Model Regularization

Overfitting, Bias-variance decomposition, L1 and L2 regularization, probabilistic interpretation

Machine Learning and Data Mining, 2020

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LAMBDA • HSE

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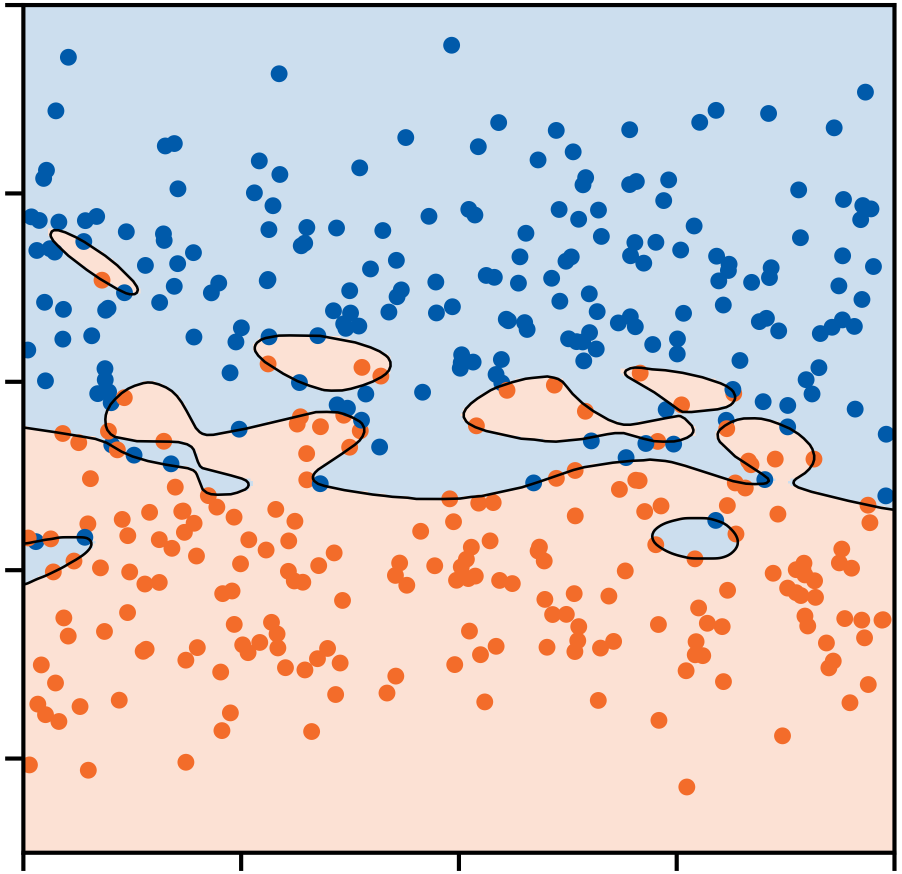
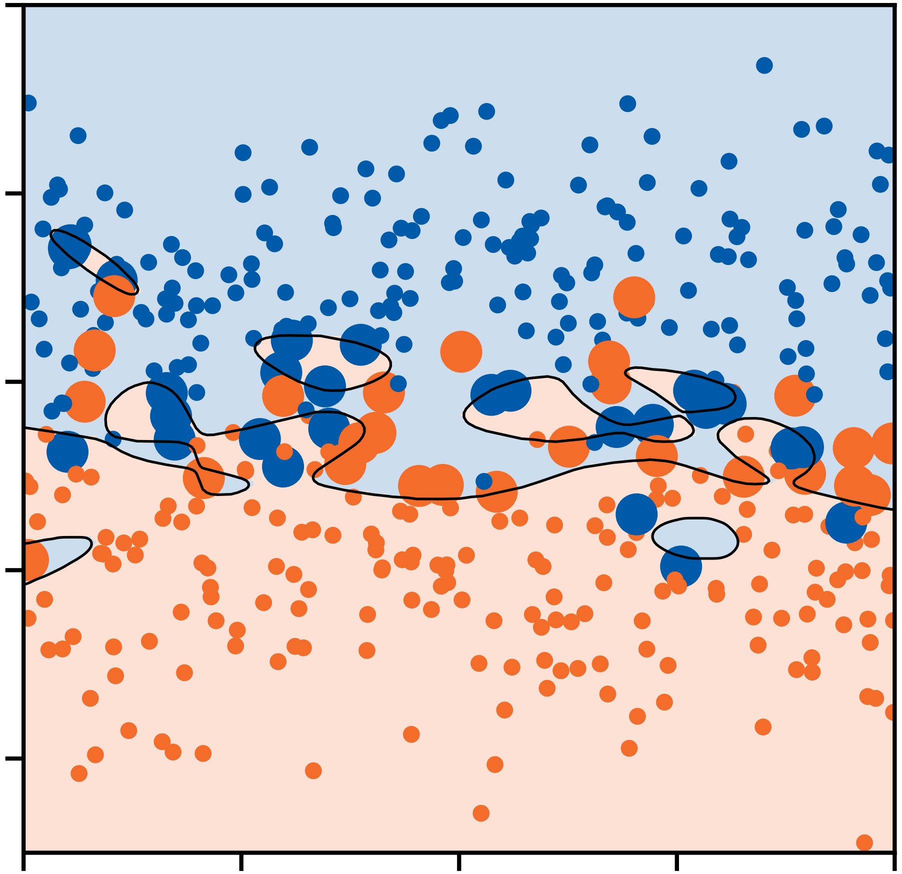
The problem of overfitting

Overfitting in classification



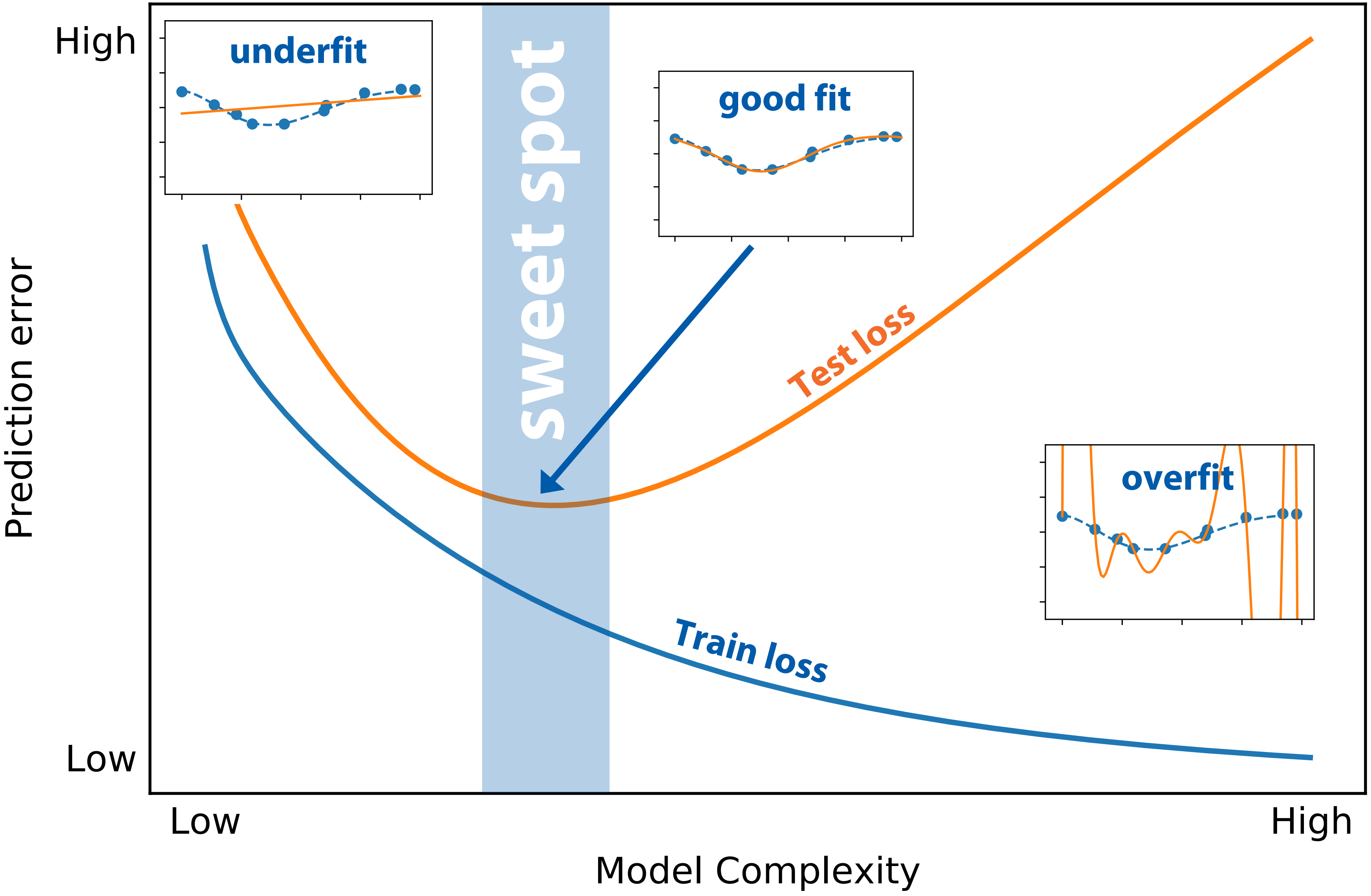
Training set



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:

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

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

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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:

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

Prediction error decomposition

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

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

Prediction error decomposition

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

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

Prediction of the "expected model"

Prediction error decomposition

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

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

Ground truth (without the noise)

Prediction error decomposition

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

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(grouping the terms, then expanding the square)

Prediction error decomposition

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

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

Variance of the model

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

Prediction error decomposition

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

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how much the “expected model” differs from the ground truth

Squared bias

Prediction error decomposition

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

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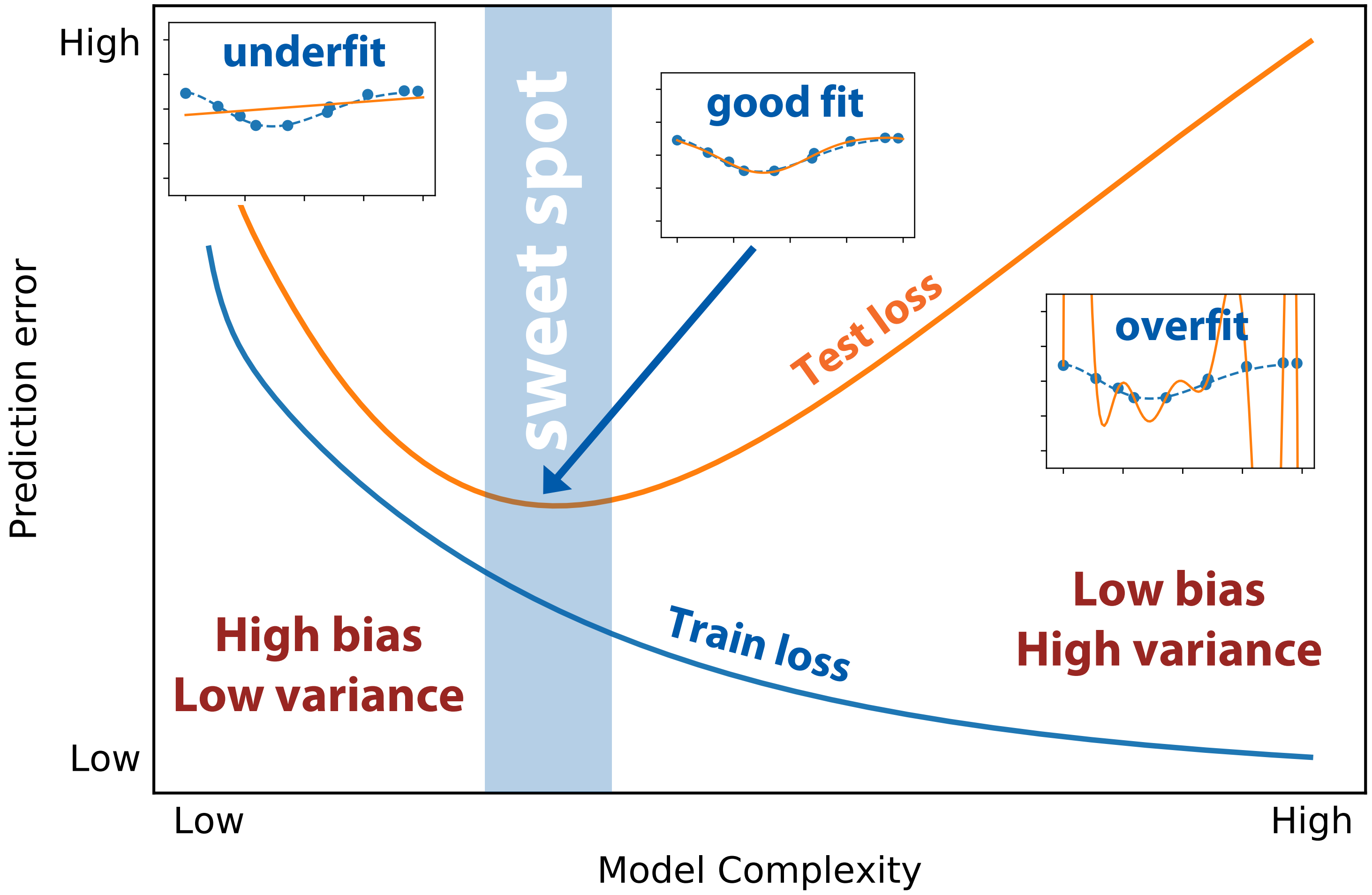
Irreducible error
$(= \mathbb{E}[\varepsilon^2] = \sigma_\varepsilon^2)$

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 $\mathop{\mathbb{E}}_{\tau}$ 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**)

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Simplification:

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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:

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

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

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

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

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.

[derivation]

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

Note that $\widehat{f}_\tau(x)$ can be thought of as a **linear transformation** to the training targets vector y_τ:

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

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

[derivation]

$$\text{variance}(x) = \mathop{\mathbb{E}}_{\tau}\left[\left(h^{\mathrm{T}}(x)y_\tau - \mathop{\mathbb{E}}_{\tau'}[h^{\mathrm{T}}(x)y_{\tau'}]\right)^2\right] = \mathop{\mathbb{E}}_{\tau}\left[\left(h^{\mathrm{T}}(x)\left(y_\tau - \mathop{\mathbb{E}}_{\tau'}[y_{\tau'}]\right)\right)^2\right]$$

$$= \mathop{\mathbb{E}}_{\tau}\left[h^{\mathrm{T}}(x)\left(y_\tau - \mathop{\mathbb{E}}_{\tau'}[y_{\tau'}]\right)\left(y_\tau - \mathop{\mathbb{E}}_{\tau'}[y_{\tau'}]\right)^{\mathrm{T}} h(x)\right]$$

$$= h^{\mathrm{T}}(x)\mathop{\mathbb{E}}_{\tau}\left[\left(y_\tau - \mathop{\mathbb{E}}_{\tau'}[y_{\tau'}]\right)\left(y_\tau - \mathop{\mathbb{E}}_{\tau'}[y_{\tau'}]\right)^{\mathrm{T}}\right] h(x)$$

$$= h^{\mathrm{T}}(x)\mathop{\mathrm{cov}}_{\tau}[y_\tau, y_\tau]\, h(x) = \sigma_\varepsilon^2 h^{\mathrm{T}}(x)h(x)$$

[derivation]

$$\text{variance}(x) = \sigma_\varepsilon^2 h^\mathrm{T}(x) h(x)$$

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

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

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

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

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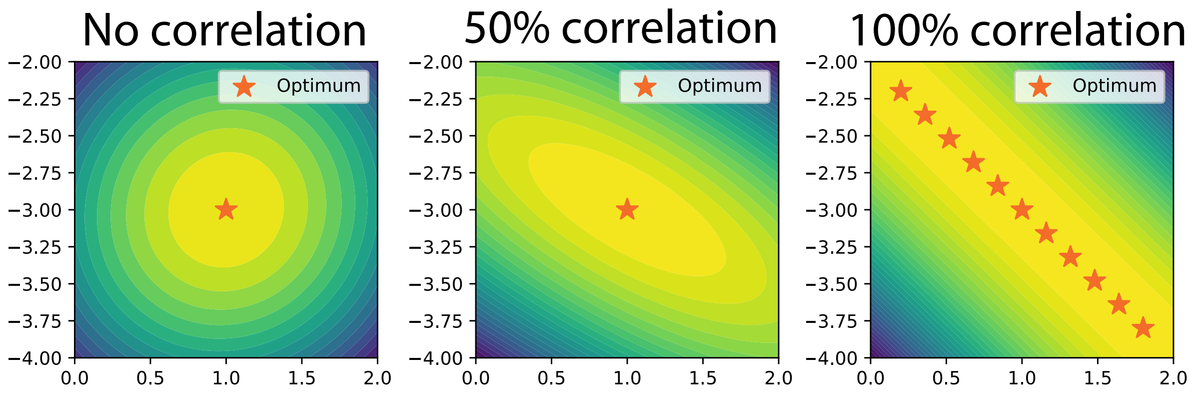
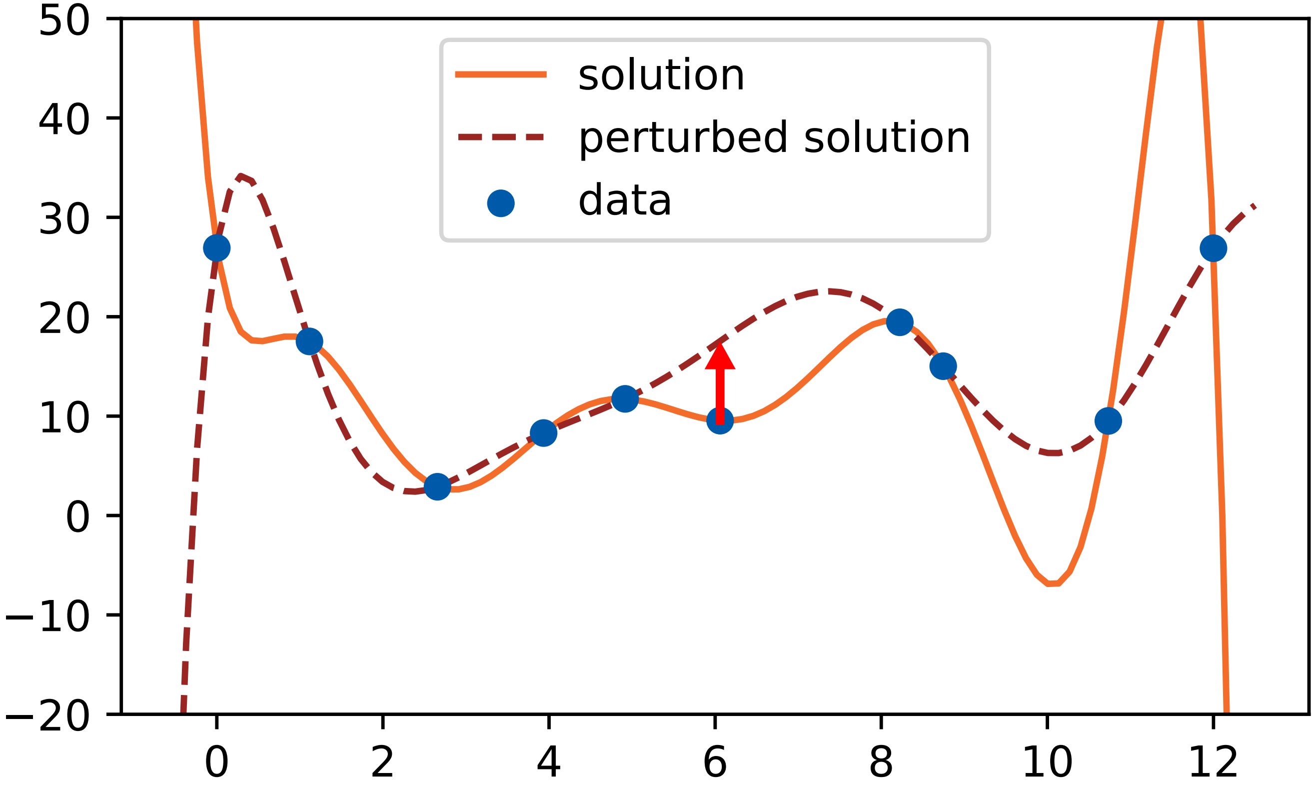
This happens when $X^{\mathrm{T}}X$ is ill-defined e.g. when the features are correlated



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 $X^{\mathrm{T}}X\ldots$

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In fact, we can do this manually:

$$X^{\mathrm{T}}X \to X^{\mathrm{T}}X + \alpha I,$$

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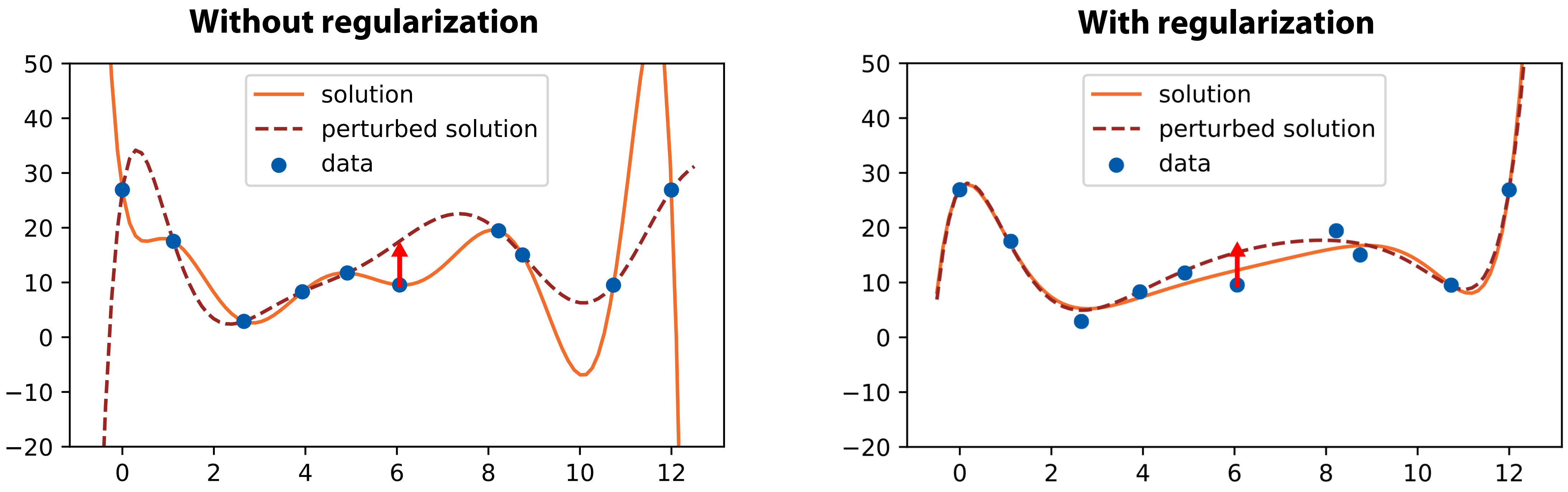
I.e. we are **changing the solution** to:

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

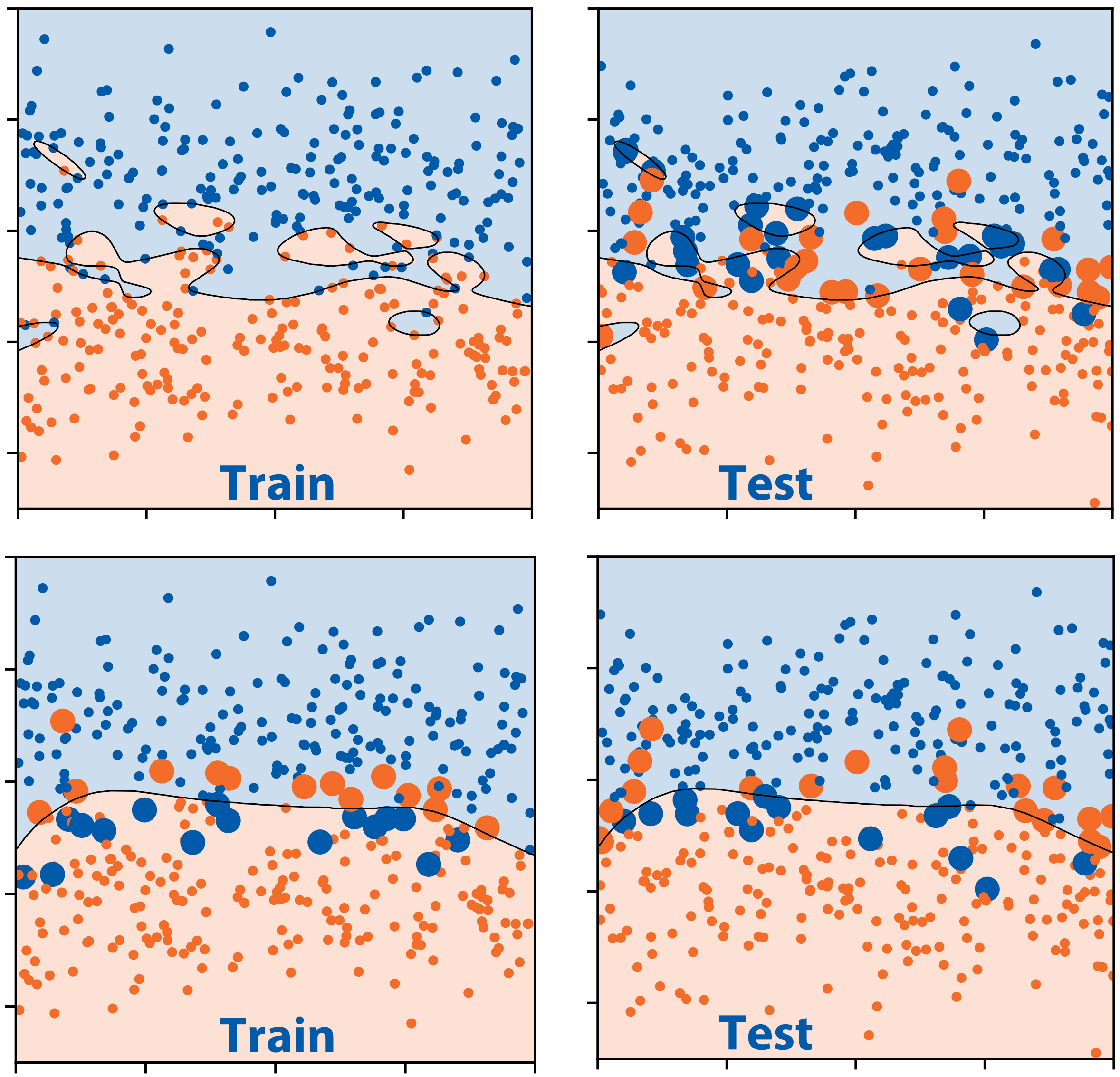
The effect of regularization



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

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

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

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:

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

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:

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

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

Such model is also called
ridge regression

Various regularization methods

L2 regularization (Ridge):

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

L2 norm:

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

L1 regularization (Lasso):

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

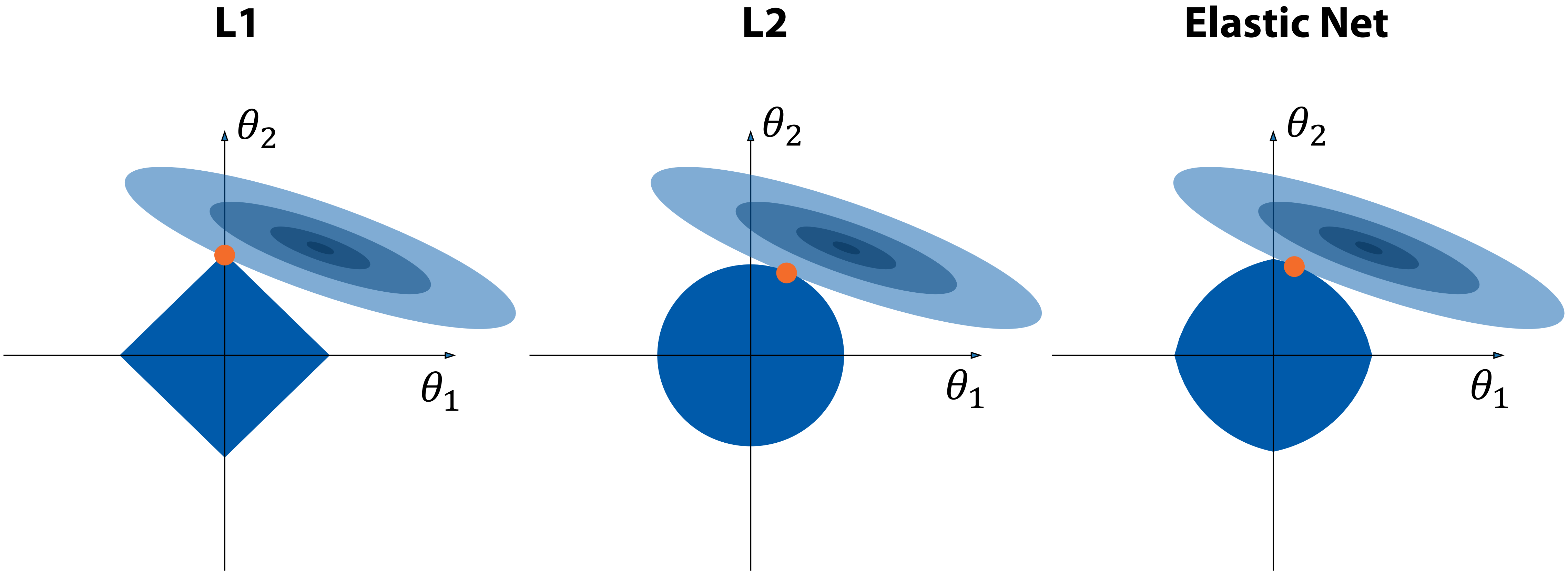
L1 norm:

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

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

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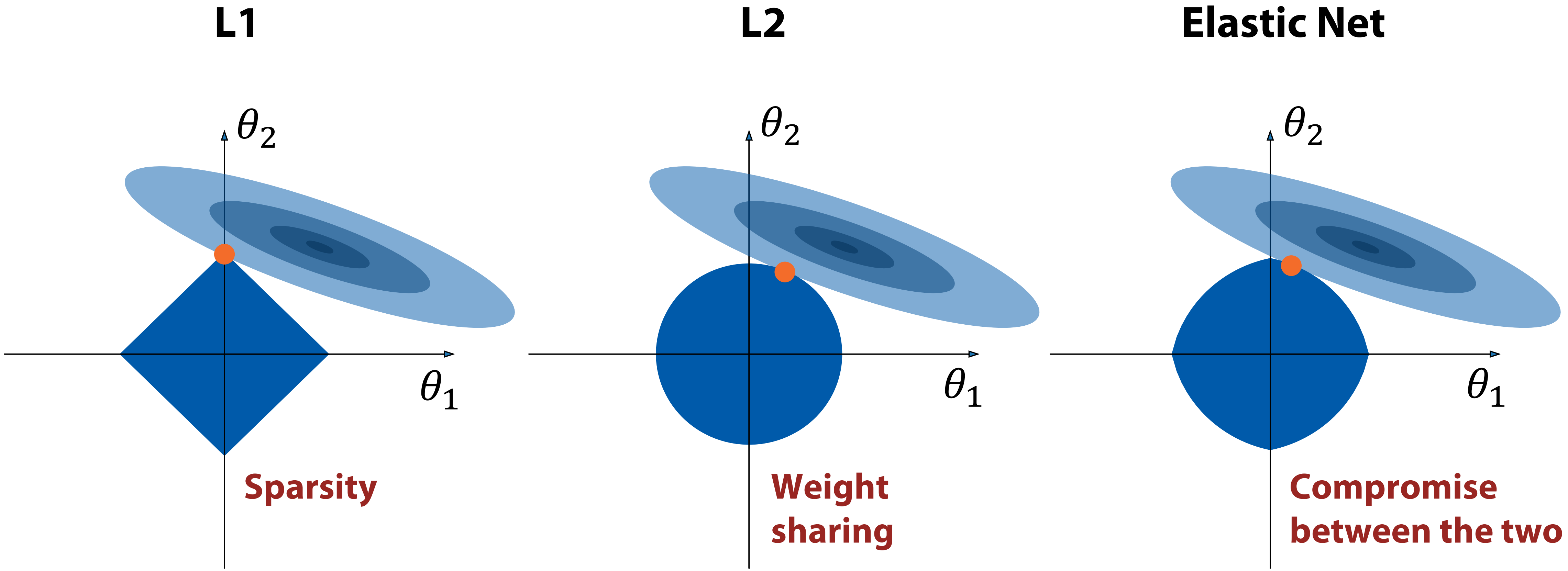

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Probabilistic view

Probabilistic model

Let's revisit our assumption about data:

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

Now we'll assume that **label noise** is **normally distributed:**

$$\varepsilon \sim \mathcal{N}(0, \sigma_\varepsilon^2)$$

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We want our model $\widehat{f}_\theta(x)$ to fit the true dependence $f(x)$, i.e. we **define a probabilistic model**:

$$y|x \sim \mathcal{N}\left(\widehat{f}_\theta(x), \sigma_\varepsilon^2\right)$$

Probabilistic model

Our model can be fitted with the **maximum likelihood** approach:

$$L = \prod_{i=1\ldots N} \mathcal{N}\left(y_i \middle| \widehat{f_\theta}(x_i), \sigma_\varepsilon^2\right) \to \max_\theta$$

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Max. likelihood = min. negative log likelihood

$$-\log L = -\sum_{i=1\ldots N} \log \mathcal{N}\left(y_i \middle| \widehat{f_\theta}(x_i), \sigma_\varepsilon^2\right)$$

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$$= -\sum_{i=1\ldots N} \left[\log \exp\left(-\frac{\left(y_i - \hat{f}_\theta(x_i)\right)^2}{2\sigma_\varepsilon^2}\right) - \log\sqrt{2\pi\sigma_\varepsilon^2}\right]$$

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$$= C \cdot \sum_{i=1\ldots N} \left(y_i - \hat{f}_\theta(x_i)\right)^2 + const$$

Probabilistic model

Our model can be fitted with the **maximum likelihood** approach:

$$L = \prod_{i=1\ldots N} \mathcal{N}\left(y_i \middle| \widehat{f_\theta}(x_i), \sigma_\varepsilon^2\right) \to \max_\theta$$

Max. likelihood = min. negative log likelihood

$$-\log L = -\sum_{i=1\ldots N} \log \mathcal{N}\left(y_i \middle| \widehat{f_\theta}(x_i), \sigma_\varepsilon^2\right)$$

$$= -\sum_{i=1\ldots N} \left[\log \exp\left(-\frac{\left(y_i - \widehat{f_\theta}(x_i)\right)^2}{2\sigma_\varepsilon^2}\right) - \log\sqrt{2\pi\sigma_\varepsilon^2}\right]$$

MSE loss ⟺ Prob. model with normal label noise!

$$= C \cdot \sum_{i=1\ldots N} \left(y_i - \widehat{f_\theta}(x_i)\right)^2 + const$$

Bayessian view

We are going to treat both data (X, y) and model parameters (θ) as random variables

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$$p(\theta|X, y) = \frac{p(y|\theta, X) \cdot p(\theta)}{\int [p(y|\theta, X) \cdot p(\theta)] d\theta}$$

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(Reminder) Bayes rule:

Our prior knowledge
about the model
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Likelihood function

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Posterior knowledge
about the model after
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"Evidence" (probability of observing this data when the parameter uncertainty is integrated out)

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(Reminder) Bayes rule:

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We'll make a point estimate (maximum a posteriori):

$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}}\, p(\theta|X, y) = \underset{\theta}{\operatorname{argmax}}\, p(y|\theta, X) \cdot p(\theta)$$

Maximum a posteriori

Maximum a posteriori estimate:

$$\hat{\theta} = \underset{\theta}{\operatorname{argmax}}\, p(y|\theta, X) \cdot p(\theta) = \underset{\theta}{\operatorname{argmin}} [- \log p(y|\theta, X) - \log p(\theta)]$$

Neg. log likelihood

Regularizer

Example

Suppose we model the data with a normal distribution:

$$y|x \sim \mathcal{N}\left(\widehat{f}_\theta(x), \sigma_\varepsilon^2\right)$$

And the prior is normal as well:

$$\theta \sim \mathcal{N}\left(0, \sigma_\theta^2 I\right)$$

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Normal prior ⟺ L2 regularization

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- Food for thought: what probabilistic model would correspond to minimizing MAE loss?

Thank you!

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