Linear Regression & Gradient Descent

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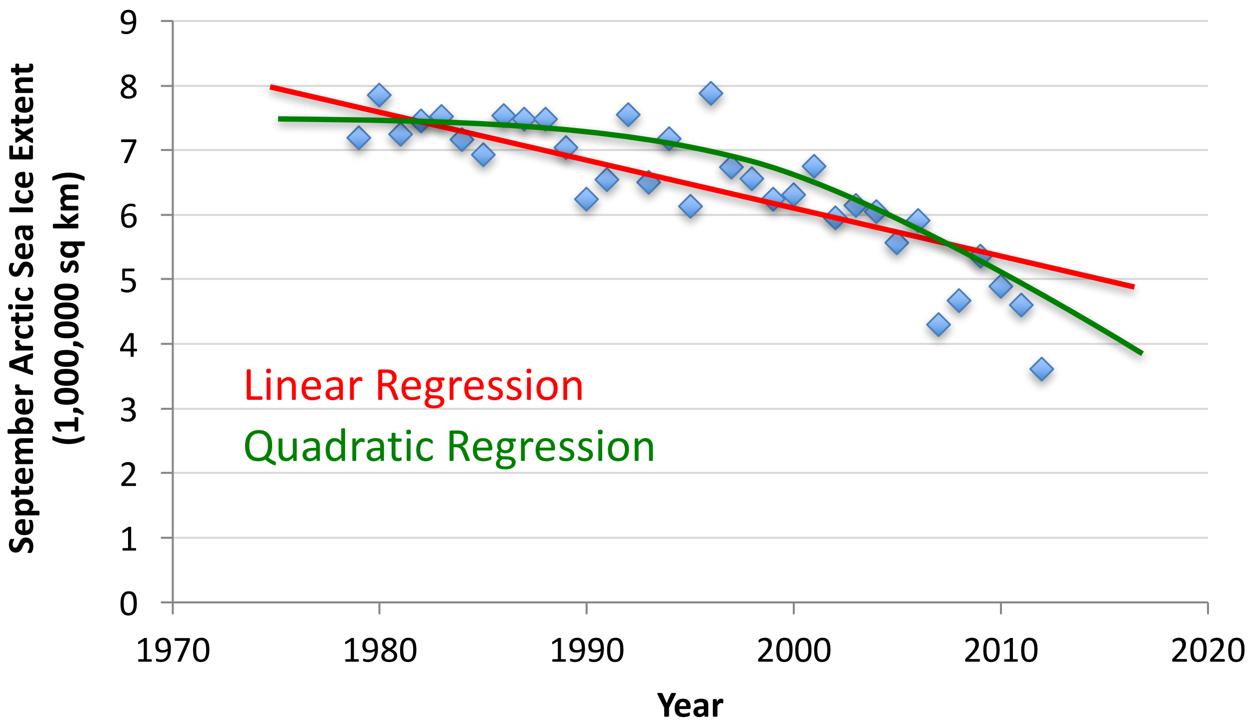
Regression

Given:

- Data $\boldsymbol{X} = \left\{ \boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(n)} \right\}$ where $\boldsymbol{x}^{(i)} \in \mathbb{R}^d$
- Corresponding labels $\boldsymbol{y} = \left\{ y^{(1)}, \ldots, y^{(n)} \right\}$ where $y^{(i)} \in \mathbb{R}$



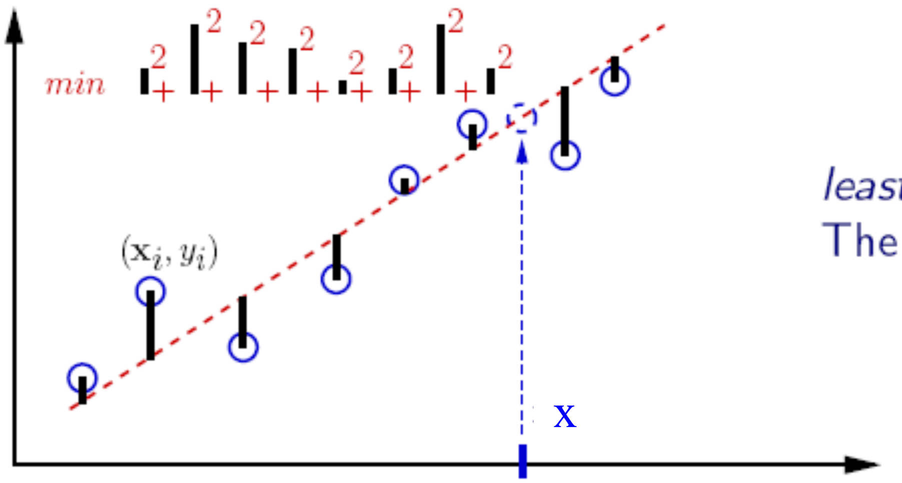
Linear Regression

- Hypothesis:

$$y = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots + \theta_d x_d = \sum_{j=0}^{d} \theta_j x_j$$

Assume $x_0 = 1$

- Fit model by minimizing sum of squared errors



least squares (LSQ)
The fitted line is used as a predictor

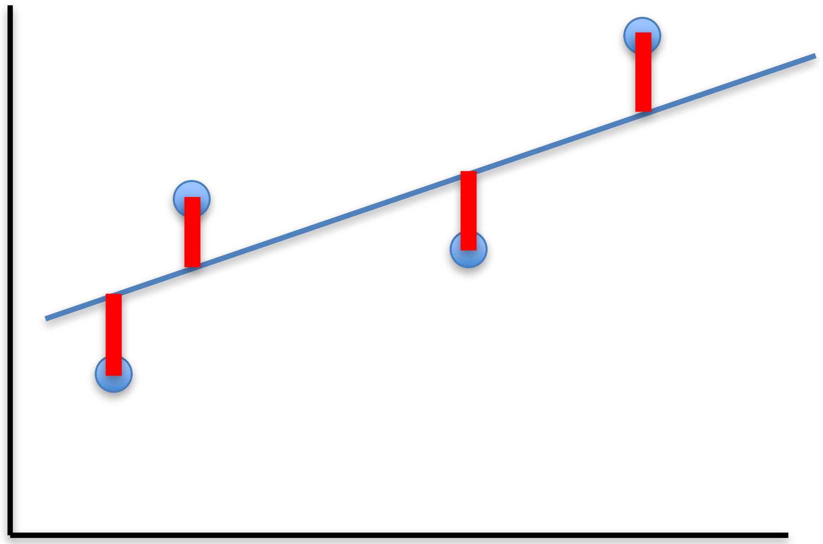
Figures are courtesy of Greg Shakhnarovich

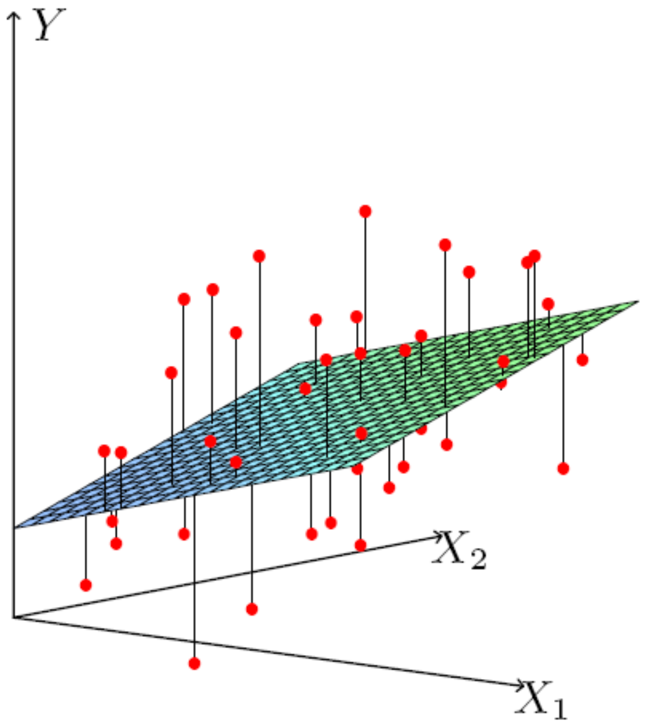
Least Squares Linear Regression

- Cost Function

$$J(\boldsymbol{\theta}) = \frac{1}{2n} \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right)^2$$

- Fit by solving $\min_{\boldsymbol{\theta}} J(\boldsymbol{\theta})$





Direct solution

- The minimum must occur at a point where the partial derivatives are zero.

$$\frac{\partial \mathcal{J}}{\partial w_j} = 0 \qquad \frac{\partial \mathcal{J}}{\partial b} = 0.$$

- If $\partial \mathcal{J} / \partial w_j \neq 0$, you could reduce the cost by changing w_j.
- This turns out to give a system of linear equations, which we can solve efficiently. **Full derivation in the readings.**
- Optimal weights:

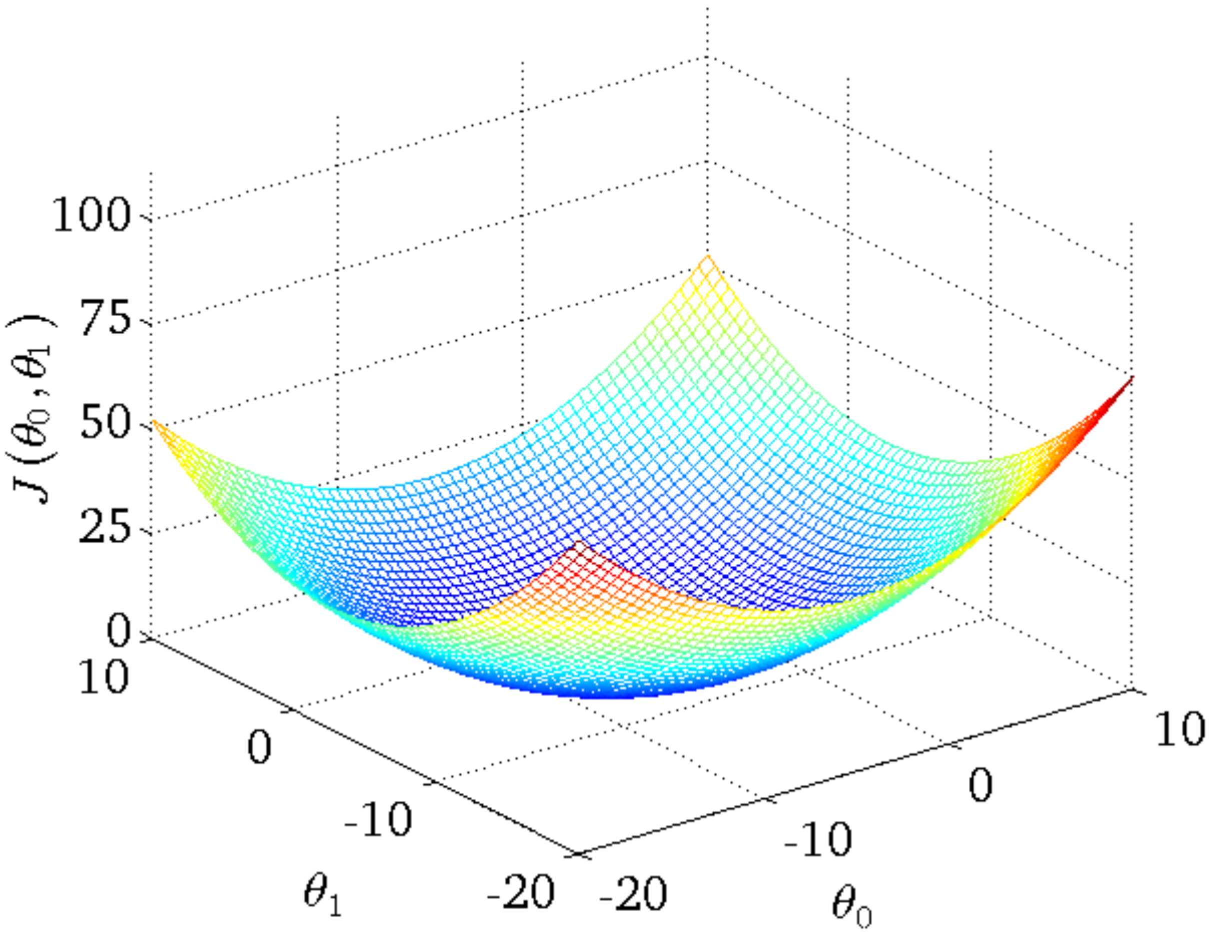
$$\mathbf{w} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{t}$$

- Linear regression is one of only a handful of models in this course that permit direct solution.

Gradient Descent

- Now let's see a second way to minimize the cost function which is more broadly applicable: gradient descent.
- Gradient descent is an iterative algorithm, which means we apply an update repeatedly until some criterion is met.
- We initialize the weights to something reasonable (e.g. all zeros) and repeatedly adjust them in the direction of steepest descent.

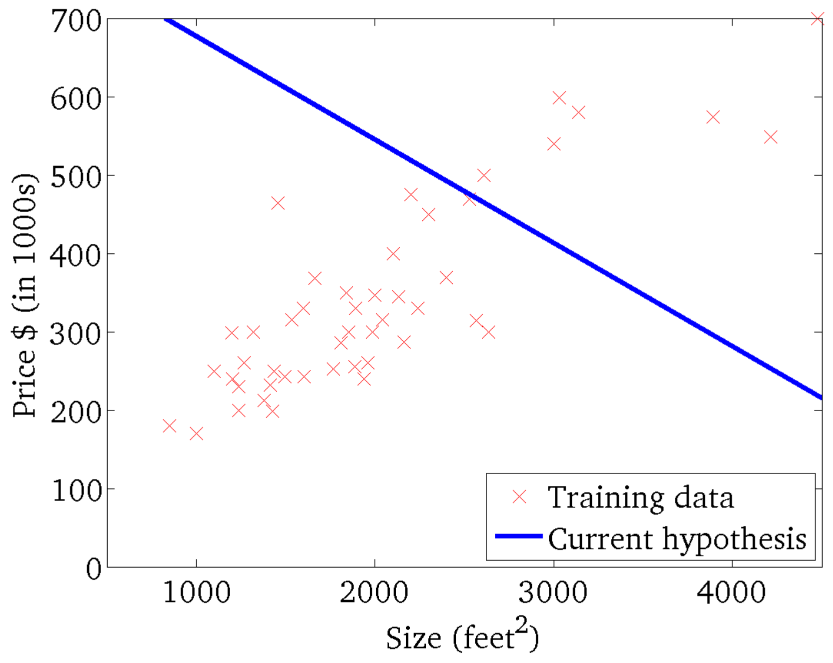
Intuition Behind Cost Function



Intuition Behind Cost Function

$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



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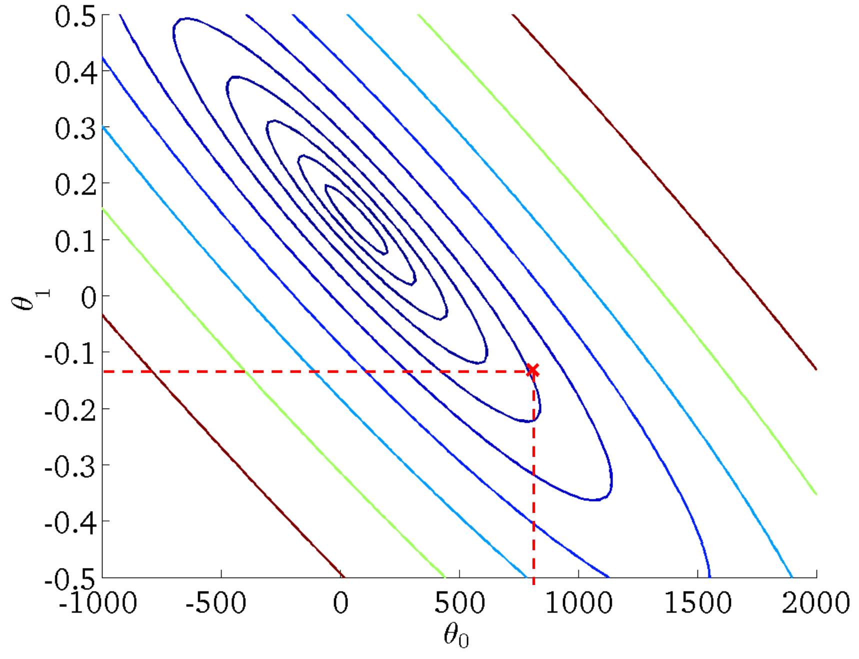
(function of the parameters θ_0, θ_1)



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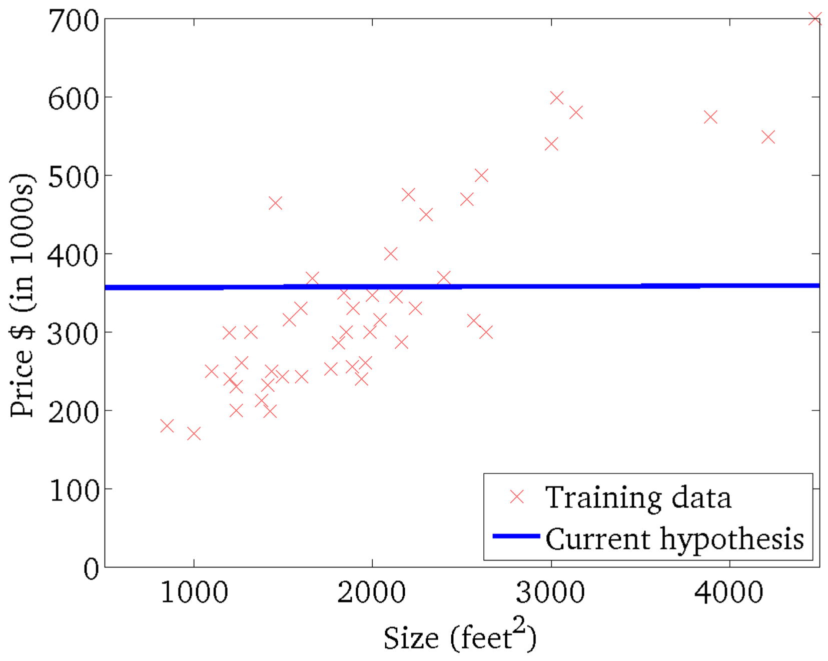

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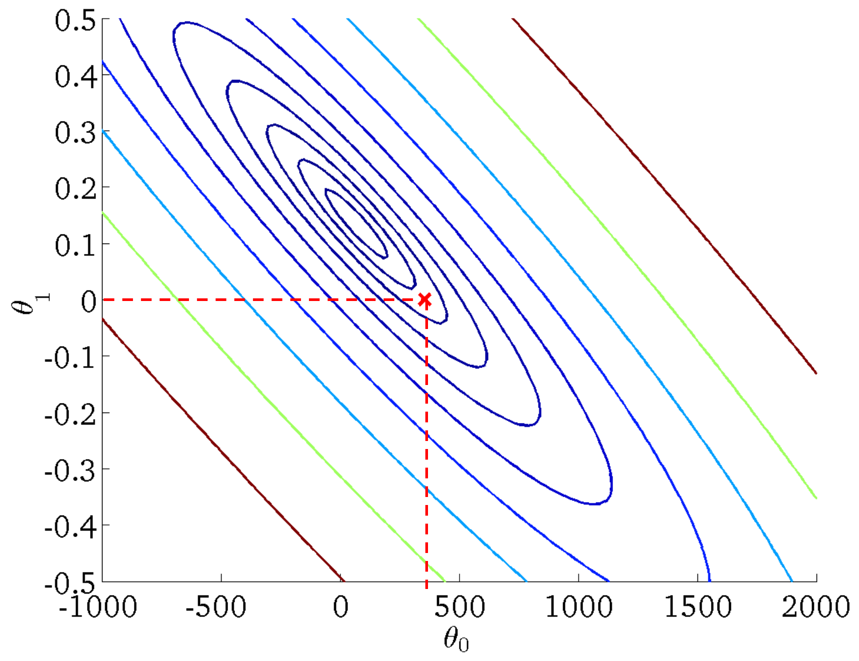

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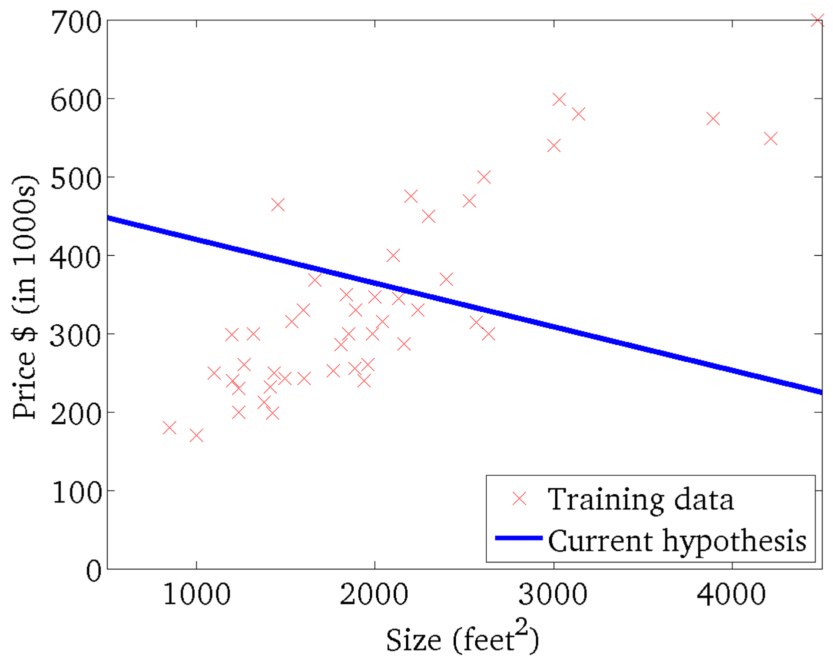

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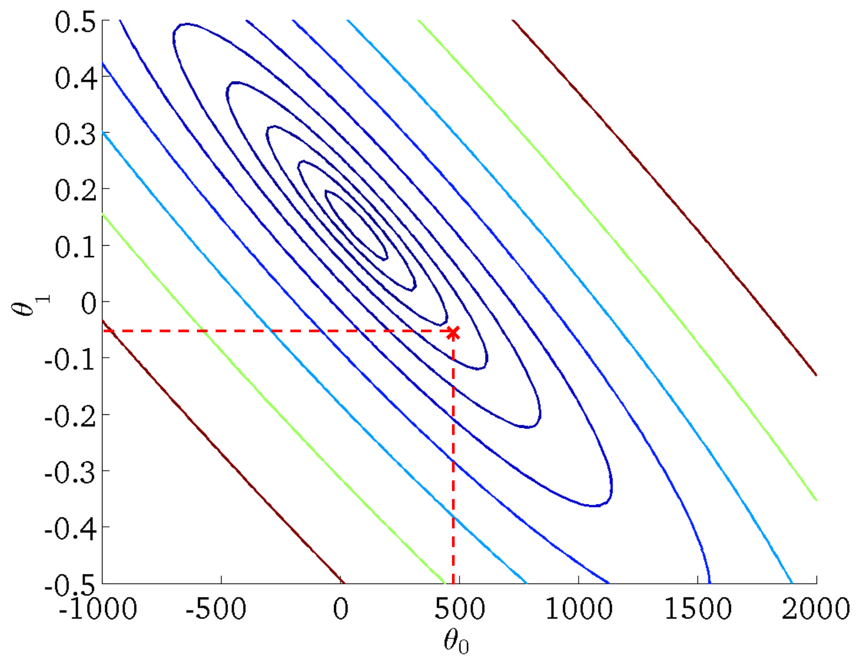

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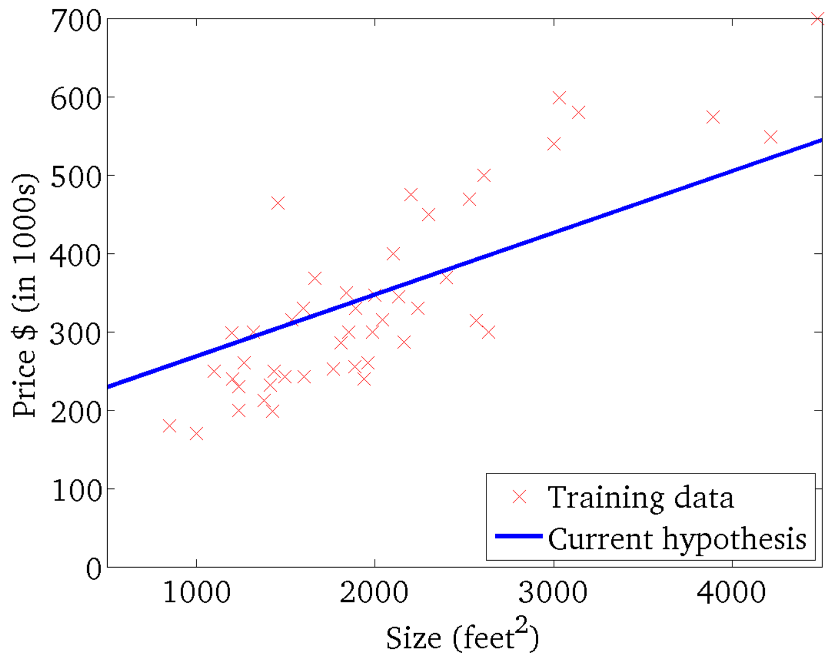

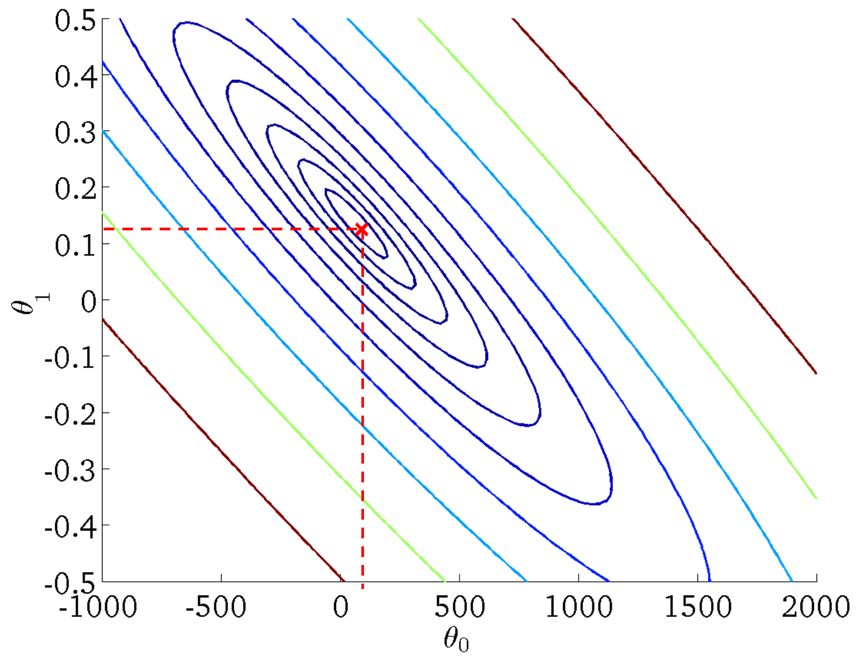

Basic Search Procedure

- Choose initial value for θ
- Until we reach a minimum:
  - Choose a new value for $\boldsymbol{\theta}$ to reduce $J(\boldsymbol{\theta})$

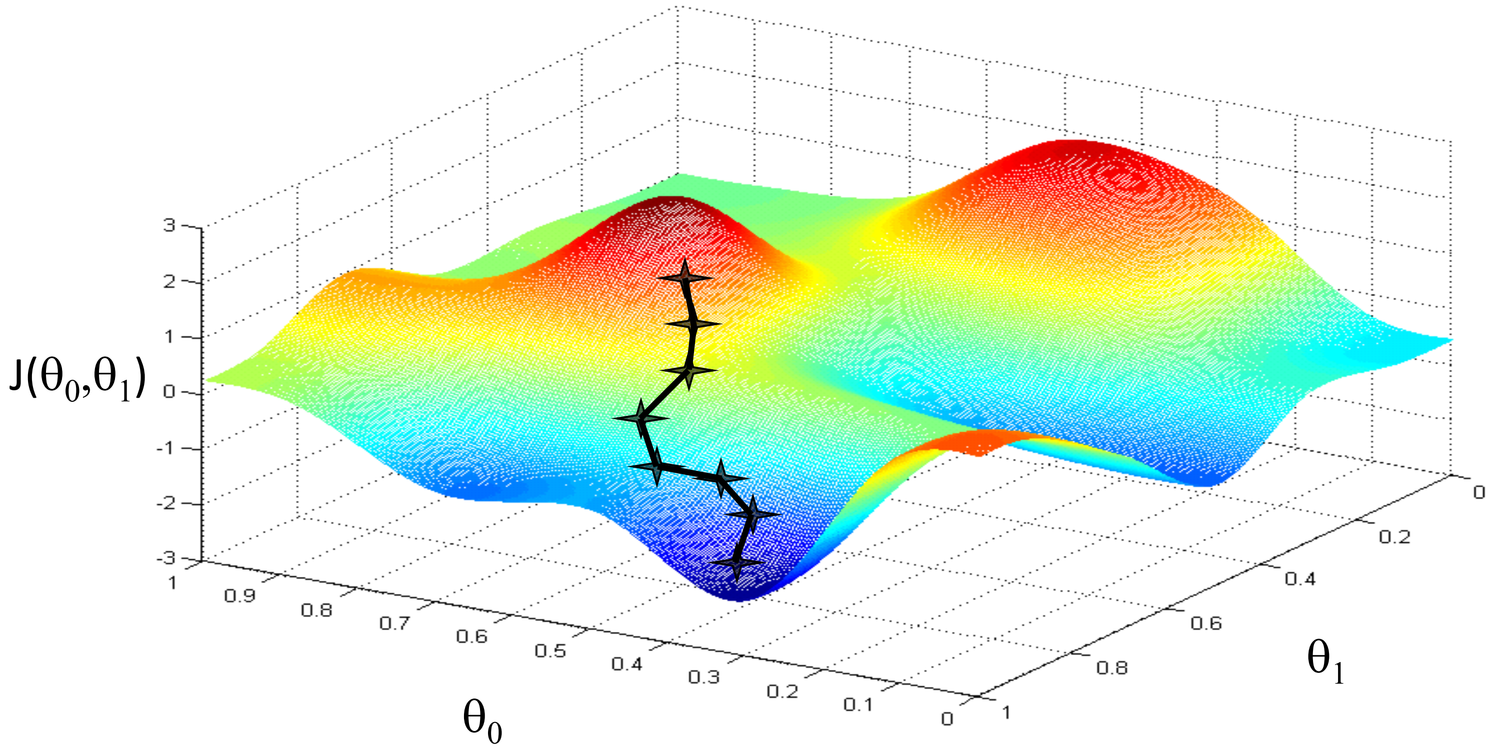

Figure by Andrew Ng

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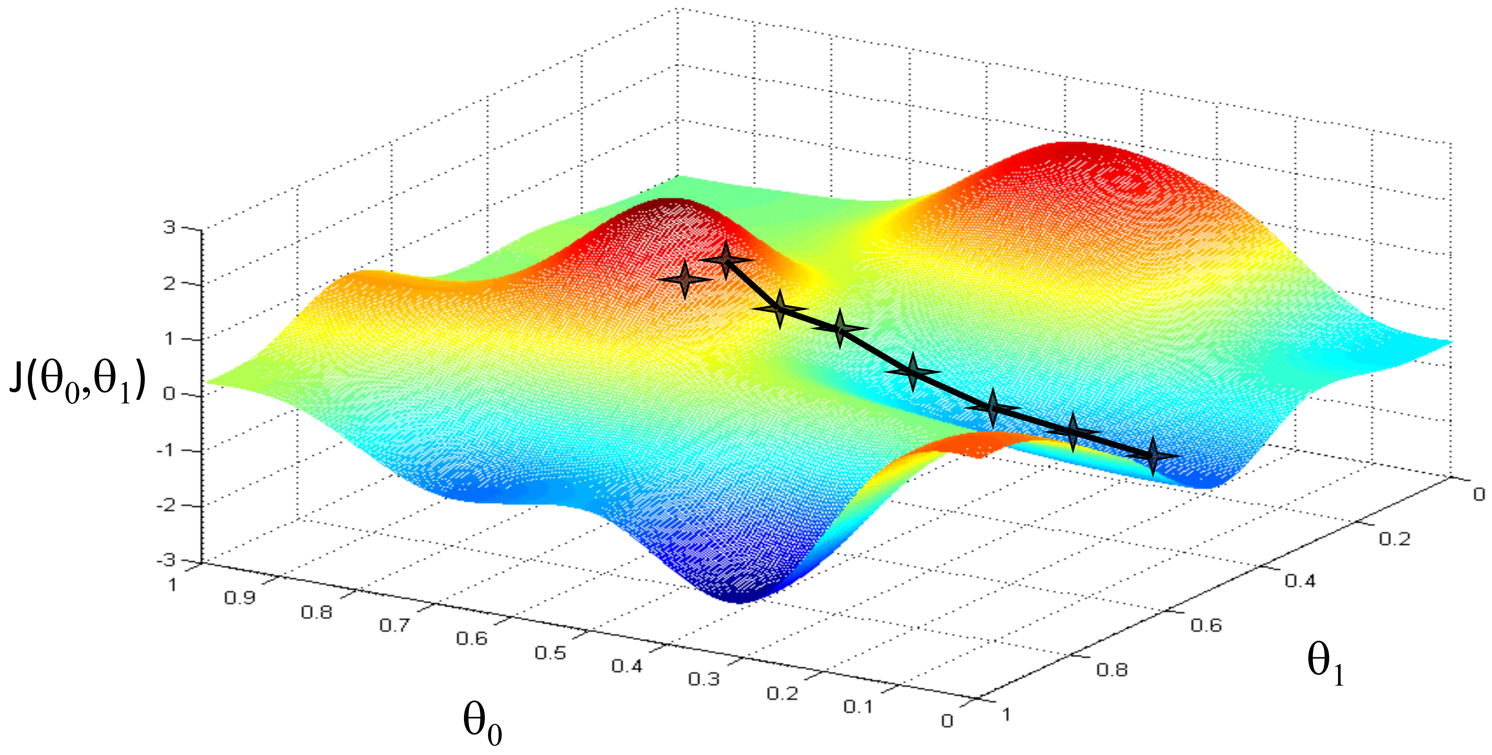

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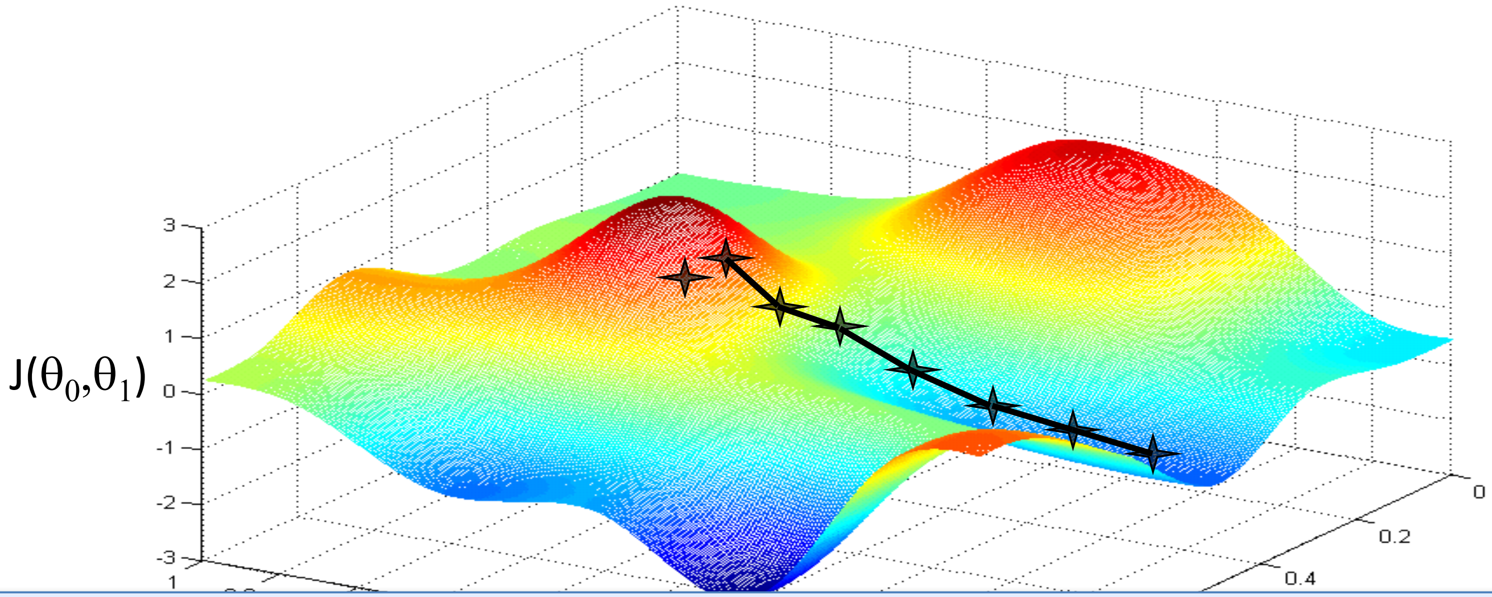


Since the least squares objective function is convex (concave), we don't need to worry about local minima in linear regression

Figure by Andrew Ng

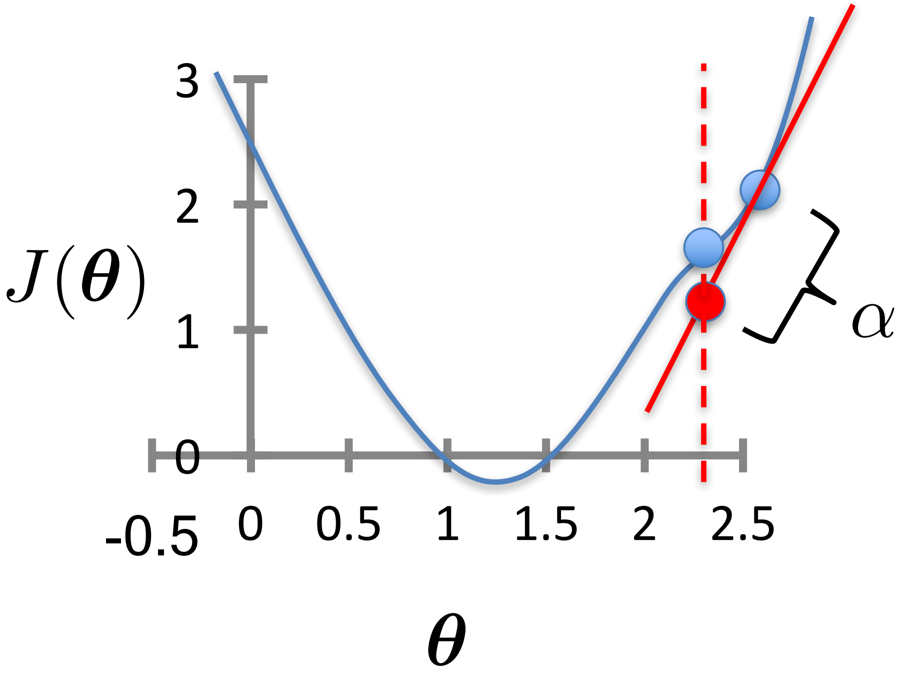
Gradient Descent

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta})$$

simultaneous update
for j = 0 ... d

learning rate (small)
e.g., α = 0.05



Gradient Descent

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

$$\theta_j \qquad \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta})$$

simultaneous update
for j = 0 ... d

For Linear Regression: $$\frac{\partial}{\partial \theta_j} J(\boldsymbol{\theta}) = \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)} \right)^2$$

$$= \frac{\partial}{\partial \theta_j} \frac{1}{2n} \sum_{i=1}^{n} \quad \sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \Bigg)^2$$

$$= \frac{1}{n} \sum_{i=1}^{n} \quad \sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \Bigg) \times \frac{\partial}{\partial \theta_j} \quad \sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \Bigg)$$

$$= \frac{1}{n} \sum_{i=1}^{n} \quad \sum_{k=0}^{d} \theta_k x_k^{(i)} - y^{(i)} \Bigg) x_j^{(i)}$$

Gradient Descent for Linear Regression

- Initialize $\boldsymbol{\theta}$
- Repeat until convergence

$$\theta_j \leftarrow \theta_j - \alpha \frac{1}{n} \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right) - y^{(i)} \right) x_j^{(i)}$$

simultaneous update for j = 0 ... d

- To achieve simultaneous update
  - At the start of each GD iteration, compute $h_{\boldsymbol{\theta}} \left(\boldsymbol{x}^{(i)} \right)$
  - Use this stored value in the update step loop

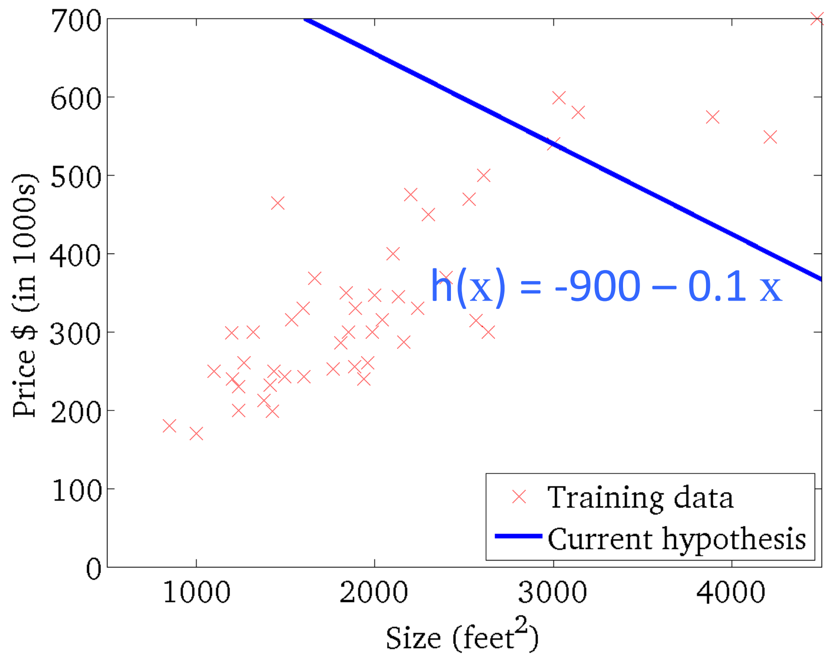
- Assume convergence when $\|\boldsymbol{\theta}_{new} - \boldsymbol{\theta}_{old}\|_2 < \epsilon$

L$_2$ norm: $\|\boldsymbol{v}\|_2 = \sqrt{\sum_i v_i^2} = \sqrt{v_1^2 + v_2^2 + \ldots + v_{|v|}^2}$

Gradient Descent

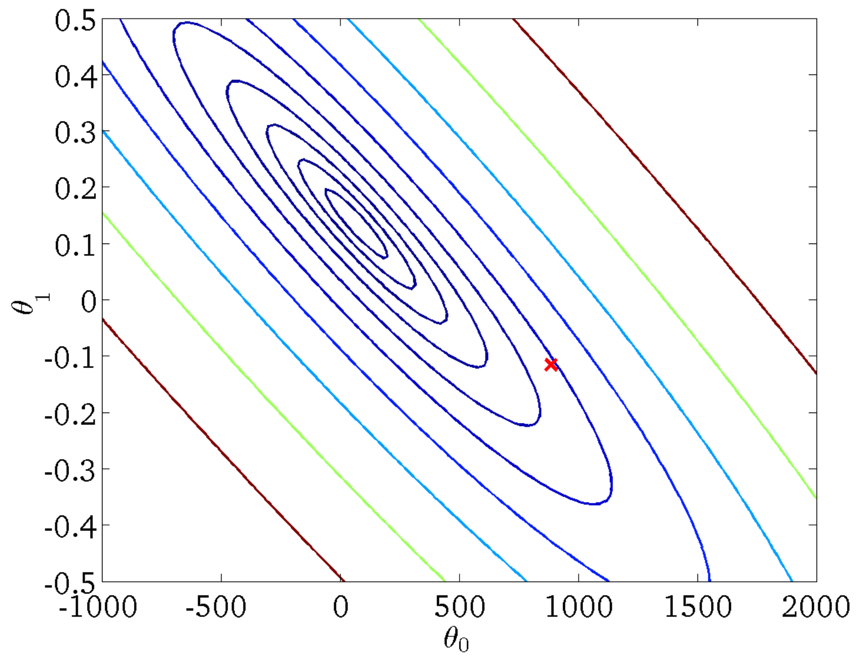
$h_\theta(x)$

(for fixed θ_0, θ_1, this is a function of x)



$J(\theta_0, \theta_1)$

(function of the parameters θ_0, θ_1)



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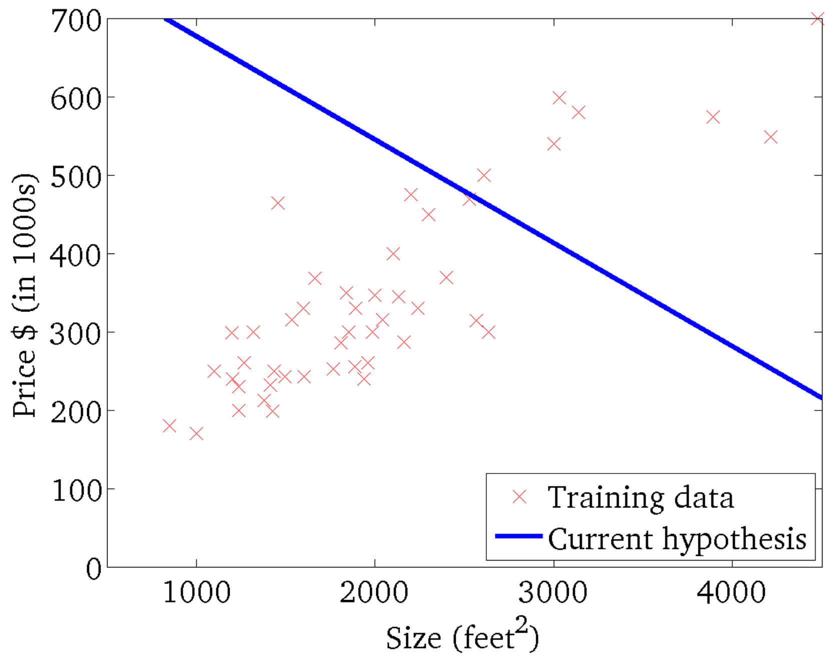

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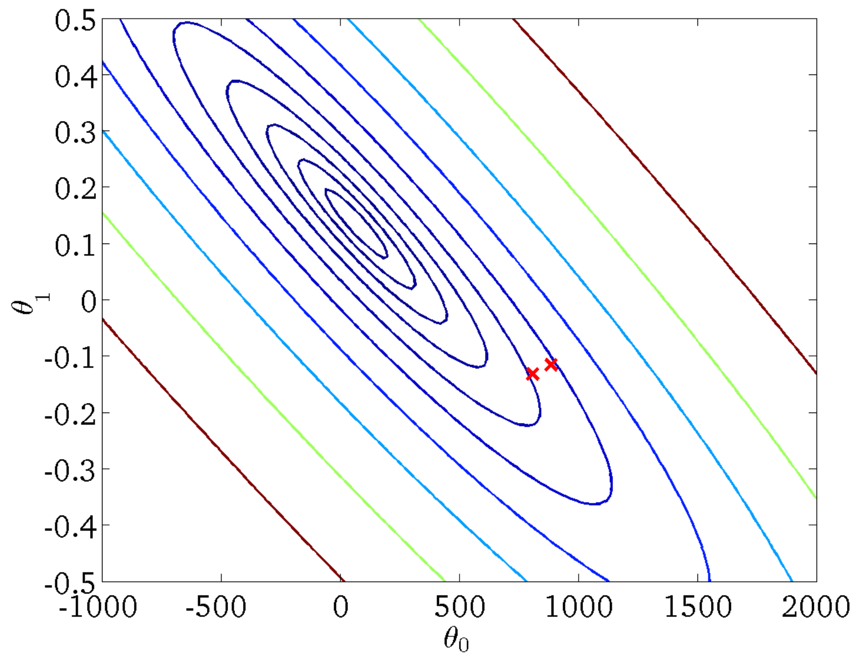

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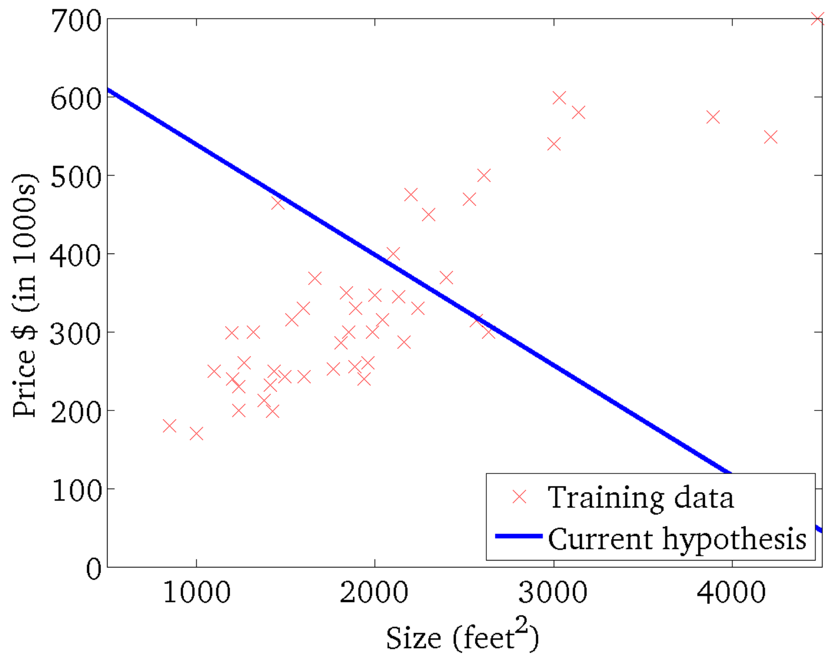

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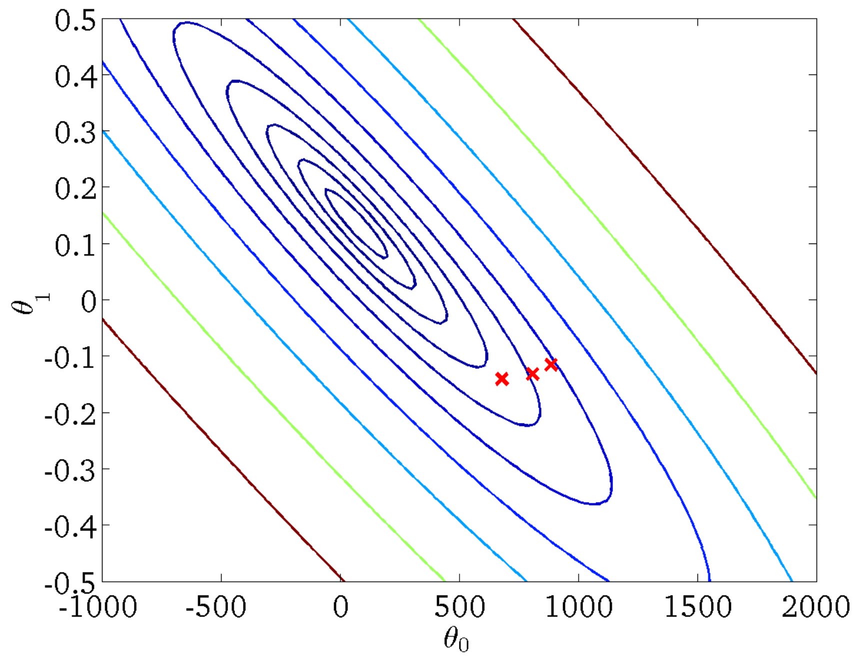

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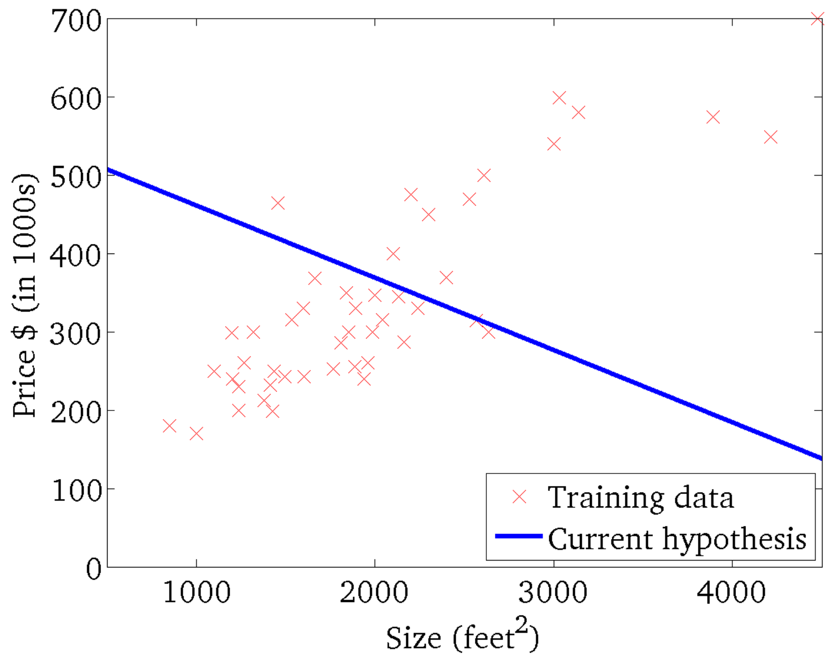

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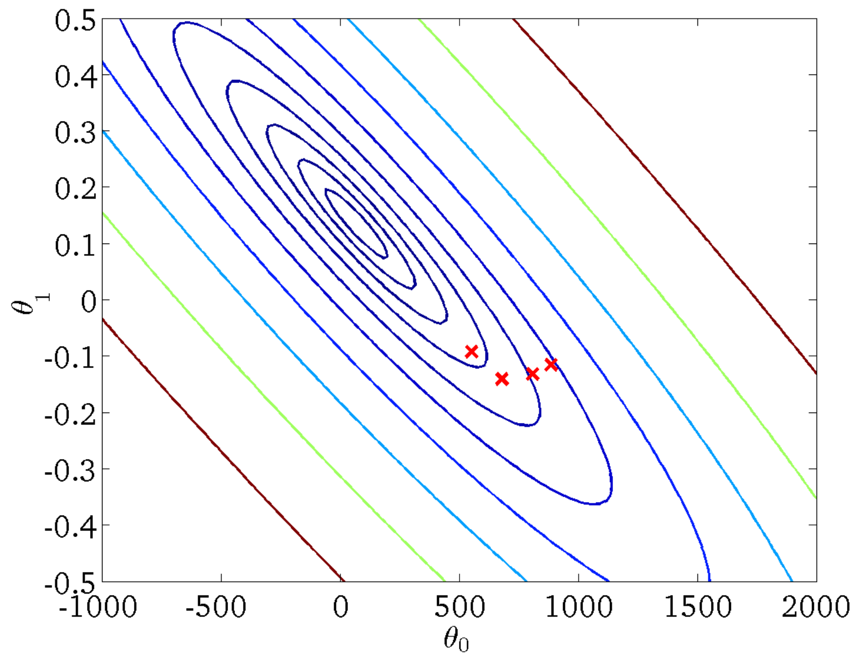

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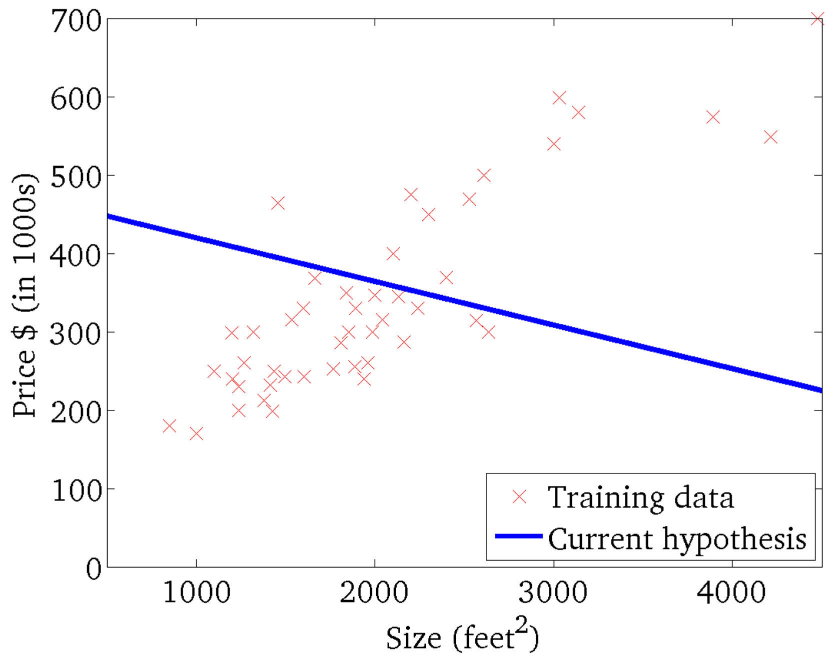

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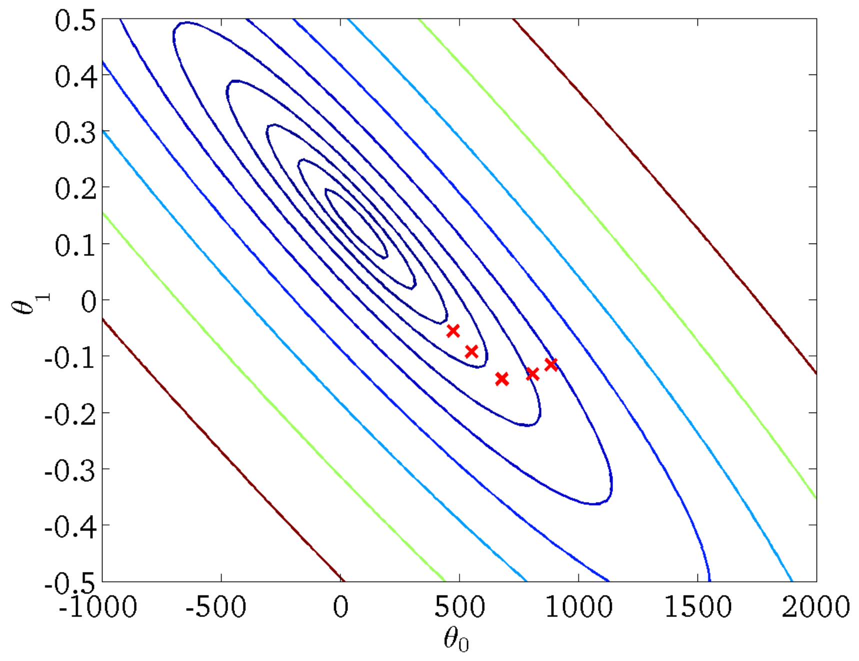

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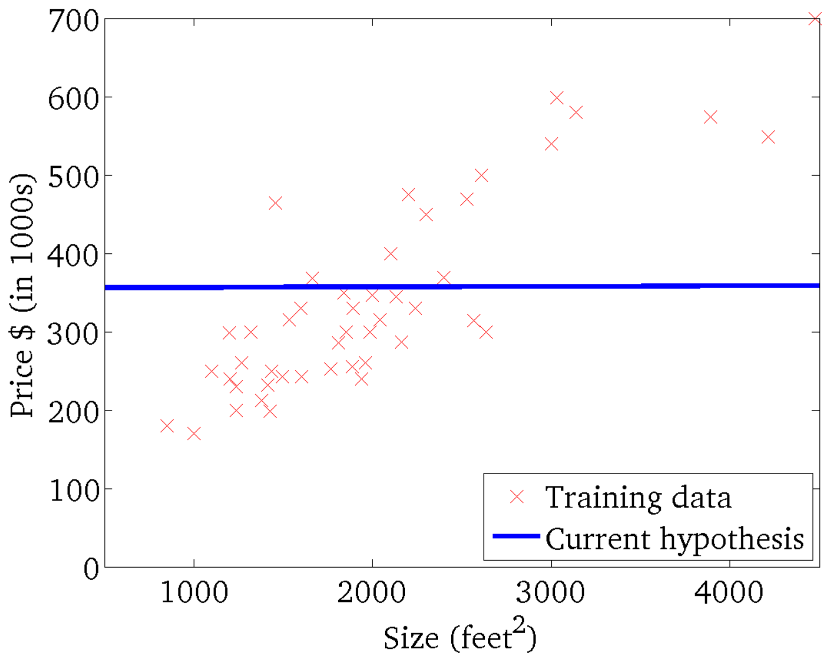

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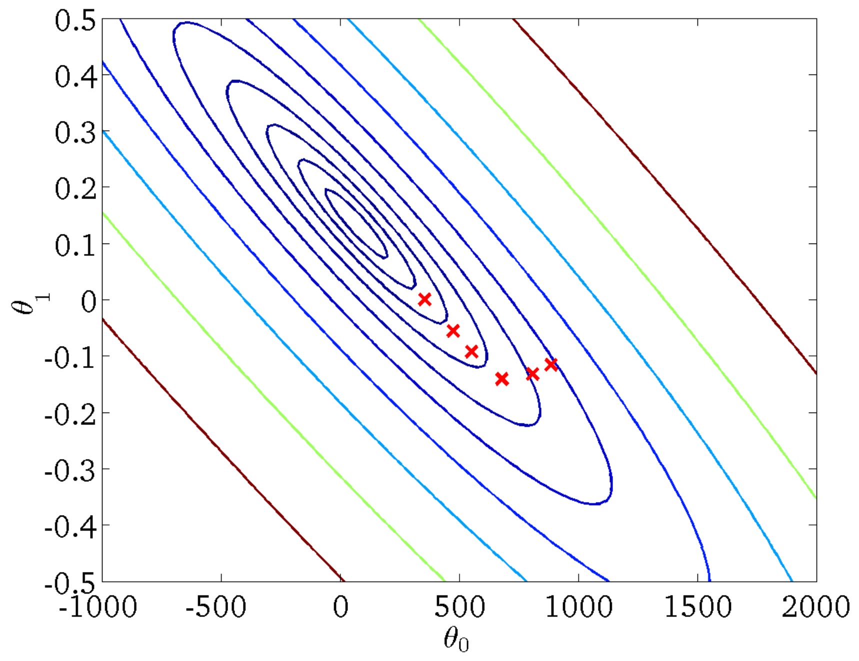

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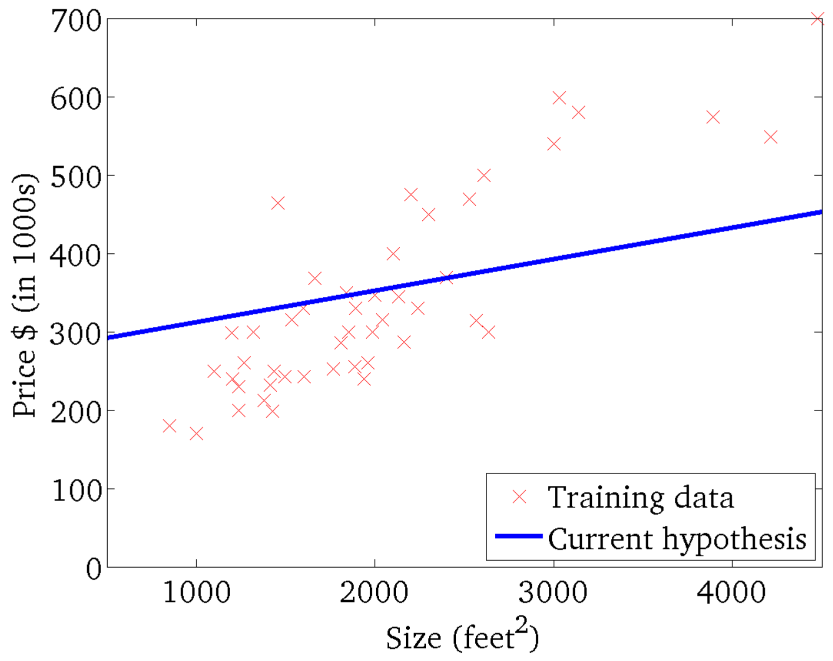

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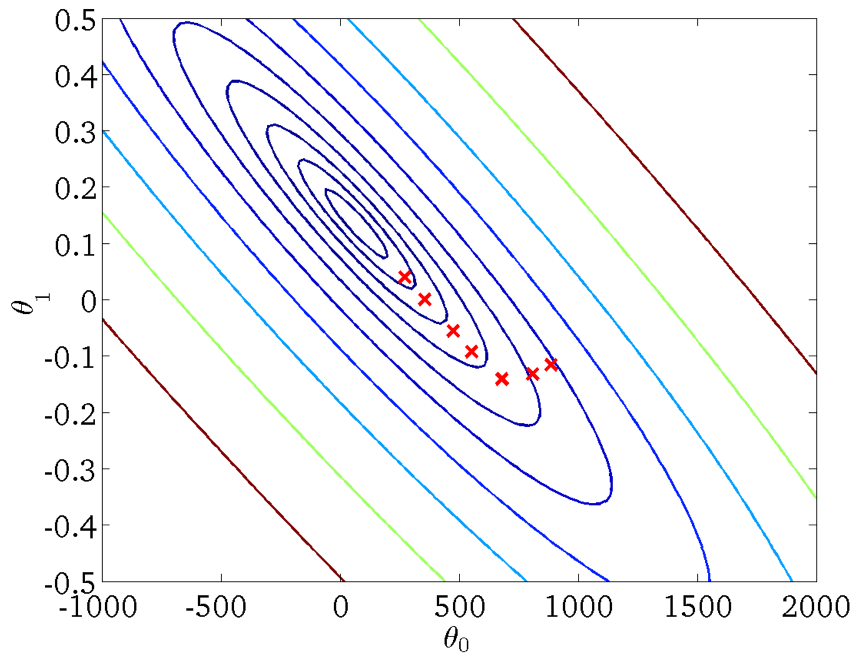

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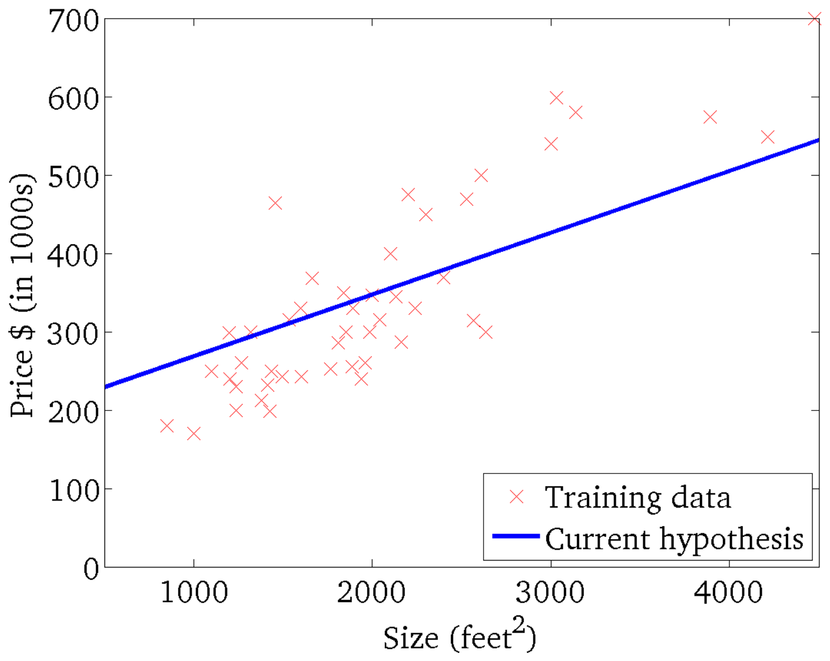

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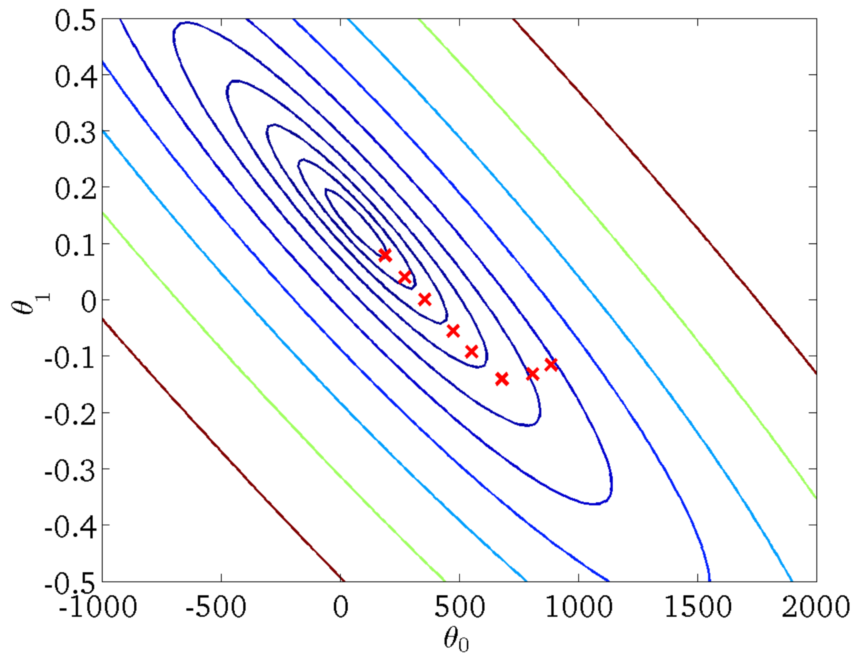

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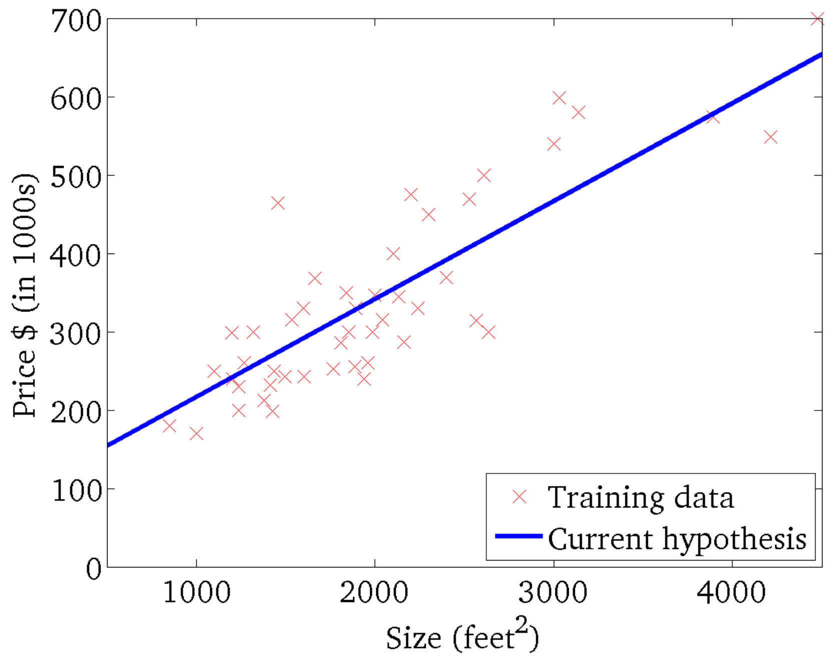

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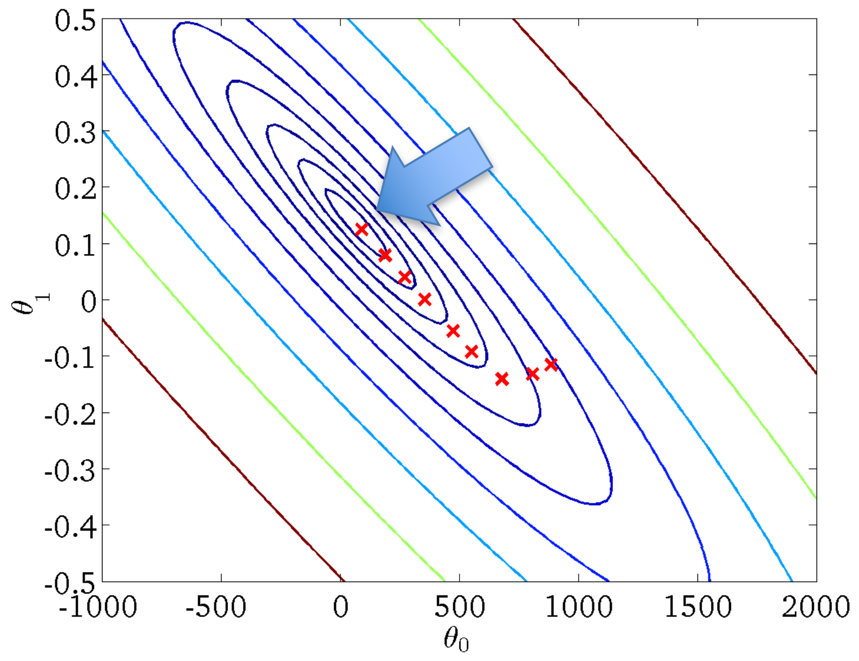
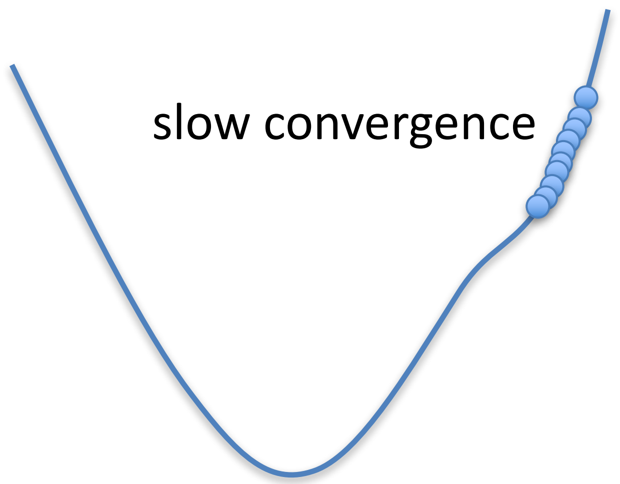
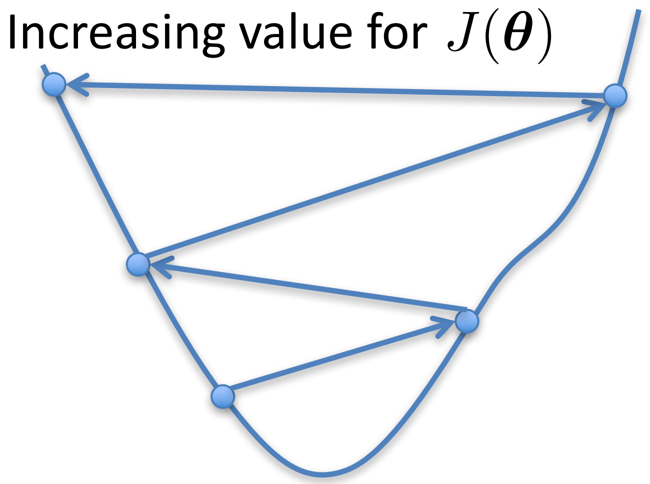


Choosing α

α too small



α too large



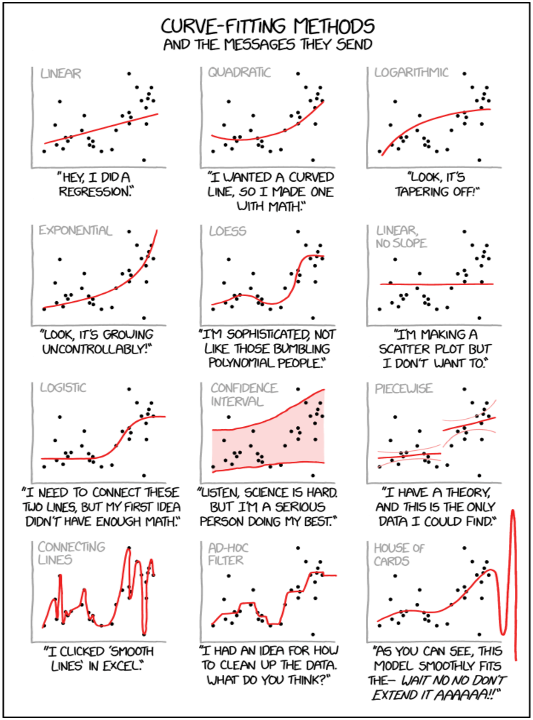
- May overshoot the minimum
- May fail to converge
- May even diverge

To see if gradient descent is working, print out $J(\boldsymbol{\theta})$ each iteration

- The value should decrease at each iteration
- If it doesn't, adjust α

Gradient descent

- Why gradient descent, if we can find the optimum directly?
  - GD can be applied to a much broader set of models
  - GD can be easier to implement than direct solutions, especially with automatic differentiation software
  - For regression in high-dimensional spaces, GD is more efficient than direct solution (matrix inversion is an $\mathcal{O}(D^3)$ algorithm).


CURVE-FITTING METHODS
AND THE MESSAGES THEY SEND
LINEAR
"HEY, I DID A REGRESSION."
QUADRATIC
"I WANTED A CURVED LINE, SO I MADE ONE WITH MATH."
LOGARITHMIC
"LOOK, IT'S TAPERING OFF!"
EXPONENTIAL
"LOOK, IT'S GROWING UNCONTROLLABLY!"
LOESS
"I'M SOPHISTICATED, NOT LIKE THOSE BUMBLING POLYNOMIAL PEOPLE."
LINEAR, NO SLOPE
"I'M MAKING A SCATTER PLOT BUT I DON'T WANT TO."
LOGISTIC
"I NEED TO CONNECT THESE TWO LINES, BUT MY FIRST IDEA DIDN'T HAVE ENOUGH MATH."
CONFIDENCE INTERVAL
"LISTEN, SCIENCE IS HARD. BUT I'M A SERIOUS PERSON DOING MY BEST."
PIECEWISE
"I HAVE A THEORY, AND THIS IS THE ONLY DATA I COULD FIND."
CONNECTING LINES
"I CLICKED 'SMOOTH LINES' IN EXCEL."
AD-HOC FILTER
"I HAD AN IDEA FOR HOW TO CLEAN UP THE DATA. WHAT DO YOU THINK?"
HOUSE OF CARDS
"AS YOU CAN SEE, THIS MODEL SMOOTHLY FITS THE– WAIT NO NO DON'T EXTEND IT AAAAAA!!"

Extending Linear Regression to More Complex Models

- The inputs **X** for linear regression can be:
  - Original quantitative inputs
  - Transformation of quantitative inputs
    - e.g. log, exp, square root, square, etc.
  - Polynomial transformation
    - example: $y = \beta_0 + \beta_1 \cdot x + \beta_2 \cdot x^2 + \beta_3 \cdot x^3$
  - Basis expansions
  - Dummy coding of categorical inputs
  - Interactions between variables
    - example: $x_3 = x_1 \cdot x_2$

This allows use of **linear** regression techniques to fit **non-linear** datasets.

Linear Basis Function Models

- Generally,

$$h_{\boldsymbol{\theta}}(\boldsymbol{x}) = \sum_{j=0}^{d} \theta_j \underbrace{\phi_j(\boldsymbol{x})}_{\text{basis function}}$$

- Typically, $\phi_0(\boldsymbol{x}) = 1$ so that θ_0 acts as a bias
- In the simplest case, we use linear basis functions :

$$\phi_j(\boldsymbol{x}) = x_j$$

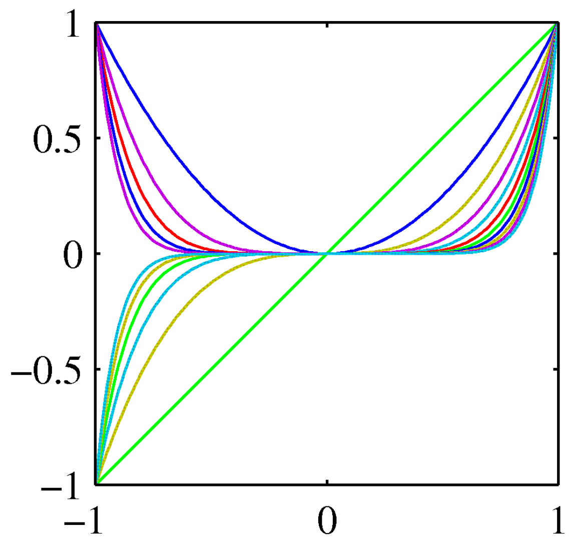
Based on slide by Christopher Bishop (PRML)

Linear Basis Function Models

- Polynomial basis functions:

$$\phi_j(x) = x^j$$

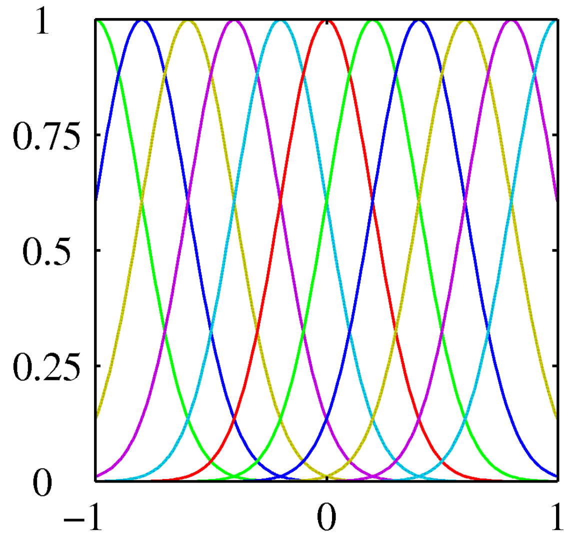
  - These are global; a small change in x affects all basis functions



- Gaussian basis functions:

$$\phi_j(x) = \exp\left\{-\frac{(x-\mu_j)^2}{2s^2}\right\}$$

  - These are local; a small change in x only affect nearby basis functions. μ_j and s control location and scale (width).



Based on slide by Christopher Bishop (PRML)

Linear Basis Function Models

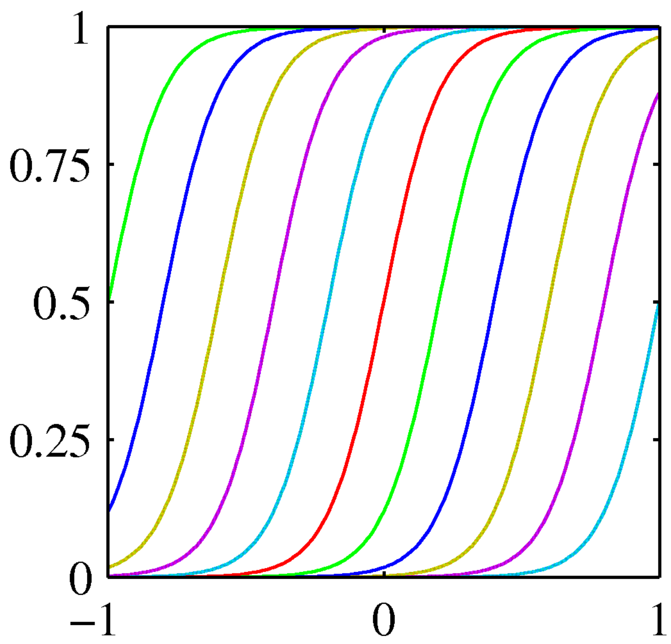
- Sigmoidal basis functions:

$$\phi_j(x) = \sigma\left(\frac{x - \mu_j}{s}\right)$$

where

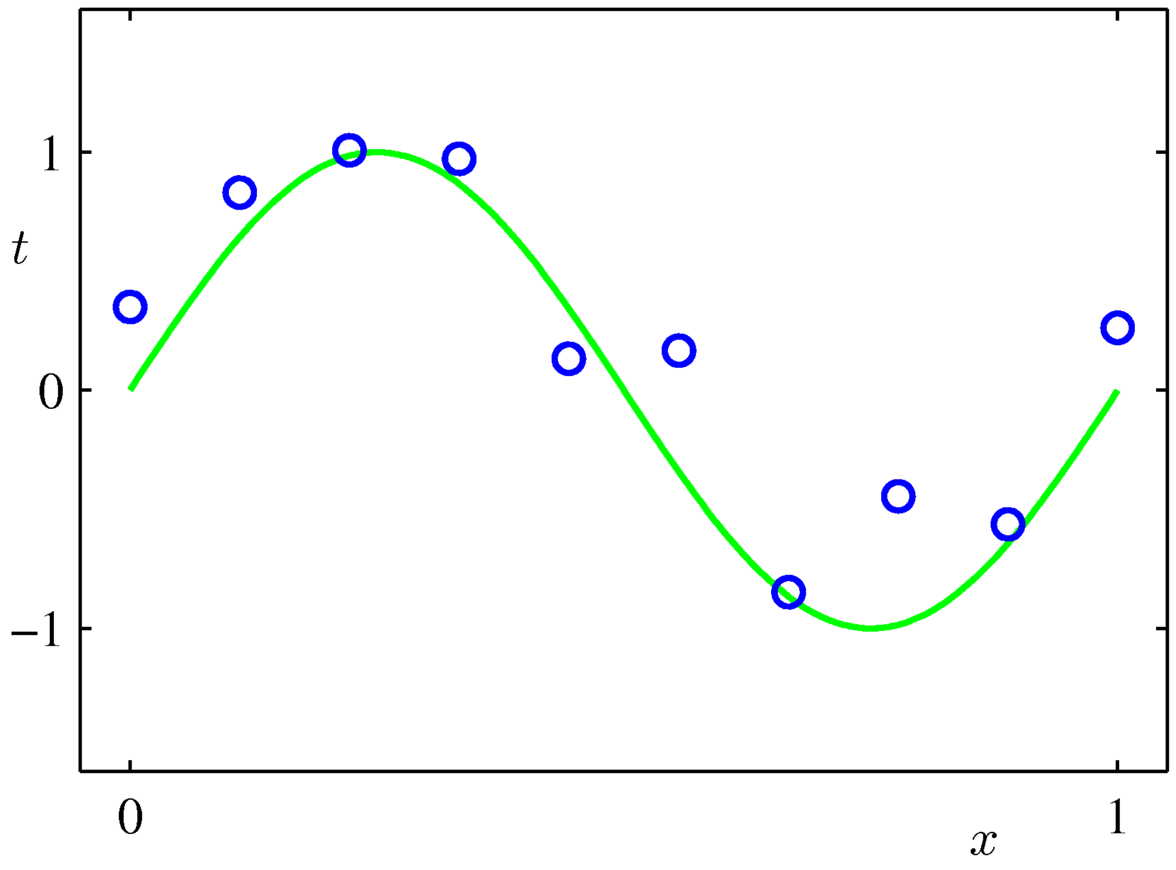
$$\sigma(a) = \frac{1}{1 + \exp(-a)}$$

  - These are also local; a small change in x only affects nearby basis functions. μ_j and s control location and scale (slope).



Based on slide by Christopher Bishop (PRML)

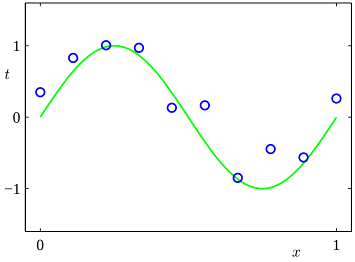
Example of Fitting a Polynomial Curve with a Linear Model



$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \ldots + \theta_p x^p = \sum_{j=0}^{p} \theta_j x^j$$

Feature mappings

- Suppose we want to model the following data



-Pattern Recognition and Machine Learning, Christopher Bishop.

- One option: fit a low-degree polynomial; this is known as polynomial regression

$$y = w_3 x^3 + w_2 x^2 + w_1 x + w_0$$

- Do we need to derive a whole new algorithm?

Feature mappings

- We get polynomial regression for free!
- Define the feature map

$$\boldsymbol{\psi}(x) = \begin{pmatrix} 1 \\ x \\ x^2 \\ x^3 \end{pmatrix}$$

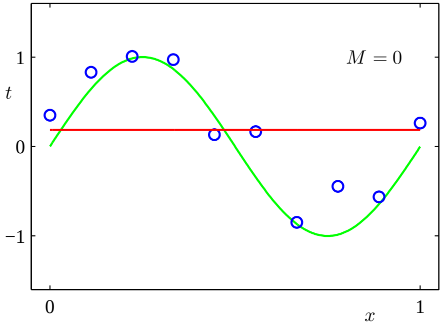
- Polynomial regression model:

$$y = \mathbf{w}^\top \boldsymbol{\psi}(x)$$

- All of the derivations and algorithms so far in this lecture remain exactly the same!

Fitting polynomials

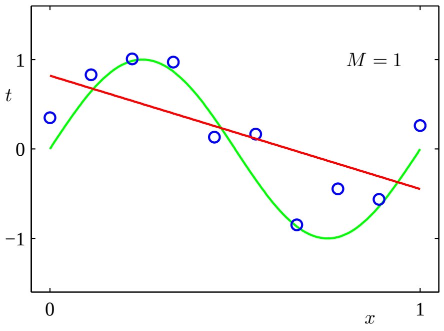
$$y = w_0$$



-Pattern Recognition and Machine Learning, Christopher Bishop.

Fitting polynomials

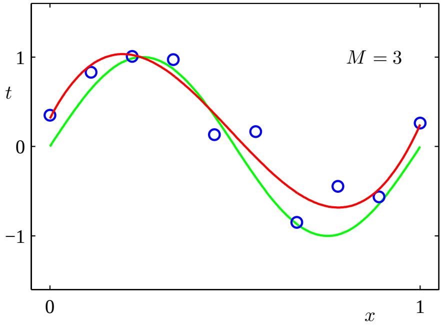
$$y = w_0 + w_1 x$$



-Pattern Recognition and Machine Learning, Christopher Bishop.

Fitting polynomials

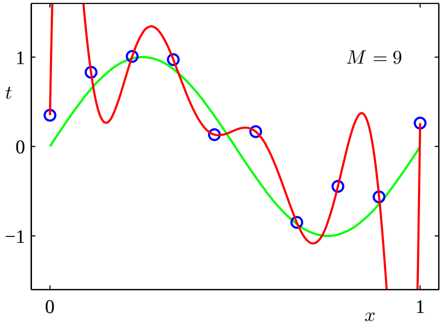
$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3$$



-Pattern Recognition and Machine Learning, Christopher Bishop.

Fitting polynomials

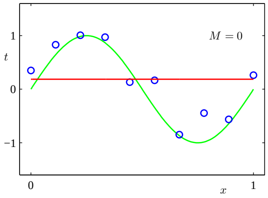
$$y = w_0 + w_1 x + w_2 x^2 + w_3 x^3 + \ldots + w_9 x^9$$



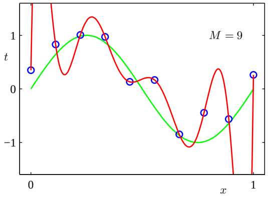
-Pattern Recognition and Machine Learning, Christopher Bishop.

Generalization

Underfitting : model is too simple — does not fit the data.

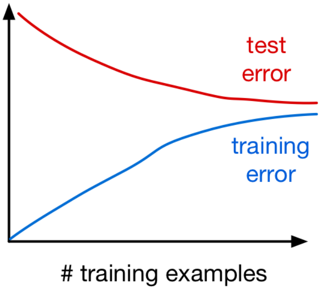


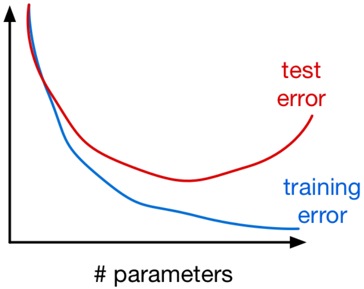
Overfitting : model is too complex — fits perfectly, does not generalize.



Generalization

- Training and test error as a function of # training examples and # parameters:





Regularization

- The degree of the polynomial is a hyperparameter, just like k in KNN. We can tune it using a validation set.
- But restricting the size of the model is a crude solution, since you'll never be able to learn a more complex model, even if the data support it.
- Another approach: keep the model large, but regularize it
    - Regularizer: a function that quantifies how much we prefer one hypothesis vs. another

Regularization

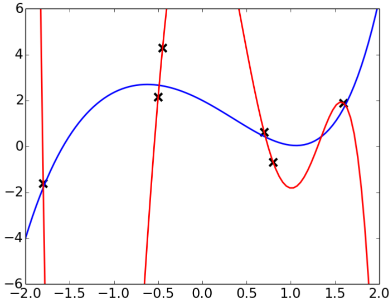
- A method for automatically controlling the complexity of the learned hypothesis

- **Idea**: penalize for large values of θ_j
  - Can incorporate into the cost function
  - Works well when we have a lot of features, each that contributes a bit to predicting the label

- Can also address overfitting by eliminating features (either manually or via model selection)

L^2 Regularization

Observation: polynomials that overfit often have large coefficients.



$$y = 0.1x^5 + 0.2x^4 + 0.75x^3 - x^2 - 2x + 2$$

$$y = -7.2x^5 + 10.4x^4 + 24.5x^3 - 37.9x^2 - 3.6x + 12$$

So let's try to keep the coefficients small.

L^2 Regularization

Another reason we want weights to be small:

- Suppose inputs x_1 and x_2 are nearly identical for all training examples. The following two hypotheses make nearly the same predictions:

$$\mathbf{w} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \qquad \mathbf{w} = \begin{pmatrix} -9 \\ 11 \end{pmatrix}$$

- But the second network might make weird predictions if the test distribution is slightly different (e.g. x_1 and x_2 match less closely).

L^2 Regularization

- We can encourage the weights to be small by choosing as our regularizer the L^2 penalty.

$$\mathcal{R}(\mathbf{w}) = \tfrac{1}{2}\|\mathbf{w}\|^2 = \frac{1}{2}\sum_j w_j^2.$$

  - Note: to be pedantic, the L^2 norm is Euclidean distance, so we're really regularizing the *squared* L^2 norm.

- The regularized cost function makes a tradeoff between fit to the data and the norm of the weights.

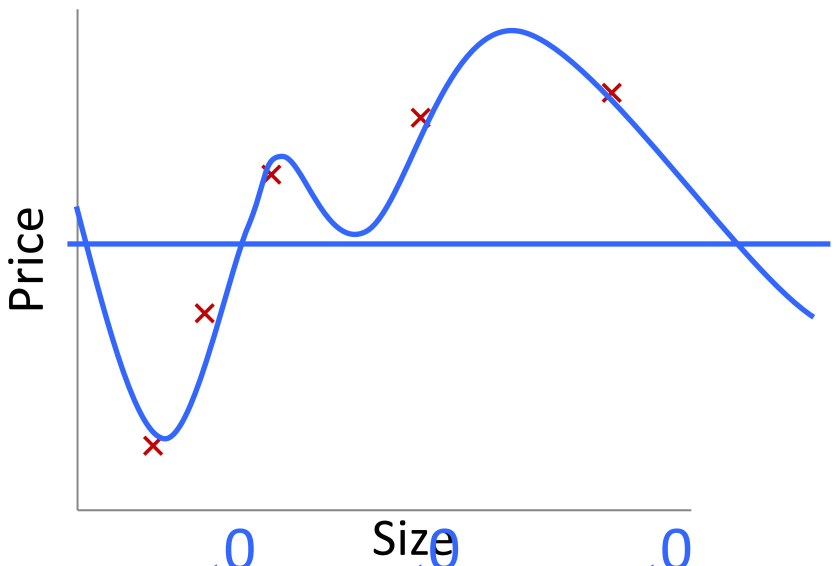
$$\mathcal{J}_{\mathrm{reg}} = \mathcal{J} + \lambda\mathcal{R} = \mathcal{J} + \frac{\lambda}{2}\sum_j w_j^2$$

- Here, λ is a hyperparameter that we can tune using a validation set.

Understanding Regularization

$$J(\boldsymbol{\theta}) = \frac{1}{2n}\sum_{i=1}^{n}\left(h_{\boldsymbol{\theta}}\left(\boldsymbol{x}^{(i)}\right) - y^{(i)}\right)^2 + \frac{\lambda}{2}\sum_{j=1}^{d}\theta_j^2$$

- What happens if we set λ to be huge (e.g., 10^{10})?

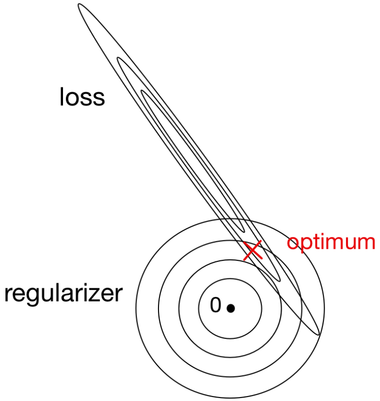


$$\theta_0 + \overset{0}{\cancel{\theta_1}}x + \overset{0}{\cancel{\theta_2}}x^2 + \overset{0}{\cancel{\theta_3}}x^3 + \overset{0}{\cancel{\theta_4}}x^4$$

Based on example by Andrew Ng

L^2 Regularization

- The geometric picture:



L^2 Regularization

- Recall the gradient descent update:

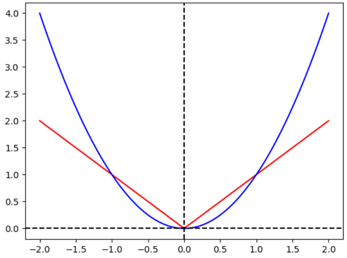
$$\mathbf{w} \leftarrow \mathbf{w} - \alpha \frac{\partial \mathcal{J}}{\partial \mathbf{w}}$$

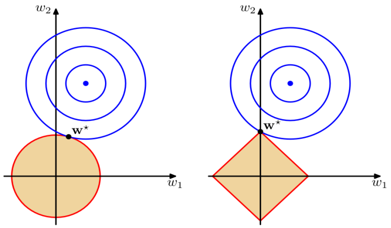
- The gradient descent update of the regularized cost has an interesting interpretation as weight decay:

$$\begin{aligned} \mathbf{w} &\leftarrow \mathbf{w} - \alpha \left(\frac{\partial \mathcal{J}}{\partial \mathbf{w}} + \lambda \frac{\partial \mathcal{R}}{\partial \mathbf{w}} \right) \\ &= \mathbf{w} - \alpha \left(\frac{\partial \mathcal{J}}{\partial \mathbf{w}} + \lambda \mathbf{w} \right) \\ &= (1 - \alpha\lambda)\mathbf{w} - \alpha \frac{\partial \mathcal{J}}{\partial \mathbf{w}} \end{aligned}$$

L^1 vs. L^2 Regularization

- The L^1 norm, or sum of absolute values, is another regularizer that encourages weights to be exactly zero. (How can you tell?)
- We can design regularizers based on whatever property we'd like to encourage.





L2 regularization

$$\mathcal{R} = \sum_i w_i^2$$

L1 regularization

$$\mathcal{R} = \sum_i |w_i|$$

— Bishop, *Pattern Recognition and Machine Learning*

Conclusion

Linear regression exemplifies recurring themes of this course:

- choose a model and a loss function
- formulate an optimization problem
- solve the optimization problem using one of two strategies
    - direct solution (set derivatives to zero)
    - gradient descent
- vectorize the algorithm, i.e. represent in terms of linear algebra
- make a linear model more powerful using features
- improve the generalization by adding a regularizer