Reducing Overfit

Supervised learning in practice

Preprocessing
Explore & prepare data

Data Visualization and Exploration

Identify patterns that can be leveraged for learning

Data Cleaning

- Missing data
- Noisy data
- Erroneous data

Scaling (Standardization)

Prepare data for use in scale-dependent algorithms.

Feature Extraction

Dimensionality reduction eliminates redundant information

Model training

Select models (hypotheses)

Select model options that may fit the data well. We'll call them "hypotheses".

Fit the model to training data

Pick the "best" hypothesis function of the options by choosing model parameters

Iteratively fine tune the model

Performance evaluation

Make a prediction on validation data

Metrics

Classification
Precision, Recall, F_1, ROC Curves (Binary), Confusion Matrices (Multiclass)

Regression
MSE, explained variance, R^2

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Scaling (Standardization)

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Model training

1 Supervised Learning Models: Linear models and KNN
(enough to get started using supervised learning)

Select model options

5 Other algorithms and concepts:

- Generative vs discriminative models
- Parametric vs nonparametric models
- Model ensembles
- Feature/representation learning (neural networks, deep learning)

4 How to control model overfit: regularization strategies for model refinement

Iteratively fine tune the model

Performance evaluation

Make a prediction on validation data

2 Evaluating model performance and comparing models

Precision, Recall, F_1,

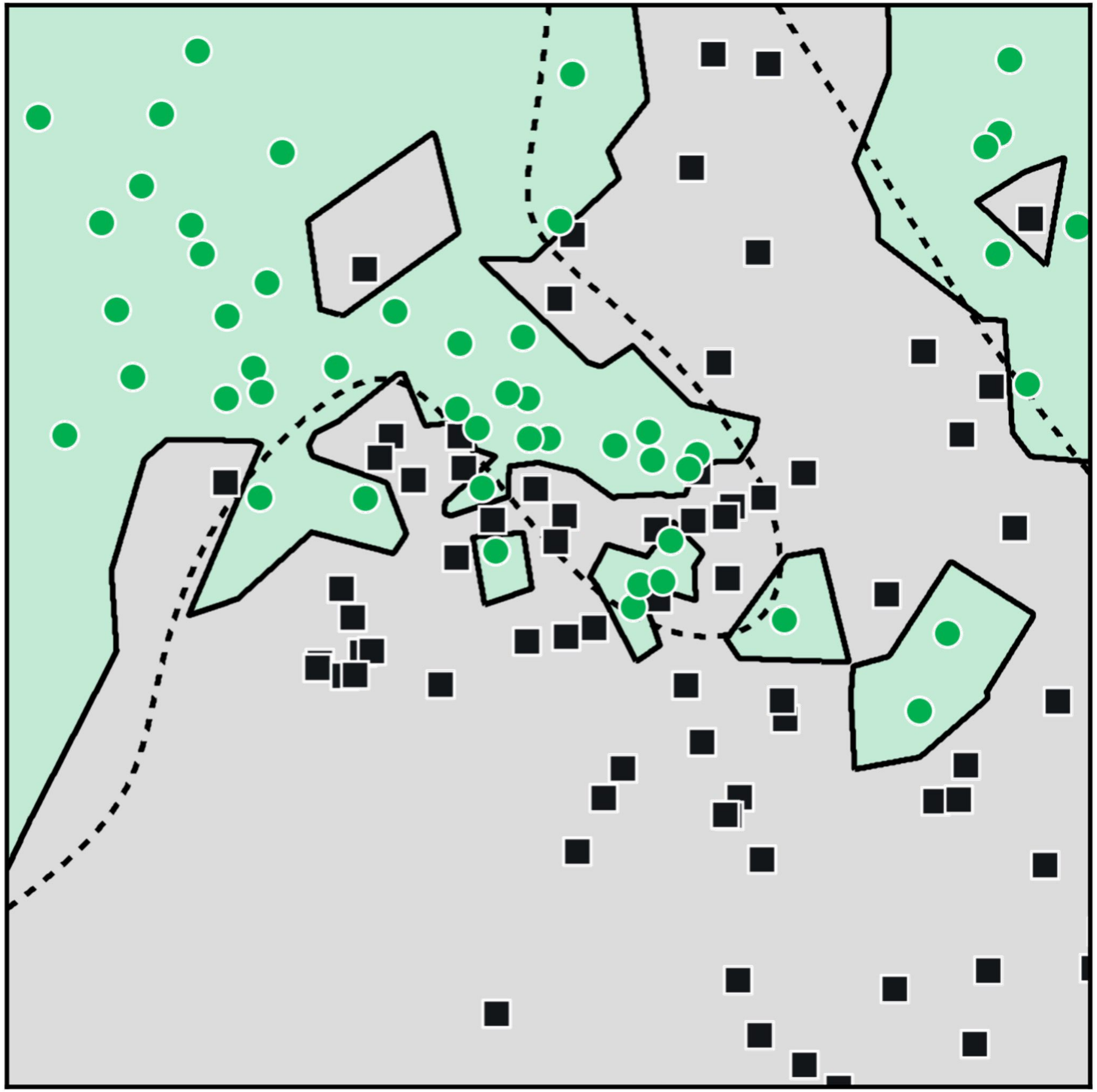
3 How to make decisions using models

Regression
MSE, explained variance, R^2

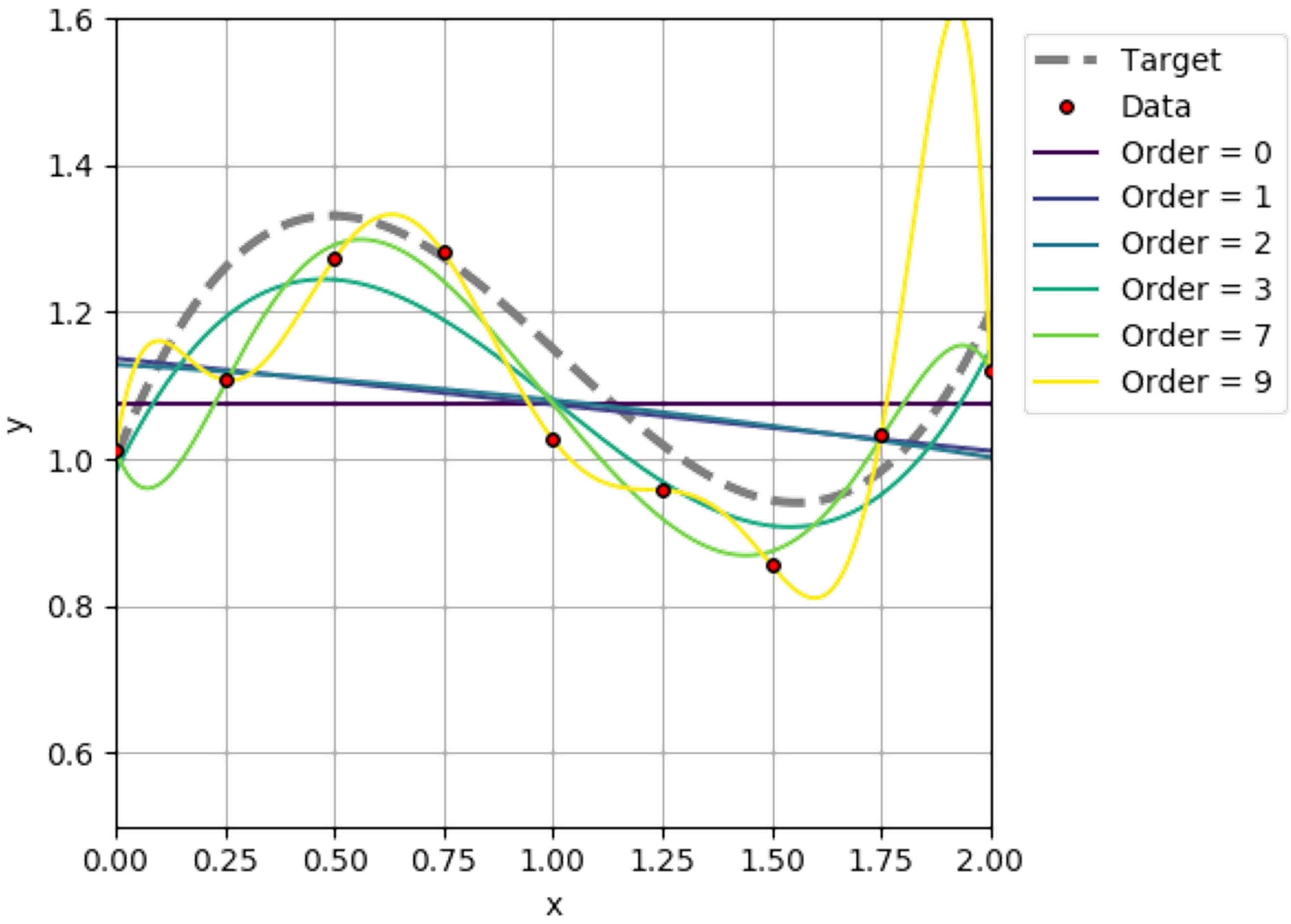
We’ve seen overfit in classification…

Overfitting to the training data

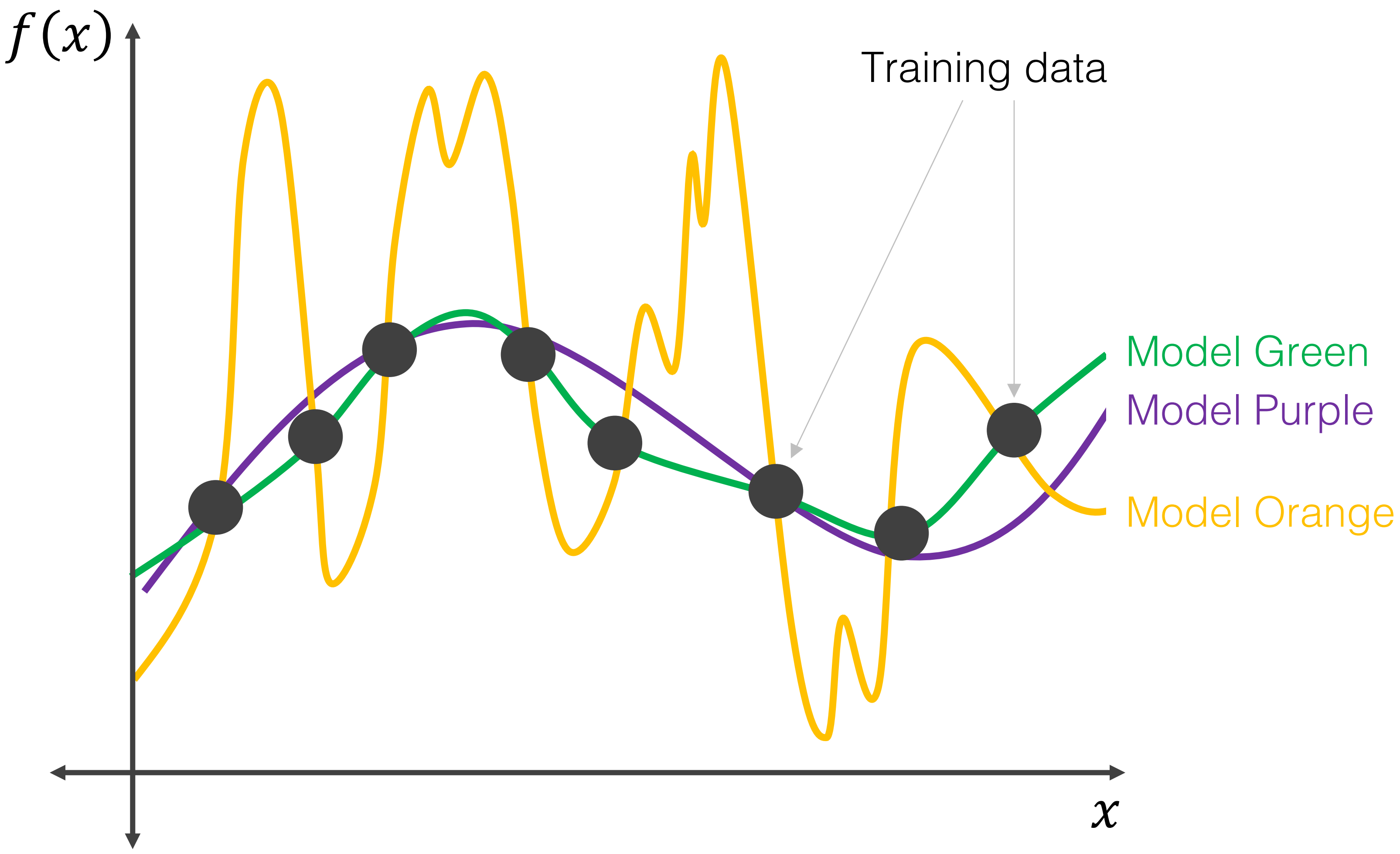
High model **variance**



…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?

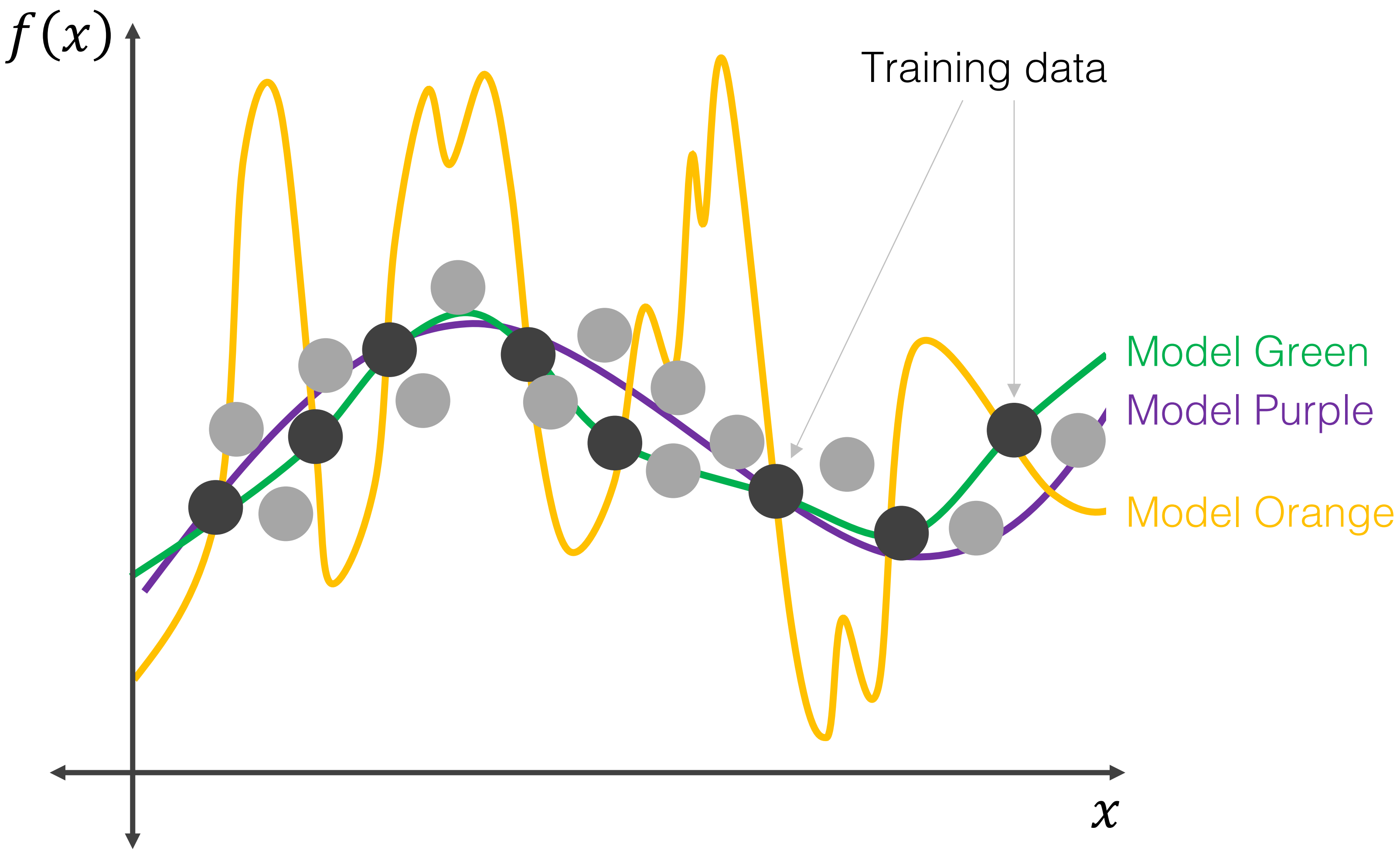
Option #1: Add more data!

cost is the biggest problem

(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

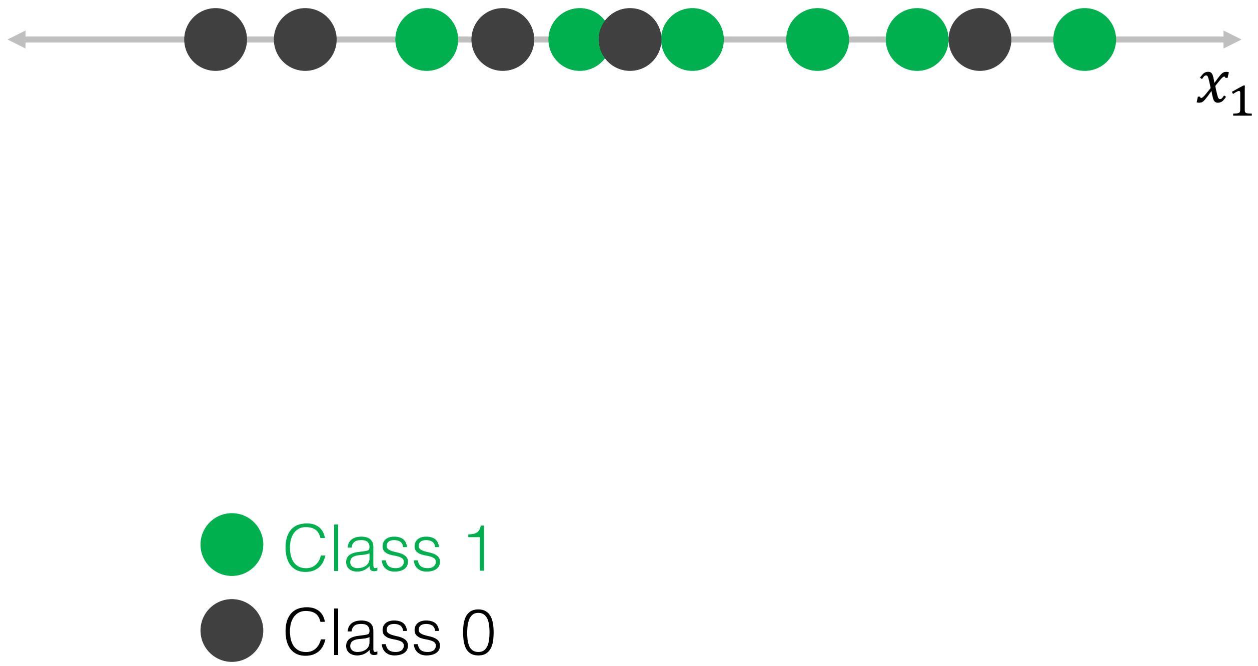
Occam's Razor / Law of Parsimony

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

Options for limiting model flexibility

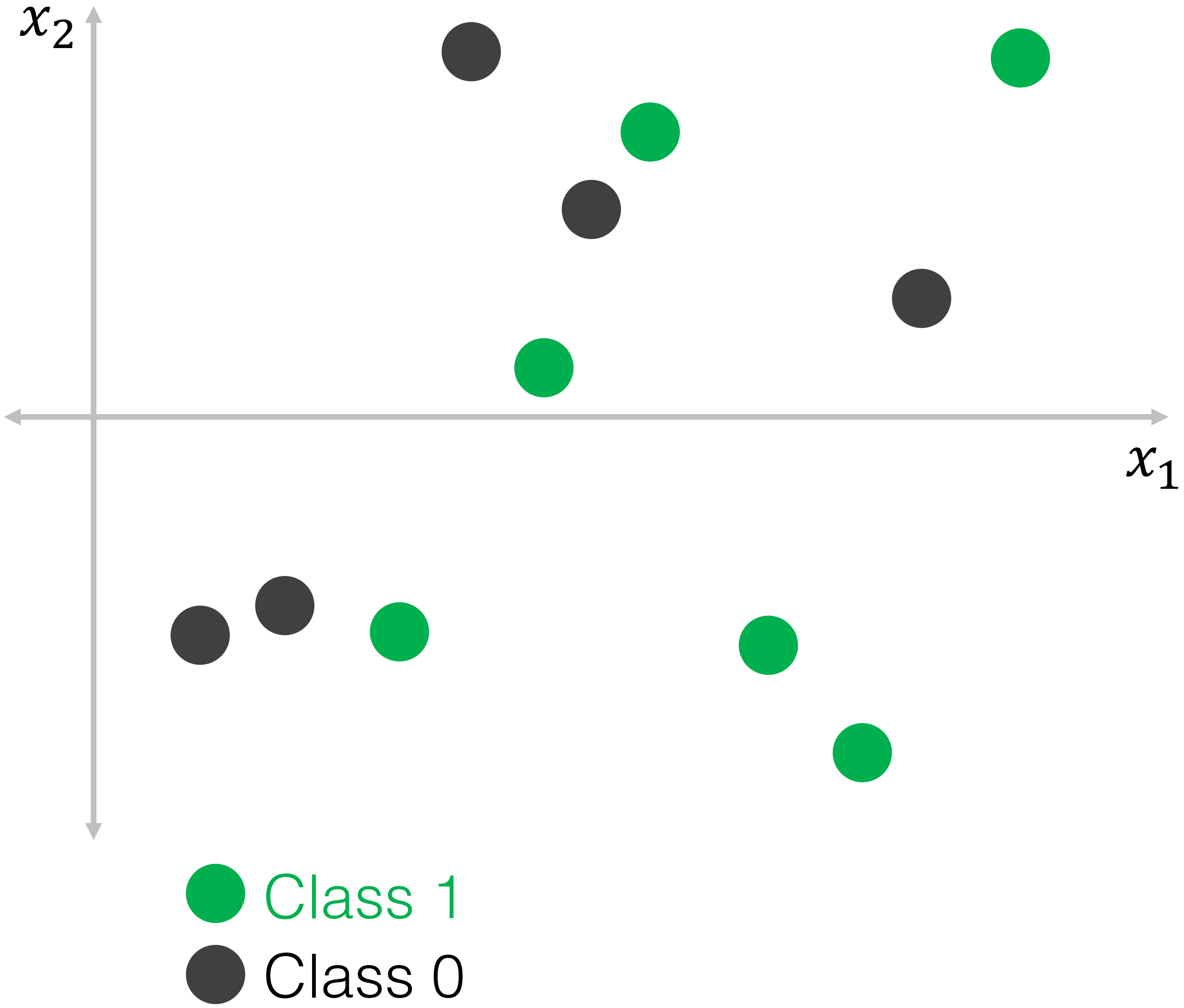
1. **Variable/feature subset selection**
2. Regularization/shrinkage
3. Dimensionality reduction

What's the problem with adding features?



Binary classification with one feature

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
try different combinitions of feature selection and decide which combination works the best
(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 best result
Forward selection the rest are trying to approximate exhaustive search
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

by adding the regularization penalty term

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

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

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

For regression:

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

penalty minimized when abs weights are minimized

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

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

Square error

regression --> Least squared error
classification --> cross-entropy or least

L_2 regularization penalty

This term causes the estimated parameter values to “shrink”

Regularization
a.k.a. shrinkage

Here we assume a regression example

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

a.k.a….

L2 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)

L1 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**)

L2 & L1 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

…other norms

Normal Rockwell (painter)

Norm Macdonald (comedian)

Norman Borlaug (agronomist)

Norm Peterson (character on Cheers)

Norm

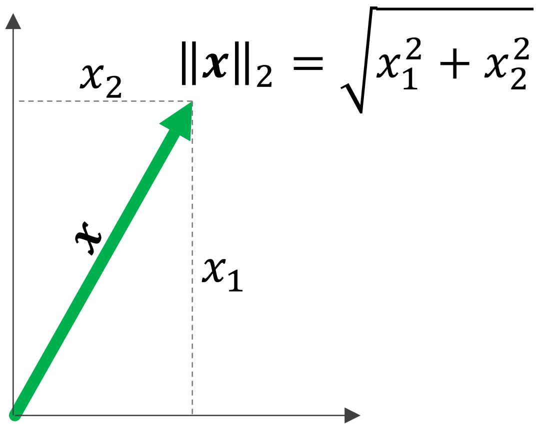
A function that assigns a positive **length or size** to a vector

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:

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

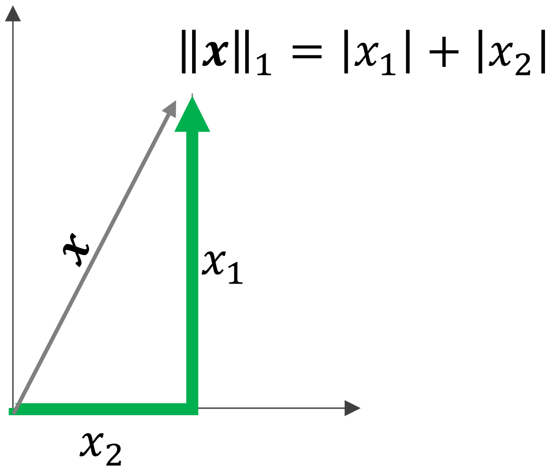


Norms

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: $\boldsymbol{w} = \begin{bmatrix} 1 \\ 3 \end{bmatrix}$

$$||\boldsymbol{w}||_1 = |w_1| + |w_2|$$
$$= |1| + |3|$$
$$= 4$$

$$||\boldsymbol{w}||_2 = \sqrt{w_1^2 + w_2^2}$$
$$= \sqrt{1^2 + 3^2}$$
$$= \sqrt{10} \approx 3.2$$

$$||\boldsymbol{w}||_\infty = \max_i |w_i|$$
$$= 3$$

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)

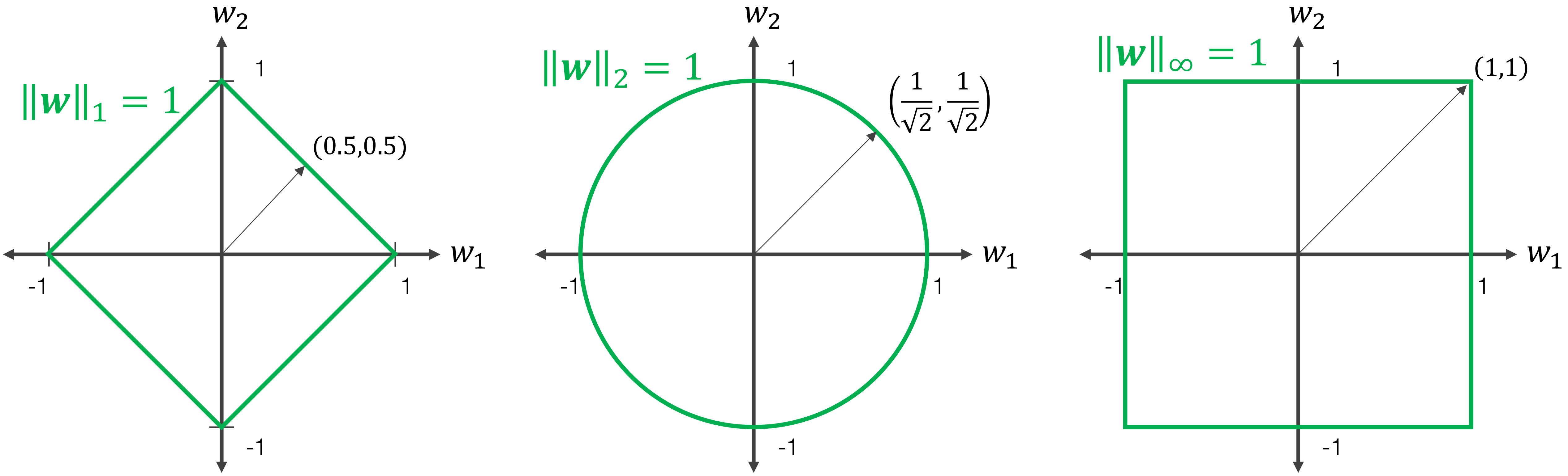
$$\|\boldsymbol{w}\|_1 = \sum_{i=1}^{n} |w_i|$$

focus on these two only

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

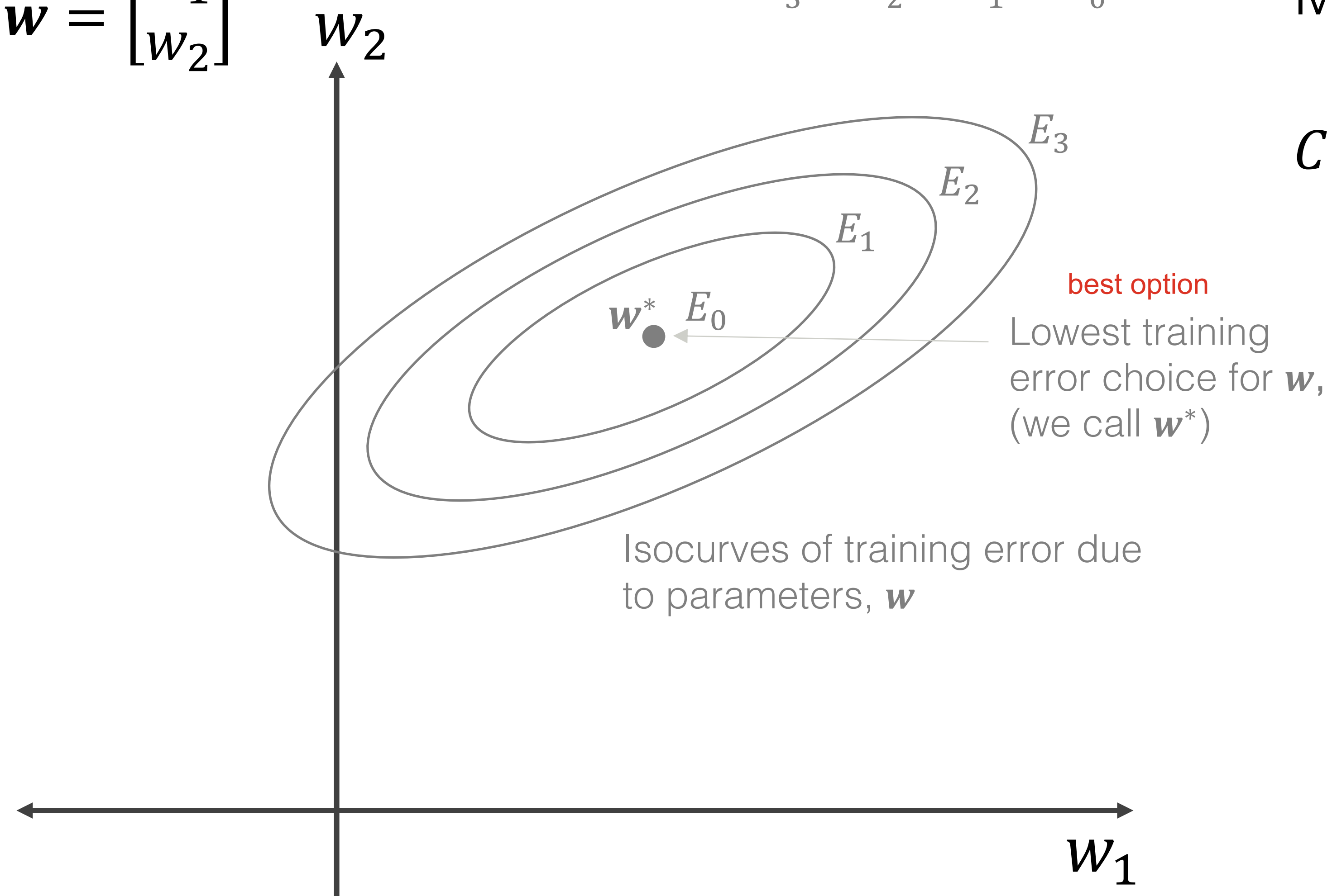
$$\|\boldsymbol{w}\|_\infty = \max_i |w_i|$$

w1+w2 = 1



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

等Error线 $E_3 > E_2 > E_1 > E_0$

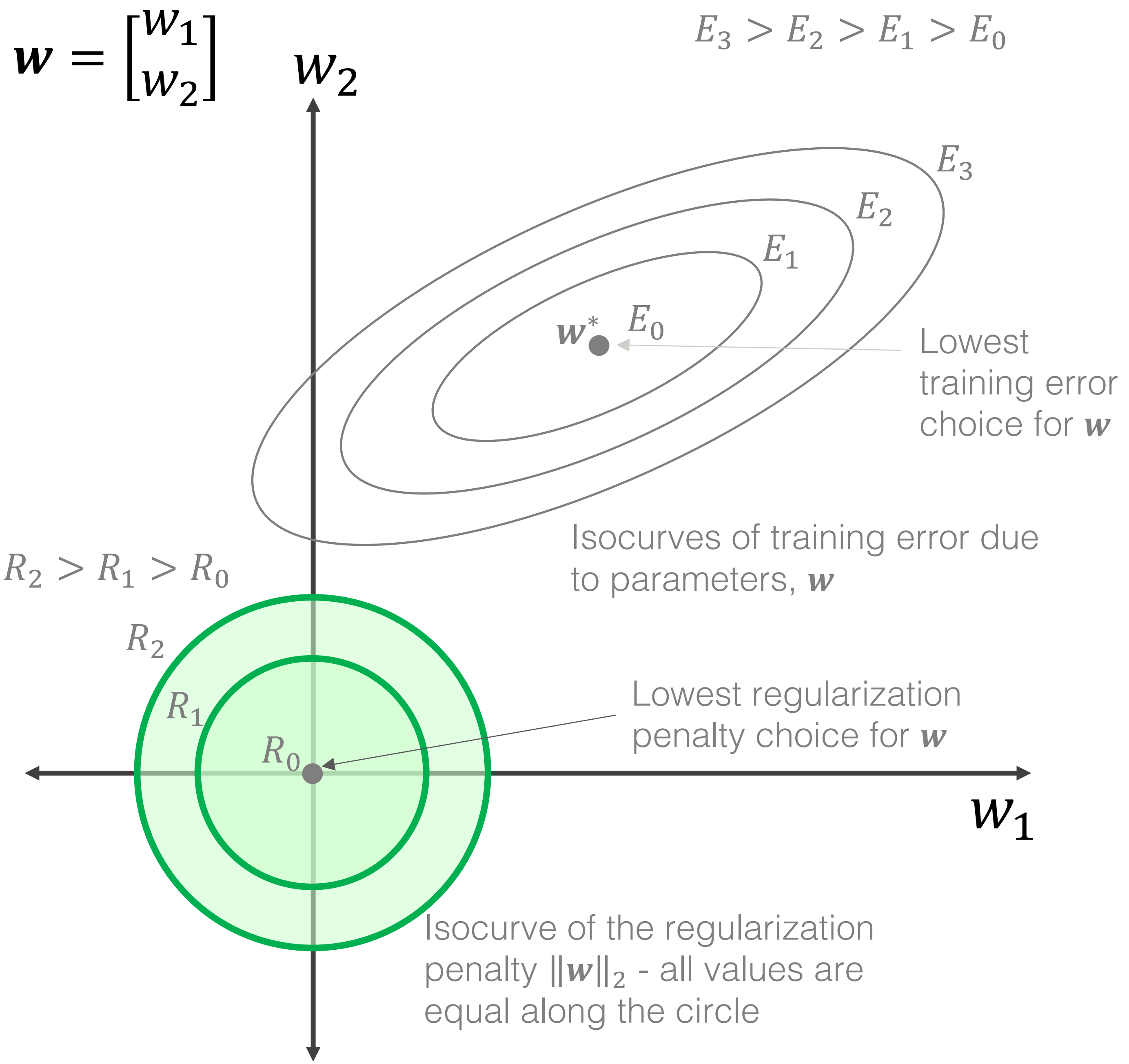


Every point in this space corresponds to a possible choice of model parameters $\boldsymbol{w}$

Minimize cost function:

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

First, let's just minimize training error

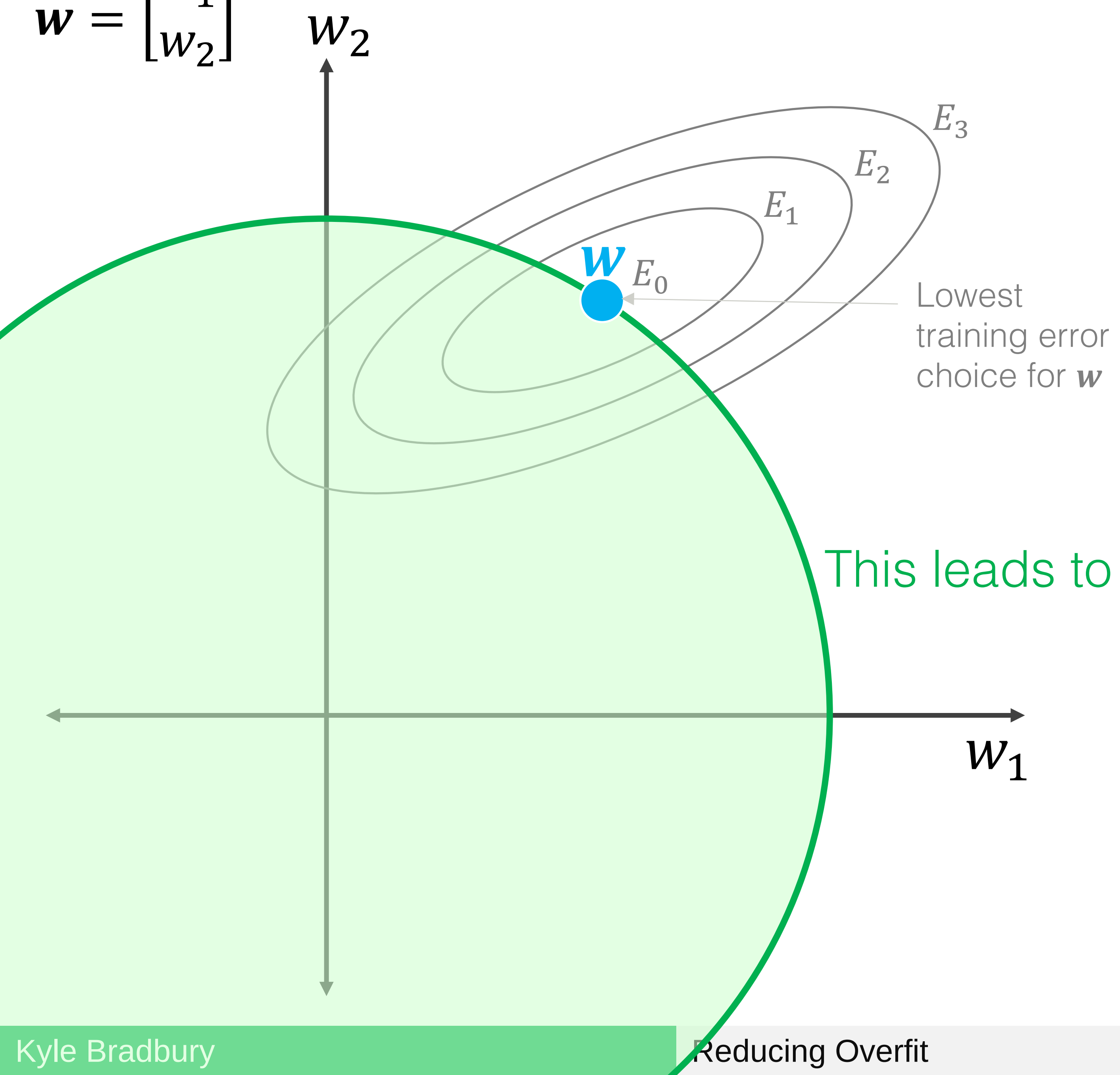


Minimize cost function:

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

Next, let's add a regularization penalty

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



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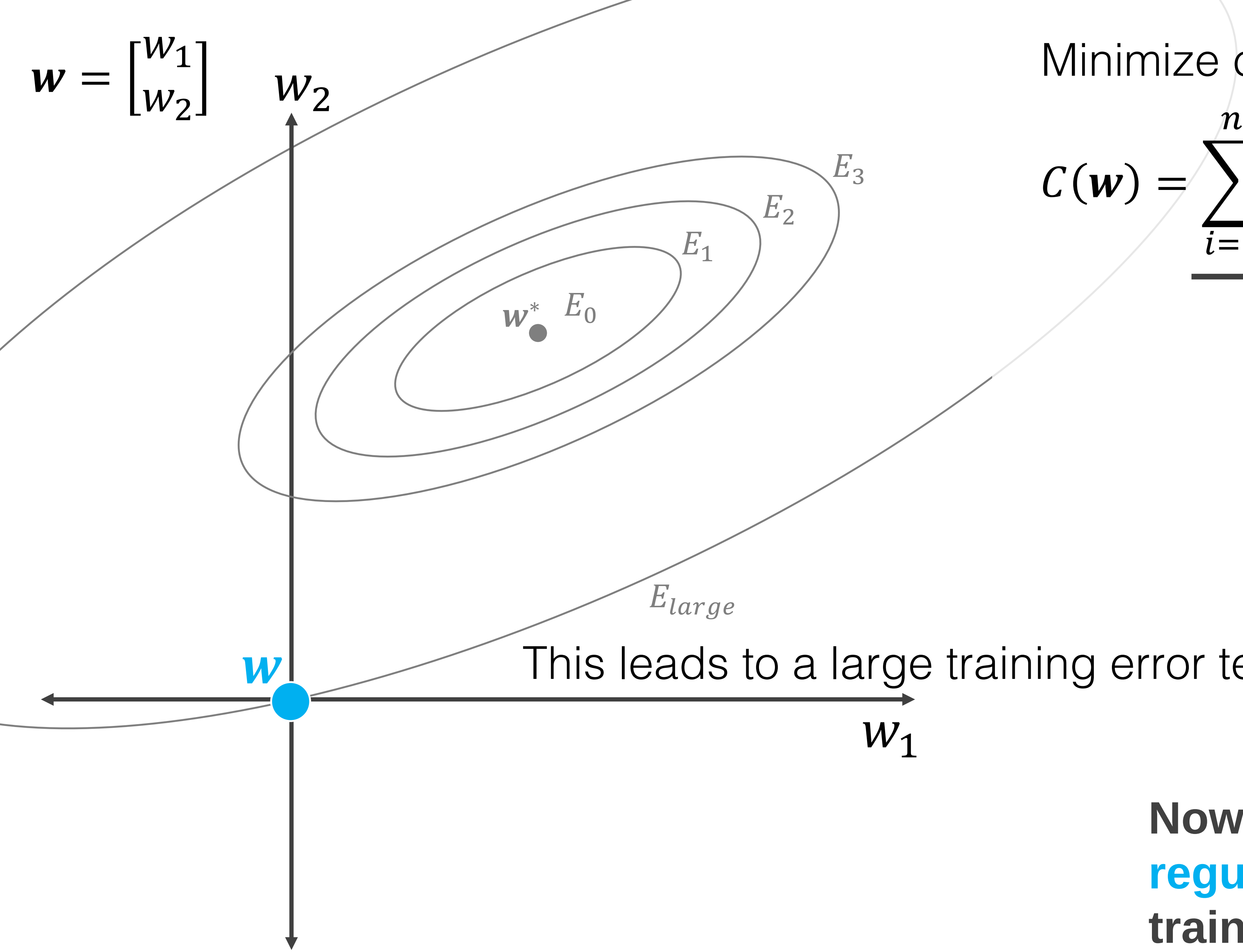
$$C(\boldsymbol{w}) = \underbrace{\sum_{i=1}^{n} \left(\hat{f}(\boldsymbol{x}_i, \boldsymbol{w}) - y_i\right)^2}_{\text{Training error}} + \underbrace{\lambda \sum_{j=1}^{p} w_j^2}_{\text{Regularization penalty}}$$

Small **Large**

This leads to a large regularization penalty

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



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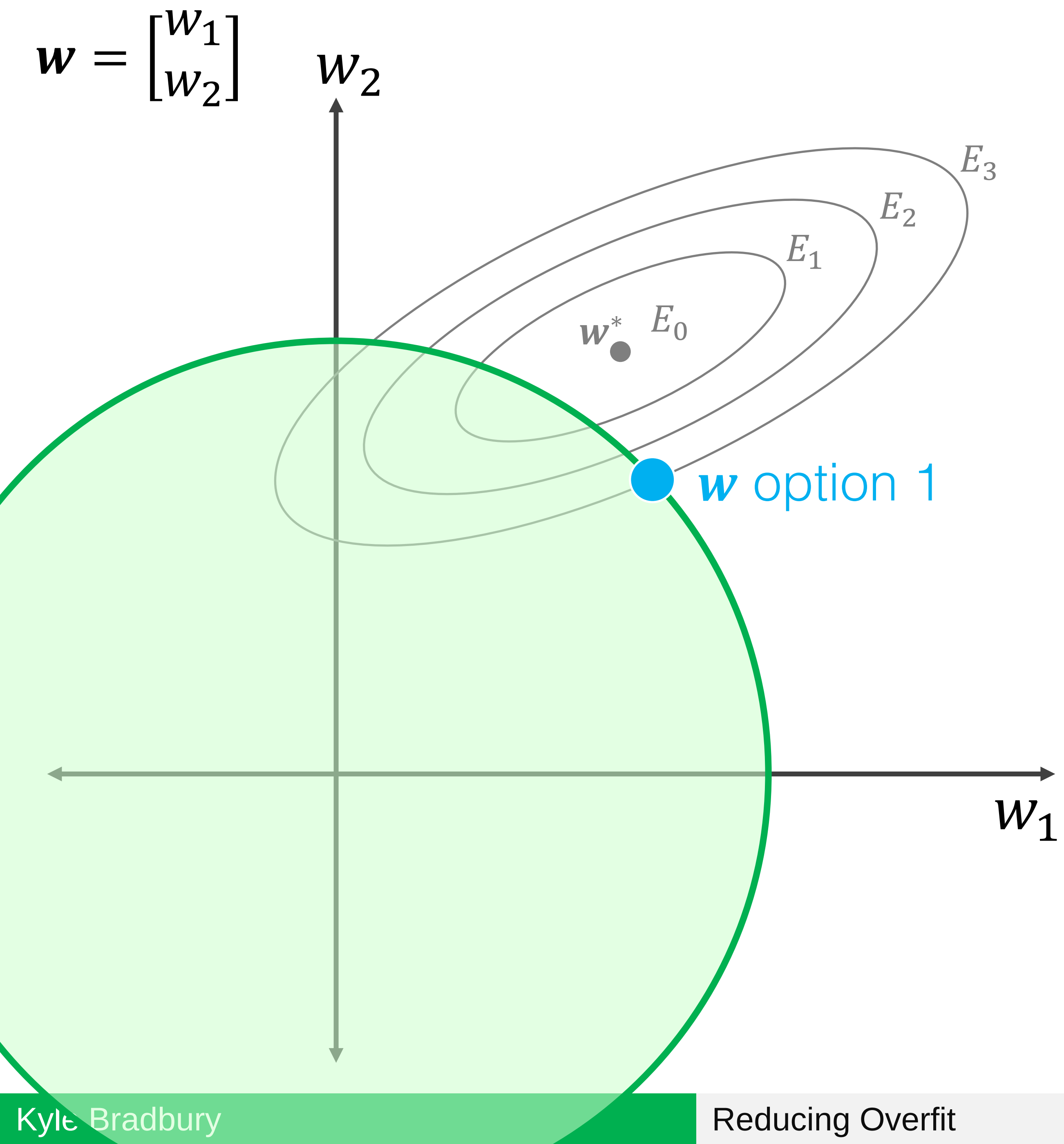
$$C(\boldsymbol{w}) = \underbrace{\sum_{i=1}^{n} \left(\hat{f}(\boldsymbol{x}_i, \boldsymbol{w}) - y_i\right)^2}_{\text{Training error}} + \underbrace{\lambda \sum_{j=1}^{p} w_j^2}_{\text{Regularization penalty}}$$

Large **Small**

This leads to a large training error term…

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



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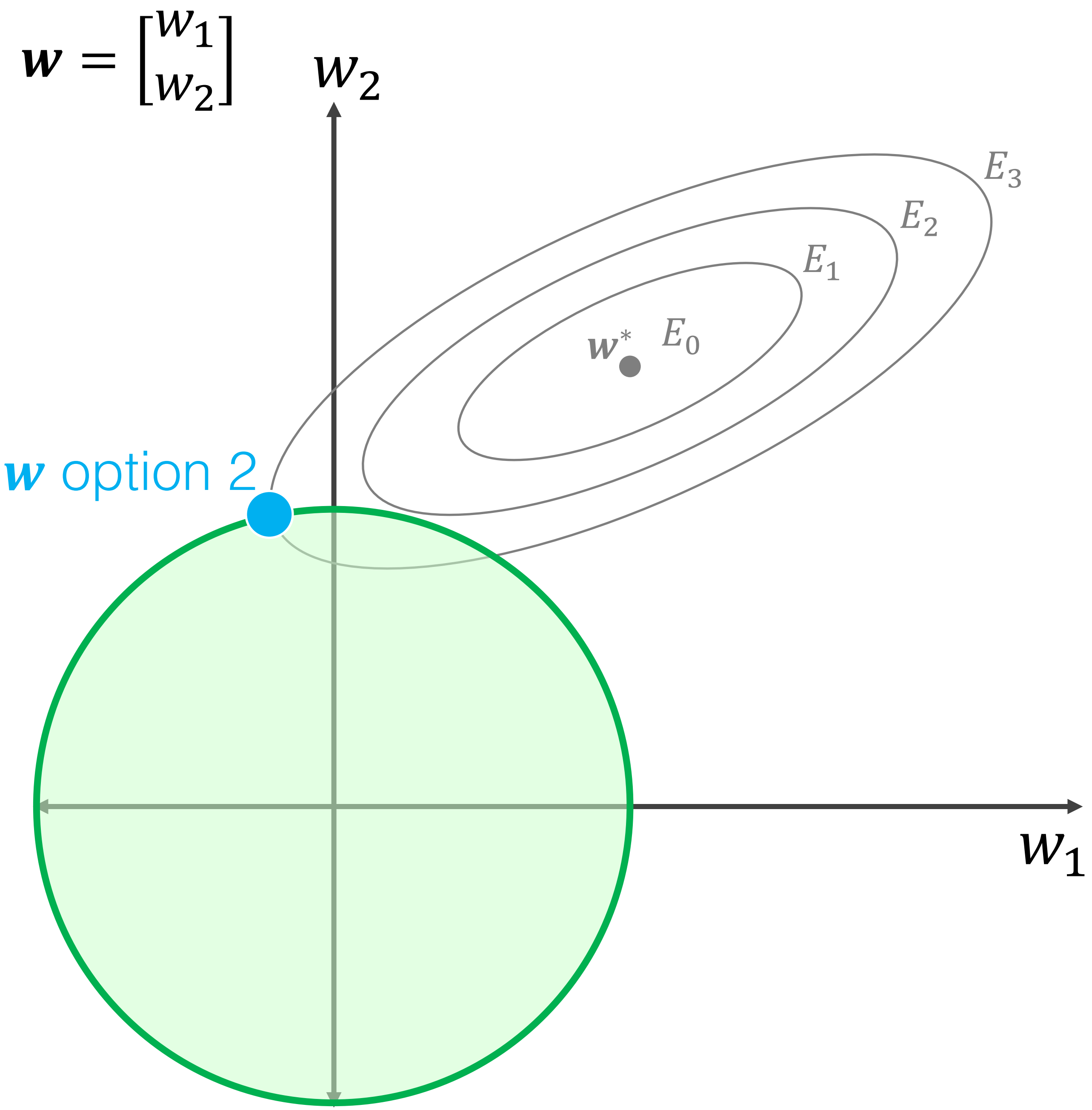
For any level of training error (assume E_3 here), there may be many parameter values that result in an equivalent training error



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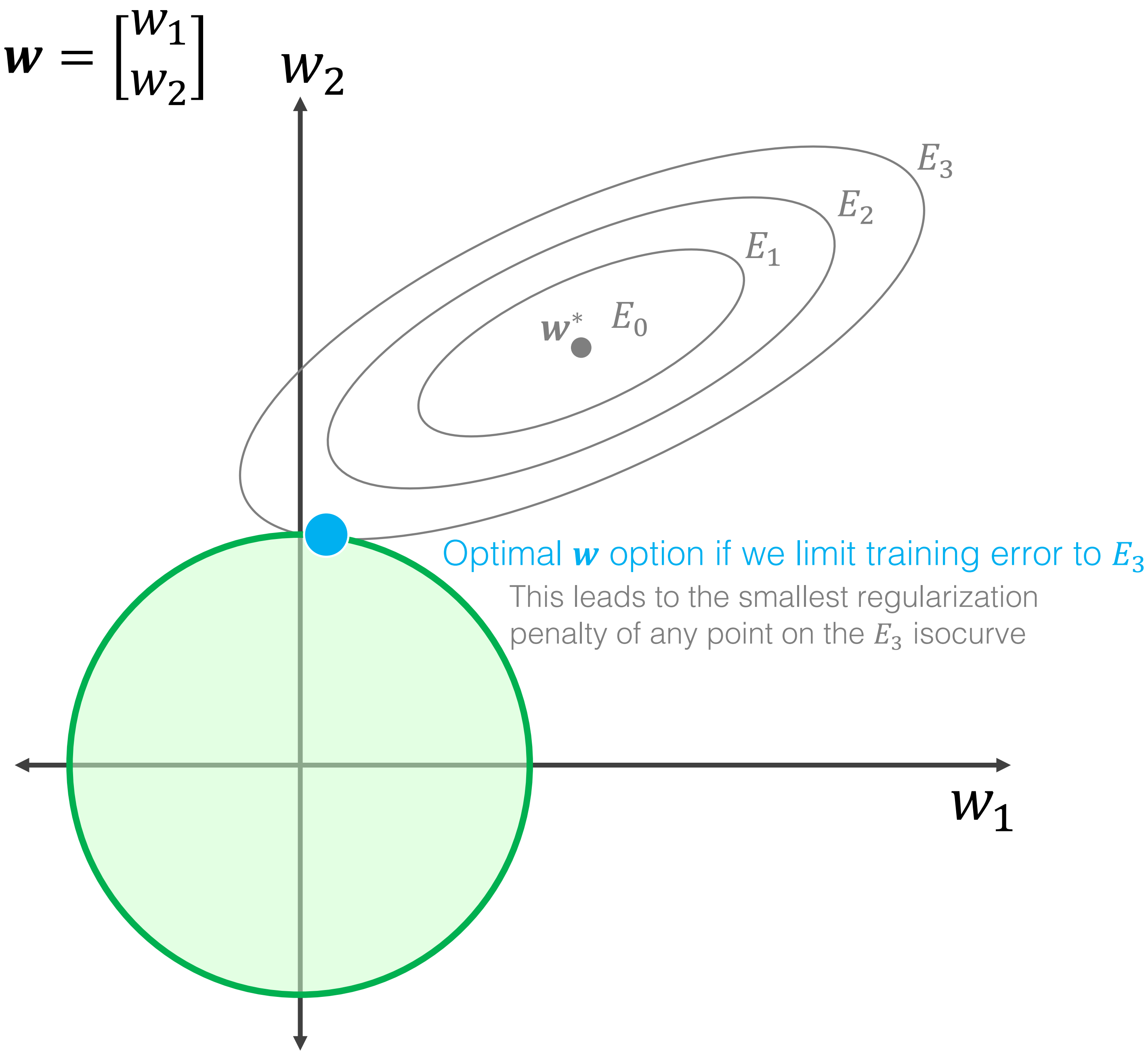
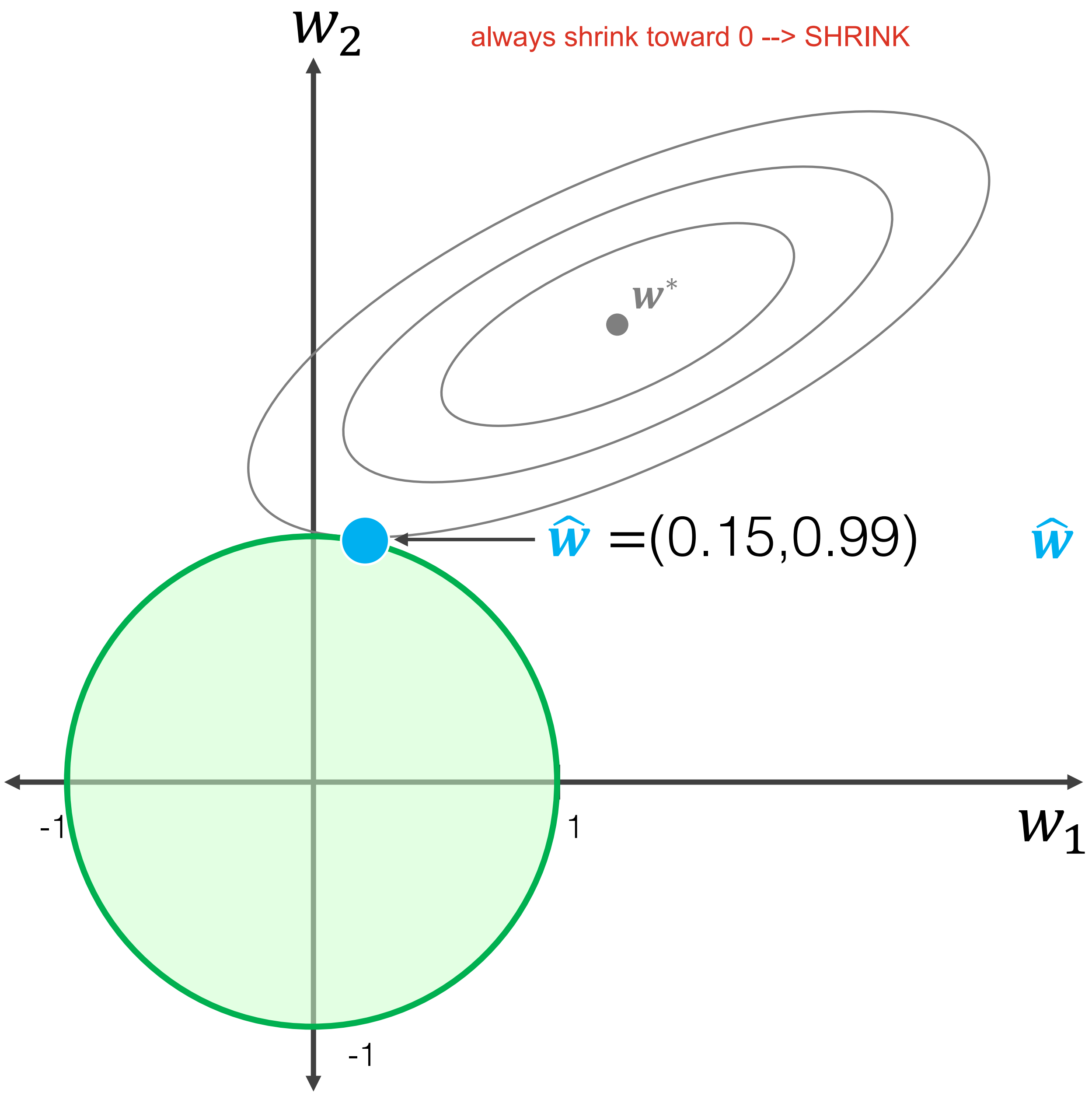


Minimize cost function:

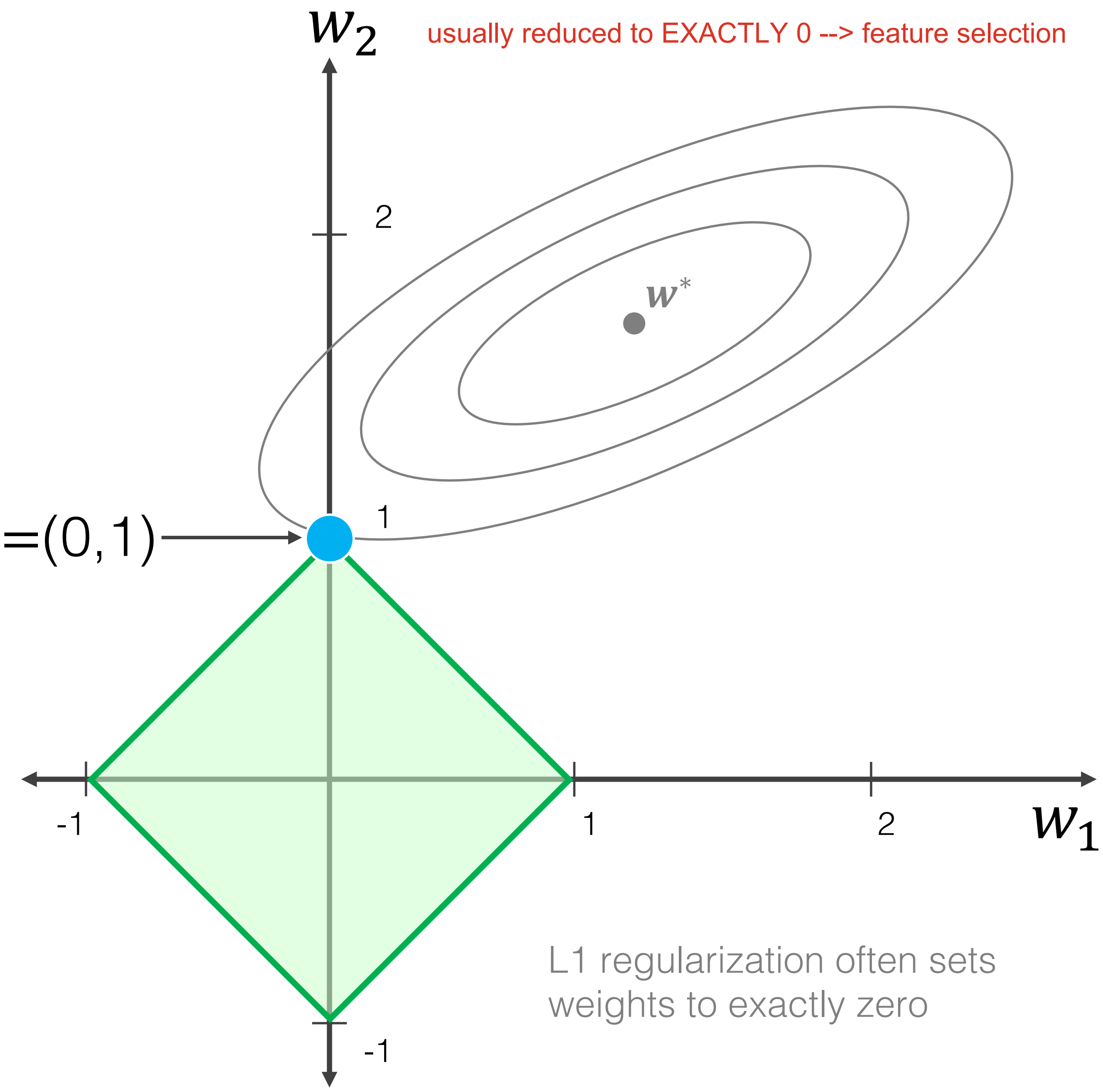
$$C(\boldsymbol{w}) = \underbrace{\sum_{i=1}^{n} \left(\hat{f}(\boldsymbol{x}_i, \boldsymbol{w}) - y_i\right)^2}_{\text{Training error}} + \underbrace{\lambda \sum_{j=1}^{p} w_j^2}_{\text{Regularization penalty}}$$

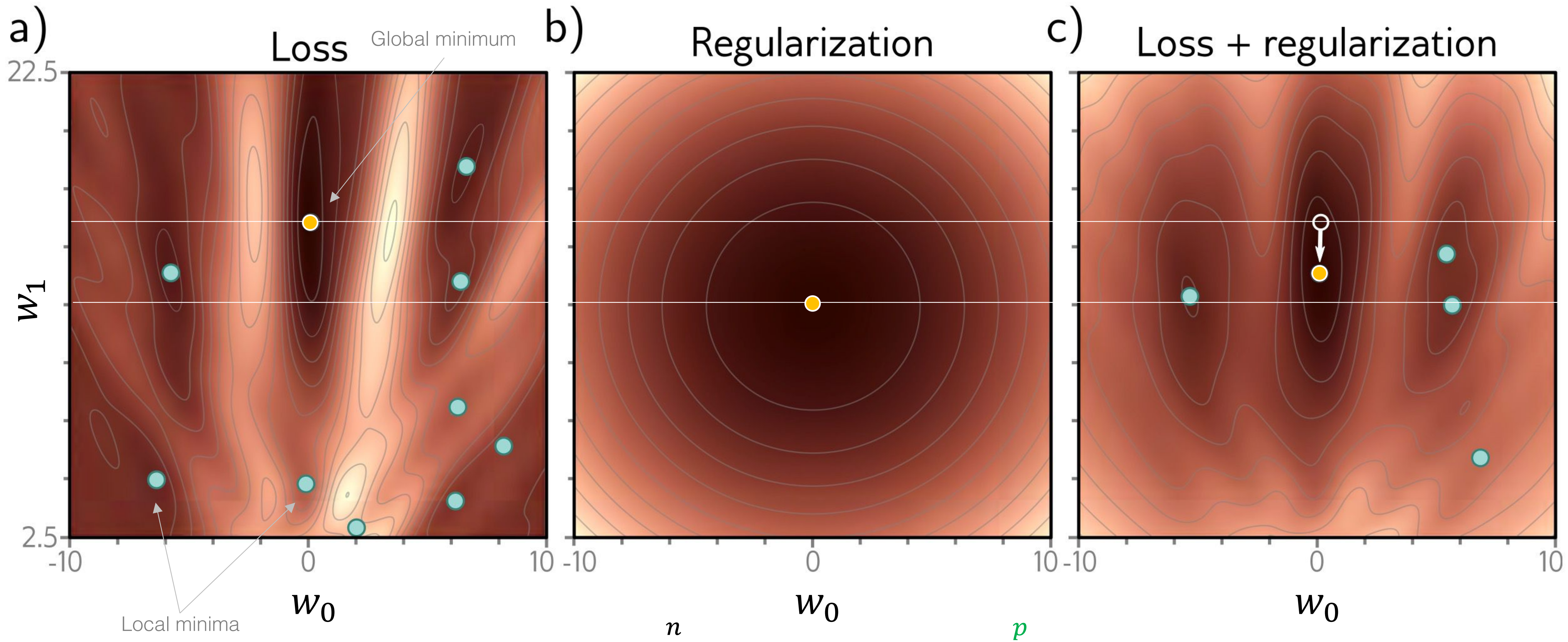
However, we can choose between the options by minimizing the regularization penalty

Ridge: L_2 regularization



LASSO: L_1 regularization





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

c **a** **b**

Visualizing Regularization in Action

Image from Prince, Understanding Deep Learning, 2023

Regularization reduces variance

Leads to smaller model parameters

L_1 regularization also performs variable selection

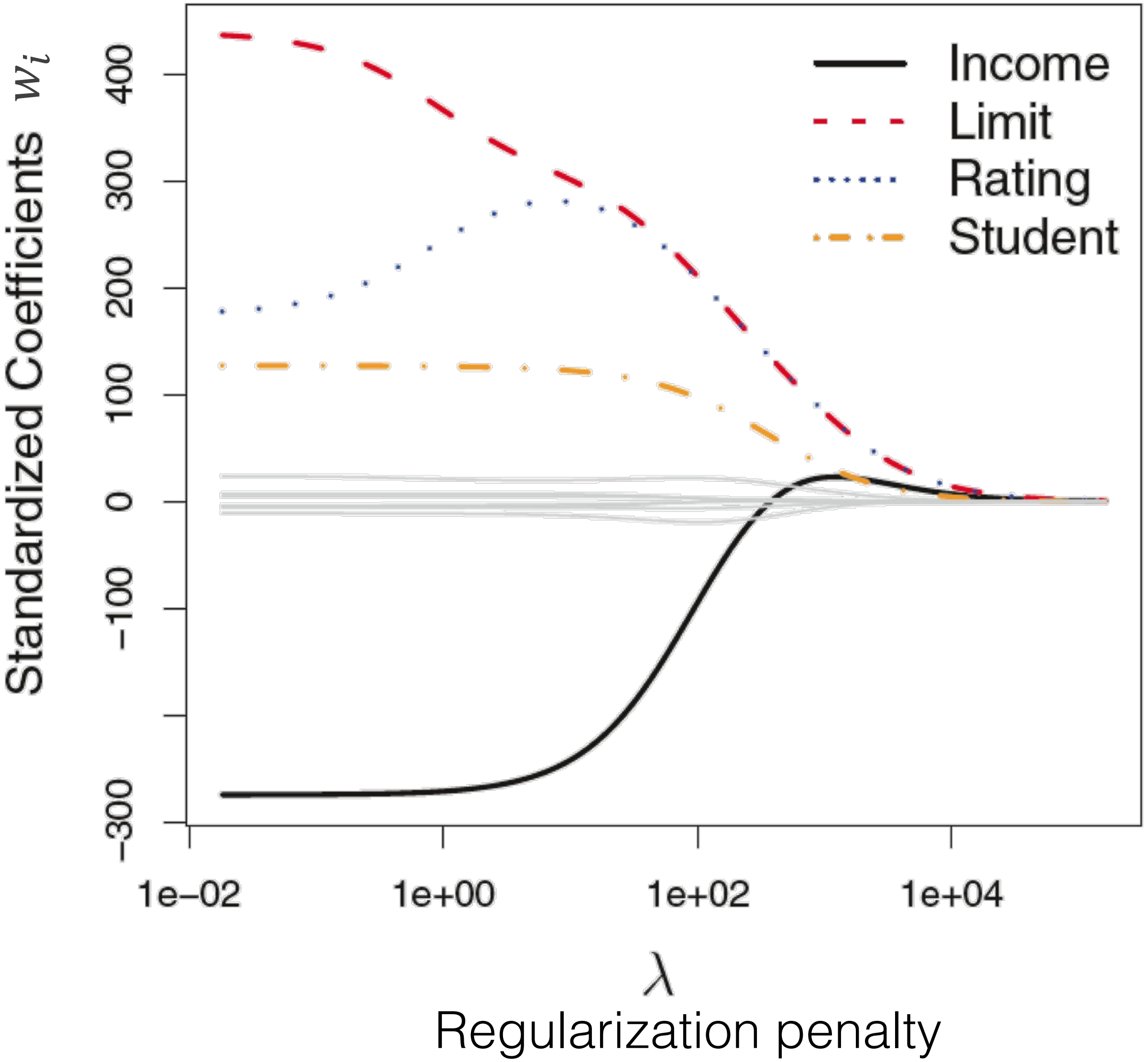
Example: predicting credit default

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

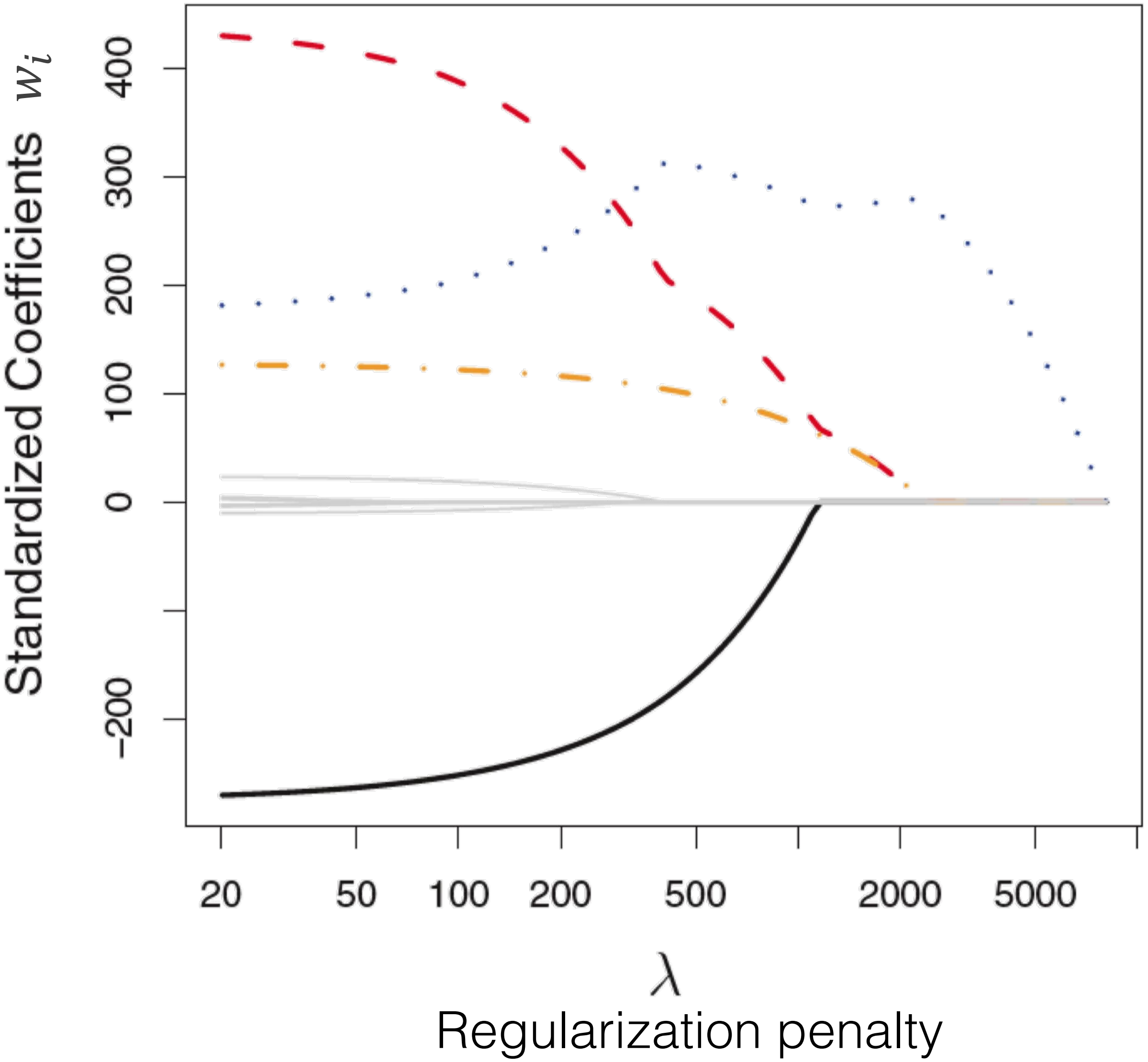
Ridge regression



everything goes towards 0

L_1 regularization

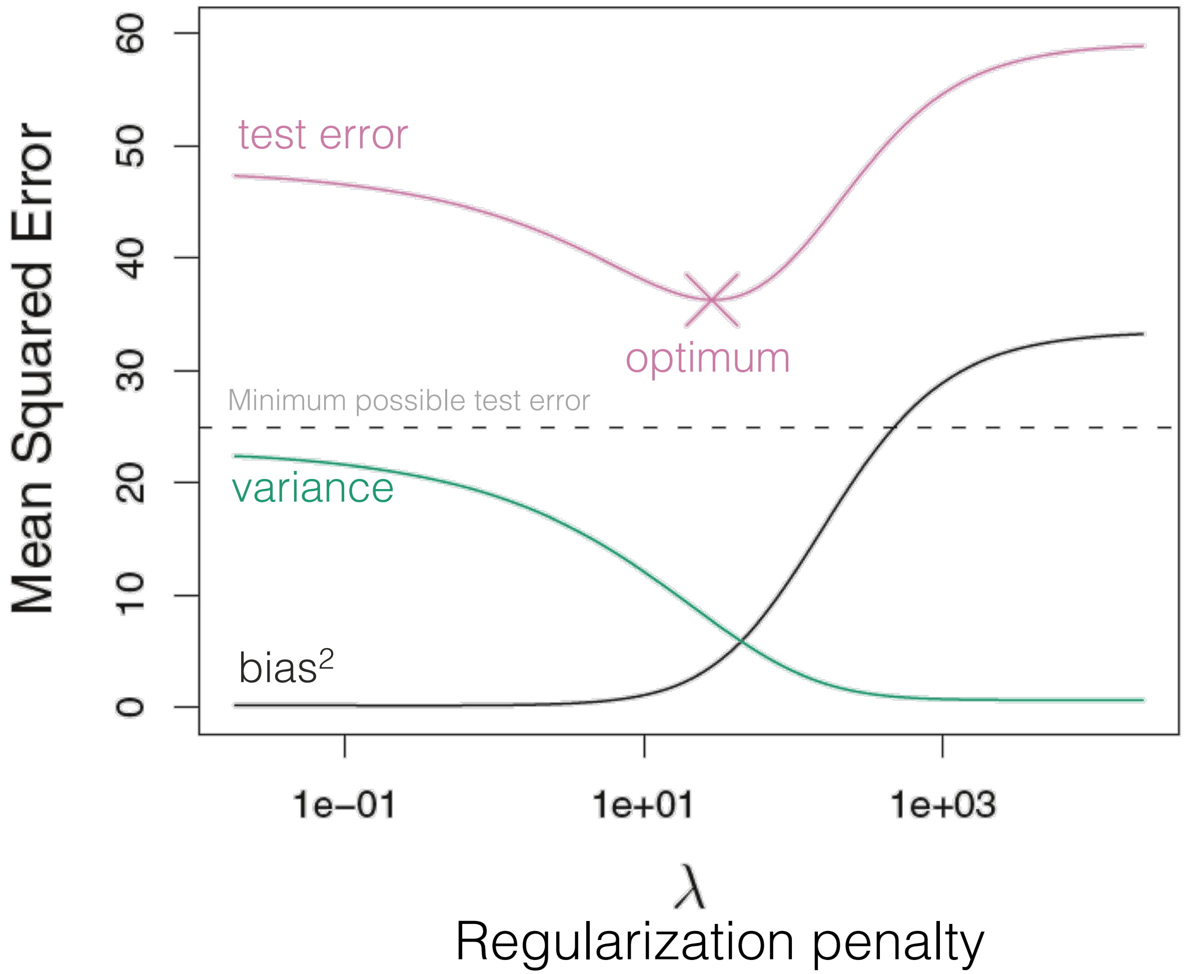
LASSO regularization



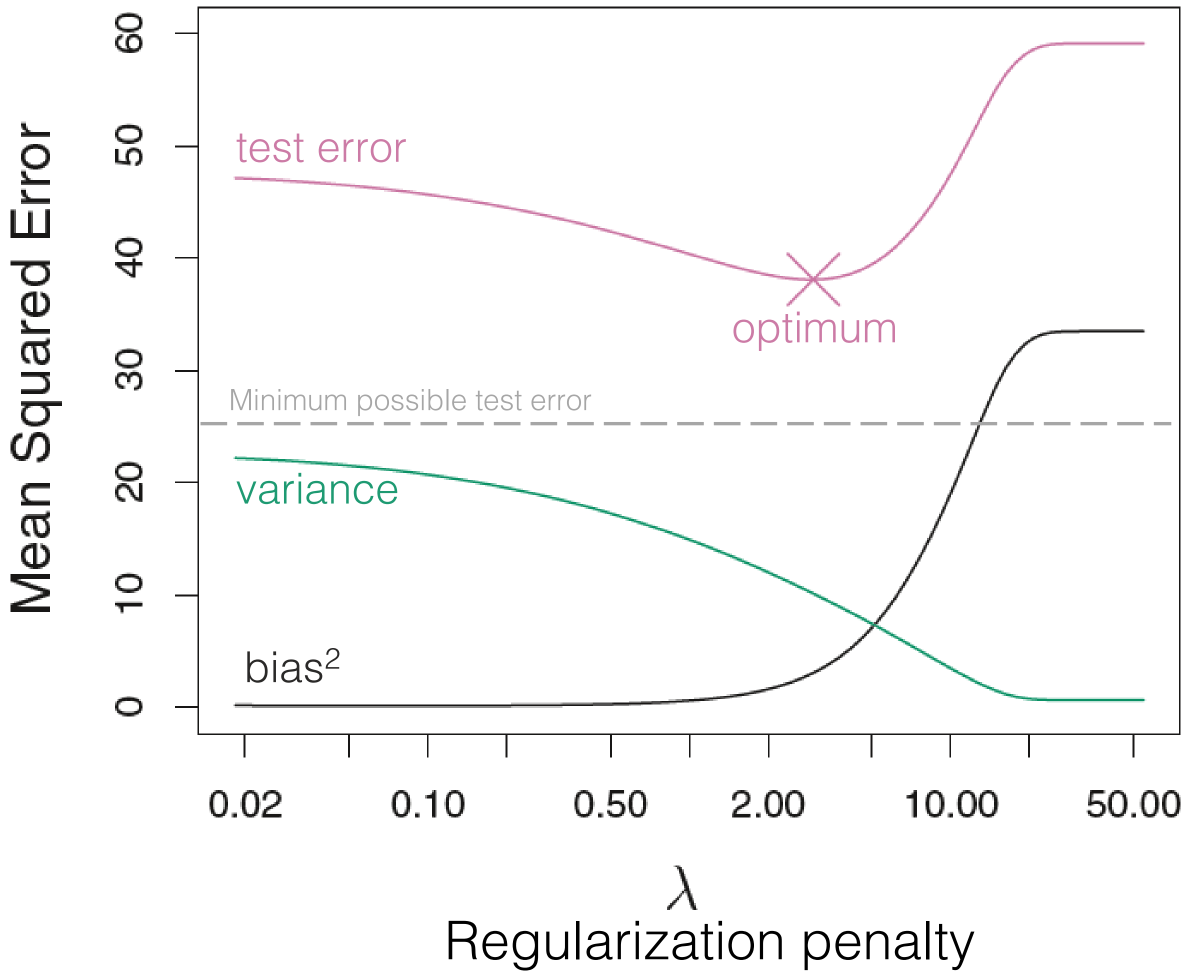
some may hit exactly 0

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

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

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 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 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

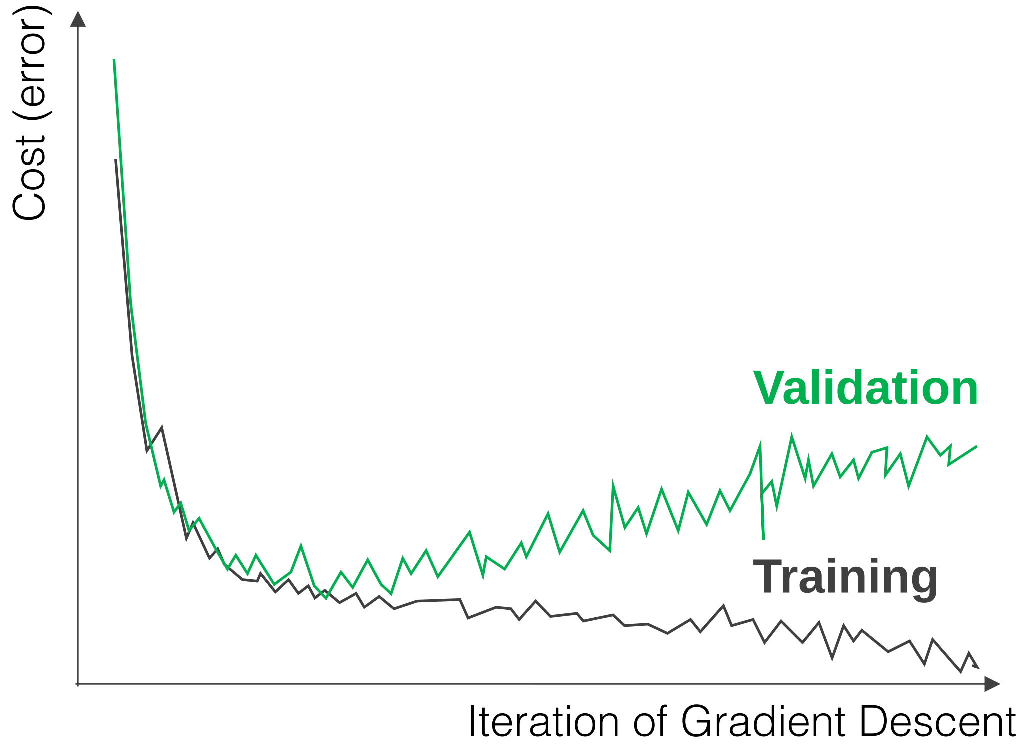
One more approach: Early Stopping

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