COMP 551 – Applied Machine Learning
Lecture 2: Linear regression

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Class web page: www.cs.mcgill.ca/~jpineau/comp551

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Today’s Quiz (informal)

Write down the 3 most useful insights you gathered from the article:

“A Few Useful Things to Know About Machine Learning”.
Supervised learning

• Given a set of **training examples**: \( x_i = < x_{i1}, x_{i2}, x_{i3}, \ldots, x_{in}, y_i > \)
  
  \( x_{ij} \) is the \( j^{th} \) feature of the \( i^{th} \) example

  \( y_i \) is the desired **output** (or **target**) for the \( i^{th} \) example.

  \( X_j \) denotes the \( j^{th} \) feature.

• We want to learn a function \( f : X_1 \times X_2 \times \ldots \times X_n \rightarrow Y \)
  
  which maps the input variables onto the output domain.

<table>
<thead>
<tr>
<th>tumor size</th>
<th>texture</th>
<th>perimeter</th>
<th>\ldots</th>
<th>outcome</th>
<th>time</th>
</tr>
</thead>
<tbody>
<tr>
<td>18.02</td>
<td>27.6</td>
<td>117.5</td>
<td></td>
<td>N</td>
<td>31</td>
</tr>
<tr>
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<td>122.8</td>
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<td>61</td>
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<tr>
<td>20.29</td>
<td>14.34</td>
<td>135.1</td>
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<td>R</td>
<td>27</td>
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Supervised learning

• Given a dataset \( X \times Y \), find a function: \( f : X \rightarrow Y \) such that \( f(x) \) is a good predictor for the value of \( y \).

• Formally, \( f \) is called the **hypothesis**.

• Output \( Y \) can have many types:
  – If \( Y = \mathbb{R} \), this problem is called **regression**.
  – If \( Y \) is a finite discrete set, the problem is called **classification**.
  – If \( Y \) has 2 elements, the problem is called **binary classification**.
Prediction problems

• The problem of predicting tumour recurrence is called: **classification**

• The problem of predicting the time of recurrence is called: **regression**

• Treat them as two separate supervised learning problems.

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<td>135.1</td>
<td>R</td>
<td>27</td>
</tr>
</tbody>
</table>

...
Variable types

- **Quantitative**, often real number measurements.
  - Assumes that similar measurements are similar in nature.

- **Qualitative**, from a set (categorical, discrete).
  - E.g. {Spam, Not-spam}

- **Ordinal**, also from a discrete set, without metric relation, but that allows ranking.
  - E.g. {first, second, third}
The i.i.d. assumption

• In supervised learning, the examples $x_i$ in the training set are assumed to be \textit{independently} and \textit{identically distributed}.

  – Independently: Every $x_i$ is freshly sampled according to some probability distribution $D$ over the data domain $X$.

  – Identically: The distribution $D$ is the same for all examples.

• Why?
Empirical risk minimization

For a given function class $F$ and training sample $S$,

- Define a notion of error (*left intentionally vague for now*):
  $$L_S(f) = \# \text{ mistakes made on the sample } S$$

- Define the Empirical Risk Minimization (ERM):
  $$\text{ERM}_F(S) = \text{argmin}_{f \in F} L_S(f)$$
  where \text{argmin} returns the function $f$ (or set of functions) that achieves the minimum loss on the training sample.

- Easier to minimize the error with i.i.d. assumption.
A regression problem

- What hypothesis class should we pick?

<table>
<thead>
<tr>
<th>Observe</th>
<th>Predict</th>
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<tbody>
<tr>
<td>X</td>
<td>Y</td>
</tr>
<tr>
<td>0.86</td>
<td>2.49</td>
</tr>
<tr>
<td>0.09</td>
<td>0.83</td>
</tr>
<tr>
<td>-0.85</td>
<td>-0.25</td>
</tr>
<tr>
<td>0.87</td>
<td>3.10</td>
</tr>
<tr>
<td>-0.44</td>
<td>0.87</td>
</tr>
<tr>
<td>-0.43</td>
<td>0.02</td>
</tr>
<tr>
<td>-1.1</td>
<td>-0.12</td>
</tr>
<tr>
<td>0.40</td>
<td>1.81</td>
</tr>
<tr>
<td>-0.96</td>
<td>-0.83</td>
</tr>
<tr>
<td>0.17</td>
<td>0.43</td>
</tr>
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Linear hypothesis

• Suppose $Y$ is a **linear function** of $X$:

$$f_W(X) = w_0 + w_1 x_1 + \ldots + w_m x_m$$

$$= w_0 + \sum_{j=1:m} w_j x_j$$

• The $w_j$ are called **parameters** or **weights**.

• To simplify notation, we add an attribute $x_0=1$ to the $m$ other attributes (also called **bias term** or **intercept**).

How should we pick the **weights**?
Least-squares solution method

• The linear regression problem: \[ f_w(X) = w_0 + \sum_{j=1:m} w_j x_j \]
  where \( m \) = the dimension of observation space, i.e. number of features.

• **Goal:** Find the best linear model given the data.

• Many different possible evaluation criteria!

• Most common choice is to find the \( w \) that minimizes:

\[
\text{Err}(w) = \sum_{i=1:n} (y_i - w^T x_i)^2
\]

(A note on notation: Here \( w \) and \( x \) are column vectors of size \( m+1 \).)
Least-squares solution for $X \in \mathbb{R}^2$

FIGURE 3.1. Linear least squares fitting with $X \in \mathbb{R}^2$. We seek the linear function of $X$ that minimizes the sum of squared residuals from $Y$.

How do we minimize (3.2)? Denote by $X$ the $N \times (p+1)$ matrix with each row an input vector (with a 1 in the first position), and similarly let $y$ be the $N$-vector of outputs in the training set. Then we can write the residual sum-of-squares as

$$RSS(\beta) = (y - X\beta)^T (y - X\beta).$$  \hspace{1cm} (3.3)

This is a quadratic function in the $p+1$ parameters. Differentiating with respect to $\beta$ we obtain

$$\frac{\partial RSS}{\partial \beta} = -2X^T (y - X\beta) \qquad \text{and} \qquad \frac{\partial^2 RSS}{\partial \beta \partial \beta^T} = 2X^T X.$$

Assuming (for the moment) that $X$ has full column rank, and hence $X^T X$ is positive definite, we set the first derivative to zero

$$X^T (y - X\beta) = 0 \quad \text{(3.5)}$$

to obtain the unique solution

$$\hat{\beta} = (X^T X)^{-1} X^T y. \quad \text{(3.6)}$$
Least-squares solution method

• Re-write in matrix notation: \[ f_w(X) = Xw \]

\[ Err(w) = (Y - Xw)^T(Y - Xw) \]

where \( X \) is the \( n \times m \) matrix of input data, \( Y \) is the \( n \times 1 \) vector of output data, \( w \) is the \( m \times 1 \) vector of weights.

• To minimize, take the derivative w.r.t. \( w \):

\[ \frac{\partial Err(w)}{\partial w} = -2 X^T (Y - Xw) \]

– You get a system of \( m \) equations with \( m \) unknowns.

• Set these equations to 0:

\[ X^T (Y - Xw) = 0 \]
Least-squares solution method

- We want to solve for $w$: $X^T (Y - Xw) = 0$

- Try a little algebra:
  
  $X^T Y = X^T X \hat{w}$

  $\hat{w} = (X^T X)^{-1} X^T Y$

  ($\hat{w}$ denotes the estimated weights)

- The fitted data:
  
  $\hat{Y} = X\hat{w} = X (X^T X)^{-1} X^T Y$

- To predict new data $X' \rightarrow Y'$:
  
  $Y' = X'\hat{w} = X' (X^T X)^{-1} X^T Y$
Example of linear regression

Example: What hypothesis class should we pick?

What is a plausible estimate of \( w \)?

Try it!
Data matrices

\[ X^T X = \]

\[
\begin{bmatrix}
0.86 & 0.09 & -0.85 & 0.87 & -0.44 & -0.43 & -1.10 & 0.40 & -0.96 & 0.17 \\
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1
\end{bmatrix}
\times
\begin{bmatrix}
0.86 & 1 \\
0.09 & 1 \\
-0.85 & 1 \\
0.87 & 1 \\
-0.44 & 1 \\
-0.43 & 1 \\
-1.10 & 1 \\
0.40 & 1 \\
-0.96 & 1 \\
0.17 & 1
\end{bmatrix}
\]

\[ = \begin{bmatrix}
4.95 & -1.39 \\
-1.39 & 10
\end{bmatrix}\]
Data matrices

\[ X^T Y = \]

\[ \begin{bmatrix}
  0.86 & 0.09 & -0.85 & 0.87 & -0.44 & -0.43 & -1.10 & 0.40 & -0.96 & 0.17 \\
  1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1
\end{bmatrix} \times \]

\[ \begin{bmatrix}
  2.49 \\
  0.83 \\
  -0.25 \\
  3.10 \\
  0.87 \\
  0.02 \\
  -0.12 \\
  1.81 \\
  -0.83 \\
  0.43
\end{bmatrix} \]

\[ = \begin{bmatrix}
  6.49 \\
  8.34
\end{bmatrix} \]
Solving the problem

\[ w = (X^T X)^{-1} X^T Y = \begin{bmatrix} 4.95 & -1.39 \\ -1.39 & 10 \end{bmatrix}^{-1} \begin{bmatrix} 6.49 \\ 8.34 \end{bmatrix} = \begin{bmatrix} 1.60 \\ 1.05 \end{bmatrix} \]

So the best fit line is \( y = 1.60x + 1.05 \).
Interpreting the solution

- Linear fit for a prostate cancer dataset
  - Features \( X = \{ \text{lcavol, lweight, age, lbph, svi, lcp, gleason, pgg45}\} \)
  - Output \( y \) = level of PSA (an enzyme which is elevated with cancer).
  - High coefficient weight (in absolute value) = important for prediction.

<table>
<thead>
<tr>
<th>Term</th>
<th>Coefficient</th>
<th>Std. Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>Intercept</td>
<td>( w_0 = 2.46 )</td>
<td>0.09</td>
</tr>
<tr>
<td>lcavol</td>
<td>0.68</td>
<td>0.13</td>
</tr>
<tr>
<td>lweight</td>
<td>0.26</td>
<td>0.10</td>
</tr>
<tr>
<td>age</td>
<td>-0.14</td>
<td>0.10</td>
</tr>
<tr>
<td>lbph</td>
<td>0.21</td>
<td>0.10</td>
</tr>
<tr>
<td>svi</td>
<td>0.31</td>
<td>0.12</td>
</tr>
<tr>
<td>lcp</td>
<td>-0.29</td>
<td>0.15</td>
</tr>
<tr>
<td>gleason</td>
<td>-0.02</td>
<td>0.15</td>
</tr>
<tr>
<td>pgg45</td>
<td>0.27</td>
<td>0.15</td>
</tr>
</tbody>
</table>
Computational cost of linear regression

• What operations are necessary?
  – Overall: 1 matrix inversion + 3 matrix multiplications
  – $X^TX$ (other matrix multiplications require fewer operations.)
    • $X^T$ is $mxn$ and $X$ is $nxm$, so we need $nm^2$ operations.
  – $(X^TX)^{-1}$
    • $X^TX$ is $mxm$, so we need $m^3$ operations.

• We can do linear regression in polynomial time, but handling large datasets (many examples, many features) can be problematic.
An alternative for minimizing mean-squared error (MSE)

• Recall the least-square solution: $$\hat{w} = (X^T X)^{-1} X^T Y$$

• What if $X$ is too big to compute this explicitly (e.g. $m \sim 10^6$)?

• Go back to the gradient step:

$$\text{Err}(w) = (Y - Xw)^T(Y - Xw)$$

$$\frac{\partial \text{Err}(w)}{\partial w} = -2 X^T (Y - Xw)$$

$$\frac{\partial \text{Err}(w)}{\partial w} = 2(X^T Xw - X^T Y)$$
Gradient-descent solution for MSE

- Consider the error function:

  - The gradient of the error is a vector indicating the direction to the minimum point.

- Instead of directly finding that minimum (using the closed-form equation), we can take small steps towards the minimum.

\[
\text{J}(w) = \frac{1}{2m} \sum_{i=1}^{m} (h_w(x_i) - y_i)^2
\]

\[
\nabla \text{J}(w) = \frac{1}{m} \sum_{i=1}^{m} (h_w(x_i) - y_i)x_i
\]

\[
w_{i+1} = w_i - \eta \nabla \text{J}(w_i)
\]

- In this case, the final solution may depend on the initial parameters.
Gradient-descent solution for MSE

• We want to produce a sequence of weight solutions, \( \mathbf{w}_0, \mathbf{w}_1, \mathbf{w}_2, \ldots \), such that: \( \text{Err}(\mathbf{w}_0) > \text{Err}(\mathbf{w}_1) > \text{Err}(\mathbf{w}_2) > \ldots \)

• The algorithm:

\[
\text{Given an initial weight vector } \mathbf{w}_0; \\
\text{Do for } k=1, 2, \ldots \ \text{ } \\
\mathbf{w}_{k+1} = \mathbf{w}_k - \alpha_k \frac{\partial \text{Err}(\mathbf{w}_k)}{\partial \mathbf{w}_k} \\
\text{End when } |\mathbf{w}_{k+1} - \mathbf{w}_k| < \varepsilon
\]

• Parameter \( \alpha_k > 0 \) is the step-size (or learning rate) for iteration \( k \).
Convergence

• Convergence depends in part on the $\alpha_k$.

• If steps are too large: the $w_k$ may oscillate forever.
  – This suggests that $\alpha_k \to 0$ as $k \to \infty$.

• If steps are too small: the $w_k$ may not move far enough to reach a local minimum.
Robbins-Monroe conditions

• The $\alpha_k$ are a Robbins-Monroe sequence if:

\[
\sum_{k=0}^{\infty} \alpha_k = \infty
\]

\[
\sum_{k=0}^{\infty} \alpha_k^2 < \infty
\]

• These conditions are sufficient to ensure convergence of the $w_k$ to a local minimum of the error function.

E.g. $\alpha_k = 1 / (k + 1)$ (averaging)

E.g. $\alpha_k = 1/2$ for $k = 1, \ldots, T$

$\alpha_k = 1/2^2$ for $k = T+1, \ldots, (T+1)+2T$

etc.
Local minima

- Convergence is **NOT** to a global minimum, only to local minimum.

- The blue line represents the error function. There is *no guarantee* regarding the amount of error of the weight vector found by gradient descent, compared to the globally optimal solution.
Convergence is **NOT** to a global minimum, only to local minimum.

For linear function approximations using Least-Mean Squares (LMS) error, this is not an issue: only **ONE** global minimum!

- Local minima affects many other function approximators.
Local minima

• Convergence is **NOT** to a global minimum, only to local minimum.

• For linear function approximations using Least-Mean Squares (LMS) error, this is not an issue: **only ONE** global minimum!
  – Local minima affects many other function approximators.

• **Repeated random restarts** can help (in all cases of gradient search).
A 3\textsuperscript{rd} optimization method: QR decomposition (optional)

- Consider the usual criteria: 
  \[ X^T(Y - Xw) = 0 \]

- Assume \( X \) can be decomposed: 
  \[ X = QR \]
  where \( Q \) is an \( nxm \) orthogonal matrix (i.e. \( Q^TQ = I \)), and \( R \) is an \( mxm \) upper triangular matrix.

- Replace \( X \) in equation above: 
  \[ (QR)^T Y = (QR)^T(QR)w \]

- Distribute the transpose: 
  \[ R^T Q^T Y = R^T Q^T Q R w \]

- Let \( Q^T Q = I \) and multiply by \( (R^T)^{-1} \) 
  \[ Q^T Y = R w \]

- Solution: \( \hat{w} = R^{-1} Q^T Y \)  
  The fitted outputs are: \( \hat{Y} = QQ^T Y \)

- This method is more numerically stable than others, and \( R^{-1} \) is fast to compute because upper triangular.

- Alternately, we can use singular value decomposition.
What you should know

- Definition and characteristics of a supervised learning problem.
- Linear regression (hypothesis class, cost function, algorithm).
- Closed-form least-squares solution method (algorithm, computational complexity, stability issues).
- Gradient descent method (algorithm, properties).
To-do

• Reproduce the linear regression example (slides 15-18), solving it using the software of your choice.

• Suggested complementary readings:
  – Ch.2 (Sec. 2.1-2.4, 2.9) of Hastie et al.
  – Ch.3 of Bishop.
  – Ch.9 of Shalev-Schwartz et al.

• Write down **midterm** date in agenda: Nov. 22, 6-8pm, Leacock 132.


• Office hours (confirmed): www.cs.mcgill.ca/~jpineau/comp551/syllabus.html