

Linear Algebra & Convex Optimization Review


CS 534: Machine Learning

Linear Algebra

Notation

- Vector: $\mathbf{x} \in \mathbb{R}^n$

Hastie et al. book notation


$$\mathbf{x} = X = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix}$$

- Matrix: $\mathbf{A} \in \mathbb{R}^{m \times n}$

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} = [\mathbf{a}_1 \quad \mathbf{a}_2 \quad \cdots \quad \mathbf{a}_n]$$

Special Matrices

- Identity Matrix:

$$\mathbf{I} \in \mathbb{R}^{n \times n}, \text{ where } I_{ij} = \begin{cases} 1, & i = j \\ 0, & i \neq j \end{cases}$$

$$\mathbf{A}\mathbf{I} = \mathbf{A} = \mathbf{I}\mathbf{A}$$

- Diagonal Matrix:

$$\mathbf{D} = \text{diag}(d_1, d_2, \dots, d_n) \text{ with } D_{ij} = \begin{cases} d_i, & i = j \\ 0, & i \neq j \end{cases}$$

Matrix Multiplication

If $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\mathbf{B} \in \mathbb{R}^{n \times p}$,

$$\mathbf{C} = \mathbf{AB} \in \mathbb{R}^{m \times p}, \text{ where } C_{ij} = \sum_{k=1}^n A_{ik} B_{kj}$$

- Properties

- Associative

$$(\mathbf{AB})\mathbf{C} = \mathbf{A}(\mathbf{BC})$$

- Distributive

$$\mathbf{A}(\mathbf{B} + \mathbf{C}) = \mathbf{AB} + \mathbf{AC}$$

Generally not
commutative so
 $\mathbf{AB} \neq \mathbf{BA}$

Transpose

- “Flip” rows and columns of a matrix

$$(A^{\top})_{ij} = A_{ji}$$

- Properties

- $(\mathbf{A}^{\top})^{\top} = \mathbf{A}$

- $(\mathbf{AB})^{\top} = \mathbf{B}^{\top} \mathbf{A}^{\top}$

- $(\mathbf{A} + \mathbf{B})^{\top} = \mathbf{A}^{\top} + \mathbf{B}^{\top}$

Trace

- Sum of the diagonal elements in a square matrix

$$\text{Tr}(\mathbf{A}) = \sum_{i=1}^n A_{ii}$$

- Properties

- $\text{Tr}(\mathbf{A}) = \text{Tr}(\mathbf{A}^\top)$

- $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{n \times n}, \text{Tr}(\mathbf{A} + \mathbf{B}) = \text{Tr}(\mathbf{A}) + \text{Tr}(\mathbf{B})$

- $\mathbf{A} \in \mathbb{R}^{n \times n}, t \in \mathbb{R}, \text{Tr}(t\mathbf{A}) = t\text{Tr}(\mathbf{A})$

$$\mathbf{AB} \in \mathbb{R}^{n \times n}, \text{Tr}(\mathbf{AB}) = \text{Tr}(\mathbf{BA})$$

Norms

- Norm is any function $f : \mathbb{R}^n \rightarrow \mathbb{R}$ that satisfies 4 properties:

- Non-negativity

$$\text{For all } \mathbf{x} \in \mathbb{R}^n, f(\mathbf{x}) \geq 0$$

- Definiteness

$$f(\mathbf{x}) = 0 \text{ if and only if } \mathbf{x} = 0$$

- Homogeneity

$$\text{For all } \mathbf{x} \in \mathbb{R}^n, t \in \mathbb{R}, f(t\mathbf{x}) = |t|f(x)$$

- Triangle Inequality

$$\text{For all } \mathbf{x}, \mathbf{y} \in \mathbb{R}^n, f(\mathbf{x} + \mathbf{y}) \leq f(\mathbf{x}) + f(\mathbf{y})$$

Common Vector Norms

- Euclidean (ℓ_2) norm

$$||\mathbf{x}||_2 = \sqrt{\sum_{i=1}^n x_i^2}$$

- ℓ_1 norm

$$||\mathbf{x}||_1 = \sum_{i=1}^n |x_i|$$

- ℓ_∞ norm

$$||\mathbf{x}||_\infty = \max_{x_i} |x_i|$$

- ℓ_p norm

$$||\mathbf{x}||_p = \left(\sum_{i=1}^n |x_i|^p \right)^{1/p}$$

Common Matrix Norms

- Frobenius norm

$$||\mathbf{A}||_F = \sqrt{\sum_{ij} |A_{ij}|^2} = \sqrt{\text{Tr}(\mathbf{A}^\top \mathbf{A})}$$

- 1-norm

$$||\mathbf{A}||_1 = \max_j \sum_i |A_{ij}|$$

- 2-norm

$$||\mathbf{A}||_2 = \sqrt{\max \text{eig}(\mathbf{A}^\top \mathbf{A})}$$

- p-norm

$$||\mathbf{A}||_p = \left(\max_{||\mathbf{x}||_p=1} ||\mathbf{Ax}||_p \right)^{1/p}$$

Linear Independence

- Set of vectors are linearly independent if no vector can be represented as a linear combination of the remaining vectors
- Linearly dependent vector:

$$\mathbf{x}_n = \sum_{i=1}^{n-1} \alpha_i \mathbf{x}_i$$

Rank

- Column rank: size of largest subset of columns of A such that constitute a linearly independent set
- Row rank: largest number of rows of A that constitute a linearly independent set
- For any matrix in real space, column rank = row rank

Rank Properties

$$\mathbf{A} \in \mathbb{R}^{m \times n}$$

- Rank vs dimension

$$\text{rank}(\mathbf{A}) \leq \min(m, n)$$

- Full rank

$$\text{rank}(\mathbf{A}) = \min(m, n)$$

- Rank of transpose

$$\text{rank}(\mathbf{A}) = \text{rank}(\mathbf{A}^\top)$$

Rank Properties (2)

- Multiplication of two matrices

$$\text{rank}(\mathbf{AB}) \leq \min(\text{rank}(\mathbf{A}), \text{rank}(\mathbf{B}))$$

- Addition of two same sized matrices

$$\text{rank}(\mathbf{A} + \mathbf{B}) \leq \text{rank}(\mathbf{A}) + \text{rank}(\mathbf{B})$$

Matrix Inverse

- Unique matrix such that

$$\mathbf{A}^{-1}\mathbf{A} = \mathbf{I} = \mathbf{A}\mathbf{A}^{-1}$$

- A is invertible and non-singular if inverse exists
- A is singular if not invertible
- A must be full rank to have an inverse

Matrix Inverse Properties

- $(\mathbf{A}^{-1})^{-1} = \mathbf{A}$
- $(\mathbf{AB})^{-1} = \mathbf{B}^{-1} \mathbf{A}^{-1}$
- $(\mathbf{A}^{-1})^{\top} = (\mathbf{A}^{\top})^{-1}$

Pseudo Inverse (Moore-Penrose)

- Generalization of inverse for non-square but full rank
- Criteria:
 - $\mathbf{A}\mathbf{A}^\dagger\mathbf{A} = \mathbf{A}$
 - $\mathbf{A}^\dagger\mathbf{A}\mathbf{A}^\dagger = \mathbf{A}^\dagger$
 - $(\mathbf{A}\mathbf{A}^\dagger)^\top = \mathbf{A}\mathbf{A}^\dagger$
 - $(\mathbf{A}^\dagger\mathbf{A})^\top = \mathbf{A}^\dagger\mathbf{A}$

Orthogonal Matrices

- Orthogonal vectors \mathbf{x} , \mathbf{y} :

$$\mathbf{x}^\top \mathbf{y} = 0$$

- Normalized vector:

$$\|\mathbf{x}\|_2 = 1$$

- Orthogonal square matrix if all columns are orthogonal to one another
- Orthonormal square matrix if orthogonal matrix and all columns are normalized

Orthogonal Properties

- Inverse of orthogonal matrix is its transpose

$$\mathbf{U}^\top \mathbf{U} = \mathbf{I} = \mathbf{U} \mathbf{U}^\top$$

- Vector operation will not change its Euclidean norm

$$\|\mathbf{U}\mathbf{x}\|_2 = \|\mathbf{x}\|_2$$

Range and Nullspace

- Span of a set of vectors is all the vectors that can be expressed as linear combination of these vectors

$$\text{span}(\{\mathbf{x}_1, \dots, \mathbf{x}_n\}) = \left\{ \mathbf{v} : \mathbf{v} = \sum_{i=1}^n \alpha_i \mathbf{x}_i \right\}$$

- Range (columnspace) is the span of the columns of the matrix

$$\mathcal{R}(\mathbf{A}) = \{\mathbf{v} \in \mathbb{R}^m : \mathbf{v} = \mathbf{A}\mathbf{x}, \mathbf{x} \in \mathbb{R}^n\}$$

- Nullspace is the set of all vectors that equal 0 when multiplied by matrix

$$\mathcal{N}(\mathbf{A}) = \{\mathbf{x} \in \mathbb{R}^n : \mathbf{A}\mathbf{x} = \mathbf{0}\}$$

Fundamental Subspaces

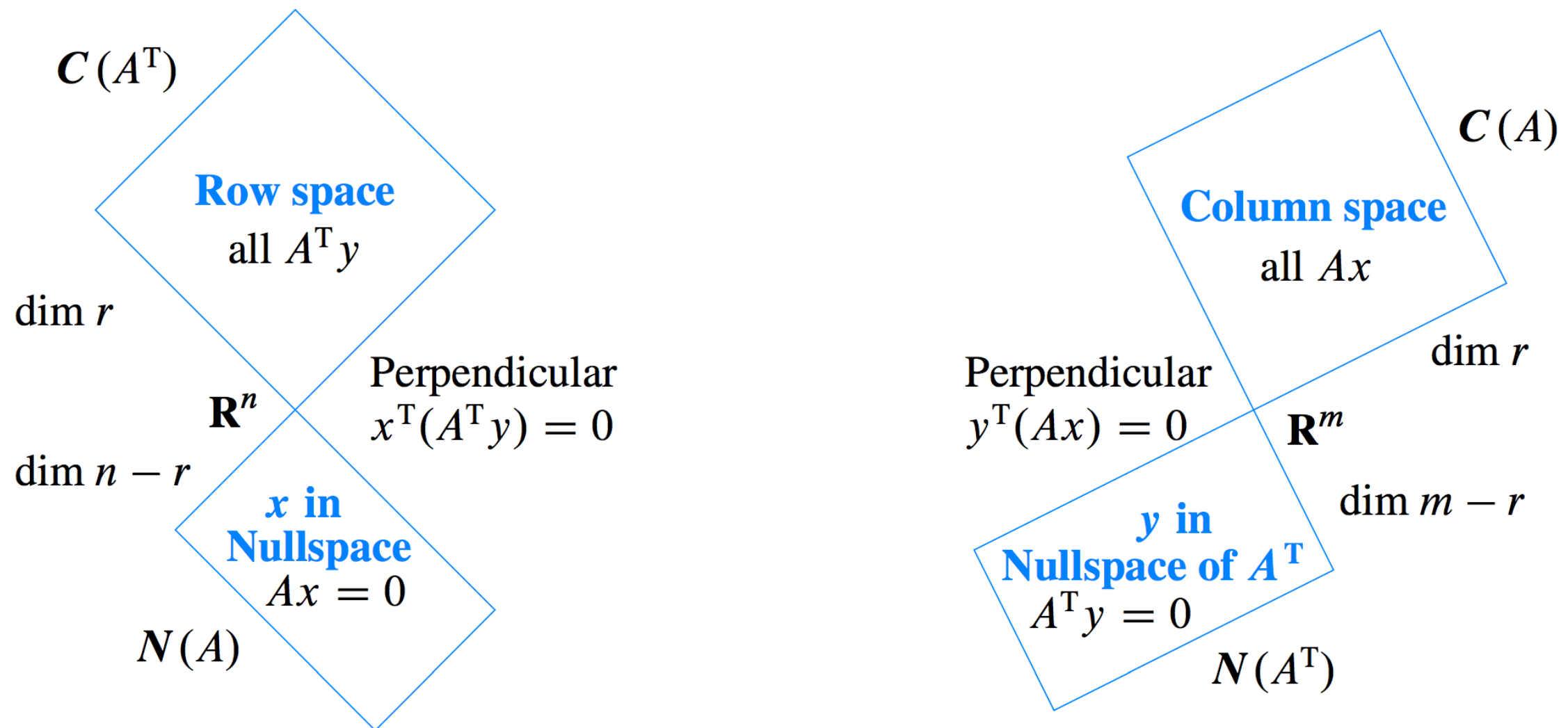


Figure 1: Dimensions and orthogonality for any m by n matrix A of rank r .

Eigenvalues and Eigenvectors

- Instrumental to systems

$$\mathbf{A}\mathbf{x} = \lambda\mathbf{x}$$

- Analogy: Matrix is a gust of wind (invisible force with visible result)
- Eigenvector is like a weathervane which tells you the direction the wind is blowing in
- Eigenvalue is just the scalar coefficient

<https://deeplearning4j.org/eigenvector>

Eigenvalue Properties

- Trace of a matrix is sum of its eigenvalues

$$\text{Tr}(\mathbf{A}) = \sum_{i=1}^n \lambda_i$$

- Determinant of matrix is equal to product of its eigenvalues

$$|\mathbf{A}| = \prod_{i=1}^n \lambda_i$$

- Rank of matrix is the number of non-zero eigenvalues
- If eigenvectors of matrix are linearly independent, then the matrix is invertible

$$\mathbf{A} = \mathbf{X}\mathbf{\Lambda}\mathbf{X}^{-1}$$

Symmetric Matrix & Eigenvectors

- Two remarkable properties from a symmetric matrix
 - Eigenvalues of the matrix are real
 - Eigenvectors of the matrix are orthonormal

$$\mathbf{A} = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^{\top}$$

- Eigenvalues are positive \rightarrow positive definite
- Eigenvalues are non-negative \rightarrow positive semidefinite

Convex Optimization Review

Optimization Problem

- Minimize a function subject to some constraints

$$\begin{aligned} \min_x \quad & f_0(x) \\ \text{s.t.} \quad & f_k(x) \leq 0, k = 1, 2, \dots, K \\ & h_j(x) = 0, j = 1, 2, \dots, J \end{aligned}$$

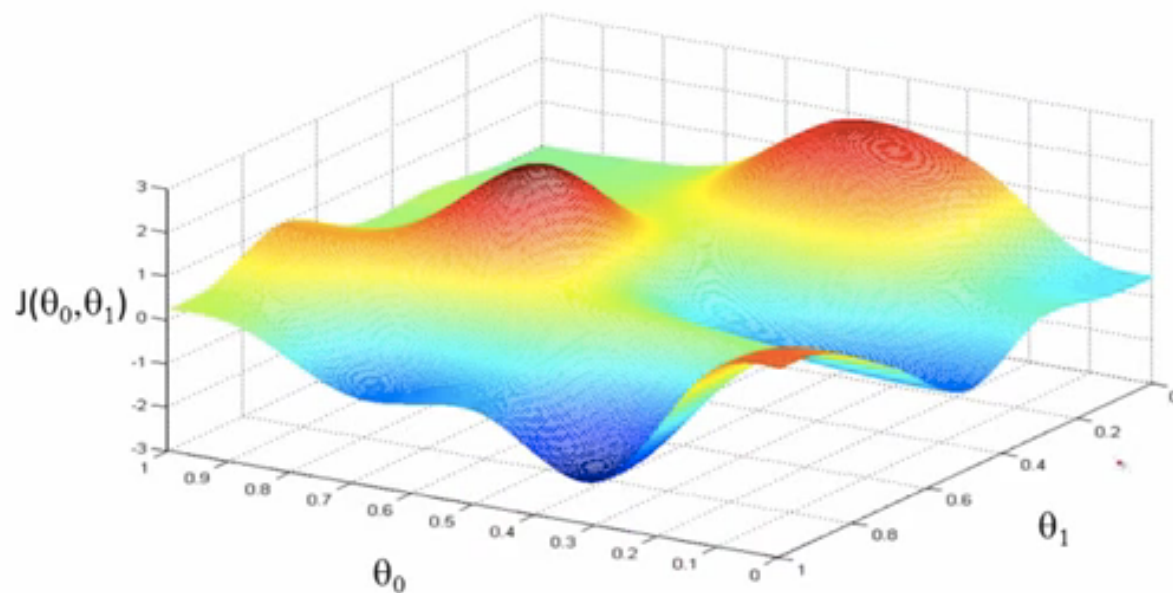
- Example: Minimize the variance of your returns while earning at least \$100 in the stock market.

Machine Learning and Optimization

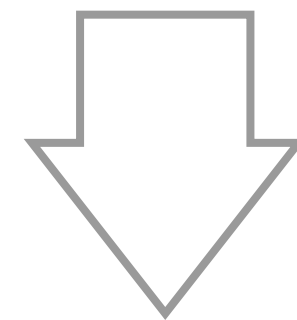
- Linear regression $\min_w ||Xw - y||^2$
- Logistic regression $\min_w \sum_i \log(1 + \exp(-y_i x_i^\top w))$
- SVM
$$\begin{aligned} \min_w \quad & ||w||^2 + C \sum_i \xi_i \\ \text{s.t.} \quad & \xi_i \geq 1 - y_i x_i^\top w \\ & \xi_i \geq 0 \end{aligned}$$
- And many more ...

Non-Convex Problems are Everywhere

- Local (non-global) minima
- All kinds of constraints



No easy solution
for these problems



Consider
convex problems

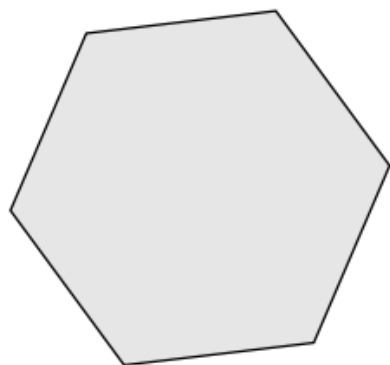
Why Convex Optimization?

- Achieves global minimum, no local traps
- Highly efficient software available
- Can be solved by polynomial time complexity algorithms
- Dividing line between “easy” and “difficult” problems

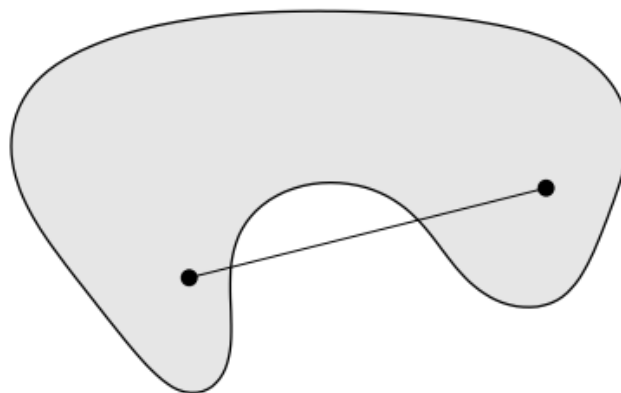
Convex Sets

Any line segment joining any two elements lies entirely in set

$$x_1, x_2 \in C, 0 \leq \theta \leq 1 \implies \theta x_1 + (1 - \theta)x_2 \in C$$



convex



non-convex



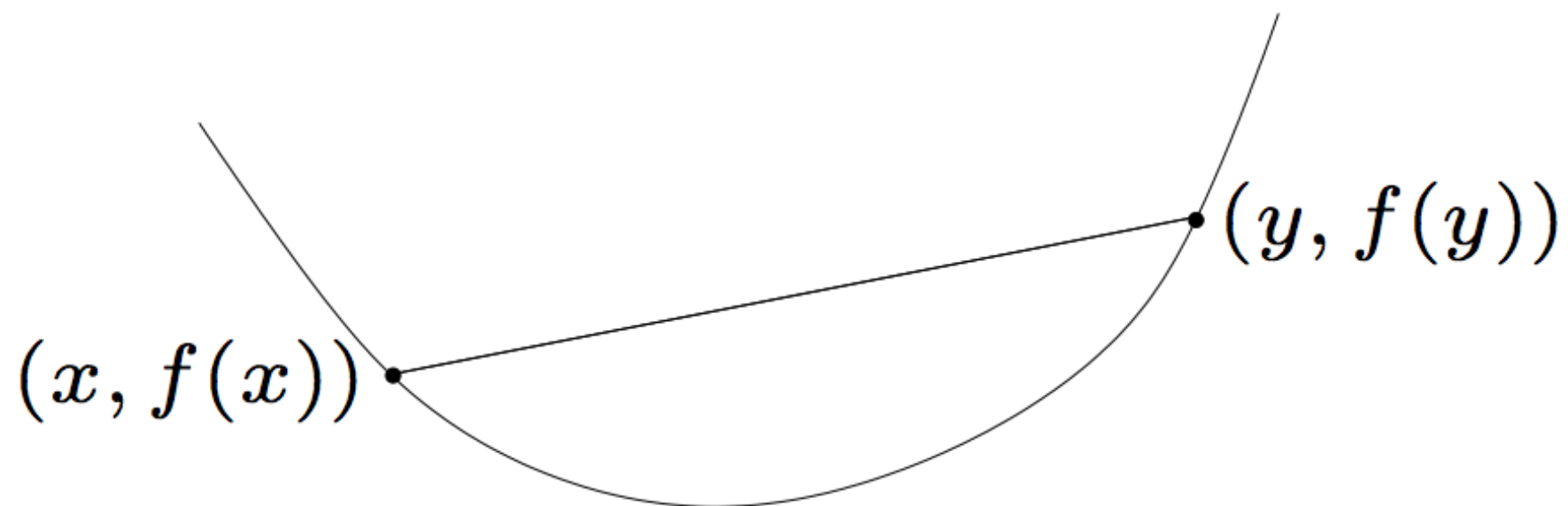
non-convex

Convex Function

$f : \mathbb{R}^n \rightarrow \mathbb{R}$ is convex if **dom** f is a convex set and

$$f(\theta x + (1 - \theta)y) \leq \theta f(x) + (1 - \theta)f(y)$$

for all $x, y \in \mathbf{dom} f, 0 \leq \theta \leq 1$



f lies below the line segment joining $f(x)$, $f(y)$

Properties of Convex Functions

- Convexity over all lines

$f(x)$ is convex $\implies f(x_0 + th)$ is convex in t for all x_0, h

- Positive multiple

$f(x)$ is convex $\implies \alpha f(x)$ is convex for all $\alpha \geq 0$

- Sum of convex functions

$f_1(x), f_2(x)$ convex $\implies f_1(x) + f_2(x)$ is convex

- Pointwise maximum

$f_1(x), f_2(x)$ convex $\implies \max\{f_1(x), f_2(x)\}$ is convex

- Affine transformation of domain

$f(x)$ is convex $\implies f(Ax + b)$ is convex

Convex Optimization Problem

Definition:

An optimization problem is **convex** if its objective is a convex function, the inequality constraints are convex, and the equality constraints are affine

$$\min_x f_0(x)$$

convex function

$$\text{s.t. } f_k(x) \leq 0, k = 1, 2, \dots, K$$

convex sets

$$h_j(x) = 0, j = 1, 2, \dots, J$$

affine constraints

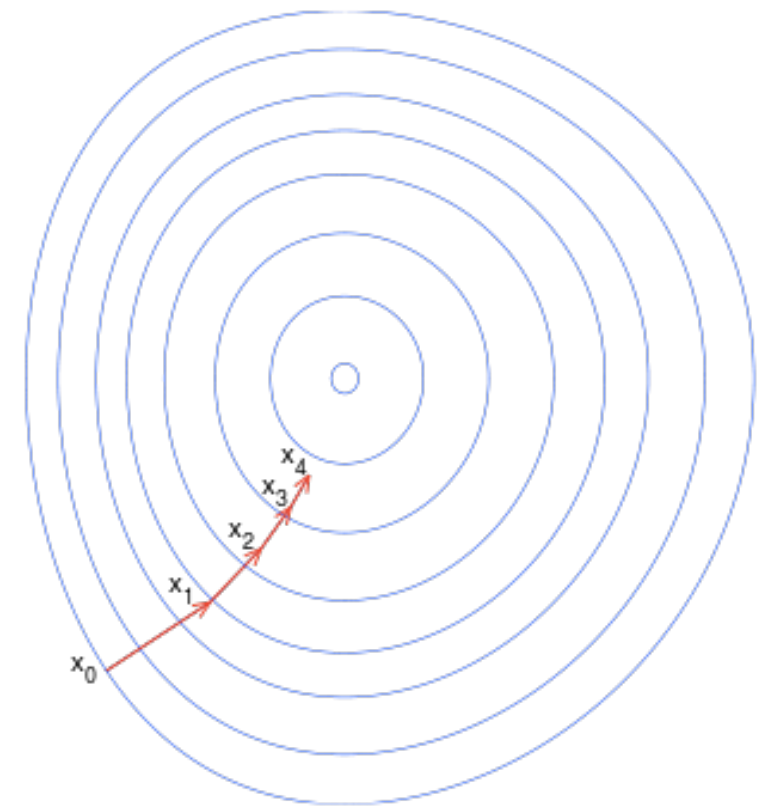
Benefits of Convexity

- Theorem: If x is a local minimizer of a convex optimization problem, it is a **global** minimizer
- Theorem: If the gradient at c is zero, then c is the global minimum of $f(x)$

$$\nabla f(c) = 0 \iff c = x^*$$

Gradient Descent (Steepest Descent)

- Simplest and extremely popular
- Main Idea: take a step proportional to the negative of the gradient
- Easy to implement
- Each iteration is relatively cheap
- Can be slow to converge

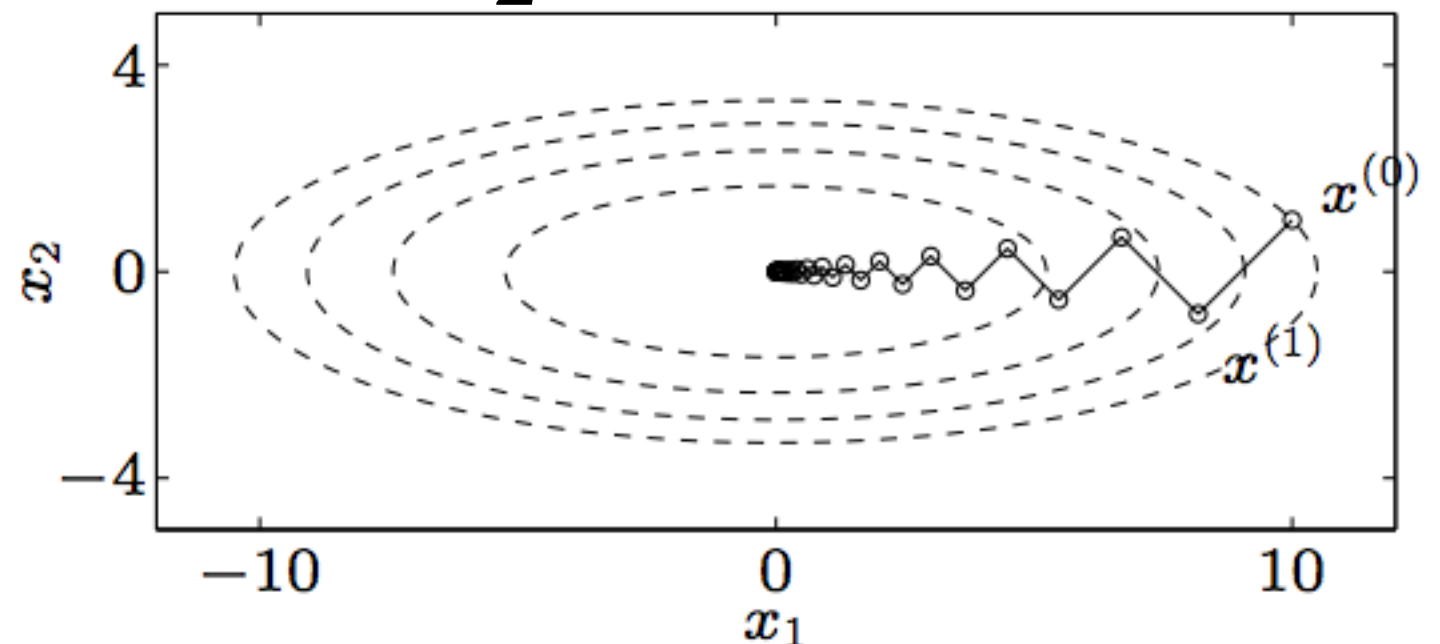


Gradient Descent Algorithm

Algorithm 1: Gradient Descent

```
while Not Converged do  
     $x^{(k+1)} = x^{(k)} - \eta^{(k)} \nabla f(x)$   
end  
return  $x^{(k+1)}$ 
```

Example: $f(x) = \frac{1}{2}(x_1^2 + \gamma x_2^2), \gamma > 0$



Some Resources for Convex Optimization

- Boyd & Vandenberghe's Book on Convex Optimization
https://web.stanford.edu/~boyd/cvxbook/bv_cvxbook.pdf
- Stephen Boyd's Class at Stanford
<http://stanford.edu/class/ee364a/>
- Vandenberghe's Class at UCLA
<http://www.seas.ucla.edu/~vandenbe/ee236b/ee236b.html>
- Ben-Tai & Nemirovski Lectures on Modern Convex Optimization
<http://epubs.siam.org/doi/book/10.1137/1.9780898718829>