COMPSCI 389
Introduction to Machine Learning

Days: Tu/Th. **Time:** 2:30 – 3:45 **Building:** Morrill 2 **Room:** 222

Topic 5.6: Linear Regression and the Optimization Perspective

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Review: Regression

- X: **Input** (also called **features**, **attributes**, **covariates**, or **predictors**)
  - Typically, X is a vector, array, or list of numbers or strings.
- Y: **Output** (also called **labels** or **targets**)
  - In regression, Y is a real number.
- An input-output pair is (X, Y).
- Let n, called the **data set size**, be the number of input-output pairs in the data set.
- Let (X_i, Y_i) denote the i^{th} input output pair.
- The complete data set is
$$(X_i, Y_i)_{i=1}^{n} = \big((X_1, Y_1), (X_2, Y_2), \dots, (X_n, Y_n)\big).$$

Review: Nearest Neighbor (Variants)

- Given a query input x_{query}, find the k nearest points in the training data.
- Return a weighted average of their labels.
  - $k = 1$ is nearest neighbor
  - $k > 1$ with all w_i equal is k-nearest neighbor
  - $k > 1$ with not all w_i equal is weighted k-nearest neighbor
- These algorithms don't pre-process the training data much.
  - They can build data structures like KD-Trees for efficiency.

Linear Regression

- Search for the **line** that is a best fit to the data.
- Different performance measures correspond to different ways of measuring the quality of a fit.
- Sample mean squared error, or the sum of the squared errors is particularly common:

$$\widehat{\mathrm{MSE}}_n\!: \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \text{ and } \mathrm{SSE}\!: \sum_{i=1}^{n}(y_i - \hat{y}_i)^2$$

  - Although not identical, the line that minimizes one also minimizes the other.
- Using sample MSE, this method is called “least squares linear regression.”

Linear Regression: What is a line?

$$y = mx + b$$

Prediction, $\hat{y}_i$ Slope, m Input, x_i y-intercept, b

"weights," or "parameters", $w = (w_1, w_2)$

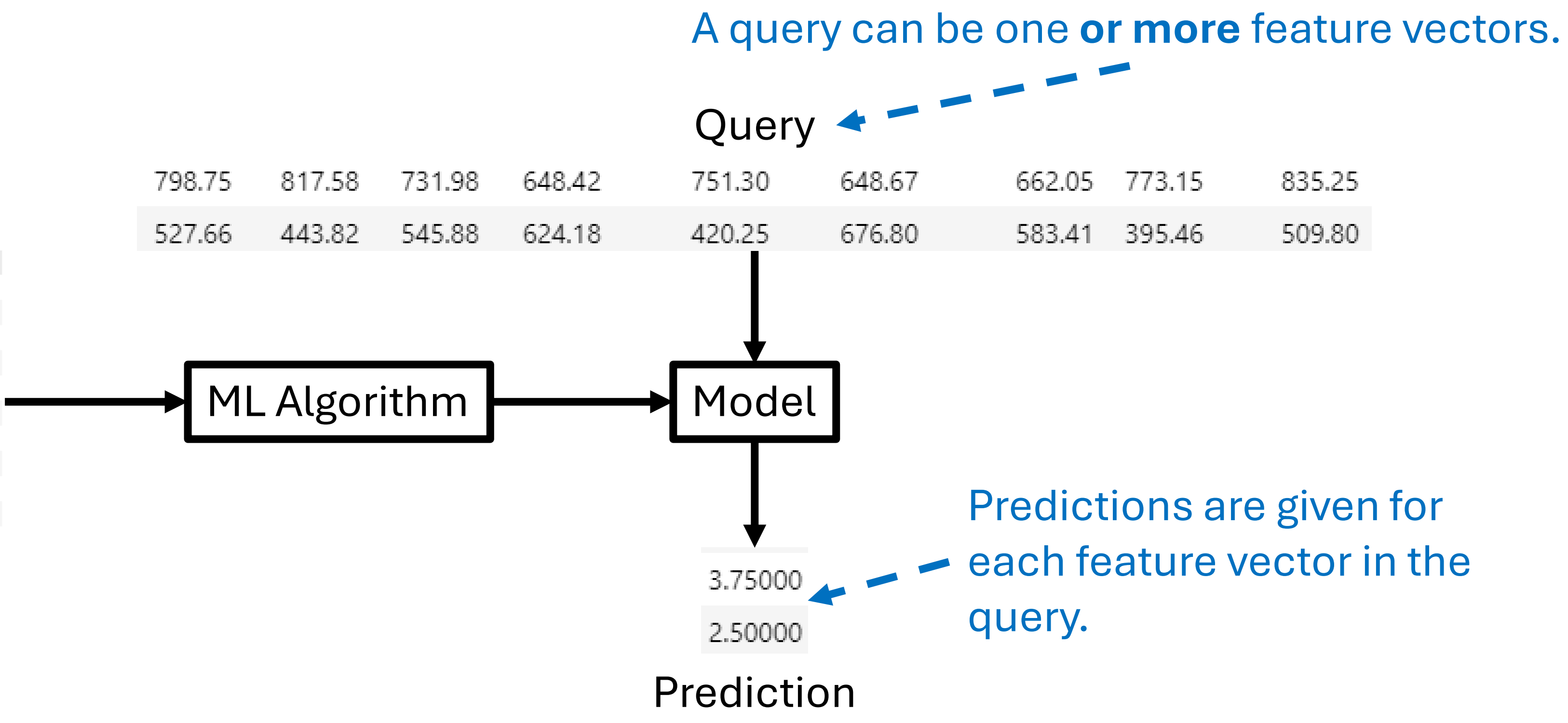
$$\hat{y} = w_1 x_i + w_2$$

Models (Review)

- A model is a mechanism that maps input data to predictions.
- ML algorithms take data sets as input and produce models as output.

	physics	biology	history	English	geography	literature	Portuguese	math	chemistry	gpa
0	622.60	491.56	439.93	707.64	663.65	557.09	711.37	731.31	509.80	1.33333
1	538.00	490.58	406.59	529.05	532.28	447.23	527.58	379.14	488.64	2.98333
2	455.18	440.00	570.86	417.54	453.53	425.87	475.63	476.11	407.15	1.97333
3	756.91	679.62	531.28	583.63	534.42	521.40	592.41	783.76	588.26	2.53333
4	584.54	649.84	637.43	609.06	670.46	515.38	572.52	581.25	529.04	1.58667
...	...	...	...	...	...	...	...	...	...	...
43298	519.55	622.20	660.90	543.48	643.05	579.90	584.80	581.25	573.92	2.76333
43299	816.39	851.95	732.39	621.63	810.68	666.79	705.22	781.01	831.76	3.81667
43300	798.75	817.58	731.98	648.42	751.30	648.67	662.05	773.15	835.25	3.75000
43301	527.66	443.82	545.88	624.18	420.25	676.80	583.41	395.46	509.80	2.50000
43302	512.56	415.41	517.36	532.37	592.30	382.20	538.35	448.02	496.39	3.16667

Data Set



Parametric Model

- A model "parameterized" by a weight vector w.
- Different settings of w result in different predictions.
- Let $\hat{y} = f_w(x)$
  - 1-dimensional linear case:

$$f_w(x) = w_1 x + w_2$$

Linear Regression: Hyperplanes

- What if we have more than one input feature?
- Let $x_i = (x_{i,1}, x_{i,2}, \ldots, x_{i,d})$ be a d-dimensional input.
  - We include the i subscript to make it clear that 1,2,… aren't referencing different input vectors, but different elements of one input vector.
- We use a *hyperplane*:

$$f_w(x_i) = w_1 x_{i,1} + w_2 x_{i,2} + \ldots + w_d x_{i,d} + w_{d+1}.$$

Slope along the first dimension

Rate of change of the prediction as the first feature increases

Slope along the second dimension
Rate of change of the prediction as the second feature increases

The **offset**, **bias**, or **intercept** term, which gives the prediction when the input features are all zero.

Linear Regression (cont.)

$$f_w(x_i) = w_1 x_{i,1} + w_2 x_{i,2} + \ \dots + w_d x_{i,d} + w_{d+1}.$$

- **Thought**: We don't want to have to keep remembering a special "intercept" term.
- **Idea**: Drop the intercept term!
  - If you want to include the intercept term, add one more feature to your data set, $x_{d+1} = 1$.
  - If d is the dimension of the input ***with*** this additional feature, we then have:
  $$f_w(x_i) = w_1 x_{i,1} + w_2 x_{i,2} + \ \dots + w_d x_{i,d}$$
  - We can write this as:
  $$f_w(x_i) = \sum_{j=1}^{d} w_j \, x_{i,j}.$$
  - This is called a **dot product** and can be written as $w \cdot x_i$ or $w^T x_i$.

Linear Regression (cont.)

$$\hat{y_i} = f_w(x_i) = \sum_{j=1}^{d} w_j \, x_{i,j}$$

- How many weights (parameters) does the model have?
    - d, the dimension of any one input vector x_i.
    - **Not** n, the number of training data points.

Linear Regression: Optimization Perspective

- Given a parametric model f_w of any form how can we find the weights w that result in the "best fit"?
- Let L be a function called a **loss function**.
  - It takes as input a model (or model weights w)
  - It also takes as input data D
  - It produces as output a real-number describing how *bad* of a fit the model is to the provided data.
- The evaluation metrics we have discussed can be viewed as loss functions. For example, the sample MSE loss function is:

$$L(w) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 = \frac{1}{n}\sum_{i=1}^{n}\left(y_i - f_w(x_i)\right)^2$$

For the sample MSE loss function, this can be *any* parametric model, not just a linear one!

- We phrase this as an **optimization problem**:

$$\operatorname{argmin}_w L(w, D)$$

Linear Regression: Optimization Perspective

$$\text{argmin}_w \, L(w, D)$$

- **Recall**: argmin returns the w that achieves the minimum value of $L(w, D)$, not the minimum value of $L(w, D)$ itself.
- This expression describes a *massive* range of ML methods.
  - Supervised, unsupervised, (batch/offline) RL
  - Deep neural networks
  - Large language models and generative AI
- Different problem settings and algorithms in ML correspond to:
  - Different loss functions
  - Different parametric models.
  - Different algorithms for approximating the best weight vector w.

Least Squares Linear Regression (cont.)

- Find the weights w that minimize

$$L(w, D) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - f_w(x_i) \right)^2$$

Number of training data points

Dimension of each input vector (number of features per row)

$$L(w, D) = \frac{1}{n} \sum_{i=1}^{n} \left(y_i - \sum_{j=1}^{d} w_j x_{i,j} \right)^2$$

Linear Regression: Least Squares Solvers

- How should one solve this problem?

$$\text{argmin}_w \ \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \sum_{j=1}^{d} w_j x_{i,j}\right)^2$$

- Answer: “Least squares solvers”
  - Algorithms based on concepts from linear algebra.
  - Extremely effective for solving problems of precisely this form.
  - Beyond the scope of this class.
  - **Only useful for this exact problem.**
    - Not effective when using other parametric models (e.g., not linear)
    - Not effective when using other loss functions / performance metrics.

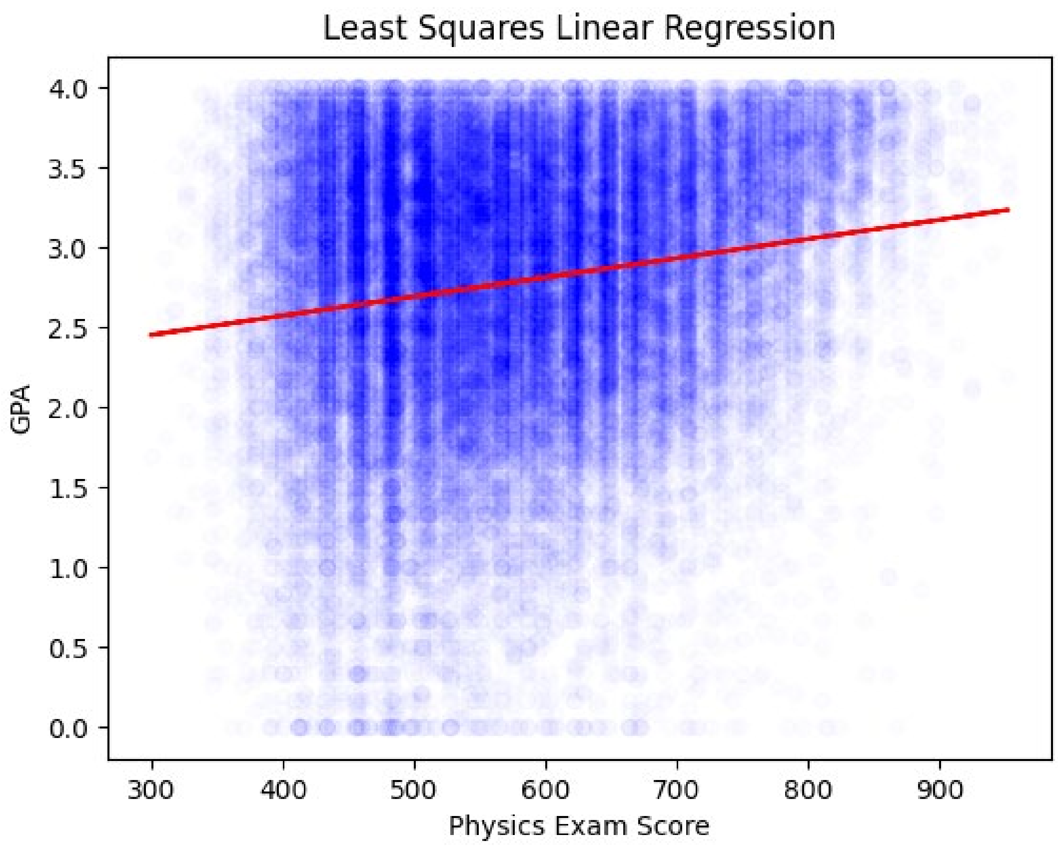
Linear Regression

- How **do we** solve this problem?

$$\operatorname{argmin}_w \frac{1}{n}\sum_{i=1}^{n}\left(y_i - \sum_{j=1}^{d} w_j x_{i,j}\right)^2$$

- We will study a different approach for solving this problem.
- It *is* less efficient.
- **It applies to almost all loss functions and parametric models of interest.**
- Method: Gradient descent.
  - Soon we will discuss gradient descent.
  - For now, assume we have some way of finding the $\operatorname{argmin}_w L(w, D)$.

Least Squares Linear Regression



Linear Regression vs Weighted k-NN for GPA Prediction

```
Weighted KNN Model:
    Average MSE: 0.571
    MSE Standard Error: 0.004

Linear Regression Model:
    Average MSE: 0.582
    MSE Standard Error: 0.004
```

Very simple method achieves nearly the same performance as a tuned-version of weighted *k*-NN!

Soon, we will consider more complex parametric models that can be even more effective.

Linear Regression Limitation

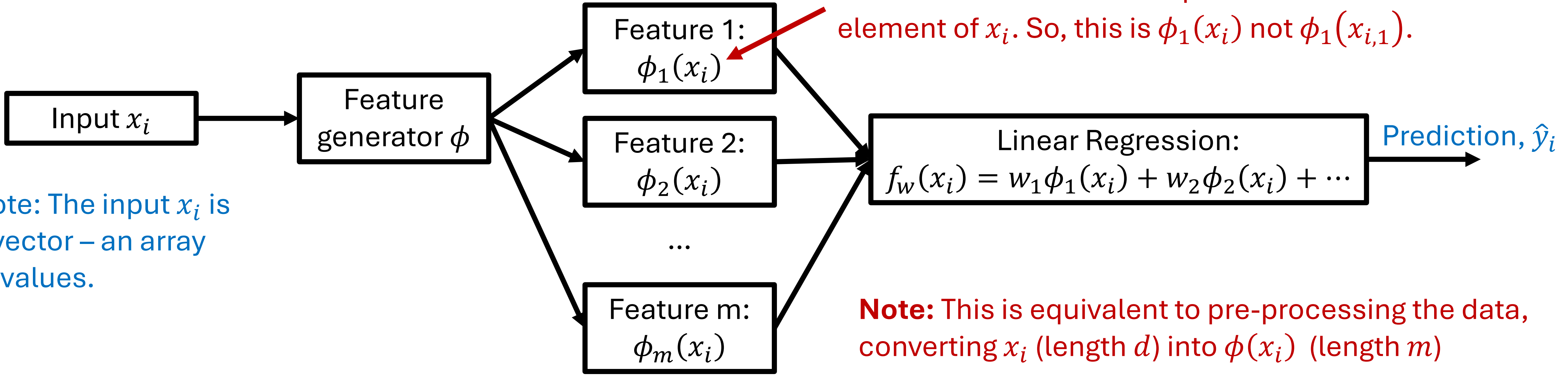
- What if the relationship between the inputs and outputs is not linear (or affine)?
  - Linear: $A_1 x_{i,1} + A_2 x_{i,2} + \cdots + A_n x_{i,n}$
  - Affine: $A_1 x_{i,1} + A_2 x_{i,2} + \cdots + A_n x_{i,n} + b$
    - Equivalent to linear with an additional feature $x_{i,n+1} = 1$.
- **Idea**: Have parametric functions that can represent more than linear functions!

Linear Parametric Model $\neq$ Linear Functions

- **Linear parametric functions** are functions $f_w(x_i)$ that are **linear functions of the weights w.**
- They need not be linear functions of the input x_i.

Each feature is a real number (not a vector or array)

Note: Each feature can depend on more than one element of x_i. So, this is $\phi_1(x_i)$ not $\phi_1(x_{i,1})$.



Note: The input x_i is a vector – an array of values.

Note: This is equivalent to pre-processing the data, converting x_i (length d) into $\phi(x_i)$ (length m)

Linear Parametric Model $\neq$Linear Functions

- **Linear parametric functions** are functions $f_w(x_i)$ that are **linear functions of the weights w**.
- They need not be linear functions of the input x_i.
- That is, a linear parametric model has the form:

$$f_w(x_i) = \sum_{j=1}^{m} w_j \phi_j(x_i)\,,$$

where ϕ takes the input vector x_i as input and produces a vector of m features as output. That is, $\phi_j(x_i)$ is the j^{th} feature output by ϕ.

- ϕ is called the **basis function, feature generator,** or **feature mapping function**.

Linear Parametric Model

$$f_w(x_i) = \sum_{j=1}^{m} w_j \phi_j(x_i)$$

- Polynomial basis
  - If $x_i \in \mathbb{R}$ then $\phi_j(x_i) = x_i^{j-1}$ so that:
    $$\phi(x_i) = \left[1, x_i, x_i^2, x_i^3, \dots, x_i^{m-1}\right]$$
  - Here $m - 1$ is the **degree** or **order** of the polynomial basis.
  - $f_w(x_i) = w_1 + w_2 x_i + w_3 x_i^2 + w_4 x_i^3 + \cdots + w_m x_i^{m-1}$
  - We are fitting a polynomial to the data!
  - This is a non-linear function of the input x_i
  - This can represent *any* smooth function (if m is big enough).
  - This is a linear function of w.