

Logistics:

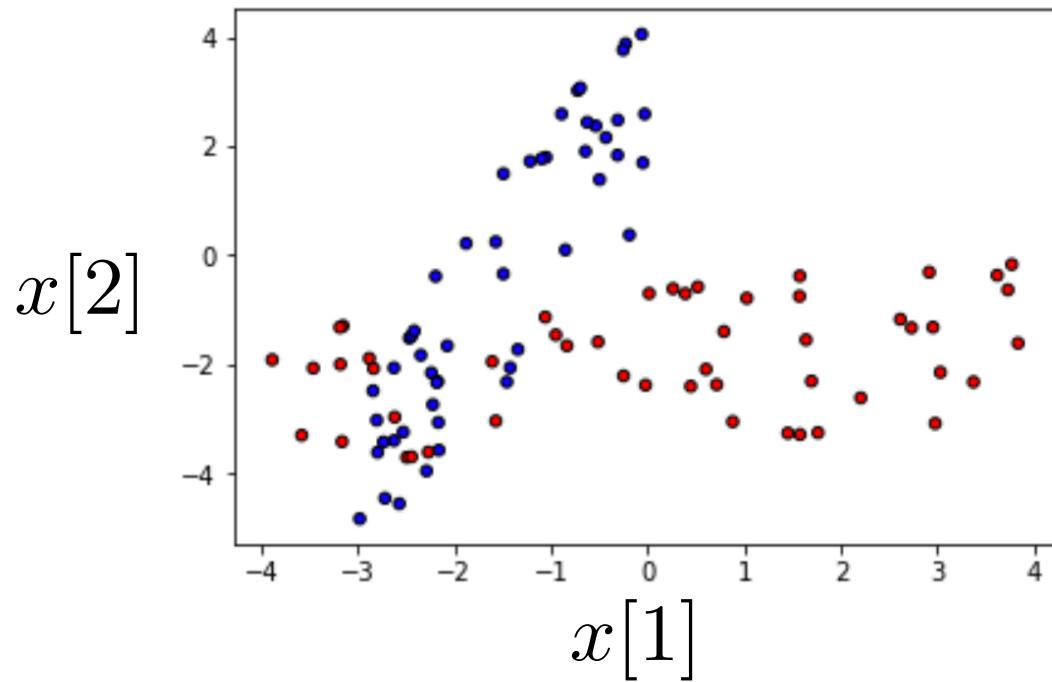
- New Office Hours now on course website. Some on zoom some in-person.
- Lectures will be recorded, published on Canvas.

Lecture 12: Classification with logistic regression (continued)

- Regression: label is continuous valued
- Classification: label is discrete valued, e.g., {0,1}
- Note that logistic regression is a classification algorithm not a regression algorithm

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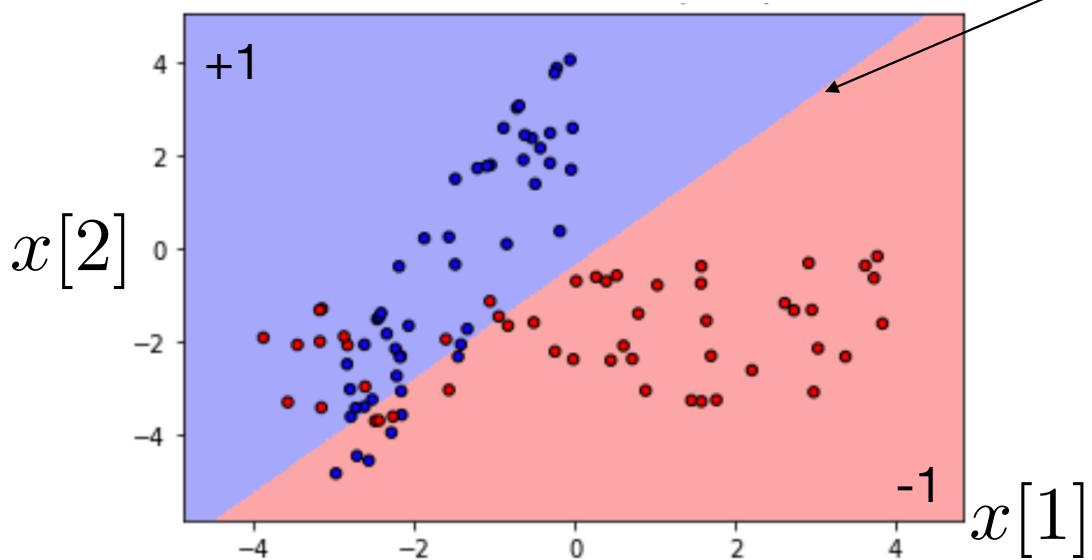
Training data for a binary classification problem



- in this example, each input is $x_i \in \mathbb{R}^2$
- Red points have label $y_i = -1$, blue points have label $y_i = 1$
- We want a predictor that maps any $x \in \mathbb{R}^2$ to a prediction $\hat{y} \in \{-1, +1\}$

Example: linear classifier trained on 100 samples

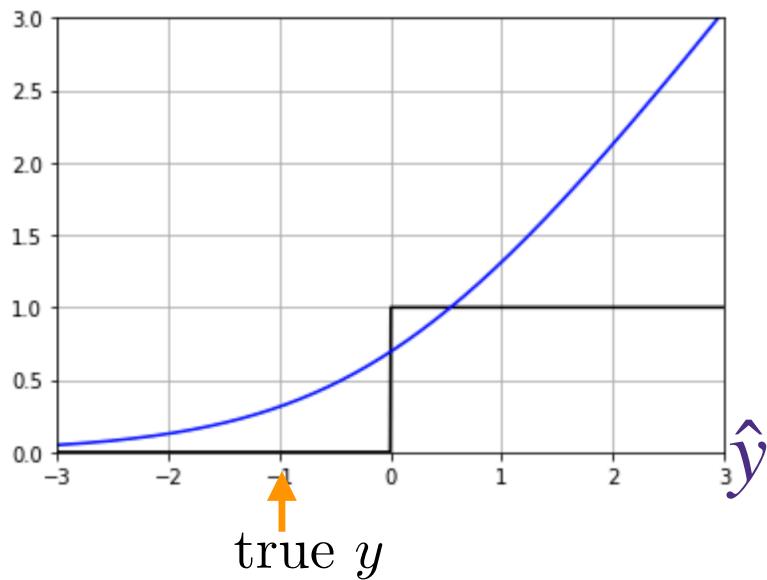
simple decision boundary at $w^T x + b = 0$



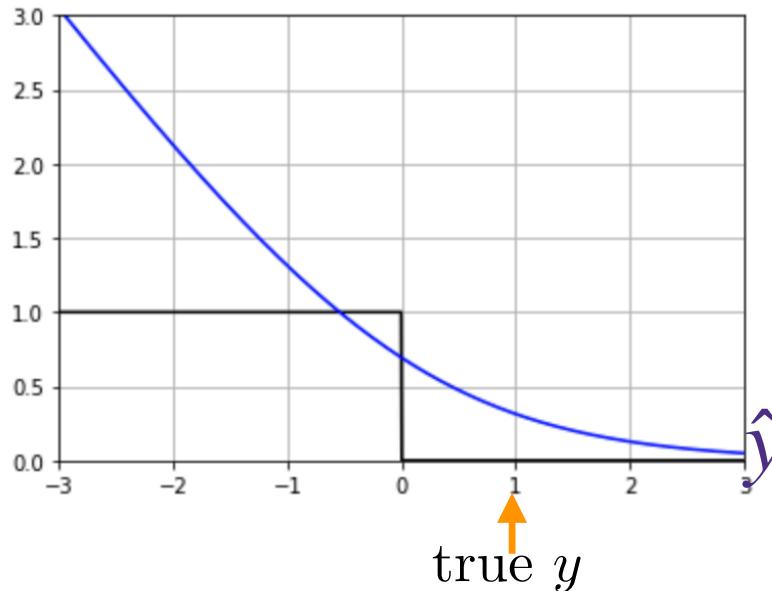
- We fit a linear model: $w_0 + w_1x[1] + w_2x[2] = 0.8 - 1.1x[1] + 0.9x[2]$
- predict using $\hat{y} = \text{sign}(0.8 - 1.1x[1] + 0.9x[2])$
- decision boundary is the line (or hyperplane in higher dimensions) defined by $0.8 - 1.1x[1] + 0.9x[2] = 0$
- note that a model $2w^T x + 2b$ has the same predictions as $w^T x + b$
- How do we find such a good linear classifier that fits the data?

Logistic loss $\ell(\hat{y}, y) = \log(1 + e^{-y\hat{y}})$

$$\ell(\hat{y}, -1) = \log(1 + e^{\hat{y}})$$



$$\ell(\hat{y}, +1) = \log(1 + e^{-\hat{y}})$$



- differentiable and convex in \hat{y}
- how do we show $\ell(\cdot, y)$ is convex?
- approximation of 0-1
- Most popular choice of a loss function for classification problems

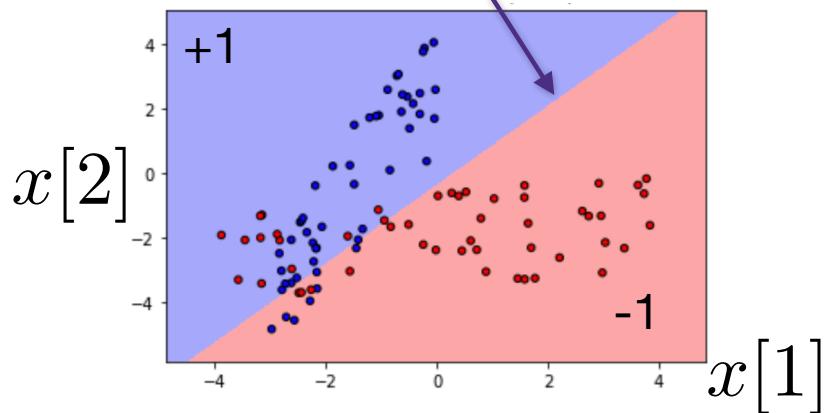
Logistic regression for binary classification

- Data $\mathcal{D} = \{(x_i \in \mathbb{R}^d, y_i \in \{-1, +1\})\}_{i=1}^n$
- Model: $\hat{y} = x^T w + b$
- Loss function: logistic loss $\ell(\hat{y}, y) = \log(1 + e^{-y\hat{y}})$
- Optimization: solve for

$$(\hat{b}, \hat{w}) = \arg \min_{b,w} \sum_{i=1}^n \log(1 + e^{-y_i(b+x_i^T w)})$$

- As this is a **smooth convex** optimization, it can be solved efficiently using gradient descent
- Prediction: $\text{sign}(b + x^T w)$

decision boundary at
 $w^T x + b = 0$



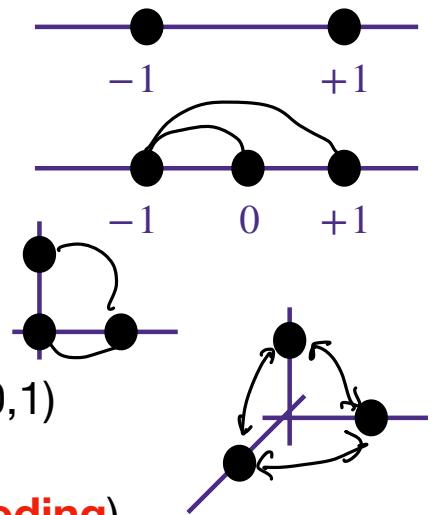
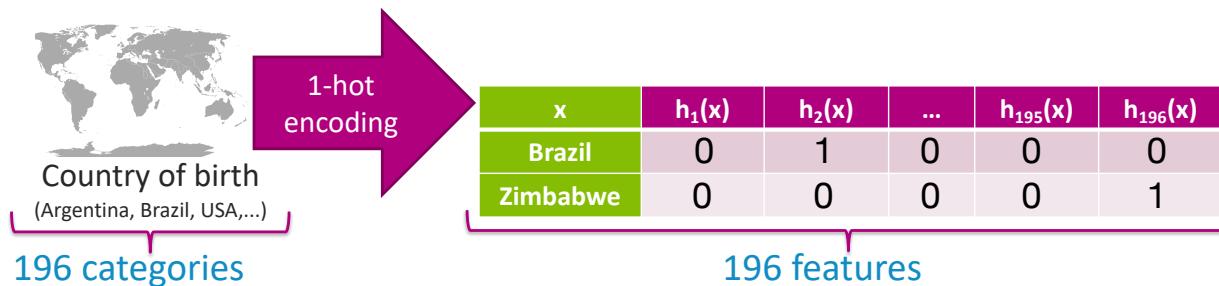
Multi-class regression

How do we encode general categorical data y ?

- so far, we considered Binary case where there are two categories
- encoding y is simple: $\{+1, -1\}$
- We output a scalar prediction $\hat{y} = b + w^T x$, and take the sign
- multi-class classification predicts categorial y
- taking values in $y \in C = \{c_1, \dots, c_k\}$
- c_j 's are called **classes** or **labels**
- examples:
 - Country of birth
(Argentina, Brazil, USA,...)
 - Zipcode
(10005, 98195,...)
 - All English words
- even though zip codes are numbers,
you don't want to use it as is
as your label y .
- a **k-class classifier** predicts y given x , but we need to represent categorical y with numerical values

Embedding c_j 's in real values

- Since we rely on optimization, which are numerical solvers, we need to **embed** raw categorical c_j 's into real valued vectors
- there are many ways to embed categorial data
 - True->1, False->-1, can we use it for all binary classification?
 - Yes->1, Maybe->0, No->-1 can we use it for all ternary classification?
 - Yes->(1,0), Maybe->(0,0), No->(0,1)
 $\nsubseteq \mathbb{R}^2$
 - Apple->(1,0,0), Orange->(0,1,0), Banana->(0,0,1)
 $\nsubseteq \mathbb{R}^K$
- we use **one-hot embedding** (a.k.a. **one-hot encoding**), because it is neutral representation with no domain knowledge
 - each class is a standard basis vector in k -dimension



Multi-class logistic regression

- **data:** categorical y in $\{c_1, \dots, c_k\}$ with k categories

we use **one-hot encoding**, s.t. $y = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$ implies that $y = c_1$

- **model:** linear vector-function makes a linear prediction $\hat{y} \in \mathbb{R}^k$

$$\hat{y}_i = f(x_i) = w^T x_i \in \mathbb{R}^k$$

with model parameter matrix $w \in \mathbb{R}^{d \times k}$ and sample $x_i \in \mathbb{R}^d$

$$f(x_i) = \begin{bmatrix} f_1(x_i) \\ f_2(x_i) \\ \vdots \\ f_k(x_i) \end{bmatrix} = \underbrace{\begin{bmatrix} w_{1,0} & w_{1,1} & w_{1,2} & \cdots \\ w_{2,0} & w_{2,1} & w_{2,2} & \cdots \\ \vdots & & & \\ w_{k,0} & w_{k,1} & w_{k,2} & \cdots \end{bmatrix}}_{w^T} \underbrace{\begin{bmatrix} 1 \\ x_i[1] \\ \vdots \\ x_i[d] \end{bmatrix}}_{x_i} = \underbrace{\begin{bmatrix} w_{1,0} + w_{1,1}x_i[1] + w_{1,2}x_i[2] + \cdots \\ w_{2,0} + w_{2,1}x_i[1] + w_{2,2}x_i[2] + \cdots \\ \vdots \\ w_{k,0} + w_{k,1}x_i[1] + w_{k,2}x_i[2] + \cdots \end{bmatrix}}_{w^T x_i}$$

$$w = [w[:, 1] \quad w[:, 2] \quad \cdots \quad w[:, k]]$$

↑
Model parameter for category 1

2 equivalent approaches for binary Logistic regression

- What we learned so far:

single model parameter $w \in \mathbb{R}^d$

$w^T x_i \approx \text{How likely is } x_i \text{ to be labeled } +1$

$$\mathbb{P}(y_i = +1 | x_i) = \frac{1}{1 + e^{-w^T x_i}} = \frac{e^{w^T x_i}}{1 + e^{w^T x_i}}$$

$$\mathbb{P}(y_i = -1 | x_i) = 1 - \mathbb{P}(y_i = +1 | x_i)$$

Maximum Likelihood Estimator

$$\underset{w \in \mathbb{R}^d}{\text{maximize}} \frac{1}{n} \sum_{i=1}^n \log \left(\frac{e^{y_i w^T x_i}}{1 + e^{y_i w^T x_i}} \right)$$

Representing the two categories as $\{-1, +1\}$ helps simplify the notations, where

$$\text{we used the fact that } \frac{e^{-w^T x}}{1 + e^{-w^T x}} = 1 - \frac{e^{w^T x}}{1 + e^{w^T x}}$$

- Another approach: two parameters $w_1, w_2 \in \mathbb{R}^d$
- $\exp(w_1^T x)$ represents how much category 1 is more likely at a data point x (relative to $w_2^T x$)
- $\exp(w_2^T x)$ represents how much category 2 is more likely at a data point x

$$\mathbb{P}(y_i = 1 | x_i) = \frac{e^{w_1^T x_i}}{e^{w_1^T x_i} + e^{w_2^T x_i}}$$

$$\mathbb{P}(y_i = 2 | x_i) = \frac{e^{w_2^T x_i}}{e^{w_1^T x_i} + e^{w_2^T x_i}}$$

$$\begin{aligned} & \underset{w}{\text{maximize}} \frac{1}{n} \sum_{i=1}^n \log(\mathbb{P}(y_i | x_i)) \\ & \underset{w_1, w_2 \in \mathbb{R}^d}{\text{maximize}} \frac{1}{n} \sum_{i=1}^n \left\{ \log \left(\frac{e^{w_{y_i}^T x_i}}{e^{w_1^T x_i} + e^{w_2^T x_i}} \right) \right\} \end{aligned}$$

Representing the two categories as $\{1, 2\}$ is inline with the notation for the parameters w_1 and w_2 , and we simplify the numerator using w_{y_i}

- Do these two approaches give different solutions?
- The second approach is more symmetric, and hence generalizes to larger classes

$$w = w_1 - w_2$$

Logistic regression

2 classes

$$\mathbb{P}(y_i = 1 | x_i) = \frac{e^{w_1^T x_i}}{e^{w_1^T x_i} + e^{w_2^T x_i}}$$

$$\mathbb{P}(y_i = 2 | x_i) = \frac{e^{w_2^T x_i}}{e^{w_1^T x_i} + e^{w_2^T x_i}}$$

$$\omega = \left[\begin{array}{c|c|c|c} w_1 & w_2 & \cdots & w_k \end{array} \right] \}^d$$

k classes

$$\mathbb{P}(y_i = 1 | x_i) = \frac{e^{w[:,1]^T x_i}}{e^{w[:,1]^T x_i} + \cdots + e^{w[:,k]^T x_i}}$$

⋮

$$\mathbb{P}(y_i = k | x_i) = \frac{e^{w[:,k]^T x_i}}{e^{w[:,1]^T x_i} + \cdots + e^{w[:,k]^T x_i}}$$

Maximum Likelihood Estimator

$$\underset{w}{\text{maximize}} \quad \frac{1}{n} \sum_{i=1}^n \log(\mathbb{P}(y_i | x_i))$$

$$\underset{w_1, w_2 \in \mathbb{R}^d}{\text{maximize}} \quad \frac{1}{n} \sum_{i=1}^n \left\{ \log \left(\frac{e^{w_{y_i}^T x_i}}{e^{w_1^T x_i} + e^{w_2^T x_i}} \right) \right\}$$

$$\underset{w \in \mathbb{R}^{d \times k}}{\text{maximize}} \quad \frac{1}{n} \sum_{i=1}^n \log \left(\frac{e^{w[:,y_i]^T x_i}}{\sum_{j=1}^k e^{w[:,j]^T x_i}} \right)$$

Predict: $\underset{1 \quad 2.}{\text{argmax}} \{ w_1^T x, w_2^T x \}$

Predict: $\underset{1 \quad 2 \quad \cdots \quad k}{\text{argmax}} \{ w_1^T x, w_2^T x, \dots, w_k^T x \}$

Gradient Descent

- how are we going to find the solution for

$$\arg \min_{b,w} \sum_{i=1}^n \ell(b + w^T x_i, y_i)$$

- e.g., Lasso, Logistic Regression do not have closed form solution for
 $\nabla_{b,w} \mathcal{L}(b, w) = 0$

W

Gradient descent

Example of a general non-convex $f(w)$

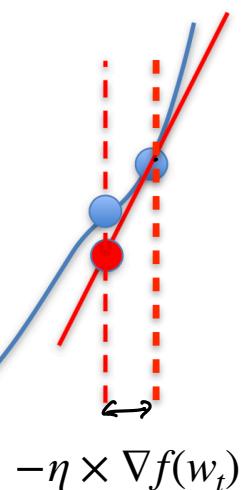
- Initialize: $w_0 = 0$

- For $t=0,1,2,\dots$

- $w_{t+1} \leftarrow w_t - \eta \cdot \nabla_w f(w_t)$



I will omit w in ∇_w when obvious



- Learning rate or step-size
- A hyper-parameter to be chosen by the analyst
- Can be fixed over the iterations,
or can also change, in which case we use η_t
to emphasize the fact that it changes over iteration t

Running example: linear regression

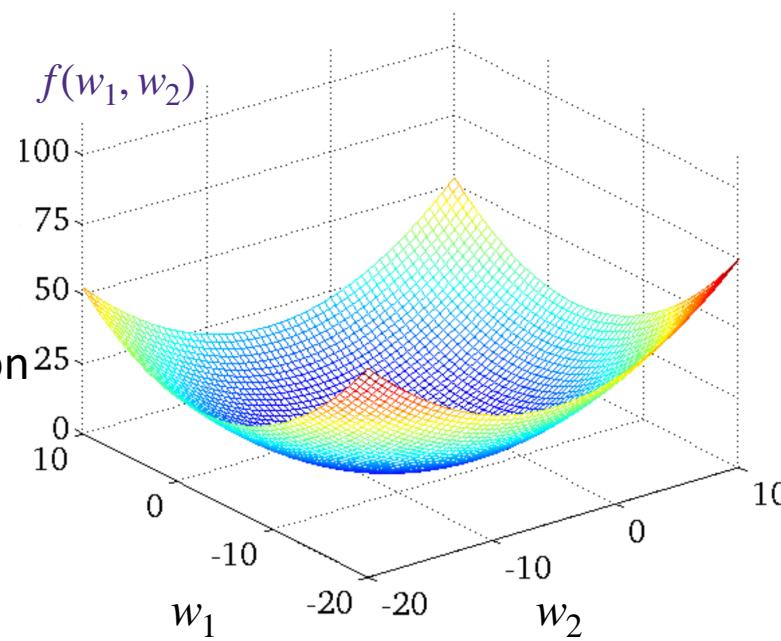
- Given data:

$$\{(x_i, y_i)\}_{i=1}^n \quad x_i \in \mathbb{R}^d \quad y_i \in \mathbb{R}$$

- Learning model parameters:

$$\hat{w}_{\text{LS}} = \arg \min_{w \in \mathbb{R}^d} \underbrace{\|\mathbf{y} - \mathbf{X}w\|_2^2}_{f(w)}$$

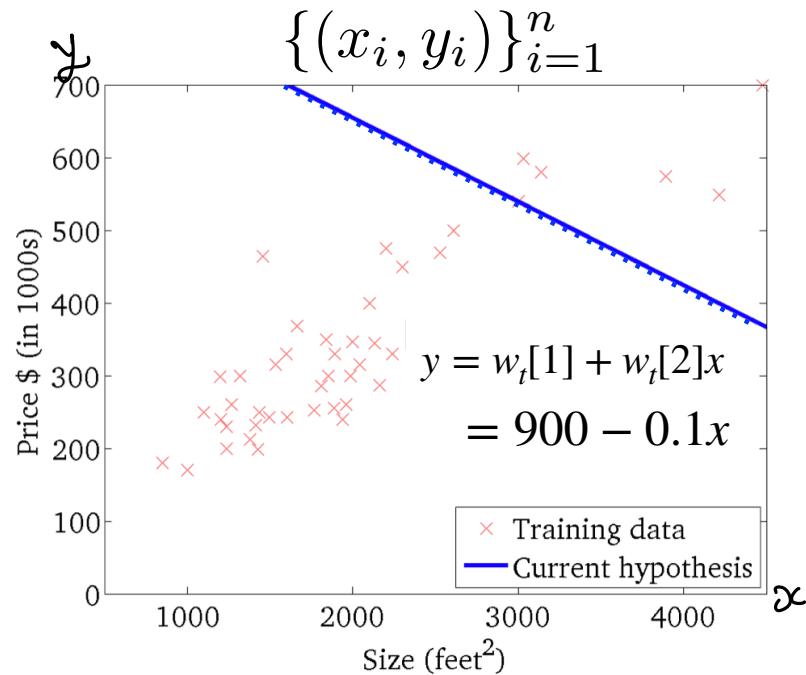
- Although we know the optimal solution in a closed form, we will use this as a running example to understand GD



- $w_0 = (900, -0.1)$

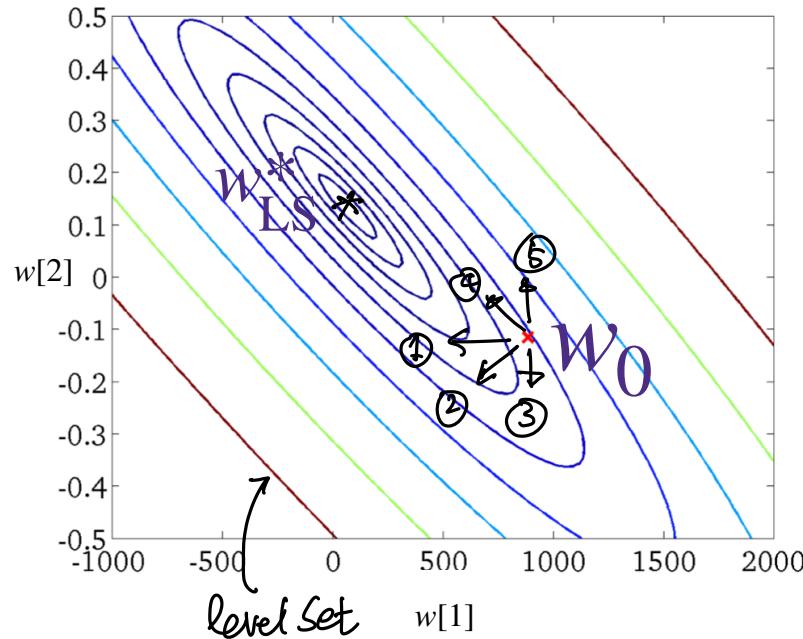
- For $t=0,1,2,\dots$

$$\bullet w_{t+1} \leftarrow w_t - \eta \cdot \nabla_w f(w_t)$$



Evolution of the predictor

- Which direction will the GD move?



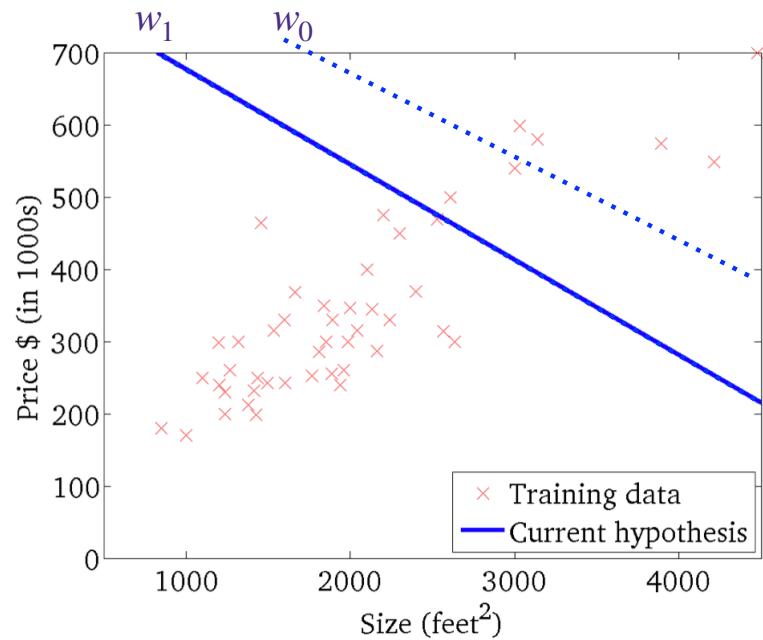
GD dynamics in the Parameter space



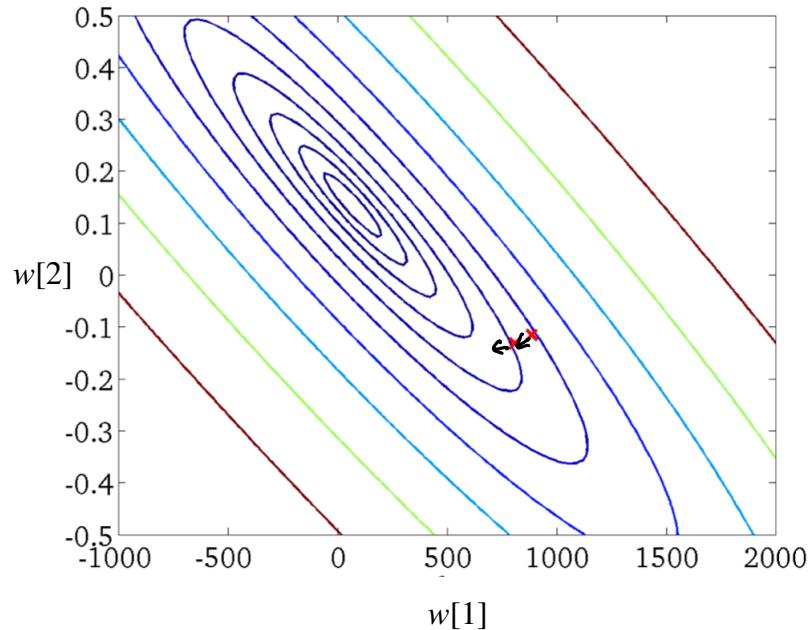
- $w_0 = (900, -0.1)$

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Evolution of the predictor

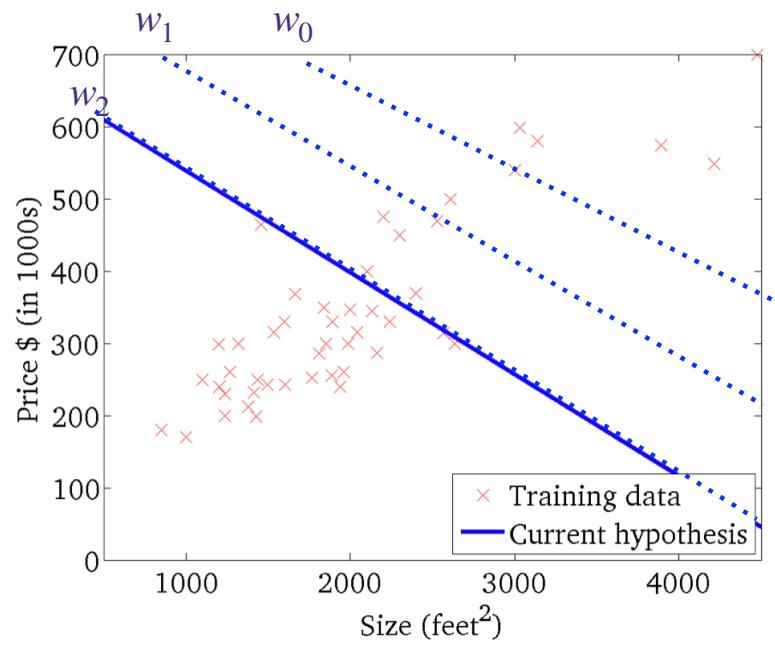


GD dynamics in the Parameter space

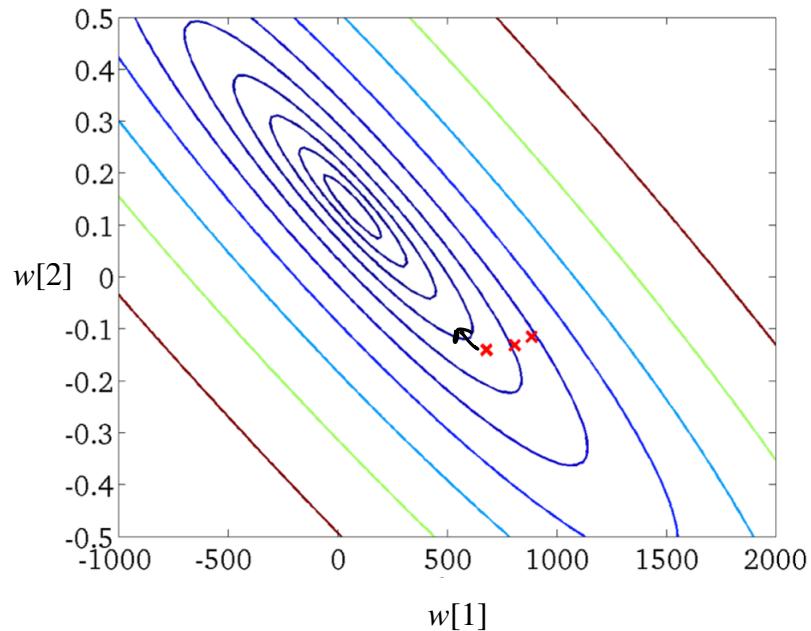
• $w_0 = (900, -0.1)$

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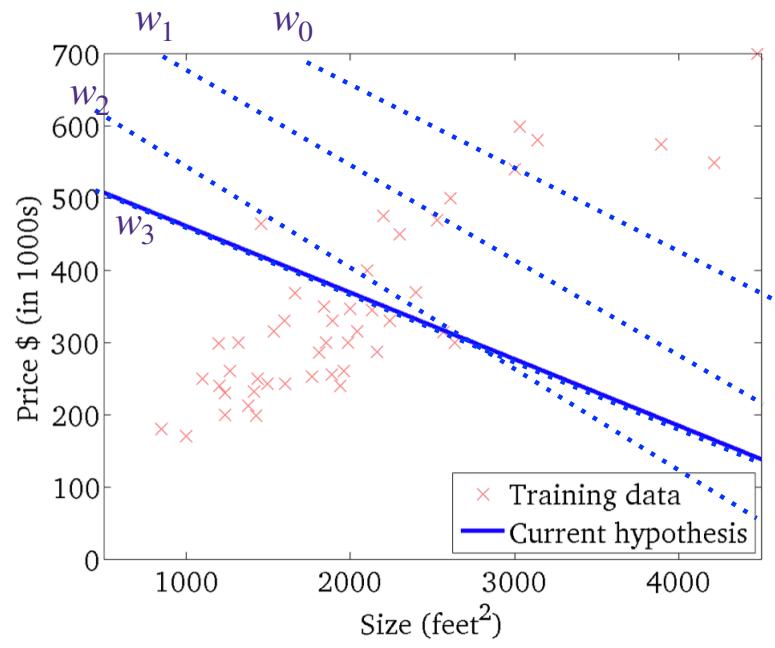


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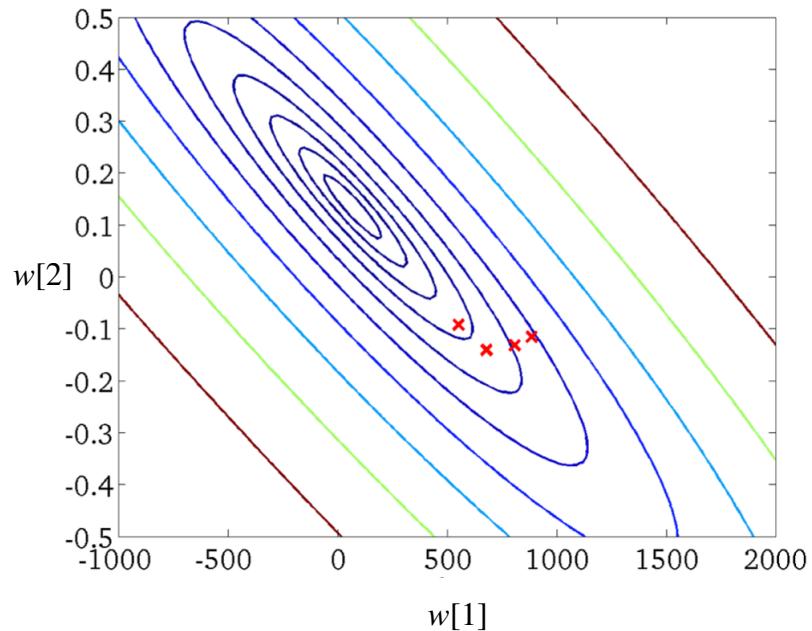
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Evolution of the predictor

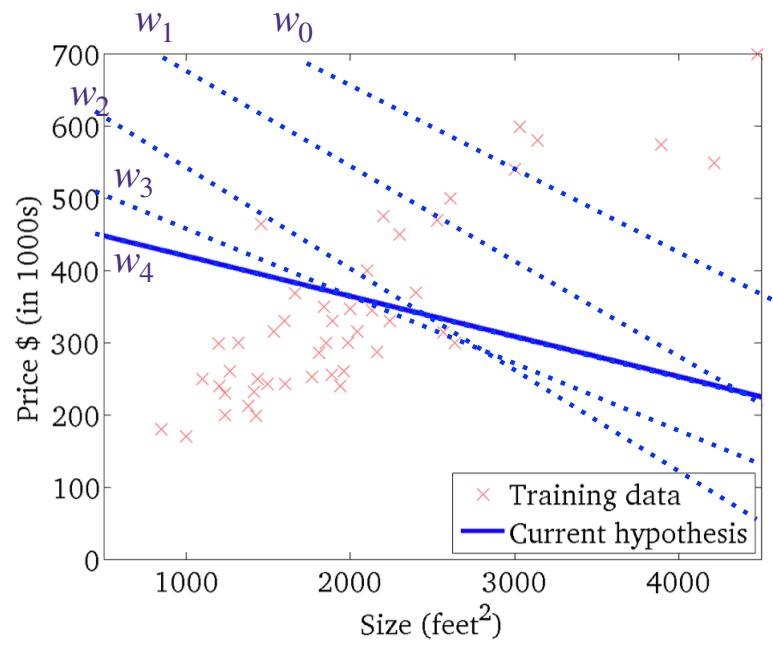


GD dynamics in the Parameter space

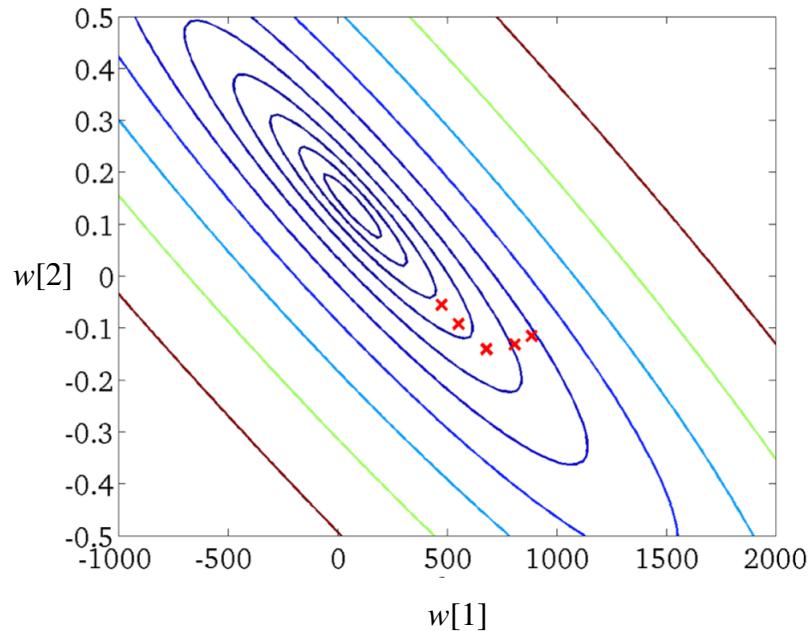
• $w_0 = (900, -0.1)$

• For $t=0,1,2,\dots$

$$\bullet w_{t+1} \leftarrow w_t - \eta \cdot \nabla_w f(w_t)$$



Evolution of the predictor

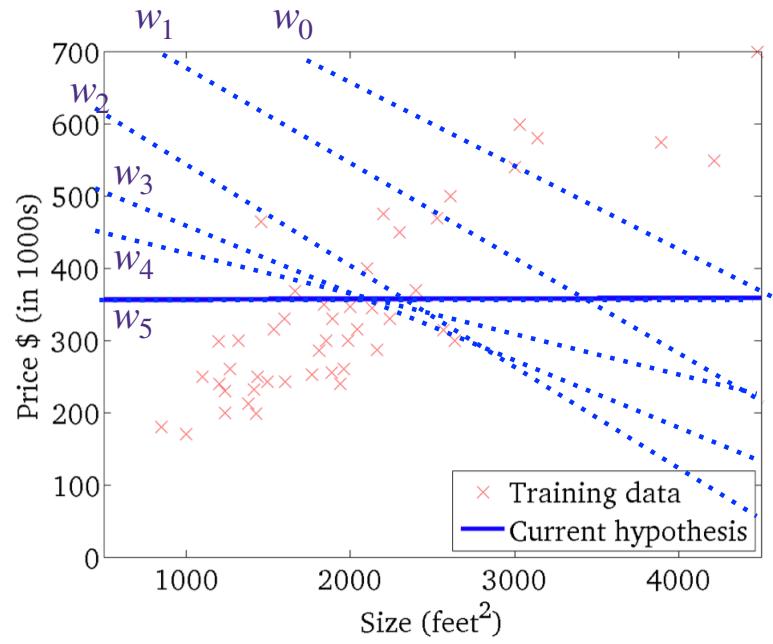


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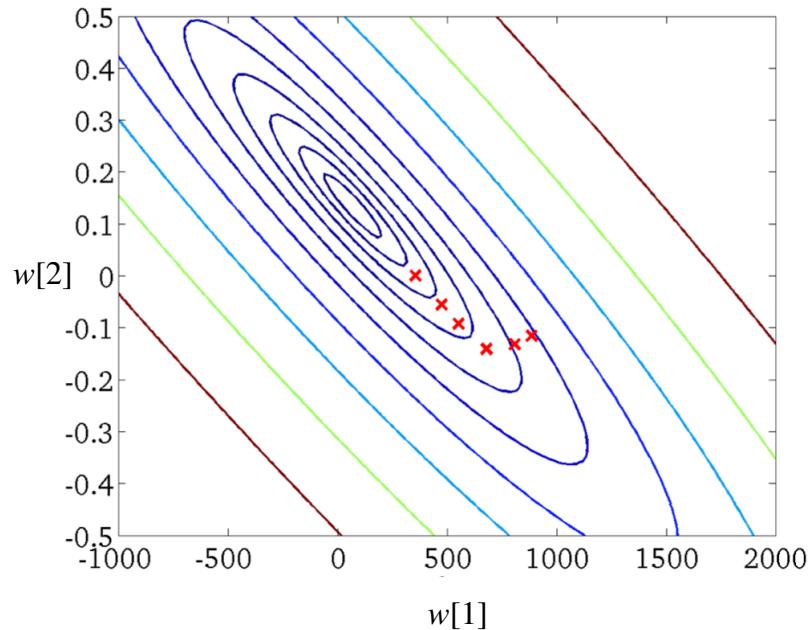
• $w_0 = (900, -0.1)$

• For $t=0,1,2,\dots$

$$\bullet w_{t+1} \leftarrow w_t - \eta \cdot \nabla_w f(w_t)$$



Evolution of the predictor

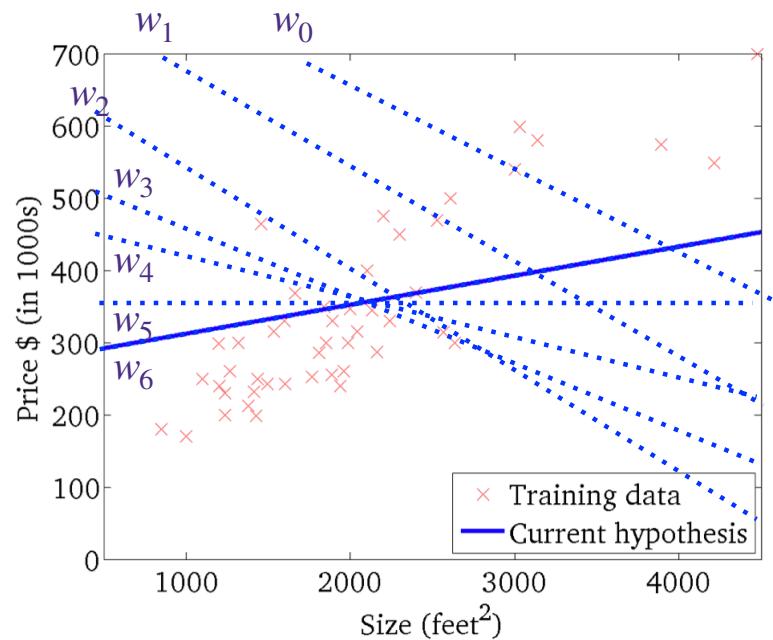


GD dynamics in the Parameter space

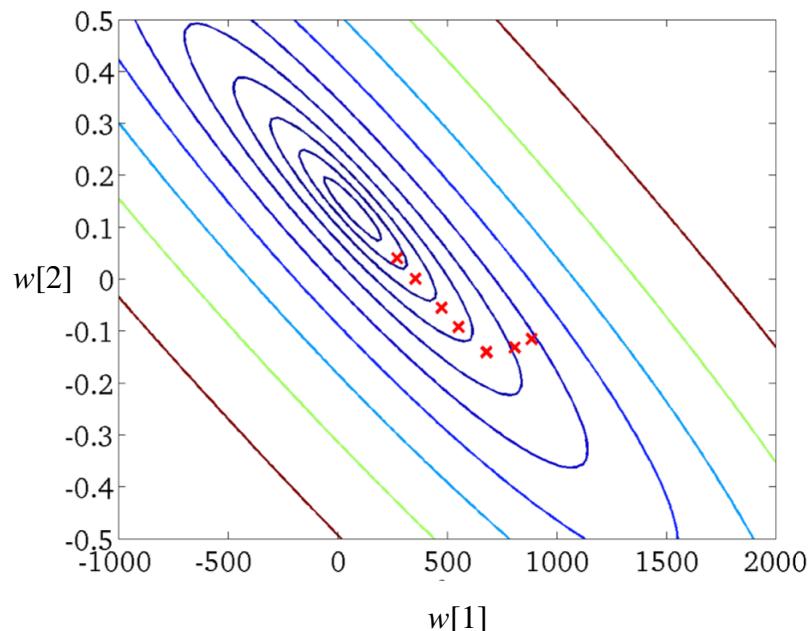
- $w_0 = (900, -0.1)$

- For $t=0,1,2,\dots$

$$\bullet w_{t+1} \leftarrow w_t - \eta \cdot \nabla_w f(w_t)$$



Evolution of the predictor

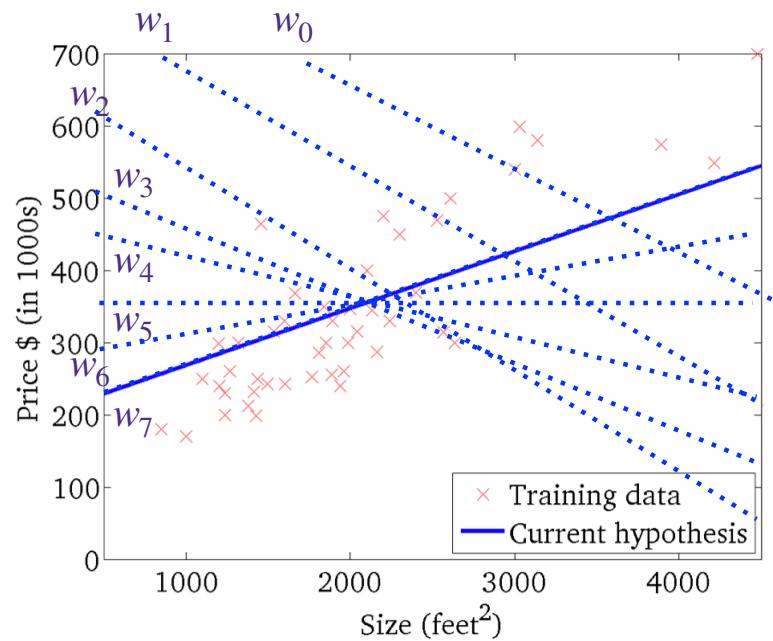


GD dynamics in the Parameter space

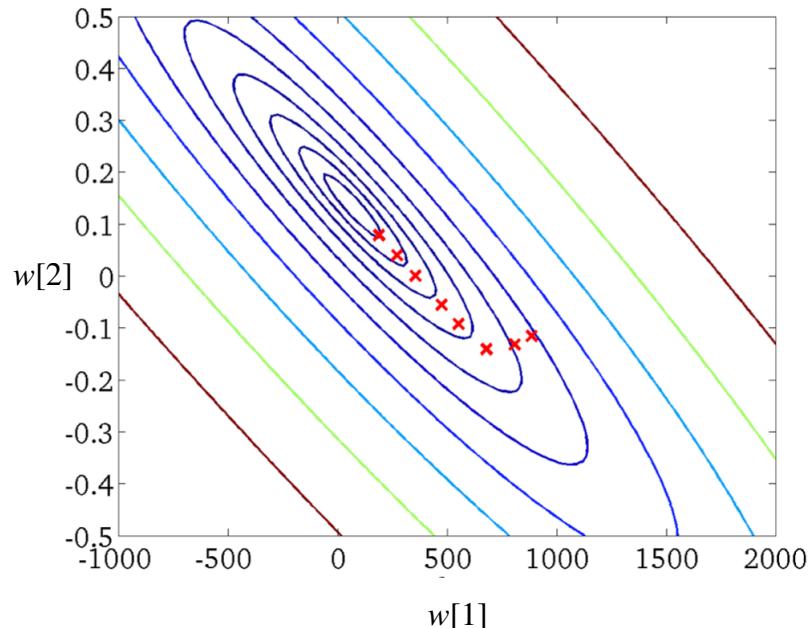
- $w_0 = (900, -0.1)$

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Evolution of the predictor

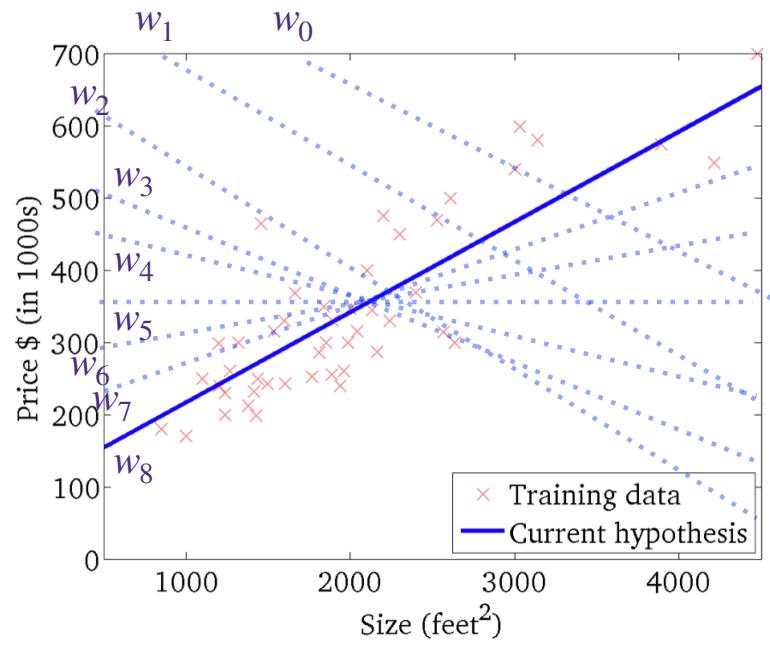


GD dynamics in the Parameter space

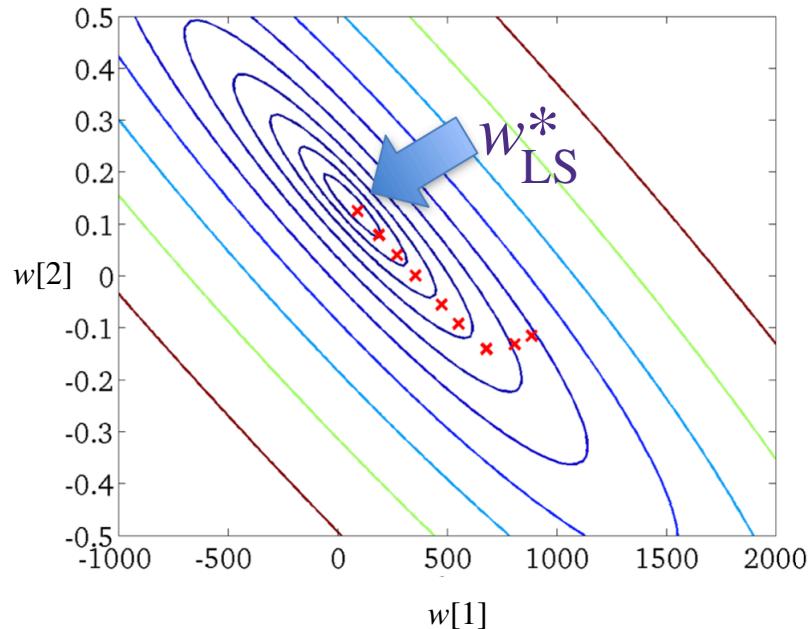
- $w_0 = (900, -0.1)$

- For $t=0,1,2,\dots$

$$\bullet w_{t+1} \leftarrow w_t - \eta \cdot \nabla_w f(w_t)$$



Evolution of the predictor



GD dynamics in the Parameter space

Gradient descent for linear regression

- In this example of linear regression, we can derive exactly the gradient descent trajectory
- Initialize: $w_0 = 0$
- For $t=0,1,2,\dots$

$$w_{t+1} \leftarrow w_t - \eta \cdot \underbrace{\nabla_w f(w_t)}_{-2 \cdot X^T (y - Xw_t)}$$

$$w_{t+1} = w_t + 2\eta X^T (y - Xw_t) = (\mathbb{I} - 2\eta X^T X)w_t + 2\eta X^T y$$

$$\begin{aligned} w_{t+1} - w^* &= (\underbrace{\mathbb{I} - 2\eta X^T X}_{\text{Matrix}}) w_t - \underbrace{(\mathbb{I} - 2\eta X^T X + 2\eta X^T X) w^*}_{\text{Matrix}} + 2\eta X^T y \\ &= (\mathbb{I} - 2\eta X^T X)(w_t - w^*) + 2\eta \left(X^T y - \underbrace{\frac{X^T X w^*}{X^T y}}_{\text{Matrix}} \right) \\ &= (\mathbb{I} - 2\eta X^T X)(w_t - w^*) \end{aligned}$$

For linear regression, we have

$$\hat{w}_{LS} = \arg \min_{w \in \mathbb{R}^d} \underbrace{\|y - Xw\|_2^2}_{f(w)}$$

$$, \quad w^* = (X^T X)^{-1} X^T y$$

Gradient descent for linear regression

- Initialize: $w_0 = 0$

- For $t=0,1,2,\dots$

- $w_{t+1} \leftarrow w_t - \eta \cdot \nabla_w f(w_t)$

For linear regression, we have

$$\hat{w}_{\text{LS}} = \arg \min_{w \in \mathbb{R}^d} \underbrace{\|\mathbf{y} - \mathbf{X}w\|_2^2}_{f(w)}$$

$$\nabla f(w_t) = -2\mathbf{X}^T(\mathbf{y} - \mathbf{X}w_t)$$

$$w_{t+1} = w_t + \eta 2\mathbf{X}^T(\mathbf{y} - \mathbf{X}w_t) = (\mathbf{I} - 2\eta\mathbf{X}^T\mathbf{X})w_t + 2\eta\mathbf{X}^T\mathbf{y}$$

Let the least-squares solution be $w^* = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$

$$\begin{aligned} w_{t+1} - w^* &= (\mathbf{I} - 2\eta\mathbf{X}^T\mathbf{X})w_t + 2\eta\mathbf{X}^T\mathbf{y} - w^* \\ &= (\mathbf{I} - 2\eta\mathbf{X}^T\mathbf{X})(w_t - w^*) + 2\eta\mathbf{X}^T\mathbf{y} - 2\eta\mathbf{X}^T\mathbf{X}w^* \\ &= (\mathbf{I} - 2\eta\mathbf{X}^T\mathbf{X})(w_t - w^*) \end{aligned}$$

Gradient Descent (GD) for Linear Regression (LR)

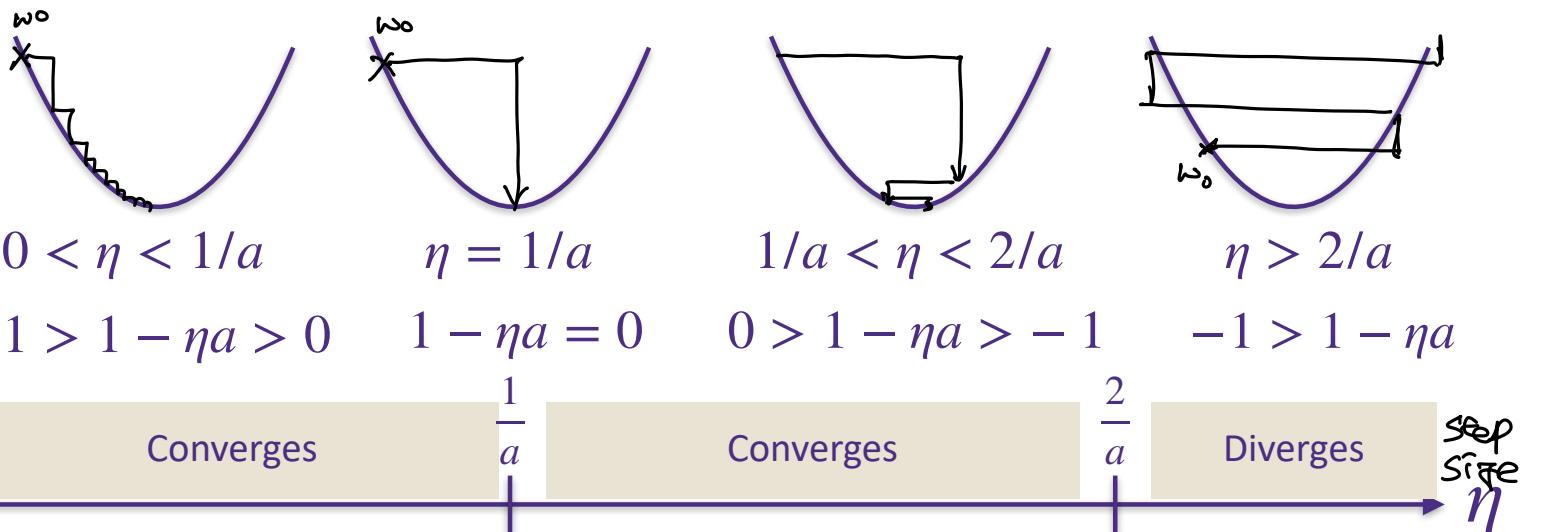
- We use this analytical derivation of GD for LR to understand how the choice of step size impacts the algorithm

$$\begin{aligned} w_{t+1} &= w_t - \eta \nabla f(w_t) \implies w_{t+1} - w^* &= (\mathbf{I} - 2\eta \mathbf{X}^T \mathbf{X})(w_t - w^*) \\ &= (\mathbb{I} - 2\eta \mathbf{X}^T \mathbf{X})^2 (w_0 - w^*) \\ &\equiv \underbrace{(\mathbb{I} - 2\eta \mathbf{X}^T \mathbf{X})^{t+1}}_{\text{step size}} \underbrace{(w_0 - w^*)}_{\text{initial error}} \end{aligned}$$

Gradient descent for linear regression

$$\begin{aligned} w_{t+1} &= w_t - \eta \nabla f(w_t) \implies w_{t+1} - w^* &= (\mathbf{I} - 2\eta \mathbf{X}^T \mathbf{X})(w_t - w^*) \\ &&= (\mathbf{I} - 2\eta \mathbf{X}^T \mathbf{X})^2(w_{t-1} - w^*) \\ &&\vdots \\ &&= (\mathbf{I} - 2\eta \mathbf{X}^T \mathbf{X})^{t+1}(w_0 - w^*) \\ &\stackrel{\text{def. } (w_0 - w^*)}{=} (1 - \eta a)^{t+1}(w_0 - w^*) \end{aligned}$$

In one dimension, $2\mathbf{X}^T \mathbf{X} = a$ is a scalar, and $w_{t+1} - w^* = (1 - \eta a)^{t+1}(w_0 - w^*)$



Gradient descent for linear regression

$$w_{t+1} = w_t - \eta \nabla f(w_t) \implies w_{t+1} - w^* = (\mathbf{I} - 2\eta \mathbf{X}^T \mathbf{X})^{t+1} (w_0 - w^*)$$

- In multi dimensions, **eigenvalues** of $\mathbf{X}^T \mathbf{X}$ are important

(you will see why I consider eigenvalues of $\mathbf{X}^T \mathbf{X}$,
instead of $\mathbf{I} - 2\eta \mathbf{X}^T \mathbf{X}$ in couple of slides)

- Let the eigenvalue decomposition of $\mathbf{I} - 2\eta \mathbf{X}^T \mathbf{X}$ be $Q^{-1} D Q$

$$\begin{aligned} w_{t+1} - w^* &= \underbrace{Q^{-1} D Q Q^{-1} D Q \cdots Q^{-1} D Q}_{t+1} \cdot (w_0 - w^*) && \text{Orthogonal matrix} \\ &= Q^{-1} \cdot D^{t+1} \cdot Q \cdot (w_0 - w^*) \\ \underline{Q} \cdot \underline{(w_{t+1} - w^*)} &= \underline{D^{t+1}} \cdot \underline{Q} \cdot \underline{(w_0 - w^*)} \\ &= \begin{bmatrix} D_{11}^{t+1} & & \\ & D_{22}^{t+1} & \\ & & \ddots \end{bmatrix} \end{aligned}$$


 $D \begin{bmatrix} D_{11} & & \\ & \ddots & \\ & & D_{nn} \end{bmatrix}$

$Q^T Q = \mathbb{I}$

Gradient descent for linear regression

$$w_{t+1} = w_t - \eta \nabla f(w_t) \implies w_{t+1} - w^* = (\mathbf{I} - 2\eta \mathbf{X}^T \mathbf{X})^{t+1} (w_0 - w^*)$$

- In multi dimensions, **eigenvalues** of $\mathbf{X}^T \mathbf{X}$ are important
(you will see why I consider eigenvalues of $\mathbf{X}^T \mathbf{X}$,
instead of $\mathbf{I} - 2\eta \mathbf{X}^T \mathbf{X}$ in couple of slides)
- Let the eigenvalue decomposition of $\mathbf{I} - 2\eta \mathbf{X}^T \mathbf{X}$ be $Q^{-1}DQ$

$$\begin{aligned} \text{Then, } w_{t+1} - w^* &= (Q^{-1}DQ)^{t+1} (w_0 - w^*) \\ &= \underbrace{Q^{-1}DQ Q^{-1}DQ \dots Q^{-1}DQ}_{t+1 \text{ times}} (w_0 - w^*) \\ &= Q^{-1} D^{t+1} Q (w_0 - w^*) \\ Q(w_{t+1} - w^*) &= D^{t+1} Q (w_0 - w^*) \end{aligned}$$

Gradient descent for linear regression

$$(*) \quad Q(w_{t+1} - w^*) = D^{t+1} Q(w_0 - w^*) \quad GR^d$$

- Where eigenvalue decomposition of $\boxed{\mathbf{I} - 2\eta \mathbf{X}^T \mathbf{X}}$ is $Q^{-1} D Q$

- Let $Q = \begin{bmatrix} - & q_1^T & - \\ - & q_2^T & - \\ & \vdots & \end{bmatrix}$, then the above multi-dimensional dynamics

of GD can be decomposed into multiple 1-d dynamics we saw before

- In direction q_1 , the error decreases multiplicatively according to

(*) written at
as series of
equations

$$\left\{ \begin{array}{l} \underline{q_1^T(w_{t+1} - w^*)} = \underline{D_{11}^{t+1}} \underline{q_1^T(w_0 - w^*)} \quad GR \\ \underline{q_2^T(w_{t+1} - w^*)} = \underline{D_{22}^{t+1}} \underline{q_2^T(w_0 - w^*)} \\ \vdots \end{array} \right.$$

Gradient descent for linear regression

$$w_{t+1} = w_t - \eta \nabla f(w_t) \implies w_{t+1} - w^* = (\mathbf{I} - 2\eta \mathbf{X}^T \mathbf{X})^{t+1} (w_0 - w^*)$$

$$\implies Q(w_{t+1} - w^*) = D^{t+1} Q (w_0 - w^*)$$

$$q_1^T (w_{t+1} - w^*) = D_{11}^{t+1} q_1^T (w_0 - w^*)$$

$$q_2^T (w_{t+1} - w^*) = D_{22}^{t+1} q_2^T (w_0 - w^*)$$

key values align
with axes defining the
oval-shaped level sets.

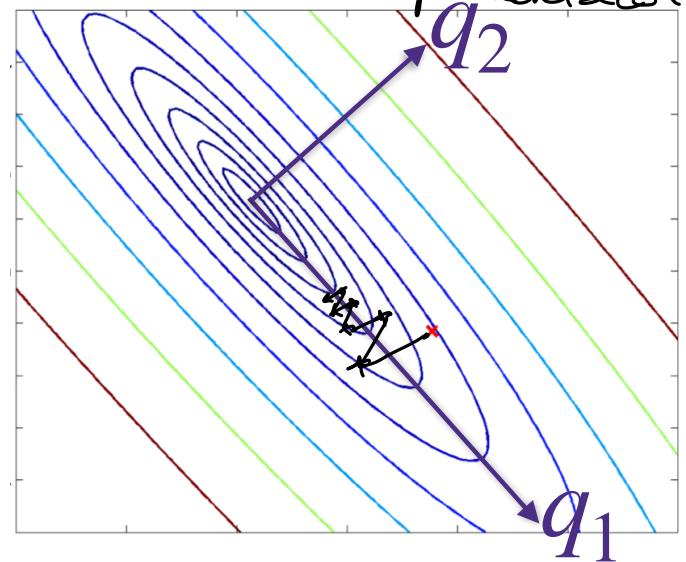
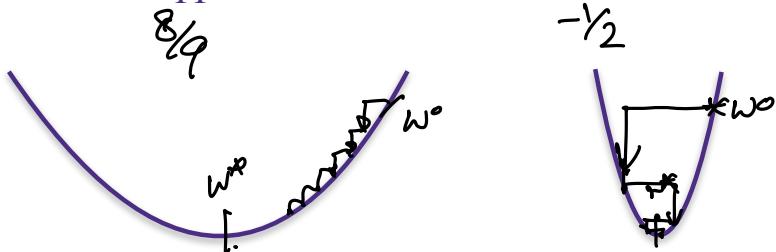
- For example suppose, the step size η is chosen such that

In direction q_1

$$0 < D_{11} < 1$$

In direction q_2

$$-1 < D_{22} < 0$$

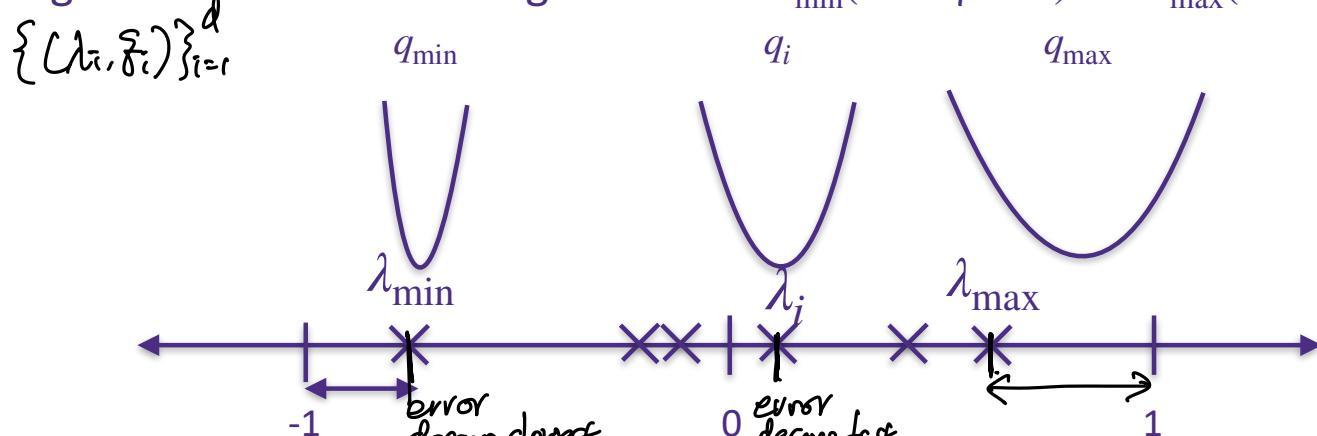


Gradient descent for linear regression

- Note that $D_{ii} := \lambda_i(\mathbf{I} - 2\eta\mathbf{X}^T\mathbf{X})$ is defined as the i -th Eigen value of the matrix $\mathbf{I} - 2\eta\mathbf{X}^T\mathbf{X}$
- Recall that in each eigen direction error evolves as

$$q_i^T(w_{t+1} - w^*) = (\lambda_i(\mathbf{I} - 2\eta\mathbf{X}^T\mathbf{X}))^{t+1} q_i^T(w_0 - w^*)$$

- We want the error to decay fast in all directions, whose bottleneck are the largest and the smallest eigen values: $\lambda_{\min}(\mathbf{I} - 2\eta\mathbf{X}^T\mathbf{X})$ and $\lambda_{\max}(\mathbf{I} - 2\eta\mathbf{X}^T\mathbf{X})$



We want to choose the learning rate η such that

$$-1 \ll \lambda_{\min}(\mathbf{I} - 2\eta\mathbf{X}^T\mathbf{X}) \leq \dots \leq \lambda_{\max}(\mathbf{I} - 2\eta\mathbf{X}^T\mathbf{X}) \ll 1$$

Gradient descent for linear regression

- We use linear algebra to answer the question:
how does the rate of error decay change with step size η
- Recall that in each eigen direction error decays as

$$q_i^T(w_{t+1} - w^*) = \lambda_i(\mathbf{I} - 2\eta \mathbf{X}^T \mathbf{X})^{t+1} q_i^T(w_0 - w^*)$$

- I will not prove the facts that $\|q_i\|_2 = 1$ and $q_i^T q_j = 0$

Claim: $\lambda_i(\mathbf{I} - 2\eta \mathbf{X}^T \mathbf{X}) = 1 - 2\eta \underbrace{\lambda_i}_{\tilde{\lambda}_i} (\mathbf{X}^T \mathbf{X})$

$\mathbf{X}^T \mathbf{X}$ has eigen decomposition
 $\tilde{\mathbf{Q}} \tilde{\mathbf{D}} \tilde{\mathbf{Q}}^T$, $\tilde{\mathbf{D}} = [\tilde{\lambda}_1, \tilde{\lambda}_2, \dots, \tilde{\lambda}_d]$

$$\begin{aligned} \mathbf{I} - 2\eta \mathbf{X}^T \mathbf{X} &= \tilde{\mathbf{Q}}^T \tilde{\mathbf{Q}} - 2\eta \tilde{\mathbf{Q}}^T \tilde{\mathbf{D}} \tilde{\mathbf{Q}} \\ &= \tilde{\mathbf{Q}}^T \underbrace{(\mathbf{I} - 2\eta \tilde{\mathbf{D}})}_{\cong D = [\tilde{\lambda}_1, \dots, \tilde{\lambda}_d]} \tilde{\mathbf{Q}} \end{aligned}$$

Claim: $\lambda_i(\mathbf{X}^T \mathbf{X}) \geq 0$

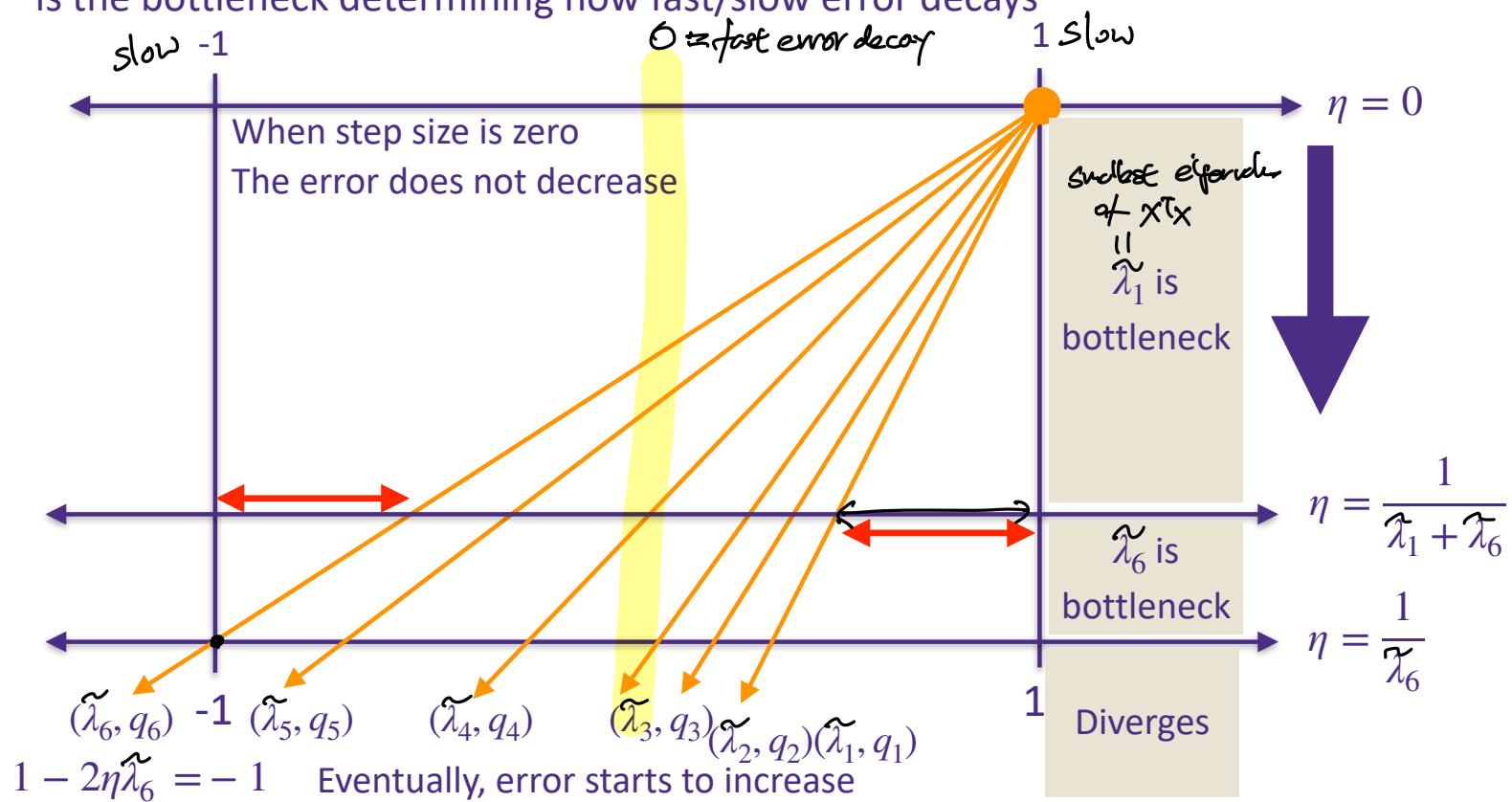
skip proof.

$$\boxed{\lambda_i = 1 - 2\eta \tilde{\lambda}_i}$$

↑ eigenvalue of $\mathbf{I} - 2\eta \mathbf{X}^T \mathbf{X}$ ↑ eigen value of $\mathbf{X}^T \mathbf{X}$

Gradient descent for linear regression

- Claim: $\lambda_i(\mathbf{I} - 2\eta \mathbf{X}^T \mathbf{X}) = \underbrace{1 - 2\eta \lambda_i(\mathbf{X}^T \mathbf{X})}_{1-2\eta\lambda_i(\mathbf{X}^T \mathbf{X})}$, and $\lambda_i(\mathbf{X}^T \mathbf{X}) \geq 0$
- We plot $\{1 - 2\eta \lambda_i(\mathbf{X}^T \mathbf{X})\}$ for increasing step sizes, the largest $|1 - 2\eta \lambda_i(\mathbf{X}^T \mathbf{X})|$
is the bottleneck determining how fast/slow error decays



Gradient descent for logistic regression

- Now we know how to find the global minimum of a logistic regression problem, numerically

Loss function: Conditional Likelihood

$$\{(x_i, y_i)\}_{i=1}^n \quad x_i \in \mathbb{R}^d, \quad y_i \in \{-1, 1\}$$

$$\widehat{w}_{MLE} = \arg \max_w \prod_{i=1}^n P(y_i | x_i, w) \quad P(Y = y | x, w) = \frac{1}{1 + \exp(-y w^T x)}$$

$$= \arg \min_w \sum_{i=1}^n \log(1 + \exp(-y_i x_i^T w))$$

$$\nabla f(w) = \sum_{i=1}^n \frac{1}{1 + \exp(-y_i x_i^T w)} \exp(-y_i x_i^T w) (-y_i x_i)$$

What is known for Gradient descent

- $f(\cdot)$ is L -smooth if $\|\nabla f(w) - \nabla f(v)\|_2 \leq L\|w - v\|_2$ for all $w, v \in \mathbb{R}^d$
- $f(\cdot)$ is μ -strongly convex if $f(w) \geq f(v) + \nabla f(v)^T(w - v) + \frac{\mu}{2}\|w - v\|_2^2$
- For L -smooth functions, with a fixed step size $\eta < 1/L$
 - if $f(w)$ is convex,

$$f(w_t) - f(w^*) \leq \frac{\|w_0 - w^*\|_2^2}{2\eta t} = \left(\frac{1}{t}\right) \text{convex rate}$$

- if $f(w)$ is μ -strongly convex,

$$f(w_t) - f(w^*) \leq (1 - \eta\mu)^t (f(w_0) - f(w^*)) = (e^{-\frac{\mu}{\eta}t}) \text{convex rate}$$

- What can we do for non-smooth function $f(w)$?
 - for example, LASSO

$$\hat{w}_{\text{Lasso}} = \arg \min_{w \in \mathbb{R}^d} \underbrace{\|\mathbf{y} - \mathbf{X}w\|_2^2 + \lambda\|w\|_1}_{f(w)}$$

Questions?
