CS57300
PURDUE UNIVERSITY

FEBRUARY 19, 2019

DATA MINING

ANNOUNCEMENT

- Assignment 3 is out
  - Implement Logistic Regression and Linear SVM for speed dating event outcome prediction
  - Due: March 8 (Friday), 11:59pm
- In-class midterm exam in two weeks
  - March 5, 4:30-5:45pm, WANG 2599

SMOOTH OPTIMIZATION

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
- What about minimizing a convex function with constraints?

USE LAGRANGE MULTIPLIERS TO SOLVE CONVEX OPTIMIZATION

- For a standard form of convex optimization problem (f_0 are f_i are convex, h_i is linear):

$$
\begin{array}{ll}
\text{minimize} & f_0(x) \\
\text{subject to} & f_i(x) \leq 0, \quad \text{for } i = 1, \ldots, m. \\
& h_i(x) = 0, \quad \text{for } i = 1, \ldots, k.
\end{array}
$$

- The Lagrangian function of it is

$$L(x, \lambda, v) = f_0(x) + \sum_{i=1}^{m} \lambda_i f_i(x) + \sum_{i=1}^{k} v_i h_i(x)$$

  - $\lambda_i \geq 0$ is the **Lagrange multiplier** for the *i*-th inequality constraint, v_i is the **Lagrange multiplier** for the *i*-th equality constraint
  - Solve the constrained optimization problem by finding the stationary point of the Lagrangian function

LOGISTIC REGRESSION LEARNING

- Logistic regression: $P(y=1|\mathbf{x}) = \dfrac{1}{1+e^{-(\mathbf{w}^T\mathbf{x}+w_0)}}$
  - Maximize (log) likelihood: $\mathsf{w} = (\mathsf{w}, w_0), \mathsf{x_i} = (\mathsf{x_i}, 1)$

$$
\begin{aligned}
logL(\mathsf{w}\,|\,D) &= \sum_{i=1}^{N} logp(y_i\,|\,\mathsf{w}) \\
&= \sum_{i=1}^{N} log[(\frac{1}{1+e^{-\mathsf{w}^\mathsf{T}\mathsf{x_i}}})^{y_i}(\frac{e^{-\mathsf{w}^\mathsf{T}\mathsf{x_i}}}{1+e^{-\mathsf{w}^\mathsf{T}\mathsf{x_i}}})^{1-y_i}] \\
&= \sum_{i=1}^{N} (y_i\mathsf{w}^\mathsf{T}\mathsf{x_i} - log(1+e^{\mathsf{w}^\mathsf{T}\mathsf{x_i}}))
\end{aligned}
$$

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

LOGISTIC REGRESSION LEARNING

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

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

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

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

Convex!

But no closed form solution!

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 $\mathbf{\Delta}(\underline{\mathbf{w}})$ (steepest downhill direction)
2. How far we go is determined by the value of $\boldsymbol{\eta}$

ILLUSTRATION OF GRADIENT DESCENT

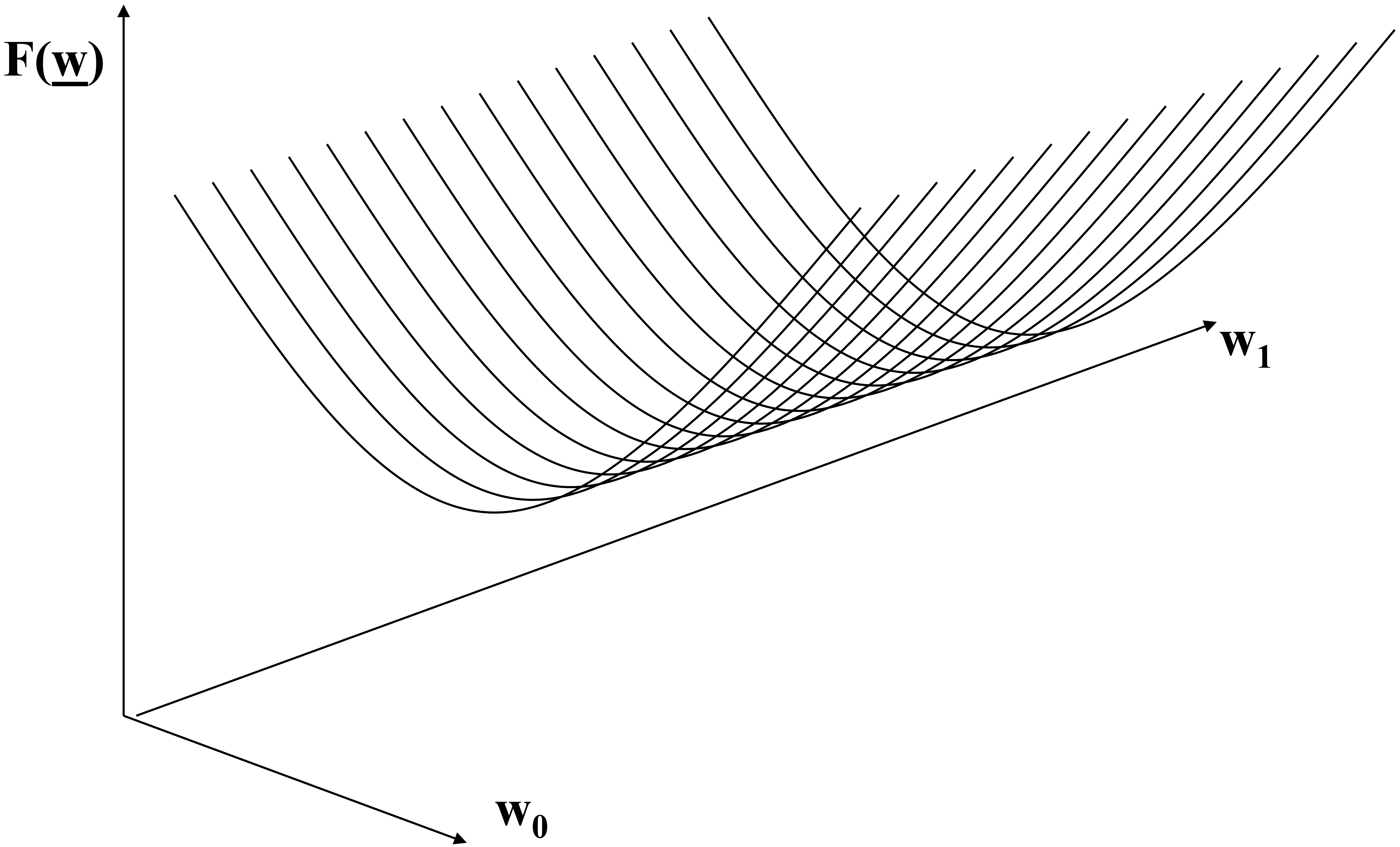
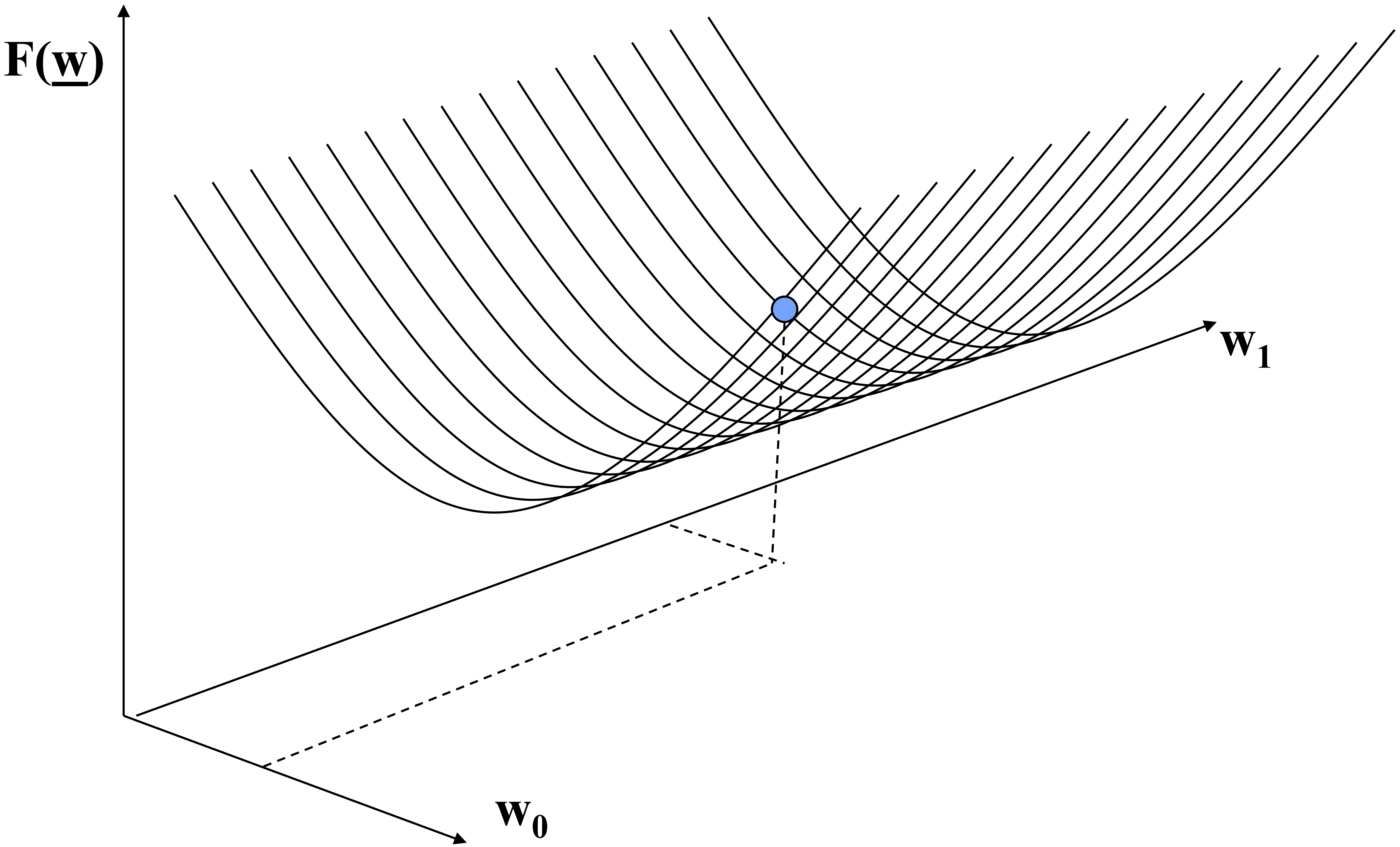


ILLUSTRATION OF GRADIENT DESCENT



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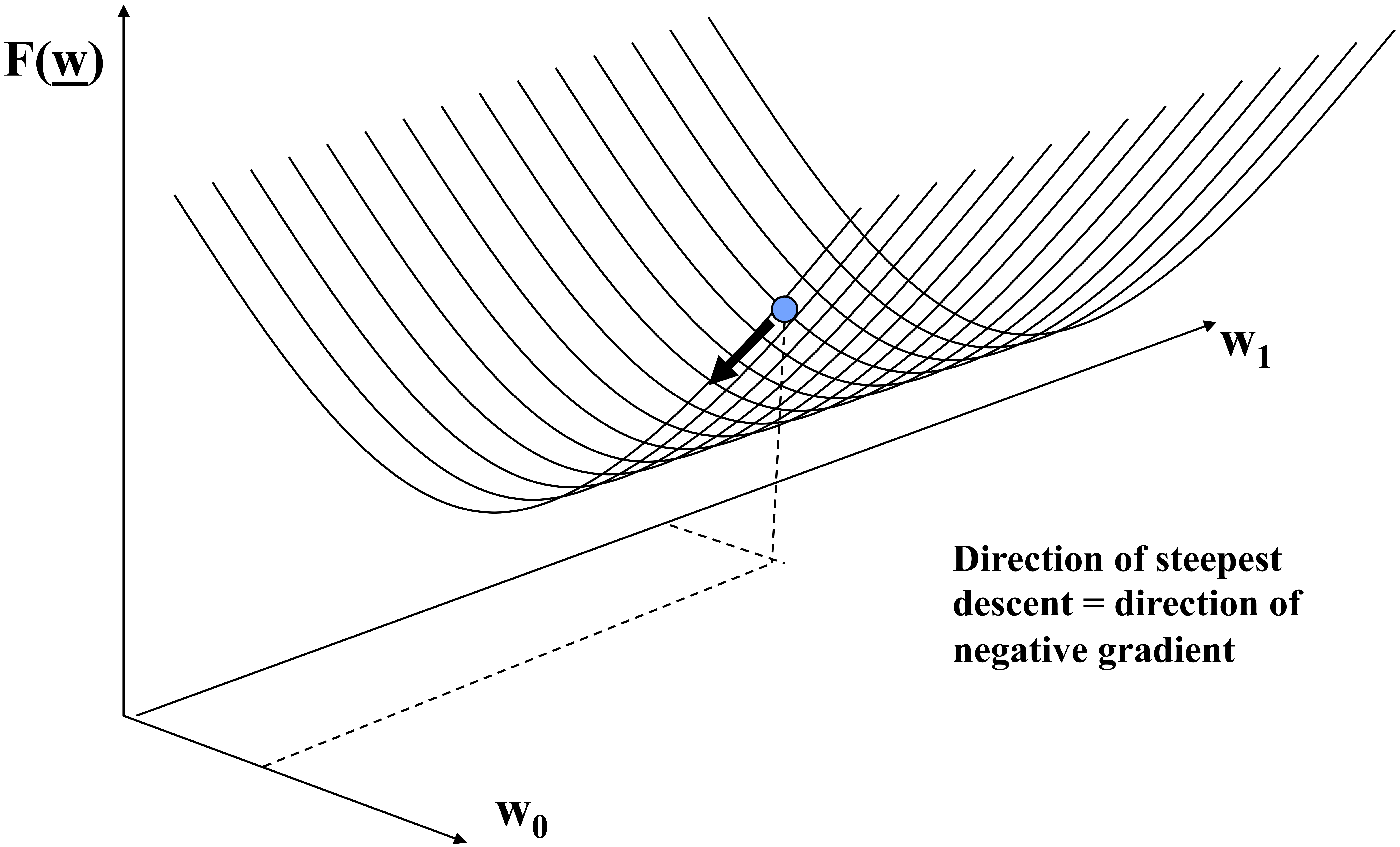

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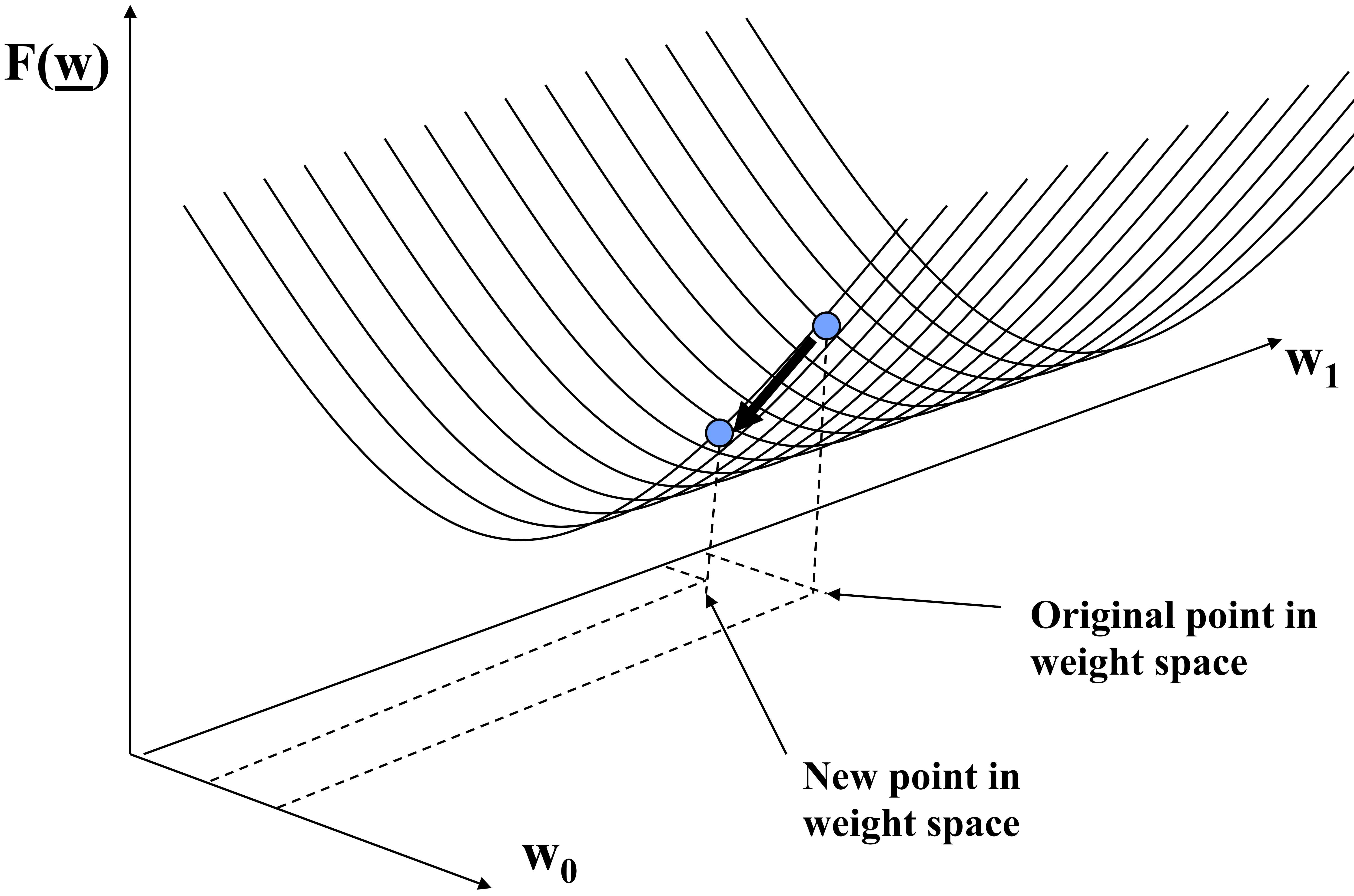


For convex functions, when gradient descent converges, the solution is global minimum.

STOPPING CRITERIA FOR GRADIENT DESCENT

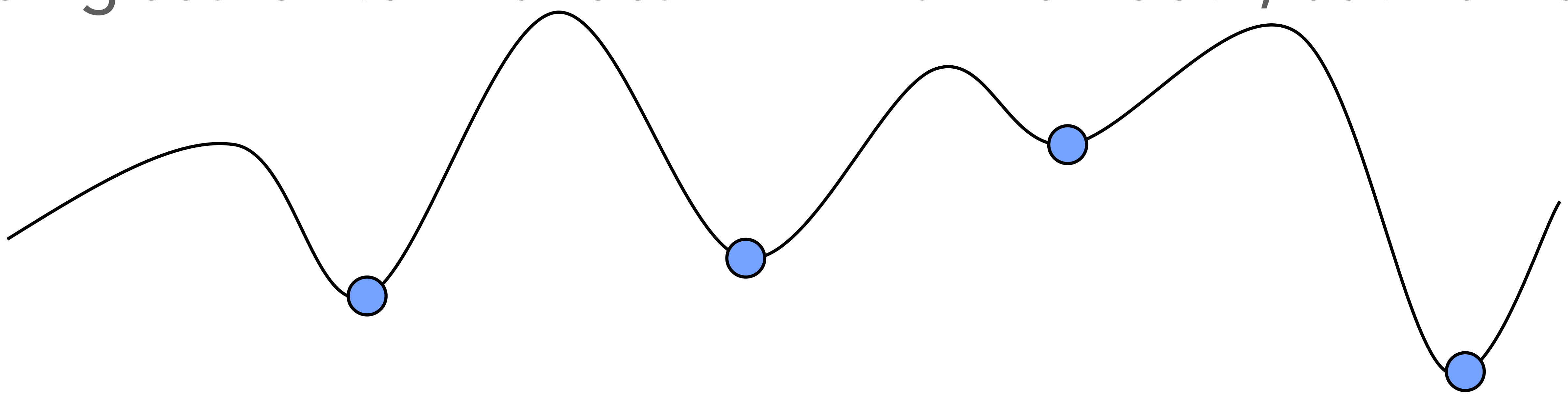
- Ideally, f′(x)=0…
- In practice…
  - $\|\nabla f(x)\| < \varepsilon$
  - $|f(x_{k+1}) - f(x_k)| < \varepsilon$
  - $\|x_{k+1} - x_k\| < \varepsilon$
  - Maximum number of iterations has been reached

GRADIENT ASCENT

- For concave functions that you want to *maximize*, take a step in direction of gradient (i.e., $w_{new} \leftarrow w_{old} + \eta\nabla(w)$)
- Otherwise same as gradient descent:
  - Start at some parameter values
  - Take derivative, move the parameters in the direction of gradient
  - Repeat until stopping criteria is met (e.g., gradient close to 0)

GRADIENT DESCENT FOR NON-CONVEX OPTIMIZATION

- Works on any objective function F(θ)
  - as long as we can evaluate the gradient Δ(θ)
  - this can be very useful for minimizing complex functions F
- Can be used in hill-climbing search to find local minima in smooth, but non-convex functions



- If function has multiple local minima, gradient descent goes to the closest local minimum:
  - solution: random restarts from multiple places in model space

LOGISTIC REGRESSION: RECAP

LOGISTIC REGRESSION

- Same parametric form as standard regression, but uses logistic function for binary classification

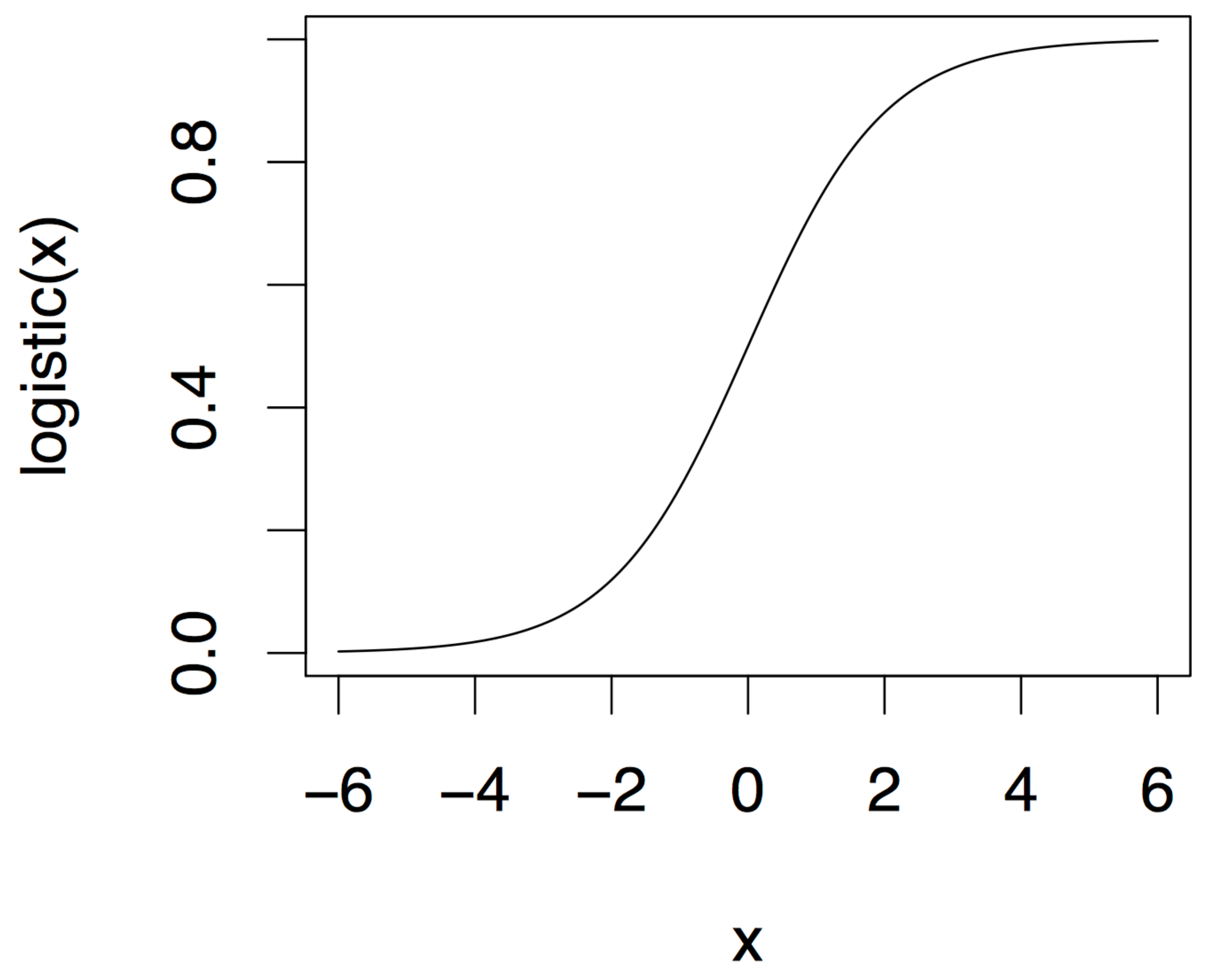
Logistic regression model:

$$P(y = 1|\mathbf{x}) = \frac{1}{1 + e^{-(\mathbf{w}^T\mathbf{x} + w_0)}}$$

- Output is the (positive) class probability rather than the binary prediction
- Logistic function transform ensures output is [0,1]

Logistic function:

$$\text{logistic}(x) := \frac{e^x}{1 + e^x} = \frac{1}{1 + e^{-x}}$$



LR EXAMPLE

$$P(BC = 1|A, I, S, CR) = \frac{1}{1 + e^{-(\mathbf{w}^T\mathbf{x})}}$$

$$\mathbf{x} = [Int, A, I, S, CR]$$
$$\mathbf{w} = [w_0, w_A, w_I, w_S, w_{CR}]$$

LR parameters = w

Intercept	Age>40	Income=high	Student=yes	Credit=fair	BuysComp?
1	0	1	0	1	0
1	0	1	0	0	0
1	0	1	0	1	1
1	1	0	0	1	1
1	1	0	1	1	1
1	1	0	1	0	0
1	0	0	1	0	1
1	0	0	0	1	0
1	0	0	1	1	1
1	1	0	1	1	1
1	0	0	1	0	1
1	0	0	0	0	1
1	0	1	1	1	1
1	1	0	0	0	0

- Score function: likelihood
- Estimate **w** with maximum likelihood estimation

LR LEARNING

- Score function: likelihood function

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

- Estimate optimal **w** using gradient descent $\dfrac{dlogL}{dw_j} = \sum_{i=1}^{N} (-y_i + P(y_i = 1 \,|\, \mathbf{w}, \mathbf{x}_i))x_{ij}$

Gradient descent:

Start at some **w**, e.g., **w**=[0,0,0,0,0]

Make predictions given current **w**: $\forall i \;\; \widehat{y_i} = P(y_i = 1|\mathbf{x}_i) = \dfrac{1}{1 + e^{-\mathbf{w}^T \mathbf{x_i}}}$

Calculate gradient for each parameter: $\forall j \;\; \dfrac{d\,logL}{d\,w_j} = \left[\sum_{i=1}^{n}(-y_i + \hat{y}_i)x_{ij}\right] = \nabla_j$

Move parameters in direction of negative gradient: $\forall j \;\; w_j^{new} = w_j - \eta \nabla_j$

Repeat until stopping criteria is met

LR PREDICTION

Intercept	Age>40	Income=high	Student=yes	Credit=fair	BuysComp?
1	0	1	0	1	0
1	0	1	0	0	0
1	0	1	0	1	1
1	1	0	0	1	1
1	1	0	1	1	1
1	1	0	1	0	0
1	0	0	1	0	1
1	0	0	0	1	0
1	0	0	1	1	1
1	1	0	1	1	1
1	0	0	1	0	1
1	0	0	0	0	1
1	0	1	1	1	1
1	1	0	0	0	0
1	**0**	**1**	**0**	**0**	**?**

- What is the probability that new person will buy a computer?

$$\mathbf{x} = [1, 0, 1, 0, 0]$$

$$\mathbf{w} = [-1.3, 1, 2, -2, 0.7]$$

$$\mathbf{x}^T \mathbf{w} = 0.7$$

$$P(BC = 1 | \mathbf{x}\ ) = \frac{1}{1 + e^{-0.7}}$$
$$= 0.668$$

DEAL WITH OVERFITTING

- Simply finding the parameter values that lead to maximum likelihood function value in the training dataset may imply overfitting!
- Solution: add a **regularization term** in the scoring function to penalize complex models
  - e.g., L2 regularization term: $\frac{\lambda}{2}\|w\|^2$
  - λ is the regularization parameter; the larger the value, the more we are in favor of simple models

LR LEARNING WITH REGULARIZATION TERM

- Score function: likelihood with L2 regularization

$$minimize \sum_{i=1}^{N} (-y_i \mathbf{w}^T \mathbf{x}_i + log(1 + e^{\mathbf{w}^T \mathbf{x}_i})) + \frac{\lambda}{2} \|\mathbf{w}\|^2$$

- Estimate optimal **w** using gradient descent

Gradient descent:

Start at some **w**, e.g., **w**=[0,0,0,0,0]

Make predictions given current **w**: $\forall i \;\; \widehat{y}_i = P(y_i = 1|\mathbf{x}_i) = \frac{1}{1+e^{-\mathbf{w}^T \mathbf{x}_i}}$

Calculate gradient for each parameter: $\forall j \;\; \frac{d\, logL}{d\, w_j} = \left[\sum_{i=1}^{n} (-y_i + \hat{y}_i) x_{ij}\right] + \lambda w_j = \nabla_j$

Move parameters in direction of negative gradient: $\forall j \;\; w_j^{new} = w_j - \eta \nabla_j$

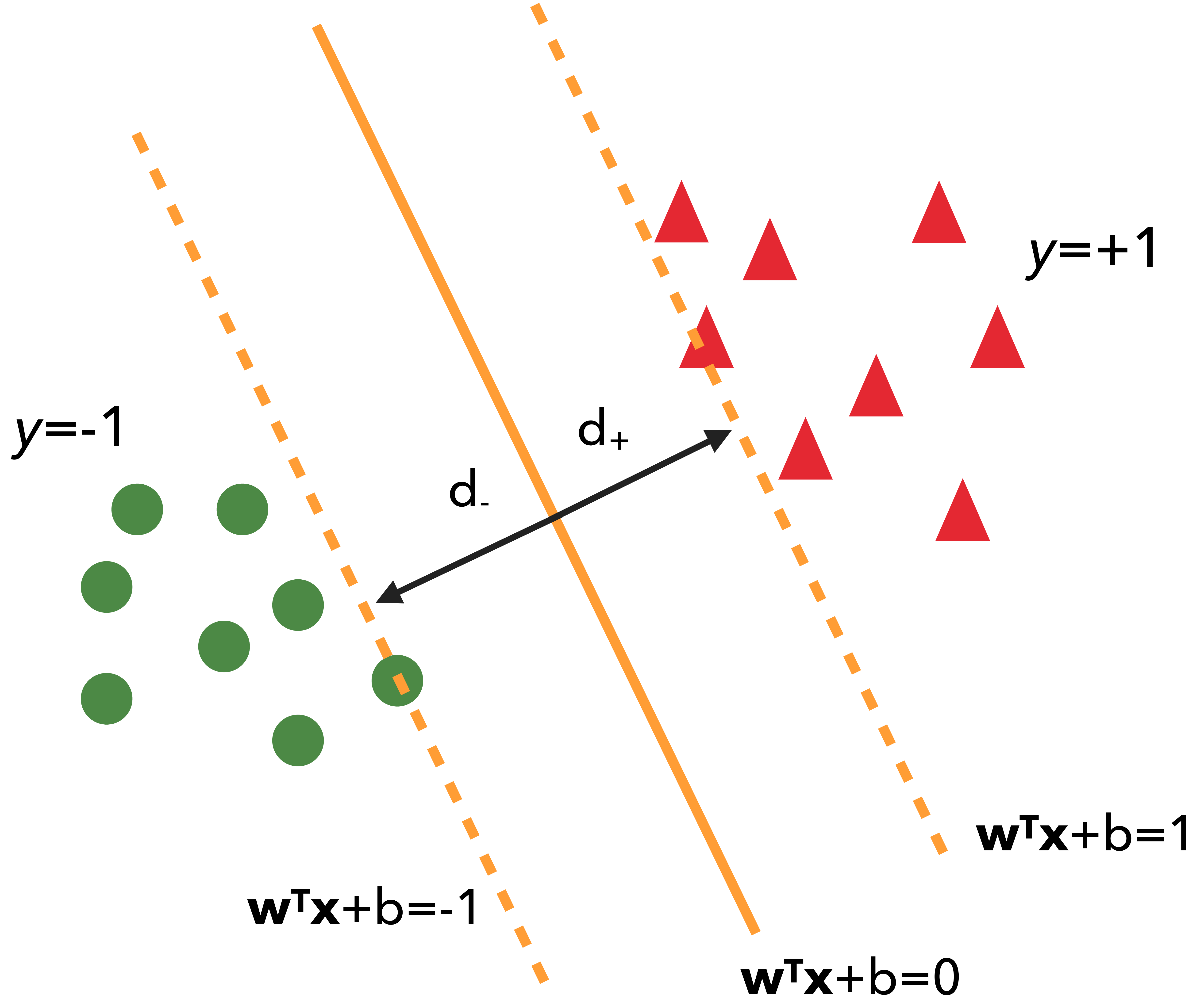
Repeat until stopping criteria is met

SVM: RECAP

SVM: KNOWLEDGE REPRESENTATION AND SCORING FUNCTION

- Linear SVM: $y = sign\left[\sum_{i=1}^{m} w_i x_i + b\right]$
- Margin = $d_+ + d_- = 2/||\mathbf{w}||$
- Optimization problem
  - max $2/||\mathbf{w}||$
  - subject to

    $y_i(\mathbf{w}^T \mathbf{x}_i + b) \geq 1, \forall i \in \{1,2,\ldots,N\}$



SVM LEARNING

- Equivalent to minimize $||\mathbf{w}||^2/2$ subject to

$$y_i(\mathbf{w}^\mathsf{T}\mathbf{x}_i + b) \geq 1, \forall i \in \{1,2,\ldots,N\}$$

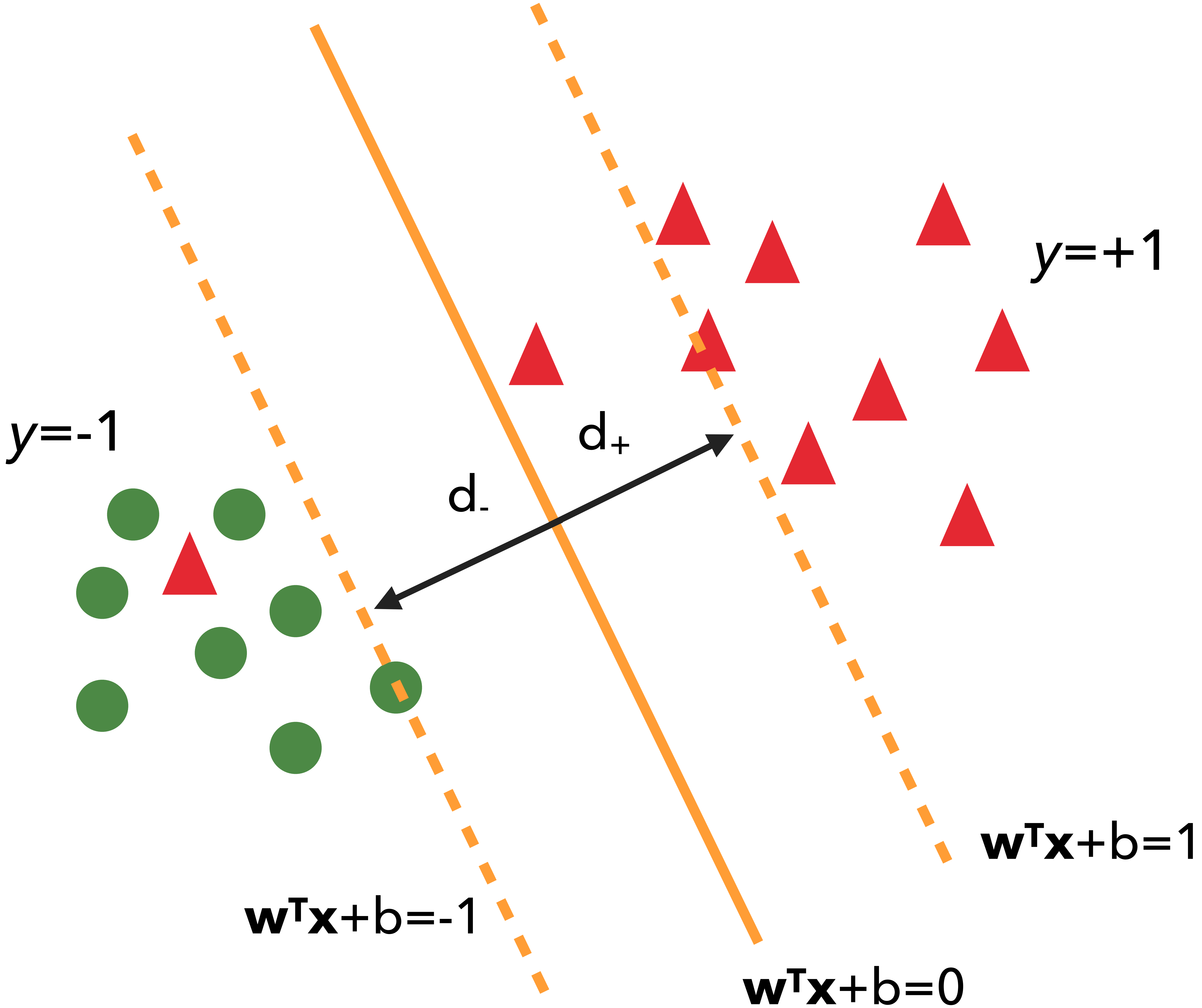
- This is a **quadratic optimization** problem subject to linear constraints, there is a unique minimum
- Lagrangian function $L(\mathbf{w}, b, \lambda_i) = \frac{1}{2}||\mathbf{w}||^2 + \sum_{i=1}^{N} \lambda_i(1 - y_i(\mathbf{w}^\mathsf{T}\mathbf{x}_\mathbf{i} + b))$

WHAT ABOUT LINEARLY NON-SEPARABLE DATA?

- Introduce slack variables $\varepsilon_i \geq 0$ such that:

  $y_i(\mathbf{w}^T\mathbf{x}_i + b) \geq 1 - \varepsilon_i, \forall i \in \{1,2,\ldots,N\}$

- ε_i measures the amount of error
  - When $0 < \varepsilon_i \leq 1$, data is between the margin, but classified correctly
  - When $\varepsilon_i > 1$, data is misclassified



“SOFT” MARGIN OPTIMIZATION

- With slack variables the score function is:

$$\min_{\mathbf{w},\xi} ||\mathbf{w}||^2 + C\sum_{i}^{N} \xi_i$$

- And new constraints:

$$y_i(x_i \cdot w + b) - (1 - \xi_i) \geq 0 \;\; \forall i$$

- If ξ are sufficiently large, then every constraint can be satisfied
- C is regularization parameter
  - Small C means constraints can be ignored in order to find large margin
  - Large C means constraints cannot be ignored and result is small margin (C=∞ enforces hard margin)

SVM OPTIMIZATION

- Constraint can be rewritten as:

$$y_i f(x_i) \geq 1 - \xi_i \quad \forall i$$

- Together with $\xi_i \geq 0$, is equivalent to:

$$\xi_i = max\Big(0, 1 - y_i f(x_i)\Big)$$

- Hence we can use the following score in unconstrained optimization:

$$\min_{\mathbf{w}} ||\mathbf{w}||^2 + C \sum_{i}^{N} \left[max\Big(0, 1 - y_i f(x_i)\Big) \right]$$

NEW OBJECTIVE

$$\min_{\mathbf{w}} ||\mathbf{w}||^2 + C \sum_{i}^{N} \left[\boxed{max\Big(0, 1 - y_i f(x_i)\Big)} \right]$$

Hinge Loss

Points are in three categories:

1. $y_i f(x_i) > 1$
   Point is outside margin.
   No contribution to loss
2. $y_i f(x_i) = 1$
   Point is on margin.
   No contribution to loss.
   As in hard margin case.
3. $y_i f(x_i) < 1$
   Point violates margin constraint.
   Contributes to loss