Symmetric Matrices

Geometric Algorithms
Lecture 25

CAS CS 132

Introduction

Objectives

1. Finish up our discussion of linear models (actually define linear models).
2. Talk briefly about symmetric matrices and eigenvalues.
3. Describe an application to constrained optimization problems.

Keywords

linear models

design matrices

general linear regression

symmetric matrices

the spectral theorem

orthogonal diagonalizability

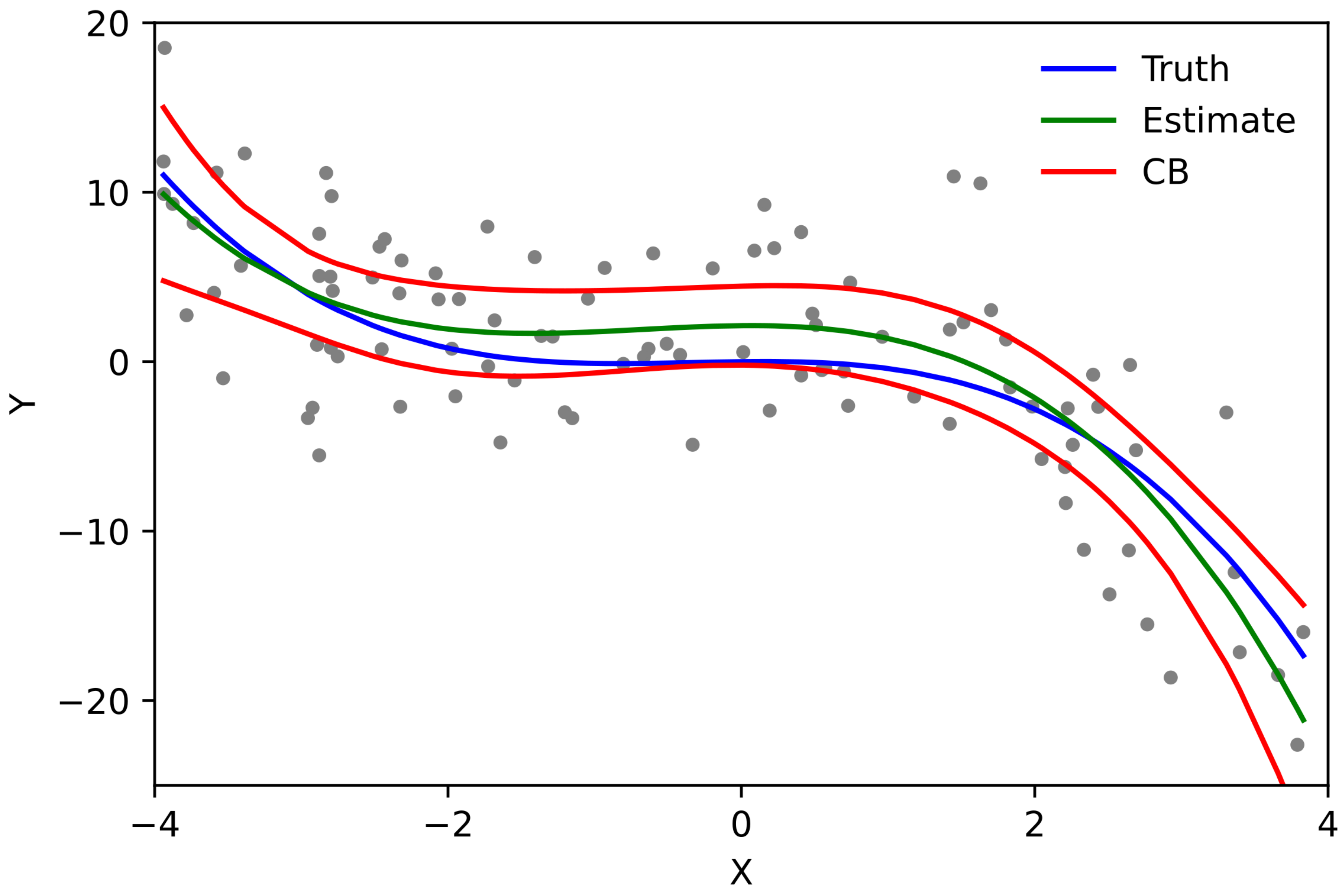
quadratic forms

definiteness

constrained optimization

Recap

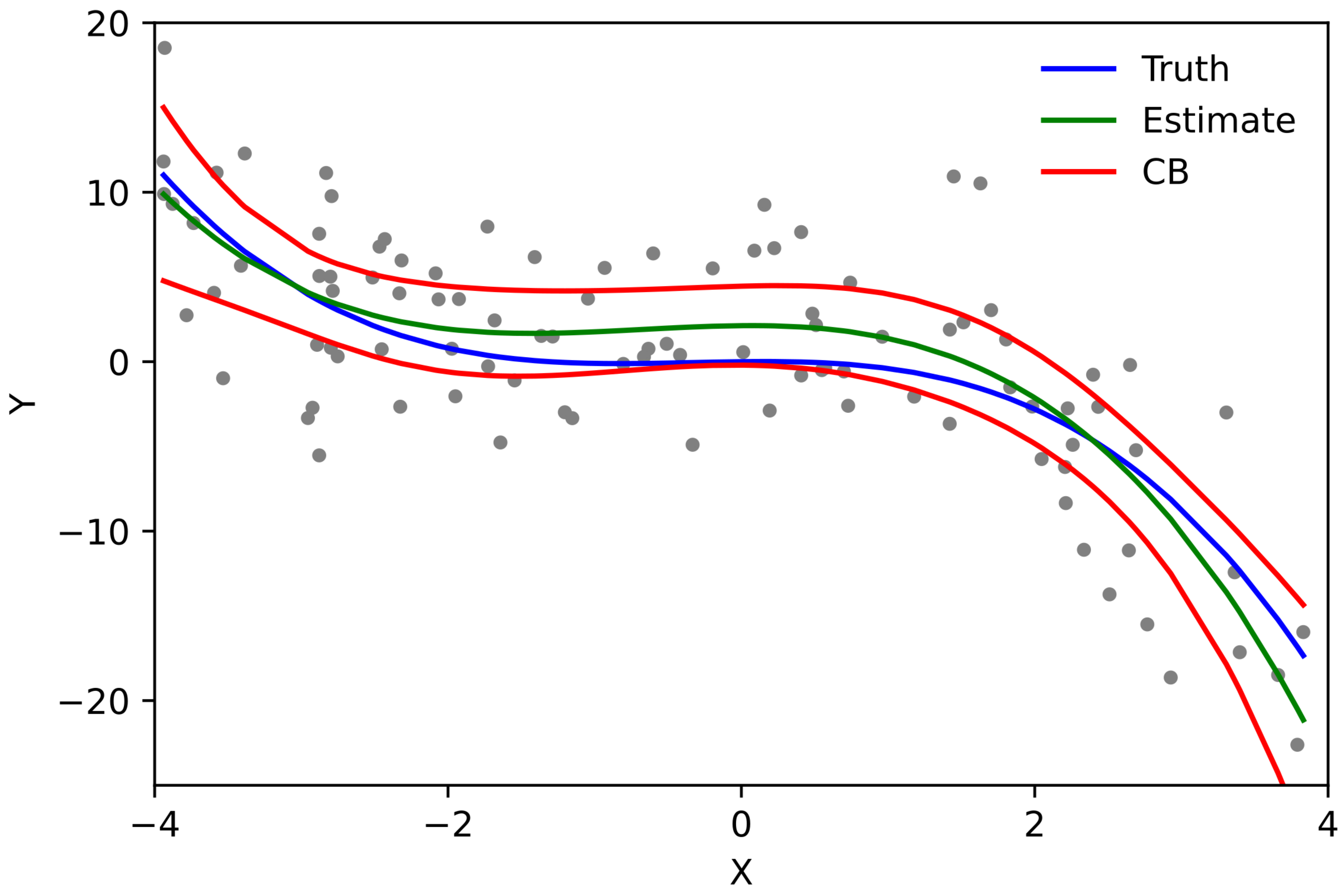
Recall: General Regression



https://commons.wikimedia.org/wiki/File:Polyreg_scheffe.svg

Recall: General Regression

Regression is the process of estimating the relationships independent and dependent variables in a dataset.



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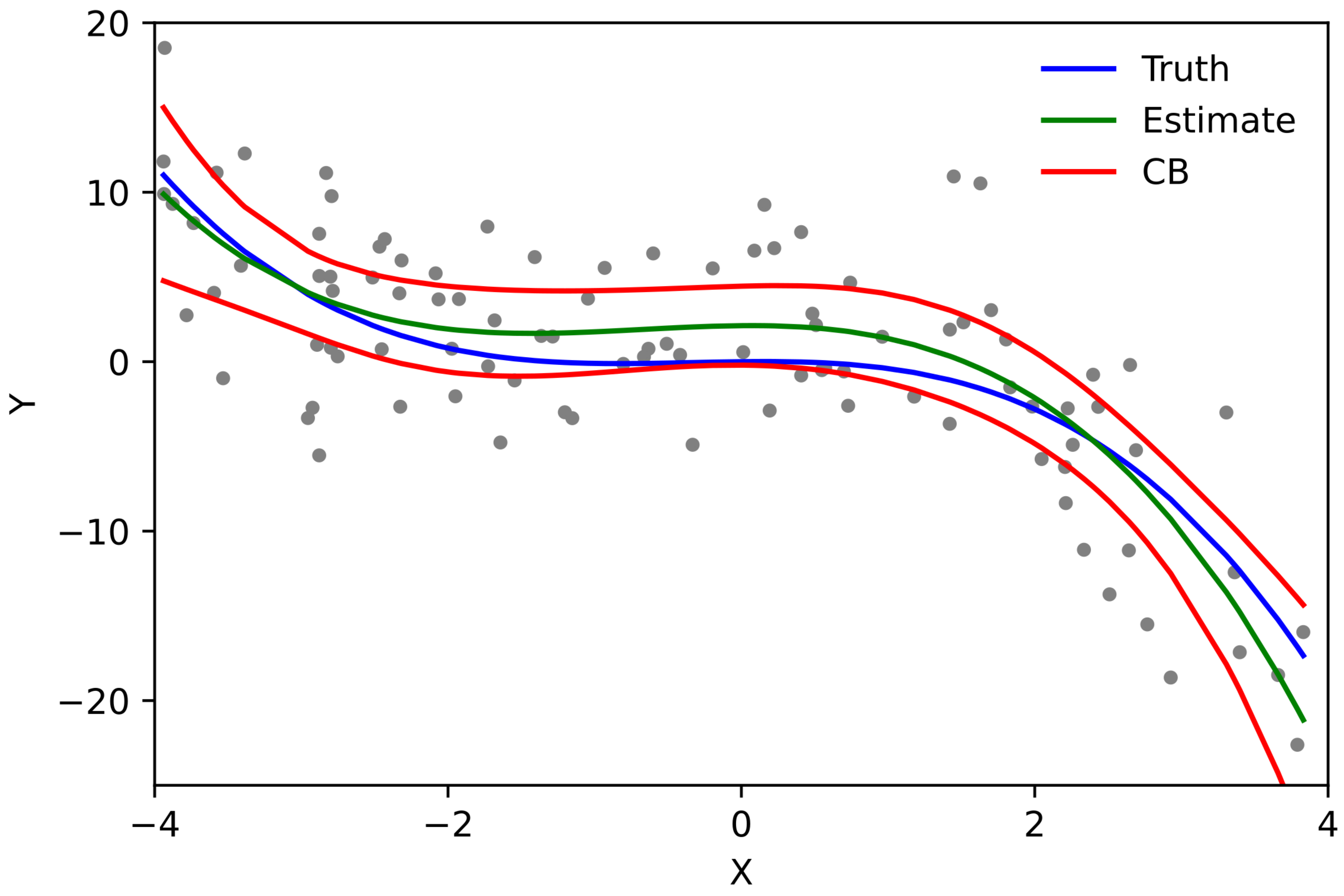

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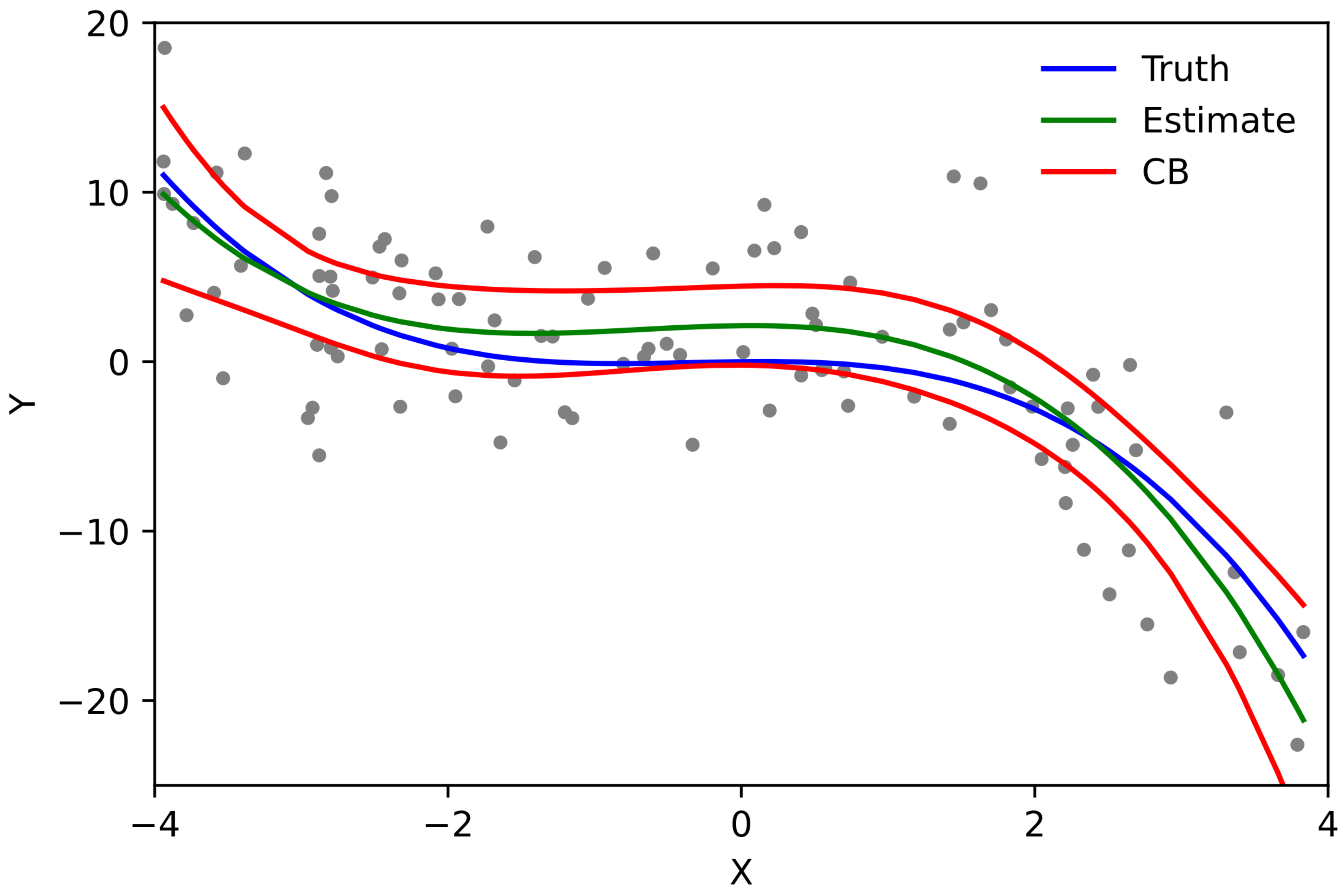
What we are estimating is a mathematical function

We think of the environment has providing us a function from our independent variables to our dependent variables.



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Recall: How To: Line of Best Fit

$$\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ \vdots & \vdots \\ 1 & x_n \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

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Problem. Find the least squares line for the dataset $\{(x_1, y_1), \ldots, (x_n, y_n)\}$.

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$y = \beta_0 + \beta_1 x$

Problem. Find the least squares line for the dataset $\{(x_1, y_1), \ldots, (x_n, y_n)\}$.

Solution. Find the least squares solution to the above equation.

Recall: "Vectors" of Generalization

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1. What if we have *more than one* independent value?

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2. What if our data is not *exactly* linear.

   e.g., polynomial regression

Recall: Plane of Best Fit

Dataset: $\{(x_1, y_1, z_1), \ldots, (x_k, y_k, z_k)\}$ where (x_i, y_i) is an longitude and latitude and z_i is an altitude.

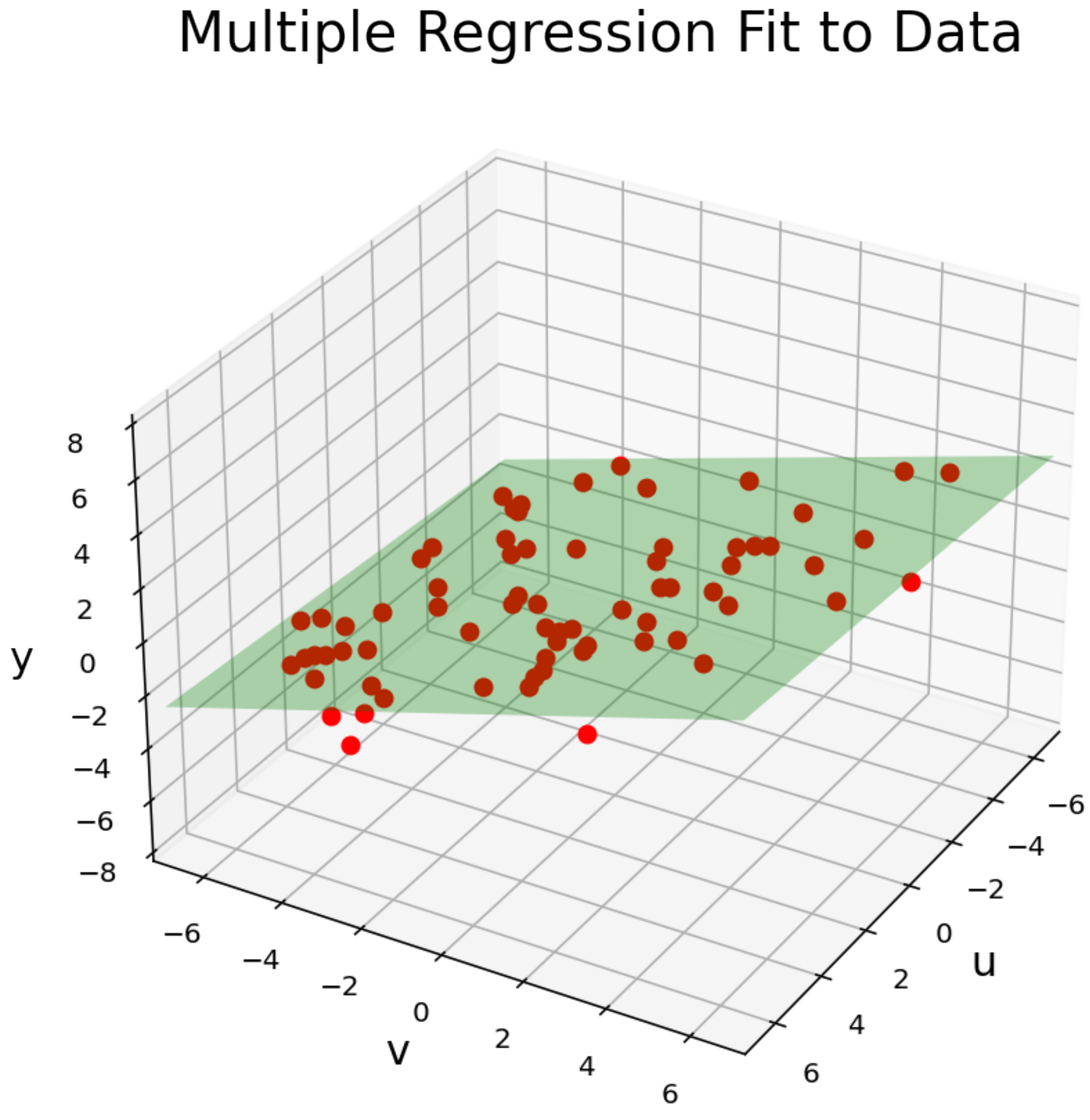
Problem: Find $\beta_0, \beta_1, \beta_2$ such that

$$f(x, y) = \beta_0 + \beta_1 x + \beta_2 y$$

which minimizes

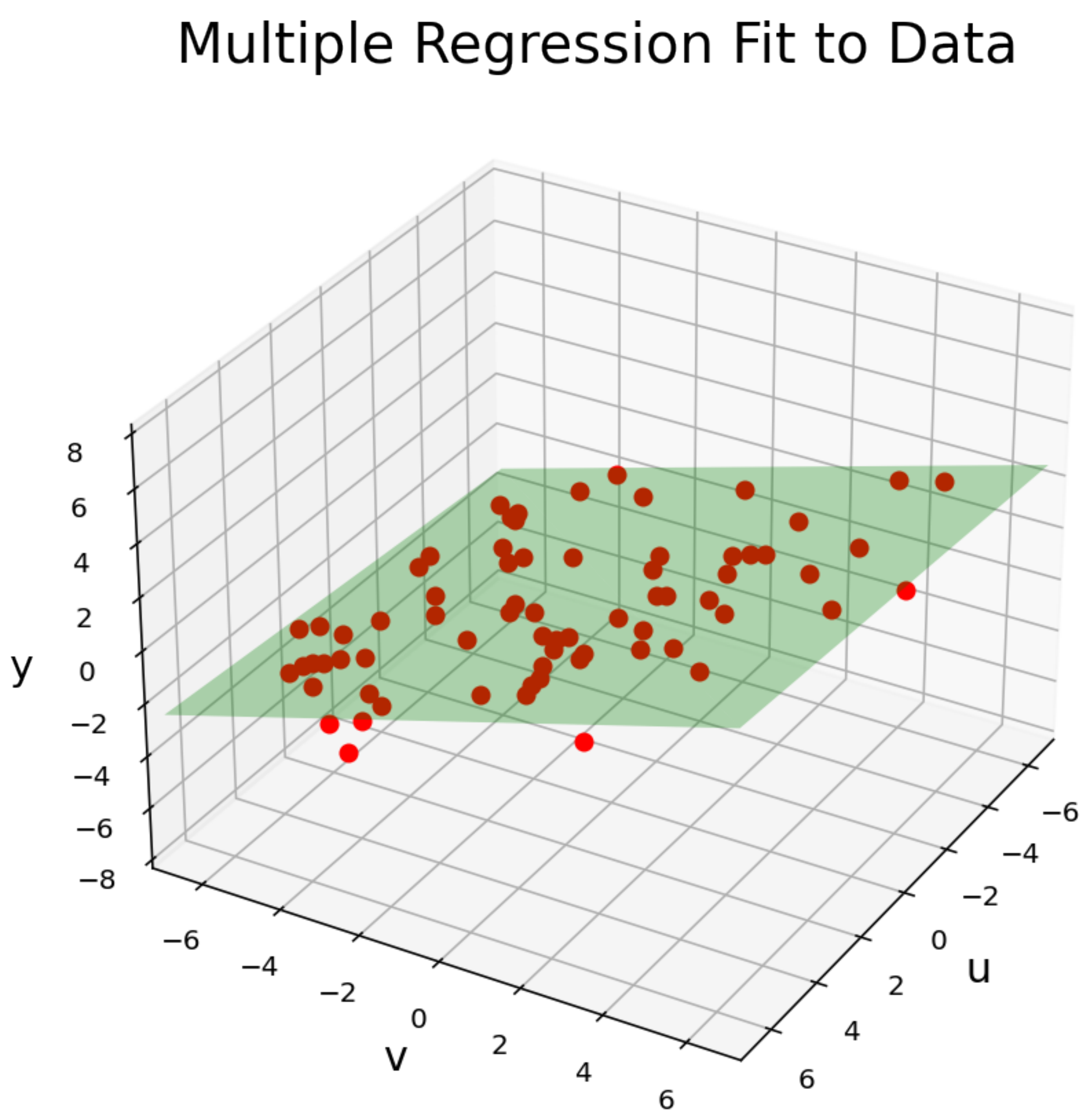
$$\sum_{i=1}^{k} (f(x_i, y_i) - z_i)^2$$

Figure 23.2



Recall: Plane of Best Fit

Figure 23.2



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recall: planes are given by linear equations

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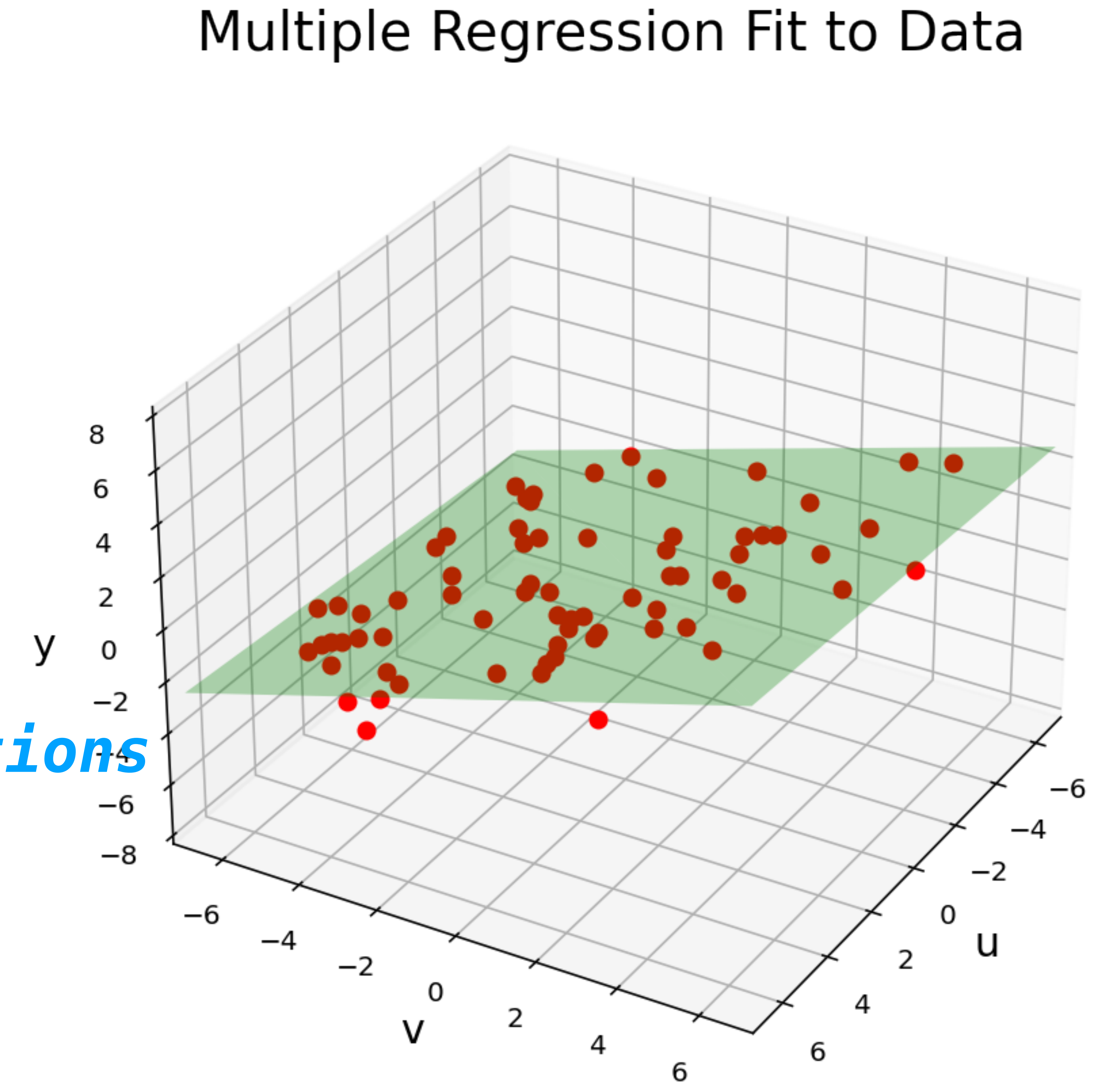

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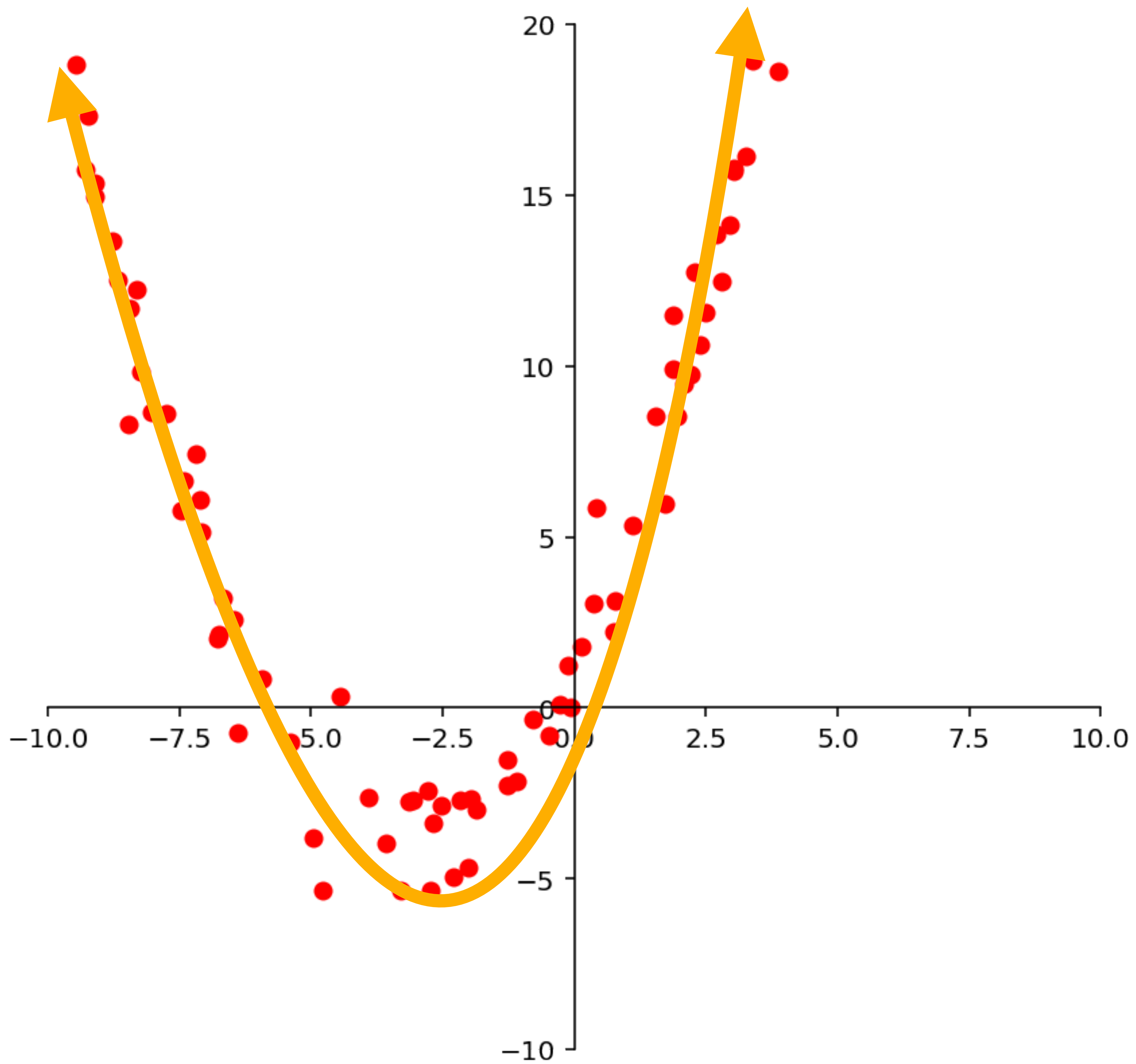

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$$\underbrace{\begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ \vdots & \vdots & \vdots \\ 1 & x_k & x_k^2 \end{bmatrix}}_{X} \underbrace{\begin{bmatrix} \beta_0 \\ \beta_1 \\ \beta_2 \end{bmatrix}}_{\vec{\beta}} = \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_k \end{bmatrix}}_{\mathbf{y}}$$

Step 2: Rewrite the system as a matrix equation.

Recall: Parabola of Best Fit

$A\vec{x} = b$

unique L.S. sol.

$\hat{b} = A\hat{x} = A(A^TA)^{-1}A^T\vec{b}$

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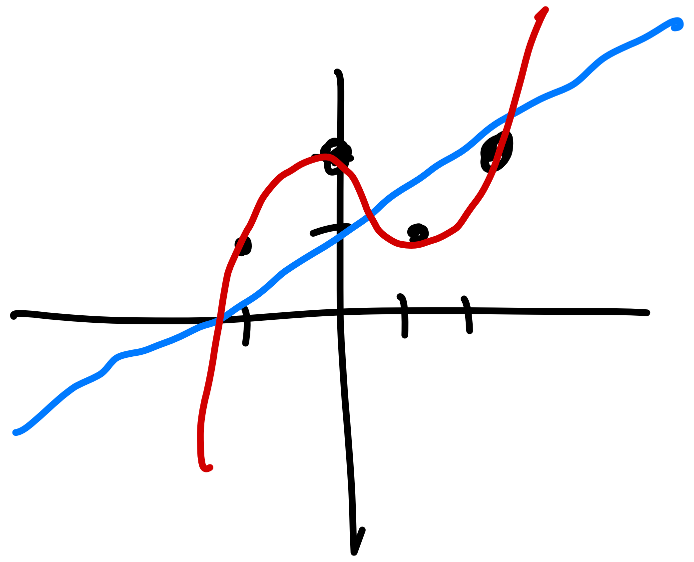
Step 3: Find the least squares solution of this system and use as the parameters of your model.

Recap Problem

$$\{(0,3),(1,1),(-1,1),(2,3)\}$$

Find the matrices X as in the previous example to find the least squares best fix parabola <u>and the least squares best fit cubic</u> for this dataset.

Answer



$\{(0,3),(1,1),(-1,1),(2,3)\}$

$$\begin{bmatrix} 1 & x_i & x_i^2 \end{bmatrix} X = \begin{bmatrix} 1 & -1 & 1 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \end{bmatrix}$$

for best-fit parabola

$$\begin{bmatrix} 1 & x_i & x_i^2 & x_i^3 \end{bmatrix} X = \begin{bmatrix} 1 & -1 & 1 & -1 \\ 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \\ 1 & 2 & 4 & 8 \end{bmatrix}$$

for best-fit cubic

Design Matrices

The Takeaway

We can use non-linear modeling functions as long as they are <u>linear in the parameters</u>.

Linear in Parameters

nonexample:

$$f(x_1, x_2) = \beta_0 \beta_1 x_1$$

$$= e^{\beta_1 x_1}$$

vectors

numbers

Definition. A function $f : \mathbb{R}^n \to \mathbb{R}$ is **linear in the parameters** $\beta_1, \ldots, \beta_k$ if it can be written as

$$f(\mathbf{x}) = \beta_1 \phi_1(\mathbf{x}) + \beta_2 \phi_2(\mathbf{x}) + \ldots + \beta_k \boxed{\phi_k(\mathbf{x})}$$

not necessarily linear

for functions $\phi_1, \ldots, \phi_k : \mathbb{R}^n \to \mathbb{R}$

Example:

$$f(x_1, x_2) = \boxed{\beta_0} \cos(x_1 x_2) + \boxed{\beta_1} e^{x^{1/3}}$$

$$f\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right)$$

An Aside: Statistical Models (Another view)

$$\mathbf{y} = X\vec{\beta} + \vec{\epsilon}$$

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(We won't use this view, this is mostly for your personal betterment, and because the notes use this notation occasionally.)

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The Takeaway (Again)

We can build <u>design matrices</u> for function which are linear in their parameters.

Linear (Regression) Model

Definition. A **linear model** with parameters $\beta_1, \ldots, \beta_k$ is a function $f : \mathbb{R}^n \to \mathbb{R}$ which is linear in the parameters $\beta_1, \ldots, \beta_k$.

The *model fitting problem* is the problem of determining which parameters fit the data "best".

General Linear Regression

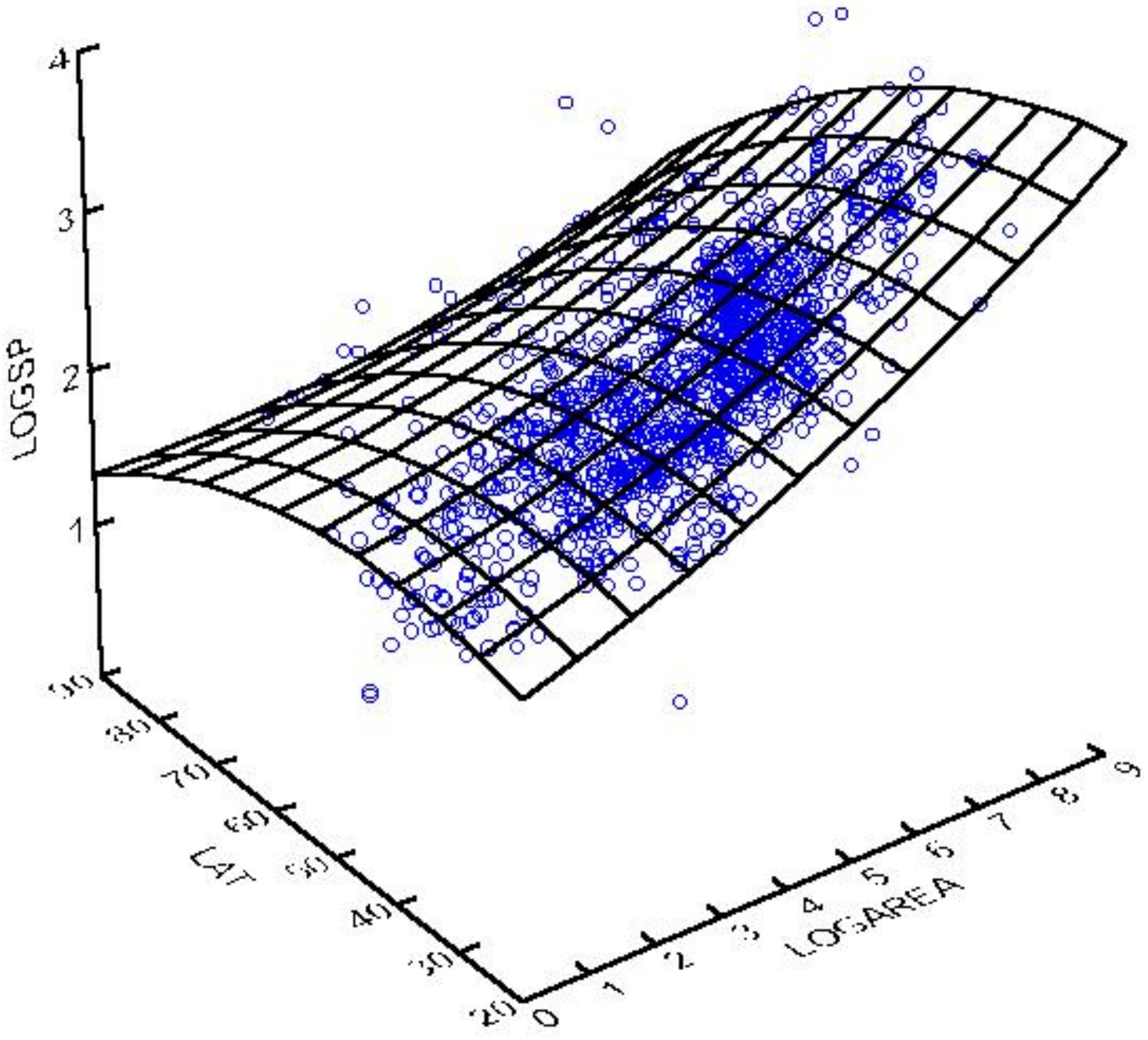
dataset: $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$ where $\mathbf{x}_i \in \mathbb{R}^n$ and $y_i \in \mathbb{R}$

Problem. Given a function

$$f_{\beta_1,\ldots,\beta_k} : \mathbb{R}^n \to \mathbb{R}$$

which is *linear in the parameters* $\beta_1, \ldots \beta_k$, find values for $\beta_1, \ldots, \beta_k$ which minimize

$$\sum_{i=1}^{k} (f_{\beta_1,\ldots,\beta_k}(\mathbf{x}_i) - y_i)^2$$



https://ordination.okstate.edu/MULTIPLE.htm

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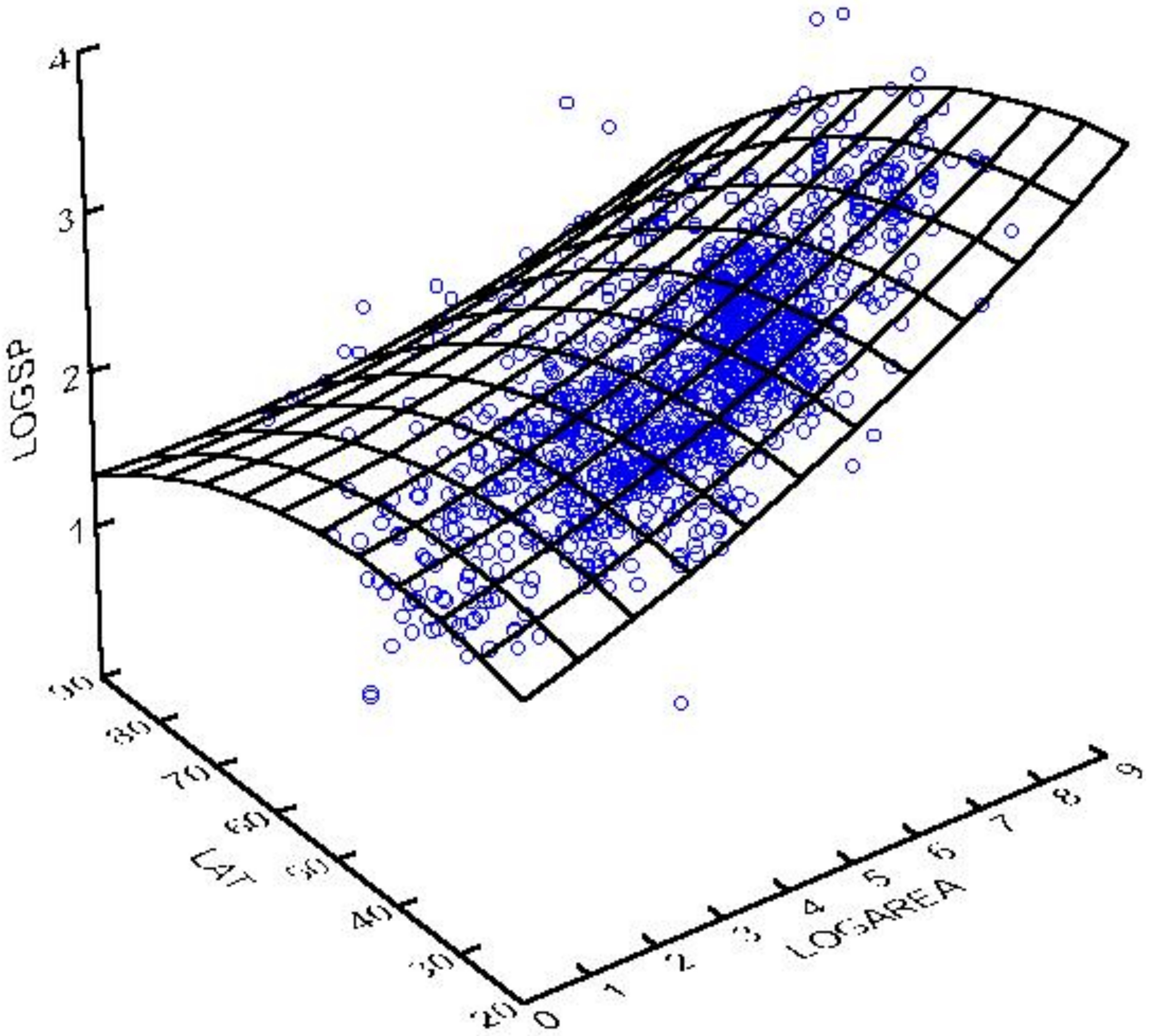
$$\sum_{i=1}^{k} \overbrace{(\underbrace{f_{\beta_1,\ldots,\beta_k}(\mathbf{x}_i)}_{\text{prediction}} - \underbrace{y_i}_{\text{observation}})}^{\text{residuals}}{}^2$$



Build a linear model which minimizes the least-squares error.

https://ordination.okstate.edu/MULTIPLE.htm

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$$\begin{aligned}
\beta_1\phi_1(\mathbf{x}_1) + \ldots + \beta_k\phi_k(\mathbf{x}_1) &= y_1 \\
\beta_1\phi_1(\mathbf{x}_2) + \ldots + \beta_k\phi_k(\mathbf{x}_2) &= y_2 \\
&\vdots \\
\beta_1\phi_1(\mathbf{x}_2) + \ldots + \beta_k\phi_k(\mathbf{x}_2) &= y_2
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Step 1: Set up an (almost assuredly inconsistent) system of linear equations in terms of the variables $\beta_1, \ldots, \beta_k$

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design matrix

$$\overset{X}{\begin{bmatrix} \phi_1(\mathbf{x}_1) & \phi_2(\mathbf{x}_1) & \ldots & \phi_k(\mathbf{x}_1) \\ \phi_1(\mathbf{x}_2) & \phi_2(\mathbf{x}_2) & \ldots & \phi_k(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{x}_m) & \phi_2(\mathbf{x}_m) & \ldots & \phi_k(\mathbf{x}_m) \end{bmatrix}} \overset{\vec{\beta}}{\begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \; \cancel{\beta_k} \\ \beta_k \end{bmatrix}} = \overset{\mathbf{y}}{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_k \end{bmatrix}}$$

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Problem. Find the design matrix for least squares regression with the function f in terms of the parameters $\beta_1, \beta_2, \ldots, \beta_k$ given the dataset $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$.

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Solution. First write $f(\mathbf{x})$ as $\beta_1\phi_1(\mathbf{x}) + \ldots + \beta_k\phi(\mathbf{x})$ where $\phi_1, \ldots, \phi_k$ are potentially non-linear functions. Then build the matrix:

$$\begin{bmatrix} \phi_1(\mathbf{x}_1) & \phi_2(\mathbf{x}_1) & \ldots & \phi_k(\mathbf{x}_1) \\ \phi_1(\mathbf{x}_2) & \phi_2(\mathbf{x}_2) & \ldots & \phi_k(\mathbf{x}_2) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_1(\mathbf{x}_m) & \phi_2(\mathbf{x}_m) & \ldots & \phi_k(\mathbf{x}_m) \end{bmatrix}$$

Question

Find the design matrix for the least squares regression with the function

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \mapsto \beta_1 \cos(x_1) + \beta_2 e^{-x_1 x_2} - \beta_1 x_3 + \beta_3$$

for the dataset

$$\mathbf{x}_1 = (0,0,0) \qquad y_1 = 5$$
$$\mathbf{x}_2 = (\pi,3,1) \qquad y_2 = 3$$

Answer: $\begin{bmatrix} 1 & 1 & 1 \\ -2 & e^{-3\pi} & 1 \end{bmatrix}$

$$f(x_1, x_2, x_3) = \boxed{\beta_1}\left(\cos(x_1) - x_3\right) + \boxed{\beta_2} e^{-x_1 x_2} + \boxed{\beta_3}$$

$$\vec{x}_1 = (0, 0, 0)$$

$$\vec{x}_2 = (\pi, 3, 1)$$

$$\begin{bmatrix} \cos(0) - 0 & e^{-0(0)} & 1 \\ \cos(\pi) - 1 & e^{-\pi 3} & 1 \end{bmatrix}$$

$$= \boxed{\begin{bmatrix} 1 & 1 & 1 \\ -2 & e^{-3\pi} & 1 \end{bmatrix}}$$

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Again, is least-squares error really what we want? What if we want to minimize something else?

Concerns for another class.

One Last Thing

Read though the extended example in the notes on "Multiple Regression in Practice."

It should be useful for Homework 12.

Symmetric Matrices

Recall: Symmetric Matrices

Definition. A square matrix A is **symmetric** if $A^T = A$.

Example:

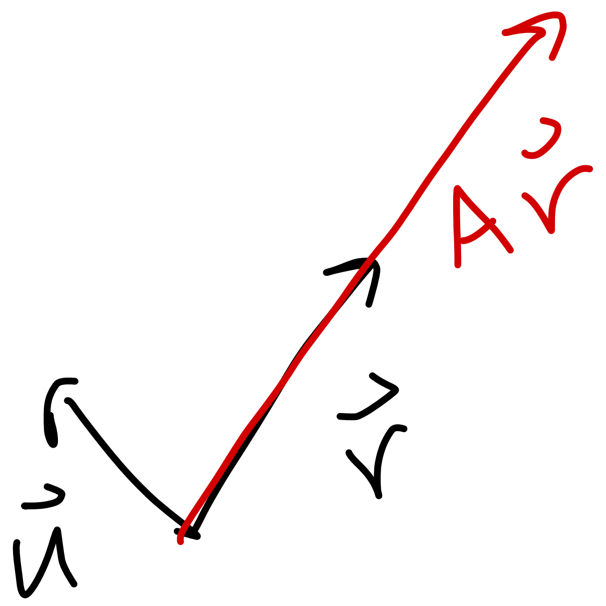
$$A_{ij} = A_{ji}$$

$$\begin{bmatrix} 1 & 0 & 2 \\ 0 & 5 & -1 \\ 2 & -1 & 4 \end{bmatrix}$$

non-example.

$$\begin{bmatrix} 1 & 0 \\ 2 & 0 \end{bmatrix}$$

Orthogonal Eigenvectors



Theorem. For a symmetric matrix A, if $\mathbf{u}$ and $\mathbf{v}$ are eigenvectors for *distinct* eigenvalues, then $\mathbf{u}$ and $\mathbf{v}$ are orthogonal.

Verify: $A\vec{u} = \lambda_1 \vec{u}$ $\quad A\vec{v} = \lambda_2 \vec{v}$

WTS: $\langle \vec{u}, \vec{v} \rangle = 0$ $\quad \langle \vec{u}, A\vec{v} \rangle = u^T A \vec{v}$

$= u^T \lambda_2 \vec{v}$

$u^T A \vec{v} = u^T A^T \vec{v} = (A\vec{u})^T \vec{v}$

$\lambda_1 \neq \lambda_2$

$$\boxed{= \lambda_1 \langle u, \vec{v} \rangle \qquad = \lambda_2 \langle u, v \rangle}$$

$\therefore \langle \vec{u}, \vec{v} \rangle = 0$

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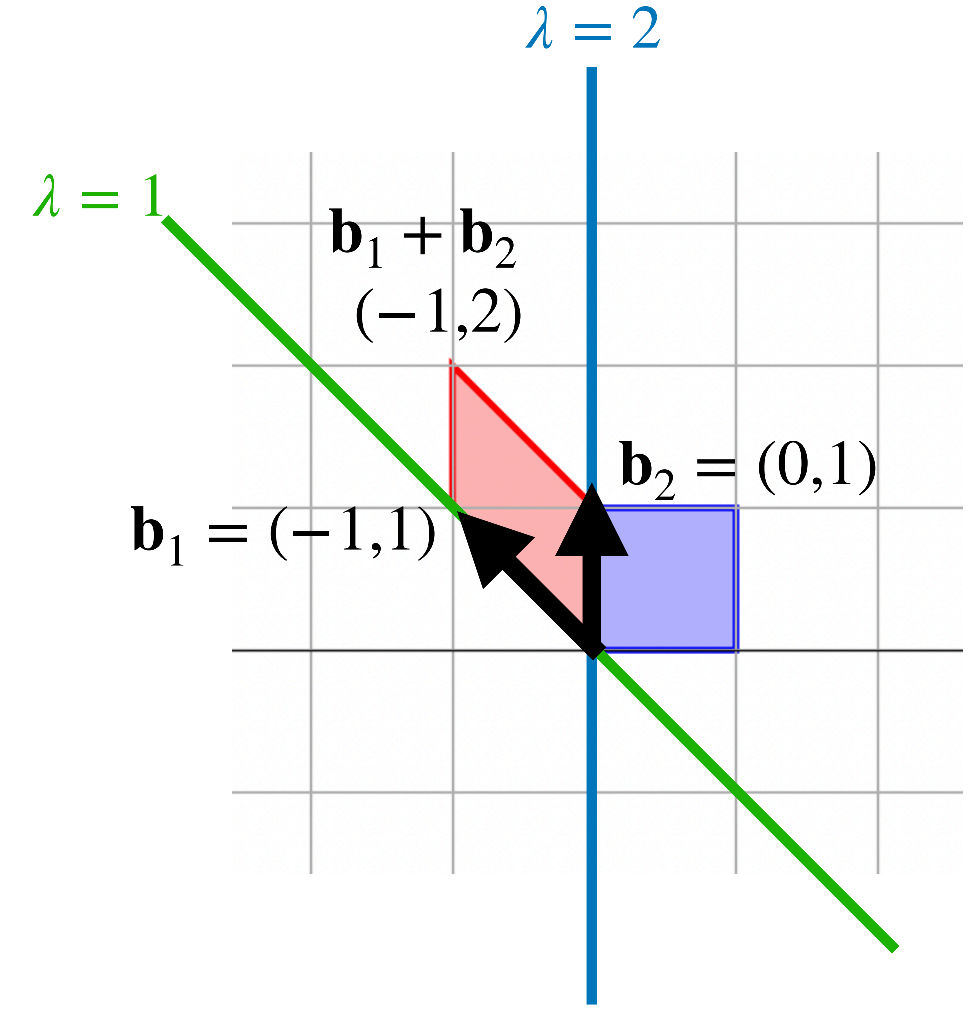
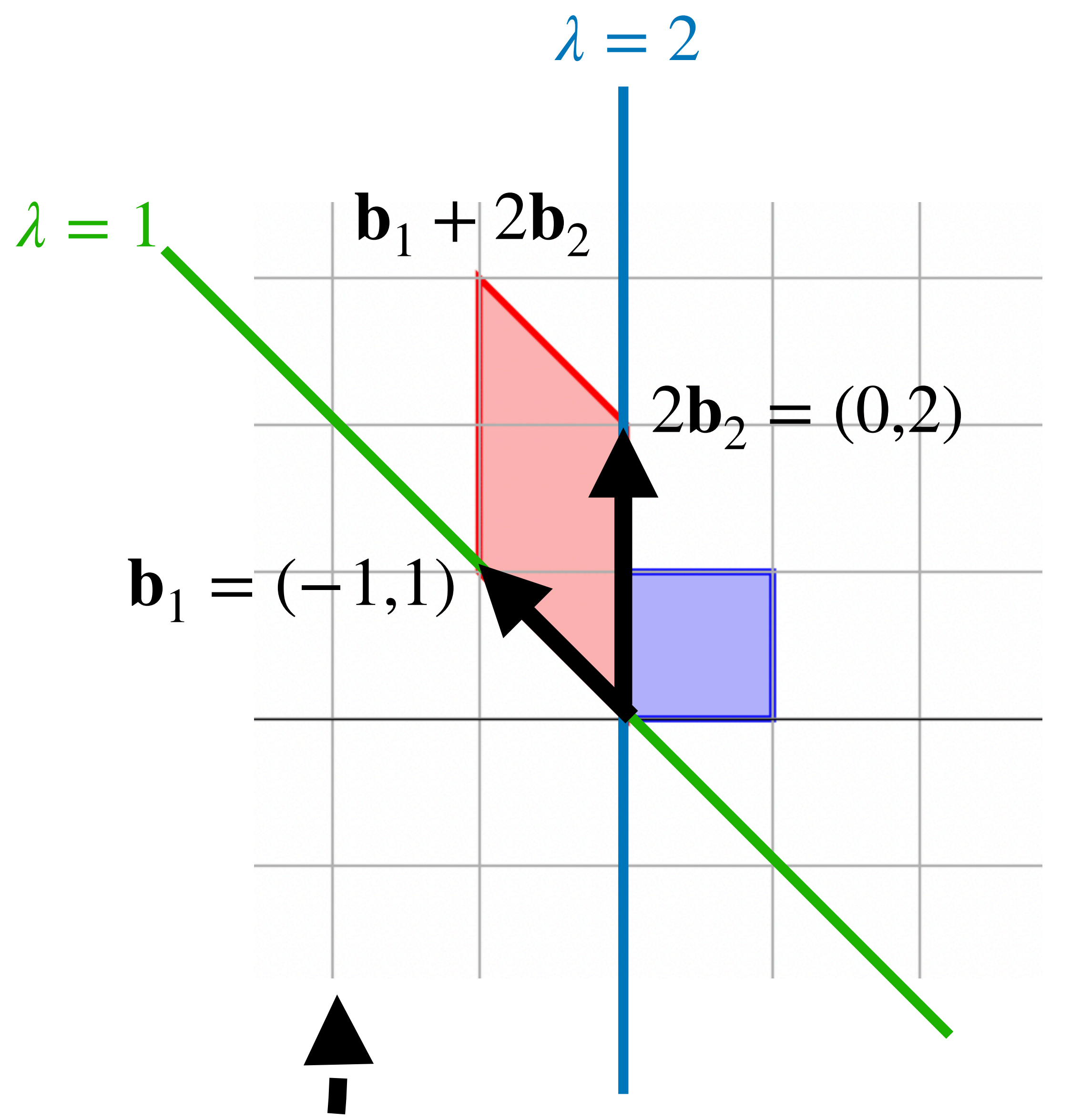
Diagonalizable matrices are the same as scaling matrices up to a change of basis.

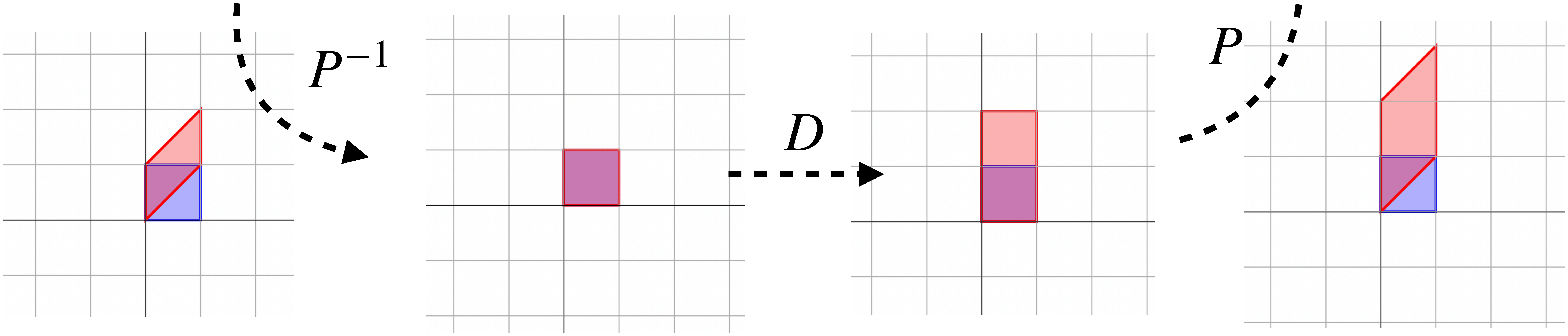
Recall: The Picture



$$A = PDP^{-1}$$

$$\begin{bmatrix} 2 & 0 \\ -1 & 1 \end{bmatrix} = \begin{bmatrix} -1 & 0 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} -1 & 0 \\ 1 & 1 \end{bmatrix}^{-1}$$





Recall: The Diagonalization Theorem

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Theorem. A is diagonalizable if and only if it has an eigenbasis.

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The idea:

Recall: The Diagonalization Theorem

$$A = \overset{\text{eigenbasis}}{P} D P^{-1}$$

Theorem. A is diagonalizable if and only if it has an eigenbasis.

The idea:

The columns of P form an <u>eigenbasis</u> for A.

Recall: The Diagonalization Theorem

$$A = \underbrace{P}_{\text{eigenbasis}}\underbrace{D}_{\text{eigenvalues}}P^{-1}$$

Theorem. A is diagonalizable if and only if it has an eigenbasis.

The idea:

The columns of P form an eigenbasis for A.

The diagonal of D are the eigenvalues for each column of P.

Recall: The Diagonalization Theorem

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Theorem. A is diagonalizable if and only if it has an eigenbasis.

The idea:

The columns of P form an <u>eigenbasis</u> for A.

The diagonal of D are the eigenvalues for each column of P.

The matrix P^{-1} is a change of basis to this eigenbasis of A.

The Spectral Theorem

Theorem. If A is symmetric, then it has an ***orthonormal*** eigenbasis.

(we won't prove this)

Symmetric matrices are diagonalizable.

But more than that, we can choose P to be ***orthogonal***.

Recall: Orthonormal Matrices

Definition. A matrix is **orthonormal** if its columns form an orthonormal set.

The notes call a square orthonormal matrix an **orthogonal** matrix.

Recall: Inverses of Orthogonal Matrices

Theorem. If an $n \times n$ matrix U is orthogonal (square orthonormal) then it is invertible and

$$U^{-1} = U^T$$

Verify:

Orthogonal Diagonalizability

Definition. A matrix A is **orthogonally diagonalizable** if there is a diagonal matrix D and matrix P such that

$$A = PDP^T = PDP^{-1}$$

P must be an <u>orthogonal matrix</u>.

Symmetric matrices are orthogonally diagonalizable

Orthogonal Diagonalizability and Symmetry

Fact. All orthogonally diagonalizable matrices are symmetric.

Verify:

$A = PDP^T$

$$\begin{aligned} A^T &= (PDP^T)^T \\ &= P^{TT}(PD)^T \\ &= P^{TT} D^T P^T \\ &= PDP^T = A \end{aligned}$$

Orthogonal Diagonalizability and Symmetry

Theorem. A matrix is orthogonally diagonalizable if and only if it is symmetric.

(You won't need to construct an orthogonal diagonalization, we'll just use NumPy.)

Quadratic Forms

Quadratic Forms

Definition. A **quadratic form** is an function of variables $x_1, \ldots, x_n$ in which every term has degree two:

$$\sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{ij} x_i x_j \qquad x_i^2 \,, \quad x_j^2$$

Quadratic forms are the quadratic versions the left-hand-sides of linear equations.

Examples

$$Q(x_1, x_2, x_3) = 2x_1^2 + 2x_3^2 + 4x_1x_3 - 2x_2x_3$$

$$Q(\vec{x}) = \vec{x}^T\vec{x} = \langle \vec{x}, \vec{x} \rangle$$

Non.examples

$$Q(x_1) = x_1^3$$

linear term

$$Q(x_1, x_2) = x_1^2 + x_1x_2 + \cancel{\boxed{x_2}}$$

Quadratic Forms and Symmetric Matrices

Fact. Every quadratic form can be represented as

$$\boxed{\mathbf{x}^T}\boxed{A\mathbf{x}} \qquad \langle x, Ax \rangle$$

where A is <u>symmetric</u>.

Example: $3x_1^2 + 7x_2^2 = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 3 & 0 \\ 0 & 7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$

$\begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 3x_1 \\ 7x_2 \end{bmatrix} = 3x_1^2 + 7x_2^2$

Example: Computing the Quadratic Form for a Matrix

$$A = \begin{bmatrix} 3 & -2 \\ -2 & 7 \end{bmatrix}$$

This means, given a symmetric matrix A, we can compute its corresponding quadratic form:

$$\begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 3 & -2 \\ -2 & 7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 3x_1 - 2x_2 \\ -2x_1 + 7x_2 \end{bmatrix}$$

$$= x_1(3x_1 - 2x_2) + x_2(-2x_1 + 7x_2) = \boxed{3x_1^2 - 4x_1x_2 + 7x_2^2}$$

$$3x_1^2 - 2x_2x_1 + (-2)x_2x_1 + 7x_2^2 =$$

Quadratic forms and Symmetric Matrices (Again)

Furthermore, we can generally say

$$\mathbf{x}^T A \mathbf{x} = \sum_{i=1}^{n} \sum_{j=1}^{n} A_{ij} x_i x_j$$

Verify:

A Slightly more Complicated Example

$$A = \begin{bmatrix} 1 & 2 & -1 \\ 2 & 3 & 0 \\ -1 & 0 & 5 \end{bmatrix}$$

Let's expand $\mathbf{x}^T A\mathbf{x}$:

Matrices from Quadratic Forms

$$Q(\mathbf{x}) = 5x_1^2 + 3x_2^2 + 2x_3^2 - x_1x_2 + 8x_2x_3$$

We can also go in the other direction. Let's express this as $\mathbf{x}^T A\mathbf{x}$:

How To: Matrices of Quadratic Forms

Problem. Given a quadratic form $Q(\mathbf{x})$, find the symmetric matrix A such that $Q(\mathbf{x}) = \mathbf{x}^T A \mathbf{x}$.

Solution.

» if $Q(\mathbf{x})$ has the term αx_i^2 then $A_{ii} = \alpha$

» if $Q(\mathbf{x})$ has the term $\alpha x_i x_j$, then $A_{ij} = A_{ji} = \dfrac{\alpha}{2}$

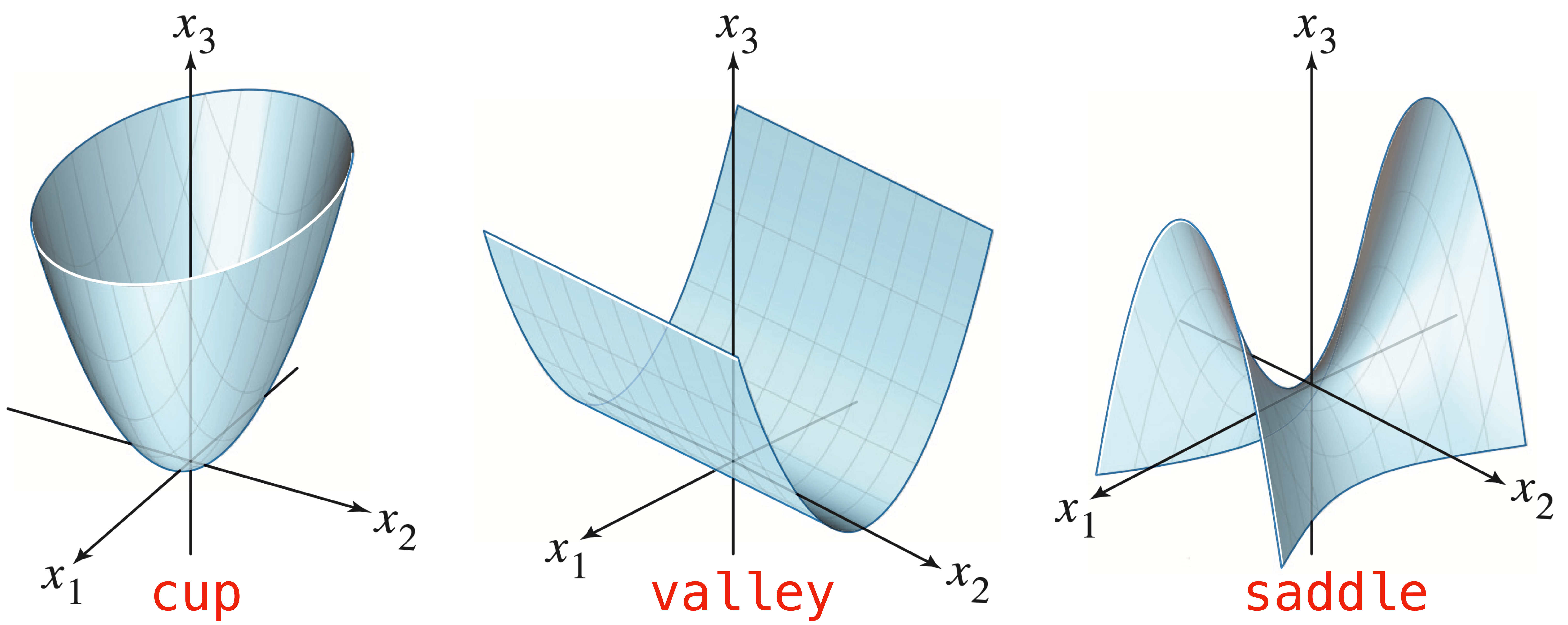
Question

$$Q(x_1, x_2, x_3, x_4) = x_1^2 + 3x_2^2 - 2x_3x_4 - 6x_4^2 + 7x_1x_3$$

Find the symmetric matrix A *such that* $Q(\mathbf{x}) = \mathbf{x}^T A\mathbf{x}$.

Answer

Shapes of of Quadratic Forms in $\mathbb{R}^3$

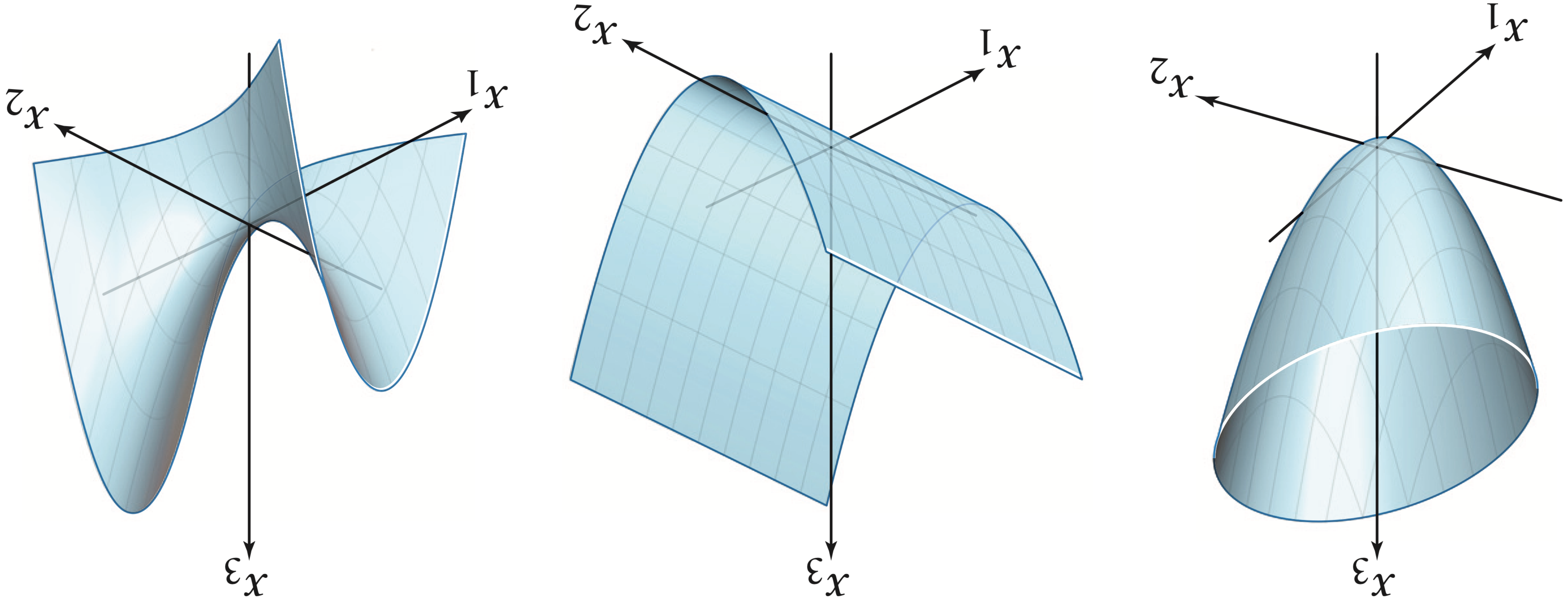


There are essentially three possible shapes (six if you include the negations).

Can we determine what shape it will be mathematically?

Linear Algebra and its Applications, Lay, Lay, McDonald

Shapes of of Quadratic Forms in $\mathbb{R}^3$



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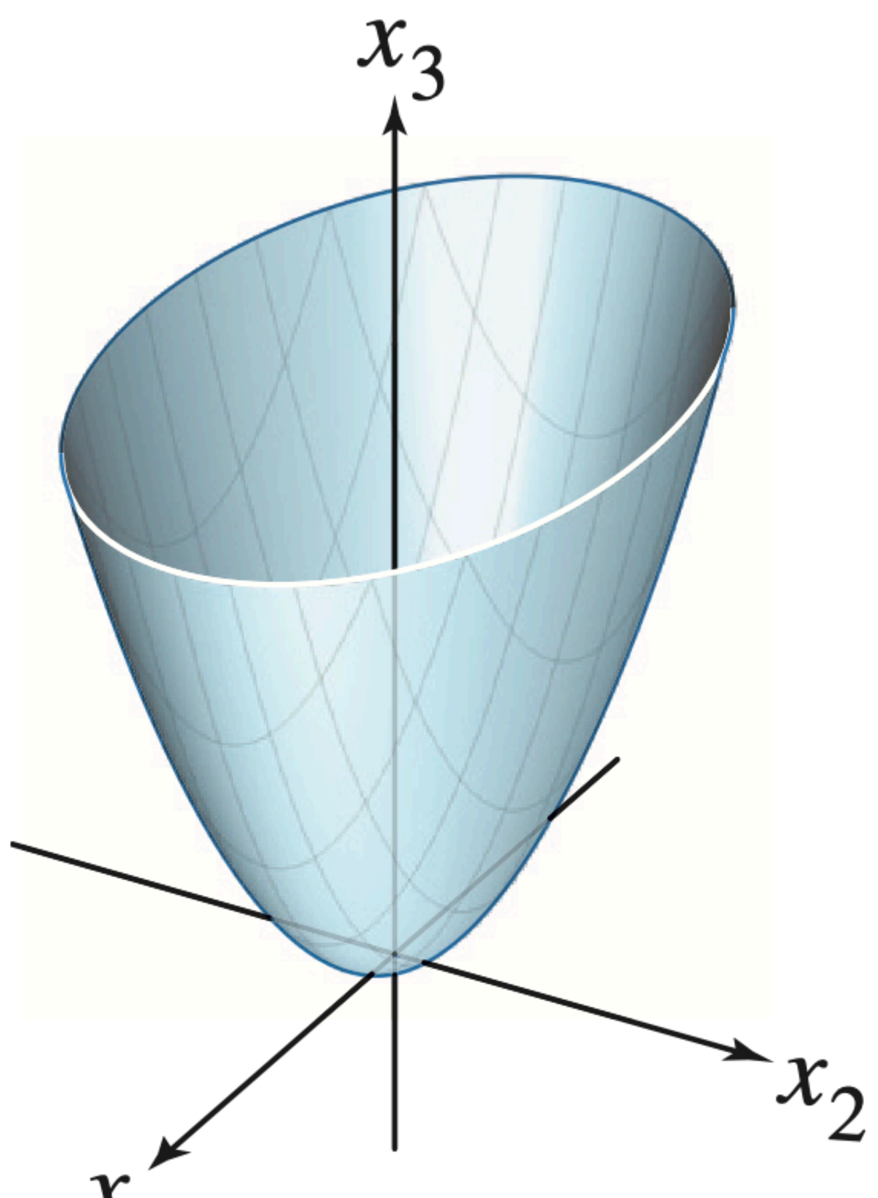
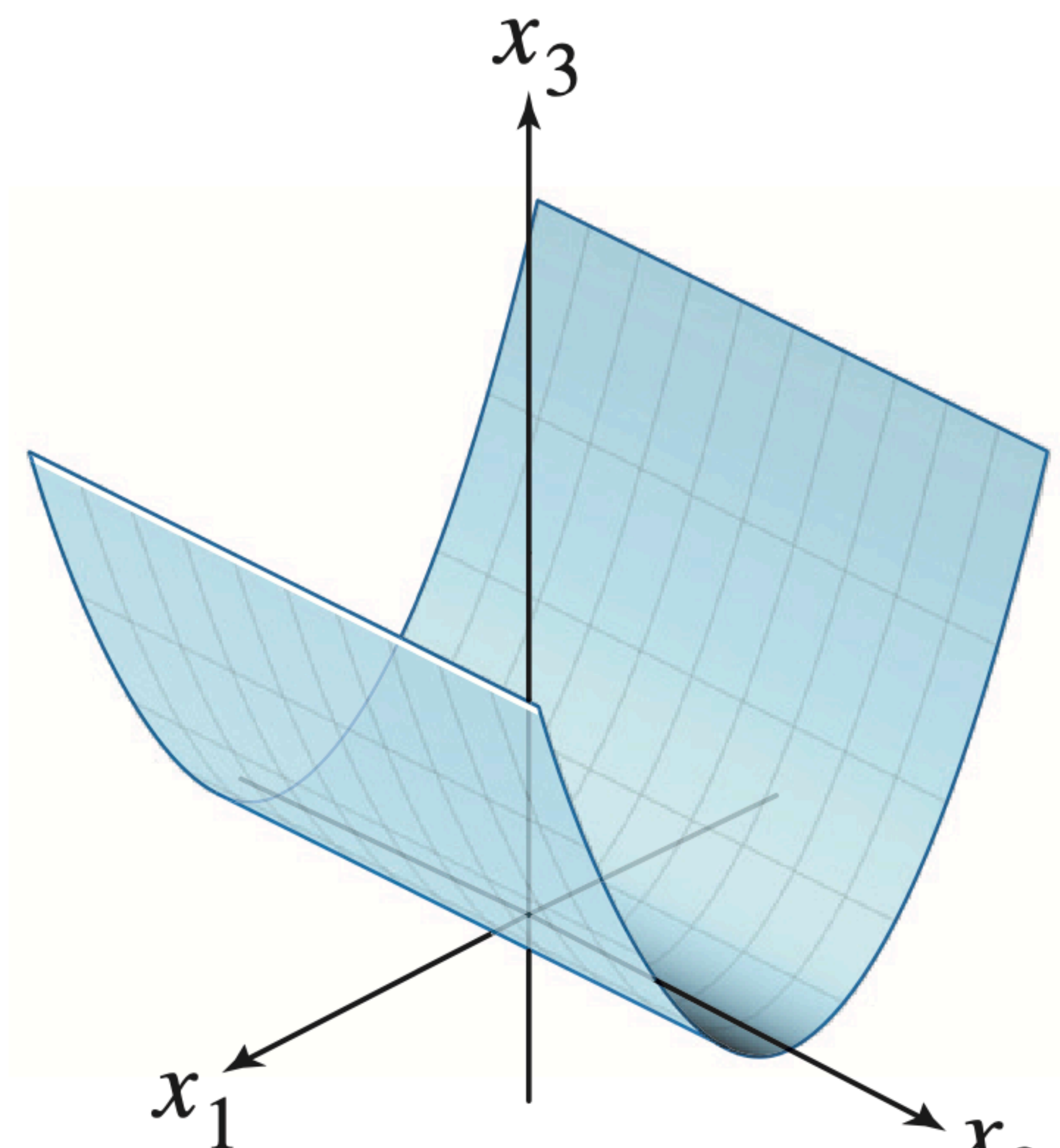
Definiteness



$Q(\mathbf{x}) > 0$



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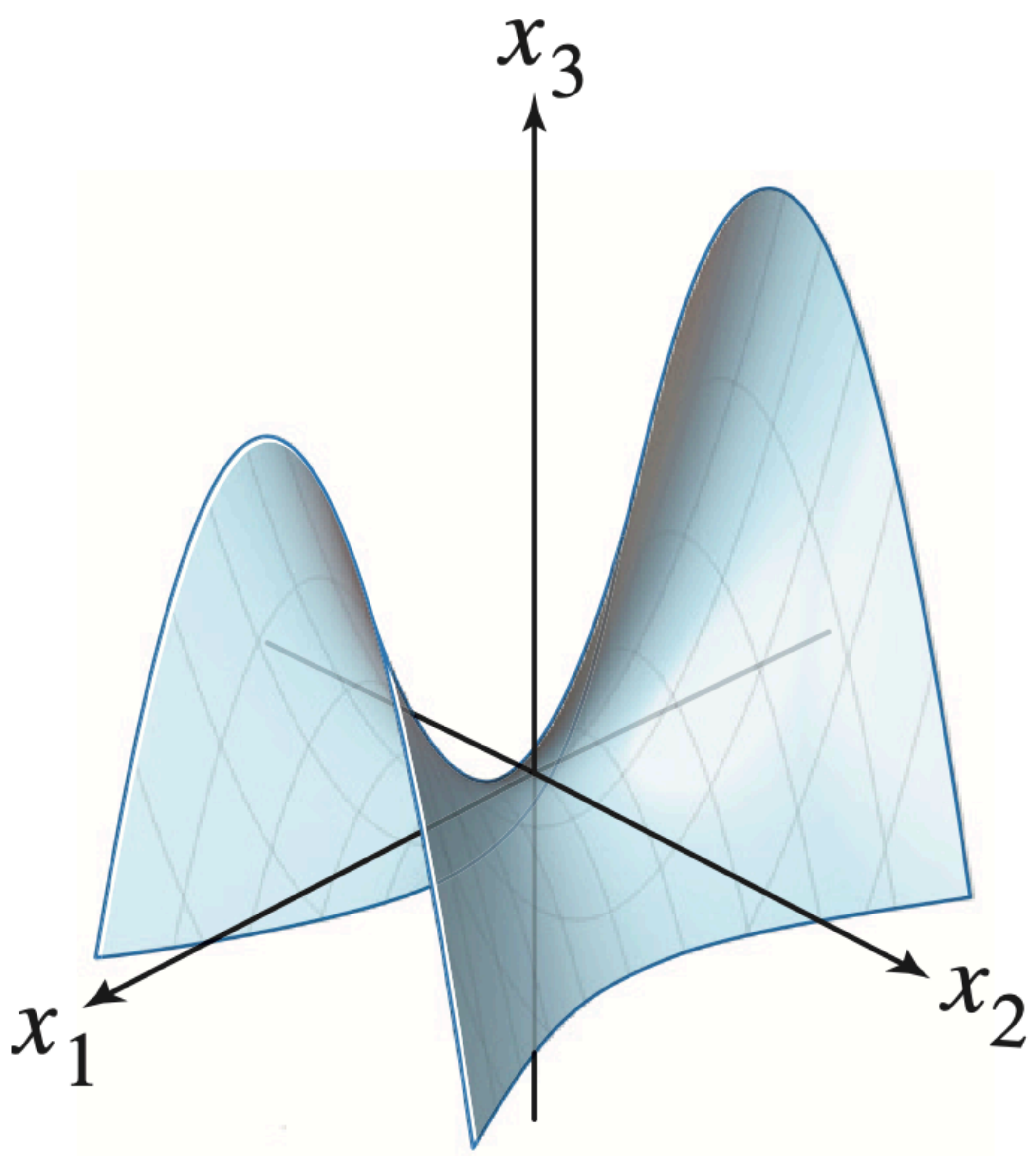
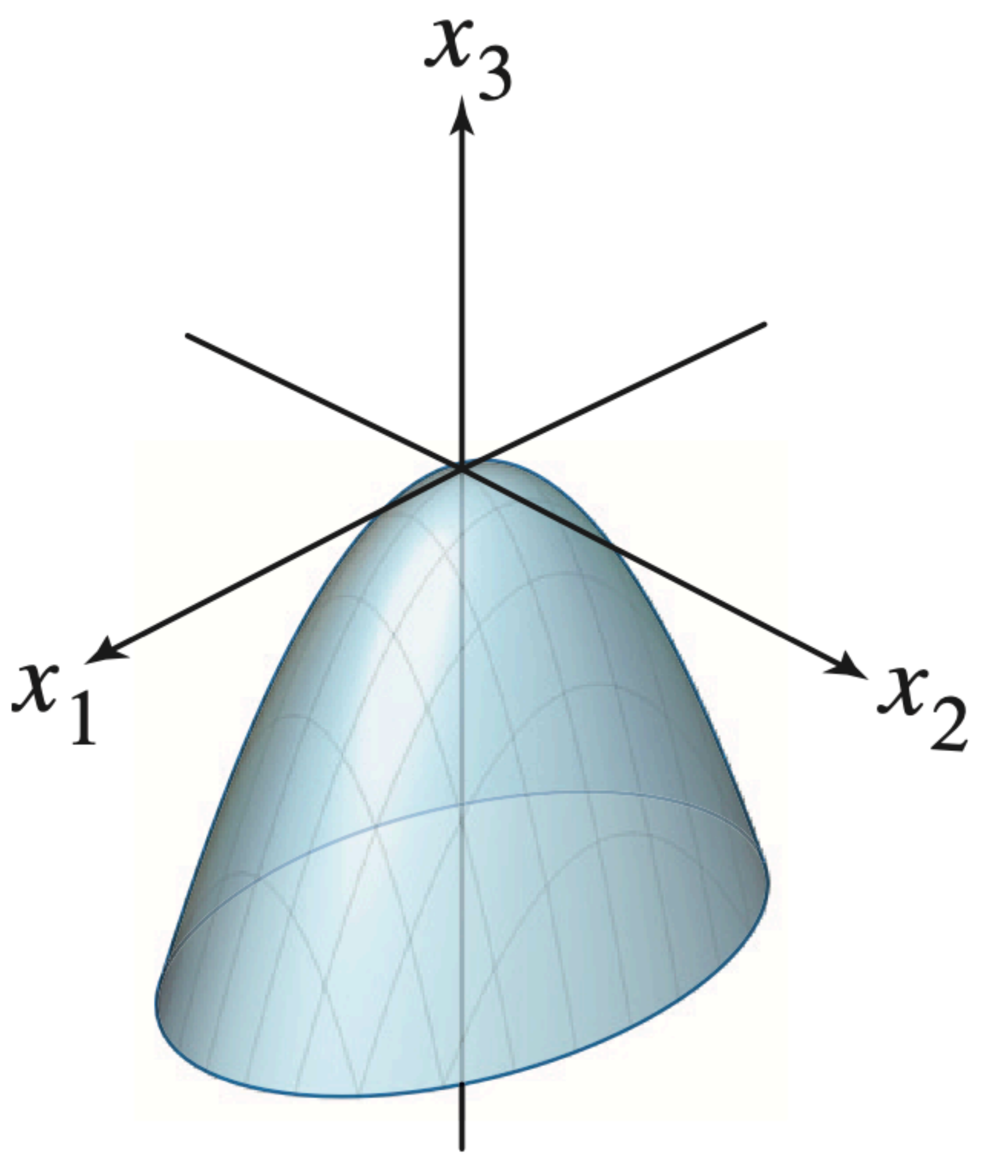


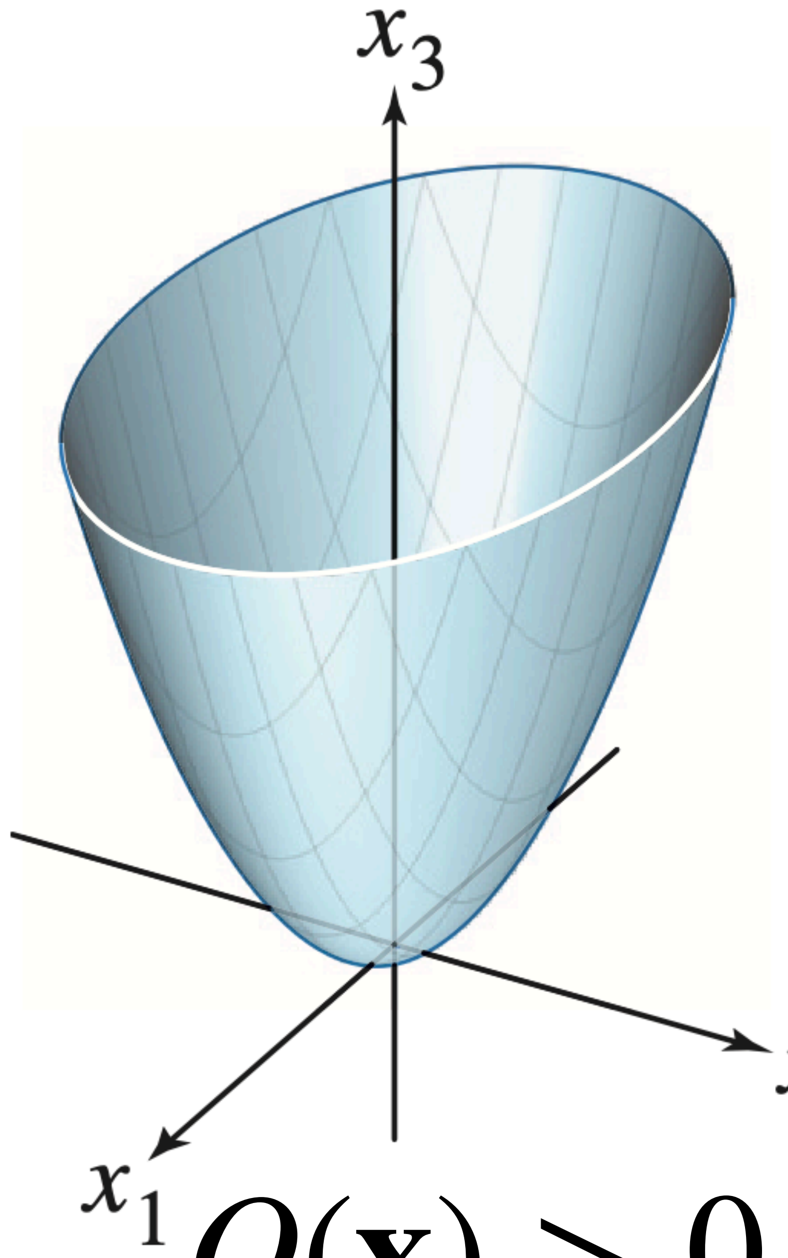
$Q(\mathbf{x})$ can be + & –



$Q(\mathbf{x}) < 0$

For $\mathbf{x} \neq \mathbf{0}$, each of the above graphs satisfy the associated properties.

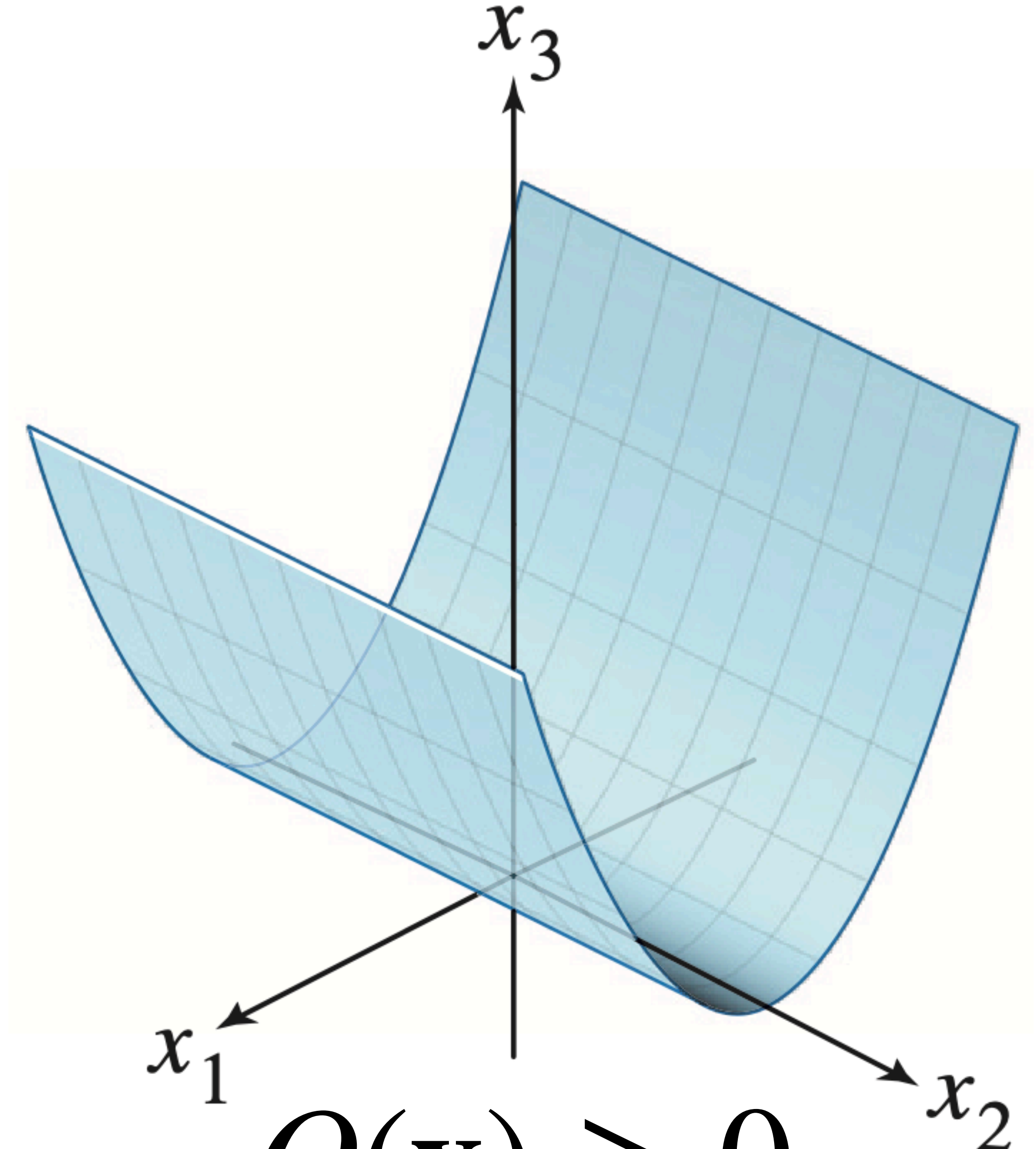
Definiteness



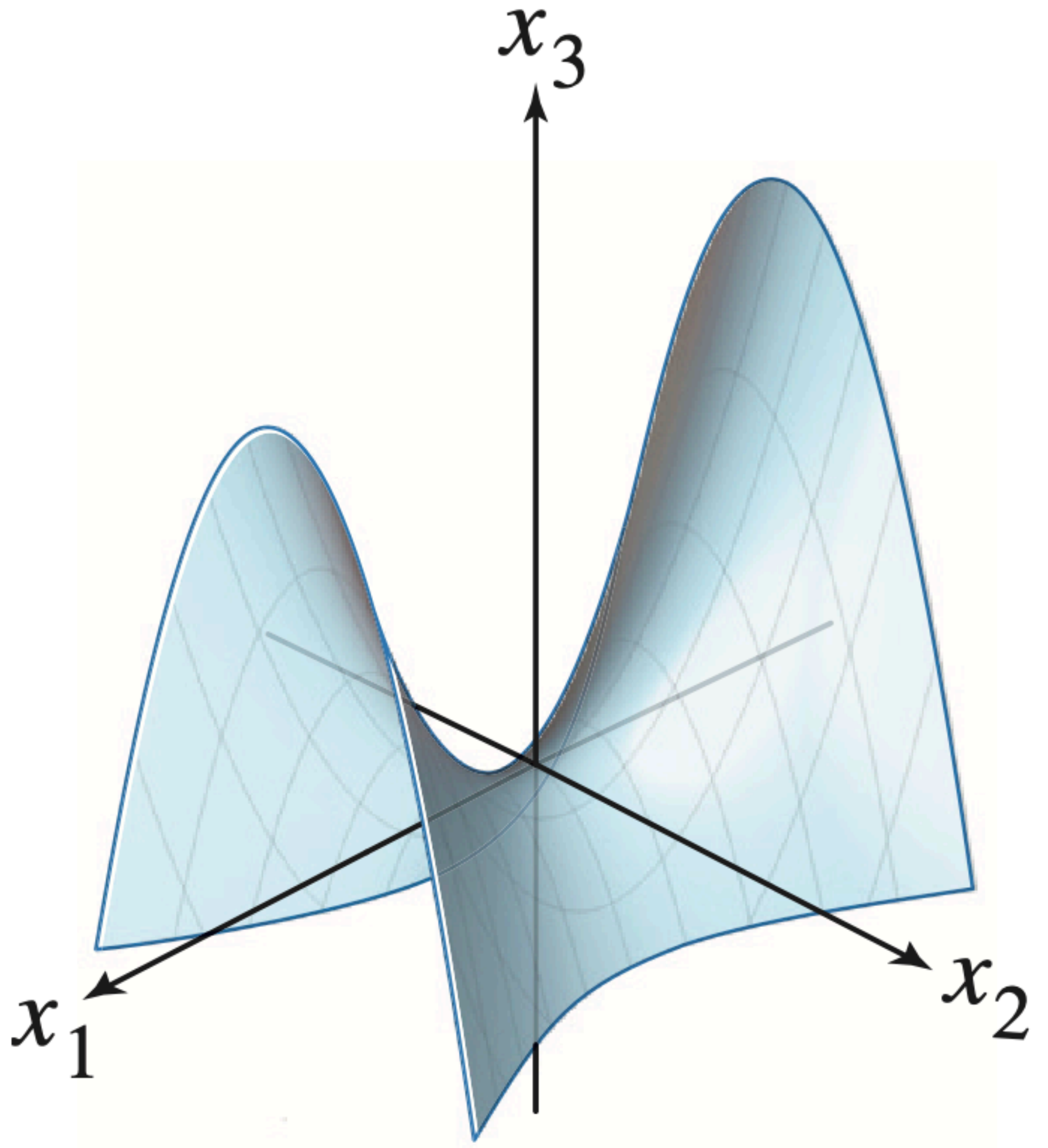
$Q(\mathbf{x}) > 0$

positive definite

positive semidefinite



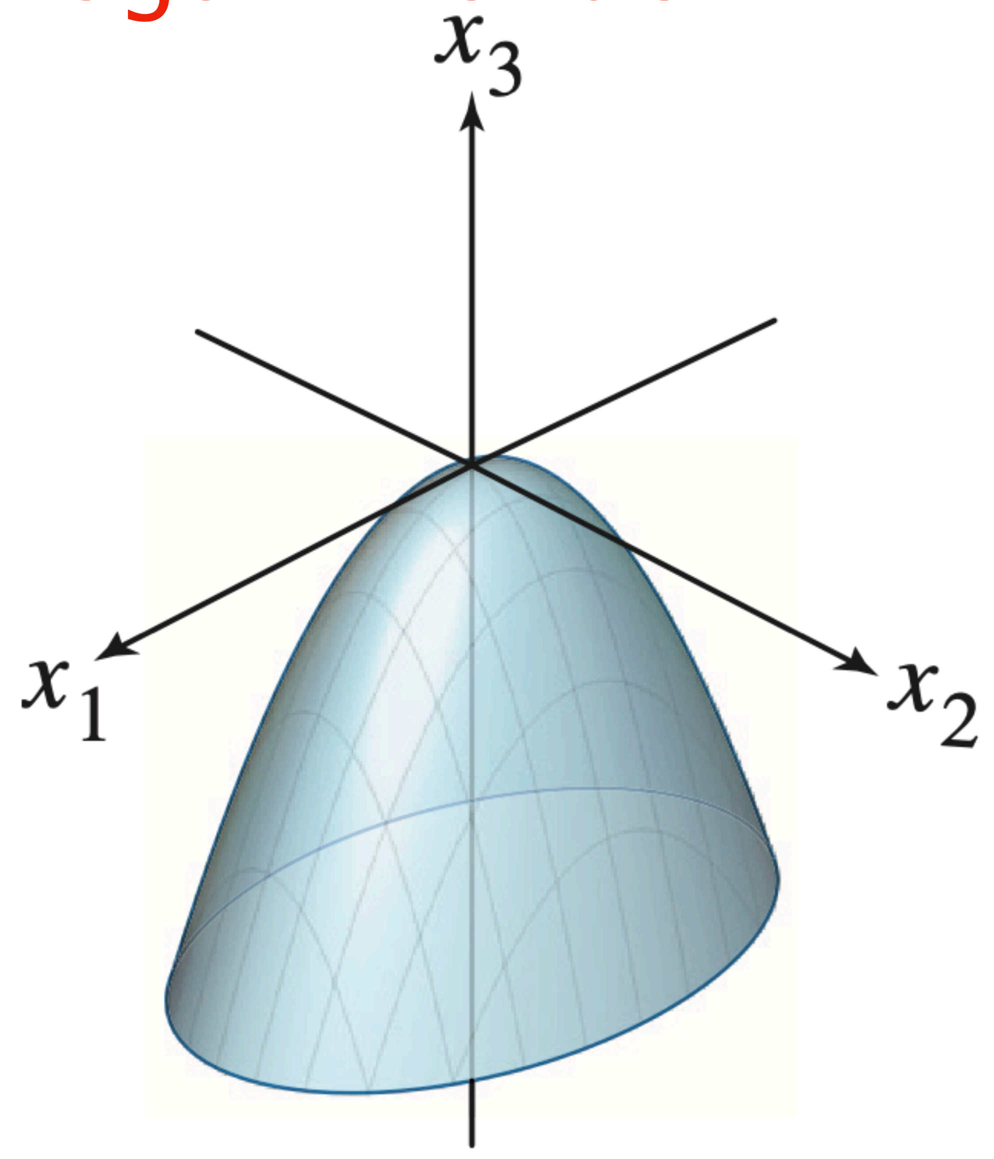
$Q(\mathbf{x}) \geq 0$



$Q(\mathbf{x})$ can be + & –

indefinite

negative definite



$Q(\mathbf{x}) < 0$

For $\mathbf{x} \neq \mathbf{0}$, each of the above graphs satisfy the associated properties.

Definiteness and Eigenvectors

Theorem. For a symmetric matrix A, the quadratic form $\mathbf{x}^T A \mathbf{x}$

- **positive definite** ≡ all positive eigenvalues
- **positive semidefinite** ≡ all nonnegative eigenvalues
- **indefinite** ≡ positive and negative eigenvalues
- **negative definite** ≡ all negative eigenvalues

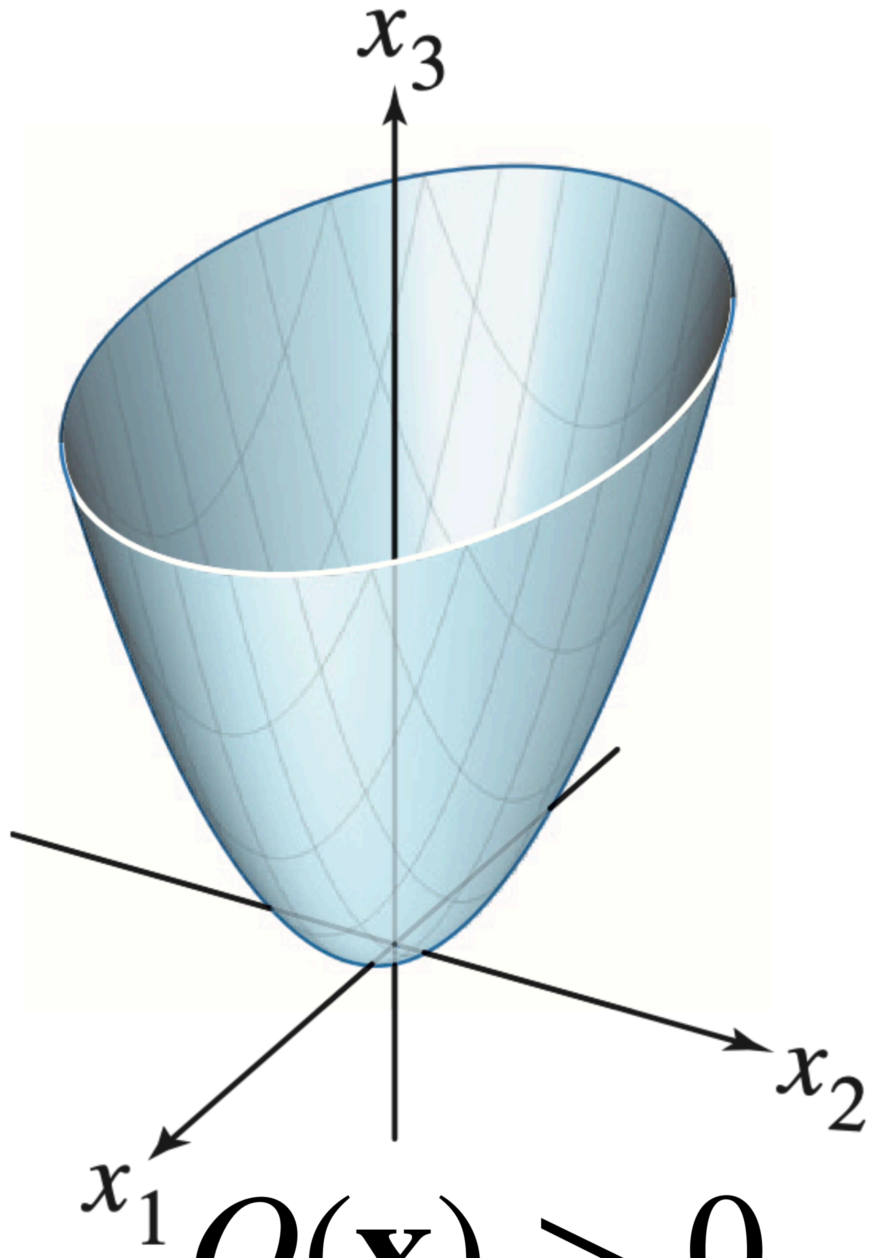
Definiteness

all nonneg. eigenvals

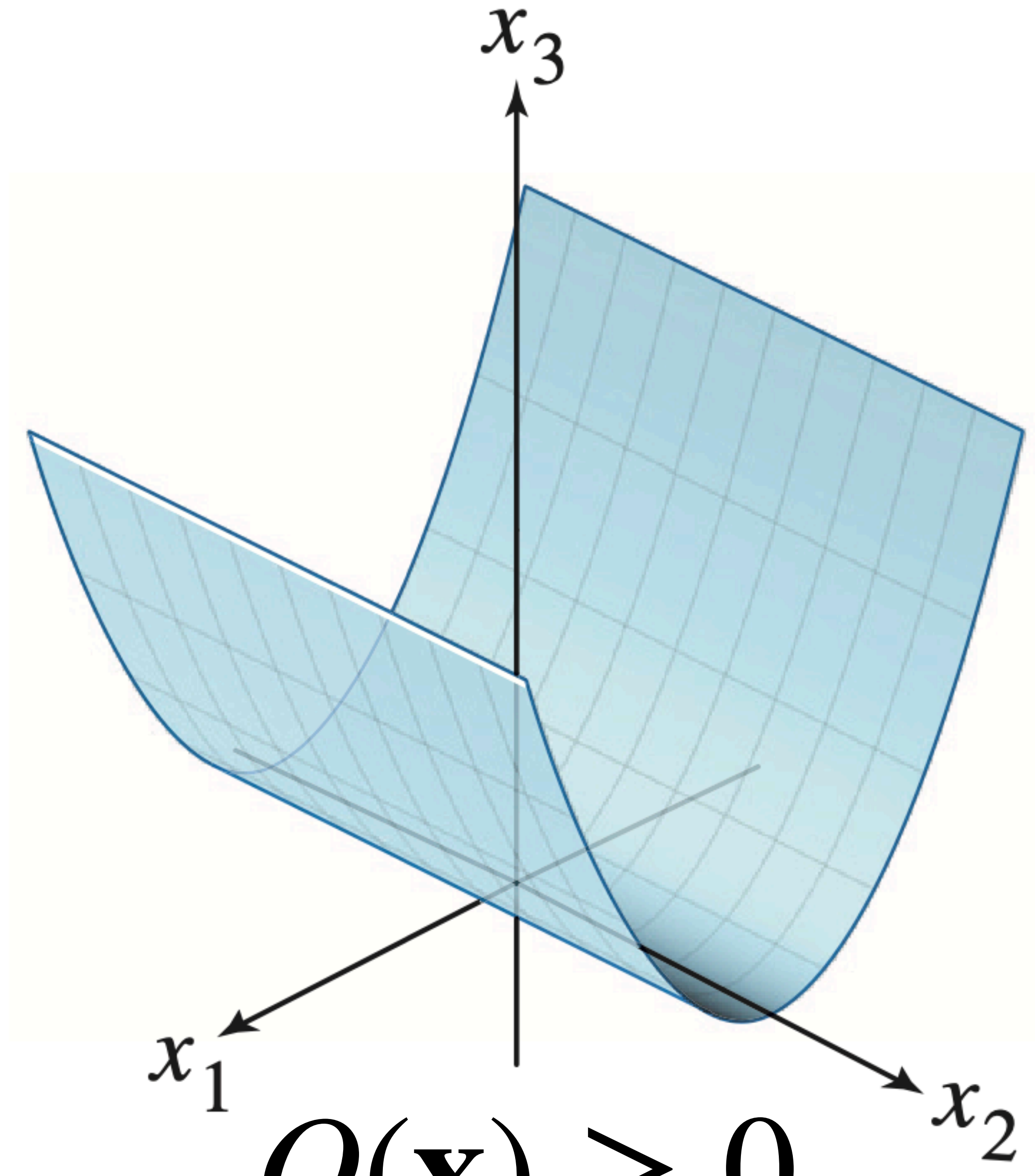
positive semidefinite

all neg. eigenvals

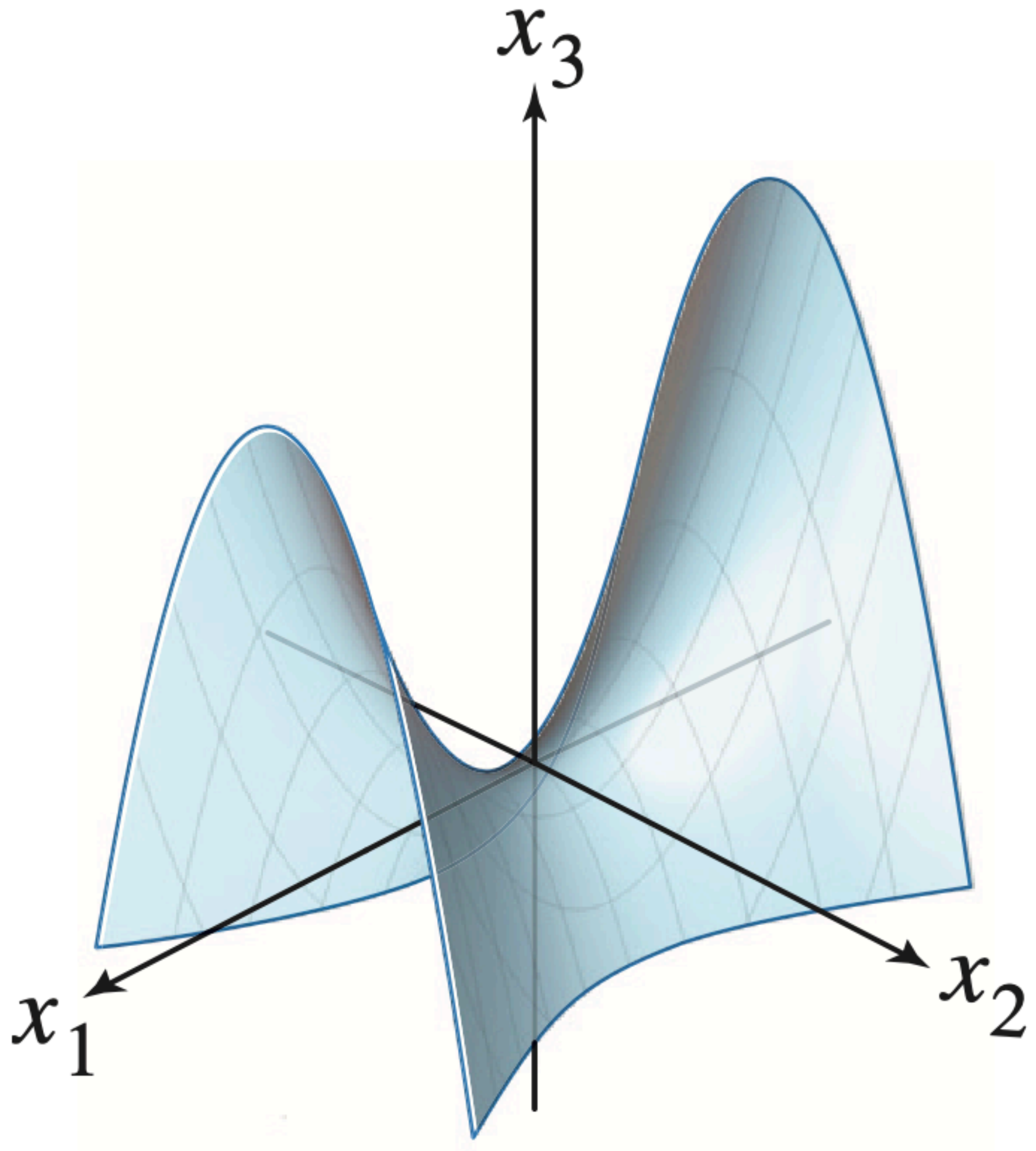
negative definite



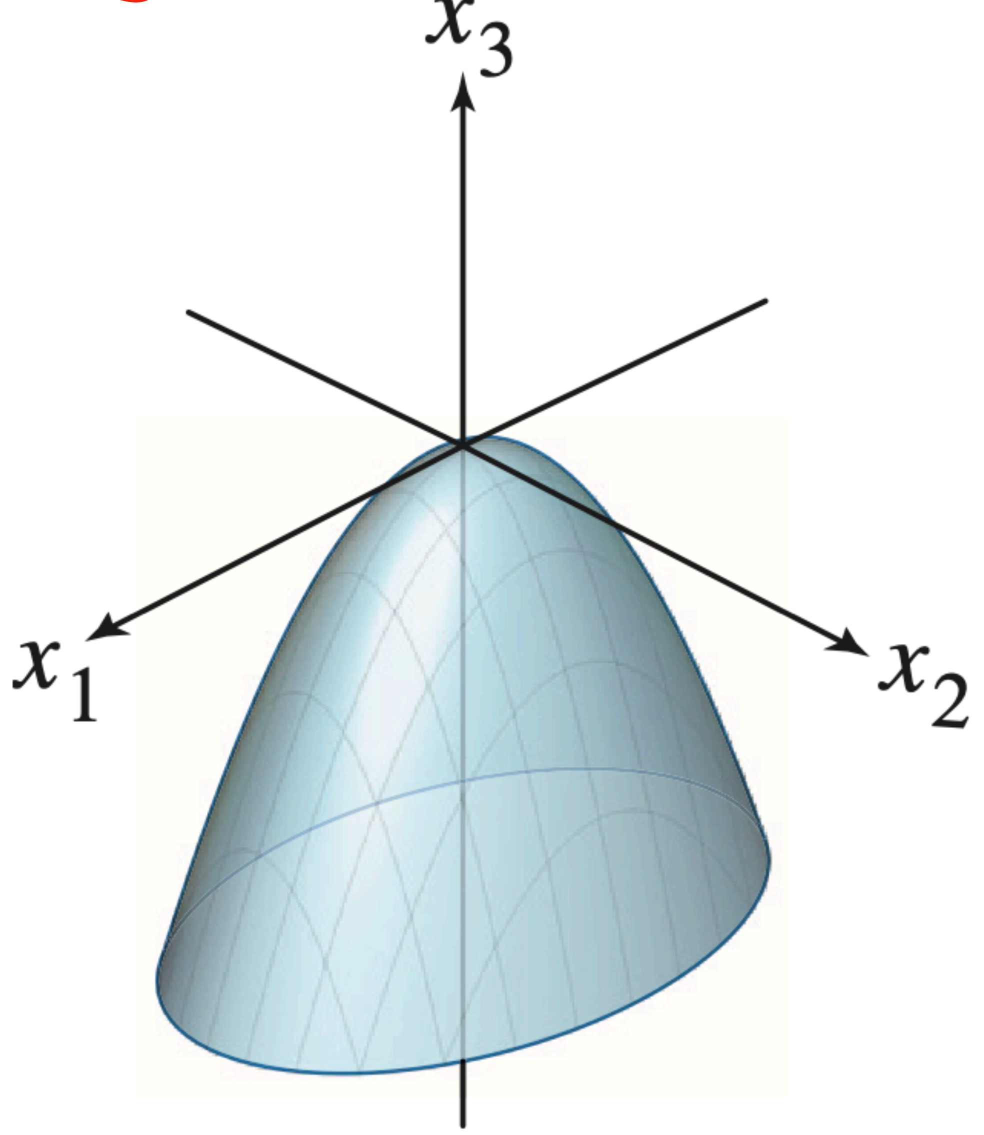
$Q(\mathbf{x}) > 0$



$Q(\mathbf{x}) \geq 0$



$Q(\mathbf{x})$ can be + & −



$Q(\mathbf{x}) < 0$

positive definite

all pos. eigenvals

indefinite

pos. and neg. eigenvals

Positive Definite Case

```
Let's think why this is for the positive definite case:
```

Example

$$Q(x_1, x_2, x_3) = 3x_1^2 + x_2^2 + 4x_2x_3 + x_3^2$$

`Let's determine which case this is:`

Constrained Optimization

In General

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Given a function $f: \mathbb{R}^n \to \mathbb{R}$ and a set of vectors X from $\mathbb{R}^n$ the **constrained minimization problem** for f over X is the problem of determining

$$\min_{\mathbf{v} \in X} f(\mathbf{v})$$

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(analogously for maximization)

In General

Given a function $f : \mathbb{R}^n \to \mathbb{R}$ and a set of vectors X from $\mathbb{R}^n$ the **constrained minimization problem** for f over X is the problem of determining

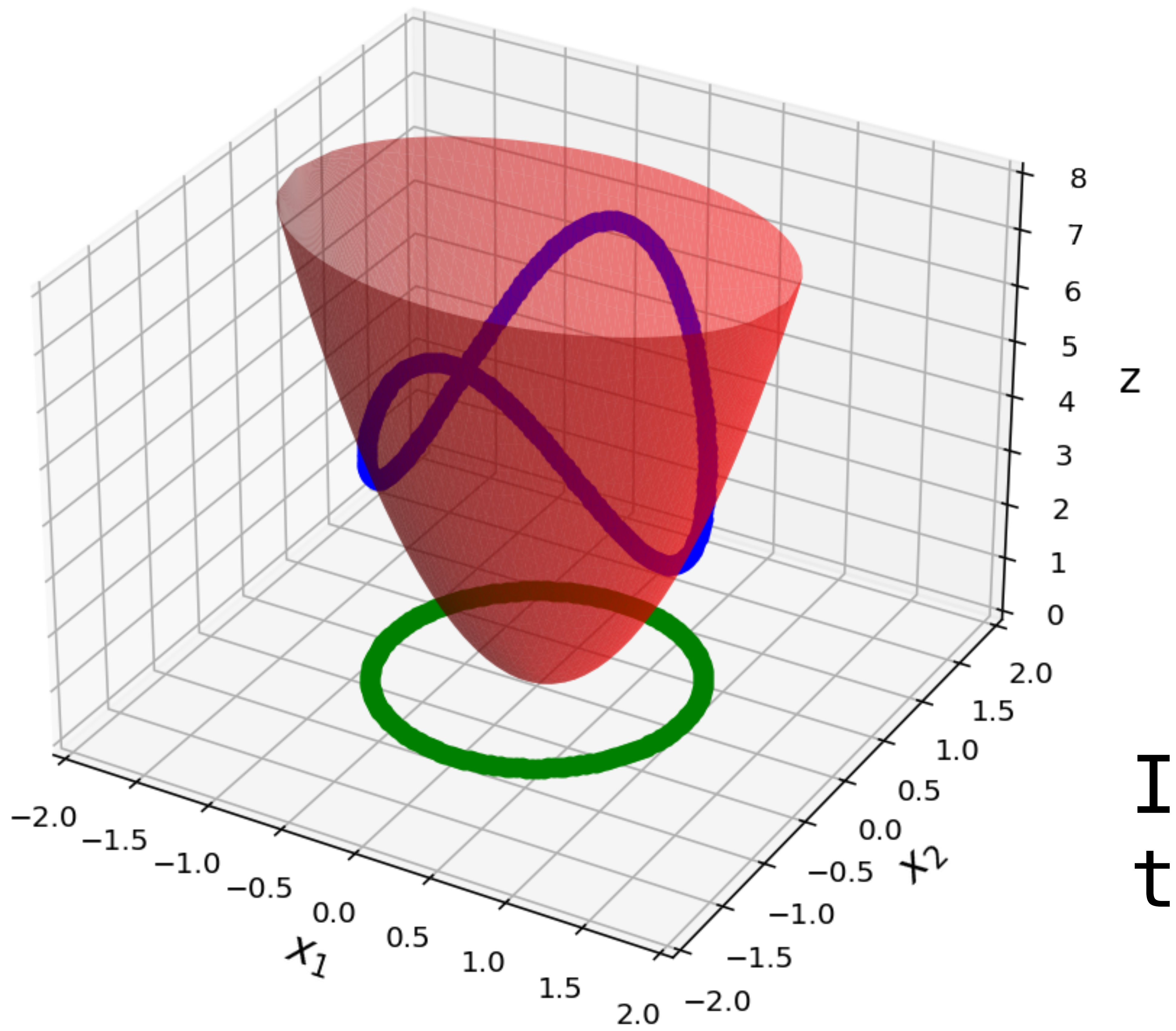
$$\min_{\mathbf{v} \in X} f(\mathbf{v})$$

(analogously for maximization)

Find the smallest value of $f(\mathbf{v})$ subject to choosing a vector in X

Constrained Optimization for Quadratic Forms and Unit Vectors

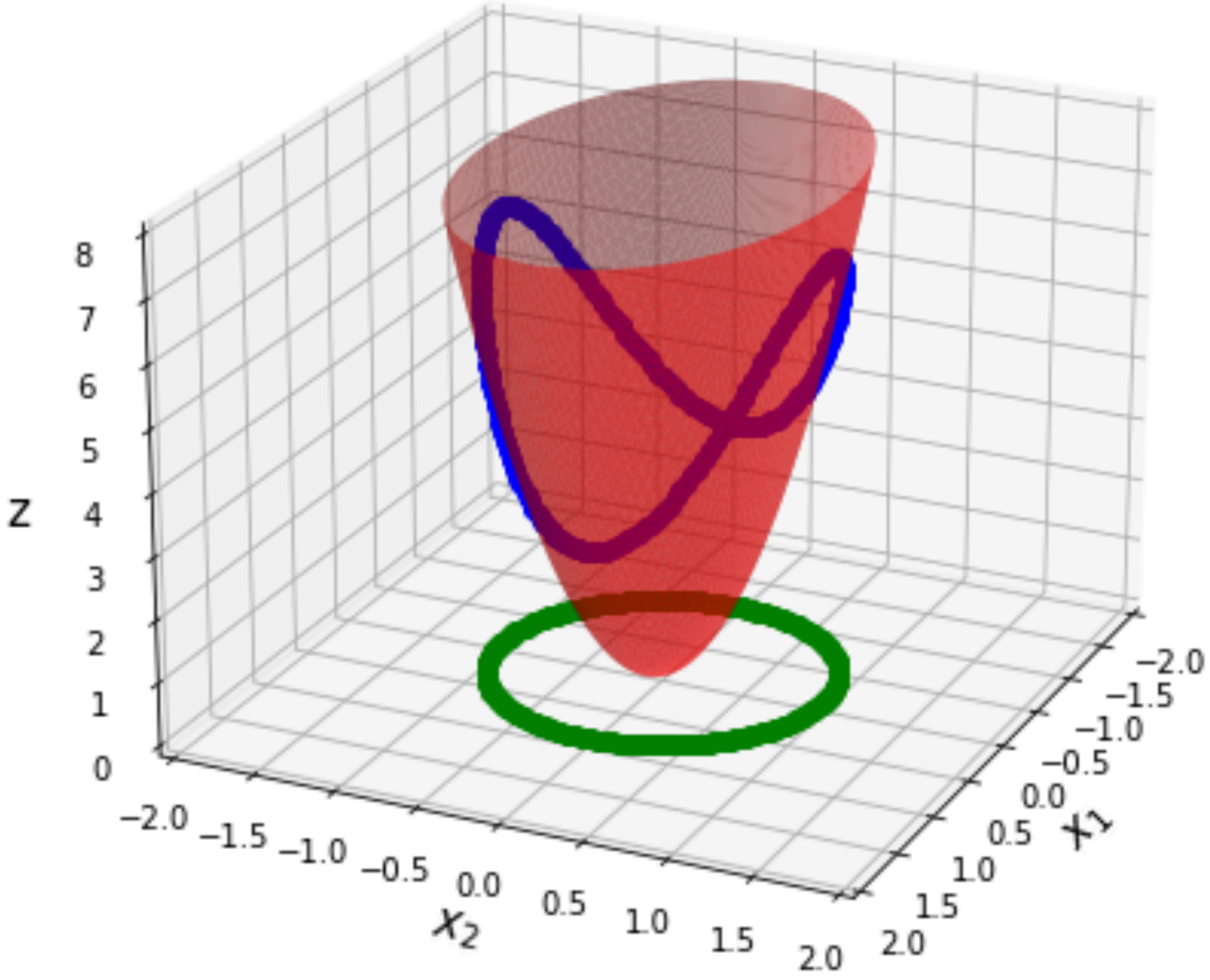
mini/maximize $\mathbf{x}^T A \mathbf{x}$ subject to $\|\mathbf{x}\| = 1$



It's common to constraint to unit vectors.

Example: $3x_1^2 + 7x_2^2$

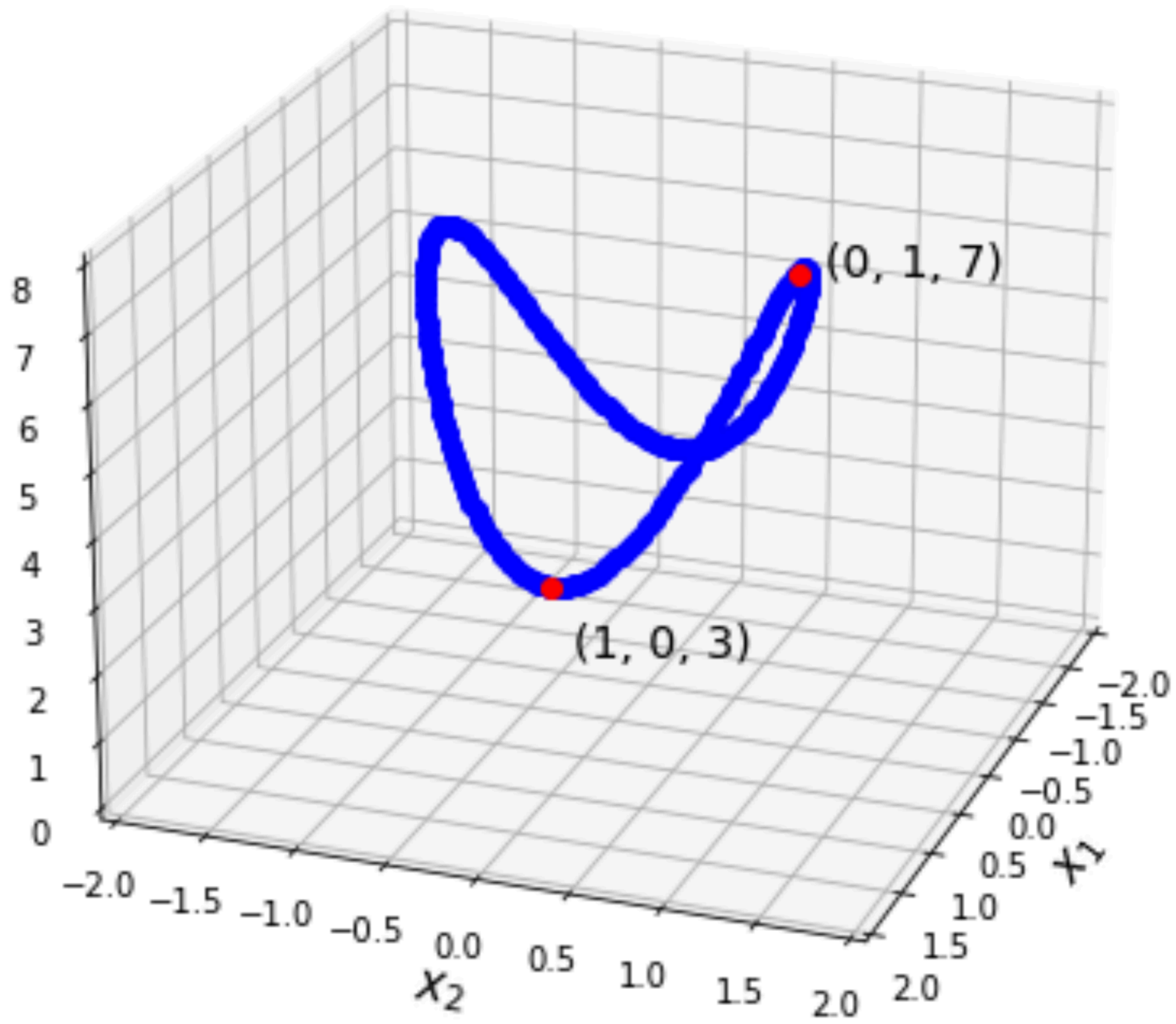
`What are the min/max values?:`



Example: $3x_1^2 + 7x_2^2$

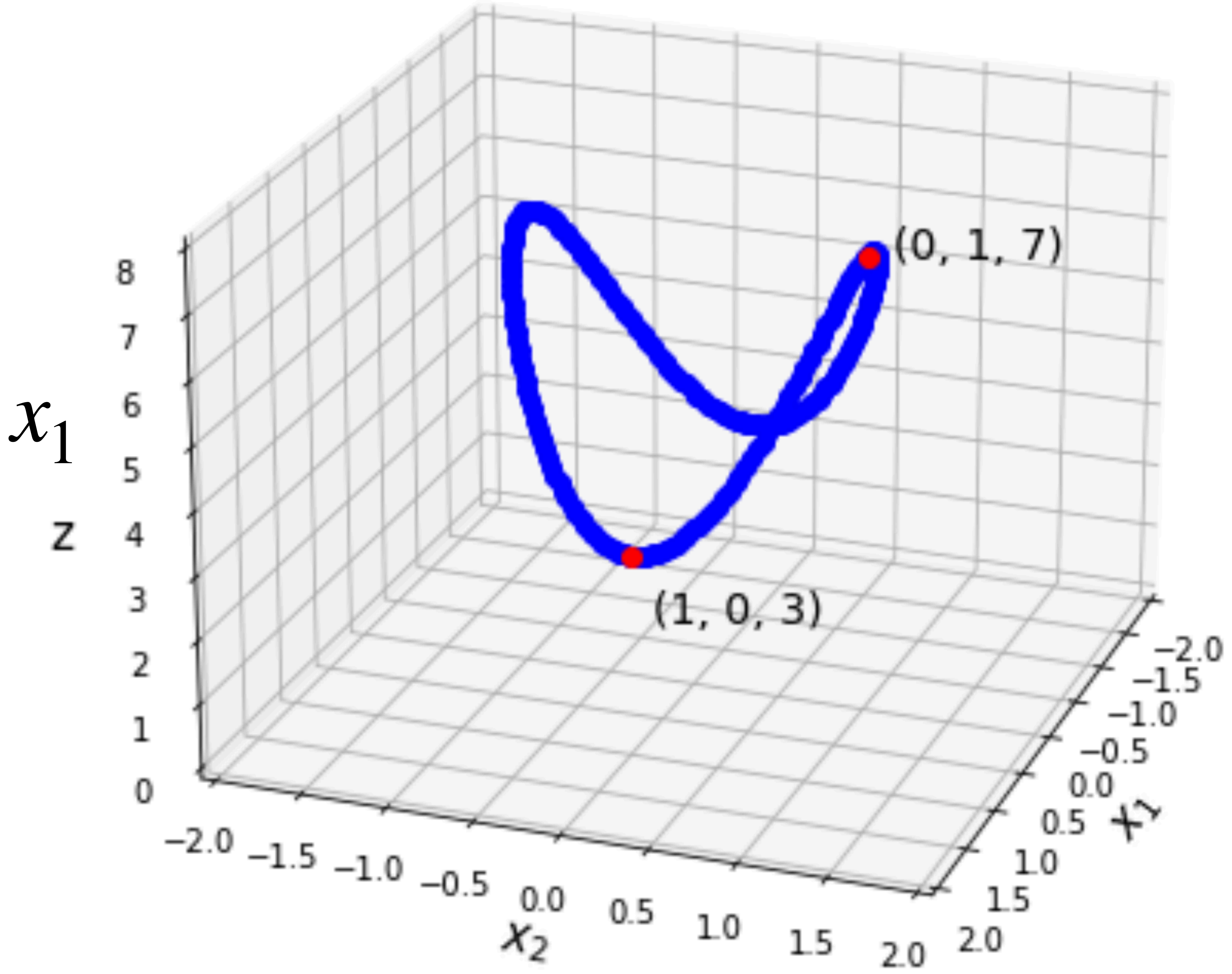
The minimum and maximum values are attained when the "weight" of the vector is distributed all on x_1 or x_2.

x_1



Example: $3x_1^2 + 7x_2^2$

```
What is the matrix?:
```



Constrained Optimization and Eigenvalues

Theorem. For a symmetric matrix A, with *largest* eigenvalue λ_1 and *smallest* eigenvalue λ_n

$$\max_{\|\mathbf{x}\|=1} \mathbf{x}^T A \mathbf{x} = \lambda_1 \qquad \min_{\|\mathbf{x}\|=1} \mathbf{x}^T A \mathbf{x} = \lambda_n$$

No matter the shape of A, this will hold.

How To: Constrained Optimization

How To: Constrained Optimization

Problem. Find the maximum value of $\mathbf{x}^T A \mathbf{x}$ subject to $\|\mathbf{x}\| = 1$.

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Solution. Find the largest eigenvalue of A, this will be the maximum value.

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Problem. Find the maximum value of $\mathbf{x}^T A \mathbf{x}$ subject to $\|\mathbf{x}\| = 1$.

Solution. Find the largest eigenvalue of A, this will be the maximum value.

(Use NumPy)

Summary

We can build models which are nonlinear functions if those functions are linear in their parameters.

We can solve constrained optimization problems using eigenvalues.