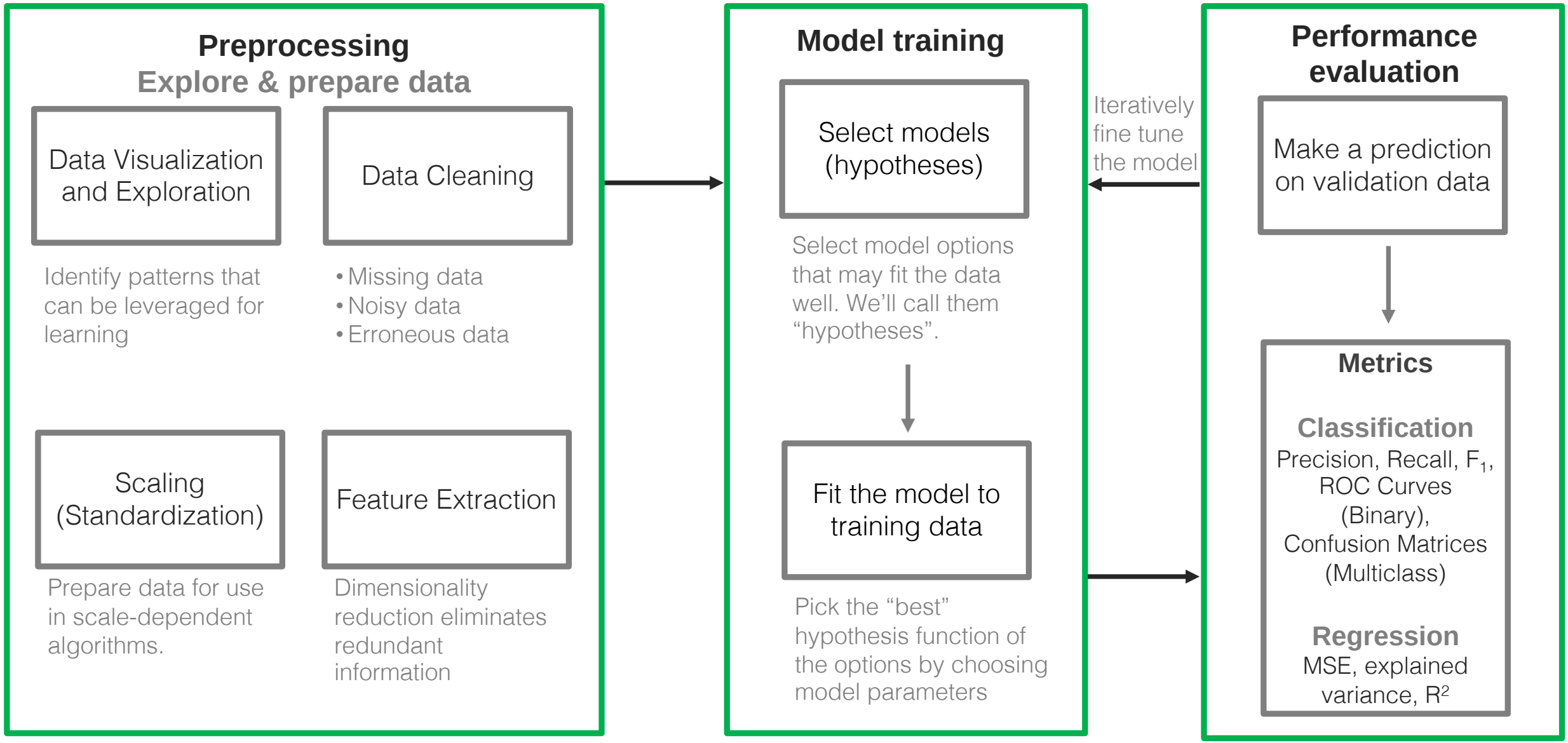
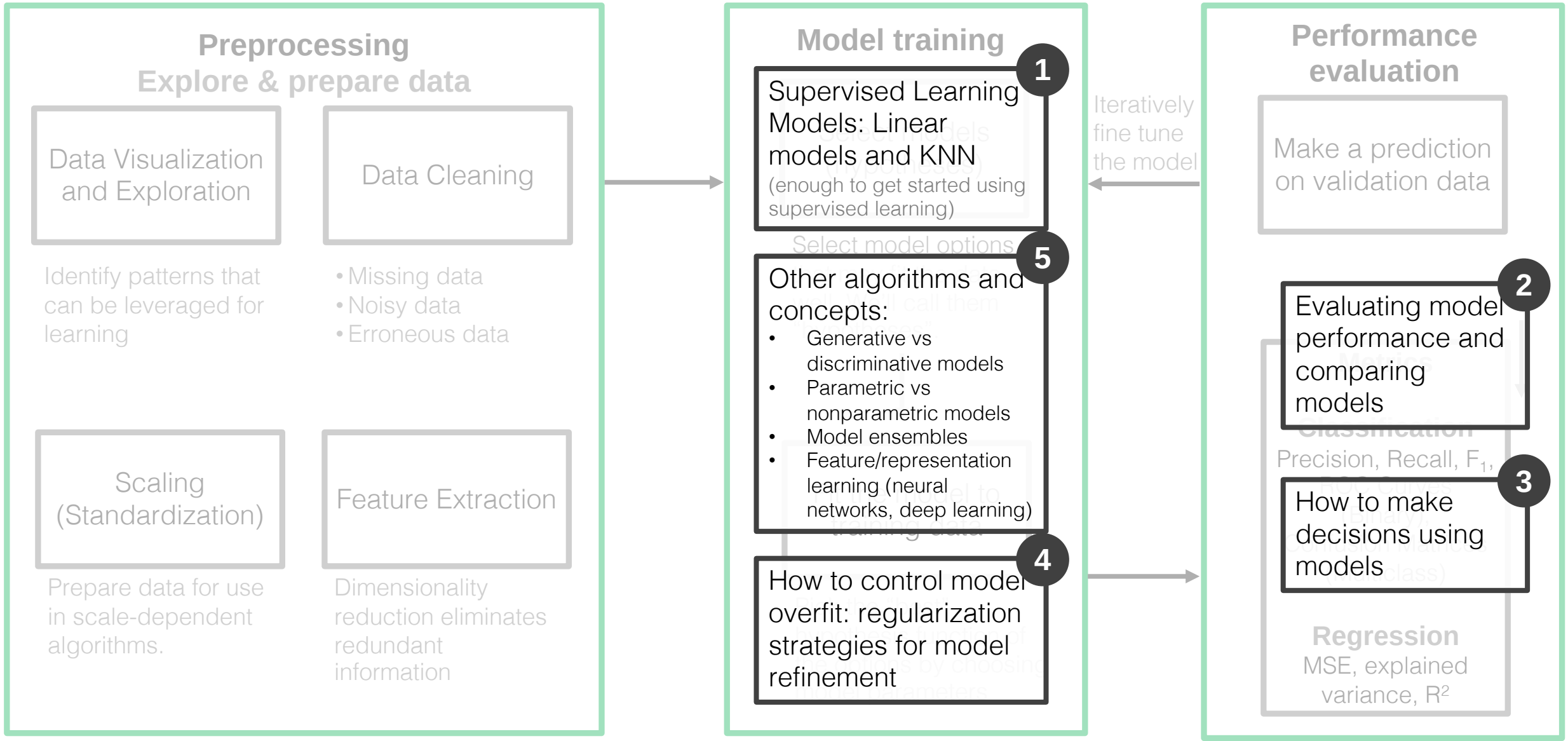
Reducing Overfit

Supervised learning in practice



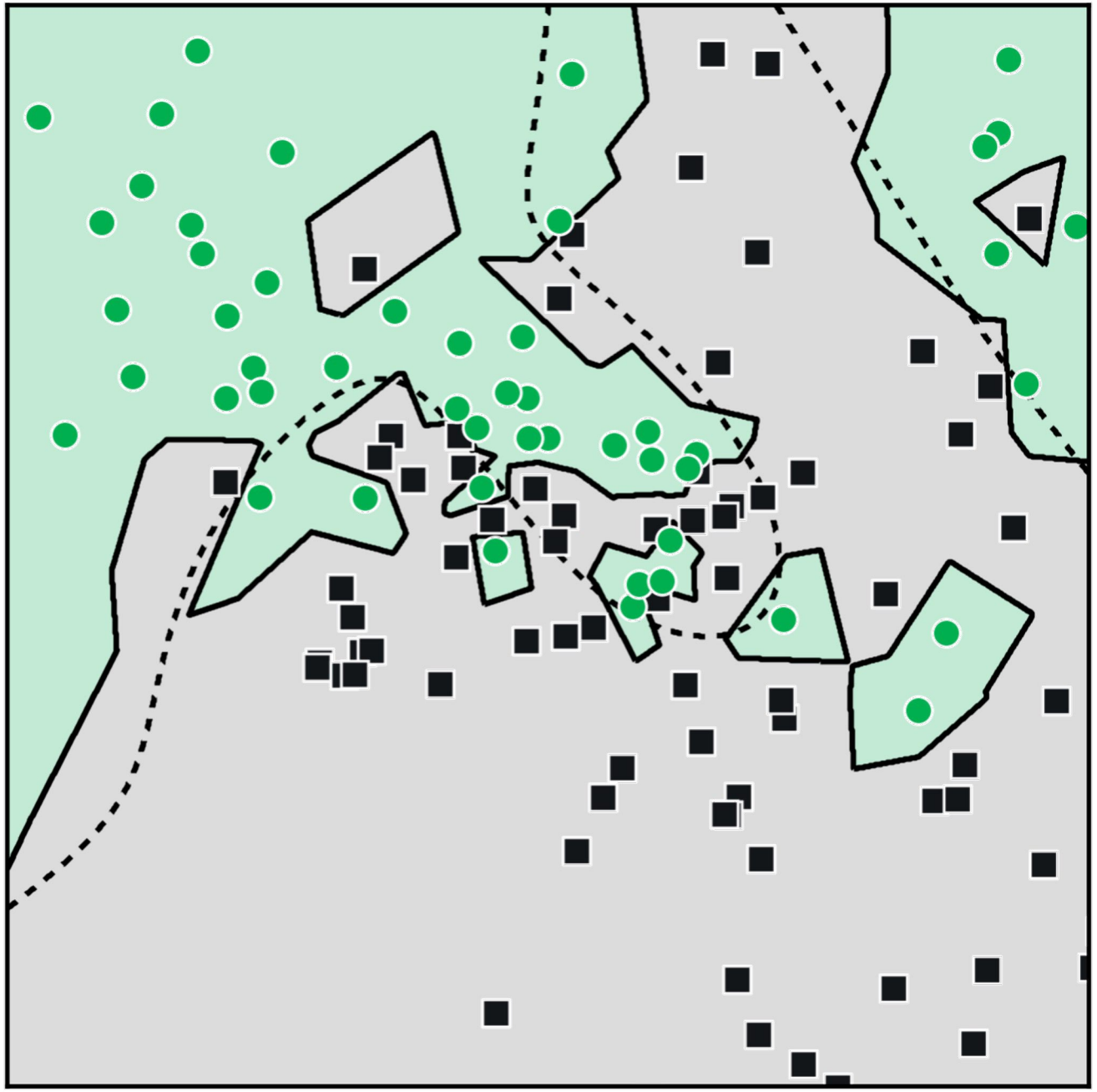
Supervised learning in practice



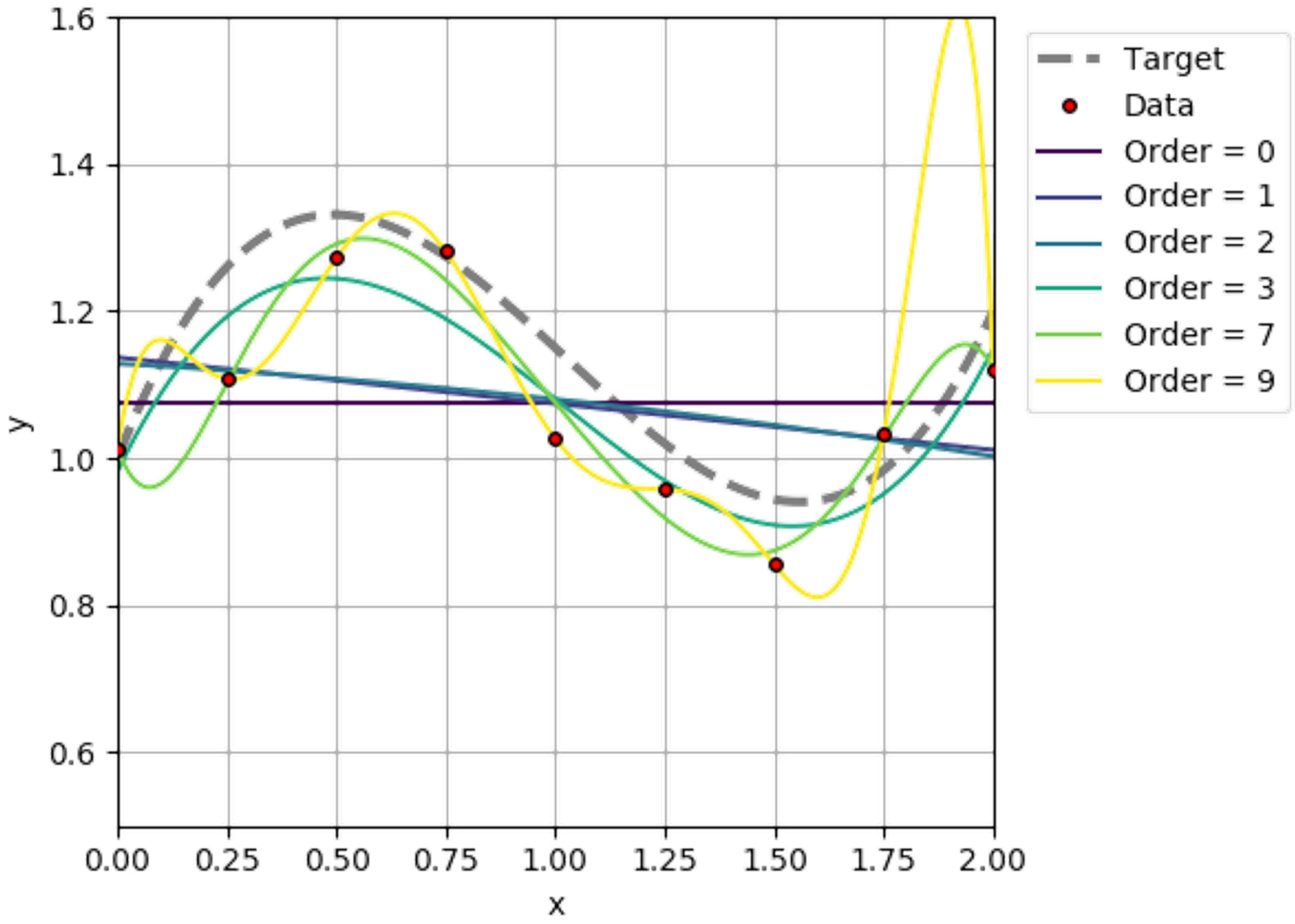
We've seen overfit in classification…

Overfitting to the training data

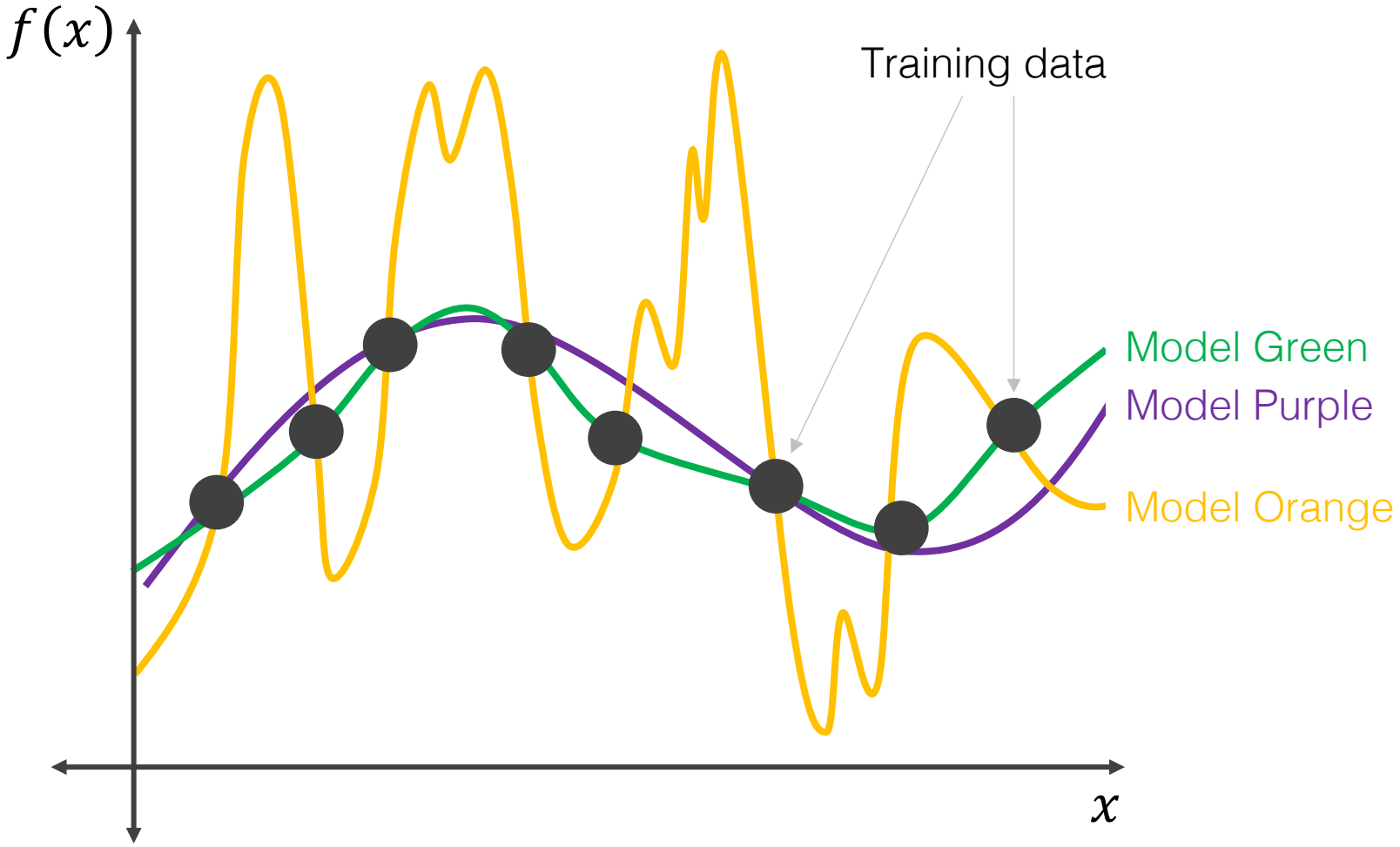
High model **variance**



…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

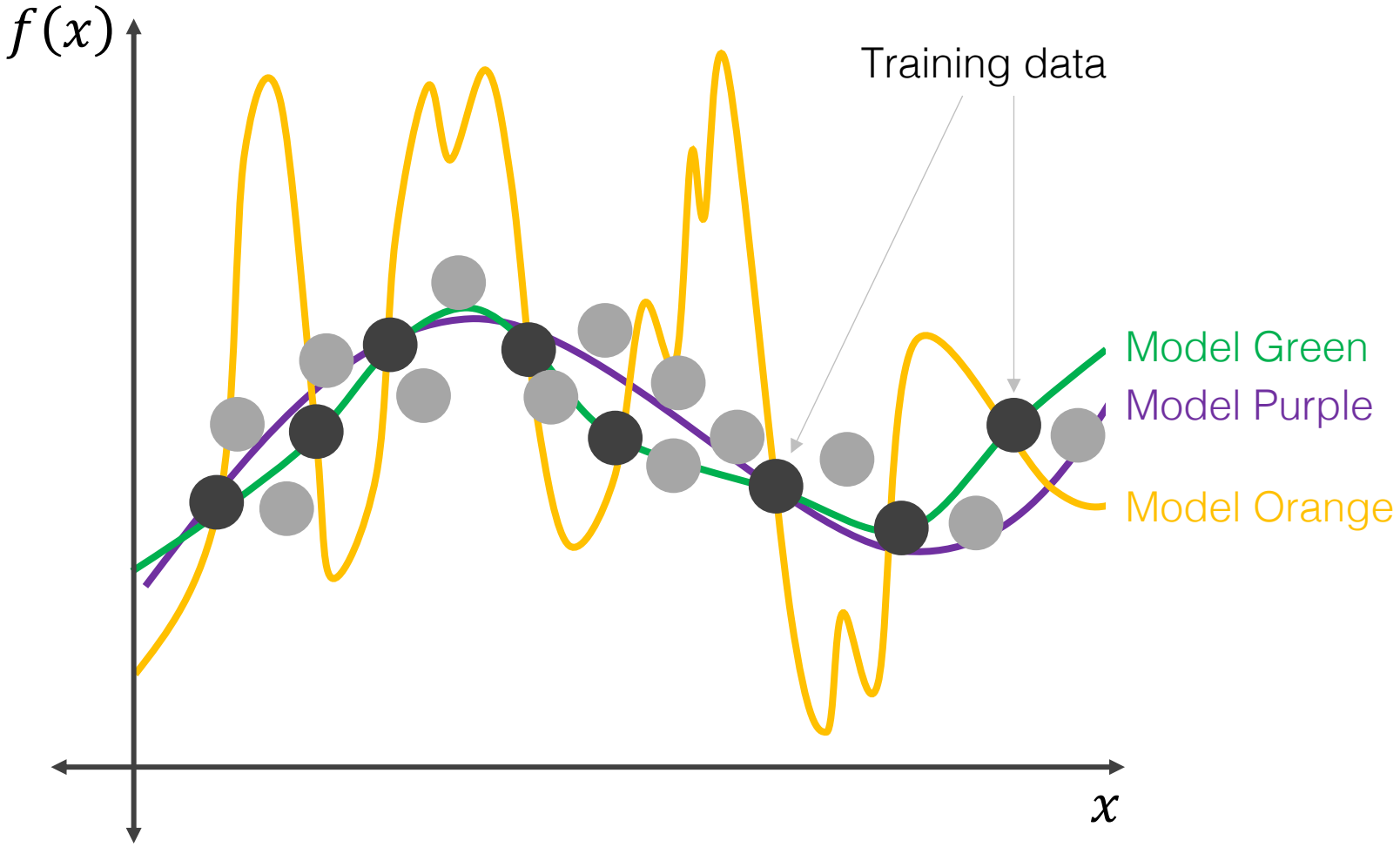
How do enable the algorithm to find solutions that generalize better?

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

…is not always an option

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

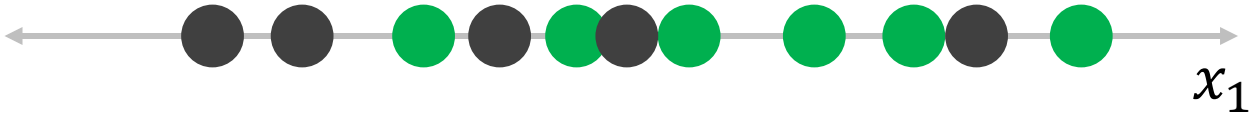
All else being equal, choose the **simpler** solution

Options for limiting model flexibility

1. **Variable/feature subset selection**
2. Regularization/shrinkage
3. Dimensionality reduction

What's the problem with adding features?

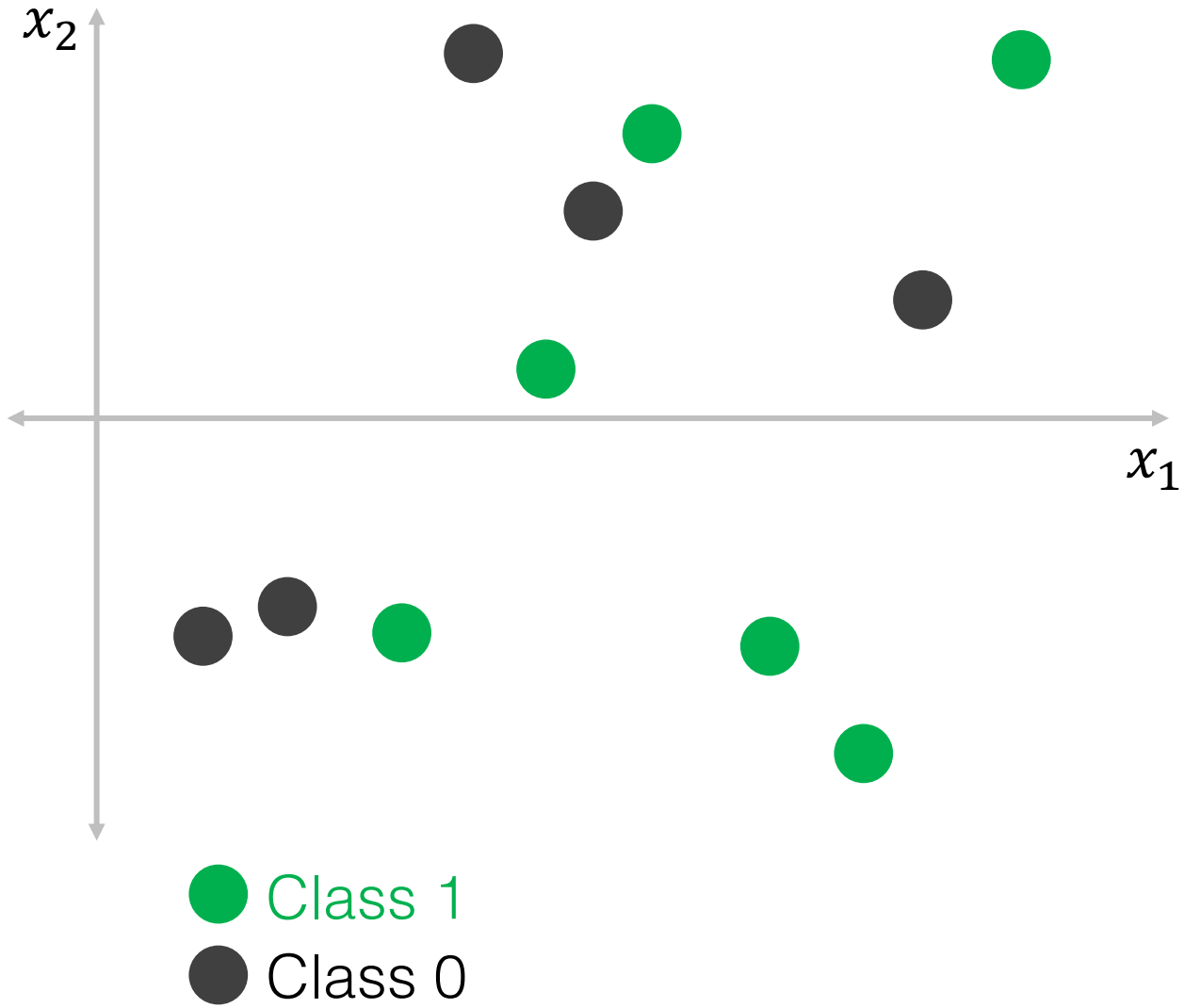
Binary classification with one feature



Class 1

Class 0

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

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

E is our cost / loss function:
- MSE for regression
- Cross entropy/log loss for classification

For regression:

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

Square error

L_2 regularization penalty

This term causes the estimated parameter values to "shrink"

Here $\hat{f}$ is our model.
For linear regression,

$$\hat{f}(\boldsymbol{x}_i, \boldsymbol{w}) = \boldsymbol{w}^T \boldsymbol{x}_i$$

Regularization

a.k.a. shrinkage

Here we assume a regression example

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

a.k.a.…

L_2 regularization

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

ridge regression or weight decay
(Tikhonov regularization)

L_1 regularization

$$C(\boldsymbol{w}) = \sum_{i=1}^{n} \left(\hat{f}(\boldsymbol{x}_i, \boldsymbol{w}) - y_i\right)^2 + \lambda \sum_{j=1}^{p} |w_j|$$

least absolute shrinkage and selection operator (**LASSO**)

L_2 & L_1 regularization

$$C(\boldsymbol{w}) = \sum_{i=1}^{n} \left(\hat{f}(\boldsymbol{x}_i, \boldsymbol{w}) - y_i\right)^2 + \lambda_1 \sum_{j=1}^{p} |w_j| + \lambda_2 \sum_{j=1}^{p} w_j^2$$

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

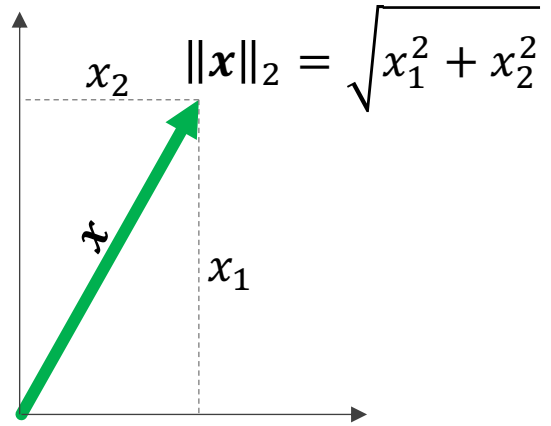
A function that assigns a positive **length or size** to a vector

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:

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

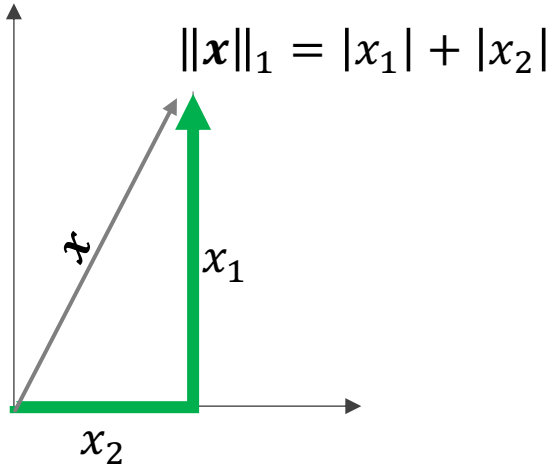


Norms

There's also the 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 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: $\boldsymbol{w} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}$

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

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

$$= 4$$

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

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

$$= \sqrt{10} \approx 3.2$$

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

$$= 3$$

Unit Norms

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

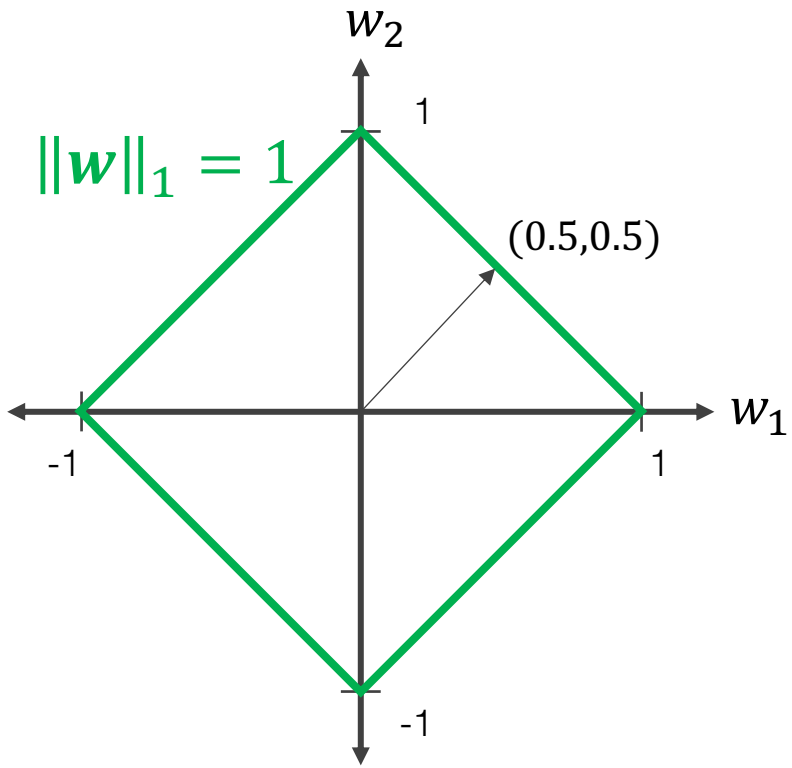
All possible values of $\boldsymbol{w}$ that have a norm of 1

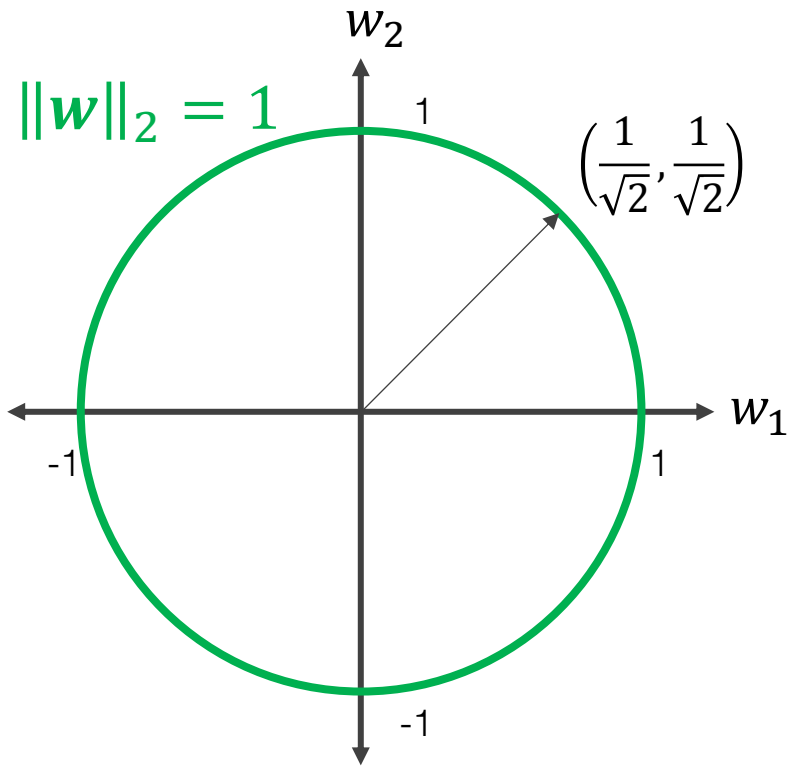
(Plotted as the green lines below)

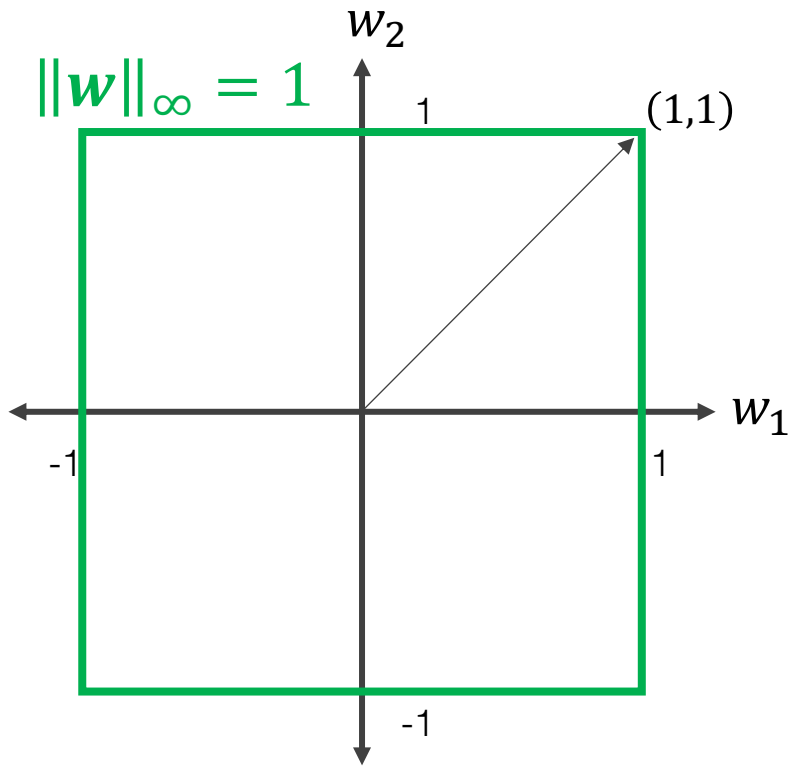
$$\|\boldsymbol{w}\|_1 = \sum_{i=1}^{n} |w_i|$$

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

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

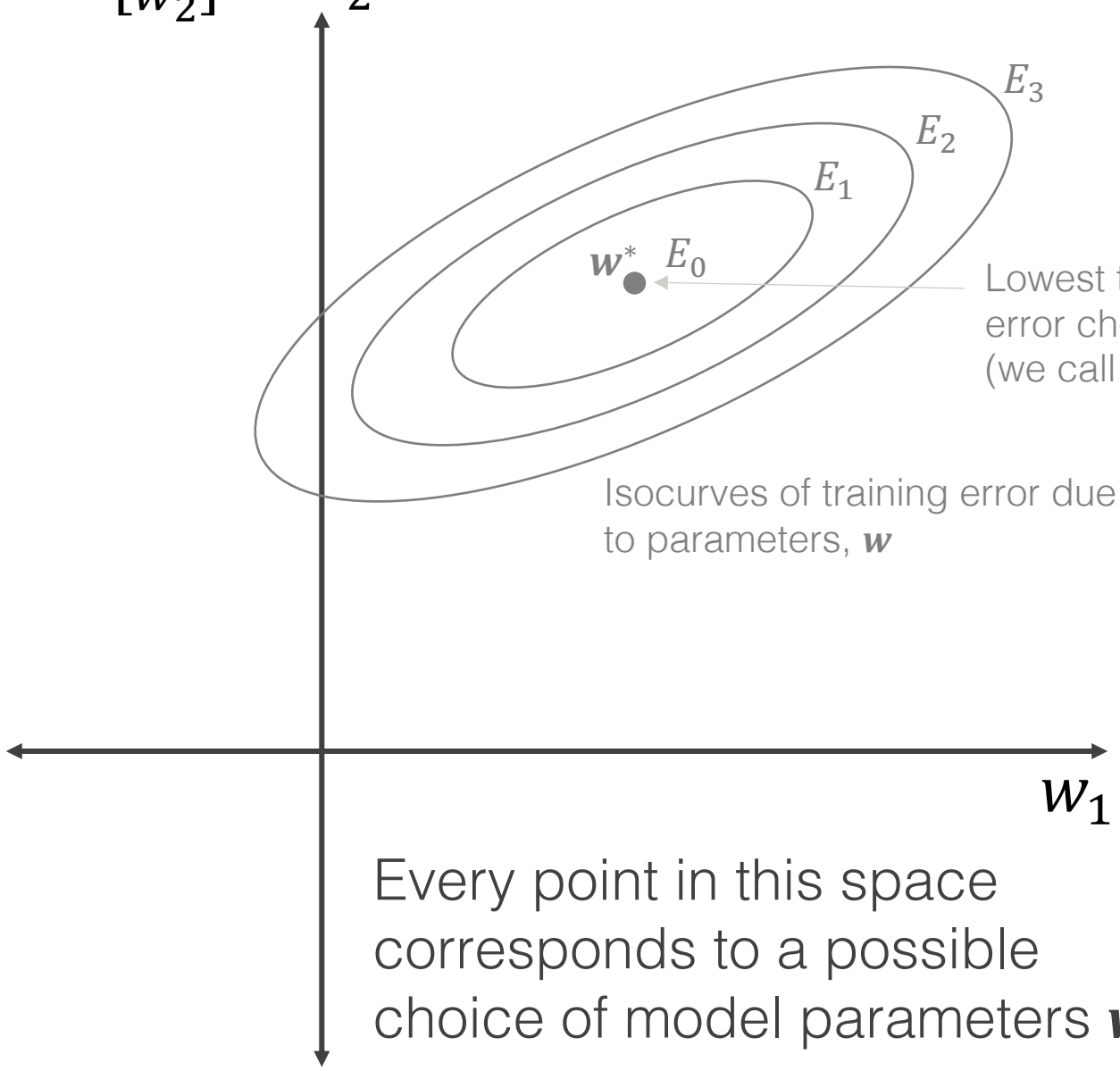






$$\boldsymbol{w} = \begin{bmatrix} w_1 \\ w_2 \end{bmatrix}$$

$E_3 > E_2 > E_1 > E_0$



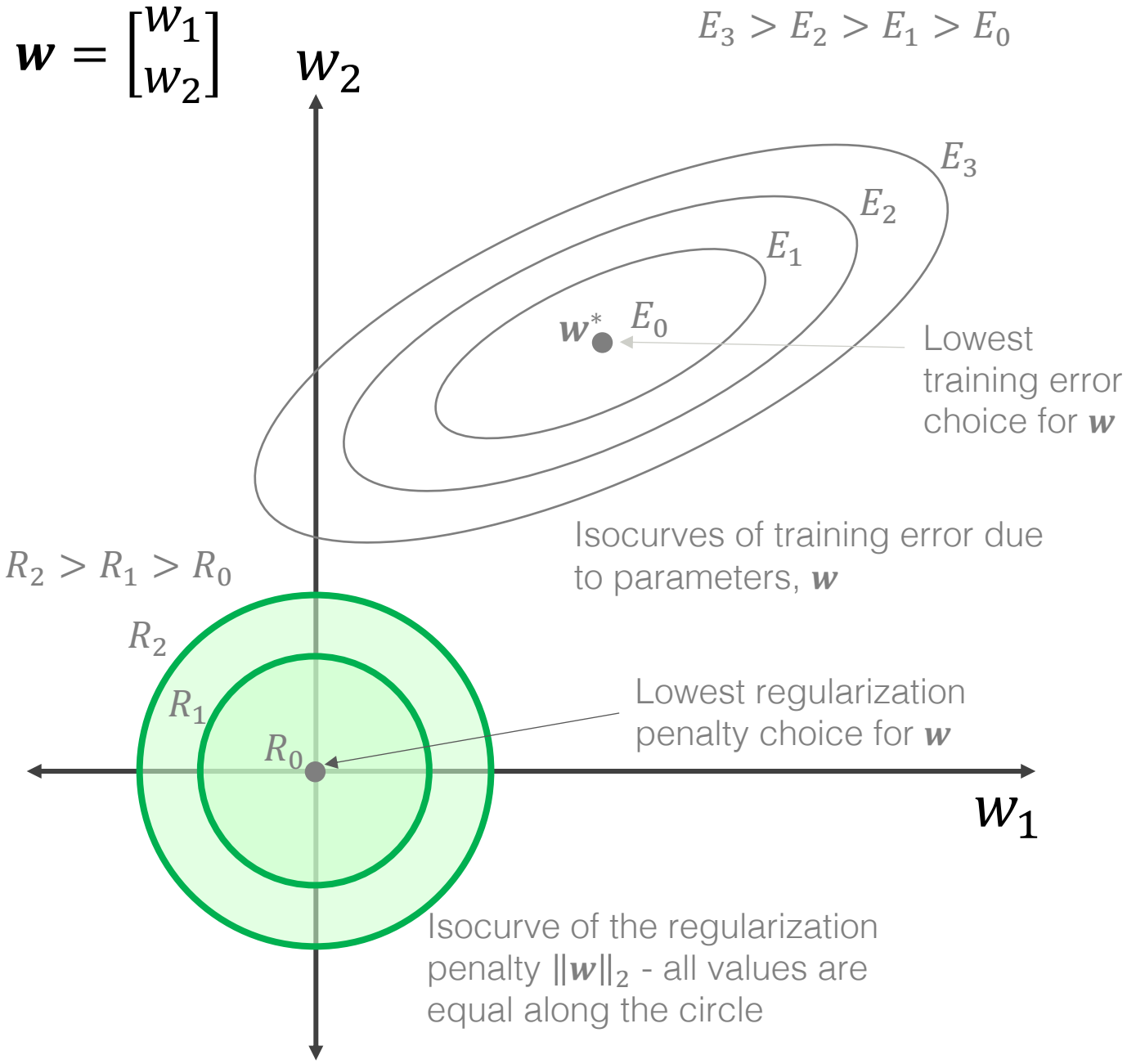
Every point in this space corresponds to a possible choice of model parameters $\boldsymbol{w}$

Minimize cost function:

$$C(\boldsymbol{w}) = \sum_{i=1}^{n} \left(\hat{f}(\boldsymbol{x}_i, \boldsymbol{w}) - y_i\right)^2$$

Training error term (E)

First, let's just minimize training error

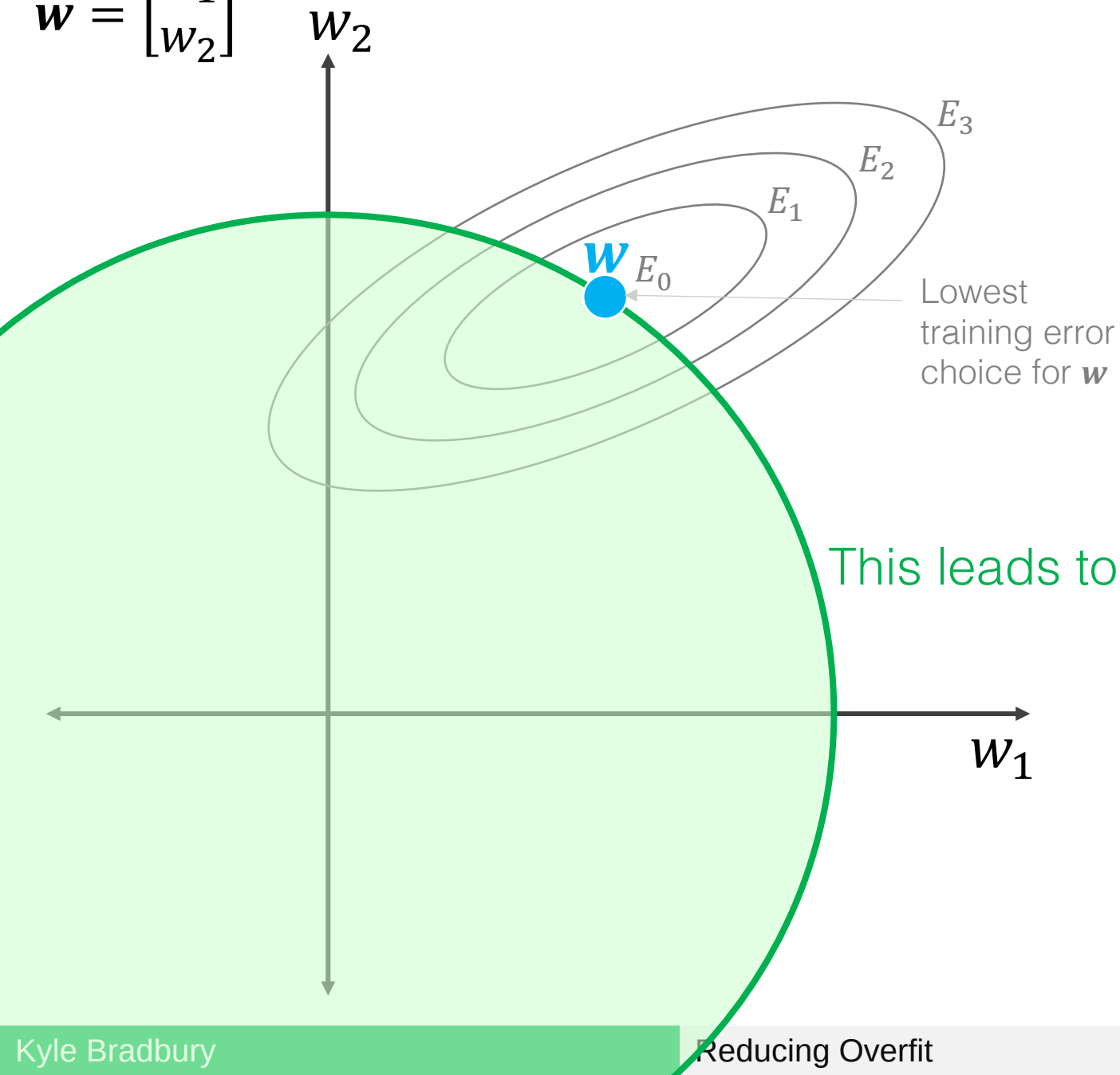


Minimize cost function:

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

Next, let's add a regularization penalty

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



Minimize cost function:

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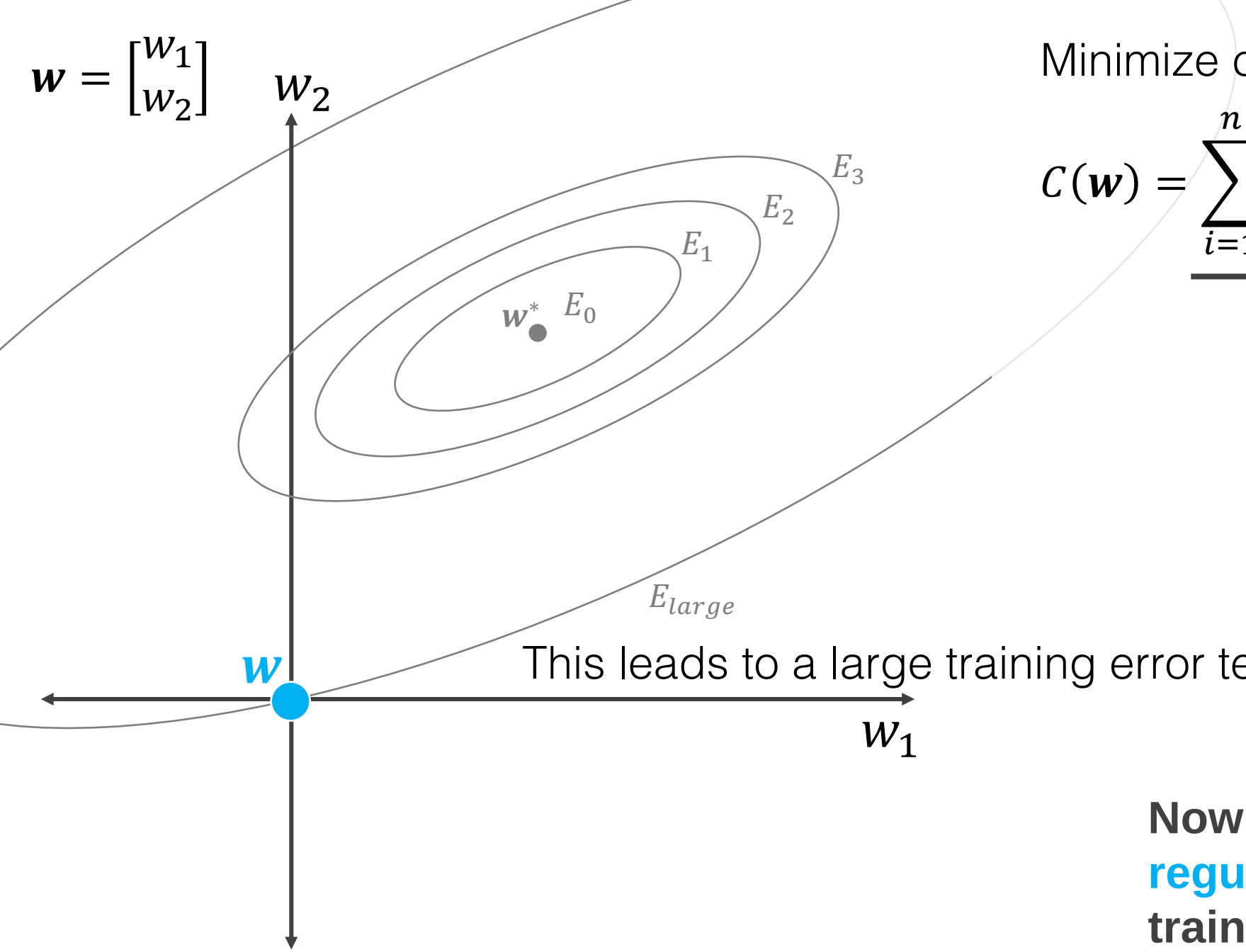
Small **Large**

This leads to a large regularization penalty

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



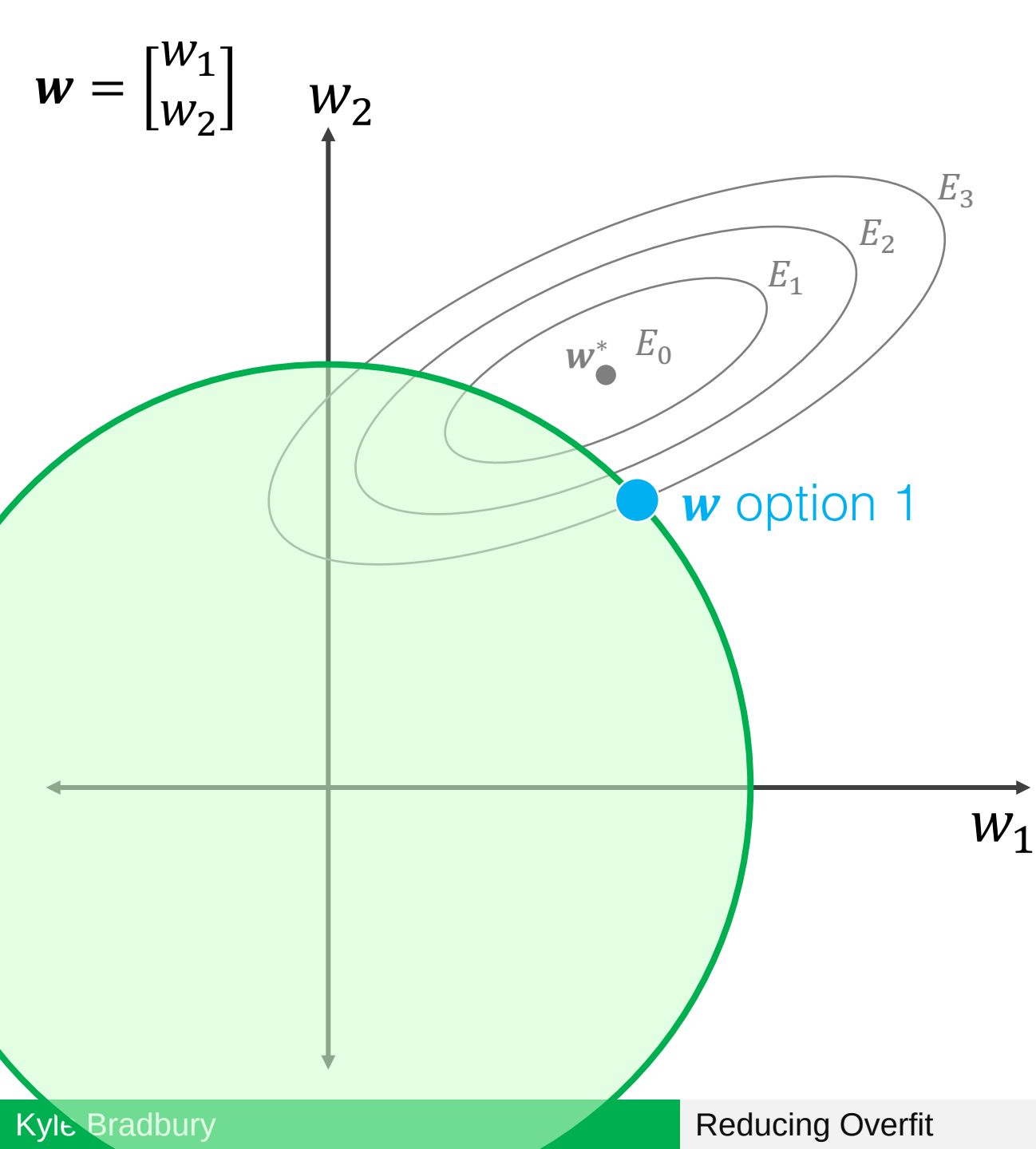
Minimize cost function:

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

Large **Small**

This leads to a large training error term…

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



Minimize cost function:

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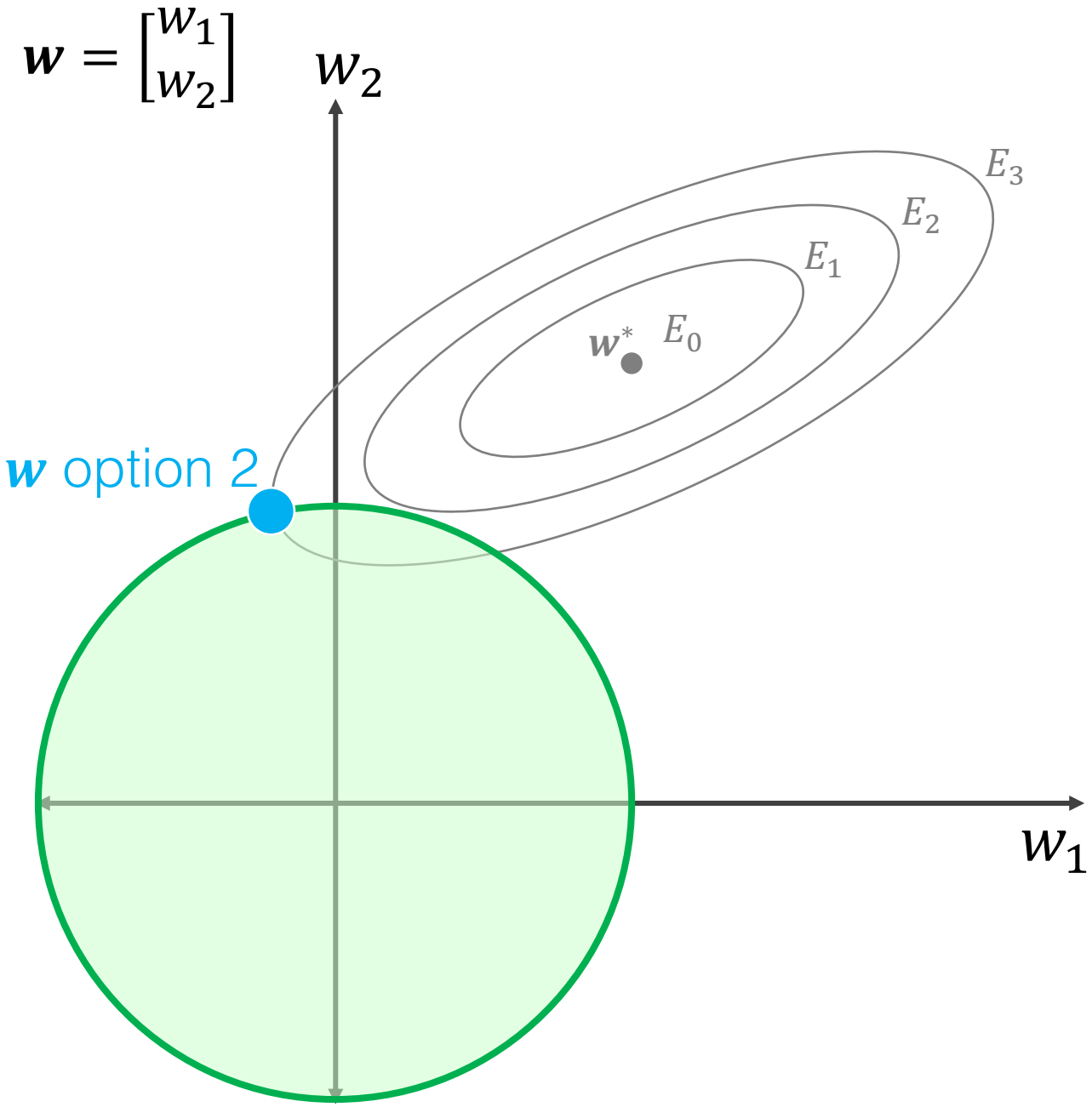
For any level of training error (assume E_3 here), there may be many parameter values that result in an equivalent training error



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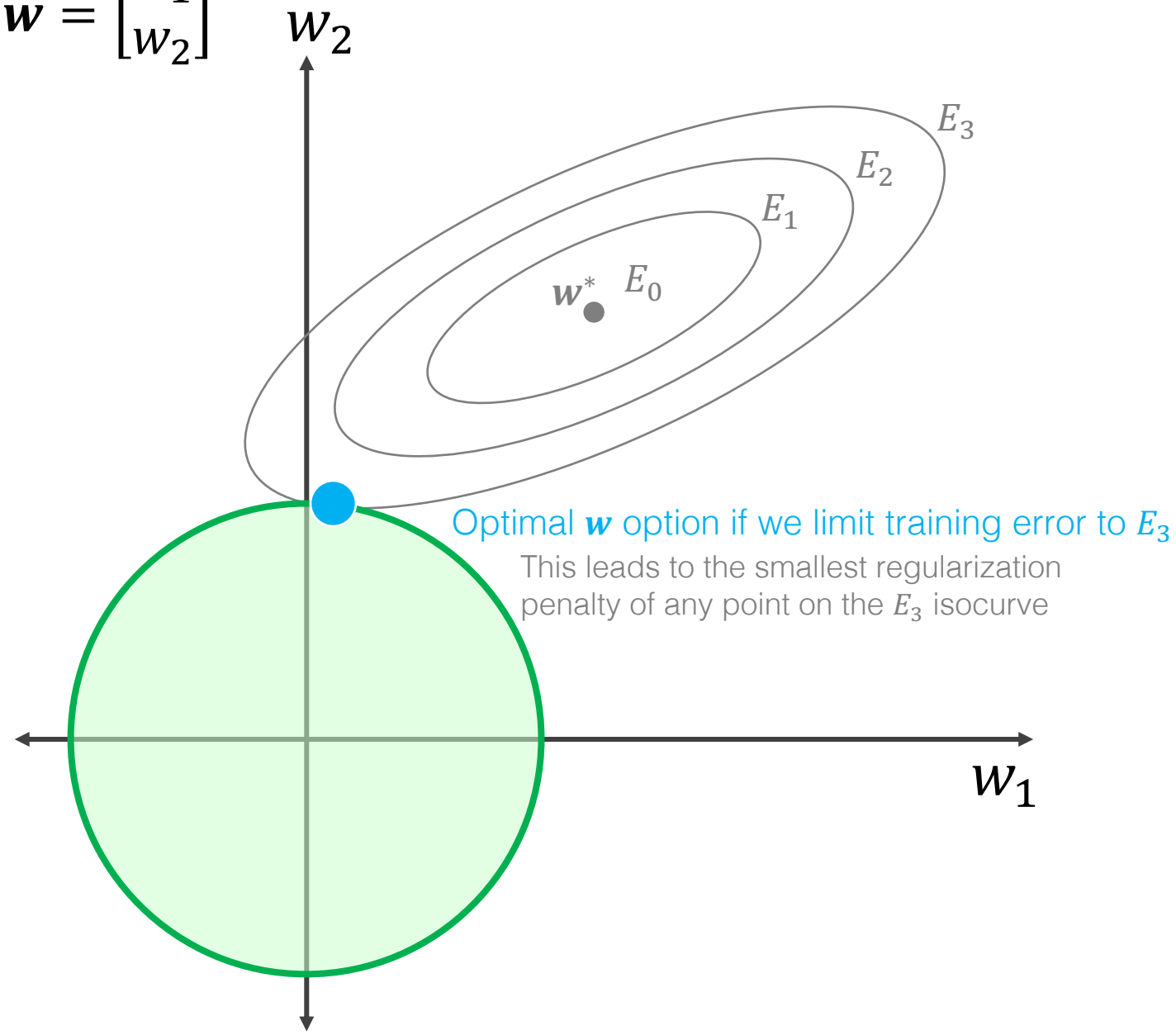
For any level of training error (assume E_3 here), there may be many parameter values that result in an equivalent training error

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



Optimal $\boldsymbol{w}$ option if we limit training error to E_3

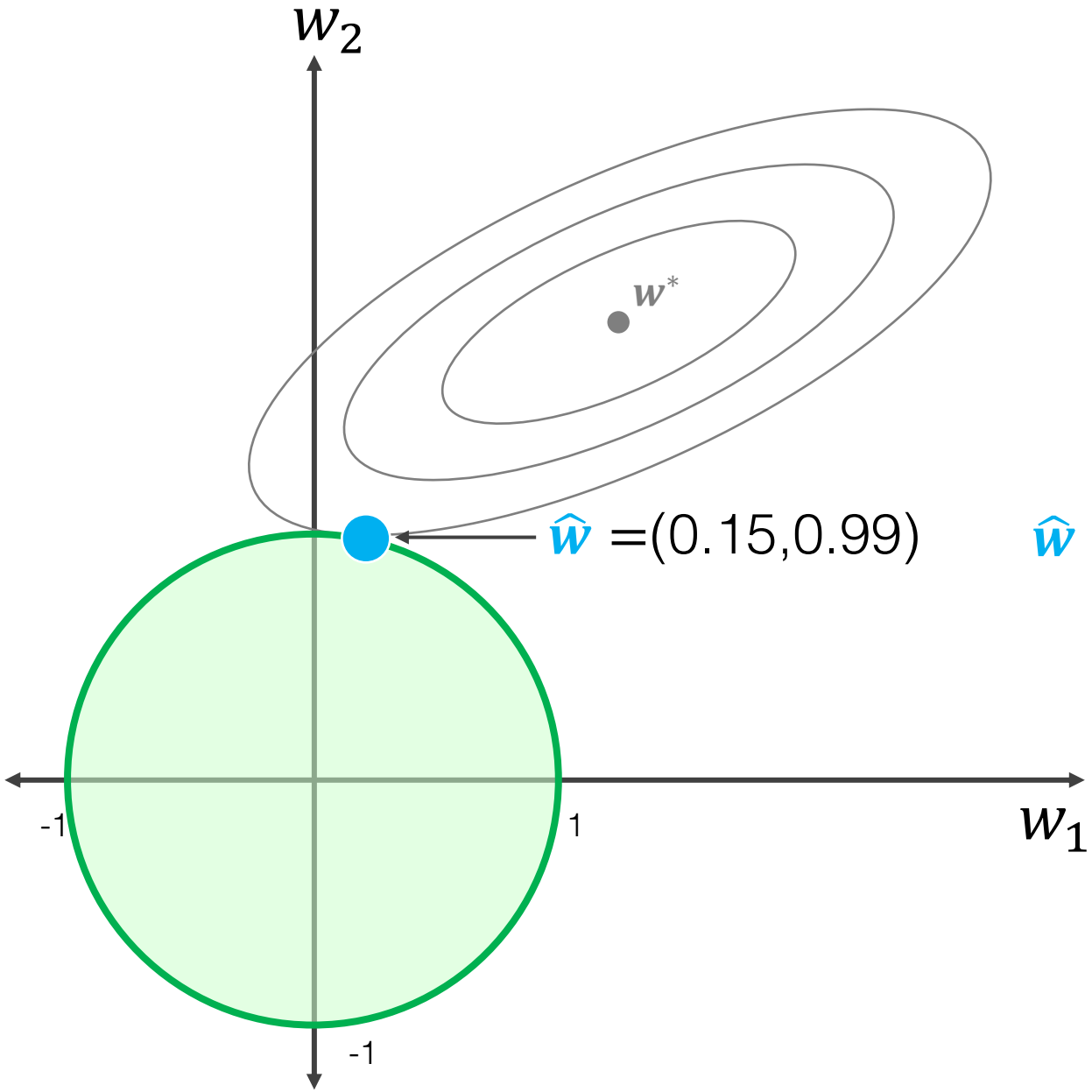
This leads to the smallest regularization penalty of any point on the E_3 isocurve

Minimize cost function:

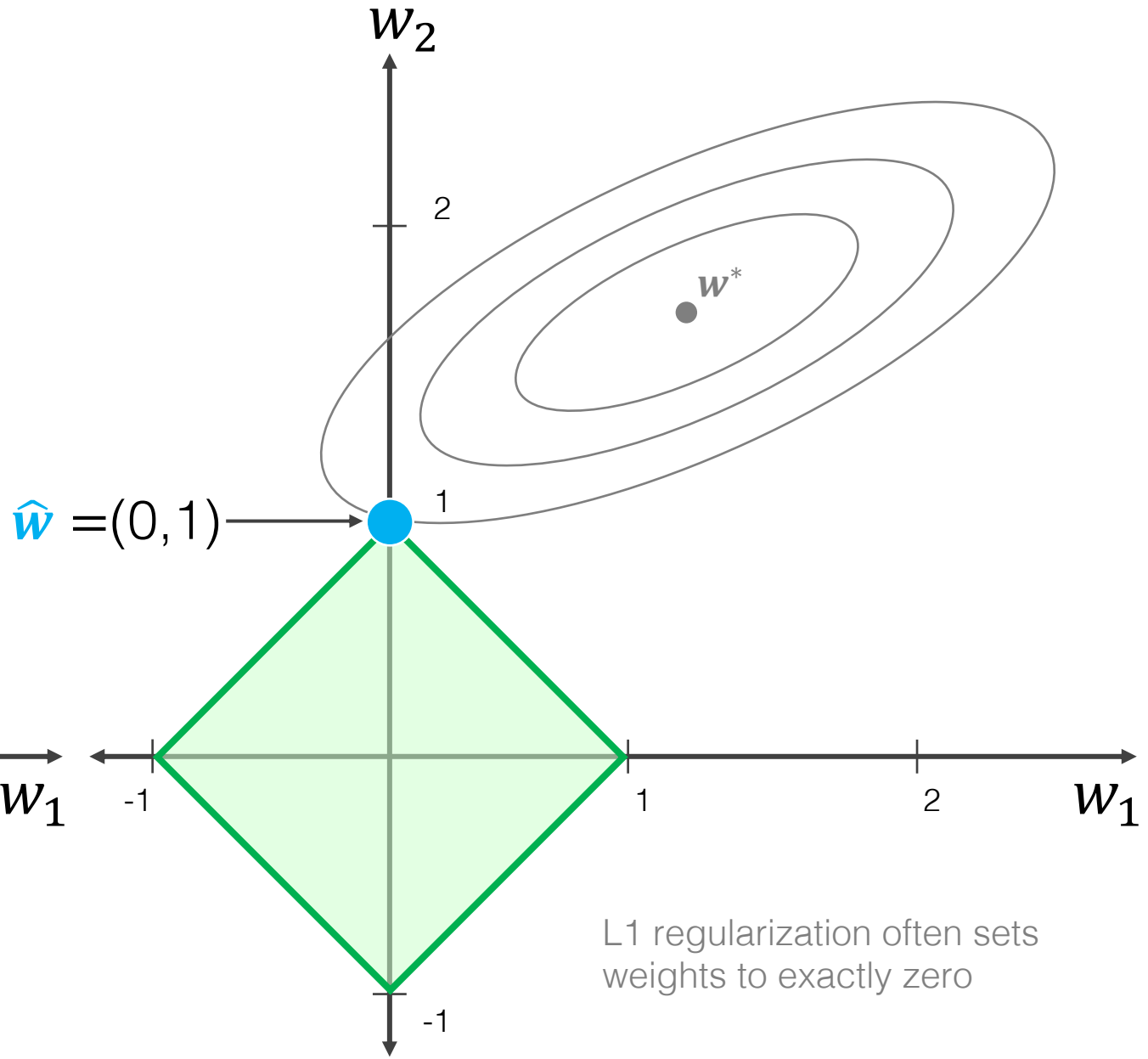
$$C(\boldsymbol{w}) = \underbrace{\sum_{i=1}^{n} \left(\hat{f}(\boldsymbol{x}_i, \boldsymbol{w}) - y_i\right)^2}_{\text{Training error}} + \underbrace{\lambda \sum_{j=1}^{p} w_j^2}_{\text{Regularization penalty}}$$

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

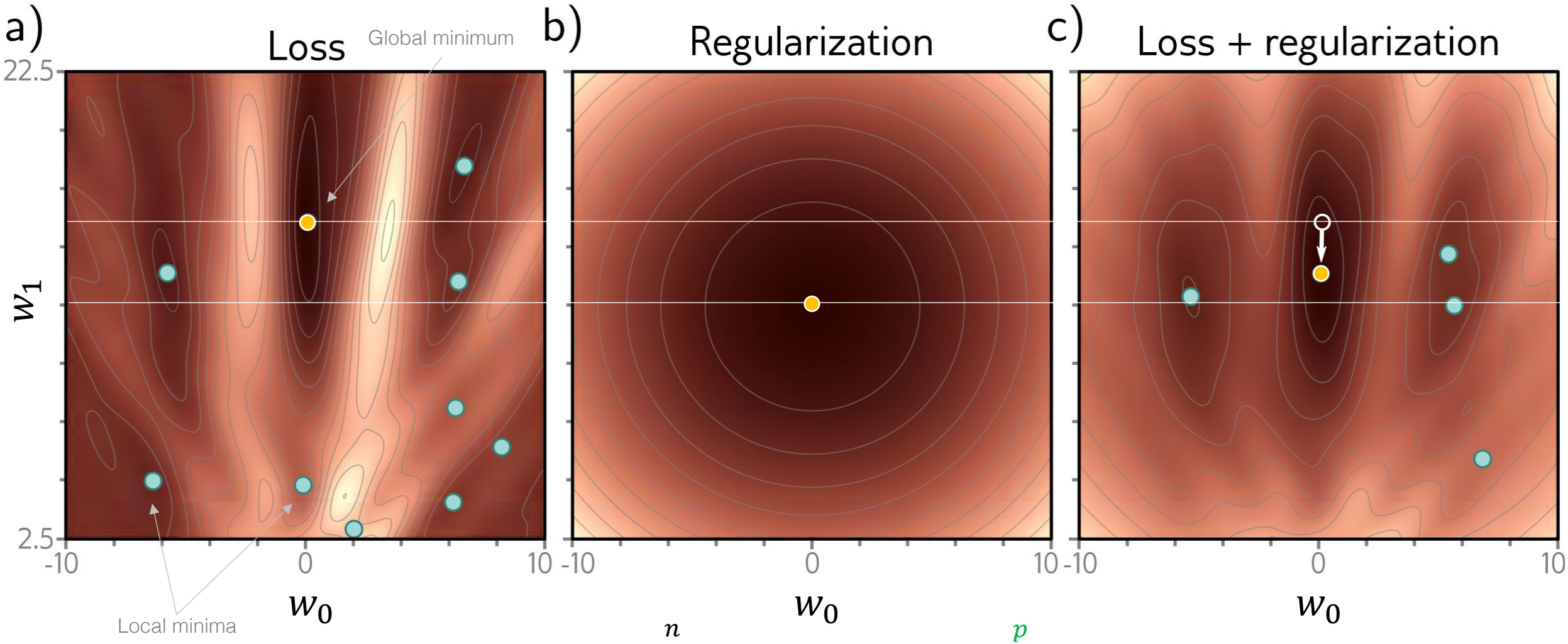
Ridge: L_2 regularization



LASSO: L_1 regularization



L1 regularization often sets weights to exactly zero



$$C(\boldsymbol{w}) = \underbrace{\sum_{i=1}^{n} \left(\hat{f}(\boldsymbol{x}_i, \boldsymbol{w}) - y_i\right)^2}_{\text{Training error (a.k.a. loss)}} + \underbrace{\lambda \sum_{j=1}^{p} w_j^2}_{\substack{\text{Regularization} \\ \text{penalty}}}$$

Visualizing Regularization in Action

Image from Prince, Understanding Deep Learning, 2023

c **a** **b**

Regularization reduces variance

Leads to smaller model parameters

L_1 regularization also performs variable selection

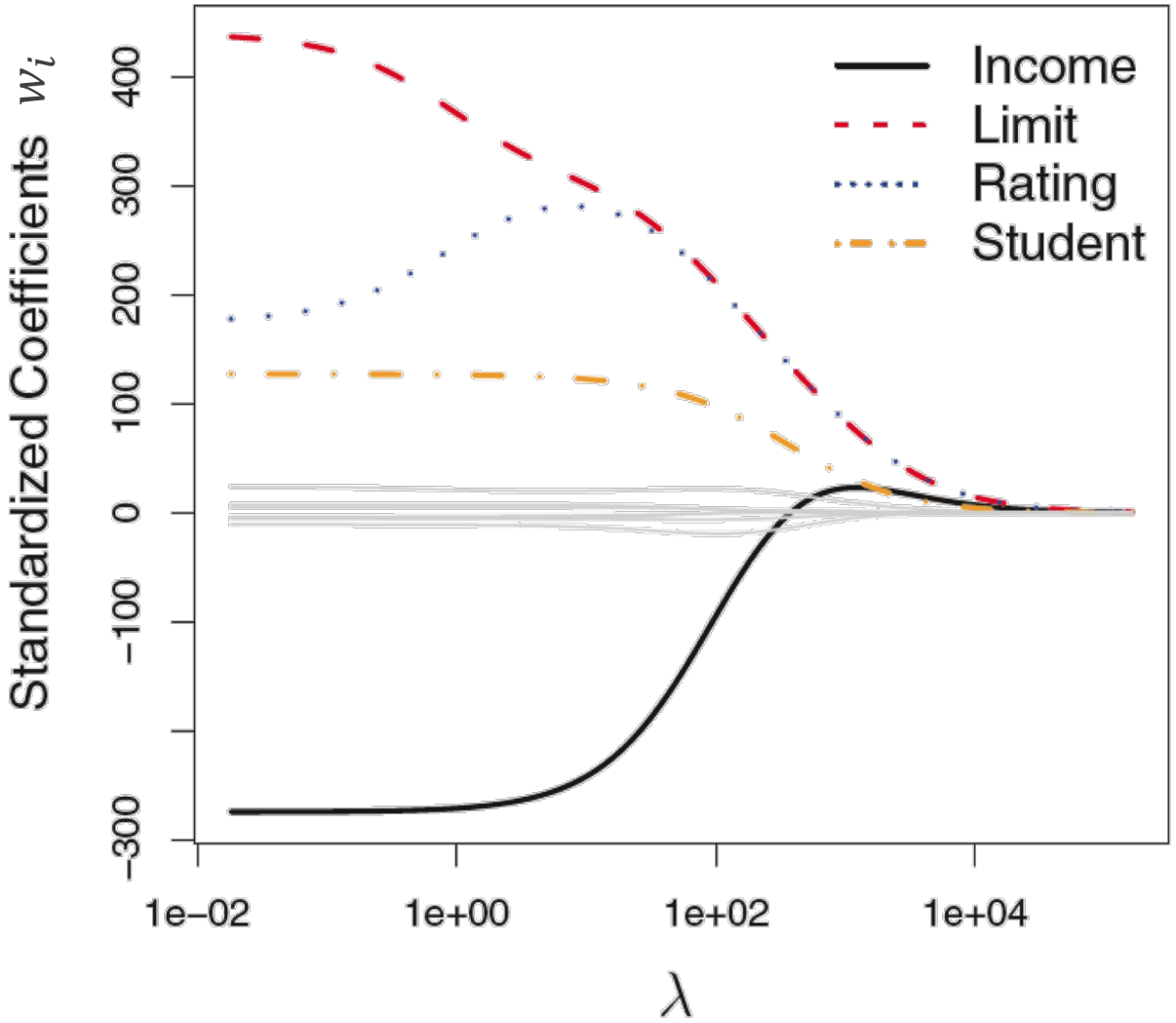
Example: predicting credit default

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

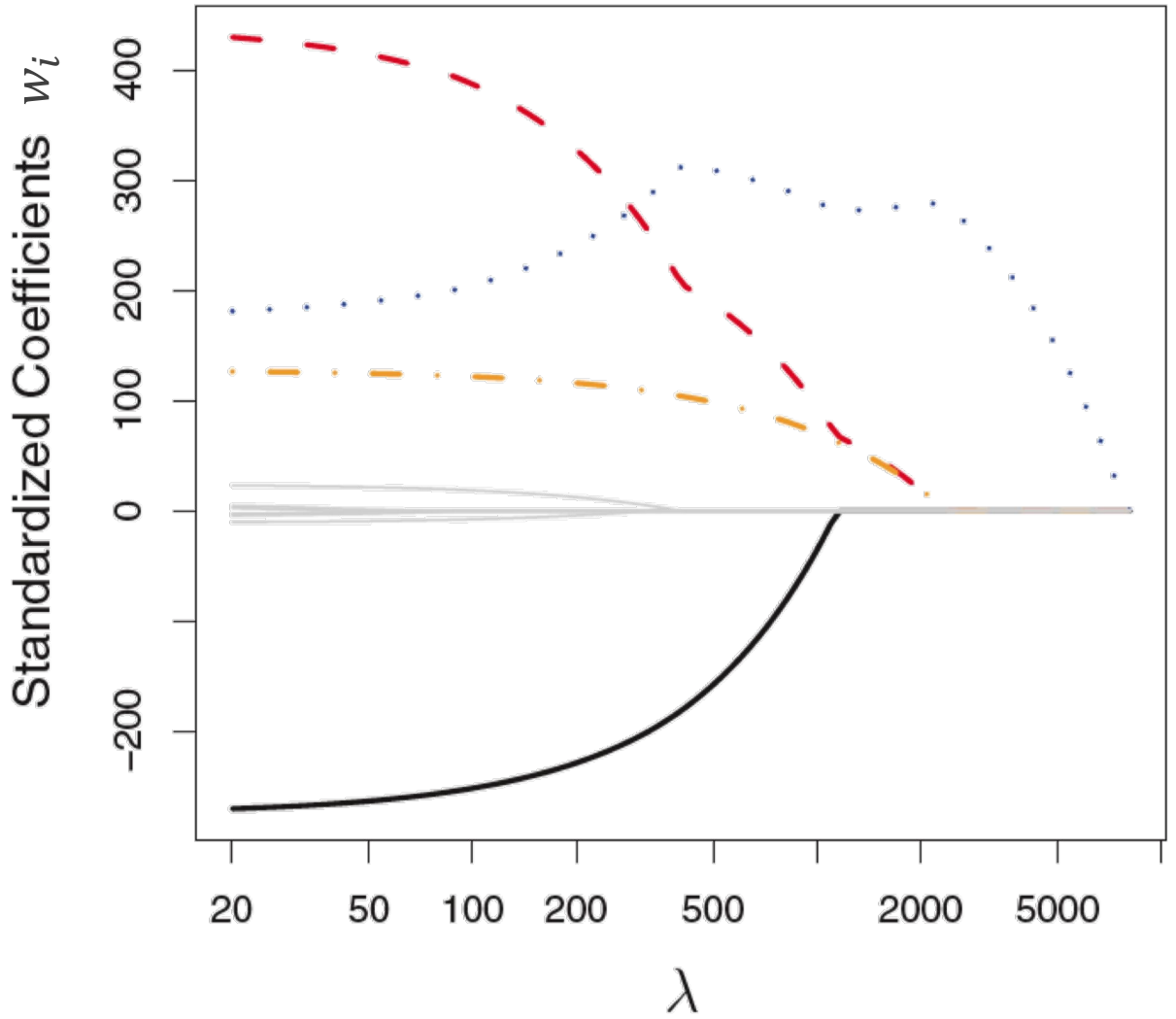
Ridge regression



Regularization penalty

L_1 regularization

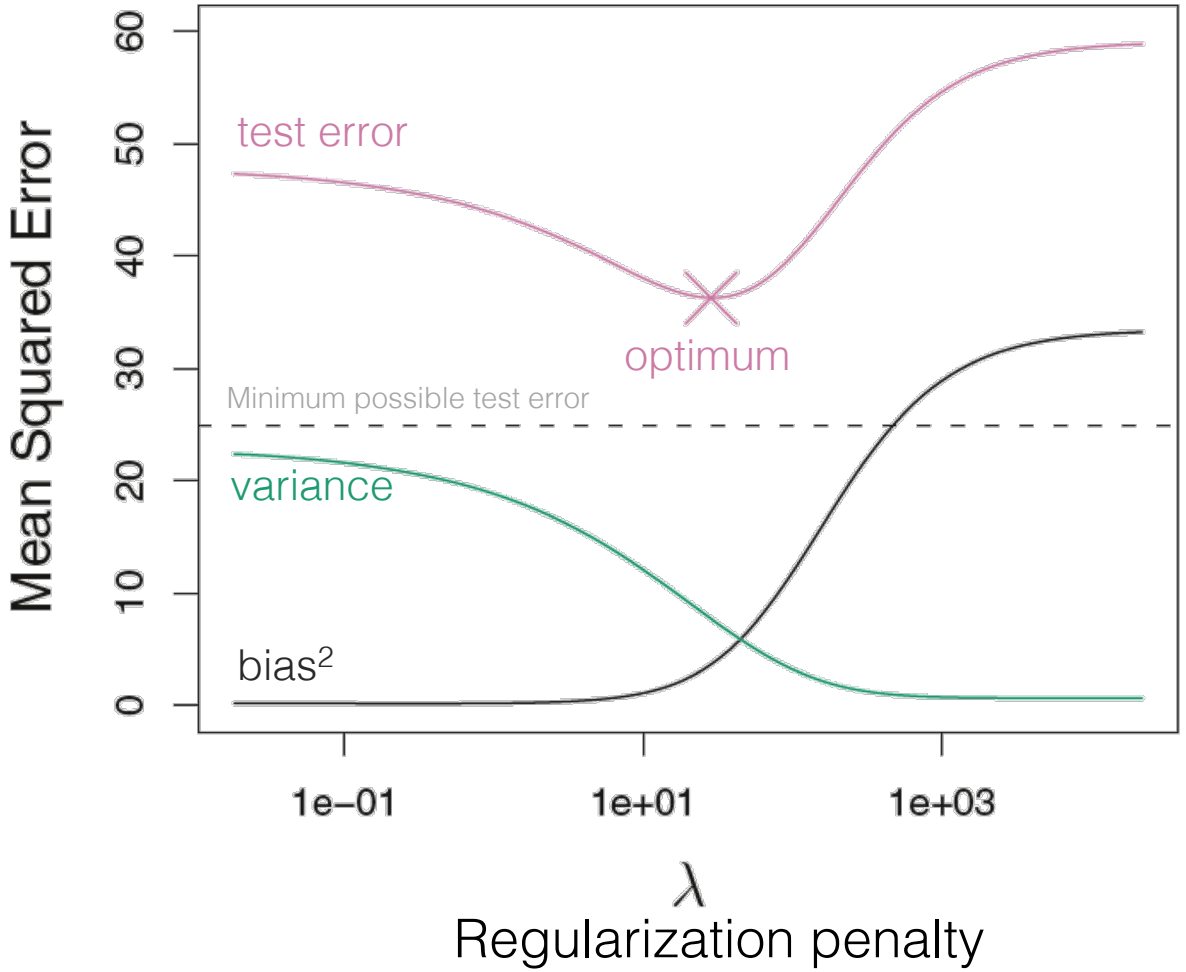
LASSO regularization



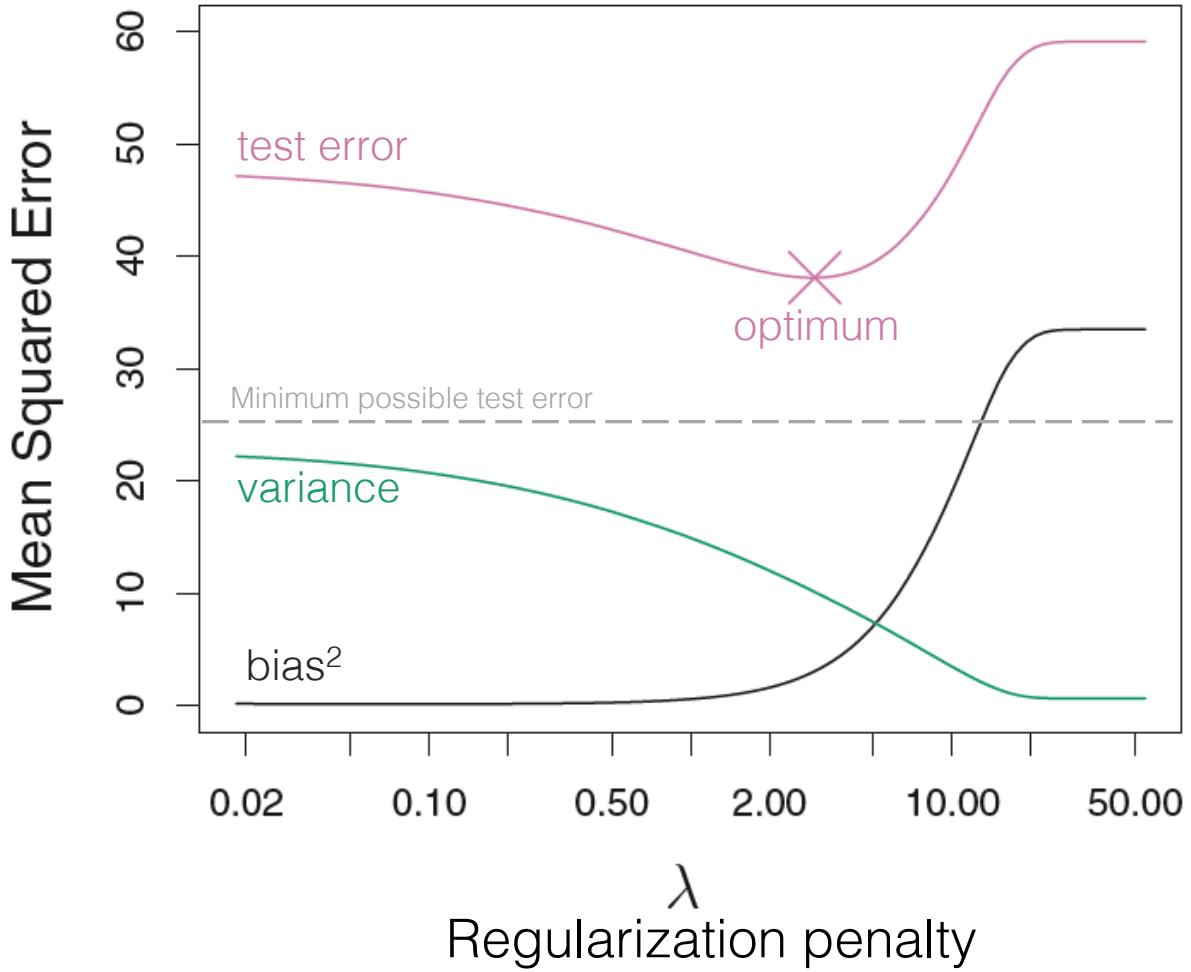
Regularization penalty

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

L_2 regularization

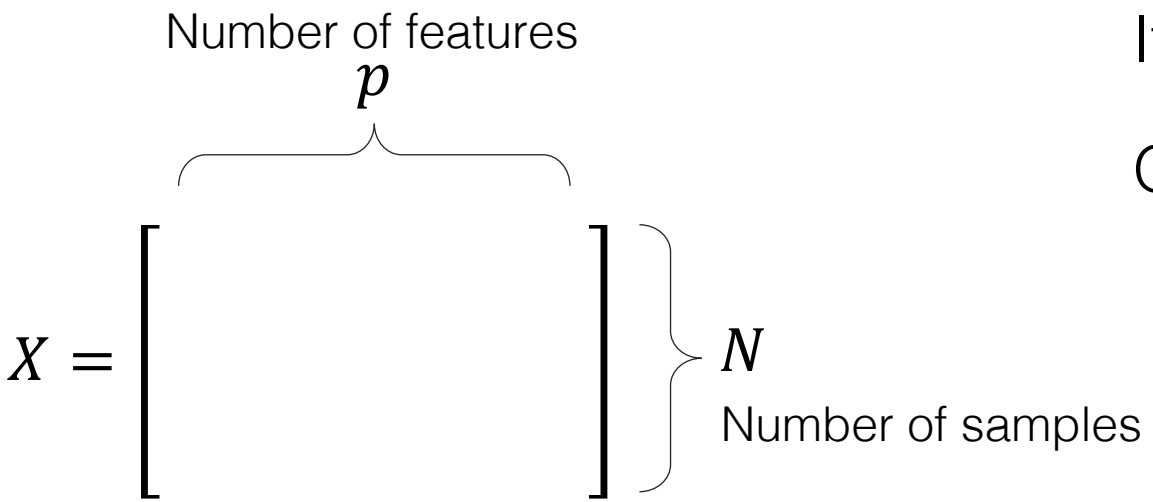


L_1 regularization



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

Underdetermined systems and OLS



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

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

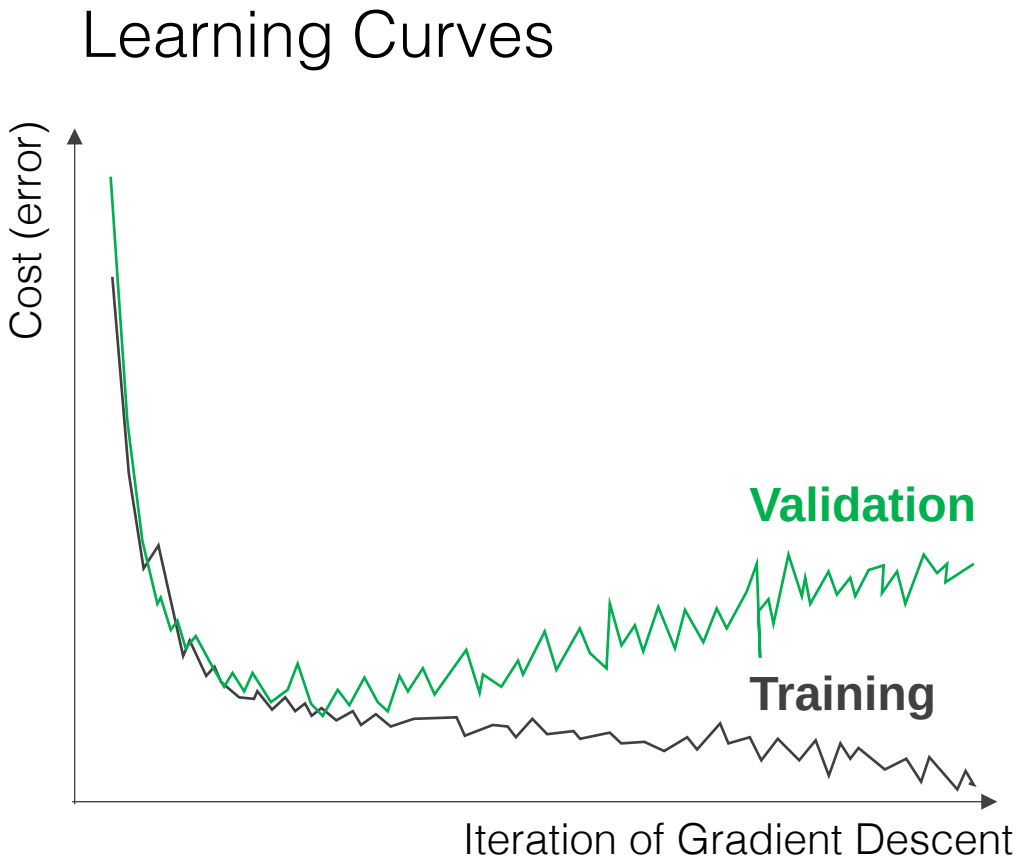
These approaches can be easily added to many cost functions

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



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