Regularized Linear Regression

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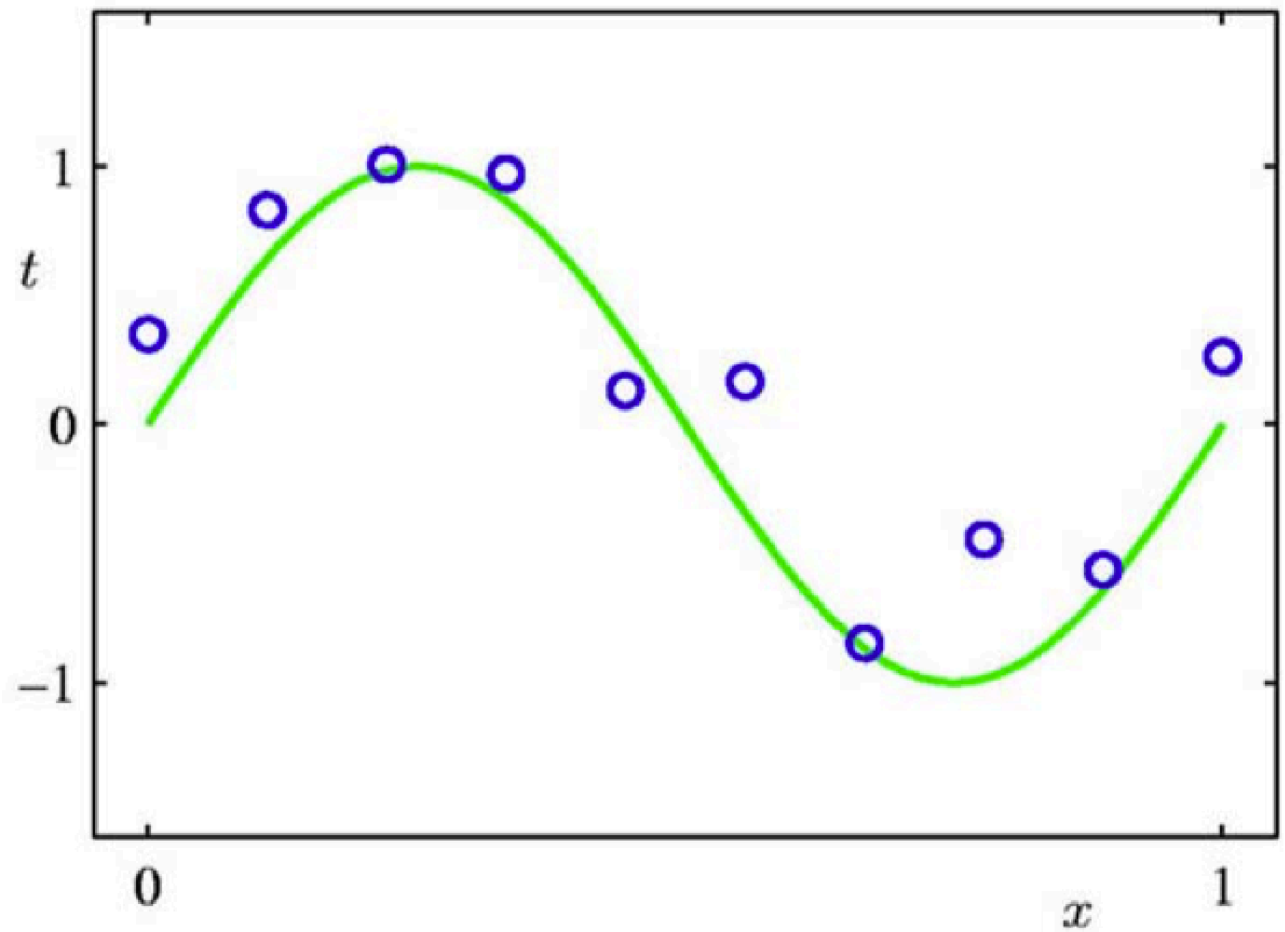
These slides are inspired based on slides from Andrew Zisserman, Jonathan Taylor, Chao Zhang and Yaser Abu-Mostafa.

Outline

- Overfitting and regularized learning
- Ridge regression
- Lasso regression
- Determining regularization strength

Regression: Recap

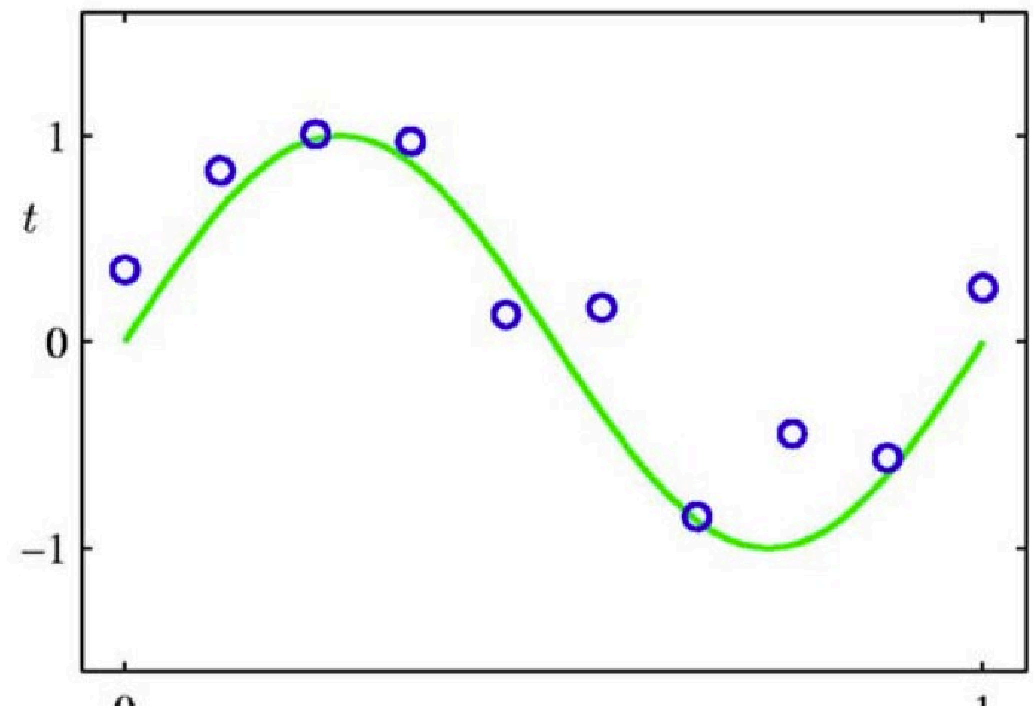


- Suppose we are given a training set of N observations

$$(x_1, \ldots, x_N) \text{ and } (y_1, \ldots, y_N)$$

- Regression problem is to estimate y(x) from this data

Regression: Recap



- Want to fit a polynomial regression model

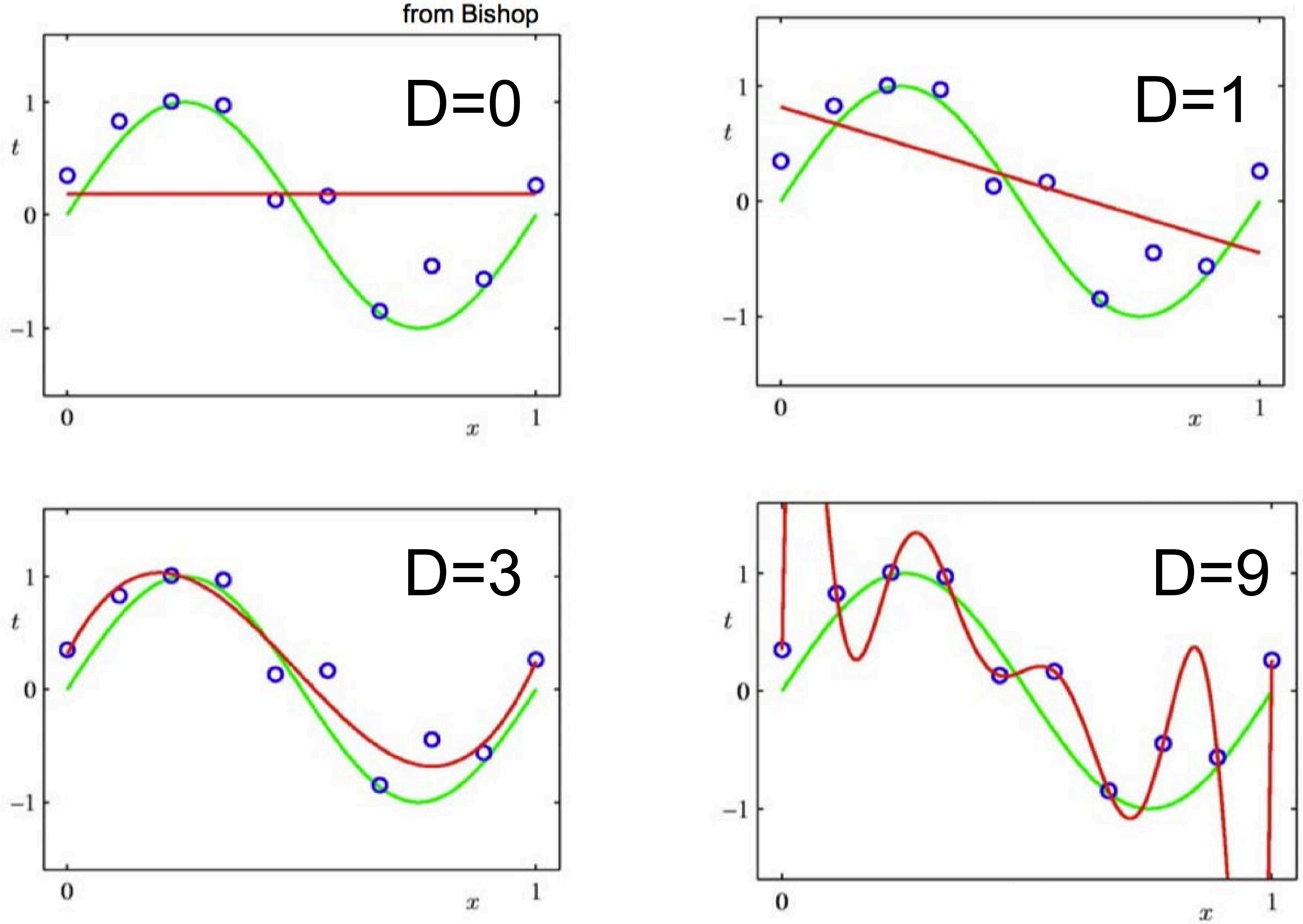
$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_d x^d + \epsilon$$

- $z = \{1, x, x^2, \ldots, x^d\} \in R^d$ and $\theta = (\theta_0, \theta_1, \theta_2, \ldots, \theta_d)^T$

$$y = z\theta$$

Which One is Better?

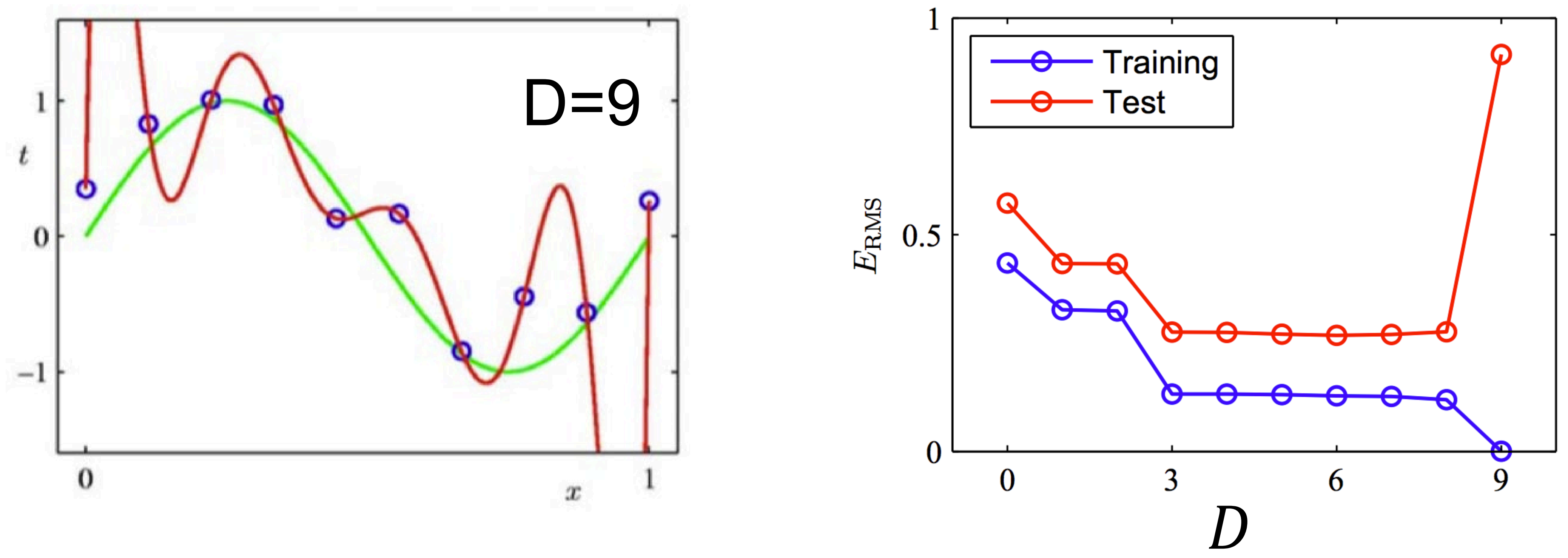
from Bishop



- Can we increase the maximal polynomial degree to very large, such that the curve passes through all training points?

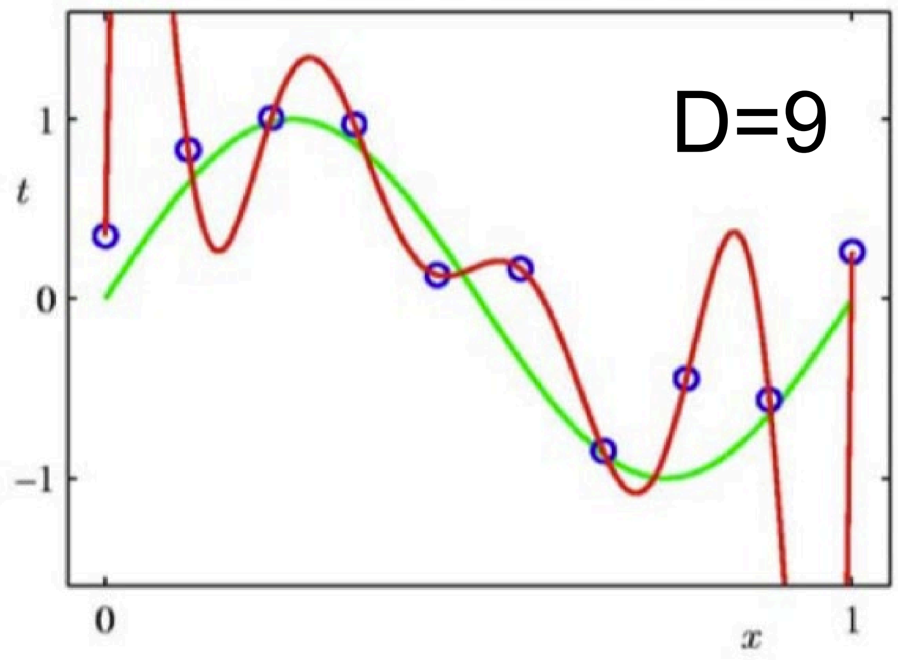
No, this can lead to **overfitting**!

The Overfitting Problem



- The training error is very low, but the error on test set is large.
- The model captures not only patterns but also noisy nuisances in the training data.

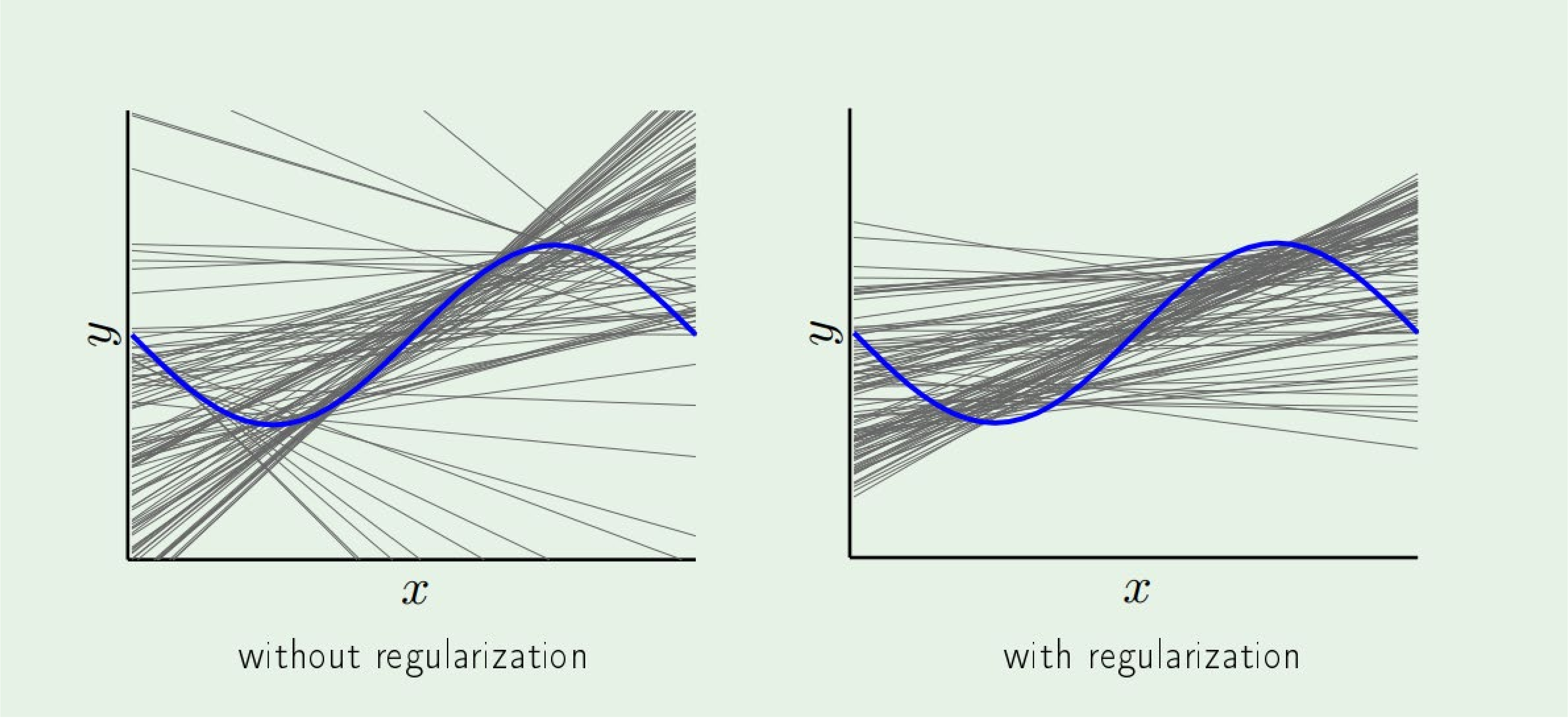
The Overfitting Problem



- In regression, overfitting is often associated with large Weights (severe oscillation)
- How can we address overfitting?

Regularization

(smart way to cure overfitting disease)

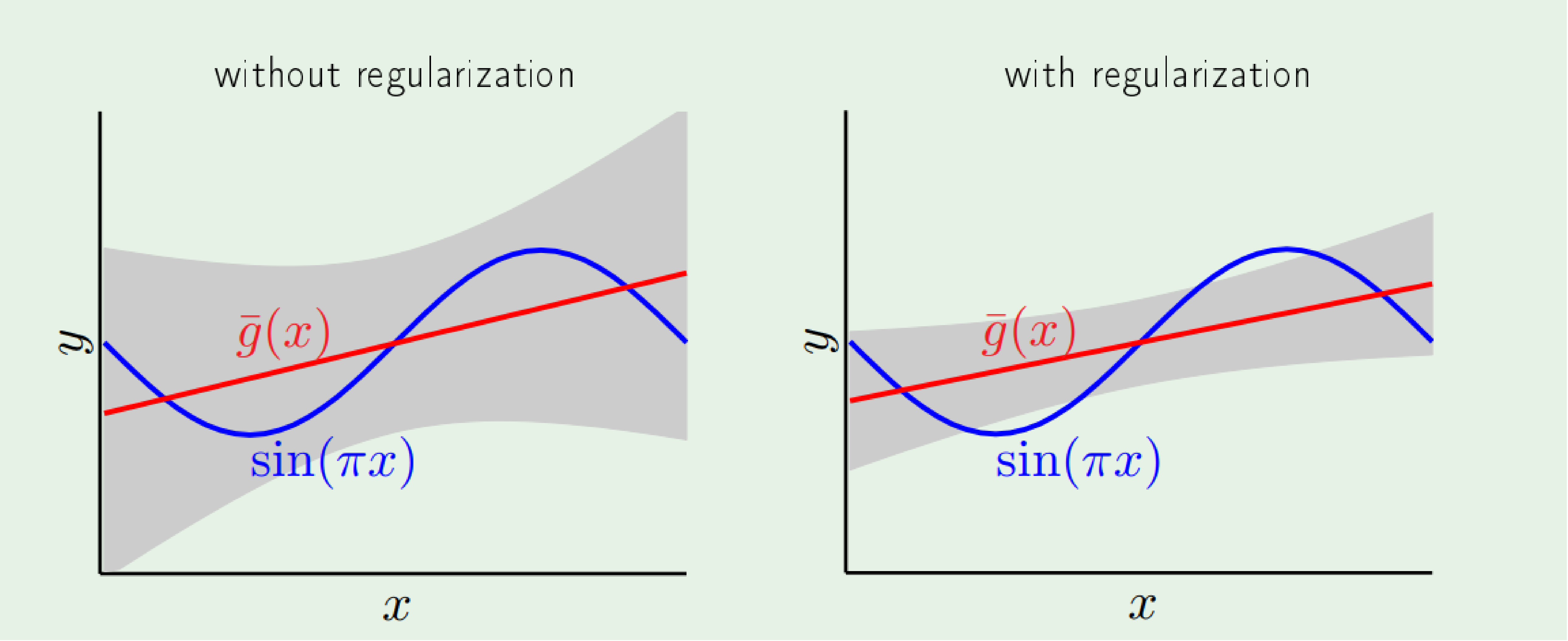


Put a brake on fitting

Fit a linear line on sinusoidal with just two data points

Who is the winner?

$\bar{g}\,(x)$: average over all lines



bias=0.21; var=1.69

bias=0.23; var=0.33

Polynomial Model

Want to fit a polynomial regression model

$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_d x^d + \epsilon$$

Let's rewrite it as:

$$y = \theta_0 + \theta_1 z_1 + \theta_2 z_2 + \cdots + \theta_d z_{\mathrm{d}} + \epsilon = \boldsymbol{z\theta}$$

Regularizing is just constraining the weights ($\boldsymbol{\theta}$)

For example: let’s do a **hard** constraining

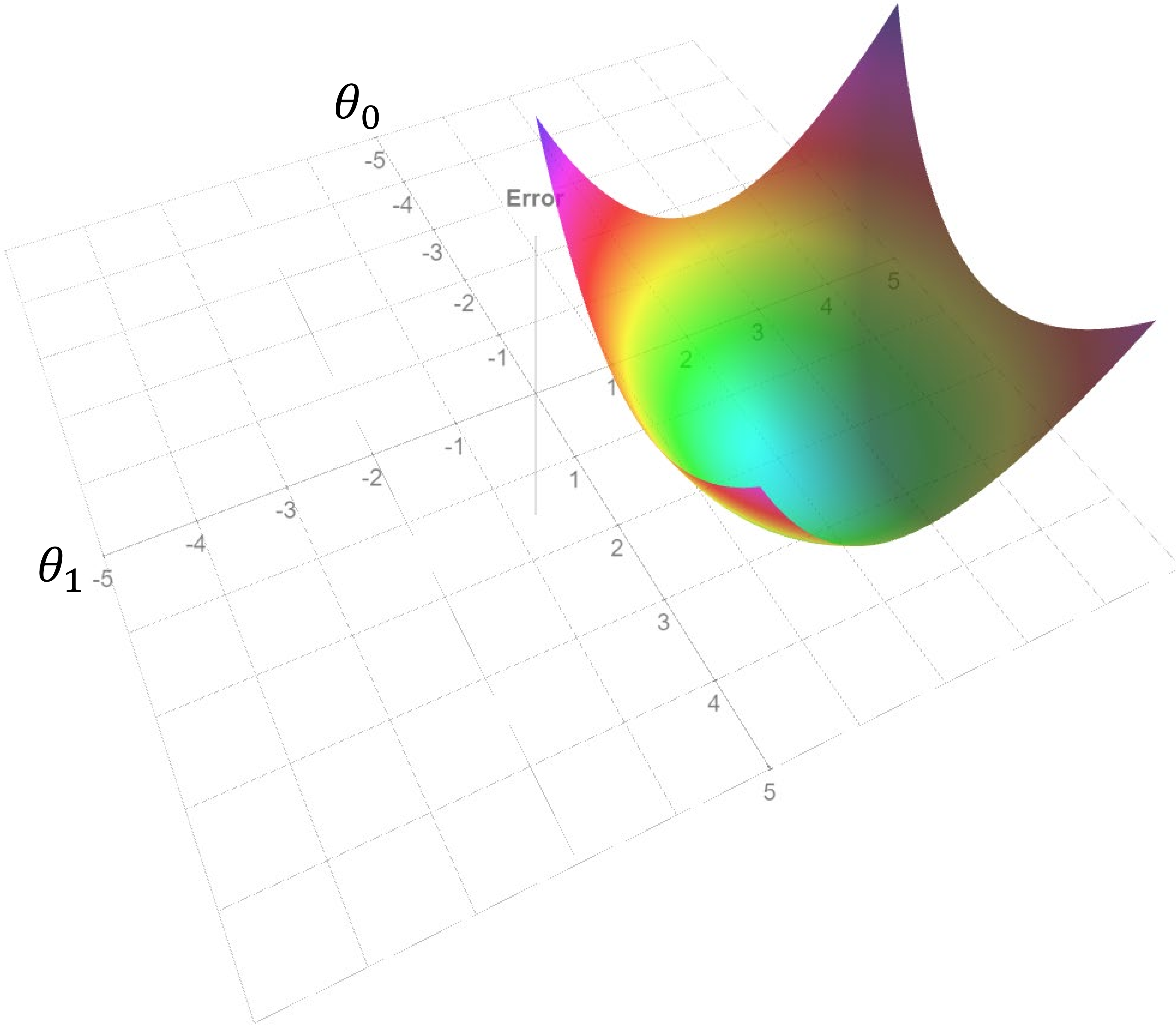
$$y = \theta_0 + \theta_1 z_1 + \theta_2 z_2 + \cdots + \theta_d z_{\mathrm{d}}$$

subject to

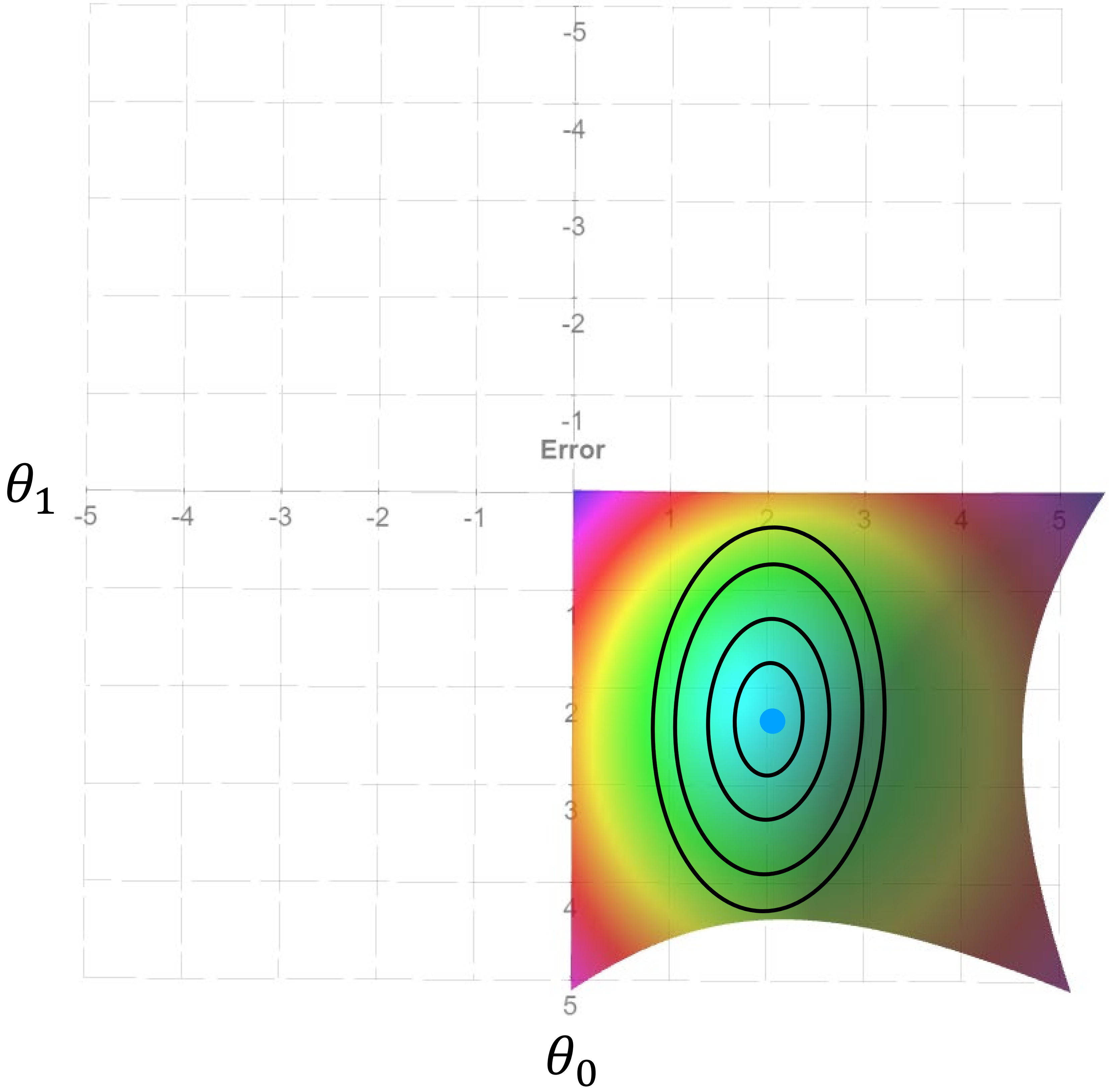
$$\theta_d = 0 \; for \; d > 2$$

$$y = \theta_0 + \theta_1 z_1 + \theta_2 z_2 + 0 + \cdots + 0$$

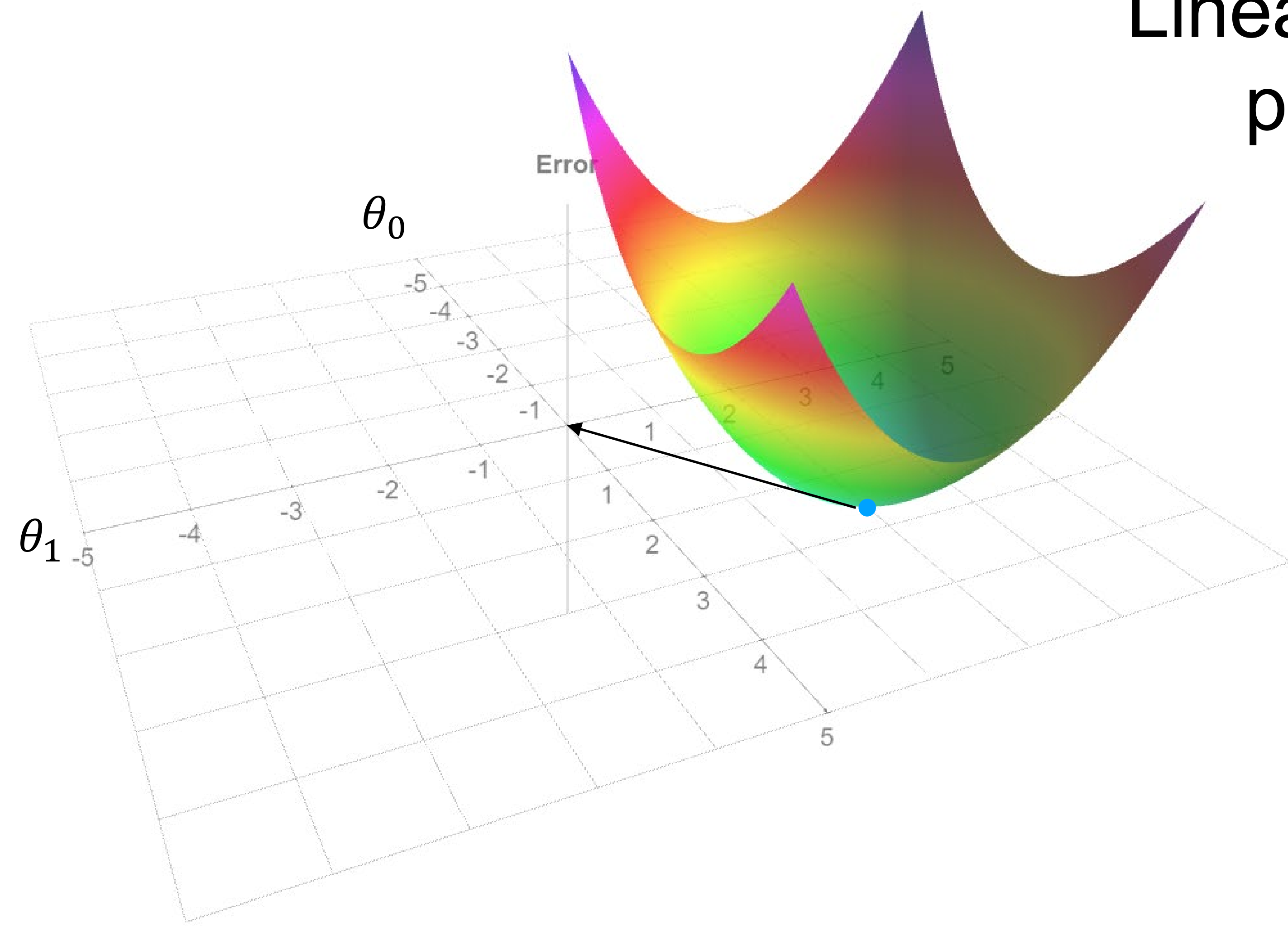
$$E(\theta) = \frac{1}{N}\sum_{i=1}^{n}\left(y^i - z_i\theta\right)^2$$

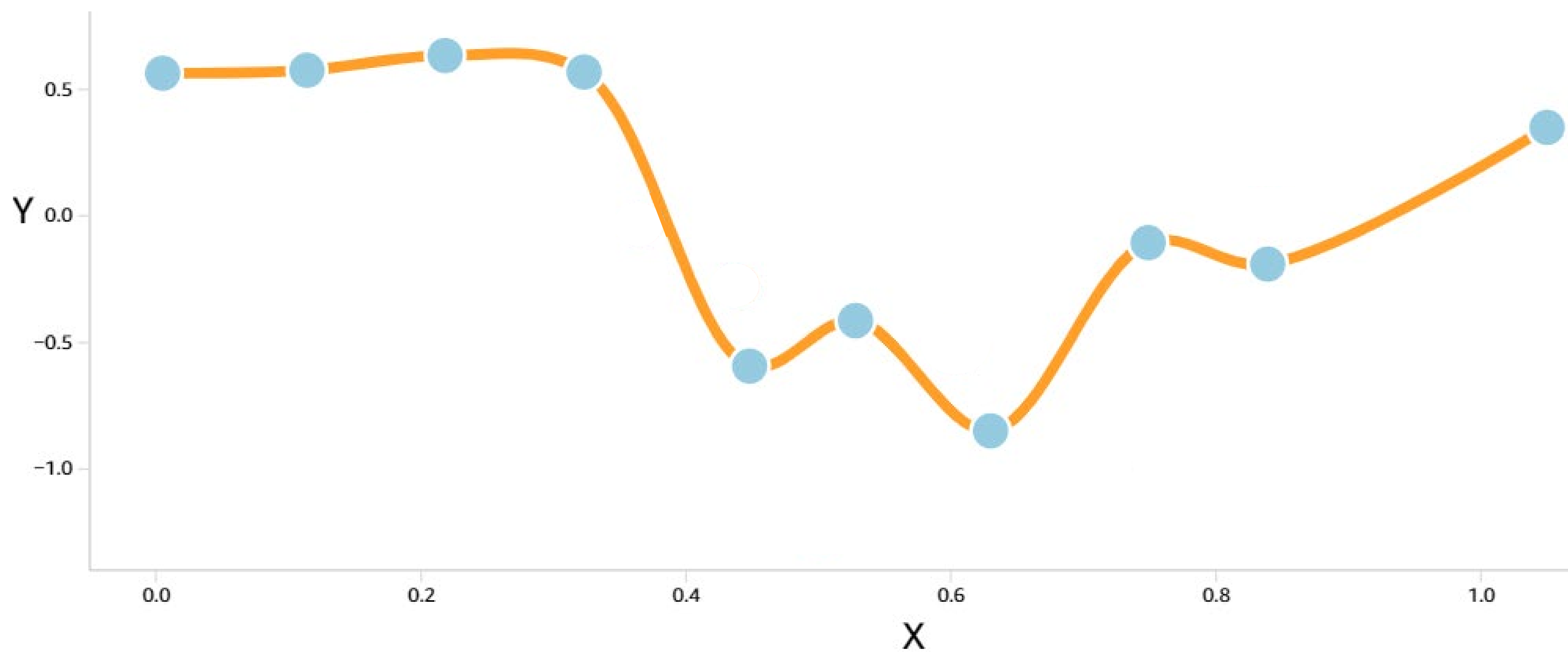


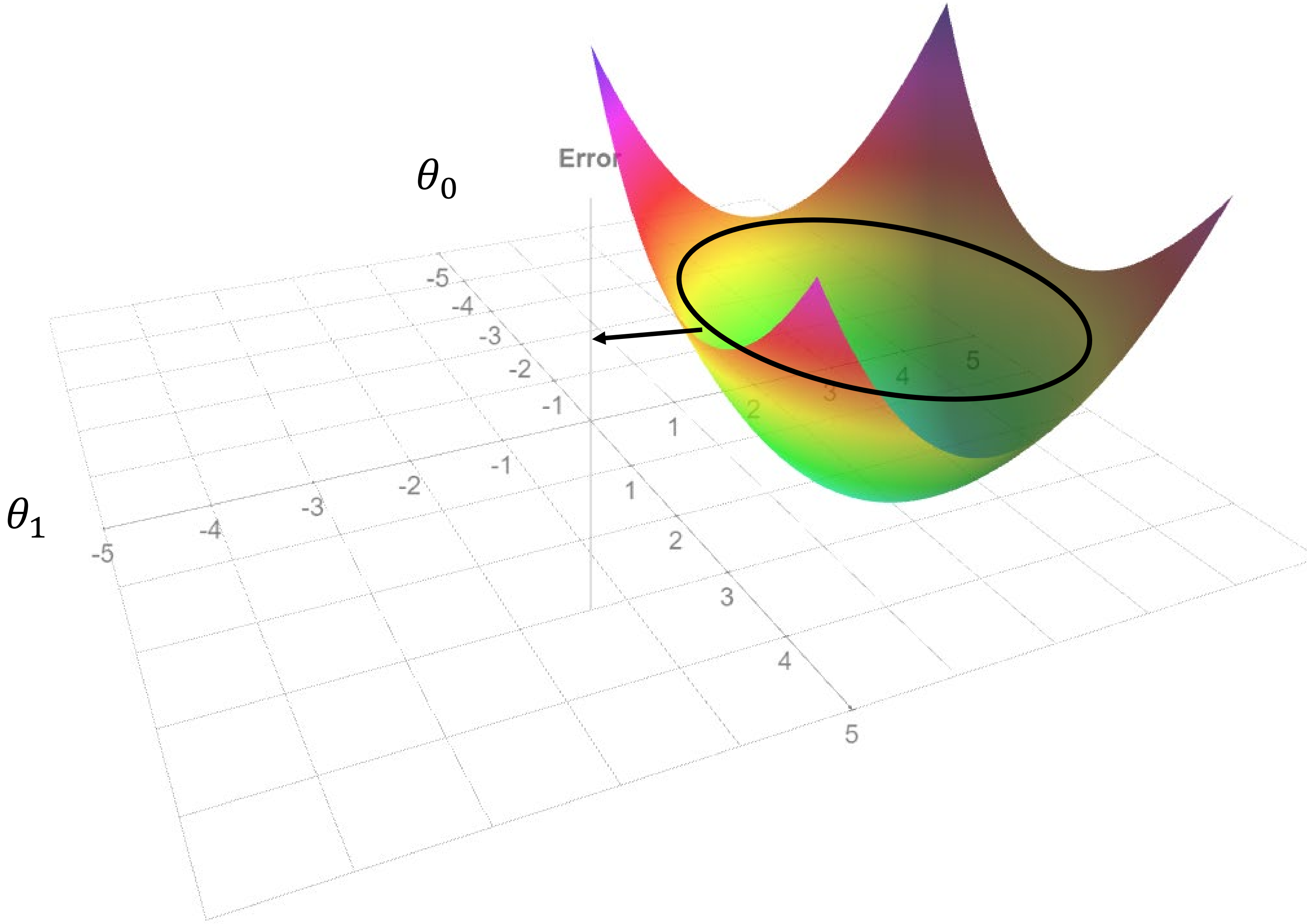
Project the same graph on x-y using contour plot

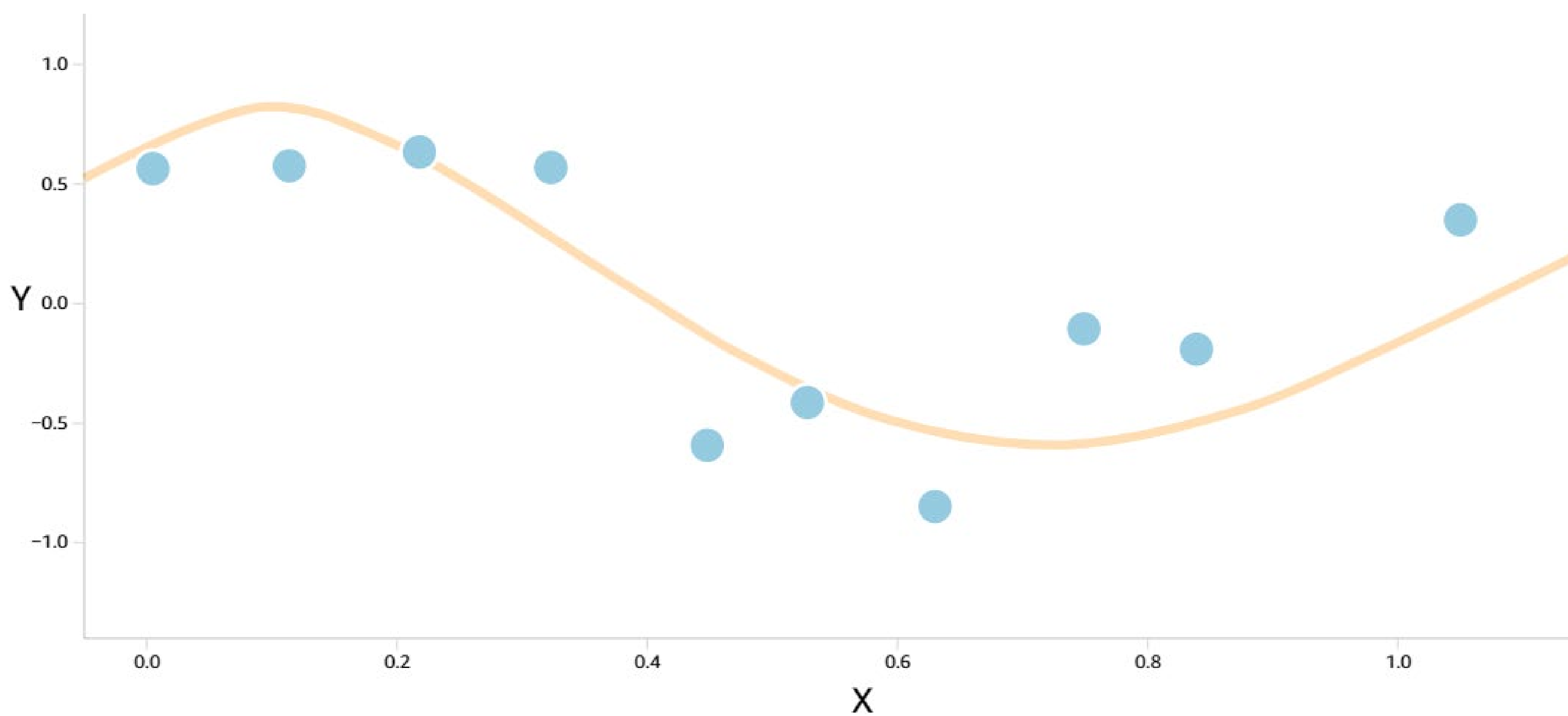


Linear regression with a very high polynomial degree solution






θ_0
θ_1
Error
-5
-4
-3
-2
-1
1
2
3
4
5

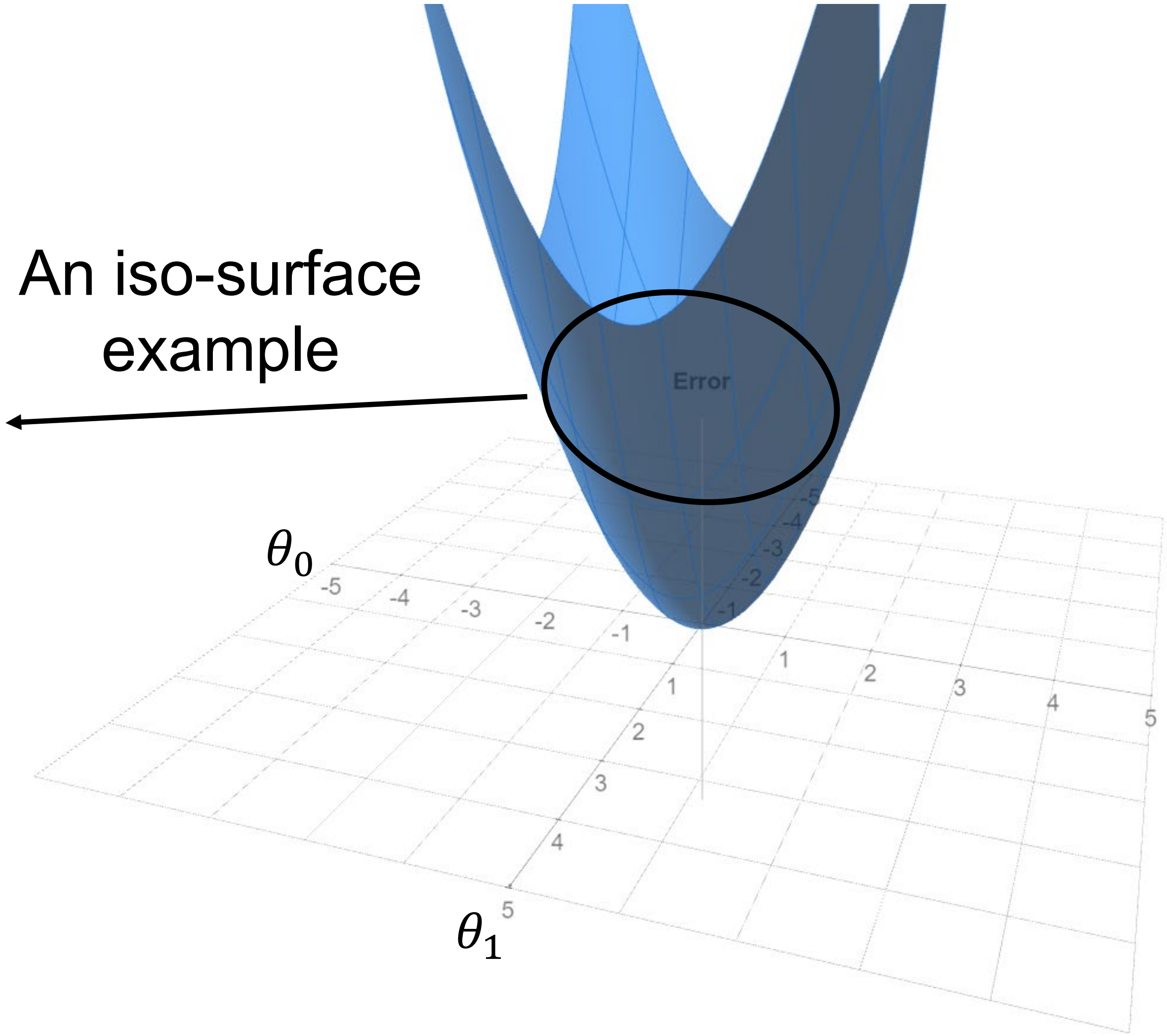

Y
X
1.0
0.5
0.0
-0.5
-1.0
0.0
0.2
0.4
0.6
0.8
1.0

How can we get an optimal solution with a positive error for a model that overfits?

We need to introduce a constraint

$$g(\theta) = \theta_0^2 + \theta_1^2 = \theta^T\theta = C$$

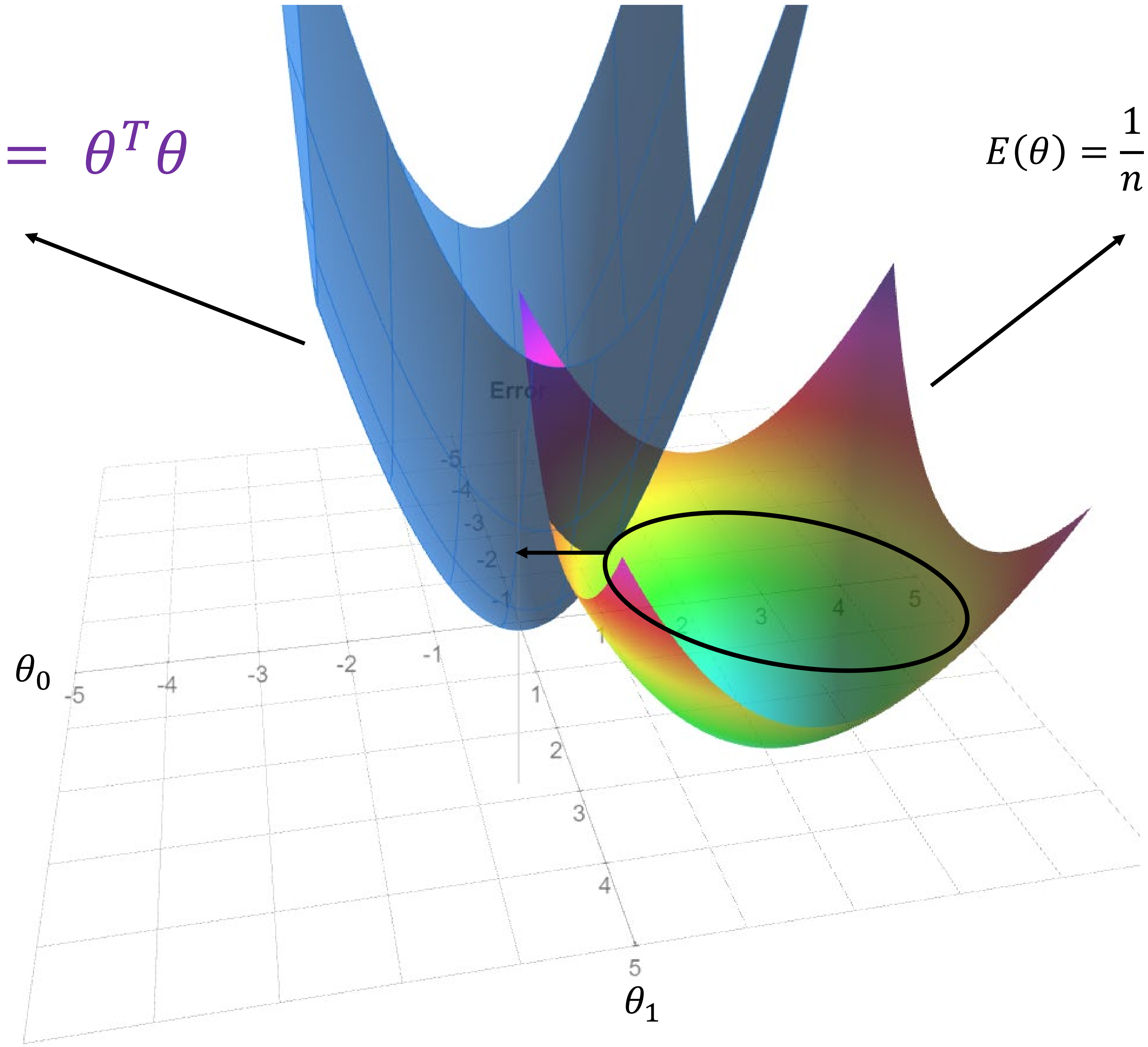
An iso-surface example



Error function together with a new introduced constraint

$$g(\theta) = \theta_0^2 + \theta_1^2 = \theta^T\theta$$

$$E(\theta) = \frac{1}{n}\sum_{i=1}^{n}\left(y^i - z_i\theta\right)^2$$



Let's define the Lagrange function

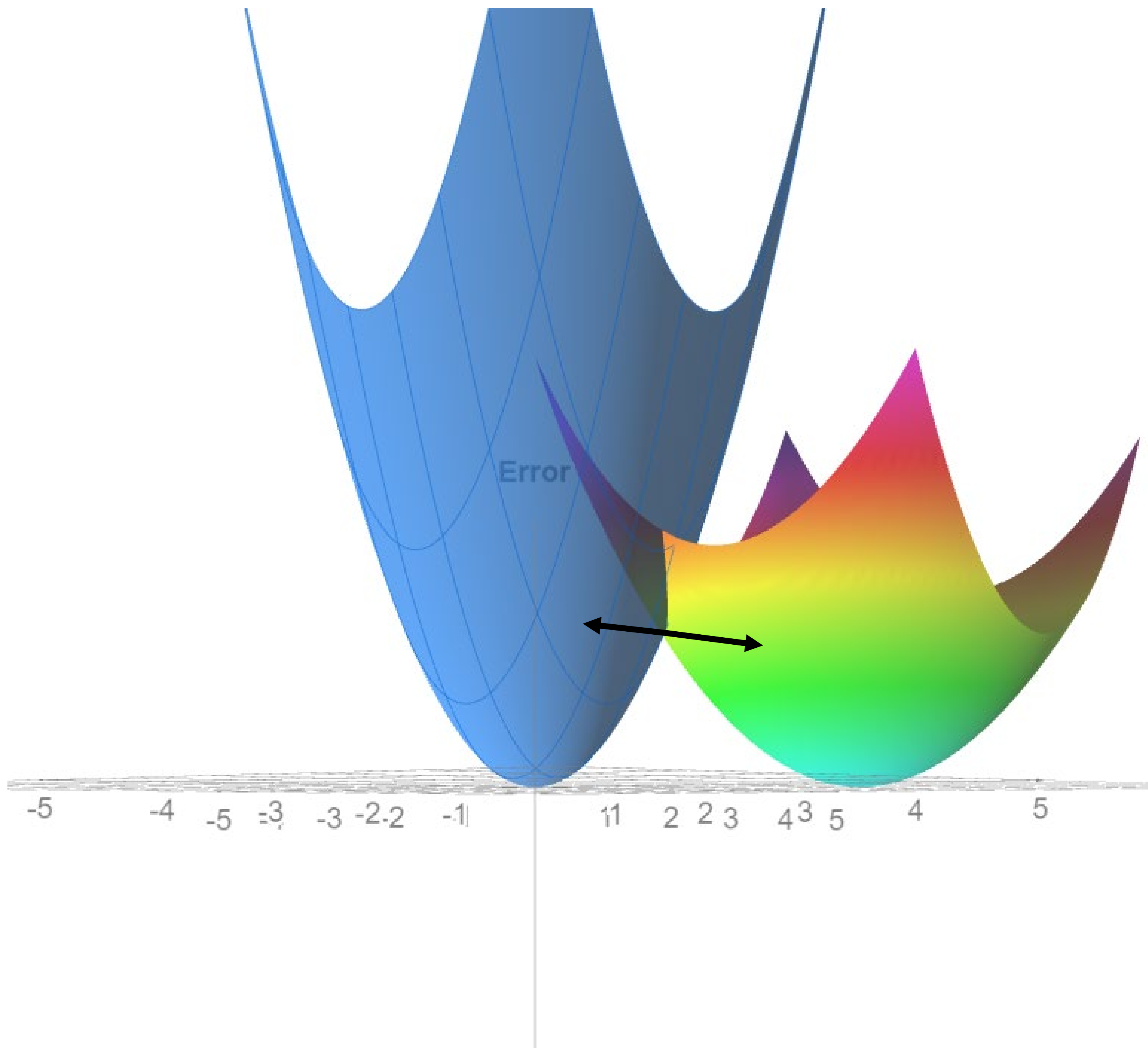
$$L(\theta, \lambda) = E(\theta) + \lambda g(\theta)$$

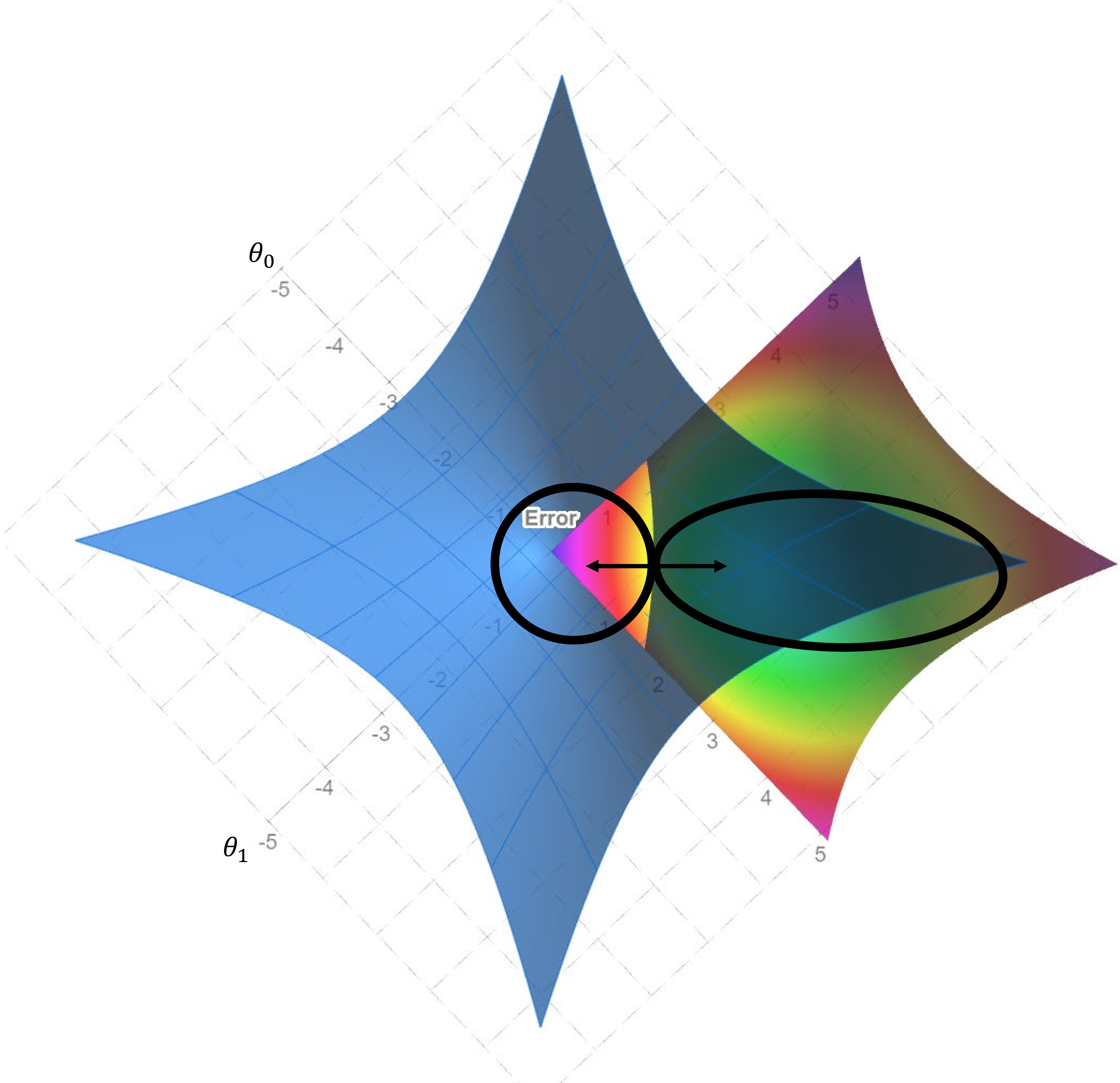
$$L(\theta, \lambda) = E(\theta) + \lambda \theta^T \theta$$

$$\nabla L(\theta, \lambda) = 0 \qquad \nabla[E(\theta) + \lambda \theta^T \theta] = 0$$

$$\nabla[E(\theta)] + \lambda \nabla[\theta^T \theta] = 0$$

How to enforce the gradient of Lagrange function to be zero





θ_0
θ_1
Error
-5
-4
-3
-2
-1
1
2
3
4
5

Let’s calculate the gradients

Gradient of constraint $g(\theta)$ $\quad$ $\nabla[\theta^T\theta] = 2\theta$

$$\nabla[E(\theta)] + \lambda\nabla[\theta^T\theta] = 0$$

$$\nabla[E(\theta)] = -\lambda\nabla[\theta^T\theta]$$

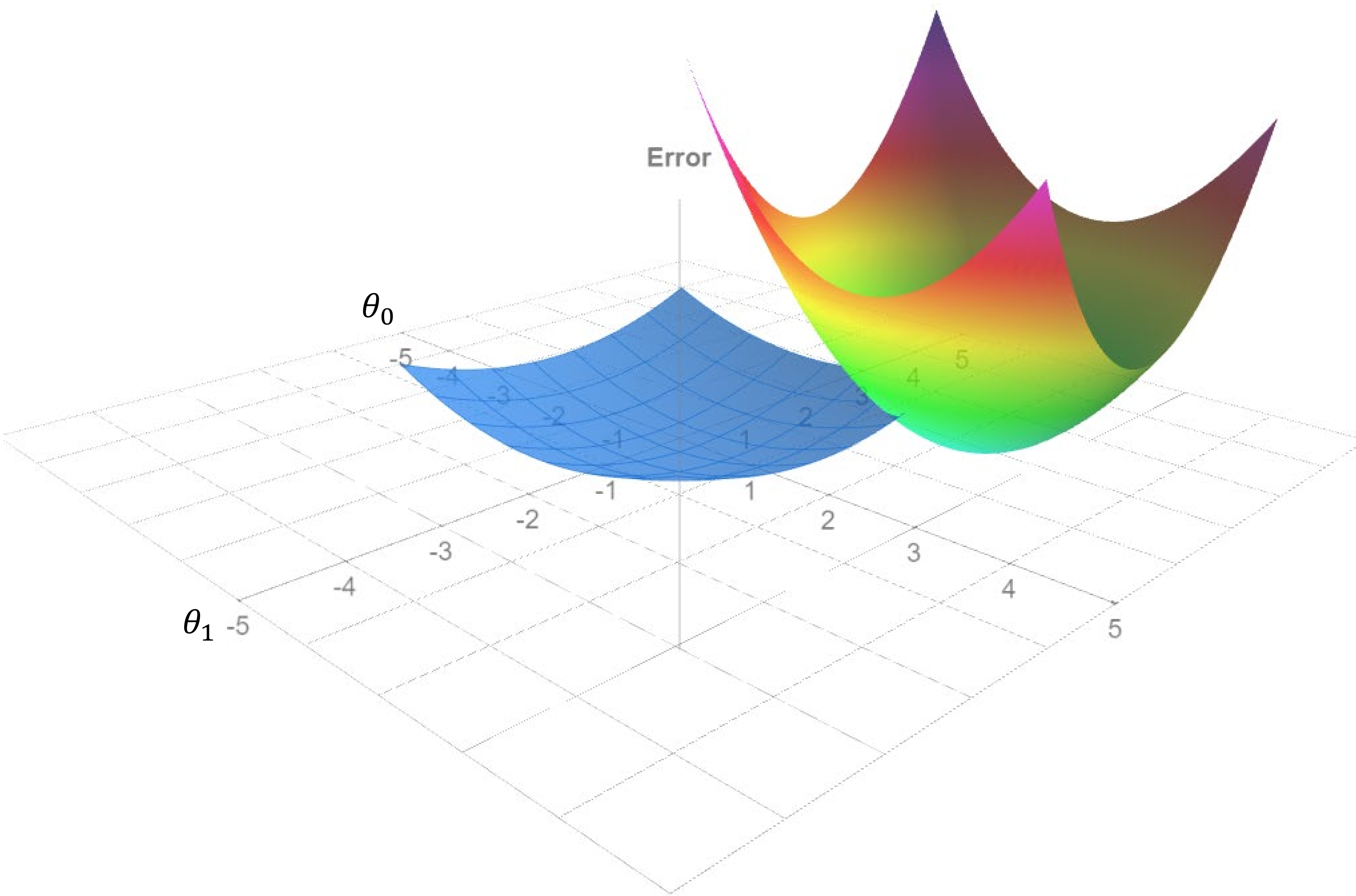
$$\nabla E(\theta) = -2\lambda\theta$$

$$\nabla E(\theta) + 2\lambda\theta = 0$$

Let’s do integration $\quad$ $E(\theta) + \lambda\theta^T\theta$

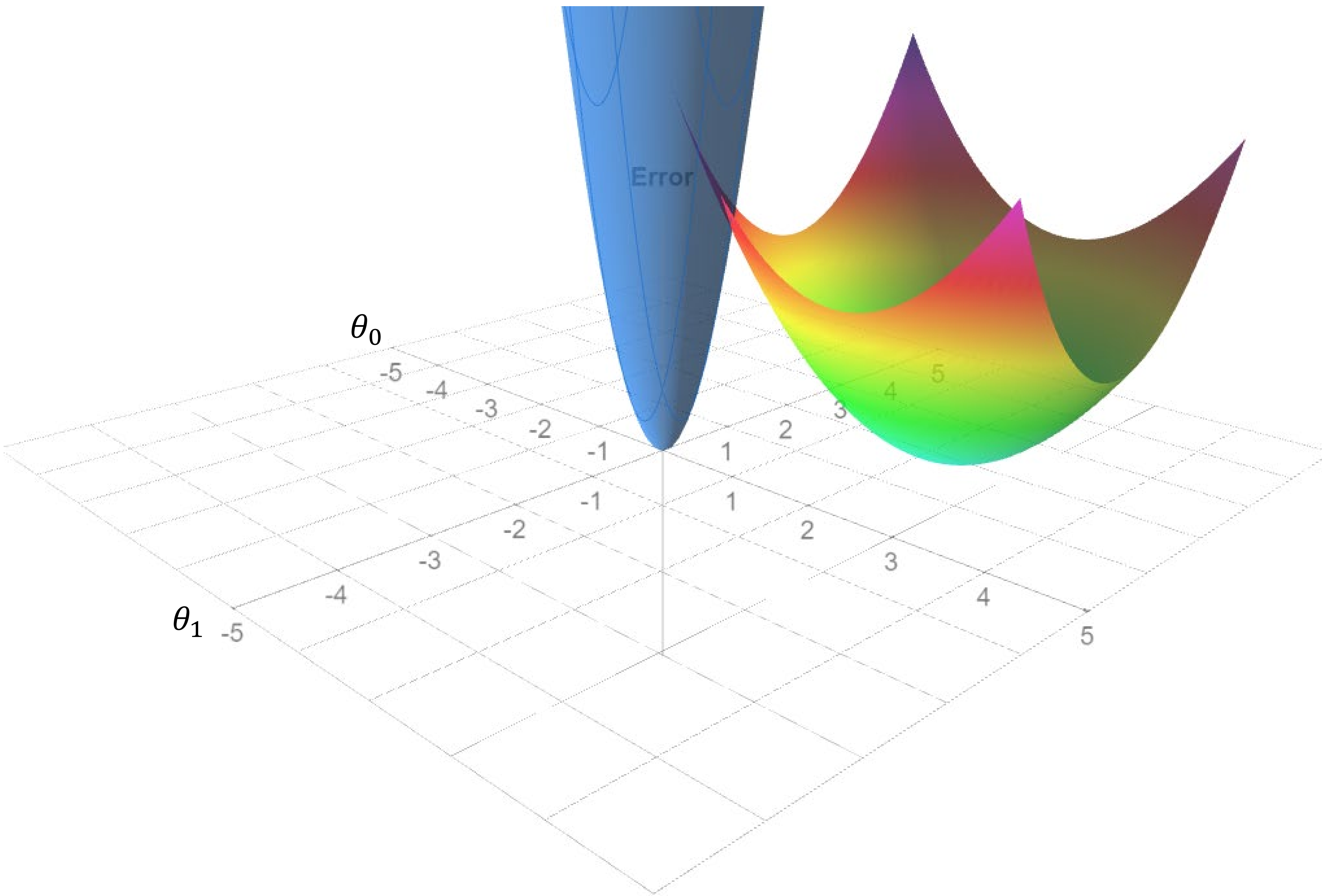
The effect of low Lambda

$$E(\theta) + \frac{\lambda}{N}\theta^T\theta$$



The effect of high Lambda

$$E(\theta) + \frac{\lambda}{N}\theta^T\theta$$



Regularized Learning

Now we know Why this term leads to the regularization of parameters

Minimize $E(\theta) + \lambda\theta^T\theta$

Regularized Error

$$\tilde{E}(\theta) = \frac{1}{N}\sum_{i=1}^{n}\left(y^i - z_i\theta\right)^2 + \frac{\lambda}{2N}\|\theta\|_2^2$$

L2 Regularization term

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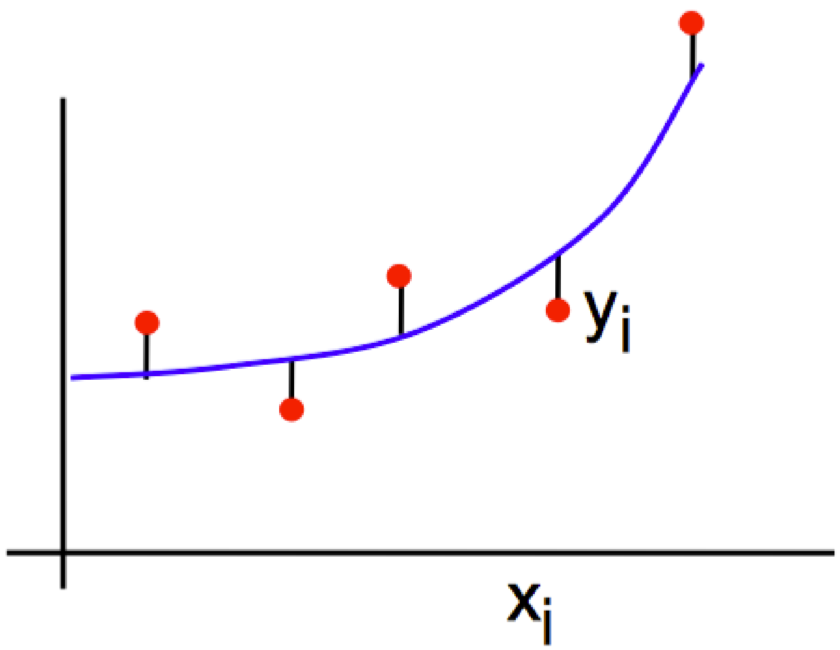
- Overfitting and regularized learning
- Ridge regression
- Lasso regression
- Determining regularization strength

Ridge Regression

$$\tilde{E}(\theta) = \frac{1}{N}\sum_{i=1}^{n}\left(y^i - z_i\theta\right)^2 + \lambda\|\theta\|_2^2$$



$$\theta_0 + \theta_1 z_1 + \theta_2 z_2 + \cdots + \theta_d z_\mathrm{d} + \epsilon = \boldsymbol{z\theta}$$

General form

$$\tilde{E}(\theta) = \frac{1}{N}\sum_{i=1}^{n}\left(y^i - z_i\theta\right)^2 + \lambda\|\theta\|_2^2$$

Matrix form

$$\tilde{E}(\theta) = \frac{1}{N}(y - z\theta)^{\mathrm{T}}(\mathrm{y} - z\theta) + \lambda\|\theta\|_2^2$$

$$\frac{\partial \tilde{E}(\theta)}{\partial \theta} = -z^T(y - z\theta) + \lambda\theta$$

$$(z^T z + \lambda I)\theta = z^T y$$

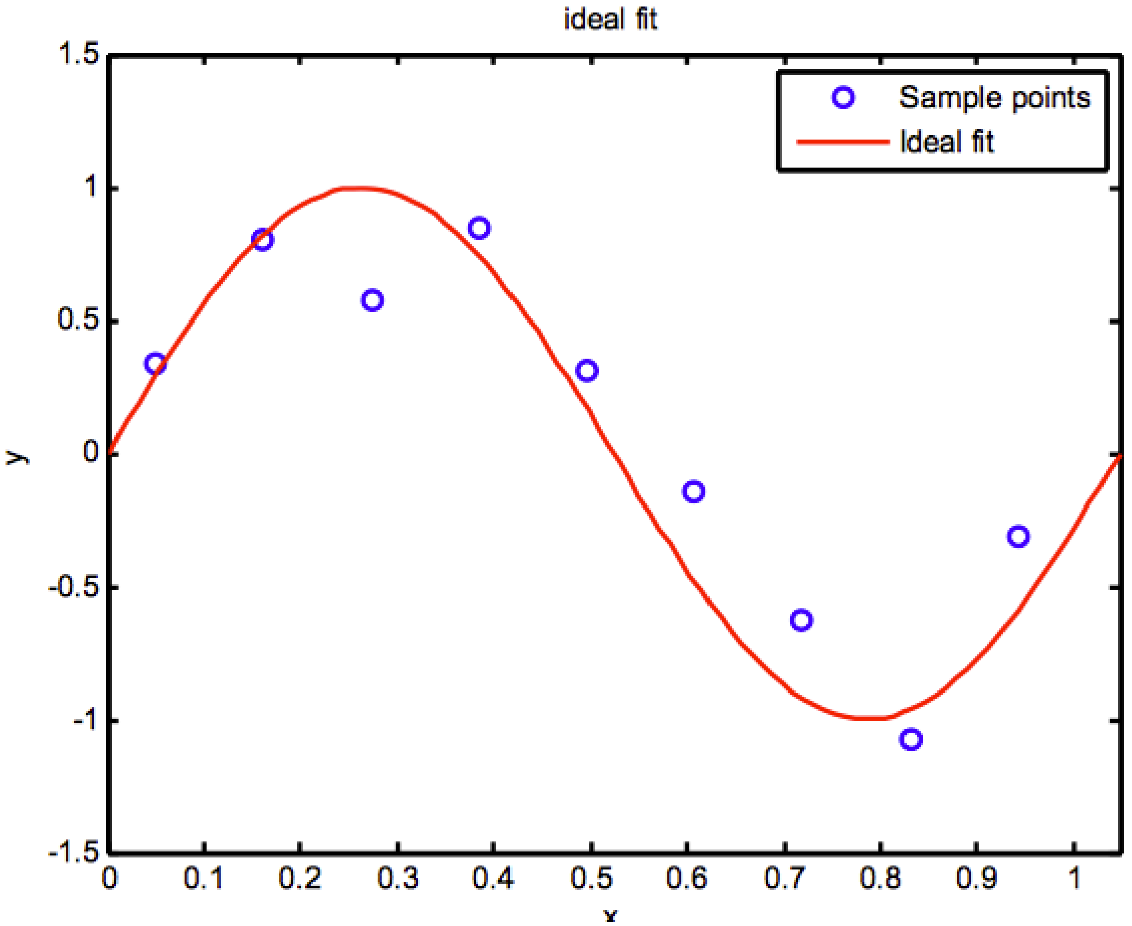
$$\theta = (z^T z + \lambda I)^{-1} z^T y$$

Ridge Regression Example

- The red curve is the true function (which is not a polynomial)

- The data points are samples from the curve with added noise in y.

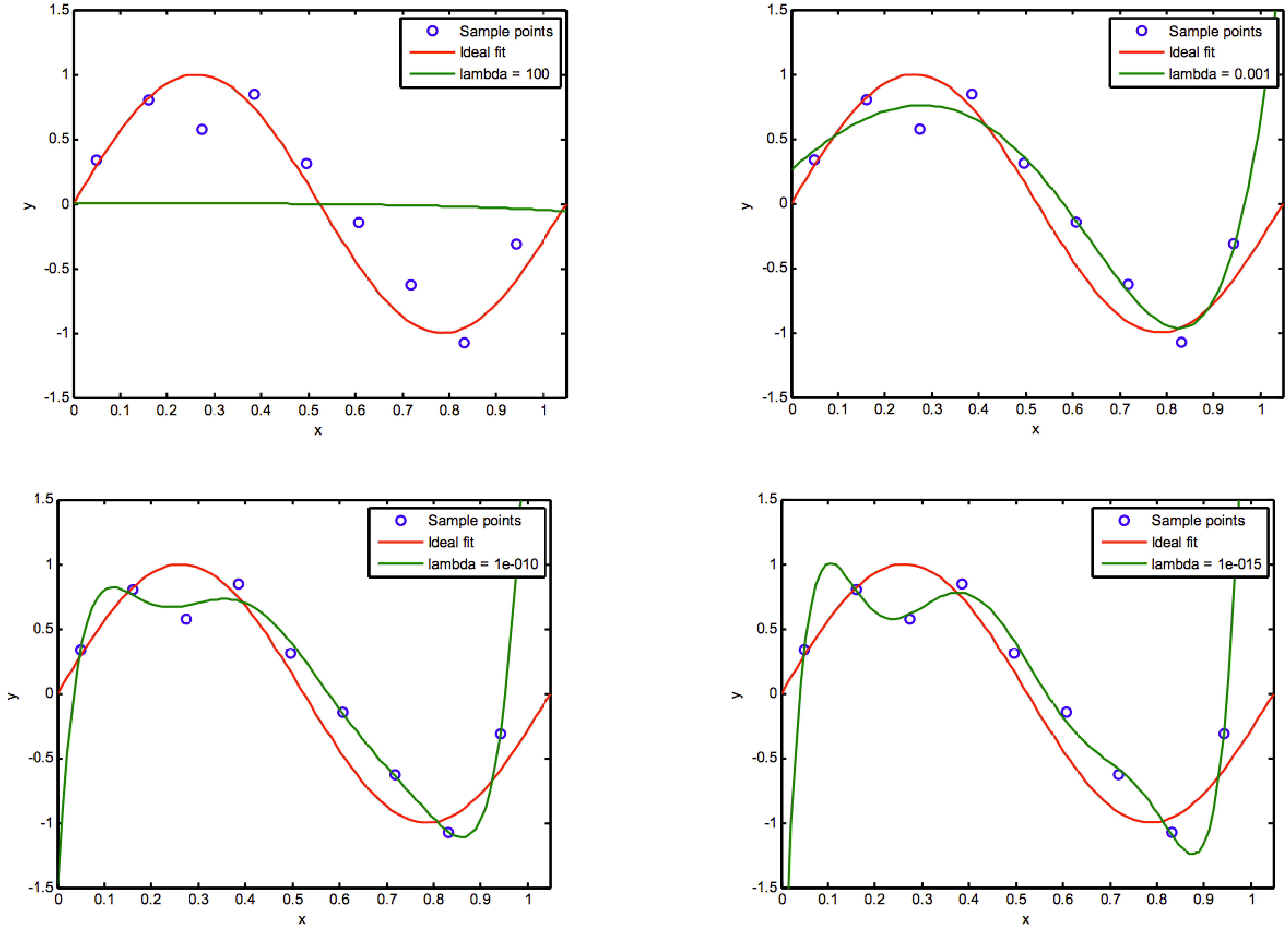
- There is a choice in both the degree, D, of the basis functions used, and in the strength of the regularization



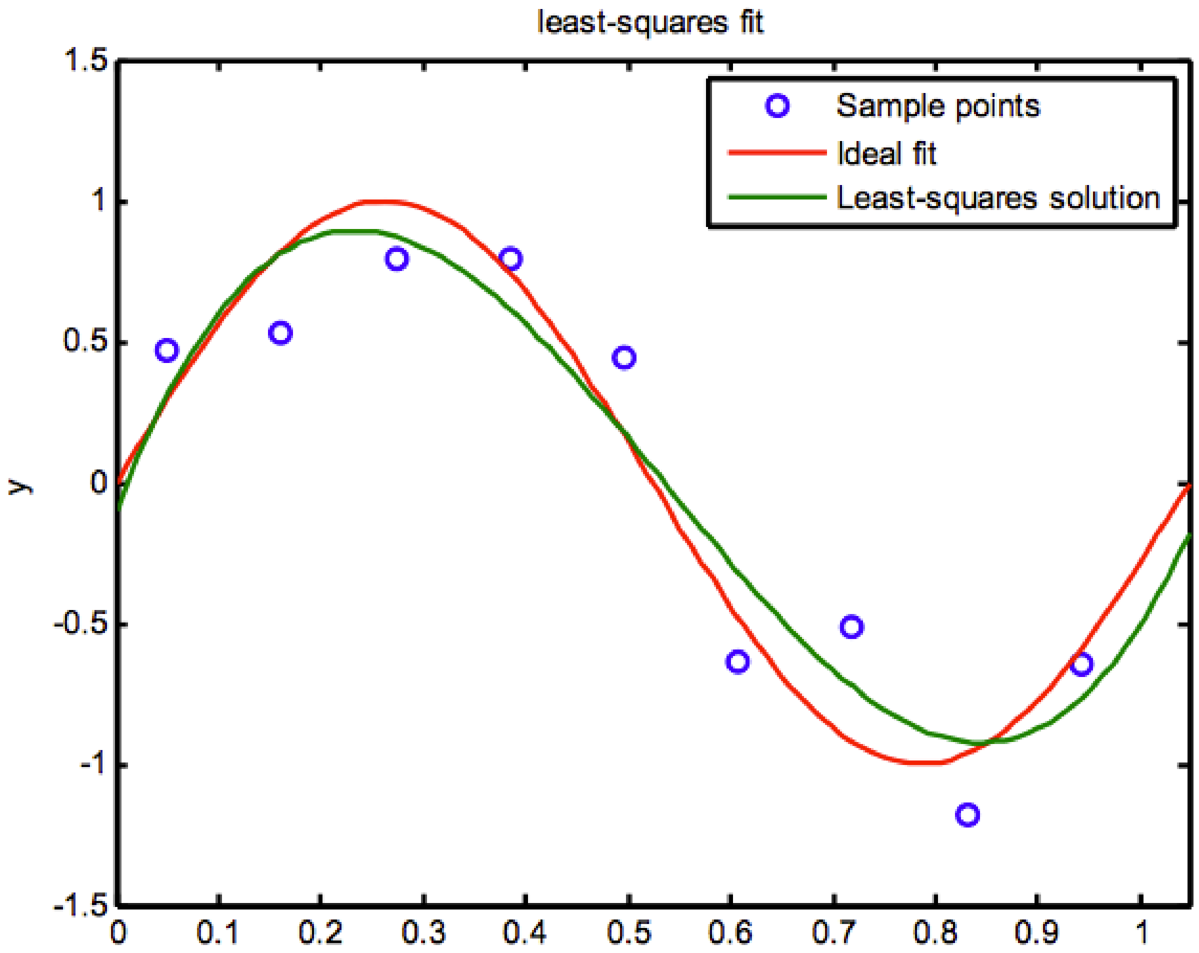
$$f(x,\theta) = z\theta \qquad\qquad z: x \to z$$

$$\tilde{E}(\theta) = \frac{1}{N}\sum_{i=1}^{n}\left(y^i - z_i\theta\right)^2 + \lambda\|\theta\|_2^2 \qquad \theta \in \mathbb{R}^{D+1}$$

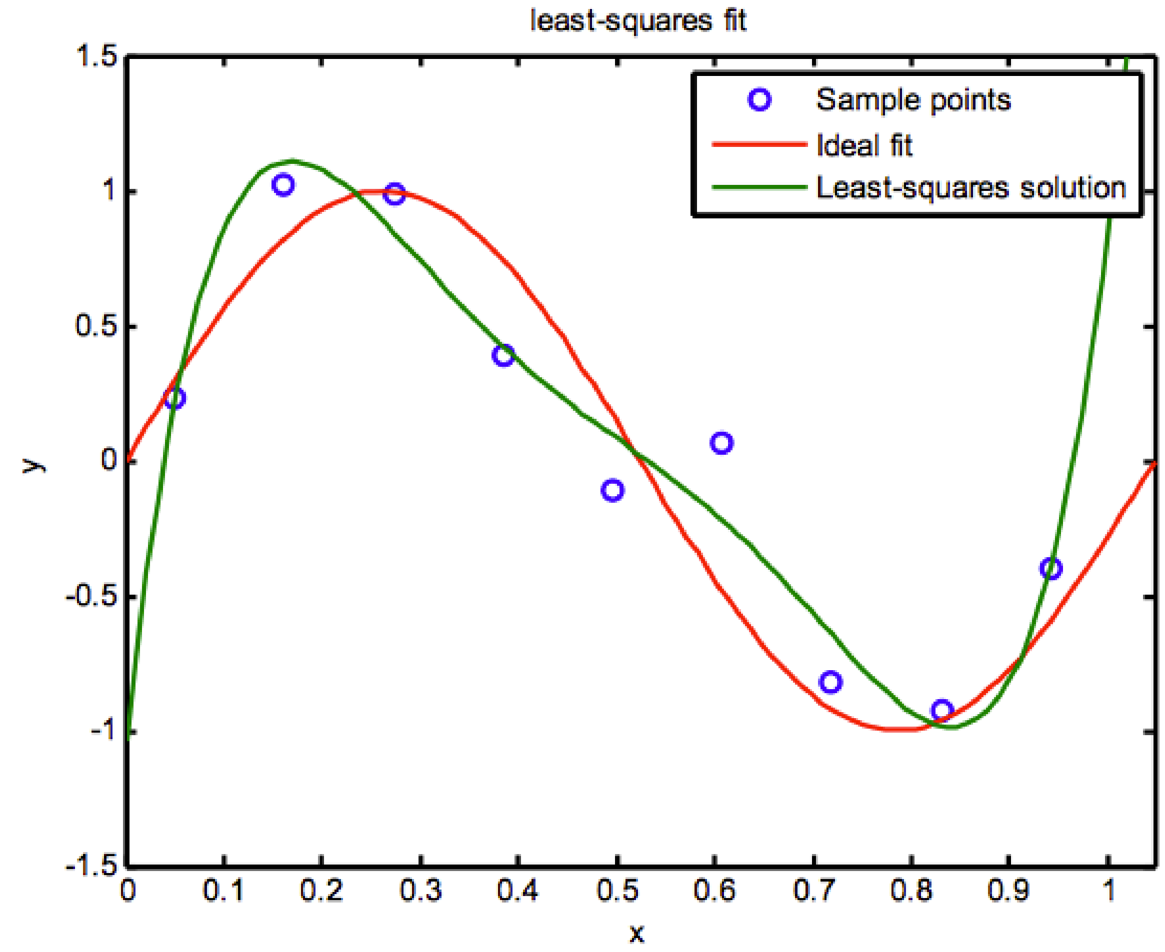
N = 9 samples, D = 7



D = 3


least-squares fit
Sample points
Ideal fit
Least-squares solution
y
1.5
1
0.5
0
-0.5
-1
-1.5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

D = 5


least-squares fit
Sample points
Ideal fit
Least-squares solution
y
x
1.5
1
0.5
0
-0.5
-1
-1.5
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1

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Regularized Regression

$$\tilde{E}(\theta) = \frac{1}{N}\sum_{i=1}^{n}\left(y^{i} - z_{i}\theta\right)^{2} + \lambda\|\theta\|_{2}^{2}$$

Squared loss\Error $\quad \frac{1}{N}\sum_{i=1}^{n}\left(y^{i} - z_{i}\theta\right)^{2}$

L2 Regularizer $\quad \lambda\|\theta\|_{2}^{2}$

Now let's look at another regularization choice.

The Lasso Regularization (L1 norm) and sparsity

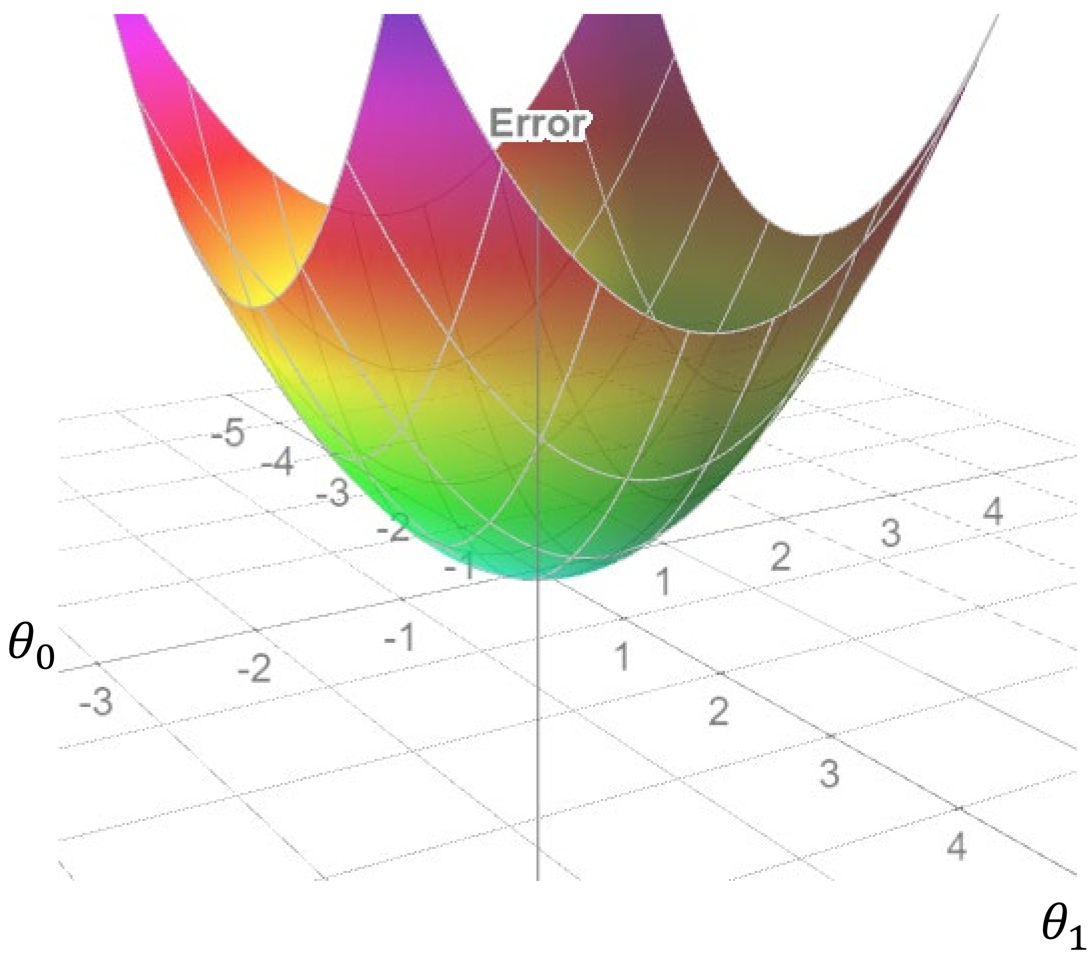
Lasso = **L**east Absolute **S**hrinkage and **S**election **O**perator

$$\tilde{E}(\theta) = \frac{1}{N}\sum_{i=1}^{n}\left(y^i - z_i\theta\right)^2 + \lambda\|\theta\|_1$$

L1 norm induces sparsity. This means that some of the weights become zero, and the feature contribution will be completely removed. L1 Regularizer could be used for feature selection

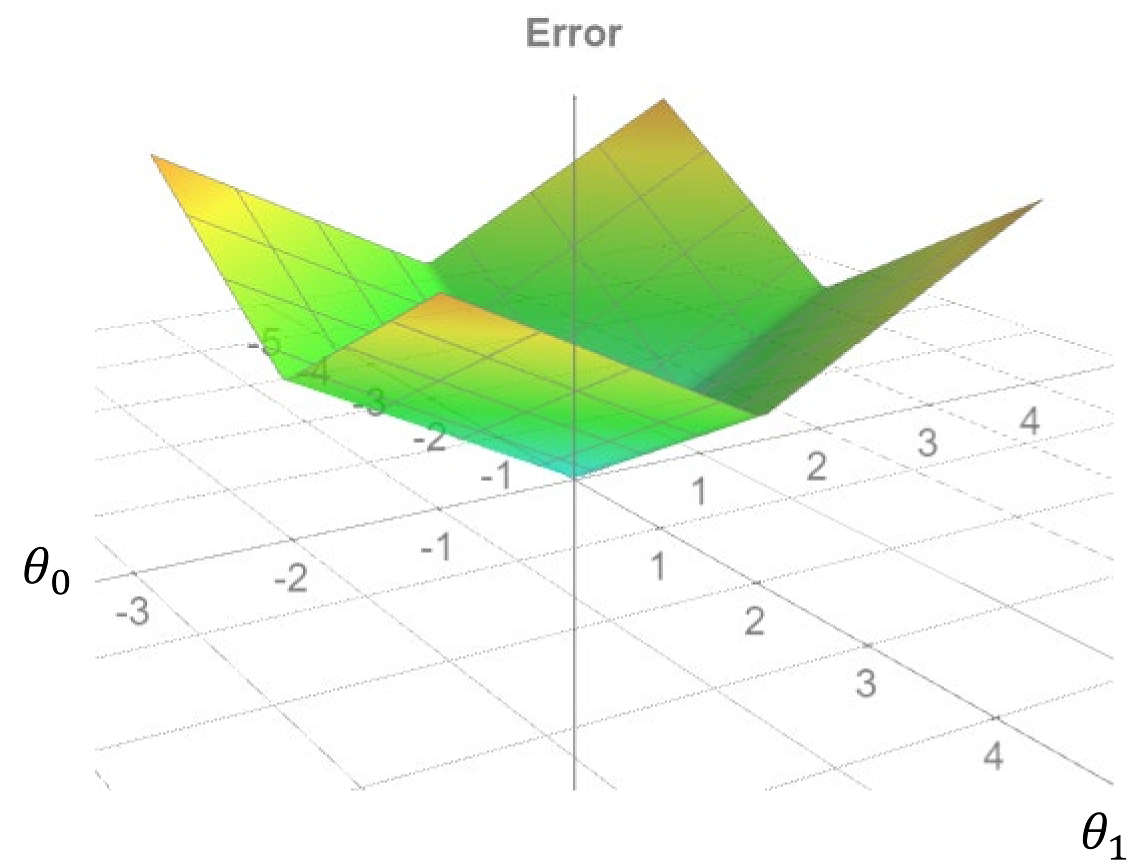
Ridge Regularizer

$$g(\theta) = \theta_0^2 + \theta_1^2 = \theta^T\theta$$



Lasso Regularizer

$$g(\theta) = \theta_0 + \theta_1 = \theta$$

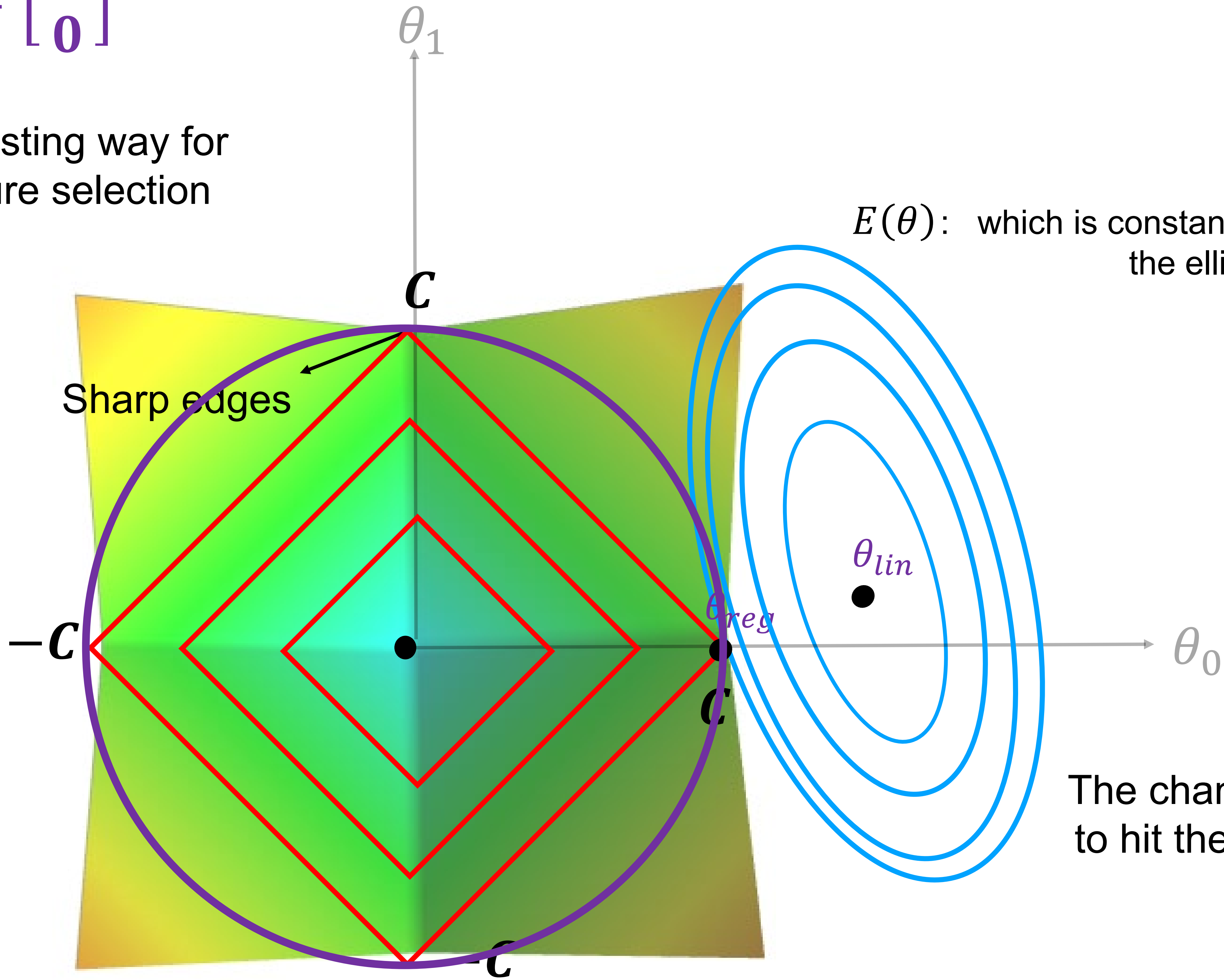


Let's say we have two parameters (θ_0 and θ_1)

$$Min\ E(\theta) = \frac{1}{N}(zw - y)^T(z\theta - y) + \lambda\|\theta\|_1$$

$$\theta = \begin{bmatrix} \theta_0 \\ \mathbf{0} \end{bmatrix}$$

Interesting way for feature selection



The chance is very high to hit the sharp corners first

Ridge versus Lasso

Ridge

$$\tilde{E}(\theta) = \frac{1}{N}(y - z\theta)^{\mathrm{T}}(\mathrm{y} - z\theta) + \lambda\|\theta\|_2^2$$

It is a convex model

Both mean squared error and L2 regularizer are differentiable.

We can get a closed form solution

Lasso

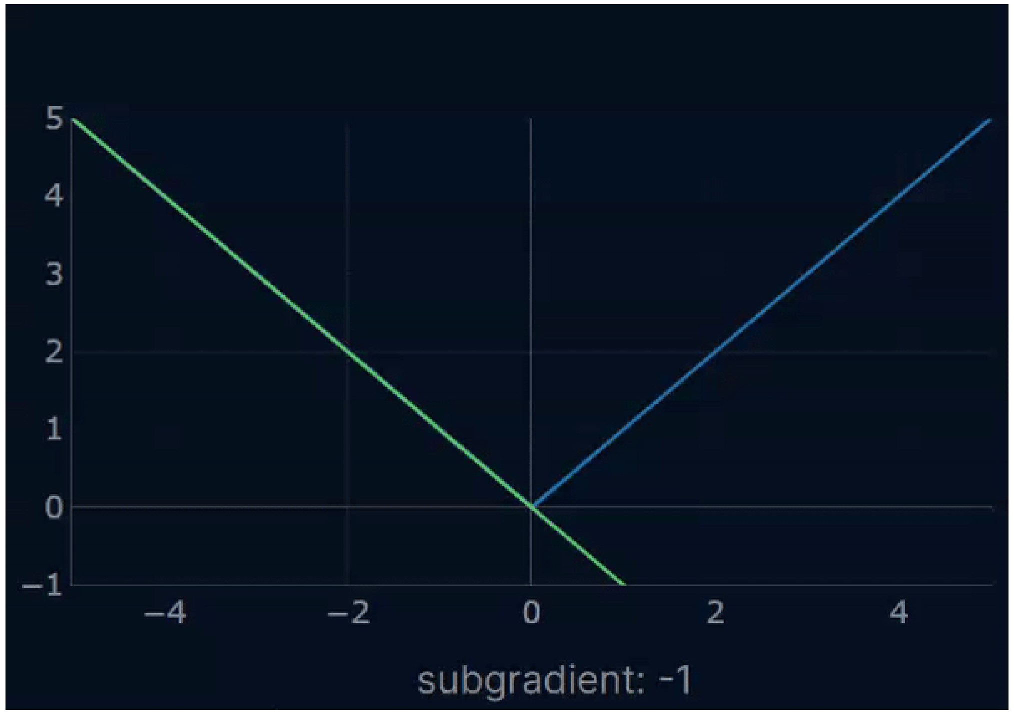
$$\tilde{E}(\theta) = \frac{1}{N}(y - z\theta)^{\mathrm{T}}(\mathrm{y} - z\theta) + \lambda\|\theta\|_1$$

It is a convex model

L1 regularizer is NOT differentiable.

We can **NOT** get a closed form solution

Sub-gradient Descend in Lasso

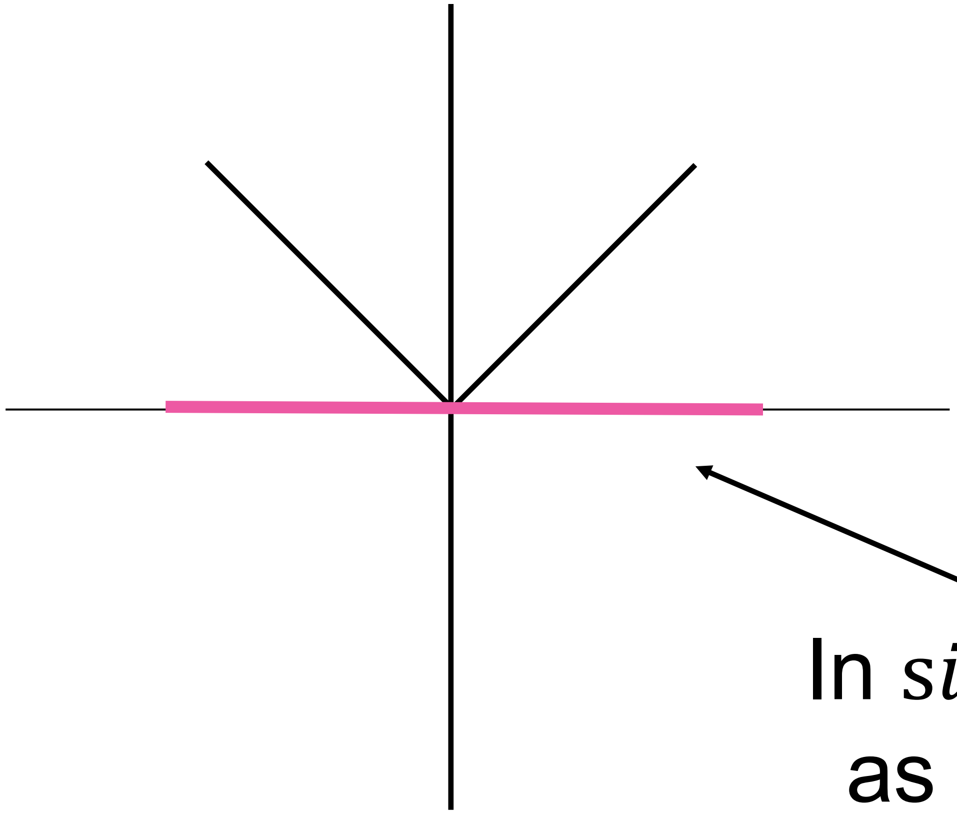


$$\tilde{E}(\theta) = \frac{1}{N}(y - z\theta)^{\mathrm{T}}(\mathrm{y} - z\theta) + \lambda\|\theta\|_1$$

$$\frac{\partial \tilde{E}(\theta)}{\partial \theta} = -z^T(y - z\theta) + \frac{\partial(\lambda\|\theta\|_1)}{\partial \theta}$$

Using Sub-gradient

$$\frac{\partial \tilde{E}(\theta)}{\partial \theta} = -z^T(y - z\theta) + \lambda sign(\theta)$$



In $sign$ function, we use this sub-gradient line as our under-estimator (below our function)

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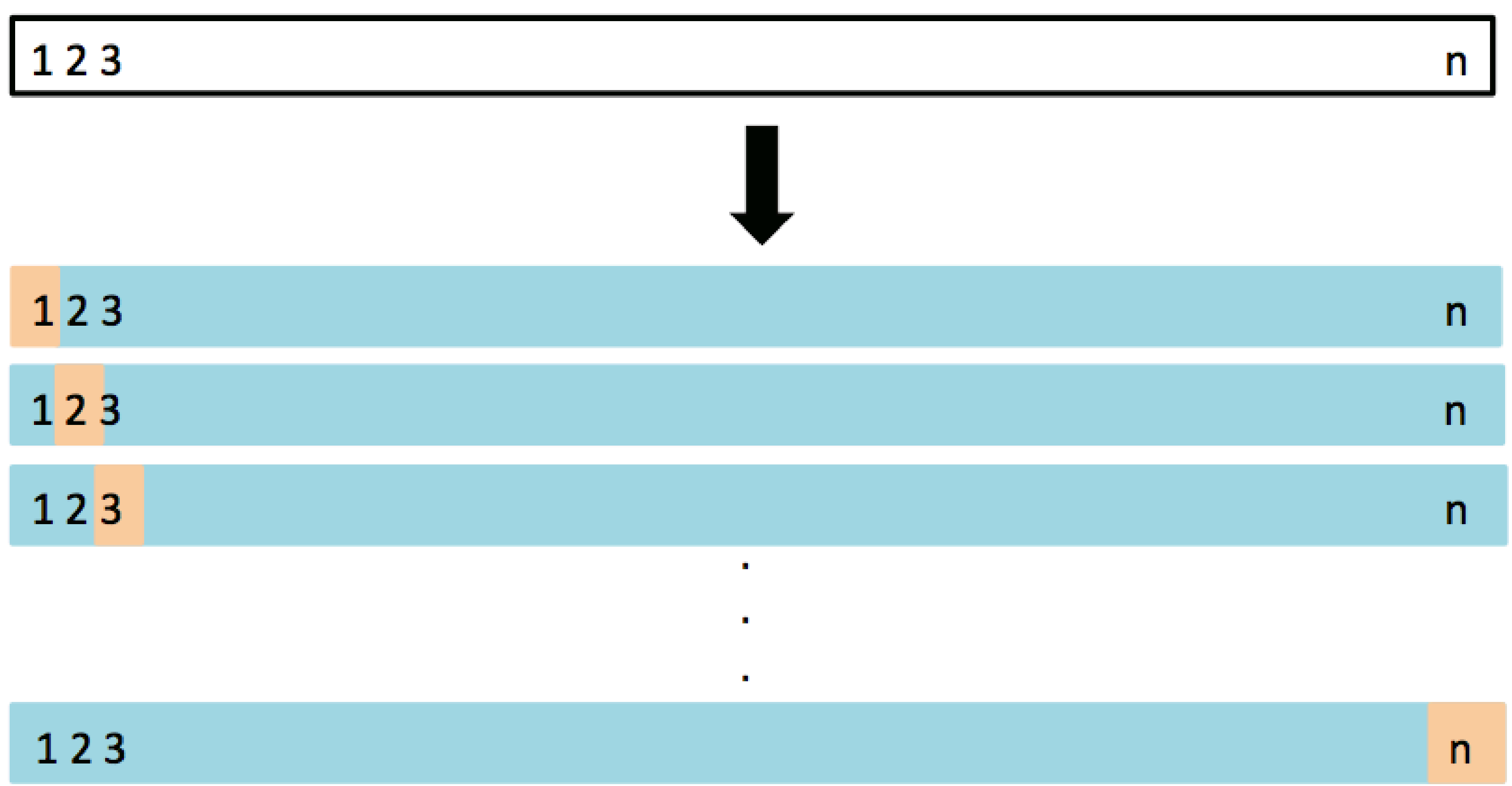
Leave-One-Out Cross Validation

For every $i = 1, \ldots, n$:

- train the model on every point except i,
- compute the test error on the held out point.

Average the test errors. $$\text{CV}_{(n)} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i^{(-i)})^2$$



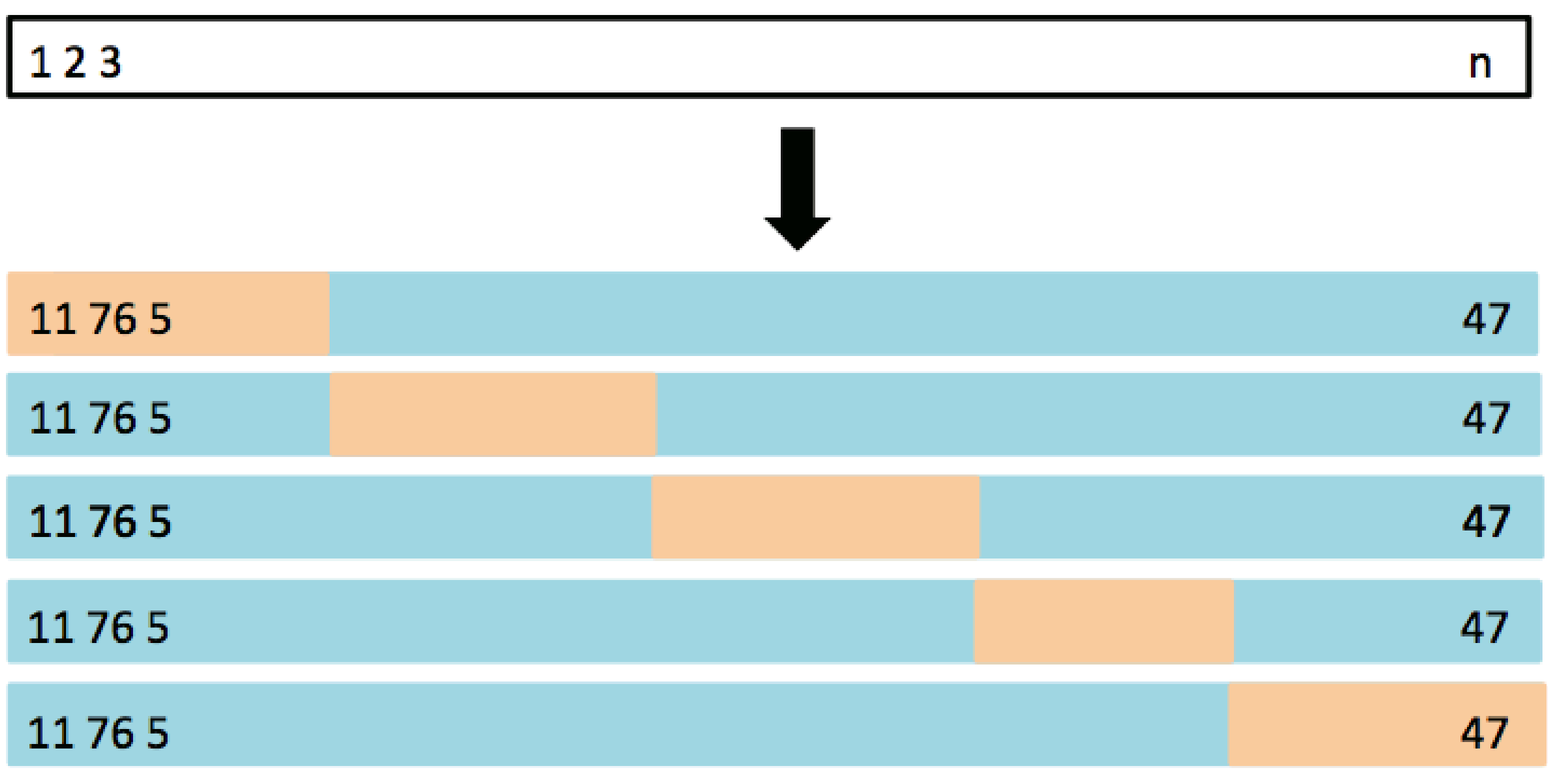
K-Fold Cross Validation

Split the data into k subsets or *folds*.

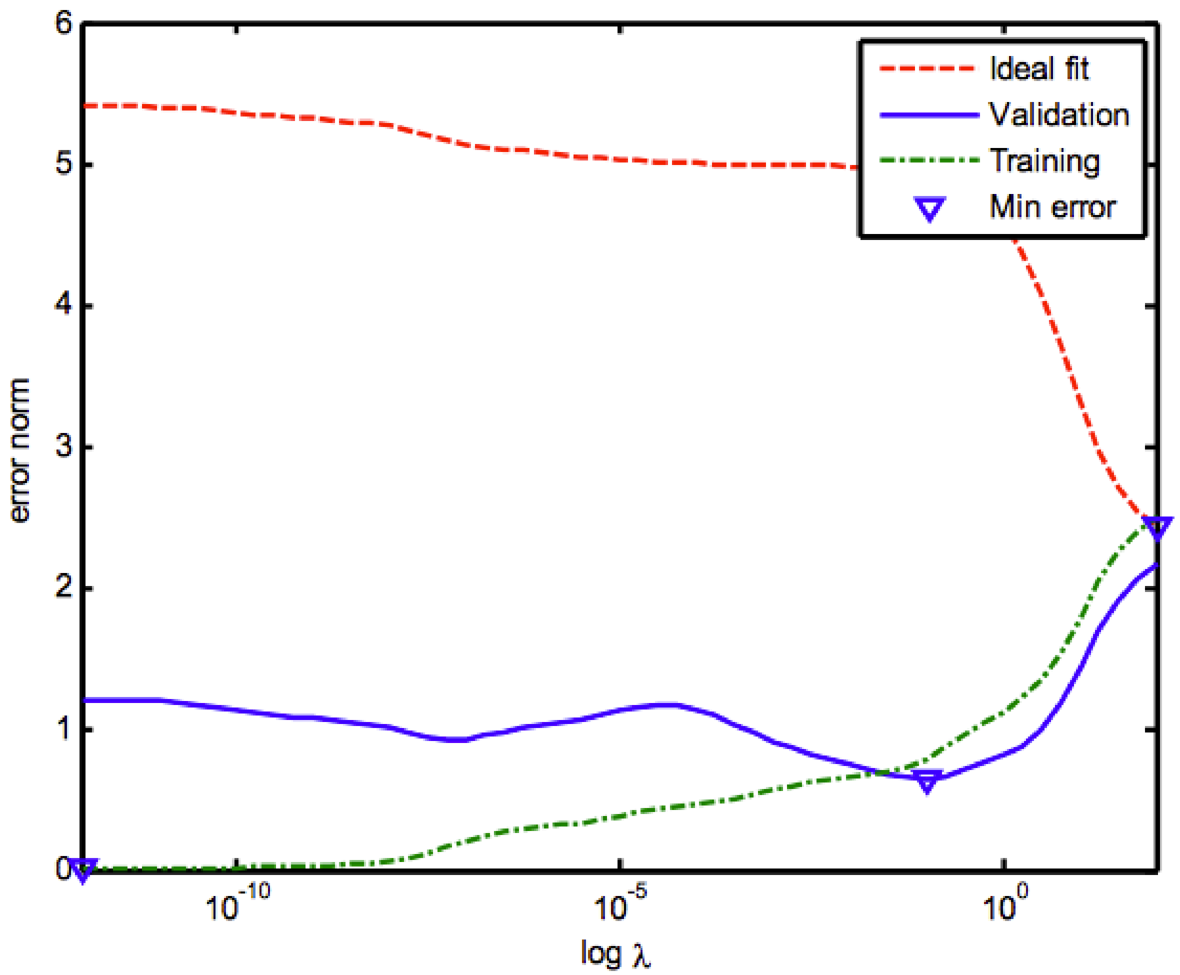
For every $i = 1, \ldots, k$:

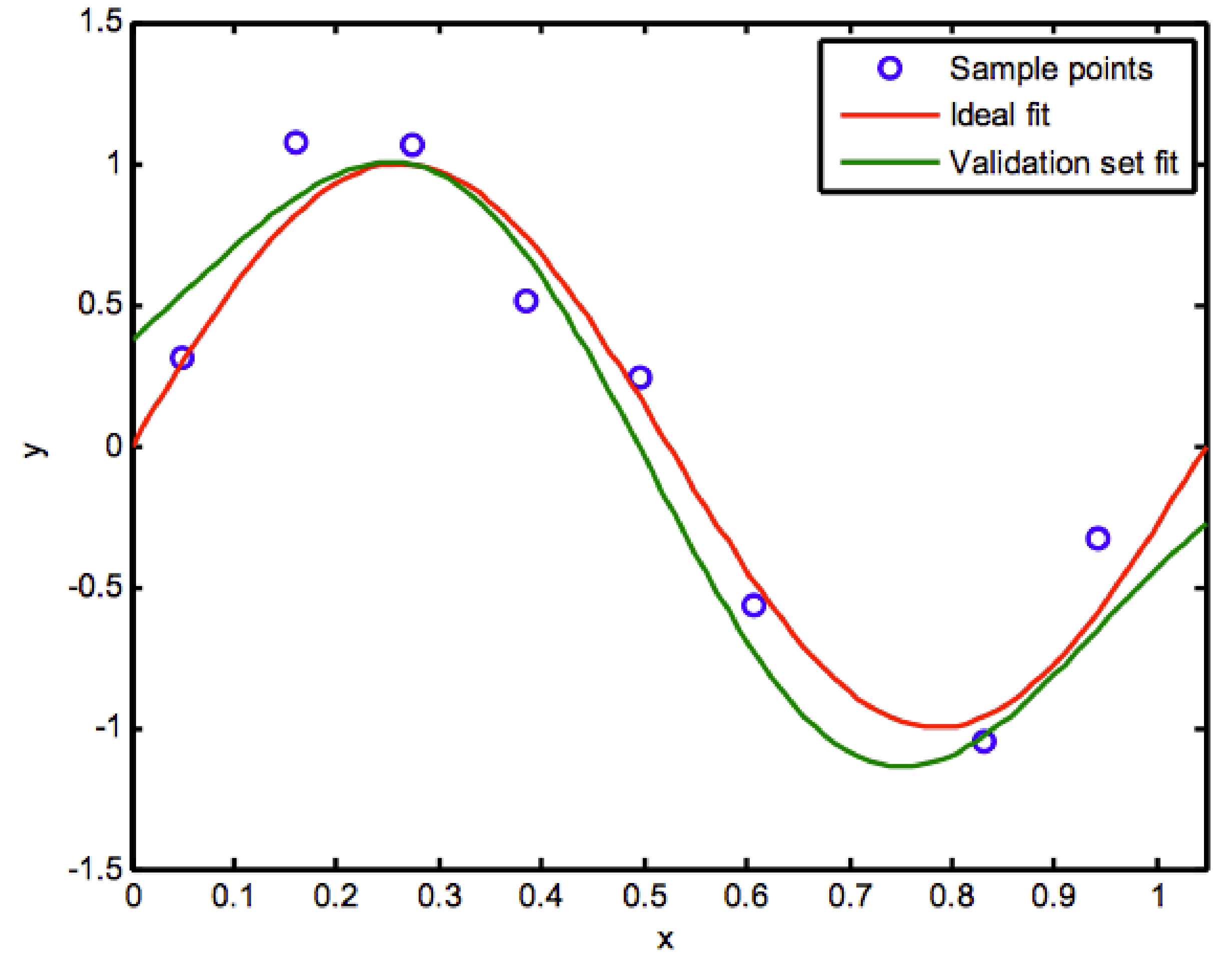
- train the model on every fold except the ith fold,
- compute the test error on the ith fold.

Average the test errors.



Choosing λ Using Validation Dataset





Pick up the lambda with the lowest mean value of rmse calculated by Cross Validation approach

Take-Home Messages

- What is overfitting
- What is regularization
- How does Ridge regression work
- Sparsity properties of Lasso regression
- How to choose the regularization coefficient λ