

Data Mining & Machine Learning

CS37300

Purdue University

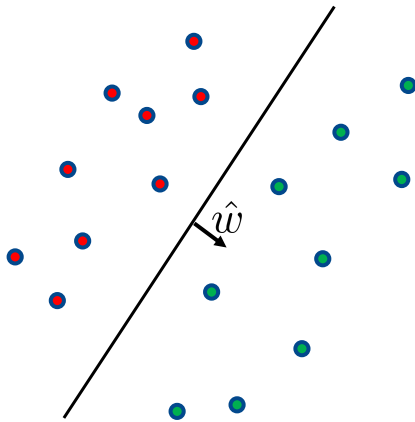
Sep 25, 2023

Today's topics

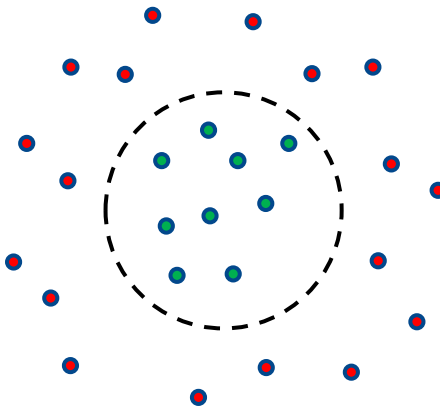
- Kernels and Kernel-SVM

Nonlinear Decision Boundaries

- Linear separators are simple



- But there are many scenarios that are separable, only non-linearly

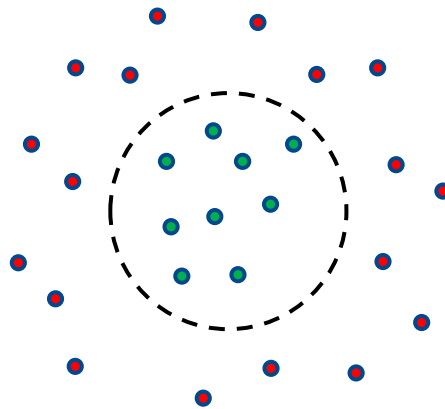


- We want to learn these with optimization based ML (SVM)

Learning Nonlinear Decision Boundaries

- We've already seen some nonlinear separators:
 - Decision Trees, KNN
- Question: How can we learn this example using SVM?

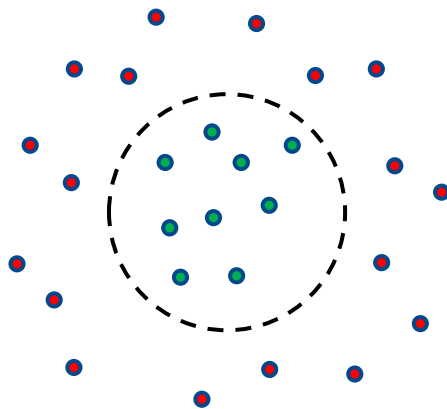
Example:



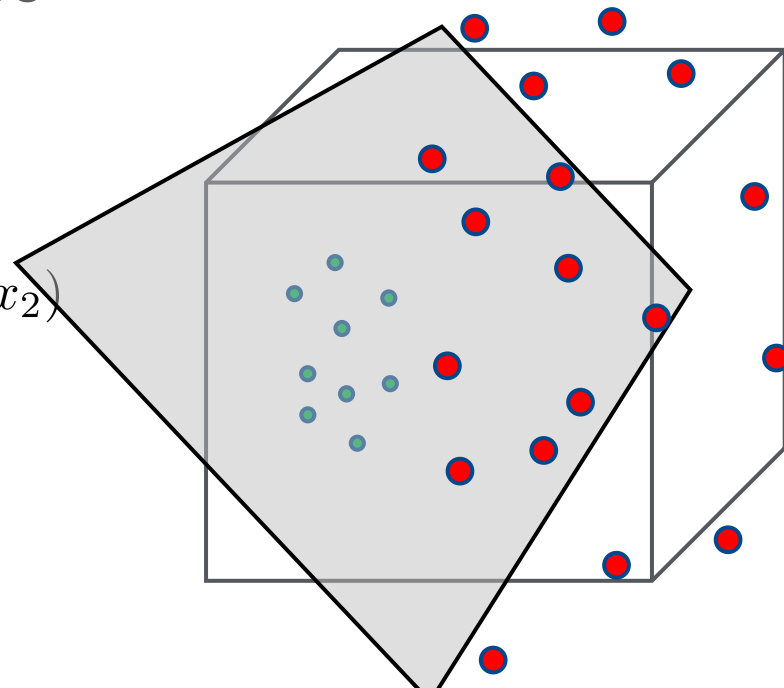
Learning Nonlinear Decision Boundaries

- We've already seen some nonlinear separators:
 - Decision Trees, KNN
- Question: How can we learn this example using SVM?
 - Map the examples into a higher-dimensional space and learn a linear separator in that space

Example:



Re-represent each $\underline{x} = (x_1, x_2)$
as 3-dimensional vector
 $\phi(\underline{x}) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$



Representing Nonlinear Decision Boundaries

- General strategy: consider a function: $\phi(x) \in \mathbb{R}^N$
 - N may be large, or even infinite
- Then learn a linear separator in the ϕ space:

$$\hat{h}(x) = \text{sign}(w^\top \phi(x)) , \quad \text{where } w \in \mathbb{R}^N$$

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$$\hat{h}(x) = \text{sign}(w^\top \phi(x)), \quad \text{where } w \in \mathbb{R}^N$$

$$\hat{w} = \underset{w \in \mathbb{R}^N : \|w\|=1}{\text{argmax}} \min_{1 \leq i \leq n} y_i (w^\top \phi(x_i))$$

Minimize $\|w\|^2$

subject to $y_i (w^\top \phi(x_i)) \geq 1, \forall i : 1 \leq i \leq n$

Representing Nonlinear Decision Boundaries

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- Two concerns:
 1. Computation and memory required to represent $\phi(x)$, w
 2. Dimension of linear separators on \mathbb{R}^N is N .
 - Concerns about overfitting

Today's lecture is mostly about the first concern.
Solution: Kernels

The Dual Form of the SVM Optimization Problem

$$\hat{w} = \operatorname{argmax}_{w: \|w\|=1} \min_{1 \leq i \leq n} y_i (w^\top x_i)$$

- Recall: The SVM **classifier** is the unique solution to a **quadratic program**:

$$\begin{array}{ll} \text{Minimize} & \|w\|^2 \\ \text{subject to} & y_i (w^\top x_i) \geq 1, \quad \forall i : 1 \leq i \leq n \end{array}$$

- We can re-express this in Lagrangian dual form:

$$\hat{w} = \sum_{i=1}^n \alpha_i y_i x_i$$

where $\alpha_1, \dots, \alpha_n$ are solutions to:

$$\begin{array}{ll} \text{Maximize} & \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n y_i y_j \alpha_i \alpha_j x_i^\top x_j \\ \text{subject to} & \alpha_i \geq 0, \quad \forall i : 1 \leq i \leq n \\ & \sum_{i=1}^n \alpha_i y_i = 0 \end{array}$$

SVM with high-dim mapping

- We could use a mapping ϕ to get a non-linear separator:

$$\hat{w} = \sum_{i=1}^n \alpha_i y_i \phi(\mathbf{x}_i)$$

where $\alpha_1, \dots, \alpha_n$ are solutions to:

$$\text{Maximize} \quad \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n y_i y_j \alpha_i \alpha_j \phi(\mathbf{x}_i)^\top \phi(\mathbf{x}_j)$$

$$\text{subject to} \quad \alpha_i \geq 0, \quad \forall i : 1 \leq i \leq n$$

$$\sum_{i=1}^n \alpha_i y_i = 0$$

- Notice training only uses ϕ when computing **inner product** $\phi(x_i)^\top \phi(x_j)$
- Instead of starting by defining ϕ , we could start by defining a function **$K(\mathbf{x}_i, \mathbf{x}_j)$** that computes an inner product, without computing ϕ :
$$K(x_i, x_j) = \phi(x_i)^\top \phi(x_j)$$
- **Kernel**: way to compute inner products without computing $\phi(\mathbf{x})$!

SVM with high-dim mapping

- We could use a mapping ϕ to get a non-linear separator:

$$\hat{w} = \sum_{i=1}^n \alpha_i y_i \phi(x_i)$$

where $\alpha_1, \dots, \alpha_n$ are solutions to:

$$\text{Maximize} \quad \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n y_i y_j \alpha_i \alpha_j \phi(x_i)^\top \phi(x_j)$$

subject to $\alpha_i \geq 0, \forall i : 1 \leq i \leq n$

$$\sum_{i=1}^n \alpha_i y_i = 0$$

- Notice training only uses ϕ when computing inner product

$$\phi(x_i)^\top \phi(x_j)$$

- And the classifier also uses an inner product (no need to compute w)

$$h_{\hat{w}}(x) = \text{sign}(\hat{w}^\top \phi(x)) = \text{sign} \left(\left(\sum_{i=1}^n \alpha_i y_i \phi(x_i) \right)^\top \phi(x) \right) = \text{sign} \left(\sum_{i=1}^n \alpha_i y_i \phi(x_i)^\top \phi(x) \right)$$

- Replace all of these with

$$K(x_i, x) = \phi(x_i)^\top \phi(x)$$

Kernel SVM

- Training time:

Solve for $\alpha_1, \dots, \alpha_n$:

$$\begin{aligned} \text{Maximize} \quad & \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i=1}^n \sum_{j=1}^n y_i y_j \alpha_i \alpha_j \mathbf{K}(\mathbf{x}_i, \mathbf{x}_j) \\ \text{subject to} \quad & \alpha_i \geq 0, \quad \forall i : 1 \leq i \leq n \\ & \sum_{i=1}^n \alpha_i y_i = 0 \end{aligned}$$

- Test time:
- Classify a new point \mathbf{x} with

$$\hat{h}(\mathbf{x}) = \text{sign} \left(\sum_{i=1}^n \alpha_i y_i \mathbf{K}(\mathbf{x}_i, \mathbf{x}) \right)$$

Kernels

Example:

Quadratic kernel: $K(\underline{u}, \underline{v}) = (\underline{u}^\top \underline{v} + 1)^2$

For $\underline{x} \in \mathbb{R}^d$, implicitly computes an inner product in $\frac{1}{2}d(d-1) + 2d + 1$ dim
e.g., For $\underline{x} \in \mathbb{R}^2$, implicitly defined ϕ :

$$\phi(\underline{x}) = \left[1, \sqrt{2}x_1, \sqrt{2}x_2, x_1^2, x_2^2, \sqrt{2}x_1x_2 \right]^\top$$

Check: $\phi(\underline{u})^\top \phi(\underline{v})$

$$\begin{aligned} &= \left[1, \sqrt{2}u_1, \sqrt{2}u_2, u_1^2, u_2^2, \sqrt{2}u_1u_2 \right] \left[1, \sqrt{2}v_1, \sqrt{2}v_2, v_1^2, v_2^2, \sqrt{2}v_1v_2 \right]^\top \\ &= 1 + 2u_1v_1 + 2u_2v_2 + u_1^2v_1^2 + u_2^2v_2^2 + 2u_1u_2v_1v_2 \\ &= (1 + u_1v_1 + u_2v_2)^2 = (1 + \underline{u}^\top \underline{v})^2 = K(\underline{u}, \underline{v}) \end{aligned}$$

The point is that we can compute this higher-dim inner product just by evaluating $K(\underline{u}, \underline{v})$: no need to compute ϕ

Kernels

- More Examples:

- Polynomial kernel: $K(\underline{u}, \underline{v}) = (\underline{u}^\top \underline{v} + 1)^p$

- Implicitly computes an inner product in $\sim d^p$ dimensions

- Gaussian kernel:

$$K(\underline{u}, \underline{v}) = e^{-\frac{\|\underline{u} - \underline{v}\|^2}{2\sigma^2}}$$

- Implicitly computes an inner product in **infinite** dimensions
- Remark: This is the most popular kernel in practice

What are “Legal” Kernels?

- A kernel $K(\cdot, \cdot)$ is a legal definition of an inner product
- Technically, this is called a **Mercer kernel**
 - A kernel should be a symmetric function: $K(u, v) = K(v, u)$
 - A kernel should also be positive semi-definite: namely,
 - For any set of data points x_1, \dots, x_n
 - And for any values $a_1, \dots, a_n \in \mathbb{R}$

$$\sum_{i=1}^n \sum_{j=1}^n a_i a_j K(x_i, x_j) \geq 0$$

- Mercer’s Theorem: For any K satisfying the above, there exists some function ϕ such that

$$K(u, v) = \phi(u)^\top \phi(v)$$

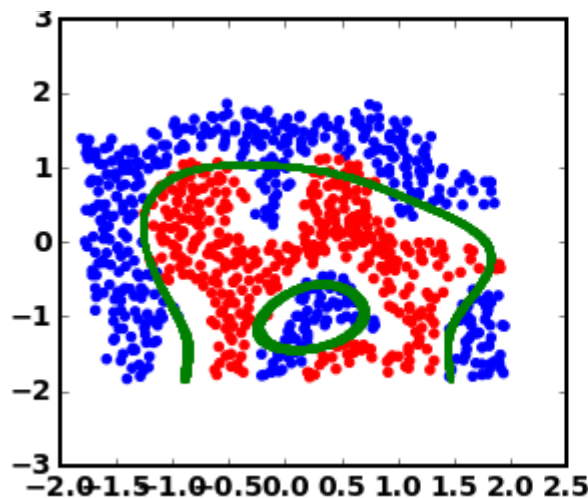
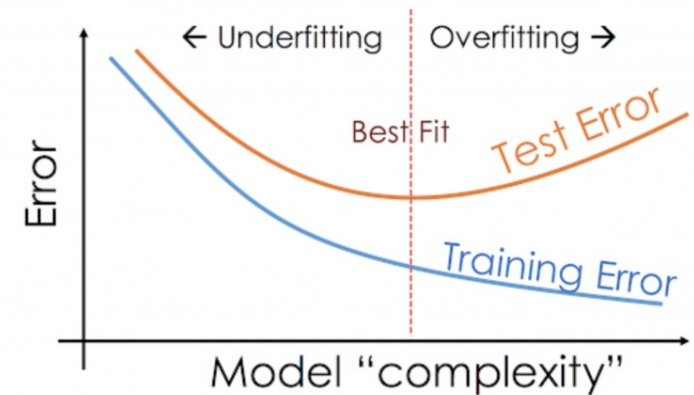
- In other words: K is a valid kernel

Example: Soft-SVM with Gaussian Kernel

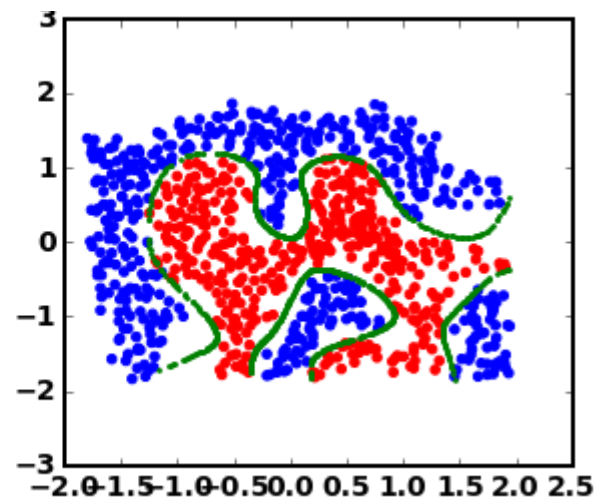
- A common choice is to use the Gaussian kernel

$$K(\underline{u}, \underline{v}) = e^{-\frac{\|\underline{u} - \underline{v}\|^2}{2\sigma^2}}$$

- σ called the **bandwidth**
- It controls smoothness of the boundary
- Gives a notion of model complexity:
- large $\sigma \rightarrow$ simple boundaries, small $\sigma \rightarrow$ complex boundaries



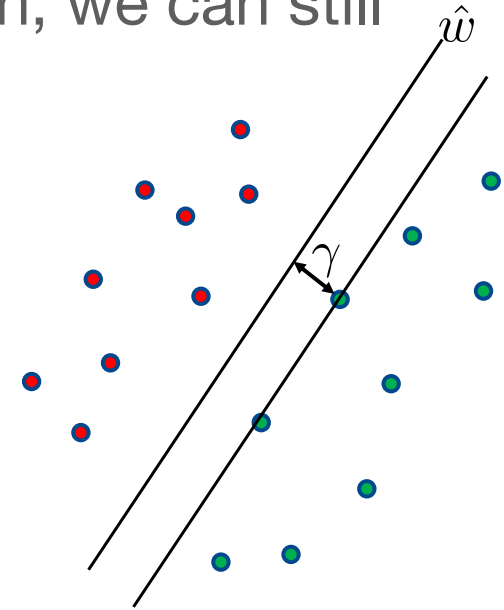
large σ



small σ

What about overfitting?

- If we're using such a high-dimensional representation, won't the dimension be large? Doesn't this lead to overfitting?
- Margin: If we can find a solution with large margin, we can still avoid overfitting.
- This is true even with kernels



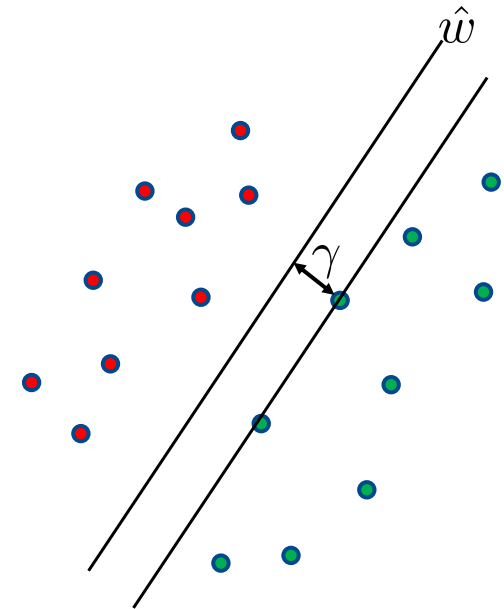
What about overfitting?

- Margin for kernel SVM:

geometric margin of classifier w :

$$\gamma = \min_{1 \leq i \leq n} y_i \left(\frac{w^\top}{\|w\|} \phi(x_i) \right)$$

Recall: The \hat{w} solution of SVM primal problem satisfies $\|\hat{w}\| = \frac{1}{\gamma}$



For kernel SVM, this means

$$\frac{1}{\gamma^2} = \|\hat{w}\|^2 = \hat{w}^\top \hat{w} = \sum_{i=1}^n \sum_{j=1}^n \alpha_i \alpha_j y_i y_j K(x_i, x_j)$$

Solve for γ to compute the margin

So we can also calculate the margin without computing ϕ , using K

Summary

- Kernel methods are a convenient family of algorithms
- They allow us to specify a non-linear representation for the classifier just by providing a kernel function, and the rest is automatic
- In this sense, they are “plug-and-play”: very easy to use
- We need to be careful that the implicit high-dimensional representation doesn't lead to overfitting
- If the solution has large margin, it can avoid overfitting
- Recall that SVM is designed to maximize the margin, so it is well-suited to this type of guarantee

Gradient descent

Logistic regression learning

$$\text{minimize} \sum_{i=1}^N (-y_i w^T x_i + \log(1 + e^{w^T x_i}))$$

$$\begin{aligned} \frac{d \log L(w|D)}{dw_j} &= \sum_{i=1}^N \left(-y_i x_{ij} + \frac{1}{1 + e^{w^T x_i}} e^{w^T x_i} x_{ij} \right) \\ &= \sum_{i=1}^N \left(-y_i + \frac{1}{1 + e^{w^T x_i}} e^{w^T x_i} \right) x_{ij} \\ &= \sum_{i=1}^N (-y_i + P(y_i = 1|w)) x_{ij} \end{aligned}$$

Convex!

But no closed form solution!

Convex optimization problems

$$\begin{array}{ll}\text{minimize} & f(x) \\ \text{subject to} & x \in C\end{array}$$

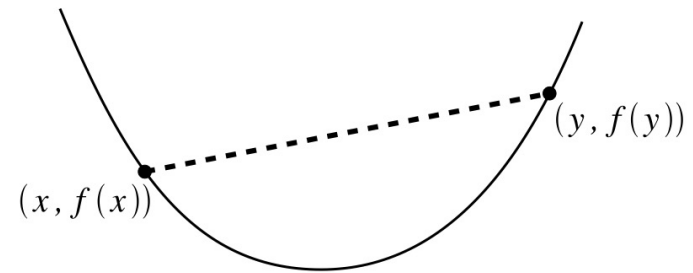
- ▶ x is the optimization variable (e.g., model parameters)
 f (e.g., score function) is a **convex function**
 C is a **convex set** (e.g., constraints on model parameters)
- ▶ For convex optimization problems, all locally optimal points are globally optimal

Convex functions

- ▶ In graph of convex function f , the line connecting two points must lie above the function:

$$f(\alpha x + (1 - \alpha)y) \leq \alpha f(x) + (1 - \alpha)f(y) \text{ for all } 0 \leq \alpha \leq 1$$

- ▶ Practical test for convexity: a twice differentiable function f of a variable is convex on an interval if and only if for any x in the interval: $f''(x) \geq 0$

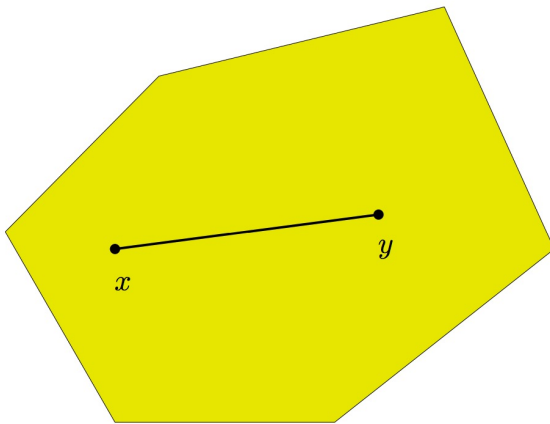


- ▶ Strictly convex if $f''(x) > 0$
- ▶ Sum of convex functions is convex; max of convex functions is convex

Convex set

- ▶ A set C is convex if for any $x, y \in C$ and any θ with $0 \leq \theta \leq 1$ we have

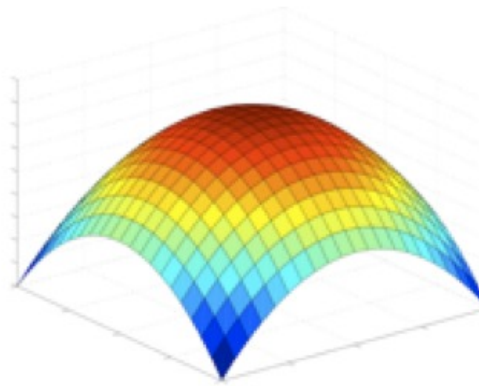
$$\theta x + (1 - \theta)y \in C$$



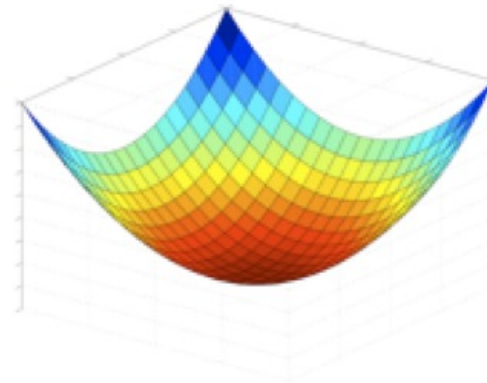
Concave vs convex

- ▶ Maximizing a concave function is equivalent to minimizing a convex function

concave



convex



Solve convex optimization problem

- ▶ Minimize a convex function without any constraints on the variables
 - ▶ If $f'(x)=0$ then x is a stationary point of f
 - ▶ If $f'(x)=0$ and $f''(x)$ is not negative then x is a local minimum of f (for convex function, this is also a global minimum)
 - ▶ If f is a strictly convex function, any stationary point of f is the unique global minimum of f

Gradient descent

- ▶ For some convex functions, we may be able to take the derivative, but it may be difficult to directly solve for parameter values
- ▶ Solution:
 - ▶ Start at some value of the parameters
 - ▶ Take derivative and use it to move the parameters in the direction of the negative gradient
 - ▶ Repeat until stopping criteria is met (e.g., gradient close to 0)

Gradient Descent Rule:

$$\underline{\mathbf{w}}_{\text{new}} = \underline{\mathbf{w}}_{\text{old}} - \eta \Delta(\underline{\mathbf{w}})$$

where

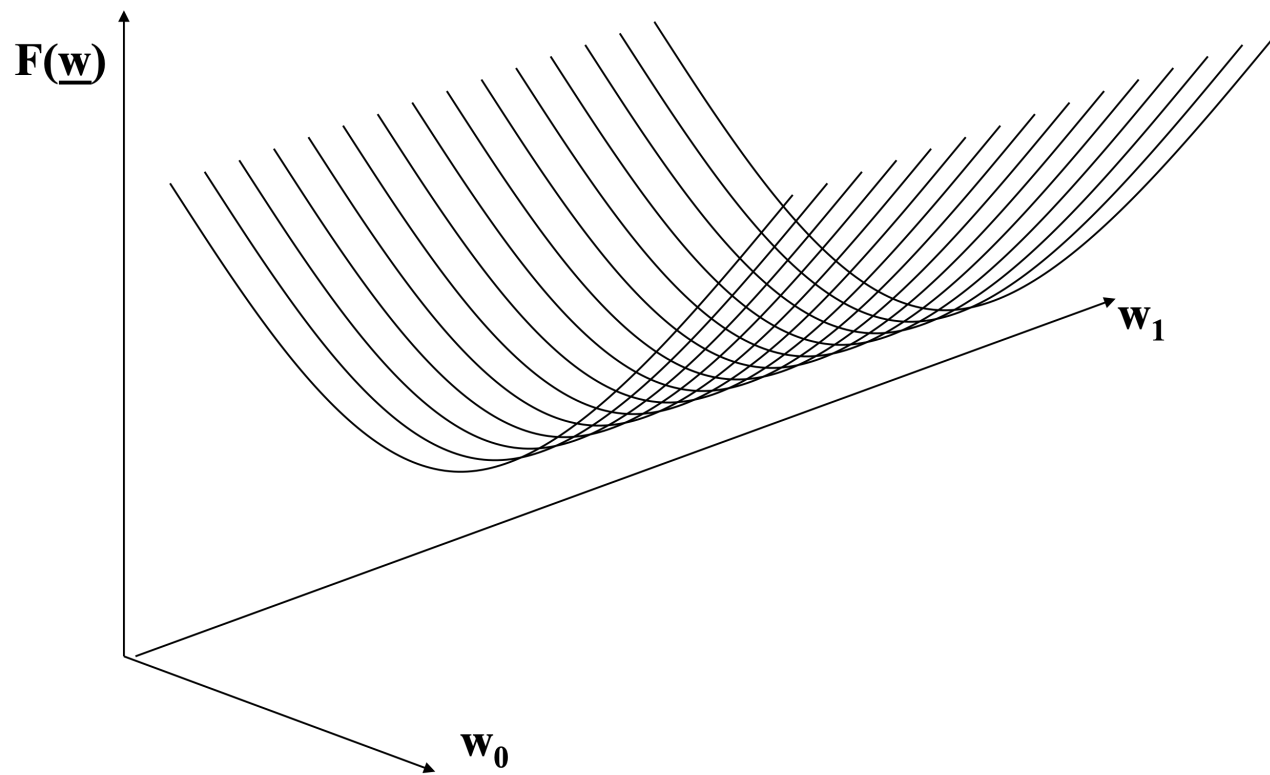
$\Delta(\underline{\mathbf{w}})$ is the gradient and

η is the learning rate (small, positive)

Notes:

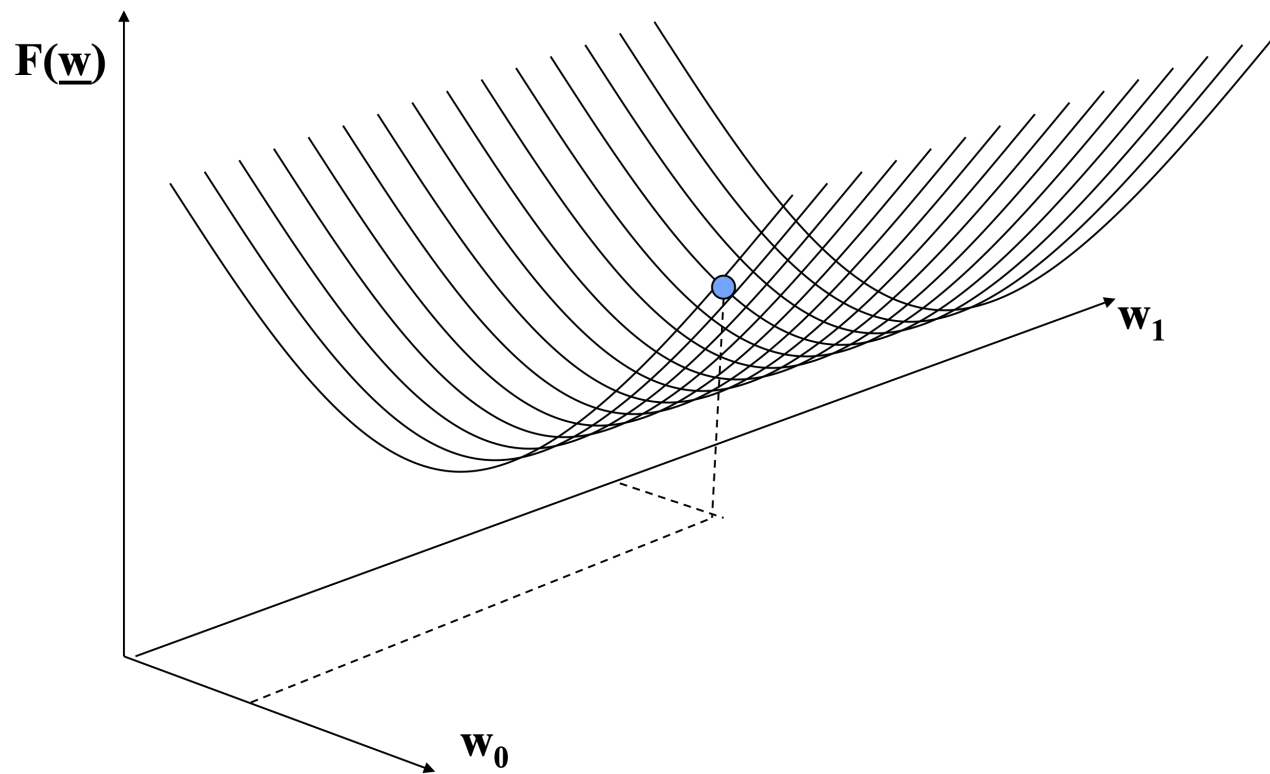
1. This moves us downhill in direction $\Delta(\underline{\mathbf{w}})$ (steepest downhill direction)
2. How far we go is determined by the value of η

Illustration of gradient descent



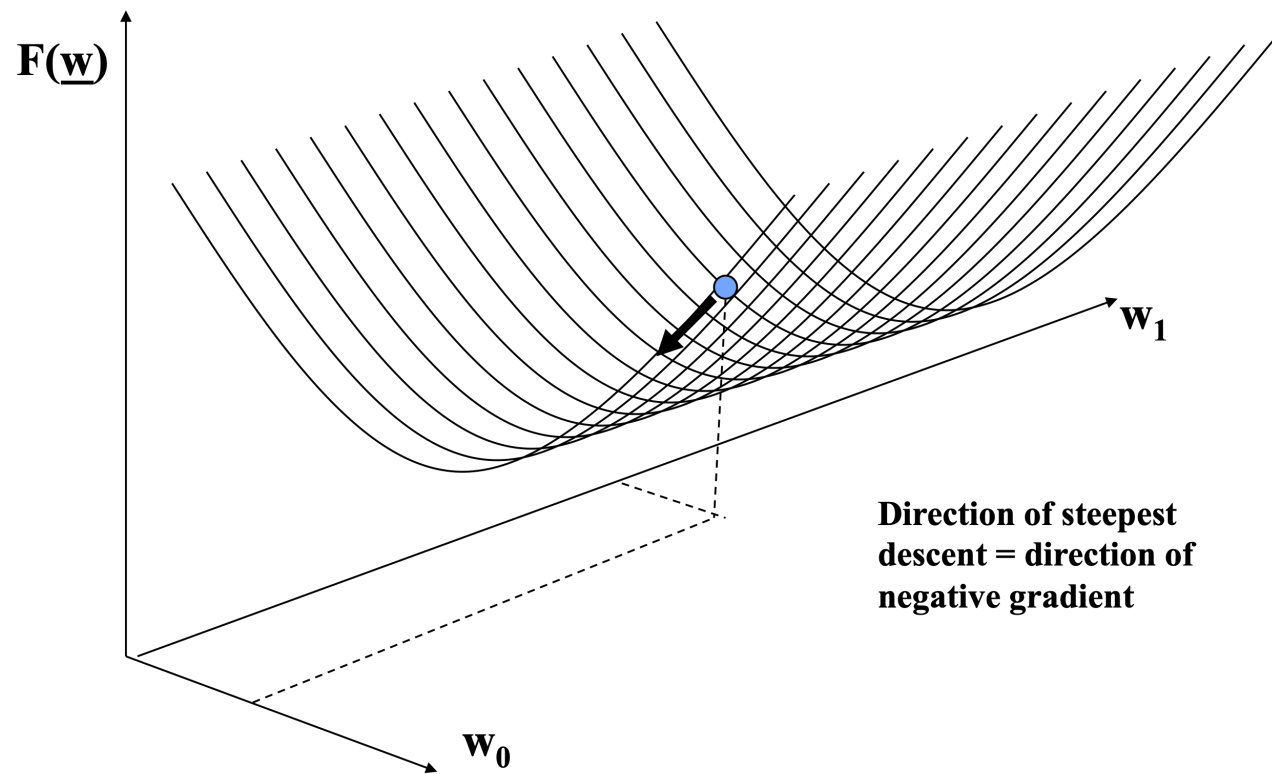
Slides adapted from CS175, UC Irvine, Padhraic Smyth

Illustration of gradient descent



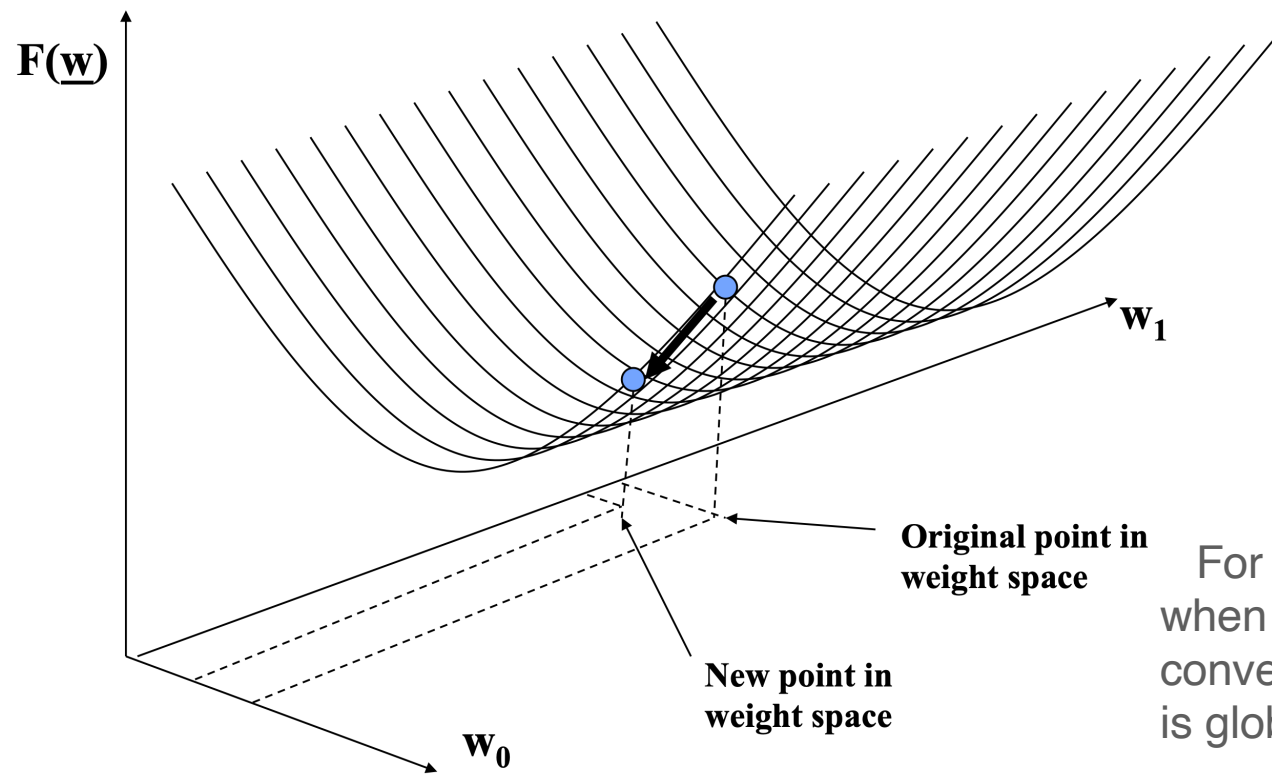
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Illustration of gradient descent



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Illustration of gradient descent



For convex functions, when gradient descent converges, the solution is global minimum.

Slides adapted from CS175, UC Irvine, Padhraic Smyth

Take-home Quiz

(Due Sept 27th at 9am on Gradescope)

- Recall the previous example in the Decision Tree lecture

age	income	student	credit rating	buys computer
<=30	high	no	fair	no
<=30	high	no	excellent	no
31...40	high	no	fair	yes
>40	medium	no	fair	yes
>40	low	yes	fair	yes
>40	low	yes	excellent	no
31...40	low	yes	excellent	yes
<=30	medium	no	fair	no
<=30	low	yes	fair	yes
>40	medium	yes	fair	yes
<=30	medium	yes	excellent	yes
31...40	medium	no	excellent	yes
31...40	high	yes	fair	yes
>40	medium	no	excellent	no

- Please construct a decision tree using information gain and full growth criteria.