Machine Learning

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   - Linear Regression, Logistic Regression, Support Vector Machines, Trees, Random Forests, Boosting, Artificial Neural Networks
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Supervised Learning

- **Linear Regression**
- Logistic Regression
- Support Vector Machines
- Trees (Decision and Regression)
- Random Forests
- Boosting
- Artificial Neural Networks

$\hat{y} = h(x, w) = w_0 + w_1 x$

Linear Regression

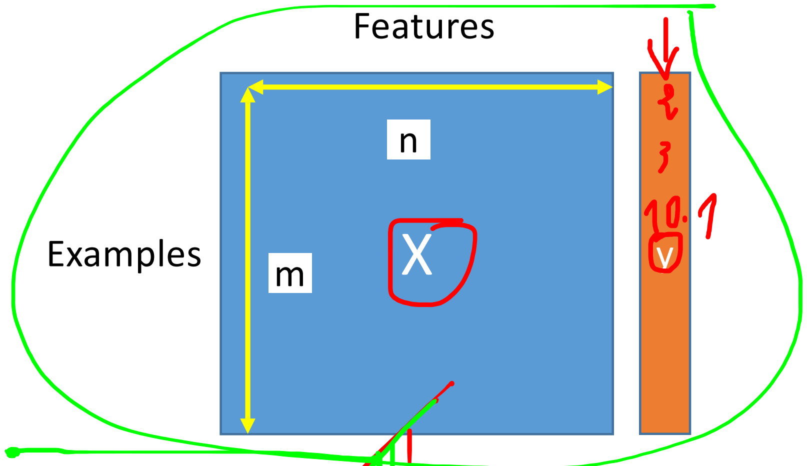
$w \begin{pmatrix} w_0 \\ w_1 \end{pmatrix}$

$\hat{y} = w_0 + w_1 x$

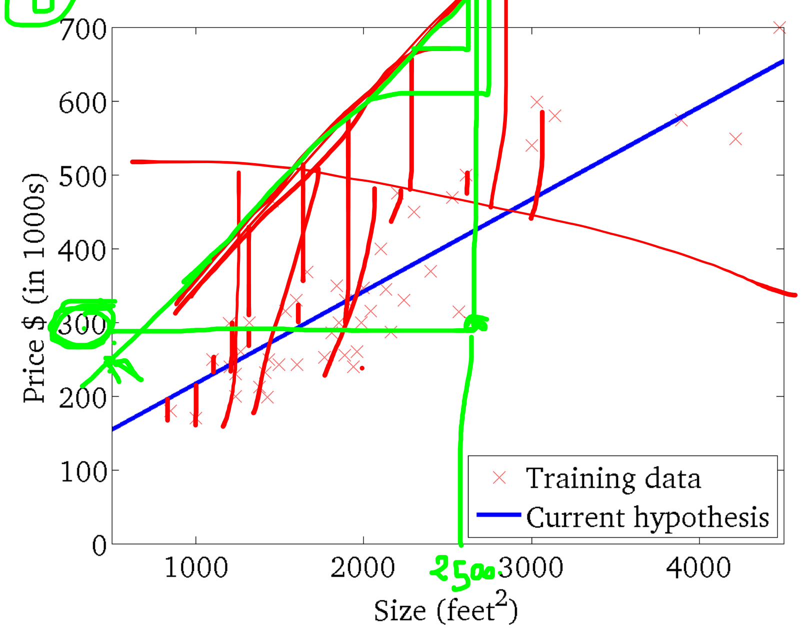
- The output y is continuous
- Fit X with a line $\hat{y} = w_0 + w_1 x$
- The best line is the line with minimum loss

$$L(w) = \frac{1}{2m} \sum_{i=1}^{m} \left(y^{(i)} - \hat{y}^{(i)}\right)^2$$

- Solved using Normal Equations
  - $W = (X^T X)^{-1} X^T y$
  - But not for big X !
- Find W iteratively using gradient descent



$\hat{y}$



Gradient Descent

(Batch) GD

X = data_input
Y = data_output
W = initialize_parameters()
for it **in** range(num_iterations):
  Yhat = h(X, W)
  L = loss(Yhat, Y)
  dW = gradient(L(W))
  $W = W - \alpha\, dW$

$$\boxed{L(w) = \frac{1}{2m}\sum_{i=1}^{m}\left(y^{(i)} - \hat{y}^{(i)}\right)^2}$$

$$= \frac{1}{2m}\sum\left(y^{(i)} - w_0 - w_1 x\right)^2$$

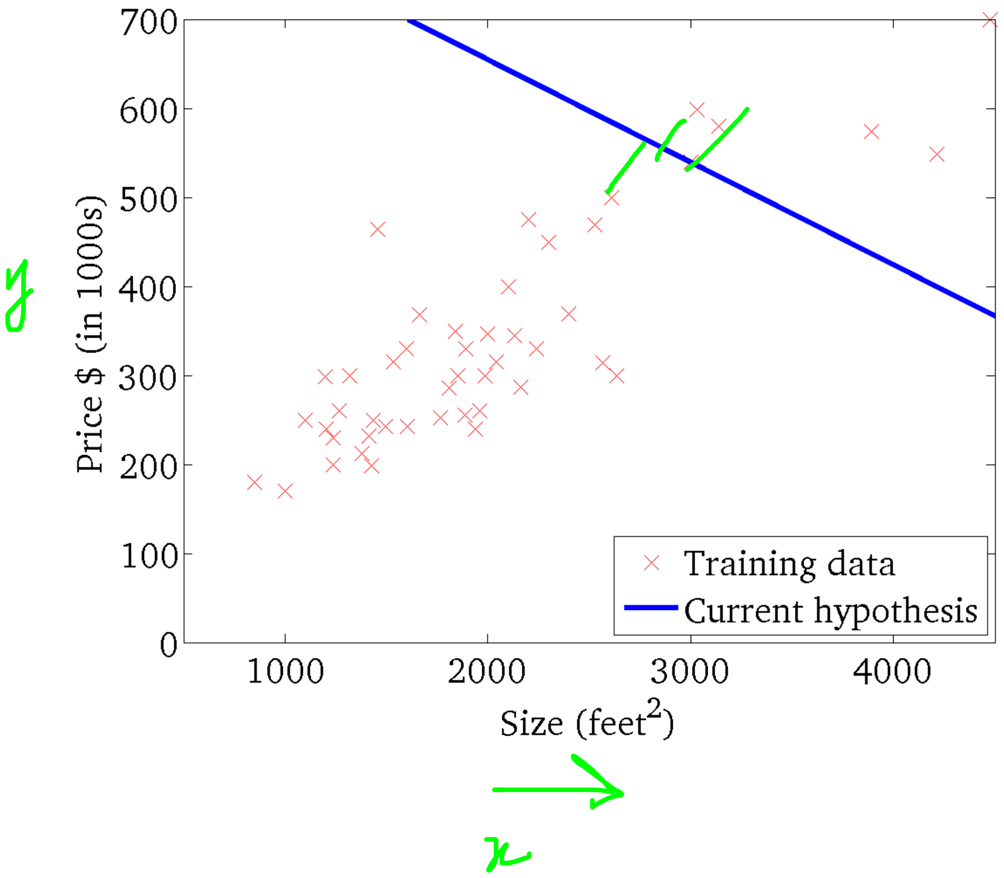
$$\left(f(x)^n\right)' \qquad n f'(x)\, f(x)^{n-1}$$

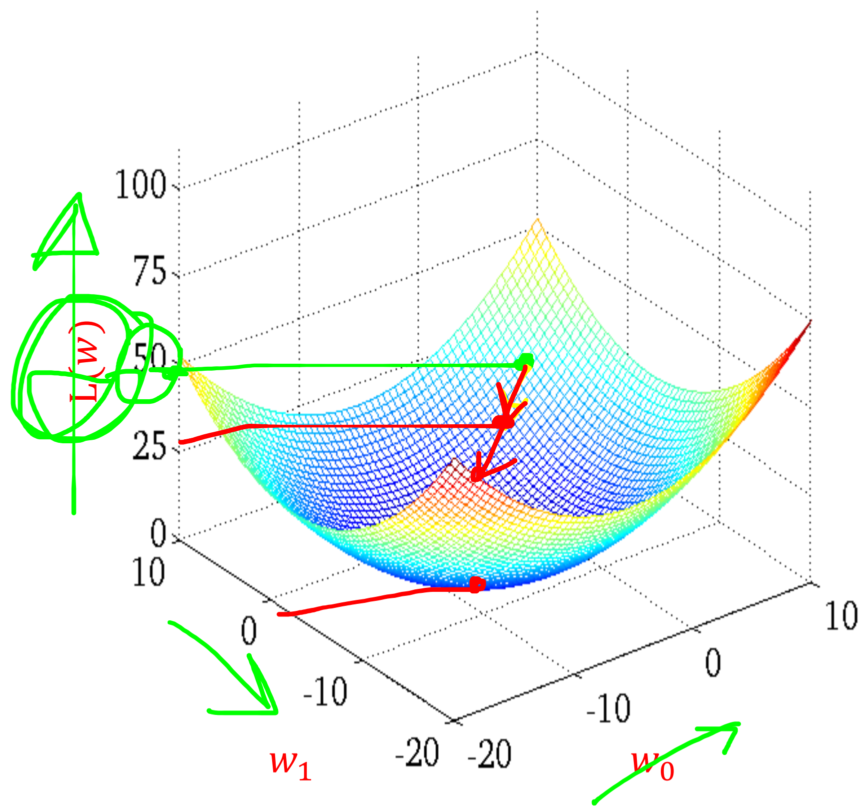
$$\frac{\partial L(w)}{\partial w_0} = -\frac{1}{\cancel{2}m}\sum \cancel{2}\left(y^{(i)} - w_0 - w_1 x\right)$$

$$\frac{\partial L(w)}{\partial w_1} = -\frac{1}{\cancel{2}m}\sum \cancel{2}\left(y^{(i)} - w_0 - w_1 x\right)x$$

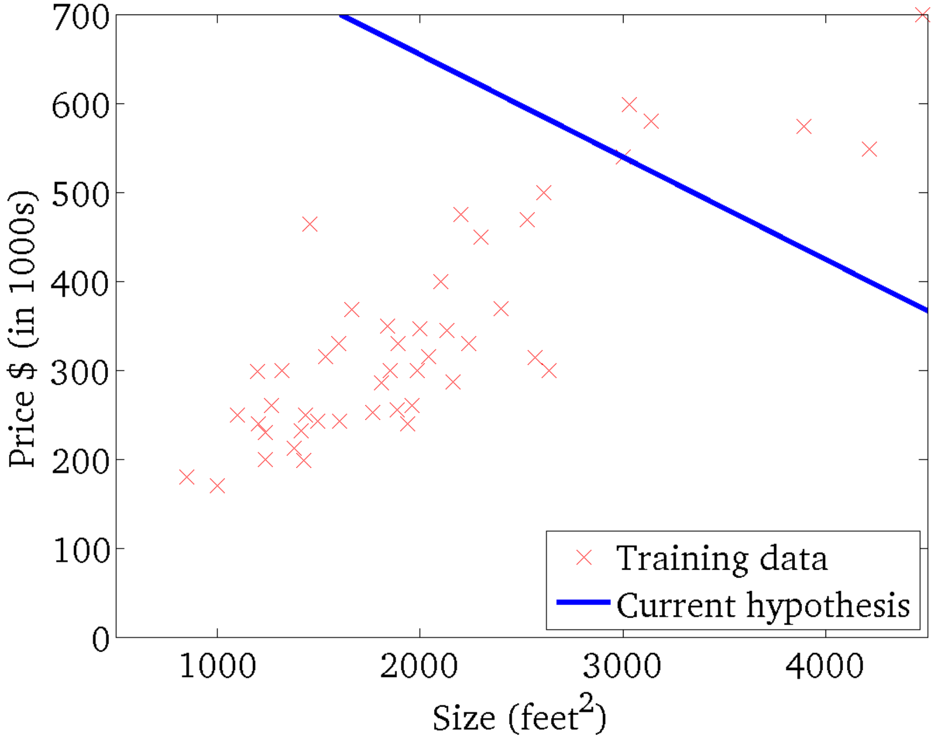
$$w_0 := w_0 - \alpha$$

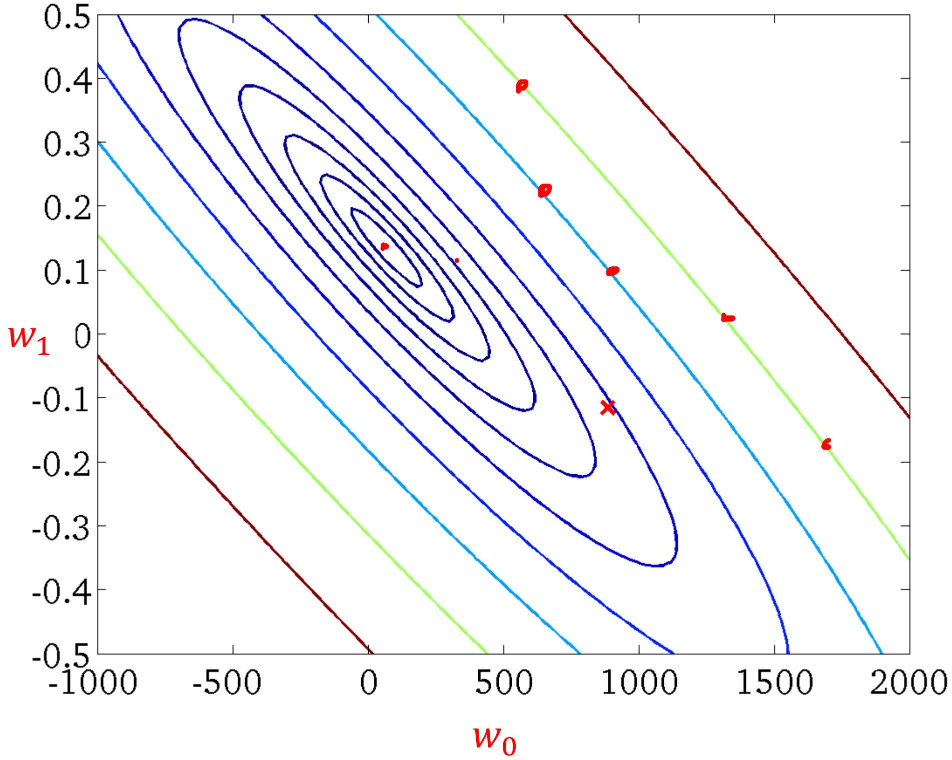
Linear Regression



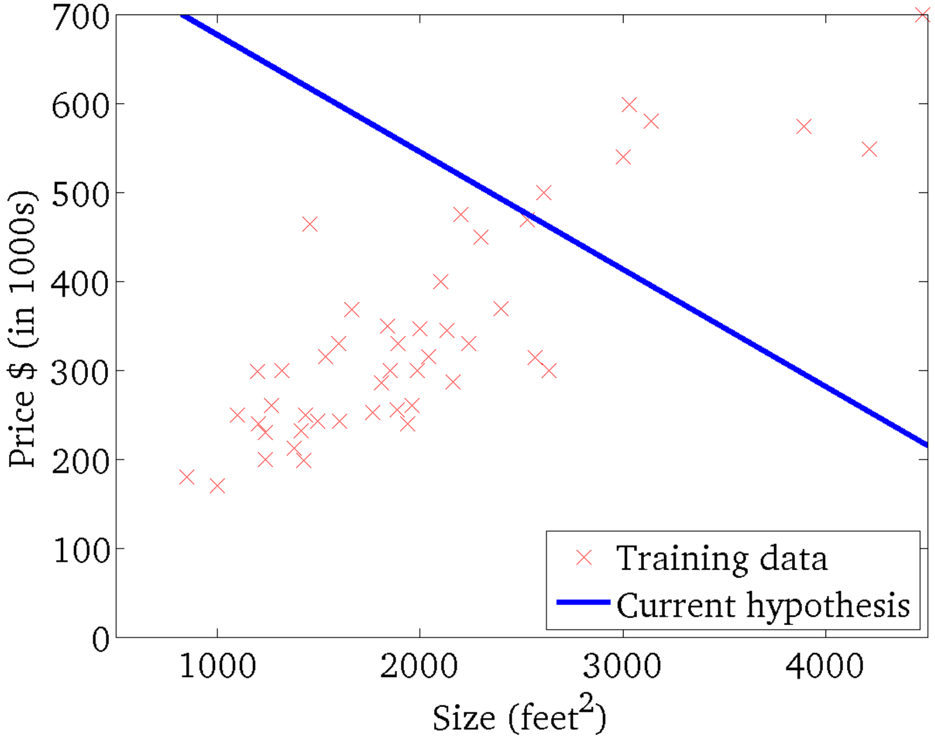


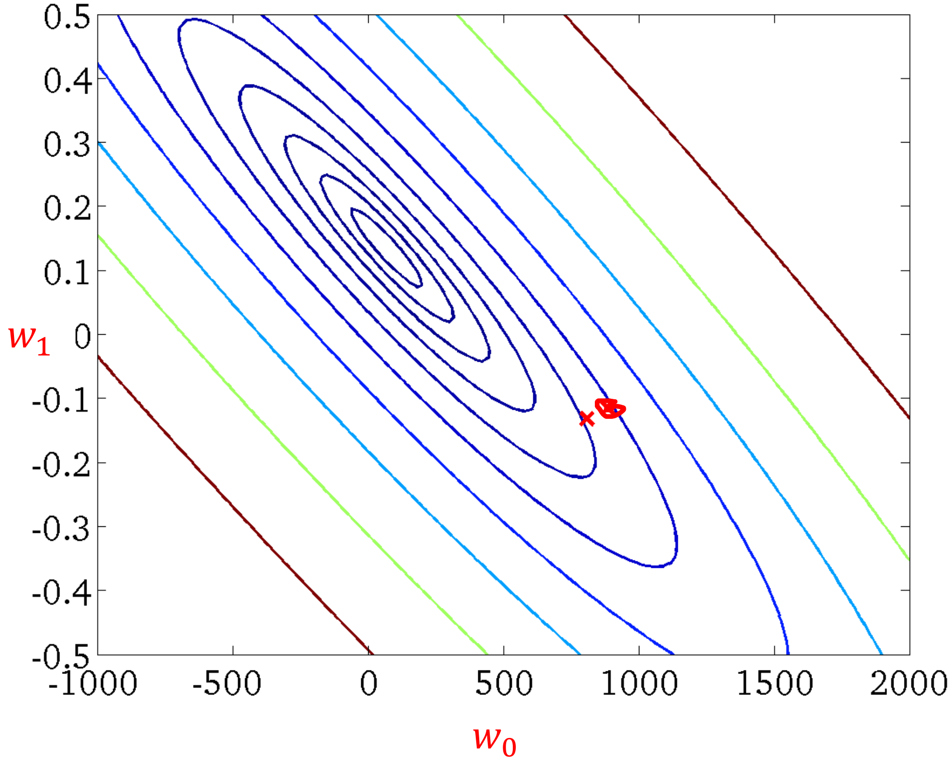
Linear Regression



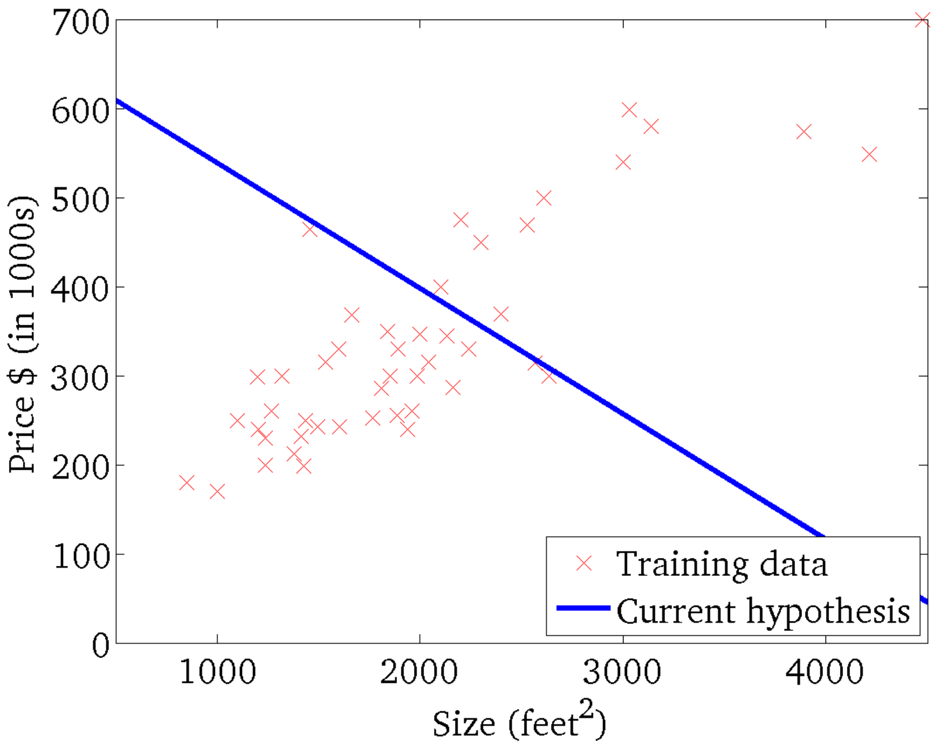


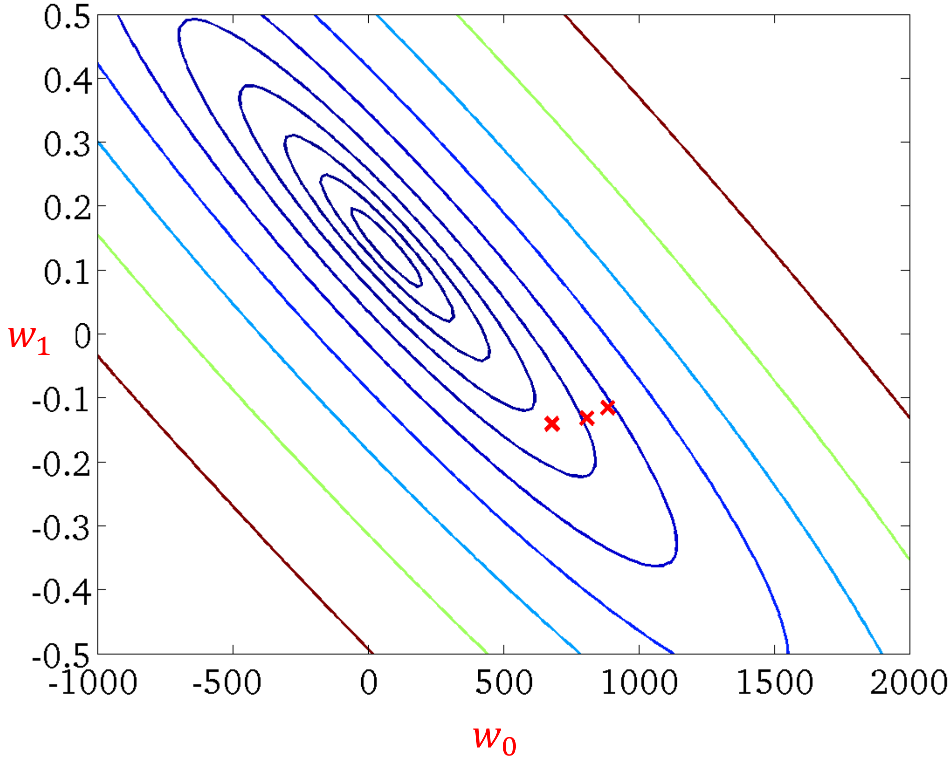
Linear Regression



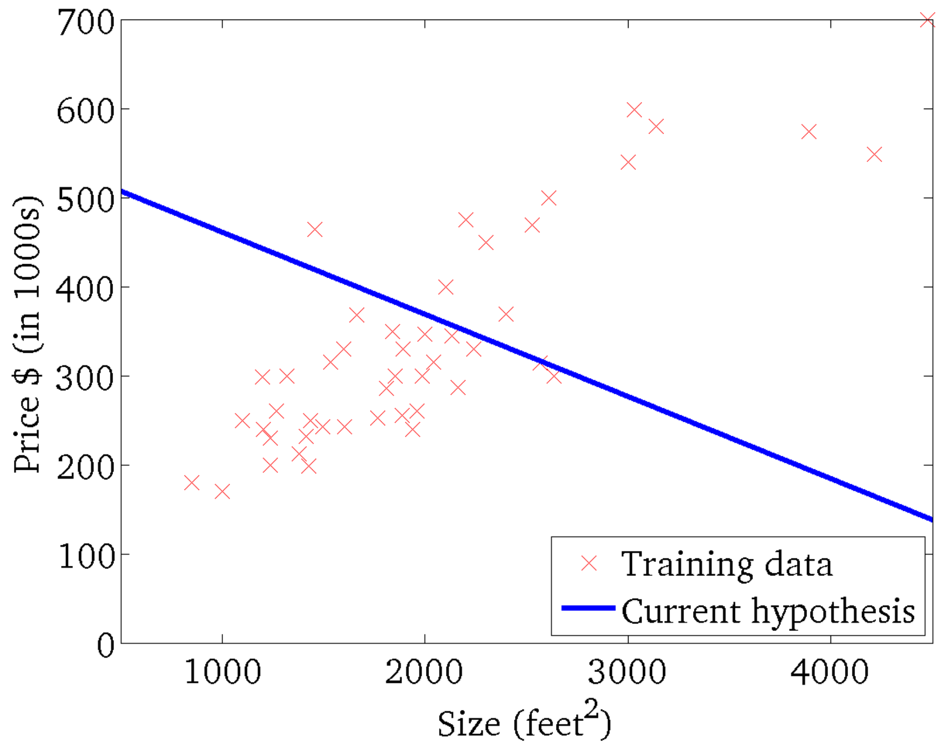


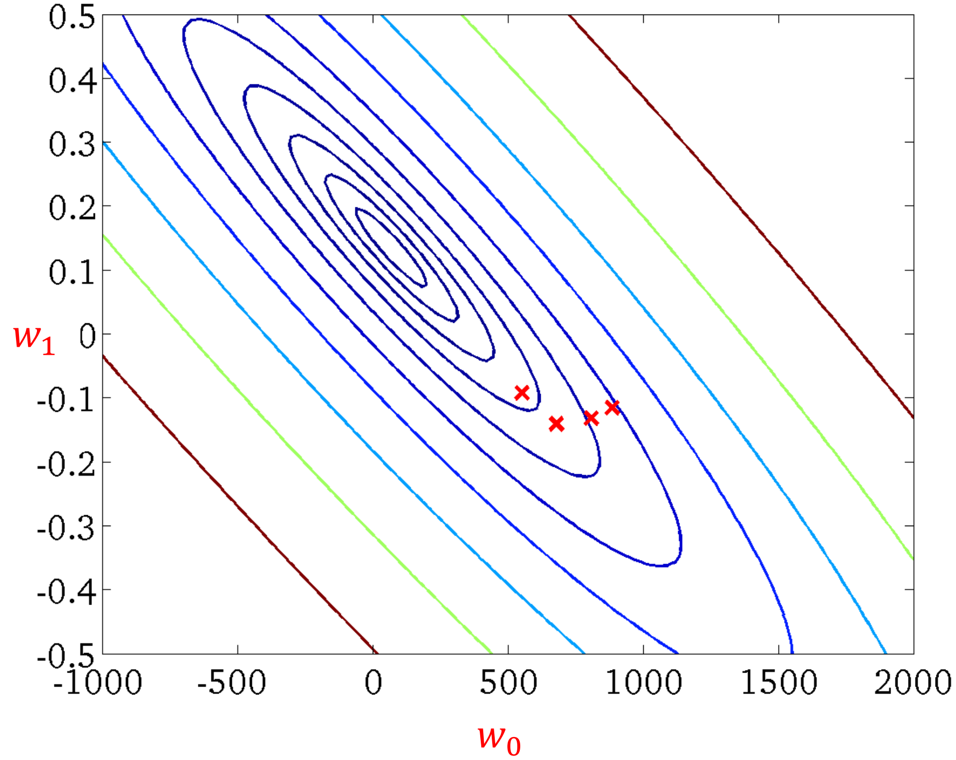
Linear Regression



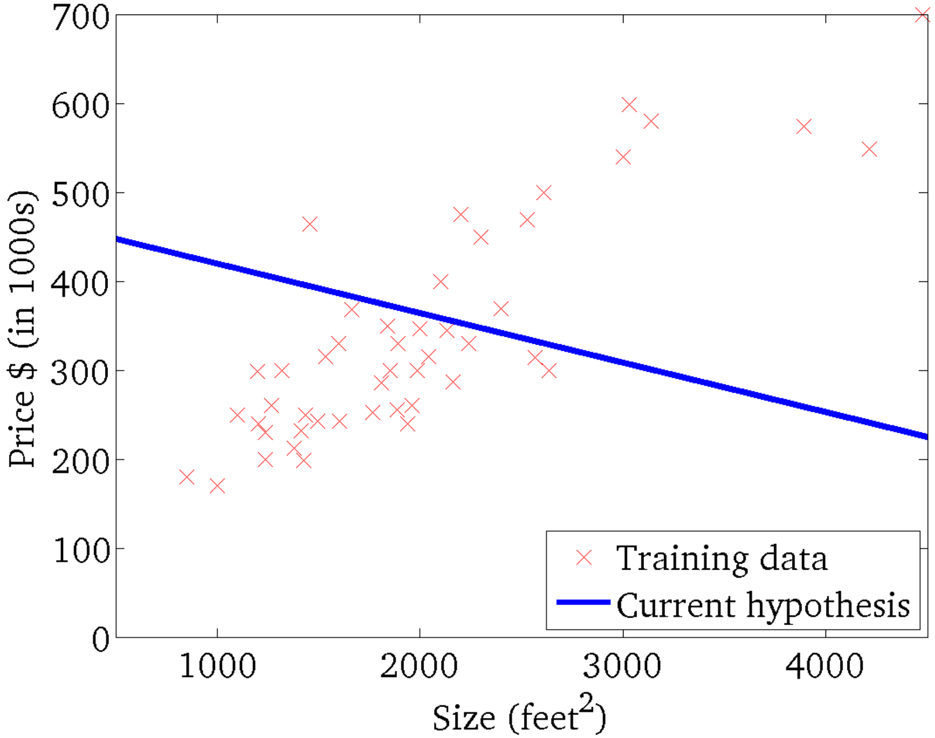


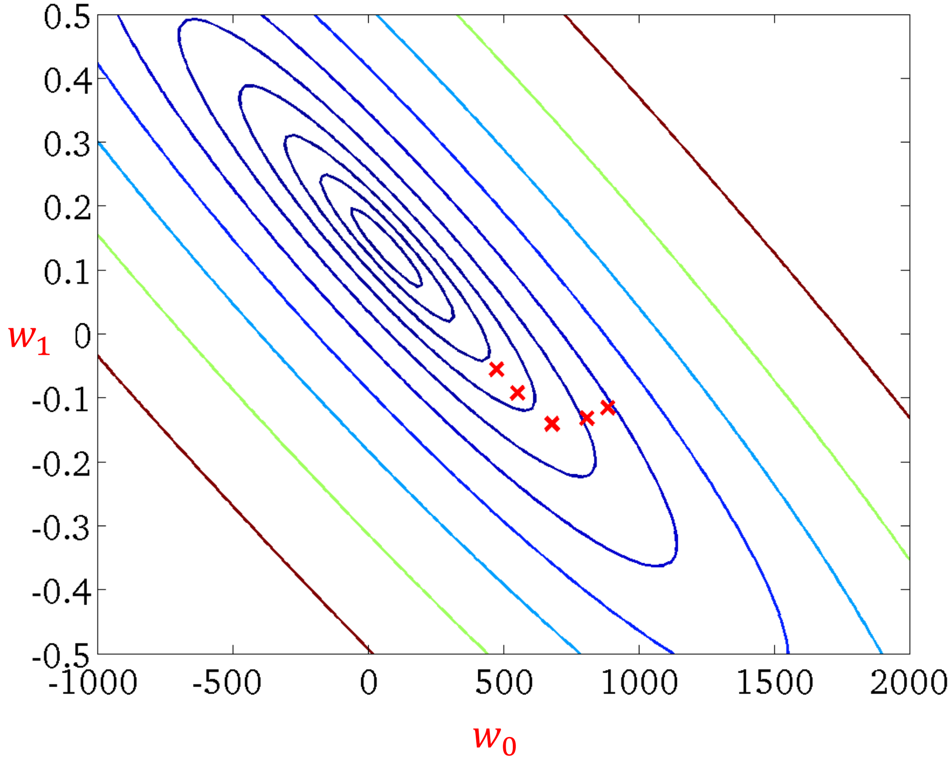
Linear Regression



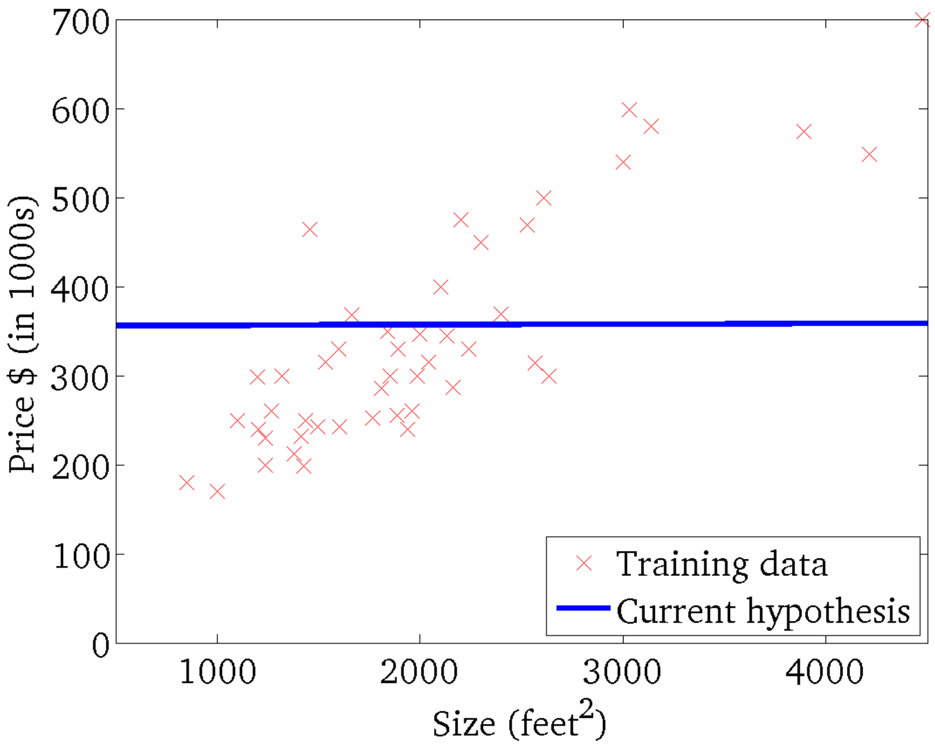


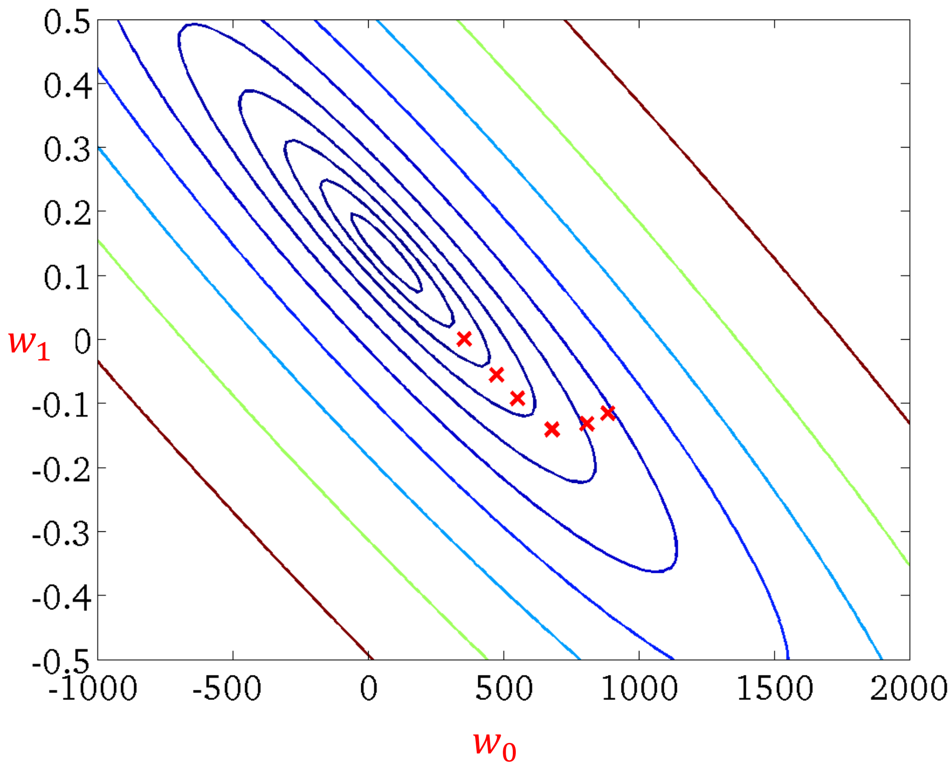
Linear Regression



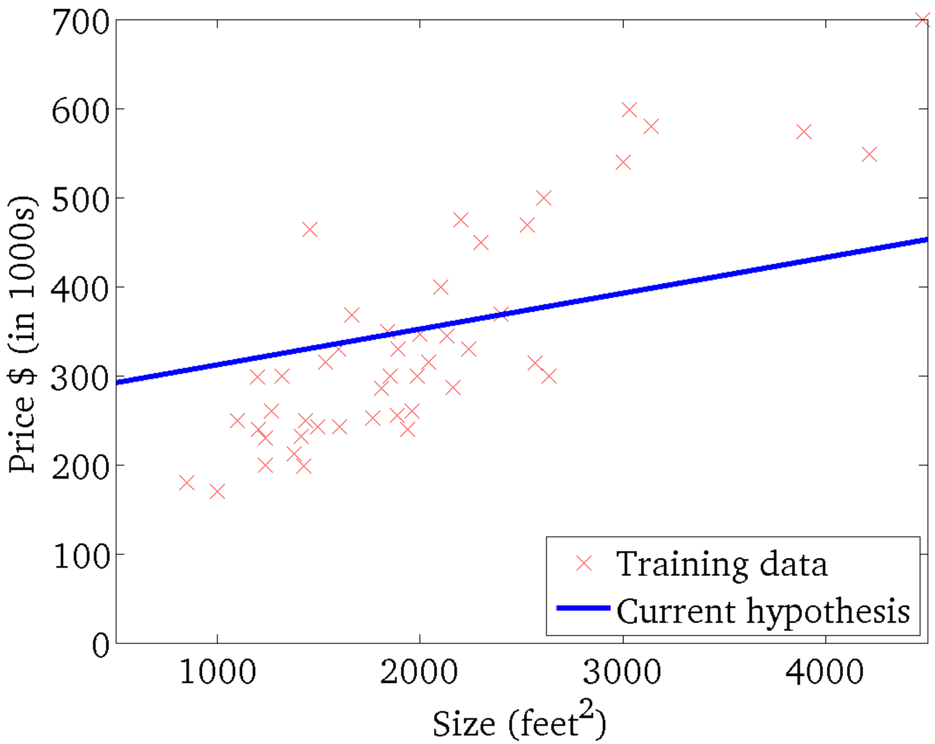


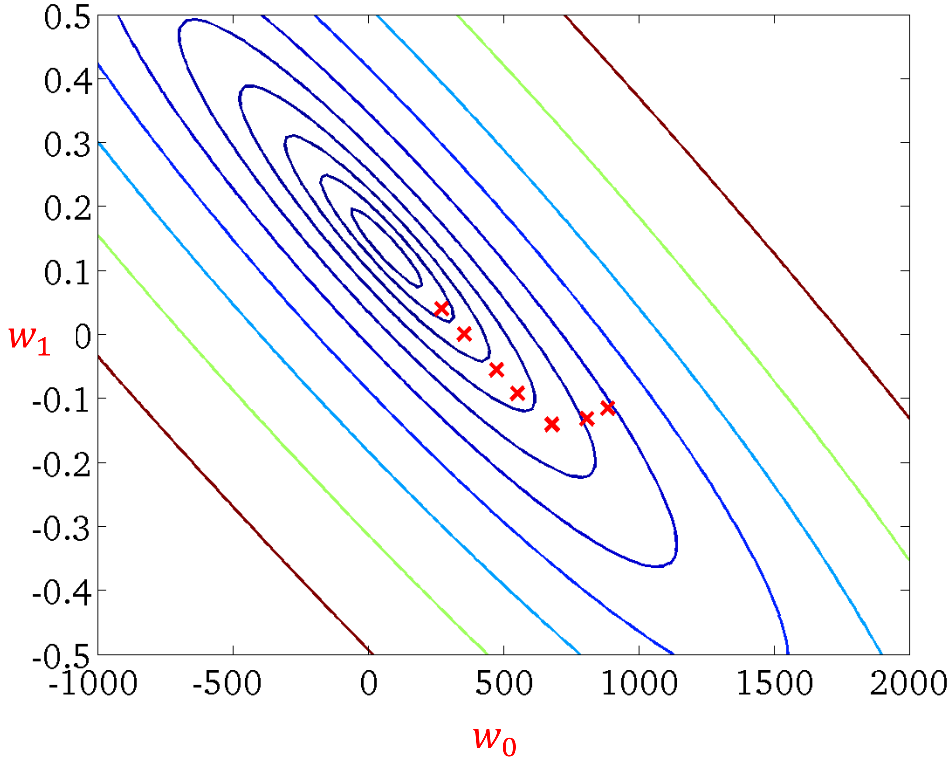
Linear Regression



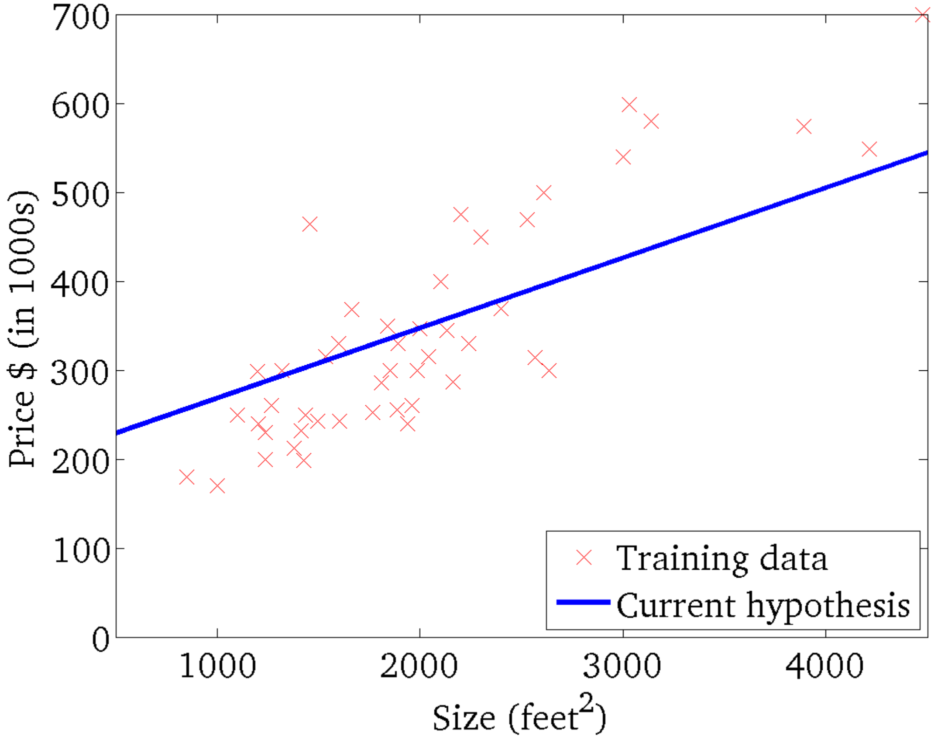


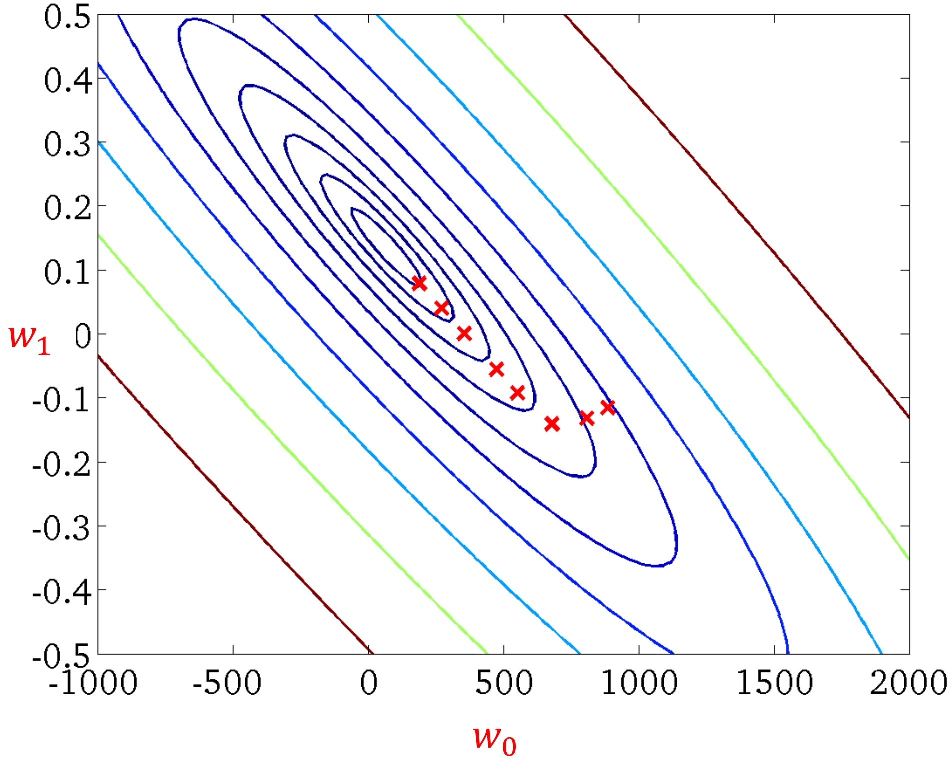
Linear Regression



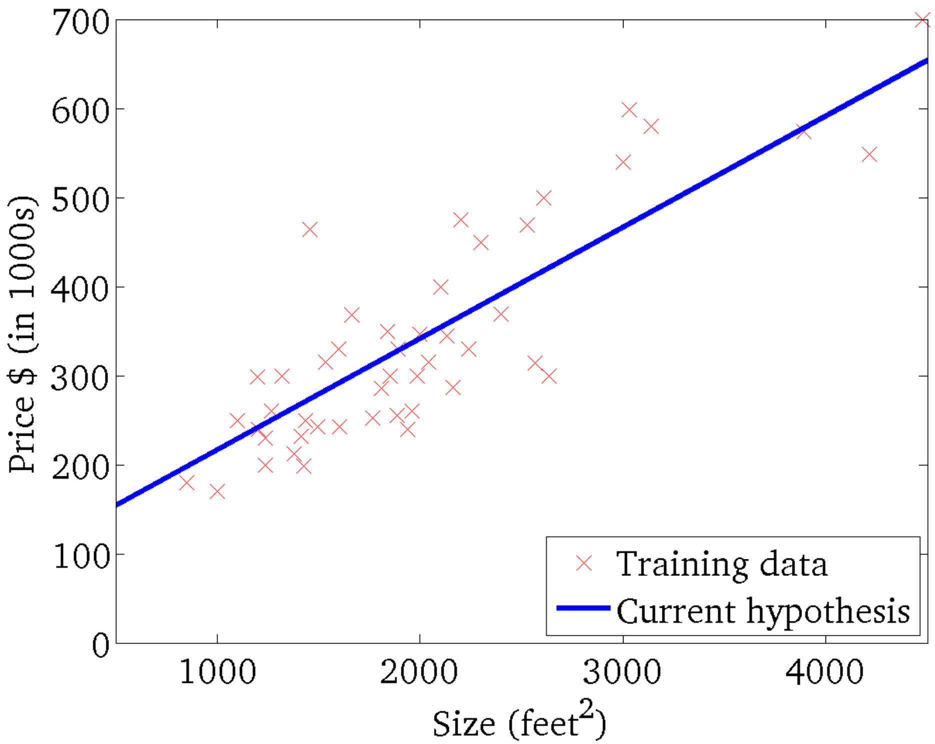


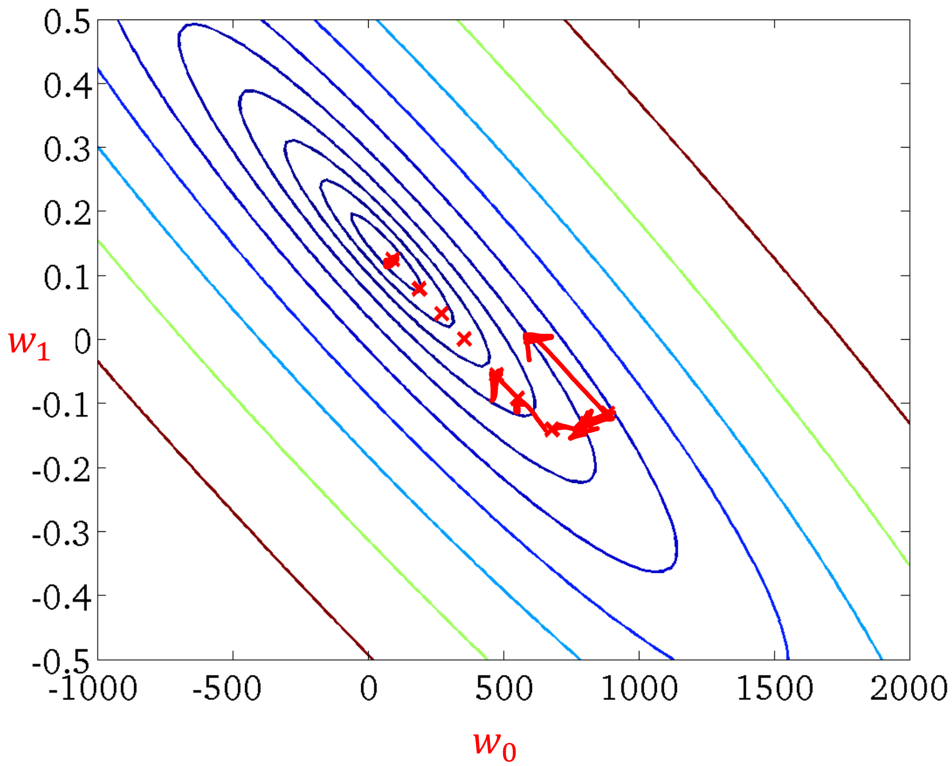
Linear Regression





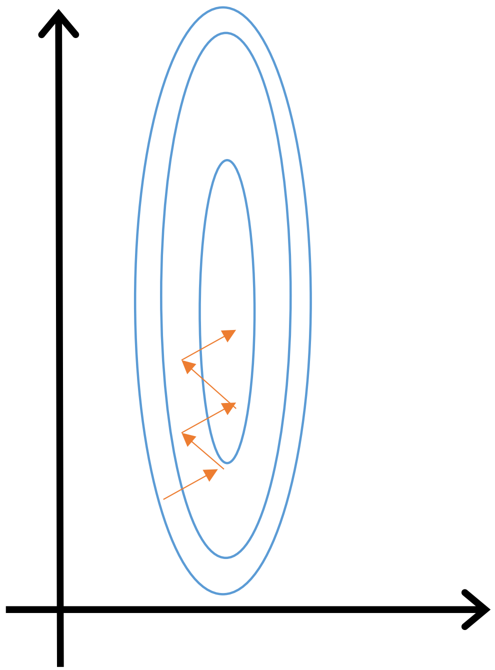
Linear Regression





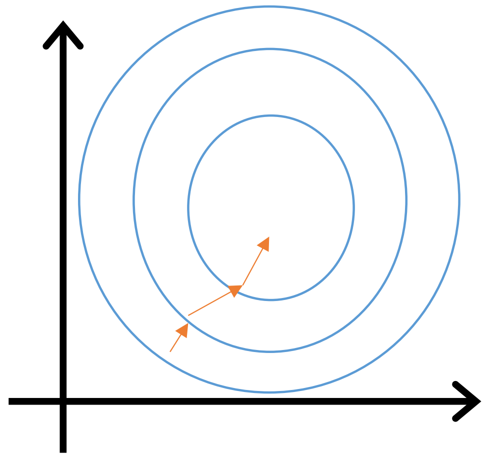
Feature Scaling

Problem: features are not on a similar scale



Solution: Mean Normalization

$$\frac{x_j - \mu_j}{\sigma_j} \qquad -1 \leq x_j \leq 1$$

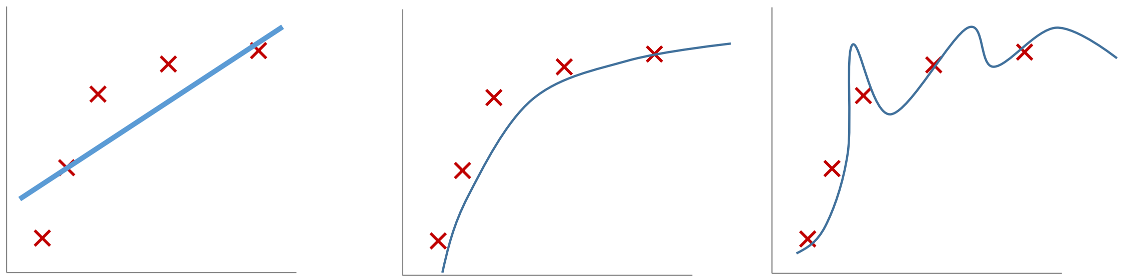


Overfitting vs. Underfitting

Underfitting
High Bias
Low variance

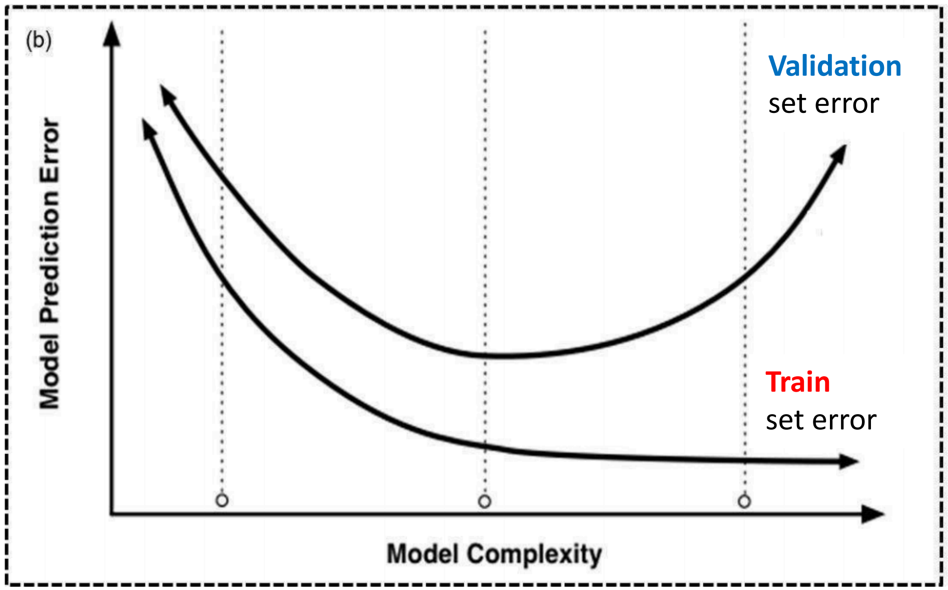
Trade-off

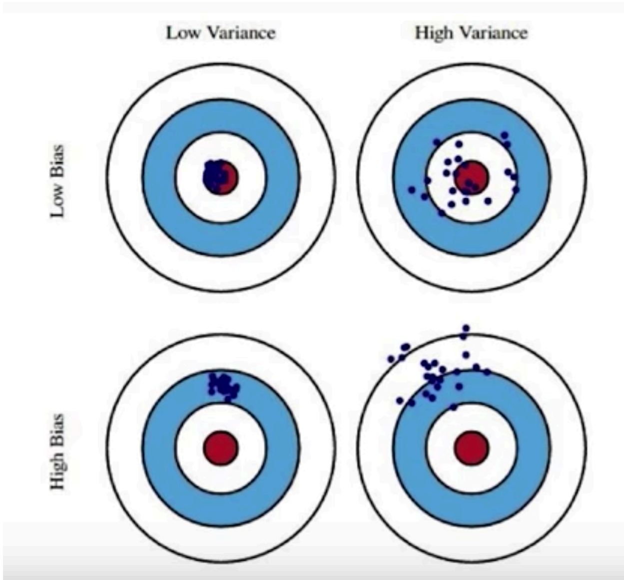
Overfitting
Low Bias
High Variance



Bias-Variance Tradeoff

Expected error (Human or Bayes optimal): **0%**	**Train** set error	1%	15%	15%	0.5%
	Validation set error	11%	16%	30%	1%
		High variance	High bias	High bias High variance	Low bias Low variance

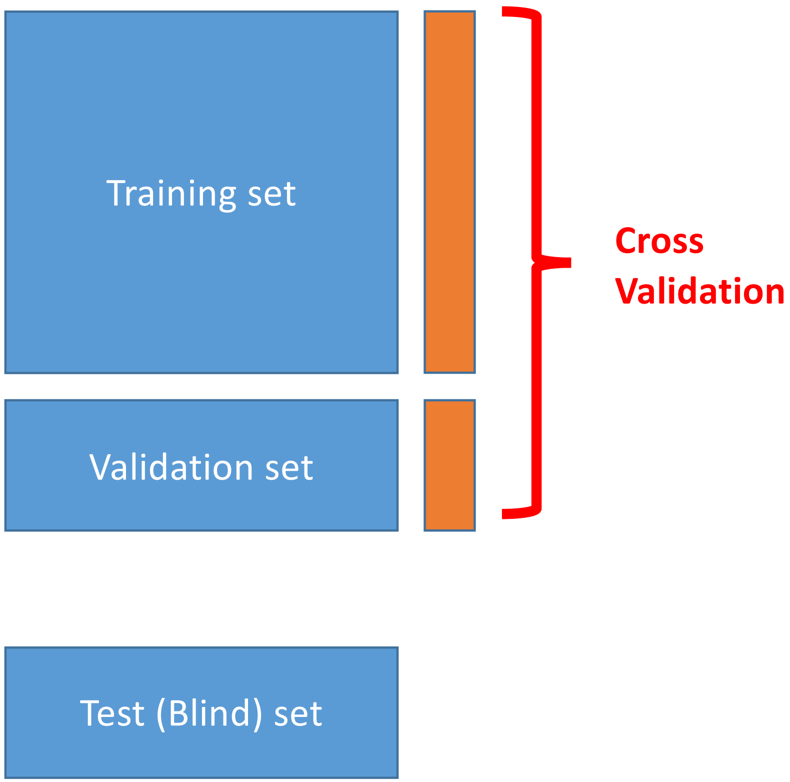


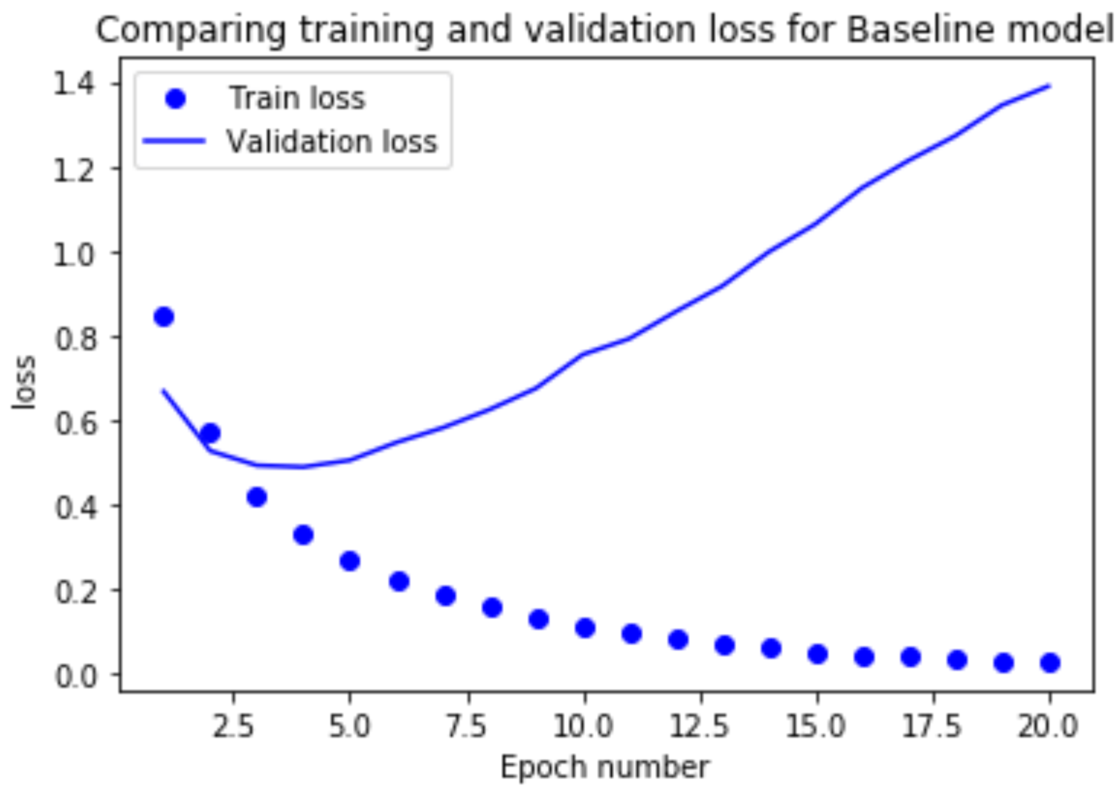


Address Overfitting

- Detect Overfitting
  - Performance analysis (Cross-Validation)
- Avoid Overfitting
  - Fewer features (Feature Selection, Dimensionality Reduction)
  - Constraint the model (Regularization : minimum loss $\mathrm{L}(w) + \lambda\, ww^T$)
  - Model Selection (Tune hyper-parameters using Grid Search)

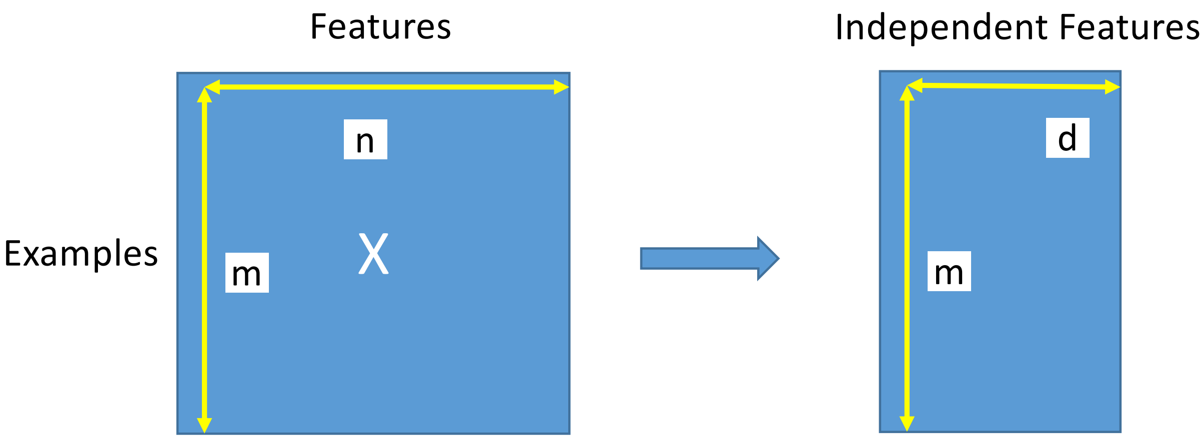
Performance Analysis

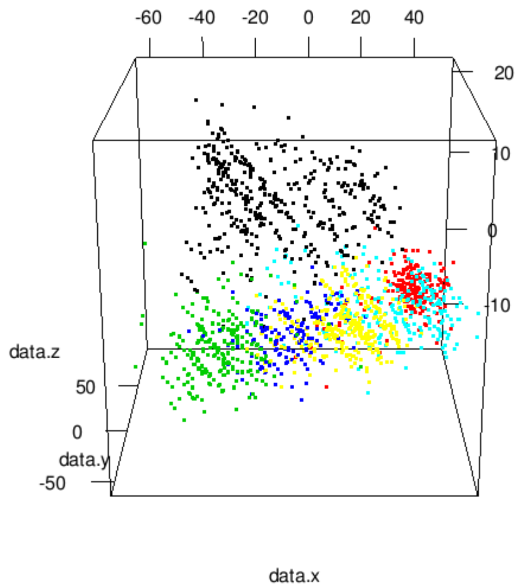




Dimensionality Reduction

- Reducing the number of features





Regularization: Ridge Regression (L_2 norm)

Linear Regression

$$\hat{y} = w_0 + w_1 x_1 + w_2 x_2$$

if λ is set to be extremely large, then w_j have to be very small.

→Algorithm results in underfitting

→Gradient Descent will fail to converge

$$\underset{w}{\text{minimize}} \quad L(w)$$

L_2 norm

$$\underset{w}{\text{minimize}} \quad L(w) + \lambda \boxed{\sum_{j=1}^{n} w_j^2}$$

Do not regularize for j=0

Training $w_0 = 1, w_1 = 2, w_2 = 0.01$

Test $w_0 = 1, w_1 = 2, w_2 = 0$

Regularization: LASSO Regression (L_1 norm)

Linear Regression

$$\hat{y} = w_0 + w_1 x_1 + w_2 x_2$$

- LASSO: Least Absolute Shrinkage and Selection Operator
- LASSO is not differentiable for every value of w, but performs best feature selection

$$\underset{w}{\text{minimize}} \quad L(w)$$

L_1 norm

$$\underset{w}{\text{minimize}} \; L(w) + \lambda \boxed{\sum_{j=1}^{n} |w_j|}$$

Do not regularize for j=0

Training $\quad w_0 = 1, w_1 = 2, w_2 = 0$

Test $\quad w_0 = 1, w_1 = 2, w_2 = 0$

Model Selection

- Hyper-Parameters Tuning
  - λ : regularization hyper-parameter
  - d: degree of polynomial
  - Alpha: learning rate
  - Etc.
- Grid Search
- Randomized search

Supervised Learning

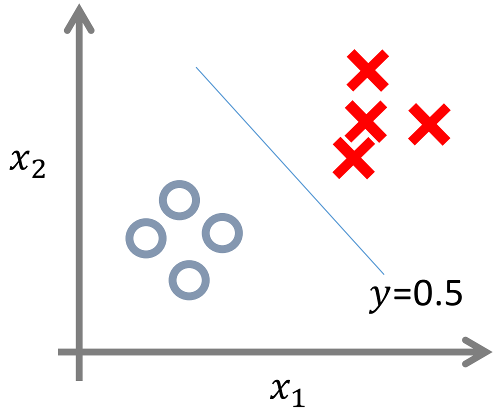
- Linear Regression
- **Logistic Regression**
- Support Vector Machines
- Trees (Decision and Regression)
- Random Forests
- Boosting
- Artificial Neural Networks

Logistic Regression

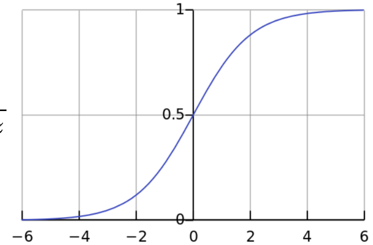
- The output y is discrete
- Classify X with a line $\hat{y} = \boldsymbol{g}(w_0 + w_1 x_1 + w_2 x_2)$
- The best line is the one with minimum loss

$$\mathrm{L}(w) = \frac{1}{m}\sum_{i=1}^{m}\left[y^{(i)}\log(\hat{y}^{(i)}) + (1 - y^{(i)})\log(1 - \hat{y}^{(i)})\right]$$

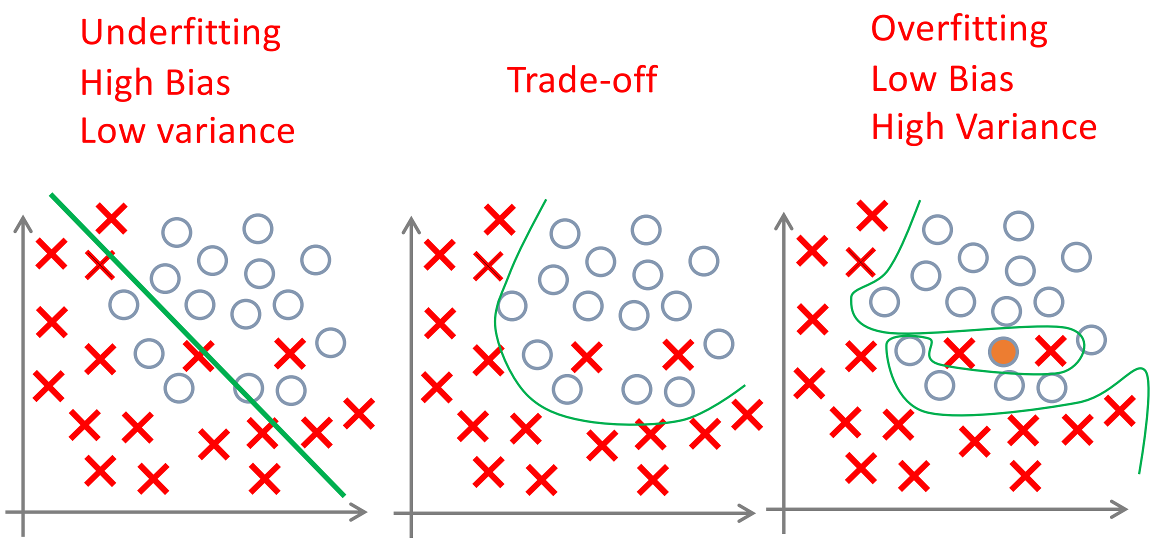
- Solved with gradient descent



$$g(z) = \frac{1}{1 + e^{-z}}$$



Overfitting vs. Underfitting



Linear and Logistic Regression

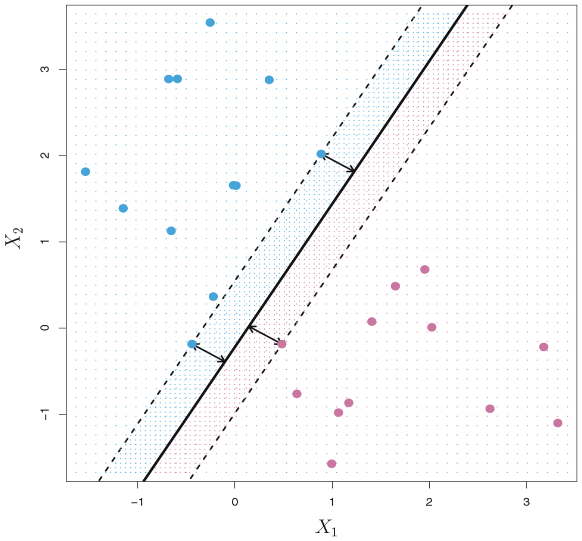
- Hyper-Parameters Tuning
  - λ : regularization hyper-parameter
  - d: degree of polynomial

Supervised Learning

- Linear Regression
- Logistic Regression
- **Support Vector Machines**
- Trees (Decision and Regression)
- Random Forests
- Boosting
- Artificial Neural Networks

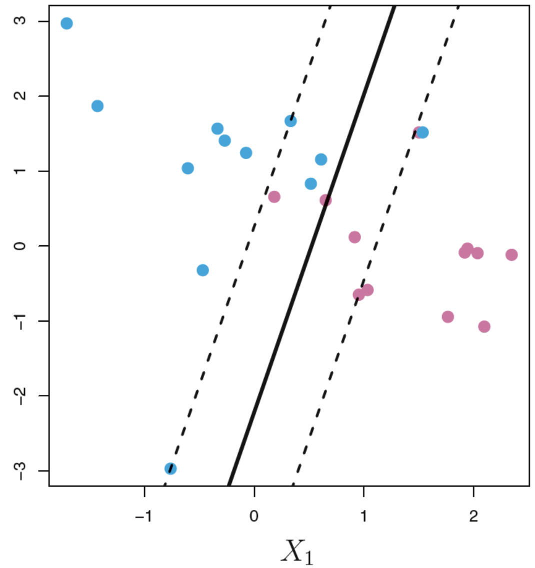
Support Vector Machines

Maximum Margin Classifier



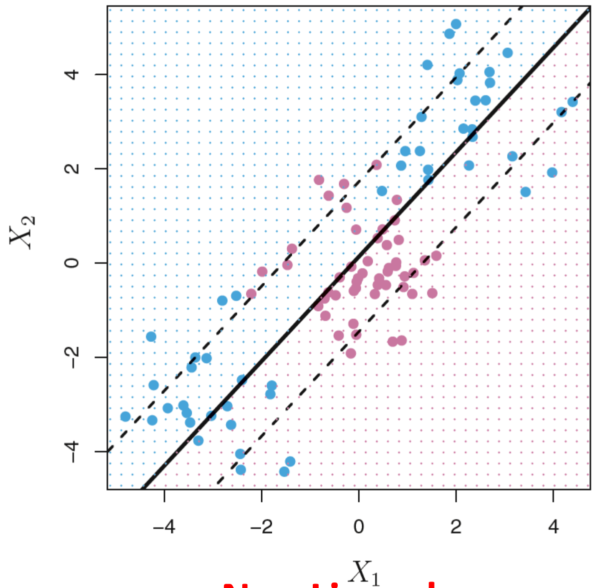
Linearly separable

Soft Margin Classifier



Slightly Linearly separable

Support Vector Machines



Non Linearly separable

Maximal Margin Classifier

- 2D: line

$$w_0 + w_1 x_1 + w_2 x_2 = 0$$

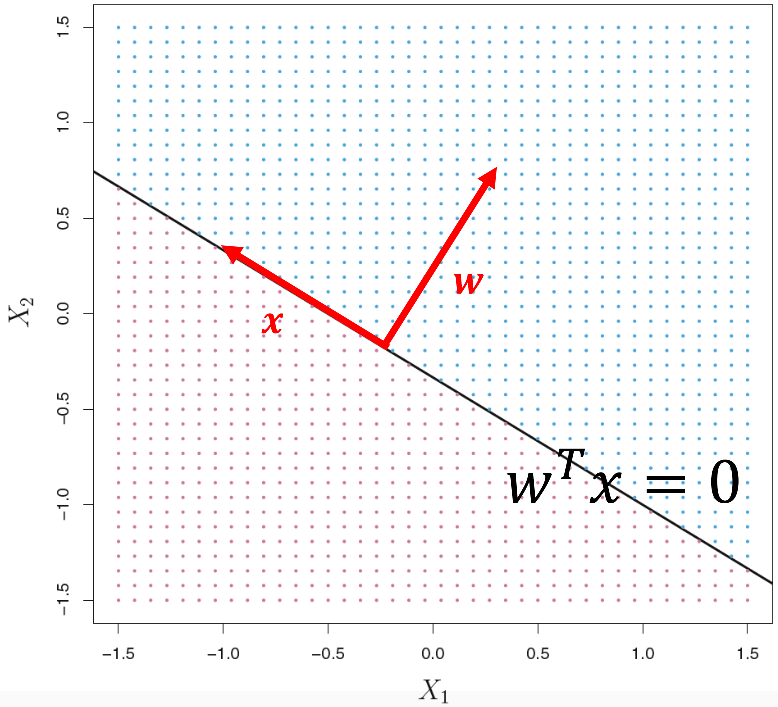
- 3D: plan

$$w_0 + w_1 x_1 + w_2 x_2 + w_3 x_3 = 0$$

- nD: Hyperplane

$$w_0 + w_1 x_1 + w_2 x_2 + \cdots + w_n x_n = 0$$

$$w^T x = 0$$



Maximal Margin Classifier

A separating hyperplane has the properties that:
for all i = 1, … m.

$$w^T x^{(i)} > 0 \;\; if \;\; y^{(i)} = +1$$
$$w^T x^{(i)} < 0 \;\; if \;\; y^{(i)} = -1$$

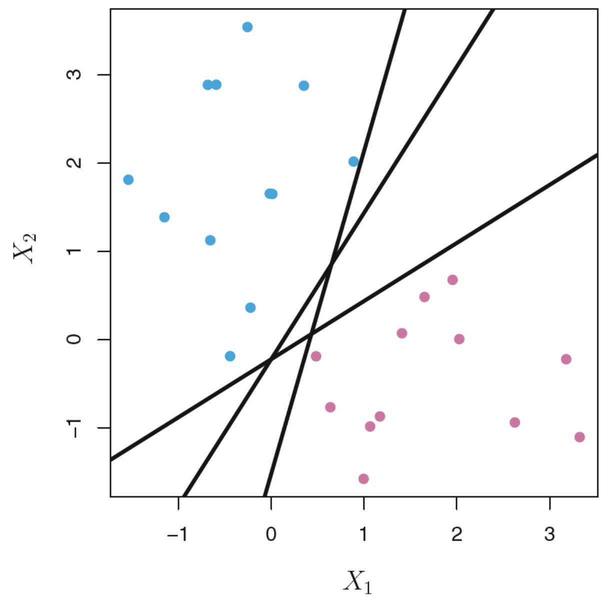
Equivalently

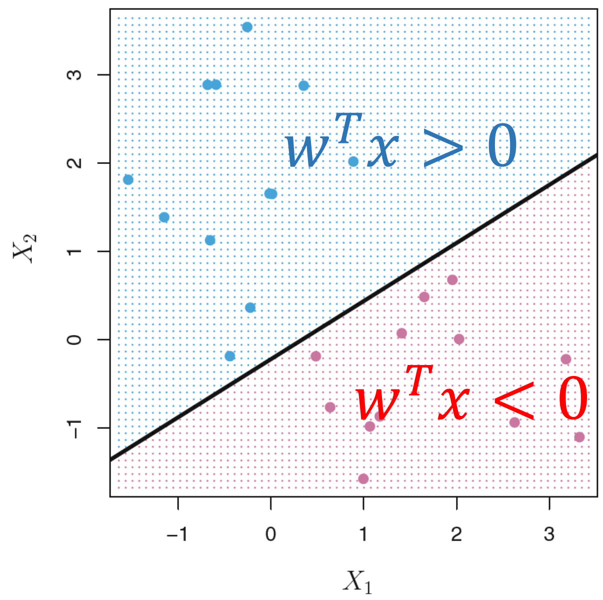
$$y^{(i)}(w^T x^{(i)}) > 0$$

$y^{(i)}$={1,-1}

2 classes

$w \begin{bmatrix} w_0 \\ w_1 \\ \dots \\ w_n \end{bmatrix}$ $\quad x^{(i)} \begin{bmatrix} x_0^{(i)} \\ x_1^{(i)} \\ \dots \\ x_n^{(i)} \end{bmatrix}$





Many hyperplanes
Which is the best?

Maximal Margin Classifier

The optimization problem

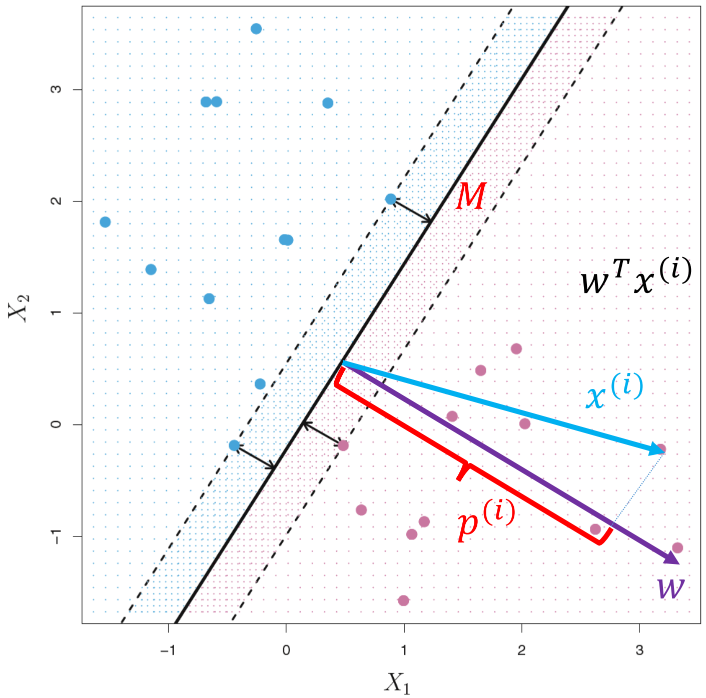
$$\underset{w}{\text{maximize}}\, M$$

Subject to: $\|w\| = \sum_{j=1}^{n} w_j^2 = 1,$

$$y^{(i)}(w^T x^{(i)}) \geq M, \forall\, i = 1 \ldots m$$

These equations ensure that each example is on the correct side of the hyperplane and at least a distance M from it.

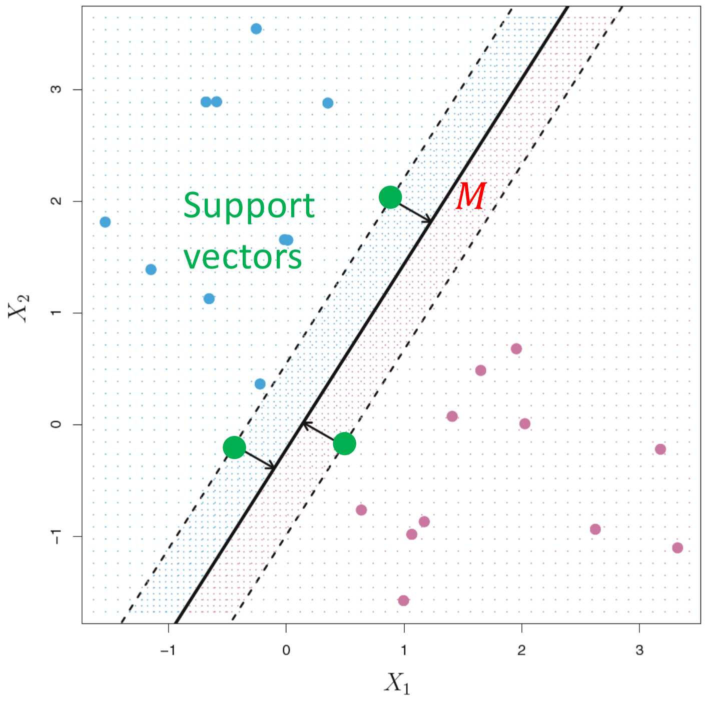
Intuitively, pick the hyperplane with Maximum margin



$w^T x^{(i)} = p^{(i)} * \|w\|$

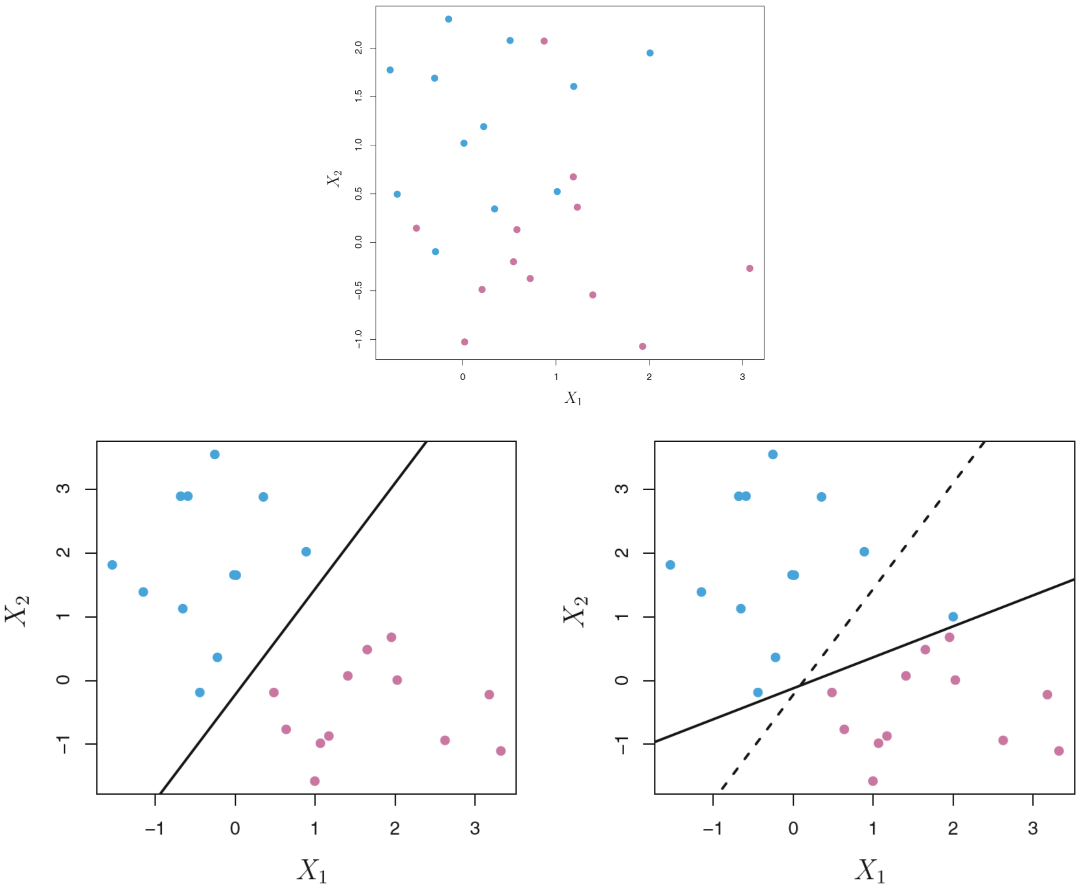
Maximal Margin Classifier

- Support vectors: examples supporting the margin (equidistant from the maximal margin hyperplane)
- If Support vectors were moved slightly, then the maximal margin hyperplane would move as well.
- The non-support vectors have no impact on the hyperplane !



Soft Margin Classifier

- The Non-linearly separable case
- Soft margin: can be violated by some of the training examples.
- It could be better to misclassify a few training examples in order to do a better job in classifying the remaining ones.



Soft Margin Classifier

The optimization problem

$$\underset{w,\epsilon}{\text{maximize}}\, M$$

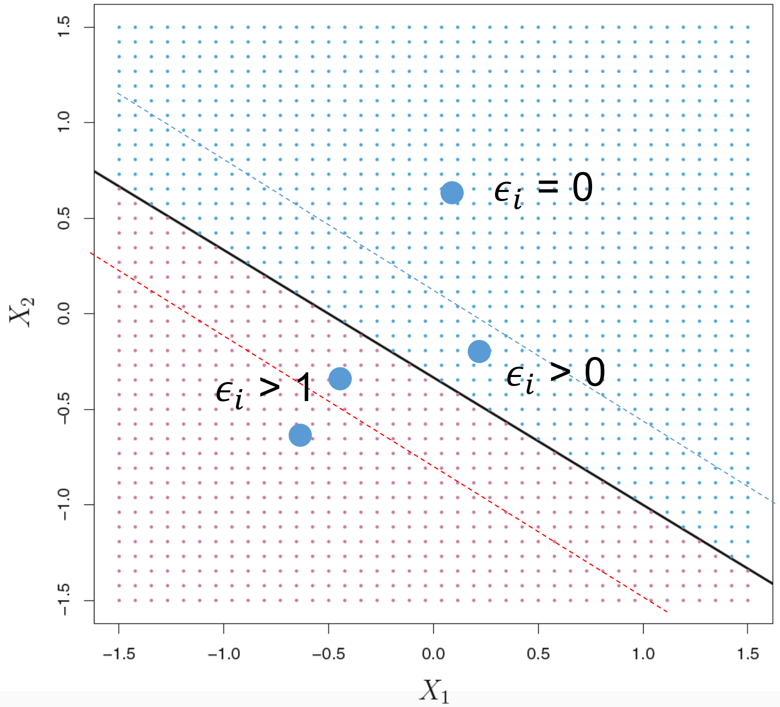
Subject to: $\|w\| = \sum_{j=1}^{n} w_j^2 = 1,$

$$y^{(i)}(w^T x^{(i)}) \geq M(1-\epsilon_i), \forall\, i = 1 \dots m$$

$$\epsilon_i \geq 0, \quad \|\epsilon\| = \sum_{i=1}^{m} \epsilon_i^2 \leq C,$$

slack variables

Hyper parameter ≥ 0



- If $\epsilon_i = 0$, then example i is on the correct side of the margin,
- If $\epsilon_i > 0$, then example i is on the wrong side of the margin.
- If $\epsilon_i > 1$, then it is on the wrong side of the hyperplane.

Soft Margin Classifier

The optimization problem

$$\underset{w,\epsilon}{\text{maximize}}\, M$$

Subject to: $\|w\| = \sum_{j=1}^{n} w_j^2 = 1,$

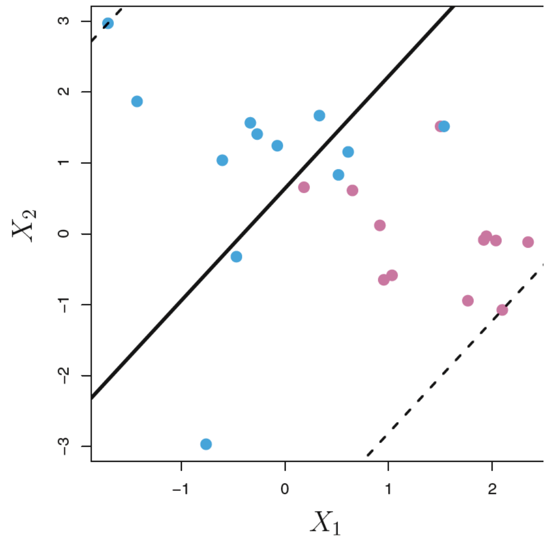
$$y^{(i)}(w^T x^{(i)}) \geq M(1 - \epsilon_i), \forall\, i = 1 \ldots m$$

$$\epsilon_i \geq 0, \quad \|\epsilon\| = \sum_{i=1}^{m} \epsilon_i^2 \leq C,$$

slack variables

Hyper parameter ≥ 0

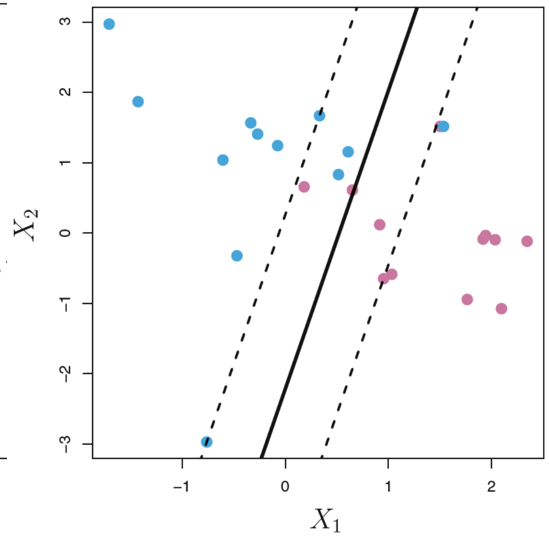
C is large



High tolerance for examples being on the wrong side of the margin ($\epsilon_i > 0$)

Underfitting:
(high bias, low variance)

C is small



Low tolerance for examples being on the wrong side of the margin ($\epsilon_i > 0$)

Overfitting:
(low bias, high variance)

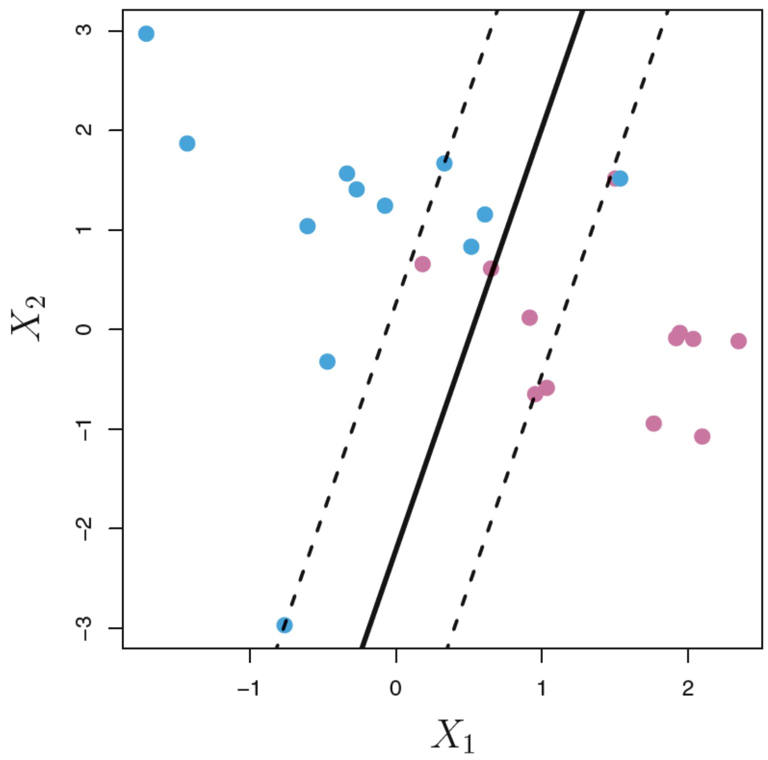
Soft Margin Classifier

- It turns out that, using quadratic programming, the solution is

$$w = \sum_{i=1}^{m} \alpha_i y^{(i)} x^{(i)}$$

and $w_0 = y^{(k)} - w^T x^{(k)}$ for any k where $C > \alpha_i > 0$

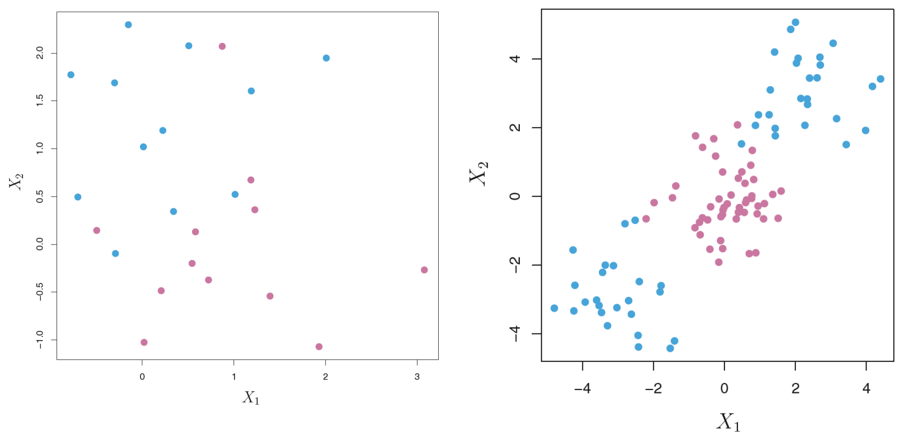
- α_i are Lagrange multipliers!
- Then, for a new $x^{(i)}$, $\hat{y}^{(i)} = sign(w^T x^{(i)})$
- $x^{(i)}$ where $\alpha_i > 0$ are called Support Vectors
- They are examples that lie directly on the margin, or on the wrong side of the margin for their class.
- Only those examples can affect the hyperplane, and hence the support vector classifier f.



Support Vector Machines

- Highly non-linearly separable case
- Use feature mapping $\varphi(x)$ to address this non-linearity.
- Example: high order polynomials

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{bmatrix} -> \varphi(x) = \begin{bmatrix} x_1 \\ x_2 \\ \dots \\ x_N \end{bmatrix}$$



N is the number of features in the new space

Support Vector Machines

The optimization problem

$$\underset{w,\epsilon}{\text{maximize}}\, M$$

Subject to: $\|w\| = \sum_{j=1}^{N} w_j^2 = 1,$

$$y^{(i)}(w^T \varphi(x^{(i)})) \geq M(1 - \epsilon_i),$$
$$\forall\ i = 1 \ldots m$$

$$\epsilon_i \geq 0, \quad \|\epsilon\| = \sum_{i=1}^{m} \epsilon_i^2 \leq C,$$

If S is the set of support vectors, then:

$$f(x) = w_0 + \sum_{i \epsilon S} \alpha_i \varphi(x)^T \varphi(x^{(i)})$$

N could be very large → the computations would become unmanageable!

→ Use Kernel Trick

Support Vector Machines

- Non linearly separable data become separable in higher space!
- So, first go to higher feature space $x -> \varphi(x)$
- To solve SVM, you have to compute the Kernel $K(u, v) = \varphi(u)^T \varphi(v)$
  - But: very costly !!!
- Kernel Trick: If you chose φ carefully, you end up getting K, without calculating the very costly dot product $\varphi(u)^T \varphi(v)$
- The solution: $w = \sum_{i=1}^{m} \alpha_i y^{(i)} \varphi\left(x^{(i)}\right)$

and $w_0 = y^{(k)} - w^T \varphi\left(x^{(k)}\right)$ for any k where $C > \alpha_k > 0$

- Instead, compute: $w\ \varphi(x) = \sum_{i=1}^{m} \alpha_i y^{(i)} K\left(x, x^{(i)}\right)$

Support Vector Machines

- Exemple
  - Assume each example $x = [x_1, x_2]^T$ is mapped to the quadratic feature space $\varphi(x) = \left[x_1^2, x_2^2, \sqrt{2}x_1x_2, \sqrt{2}x_1, \sqrt{2}x_2, 1\right]^T$
  - We can then show that $K(x, x') = \varphi(x)^T \varphi(x') = (1 + x^T x')^2$
  - In this way, the computation in the higher dimensional space is performed implicitly in the original input space !

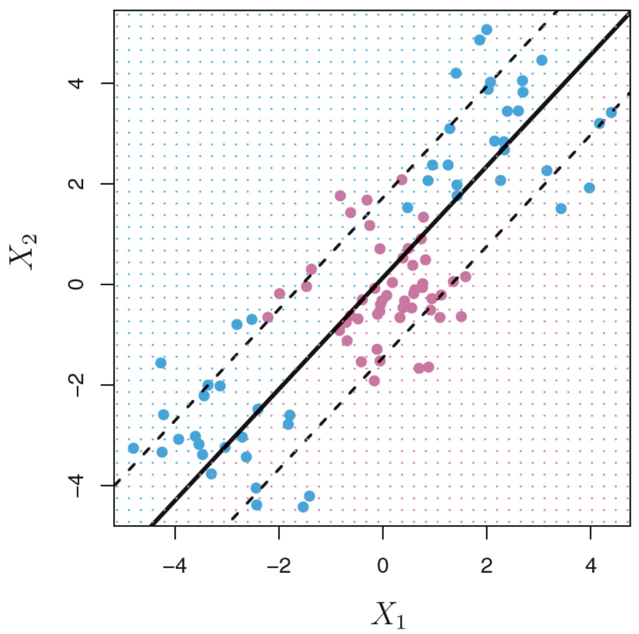
Support Vector Machines

- Kernel Examples
  - Linear Kernel $K(u, v) = u^T v$,
  - Polynomial Kernel: $K(u, v) = (c + u^T v)^d$,
  - Radial Basis Function (RBF) Kernel (Gaussian Kernel) :

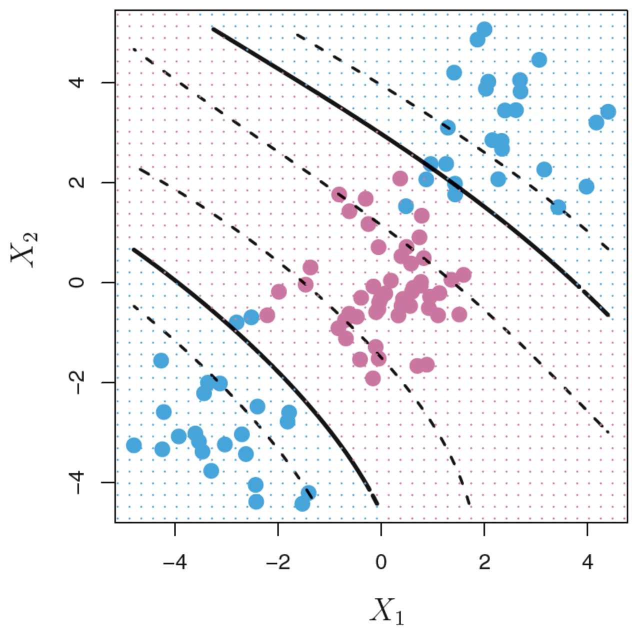
    $$K(u, v) = \exp(-\gamma \|u - v\|^2),$$ (infinite feature space!)
  - And many others: Sigmoid Kernel, String kernel, chi-square kernel, histogram intersection kernel, etc.

    (d, c and γ are hyper-parameters)
- Kernels need to satisfy technical conditions called "Mercer's conditions"

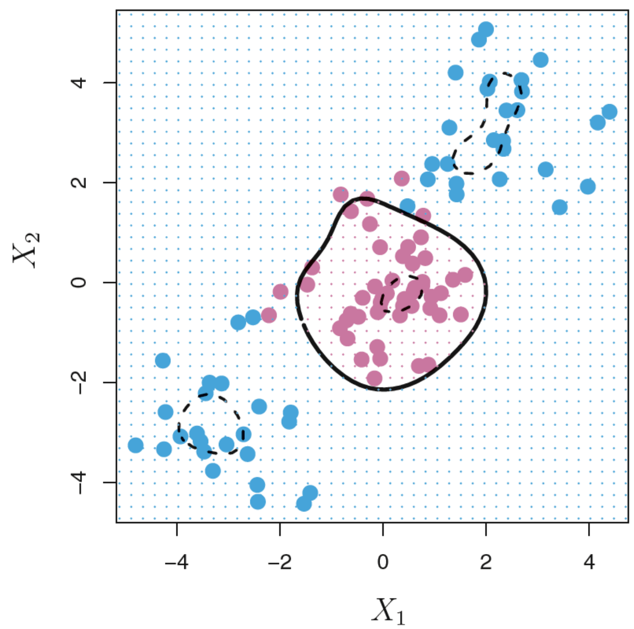
Support Vector Machines



Linear Kernel



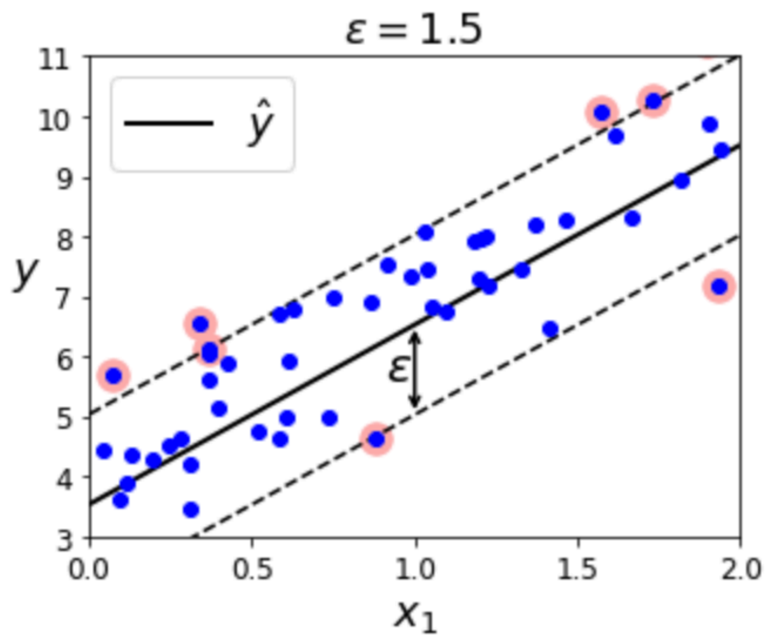
Polynomial Kernel
d=3



Radial Kernel
γ =0.1

Support Vector Machines

- Regression
  - Fit as many points as possible on the street while limiting margin violations.
  - The width of the street is controlled by a hyper-parameter ε



Support Vector Machines

- Hyper-Parameters Tuning
  - C, d: polynomial Kernel
  - γ: RBF kernel
  - ε: for regression
  - Etc.