Lecture 5 – Cross-validation and the bias-variance trade-off

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Summary of Lecture 4 (I/III)

Linear Discriminant Analysis (LDA) models the conditional class probabilities as

$$p(y = m \,|\, \mathbf{x}) = \frac{p(\mathbf{x} \,|\, y = m)p(y = m)}{\sum_{j=1}^{M} p(\mathbf{x} \,|\, y = j)p(y = j)}.$$

where

- $p(y = m) = \pi_m$ is the *prior* probability of class m.
- $p(\mathbf{x} \,|\, y = m) = \mathcal{N}(\mathbf{x} \,|\, \boldsymbol{\mu}_m, \boldsymbol{\Sigma})$ is the probability density of $\mathbf{x}$ for an observation that comes from the mth class.

The **parameters** are: $\pi_1, \ldots, \pi_M, \boldsymbol{\mu}_1, \ldots, \boldsymbol{\mu}_M, \boldsymbol{\Sigma}$

Summary of Lecture 4 (II/III)

The parameters are estimated as the class frequencies and (within class) sample means and covariances, respectively,

$$\widehat{\pi}_m = \frac{n_m}{n} \qquad m = 1, \ldots, M,$$

$$\widehat{\boldsymbol{\mu}}_m = \frac{1}{n_m} \sum_{i:y_i=m} \mathbf{x}_i, \qquad m = 1, \ldots, M,$$

$$\widehat{\boldsymbol{\Sigma}} = \frac{1}{n-M} \sum_{m=1}^{M} \sum_{i:y_i=j} (\mathbf{x}_i - \widehat{\boldsymbol{\mu}}_m)(\mathbf{x}_i - \widehat{\boldsymbol{\mu}}_m)^{\mathsf{T}}.$$

The LDA classifier assigns a test input $\mathbf{x}_\star$ to class m with the maximum predicted probability $p(y = m \,|\, \mathbf{x}_\star)$. LDA is a **linear classifier**.

Summary of Lecture 4 (III/III)

Parametric models are specified using a fixed-dimensional vector of parameters.

Non-parametric models allow the flexibility of the model to grow with data.

One non-parametric model is the k-**nearest neighbor classifier**.

Given training data $\mathcal{T} = \{(\mathbf{x}_i, y_i)\}_{i=1}^n$, for a test input $\mathbf{x}_\star$,

1. Identify the k training inputs $\mathbf{x}_i$ closest to $\mathbf{x}_\star$.
2. Classify $\mathbf{x}_\star$ according to a majority vote among these k training samples.

Evaluating a supervised machine learning method

Evaluating performance

Training/learning: Minimizes the average loss on training data. Loss functions differ between methods and the values can not directly be compared.

We would like to evaluate already trained models with respect to hyperparameters (eg. regularization parameter γ or k in k-NN) but also different methods (LDA, logistic regression, neural net).

Error function

$$E\big(\widehat{y}(\mathbf{x})\big), y) = \begin{cases} \mathbb{I}\{\widehat{y}(\mathbf{x}) = y\} & \text{(classification)} \\ \big(\widehat{y}(\mathbf{x}) - y\big)^2 & \text{(regression)} \end{cases}$$

Note: Error function not necessarily the same as loss function.

Evaluating performance

Let $\mathcal{T} = \{(x_i, y_i)\}_{i=1}^n$ be training data.

Training error

$$E_{\text{train}} = \frac{1}{n} \sum_{i=1}^{n} E\big(\widehat{y}(\mathbf{x}_i), y_i\big)$$

Measures how well a predictor $\widehat{y}$ performs on training data, but we are interested in new data. Let $p(\mathbf{x}, y)$ be the joint distribution over data.

Expected new data error

$$E_{\text{new}} = \mathbb{E}_\star \left[E\big(\widehat{y}(x_\star), y_\star\big) \right] = \int E\big(\widehat{y}(x_\star), y_\star\big) p(x_\star, y_\star) dx_\star dy_\star$$

Impossible to compute since $p(\mathbf{x}, y)$ is unknown, but minimizing E_{new} is our ultimate goal.

Maybe we can learn it?

Approximating integrals

By the law of large numbers, we can approximate integrals using samples:

$$\mathbb{E}\left[h(\mathbf{x})\right] = \int h(\mathbf{x})p(\mathbf{x})d\mathbf{x} \approx \frac{1}{n}\sum_{i=1}^{n} h(\mathbf{x}_i), \quad \mathbf{x}_i \overset{\text{i.i.d.}}{\sim} p(\mathbf{x}_i),\ i = 1, \ldots, n$$

With samples from $p(\mathbf{x}, y)$, we can estimate E_{new}!

Note: Important that samples come from real world, "in-production" distribution.

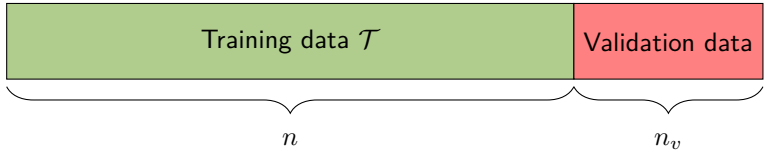
Training data are (or should be) n samples from $p(\mathbf{x}, y)$.

Approximate $E_{\text{new}} \overset{?}{\approx} E_{\text{train}}$? **NO!**

Training data is part of the predictor $\widehat{y}(\mathbf{x}; \mathcal{T})$!

Estimating E_{new}: hold-out validation data

Split data in **training data** and **validation data**.



Hold-out validation error:

$$E_{\text{new}} \approx E_{\text{hold-out}} = \frac{1}{n_v} \sum_{i=1}^{n_v} E\big(\widehat{y}(\mathbf{x}_i; \mathcal{T}), y_i\big)$$

\+ Simple
! Good estimate of E_{new} requires the validation set to be large
! Good predictor $\widehat{y}$ requires the training set to be large
– Not all data is used for learning

Always split **randomly** between training and validation data!

Estimating E_{new}: k-fold cross-validation

Split data in k batches and hold out batch ℓ when estimating model. Use batch ℓ to estimate E_{new} and average over all k estimates. Estimate final model using whole dataset.

k-fold cross-validation error

$$E_{\text{new}} \approx E_{\text{k-fold}} = \frac{1}{k} \sum_{\ell=1}^{k} E_{\text{hold-out}}^{(\ell)}$$

+ Gives a better estimate of E_{new}
– Computationally more demanding than the hold-out data approach

Using a test set

An important use of $E_{\text{k-fold}}$ is to choose between models or select hyperparameters (k in k-NN or λ in regularization). If a good estimate of E_{new} is important:

We can no longer use $E_{\text{k-fold}}$ to estimate E_{new}!

Set aside a test set and use **only** to estimate E_{new}.

Flavors of cross-validation

- k-fold cross-validation: Typically $k \approx 10$
- Leave-one-out cross-validation: k-fold cross-validation with $k = n$
- Monte Carlo cross-validation: Random selection of validation set at each iteration

Understanding E_{new}

Collecting data is a random process where $\mathcal{T}$ is sampled from $p(\mathbf{x}, y)$. Because $\mathcal{T}$ is random, so is our learned model $\widehat{y}(\mathbf{x}; \mathcal{T})$.

To better understand the behavior of E_{new}, we need to introduce

$$\bar{E}_{\text{train}} = \mathbb{E}_{\mathcal{T}}\left[E_{\text{train}}\right],$$
$$\bar{E}_{\text{new}} = \mathbb{E}_{\mathcal{T}}\left[E_{\text{new}}\right],$$

where $\mathbb{E}_{\mathcal{T}}[\cdot]$ is the average over **training data** $\mathcal{T}$.

Note: k-fold cross-validation estimates $\bar{E}_{new}$ rather than E_{new}.

It usually holds that

$$\bar{E}_{\text{train}} < \bar{E}_{\text{new}}.$$

On average, a method usually performs better on training data than new data.

Model complexity

Since $\bar{E}_{\text{train}} < \bar{E}_{\text{new}}$, define generalization gap:

$$\bar{E}_{\text{new}} = \bar{E}_{\text{train}} + \textbf{generalization gap}$$

A models ability to adapt to patterns in the data, we call the **model complexity**[1].

Model complexity ↗
- ↘ $\bar{E}_{\text{train}}$
- ↗ Generalization gap

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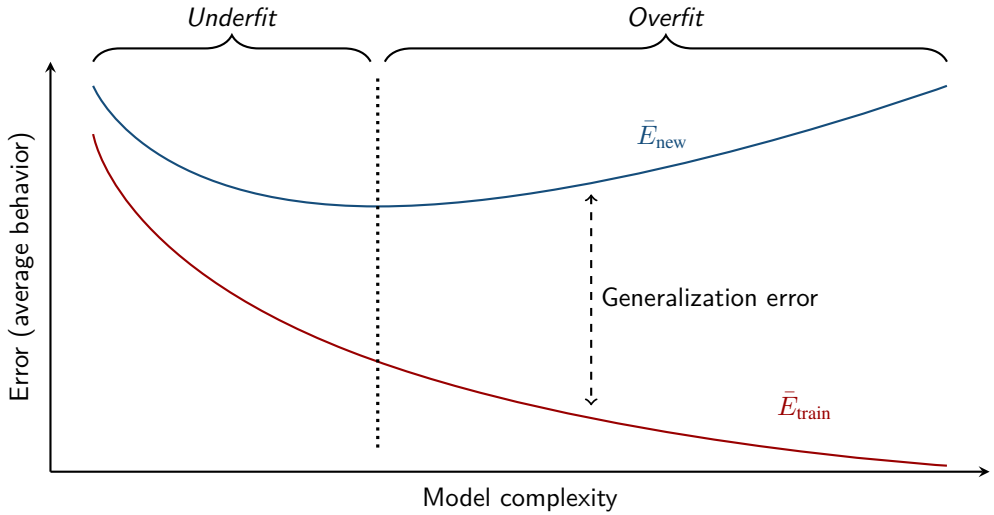
- ↗ $\bar{E}_{\text{train}}$
- ↘ Generalization gap

$\bar{E}_{\text{new}}$ usually attains a minimum at some intermediate complexity.

[1] A formal definition is possible. We will not do that in this course.

Model complexity, $\bar{E}_{\text{train}}$ and $\bar{E}_{\text{new}}$



Example: cross-validation for model selection

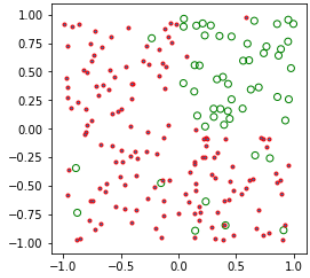
All models are wrong, but some are useful. — *George Box*

Example: cross-validation for model selection

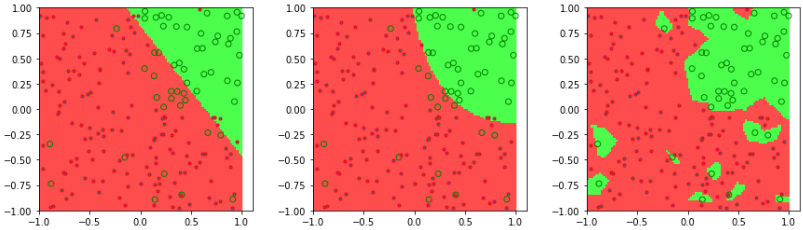
Binary classification, $p = 2$.
Evaluate the following methods

- logistic regression
- QDA
- k-NN

We would like to pick the method with lowest E_{new}.
Since we only have the data, we can only *estimate* E_{new}.



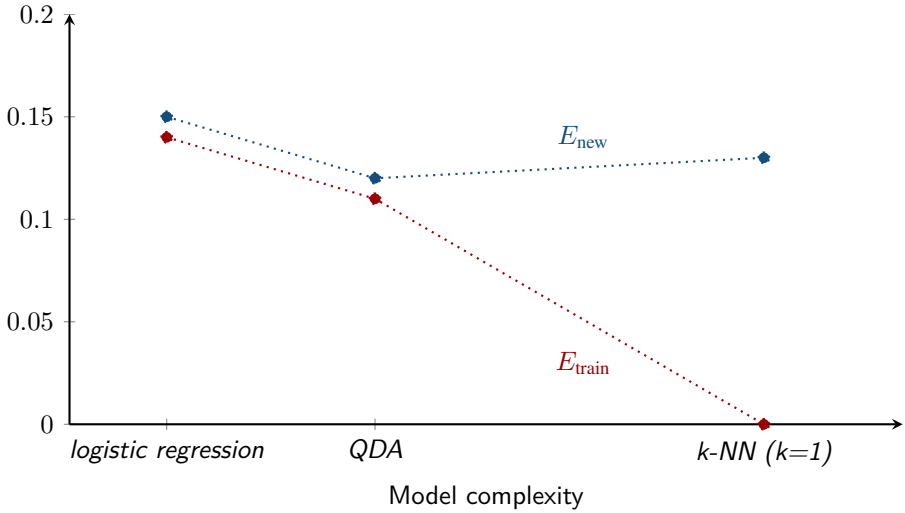
Example: cross-validation for model selection



	logistic regression	QDA	k-NN ($k = 1$)
E_{train}	0.14	0.11	0.0
E_{new}[2]	0.15	0.12	0.13

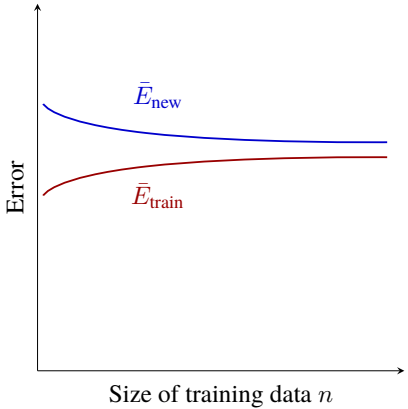
[2] Estimated using cross-validation

Example: cross-validation for model selection

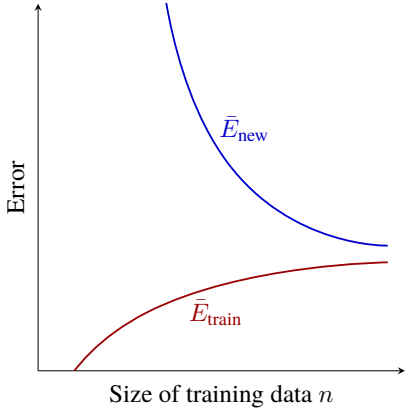


Generalization error and training data size

In general, more training data n decreases the generalization error.
However, $\bar{E}_{\text{train}}$ typically increases with n.



Low model complexity



High model complexity

Digging even deeper to understand E_{new}

Let us focus on the regression setting.
Assume that "the real world" works as

$$y = f_0(\mathbf{x}) + \epsilon, \text{ where } \begin{cases} \epsilon \text{ random, independent of } \mathbf{x} \\ \mathbb{E}[\epsilon] = 0, \\ \mathbb{E}\left[\epsilon^2\right] = \sigma^2. \end{cases}$$

Denote the **average trained model**

$$\bar{f}(\mathbf{x}) \triangleq \mathbb{E}_{\mathcal{T}}\left[\widehat{y}(\mathbf{x}; \mathcal{T})\right].$$

The average model if we could re-train the model on new data an infinite number of times.

Bias-variance decomposition

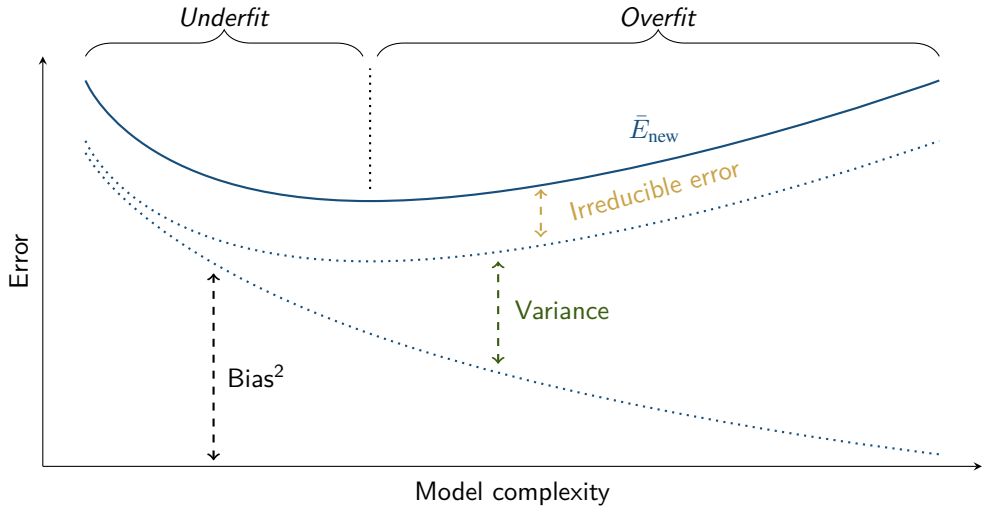
$$\begin{aligned}\bar{E}_{\text{new}} &= \mathbb{E}_{\mathcal{T}}\left[\mathbb{E}_{\star}\left[\left(\widehat{y}(\mathbf{x}_{\star};\mathcal{T}) - y_{\star}\right)^2\right]\right] = \mathbb{E}_{\star}\left[\mathbb{E}_{\mathcal{T}}\left[\left(\widehat{y}(\mathbf{x}_{\star};\mathcal{T}) - f_0(\mathbf{x}_{\star}) - \epsilon\right)^2\right]\right] \\ &= \mathbb{E}_{\star}\left[\mathbb{E}_{\mathcal{T}}\left[\left(\widehat{y}(\mathbf{x}_{\star};\mathcal{T}) - \bar{f}(\mathbf{x}_{\star}) + \bar{f}(\mathbf{x}_{\star}) - f_0(\mathbf{x}_{\star}) - \epsilon\right)^2\right]\right] \\ &= \underbrace{\mathbb{E}_{\star}\left[\mathbb{E}_{\mathcal{T}}\left[\left(\widehat{y}(\mathbf{x}_{\star};\mathcal{T}) - \bar{f}(\mathbf{x}_{\star})\right)^2\right]\right]}_{\text{Variance}} + \underbrace{\mathbb{E}_{\star}\left[\left(\bar{f}(\mathbf{x}_{\star}) - f_0(\mathbf{x}_{\star})\right)^2\right]}_{\text{Bias}^2} + \underbrace{\sigma^2}_{\substack{\text{Irreducible} \\ \text{error}}}\end{aligned}$$

Technical interpretation:

- **Bias²** $\mathbb{E}_{\star}\left[\left(\bar{f}(\mathbf{x}_{\star}) - f_0(\mathbf{x}_{\star})\right)^2\right]$: The part of $\bar{E}_{\text{new}}$ that is due to the fact that the model cannot represent the true f_0.
- **Variance** $\mathbb{E}_{\star}\left[\mathbb{E}_{\mathcal{T}}\left[\left(\widehat{y}(\mathbf{x}_{\star};\mathcal{T}) - \bar{f}(\mathbf{x}_{\star})\right)^2\right]\right]$: The part of $\bar{E}_{\text{new}}$ that is due to the variability in the training dataset.

Intuitive interpretation:

- **Bias**: The inability of a method to describe the complicated patterns we would like it to describe. Low model complexity.
- **Variance**: How sensitive a method is to the training data. High model complexity.



Finding a balanced fit (neither over- nor underfit) is called the **the bias-variance tradeoff**.

Regression example

The data ($n = 10$) comes from

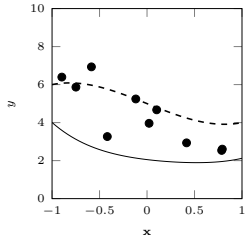
$$y = 5 - 2x + x^3 + \varepsilon, \quad \varepsilon \sim \mathcal{N}(0, 1),$$

and our regression model is

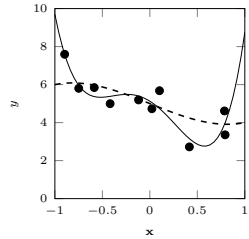
$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \theta_3 x^3 + \theta_4 x^4 + \varepsilon.$$

We use ridge regression to tune model complexity/bias-variance.

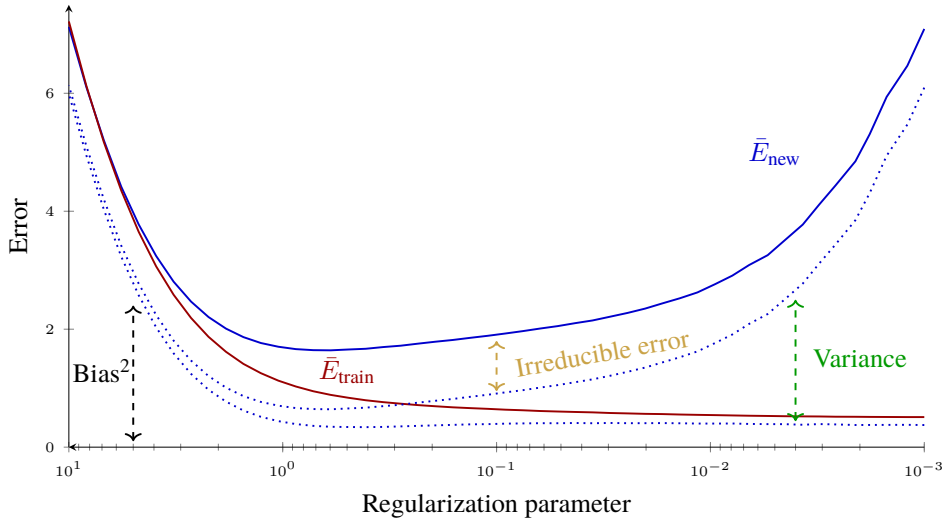
$\gamma = 10$



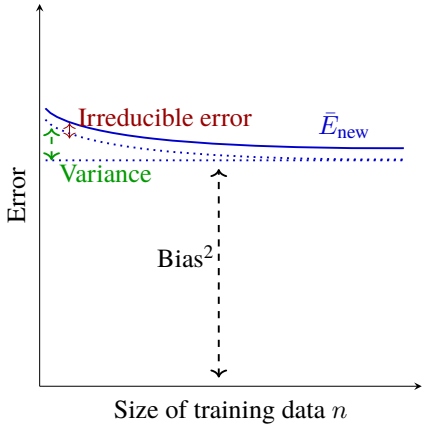
$\gamma = 0.001$



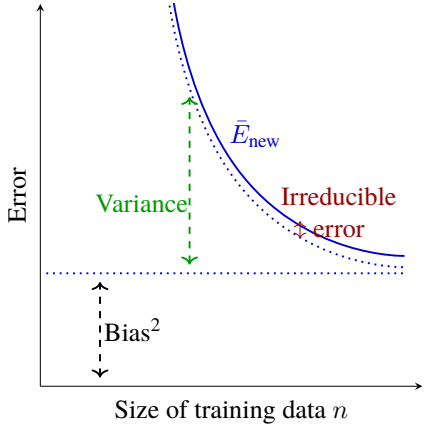
Regression example



Bias, variance and training data size



Low model complexity



High model complexity

Make the tradeoff

Some methods for **decreasing the model complexity/increasing the bias/ decreasing the variance**:

- Increase k in k-NN
- Regularization
- Bagging
- Early stopping (for methods trained using optimization, notably deep learning)
- Dropout (deep learning)

Warning! θ_0 in linear regression (and later deep learning) is sometimes called "bias term". That is **completely unrelated** to bias in this context.

A few concepts to summarize lecture 5

$E(y, \widehat{y})$**:** Error function which compares predictions $\widehat{y}$ to true output y: MSE for regression, misclassification for classification.

E_{train}**:** The training data error (E_{train} small $=$ the method fits the training data well).

E_{new}**:** The expected new data error; how well a method will perform when faced with an endless stream of new data.

Cross-validation: A method for estimating E_{new} using the training data.

Model complexity: How prone a method is to adapt to complicated patterns in the training data.

Overfitting: When a given method yields a smaller E_{train} and larger E_{new} than a model with lower model complexity would have done. That happens because the method/model is capturing patterns in the training data caused by random chance rather than true properties of the underlying function.

Bias: The inability of a method to describe the true patterns in the classification or regression problem. Low model complexity.

Variance: Sensitivity to random effects (noise) in the training data. High model complexity.