

Multiple Regression - Linear Regression with multiple features

Linear fit might not be the best fit to the data.

The data can be fit with a quadratic function or even a polynomial function.

- Simple Linear Regression - function $f(x) = w(0) + w(1) x$; Model $y(i) = w(0) + w(1) x(i) + \epsilon(i)$
- Quadratic function - $f(x) = w(0) + w(1) x + w(2) x^2$
- Higher order polynomial - $f(x) = w(0) + w(1) x + w(2) x^2 + \dots + w(p) x^p$

Polynomial regression

Model:

$$y_i = w_0 + w_1 x_i + w_2 x_i^2 + \dots + w_p x_i^p + \epsilon_i$$

treat as different features

feature 1 = 1 (constant) parameter 1 = w_0

feature 2 = x parameter 2 = w_1

feature 3 = x^2 parameter 3 = w_2

...

feature $p+1 = x^p$ parameter $p+1 = w_p$

In the polynomial regression each function of the input is treated as a separate feature.

Example : Detrending

- A dataset - log(house price) v/s Month
- Analysis captures : The house prices increase with time (linear relationship); The house prices lower in Nov-Dec (Seasonal);
- Therefore - Seasonal and Linear with time.

Model:

$$y_i = w_0 + w_1 t_i + w_2 \sin(2\pi t_i / 12 - \Phi) + \epsilon_i$$

Linear trend

Unknown phase/shift

Seasonal component =
Sinusoid with period 12
(resets annually)



Trigonometric identity: $\sin(a-b) = \sin(a)\cos(b) - \cos(a)\sin(b)$

$$\rightarrow \sin(2\pi t_i / 12 - \Phi) = \sin(2\pi t_i / 12)\cos(\Phi) - \cos(2\pi t_i / 12)\sin(\Phi)$$

Equivalently,

$$y_i = w_0 + w_1 t_i + w_2 \sin(2\pi t_i / 12) + w_3 \cos(2\pi t_i / 12) + \epsilon_i$$

feature 1 = 1 (constant)

feature 2 = t

feature 3 = $\sin(2\pi t/12)$

feature 4 = $\cos(2\pi t/12)$

- The dataset is fit with a 5th order polynomial.

Generic Model :

Model:

$$y_i = w_0 h_0(x_i) + w_1 h_1(x_i) + \dots + w_D h_D(x_i) + \epsilon_i$$

$$= \sum_{j=0}^D w_j h_j(x_i) + \epsilon_i$$

j^{th} feature

j^{th} regression coefficient
or weight

General notation

Output: y ← scalar

Inputs: $\mathbf{x} = (x[1], x[2], \dots, x[d])$

← d-dim vector

Notational conventions:

$x[j]$ = j^{th} input (scalar)

$h_j(\mathbf{x})$ = j^{th} feature (scalar)

\mathbf{x}_i = input of i^{th} data point (vector)

$x_i[j]$ = j^{th} input of i^{th} data point (scalar)

More on notation

observations $(\mathbf{x}_i, y_i) : N$

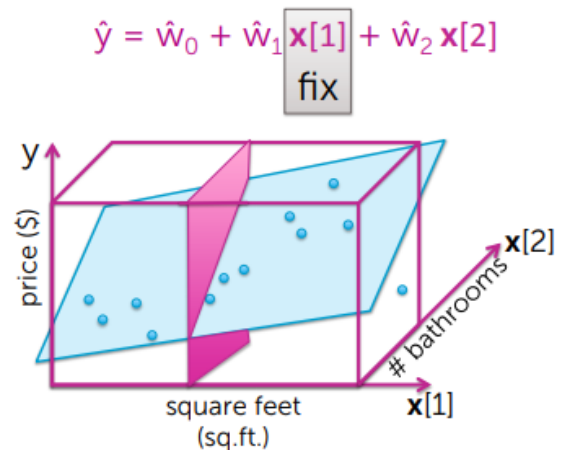
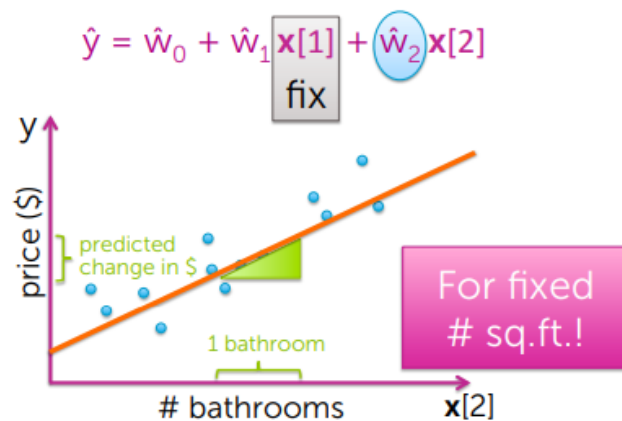
inputs $\mathbf{x}[j] : d$

features $h_j(\mathbf{x}) : D$

Interpreting the coefficients:

- While a model has multiple features the when interpreting the coefficient need to consider fix all the other inputs to the model and look at the focus feature.
- In case a house data - depends on features -> sqft of house and # of bathrooms.
- $x[1]$ -> sqft, $x[2]$ -> # bathrooms

Interpreting the coefficients – Two linear features



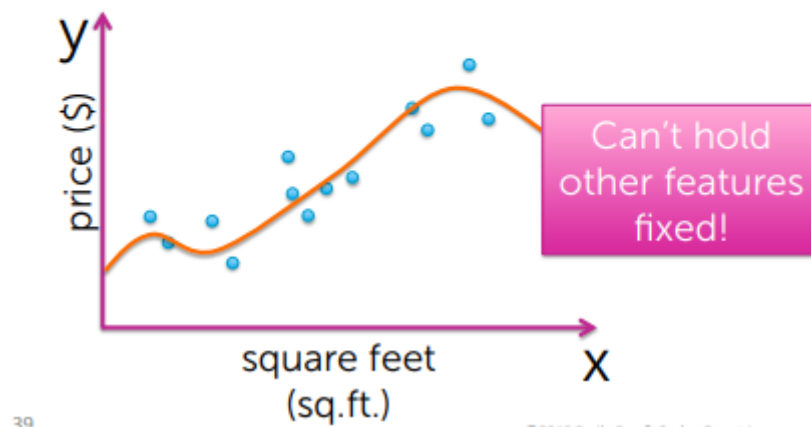
Interpreting the coefficients – Multiple linear features

$\hat{y} = \hat{w}_0 + \hat{w}_1 \mathbf{x}[1] + \dots + \hat{w}_j \mathbf{x}[j] + \dots + \hat{w}_d \mathbf{x}[d]$

fix fix fix fix

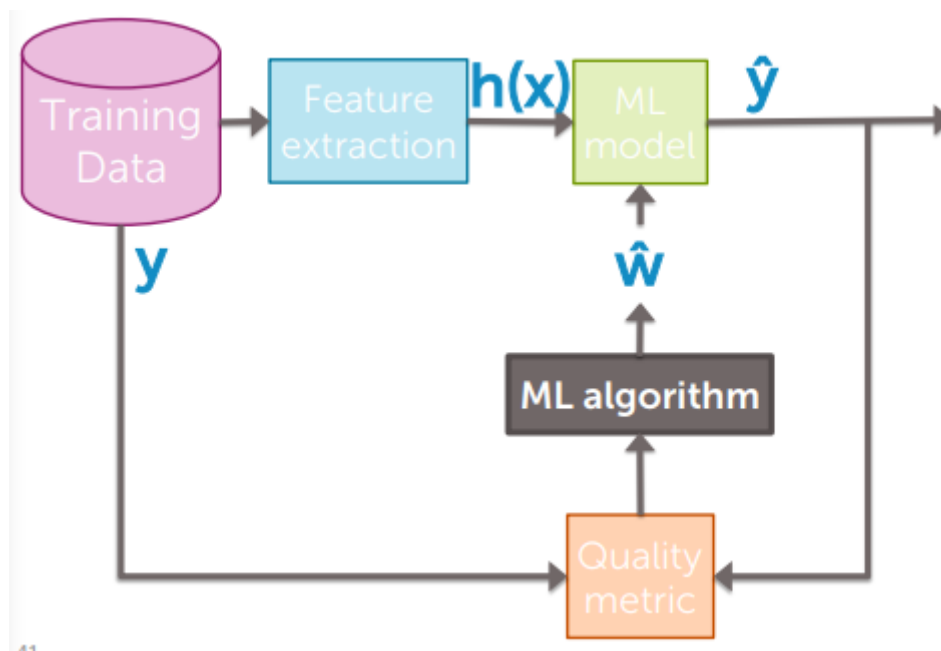
Interpreting the coefficients- Polynomial regression

$$\hat{y} = \hat{w}_0 + \hat{w}_1 x + \dots + \hat{w}_j x^j + \dots + \hat{w}_p x^p$$



In case of polynomial regression, since the model consist of powers of a single feature it is not possible to hold the other values still while focussing on one co-efficient.

Algorithms associated with Multiple Regression:



1. Closed form solution
2. Gradient descent

Step 1 : Rewrite in matrix notation:

- $w(j)$ -> parameters / co-efficients; -> vector
- $h(j)$ -> features of input; -> vector

For observation i

$$y_i = \sum_{j=0}^D w_j h_j(x_i) + \epsilon_i$$

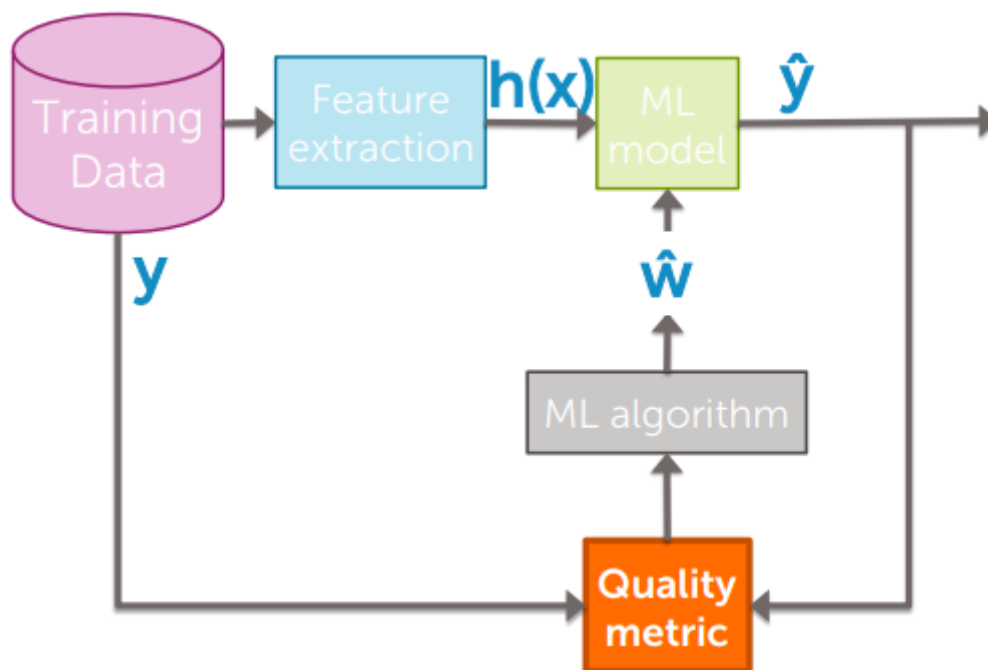
$$\begin{aligned} \mathbf{y} &= \begin{bmatrix} w_0 & w_1 & w_2 & \dots & w_D \end{bmatrix} \begin{bmatrix} h_0(x_i) \\ h_1(x_i) \\ h_2(x_i) \\ \vdots \\ h_D(x_i) \end{bmatrix} + \epsilon_i \\ &= \underbrace{w_0 h_0(x_i) + w_1 h_1(x_i) + \dots + w_D h_D(x_i)}_{\text{scalar}} + \epsilon_i \\ &= \mathbf{w}^T \mathbf{h}(x_i) + \epsilon_i \end{aligned}$$

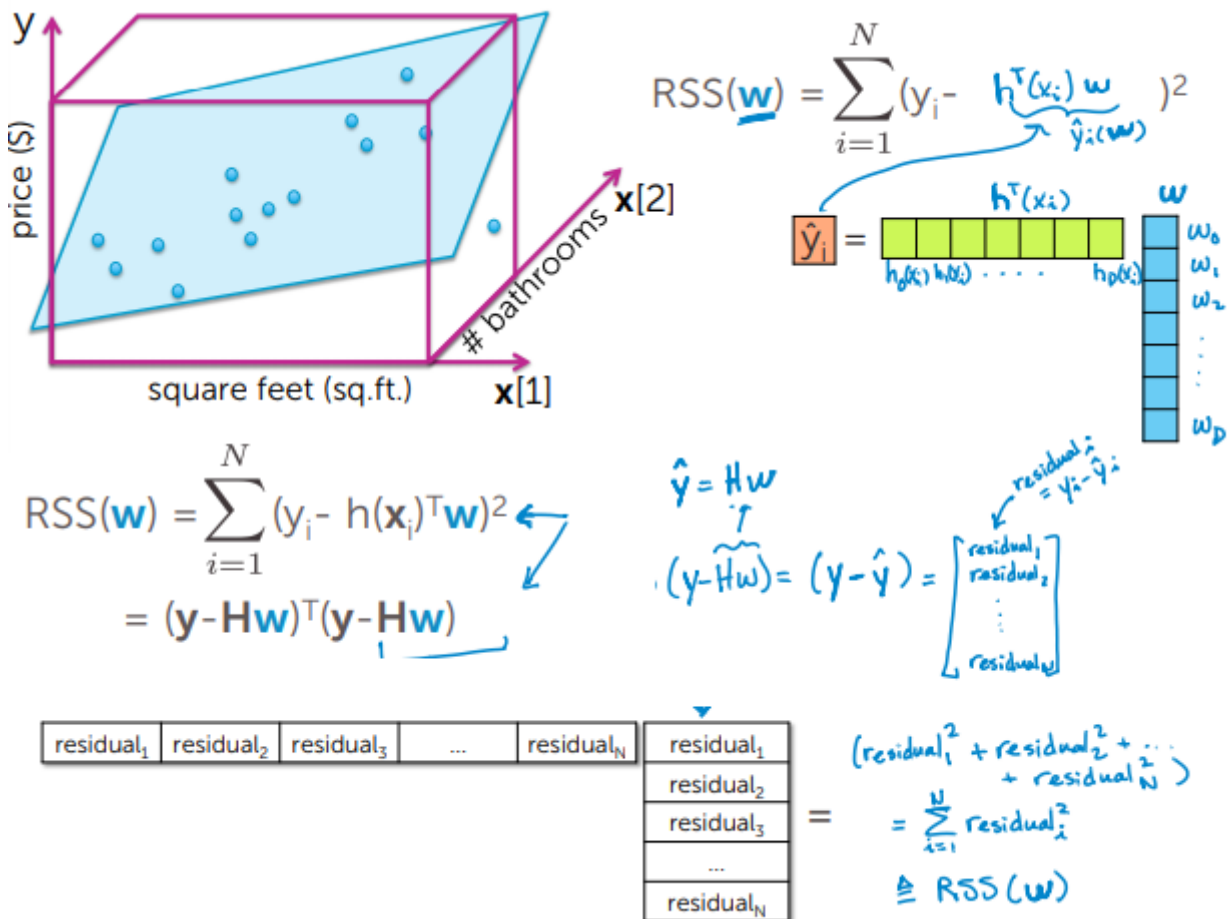
For all observations together

$$\begin{aligned} \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_N \end{bmatrix} &= \begin{bmatrix} h_0(x_1) & h_1(x_1) & h_2(x_1) & \dots & h_D(x_1) \\ h_0(x_2) & h_1(x_2) & h_2(x_2) & \dots & h_D(x_2) \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ h_0(x_N) & h_1(x_N) & h_2(x_N) & \dots & h_D(x_N) \end{bmatrix} \begin{bmatrix} w_0 \\ w_1 \\ w_2 \\ \vdots \\ w_D \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \vdots \\ \epsilon_N \end{bmatrix} \\ &\Rightarrow \mathbf{y} = \mathbf{H} \mathbf{w} + \boldsymbol{\epsilon} \end{aligned}$$

- The green-box - is a stack of all features per observation.

Step 2 : Compute the cost:





Step 3 : Take the gradient:

Gradient of RSS

$$\nabla RSS(\mathbf{w}) = \nabla [(\mathbf{y} - \mathbf{H}\mathbf{w})^T (\mathbf{y} - \mathbf{H}\mathbf{w})]$$

$$= -2\mathbf{H}^T (\mathbf{y} - \mathbf{H}\mathbf{w})$$

Why? By analogy to 1D case:

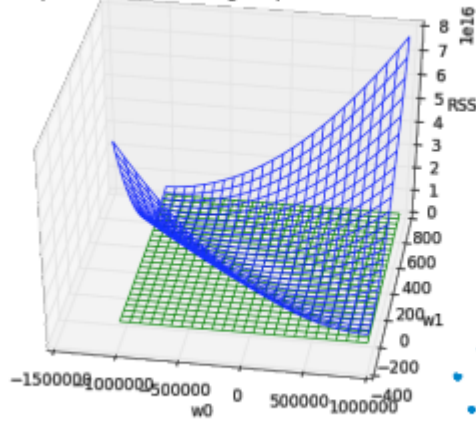
$$\frac{d}{dw} (y - hw)(y - hw) = \frac{d}{dw} (y - hw)^2 = 2 \cdot (y - hw)' (-h) = -2h(y - hw)$$

↑
scalars

Approach - 1 : Closed form

- Set the gradient = 0;

3D plot of RSS with tangent plane at minimum



$$\nabla \text{RSS}(\mathbf{w}) = -2\mathbf{H}^T(\mathbf{y} - \mathbf{H}\mathbf{w}) = 0$$

Solve for \mathbf{w} :

$$-\cancel{2}\mathbf{H}^T\mathbf{y} + \cancel{2}\mathbf{H}^T\mathbf{H}\hat{\mathbf{w}} = 0$$

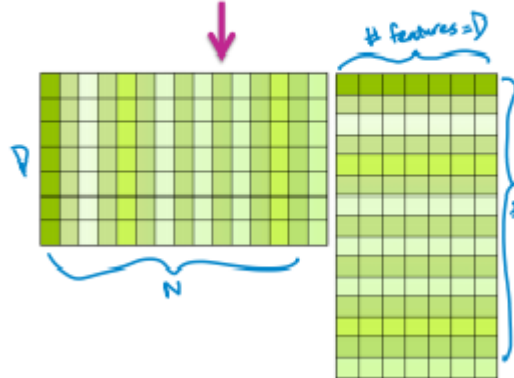
$$\mathbf{H}^T\mathbf{H}\hat{\mathbf{w}} = \mathbf{H}^T\mathbf{y}$$

$$(\mathbf{H}^T\mathbf{H})^{-1}\mathbf{H}^T\mathbf{H}\hat{\mathbf{w}} = (\mathbf{H}^T\mathbf{H})^{-1}\mathbf{H}^T\mathbf{y}$$

$$\hat{\mathbf{w}} = (\mathbf{H}^T\mathbf{H})^{-1}\mathbf{H}^T\mathbf{y}$$

$$\begin{aligned} \bullet \mathbf{A}^{-1}\mathbf{A} &= \mathbf{I} \\ \bullet \mathbf{I}\mathbf{v} &= \mathbf{v} \end{aligned}$$

$$\hat{\mathbf{w}} = (\mathbf{H}^T\mathbf{H})^{-1}\mathbf{H}^T\mathbf{y}$$



Invertible if:
In most cases is $N > D$

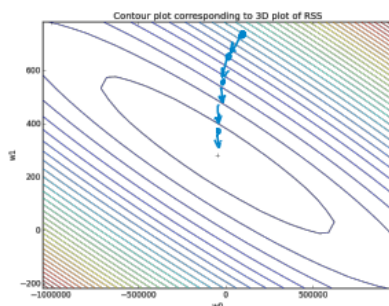
really, # of linearly ind. observations

Complexity of inverse:

$$O(D^3)$$

- $\mathbf{H}^T * \mathbf{H} \rightarrow$ matrix result is square matrix of dimension $\rightarrow D \times D$;
- The above matrix $D \times D$ is invertible if the $N > D$;
- Where $N \rightarrow$ number of observations; $D \rightarrow$ number of features;

Approach - 2 : Gradient Descent

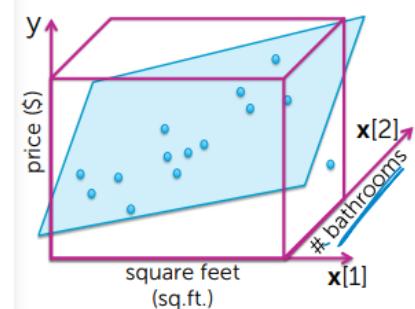


while not converged

$$\mathbf{w}^{(t+1)} \leftarrow \mathbf{w}^{(t)} - \eta \nabla \text{RSS}(\mathbf{w}^{(t)})$$

$$-2\mathbf{H}^T(\mathbf{y} - \mathbf{H}\mathbf{w})$$

$$\leftarrow \mathbf{w}^{(t)} + 2\eta \mathbf{H}^T(\mathbf{y} - \mathbf{H}\mathbf{w}^{(t)})$$

Update to j^{th} feature weight:

$$w_j^{(t+1)} \leftarrow w_j^{(t)} + 2\eta \sum_{i=1}^N h_j(\mathbf{x}_i)(y_i - \hat{y}_i(\mathbf{w}^{(t)}))$$

If underestimating impact of # bath ($w_j^{(t)}$ is too small)
then $(y_i - \hat{y}_i(\mathbf{w}^{(t)}))$ on average weighted by # bath will be positive
 $\Rightarrow w_j^{(t+1)} > w_j^{(t)}$ (increase)

$$\text{RSS}(\mathbf{w}) = \sum_{i=1}^N (y_i - \mathbf{h}(\mathbf{x}_i)^T \mathbf{w})^2$$

$$= \sum_{i=1}^N (y_i - w_0 h_0(\mathbf{x}_i) - w_1 h_1(\mathbf{x}_i) - \dots - w_p h_p(\mathbf{x}_i))^2$$

Partial with respect to w_j

$$\sum_{i=1}^N 2(y_i - w_0 h_0(\mathbf{x}_i) - w_1 h_1(\mathbf{x}_i) - \dots - w_p h_p(\mathbf{x}_i)) \cdot (-h_j(\mathbf{x}_i))$$

$$= -2 \sum_{i=1}^N h_j(\mathbf{x}_i)(y_i - \mathbf{h}(\mathbf{x}_i)^T \mathbf{w})$$

Update to j^{th} feature weight:

$$w_j^{(t+1)} \leftarrow w_j^{(t)} - \eta \left(-2 \sum_{i=1}^N h_j(\mathbf{x}_i)(y_i - \mathbf{h}(\mathbf{x}_i)^T \mathbf{w}^{(t)}) \right)$$

- initialize $\mathbf{w}(1) = 0$ (randomly) @ $t=1$
- while $\|\nabla \text{RSS}(\mathbf{w}(t))\| > \epsilon$

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- for j=0,...,D
- partial[j] = -2 * Σ[i = 1-> N] h(j) (x(i)) (y(i) - y(hat)(i)(w(t)))
- w(j)(t+1) <-- w(j)(t) - η * partial[j]
- t <-- t + 1

```

Quiz :

- 1 point
1. Which of the following is **NOT** a linear regression model. *Hint: remember that a linear regression model is always linear in the parameters, but may use non-linear features.*
- ☐ $y = w_0 + w_1 x$
☐ $y = w_0 + w_1 x^2$
☐ $y = w_0 + w_1 \log(x)$
☒ $y = w_0 w_1 + \log(w_1) x$
-
- 1 point
2. Your estimated model for predicting house prices has a large positive weight on 'square feet living'. This implies that if we remove the feature 'square feet living' and refit the model, the new predictive performance will be **worse** than before.
- ☐ True
☒ False
-
- 1 point
3. *Complete the following:* Your estimated model for predicting house prices has a positive weight on 'square feet living'. You then add 'lot size' to the model and re-estimate the feature weights. The new weight on 'square feet living' [_____] be positive.
- ☐ will not
☐ will definitely
☒ might

1
point

4. If you double the value of a given feature (i.e. a specific column of the feature matrix), what happens to the least-squares estimated coefficients for every **other** feature? (assume you have no other feature that depends on the doubled feature i.e. no interaction terms).
- ☐ They double
☐ They halve
☒ They stay the same
☐ It is impossible to tell from the information provided

1
point

5. Gradient descent/ascent is...
- ☐ A model for predicting a continuous variable
☒ An algorithm for minimizing/maximizing a function
☐ A theoretical statistical result
☐ An approximation to simple linear regression
☐ A modeling technique in machine learning

1
point

6. Gradient descent/ascent allows us to...
- ☐ Predict a value based on a fitted function
☐ Estimate model parameters from data
☒ Assess performance of a model on test data

1
point

7. Which of the following statements about step-size in gradient descent is/are **TRUE** (select all that apply)
- ☐ It's important to choose a very small step-size
☐ The step-size doesn't matter
☒ If the step-size is too large gradient descent may not converge
☒ If the step size is too small (but not zero) gradient descent may take a very long time to converge

1
point

8. Let's analyze how many computations are required to fit a multiple linear regression model *using the closed-form solution* based on a data set with 50 observations and 10 features. In the videos, we said that computing the inverse of the 10×10 matrix $H^T H$ was on the order of D^3 operations. Let's focus on forming this matrix **prior** to inversion. How many multiplications are required to form the matrix $H^T H$?

Please enter a number below.

5000

- 8th question -> Matrix multiplication between -> 23×32 matrix has -> $3 \times 2 \times 2 = 12$ multiplications performed;
- Matrix $H \times H^T = (N \times D) \times (D \times N) \Rightarrow N \times N$;
- Matrix -> 50 observation (N), 10 features (D) =>
- $H^T H \Rightarrow \# \text{ multiplication} \Rightarrow DN \times ND \Rightarrow ND^2 = 50 \times 10^2 = 5000$;

1
point

9. More generally, if you have D features and N observations what is the total complexity of computing $(H^T H)^{-1}$?

- ☐ $O(D^3)$
- ☐ $O(ND^3)$
- ☒ $O(ND^2 + D^3)$
- ☐ $O(ND^2)$
- ☐ $O(N^2 D + D^3)$
- ☐ $O(N^2 D)$

- Mutliptication complexity -> $N \cdot D^2$;
- Inversion complexity -> D^3
- Total complexity = $O(N \cdot D^2 + D^3)$;

In []: