Data Mining & Machine Learning

CS37300
Purdue University

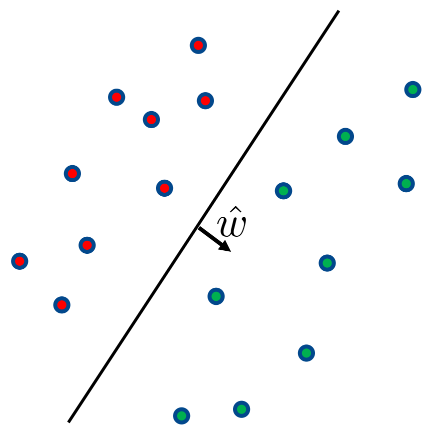
Sep 25, 2023

Today's topics

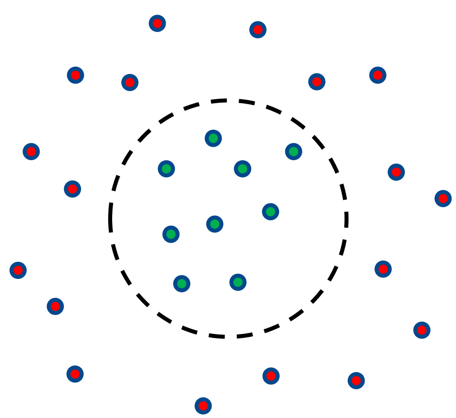
- Kernels and Kernel-SVM

Nonlinear Decision Boundaries

- Linear separators are simple



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

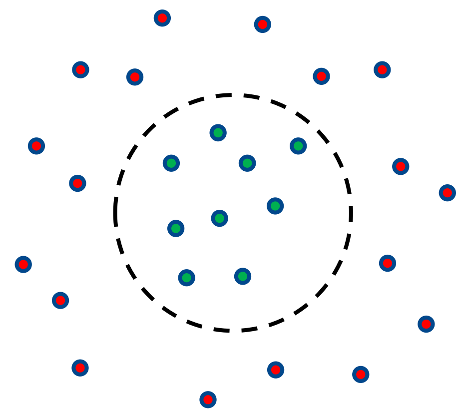


- We want to learn these with optimization based ML (SVM)

Learning Nonlinear Decision Boundaries

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

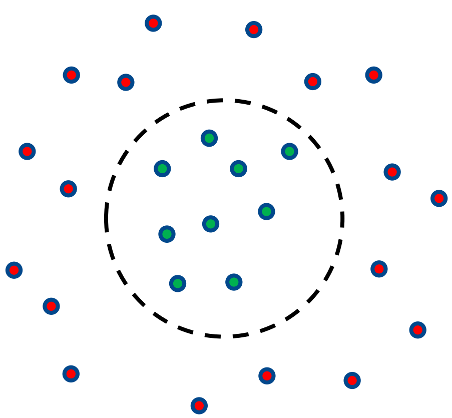
Example:



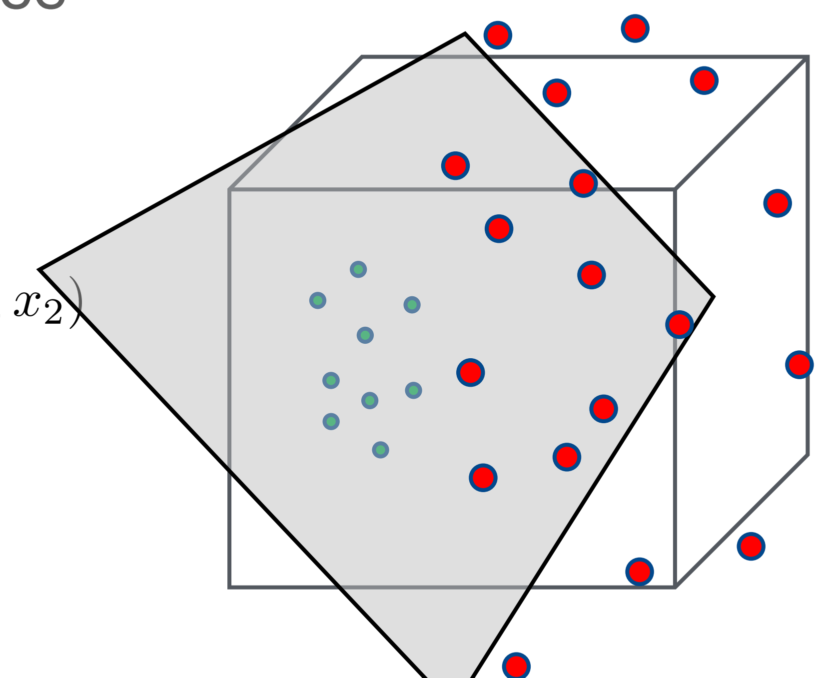
Learning Nonlinear Decision Boundaries

- 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 $\phi(\underline{x}) = (x_1^2, x_2^2, \sqrt{2}x_1 x_2)$



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:

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

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$$\hat{w} = \underset{w \in \mathbb{R}^N : \|w\|=1}{\operatorname{argmax}} \quad \min_{1 \le i \le n} y_i \left(w^\top \phi(x_i)\right)$$

$$\boxed{\begin{array}{ll} \text{Minimize} & \|w\|^2 \\ \text{subject to} & y_i \left(w^\top \phi(x_i)\right) \ge 1, \ \forall i : \ 1 \le i \le n \end{array}}$$

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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.
     $\rightarrow$ Concerns about overfitting

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

The Dual Form of the SVM Optimization Problem

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

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

$$\boxed{\begin{array}{ll} \text{Minimize} & \|w\|^2 \\ \text{subject to} & y_i \left(w^\top x_i \right) \ge 1, \ \forall i : \ 1 \le i \le n \end{array}}$$

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

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

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

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

SVM with high-dim mapping

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

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

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- 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 $K(x_i, x_j)$ 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 $\phi(x)$!

SVM with high-dim mapping

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

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

- 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)

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

- Replace all of these with

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

Kernel SVM

- Training time:

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

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

- Test time:

- Classify a new point x with

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

Kernels

Example:

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

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 :

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

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

$$= \left[1, \sqrt{2}u_1, \sqrt{2}u_2, u_1^2, u_2^2, \sqrt{2}u_1 u_2\right] \left[1, \sqrt{2}v_1, \sqrt{2}v_2, v_1^2, v_2^2, \sqrt{2}v_1 v_2\right]^\top$$

$$= 1 + 2u_1 v_1 + 2u_2 v_2 + u_1^2 v_1^2 + u_2^2 v_2^2 + 2u_1 u_2 v_1 v_2$$

$$= (1 + u_1 v_1 + u_2 v_2)^2 = \left(1 + \underline{u}^\top \underline{v}\right)^2 = K(\underline{u}, \underline{v})$$

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

Kernels

- More Examples:
  - Polynomial kernel: $K(\underline{u}, \underline{v}) = \left(\underline{u}^\top \underline{v} + 1\right)^p$
    - 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(·,·) 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 $x_1,\ldots,x_n$
    - And for any values $a_1, \ldots, a_n \in \mathbb{R}$

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

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

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

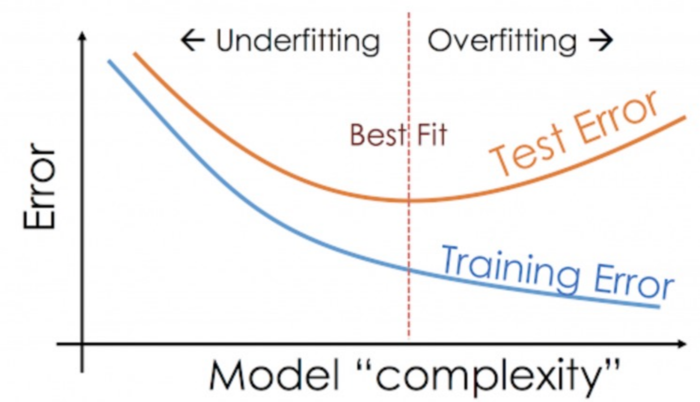
- In other words: K is a valid kernel

Example: Soft-SVM with Gaussian Kernel

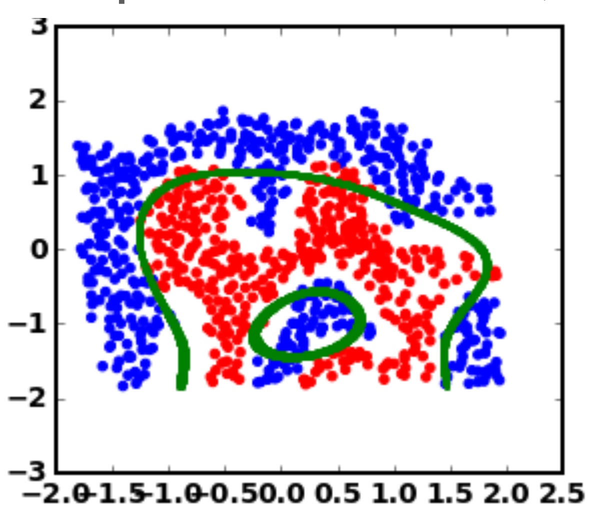
- A common choice is to use the Gaussian kernel

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

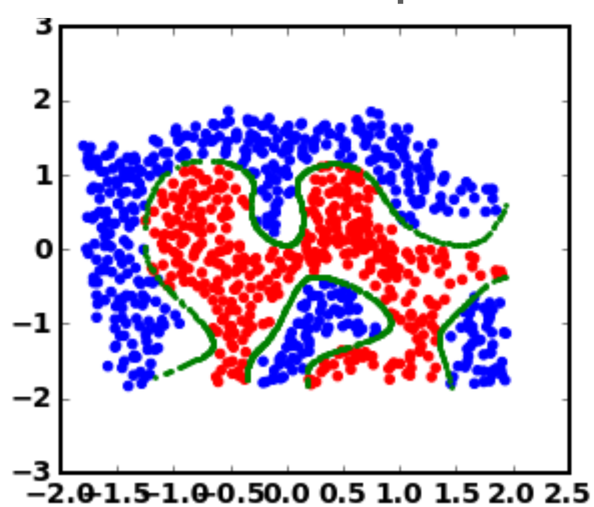
- σ called the **bandwidth**
- It controls smoothness of the boundary
- Gives a notion of model complexity:



- large σ → simple boundaries, small σ → complex boundaries



large σ



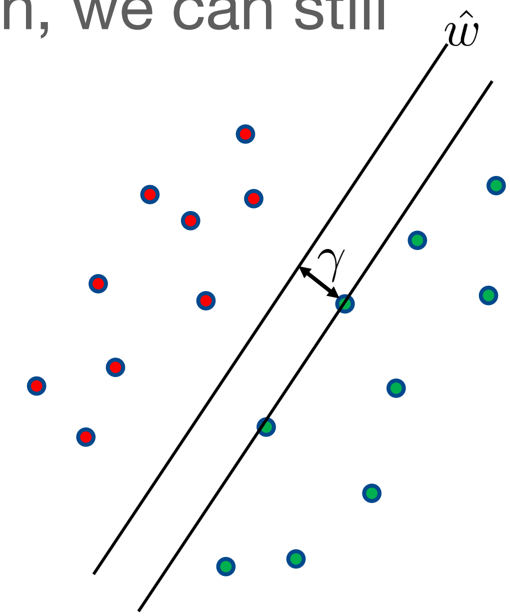
small σ

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

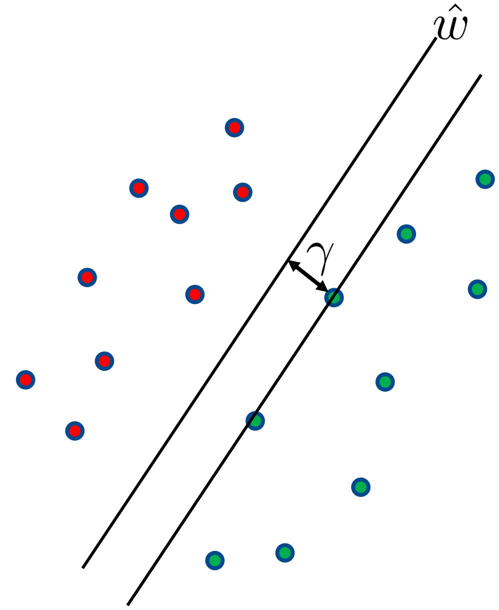


What about overfitting?

- 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

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

$$\frac{dlogL(w|D)}{dw_j} = \sum_{i=1}^{N} (-y_i x_{ij} + \frac{1}{1 + e^{w^T x_i}} e^{w^T x_i} x_{ij})$$

$$= \sum_{i=1}^{N} (-y_i + \frac{1}{1 + e^{w^T x_i}} e^{w^T x_i}) x_{ij}$$

$$= \sum_{i=1}^{N} (-y_i + P(y_i = 1 | w)) x_{ij}$$

Convex!

But no closed form solution!

Convex optimization problems

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

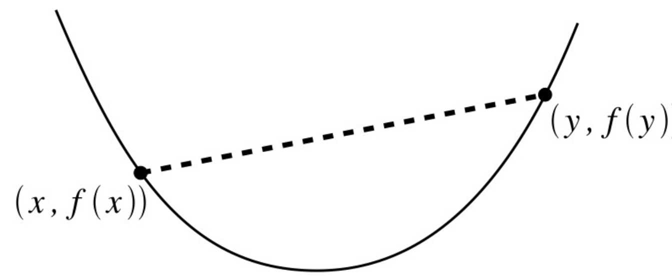
- *x* is the optimization variable (*e.g., model parameters*)
  f (*e.g., score function*) is a **convex function**
  C is a **convex set** (*e.g., constraints on model parameters*)
- For convex optimization problems, all locally optimal points are globally optimal

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 an only if for any x in the interval: $f''(x) \geq 0$
  - Strictly convex if $f''(x) > 0$

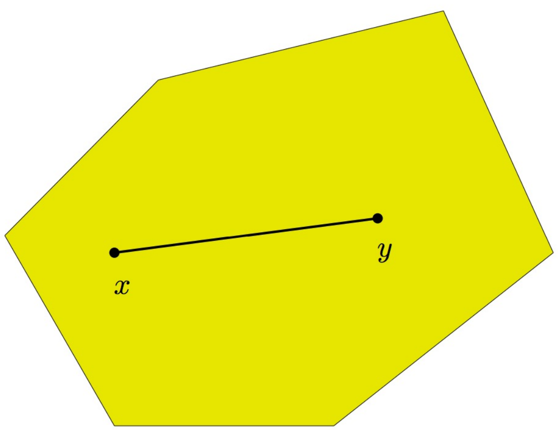


- Sum of convex functions is convex; max of convex functions is convex

Convex set

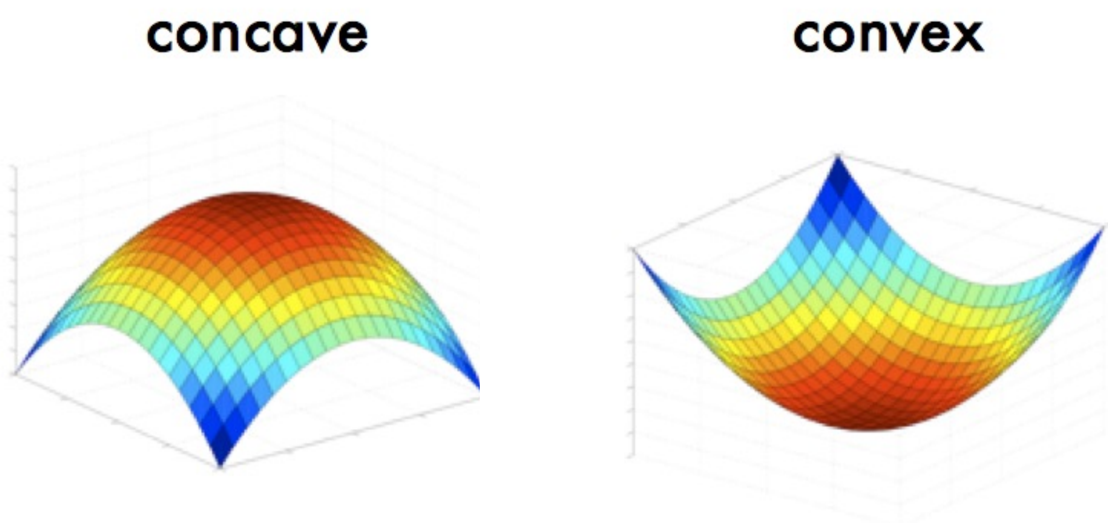
- A set C is convex if for any $x, y \in C$ and any θ with $0 \leq \theta \leq 1$ we have

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



Concave vs convex

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



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)

<u>Gradient Descent Rule:</u>

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

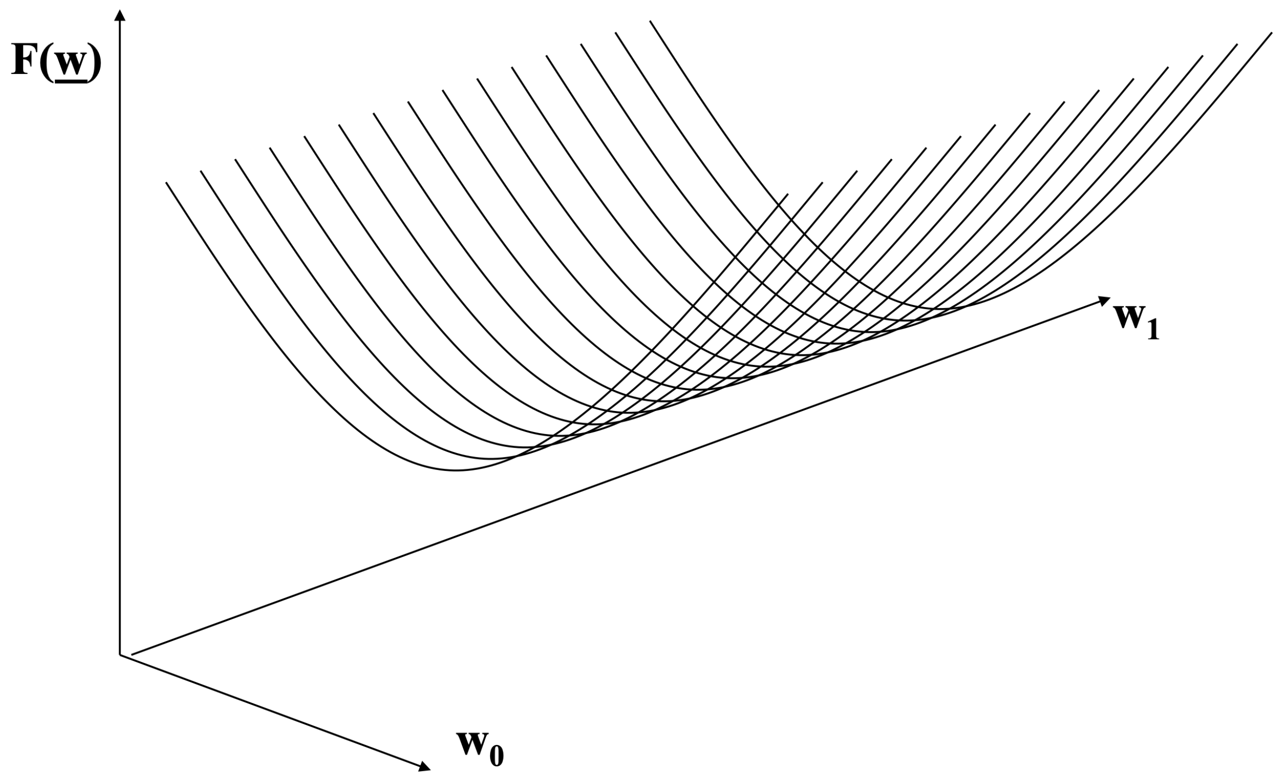
where

$\Delta(\underline{w})$ 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, UCIrvine, Padhraic Smyth

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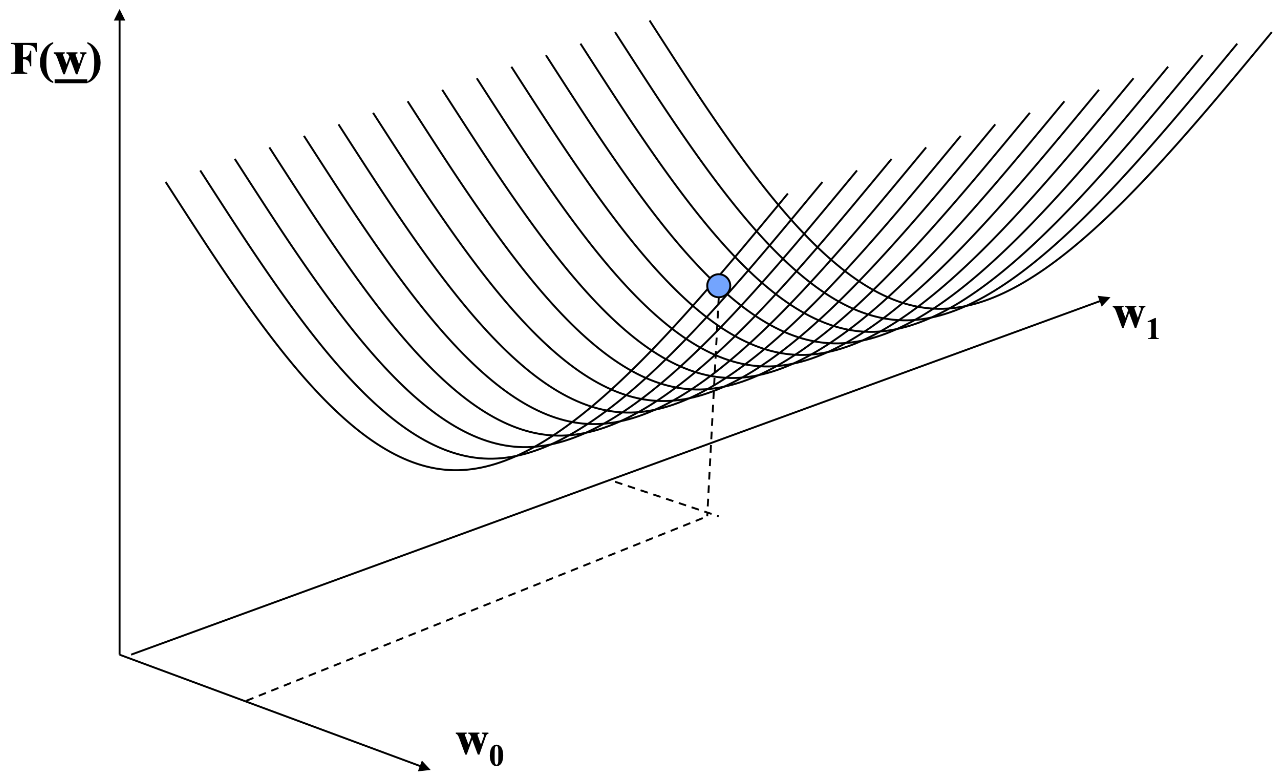

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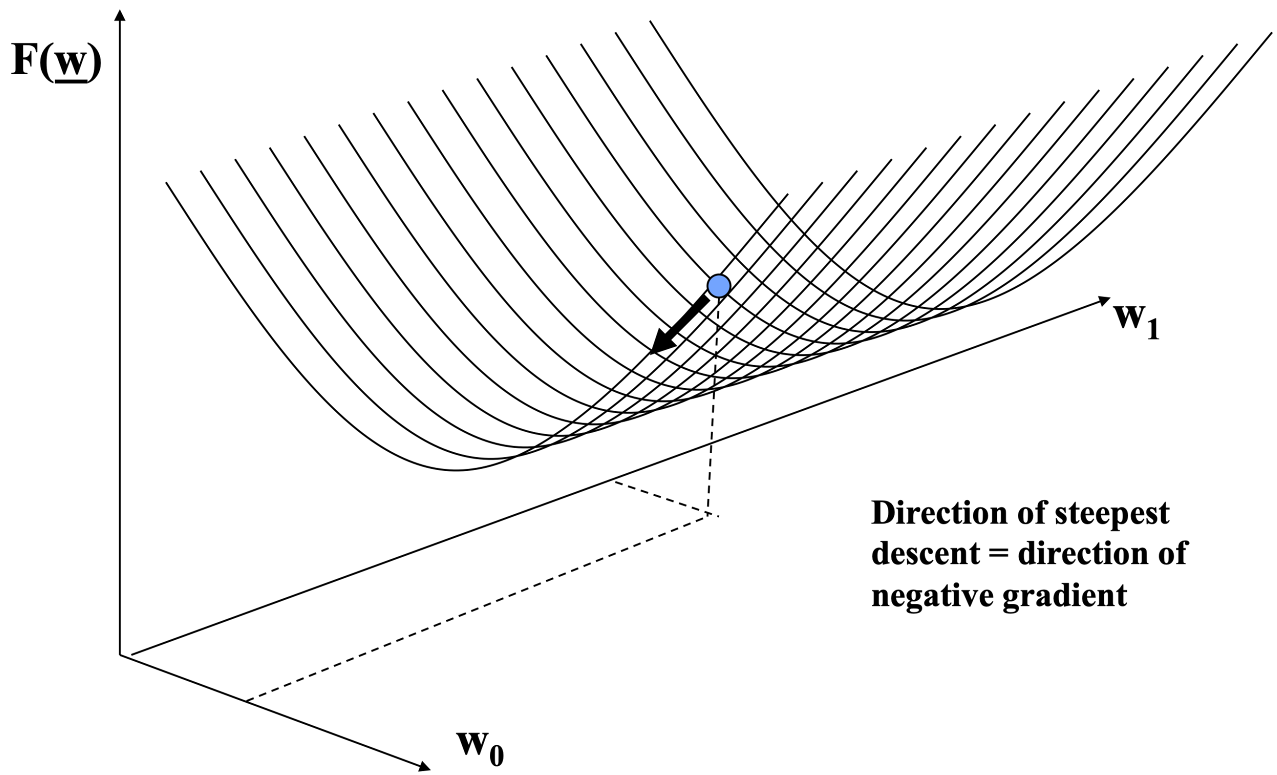

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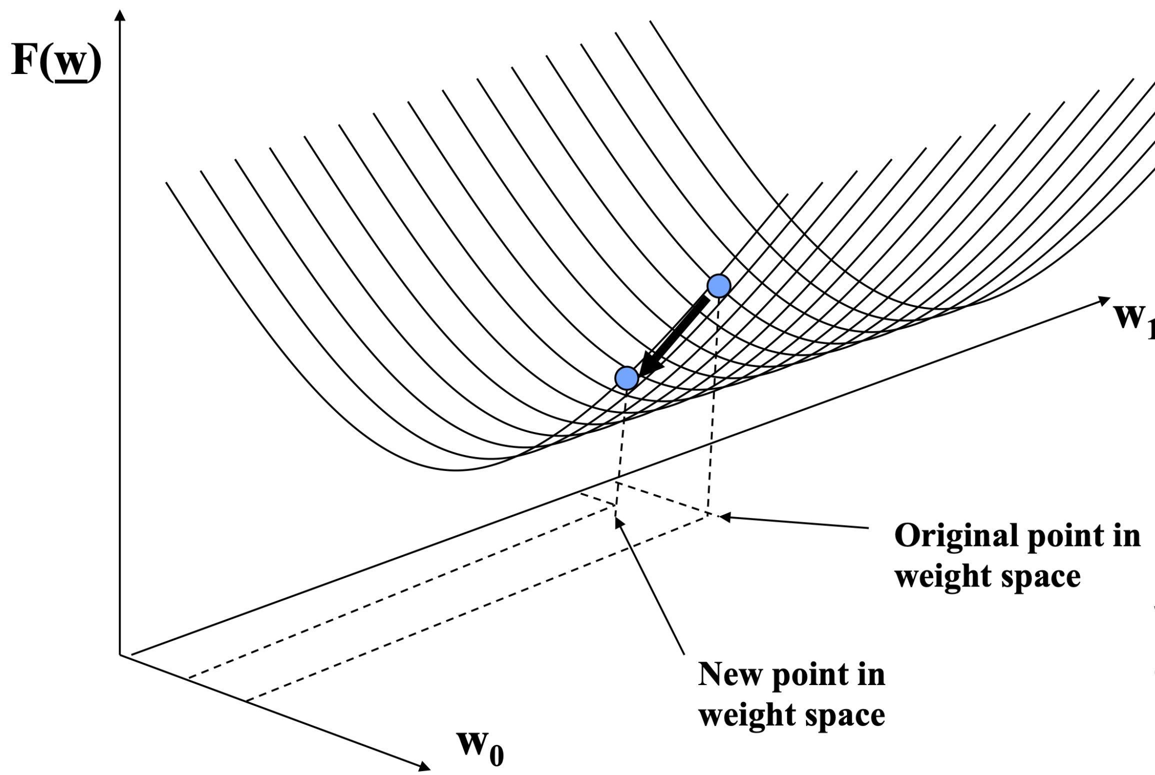

For convex functions, when gradient descent converges, the solution is global minimum.

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