Lecture 5. Regularisation & Bias-variance Trade-off

COMP90051 Statistical Machine Learning

Lecturer: Jean Honorio

This lecture

- How irrelevant features make optimisation ill-posed
- Regularising linear regression
  - Ridge regression
  - The lasso
  - Connections to Bayesian MAP
- Regularising non-linear regression
- Bias-variance

Regularisation

Process of introducing additional information in order to solve an ill-posed problem or to prevent overfitting

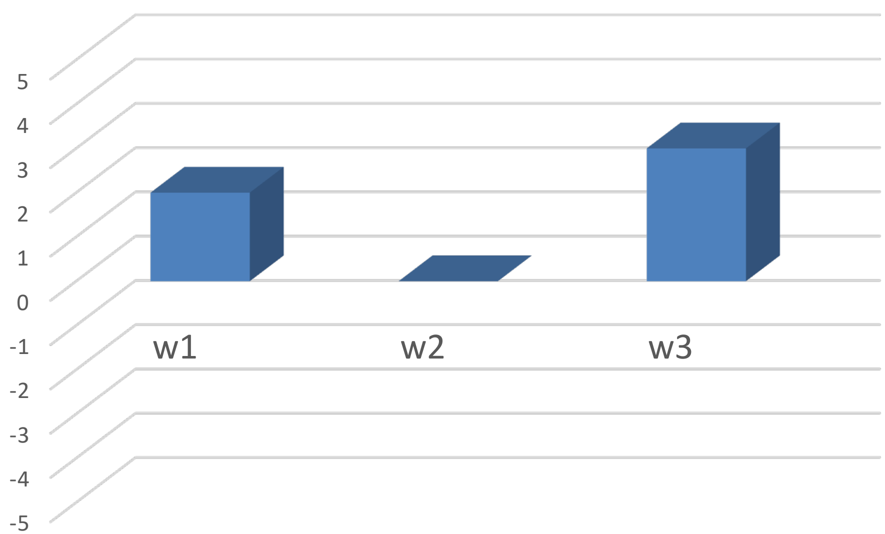
- Major technique & theme, throughout ML
- Addresses one or more of the following related problems
  - Avoids ill-conditioning (a computational problem)
  - Avoids overfitting (a statistical problem)
  - Introduce prior knowledge into modelling
- This is achieved by augmenting the objective function
- In this lecture: we cover the first two aspects. We will cover more of regularisation throughout the subject

The Problem with Irrelevant Features

Linear regression on rank-deficient data.

Example 1: Feature importance

- Linear model on three features
  - $\mathbf{X}$ is matrix on $n = 4$ instances (rows)
  - Model: $y = w_1x_1 + w_2x_2 + w_3x_3 + w_0$

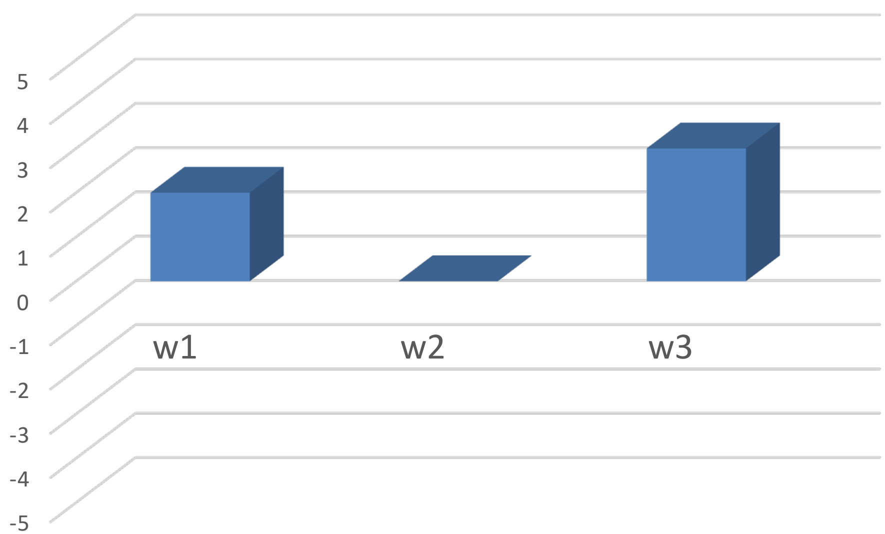


Question: Which feature is more important?

Example 1: Irrelevant features

- Linear model on three features, first two same
  - $\mathbf{X}$ is matrix on $n = 4$ instances (rows)
  - Model: $y = w_1x_1 + w_2x_2 + w_3x_3 + w_0$
  - First two columns of $\boldsymbol{X}$ identical
  - Feature 2 (or 1) is **irrelevant**

3	3	7
6	6	9
21	21	79
34	34	2



- Effect of perturbations on model predictions?
  - Add Δ to w_1
  - Subtract Δ from w_2

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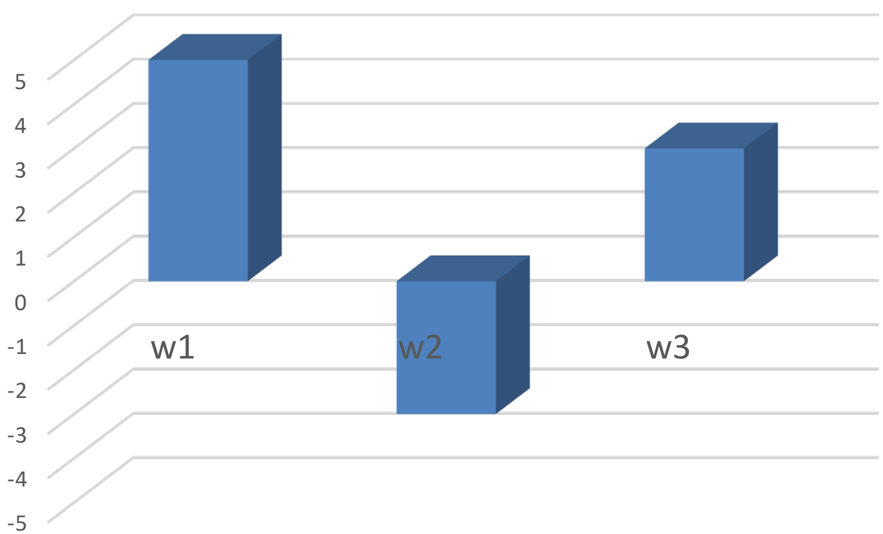

- Effect of perturbations on model predictions?
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Problems with irrelevant features

- In example, suppose $[\hat{w}_0, \hat{w}_1, \hat{w}_2, \hat{w}_3]'$ is "optimal"
- For any δ new $[\hat{w}_0, \hat{w}_1 + \delta, \hat{w}_2 - \delta, \hat{w}_3]'$ get
  - *Same* predictions!
  - *Same* sum of squared errors!
- Problems this highlights
  - The solution is not unique
  - Lack of interpretability
  - Optimising to learn parameters is ill-posed problem

Irrelevant (co-linear) features in general

- Extreme case: features complete clones
- For linear models, more generally
  - Feature $\mathbf{X}_{\cdot j}$ is irrelevant if
  - $\mathbf{X}_{\cdot j}$ is a linear combination of other columns

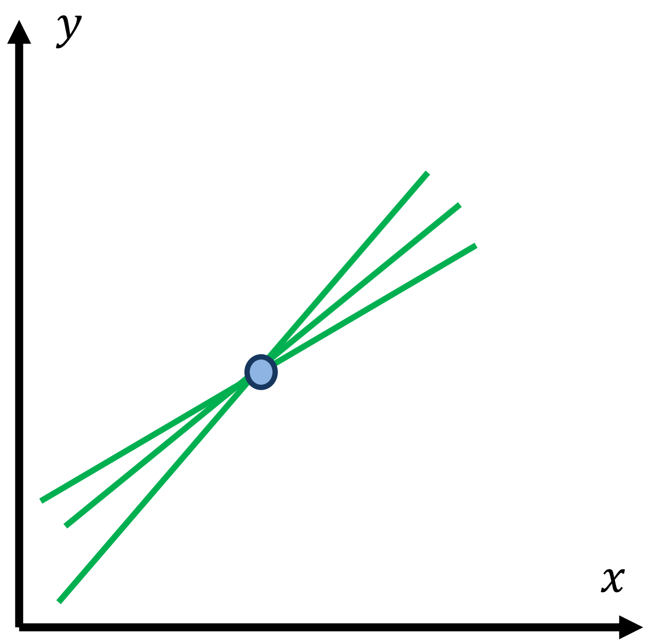
$$\mathbf{X}_{\cdot j} = \sum_{l \neq j} \alpha_l \mathbf{X}_{\cdot l}$$

  … for some scalars α_l. Also called multicollinearity
  - Equivalently: Some eigenvalue of $\mathbf{X}'\mathbf{X}$ is zero
- Even *near*-irrelevance/colinearity can be problematic
  - V small eigenvalues of $\mathbf{X}'\mathbf{X}$
- Not just a pathological extreme; *easy to happen!*

$\mathbf{X}_{\cdot j}$ denotes the j-th column of X

Example 2: Lack of data

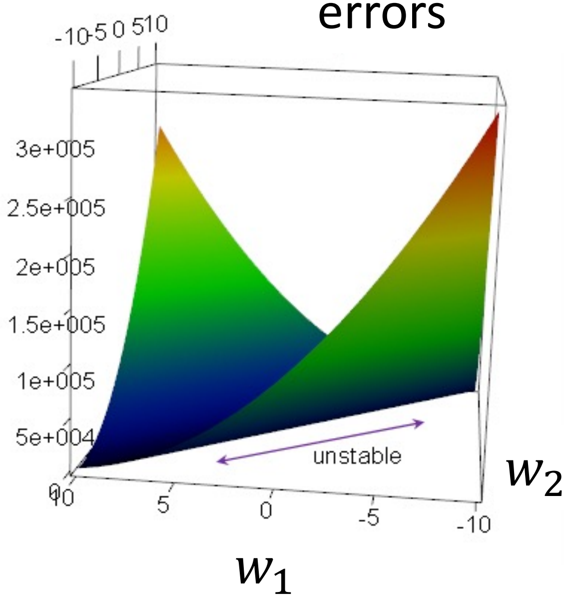
- Extreme example:
  - Model has two parameters (slope and intercept)
  - Only one data point
- Underdetermined system



Ill-posed problems

- In both examples, finding the best parameters becomes an ill-posed problem
- This means that the problem solution is not defined
  - In our case w_1 and w_2 cannot be uniquely identified
- Remember normal equations solution of linear regression: $\hat{\boldsymbol{w}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$
- With irrelevant/multicolinear features, matrix $\mathbf{X}'\mathbf{X}$ has no inverse

sum of squared errors



convex, but not strictly convex

Mini Summary

- Irrelevant features as collinearity
- Leads to
  * Ill-posed optimisation for linear regression
  * Broken interpretability
- Multiple intuitions: algebraic, geometric

- Next: Regularisation to the rescue!

Regularisation in Linear Models

Ridge regression and the Lasso

Re-conditioning the problem

- Regularisation: introduce an additional condition into the system
- The original problem is to minimise $\|\mathbf{y}-\mathbf{X}\mathbf{w}\|_2^2$
- The regularised problem is to minimise

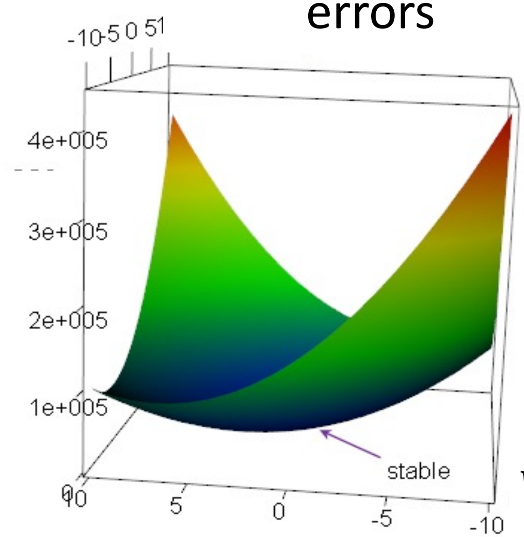
$$\|\mathbf{y}-\mathbf{X}\mathbf{w}\|_2^2 + \lambda\|\mathbf{w}\|_2^2 \text{ for } \lambda > 0$$

- The solution is now

$$\hat{\mathbf{w}} = \left(\mathbf{X}'\mathbf{X} + \lambda\mathbf{I}\right)^{-1}\mathbf{X}'\mathbf{y}$$

- This formulation is called ridge regression
  - Turns the ridge into a deep, singular valley
  - Adds λ to eigenvalues of $\mathbf{X}'\mathbf{X}$: makes invertible

sum of squared errors



w_2

w_1

strictly convex

Regulariser as a prior

- Without regularisation, parameters found based entirely on the information contained in the training set $\mathbf{X}$
  - Regularisation introduces additional information
- Recall our probabilistic model $Y = \mathbf{x}'\mathbf{w} + \varepsilon$
  - Here Y and ε are random variables, where ε denotes noise
- Now suppose that $\mathbf{w}$ is also a random variable (denoted as $\mathbf{W}$) with a Normal prior distribution

$$\mathbf{W} \sim \mathcal{N}\left(\mathbf{0}, \frac{1}{\lambda}\mathbf{I}\right) \quad \text{or equivalently} \quad W_i \sim \mathcal{N}\left(0, \frac{1}{\lambda}\right)$$

  - I.e. we expect small weights and that no one feature dominates
  - Is this always appropriate? E.g. data centring and scaling
  - We could encode much more elaborate problem knowledge

Computing posterior using Bayes rule

- The prior is then used to compute the posterior

posterior

likelihood

prior

$$p(\mathbf{w}|\mathbf{X},\mathbf{y}) = \frac{p(\mathbf{y}|\mathbf{X},\mathbf{w})p(\mathbf{w})}{p(\mathbf{y}|\mathbf{X})}$$

marginal likelihood

- Instead of maximum likelihood (MLE), take ***maximum a posteriori*** estimate (MAP)

- Apply log trick, so that

$$\log(posterior) = \log(likelihood) + \log(prior) - \cancel{\log(marg)}$$

this term doesn't affect optimisation

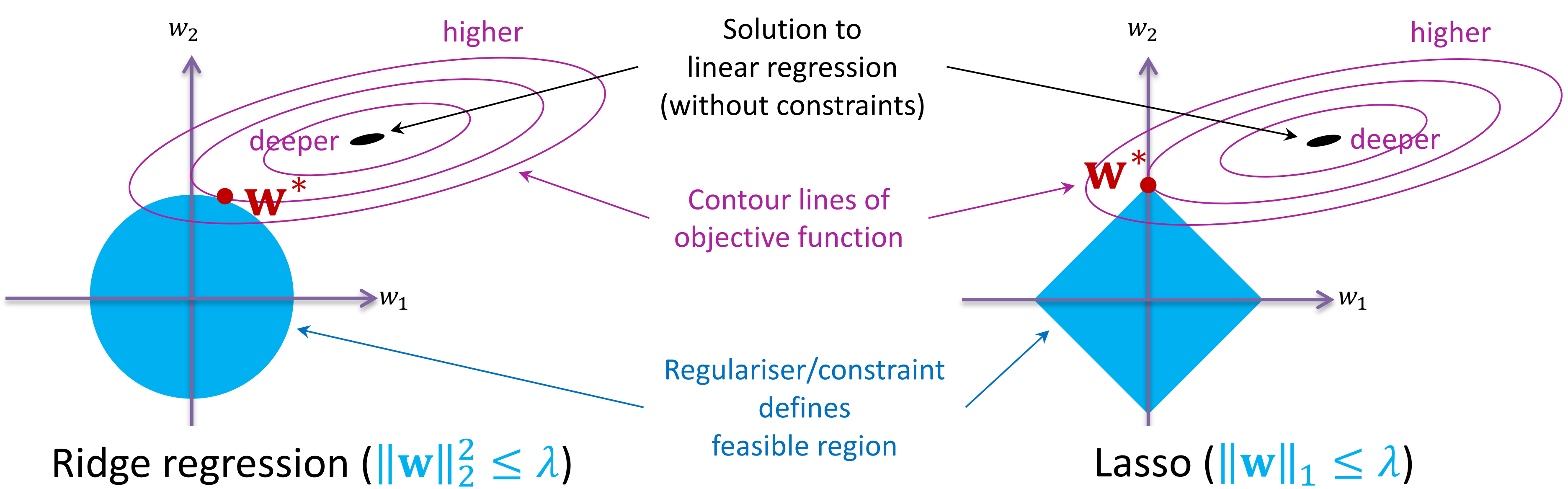
- Arrive at the problem of minimising

$$\|\mathbf{y} - \mathbf{Xw}\|_2^2 + \lambda\|\mathbf{w}\|_2^2$$

Regulariser as a constraint

- For illustrative purposes, consider a *modified problem*:

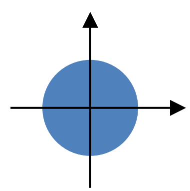
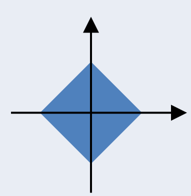
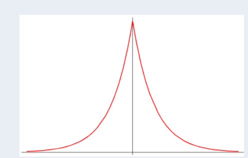
  minimise $\|\mathbf{y}-\mathbf{X}\mathbf{w}\|_2^2$ *subject to* $\|\mathbf{w}\|_2^2 \leq \lambda$ for $\lambda > 0$



- Lasso (L_1 regularisation) encourages solutions to sit on the axes

  → Some of the weights are set to zero → Solution is sparse

Regularised linear regression

Algorithm	Minimises	Regulariser	Solution	Prior
Linear regression	$\|\mathbf{y}-\mathbf{X}\mathbf{w}\|_2^2$	None	$(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{y}$ (if inverse exists)	None
Ridge regression	$\|\mathbf{y}-\mathbf{X}\mathbf{w}\|_2^2 + \lambda\|\mathbf{w}\|_2^2$	L_2 norm 	$(\mathbf{X}'\mathbf{X}+\lambda\mathbf{I})^{-1}\mathbf{X}'\mathbf{y}$	Gaussian prior $e^{-\lambda\|\mathbf{w}\|_2^2}$ 
Lasso	$\|\mathbf{y}-\mathbf{X}\mathbf{w}\|_2^2 + \lambda\|\mathbf{w}\|_1$	L_1 norm 	No closed-form, but solutions are sparse and suitable for high-dimensional data	Laplacian prior $e^{-\lambda\|\mathbf{w}\|_1}$ 

Mini Summary

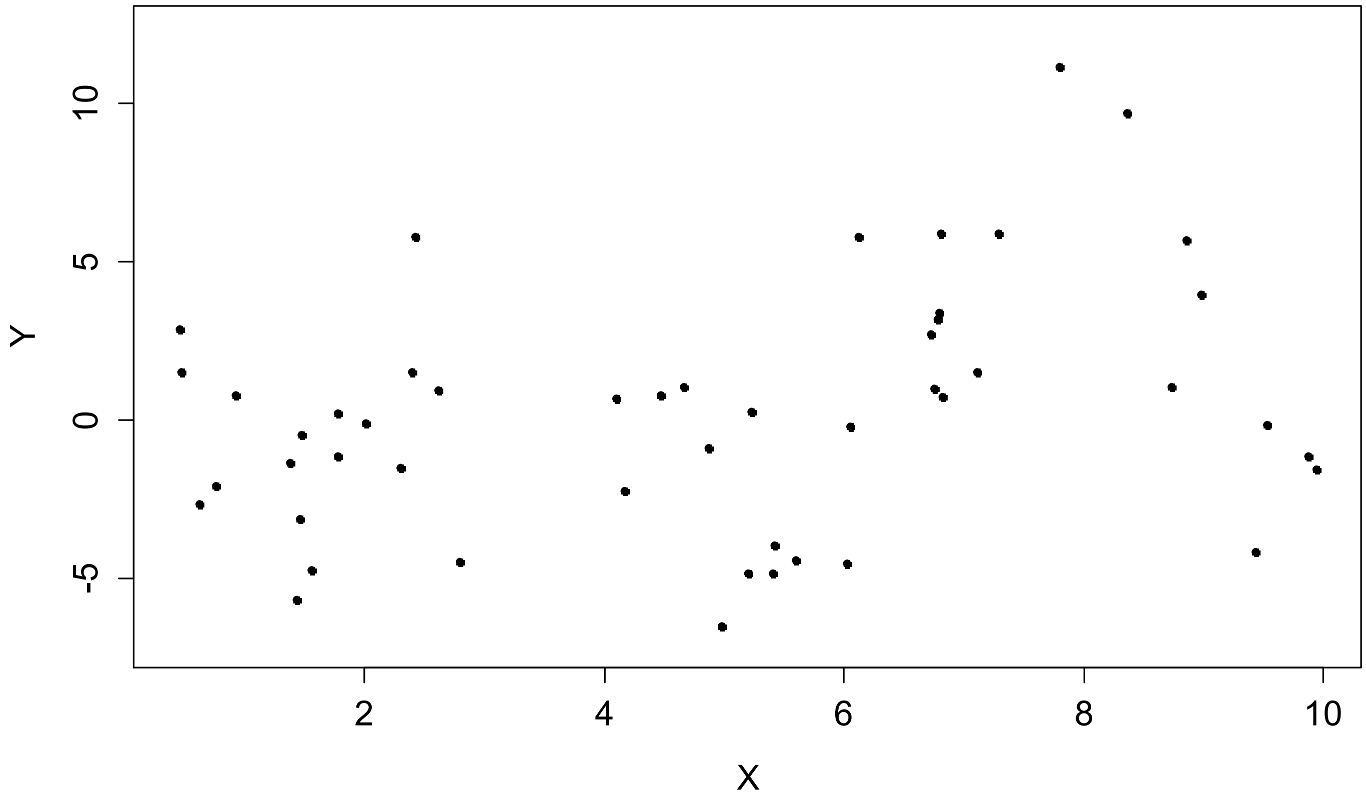
- L_2 regularisation: Ridge regression
  - Re-conditions the optimisation
  - Equivalent to MAP with Gaussian prior on weights
- L_1 regularisation: The Lasso
  - Particularly favoured in high-dimensional, low-example regimes

- Next: Regularisation and non-linear regression

Regularisation in Non-Linear Models

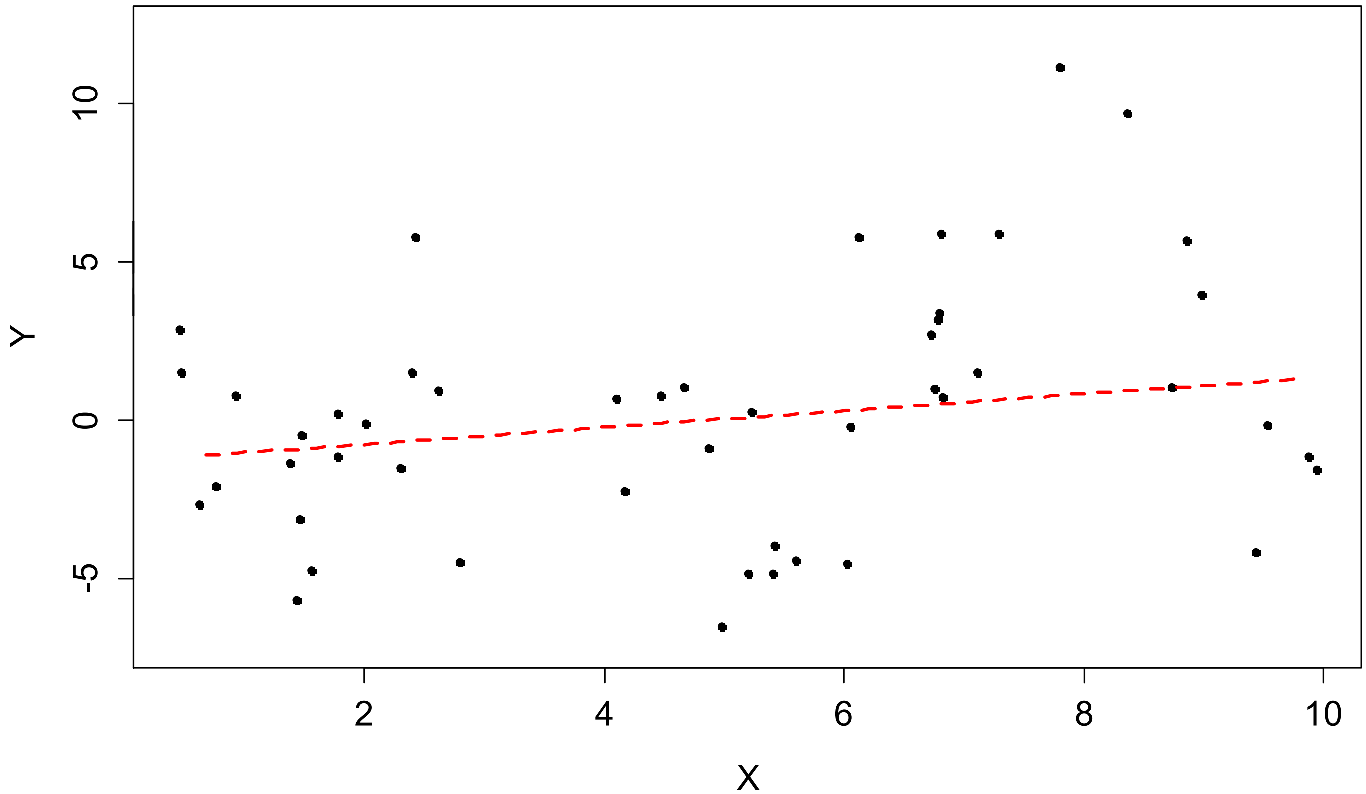
Model selection in ML

Example regression problem



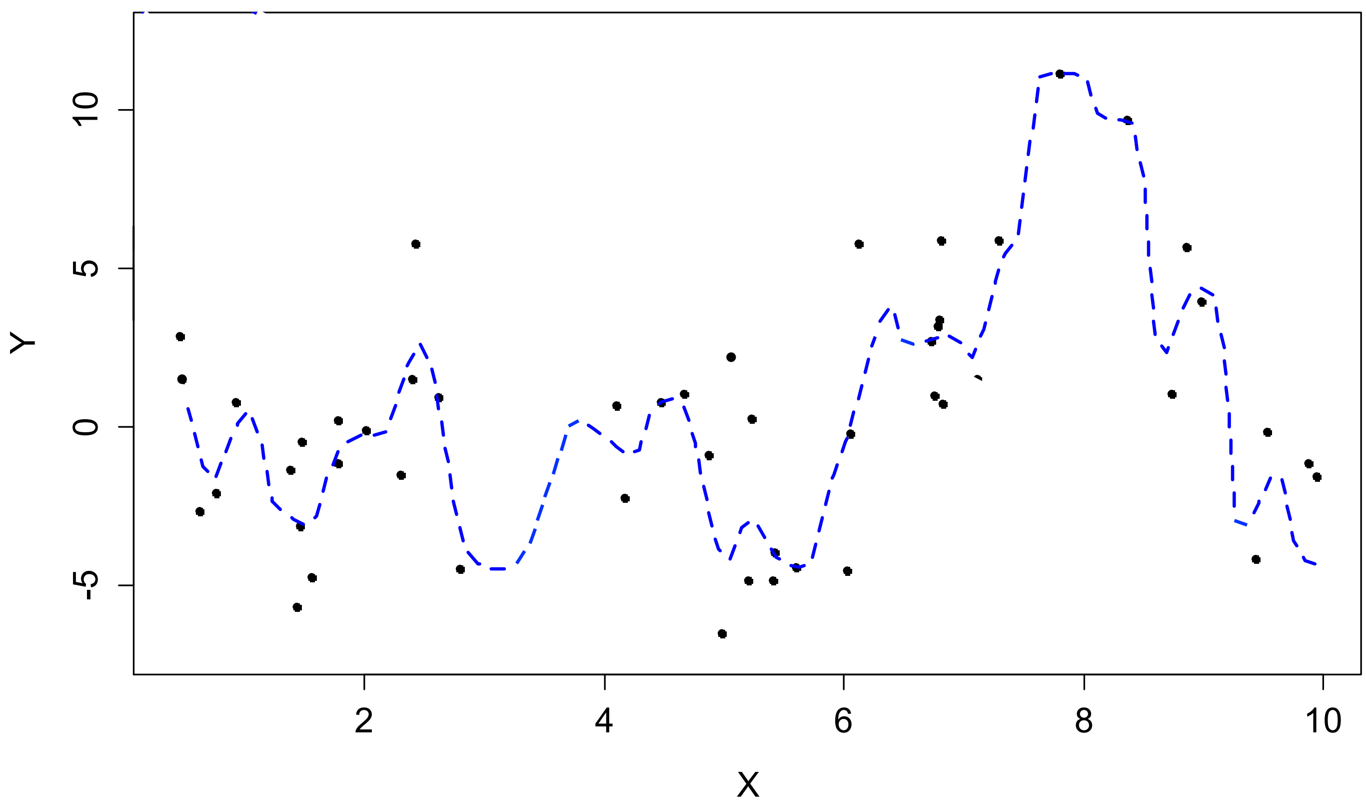
How complex a model should we use?

Underfitting (linear regression)



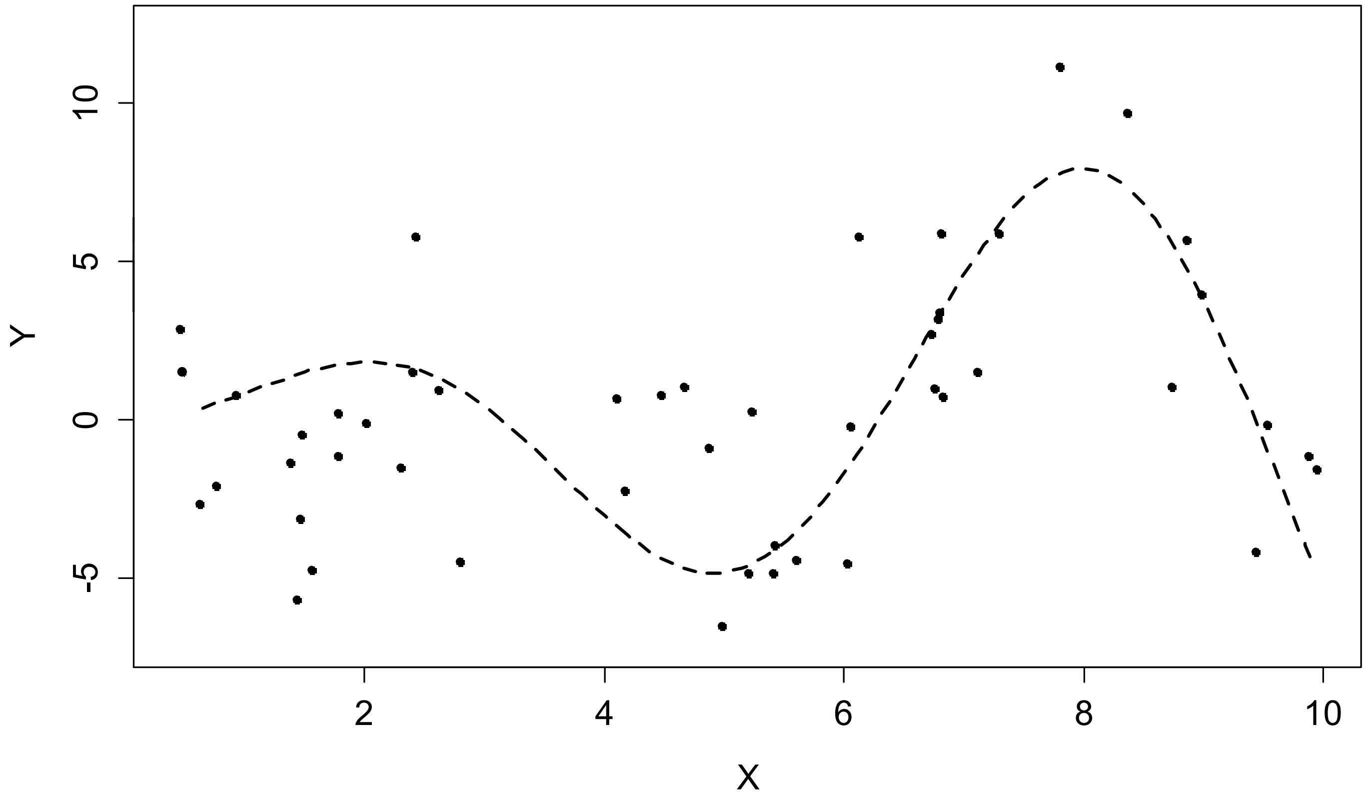
Model class Θ can be **too simple** to possibly fit true model.

Overfitting (non-parametric smoothing)



Model class Θ can be **so complex** it can fit true model + noise

Actual model ($x \sin x$)



The **right model class** Θ will sacrifice some training error, for test error.

Approach: Explicit model selection

- Try different classes of models. Example, try polynomial models of various degree d (linear, quadratic, cubic, …)
- Use held out validation (cross validation) to select the model

1. Split training data into D_{train} and $D_{validate}$ sets
2. For each degree d we have model f_d
   1. Train f_d on D_{train}
   2. Test f_d on $D_{validate}$
3. Pick degree $\hat{d}$ that gives the best test score
4. Re-train model $f_{\hat{d}}$ using all data

Approach: Regularisation

- Augment the problem:

$$\hat{\boldsymbol{\theta}} \in \underset{\boldsymbol{\theta}\in\Theta}{\operatorname{argmin}}\big(L(data, \boldsymbol{\theta}) + \lambda R(\boldsymbol{\theta})\big)$$

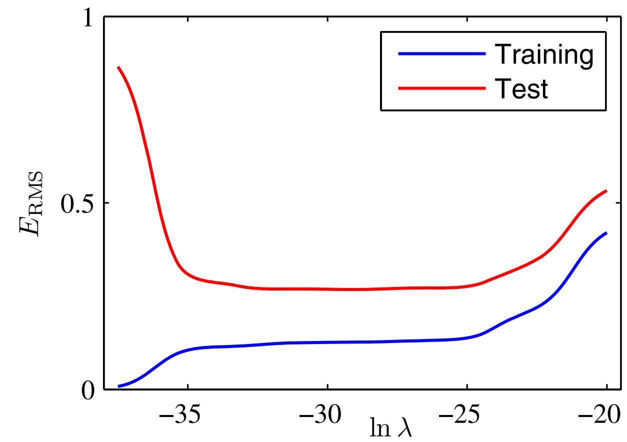
- E.g., ridge regression

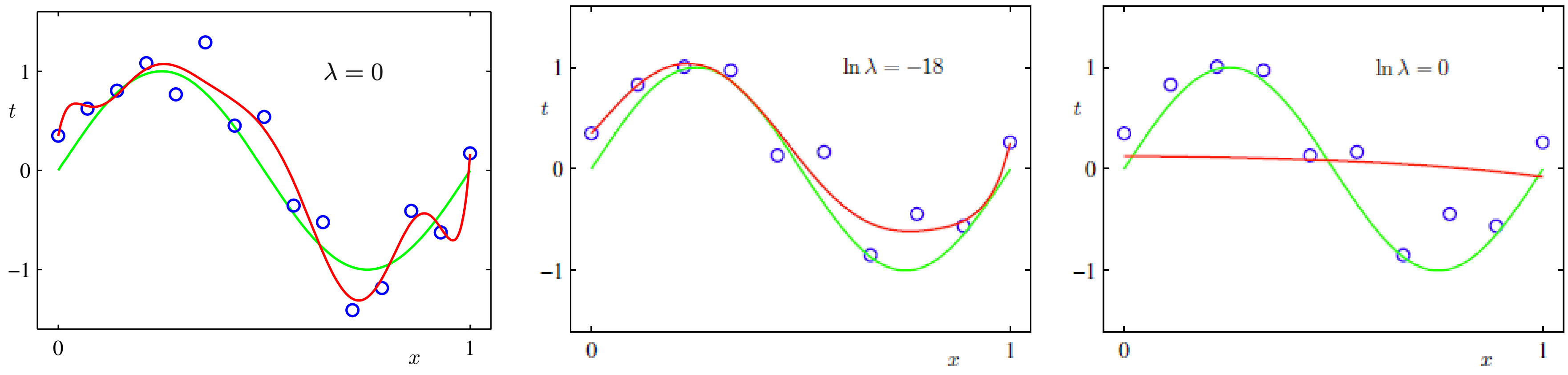
$$\hat{\boldsymbol{w}} \in \underset{\boldsymbol{w}\in W}{\operatorname{argmin}}\|\mathbf{y} - \mathbf{X}\mathbf{w}\|_2^2 + \lambda\|\mathbf{w}\|_2^2$$

- Note that regulariser $R(\boldsymbol{\theta})$ does not depend on data
- Use held out validation/cross validation to choose λ

Example: Polynomial regression

- 9th-order polynomial regression
  - model of form
    $$\hat{f} = w_0 + w_1\, x + \ \dots + w_9 x^9$$
  - regularised with $\lambda \|\mathbf{w}\|_2^2$ term





Figures from Bishop pp7-9,150

Mini Summary

- Overfitting vs underfitting
- Effect of regularisation on nonlinear regression
  - Controls balance of over- vs underfitting
  - Controlled in this case by the penalty hyperparameter

- Next: Bias-variance view for regression

Bias-variance trade-off

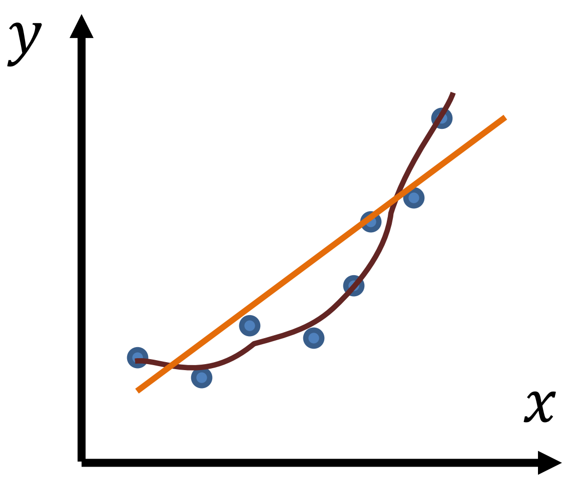
Train error, test error and model complexity in **supervised regression**

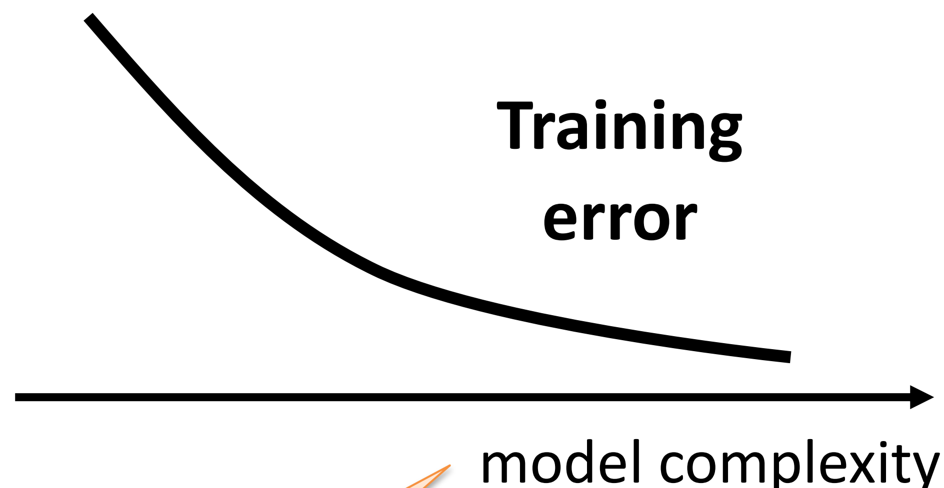
Assessing generalisation

- Supervised learning: train the model on existing data, then make predictions on new data
- Training the model: ERM / minimisation of training error
- Generalisation capacity is captured by risk / test error
- Model complexity is a major factor that influences the ability of the model to generalise **(vague still)**
- In this section, our aim is to explore error in the context of supervised regression. One way to decompose it.

Training error and model complexity

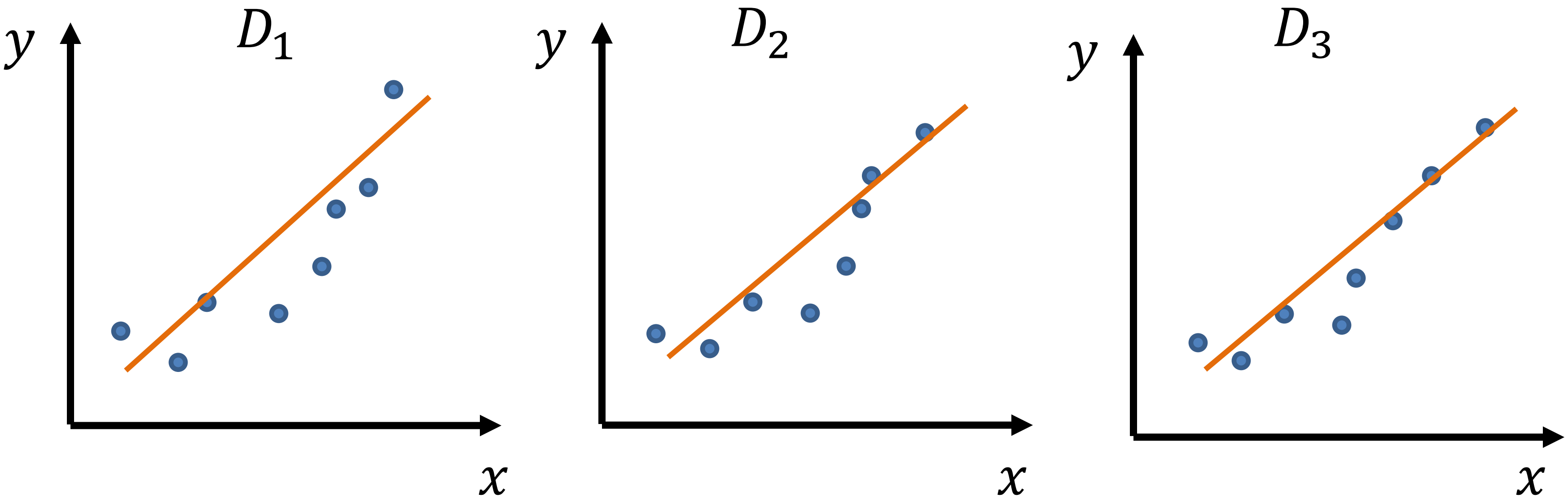
- More complex model → training error goes down
- Finite number of points → usually can reduce training error to 0 (is it always possible?)



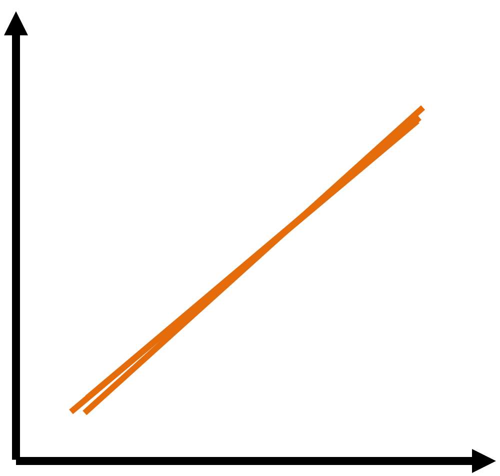


What is this?

Training data as a random variable



- Putting the three lines one on top of the other...



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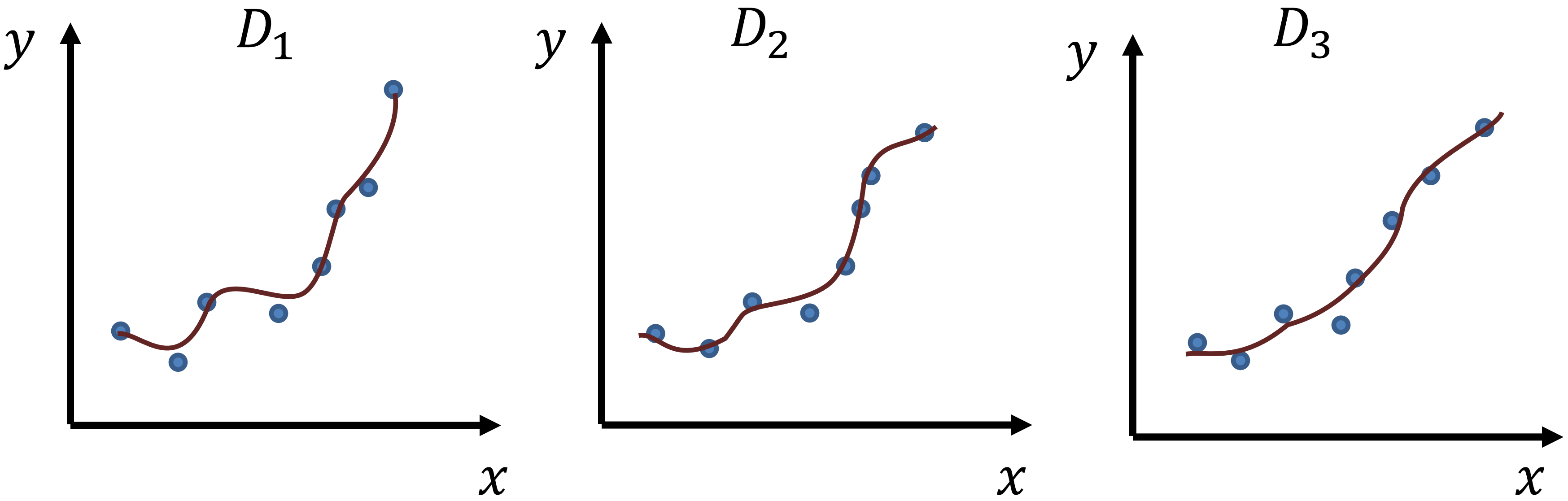
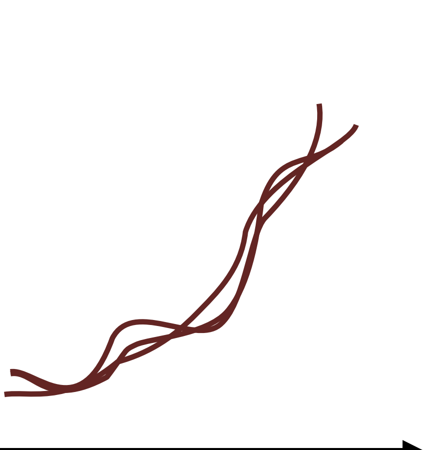
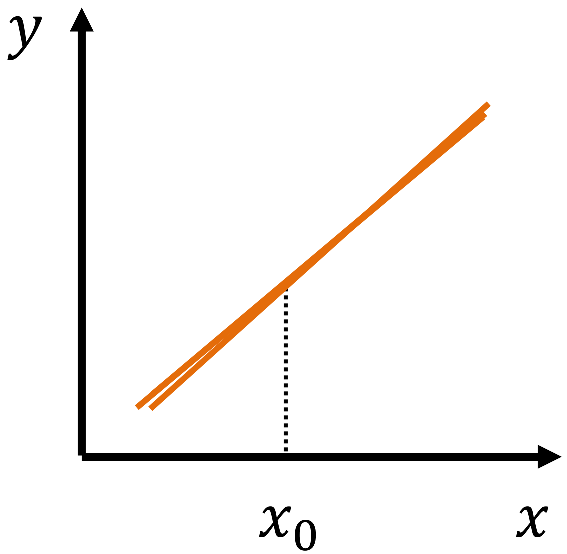


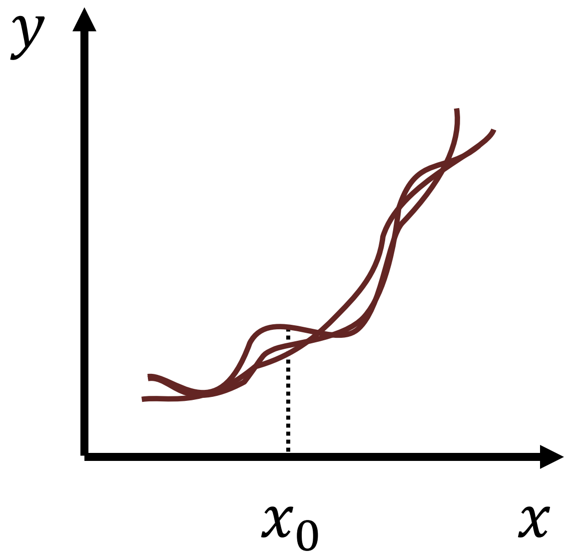
- Putting the three curves one on top of the other...



Intuition: Model complexity and variance

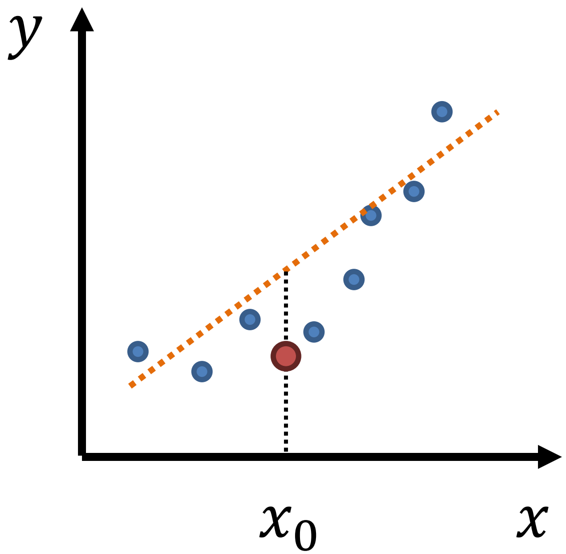
- simple model ➔ low variance
- complex model ➔ high variance

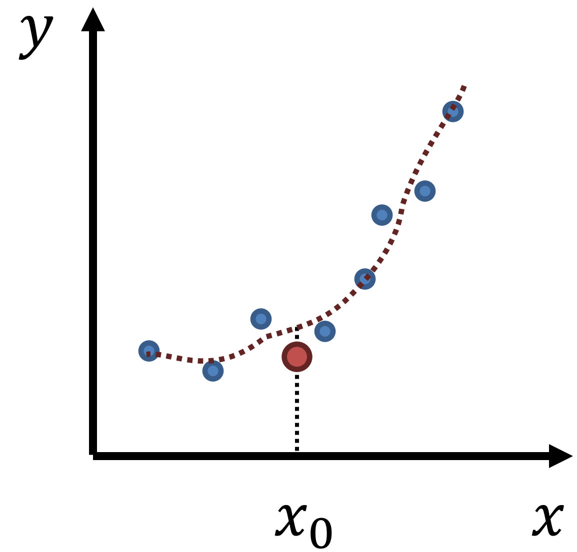




Intuition: Model complexity and variance

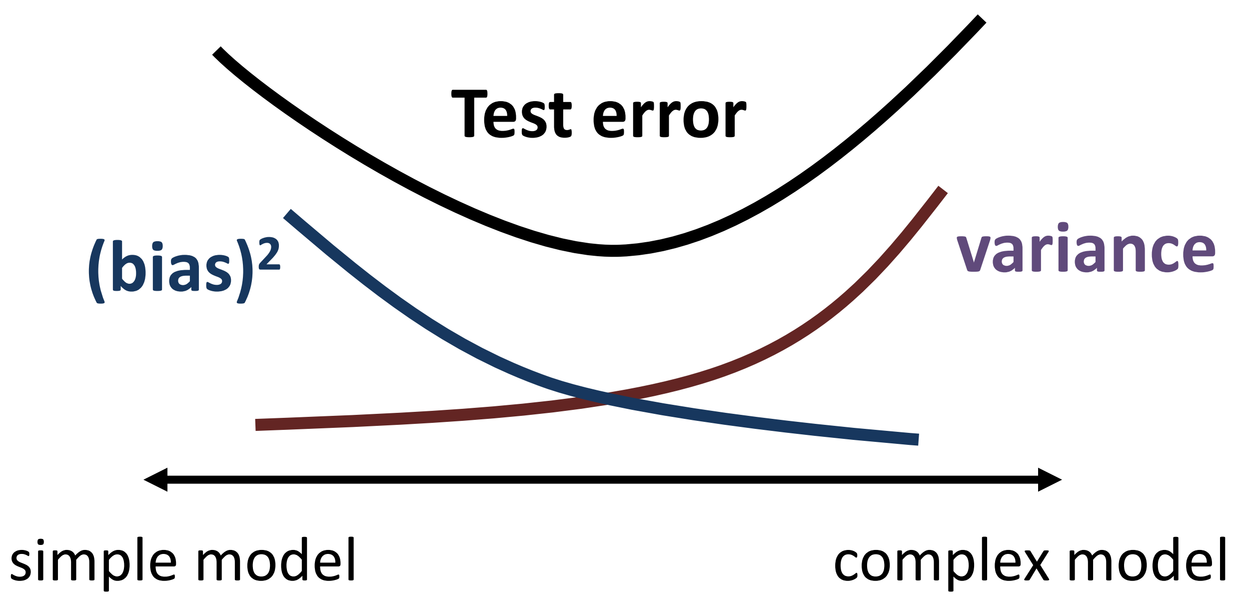
- simple model ➔ high bias
- complex model ➔ low bias





Bias-variance trade-off

- simple model ➔ high bias, low variance
- complex model ➔ low bias, high variance



(Another) Bias-variance decomposition

- Training data $\boldsymbol{D} = \{\boldsymbol{x}_1, y_1, \dots, \boldsymbol{x}_n, y_n\}$, test point $\boldsymbol{x}_0$
- Squared loss for **supervised-regression** predictions

$$l\left(Y, \hat{f}_{\boldsymbol{D}}(\boldsymbol{x}_0)\right) = \left(Y - \hat{f}_{\boldsymbol{D}}(\boldsymbol{x}_0)\right)^2$$

Classification later on

- Lemma: Bias-variance decomposition

$$\mathbb{E}\left[l\left(Y, \hat{f}_{\boldsymbol{D}}(\boldsymbol{x}_0)\right)\right] = \left(\mathbb{E}[Y] - \mathbb{E}[\hat{f}]\right)^2 + Var[\hat{f}] + Var[Y]$$

Risk / test error for $\boldsymbol{x}_0$ **(bias)²** **variance** **irreducible error**

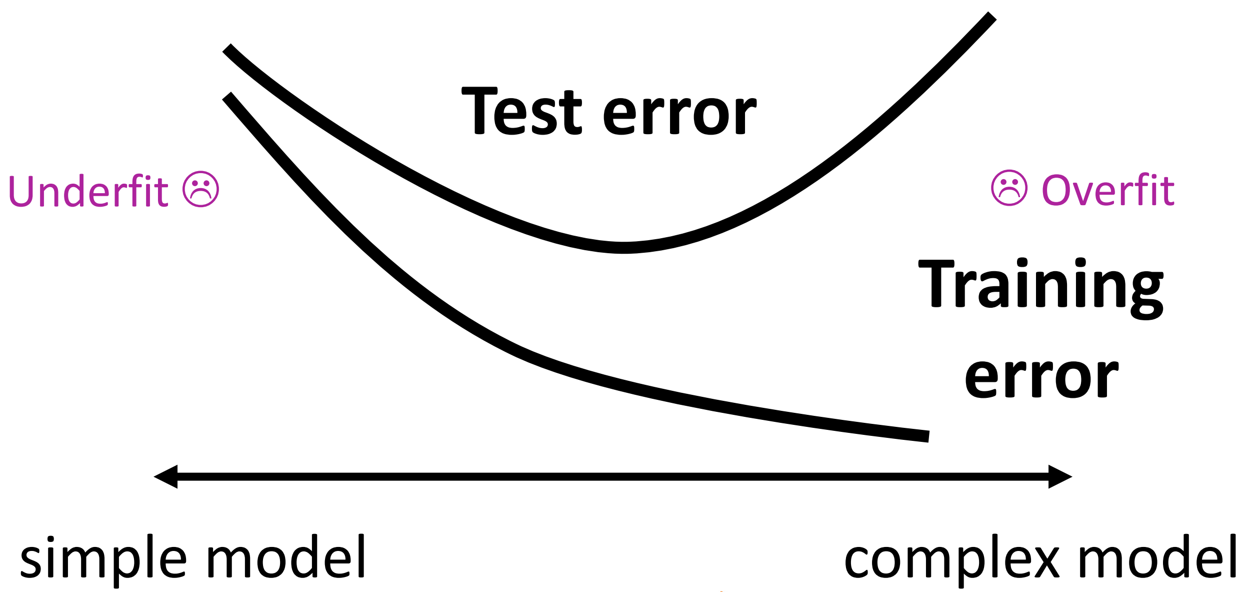
Proof sketch (outside scope of COMP90051)

- Here $\hat{f} = \hat{f}_{\boldsymbol{D}}(\boldsymbol{x}_0)$ to de-clutter notation
- $\mathbb{E}\left[\left(Y - \hat{f}\right)^2\right] = \mathbb{E}\left[Y^2 + \hat{f}^2 - 2Y\hat{f}\right]$
- $= \mathbb{E}[Y^2] + \mathbb{E}\left[\hat{f}^2\right] - 2\mathbb{E}\left[Y\hat{f}\right]$
- $= \mathrm{Var}[Y] + \mathbb{E}[Y]^2 + \mathrm{Var}\left[\hat{f}\right] + \mathbb{E}\left[\hat{f}\right]^2 - 2\mathbb{E}[Y]\mathbb{E}\left[\hat{f}\right]$
- $= \mathrm{Var}[Y] + \mathrm{Var}\left[\hat{f}\right] + \left(\mathbb{E}[Y]^2 - 2\mathbb{E}[Y]\mathbb{E}\left[\hat{f}\right] + \mathbb{E}\left[\hat{f}\right]^2\right)$
- $= \mathrm{Var}[Y] + \mathrm{Var}\left[\hat{f}\right] + \left(\mathbb{E}[Y] - \mathbb{E}\left[\hat{f}\right]\right)^2$

- Property of variance: $\mathrm{Var}[Y] = \mathbb{E}[Y^2]$ - $\mathbb{E}[Y]^2$
- Same for $\hat{f}$

- $\mathbb{E}$ with respect to D and Y only
- D independent of Y
- Thus $\hat{f}$ independent of Y

Test error and training error



But how to measure model family complexity?

Mini Summary

- Supervised regression: square-loss risk decomposes to bias, variance and irreducible terms
- This trade-off mirrors under/overfitting
- Controlled by “model complexity”
  - But we’ve been vague about what this means!?

- Next lectures: Bounding generalisation error in ML