Academy of PhD Training in Statistics
Statistical Machine Learning

Louis J.M. Aslett (louis.aslett@durham.ac.uk)

Supervised Learning
This Section

- Gentle introduction to supervised learning
- Formalise the problem setting
- Formalise the approach to learning
- Defining errors and optimal predictors
- Error decompositions
- Consistency
- Model fitting
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*Brace yourself ... a lot of things to define coming up ...*
Notation

• **Scalars**: $x, x_i, x_{ij}, y_i, \beta_i, ...$

• **Vectors**: $x, y, \beta, ...$
  - follow the standard convention that all are column vectors
  - transpose $x^T$ is row vector
  - $x_i$ indicates a vector, the elements of which are $x_{ij}$

• **Matrices**: $X, Y, ...$
  - matrix transpose: $X^T$
  - $i$-th row entries: $x_i$ (as column vector)
  - $j$-th column entries: $x_{.j}$
  - $(i, j)$-th element: $x_{ij}$
• Random variables: $X, Y, \varepsilon, \ldots$
  • clear from context whether a random scalar/vector/matrix/…
  • clear from context whether Greek letters are random variables
  • the probability measure associated with a random variable $X$ is $\pi_X$.

• Spaces: $\mathcal{X}, \mathcal{Y}, \mathbb{R}, \mathbb{Z}, \mathbb{R}^d = \mathbb{R} \times \cdots \times \mathbb{R}$, …

• Estimator: denoted by a hat, $\hat{f}(\cdot), \hat{\beta}, \ldots$

• Functions:
  • $\mathbb{1}\{A\}$ is the indicator function for $A$ being true.
  • if $f(x)$ has vector valued output, then $f_j(x)$ denotes the $j$-th component of the output.
  • where necessary an arbitrary function, $f(x)$, will be distinguished from a probability density function (pdf), $f_X(x)$, by the presence or absence of a random variable subscript.
  • the cumulative distribution function (cdf) is denoted $F_X(x)$. 
• Other:
  • \( A := B \) reads “\( A \) is defined to be \( B \)”.
  • For a finite set \( \mathcal{I} \), \(|\mathcal{I}|\) denotes the cardinality of the set.

Note: we avoid excessive formality and write \( \min \ldots \), implicitly assuming minimum exists; likewise, \( E[ \ ] \) makes an implicit assumption that it exists.
The most common supervised machine learning problems fall broadly under three types (Vapnik, 1998):

- **Regression** models a *quantitative* outcome.
  - What value is a house based on geographic/house information;
  - How long until a patient is discharged from hospital?

- **Classification** models a *qualitative* outcome.
  - Medics predicting a disease from test results;
  - Is the email just sent to my address spam?
  - Bank predicting if borrower will default;
  - Identifying a number from image of handwritten value.

- **Density estimation** models a full *probability distribution*.
Problem setting (II)

Premise: we have access to a set of $n$ observations of

- **features / predictors** from some space $\mathcal{X}$, eg:
  - $\mathcal{X} \subset \mathbb{R}^d$
  - or, $\mathcal{X}$ can be a tensor in deep learning

- and corresponding **outcomes / responses / targets** from some space $\mathcal{Y}$, eg:
  - $\mathcal{Y} \subset \mathbb{R}$ $\implies$ regression;
  - or, $\mathcal{Y} = \{1, \ldots, g\}$ where $g \geq 2$ $\implies$ classification;
  - or, for $g = 2$ often take $\mathcal{Y} = \{0, 1\}$
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Dataset is $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\} \subset (\mathcal{X} \times \mathcal{Y})^n$, where $x_i$ is a vector of length $d$,

$$x_i = (x_{i1}, \ldots, x_{id})^T \in \mathcal{X}$$

All observations of single feature $x_j$, $x_j = (x_{1j}, \ldots, x_{nj})^T$
Objective is to learn relationship between features and response:

Regression: \[ Y = f(X) + \varepsilon \]

\( \varepsilon \) is random error term, assumed mean zero.
Problem setting: objective

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where \( p_i = \mathbb{P}(Y = i \mid X = x) \).
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**Density Estimation:** \( (Y \mid X = x) \sim \mathbb{P}(Y \mid X = x) \)

possibly by jointly modelling \( \mathbb{P}(X, Y) \)
“A mathematician is a machine for turning coffee into theorems”
Example 2D regression

Figure 1: From “An Introduction to Statistical Learning”.
Example 3D regression

Figure 2: From “An Introduction to Statistical Learning”.
Example 3D regression

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Example 3D regression

Figure 2: From “An Introduction to Statistical Learning”.
Example classification (I)

- versicolor
- setosa
- virginica

Species

Petal.Length

2 4 6
Example classification (II)

![Graph showing Petal Length vs Species (setosa, versicolor, virginica)]
Example classification (III)
Problem setting: summary

- Focus is heavily on prediction and predictive accuracy for future observations
- Assume in future we have access to $x$, but not $y$
- The “model” setting is very general, we usually directly tackle estimation of $\hat{f}$
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- Assume in future we have access to $x$, but not $y$
- The “model” setting is very general, we usually directly tackle estimation of $\hat{f}$

Important aside: we are going to be interested in the random inputs scenario, not the fixed inputs one that is often studied in classical statistics setting.
Loss functions

Given fitted model $\hat{f}(\cdot)$ and newly observed feature vector $x$, denote the prediction $\hat{y} := g_{\hat{f}}(x)$.

We want to minimise the loss we suffer when predicting $\hat{y}$ and actually observing $y$. To do so, define a loss function,

$$L : \mathcal{Y} \times \mathcal{Y} \rightarrow [0, \infty)$$

which measures the discrepancy between prediction and reality.
Loss functions

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which measures the discrepancy between prediction and reality.

For classification, often

$$\mathcal{L} : \mathcal{Y} \times [0, 1]^g \rightarrow [0, \infty)$$
Loss functions: regression

- Square loss, $\mathcal{L}(y, \hat{y}) = (y - \hat{y})^2$

- Absolute loss, $\mathcal{L}(y, \hat{y}) = |y - \hat{y}|$

- Quantile loss, (sometimes called pinball loss),

$$
\mathcal{L}(y, \hat{y}) = \begin{cases} 
(1 - \alpha)(\hat{y} - y) & \text{if } y \leq \hat{y} \\
\alpha(y - \hat{y}) & \text{if } y > \hat{y} 
\end{cases}
$$

where $\alpha \in (0, 1)$ is the target quantile.
Loss functions: classification

- 0-1 loss, $\mathcal{L}(y, \hat{y}) = \mathbb{1}\{y \neq \hat{y}\}$

- Cross entropy loss, $\mathcal{L}(y, \hat{p}) = -\sum_{j=1}^{g} \mathbb{1}\{y = j\} \log \hat{p}_j = -\log \hat{p}_y$

- Brier score loss, $\mathcal{L}(y, \hat{p}) = \sum_{j=1}^{g} (\mathbb{1}\{y = j\} - \hat{p}_j)^2$

- Exponential loss (binary+scoring setting, $y \in \{-1, 1\}$), $\mathcal{L}(y, \hat{f}(x)) = \exp(-y \hat{f}(x))$
The *generalisation error* (sometimes called *generalisation risk*) of a model $\hat{f}(\cdot)$, with respect to a loss $\mathcal{L}$, is the expected loss of a future prediction $g_{\hat{f}}(\cdot)$ with respect to the true data generating measure $\pi_{XY}$,

$$
\mathcal{E}(\hat{f}) := \mathbb{E}_{XY} \left[ \mathcal{L}(Y, g_{\hat{f}}(X)) \right]
$$
The **generalisation error** (sometimes called **generalisation risk**) of a model $\hat{f}(\cdot)$, with respect to a loss $L$, is the expected loss of a future prediction $g_{\hat{f}}(\cdot)$ with respect to the true data generating measure $\pi_{XY}$,

$$\mathcal{E}(\hat{f}) := \mathbb{E}_{XY} \left[ L(Y, g_{\hat{f}}(X)) \right]$$

**Note:** $\hat{f}$ is *not* a random variable ... assumes a fixed fitted model already.
The estimated generalisation error based on dataset $\mathcal{D} = ((x_1, y_1), \ldots, (x_m, y_m))$, where $(x_i, y_i) \overset{iid}{\sim} \pi_{XY}$ is,

$$\hat{E}_D(\hat{f}) := \frac{1}{m} \sum_{i=1}^{m} L(y_i, g_{\hat{f}}(x_i)) \approx \mathcal{E}(\hat{f})$$
The estimated generalisation error based on dataset $\mathcal{D} = ((x_1, y_1), \ldots, (x_m, y_m))$, where $(x_i, y_i) \overset{iid}{\sim} \pi_{XY}$ is,

$$\hat{E}_D(\hat{f}) := \frac{1}{m} \sum_{i=1}^{m} \mathcal{L}(y_i, g_{\hat{f}}(x_i)) \approx \mathcal{E}(\hat{f})$$

$$\text{Var} \left( \hat{E}_D(\hat{f}) \right) \approx \frac{1}{m(m-1)} \sum_{i=1}^{m} \left( \mathcal{L}(y_i, g_{\hat{f}}(x_i)) - \hat{E}_D(\hat{f}) \right)^2$$
Estimated generalisation error

The *estimated generalisation error* based on dataset $\mathcal{D} = ((x_1, y_1), \ldots, (x_m, y_m))$, where $(x_i, y_i) \overset{iid}{\sim} \pi_{XY}$ is,

$$\hat{E}_\mathcal{D}(\hat{f}) := \frac{1}{m} \sum_{i=1}^{m} \mathcal{L}(y_i, g\hat{f}(x_i)) \approx \mathcal{E}(\hat{f})$$

$$\text{Var} \left( \hat{E}_\mathcal{D}(\hat{f}) \right) \approx \frac{1}{m(m-1)} \sum_{i=1}^{m} \left( \mathcal{L}(y_i, g\hat{f}(x_i)) - \hat{E}_\mathcal{D}(\hat{f}) \right)^2$$

- $\mathcal{D}$ = data used to fit $\hat{f} \implies$ training/apparent error
- $\mathcal{D}$ = different iid data from $\pi_{XY} \implies$ test error
Example in notes
Training/apparent error

Problems with training/apparent error

1. estimate is constrained to the same predictor/feature values as in the data that was used to fit the model;

2. model fitting specifically adapted to the particular responses in the training data, so the error not representative of future responses, even when made at same predictor values.

So ...

- training/apparent error is biased (point 2); and
- estimating subtly different quantity (point 1)! In-sample fixed inputs error:

\[
\text{Err} := \mathbb{E}_{Y \mid X=x_i} \left[ \mathcal{L}(Y, g^\hat{f}(x_i)) \right] \quad \hat{\text{Err}} := \frac{1}{n} \sum_{i=1}^{n} \mathcal{L}(y_i, g^\hat{f}(x_i))
\]
What to predict?

Note, by total law of expectation:

\[
\mathcal{E}(f) = \mathbb{E}_{XY} \left[ \mathcal{L}(Y, g_f(X)) \right] \\
= \mathbb{E}_X \left[ \mathbb{E}_{Y \mid X} \left[ \mathcal{L}(Y, g_f(X)) \mid X = x \right] \right]
\]

∴ pointwise solution to minimise generalisation error means we should ideally choose for our prediction function \( g_f(X) \) to predict:

\[
g^*(x) := \arg \min_{z \in Y} \mathbb{E}_{Y \mid X} \left[ \mathcal{L}(Y, z) \mid X = x \right]
\]

This is the so-called Bayes predictor.
Bayes predictor: 0-1 loss

\[ g^*(x) = \arg\min_{z \in \mathcal{Y}} \mathbb{E} \left[ \mathbb{1}\{Y \neq z\} \mid X = x \right] \]

\[ = \arg\min_{z \in \mathcal{Y}} \mathbb{P} (Y \neq z \mid X = x) \]

\[ = \arg\min_{z \in \mathcal{Y}} 1 - \mathbb{P} (Y = z \mid X = x) \]

\[ = \arg\max_{z \in \mathcal{Y}} \mathbb{P} (Y = z \mid X = x) \]

\[ \therefore (Y \mid X = x) \sim \text{Categorical} \left( (p_1, \ldots, p_g) = f(x) \right) \]
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\]

\[
\implies g^*(x) = \arg \max_{j \in \{1, \ldots, g\}} f_j(x)
\]
Bayes predictor: 0-1 loss

\[ g^*(x) = \arg\min_{z \in Y} \mathbb{E} [\mathbb{1}\{Y \neq z\} | X = x] \]

\[ = \arg\min_{z \in Y} \mathbb{P} (Y \neq z | X = x) \]

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\[ \implies g^*(x) = \arg \max_{j \in \{1, \ldots, g\}} f_j(x) \]

\[ \implies g_f(x) = \arg \max_{j \in \{1, \ldots, g\}} \hat{f}_j(x) \]
Bayes predictor: square loss

Similarly,

\[ g^*(x) = \arg \min_{z \in \mathcal{Y}} \mathbb{E} \left[ (Y - z)^2 \mid X = x \right] \]

\[ = \arg \min_{z \in \mathcal{Y}} \mathbb{E} \left[ ((Y - \mathbb{E} [Y \mid X = x]) + (\mathbb{E} [Y \mid X = x] - z))^2 \mid X = x \right] \]

\[ = \mathbb{E} [Y \mid X = x] \]

\[ \therefore \quad Y = f(X) + \varepsilon, \varepsilon \text{ zero mean} \]

\[ \implies g^*(x) = f(x) \]

\[ \implies g_{\hat{f}}(x) = \hat{f}(x) \]
Bayes error & excess risk

The *Bayes error* is the generalisation error which arises when using the Bayes predictor,

$$\mathcal{E}^* = \mathbb{E}_X \left[ \inf_{z \in Y} \mathbb{E}_Y | X [\mathcal{L}(Y, z) | X = x] \right]$$

Best performance one could hope to achieve!
The **Bayes error** is the generalisation error which arises when using the Bayes predictor,

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Best performance one could hope to achieve! *Never achievable!*

The excess risk is the increase in generalisation error above the Bayes error suffered by a given fitted model $\hat{f}$, that is, $\mathcal{E}(\hat{f}) - \mathcal{E}^*$. 
Error decompositions

\[ \mathcal{E}(\hat{f}) = \mathbb{E}(\hat{f}) - \mathbb{E}(f) \]

reducible error

\[ \mathbb{E}(f) - \hat{f} \]

irreducible error

\[ \mathbb{E}(f) - \mathbb{E}(\hat{f}) \]
Error decompositions

\[ \mathcal{E}(\hat{f}) = \mathcal{E}(\hat{f}) \]
Error decompositions

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Error decompositions

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\[ \text{estimation error} \]
Error decompositions

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\[ = \mathcal{E}(\hat{f}) - \inf_{f \in \mathcal{F}} \mathcal{E}(f) + \inf_{f \in \mathcal{F}} \mathcal{E}(f) - \mathcal{E}^* + \mathcal{E}^* \]

\[
\begin{align*}
\text{estimation error} & \quad \text{approximation error} \\
\end{align*}
\]
Error decompositions

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- estimation error
- approximation error
- reducible error (≡ excess risk)
Error decompositions

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- **Reduction error**
  - estimation error
  - approximation error
  - irreducible error (\(\equiv\) excess risk)
Error decompositions

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- estimation error
- approximation error
- reducible error (≡excess risk)

\[ \mathbb{E}[(Y - \hat{f}(X))^2] = \mathbb{E}\left[\left(f(X) - \hat{f}(X)\right)^2\right] + \text{Var}(\varepsilon) \]

- reducible error
- irreducible error
Recap

Take a breath:

- Loss functions to assess quality of prediction
Recap

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But ... so far, everything predicated on fixed, already fitted \( \hat{f} \)!
Training data

So far, model dependency on data \( \mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\} \) “hidden” to simplify notation and data fixed realisation.

\( \hat{f}(x) \) could be written \( \hat{f}(x \mid \mathcal{D}) \) to stress it is a model fitted to that data ... change the data, model changes (obviously!)
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So far, model dependency on data $\mathcal{D} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ “hidden” to simplify notation and data fixed realisation.

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$$D_n := ((X_1, Y_1), \ldots, (X_n, Y_n))$$

defined to be the random variable for $n$ observations from joint distribution

$$\pi_{XY}^n := \pi_{XY} \times \cdots \times \pi_{XY}^{n \text{ times}}$$

So, $\hat{f}(x \mid \mathcal{D}_n)$ is realisation of $\hat{f}(x \mid D_n)$
$X \sim \text{Unif}(-1, 1.1), (Y \mid X = x) \sim \mathcal{N}(\mu = 5x^3 + 2x^2 - 2x, \sigma = 1)$
Generalisation error and model complexity

![Graph showing generalisation error and model complexity](image-url)
The *double descent* phenomenon

![Graph showing the double descent phenomenon](image)

- Model complexity
- Generalisation error
- Data
  - Test
  - Train

Interpolation threshold
Expected (prediction) error

The *expected error* of a learning algorithm which learns $\hat{f} \in \mathcal{F}$ given data sample $D_n \sim \pi^n_{XY}$ is,

$$\bar{E}_n := \mathbb{E}_{D_n} \left[ \mathcal{E}(\hat{f}) \right] = \mathbb{E}_{D_n} \left[ \mathbb{E}_{XY} \left[ \mathcal{L}(Y, g_{\hat{f}}(X | D_n)) \right] \right]$$
Expected (prediction) error

The expected error of a learning algorithm which learns \( \hat{f} \in \mathcal{F} \) given data sample \( D_n \sim \pi^n_{XY} \) is,

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\]

Sometimes more interested in the expected prediction error of a learning algorithm at a particular predictor value \( X = x \),

\[
\bar{E}_n(x) := \mathbb{E}_{D_n} \left[ \mathbb{E}_{Y \mid X=x} \left[ \mathcal{L}(Y, g_{\hat{f}}(X \mid D_n)) \right] \right]
\]

where now the inner expectation is conditioned on the predictor.
Consistency

A learning algorithm is *consistent* for $\pi_{XY}$ if it is asymptotically Bayes error efficient.

i.e. if the expected error converges to the Bayes error in the limit as the sample size grows,

$$\mathbb{E}_{D_n} \left[ \mathbb{E}_{XY} \left[ \mathcal{L}(Y, g_f(X \mid D_n)) \right] \right] \rightarrow \mathcal{E}^* \text{ as } n \rightarrow \infty$$
Consistency

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A learning algorithm is *universally consistent* if it is consistent for all data generating measures \( \pi_{XY} \).
A learning algorithm is *consistent* for $\pi_{XY}$ if it is asymptotically Bayes error efficient.

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A learning algorithm is *universally consistent* if it is consistent for all data generating measures $\pi_{XY}$.

**The catch:** universally consistent methods can be very data hungry, so often underperform non-universally consistent methods in finite data regime!
Learning curves
Table 1: Relationship between types of error

<table>
<thead>
<tr>
<th></th>
<th>Fixed inputs</th>
<th>Random inputs</th>
</tr>
</thead>
<tbody>
<tr>
<td>Fixed training set</td>
<td>Err(·)</td>
<td>$\mathcal{E}(\cdot)$</td>
</tr>
<tr>
<td>Random training set</td>
<td>*</td>
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</tr>
</tbody>
</table>
Full error decomposition (I)

For square loss, taking expectations wrt $D_n$ of the earlier decomposition:

$$\bar{\mathcal{E}}_n = \mathbb{E}_{D_n} \mathbb{E}_{XY} \left[ (Y - \hat{f}(X))^2 \right] = \mathbb{E}_{D_n} \mathbb{E}_{XY} \left[ (f(X) - \hat{f}(X))^2 \right] + \mathbb{E}_{D_n} \text{Var}_{XY}(\varepsilon)$$
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$$\mathbb{E}_{D_n} \mathbb{E}_{XY} \left[ (f(X) - \hat{f}(X))^2 \right] = \underbrace{\mathbb{E}_{XY} \mathbb{E}_{D_n}}_{\text{Fubini-Tonelli Theorem}} \left[ (f(X) - \hat{f}(X))^2 \right]$$
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\tilde{\mathcal{E}}_n = \mathbb{E}_{D_n} \mathbb{E}_{XY} \left[ (Y - \hat{f}(X))^2 \right] = \mathbb{E}_{D_n} \mathbb{E}_{XY} \left[ (f(X) - \hat{f}(X))^2 \right] + \mathbb{E}_{D_n} \text{Var}_{XY}(\varepsilon)
$$

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$$

\text{Fubini-Tonelli Theorem}

$$
= \mathbb{E}_{XY} \mathbb{E}_{D_n} \left[ \left( (f(X) - \mathbb{E}_{D_n} \hat{f}(X)) + (\mathbb{E}_{D_n} \hat{f}(X) - \hat{f}(X)) \right)^2 \right] \quad \text{just } \pm \text{ same term}
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\[ = \mathbb{E}_{XY} \mathbb{E}_{D_n} \left[ (f(X) - \mathbb{E}_{D_n} \hat{f}(X))^2 + \left( \mathbb{E}_{D_n} \hat{f}(X) - \hat{f}(X) \right)^2 \right. \]

\[ + \left. 2 \left( f(X) - \mathbb{E}_{D_n} \hat{f}(X) \right) \left( \mathbb{E}_{D_n} \hat{f}(X) - \hat{f}(X) \right) \right] \]
Full error decomposition (II)

\[ \mathbb{E}_{XY} \mathbb{E}_{D_n} \left[ 2 \left( f(X) - \mathbb{E}_{D_n} \hat{f}(X) \right) \left( \mathbb{E}_{D_n} \hat{f}(X) - \hat{f}(X) \right) \right] \]

constant wrt training data

\[ = 0 \]
Full error decomposition (II)

\[
\mathbb{E}_{X,Y} \mathbb{E}_{D_n} \begin{bmatrix}
2 \left( f(X) - \mathbb{E}_{D_n} \hat{f}(X) \right) \left( \mathbb{E}_{D_n} \hat{f}(X) - \hat{f}(X) \right)
\end{bmatrix}
\begin{cases}
\text{constant wrt training data}
\end{cases}
\]

\[
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\[
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\]
Full error decomposition (III)

\[ \bar{\mathcal{E}}_n = \mathbb{E}_{XY} \mathbb{E}_{Dn} \left[ (f(X) - \mathbb{E}_{Dn} \hat{f}(X))^2 \right] \]

squared bias of model

\[ + \mathbb{E}_{XY} \mathbb{E}_{Dn} \left[ \left( \mathbb{E}_{Dn} \hat{f}(X) - \hat{f}(X) \right)^2 \right] \]

variance of model fit

\[ + \text{Var}_{XY}(\epsilon) \]

irreducible error
Full error decomposition (III)

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\]

This is a lot more complicated in the non-square loss case, but similar decompositions can be derived.
Bias, variance and irreducible error

**Bias**

How well could my model, \( \hat{f}(\cdot) \), possibly approximate the true deterministic part of the relationship, \( f(\cdot) \), assuming I could see as much data as I like?

**Variance**

How sensitive is the fitting of my model, \( \hat{f}(\cdot) \), to the actual finite amount of data I have to learn from?

**Irreducible error**

How much “true” randomness is there inherent to the problem which we could never hope to deterministically model?
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Irreducible error

How much “true” randomness is there inherent to the problem which we could never hope to deterministically model?

Maybe just need very flexible models than can be accurately fitted to problems with little inherent randomness? As we saw, these things all interact in a difficult way.
Model fitting

Broadly three categories of ML model:

1. Full probabilistic model;

2. Parametric family without explicit probabilistic structure;

3. Local method constructing non-parametric empirical estimator;
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   → empirical estimate of Bayes predictor
Model fitting: ERM

\( \mathcal{F} \) a model family (or hypothesis space) parameterised by \( \theta \in \Theta \).

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\mathcal{F} = \{ f(\cdot|\theta) : \theta \in \Theta \}
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\]

Assume dataset \( \mathcal{D} = ((x_1, y_1), \ldots, (x_n, y_n)) \overset{iid}{\sim} \pi^n_{XY} \).

Fit a model \( \hat{f} \in \mathcal{F} \) to \( \mathcal{D} \) using empirical risk minimisation of a loss function \( \mathcal{L}(\cdot, \cdot) \) as

\[
\hat{f}(\cdot) = f(\cdot | \hat{\theta}) \text{ where } \hat{\theta} = \arg \min_{\theta \in \Theta} \sum_{(x,y) \in \mathcal{D}} \mathcal{L}(y, f(x | \theta))
\]
Model fitting: local methods

Imagining target loss of interest is squared loss, we know optimal Bayes predictor is:

$$g^*(x) = \mathbb{E}[Y \mid X = x]$$

Local methods just estimate this value directly using data “local” (under some metric) to $x$. 
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- conceptually simple
- easy to implement
- hard to scale with dimensionality
- easy to overfit
Do **not** blindly perform ERM if ∃ plausible probabilistic model!

Unsurprisingly, *if* assumptions of full probabilistic model are approximately satisfied, then full likelihood or Bayesian methods usually give better model fit and better predictive performance.
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**Trivial Example:** \( Y \sim N(\mu, \sigma^2) \)

- Variance of mean: \( \frac{\sigma^2}{n} \)
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\( \implies \) favour computing mean (min sq loss) versus computing median (min abs loss) for either sq or abs loss!
Regularisation

Note standard approaches to regularisation (see APTS High-dim stats module) apply to machine learning too:

$$\arg\min_{\theta \in \Theta} \sum_{(x,y) \in D} L(y, f(x | \theta)) + \lambda C(\theta)$$

where $C(\theta)$ measures model complexity; $\lambda$ controls extent of regularisation.

eg, ridge regression, $C(\theta) = \|\theta\|_2^2$; or lasso regression, $C(\theta) = \|\theta\|_1$
Proper scoring rules (I)

Not all losses created equally!

As statisticians, we should care if whole probabilistic forecast is good, not just point estimate. Losses which are proper scoring rules (Gneiting and Raftery, 2007) ensure *calibration*. 
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Let $\mathcal{P}$ be the space of probability distributions on $\mathcal{Y}$. *Scoring rule* is function

$$S: \mathcal{P} \times \mathcal{Y} \rightarrow \mathbb{R}$$

giving numerical value to probabilistic prediction $P \in \mathcal{P}$ and associated outcome $y \in \mathcal{Y}$. 
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giving numerical value to probabilistic prediction $P \in \mathcal{P}$ and associated outcome $y \in Y$.

A scoring rule is said to be a proper scoring rule if

$$\mathbb{E}_{Y | X} S(\pi_{Y | X}, Y) \geq \mathbb{E}_{Y | X} S(P, Y) \forall P \in \mathcal{P}$$

The rule is said to be strictly proper when equality occurs if and only if $P \equiv \pi_{Y | X}$. 
Regression:
- square loss: proper
- absolute loss: proper
- likelihood: strictly proper

Classification:
- 0-1 loss: proper
- cross entropy: strictly proper
- Brier: strictly proper
Proper scoring rules: example (based on Štrumbelj, 2018)
Limitations

“Remember that all models are wrong; the practical question is how wrong do they have to be to not be useful.”
— Box and Draper (1987), pp.74

“[…] all models are approximations. Essentially, all models are wrong, but some are useful. However, the approximate nature of the model must always be borne in mind.”
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Wolpert (1996) “no free lunch theorems”: for any learning method there exists a π_{XY} for which it will be arbitrarily bad.
Theorem 7.1, Devroye et al. (1996)

Let $\varepsilon > 0$ be an arbitrarily small real value. For any integer $n$ and classification rule $g_n$, there exists a distribution $\pi_{XY}$ (for $Y$ binary) with Bayes error zero, $\mathcal{E}^* = 0$, such that

$$\bar{\mathcal{E}}_n = \mathbb{E}_{D_n} \left[ \mathbb{E}_{XY} [L(Y, g_n(X | D_n))] \right] \geq \frac{1}{2} - \varepsilon$$

when $L$ is 0-1 loss.

That is, for any sample size $n$ there exists a distribution $\pi_{XY}$ for which the learning method performs arbitrarily badly.
References I


