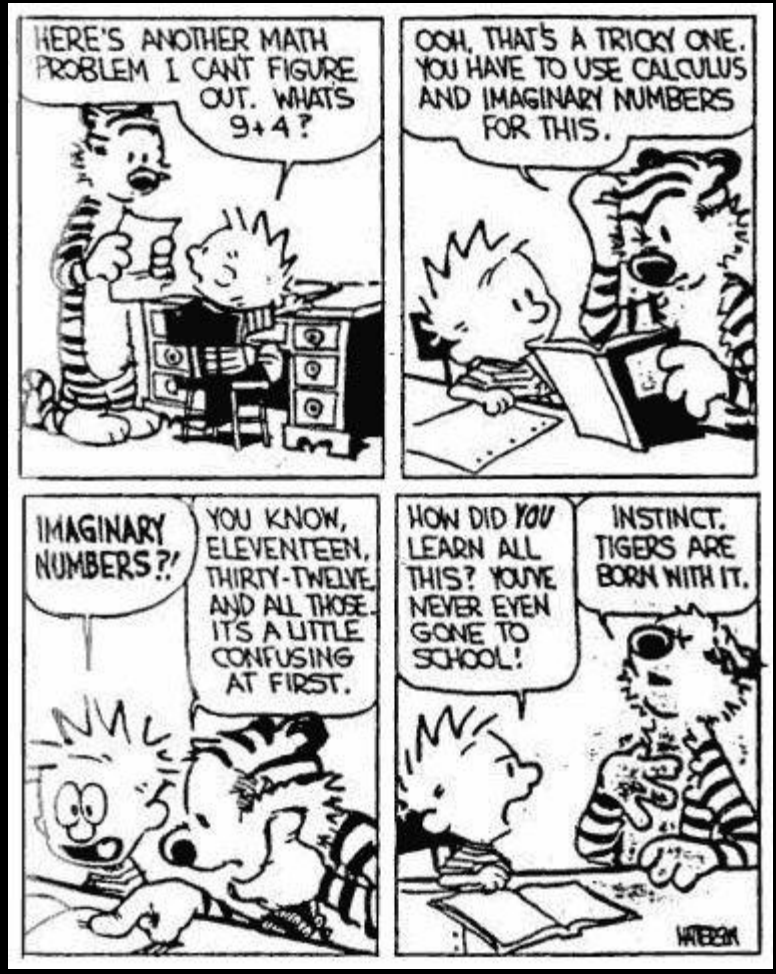


INFO 251: Applied Machine Learning

Gradient Descent

Announcements

- PS3 due in one week
- Grab a pen and paper for today's lecture

Course Outline

- Causal Inference and Research Design
  - Experimental methods
  - Non-experiment methods
- Machine Learning
  - Design of Machine Learning Experiments
  - **Linear Models and Gradient Descent**
  - Non-linear models
  - Neural models
  - Unsupervised Learning
  - Practicalities, Fairness, Bias
- Special topics

Key Concepts (previous lecture)

- Decision boundaries
- Voronoi diagrams
- (*K*-)Nearest Neighbors
- Similarity and Distance metrics
- Normalization and Standardization
- Feature weighting

Key Concepts (today's lecture)

- Cost Functions
- Gradient Descent
- Local and global minima
- Convex functions
- Incremental vs. Batch GD
- Learning rates
- Feature scaling

Outline

- **Cost functions**
- Gradient descent
- Feature scaling

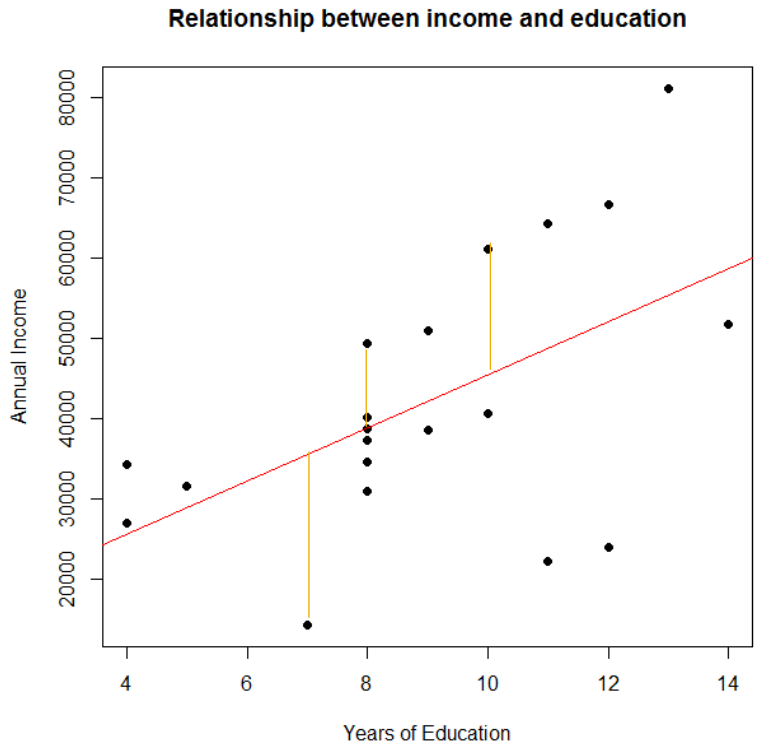
Regression: Probabilistic interpretation

- Probabilistic Formulation (generic function)
  - We make a prediction of Y using some function f(X)
  - To choose the best model:
    - Define a loss function J(Y, f(X))
    - Minimize the expected loss across the joint distribution P(X,Y)

- Linear regression:
  - f is a linear function (e.g., $\alpha + \beta X$)
  - Minimize squared-error loss E(Y-f(X))2

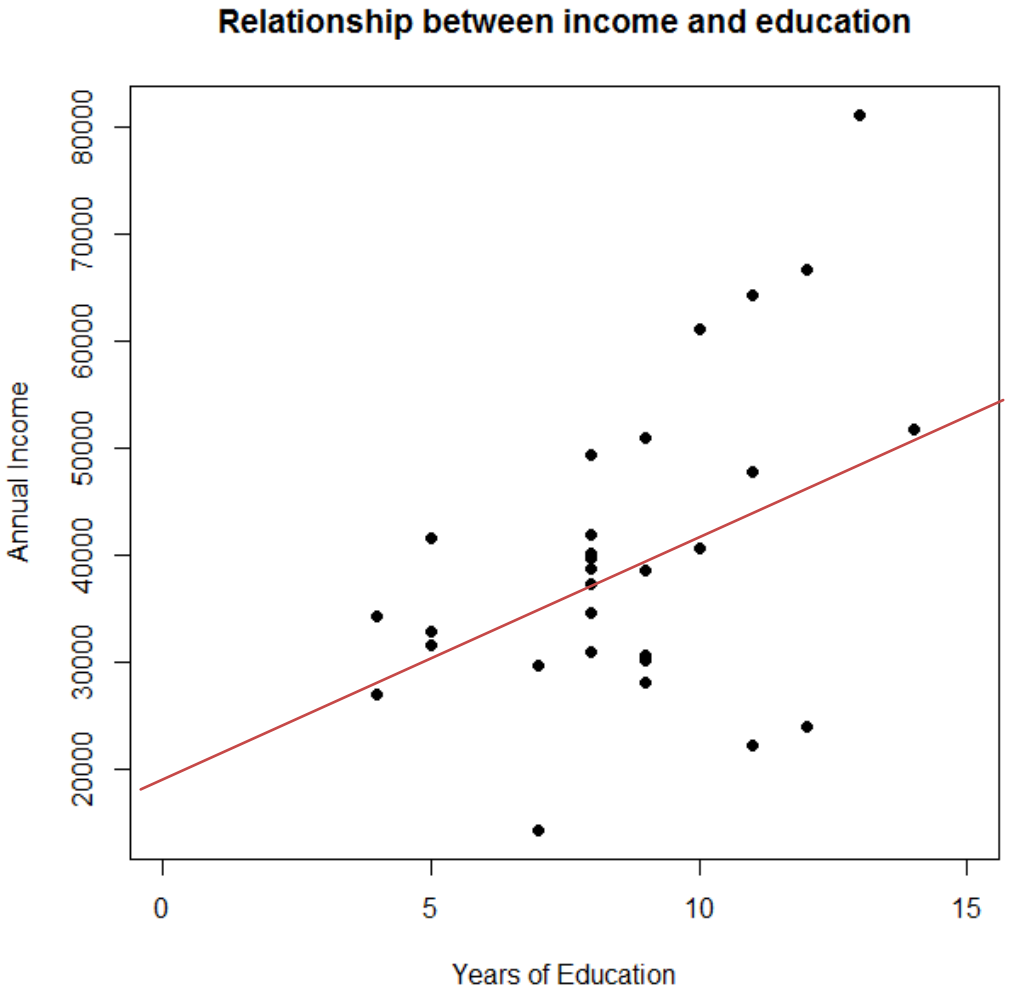
Linear Regression

- OLS as Maximum Likelihood Estimation:
  - $Y_i = \alpha + \beta X_i + \epsilon_i$
  - Idea: Choose α and β so that $\alpha + \beta X_i$ is "as close as possible" to Y_i for training data
- In other words
  - $\min_{\alpha,\beta} \sum_{i=1}^{N} (\alpha + \beta X_i - Y_i)^2$
- In general, we are minimizing a **Cost Function** *J*
  - $\min_{\alpha,\beta} J(\alpha, \beta)$
  - In the case of OLS, we use a "squared error" cost function
  - $J(\alpha, \beta) = \frac{1}{2N} \sum_{i=1}^{N} (\alpha + \beta X_i - Y_i)^2$



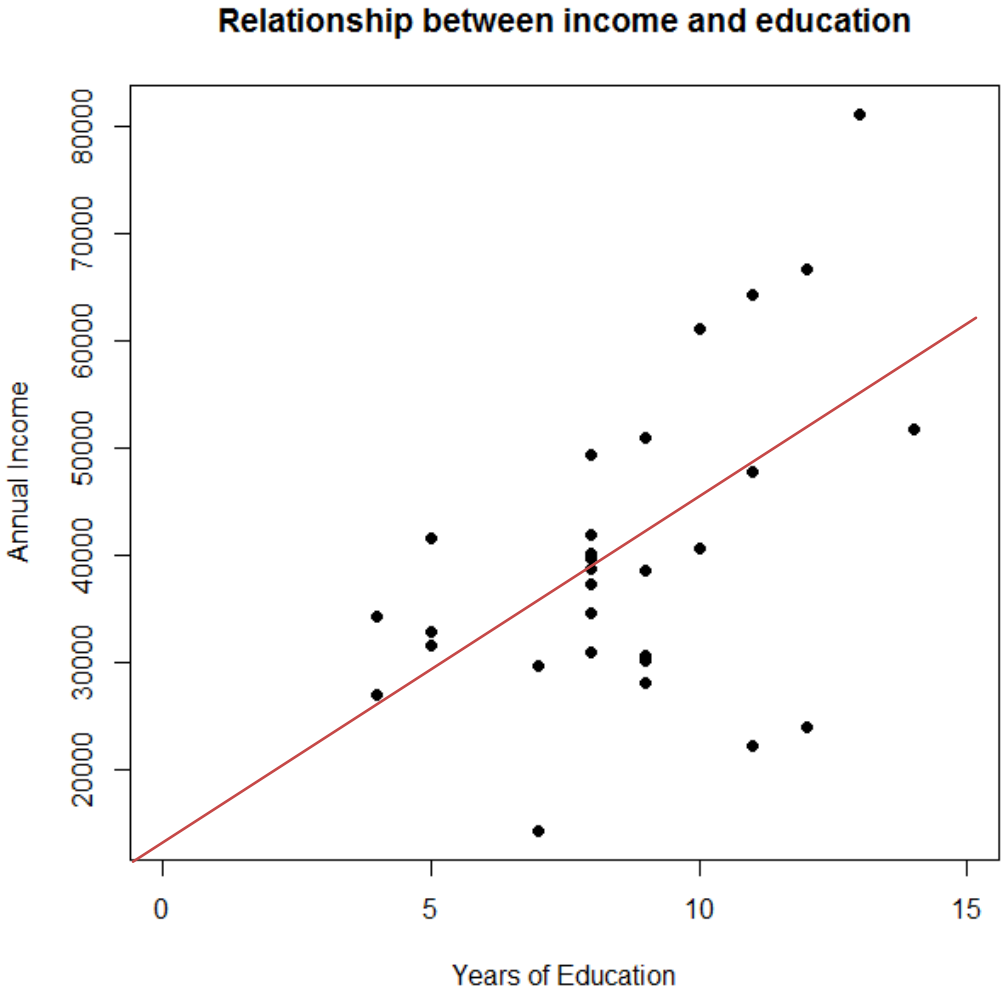
General formulation (OLS)

- Model ("hypothesis")
  - $Y_i = \alpha + \beta X_i$
- Parameters
  - α, β
- Cost Function
  - $J(\alpha, \beta) = \frac{1}{2N} \sum_{i=1}^{N} (\alpha + \beta X_i - Y_i)^2$
- Objective
  - $\min_{\alpha,\beta} J(\alpha, \beta)$



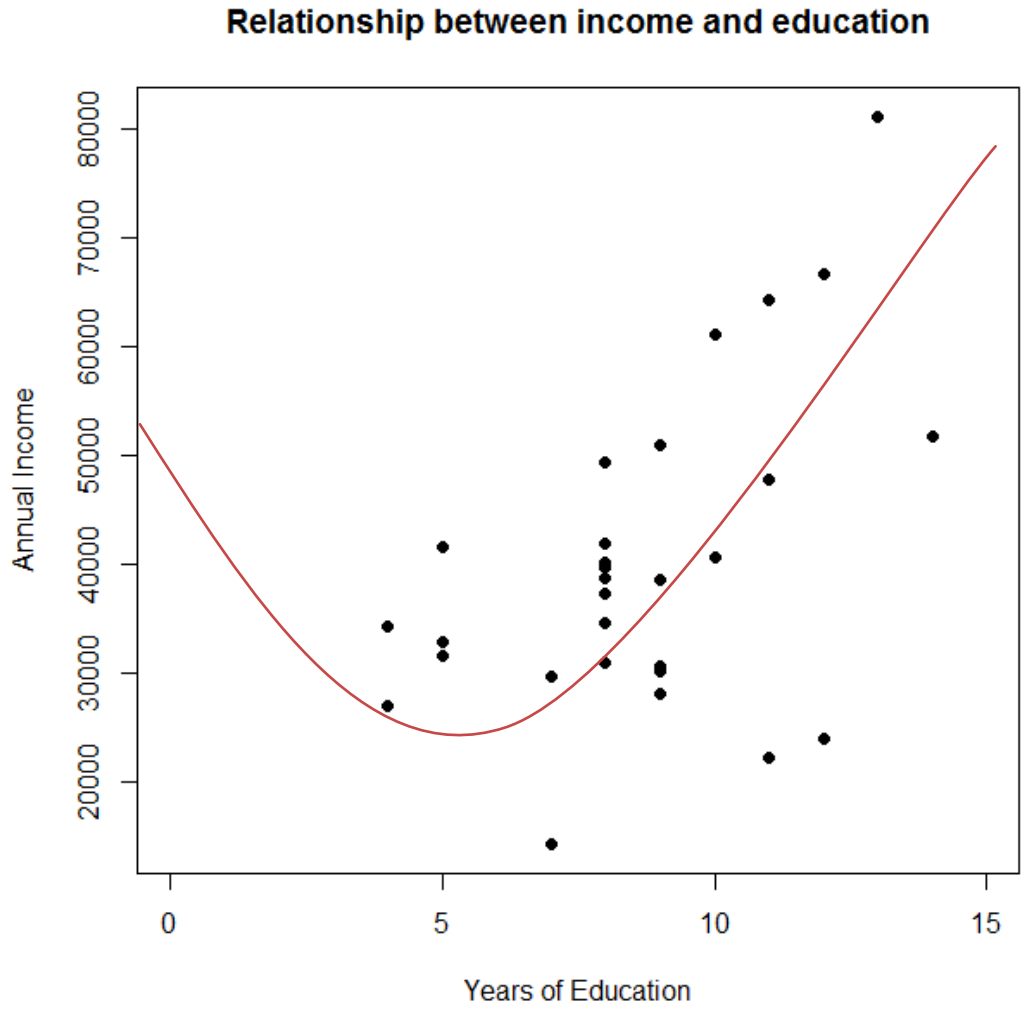
OLS with no intercept

- Model ("hypothesis")
  - $Y_i = \beta X_i$
- Parameters
  - β
- Cost Function
  - $J(\beta) = \frac{1}{2N}\sum_{i=1}^{N}(\beta X_i - Y_i)^2$
- Objective
  - $\min_{\beta} J(\beta)$



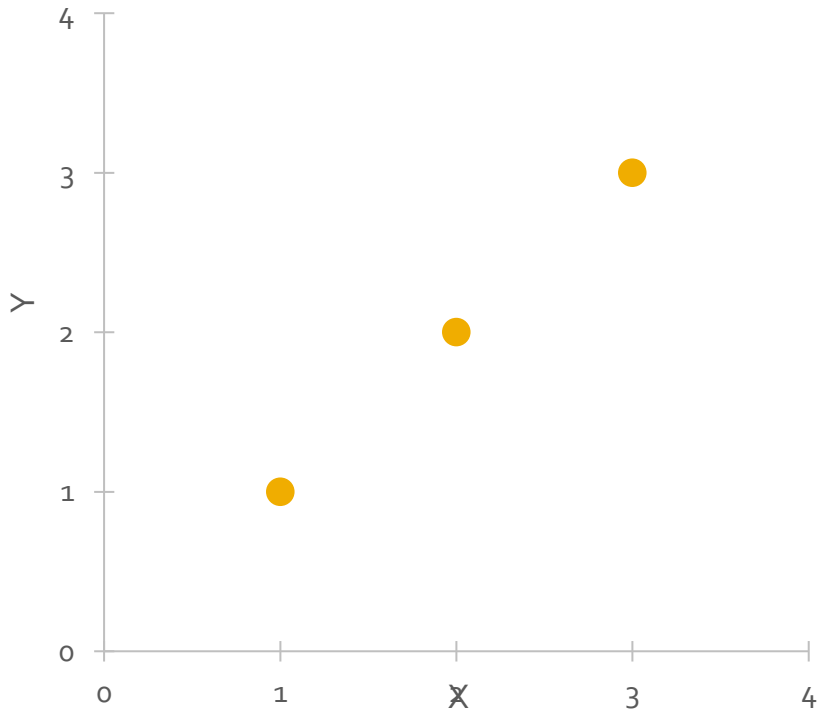
Fill in the blanks

- Model ("hypothesis")
  - Income depends on education, and also on eduction^2, i.e. nonlinearities exist
  - $Y_i = \alpha + \beta X_i + \gamma X_i^2$
- Parameters
  - α, β, γ
- Cost Function
  - Use "absolute error" cost function
  - $J(\alpha, \beta, \gamma) = \frac{1}{N}\sum_{i=1}^{N} |\alpha + \beta X_i + \gamma X_i^2 - Y_i|$
- Objective
  - $\min_{\alpha,\beta,\gamma} J(\alpha, \beta, \gamma)$



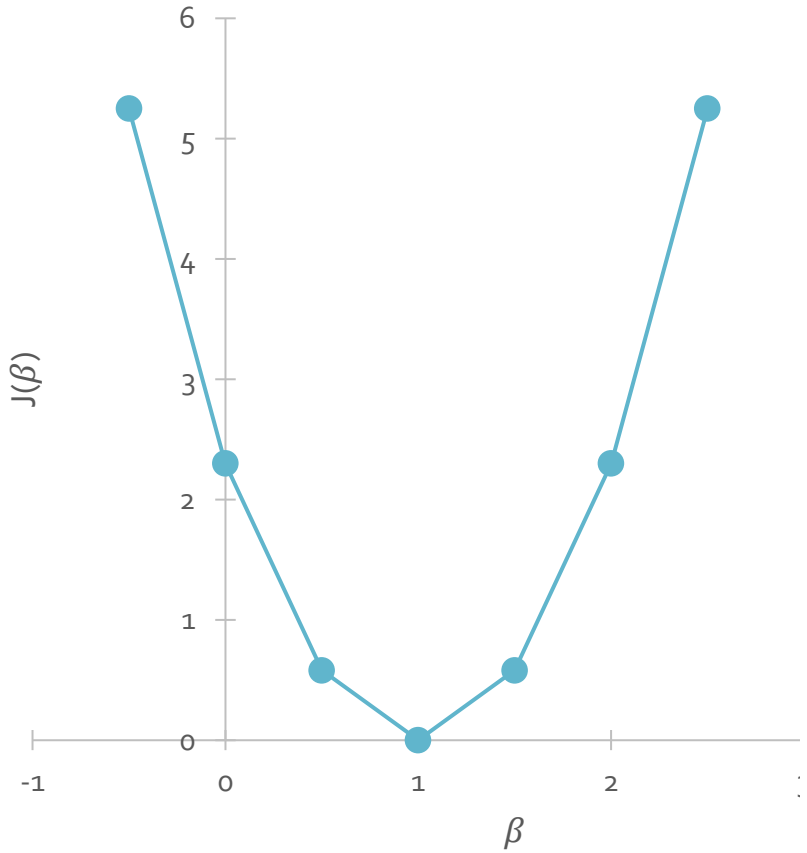
Exercise: Computing Cost

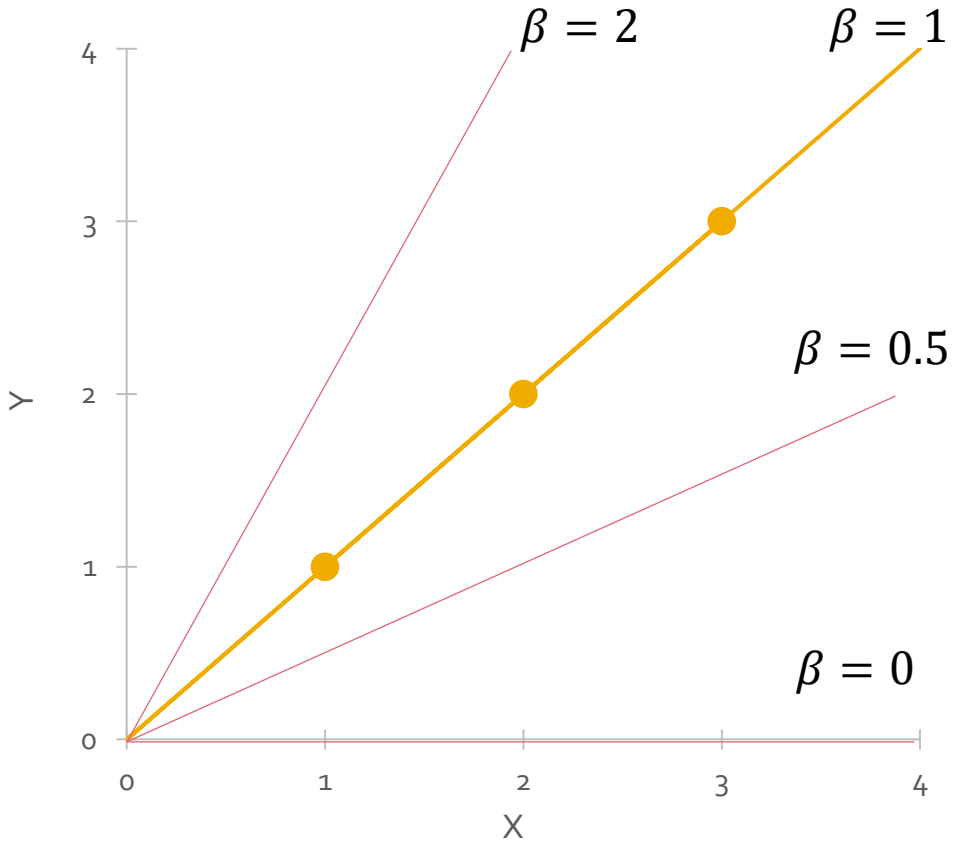
- Assume our data look like this ($N = 3$)
  - $X_1 = 1, \;\; Y_1 = 1$
  - $X_2 = 2, \;\; Y_2 = 2$
  - $X_3 = 3, \;\; Y_3 = 3$
- Our model is $Y_i = \beta X_i$
  - Our cost function is squared error: $J(\beta) = \frac{1}{2N}\sum_{i=1}^{N}(\beta X_i - Y_i)^2$
- Your task is to compute $J(\beta)$, given these 3 points, for:
  - $\beta = 1$
  - $\beta = 0$
  - $\beta = 2$
  - $\beta = 0.5$ (you might need a calculator)
- Draw a plot of $J(\beta)$ as a function of β



Visualizing Cost (1 parameter)

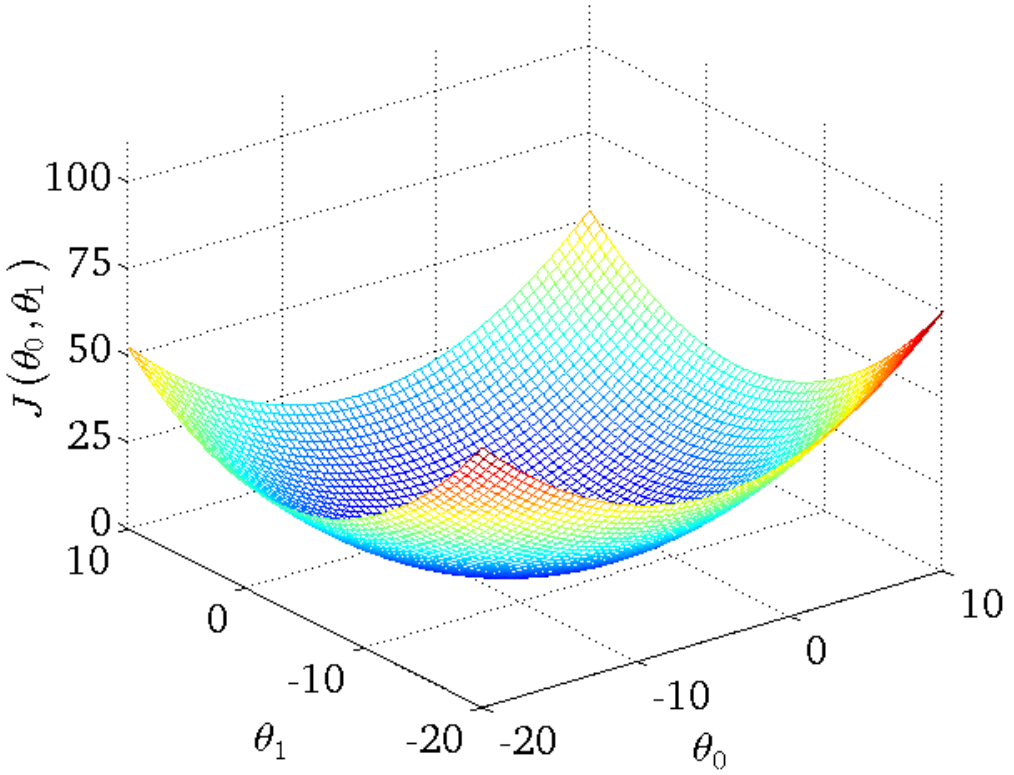
- Where is $J(\beta)$ minimized?





Visualizing Cost (2 parameters)

- Generalizing to a multi-dimensional loss surface
  - Model ("hypothesis"): $Y_i = \theta_1 + \theta_2 X_i$
  - Objective: $\min_{\theta_1,\theta_2} J(\theta_1, \theta_2)$



Outline

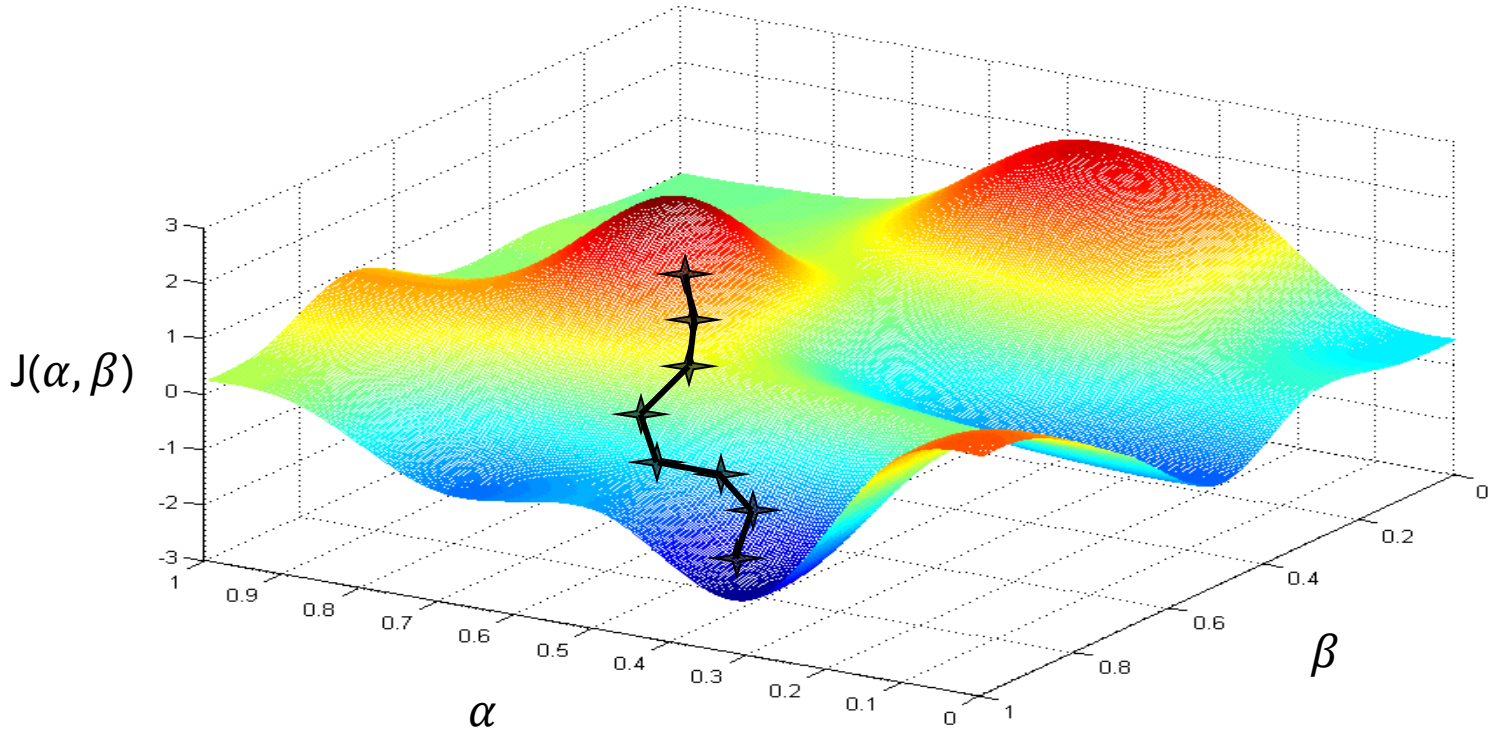
- Cost functions
- **Gradient descent**
- Feature scaling

Gradient Descent

- Gradient descent provides a principled method/algorithm to minimize the cost function J

- Idea: to solve $\min_{\alpha,\beta} J(\alpha, \beta)$
  - Initialize α, β
  - Change α, β in some way that reduces $J(\alpha, \beta)$
  - Eventually we will end up at a minimum

Gradient Descent: Visualization



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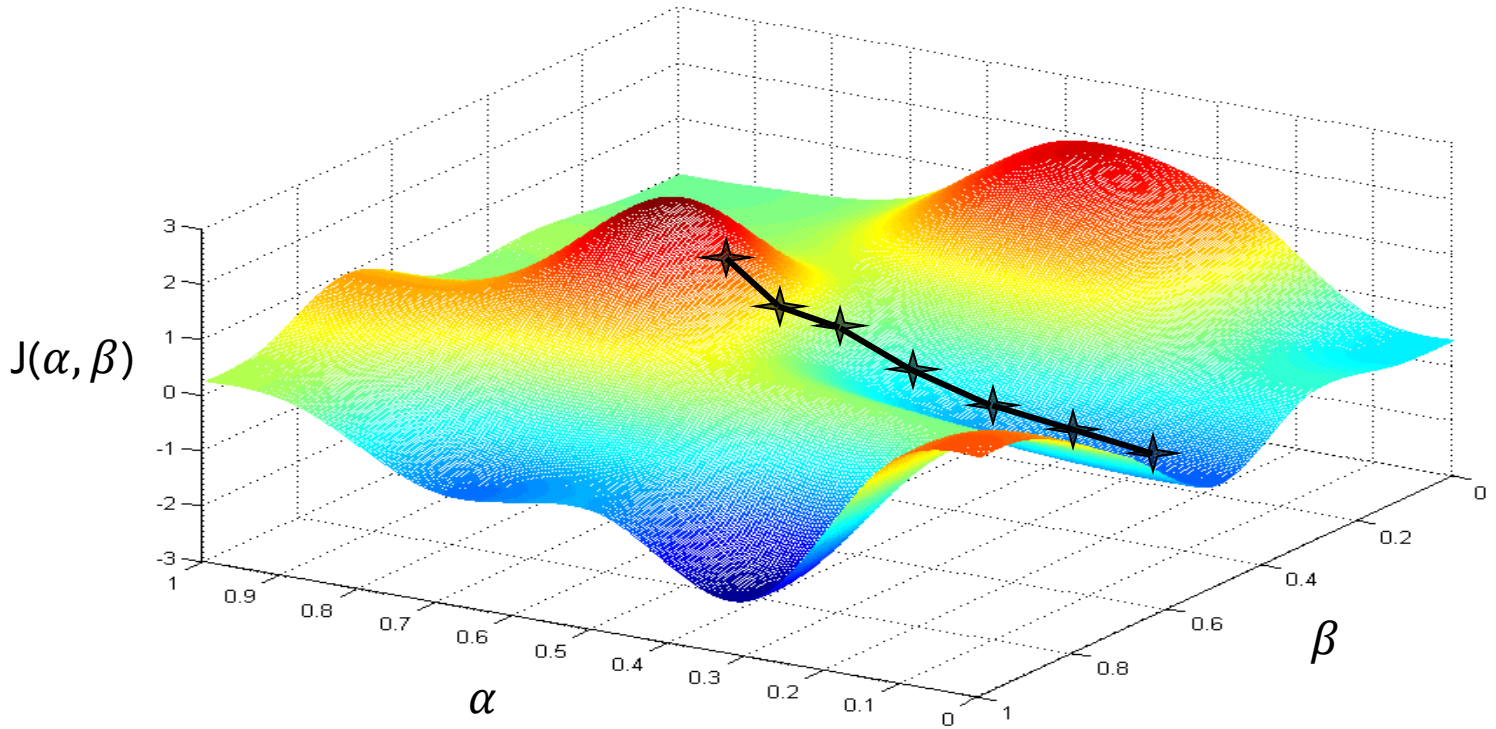
Local Minima



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Gradient Descent Algorithm

- In pseudo-code:

```
Choose an initial vector of parameters α, β
Choose learning rate R
Repeat until convergence (i.e., until an approximate minimum is obtained):
    For each example i in training set:
```

$$\alpha \leftarrow \alpha - R\frac{\partial}{\partial \alpha}J(\alpha,\beta)$$

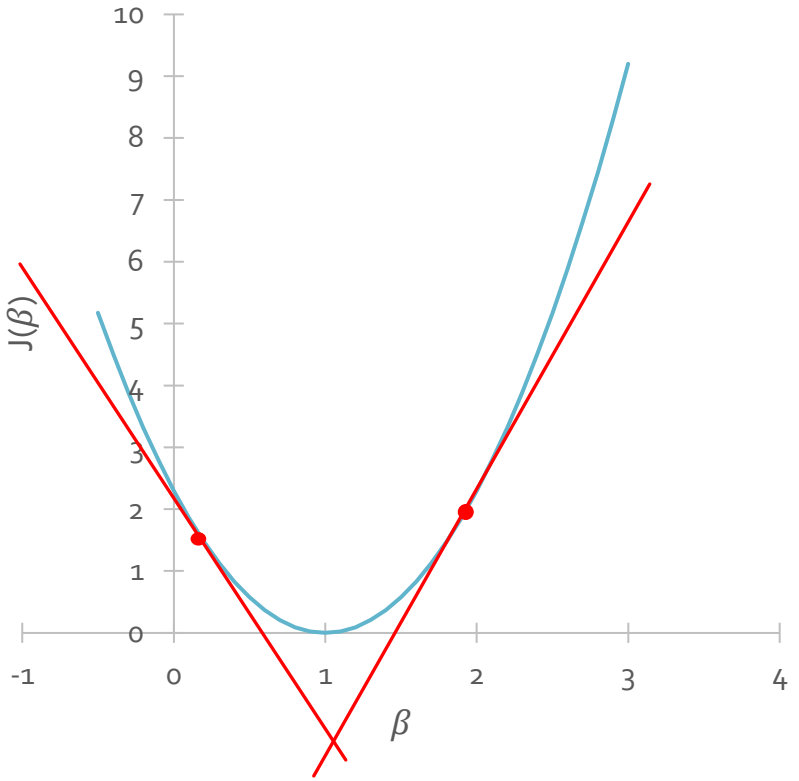
$$\beta \leftarrow \beta - R\frac{\partial}{\partial \beta}J(\alpha,\beta)$$

Simultaneous update

- With multiple predictors/regressors…
  - $Y_i = \alpha + \beta_1 X_{i1} + \beta_2 X_{i2} + \ \ldots + \beta_k X_{ik}$

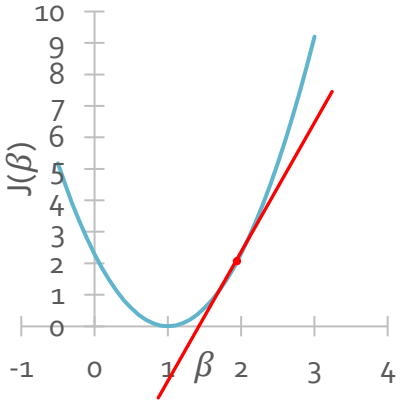
Gradient Descent: Derivative

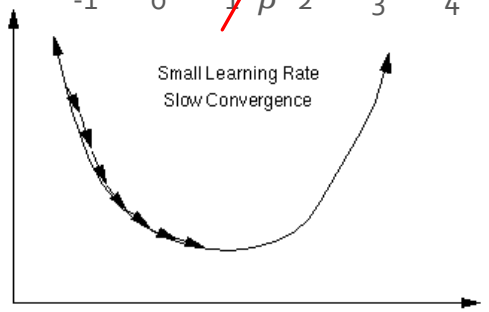
- In 1-Dimension
- Update Rule:
  - $\beta \leftarrow \beta - R \frac{\partial}{\partial \beta} J(\alpha, \beta)$
- Initialize β at 1.9
  - What's the derivative $\frac{\partial}{\partial \beta} J(\alpha, \beta)$?
  - How does β update?
- Initialize β at 0.2
  - What's the derivative $\frac{\partial}{\partial \beta} J(\alpha, \beta)$?
  - How does β update?

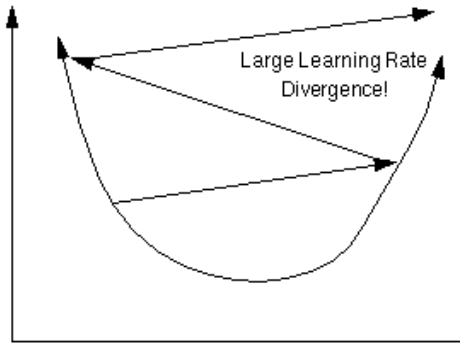


Gradient Descent: Learning Rate

- $\beta <- \beta - R\frac{\partial}{\partial \beta} J(\alpha, \beta)$
- What does R do?
- Small R:
  - Gradient descent can be slow
- Large R:
  - Can overshoot the minimum
  - May fail to converge
  - May diverge!







Gradient Descent: Convergence

- Do we need to change the learning rate?

```
Choose an initial vector of parameters α, β
Choose learning rate R
Repeat until convergence:
    For each example i:
        α <- α - R∂/∂α J(α,β)
        β <- β - R∂/∂β J(α,β)
```

- No! Gradient descent can converge to a local minimum, even with the learning rate fixed
  - As we approach a local minimum, gradient descent takes smaller steps

Gradient Descent: Regression

- Gradient Descent

  `Repeat until convergence:`

  $\alpha \leftarrow \alpha - R \frac{\partial}{\partial \alpha} J(\alpha, \beta)$

  $\beta \leftarrow \beta - R \frac{\partial}{\partial \beta} J(\alpha, \beta)$

- Regression cost function
  - $J(\alpha, \beta) = \frac{1}{2N} \sum_{i=1}^{N} (\alpha + \beta X_i - Y_i)^2$
- The missing pieces: $\frac{\partial}{\partial \alpha} J(\alpha, \beta)$ and $\frac{\partial}{\partial \beta} J(\alpha, \beta)$
  - $\frac{\partial}{\partial \alpha} J(\alpha, \beta) = \frac{\partial}{\partial \alpha} \frac{1}{2N} \sum_{i=1}^{N} (\alpha + \beta X_i - Y_i)^2$
  - $\frac{\partial}{\partial \beta} J(\alpha, \beta) = \frac{\partial}{\partial \beta} \frac{1}{2N} \sum_{i=1}^{N} (\alpha + \beta X_i - Y_i)^2$

Gradient Descent: Regression

- Partial derivatives:

$$\frac{\partial}{\partial \alpha} J(\alpha, \beta) = \frac{\partial}{\partial \alpha} \frac{1}{2N} \sum_{i=1}^{N} \left(\hat{Y}_i - Y_i\right)^2$$
$$= \frac{\partial}{\partial \alpha} \frac{1}{2N} \sum_{i=1}^{N} (\alpha + \beta X_i - Y_i)^2$$
$$= \frac{1}{2N} \sum_{i=1}^{N} \frac{\partial}{\partial \alpha} (\alpha + \beta X_i - Y_i)^2$$
$$= \frac{1}{2N} \sum_{i=1}^{N} 2(\alpha + \beta X_i - Y_i) \frac{\partial}{\partial \alpha} (\alpha + \beta X_i - Y_i)$$
$$= \frac{1}{N} \sum_{i=1}^{N} (\alpha + \beta X_i - Y_i)$$
$$= \frac{1}{N} \sum_{i=1}^{N} \left(\hat{Y}_i - Y_i\right)$$

$$\frac{\partial}{\partial \beta} J(\alpha, \beta) = \frac{\partial}{\partial \beta} \frac{1}{2N} \sum_{i=1}^{N} \left(\hat{Y}_i - Y_i\right)^2$$
$$= \frac{1}{2N} \sum_{i=1}^{N} \frac{\partial}{\partial \beta} (\alpha + \beta X_i - Y_i)^2$$
$$= \frac{1}{2N} \sum_{i=1}^{N} 2(\alpha + \beta X_i - Y_i) \frac{\partial}{\partial \beta} (\alpha + \beta X_i - Y_i)$$
$$= \frac{1}{N} \sum_{i=1}^{N} (\alpha + \beta X_i - Y_i)(X_i)$$
$$= \frac{1}{N} \sum_{i=1}^{N} \left(\hat{Y}_i - Y_i\right) X_i$$

Gradient Descent: Regression

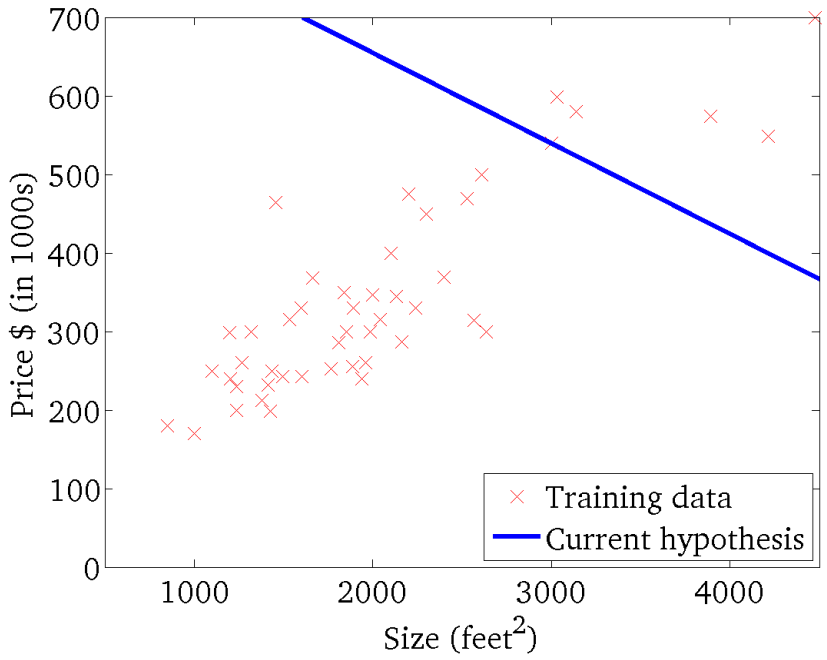
- Gradient Descent Algorithm (linear regression)

  `Repeat until convergence:`

  $\alpha \leftarrow \alpha - R\frac{1}{N}\sum_{i=1}^{N}(\alpha + \beta X_i - Y_i)$

  $\beta \leftarrow \beta - R\frac{1}{N}\sum_{i=1}^{N}(\alpha + \beta X_i - Y_i)X_i$

Gradient Descent: In Action



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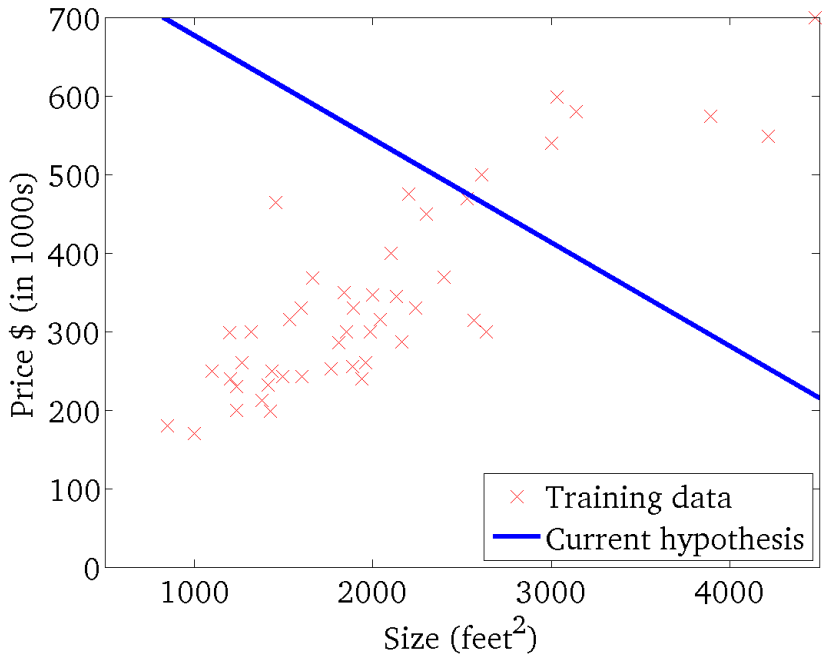
Gradient Descent: In Action



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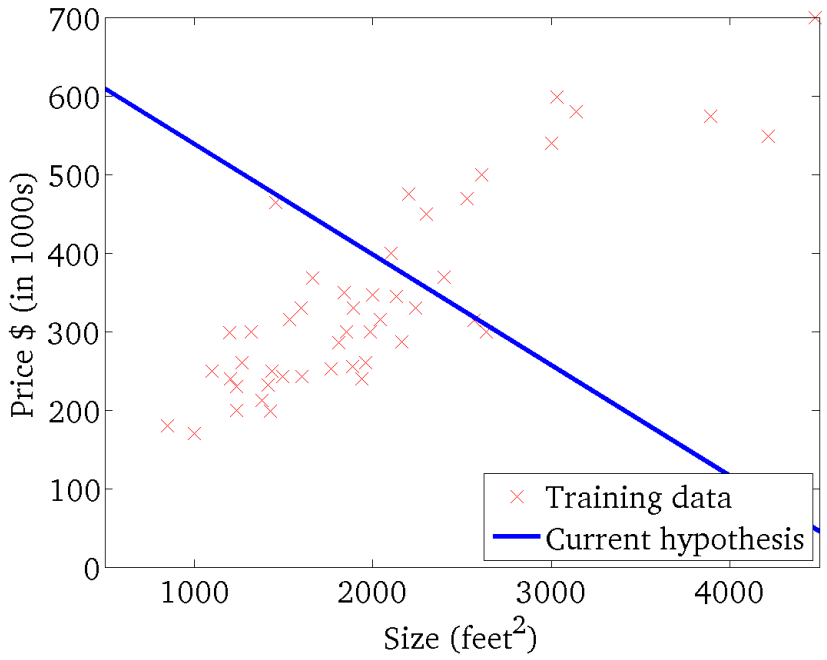
Gradient Descent: In Action



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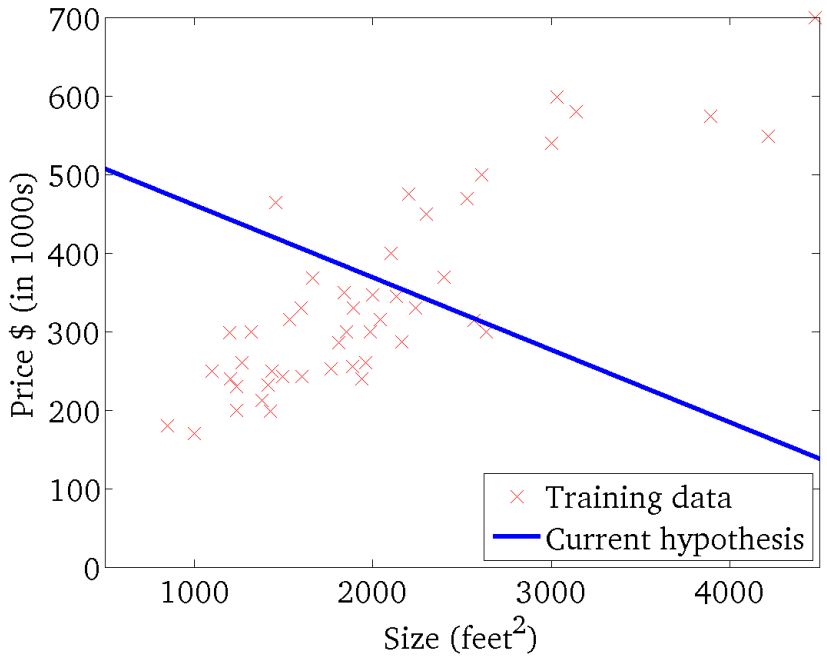
Gradient Descent: In Action



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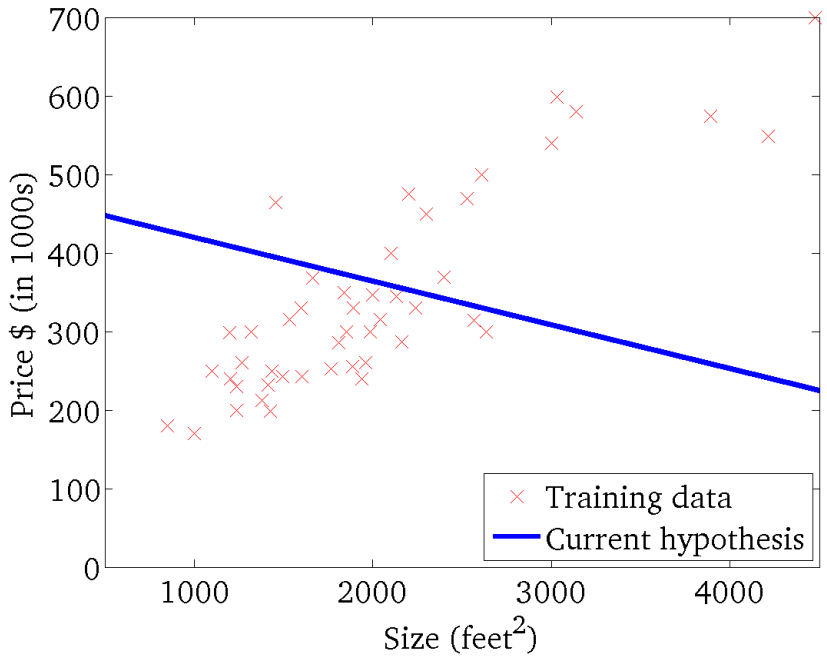
Gradient Descent: In Action



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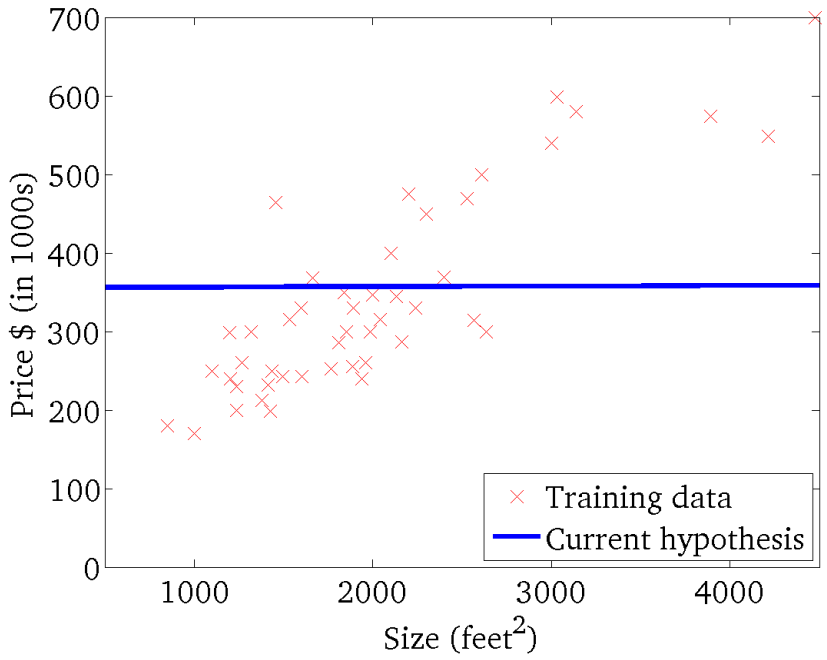
Gradient Descent: In Action



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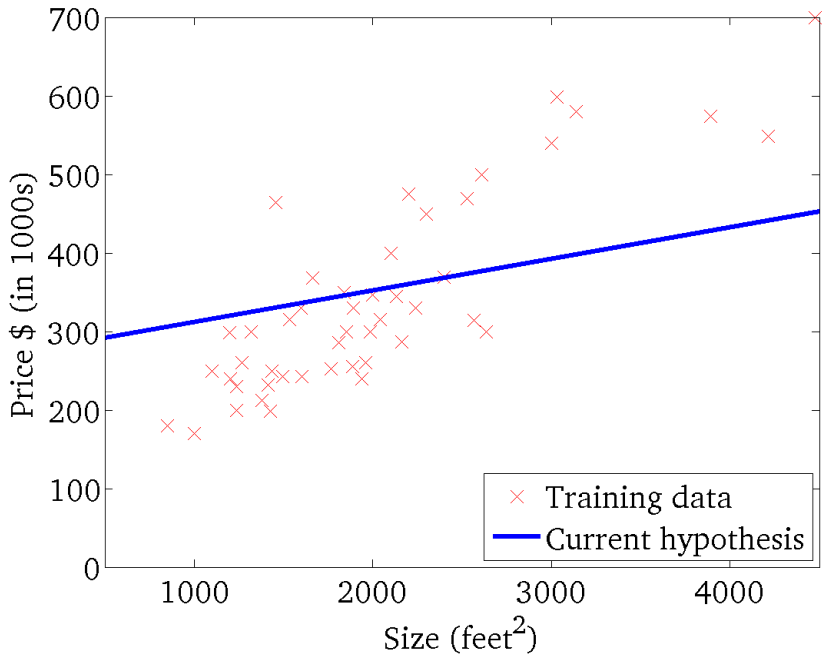
Gradient Descent: In Action



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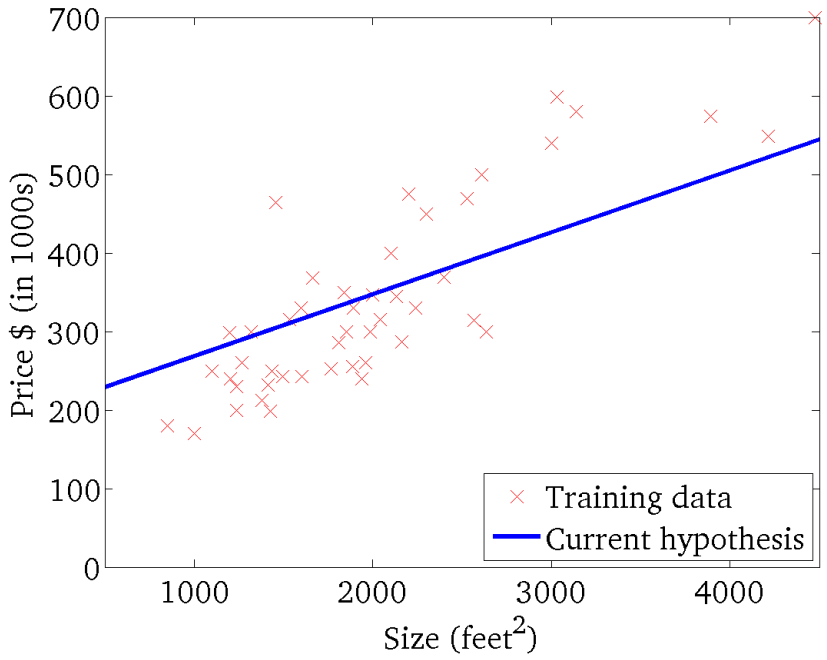
Gradient Descent: In Action



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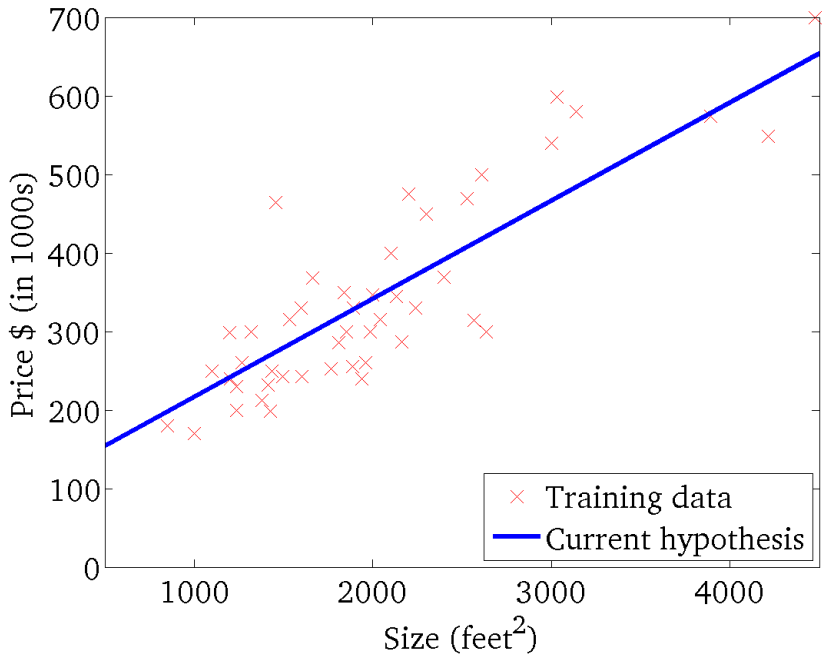
Gradient Descent: In Action



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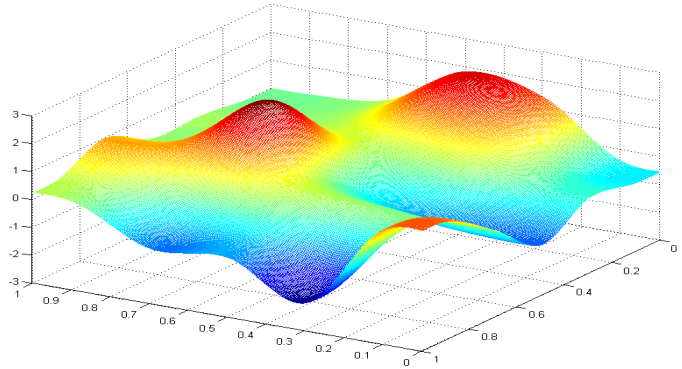
Outline

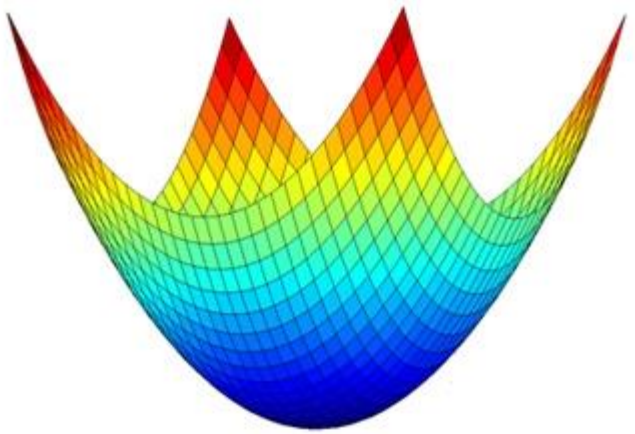
- Cost functions
- Gradient descent
  - **Local Minima**
  - Batch and Incremental versions
- Feature scaling

Local Minima?

- What about local minima in gradient descent for regression?



- No problem!
- Cost function in regression is **convex**
  - Convex: a continuous function where the midpoint of any interval doesn't exceed the mean of the endpoints
  - (second derivative is non-negative)



Incremental vs. Batch Gradient Descent

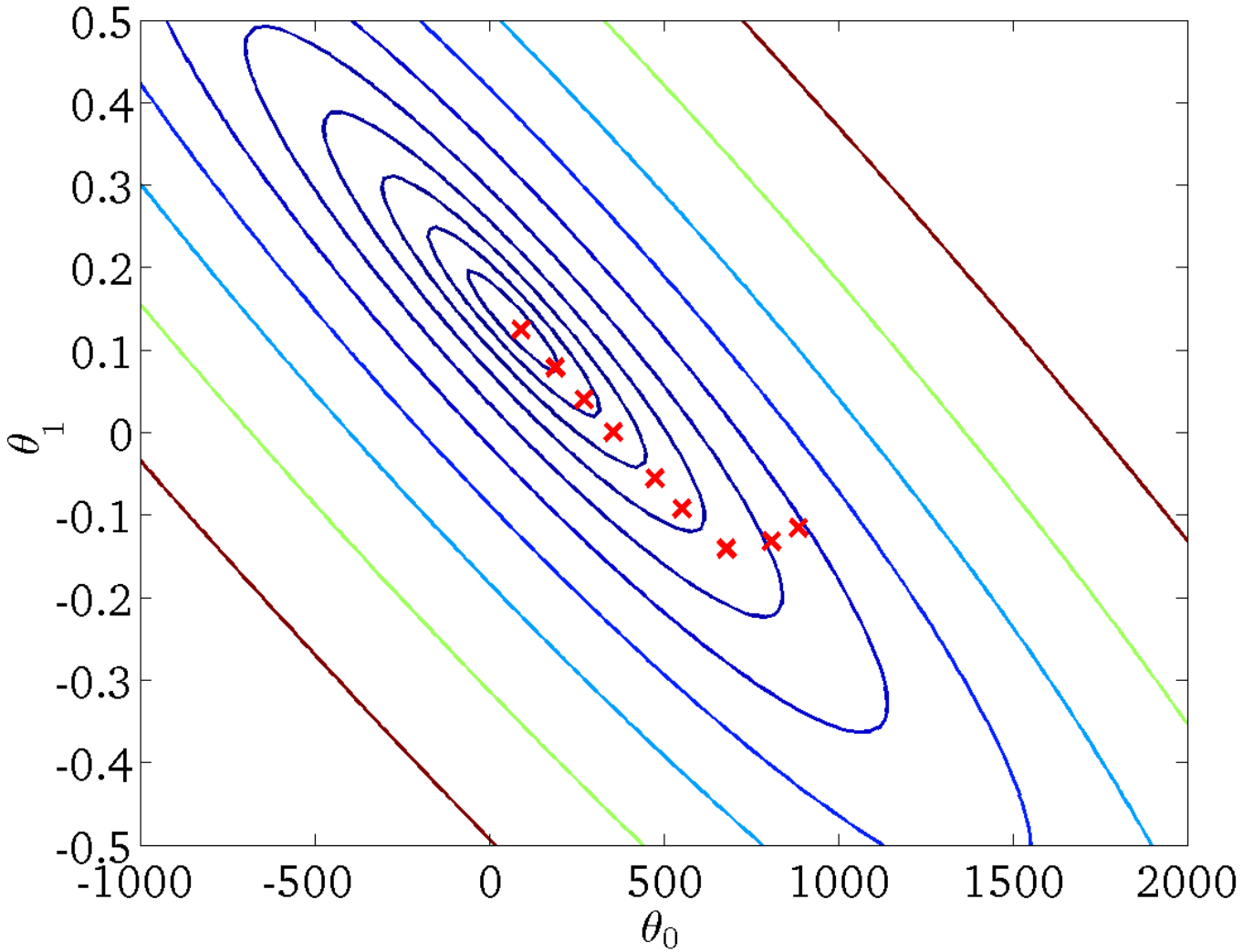
- In "Batch" gradient descent

```
Repeat until convergence:
    Compute ∇α = ∂/∂α J(α, β)          // global gradient
    Compute ∇β = ∂/∂β J(α, β)

    α <- α - R∇α                       // update once
    β <- β - R∇β
```

- Note: each step uses all training examples!

Batch Gradient Descent



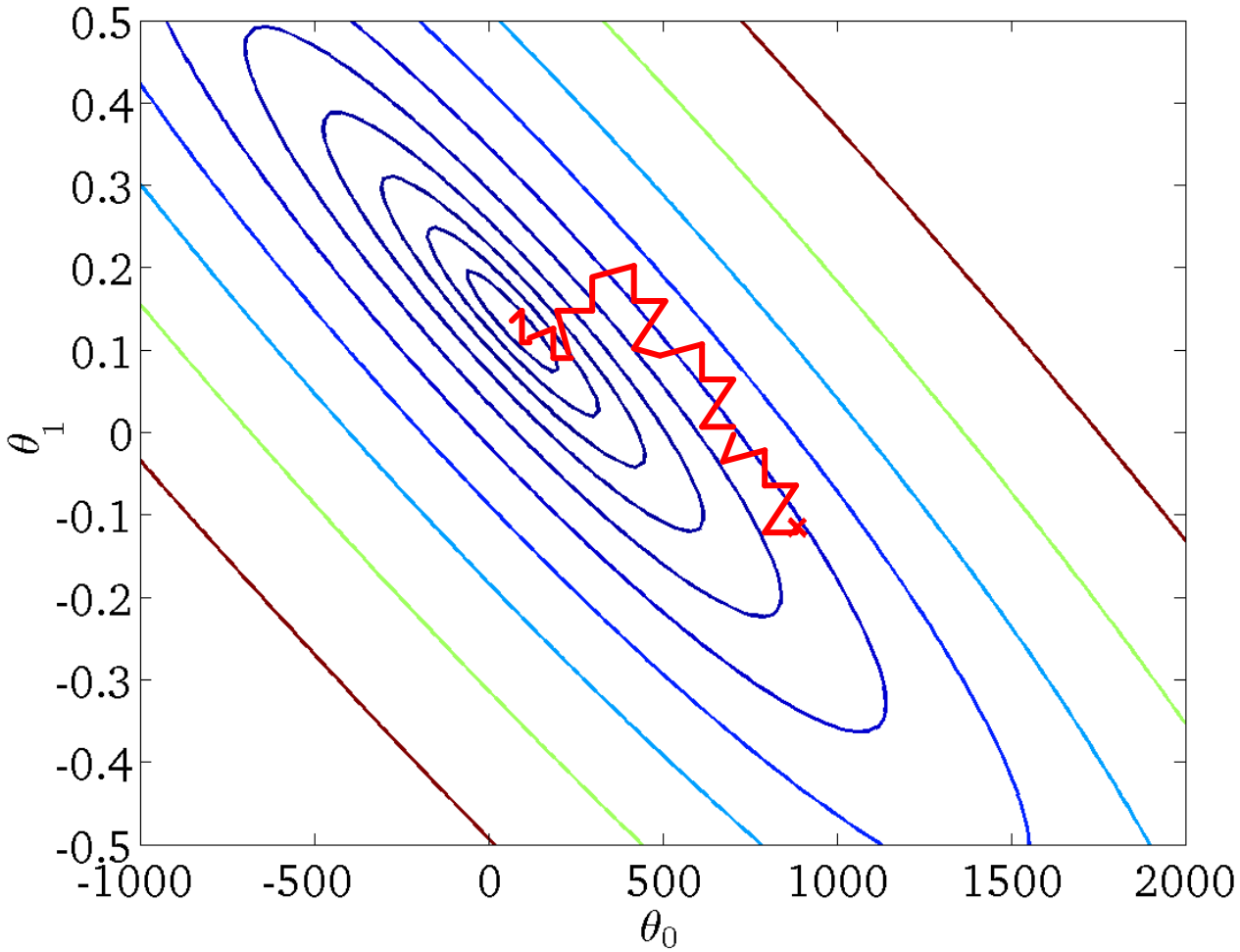
Incremental vs. Batch Gradient Descent

- "Iterative" (stochastic) version of gradient descent:

```
Repeat until an approximate minimum is obtained:
    Randomly shuffle examples in the training set
    For each example i:
        α <- α - R∂/∂α J(α,β)        // evaluate ∂/∂α J(α,β) at x_i
              and update α
        β <- β - R∂/∂β J(α,β)        // evaluate ∂/∂α J(α,β) at x_i
              and update β
```

- The parameters are adjusted with each training instance, iteratively

Stochastic Gradient Descent



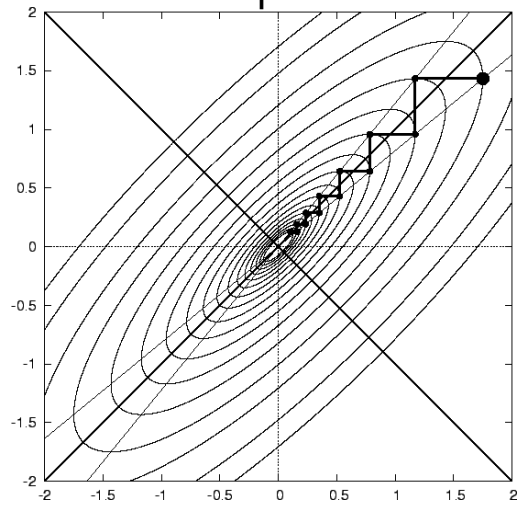
Outline

- Cost functions
- Gradient descent
- **Feature scaling**

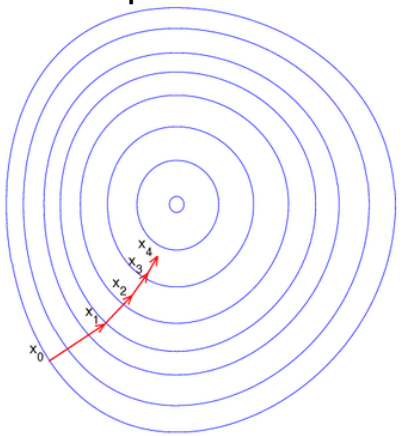
Feature scaling

- In gradient descent, we "take a step" in the direction where the decrease in cost is greatest
- When some features (axes) are on different scales, gradient descent can be inefficient
  - Putting different features on same scale can make gradient descent much faster

Not Proportional



Proportional



Feature scaling

- Feature scaling is an important pre-processing step for many common machine learning algorithms
  - Standardization: (mean 0 standard dev. 1)

$$x'_{ik} = \frac{x_{ik} - \bar{x}_k}{s_k}$$

    - s_k is standard deviation of x_k, or range (max-min) of x_k
  - Also common: force feature to be roughly between -1 and 1:

$$x'_{ik} = \frac{x_{ik}}{\max(|x_k|)}$$

Key Concepts (today's lecture)

- Cost Functions
- Gradient Descent
- Local and global minima
- Convex functions
- Incremental vs. Batch GD
- Learning rates
- Feature scaling