THE UNIVERSITY of EDINBURGH
informatics

Applied Machine Learning (AML)

Generalisation

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Generalisation

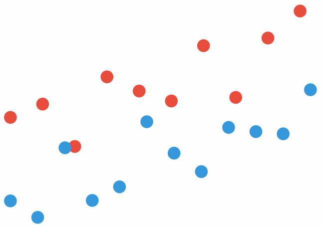
Outline

- What is Generalisation?
- How do we characterise/measure it?
- What can we do to improve it?

Generalisation

What is Generalisation?

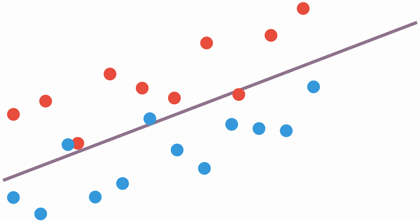
Generalisation



Machine Learning

- observe data

Generalisation



Machine Learning

- observe data
- learn to model observed data (*training* data)

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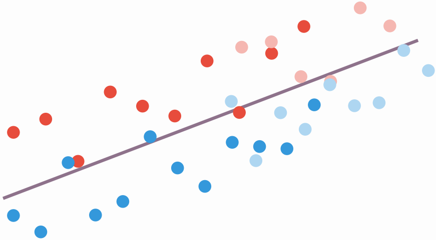

Machine Learning

- observe data
- learn to model observed data (*training* data)
- generalise to unseen, novel data (*test* data)

Reasoning about Generalisation

Overfitting

Underfitting

Reasoning about Generalisation

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- Fit training data well; unseen data poorly

Underfitting

- Fits both training and unseen data poorly

Reasoning about Generalisation

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- Reason: accidental regularities

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Capacity $\approx$ # model parameters

Overfitting vs. Underfitting: Example

Regression

Figures: C. Bishop - PRML

Overfitting vs. Underfitting: Example

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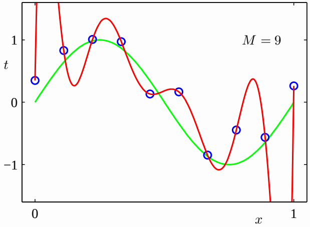

model too flexible:
fits noise

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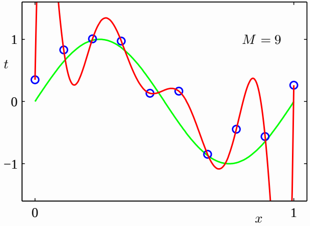

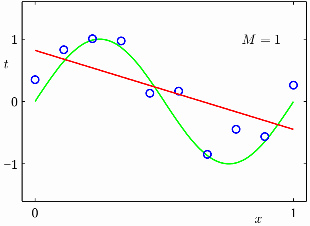

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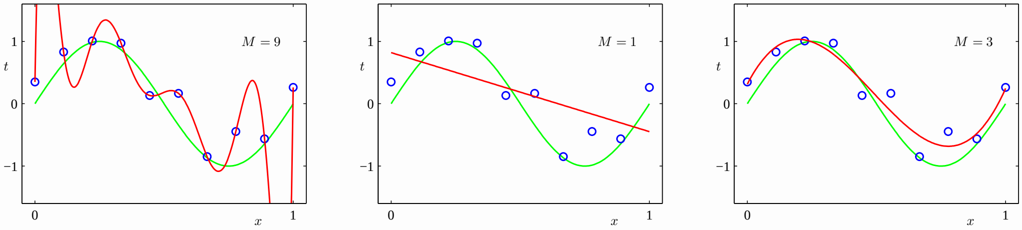

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model just right

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Reasoning about Generalisation: Qualitative

Training Data

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- More $\Longrightarrow$ better generalisation
  - close training example likely

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Model Parameters

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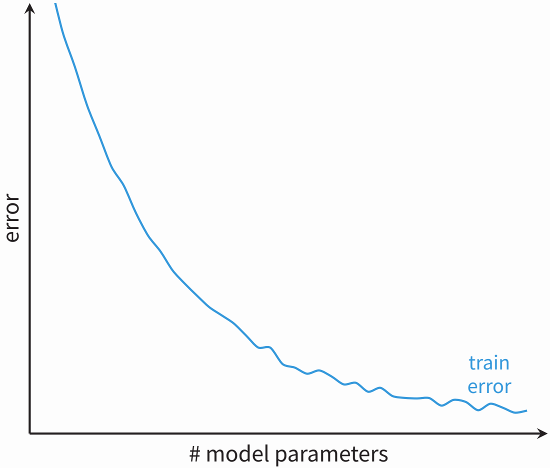
  - better flexibility



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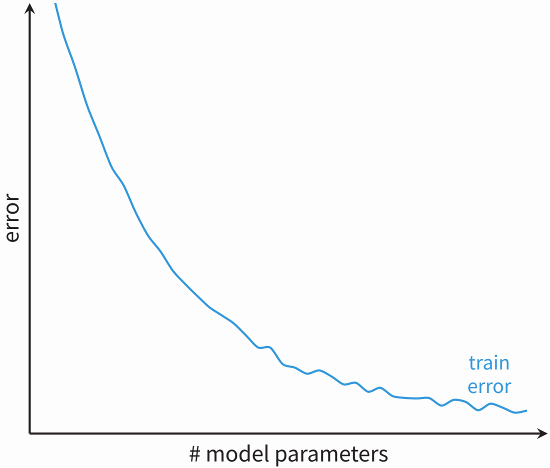

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Model Parameters

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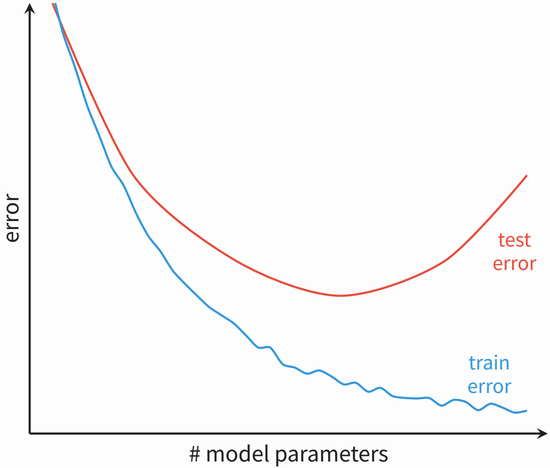

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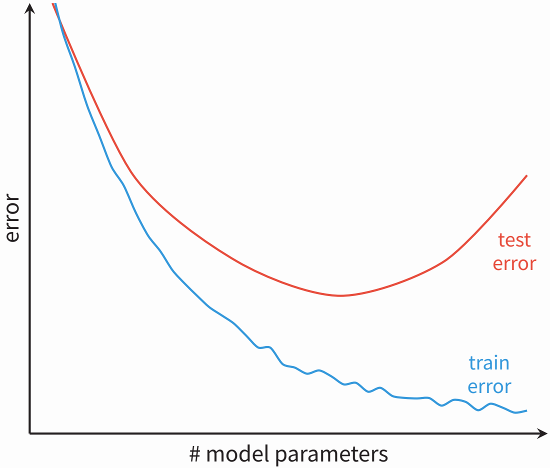

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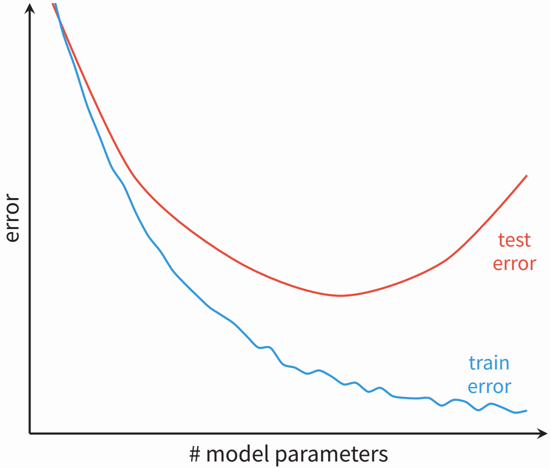

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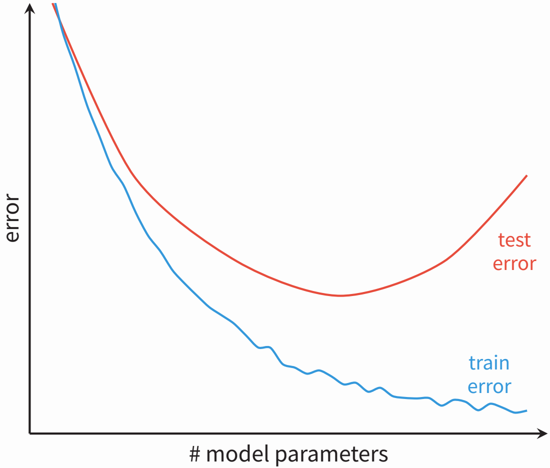

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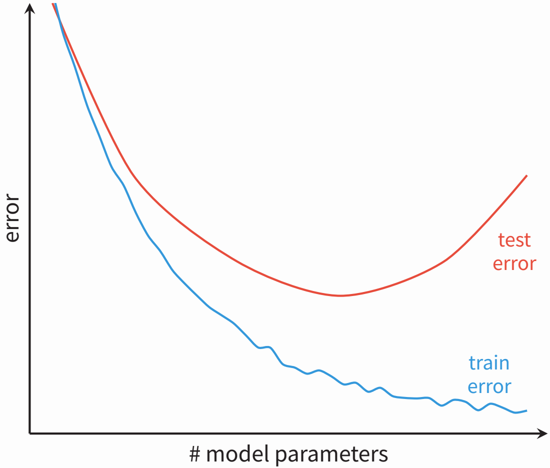

Goldilocks Zone: Sufficient capacity to learn true regularities, but not enough to memorise or exploit accidental regularities.

Tuning Model Capacity

Data requirements

- Different data requires different capacity

Figures: Stable Diffusion (Huggingface)

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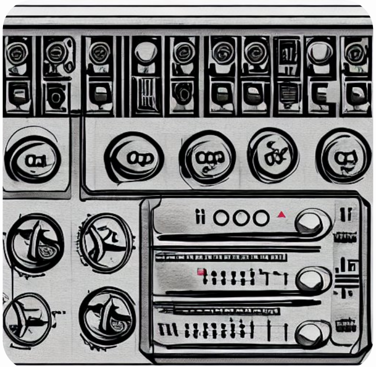

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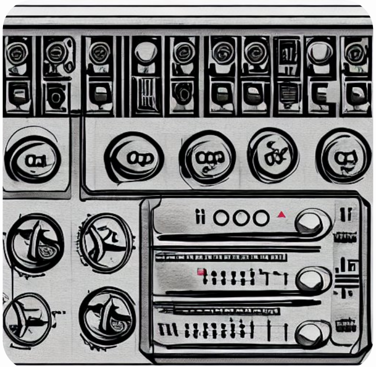

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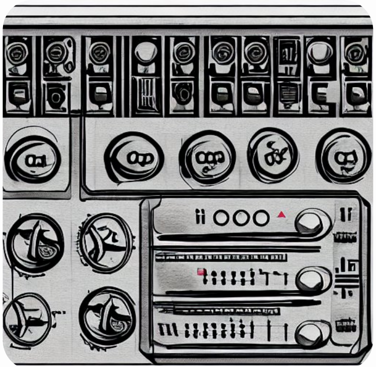

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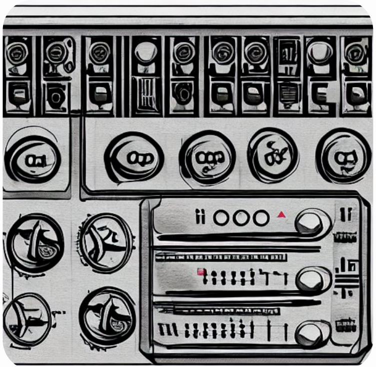

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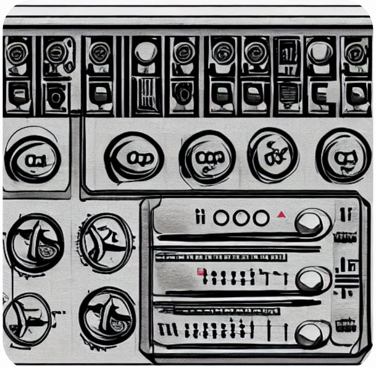

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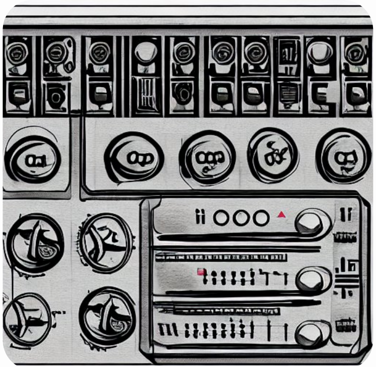

Tune to minimise generalisation error

Figures: Stable Diffusion (Huggingface)

Generalisation

Measuring Generalisation

Beyond Fitting Training Data

Optimising an error function defined as the average loss over *training* set:

$$\frac{1}{N}\sum_{i=1}^{N}\mathcal{L}\big(\hat{y}_i, y_i\big), \text{where } \hat{y}_i = f(\boldsymbol{x}_i; \boldsymbol{w})$$

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Want

- not just fit training data well
- generalise to *novel* and *unseen* instances

Setup to Estimate Generalisation

Need to estimate error on test data *without* training on test data!

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- tune hyper-parameters on $\mathcal{D}_{\text{val}}$

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- use model trained with 'best' hyper-parameters $\longrightarrow$ test error on test data

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- typically used for ‘big’ data; hard to cross validate with partitions

Modelling Generalisation Error

Setup

$$\mathcal{D} \coloneqq \{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_N, y_N)\} \sim p_{\mathcal{D}}(\boldsymbol{x}, y)$$

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Targets need not be unique

$$y \sim p_{\mathcal{D}}(y|\boldsymbol{x})$$

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$$y \sim p_{\mathcal{D}}(y|\boldsymbol{x})$$

House 1 = $\boldsymbol{x}_1$ = {3BHK, `garden`=T, `sqft`=1600} y_1 = sale price = 425K
House 2 = $\boldsymbol{x}_2$ = {3BHK, `garden`=T, `sqft`=1600} y_2 = sale price = 415K

Modelling Generalisation Error

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Model prediction

$$\hat{y} \sim p_{\boldsymbol{w}}(\hat{y}|\boldsymbol{x})$$

Bias and Variance

Expected Target Error

Targets sampled as $y \sim p_{\mathcal{D}}(y|\boldsymbol{x})$.

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Bias and Variance

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$$\begin{aligned}\mathbb{E}\big[(\hat{y}-y)^2|\boldsymbol{x}\big] &= \mathbb{E}\big[\hat{y}^2 - 2\hat{y}y + y^2|\boldsymbol{x}\big] \\ &= \hat{y}^2 - 2\hat{y}\,\mathbb{E}[y|\boldsymbol{x}] + \mathbb{E}\big[y^2|\boldsymbol{x}\big] \qquad \text{(linearity of expectation)}\end{aligned}$$

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&= \hat{y}^2 - 2\hat{y}\,\mathbb{E}[y|\boldsymbol{x}] + \mathbb{E}\left[y^2|\boldsymbol{x}\right] && \text{(linearity of expectation)} \\
&= \hat{y}^2 - 2\hat{y}\,\mathbb{E}[y|\boldsymbol{x}] + \mathbb{E}[y|\boldsymbol{x}]^2 + \mathrm{Var}[y|\boldsymbol{x}] && \text{(expression for variance)}
\end{aligned}$$

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&= (\hat{y} - \mathbb{E}[y|\boldsymbol{x}])^2 + \mathrm{Var}[y|\boldsymbol{x}]
\end{aligned}$$

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&= (\hat{y} - \mathbb{E}[y|\boldsymbol{x}])^2 + \mathrm{Var}[y|\boldsymbol{x}] \\
&\triangleq \underbrace{(\hat{y} - y_\star)^2}_{\text{residual}} + \underbrace{\mathrm{Var}[y|\boldsymbol{x}]}_{\text{Bayes error}}
\end{aligned}$$

Bias and Variance

Expected Test Error

Assume model $(p_{\boldsymbol{w}})$ trained on $\mathcal{D} \sim p_{\mathcal{D}}(\boldsymbol{x}, y)$; compute predictions on $\boldsymbol{x}$.

Predictions generated as $\hat{y} \sim p_{\boldsymbol{w}}(\hat{y}|\boldsymbol{x})$.

Bias and Variance

Expected Test Error

Assume model $(p_{\boldsymbol{w}})$ trained on $\mathcal{D} \sim p_{\mathcal{D}}(\boldsymbol{x}, y)$; compute predictions on $\boldsymbol{x}$.

Predictions generated as $\hat{y} \sim p_{\boldsymbol{w}}(\hat{y}|\boldsymbol{x})$.

$$\mathbb{E}\left[(\hat{y} - y)^2\right] = \mathbb{E}\left[(\hat{y} - y_\star)^2\right] + \mathrm{Var}[y]$$

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\end{aligned}$$

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&= y_\star^2 - 2y_\star\,\mathbb{E}[\hat{y}] + \mathbb{E}[\hat{y}]^2 + \mathrm{Var}[\hat{y}] + \mathrm{Var}[y] && \text{(expression for variance)}
\end{aligned}
$$

Bias and Variance

Expected Test Error

Assume model (p_w) trained on $\mathcal{D} \sim p_{\mathcal{D}}(\boldsymbol{x}, y)$; compute predictions on $\boldsymbol{x}$.

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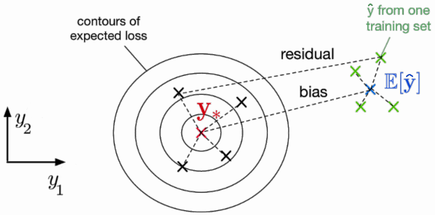
&= \underbrace{(y_\star - \mathbb{E}[\hat{y}])^2}_{\text{bias}} + \underbrace{\mathrm{Var}[\hat{y}]}_{\text{variance}} + \underbrace{\mathrm{Var}[y]}_{\text{Bayes error}}
\end{aligned}
$$

Bias and Variance: Schematic



Figures: Roger Grosse - Generalization

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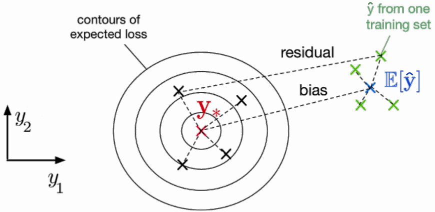

Generalisation Error:

average squared length of *residual* $\|\hat{y} - y\|^2$

Bias:

average squared length of *bias* $\|y_\star - \mathbb{E}[\hat{y}]\|^2$

Variance: spread of green $\times$'s

Bayes error: spread of black $\times$'s

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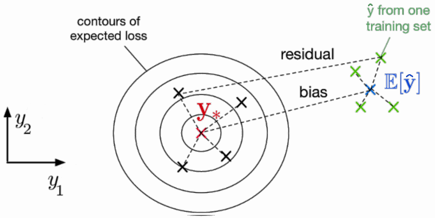

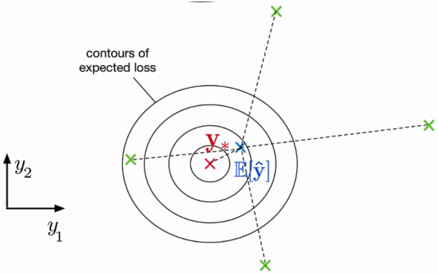

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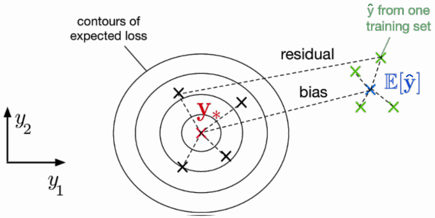

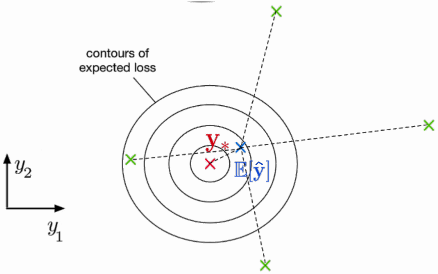

Figures: Roger Grosse - Generalization

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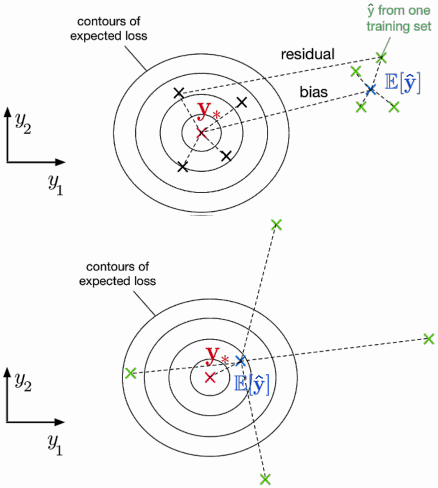

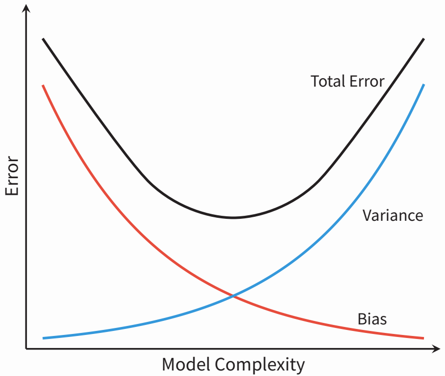

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Generalisation

Improving Generalisation

Strategies for Improving Generalisation

Primarily concerned with reducing overfitting.

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- Reducing capacity
- Early stopping
- Ensembles
- Regularisation

- Model capacity – hyper-parameter
- E.g. degree M of polynomial, # NN layers
- tune on a validation set

Note: Dangerous as can simplify model too much!

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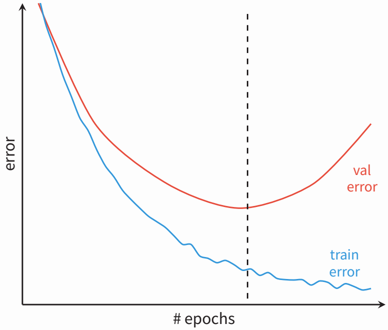

Stop training when generalisation error starts to increase

Strategies for Improving Generalisation

Primarily concerned with reducing overfitting.

- Reducing capacity
- Early stopping
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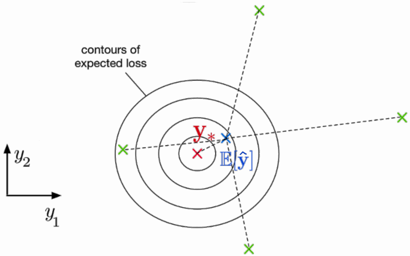
- Regularisation

- Train different models on random subsets of training data …similar to cross validation
- Averaging predictions from multiple models reduces variance

Ensemble: set of trained models whose predictions are combined



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Key Idea

Penalise parameters that may be pathological and unlikely to generalise well, by adding a “complexity” cost.

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$$\mathcal{J}(\boldsymbol{w}) = \underbrace{\frac{1}{N}\sum_{i=1}^{N}\mathcal{L}(f(\boldsymbol{x};\boldsymbol{w}),y)}_{\text{train loss}} + \underbrace{\mathcal{R}(\boldsymbol{w})}_{\text{regulariser}}$$

⋆ Requires model parameters to be *continuous*

Regularisation: Linear Regression

Intuition

Penalising polynomials with *large* coefficients, should get less “wiggly” solutions.

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$$\nabla_{\boldsymbol{w}} \mathcal{J} = \frac{1}{N} \sum_{i=1}^{N} \nabla_{\boldsymbol{w}} \mathcal{L}^i + \nabla_{\boldsymbol{w}} \mathcal{R}$$

$$\begin{aligned} \boldsymbol{w} &= \boldsymbol{w} - \eta \left(\nabla_{\boldsymbol{w}} \mathcal{L}^i + \nabla_{\boldsymbol{w}} \mathcal{R} \right) \qquad \text{(SGD)} \\ &= \boldsymbol{w} - \eta \left(\nabla_{\boldsymbol{w}} \mathcal{L}^i + 2\lambda \boldsymbol{w} \right) \\ &= (1 - 2\eta\lambda)\boldsymbol{w} - \eta \nabla_{\boldsymbol{w}} \mathcal{L}^i \end{aligned}$$

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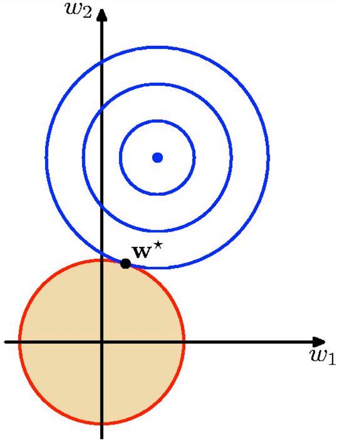
Each iteration shrinks weights by factor $(1 - 2\eta\lambda)$: *weight decay*

Regularisation: Schematic



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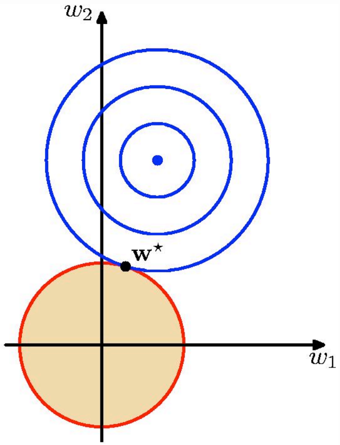

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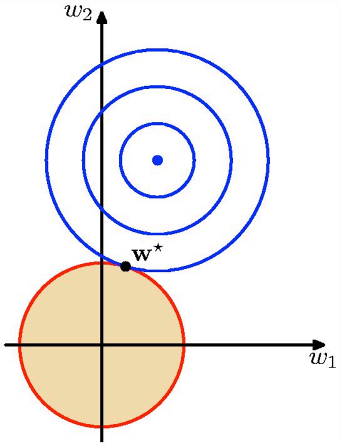

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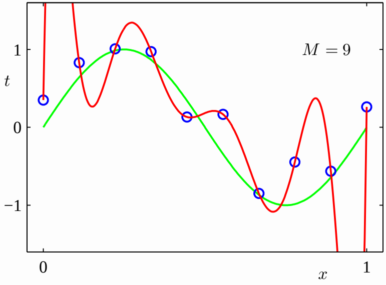
- Joint minimum on line between minimum of error and origin

  ...also called *ridge* regression

Regularisation: Example



Figures: C. Bishop - PRML

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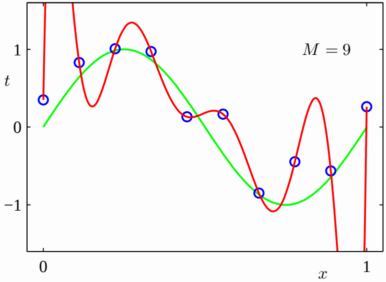

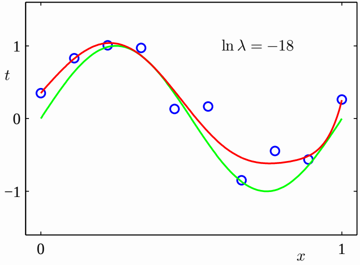

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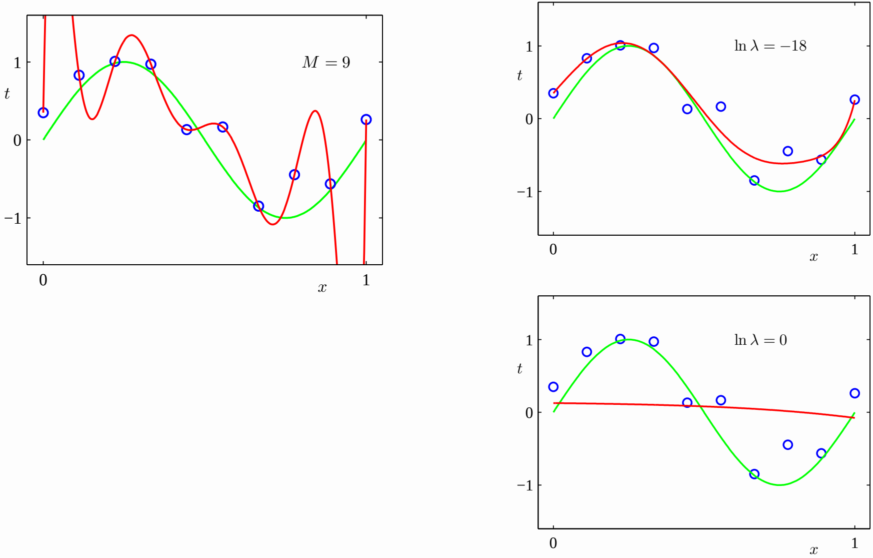

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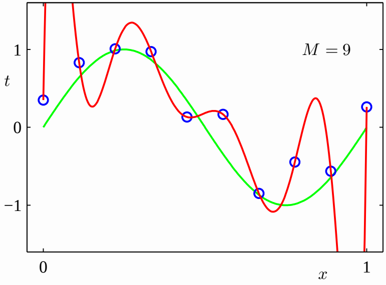

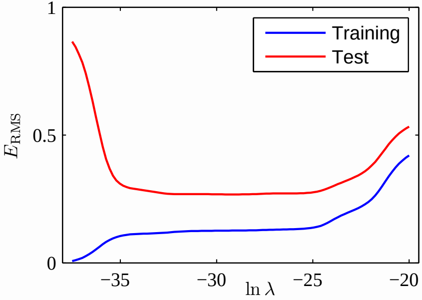

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Materials credit: Roger Grosse - Generalization

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