Lecture 4: Linear Regression (Part 3)

CIS 4190/5190

Spring 2023

Administrivia

- Class roster is now stable, and add/drop deadline has passed.
- HW1 due **tonight 8 p.m.**, and HW2 will be posted tonight/tomorrow morning, on linear regression.
  - Class late policy reminder: 0.5% points for every late hour, up to a max of 48 hours.
- TA office hours:
  - Any changes will be posted to the TA office hours thread on EdSTEM, at least 48 hours ahead of time.
  - We are moving the 3 p.m. OH on Monday and Wed to 3.30 p.m. to avoid clashing. More news on that soon.
- Recitations tomorrow at 5 p.m. on Python, Numpy, Pandas, Scikit-Learn. See EdSTEM post.

- No quiz for week 1. We'll fix the webpage.

Last Lecture Summary

- The Train/Test Split Protocol for Measuring Underfitting / Overfitting
- Bias and variance as functions of a model class
  - Tuning them by selecting hypothesis spaces / feature maps
  - Tuning them by modifying the loss function
    - $L_{\text{new}}(\beta; Z) = L(\beta; Z) + \lambda \cdot R(\beta)$

- Today:
  - Selecting hyperparameters like λ
  - Finally unveil the mystery about how to find $\hat{\beta}(Z) = \arg\min_{\beta} L(\beta; Z)$

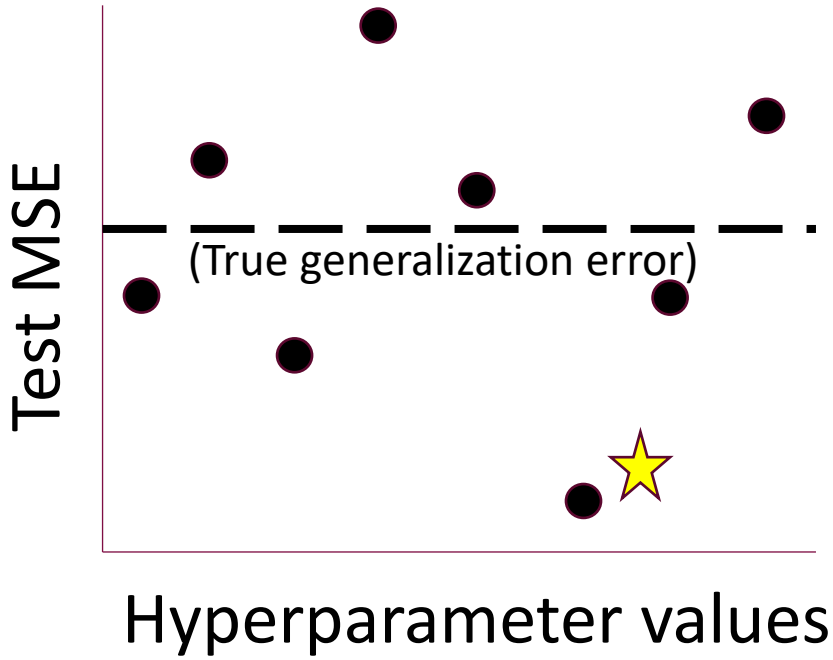
Cross-Validation for Model Selection

Hyperparameter Tuning, or “Model Selection”

- λ is a **hyperparameter** that must be tuned (satisfies $\lambda \geq 0$)
- **Naïve strategy:** Try a few different candidates λ_t and choose the one that minimizes the test loss

Test Data Contamination

- Suppose you have tried 100 different hyperparameter values, that all haver the same value of generalization MSE, if evaluated on the *full* data distribution.
- But the test dataset is only a finite sample of this distribution, so test MSE is a noisy estimate of true generalization MSE. For example



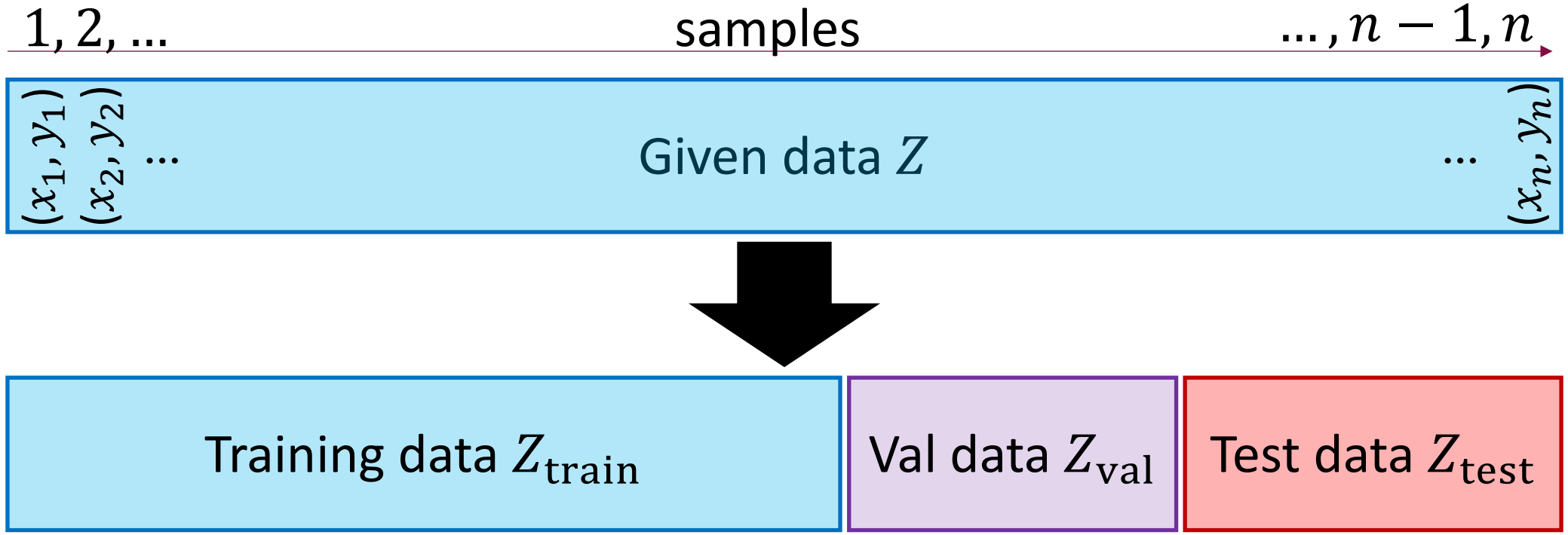
Note how, in selecting based on test MSE, you have “overfit” your hyperparameter choice to your test set!

Hyperparameter Tuning, or “Model Selection”

- λ is a **hyperparameter** that must be tuned (satisfies $\lambda \geq 0$)
- **Naïve strategy:** Try a few different candidates λ_t and choose the one that minimizes the test loss
- **Problem:** We may overfit the test set!
  - Major problem if we have more hyperparameters
- **Solution:** A new subset of data just for selecting hyperparameters

Train/Val/Test Split Protocol for Model Selection

- **Goal:** Choose best hyperparameter λ
  - Can also compare different model families, feature maps, etc.
- **Solution:** Optimize λ on a **held-out validation data**
  - **Rule of thumb:** 60/20/20 split (usually shuffle before splitting)



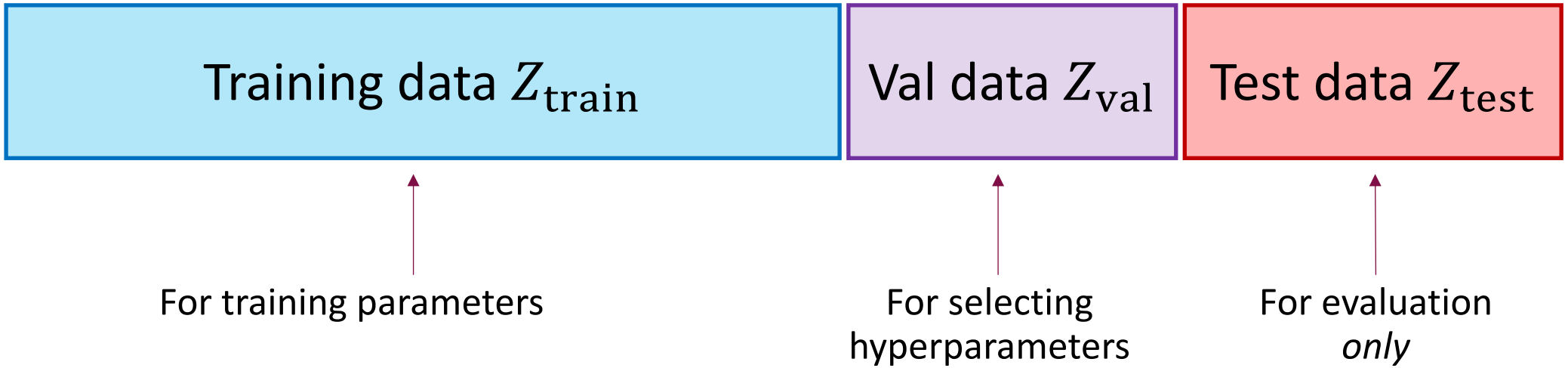
Basic Cross Validation Algorithm: "Holdout"

- **Step 1:** Split Z into Z_{train}, Z_{val}, and Z_{test}

- **Step 2:** For $t \in \{1, \ldots, h\}$ hyperparameter choices:
  - **Step 2a:** Run linear regression with Z_{train} and λ_t to obtain $\hat{\beta}(Z_{\text{train}}, \lambda_t)$
  - **Step 2b:** Evaluate validation loss $L_{\text{val}}^t = L\left(\hat{\beta}(Z_{\text{train}}, \lambda_t); Z_{\text{val}}\right)$

- **Step 3:** Use best λ_t
  - Choose $t' = \arg\min_t L_{\text{val}}^t$ with lowest validation loss
  - Re-run linear regression with Z_{train} and $\lambda_{t'}$ to obtain $\hat{\beta}(Z_{\text{train}}, \lambda_{t'})$

Cross Validation Hygiene



- The moment that test data is used for hyperparameter selection or to iterate on ML design choices, it should be treated as "contaminated".
- Remember: Performance on contaminated test data is an overly ***optimistic*** estimate of the "true" test performance.

Q: What about validation data performance then?

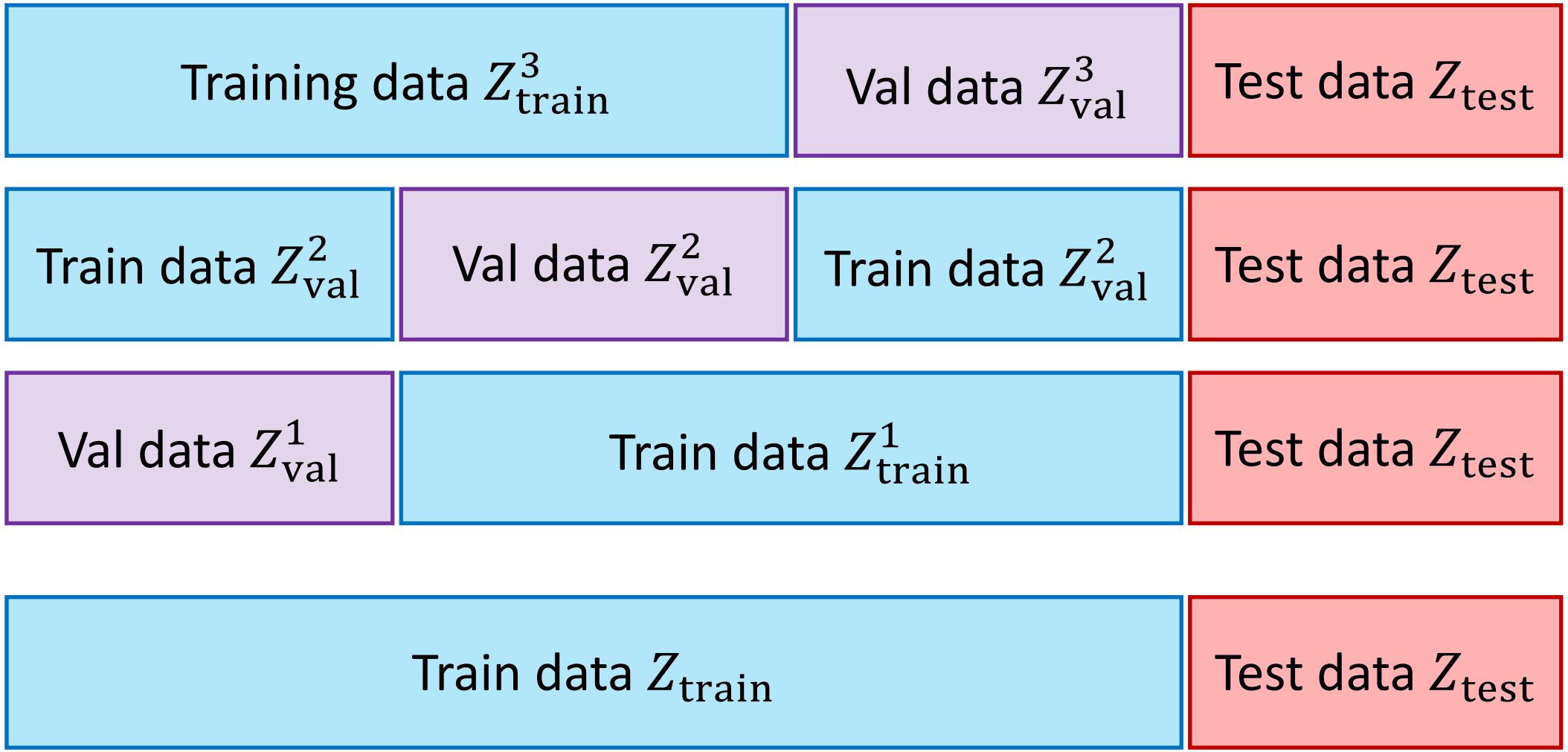
(yes, this is also overly optimistic)

Alternative Cross-Validation Algorithms

- If Z is small, then splitting it can reduce performance
  - Can use $Z_{\text{train}} \cup Z_{\text{val}}$ in Step 3

- **Alternative more thorough CV strategy:** "k-fold" cross-validation
  - Split Z into Z_{train} and Z_{test}
  - Split Z_{train} into k disjoint sets Z_{val}^{s}, and let $Z_{\text{train}}^{s} = \cup_{s' \neq s} Z_{\text{val}}^{s}$
  - Use λ' that works best on average across $s \in \{1, \ldots, k\}$ with Z_{train}
  - Chooses better λ' than above strategy

Example: $k = 3$-Fold Cross Validation



Compute vs. accuracy tradeoff: As $k \rightarrow N$, model selection becomes more accurate, but algorithm becomes more computationally expensive

Note: What Exactly Are "Hyperparameters"?

- Cross-Validation is a general, systematic trial-and-error procedure for selecting hyperparameters.
- Other hyperparameters too, not *just* the regularization λ.
- "Hyperparameters" are ML system properties / design choices that are not directly set in the optimization problem.

$$\hat{\beta}(Z) = \arg\min_{\beta} L(\beta; Z)$$

- Examples of other hyperparameters you could set with cross-validation:
  - choice of feature maps in linear regression.
  - data selection and other preprocessing procedures (coming up soon).
  - linear regression versus another ML algorithm, altogether.

Minimizing the MSE Loss

- Recall that linear regression minimizes the loss

$$L(\beta; Z) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2$$

- **Closed-form solution:** Compute a matrix expression derived using calculus

- **Iterative Optimization-based solution:** Search over candidate β

Vectorizing Linear Regression

Vectorizing Linear Regression

$$\begin{bmatrix} f_\beta(x_1) \\ \vdots \\ f_\beta(x_n) \end{bmatrix}$$

Vectorizing Linear Regression

$$\begin{bmatrix} f_\beta(x_1) \\ \vdots \\ f_\beta(x_n) \end{bmatrix} = \begin{bmatrix} \beta^\top x_1 \\ \vdots \\ \beta^\top x_n \end{bmatrix}$$

Vectorizing Linear Regression

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$$\approx$$

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

Vectorizing Linear Regression

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$\approx$

$$\begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = Y$$

Summary: $Y \approx X\beta$

Note: n equations, d variables

Vectorizing Linear Regression

$$Y \approx X\beta$$

$$Y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \qquad X = \begin{bmatrix} x_{1,1} & \cdots & x_{1,d} \\ \vdots & \ddots & \vdots \\ x_{n,1} & \cdots & x_{n,d} \end{bmatrix} \qquad \beta = \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_d \end{bmatrix}$$

Vectorizing Mean Squared Error

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$$L(\beta; Z)$$

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$$L(\beta; Z) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2$$

Vectorizing Mean Squared Error

$$L(\beta; Z) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2 = \frac{1}{n}\|Y - X\beta\|_2^2$$

$$Y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} \qquad X\beta = \begin{bmatrix} f_\beta(x_1) \\ \vdots \\ f_\beta(x_n) \end{bmatrix}$$

$$\|z\|_2^2 = \sum_{i=1}^{n} z_i^2$$

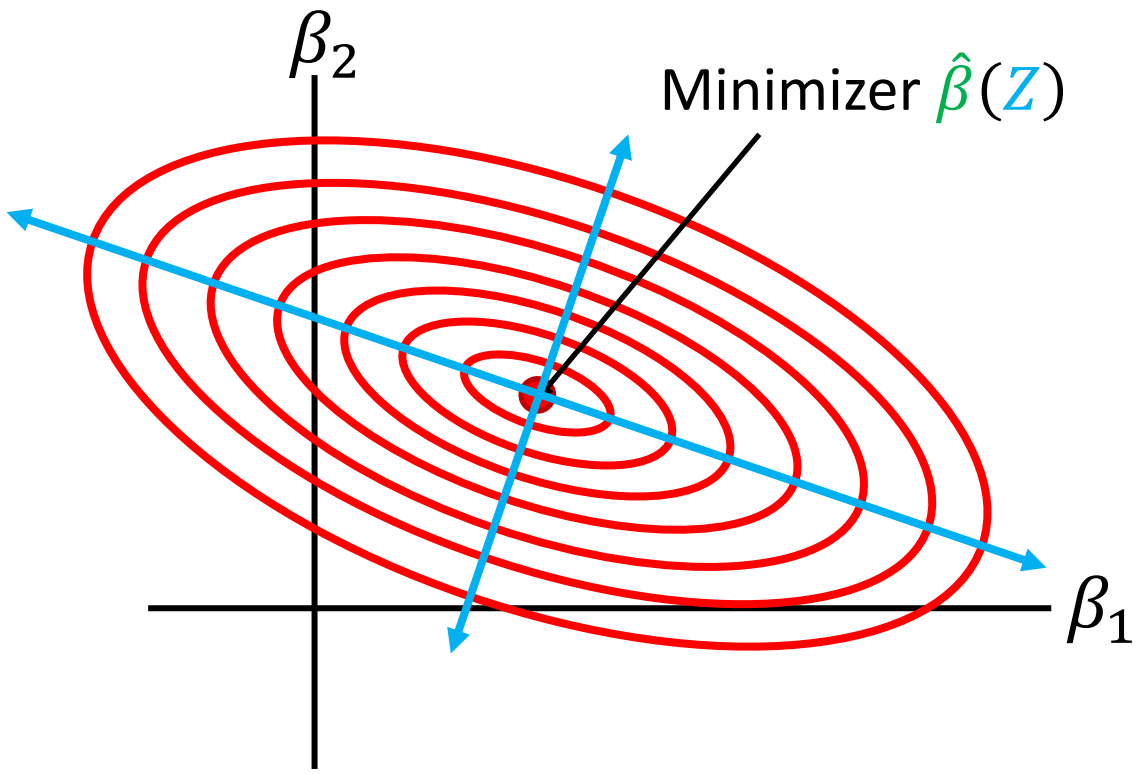
Intuition on Vectorized Linear Regression

- Rewriting the vectorized loss:

$$n \cdot L(\beta; Z) = \|Y - X\beta\|_2^2 = \|Y\|_2^2 - 2Y^\top X\beta + \|X\beta\|_2^2$$
$$= \|Y\|_2^2 - 2Y^\top X\beta + \beta^\top (X^\top X)\beta$$

- **Side note:** Quadratic function of β with leading "coefficient" $X^\top X$
  - In one dimension, "width" of parabola $ax^2 + bx + c$ is a^{-1}
  - In multiple dimensions, "width" along direction v_i is λ_i^{-1}, where v_i is an eigenvector of $X^\top X$ with eigenvalue λ_i
    - Large width (small λ_i) along a direction v_i implies that parameter values along that direction affect the loss value less.
    - This will be interesting to us later in class ("PCA")

Intuition on Vectorized Linear Regression



Directions/magnitudes are given by eigenvectors/eigenvalues of $X^\top X$

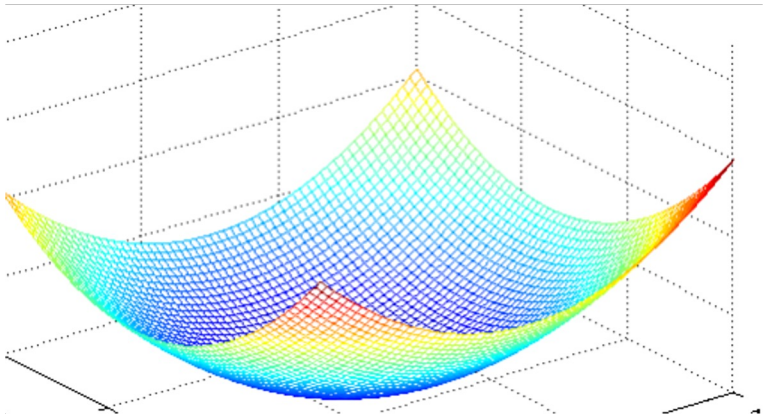
Strategy 1: Closed-Form Solution

- Recall that linear regression minimizes the loss:

$$L(\beta; Z) = \frac{1}{n}\|Y - X\beta\|_2^2$$

- Minimum solution has gradient equal to zero:

$$\nabla_\beta L\left(\hat{\beta}(Z); Z\right) = 0$$



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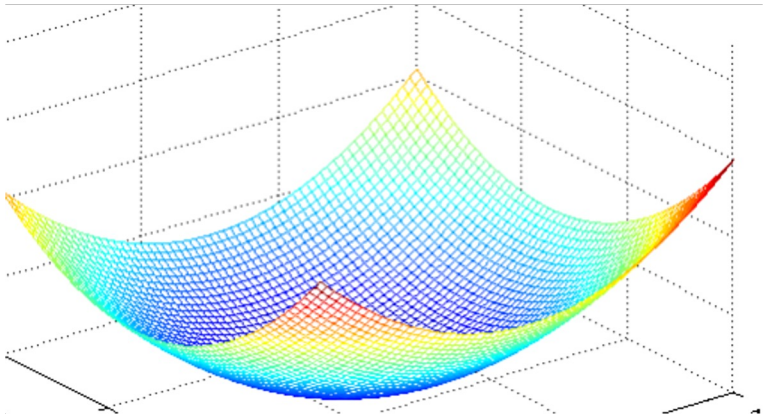

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- The gradient is

$$\nabla_{\beta} L(\beta; Z)$$

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Strategy 1: Closed-Form Solution

- The gradient is

$$\nabla_\beta L(\beta; Z) = \nabla_\beta \frac{1}{n} \|Y - X\beta\|_2^2 = \nabla_\beta \frac{1}{n} (Y - X\beta)^\top (Y - X\beta)$$

$$= \frac{2}{n} \left[\nabla_\beta (Y - X\beta)^\top\right] (Y - X\beta)$$

$$= -\frac{2}{n} X^\top (Y - X\beta)$$

$$= \boxed{-\frac{2}{n} X^\top Y + \frac{2}{n} X^\top X\beta}$$

Strategy 1: Closed-Form Solution

- The gradient is

$$\nabla_\beta L(\beta; Z) = \nabla_\beta \frac{1}{n}\|Y - X\beta\|_2^2 = -\frac{2}{n}X^\top Y + \frac{2}{n}X^\top X\beta$$

- Setting $\nabla_\beta L(\hat{\beta}; Z) = 0$, we have $X^\top X\hat{\beta} = X^\top Y$

Compare this to: $Y \approx X\beta$

- Assuming $X^\top X$ is invertible, we have

$$\hat{\beta}(Z) = \underbrace{(X^\top X)^{-1}X^\top}Y$$

This is called the "pseudoinverse" of X

Strategy 1: Closed-Form Solution

- Setting $\nabla_\beta L\left(\hat{\beta}; Z\right) = 0$, we have $X^\top X\hat{\beta} = X^\top Y$
- Assuming $X^\top X$ is invertible, we have

$$\hat{\beta}(Z) = (X^\top X)^{-1} X^\top Y$$

Note on Invertibility

- Closed-form solution only **unique** if $X^\top X$ (size dxd) is invertible
  - Otherwise, **multiple solutions exist** to $X^\top X\hat{\beta} = X^\top Y$
  - **Intuition:** Underconstrained system of linear equations

- **Example:**

$$\begin{bmatrix} 1 & 1 \\ 2 & 2 \end{bmatrix} \begin{bmatrix} \hat{\beta}_1 \\ \hat{\beta}_2 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \end{bmatrix}$$

  - In this case, any $\hat{\beta}_2 = 2 - \hat{\beta}_1$ is a solution

When Can this Happen?

- **Case 1**
  - Fewer data examples than feature dimension (i.e., $n < d$)
    - Remember: we are solving something like $Y \approx X\beta$
  - **Solution:** Remove features so $d \leq n$
  - **Solution:** Collect more data until $d \leq n$

- **Case 2:** Some feature is a linear combination of the others
  - **Special case (duplicated feature):** For some j and j', $x_{i,j} = x_{i,j'}$ for all i
  - **Solution:** Remove linearly dependent features
  - **Solution:** Use L_2 regularization (we will soon see why)

Shortcomings of Closed-Form Solution

- Computing $\hat{\beta}(Z) = (X^\top X)^{-1} X^\top Y$ can be challenging

- **Computing $(\boldsymbol{X}^\top \boldsymbol{X})^{-1}$ is $\boldsymbol{O}(\boldsymbol{d}^3)$**
  - $d = 10^4$ features → $O(10^{12})$
  - Even storing $X^\top X$ requires a lot of memory

- **Numerical accuracy issues due to "ill-conditioning"**
  - $X^\top X$ is "barely" invertible
  - Then, $(X^\top X)^{-1}$ has large variance along some dimension
  - Regularization helps (more on this later)

Iterative Optimization Algorithms

- Recall that linear regression minimizes the loss

$$L(\beta; Z) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \beta^\top x_i)^2$$

- Iteratively optimize β
  - Initialize $\beta_1 \leftarrow \text{Init}(\dots)$
  - For some number of iterations T, update $\beta_t \leftarrow \text{Step}(\dots)$
  - Return β_T

Iterative Optimization Algorithms

- **Global search**: Try random values of β and choose the best
  - I.e., β_t independent of β_{t-1}
  - Very unstructured, can take a long time (especially in high dimension d)!

- **Local search**: Start from some initial β and make local changes
  - I.e., β_t is computed based on β_{t-1}
  - What is a “local change”, and how do we find good one?

Strategy 2: Gradient Descent

- **Gradient descent:** Update β based on **gradient** $\nabla_\beta L(\beta; Z)$ of $L(\beta; Z)$:

$$\beta_{t+1} \leftarrow \beta_t - \alpha \cdot \nabla_\beta L(\beta_t; Z)$$

- **Intuition:** The gradient is the direction along which $L(\beta; Z)$ changes most quickly as a function of β

- $\alpha \in \mathbb{R}$ is a hyperparameter called the **learning rate**
  - More on this later

Strategy 2: Gradient Descent

- Choose initial value for β
- Until we reach a minimum:
  - Choose a new value for β to reduce $L(\beta; Z)$

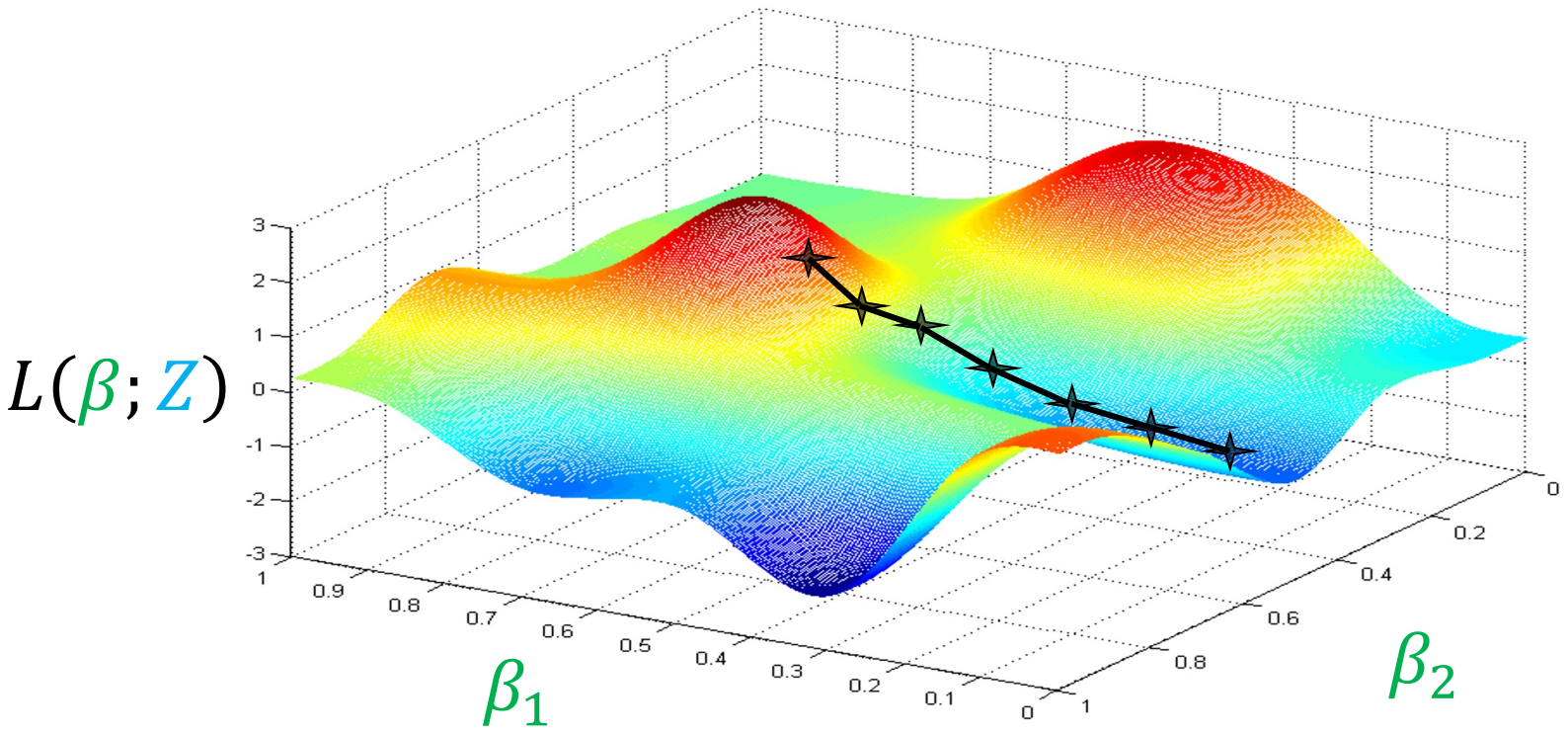

Figure by Andrew Ng

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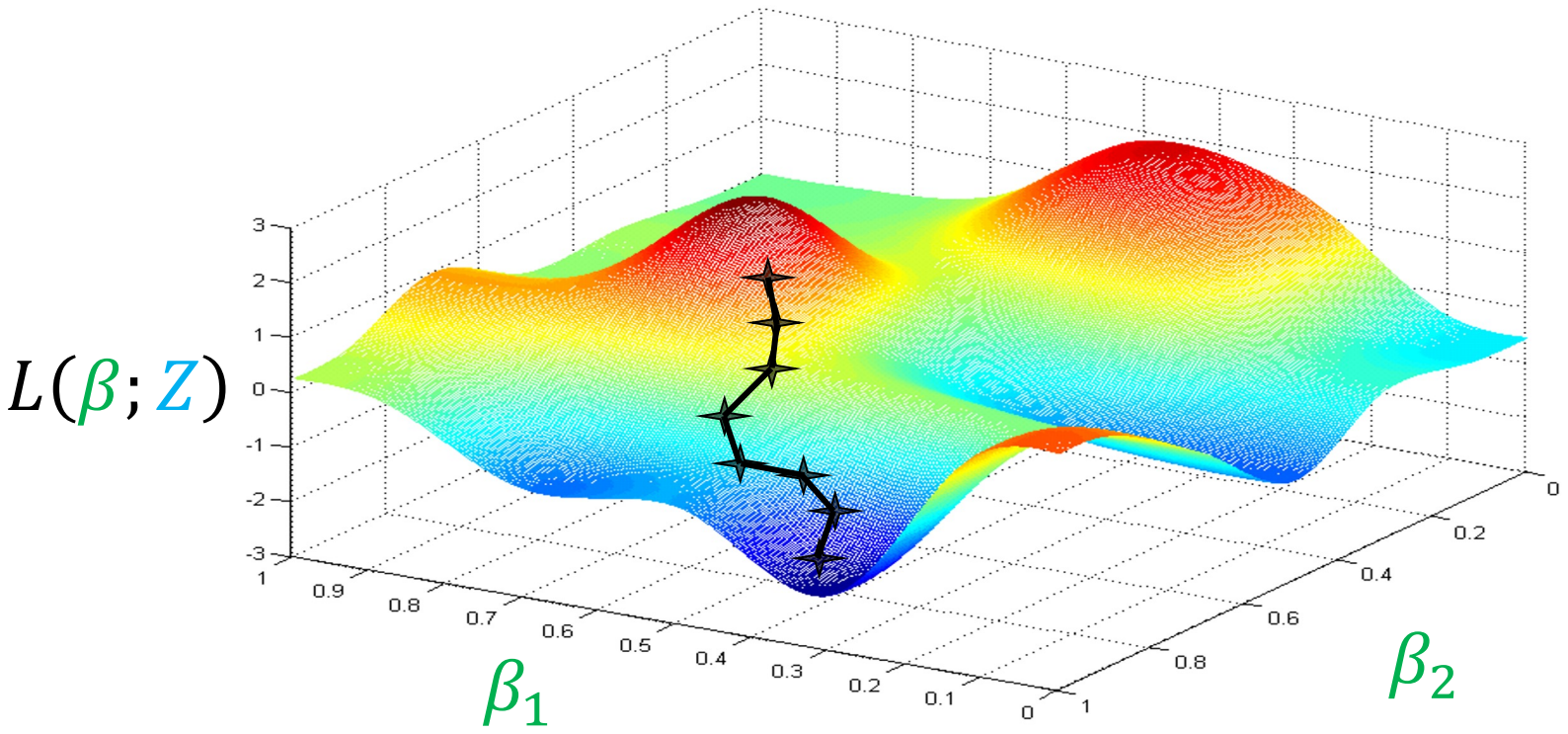

Figure by Andrew Ng

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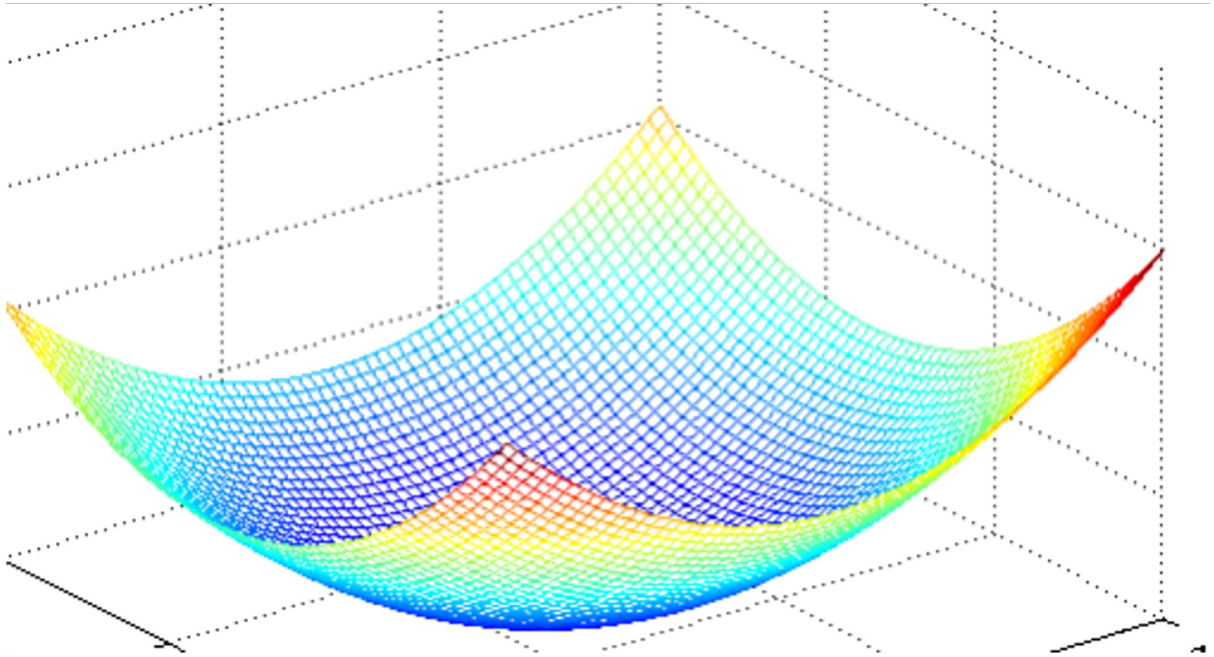


Linear regression loss is convex, so no local minima

Figure by Andrew Ng

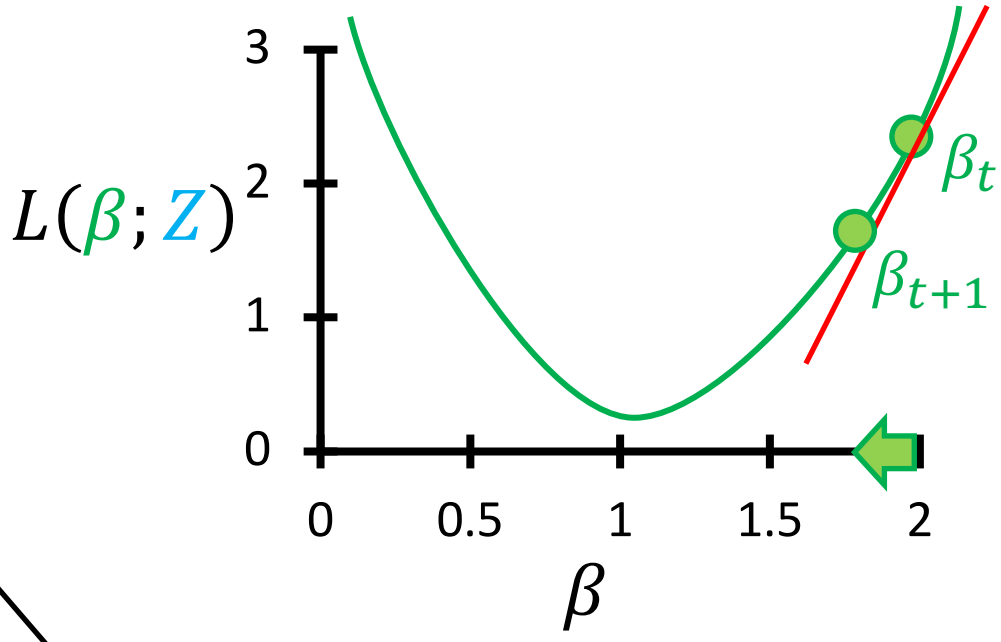
Strategy 2: Gradient Descent

Indexing iteration now, rather than parameter vector element

- Initialize $\beta_1 = \vec{0}$
- Repeat until convergence:

$$\beta_{t+1} \leftarrow \beta_t - \alpha \cdot \nabla_\beta L(\beta_t; Z)$$

- For linear regression, know the gradient from strategy 1



For in-place updates $\beta \leftarrow \beta - \alpha \cdot \nabla_\beta L(\beta; Z)$, compute all components of $\nabla_\beta L(\beta; Z)$ before modifying β

Strategy 2: Gradient Descent

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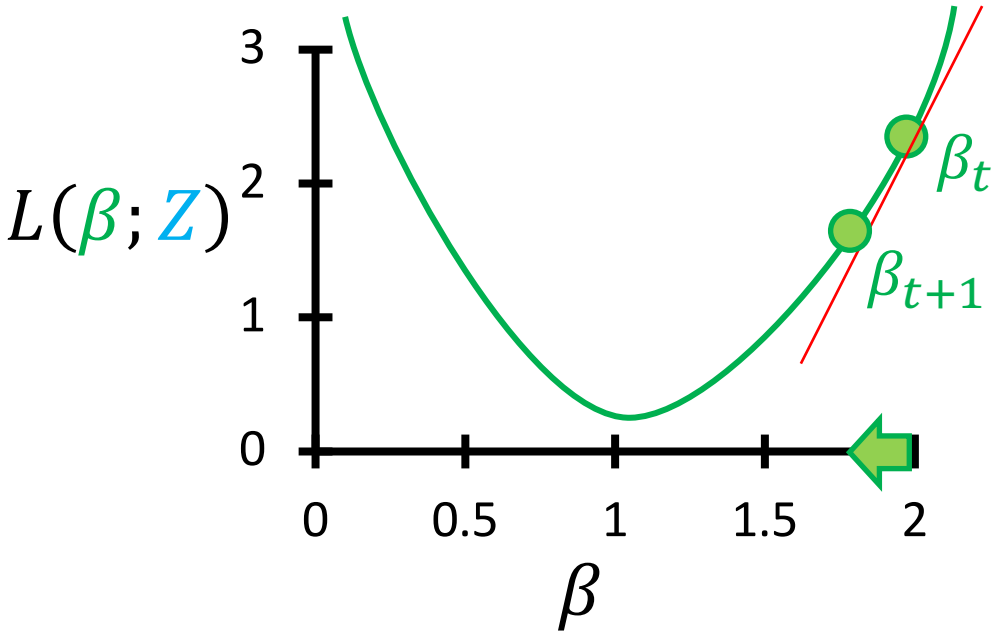

Strategy 2: Gradient Descent

- Initialize $\beta_1 = \vec{0}$
- Repeat until $\|\beta_t - \beta_{t+1}\|_2 \leq \epsilon$:

Hyperparameter defining convergence

$$\beta_{t+1} \leftarrow \beta_t - \alpha \cdot \nabla_\beta L(\beta_t; Z)$$

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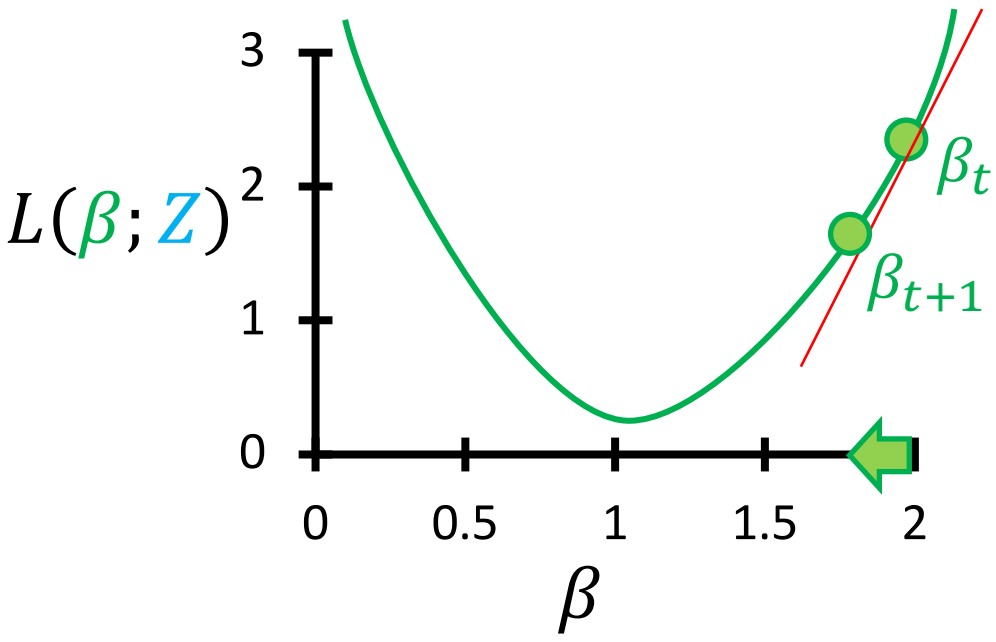


Aside: Gradient As Sum of Sample-Wise Gradients

$$-\frac{2}{n}X^\top Y + \frac{2}{n}X^\top X\beta$$

(Equivalent to our earlier matrix expression of gradient)

- By linearity of the gradient, we have

$$\nabla_\beta L(\beta; Z) = \sum_{i=1}^{n} \nabla_\beta (y_i - \beta^\top x_i)^2 = \sum_{i=1}^{n} 2(y_i - \beta^\top x_i)x_i$$

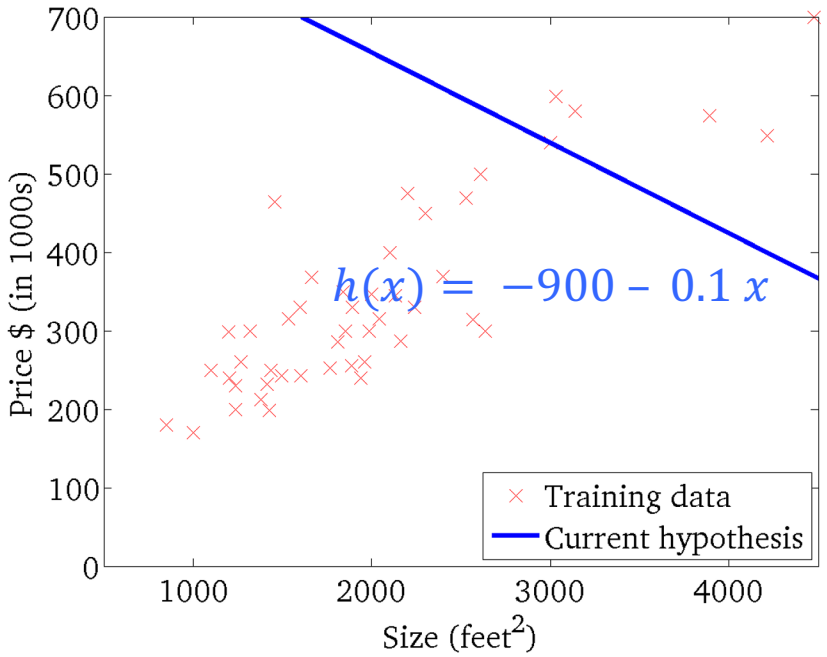
- The gradient term induced by a single training data sample is:

$$\nabla_\beta (y_i - \beta^\top x_i)^2 = 2(y_i - \beta^\top x_i)x_i$$

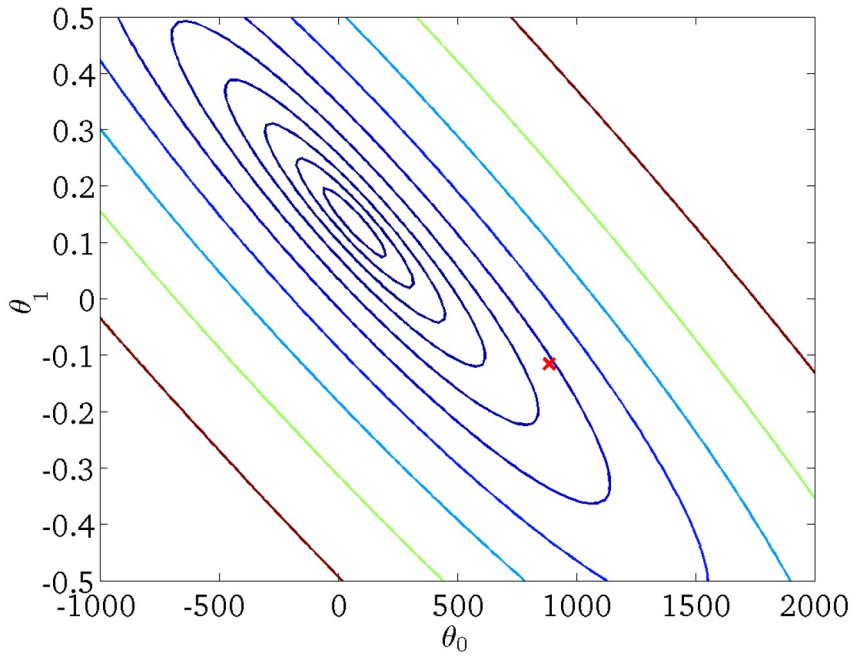
- I.e., the current error $y_i - \beta^\top x_i$ times the feature vector x_i

"Large error samples induce large changes to β, proportional to their feature values."

Strategy 2: Gradient Descent



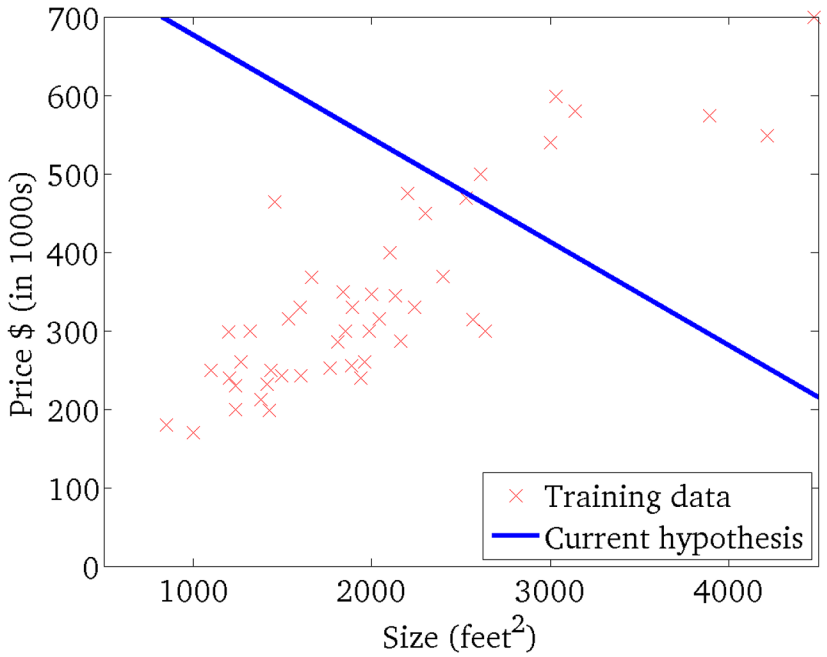
$f_\beta(x)$



$L(\beta; Z)$

Slide by Andrew Ng

Strategy 2: Gradient Descent



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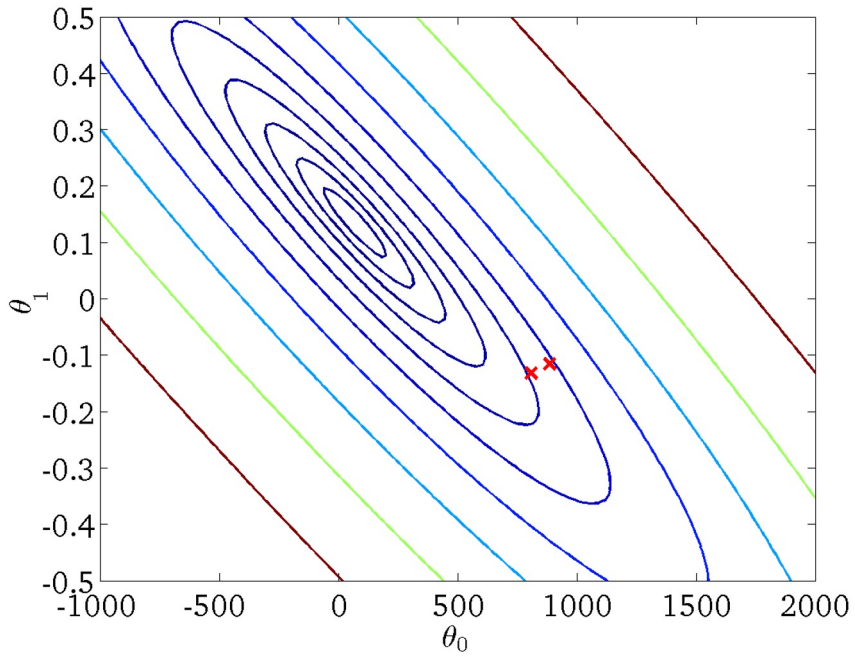

$L(\beta; Z)$

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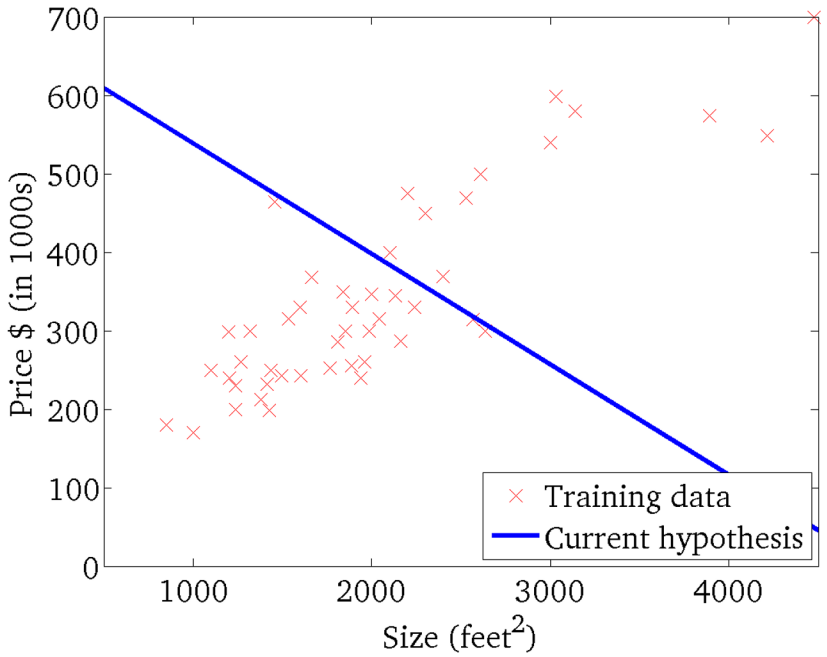
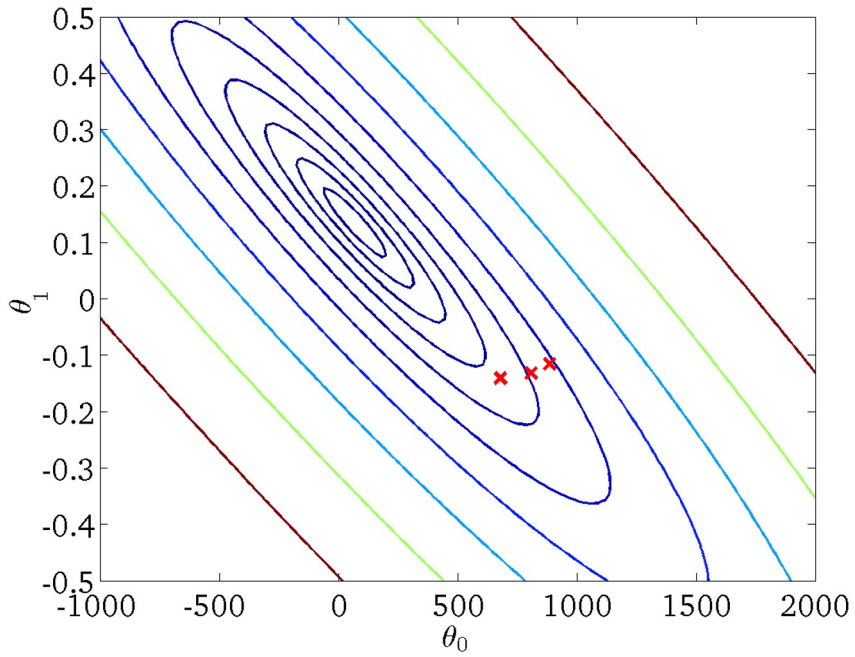


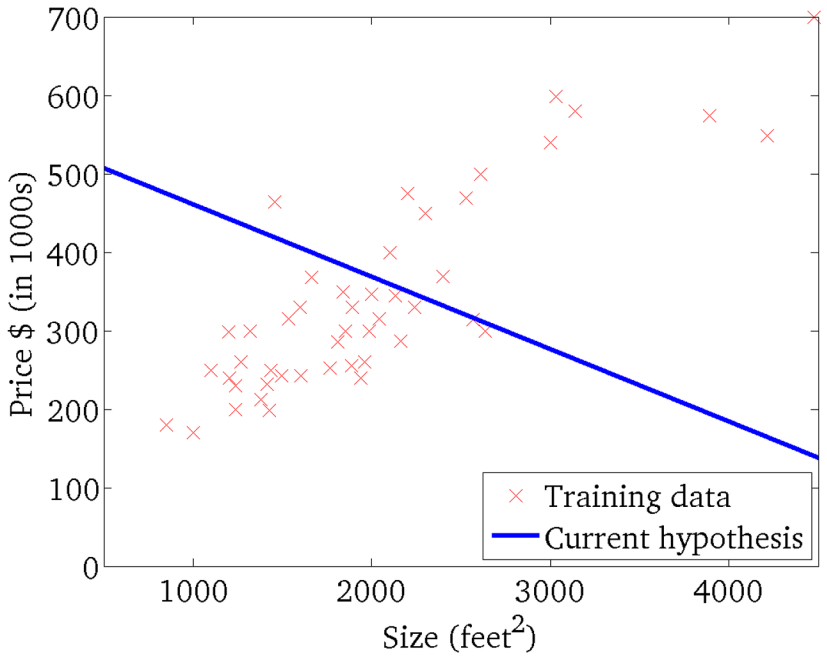
$f_\beta(x)$



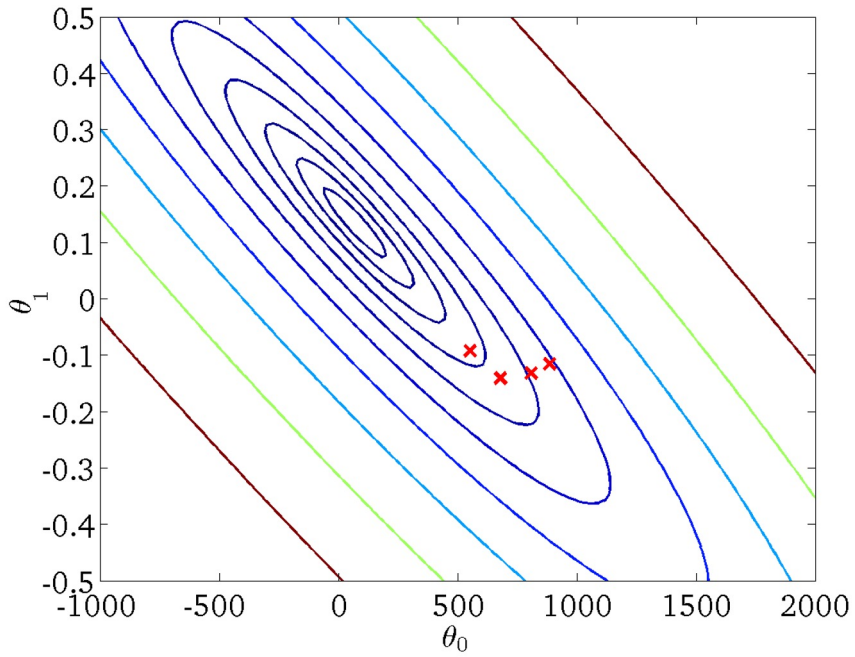
$L(\beta; Z)$

Slide by Andrew Ng

Strategy 2: Gradient Descent



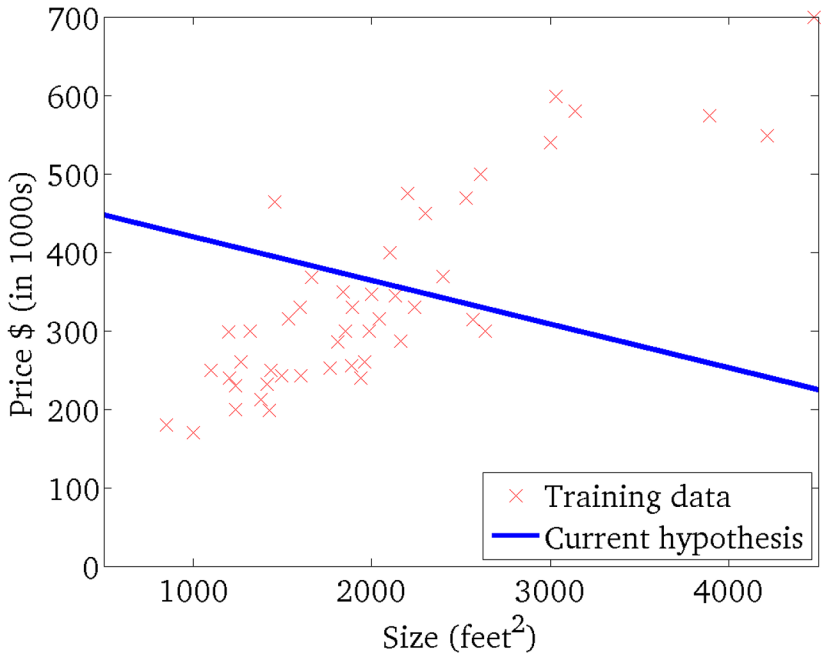
$f_\beta(x)$



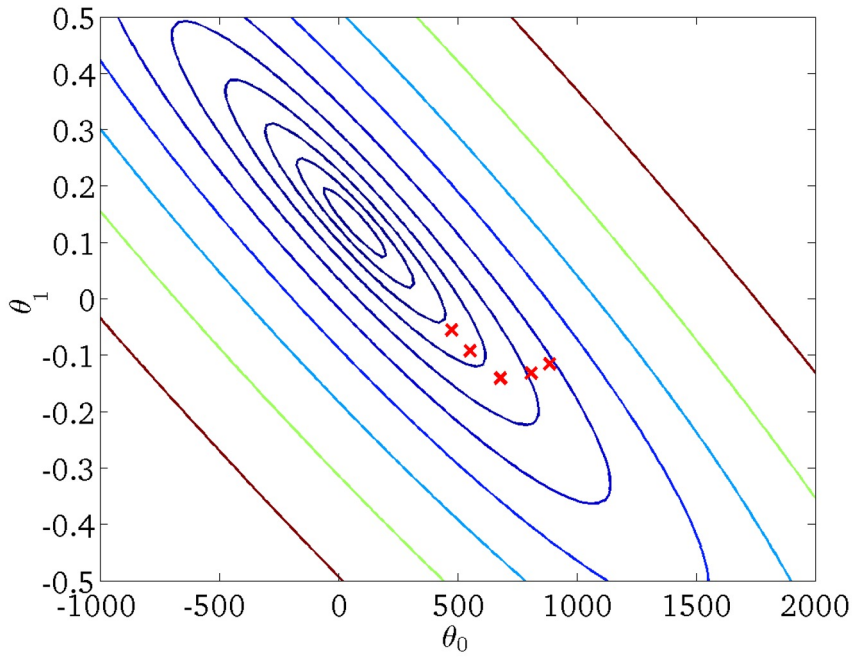
$L(\beta; Z)$

Slide by Andrew Ng

Strategy 2: Gradient Descent



$f_\beta(x)$



$L(\beta; Z)$

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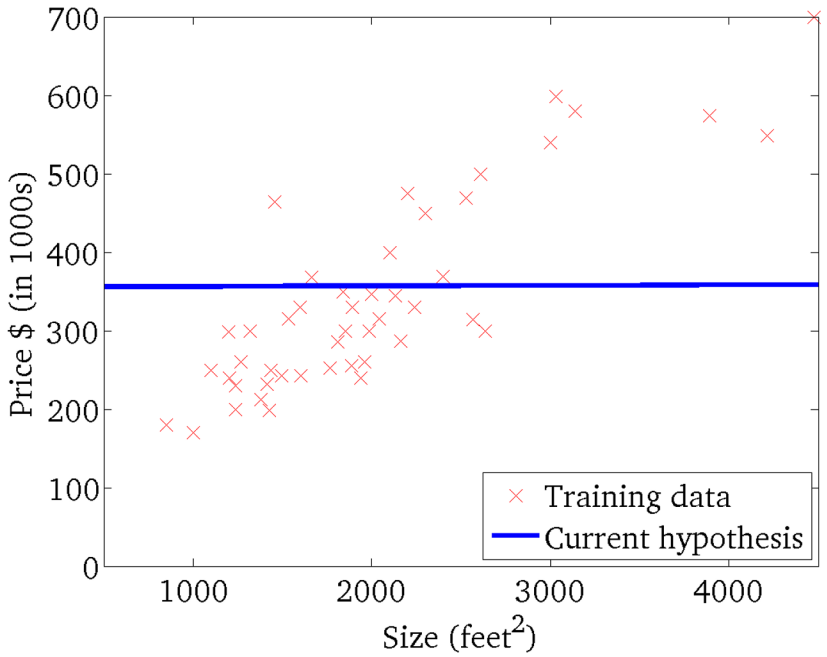
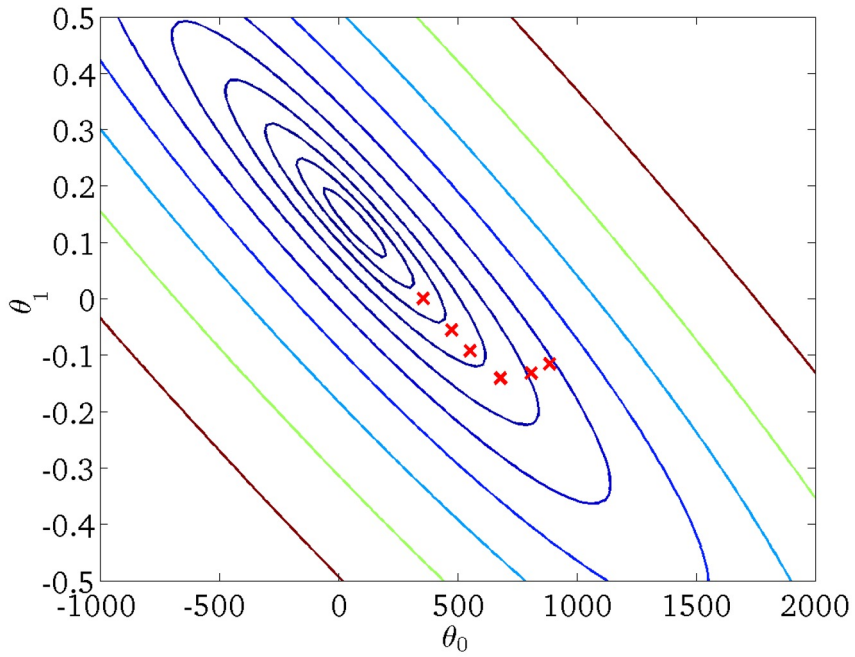
Strategy 2: Gradient Descent



$f_\beta(x)$



$L(\beta; Z)$

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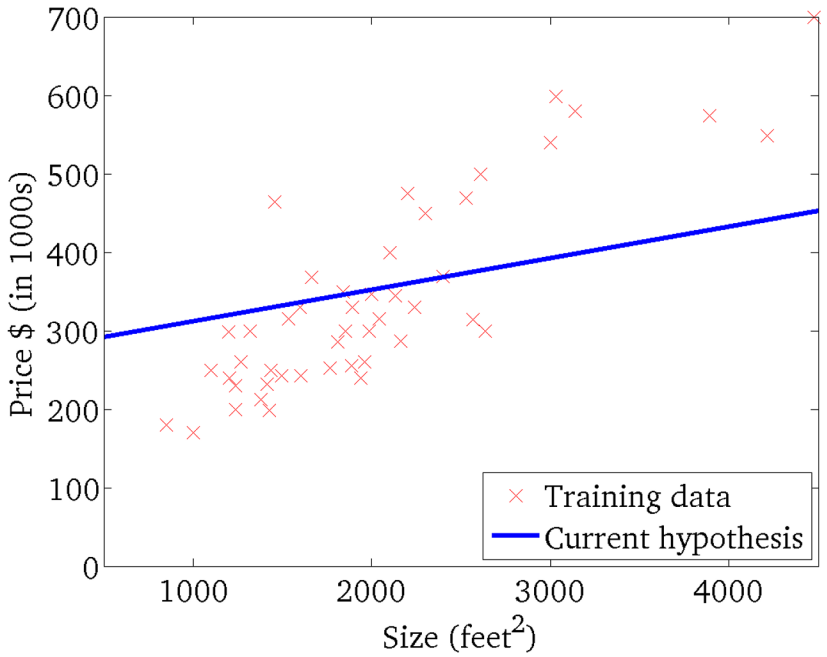
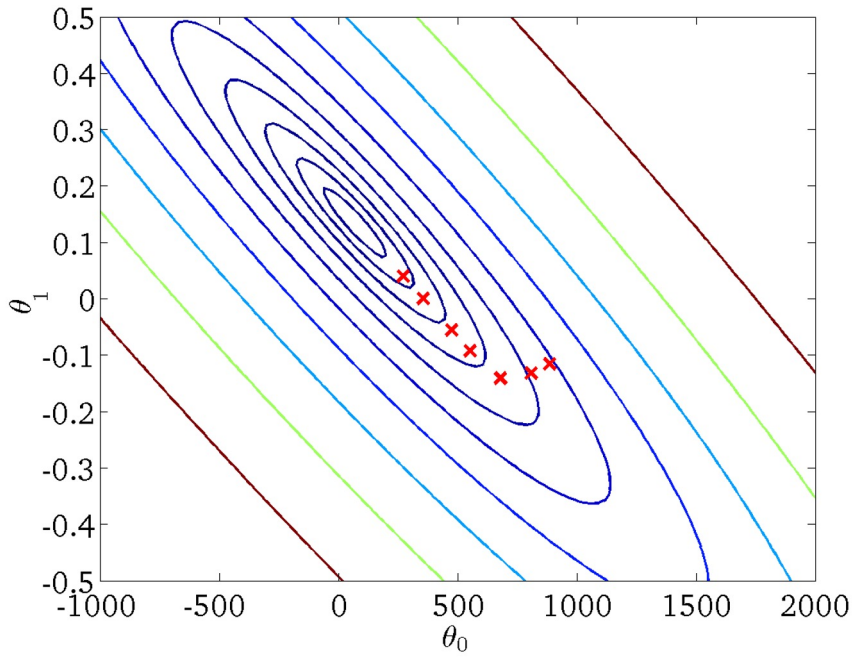
Strategy 2: Gradient Descent



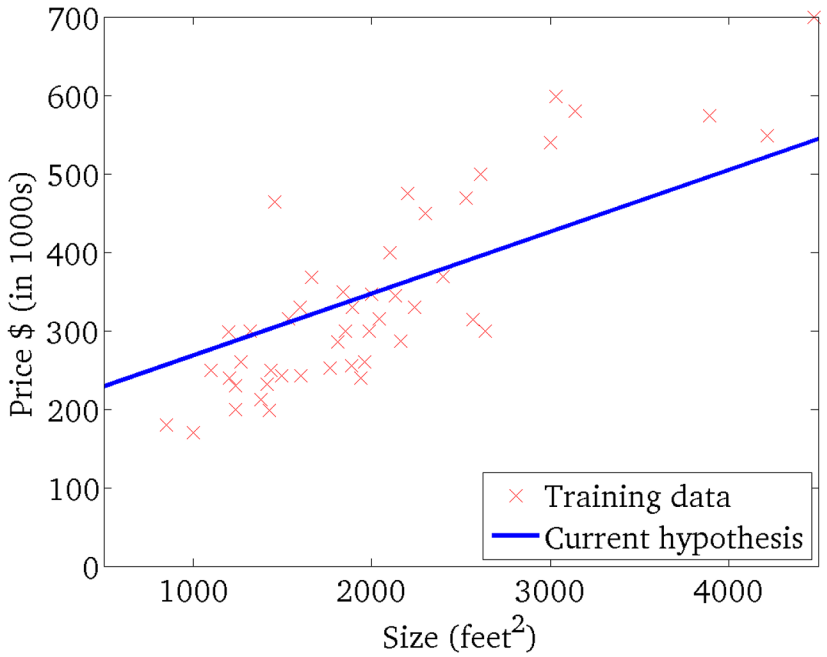
$f_\beta(x)$



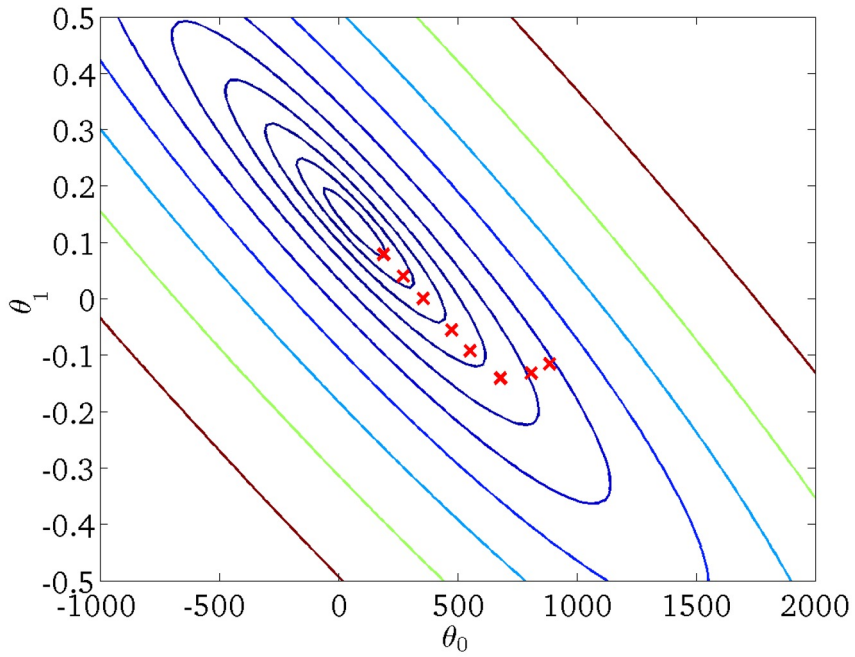
$L(\beta; Z)$

Slide by Andrew Ng

Strategy 2: Gradient Descent



$f_\beta(x)$



$L(\beta; Z)$

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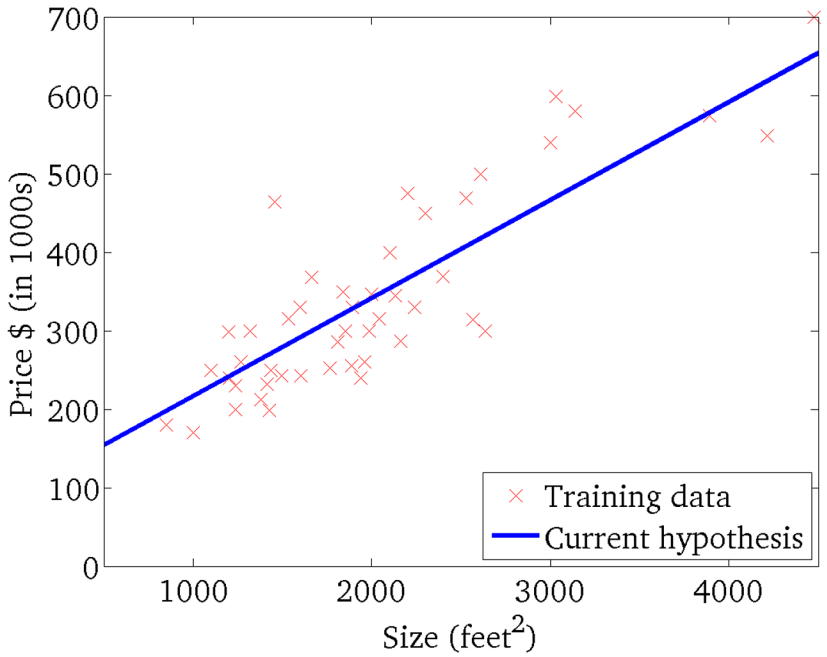
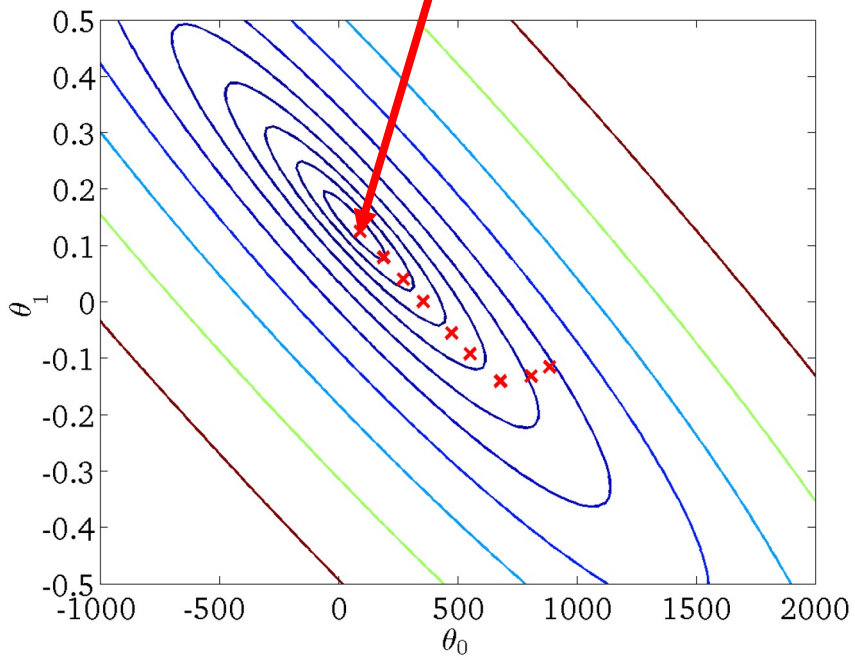
Strategy 2: Gradient Descent



$f_\beta(x)$

Minimizer of loss function



$L(\beta; Z)$

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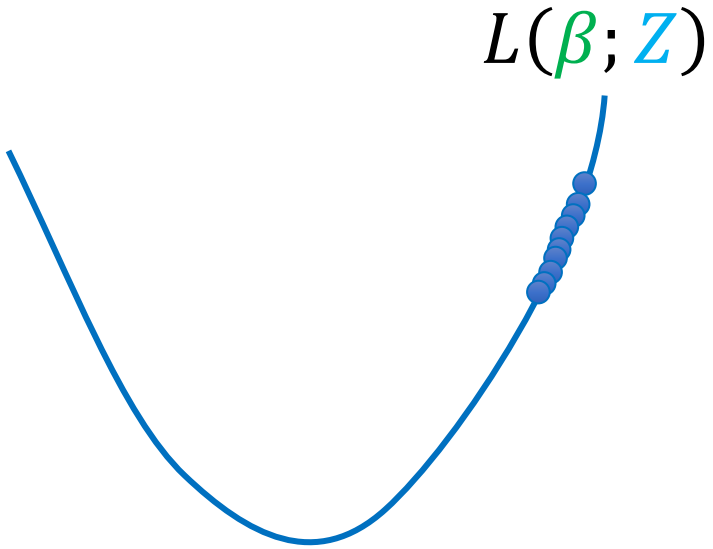
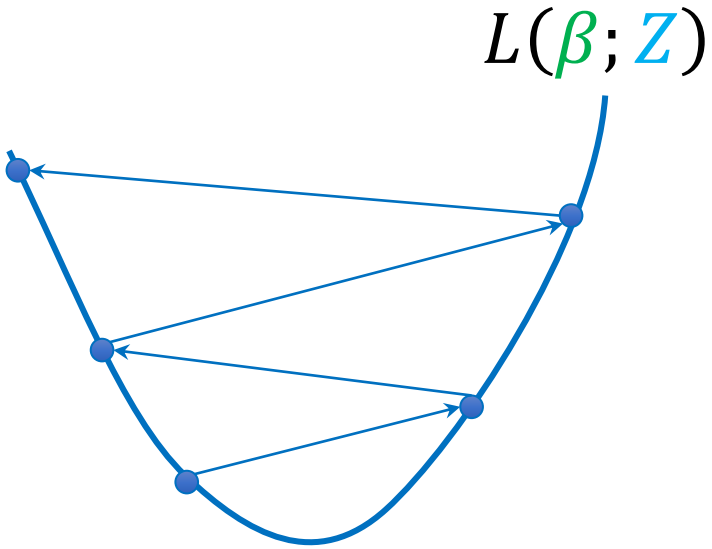
Choice of Learning Rate α



Problem: α too small

- $L(\beta; Z)$ decreases slowly



Problem: α too large

- $L(\beta; Z)$ increases!

Plot $L(\beta_t; Z_{\text{train}})$ vs. t to diagnose these problems

Choice of Learning Rate α

- α is a hyperparameter for gradient descent that we need to choose
  - Can set just based on training data

- **Rule of thumb**
  - α **too small:** Loss decreases slowly
  - α **too large:** Loss increases!

- Try rates $\alpha \in \{1.0, 0.1, 0.01, \ldots\}$ (can tune further once one works)

Comparison of Strategies

- **Closed-form solution**
  - No hyperparameters
  - Slow if n or d are large

- **Gradient descent**
  - Need to tune α
  - Scales to large n and d

- For linear regression, there are better optimization algorithms, but gradient descent is very general
  - Accelerated gradient descent is an important tweak that improves performance in practice (and in theory)

Loss Minimization View of ML

- **Two design decisions**
  - **Model family:** What are the candidate models f? (E.g., linear functions)
  - **Loss function:** How to define "approximating"? (E.g., MSE loss)

Loss Minimization View of ML

- **Three design decisions**
  - **Model family:** What are the candidate models f? (E.g., linear functions)
  - **Loss function:** How to define "approximating"? (E.g., MSE loss)
  - **Optimizer:** How do we minimize the loss? (E.g., gradient descent)