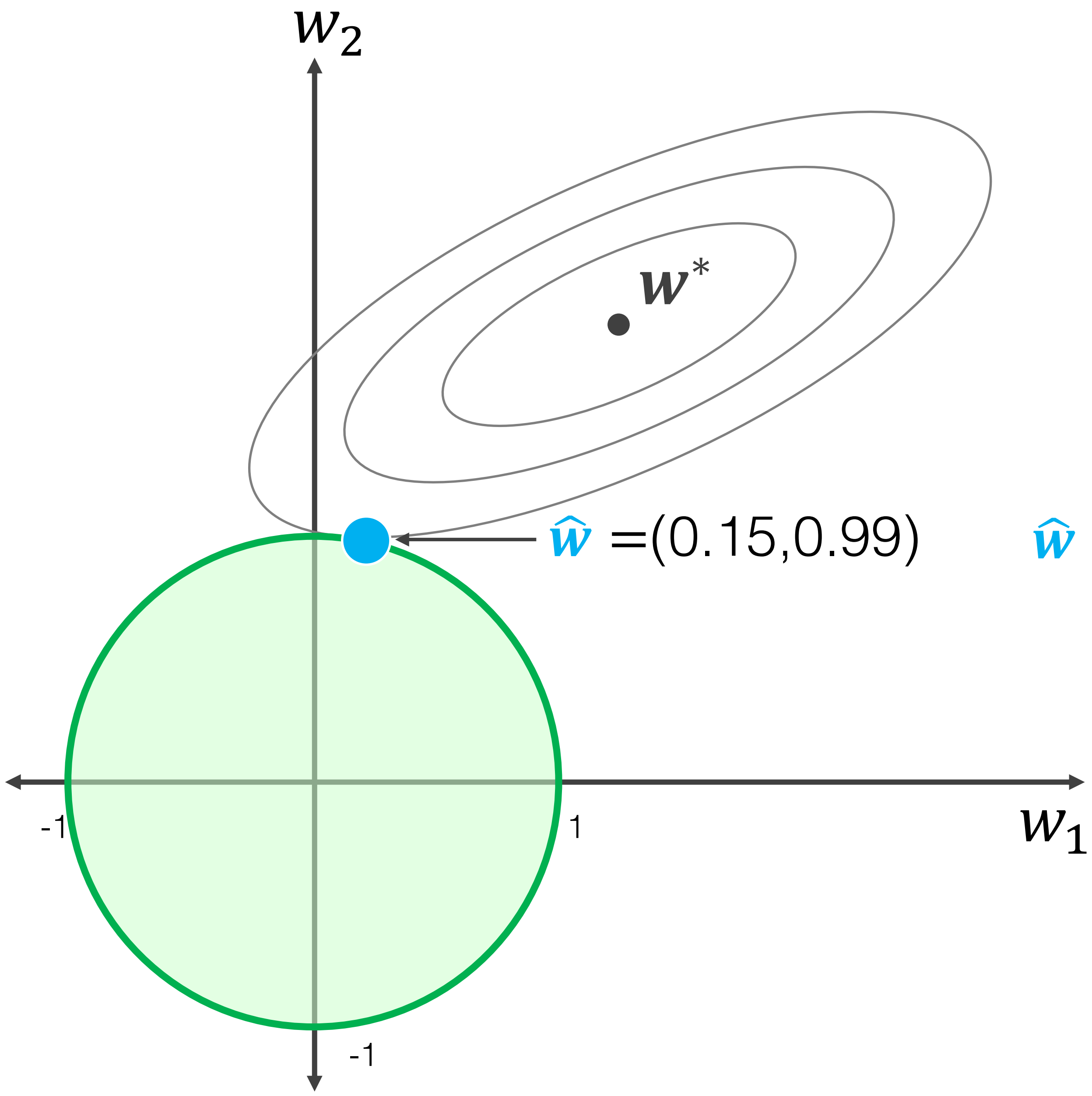
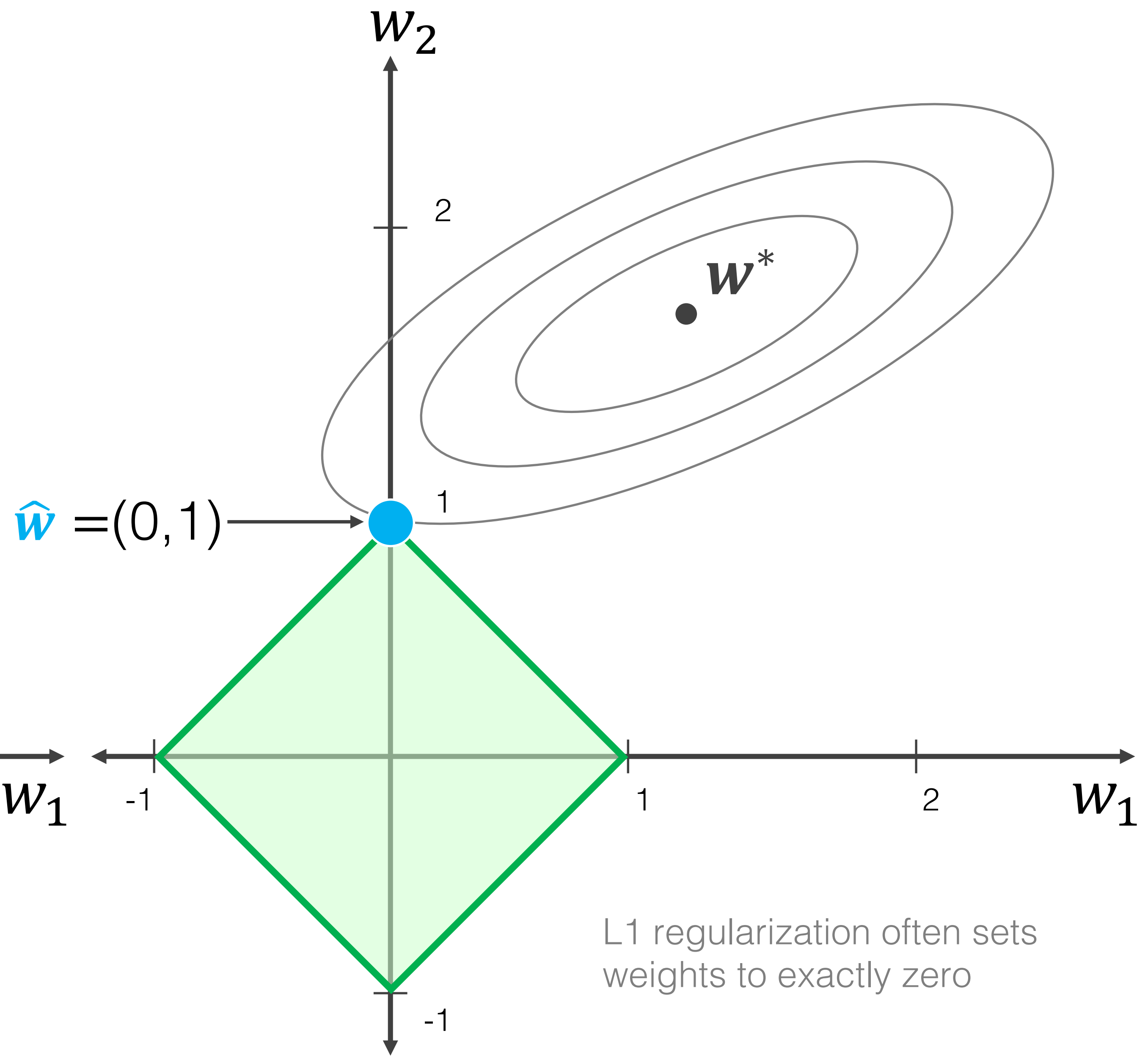
However, we can choose between the options by minimizing the regularization penalty

Ridge: L_2 regularization



LASSO: L_1 regularization



L1 regularization often sets weights to exactly zero

Regularization reduces variance

Leads to smaller model parameters

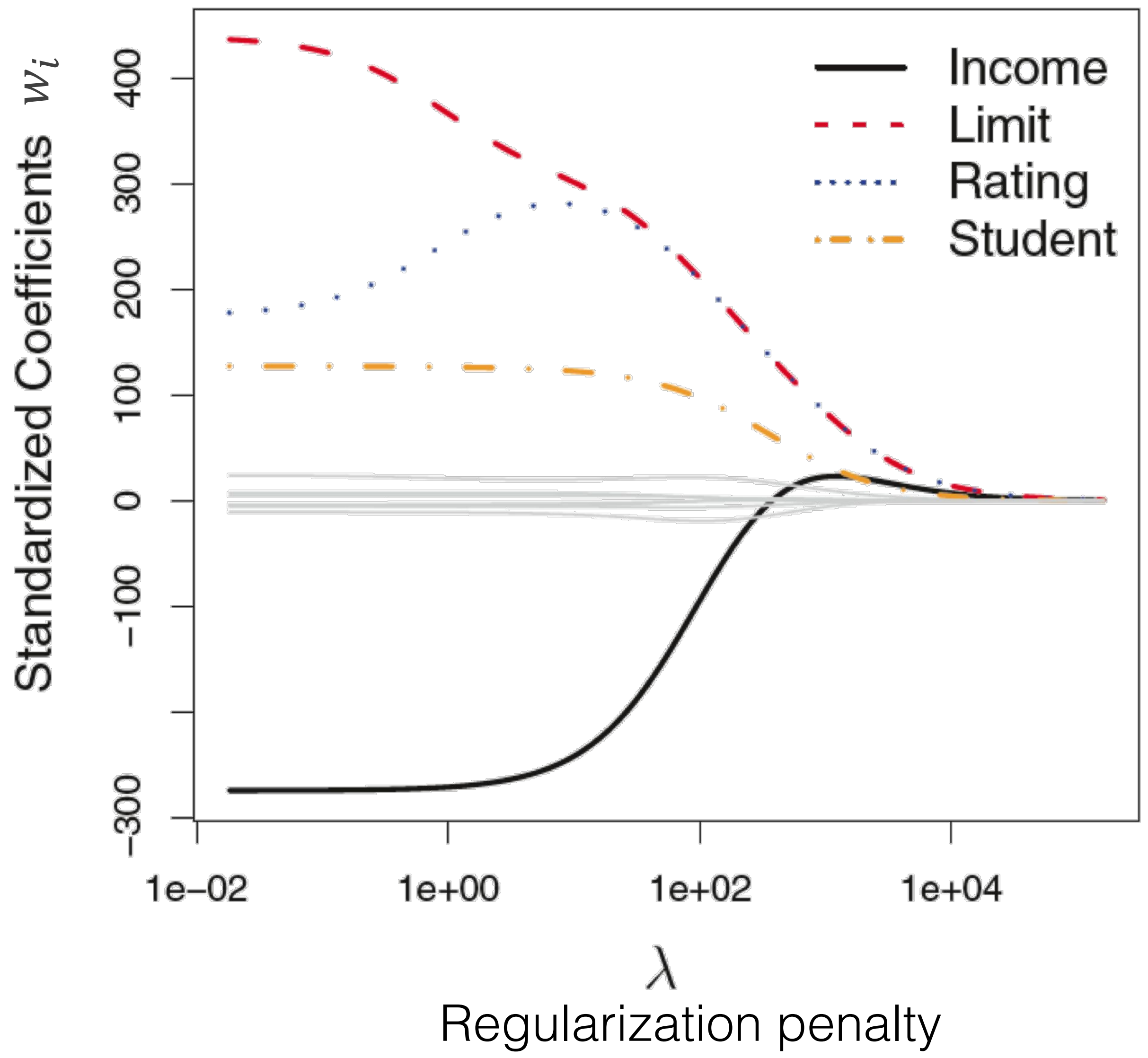
L_1 regularization also performs variable selection

Example: predicting credit default

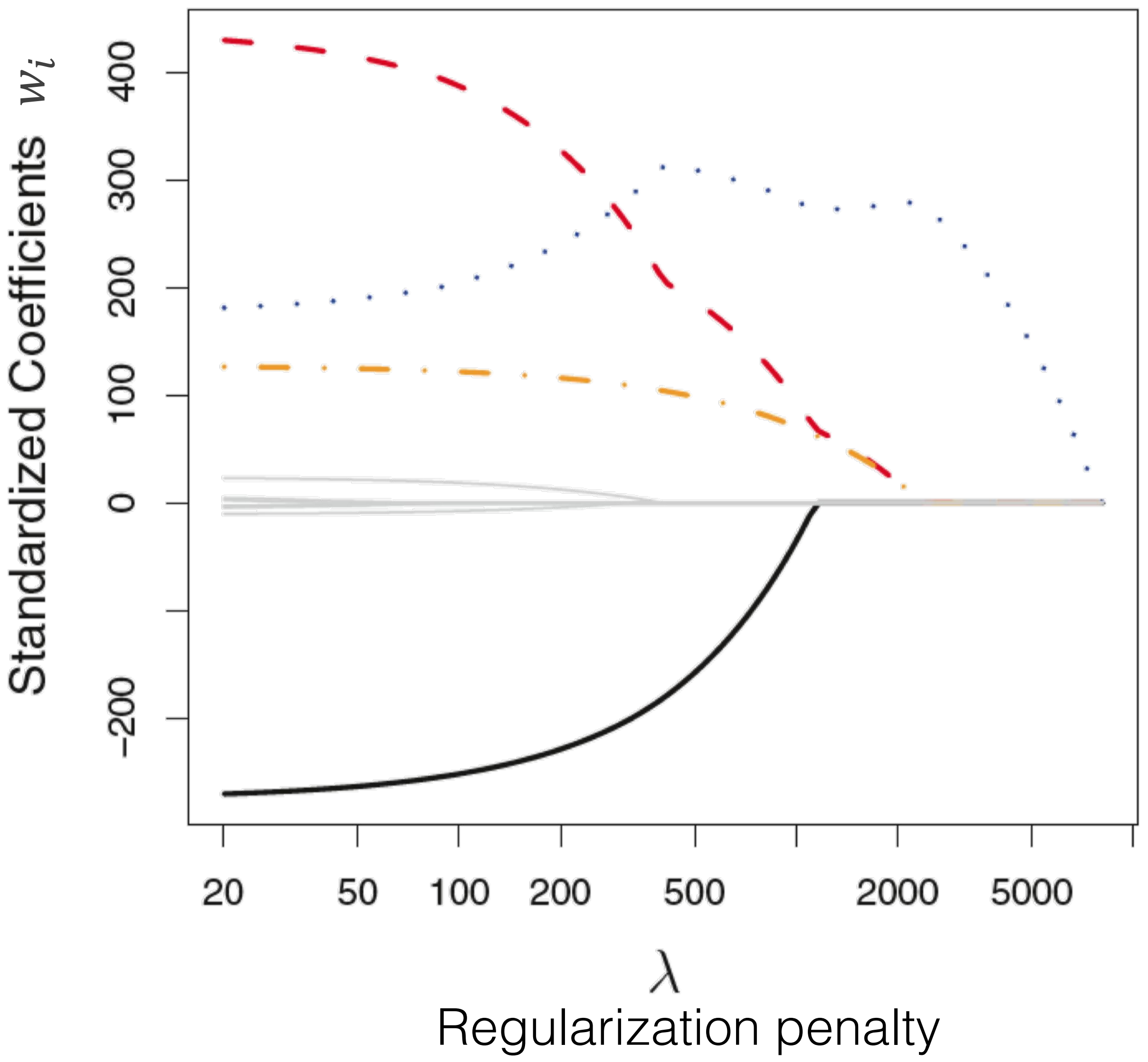
11 features to use to predict default:

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

L_2 regularization
Ridge regression

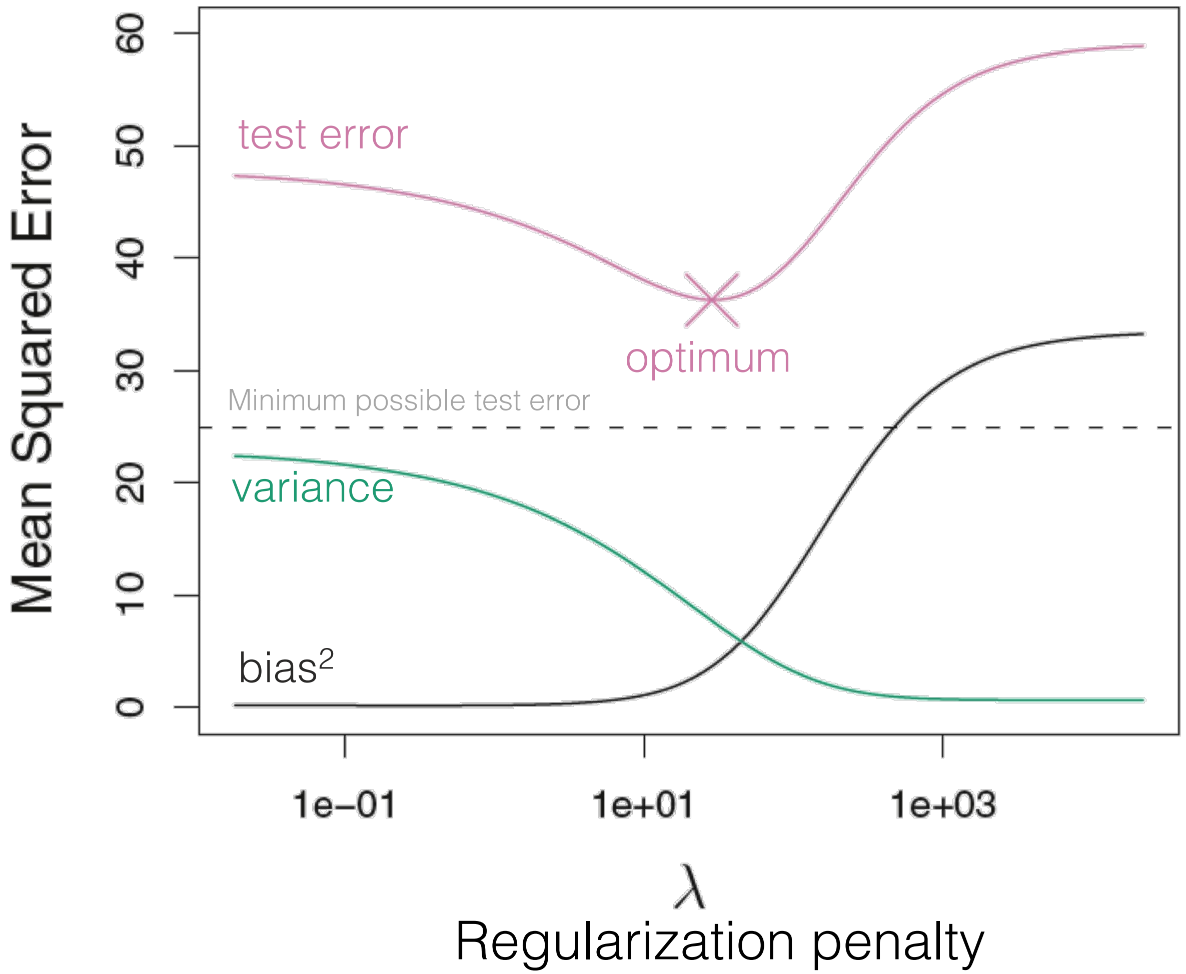


L_1 regularization
LASSO regularization

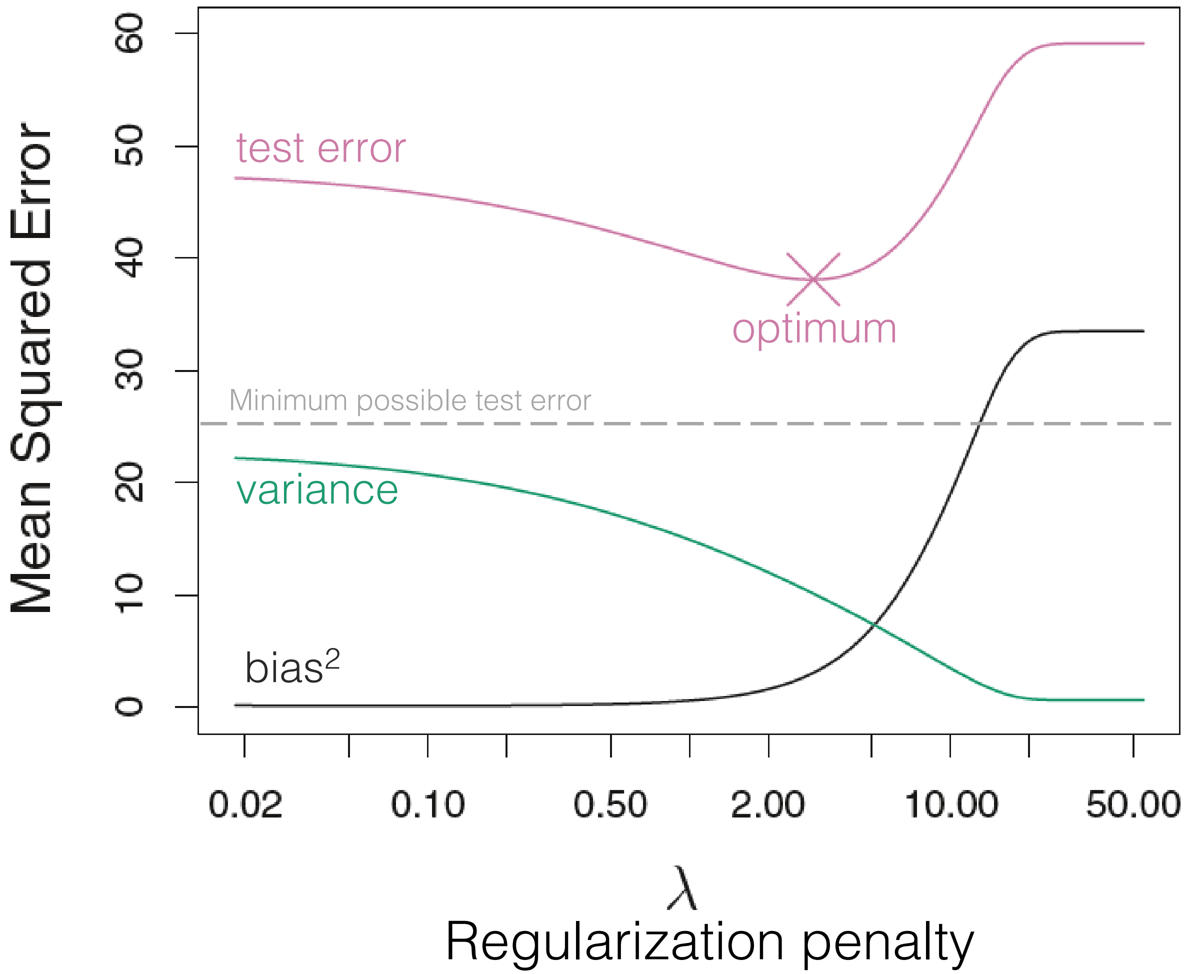


Images from James et al., An Introduction to Statistical Learning

L_2 regularization



L_1 regularization



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Underdetermined systems and OLS

$$X = \overbrace{\begin{bmatrix} \quad & \quad & \quad \\ & & \\ & & \end{bmatrix}}^{\substack{\text{Number of features} \\ p}} \left.\vphantom{\begin{bmatrix} \\ \\ \\ \end{bmatrix}}\right\} \begin{array}{l} N \\ \text{Number of samples} \end{array}$$

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 λ

- λ 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 approximate generalization performance and optimize hyperparameters	Used to evaluate generalization performance of the final model(s)

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)

LASSO selects among redundant features

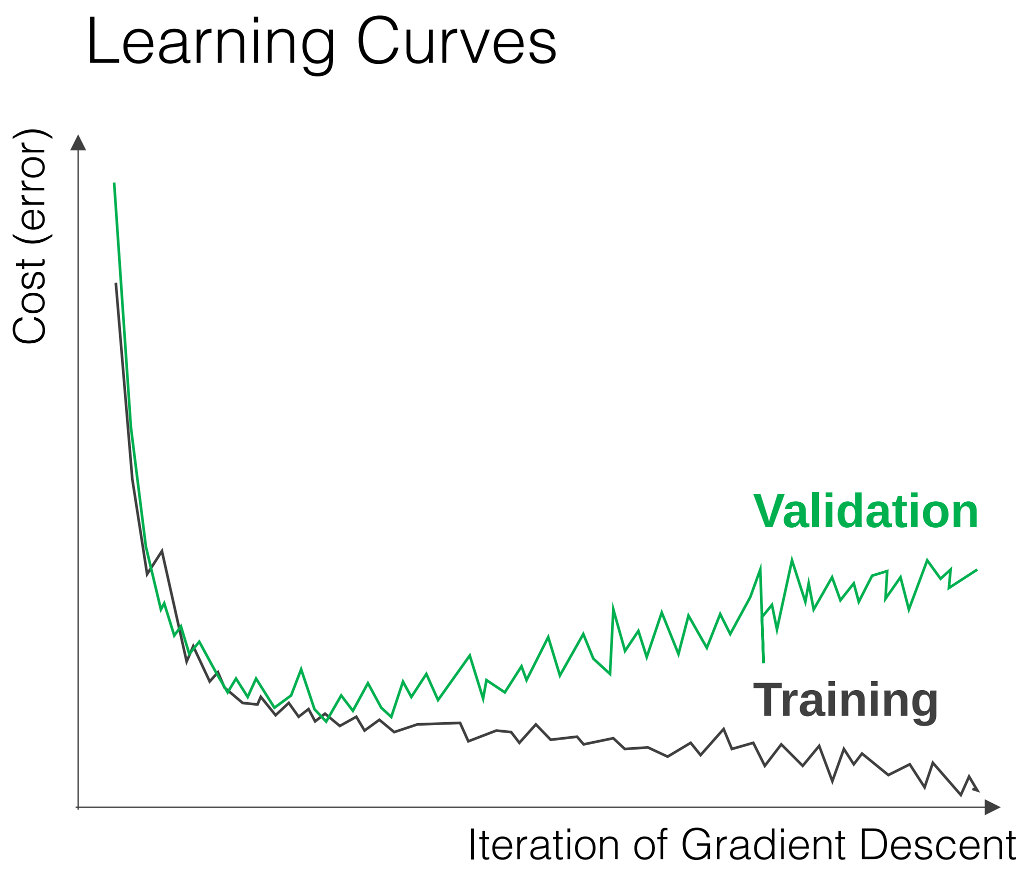
You can use a little of both via elastic net regularization

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



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