Model Regularization

Overfitting, Bias-variance decomposition, L1 and L2 regularization

Machine Learning and Data Mining, 2025

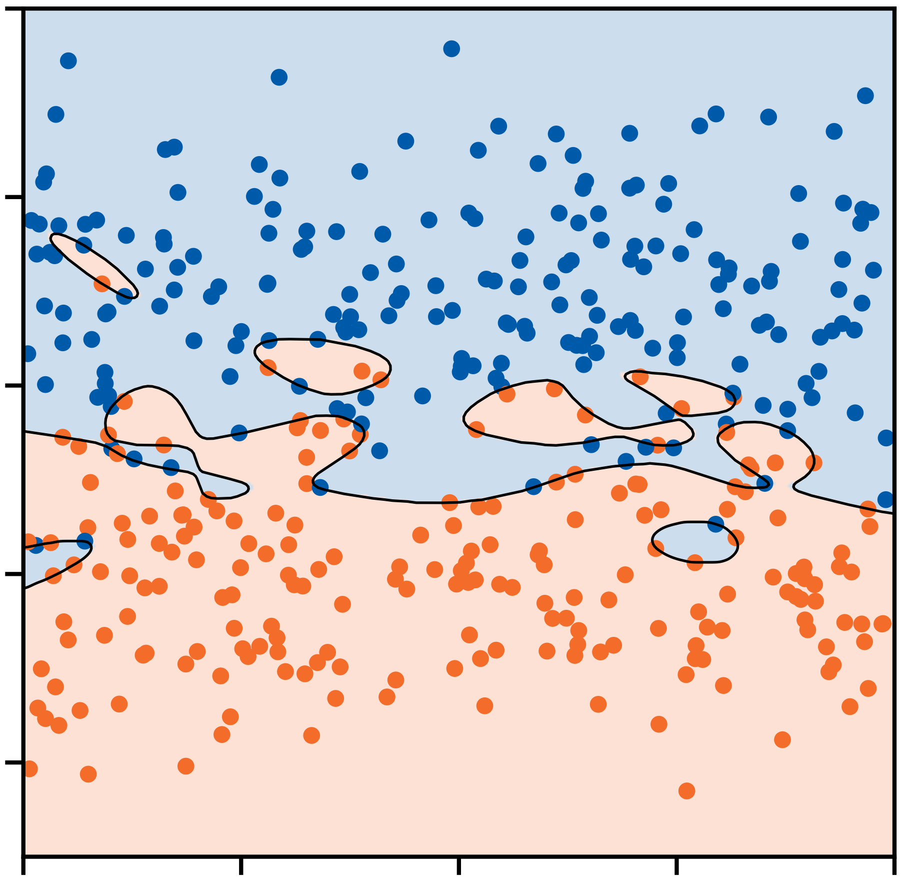
Majid Sohrabi

National Research University Higher School of Economics

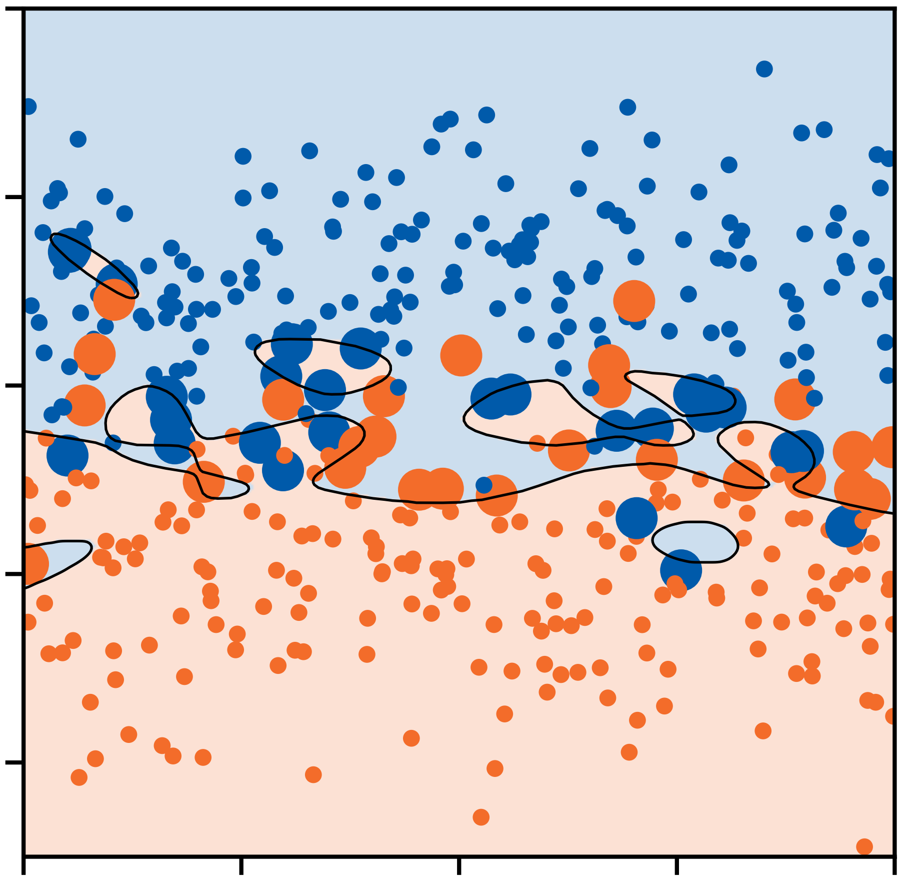
September 17, 2025

The problem of overfitting

Overfitting in classification



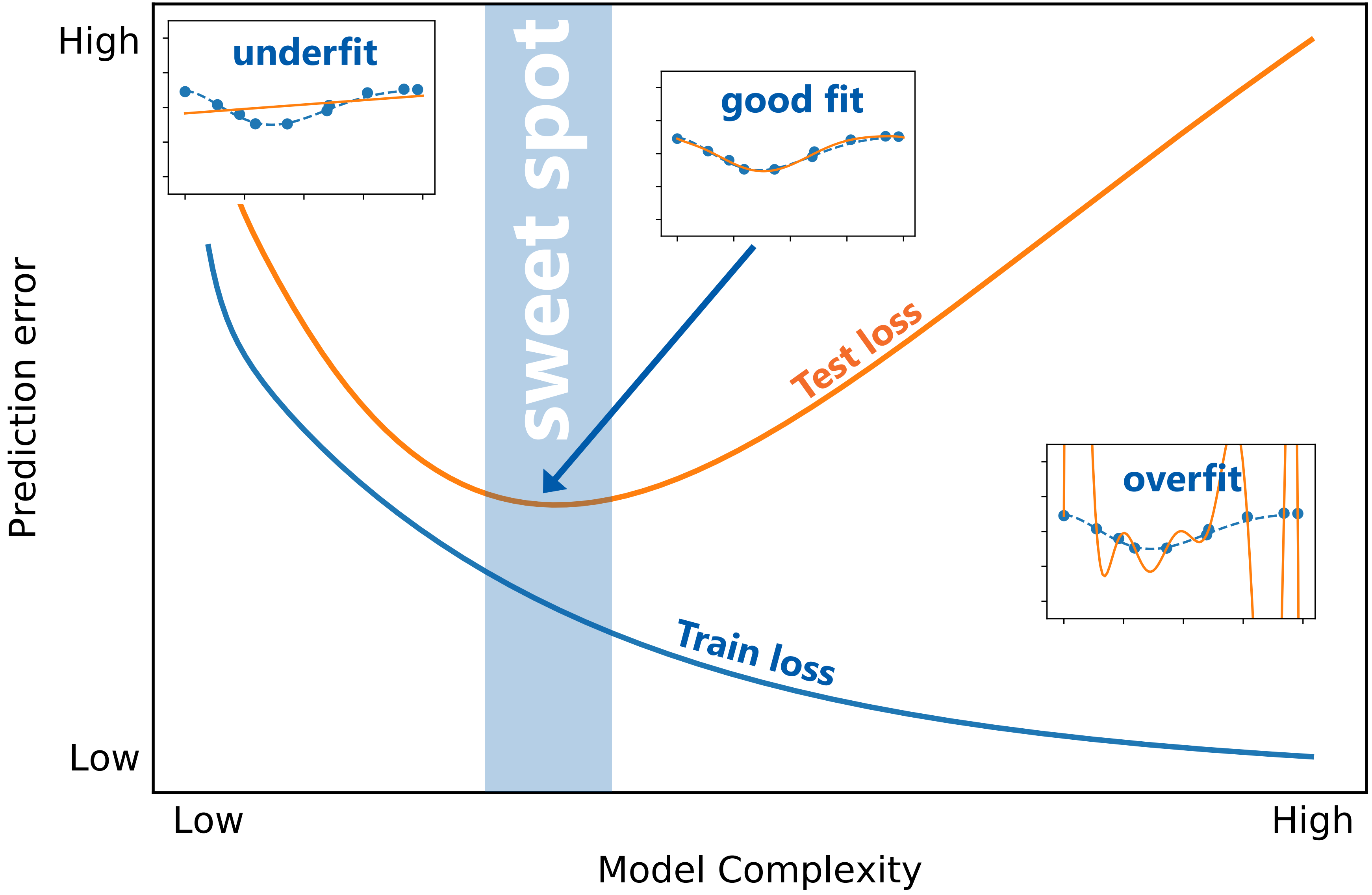
Training set



Test set

Large points =
classification error

How to check whether a model is good?



Check the loss on the **test data** – i.e. data that the learning algorithm hasn't seen

The goal is to find the **right level of limitations** – not too strict, not too loose

Prediction error decomposition

Prediction error decomposition

Assume there's the following (unknown) **relation between the features and targets**

$$y = f(x) + \varepsilon$$

where ε is some random noize:

$$\mathbb{E}[\varepsilon] = 0$$

$$\mathbb{D}[\varepsilon] = \sigma_\varepsilon^2$$

Prediction error decomposition

Assume there's the following (unknown) **relation between the features and targets**

$$y = f(x) + \varepsilon$$

where ε is some random noize:

$$\mathbb{E}[\varepsilon] = 0$$

$$\mathbb{D}[\varepsilon] = \sigma_\varepsilon^2$$

Let's denote our training set as τ.

We want to study the **expected squared error** for the model $\hat{f}_\tau$ trained on it:

$$\text{exp. sq. err}(x) = \mathop{\mathbb{E}}_{\tau, y|x}\left[\left(\hat{f}_\tau(x) - y\right)^2\right]$$

Prediction error decomposition

$$\mathrm{exp.sq.err}(x) = \mathop{\mathbb{E}}_{\tau,y|x}\left[\left(\hat{f}_\tau(x) - y\right)^2\right]$$

$$= \mathop{\mathbb{E}}_{\tau,y|x}\left[\left(\hat{f}_\tau(x) \qquad\qquad\qquad\qquad\qquad\qquad - y\right)^2\right]$$

Prediction error decomposition

$$\text{exp. sq. err}(x) = \underset{\tau,y|x}{\mathbb{E}}\left[\left(\hat{f}_\tau(x) - y\right)^2\right]$$

$$= \underset{\tau,y|x}{\mathbb{E}}\left[\left(\hat{f}_\tau(x) - \underset{\tau'}{\mathbb{E}}\left[\hat{f}_{\tau'}(x)\right] + \underset{\tau'}{\mathbb{E}}\left[\hat{f}_{\tau'}(x)\right] - y\right)^2\right]$$

Prediction of the "expected model"

Prediction error decomposition

$$\mathrm{exp.sq.err}(x) = \mathop{\mathbb{E}}_{\tau,y|x}\left[\left(\hat{f}_\tau(x) - y\right)^2\right]$$

$$= \mathop{\mathbb{E}}_{\tau,y|x}\left[\left(\hat{f}_\tau(x) - \mathop{\mathbb{E}}_{\tau'}\left[\hat{f}_{\tau'}(x)\right] + \mathop{\mathbb{E}}_{\tau'}\left[\hat{f}_{\tau'}(x)\right] - f(x) + f(x) - y \right)^2\right]$$

Ground truth (without the noise)

Prediction error decomposition

$$\text{exp. sq. err}(x) = \mathop{\mathbb{E}}_{\tau,y|x}\left[\left(\hat{f}_\tau(x) - y\right)^2\right]$$

$$= \mathop{\mathbb{E}}_{\tau,y|x}\left[\left(\left(\hat{f}_\tau(x) - \mathop{\mathbb{E}}_{\tau'}\left[\hat{f}_{\tau'}(x)\right]\right) + \left(\mathop{\mathbb{E}}_{\tau'}\left[\hat{f}_{\tau'}(x)\right] - f(x)\right) + (f(x) - y)\right)^2\right]$$

(grouping the terms, then expanding the square)

Prediction error decomposition

$$\text{exp. sq. err}(x) = \underset{\tau,y|x}{\mathbb{E}}\left[\left(\hat{f}_\tau(x) - y\right)^2\right]$$

$$= \underset{\tau,y|x}{\mathbb{E}}\left[\left(\left(\hat{f}_\tau(x) - \underset{\tau'}{\mathbb{E}}[\hat{f}_{\tau'}(x)]\right) + \left(\underset{\tau'}{\mathbb{E}}[\hat{f}_{\tau'}(x)] - f(x)\right) + (f(x) - y)\right)^2\right]$$

(easy to show that all the cross term expectations are 0)

$$= \underset{\tau}{\mathbb{E}}\left[\left(\hat{f}_\tau(x) - \underset{\tau'}{\mathbb{E}}[\hat{f}_{\tau'}(x)]\right)^2\right] + \left(\underset{\tau'}{\mathbb{E}}[\hat{f}_{\tau'}(x)] - f(x)\right)^2 + \underset{y|x}{\mathbb{E}}[(f(x) - y)^2]$$

Variance of the model

i.e. how "unstable" the model is wrt the noise in the training data

Prediction error decomposition

$$\text{exp. sq. err}(x) = \mathop{\mathbb{E}}_{\tau,y|x}\left[\left(\hat{f}_\tau(x) - y\right)^2\right]$$

$$= \mathop{\mathbb{E}}_{\tau,y|x}\left[\left(\left(\hat{f}_\tau(x) - \mathop{\mathbb{E}}_{\tau'}[\hat{f}_{\tau'}(x)]\right) + \left(\mathop{\mathbb{E}}_{\tau'}[\hat{f}_{\tau'}(x)] - f(x)\right) + (f(x) - y)\right)^2\right]$$

(easy to show that all the cross term expectations are 0)

$$= \mathop{\mathbb{E}}_{\tau}\left[\left(\hat{f}_\tau(x) - \mathop{\mathbb{E}}_{\tau'}[\hat{f}_{\tau'}(x)]\right)^2\right] + \left(\mathop{\mathbb{E}}_{\tau'}[\hat{f}_{\tau'}(x)] - f(x)\right)^2 + \mathop{\mathbb{E}}_{y|x}[(f(x) - y)^2]$$

how much the "expected model" differs from the ground truth

Squared bias

Prediction error decomposition

$$\text{exp. sq. err}(x) = \mathop{\mathbb{E}}_{\tau,y|x}\left[\left(\hat{f}_\tau(x) - y\right)^2\right]$$

$$= \mathop{\mathbb{E}}_{\tau,y|x}\left[\left(\left(\hat{f}_\tau(x) - \mathop{\mathbb{E}}_{\tau'}[\hat{f}_{\tau'}(x)]\right) + \left(\mathop{\mathbb{E}}_{\tau'}[\hat{f}_{\tau'}(x)] - f(x)\right) + (f(x) - y)\right)^2\right]$$

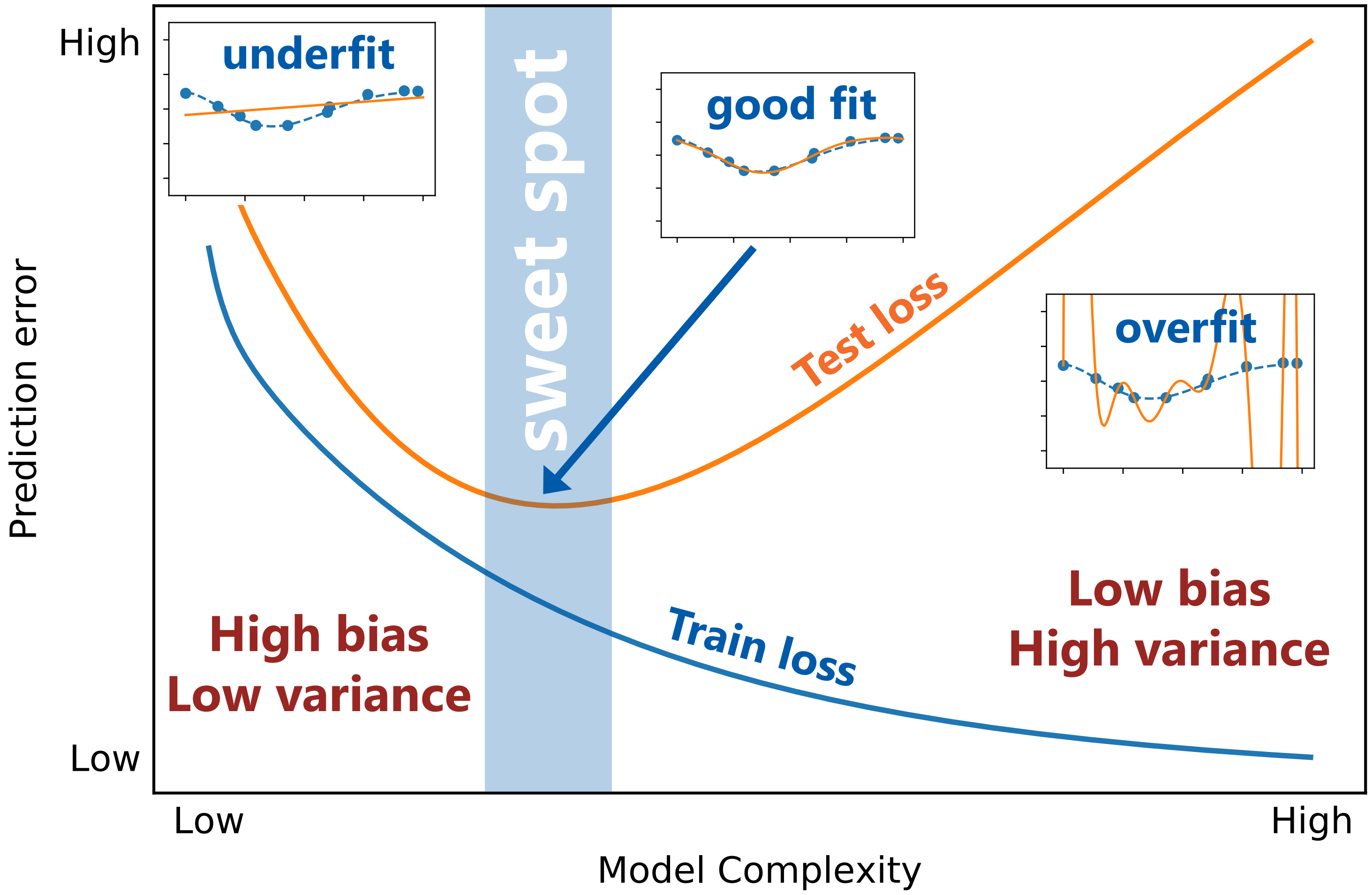
(easy to show that all the cross term expectations are 0)

$$= \mathop{\mathbb{E}}_{\tau}\left[\left(\hat{f}_\tau(x) - \mathop{\mathbb{E}}_{\tau'}[\hat{f}_{\tau'}(x)]\right)^2\right] + \left(\mathop{\mathbb{E}}_{\tau'}[\hat{f}_{\tau'}(x)] - f(x)\right)^2 + \mathop{\mathbb{E}}_{y|x}[(f(x) - y)^2]$$

Irreducible error

$(= \mathbb{E}[\varepsilon^2] = \sigma_\varepsilon^2)$

Bias-variance tradeoff



Typically there's a **tradeoff** between the two sources of error

Example: bias and variance of a linear model

Bias and variance error components can be calculated analytically for linear models

Simplification:

for each expectation term $\underset{\tau}{\mathbb{E}}$ let's consider **the features fixed**, i.e. $X_\tau \equiv X$ (the design matrix is constant), and only the **target vector y_τ is random**)

Example: bias and variance of a linear model

Bias and variance error components can be calculated analytically for linear models

Simplification:

for each expectation term $\underset{\tau}{\mathbb{E}}$ let's consider **the features fixed**, i.e. $X_\tau \equiv X$ (the design matrix is constant), and only the **target vector y_τ is random**)

Recall the solution for the linear regression model with the MSE loss:

$$\hat{f}_\tau(x) = \theta_\tau^{\mathrm{T}} x = x^{\mathrm{T}} \theta_\tau$$

$$\theta_\tau = \left(X^{\mathrm{T}} X\right)^{-1} X^{\mathrm{T}} y_\tau$$

Example: bias and variance of a linear model

Let's look at the **bias term** from the error decomposition:

$$\text{bias}(x) = \mathbb{E}_{\tau}\left[\widehat{f}_{\tau}(x)\right] - f(x)$$

Example: bias and variance of a linear model

Let's look at the **bias term** from the error decomposition:

$$\text{bias}(x) = \mathbb{E}_{\tau}\left[\hat{f}_{\tau}(x)\right] - f(x) = \mathbb{E}_{\tau}\left[x^{\mathrm{T}}\left(X^{\mathrm{T}}X\right)^{-1}X^{\mathrm{T}}y_{\tau}\right] - x^{\mathrm{T}}\theta_{\text{true}}$$

We'll also assume that the **true dependence is linear** indeed

Example: bias and variance of a linear model

Let's look at the **bias term** from the error decomposition:

$$\mathrm{bias}(x) = \mathbb{E}_{\tau}\left[\widehat{f}_{\tau}(x)\right] - f(x) = \mathbb{E}_{\tau}\left[x^{\mathrm{T}}\left(X^{\mathrm{T}}X\right)^{-1}X^{\mathrm{T}}y_{\tau}\right] - x^{\mathrm{T}}\theta_{\mathrm{true}}$$

$$= x^{\mathrm{T}}\left(X^{\mathrm{T}}X\right)^{-1}X^{\mathrm{T}}\mathbb{E}_{\tau}[y_{\tau}] - x^{\mathrm{T}}\theta_{\mathrm{true}}$$

Example: bias and variance of a linear model

Let's look at the **bias term** from the error decomposition:

$$\text{bias}(x) = \mathop{\mathbb{E}}_{\tau}\left[\widehat{f}_{\tau}(x)\right] - f(x) = \mathop{\mathbb{E}}_{\tau}\left[x^{\mathrm{T}}\left(X^{\mathrm{T}}X\right)^{-1}X^{\mathrm{T}}y_{\tau}\right] - x^{\mathrm{T}}\theta_{\text{true}}$$

$$= x^{\mathrm{T}}\left(X^{\mathrm{T}}X\right)^{-1}X^{\mathrm{T}}\mathop{\mathbb{E}}_{\tau}[y_{\tau}] - x^{\mathrm{T}}\theta_{\text{true}}$$

$$= x^{\mathrm{T}}\left(X^{\mathrm{T}}X\right)^{-1}X^{\mathrm{T}}X\theta_{\text{true}} - x^{\mathrm{T}}\theta_{\text{true}}$$

Example: bias and variance of a linear model

Let's look at the **bias term** from the error decomposition:

$$\mathrm{bias}(x) = \mathbb{E}_{\tau}\left[\hat{f}_{\tau}(x)\right] - f(x) = \mathbb{E}_{\tau}\left[x^{\mathrm{T}}\left(X^{\mathrm{T}}X\right)^{-1}X^{\mathrm{T}}y_{\tau}\right] - x^{\mathrm{T}}\theta_{\mathrm{true}}$$

$$= x^{\mathrm{T}}\left(X^{\mathrm{T}}X\right)^{-1}X^{\mathrm{T}}\mathbb{E}_{\tau}[y_{\tau}] - x^{\mathrm{T}}\theta_{\mathrm{true}}$$

$$= x^{\mathrm{T}}\left(X^{\mathrm{T}}X\right)^{-1}X^{\mathrm{T}}X\theta_{\mathrm{true}} - x^{\mathrm{T}}\theta_{\mathrm{true}}$$

Example: bias and variance of a linear model

Let's look at the **bias term** from the error decomposition:

$$\mathrm{bias}(x) = \mathop{\mathbb{E}}_{\tau}\left[\widehat{f}_{\tau}(x)\right] - f(x) = \mathop{\mathbb{E}}_{\tau}\left[x^{\mathrm{T}}\left(X^{\mathrm{T}}X\right)^{-1}X^{\mathrm{T}}y_{\tau}\right] - x^{\mathrm{T}}\theta_{\mathrm{true}}$$

$$= x^{\mathrm{T}}\left(X^{\mathrm{T}}X\right)^{-1}X^{\mathrm{T}}\mathop{\mathbb{E}}_{\tau}[y_{\tau}] - x^{\mathrm{T}}\theta_{\mathrm{true}}$$

$$= x^{\mathrm{T}}\left(X^{\mathrm{T}}X\right)^{-1}X^{\mathrm{T}}X\theta_{\mathrm{true}} - x^{\mathrm{T}}\theta_{\mathrm{true}}$$

$$= x^{\mathrm{T}}\theta_{\mathrm{true}} - x^{\mathrm{T}}\theta_{\mathrm{true}} = 0$$

I.e. linear regression model is **unbiased**

as long as the true dependence is linear

Example: bias and variance of a linear model

Now let's look at the **variance term**:

$$\text{variance}(x) = \mathop{\mathbb{E}}_{\tau}\left[\left(\hat{f}_{\tau}(x) - \mathop{\mathbb{E}}_{\tau'}[\hat{f}_{\tau'}(x)]\right)^2\right]$$

It can then be shown that:

$$\text{variance}(x) = \sigma_{\varepsilon}^2 x^{\mathrm{T}}\left(X^{\mathrm{T}}X\right)^{-1}x$$

So the variance error component is a **quadratic form**, defined by the $\left(X^{\mathrm{T}}X\right)^{-1}$ matrix.

Example: bias and variance of a linear model

We can diagonalize $X^{\mathrm{T}}X$:

$$\text{variance}(x) = \sigma_\varepsilon^2 x^{\mathrm{T}}\left(X^{\mathrm{T}}X\right)^{-1}x = \sigma_\varepsilon^2 \tilde{x}^{\mathrm{T}}\Lambda^{-1}\tilde{x}$$

where $\Lambda = \mathrm{diag}\{\lambda_1, \ldots, \lambda_d\}$ is the matrix of eigenvalues of $X^{\mathrm{T}}X$.

Example: bias and variance of a linear model

We can diagonalize $X^{\mathrm{T}}X$:

$$\mathrm{variance}(x) = \sigma_\varepsilon^2 x^{\mathrm{T}}\left(X^{\mathrm{T}}X\right)^{-1}x = \sigma_\varepsilon^2 \tilde{x}^{\mathrm{T}}\Lambda^{-1}\tilde{x}$$

where $\Lambda = \mathrm{diag}\{\lambda_1, \dots, \lambda_d\}$ is the matrix of eigenvalues of $X^{\mathrm{T}}X$.

This means that **small eigenvalues amplify the model variance**.

Example: bias and variance of a linear model

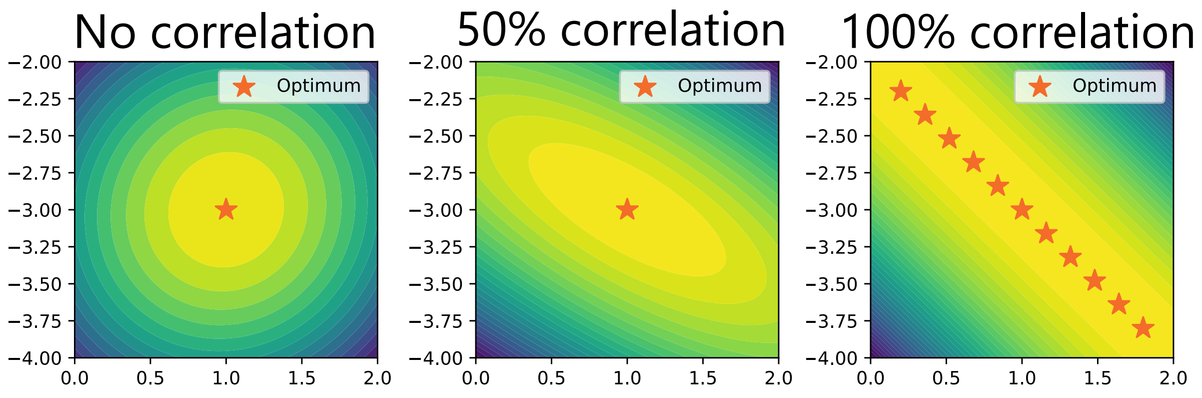
We can diagonalize $X^{\mathrm{T}}X$:

$$\text{variance}(x) = \sigma_\varepsilon^2 x^{\mathrm{T}}\left(X^{\mathrm{T}}X\right)^{-1}x = \sigma_\varepsilon^2 \tilde{x}^{\mathrm{T}}\Lambda^{-1}\tilde{x}$$

where $\Lambda = \mathrm{diag}\{\lambda_1, \dots, \lambda_d\}$ is the matrix of eigenvalues of $X^{\mathrm{T}}X$.

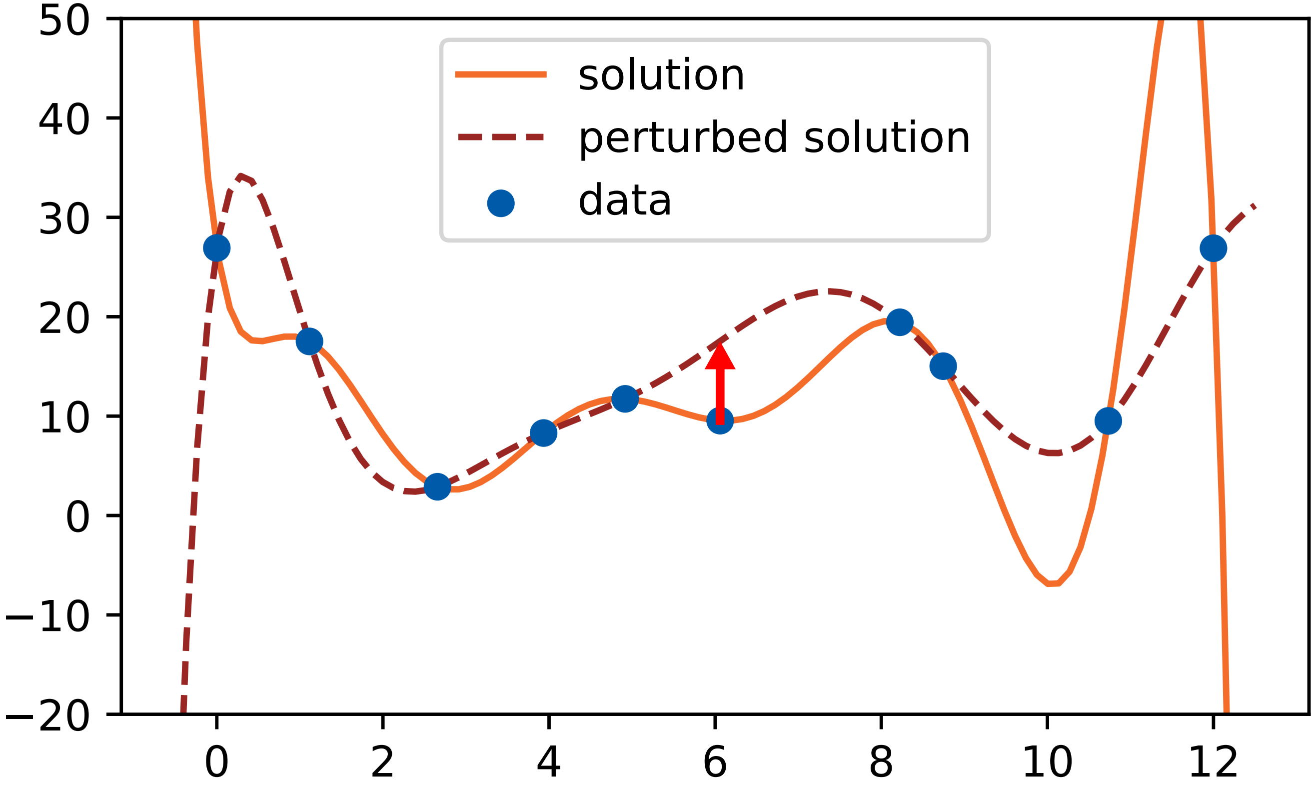
This means that **small eigenvalues amplify the model variance**.

This happens when $X^{\mathrm{T}}X$ is ill-defined e.g. when the features are correlated



MSE loss values
as a function
of model parameters

High-variance model



Small perturbation in data

⇩

Large change in prediction

Regularization

How can we reduce the variance?

If only we could **increase the eigenvalues** of $X^{\mathrm{T}}X$…

How can we reduce the variance?

If only we could **increase the eigenvalues** of $X^{\mathrm{T}}X$...

In fact, we can do this manually:

$$X^{\mathrm{T}}X \to X^{\mathrm{T}}X + \alpha I,$$
$$\alpha > 0 \in \mathbb{R},$$
$$I \text{ – unit } d \text{ by } d \text{ matrix}$$

How can we reduce the variance?

If only we could **increase the eigenvalues** of $X^{\mathrm{T}}X$...

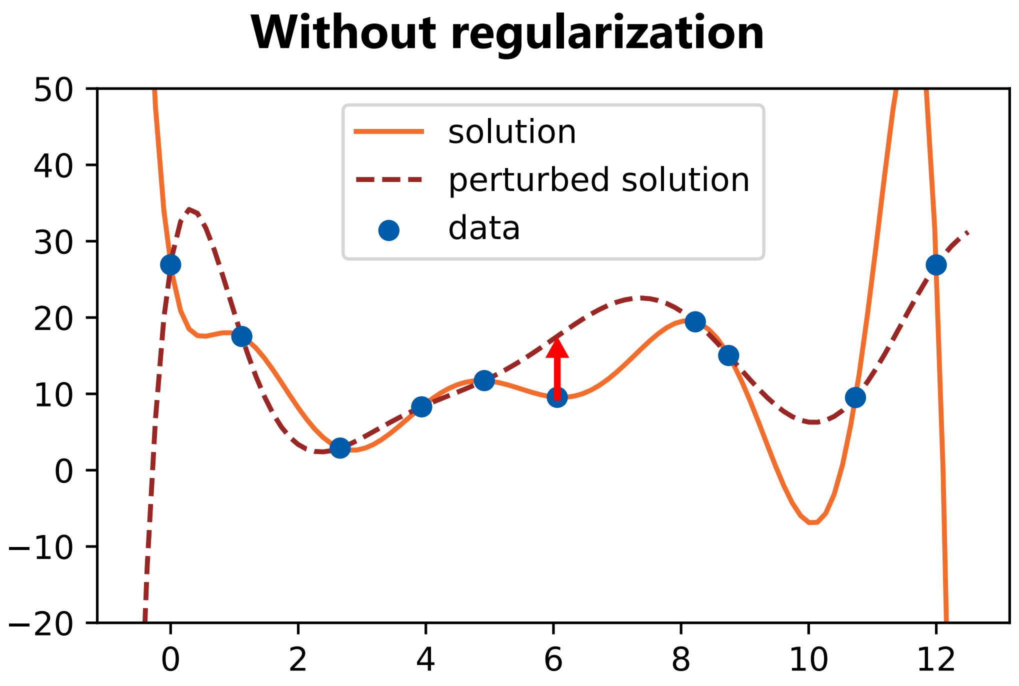
In fact, we can do this manually:

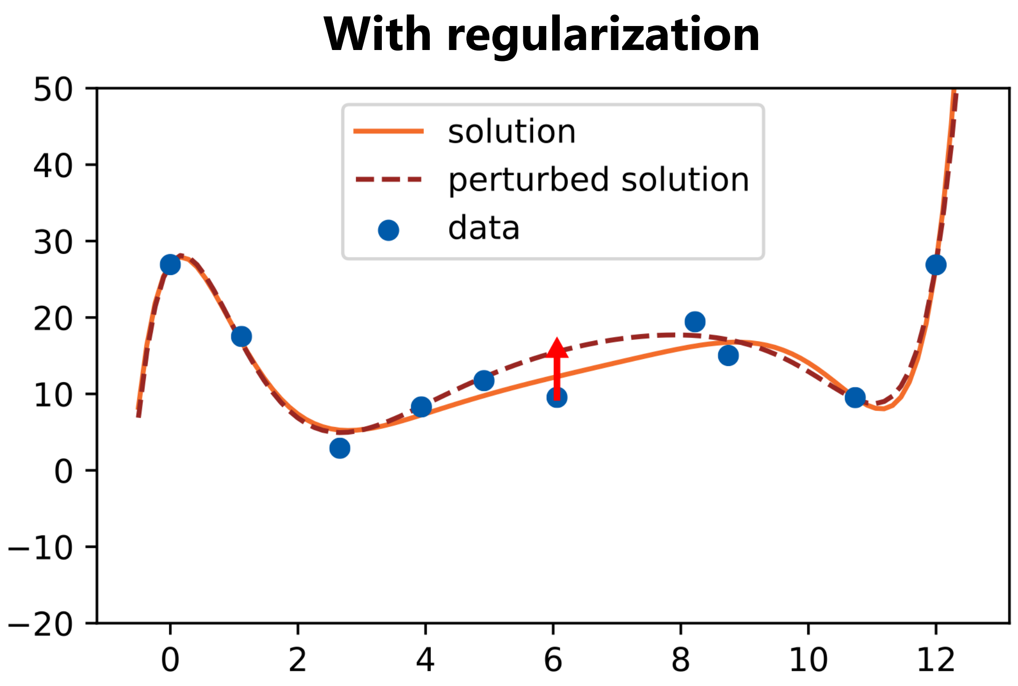
$$X^{\mathrm{T}}X \to X^{\mathrm{T}}X + \alpha I,$$
$$\alpha > 0 \in \mathbb{R},$$
$$I \text{ – unit } d \text{ by } d \text{ matrix}$$

I.e. we are **changing the solution** to:

$$\widehat{f}_\tau(x) = x^{\mathrm{T}}\left(X^{\mathrm{T}}X + \alpha I\right)^{-1} X^{\mathrm{T}} y_\tau$$

The effect of regularization





Note: the regularized model is **no longer unbiased**!

I.e. we **increased bias to reduce variance**

What problem did we solve?

We have the solution:

$$\widehat{f_\tau}(x) = x^{\mathrm{T}}\left(X^{\mathrm{T}}X + \alpha I\right)^{-1} X^{\mathrm{T}} y_\tau$$

Let's reverse engineer the loss function it optimizes:

What problem did we solve?

We have the solution:

$$\widehat{f}_\tau(x) = x^{\mathrm{T}}\left(X^{\mathrm{T}}X + \alpha I\right)^{-1}X^{\mathrm{T}}y_\tau$$

Let's reverse engineer the loss function it optimizes:

$$\theta_\tau = \left(X^{\mathrm{T}}X + \alpha I\right)^{-1}X^{\mathrm{T}}y_\tau$$

What problem did we solve?

We have the solution:

$$\widehat{f_\tau}(x) = x^{\mathrm{T}}\left(X^{\mathrm{T}}X + \alpha I\right)^{-1}X^{\mathrm{T}}y_\tau$$

Let's reverse engineer the loss function it optimizes:

$$\theta_\tau = \left(X^{\mathrm{T}}X + \alpha I\right)^{-1}X^{\mathrm{T}}y_\tau$$

$$\left(X^{\mathrm{T}}X + \alpha I\right)\theta_\tau = X^{\mathrm{T}}y_\tau$$

What problem did we solve?

We have the solution:

$$\widehat{f}_\tau(x) = x^{\mathrm{T}}\left(X^{\mathrm{T}}X + \alpha I\right)^{-1}X^{\mathrm{T}}y_\tau$$

Let's reverse engineer the loss function it optimizes:

$$\theta_\tau = \left(X^{\mathrm{T}}X + \alpha I\right)^{-1}X^{\mathrm{T}}y_\tau$$

$$\left(X^{\mathrm{T}}X + \alpha I\right)\theta_\tau = X^{\mathrm{T}}y_\tau$$

$$X^{\mathrm{T}}(X\theta_\tau - y_\tau) + \alpha\theta_\tau = 0$$

What problem did we solve?

We have the solution:

$$\widehat{f}_\tau(x) = x^{\mathrm{T}}\left(X^{\mathrm{T}}X + \alpha I\right)^{-1} X^{\mathrm{T}} y_\tau$$

Let's reverse engineer the loss function it optimizes:

$$\theta_\tau = \left(X^{\mathrm{T}}X + \alpha I\right)^{-1} X^{\mathrm{T}} y_\tau$$

$$\left(X^{\mathrm{T}}X + \alpha I\right)\theta_\tau = X^{\mathrm{T}} y_\tau$$

$$X^{\mathrm{T}}(X\theta_\tau - y_\tau) + \alpha\theta_\tau = 0$$

In fact this is the $\partial/\partial\theta_\tau \mathcal{L} = 0$ equation for:

$$\mathcal{L} = \|X\theta_\tau - y_\tau\|^2 + \alpha\|\theta_\tau\|^2$$

What problem did we solve?

$$\mathcal{L} = \|X\theta_\tau - y_\tau\|^2 + \alpha\|\theta_\tau\|^2$$

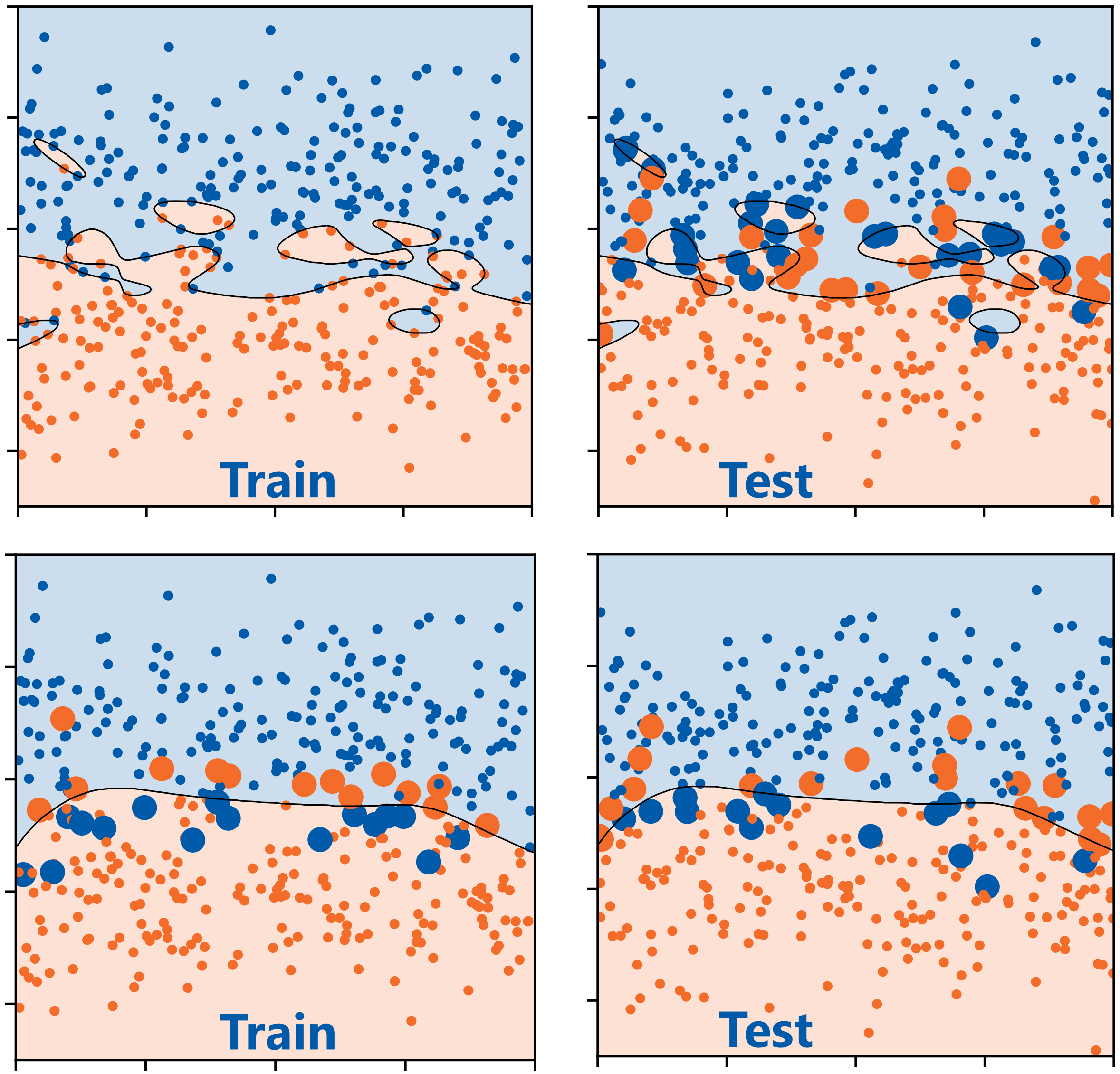
In other words, this linear model:

$$\widehat{f}_\tau(x) = x^{\mathrm{T}}\left(X^{\mathrm{T}}X + \alpha I\right)^{-1}X^{\mathrm{T}}y_\tau$$

minimizes **MSE loss** with **L2 penalty term** on the model parameters.

Such model is also called
ridge regression

Example: L2-regularized classification



Without regularization

With regularization

By regularizing the model we **increase the train loss** and **decrease the test loss**

This improves the **generalizability** of the model

Various regularization methods

L2 regularization (Ridge):

$$\mathcal{L} = \|X\theta_\tau - y_\tau\|^2 + \alpha\|\theta_\tau\|^2$$

L2 norm:

$$\|x\|^2 \equiv \sum_{i=1\ldots d} x_i^2$$

L1 regularization (Lasso):

$$\mathcal{L} = \|X\theta_\tau - y_\tau\|^2 + \alpha\|\theta_\tau\|_1$$

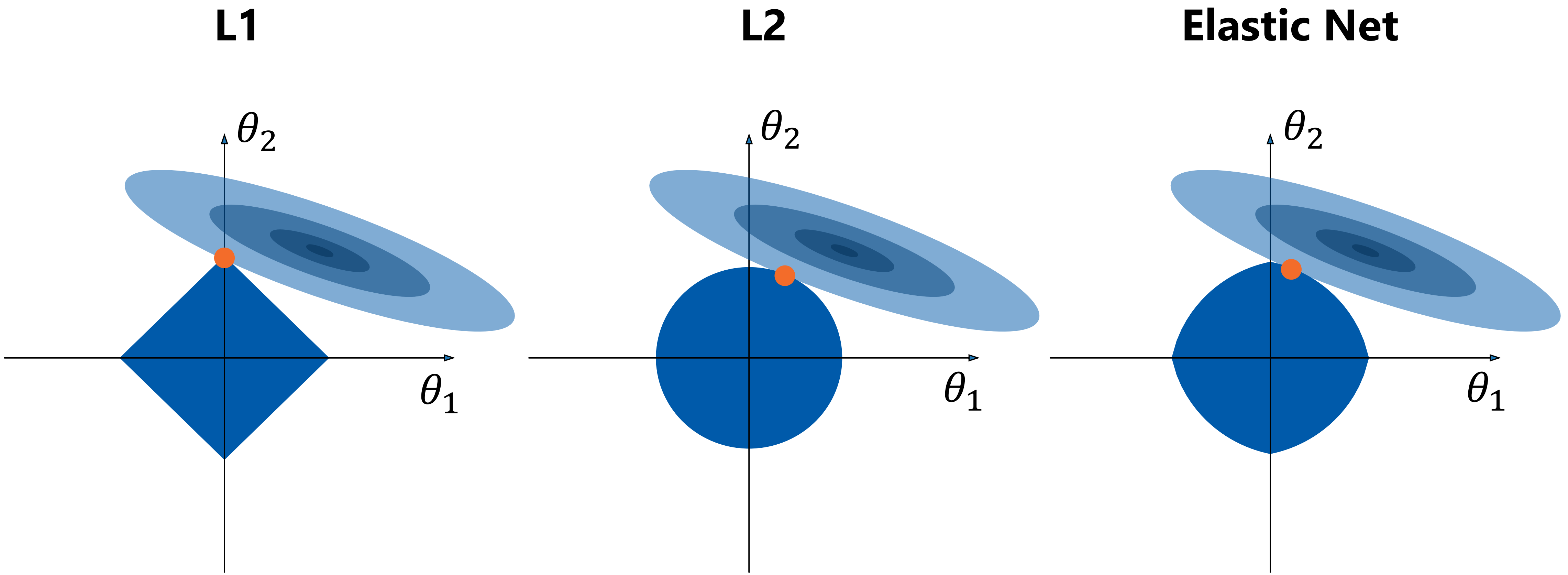
L1 norm:

$$\|x\|_1 \equiv \sum_{i=1\ldots d} |x_i|$$

Elastic net:

$$\mathcal{L} = \|X\theta_\tau - y_\tau\|^2 + \alpha\|\theta_\tau\|^2 + \beta\|\theta_\tau\|_1$$

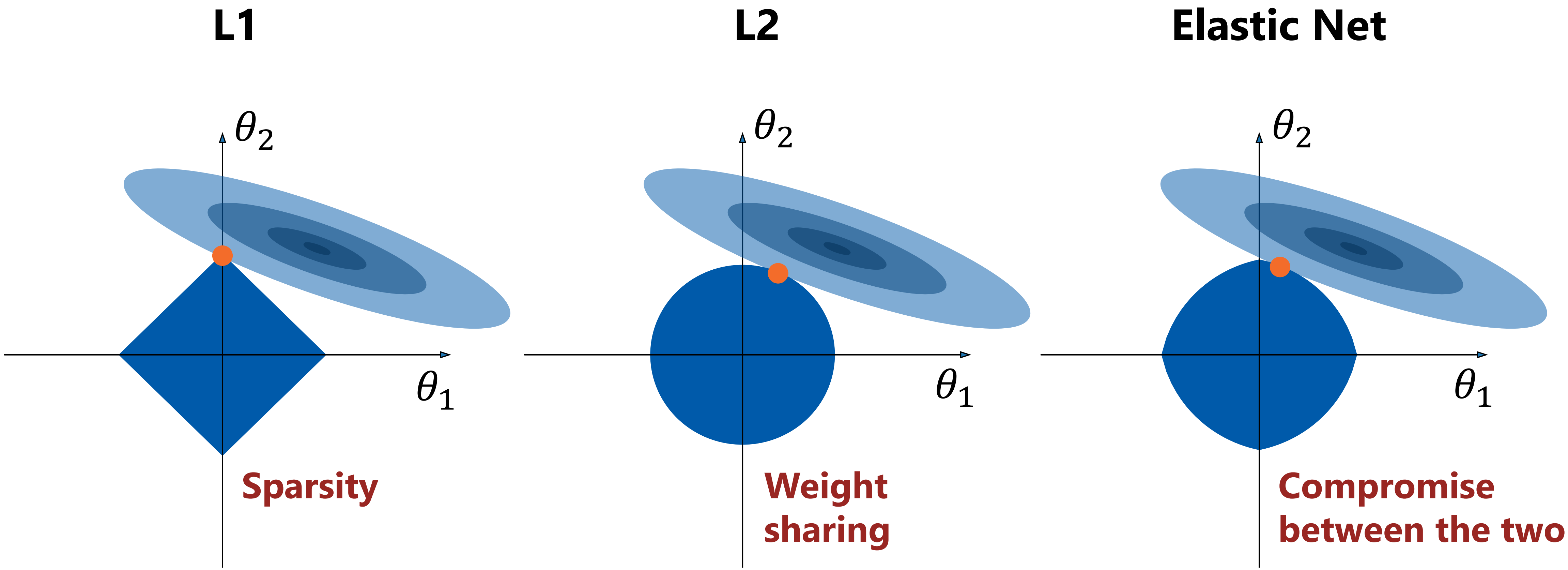
Properties of different regularization methods



They all drive the weights towards **smaller values**

Yet they **induce different properties** of the solution

Properties of different regularization methods



They all drive the weights towards **smaller values**

Yet they **induce different properties** of the solution

Summary

Prediction error can be decomposed into components corresponding to **model bias and variance**

Summary

Prediction error can be decomposed into components corresponding to **model bias and variance**

Linear regression is **unbiased**, while its variance is large when $X^{\mathrm{T}}X$ matrix is **ill-defined**

Summary

Prediction error can be decomposed into components corresponding to **model bias and variance**

Linear regression is **unbiased**, while its variance is large when $X^{\mathrm{T}}X$ matrix is **ill-defined**

Typically regularization reduces the variance with the price of **increasing the bias**

Summary

Prediction error can be decomposed into components corresponding to **model bias and variance**

Linear regression is **unbiased**, while its variance is large when $X^{\mathrm{T}}X$ matrix is **ill-defined**

Typically regularization reduces the variance with the price of **increasing the bias**

Different regularization techniques induce different properties of the solution

Thank you!

msohrabi@hse.ru

Majid Sohrabi