Lecture 3

Tian Han

Outline

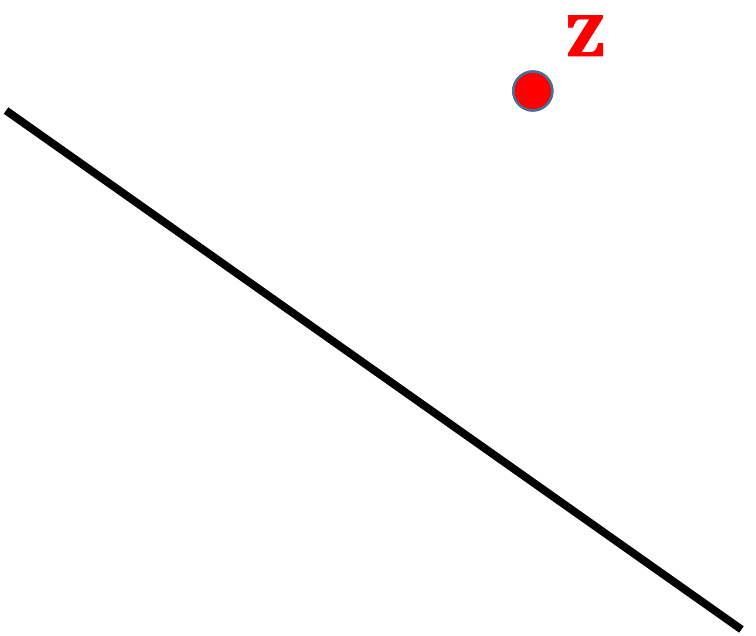
- Support Vector Machine (SVM)
- Regularization
- Convex optimization basics

Support Vector Machine (SVM)

Project a Point onto a Hyperplane

Project a Point onto a Hyperplane

Question: how to project $\mathbf{z}$ onto the hyperplane?

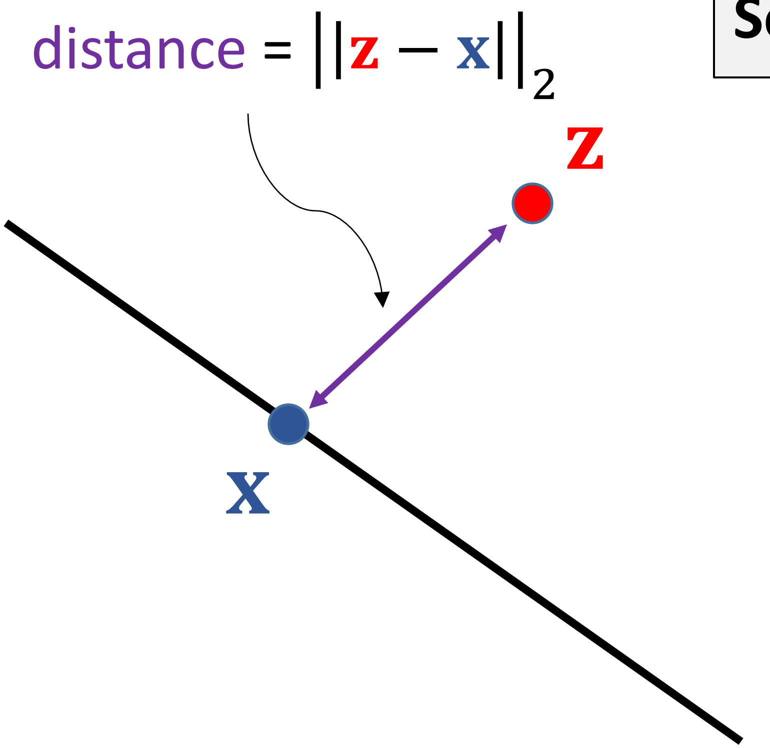


Hyperplane $\mathbf{w}^T\mathbf{x} + b = 0$

Project a Point onto a Hyperplane

Question: how to project $\mathbf{z}$ onto the hyperplane?

Solution: find $\mathbf{x}$ on the hyperplane such that $||\mathbf{z}-\mathbf{x}||_2^2$ is minimized.



Hyperplane $\mathbf{w}^T\mathbf{x}+b=0$

- $\min_{\mathbf{x}} ||\mathbf{z}-\mathbf{x}||_2^2$; s.t. $\mathbf{w}^T\mathbf{x}+b=0$

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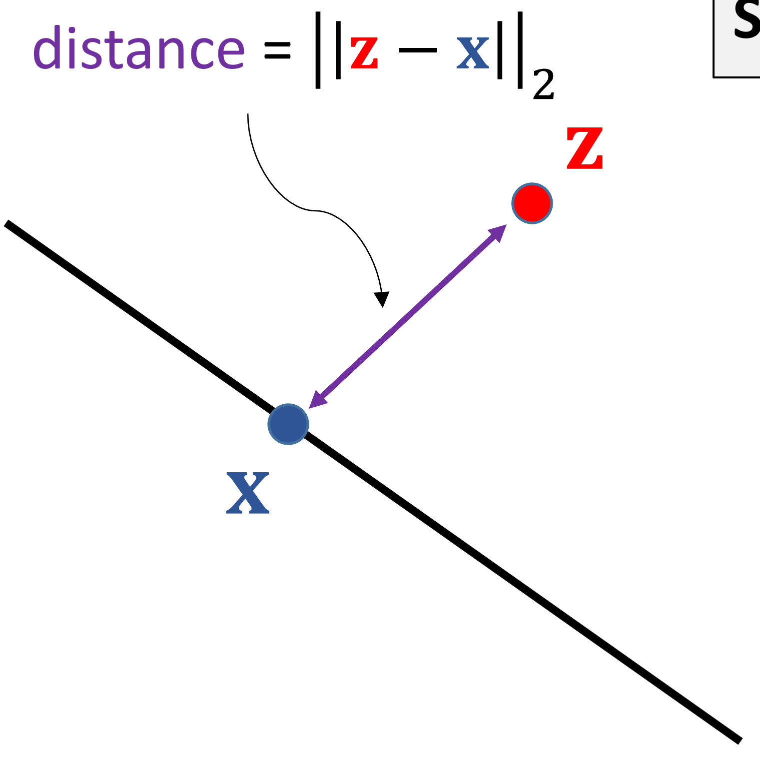


Hyperplane $\mathbf{w}^T\mathbf{x}+b=0$

- $\min_{\mathbf{x}} ||\mathbf{z}-\mathbf{x}||_2^2; \quad$ s.t. $\mathbf{w}^T\mathbf{x}+b=0$
- Solve the problem using the Lagrange multiplier:

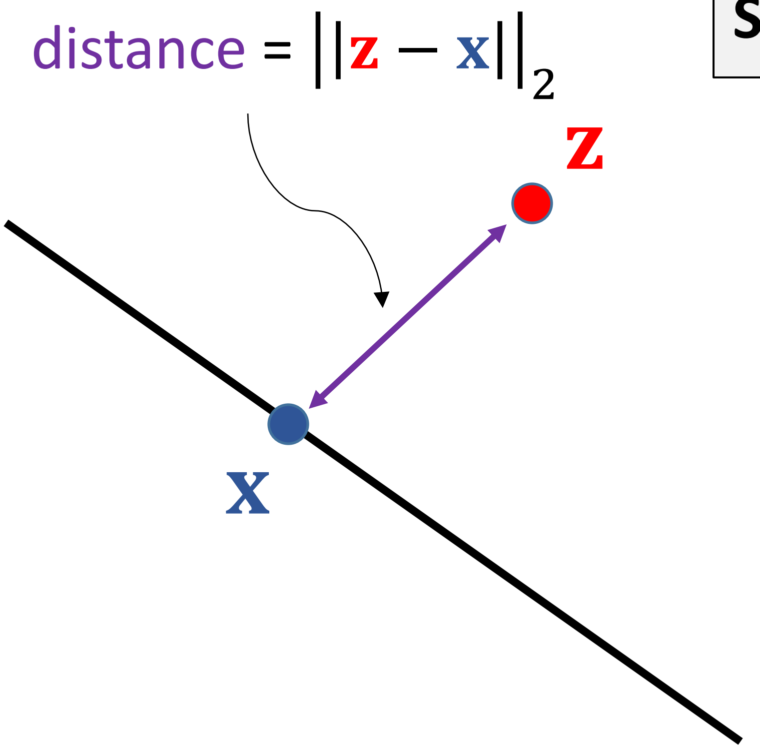
$$\begin{cases} \dfrac{\partial ||\mathbf{z}-\mathbf{x}||_2^2}{\partial \mathbf{x}} + \lambda \dfrac{\partial\,(\mathbf{w}^T\mathbf{x}+b)}{\partial \mathbf{x}} = 0; \\ \mathbf{w}^T\mathbf{x}+b=0. \end{cases}$$

- Solution: $\mathbf{x} = \mathbf{z} - \frac{\mathbf{w}^T\mathbf{z}+b}{||\mathbf{w}||_2^2}\mathbf{w}$

Project a Point onto a Hyperplane

Question: how to project $\mathbf{z}$ onto the hyperplane?

Solution: find $\mathbf{x}$ on the hyperplane such that $\|\mathbf{z} - \mathbf{x}\|_2^2$ is minimized.



Hyperplane $\mathbf{w}^T\mathbf{x} + b = 0$

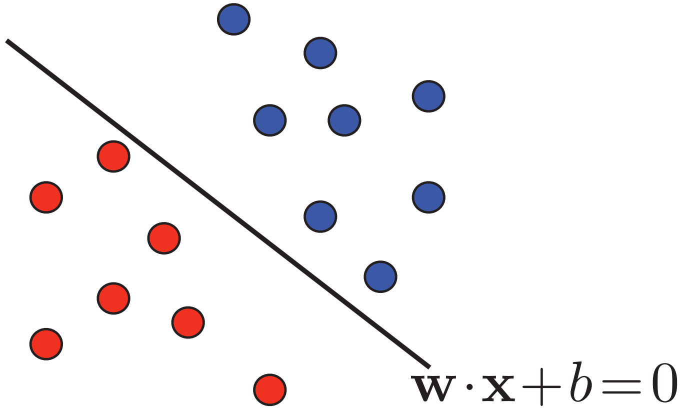
- Solution: $\mathbf{x} = \mathbf{z} - \frac{\mathbf{w}^T\mathbf{z}+b}{\|\mathbf{w}\|_2^2}\mathbf{w}$
- The ℓ_2 distance between $\mathbf{z}$ and the hyperplane is

$$\boxed{\|\mathbf{z} - \mathbf{x}\|_2 = \frac{|\mathbf{w}^T\mathbf{z}+b|}{\|\mathbf{w}\|_2}.}$$

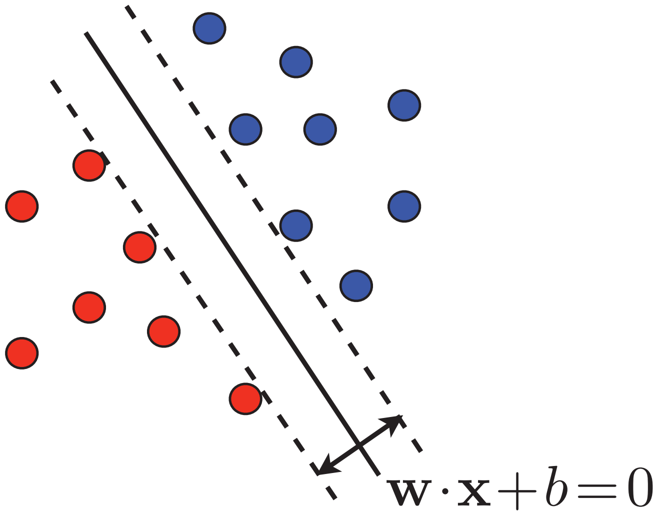
Support Vector Machine (SVM)

Support Vector Machine (SVM)

Separate data by a hyperplane (assume the data are separable)



An arbitrary hyperplane.



The hyperplane that maximizes the margin.

The figure is from the book *"Foundations of Machine Learning"*

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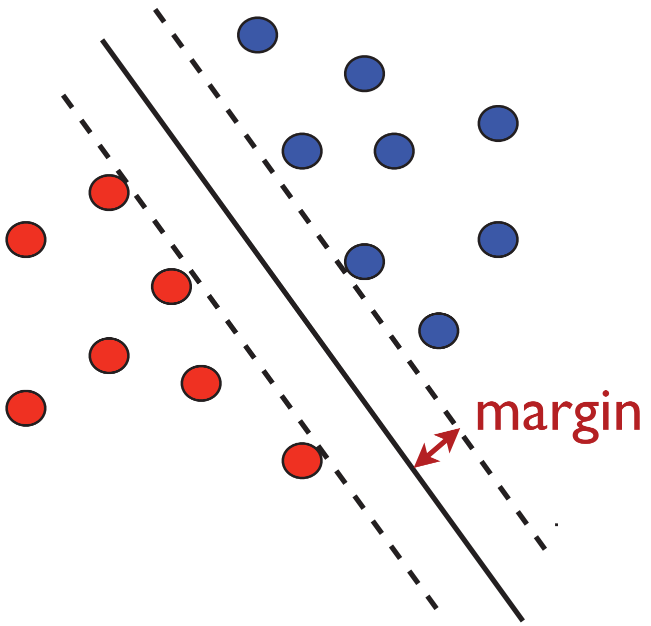

Hyperplane $\mathbf{w}^T\mathbf{x} + b = 0$

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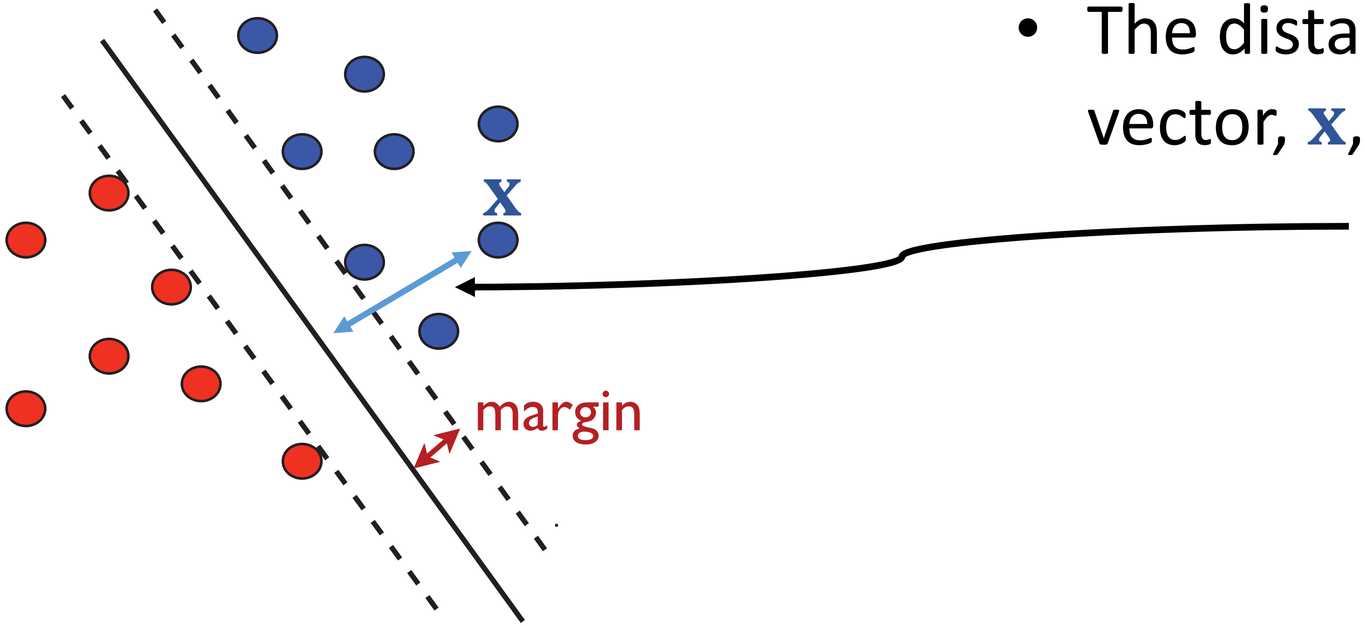

Hyperplane $\mathbf{w}^T\mathbf{x} + b = 0$

- The distance between any feature vector, $\mathbf{x}$, and the hyperplane is

$$\text{dist} = \frac{|\mathbf{w}^T\mathbf{x}+b|}{||\mathbf{w}||_2}.$$

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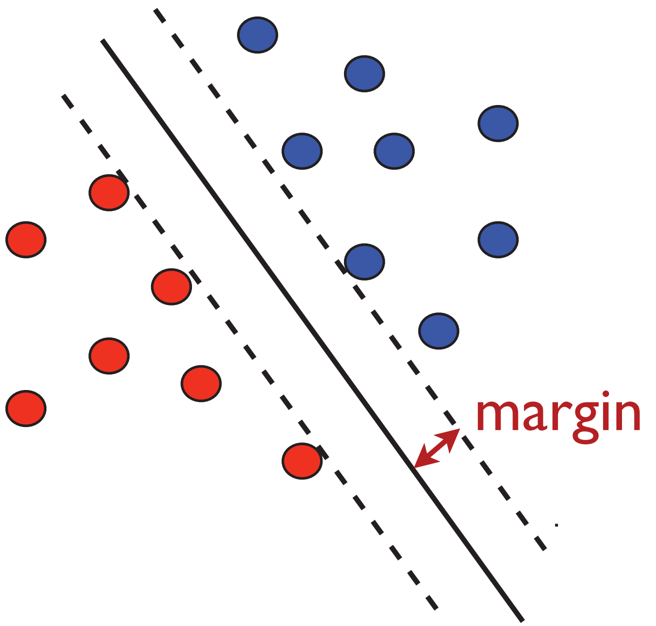

Hyperplane $\mathbf{w}^T\mathbf{x} + b = 0$

- The distance between any feature vector, $\mathbf{x}$, and the hyperplane is
$$\text{dist} = \frac{|\mathbf{w}^T\mathbf{x}+b|}{||\mathbf{w}||_2}.$$
- The margin is the smallest distance:
$$\min_j \frac{|\mathbf{w}^T\mathbf{x}_j+b|}{||\mathbf{w}||_2}$$

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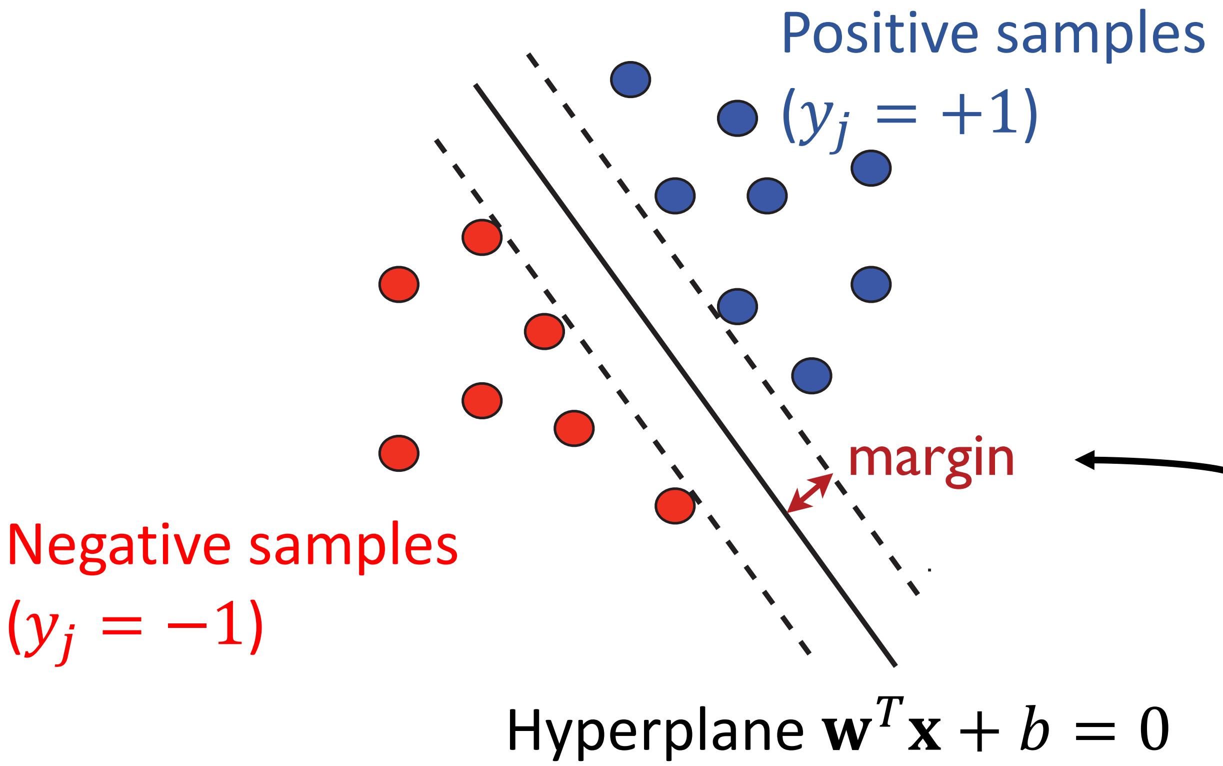

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- The margin is the smallest distance:

$$\min_j \frac{|\mathbf{w}^T\mathbf{x}_j+b|}{||\mathbf{w}||_2} = \min_j \frac{y_j(\mathbf{w}^T\mathbf{x}_j+b)}{||\mathbf{w}||_2}$$

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Support Vector Machine (SVM)

Margin = $\min_j \frac{y_j(\mathbf{w}^T\mathbf{x}_j+b)}{||\mathbf{w}||_2}$; we want to maximize the margin.

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Define $\bar{\mathbf{x}}_j = \left[\mathbf{x}_j ; 1 \right] \in \mathbb{R}^{d+1}$

Define $\bar{\mathbf{w}} = [\mathbf{w}, b] \in \mathbb{R}^{d+1}$

➔ $\boxed{\mathbf{x}_j^T \mathbf{w} + b = \bar{\mathbf{x}}_j^T \bar{\mathbf{w}}}$

Support Vector Machine (SVM)

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$\Downarrow$

Support Vector Machine (SVM): $\max_{\mathbf{w}} \min_j \frac{y_j \mathbf{w}^T \mathbf{x}_j}{||\mathbf{w}||_2}$

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$$= \operatorname{argmax}_{\mathbf{w}} \frac{1}{||\mathbf{w}||_2}, \qquad \text{s.t.} \quad \left(\min_{j} \; y_j \mathbf{w}^T \mathbf{x}_j\right) = 1$$

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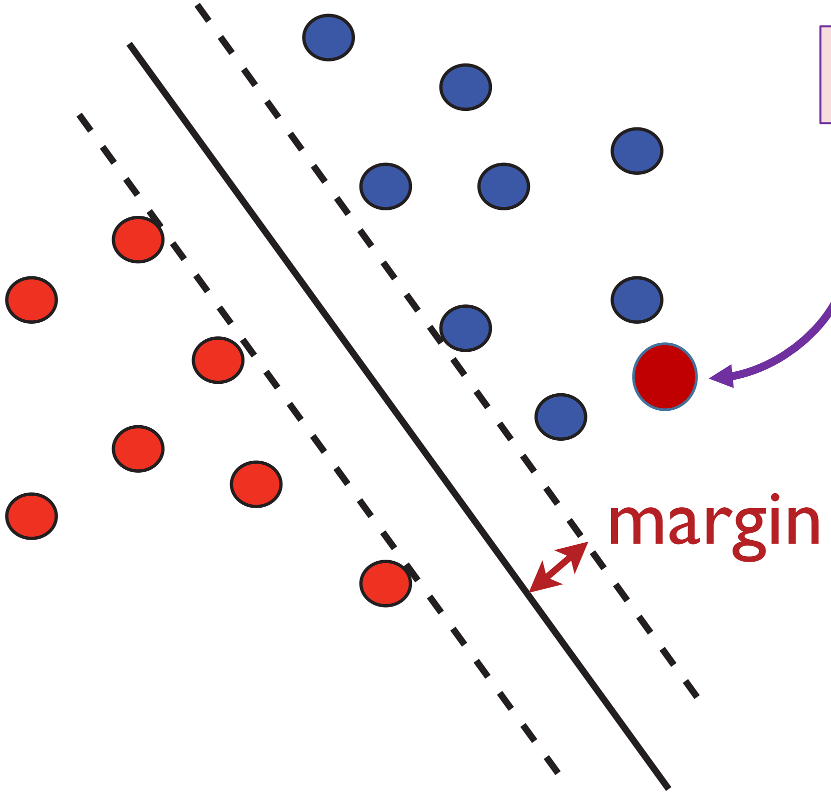
Support Vector Machine (SVM)

$$\min_{\mathbf{w}} \|\mathbf{w}\|_2^2, \quad \text{s.t.} \quad y_j \mathbf{w}^T \mathbf{x}_j \geq 1 \ \text{ for all } j \in \{1, \cdots, n\}.$$

Equivalent form of SVM

Support Vector Machine (SVM)

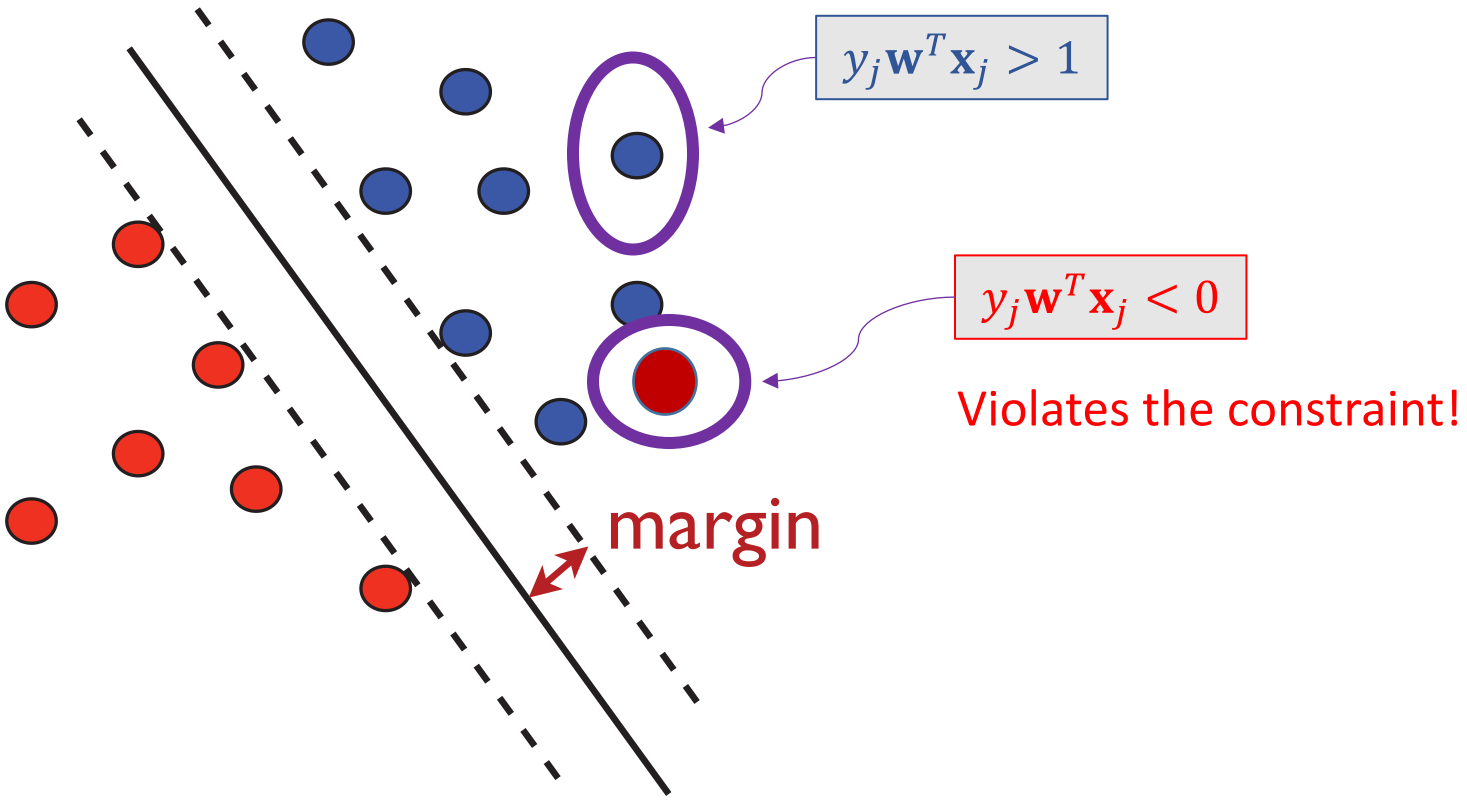
$$\min_{\mathbf{w}} \|\mathbf{w}\|_2^2, \quad \text{s.t.} \quad y_j \mathbf{w}^T \mathbf{x}_j \geq 1 \ \text{ for all } j \in \{1, \cdots, n\}.$$



What if the data is inseparable?

Support Vector Machine (SVM)

$$\min_{\mathbf{w}} \|\mathbf{w}\|_2^2, \quad \text{s.t.} \quad y_j \mathbf{w}^T \mathbf{x}_j \geq 1 \text{ for all } j \in \{1, \cdots, n\}.$$



Support Vector Machine (SVM)

$$\min_{\mathbf{w}} ||\mathbf{w}||_2^2, \quad \text{s.t.} \quad 1 - y_j \mathbf{w}^T \mathbf{x}_j \leq 0 \ \text{ for all } j \in \{1, \cdots, n\}.$$

$\Downarrow$ **Relax**

$$\min_{\mathbf{w}, \xi_j} ||\mathbf{w}||_2^2 + \lambda \sum_j [\xi_j]_+, \quad \text{s.t.} \quad 1 - y_j \mathbf{w}^T \mathbf{x}_j = \xi_j \ \text{ for all } j \in \{1, \cdots, n\}.$$

- $[\xi_j]_+ = \max\{\xi_j, 0\}$

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- $[\xi_j]_+ = \max\{\xi_j, 0\}$
- $\xi_j \leq 0$ means the constraint $1 - y_j \mathbf{w}^T \mathbf{x}_j \leq 0$ is satisfied
  ➔ no penalty!
- $\xi_j > 0$ means the constraint is violated (because the data is inseparable)
  ➔ penalize the violation ξ_j.

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$\Updownarrow$ **Equivalent**

$$\min_{\mathbf{w}, b} ||\mathbf{w}||_2^2 + \lambda \sum_j [1 - y_j \mathbf{w}^T \mathbf{x}_j]_+.$$

Comparisons

SVM: $\min_{\mathbf{w}} ||\mathbf{w}||_2^2 + \lambda \sum_j g(y_j \mathbf{w}^T \mathbf{x}_j)$.

Hinge loss: $g(z) = [1 - z]_+$.

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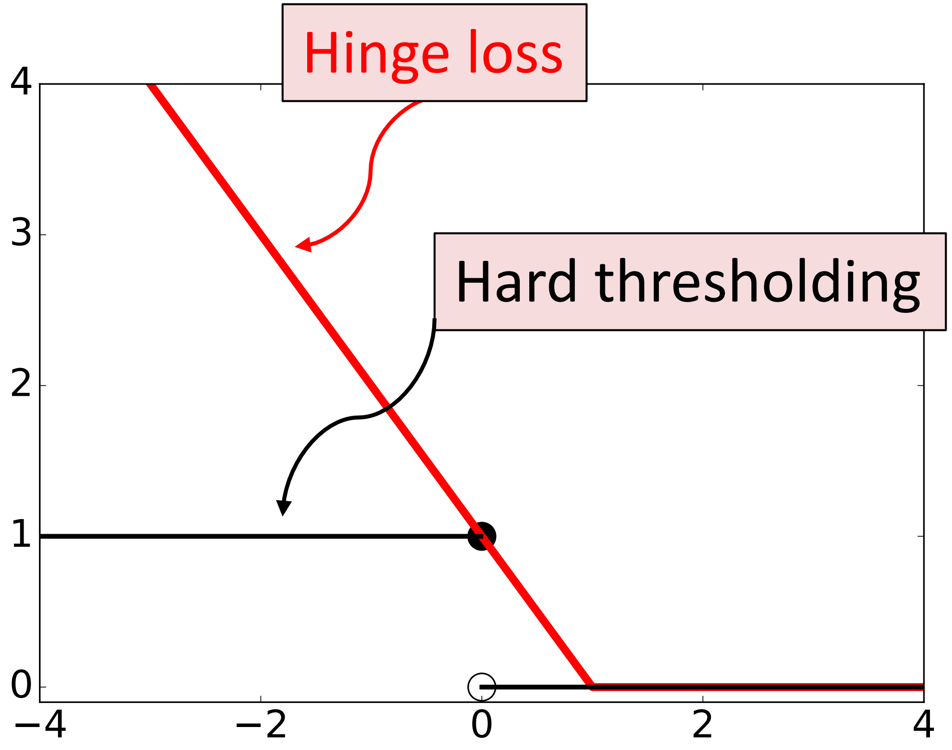

Hard thresholding: $h(\mathrm{z}) = \begin{cases} 1, & \text{if } z < 0; \\ 0, & \text{if } z \geq 0. \end{cases}$

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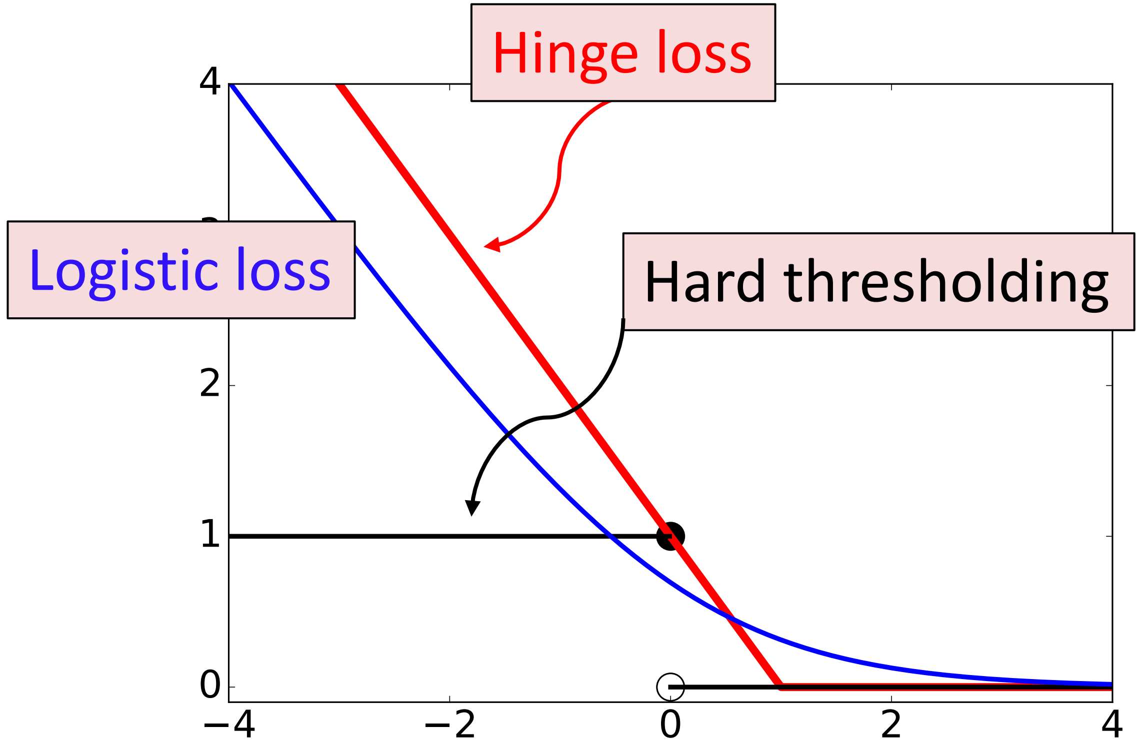

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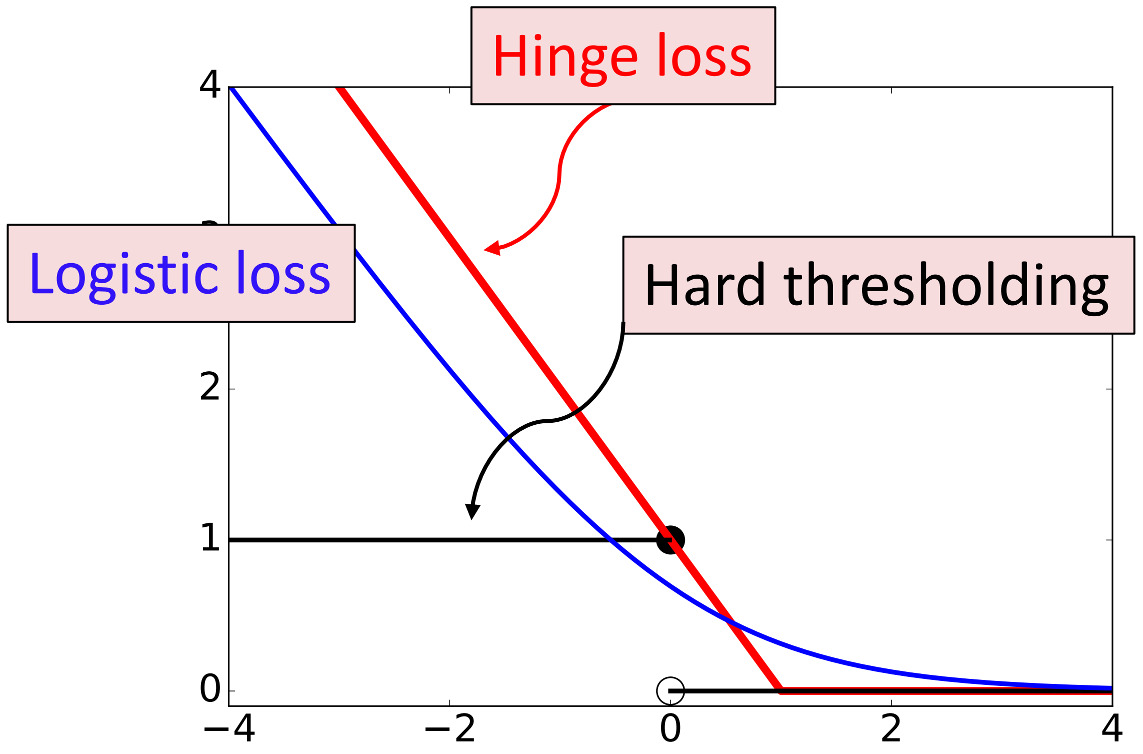
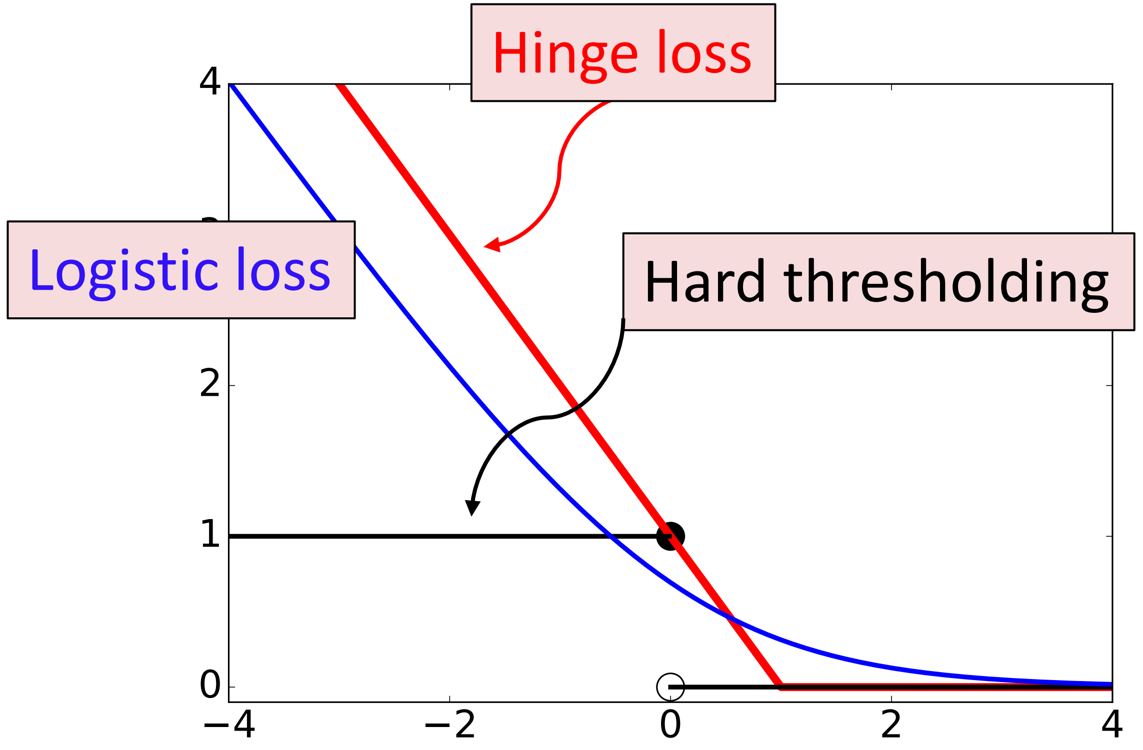
Logistic loss: $l(z) = \log(1 + e^{-z}).$

Comparisons



- Convexity
  - Hinge loss and logistic loss are convex.
  - Global optima can be efficiently found.
- Smoothness
  - Hinge loss is non-smooth.
  - Logistic loss is smooth.

Comparisons



- Convexity
  - Hinge loss and logistic loss are convex.
  - Global optima can be efficiently found.
- Smoothness
  - Hinge loss is non-smooth.
  - Logistic loss is smooth.
- Logistic regression is easier to solve than SVM.
  - GD for logistic regression has linear convergence.
  - Algorithms for SVM have sub-linear convergence.

Regularizations

The ℓ_2-Norm Regularization

Linear Regression

Input: feature matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ and labels $\mathbf{y} \in \mathbb{R}^{n}$.

Output: vector $\mathbf{w} \in \mathbb{R}^{d}$ such that $\mathbf{X}\mathbf{w} \approx \mathbf{y}$.

Task

Linear Regression

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Task

- Least squares regression:

$$\min_{\mathbf{w}} \ \frac{1}{n}\left|\left|\mathbf{X}\mathbf{w} - \mathbf{y}\right|\right|_2^2.$$

Methods

- Ridge regression:

$$\min_{\mathbf{w}} \ \frac{1}{n}\left|\left|\mathbf{X}\mathbf{w} - \mathbf{y}\right|\right|_2^2 + \gamma \left|\left|\mathbf{w}\right|\right|_2^2.$$

Loss Function

Regularization

Ridge Regression: Algorithms

- **Analytical solution:** $\mathbf{w}^\star = (\mathbf{X}^T\mathbf{X} + n\gamma\mathbf{I}_d)^{-1}\mathbf{X}^T\mathbf{y}$.
  - Time complexity: $O(nd^2 + d^3)$.

Ridge Regression: Algorithms

- **Analytical solution:** $\mathbf{w}^\star = (\mathbf{X}^T\mathbf{X} + n\gamma\mathbf{I}_d)^{-1}\mathbf{X}^T\mathbf{y}$.
  - Time complexity: $O(nd^2 + d^3)$.
- Derivations:
  - The objective function is $Q(\mathbf{w}) = \frac{1}{n}\,||\mathbf{Xw} - \mathbf{y}||_2^2 + \gamma\,||\mathbf{w}||_2^2$.
  - The gradient is $\nabla Q(\mathbf{w}) = \frac{2}{n}\mathbf{X}^T(\mathbf{Xw} - \mathbf{y}) + 2\gamma\mathbf{w}$.
  - Set $\nabla Q(\mathbf{w}^\star) = 0$ leads to $\frac{2}{n}(\mathbf{X}^T\mathbf{X} + n\gamma\mathbf{I}_d)\mathbf{w}^\star = \frac{2}{n}\mathbf{X}^T\mathbf{y}$.
- Time complexity:
  - $O(nd^2)$ time for the multiplication $\mathbf{X}^T\mathbf{X}$.
  - $O(d^3)$ time for the inversion of the $d\times d$ matrix $\mathbf{X}^T\mathbf{X} + n\gamma\mathbf{I}_d$.

Ridge Regression: Algorithms

- **Conjugate gradient (CG)**
  - $O\left(\sqrt{\kappa}\log\frac{n}{\epsilon}\right)$ iterations to reach ϵ precision.
  - Hessian matrix: $\nabla^2 Q(\mathbf{w}) = \frac{2}{n}(\mathbf{X}^T\mathbf{X} + n\gamma\mathbf{I}_d)$.
  - $\kappa = \frac{\lambda_{\max}(\mathbf{X}^T\mathbf{X}) + n\gamma}{\lambda_{\min}(\mathbf{X}^T\mathbf{X}) + n\gamma}$ is the condition number of the Hessian.

Usefulness of Regularization

Question: Why do we use the ℓ_2-norm regularization?

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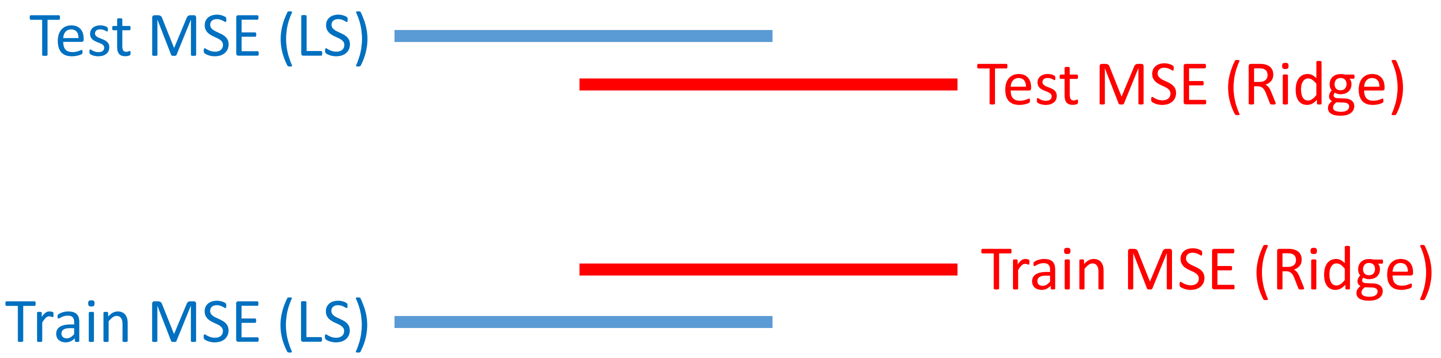
- Reason 1: easier to optimize.
  - Conjugate gradient (CG) requires $O\left(\sqrt{\kappa}\log\frac{n}{\epsilon}\right)$ iterations to reach ϵ precision.
  - Least squares: $\kappa = \frac{\lambda_{\max}(\mathbf{X}^T\mathbf{X})}{\lambda_{\min}(\mathbf{X}^T\mathbf{X})}$.
  - Ridge regression: $\kappa = \frac{\lambda_{\max}(\mathbf{X}^T\mathbf{X}) + n\gamma}{\lambda_{\min}(\mathbf{X}^T\mathbf{X}) + n\gamma}$. ($\gamma \uparrow$, $\kappa \downarrow$).
  - ➡ CG converges faster as γ increases.

Usefulness of Regularization

Question: Why do we use the ℓ_2-norm regularization?

- Reason 1: easier to optimize.
- Reason 2: better generalization.
  - Least squares has better training error (due to the optimality).
  - Ridge regression makes better prediction on test set.



The ℓ_1-Norm Regularization

Motivations

$$\mathbf{x} \in \mathbb{R}^d \xrightarrow{\text{prediction}} y \in \mathbb{R}$$

Fact 1: y can be independent of some of the d feature.

Fact 2: if $d \gg n$, linear models are likely to overfit.

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Example: Use genomic data to predict disease.

- d is huge: human have 20K protein-coding genes.
- n is small: tens or hundreds of human participants in an experiment.
- Most genes are irrelevant to a specific disease.

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Fact 1: y can be independent of some of the d feature.

Fact 2: if $d \gg n$, linear models are likely to overfit.

Goal 1: Select the features relevant to y.

Goal 2: Prevent overfitting for large d, small n problems.

The ℓ_1-Norm Constraint

- LASSO: $\min_{\mathbf{w}} \frac{1}{2n} ||\mathbf{Xw} - \mathbf{y}||_2^2 ;$ $\boxed{\text{s.t. } ||\mathbf{w}||_1 \leq t.}$

The feasible set $\left\{\mathbf{w}: \; ||\mathbf{w}||_1 \leq t\right\}$ is convex.

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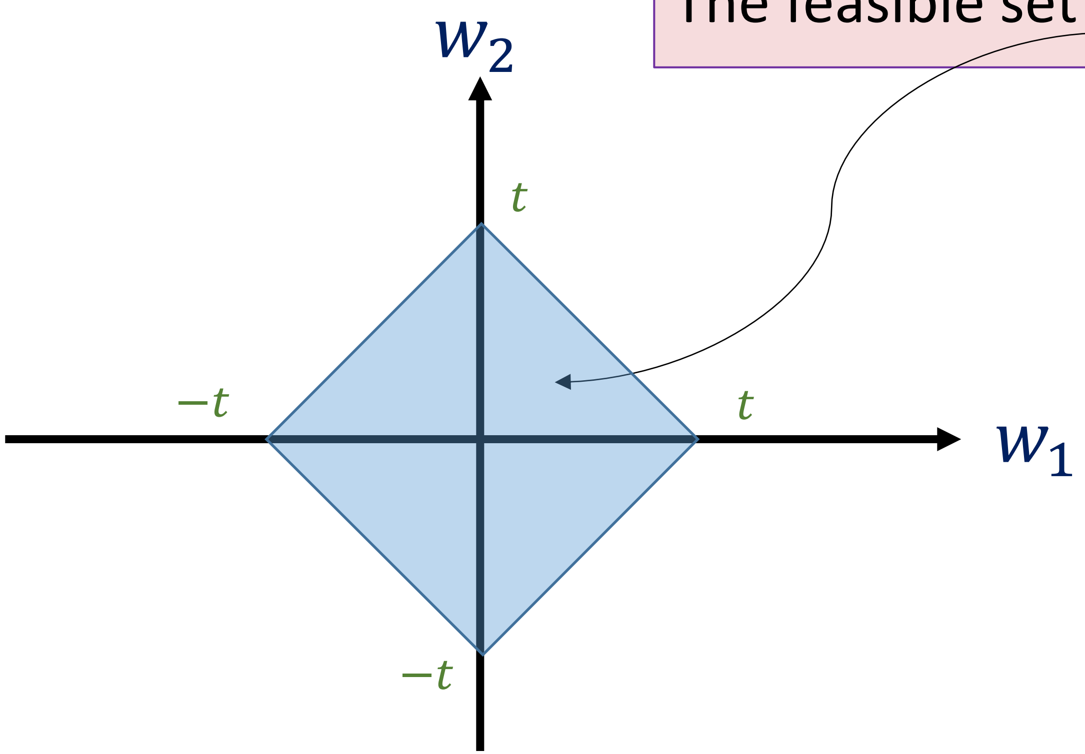

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  - It is a convex optimization model.
  - The optimal solution $\mathbf{w}^\star$ is **sparse** (i.e., most entries are zeros).
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  - Smaller t ➔ sparser $\mathbf{w}^\star$.
  - Sparsity ⬌ feature selection. Why?
    - Let $\mathbf{x}'$ be a test feature vector.
    - The prediction is $\mathbf{x}'^T \mathbf{w}^\star = w_1^\star x_1' + w_2^\star x_2' + \cdots + w_d^\star x_d'$.
    - If $w_1^\star = 0$, then the prediction is independent of x_1'.

The ℓ_1-Norm Regularization

- LASSO: $\min_{\mathbf{w}} \frac{1}{2n} ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2; \quad \text{s.t.} \; ||\mathbf{w}||_1 \leq t.$

- **Another form:** $\min_{\mathbf{w}} \quad \frac{1}{2n} ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2 \; + \; \gamma ||\mathbf{w}||_1.$

Loss Function

Regularization

Summary

Regularized ERM

- Regularized empirical risk minimization:

$$\min_{\mathbf{w}\in\mathbb{R}^d} \quad \frac{1}{n}\sum_{i=1}^{n} L(\mathbf{w};\ \mathbf{x}_i, y_i) \quad + \quad R(\mathbf{w}).$$

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Loss Function

- Linear regression: $L(\mathbf{w};\ \mathbf{x}_i, y_i) = \frac{1}{2}(\mathbf{w}^T\mathbf{x}_i - y_i)^2$
- Logistic regression: $L(\mathbf{w};\ \mathbf{x}_i, y_i) = \log(1 + \exp(-y_i\mathbf{w}^T\mathbf{x}_i))$
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Regularized ERM

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Regularization

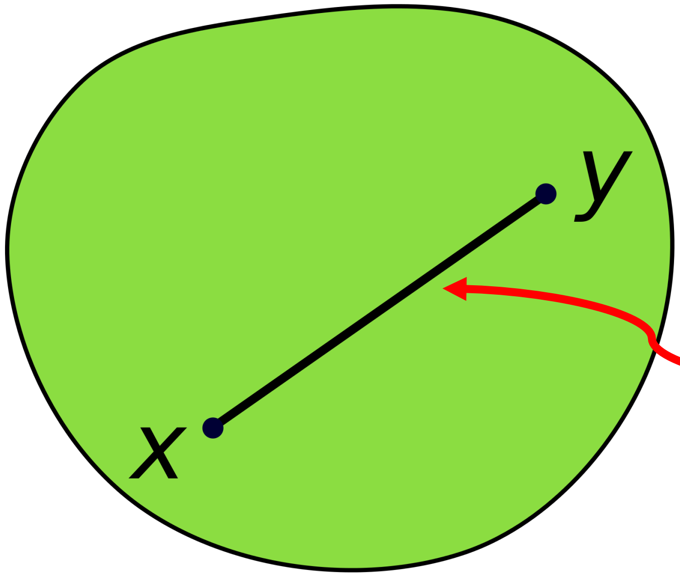
- ℓ_1-norm: $R(\mathbf{w}) = \gamma\|\mathbf{w}\|_1$
- ℓ_2-norm: $R(\mathbf{w}) = \gamma\|\mathbf{w}\|_2^2$
- Elastic net: $R(\mathbf{w}) = \gamma_1\|\mathbf{w}\|_1 + \gamma_2\|\mathbf{w}\|_2^2$

Basics of Convex Optimization

Convex Sets

Convex Set

Definition (Convex Set).
A set $\mathcal{C}$ is convex if and only if for any $\mathbf{x}, \mathbf{y} \in \mathcal{C}$ and any $\eta \in (0, 1)$, the point $\eta\mathbf{x} + (1-\eta)\mathbf{y}$ is also in $\mathcal{C}$.



A convex set $\mathcal{C}$.

By definition, the line segment between $\mathbf{x}$ and $\mathbf{y}$ is in $\mathcal{C}$.

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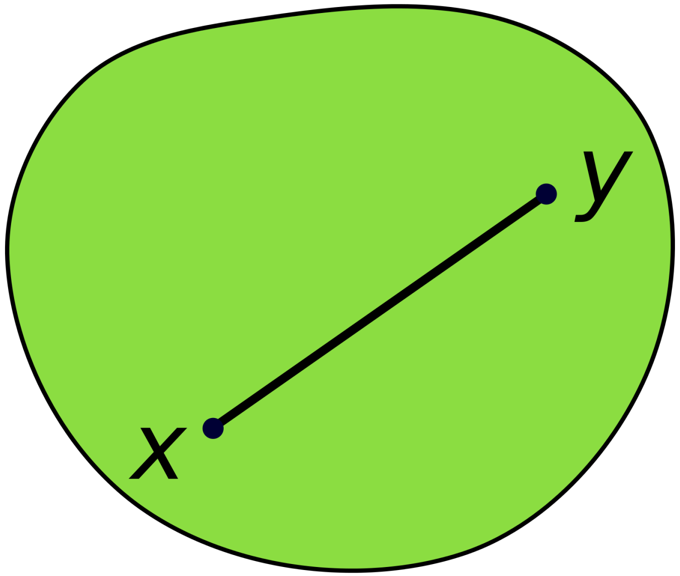

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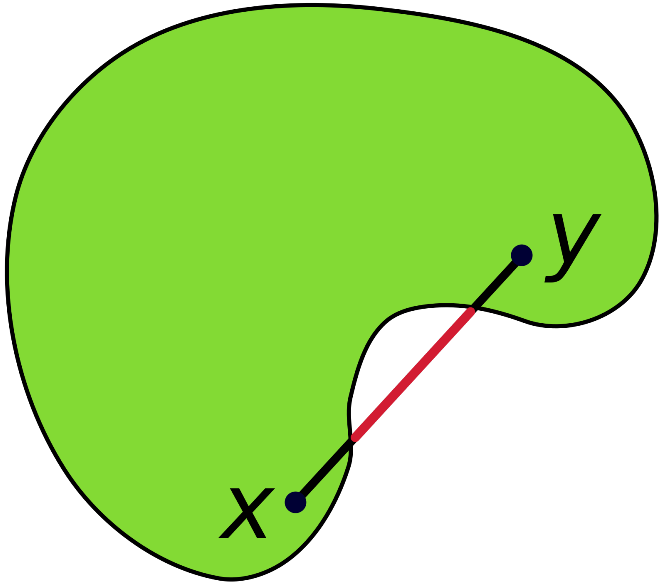

A non-convex set.

Convex Set: Examples

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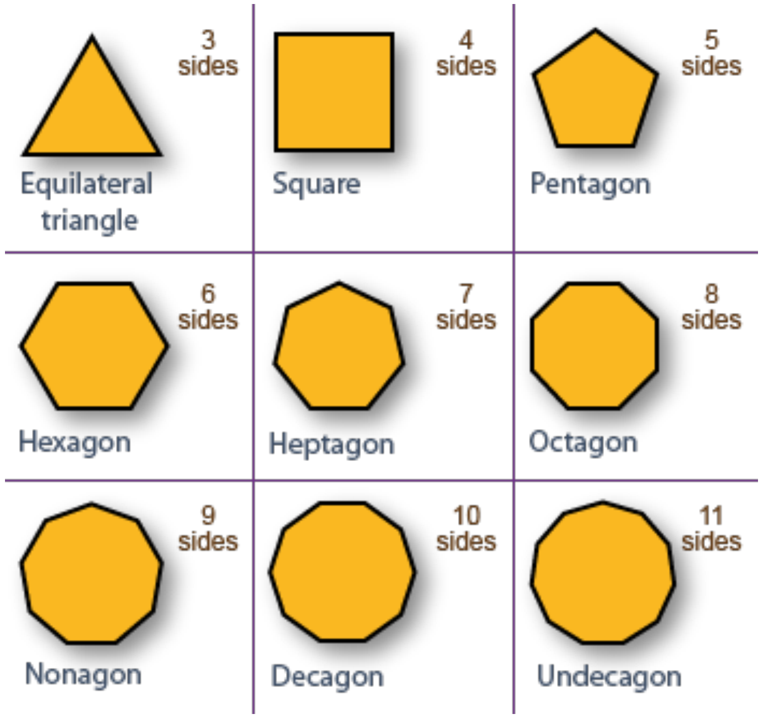
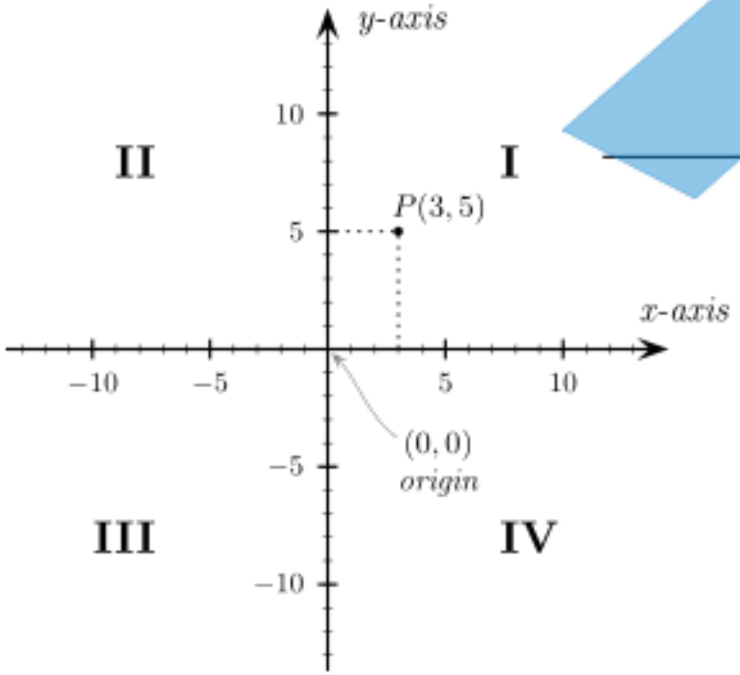
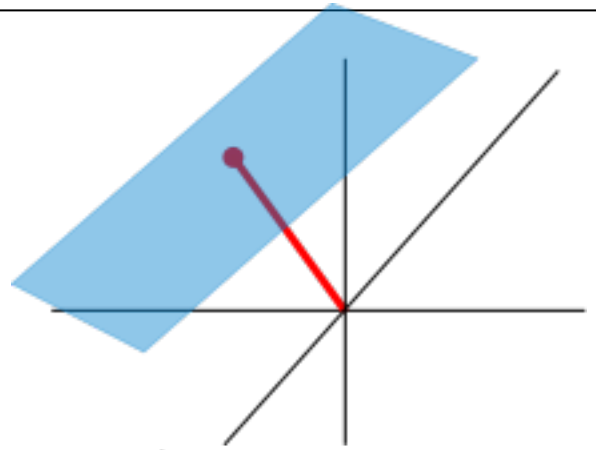
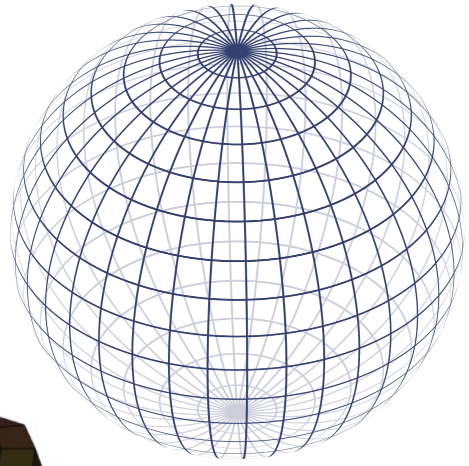
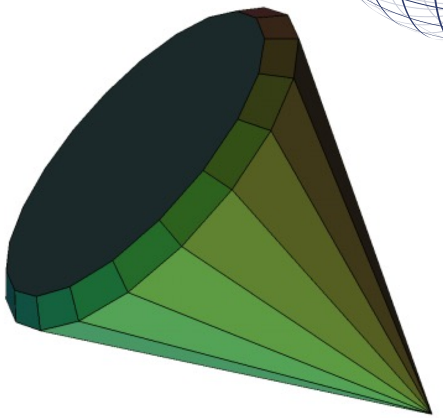




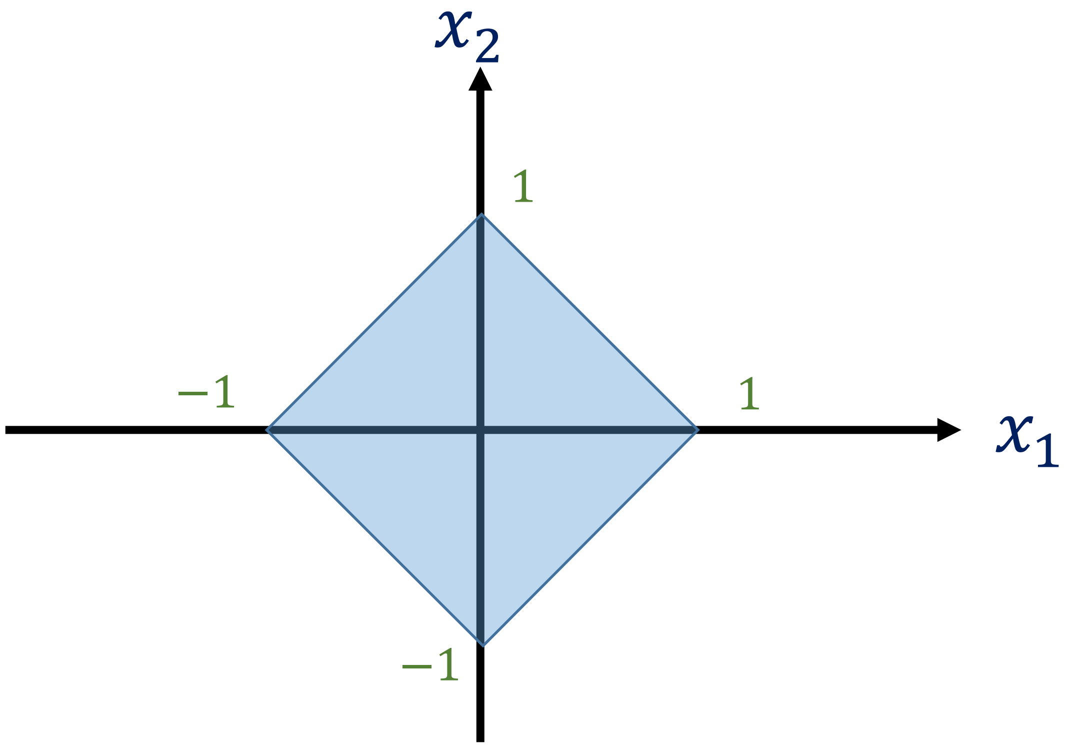






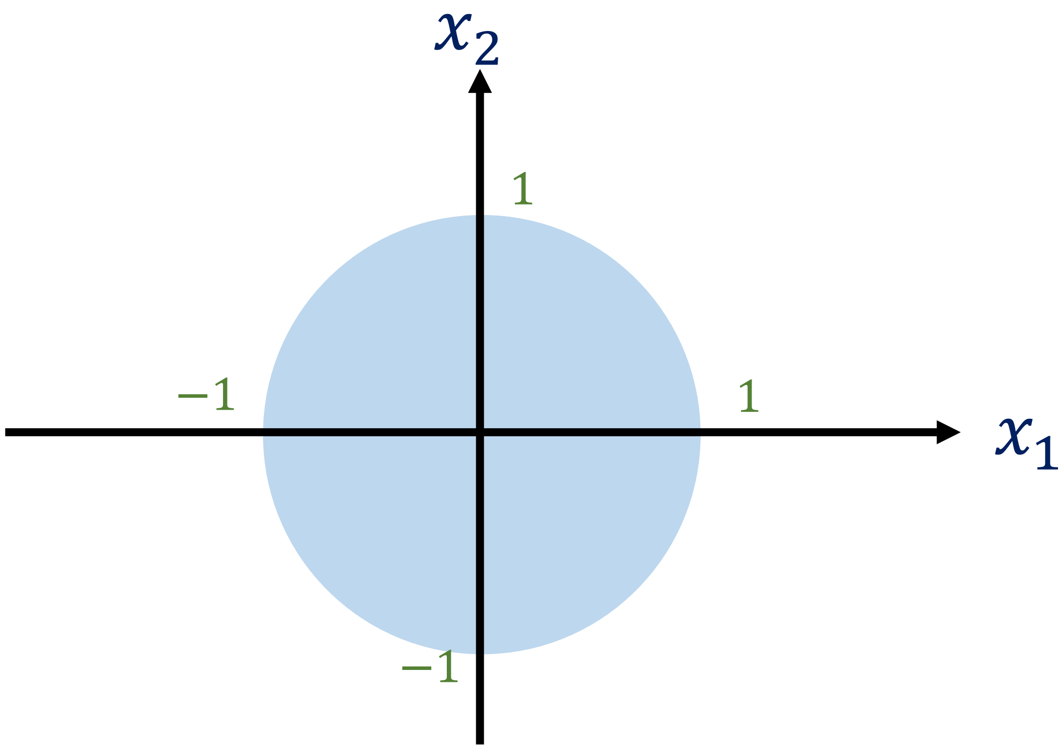
Convex Set: Examples

Example: The ℓ_1-norm ball $\left\{\mathbf{x}: \ \ ||\mathbf{x}||_1 \leq 1\right\}$.



Convex Set: Examples

Example: The ℓ_2-norm ball $\left\{\mathbf{x}:\ \ ||\mathbf{x}||_2 \leq 1\right\}$.



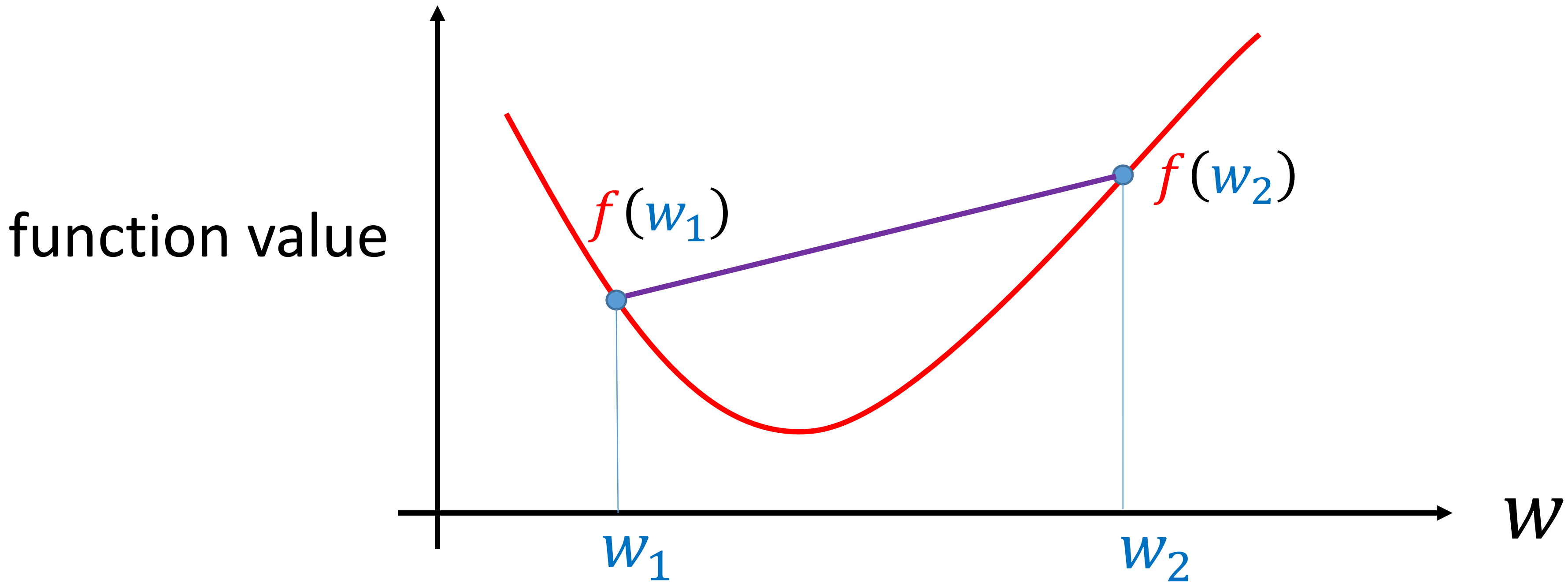
Convex Functions

Convex Function

Definition (Convex Function).

- Let $\mathcal{C}$ be a convex set and $f: \mathcal{C} \mapsto \mathbb{R}$ be a function.
- f is convex if for any $\mathbf{w}_1, \mathbf{w}_2 \in \mathcal{C}$ and any $\eta \in (0,1)$,

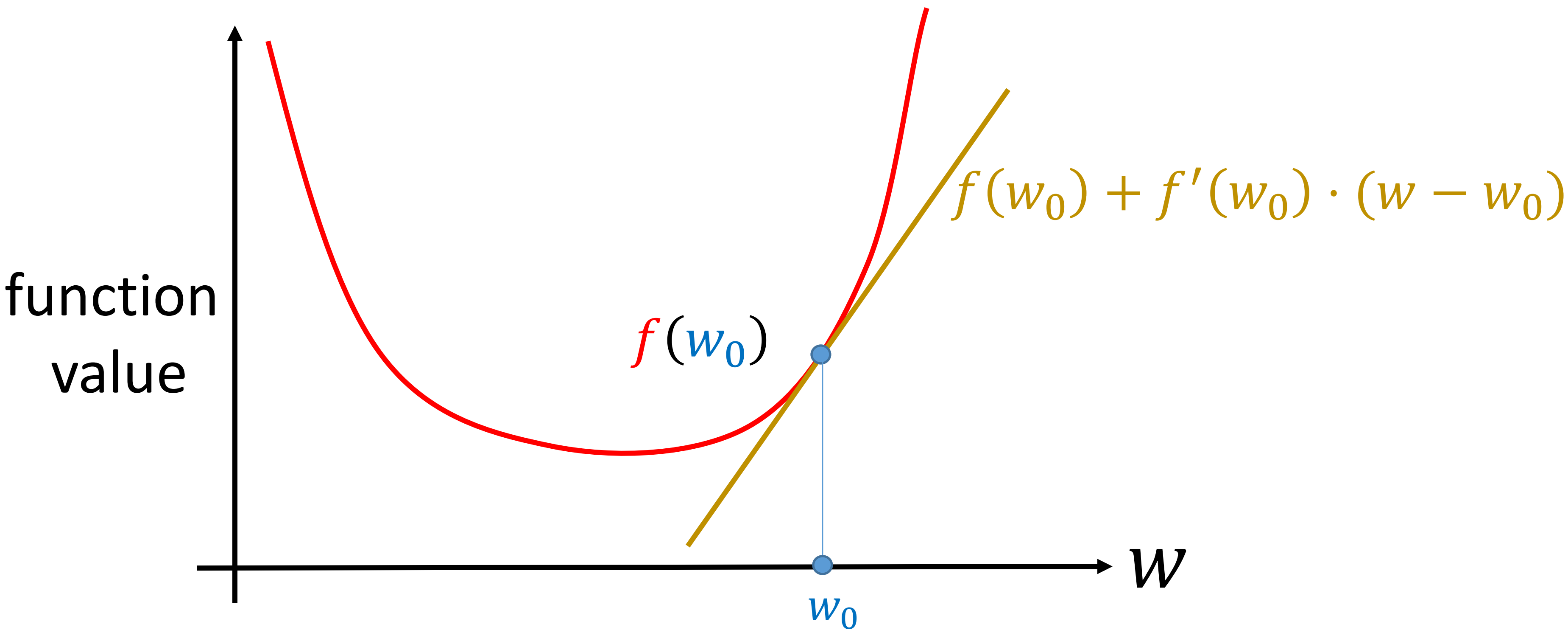
$$f(\eta \mathbf{w}_1 + (1-\eta)\mathbf{w}_2) \ \leq \ \eta f(\mathbf{w}_1) + (1-\eta) f(\mathbf{w}_2).$$



Convex Function: Properties

Properties of convex function:

1. $f(\mathbf{w}_0) + \nabla f(\mathbf{w}_0)^T(\mathbf{w} - \mathbf{w}_0) \leq f(\mathbf{w})$. (Assume f is differentiable).



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1. $f(\mathbf{w}_0) + \nabla f(\mathbf{w}_0)^T(\mathbf{w} - \mathbf{w}_0) \leq f(\mathbf{w})$. (Assume f is differentiable).
2. The Hessian matrix is everywhere positive semi-definite: $\nabla^2 f(\mathbf{w}) \succcurlyeq \mathbf{0}$.
   - Assume f is twice differentiable.
   - $\mathbf{H} \in \mathbb{R}^{d \times d}$ is positive semi-definite $\Longleftrightarrow$ for all $\mathbf{x} \in \mathbb{R}^d$, $\mathbf{x}^T \mathbf{H} \mathbf{x} \geq 0$.

Convex Functions

Question: Are they convex functions?

- $f(w) = w^2 + w - 1,\;\;$ for $w \in \mathbb{R}$.
- $f(w) = w^4,\;\;$ for $w \in \mathbb{R}$.
- $f(w) = \log_e w,\;\;$ for $w > 0$.
- $f(\mathbf{w}) = \frac{1}{2}||\mathbf{w}||_2^2,\;\;$ for $\mathbf{w} \in \mathbb{R}^d$.
- $f(\mathbf{w}) = \frac{1}{2}||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2,\;\;$ for $\mathbf{w} \in \mathbb{R}^d$.

Convex Function: Property

Property: Combination of convex functions is convex function.

- Let $f_1, \cdots, f_k$ be convex functions.
- Then $f(\mathbf{w}) = \lambda_1 f_1(\mathbf{w}) + \cdots + \lambda_k f_k(\mathbf{w})$ is convex function for $\lambda_i \geq 0$.

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Example:

- $f_1(\mathbf{w}) = \|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2$ is convex function.
- $f_2(\mathbf{w}) = \|\mathbf{w}\|_2^2$ is convex function.
- $\Rightarrow$ $f_1(\mathbf{w}) + \lambda f_2(\mathbf{w}) = \|\mathbf{X}\mathbf{w} - \mathbf{y}\|_2^2 + \lambda\|\mathbf{w}\|_2^2$ is convex function.

Convex Optimization

Convex Optimization

Definition (Convex Optimization).

- Optimization: $\min_{\mathbf{w}} f(\mathbf{w})\,; \quad \text{s.t. } \mathbf{w} \in \mathcal{C}.$
- It is convex optimization if it has two properties:
  1. $\mathcal{C}$ (feasible set) is convex set,
  2. f (objective function) is convex function.

Convex Optimization: Examples

- Least squares regression: $\min_{\mathbf{w}} \; ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2.$

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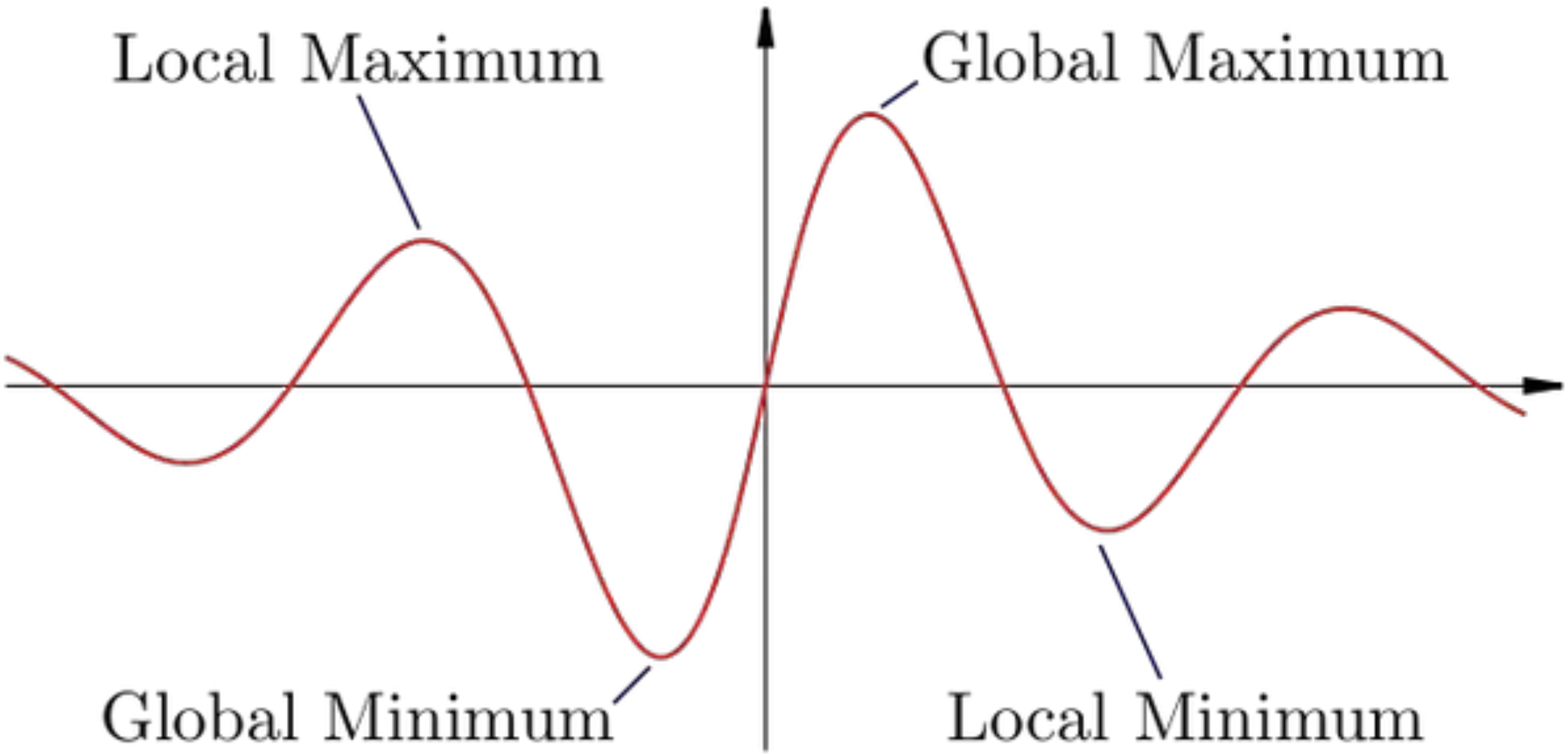
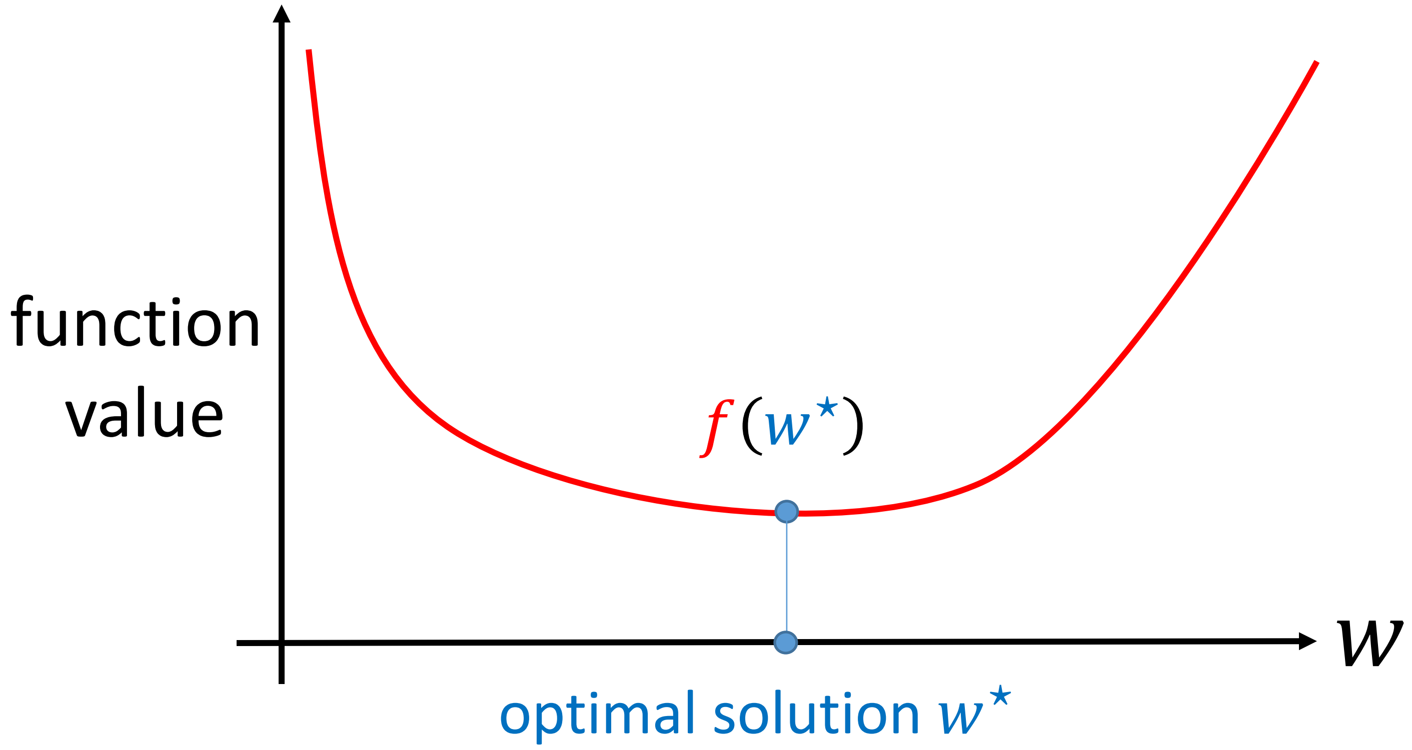
- LASSO: $\min_{\mathbf{w}} \; ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2; \quad s.t. \; ||\mathbf{w}||_1 \leq t$.

Local and Global Optima



Convex Optimization: Properties

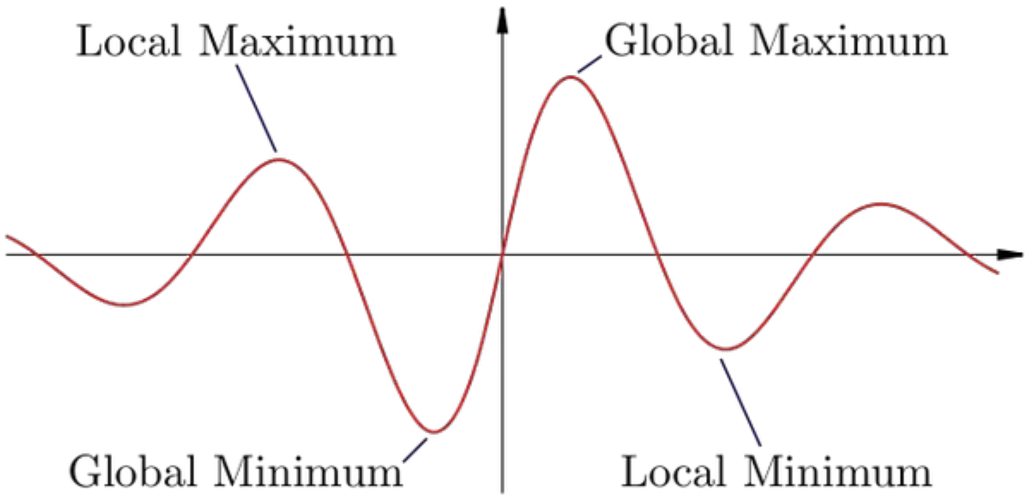
Property: For convex optimization, every local minimum is global minimum.



Optimization: Properties

First-order optimality condition (necessary condition):

- Consider the unconstrained optimization: $\min_{\mathbf{w}} f(\mathbf{w})$.
- If $\mathbf{w}^\star$ is local minimum, then the gradient $\frac{\partial f(\mathbf{w})}{\partial \mathbf{w}}$ at $\mathbf{w}^\star$ is zero.



Convex Optimization: Properties

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- If $\mathbf{w}^\star$ is local minimum, then the gradient $\frac{\partial\, f(\mathbf{w})}{\partial\, \mathbf{w}}$ at $\mathbf{w}^\star$ is zero.

Property of convex optimization (sufficient condition):

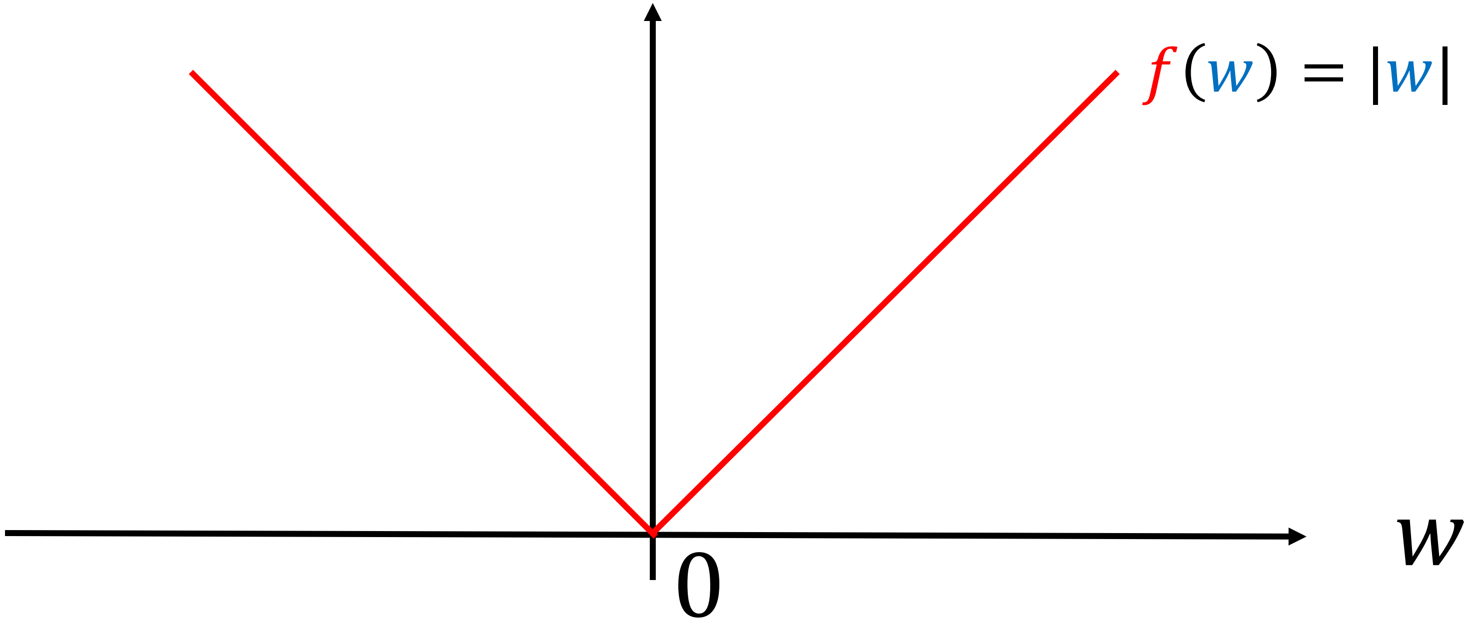
- Let $\min_{\mathbf{w}} f(\mathbf{w})$ be convex optimization.
- If $\frac{\partial\, f(\mathbf{w})}{\partial\, \mathbf{w}}$ at $\mathbf{w}^\star$ is zero, then $\mathbf{w}^\star$ is global minimum.

Subgradient and Subdifferential

Non-Differentiable Functions

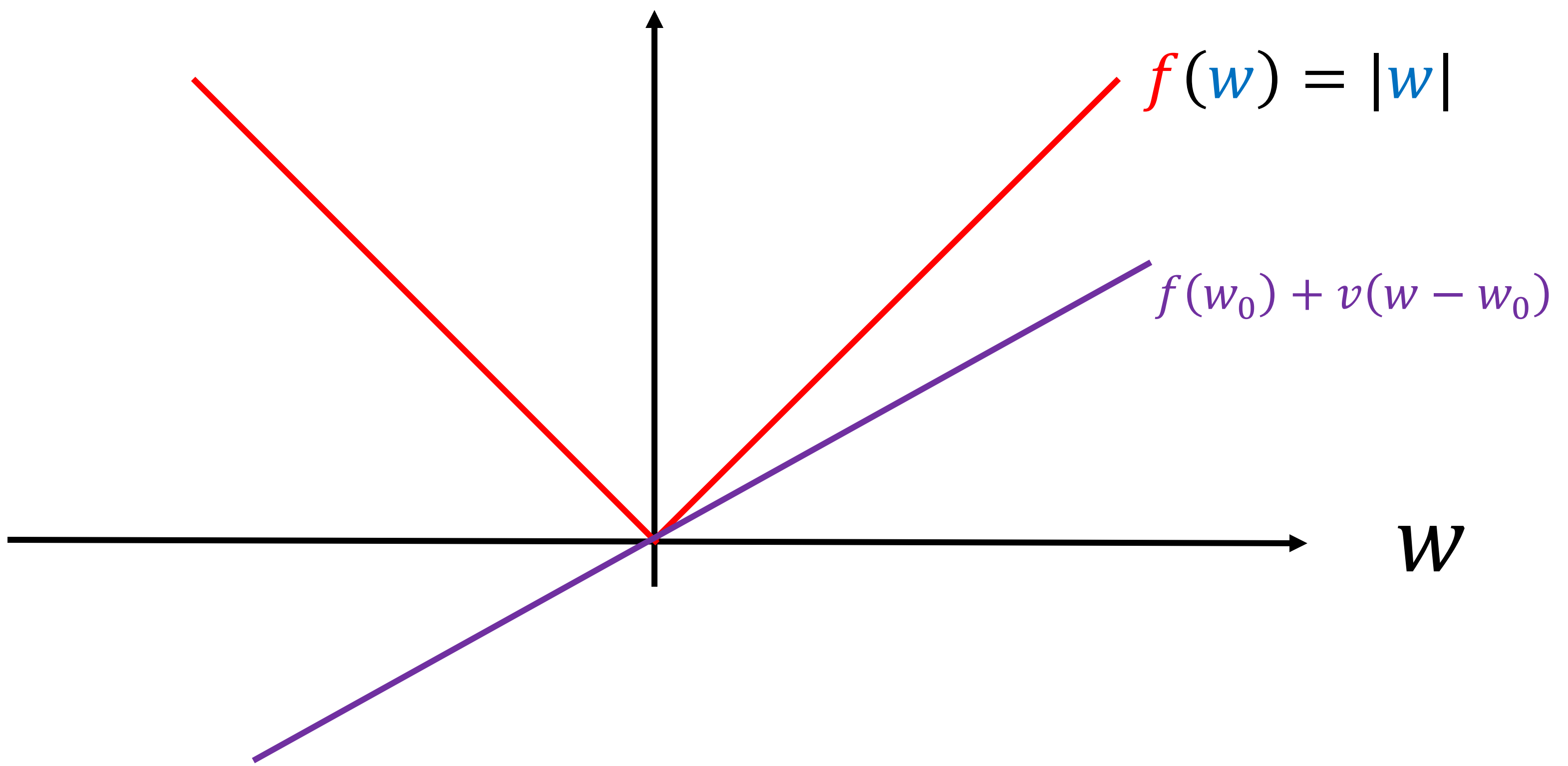
- Example of non-differentiable functions: $f(w) = |w|$

$$\frac{\partial f}{\partial w} = \begin{cases} +1, & \text{if } w > 0; \\ \text{undefined}, & \text{if } w = 0; \\ -1, & \text{if } w < 0. \end{cases}$$



Subgradient of Convex Function

Definition (Subgradient). A vector $\mathbf{v}$ is called a subgradient of f at $\mathbf{w}_0$ if for any $\mathbf{w}$, $f(\mathbf{w}) \geq f(\mathbf{w}_0) + \mathbf{v}^T(\mathbf{w} - \mathbf{w}_0)$.



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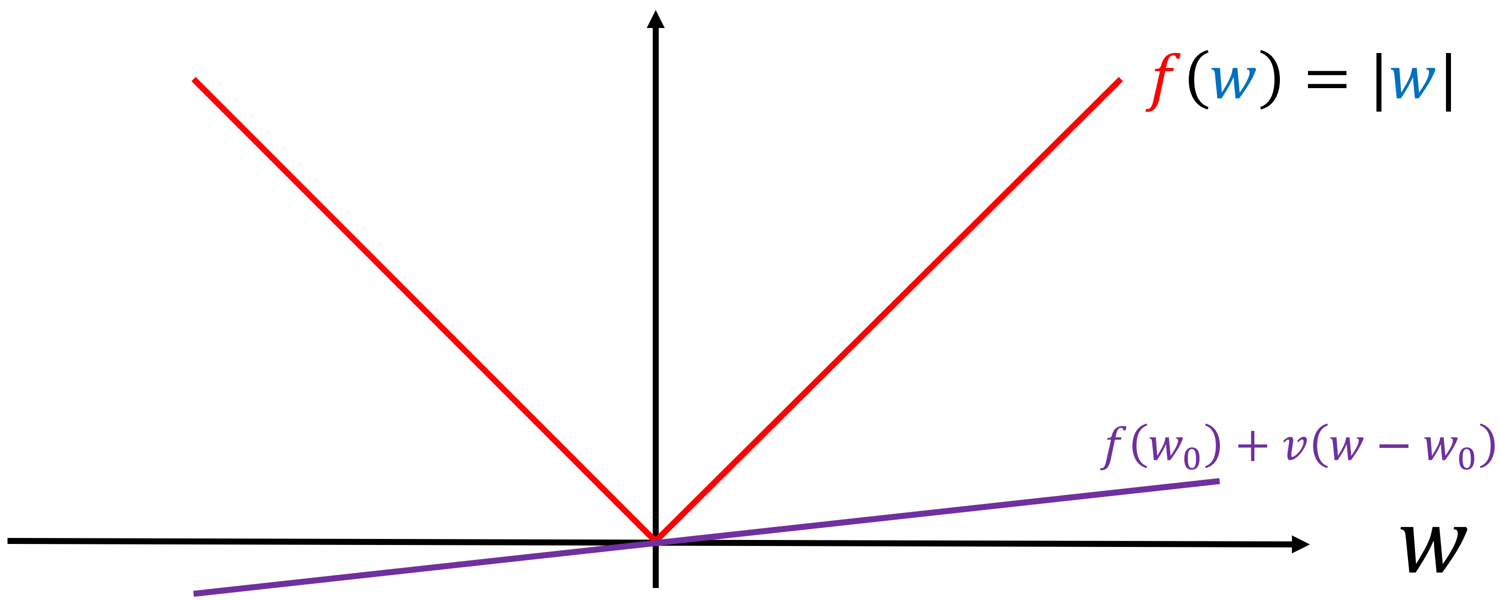

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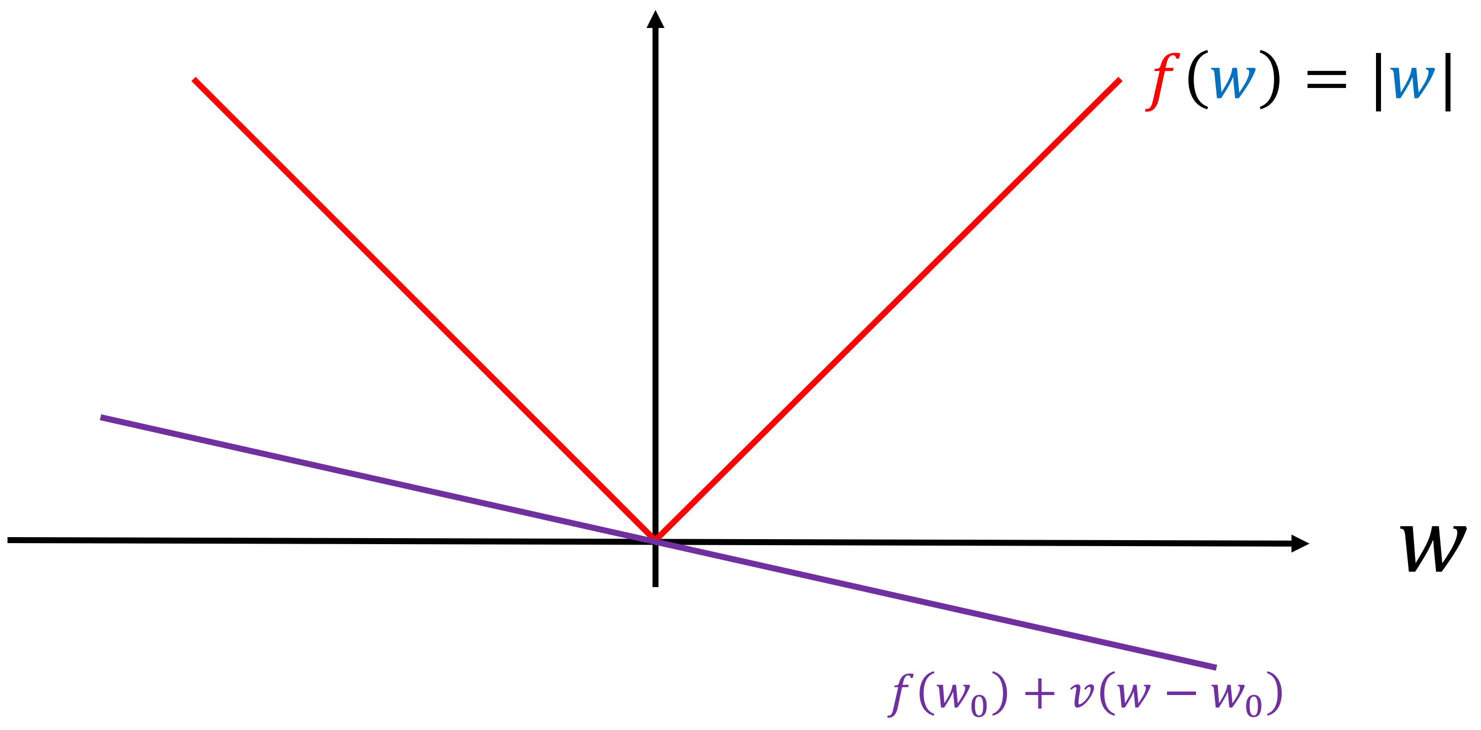

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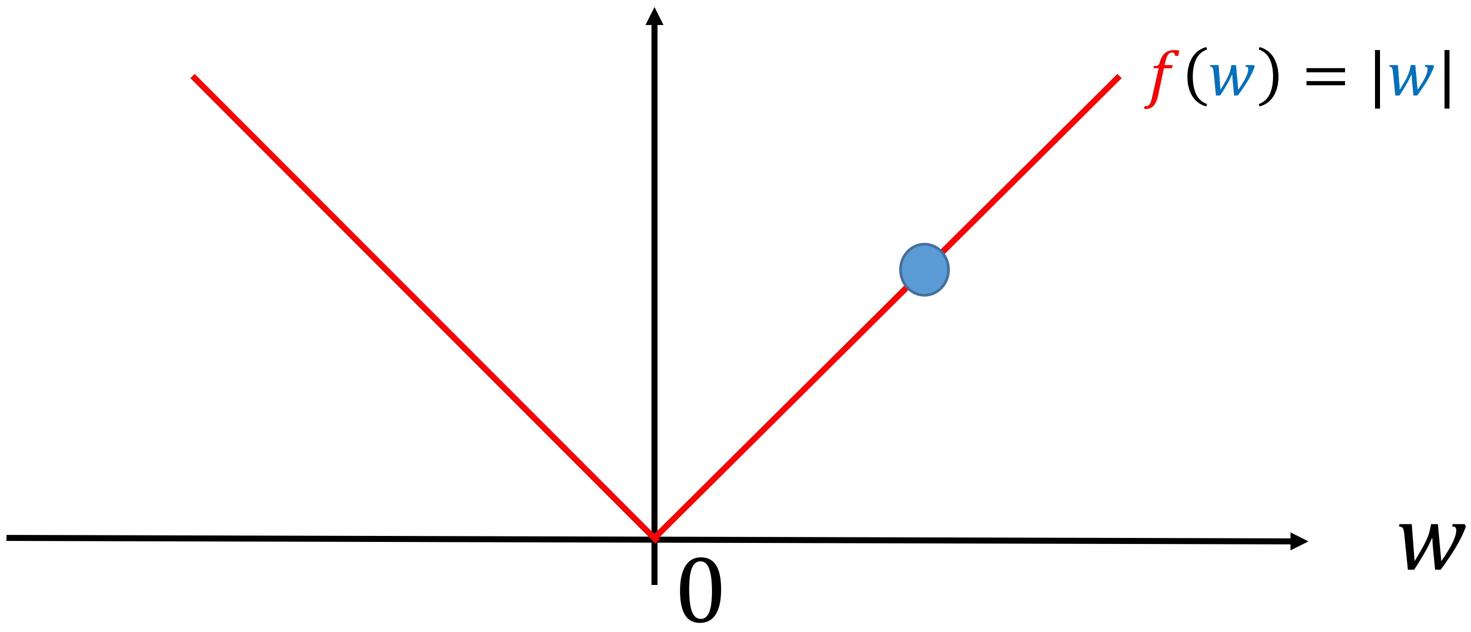
Example: $f(w) = |w|$

- $\partial f(3) = \{1\}$.



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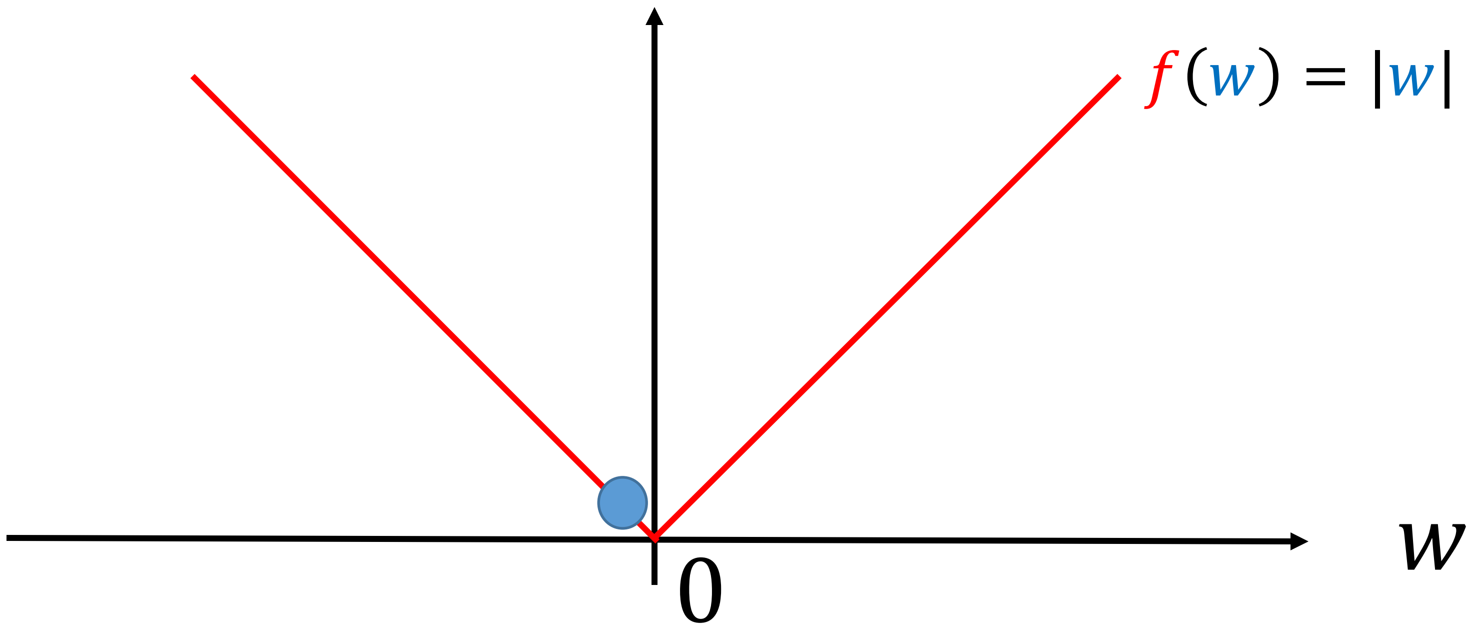

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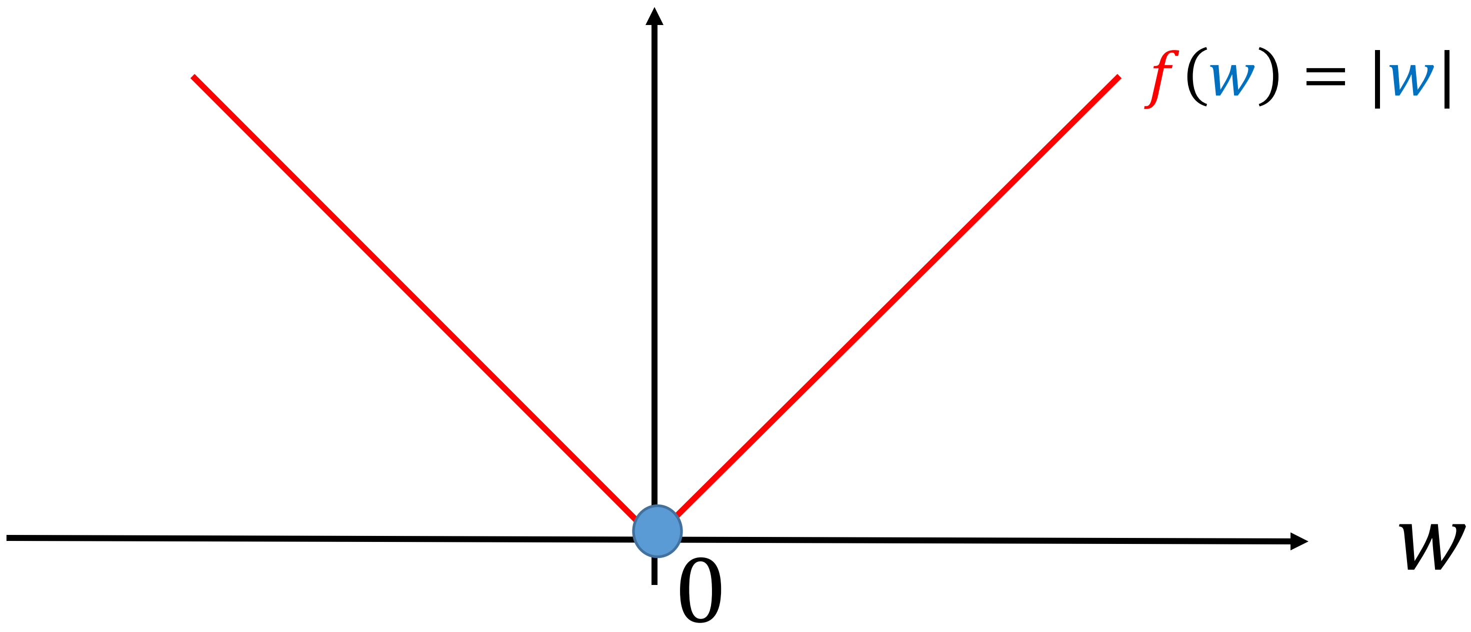
- $\partial f(0) = [-1, 1]$.



A Property of Convex Optimization

Let f be a convex function.

Property: $\mathbf{w}^\star = \min_{\mathbf{w}} f(\mathbf{w}) \iff 0 \in \partial f(\mathbf{w}^\star)$.

Example: $\min_{w} \{f(w) = |w + 5|\}$

- $\partial f(-5) = [-1, 1]$.
- Obviously $0 \in \partial f(-5)$.
- $w^\star = -5$ minimizes f .