Reducing Overfit

Lecture 9

Challenge

You have a dataset with n = 1,500 samples (observations)

Each observation has p = 30,603 predictors (features)

You're asked to develop a classifier for the data

p >> n ….what do you do?

This is exactly the case of the Kaggle competition!

Our quest to **generalize**…

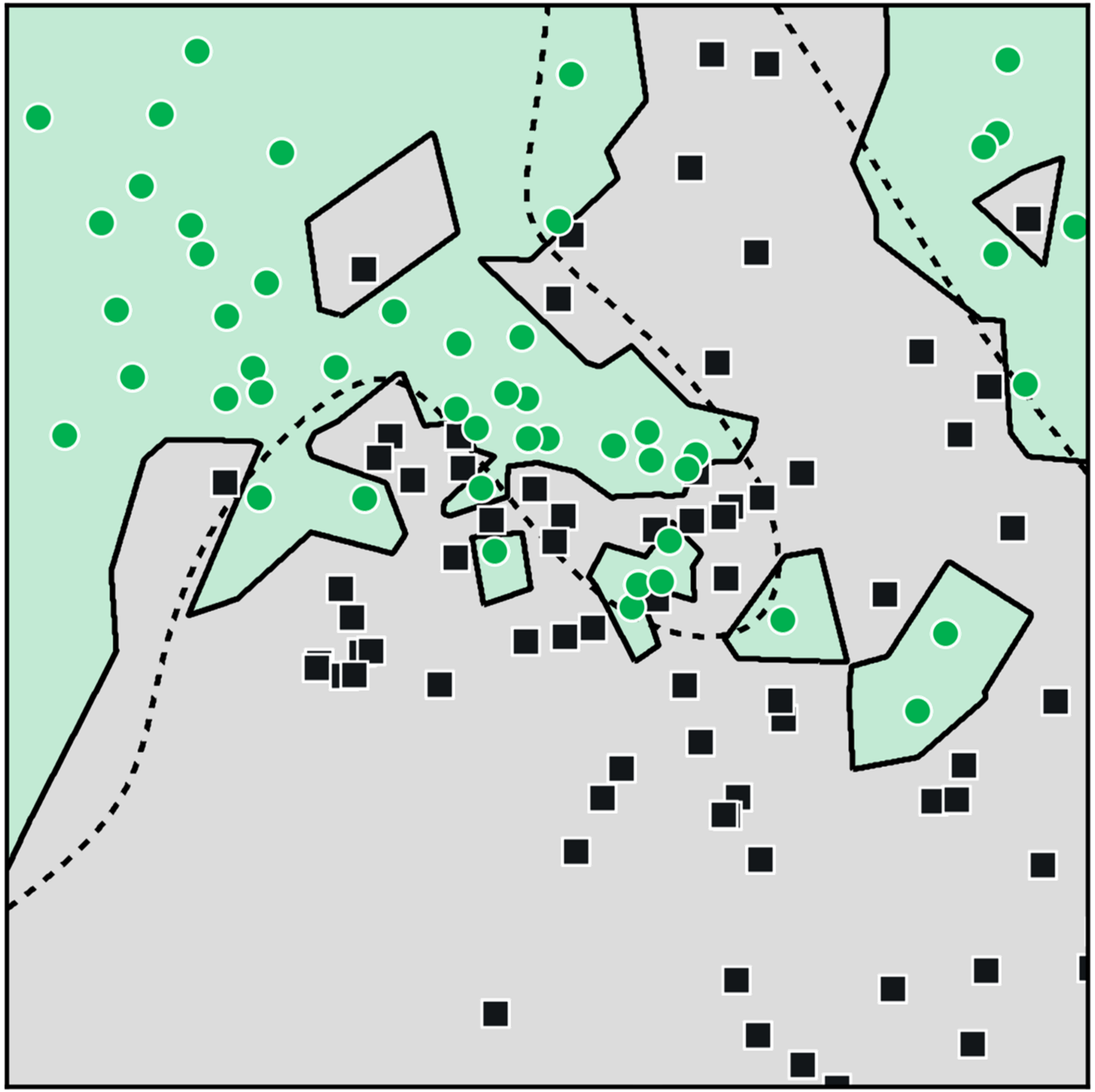
…is our quest to **prevent overfit**

1. Use cross validated performance evaluation to accurately measure generalization performance

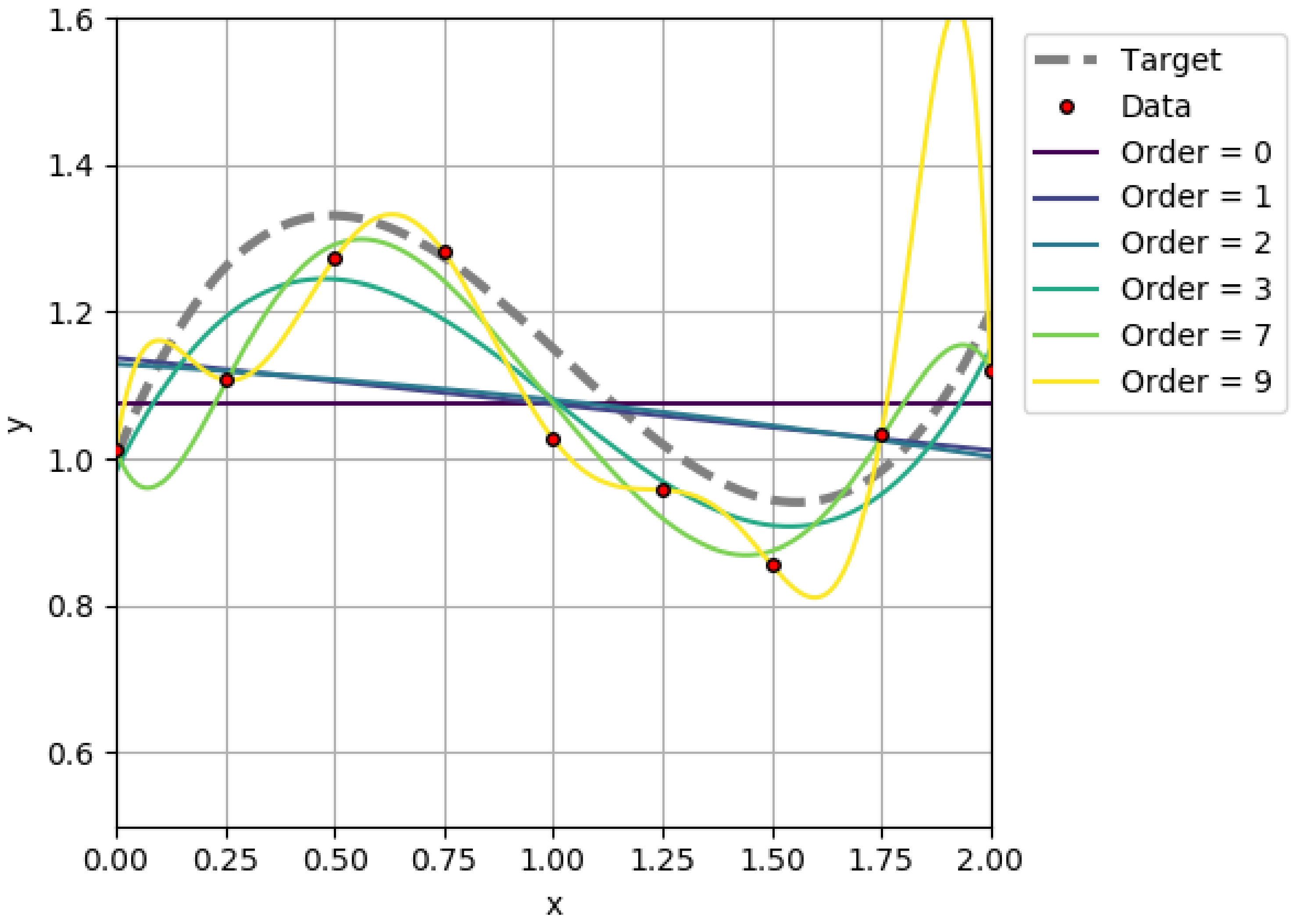
2. Reduce the flexibility models as needed

Our problem…

Overfitting to the training data



Overfitting to the training data



Overfitting and high model variance are related… we want to reduce both!

Our tool…

Image from Speckyboy.com

Occam's Razor / Law of Parsimony

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

Options

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

These all reduce p and model flexibility

Benefits of reducing 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

Wrapper methods

Filter methods

Embedded methods

Variable subset selection:
wrapper methods for feature selection

Search for subsets of features that perform well

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

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

embedded methods for feature selection

Reduce the variance by simplifying the model during training

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

$$L(\boldsymbol{w}) = \sum_{i=1}^{n} (\boldsymbol{w}^T \boldsymbol{x}_i - y_n)^2 + \lambda \sum_{i=1}^{p} w_i^2$$

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

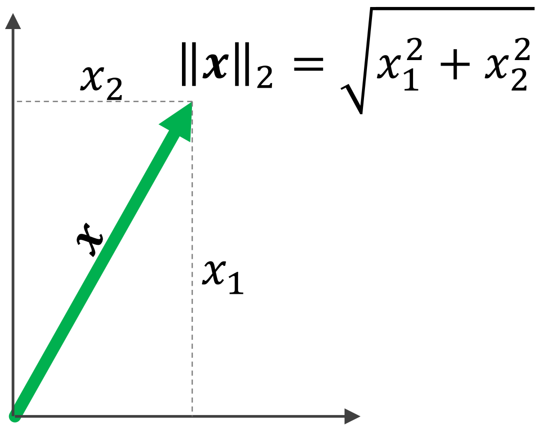
A function that assigns a positive **length or size** to a vector

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:

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

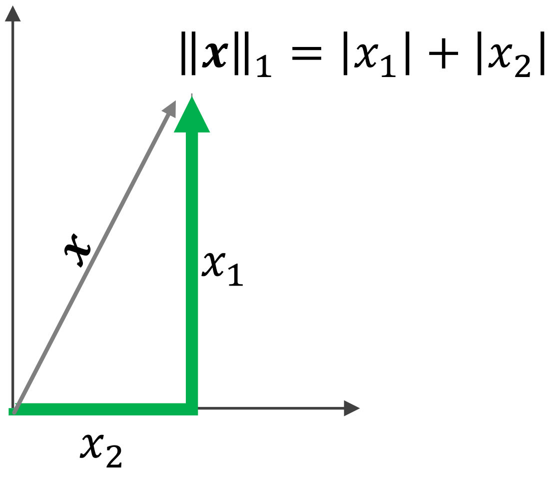


Norms

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**:

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

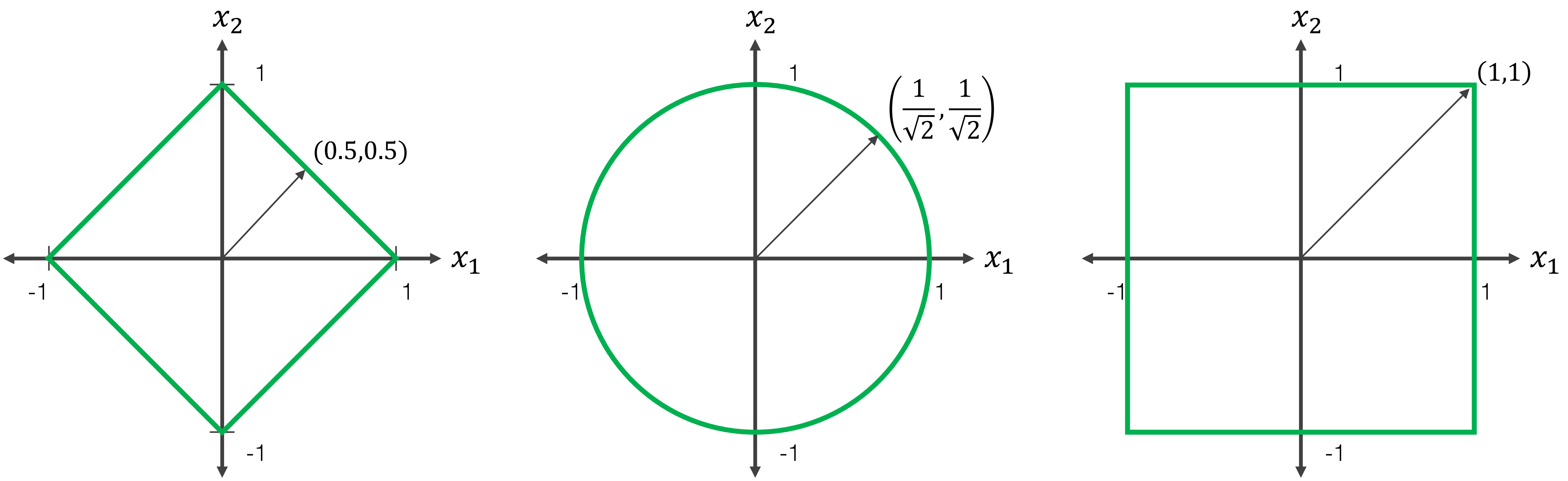
In the limit, the **infinity norm** is the maximum entry of the vector $\boldsymbol{x}$:

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

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

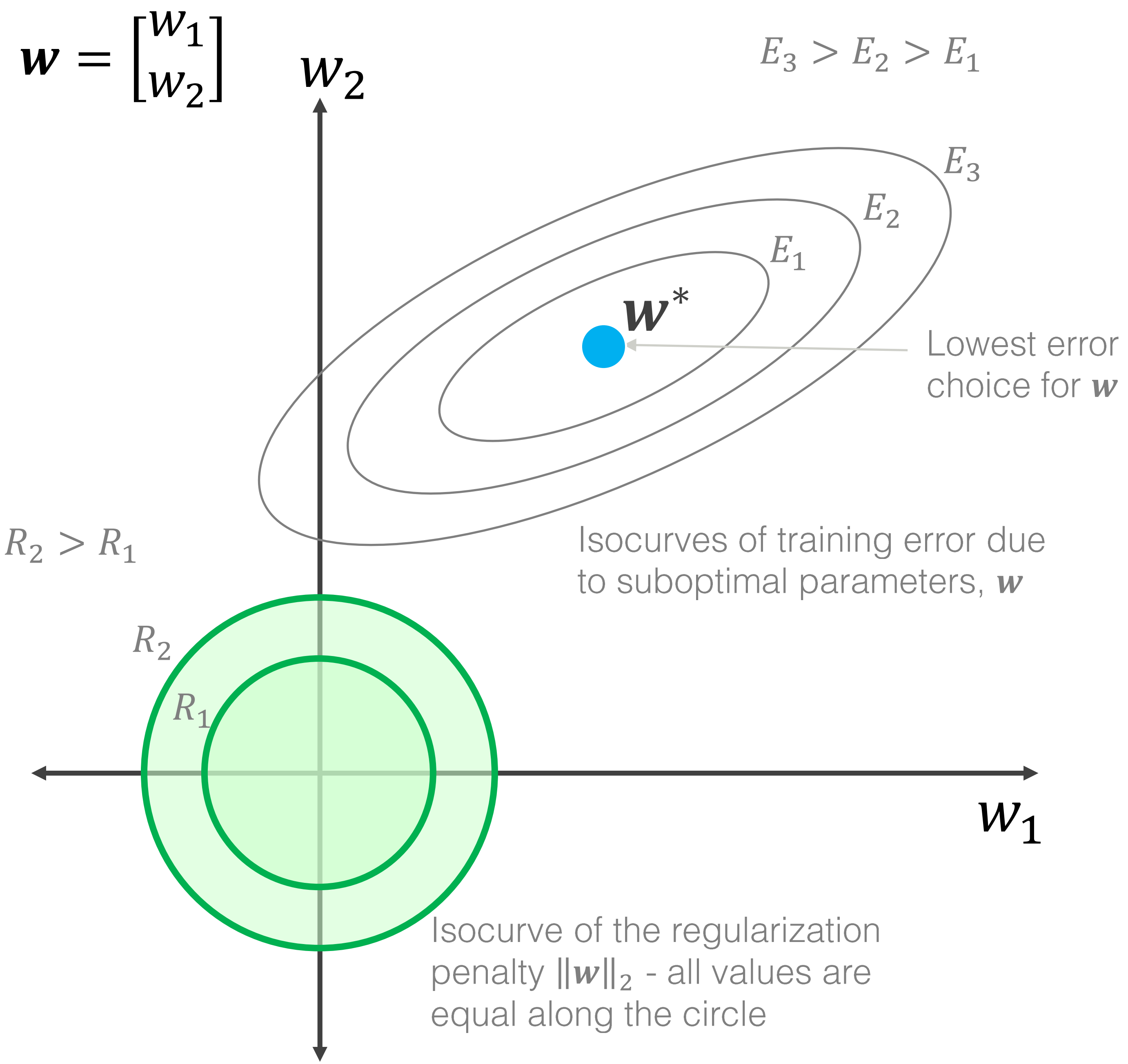
Adjust the **cost/loss function** to penalize larger parameter values

a.k.a....

L_2 regularization $$L(\boldsymbol{w}) = \sum_{i=1}^{n} (\boldsymbol{w}^T \boldsymbol{x}_i - y_n)^2 + \lambda \sum_{i=1}^{p} w_i^2$$ **ridge regression** or weight decay

L_1 regularization $$L(\boldsymbol{w}) = \sum_{i=1}^{n} (\boldsymbol{w}^T \boldsymbol{x}_i - y_n)^2 + \lambda \sum_{i=1}^{p} |w_i|$$ least absolute shrinkage and selection operator (**LASSO**)

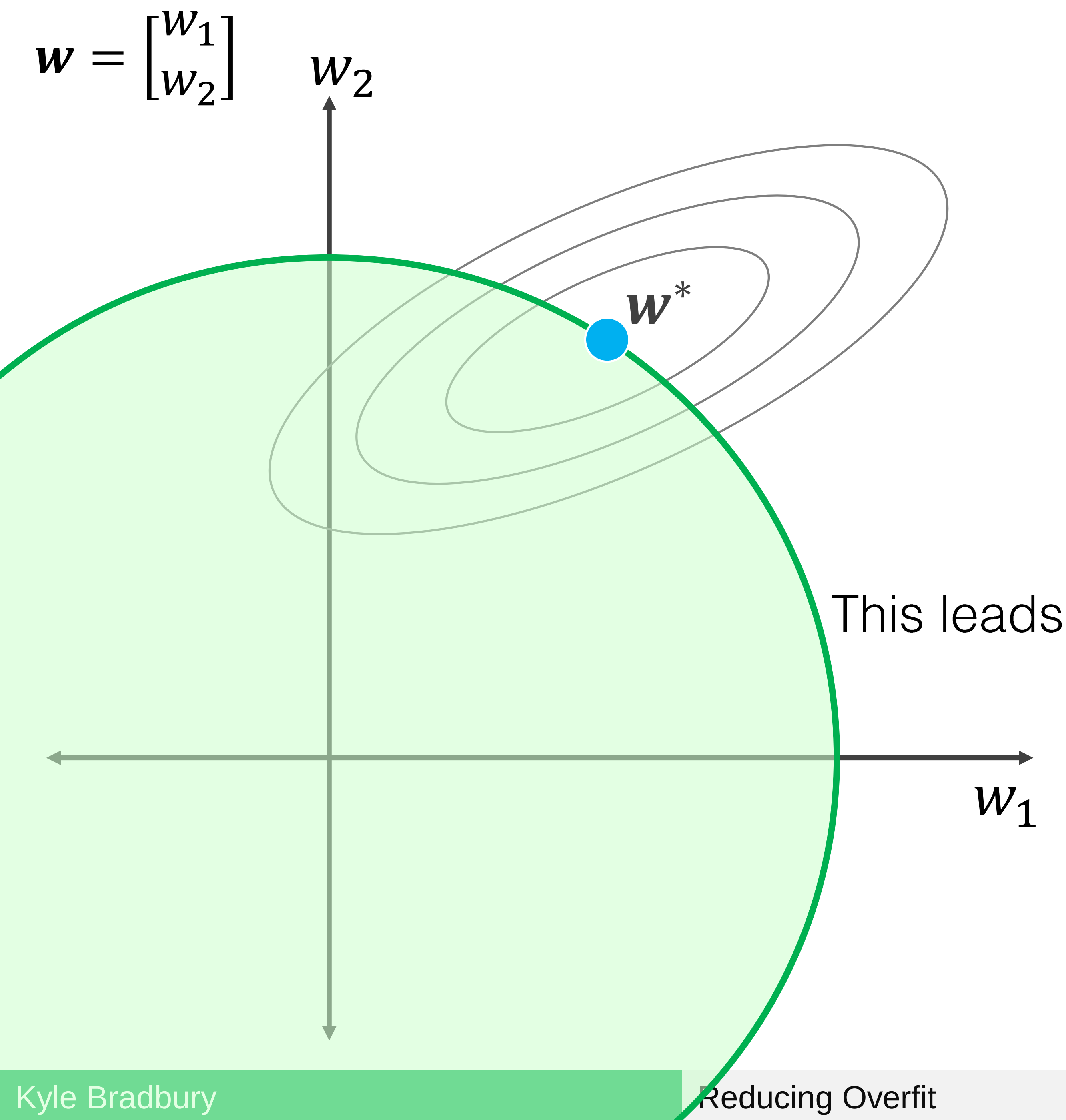
L_2 & L_1 regularization $$L(\boldsymbol{w}) = \sum_{i=1}^{n} (\boldsymbol{w}^T \boldsymbol{x}_i - y_n)^2 + \lambda_1 \sum_{i=1}^{p} |w_i| + \lambda_2 \sum_{i=1}^{p} w_i^2$$ **elastic net** regularization



Trying to minimize my loss function:

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

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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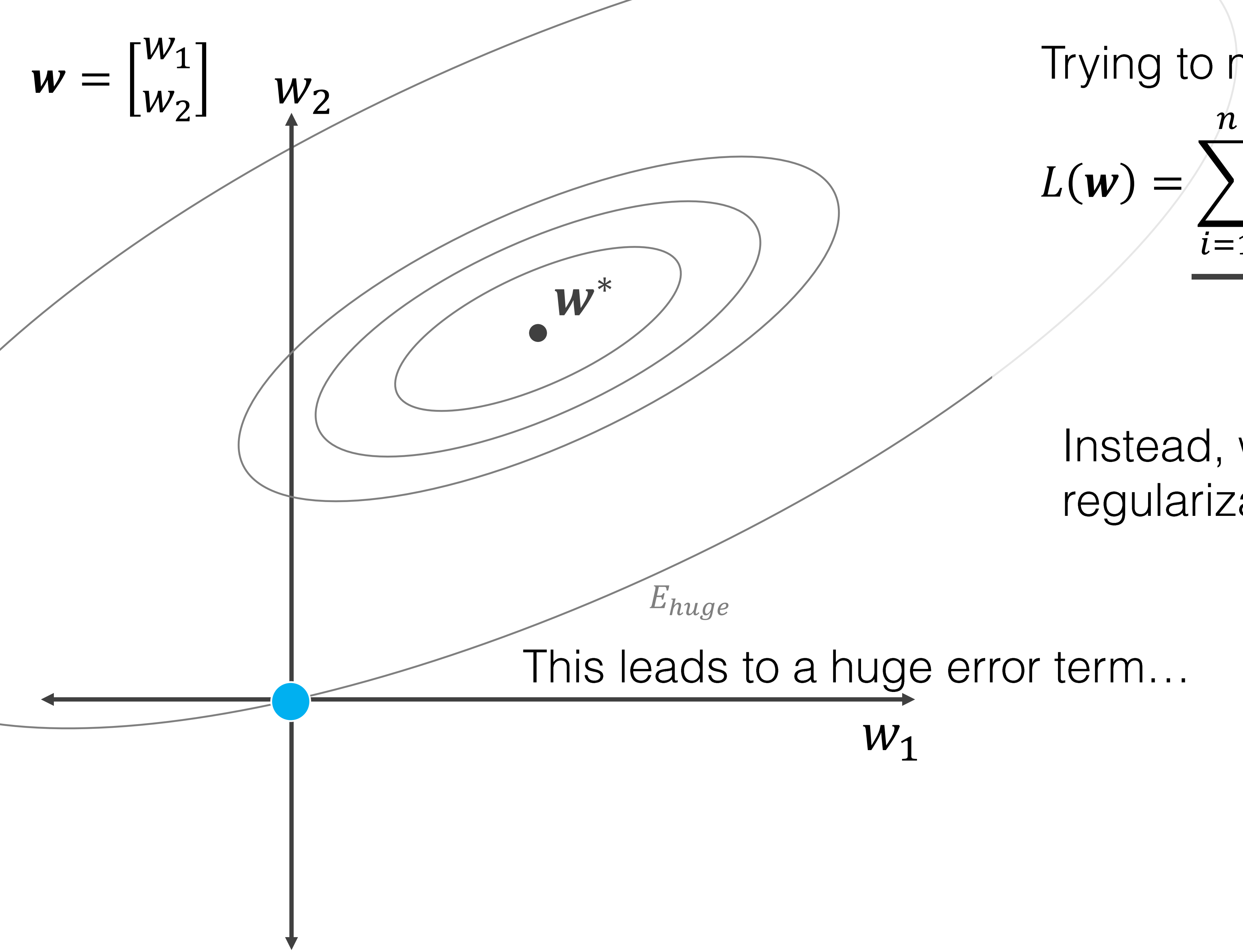
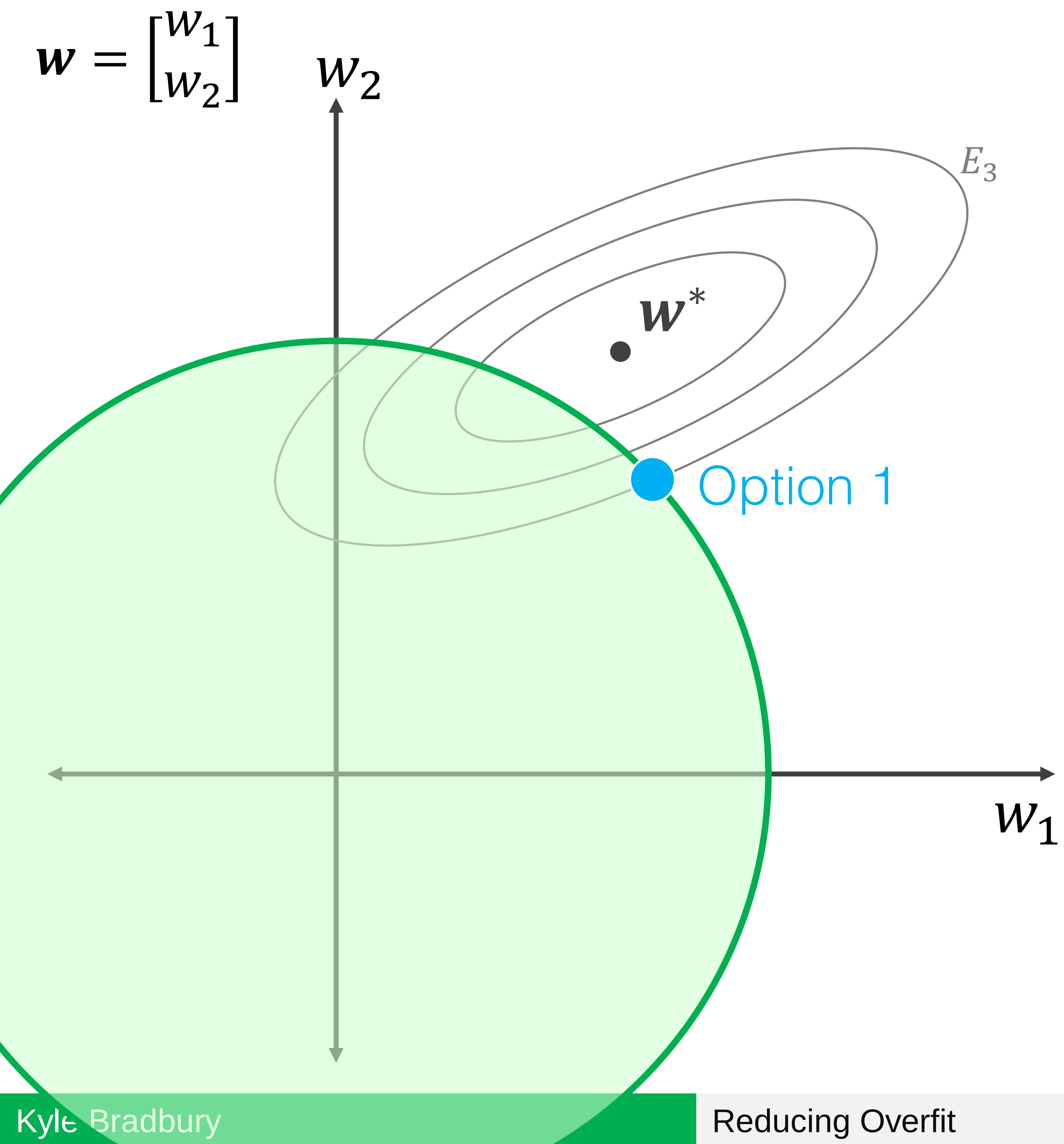


Instead, we could just minimize the regularization penalty

This leads to a huge error term…



Trying to minimize my loss function:

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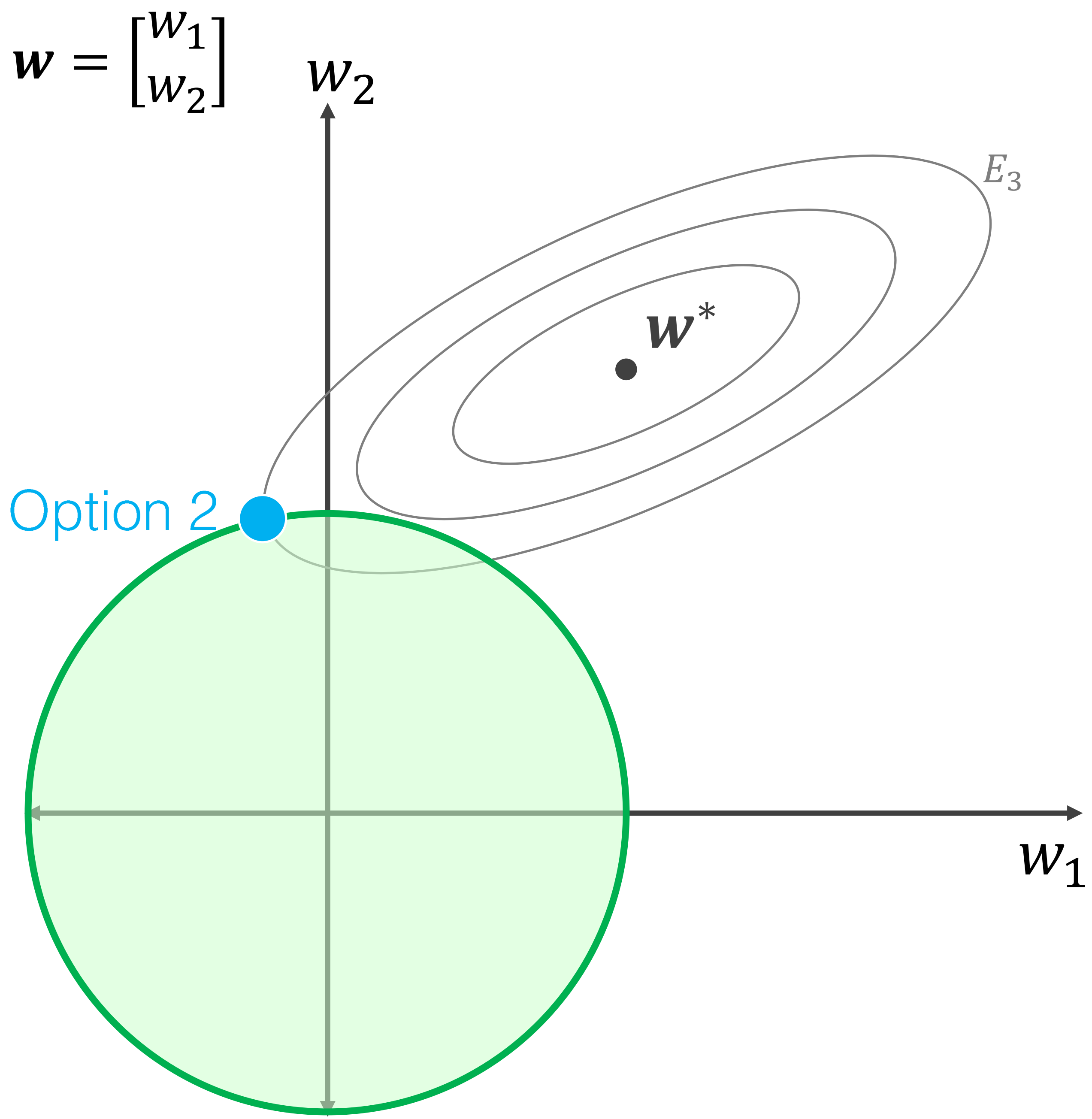
For any level of error (assume E_3 here), there may be a number of parameter values that result in an equal error term



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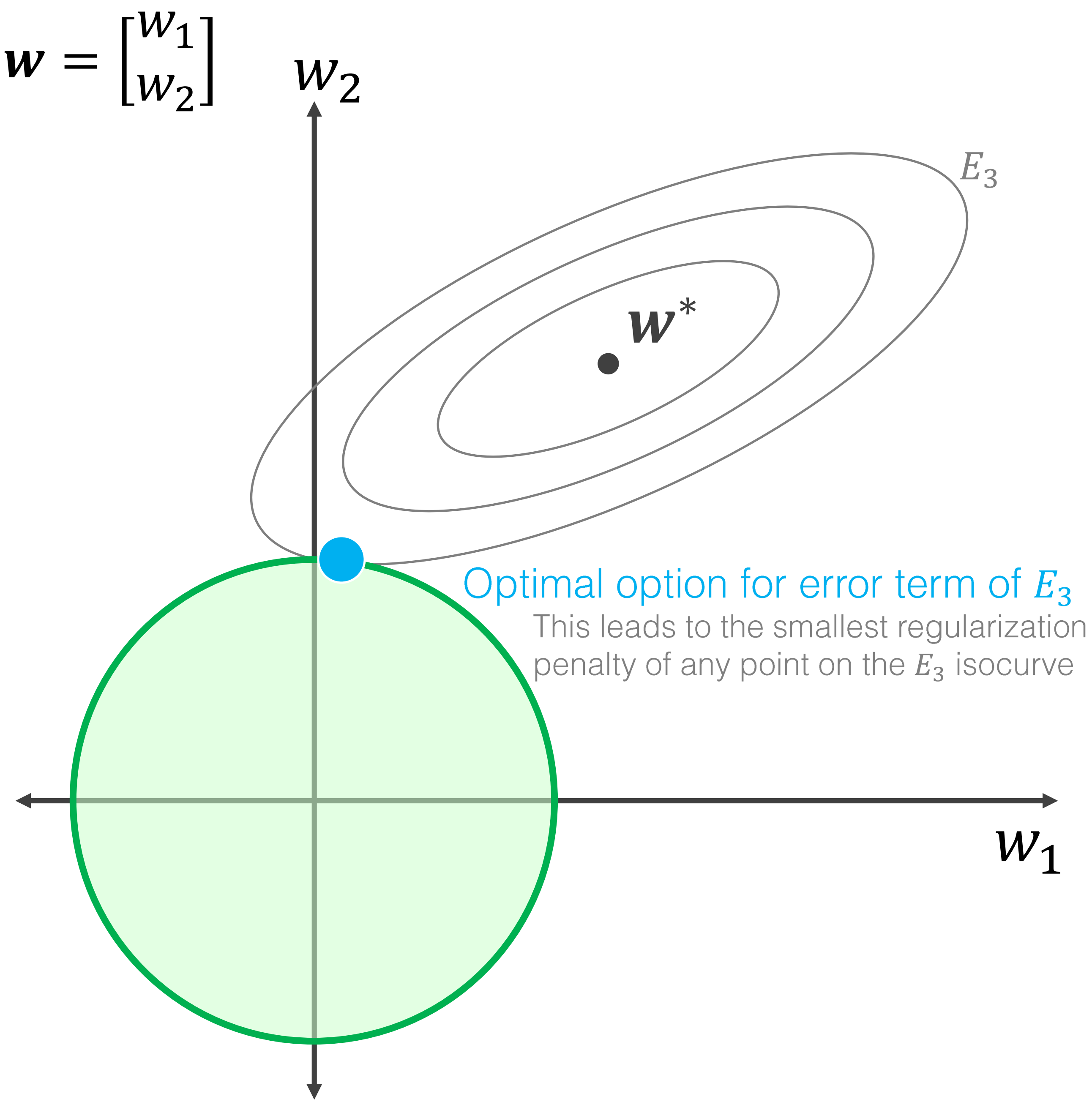

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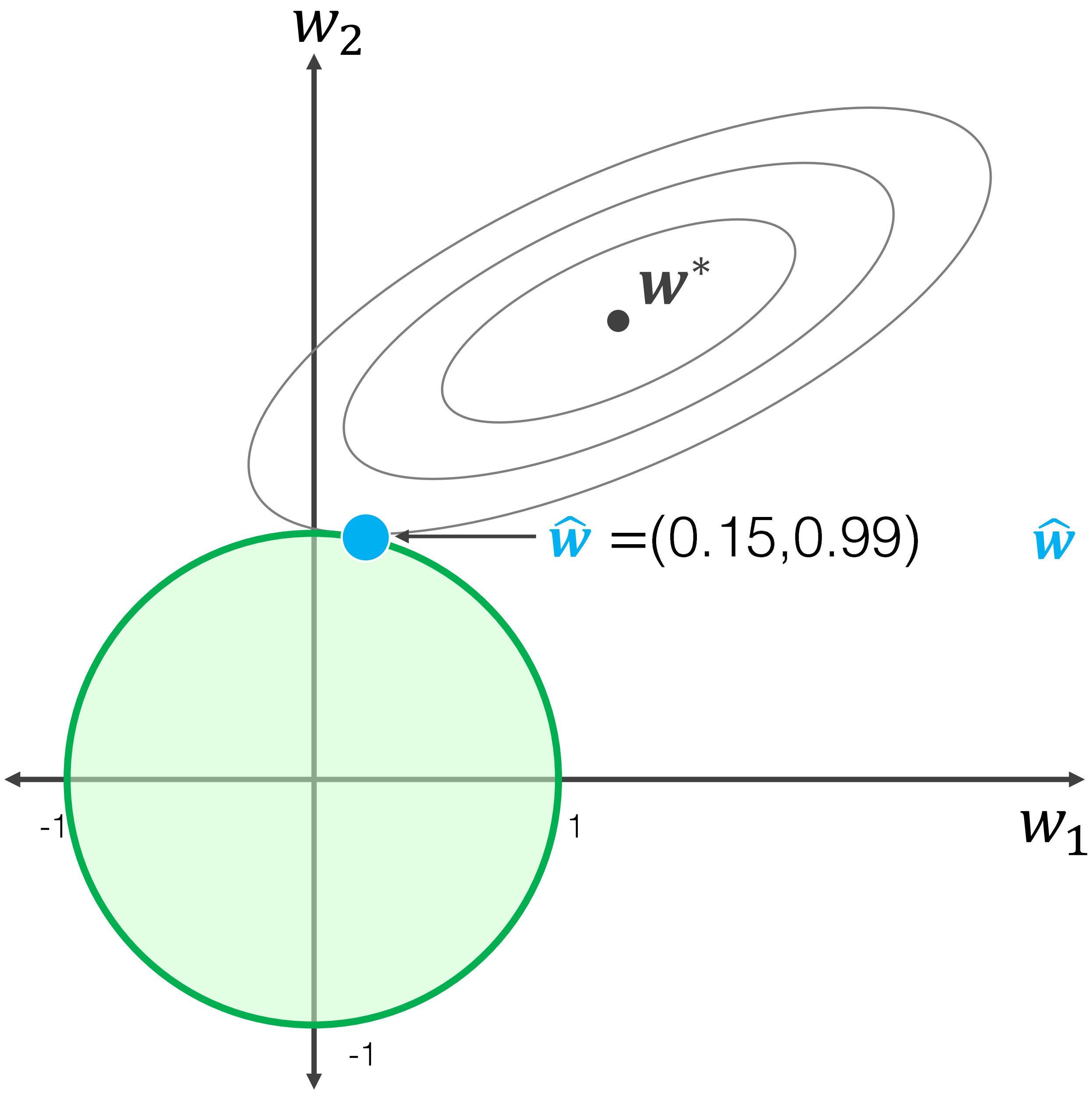
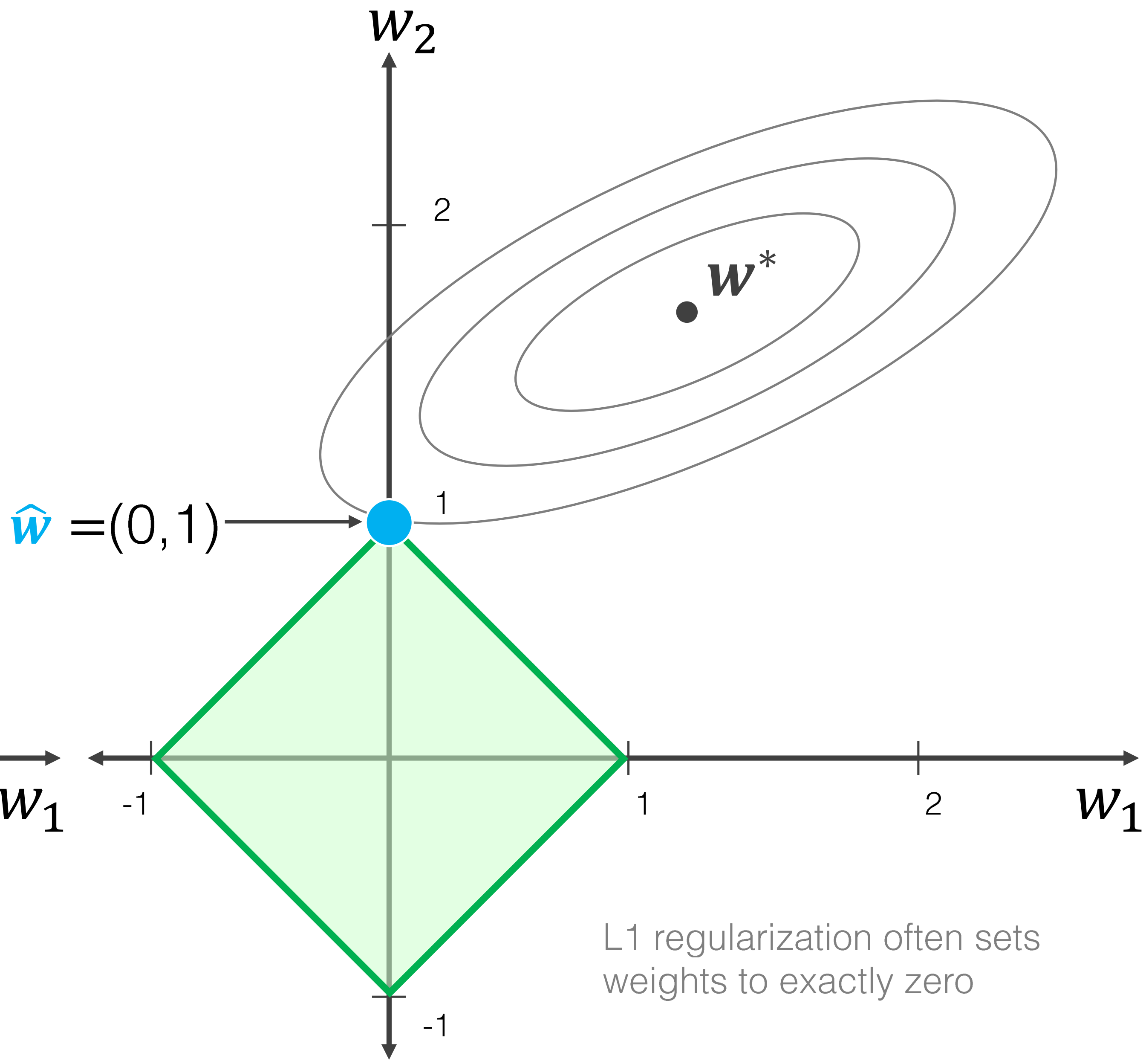
However, we can choose between the options by minimizing the regularization penalty

Ridge: L_2 regularization



LASSO: L_1 regularization



Regularization reduces variance

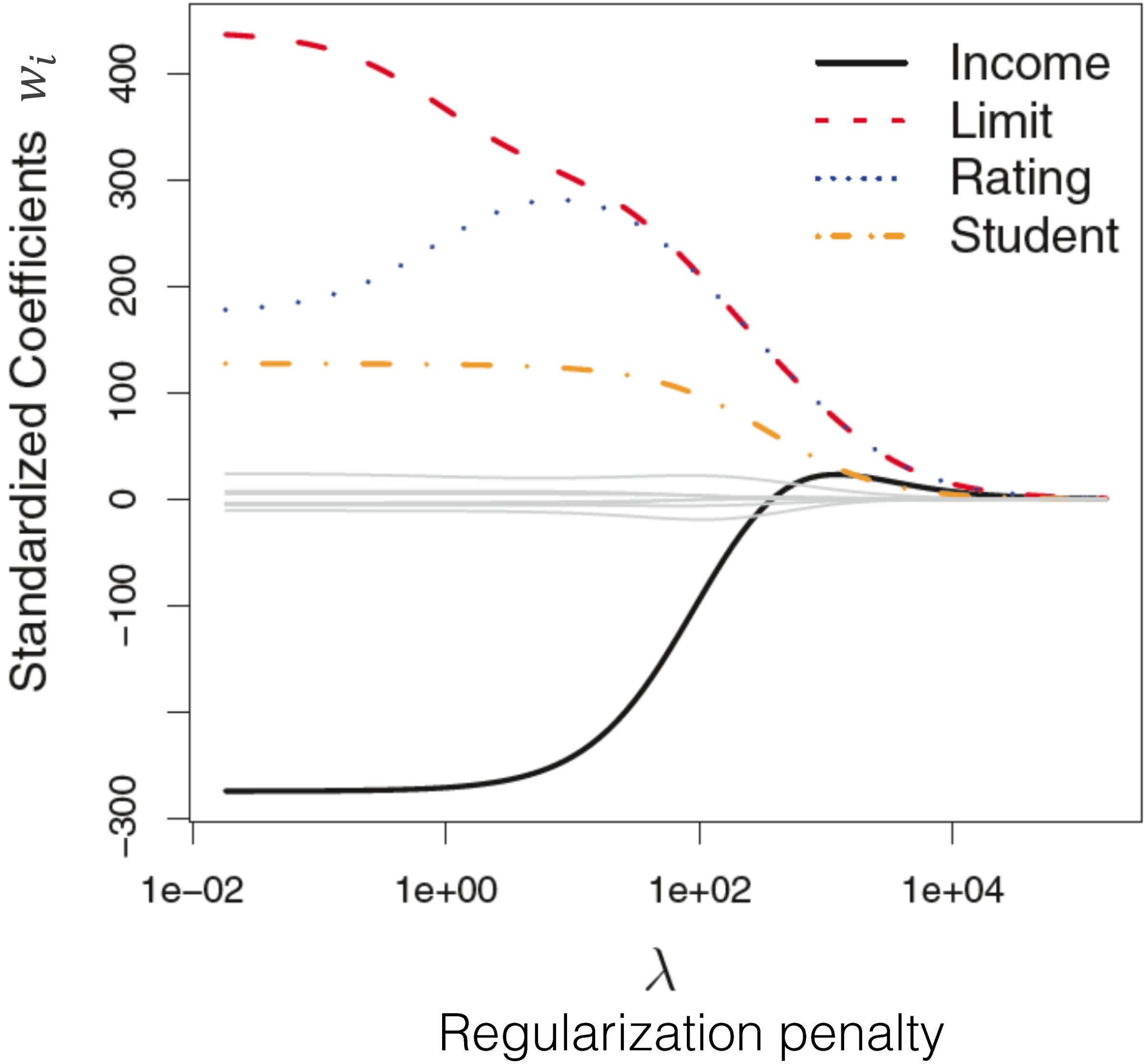
L_1 regularization also performs variable selection

Predicting credit default

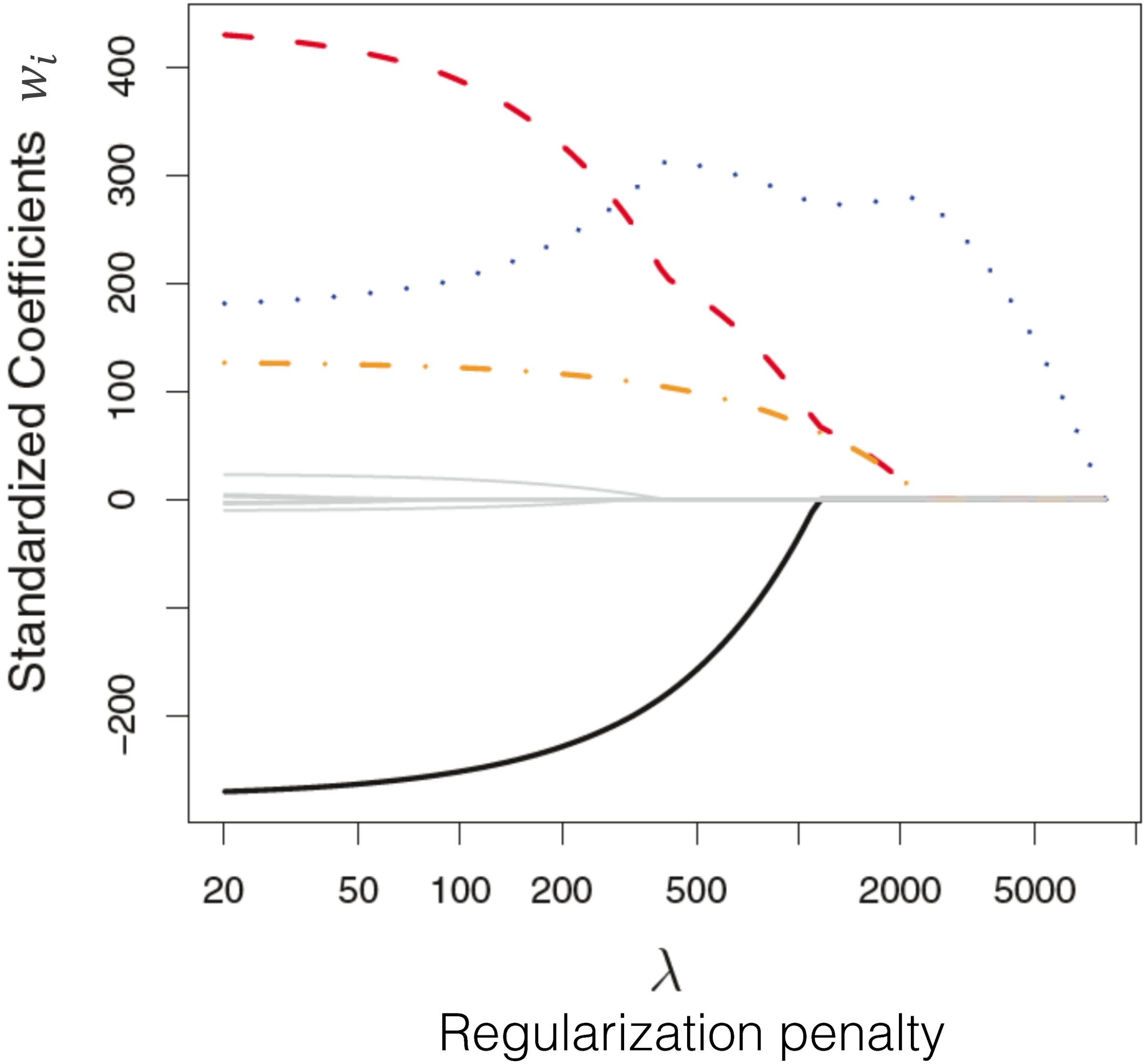
11 features to use to predict default:

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

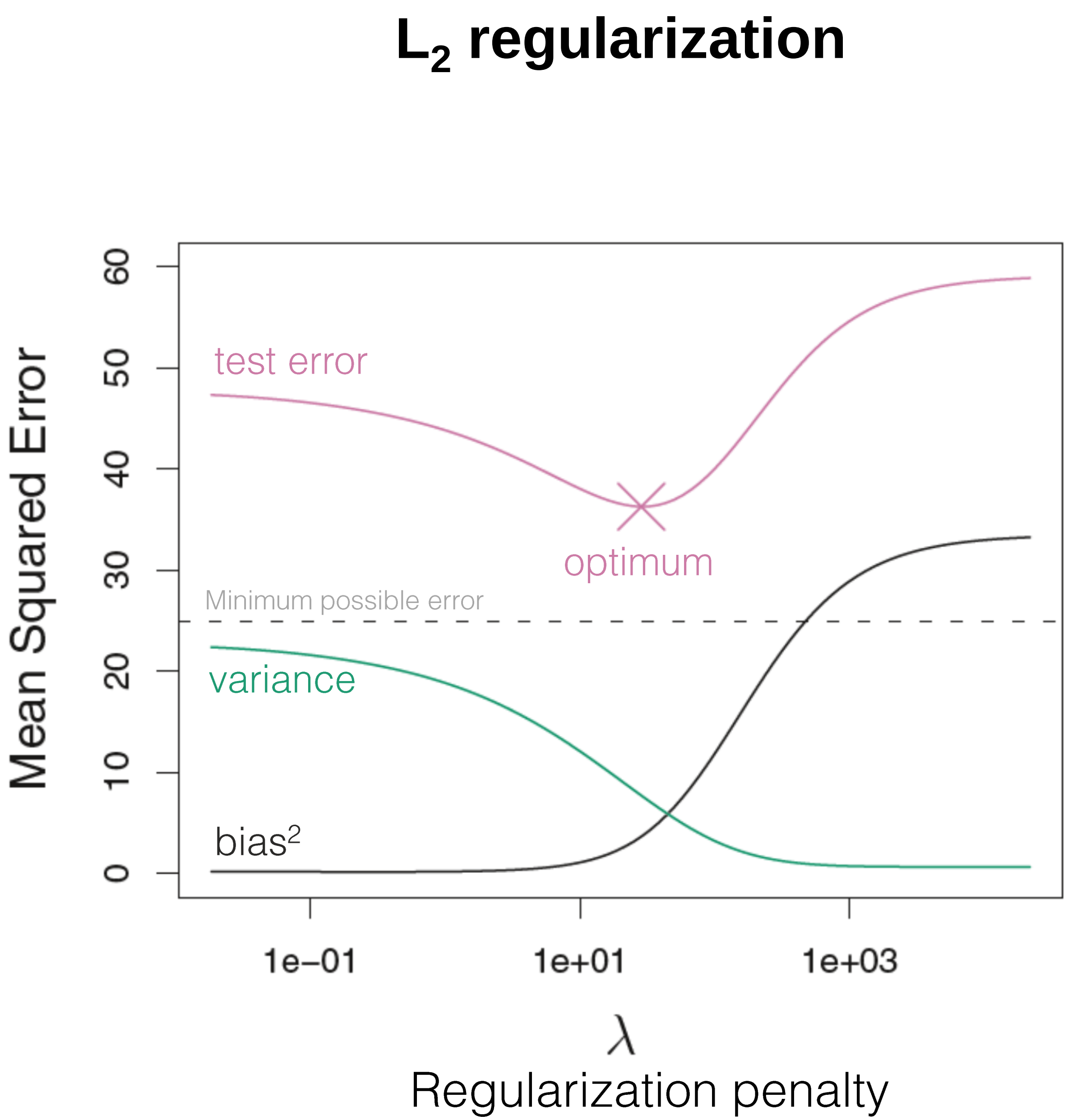
L_2 regularization
Ridge regression

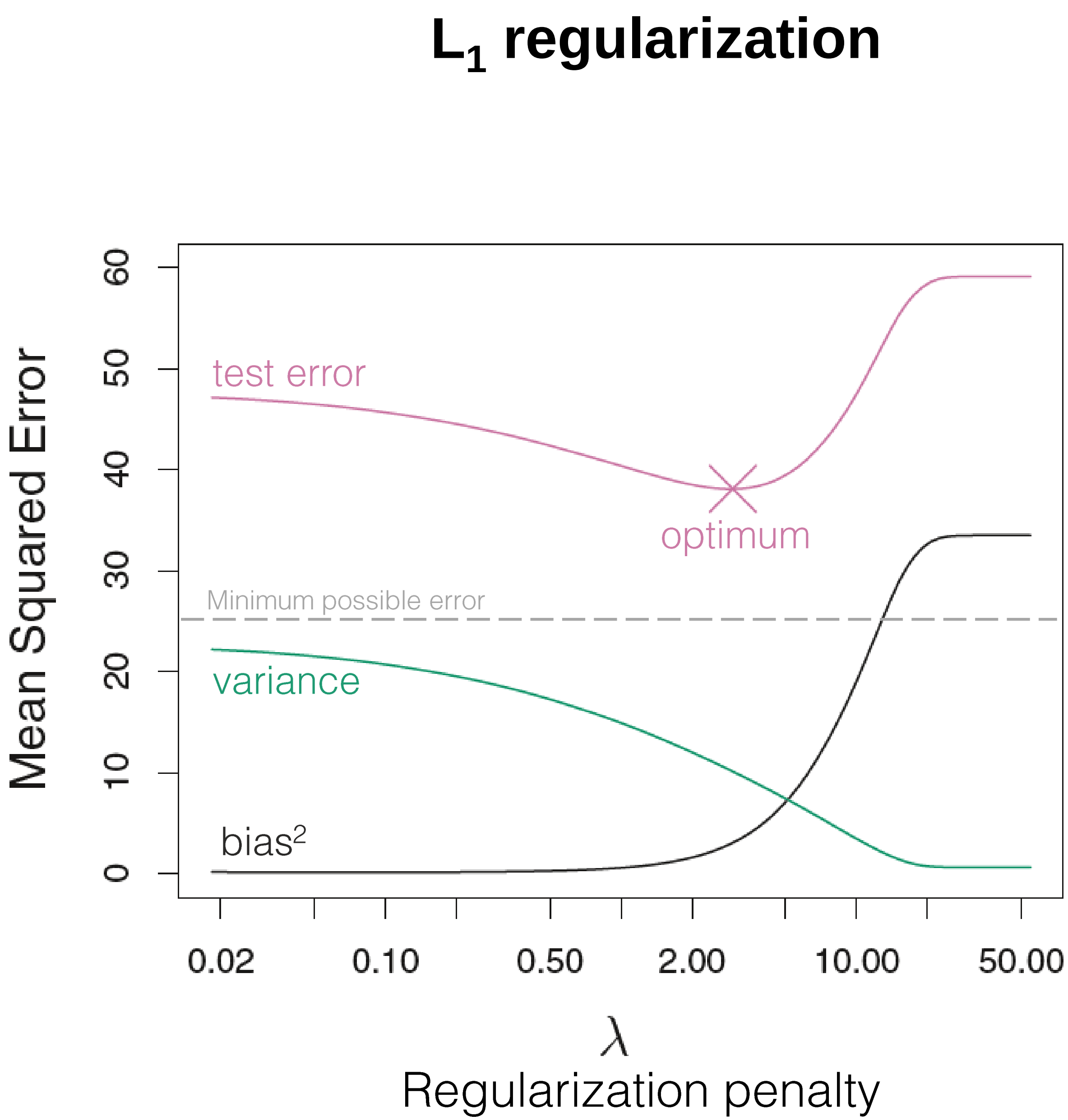


L_1 regularization
LASSO regularization



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





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Underdetermined systems and OLS

$$\begin{array}{c} \text{Number of features} \\ \overbrace{\hspace{4cm}}^{p} \\ X = \left[\hspace{4cm} \right] \end{array} \left.\vphantom{\begin{array}{c}a\\a\\a\\a\\a\end{array}}\right\} N \quad \text{Number of samples}$$

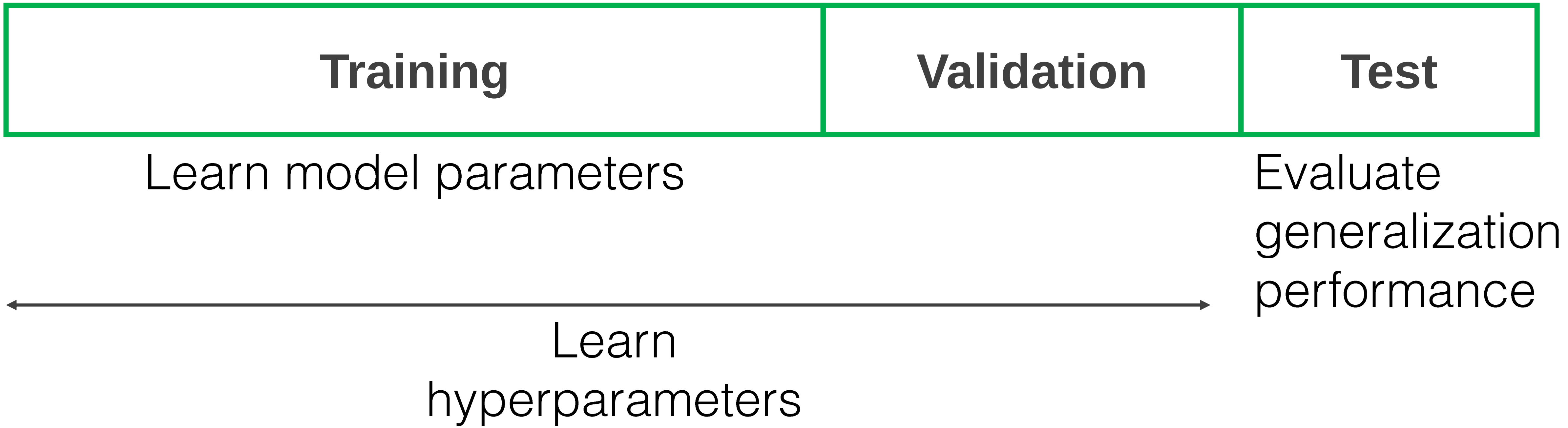
If $p > N$, then the system is **underdetermined**

Often means there are infinitely many solutions

Ridge regression makes this problem solvable

Choosing the parameter λ

- λ is a hyperparameter
- Include a training, validation, and test set
- Can apply cross validation



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

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