Math for Machine Learning

Week 1.1: Vectors, matrices, and least squares regression

By: Samuel Deng

Lesson Overview

Vectors and matrices (an ML view). A single datapoint/sample in ML is represented as a vector $\mathbf{x} \in \mathbb{R}^d$. A collection of samples is represented as a matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$.

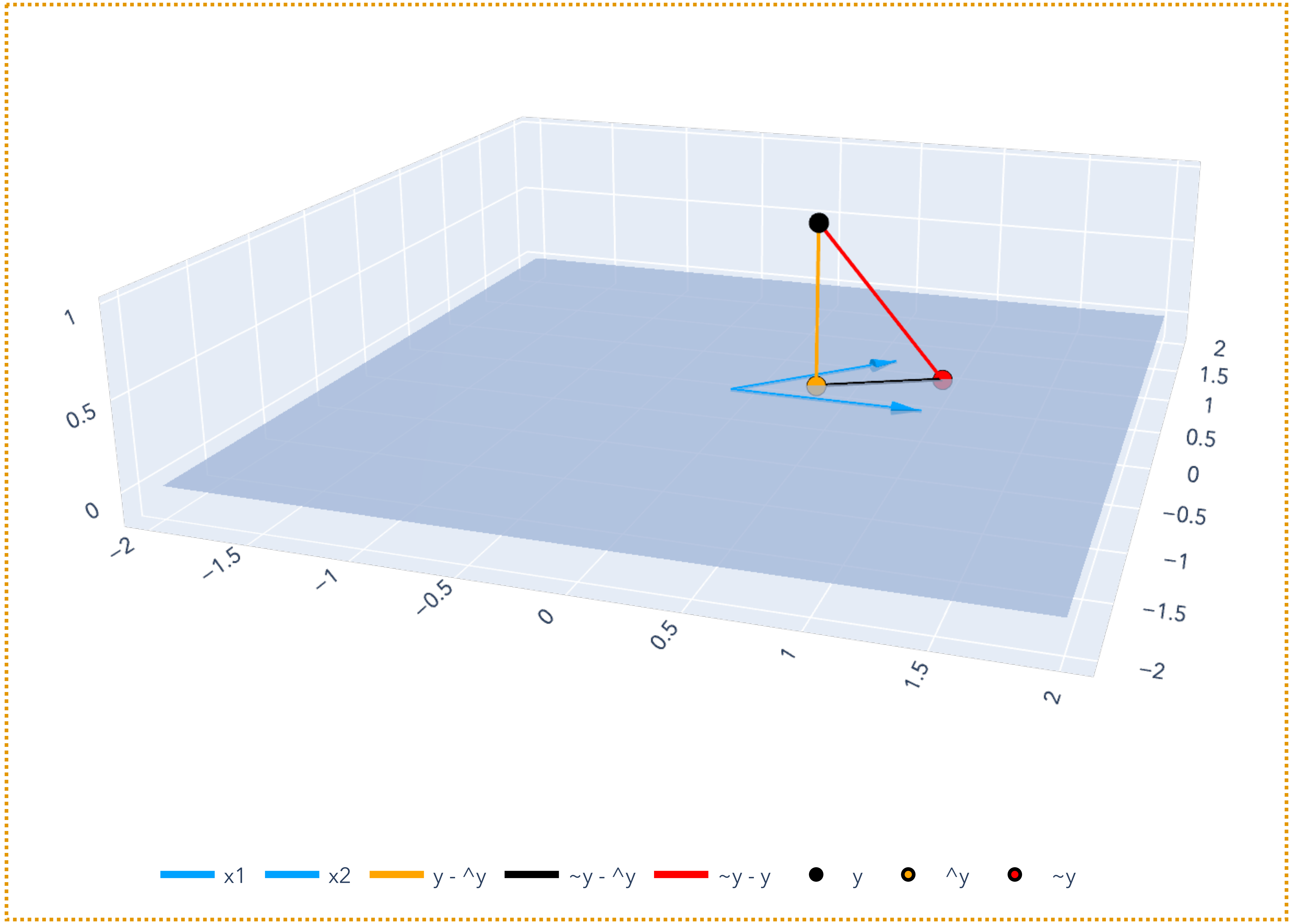
Regression (the basic ML problem). The basic problem in machine learning is regression: constructing a "best-fit" model from a collection of observed data $\mathbf{x} \in \mathbb{R}^d$ and labels $y \in \mathbb{R}$: $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)$.

Linear independence. Linearly independent vectors are vectors that are not redundant; linearly dependent vectors can be expressed as simple (linear) combinations of other vectors.

Span. The span of a set of vectors includes all vectors we can form by simple (linear) combinations of the vectors in the set.

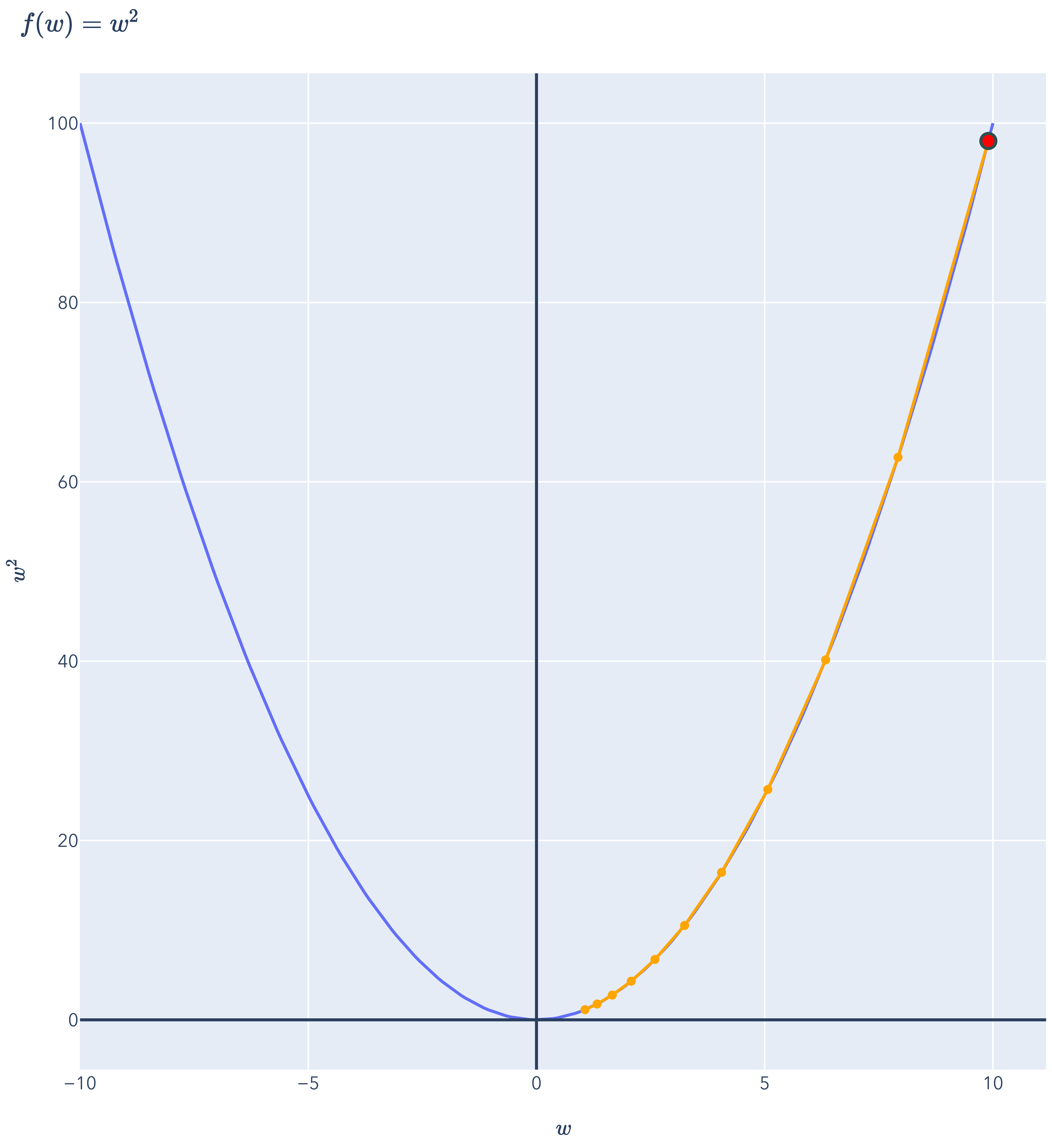
Lesson Overview

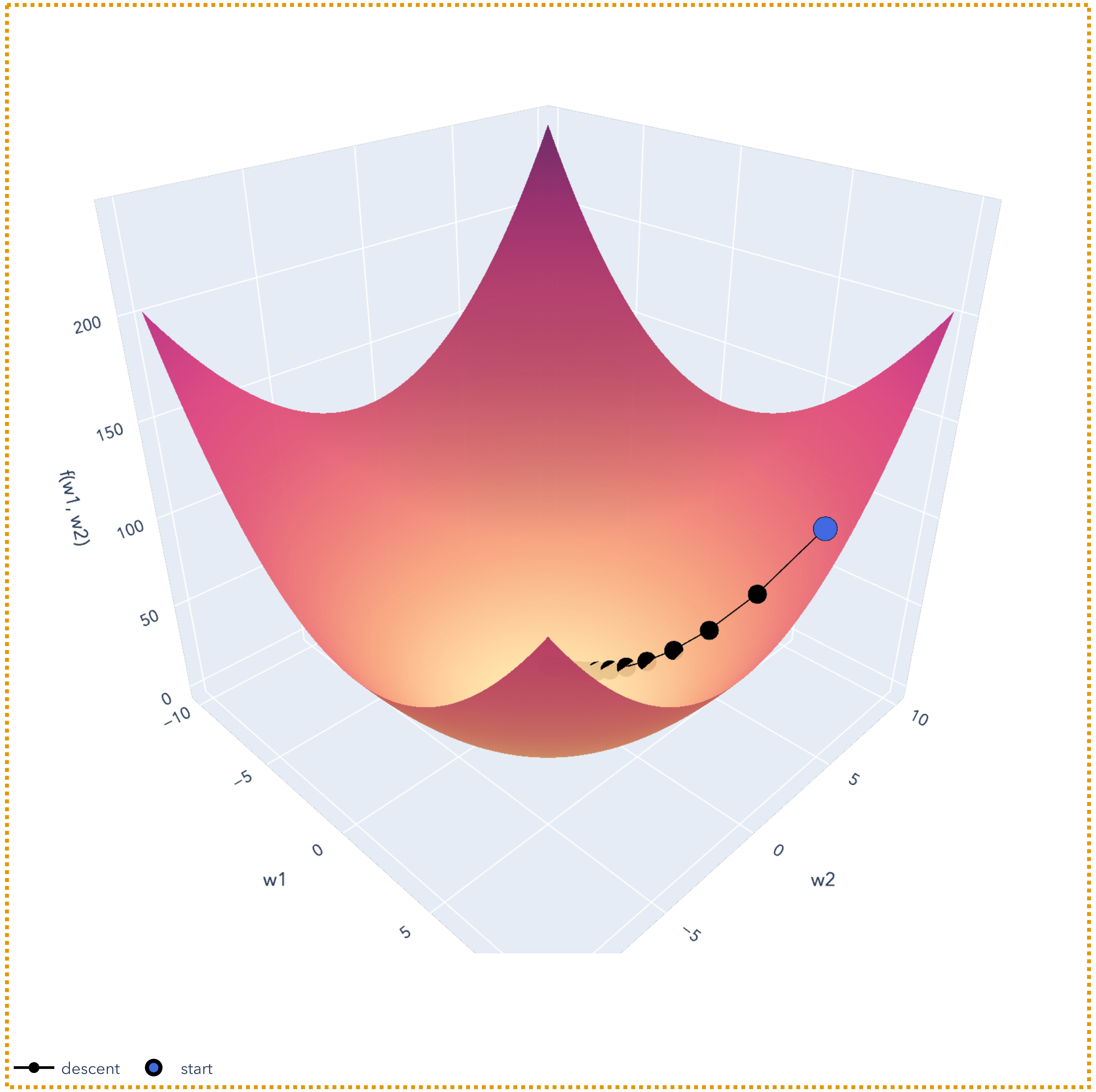
Big Picture: Least Squares



Lesson Overview

Big Picture: Gradient Descent





Vectors & Matrices

Vectors

Review from linear algebra

A vector is a list of numbers. We write $\mathbf{x} \in \mathbb{R}^d$ as:

$$\mathbf{x} := \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix} \text{ or } \mathbf{x} := (x_1, \ldots, x_d).$$

By convention, our vectors will be *column vectors*. A *row vector* looks like:

$$\mathbf{x}^\top = [x_1 \quad \cdots \quad x_d]$$

Vectors

Review from linear algebra

In $\mathbb{R}^n$, a special set of vectors is the unit basis vectors:

$$\mathbf{e}_1 = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \ldots, \mathbf{e}_n = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{bmatrix}$$

Vectors

Review from linear algebra

Vectors can interchangeably thought of as *points:*

or “*arrows*”*:*

Matrices

Review from linear algebra

A matrix is a box of numbers, or a list of vectors. We write $\mathbf{X} \in \mathbb{R}^{n \times d}$ as:

$$\mathbf{X} = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{x}_1 & \cdots & \mathbf{x}_d \\ \downarrow & & \downarrow \end{bmatrix} \quad \text{or} \quad \mathbf{X} = \begin{bmatrix} \leftarrow & \mathbf{x}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_n^\top & \rightarrow \end{bmatrix}.$$

Matrices

Review from linear algebra

A matrix is a box of numbers, or a list of vectors. We write $\mathbf{X} \in \mathbb{R}^{n \times d}$ as:

$$\mathbf{X} = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{x}_1 & \cdots & \mathbf{x}_d \\ \downarrow & & \downarrow \end{bmatrix} \quad \text{or} \quad \mathbf{X} = \begin{bmatrix} \leftarrow & \mathbf{x}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_n^\top & \rightarrow \end{bmatrix}.$$

Column definition: stack column vectors $\mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n$ side-by-side next to each other.

Row definition: take (by convention, column) vectors $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$, turn them into rows $\mathbf{x}_1^\top, \ldots, \mathbf{x}_n^\top \in \mathbb{R}^{1 \times d}$, and stack them on top of each other.

Matrices

Transpose

For a matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$, its transpose is the matrix $\mathbf{X}^\top \in \mathbb{R}^{d \times n}$ obtained from swapping $X^\top_{ij} = X_{ji}$ for all $i \in [d], j \in [n]$.

$$\mathbf{X} = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{x}_1 & \cdots & \mathbf{x}_d \\ \downarrow & & \downarrow \end{bmatrix} \quad \text{or} \quad \mathbf{X} = \begin{bmatrix} \leftarrow & \mathbf{x}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_n^\top & \rightarrow \end{bmatrix}.$$

$$\mathbf{X}^\top = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{x}_1 & \cdots & \mathbf{x}_n \\ \downarrow & & \downarrow \end{bmatrix} \quad \text{or} \quad \mathbf{X}^\top = \begin{bmatrix} \leftarrow & \mathbf{x}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_d^\top & \rightarrow \end{bmatrix}.$$

Multiplication

Vector-vector "multiplication"

Given two vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^d$, their dot product (Euclidean inner product) is:

$$\mathbf{x}^\top \mathbf{y} := x_1 y_1 + \ldots + x_d y_d.$$

More generally, an inner product between two vectors is written as $\langle \mathbf{x}, \mathbf{y} \rangle$. If not specified otherwise, we will use the dot product as default in this course.

Multiplication

Properties of the inner product

For any two vectors $\mathbf{v}, \mathbf{w} \in \mathbb{R}^d$ the inner product obeys the following:

1. **Symmetry.** $\langle \mathbf{v}, \mathbf{w} \rangle = \langle \mathbf{w}, \mathbf{v} \rangle$.

2. **Positive definiteness.** $\langle \mathbf{v}, \mathbf{v} \rangle \geq 0$, and $\langle \mathbf{v}, \mathbf{v} \rangle = 0$ if and only if $\mathbf{v} = \mathbf{0}$.

(note $\langle \mathbf{v}, \mathbf{v} \rangle = \|\mathbf{v}\|^2$, the squared norm of any vector)

3. **Linearity.** Let $\alpha \in \mathbb{R}$ be a scalar and $\mathbf{u} \in \mathbb{R}^d$ be another vector. Then:

$$\langle \alpha \mathbf{u} + \mathbf{v}, \mathbf{w} \rangle = \alpha \langle \mathbf{u}, \mathbf{w} \rangle + \langle \mathbf{v}, \mathbf{w} \rangle \,.$$

Multiplication

Vector-vector "multiplication"

<u>Example.</u> Compute the dot product between $\mathbf{x} = (2,5,3)$ and $\mathbf{y} = (-1,0,3)$.

Multiplication

Matrix-vector multiplication (column view)

To multiply a matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ and a vector $\mathbf{w} \in \mathbb{R}^d$, we can think of the *column view*:

$$\mathbf{X}\mathbf{w} = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{x}_1 & \dots & \mathbf{x}_d \\ \downarrow & & \downarrow \end{bmatrix} \begin{bmatrix} w_1 \\ \vdots \\ w_d \end{bmatrix} = w_1 \begin{bmatrix} \uparrow \\ \mathbf{x}_1 \\ \downarrow \end{bmatrix} + \ldots + w_d \begin{bmatrix} \uparrow \\ \mathbf{x}_d \\ \downarrow \end{bmatrix}.$$

The result is $\mathbf{X}\mathbf{w} \in \mathbb{R}^n$.

Interpretation: $\mathbf{X}\mathbf{w}$ is a *linear combination* of the columns of $\mathbf{X}$.

Multiplication

Matrix-vector multiplication (equation view)

To multiply a matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ and a vector $\mathbf{w} \in \mathbb{R}^d$, we can think of the *equation view*:

$$\mathbf{X}\mathbf{w} = \begin{bmatrix} \leftarrow & \mathbf{x}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_n^\top & \rightarrow \end{bmatrix} \begin{bmatrix} \uparrow \\ \mathbf{w} \\ \downarrow \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1^\top \mathbf{w} \\ \vdots \\ \mathbf{x}_n^\top \mathbf{w} \end{bmatrix}$$

The result is $\mathbf{X}\mathbf{w} \in \mathbb{R}^n$.

Interpretation: $\mathbf{X}\mathbf{w}$ compiles the “right-hand sides” of a *system of linear equations*.

Multiplication

Matrix-vector multiplication

Example. Compute the matrix-vector product:

$$\mathbf{Xw} = \begin{bmatrix} 1 & -1 & 2 \\ 0 & 2 & 3 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 1 \\ -1 \end{bmatrix}$$

Multiplication

Matrix-matrix multiplication (matrix-vector view)

To multiply two matrices $\mathbf{U} \in \mathbb{R}^{n \times r}$ and $\mathbf{V} \in \mathbb{R}^{r \times d}$, we just think of *$d$ different matrix-vector products:*

$$\mathbf{U}\mathbf{V} = \mathbf{U} \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{v}_1 & \cdots & \mathbf{v}_d \\ \downarrow & & \downarrow \end{bmatrix} = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{U}\mathbf{v}_1 & \cdots & \mathbf{U}\mathbf{v}_d \\ \downarrow & & \downarrow \end{bmatrix}$$

The result is $\mathbf{X} = \mathbf{U}\mathbf{V} \in \mathbb{R}^{n \times d}$.

Multiplication

Matrix-matrix multiplication (inner product/entry view)

To multiply two matrices $\mathbf{U} \in \mathbb{R}^{n\times r}$ and $\mathbf{V} \in \mathbb{R}^{r\times d}$, we just think of *nd different inner products:*

$$\mathbf{UV} = \begin{bmatrix} \leftarrow & \mathbf{u}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{u}_n^\top & \rightarrow \end{bmatrix} \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{v}_1 & \dots & \mathbf{v}_d \\ \downarrow & & \downarrow \end{bmatrix} = \begin{bmatrix} \mathbf{u}_1^\top \mathbf{v}_1 & \dots & \mathbf{u}_1^\top \mathbf{v}_d \\ \vdots & \ddots & \vdots \\ \mathbf{u}_n^\top \mathbf{v}_1 & \dots & \mathbf{u}_n^\top \mathbf{v}_d \end{bmatrix}$$

$$(\mathbf{UV})_{ij} = \mathbf{u}_i^\top \mathbf{v}_j \text{ for all } i \in [n], j \in [d].$$

The result is $\mathbf{X} = \mathbf{UV} \in \mathbb{R}^{n\times d}$.

Multiplication

Matrix-matrix multiplication (outer product view)

To multiply two matrices $\mathbf{U} \in \mathbb{R}^{n \times r}$ and $\mathbf{V} \in \mathbb{R}^{r \times d}$, we just think of *summing r different outer products ($n \times d$ matrices):*

$$\mathbf{U}\mathbf{V} = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{u}_1 & \dots & \mathbf{u}_r \\ \downarrow & & \downarrow \end{bmatrix} \begin{bmatrix} \leftarrow & \mathbf{v}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{v}_r^\top & \rightarrow \end{bmatrix} = \begin{bmatrix} \uparrow \\ \mathbf{u}_1 \\ \downarrow \end{bmatrix} [\leftarrow \ \ \mathbf{v}_1 \ \ \rightarrow] + \dots + \begin{bmatrix} \uparrow \\ \mathbf{u}_r \\ \downarrow \end{bmatrix} [\leftarrow \ \ \mathbf{v}_r \ \ \rightarrow]$$

The result is $\mathbf{X} = \mathbf{U}\mathbf{V} \in \mathbb{R}^{n \times d}$.

Matrices

Inverses and Identity Matrix

A square matrix $\mathbf{X} \in \mathbb{R}^{d \times d}$ is invertible if there exists a matrix $\mathbf{X}^{-1} \in \mathbb{R}^{d \times d}$ (the inverse) such that:

$$\mathbf{X}^{-1}\mathbf{X} = \mathbf{X}\mathbf{X}^{-1} = \mathbf{I},$$

where $\mathbf{I} \in \mathbb{R}^{d \times d}$ is the identity matrix:

$$\mathbf{I} := \begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ 0 & 0 & 1 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & 1 \end{bmatrix}.$$

Regression

Regression

The main problem of our course

Collect d measurements $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$ for n students…

where $y_i \in \mathbb{R}$ denotes the test score of a student.

Given the measurements for a new student, $\mathbf{x}_0 \in \mathbb{R}^d$, what is their test score?

Regression

The main problem of our course

We observe n samples of training (observed) features $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$, with labels $y_1, \ldots, y_n \in \mathbb{R}$.

$$\mathbf{x}_i = \begin{bmatrix} x_{i1} \\ \vdots \\ x_{id} \end{bmatrix}$$

<u>**Goal:**</u> Given a new unlabelled sample, $\mathbf{x}_0$, make a prediction $\hat{y}$ such that $\hat{y} \approx y_0$.

Regression

The main problem of our course

<u>Goal:</u> Given a new unlabelled sample, $\mathbf{x}_0$, make a prediction $\hat{y}$ such that $\hat{y} \approx y_0$.

To do this, we will construct a *model* for the observed data.

A *linear model* is represented with a <u>weight vector</u> $\mathbf{w} \in \mathbb{R}^d$. To make a prediction with the weight vector, we take an inner product.

$$\hat{y} = \langle \mathbf{w}, \mathbf{x}_0 \rangle = w_1 x_{01} + \ldots w_d x_{0d}.$$

Regression

The main problem of our course

How do we construct the weight vector $\mathbf{w} \in \mathbb{R}^d$?

Learn it from the observed data $(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)$.

For some weight vector $\mathbf{w} \in \mathbb{R}^d$, its predictions on the observed data are:

$$\begin{bmatrix} \hat{y}_1 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \hat{\mathbf{y}} = \mathbf{X}\mathbf{w} = \begin{bmatrix} \leftarrow & \mathbf{x}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_n^\top & \rightarrow \end{bmatrix} \begin{bmatrix} \uparrow \\ \mathbf{w} \\ \downarrow \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1^\top \mathbf{w} \\ \vdots \\ \mathbf{x}_n^\top \mathbf{w} \end{bmatrix} = \begin{bmatrix} \langle \mathbf{x}_1, \mathbf{w} \rangle \\ \vdots \\ \langle \mathbf{x}_n, \mathbf{w} \rangle \end{bmatrix}$$

Regression

The main problem of our course

For some weight vector $\mathbf{w} \in \mathbb{R}^d$, its predictions on the observed data are:

$$\begin{bmatrix} \hat{y}_1 \\ \vdots \\ \hat{y}_n \end{bmatrix} = \hat{\mathbf{y}} = \mathbf{X}\mathbf{w} = \begin{bmatrix} \leftarrow & \mathbf{x}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_n^\top & \rightarrow \end{bmatrix} \begin{bmatrix} \uparrow \\ \mathbf{w} \\ \downarrow \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1^\top \mathbf{w} \\ \vdots \\ \mathbf{x}_n^\top \mathbf{w} \end{bmatrix} = \begin{bmatrix} \langle \mathbf{x}_1, \mathbf{w} \rangle \\ \vdots \\ \langle \mathbf{x}_n, \mathbf{w} \rangle \end{bmatrix}$$

Regression

The main problem of our course

<u>Goal:</u> Given a new unlabelled sample, $\mathbf{x}_0$, make a prediction $\hat{y}$ such that $\hat{y} \approx y_0$.

If the new sample $(\mathbf{x}_0, y_0)$ is "distributed like" the training samples $\mathbf{X} \in \mathbb{R}^{n \times d}$ and $\mathbf{y} \in \mathbb{R}^n$, then it's not a bad idea to find $\mathbf{w} \in \mathbb{R}^d$ so:

$$\mathbf{X}\mathbf{w} = \hat{\mathbf{y}} \approx \mathbf{y}.$$

This will be our new goal!

Regression

Setup (Example View)

<u>Observed:</u> Matrix of *training samples* $\mathbf{X} \in \mathbb{R}^{n \times d}$ and vector of *training labels* $\mathbf{y} \in \mathbb{R}^n$.

$$\mathbf{X} = \begin{bmatrix} \leftarrow & \mathbf{x}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_n^\top & \rightarrow \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \text{ where } \mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d.$$

<u>Unknown:</u> *Weight vector* $\mathbf{w} \in \mathbb{R}^d$ with weights $w_1, \ldots, w_d$.

<u>Goal:</u> For each $i \in [n]$, we predict: $\hat{y}_i = \mathbf{w}^\top \mathbf{x}_i = w_1 x_{i1} + \ldots + w_d x_{id} \in \mathbb{R}$.

Choose a weight vector that "fits the training data": $\mathbf{w} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

$$\mathbf{X}\mathbf{w} = \hat{\mathbf{y}} \approx \mathbf{y}\,.$$

Regression

Setup (Feature View)

<u>Observed:</u> Matrix of *training samples* $\mathbf{X} \in \mathbb{R}^{n \times d}$ and vector of *training labels* $\mathbf{y} \in \mathbb{R}^n$.

$$\mathbf{X} = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{x}_1 & \cdots & \mathbf{x}_d \\ \downarrow & & \downarrow \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \text{ where } \mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n.$$

<u>Unknown:</u> *Weight vector* $\mathbf{w} \in \mathbb{R}^d$ with weights $w_1, \ldots, w_d$.

Choose a weight vector that "fits the training data": $\mathbf{w} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

$$\mathbf{X}\mathbf{w} = \hat{\mathbf{y}} \approx \mathbf{y}\,.$$

Regression

Caveat

Choose a weight vector that "fits the training data": $\mathbf{w} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

$$\mathbf{X}\mathbf{w} = \hat{\mathbf{y}} \approx \mathbf{y}\,.$$

In general, it may not be the case that $\mathbf{y} = \mathbf{X}\mathbf{w}$ for any $\mathbf{w} \in \mathbb{R}^d$ (the labels y_i don't have a perfect linear relationship with the $\mathbf{x}_i$).

Regression

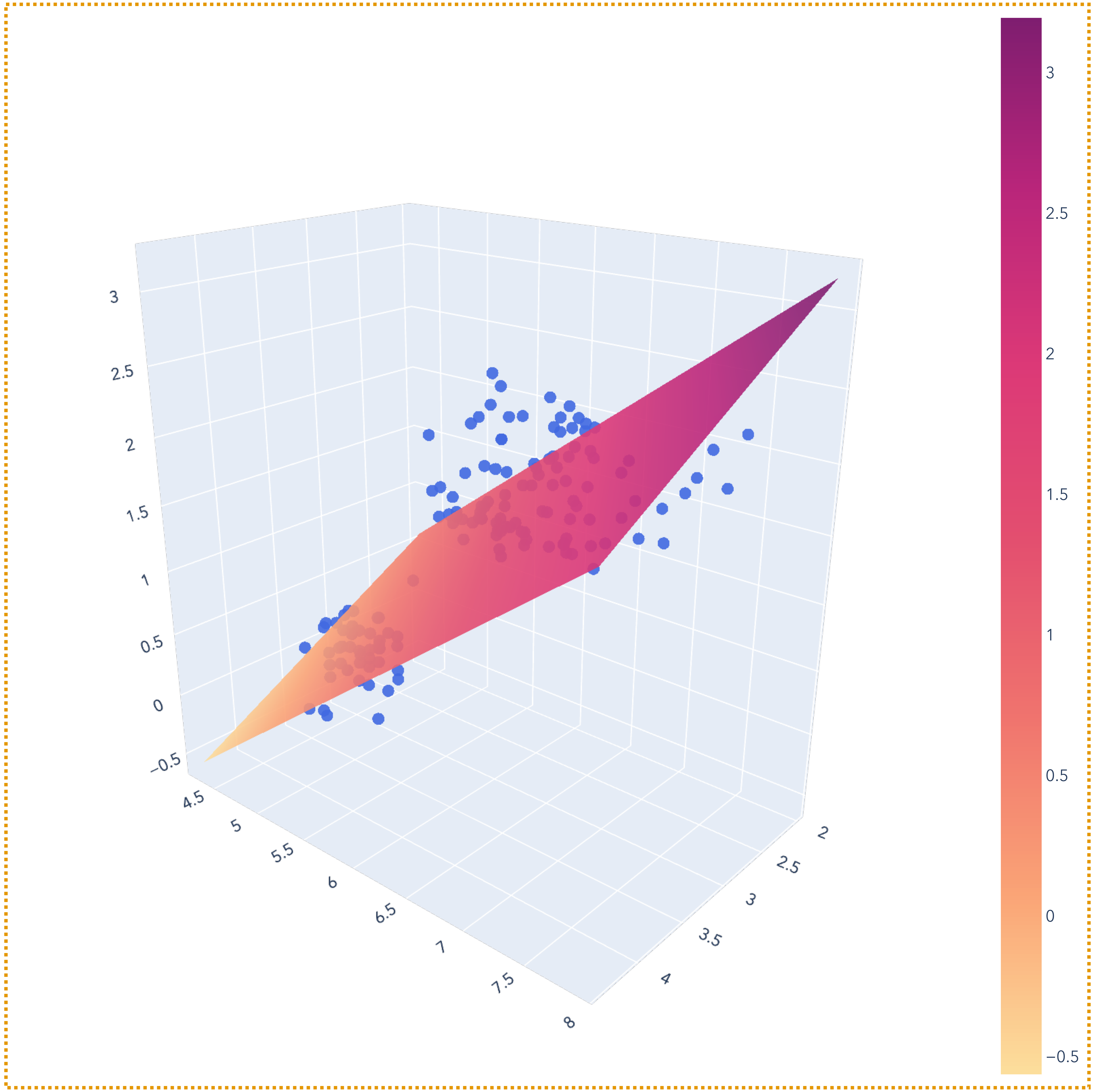
Example: $d = 1$

$$\mathbf{X} = \begin{bmatrix} \vdots \\ 14.07 \\ 17.51 \\ 22.42 \\ 26.88 \\ \vdots \end{bmatrix} \mathbf{y} = \begin{bmatrix} \vdots \\ 2.5 \\ 3 \\ 3.48 \\ 3.12 \\ \vdots \end{bmatrix}$$

Regression

Example: $d = 2$

$$\mathbf{X} = \begin{bmatrix} \vdots & \vdots \\ 3.4 & 5.4 \\ 2.9 & 6.4 \\ 3.3 & 6.7 \\ 2.6 & 7.7 \\ \vdots & \vdots \end{bmatrix} \mathbf{y} = \begin{bmatrix} \vdots \\ 0.4 \\ 1.3 \\ 2.1 \\ 2.3 \\ \vdots \end{bmatrix}$$



Least Squares

A Solution to Regression

Regression

Setup (Example View)

Observed: Matrix of *training samples* $\mathbf{X} \in \mathbb{R}^{n \times d}$ and vector of *training labels* $\mathbf{y} \in \mathbb{R}^n$.

$$\mathbf{X} = \begin{bmatrix} \leftarrow & \mathbf{x}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_n^\top & \rightarrow \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \text{ where } \mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d.$$

Unknown: *Weight vector* $\mathbf{w} \in \mathbb{R}^d$ with weights $w_1, \ldots, w_d$.

Goal: For each $i \in [n]$, we predict: $\hat{y}_i = \mathbf{w}^\top \mathbf{x}_i = w_1 x_{i1} + \ldots + w_d x_{id} \in \mathbb{R}$.

Choose a weight vector that "fits the training data": $\mathbf{w} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

$$\mathbf{X}\mathbf{w} = \hat{\mathbf{y}} \approx \mathbf{y}\,.$$

Ordinary Least Squares

Notion of Error

In general, it may not be the case that $\mathbf{y} = \mathbf{X}\mathbf{w}$ for any $\mathbf{w} \in \mathbb{R}^d$ (the labels y_i don't have a perfect linear relationship with the $\mathbf{x}_i$).

The residual $r_i(\mathbf{w})$ of the ith prediction with $\mathbf{w} \in \mathbb{R}^d$ is

$$r_i(\mathbf{w}) := \hat{y}_i - y_i = \langle \mathbf{w}, \mathbf{x}_i \rangle - y_i.$$

We can write this as a vector $\mathbf{r} \in \mathbb{R}^n$.

The *sum of squared residuals* is

$$SSR := \sum_{i=1}^{n} r_i(\mathbf{w})^2 = r_1(\mathbf{w})^2 + \ldots + r_n(\mathbf{w})^2.$$

Norms and Inner Products

Euclidean Norm

Recall the notion of "length" from $\mathbb{R}^2$. For a vector $\mathbf{x} = (x_1, x_2) \in \mathbb{R}^2$,

$$\|\mathbf{x}\|_2 := \sqrt{x_1^2 + x_2^2}.$$

Generalizing this, for $\mathbf{x} \in \mathbb{R}^n$, the Euclidean norm ($\ell_2$-norm) is:

$$\|\mathbf{x}\|_2 := \sqrt{x_1^2 + \ldots + x_n^2} = \sqrt{\mathbf{x}^\top \mathbf{x}}.$$

$$\|\mathbf{x}\|_2^2 = \mathbf{x}^\top \mathbf{x}.$$

Ordinary Least Squares

Notion of Error

Residual: $r_i(\mathbf{w}) := \hat{y}_i - y_i = \langle \mathbf{w}, \mathbf{x}_i \rangle - y_i$, or $\mathbf{r} \in \mathbb{R}^n$.

The *sum of squared residuals* is

$$SSR := \sum_{i=1}^{n} r_i(\mathbf{w})^2 = r_1(\mathbf{w})^2 + \ldots + r_n(\mathbf{w})^2 .$$

$$SSR = \|\mathbf{r}\|^2 = \|\hat{\mathbf{y}} - \mathbf{y}\|^2 = \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2.$$

Ordinary Least Squares

Principle of Least Squares

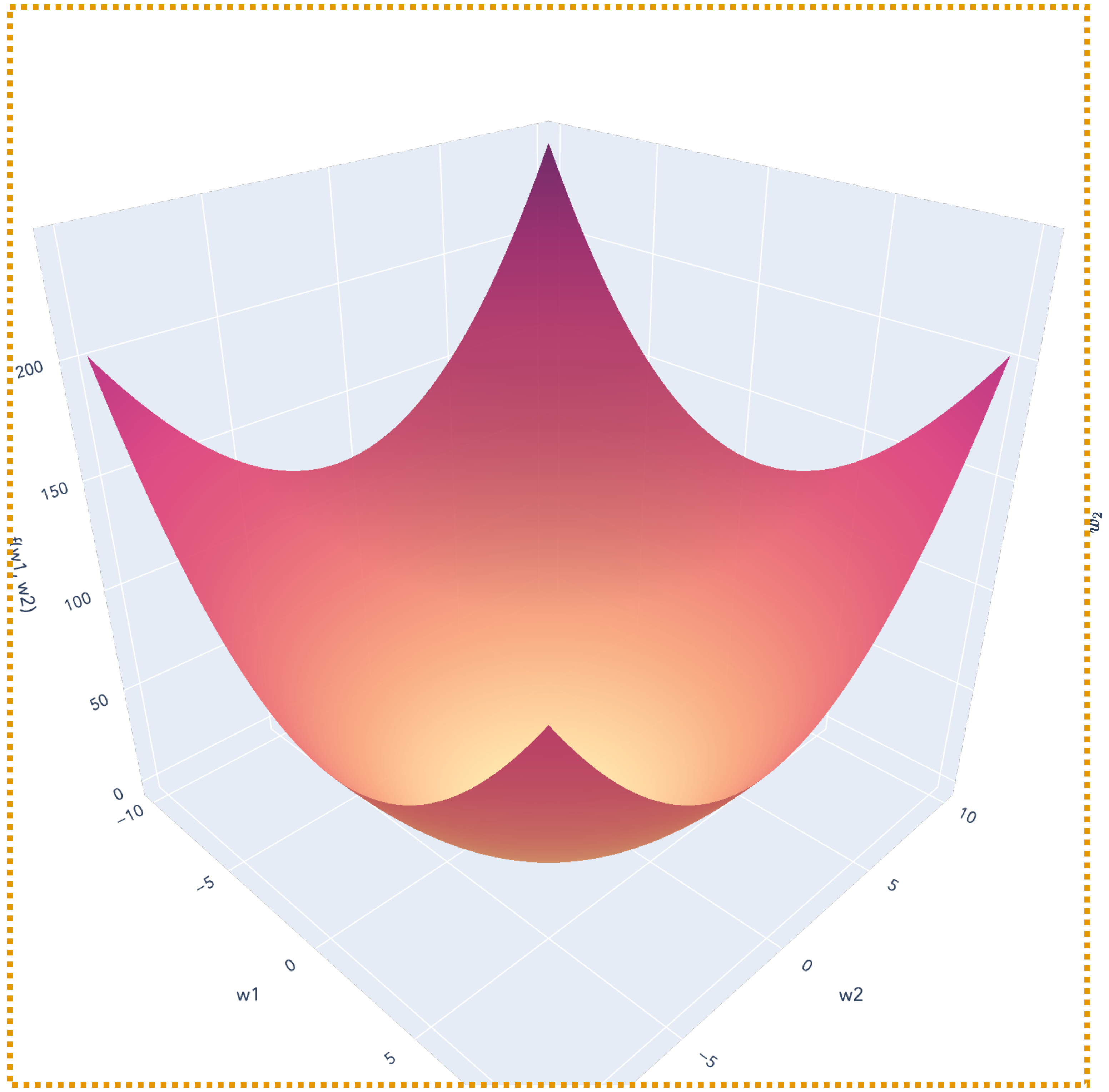
<u>Goal:</u> Find the $\mathbf{w} \in \mathbb{R}^d$ that minimizes the sum of squared residuals:

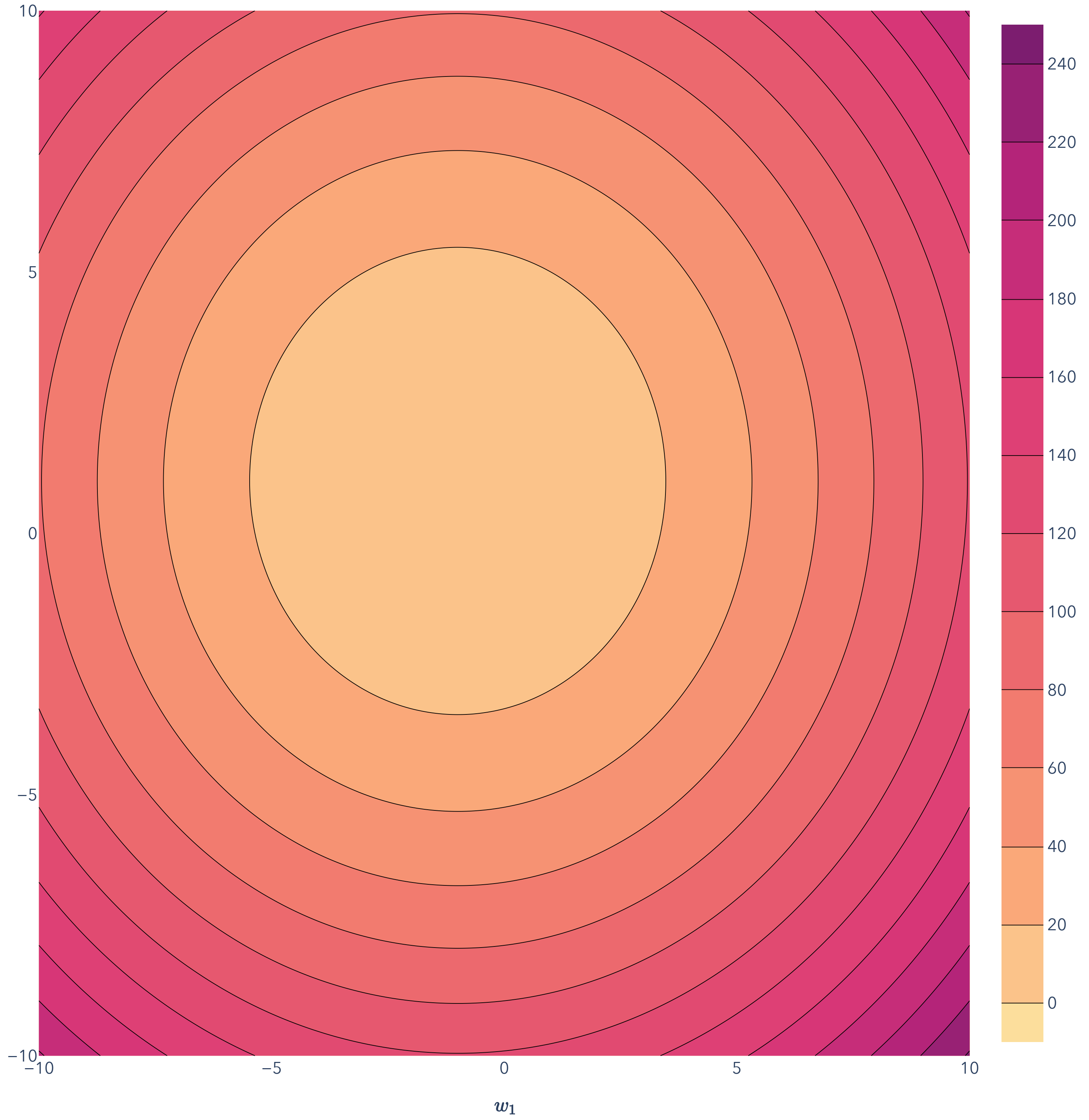
$$\|\mathbf{r}\|^2 = \|\hat{\mathbf{y}} - \mathbf{y}\|^2 = \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2.$$

Ordinary Least Squares

Sum of Squared Residuals

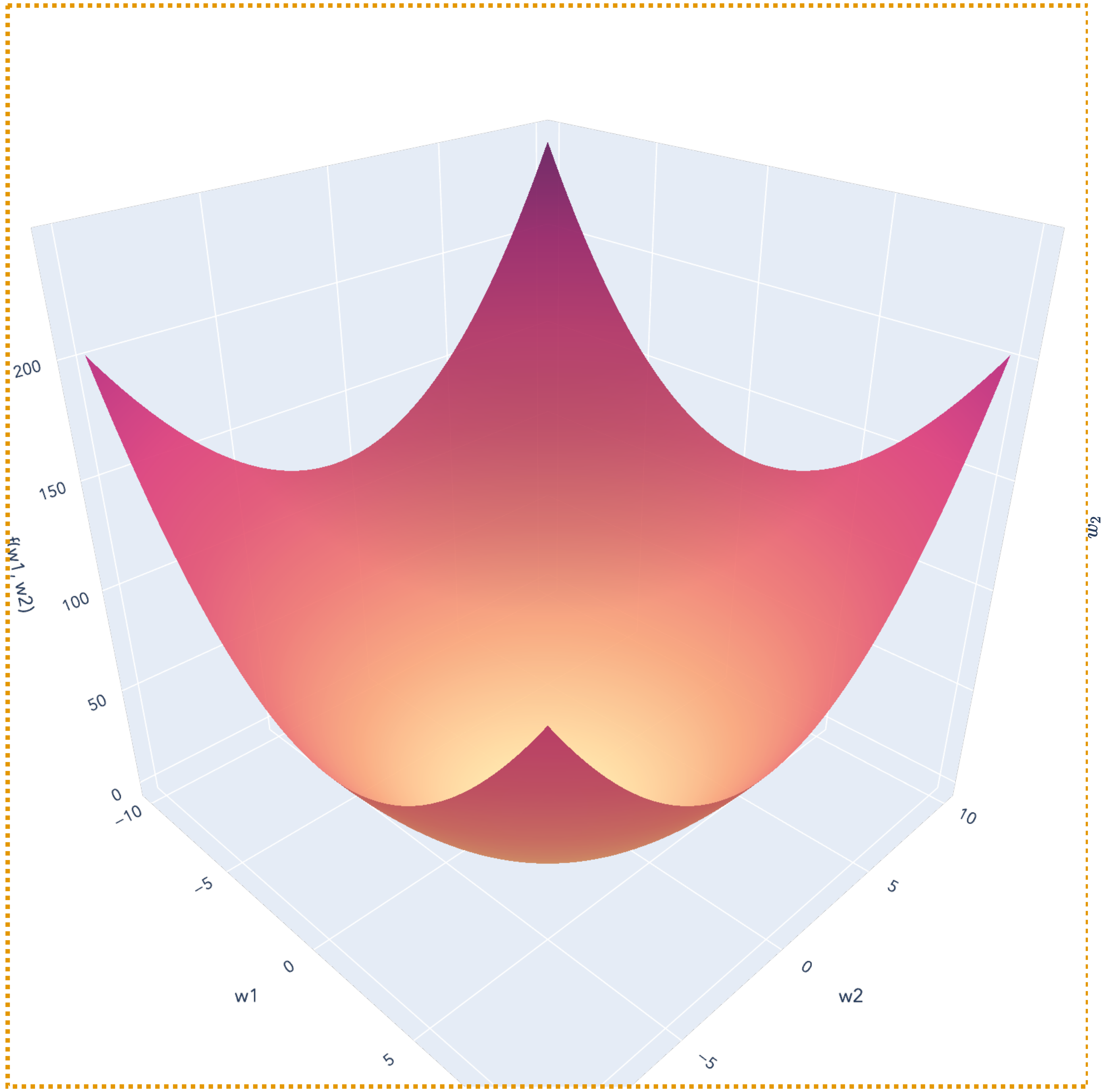
<u>Example:</u> If $\mathbf{X} \in \mathbb{R}^{n \times 2}$ and $\mathbf{y} \in \mathbb{R}^n$, what can $SSR(\mathbf{w}) = \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$ look like?

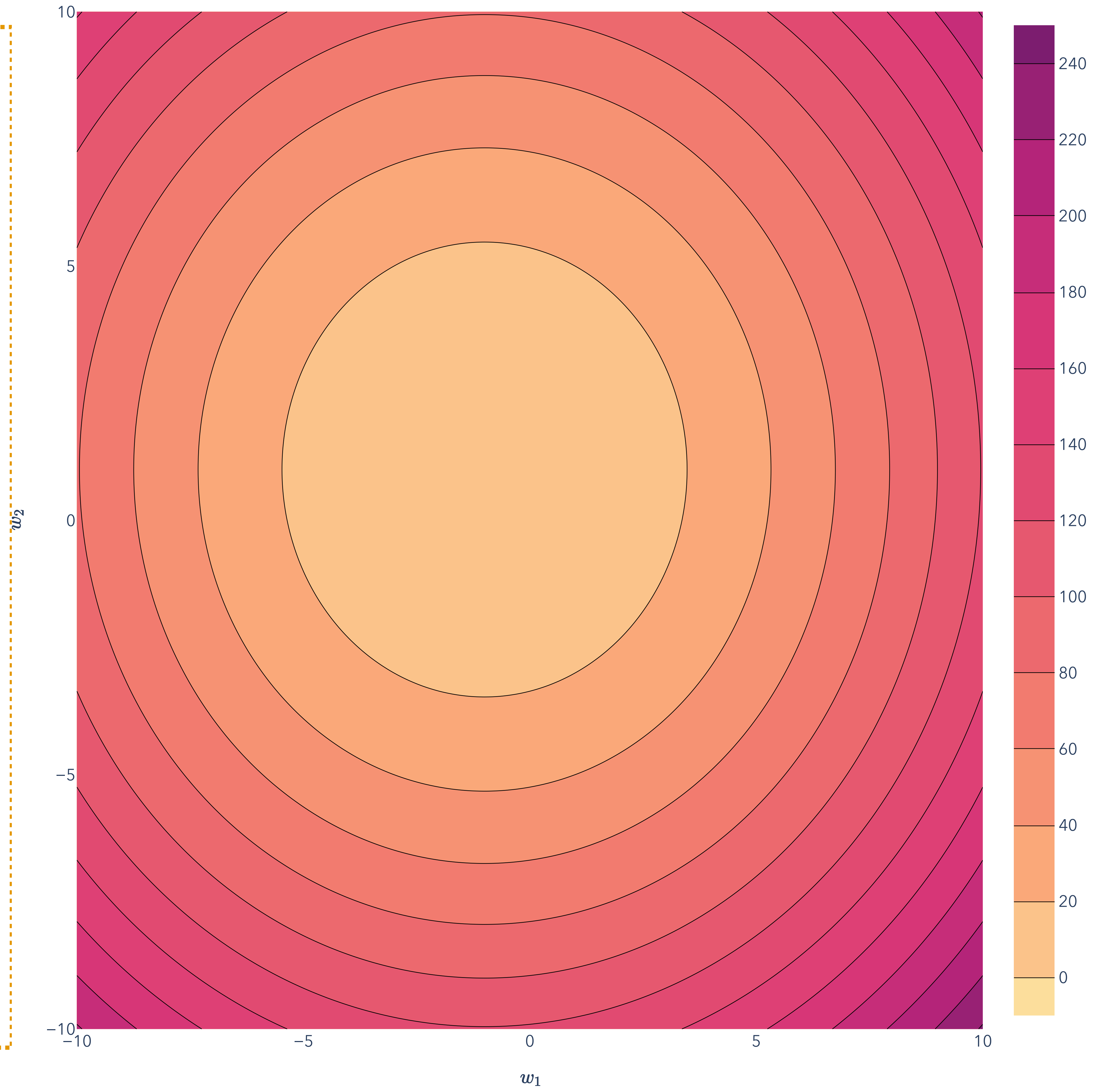




Ordinary Least Squares

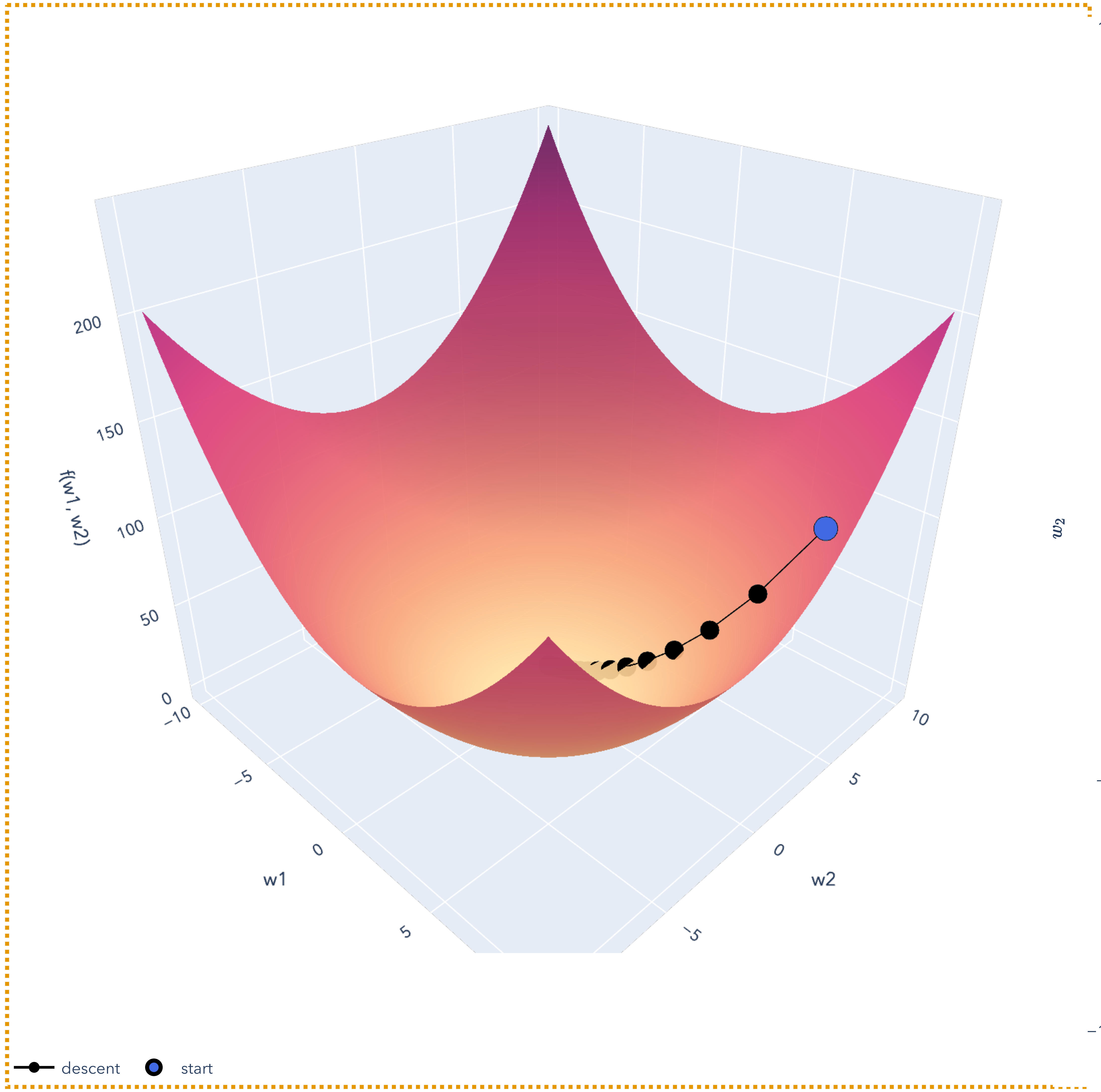
Sum of Squared Residuals

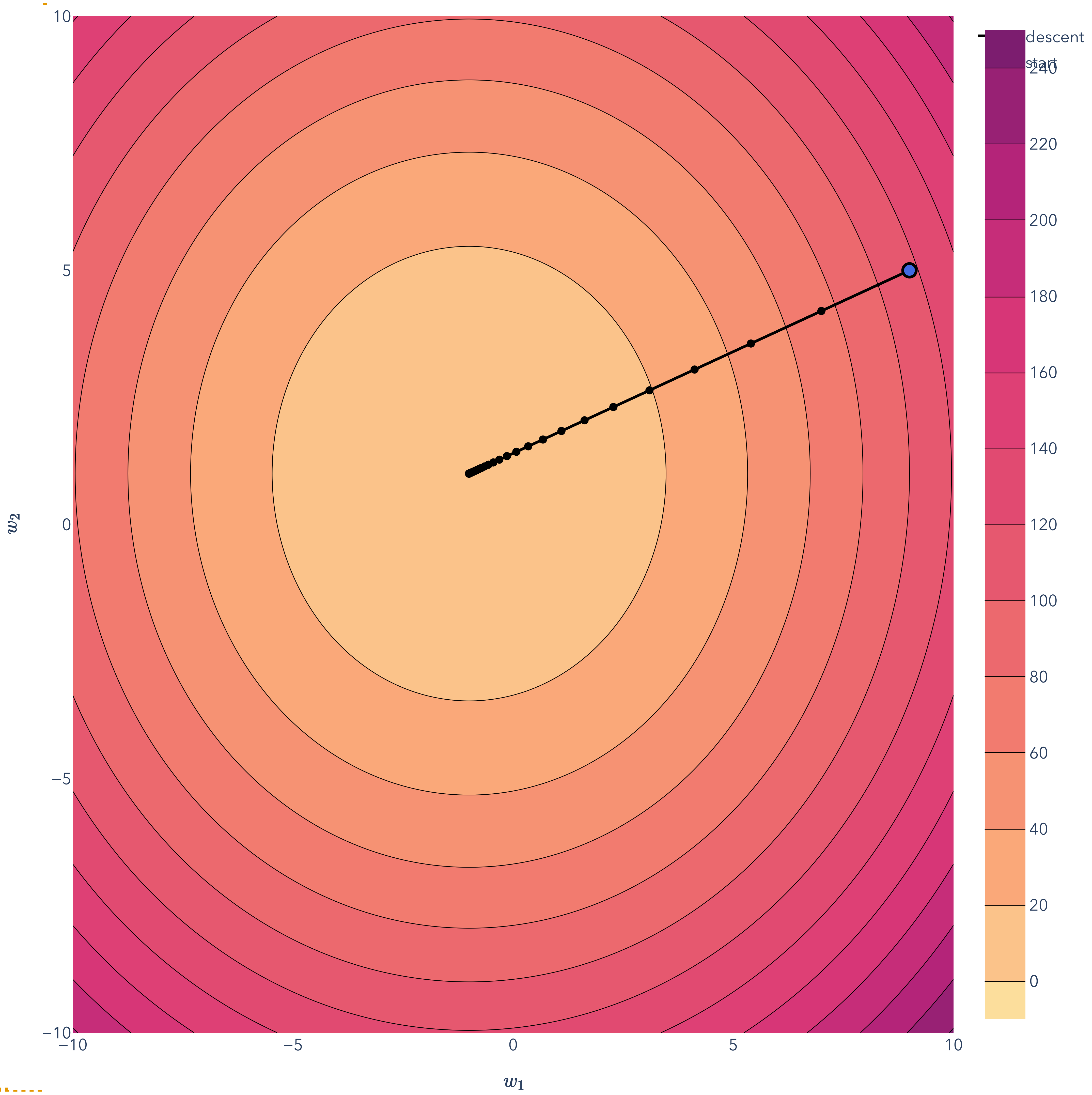




Ordinary Least Squares

Sum of Squared Residuals





Regression

Setup (Feature View)

<u>Observed:</u> Matrix of *training samples* $\mathbf{X} \in \mathbb{R}^{n \times d}$ and vector of *training labels* $\mathbf{y} \in \mathbb{R}^n$.

$$\mathbf{X} = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{x}_1 & \cdots & \mathbf{x}_d \\ \downarrow & & \downarrow \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}, \text{ where } \mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n.$$

<u>Unknown:</u> *Weight vector* $\mathbf{w} \in \mathbb{R}^d$ with weights $w_1, \ldots, w_d$.

Choose a weight vector that "fits the training data": $\mathbf{w} \in \mathbb{R}^d$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

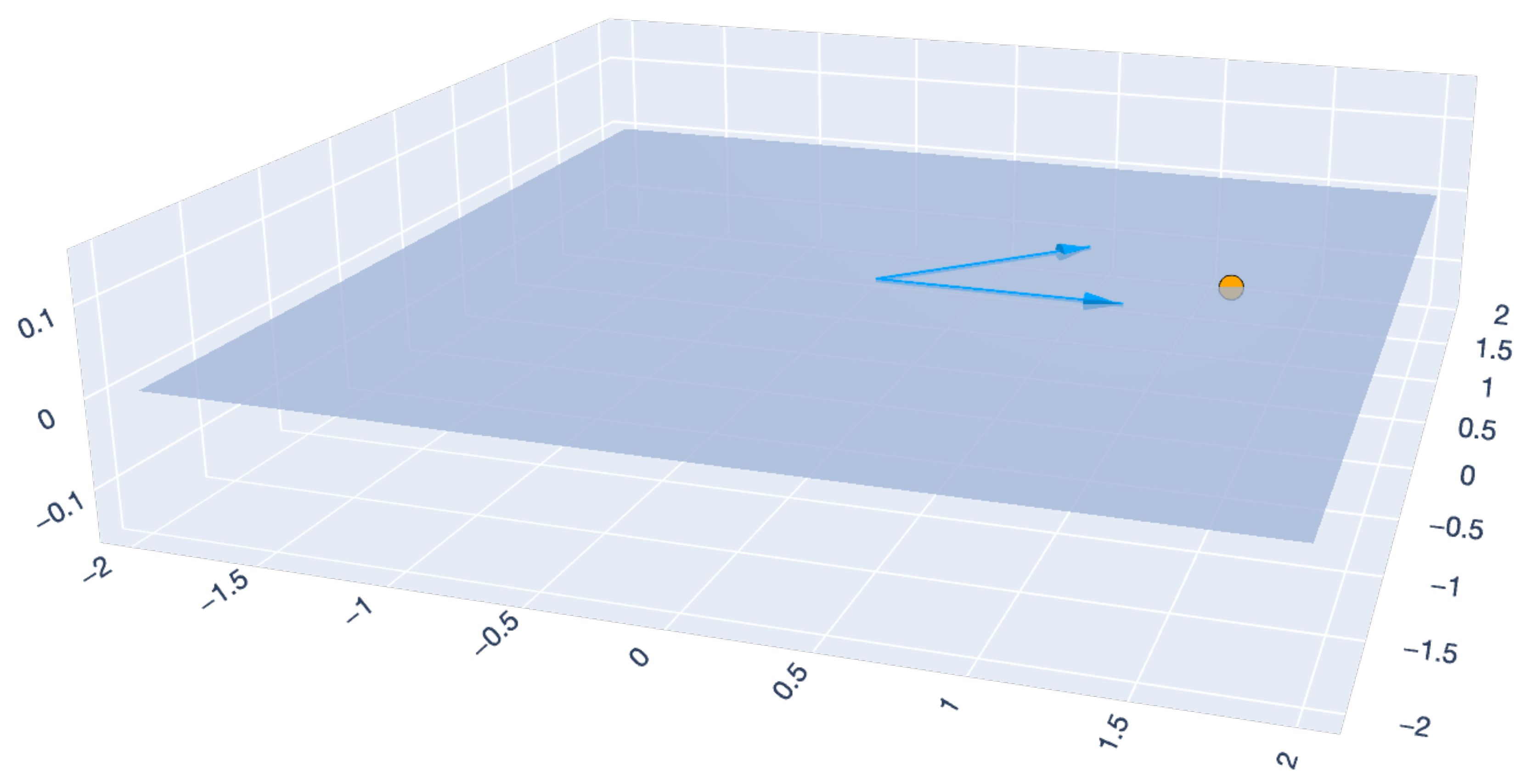
$$\mathbf{X}\mathbf{w} = \hat{\mathbf{y}} \approx \mathbf{y}\,.$$

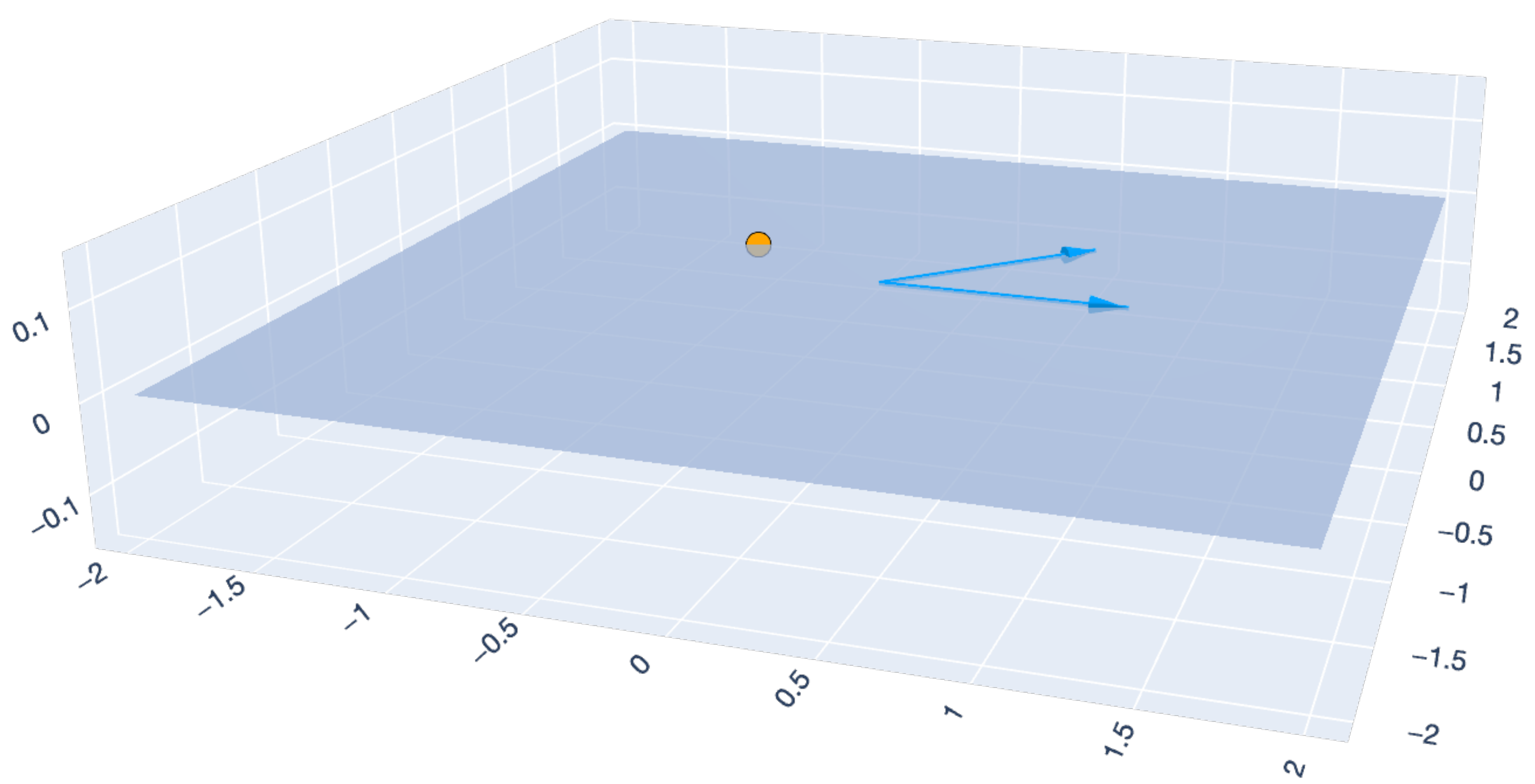
Ordinary Least Squares

Geometry of Least Squares

Let $n = 3$ and $d = 2$. In this case $\hat{\mathbf{y}} \in \mathbb{R}^3$ is a *linear combination* of columns $\mathbf{x}_1$ and $\mathbf{x}_2$.

$$\hat{\mathbf{y}} = \mathbf{X}\mathbf{w} = w_1\mathbf{x}_1 + w_2\mathbf{x}_2 \in \mathbb{R}^3$$

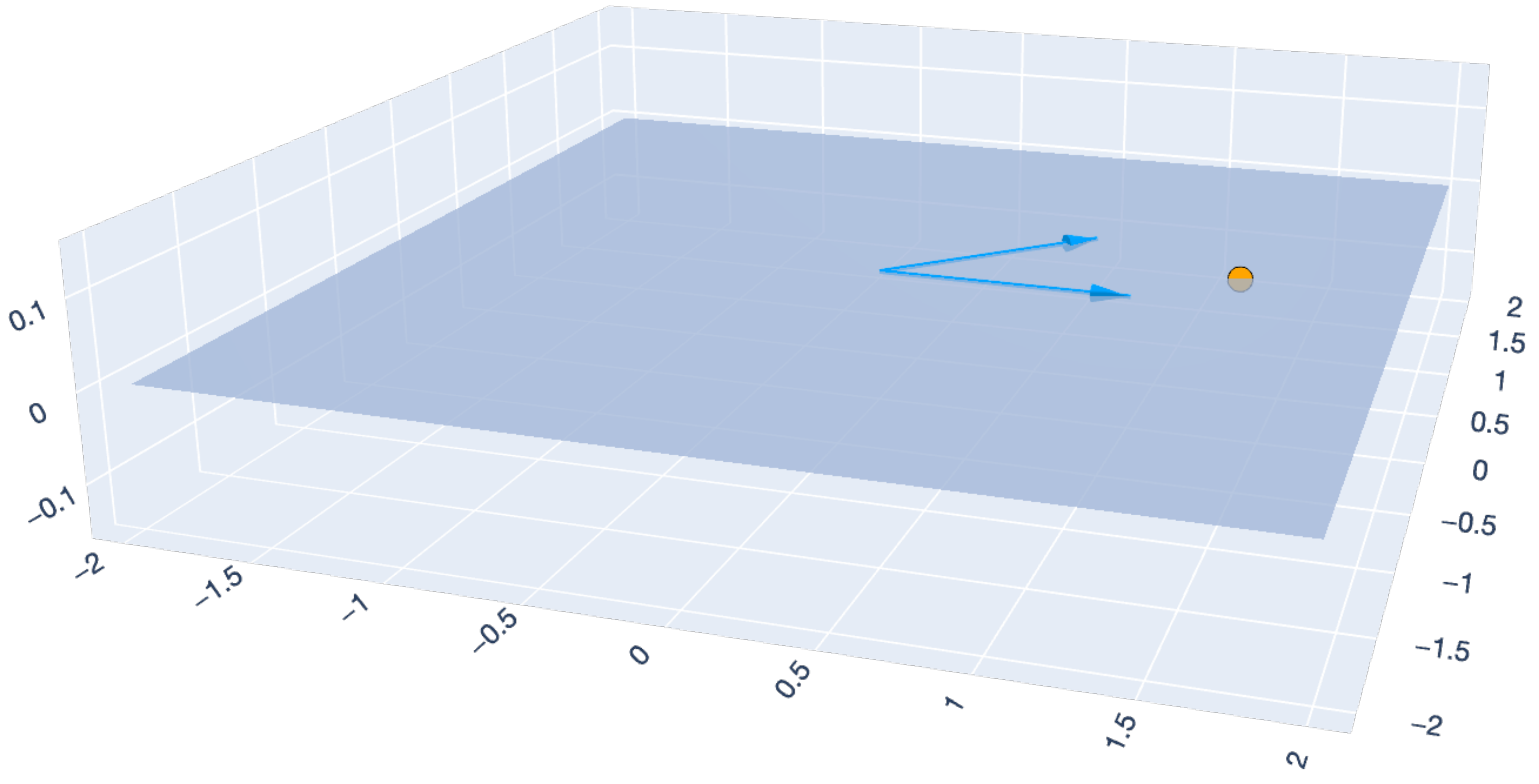




Span

Idea

For a collection of vectors $\mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n$, the span is…



Span

Definition

For a collection of vectors $\mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n$, the span is the set of vectors we can attain through linear combinations of $\mathbf{x}_1, \ldots, \mathbf{x}_d$:

$$\text{span}(\mathbf{x}_1, \ldots, \mathbf{x}_d) = \left\{ \mathbf{y} \in \mathbb{R}^n : \mathbf{y} = \sum_{i=1}^{d} \alpha_i \mathbf{x}_i, \alpha_i \in \mathbb{R} \right\}.$$

Span

Examples

$$\operatorname{span}\left(\begin{bmatrix}1\\0\end{bmatrix}\right)$$

$$\operatorname{span}\left(\begin{bmatrix}2\\1\end{bmatrix}, \begin{bmatrix}0\\-1\end{bmatrix}\right)$$

$$\operatorname{span}\left(\begin{bmatrix}1\\0\\0\end{bmatrix}, \begin{bmatrix}0\\-2\\0\end{bmatrix}, \begin{bmatrix}1\\0\\1\end{bmatrix}\right)$$

Ordinary Least Squares

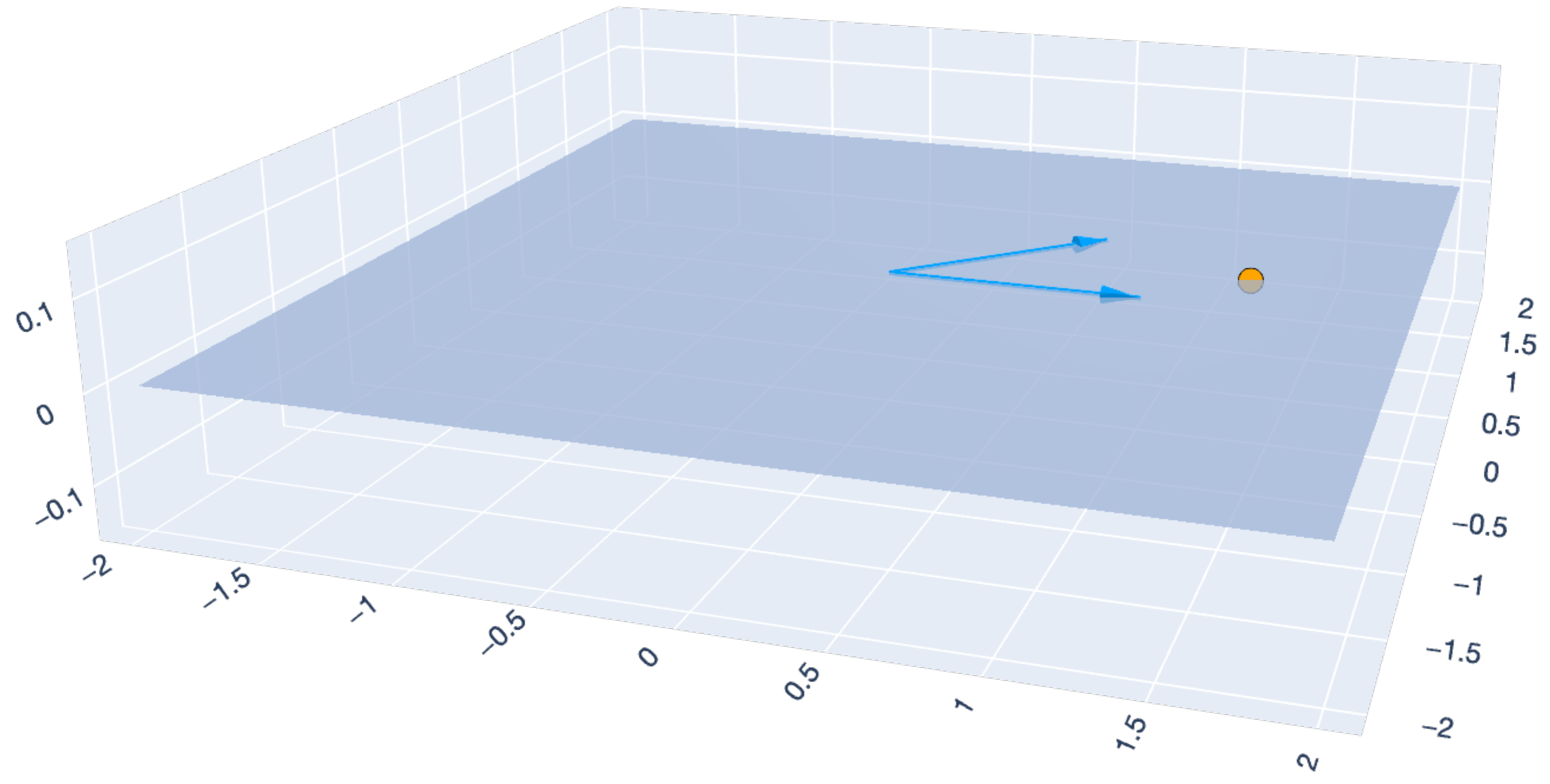
Geometry of Least Squares

Let $n = 3$ and $d = 2$. In this case $\hat{\mathbf{y}} \in \mathbb{R}^3$ is a *linear combination* of columns $\mathbf{x}_1$ and $\mathbf{x}_2$.

$$\hat{\mathbf{y}} = \mathbf{X}\mathbf{w} = w_1\mathbf{x}_1 + w_2\mathbf{x}_2 \in \mathbb{R}^3$$

Let $\mathrm{col}(\mathbf{X}) := \{\mathbf{x}_1, \ldots, \mathbf{x}_d\}$ be the *columnspace* of $\mathbf{X} \in \mathbb{R}^{n\times d}$. Then,

$$\hat{\mathbf{y}} \in \mathrm{span}(\mathrm{col}(\mathbf{X})).$$



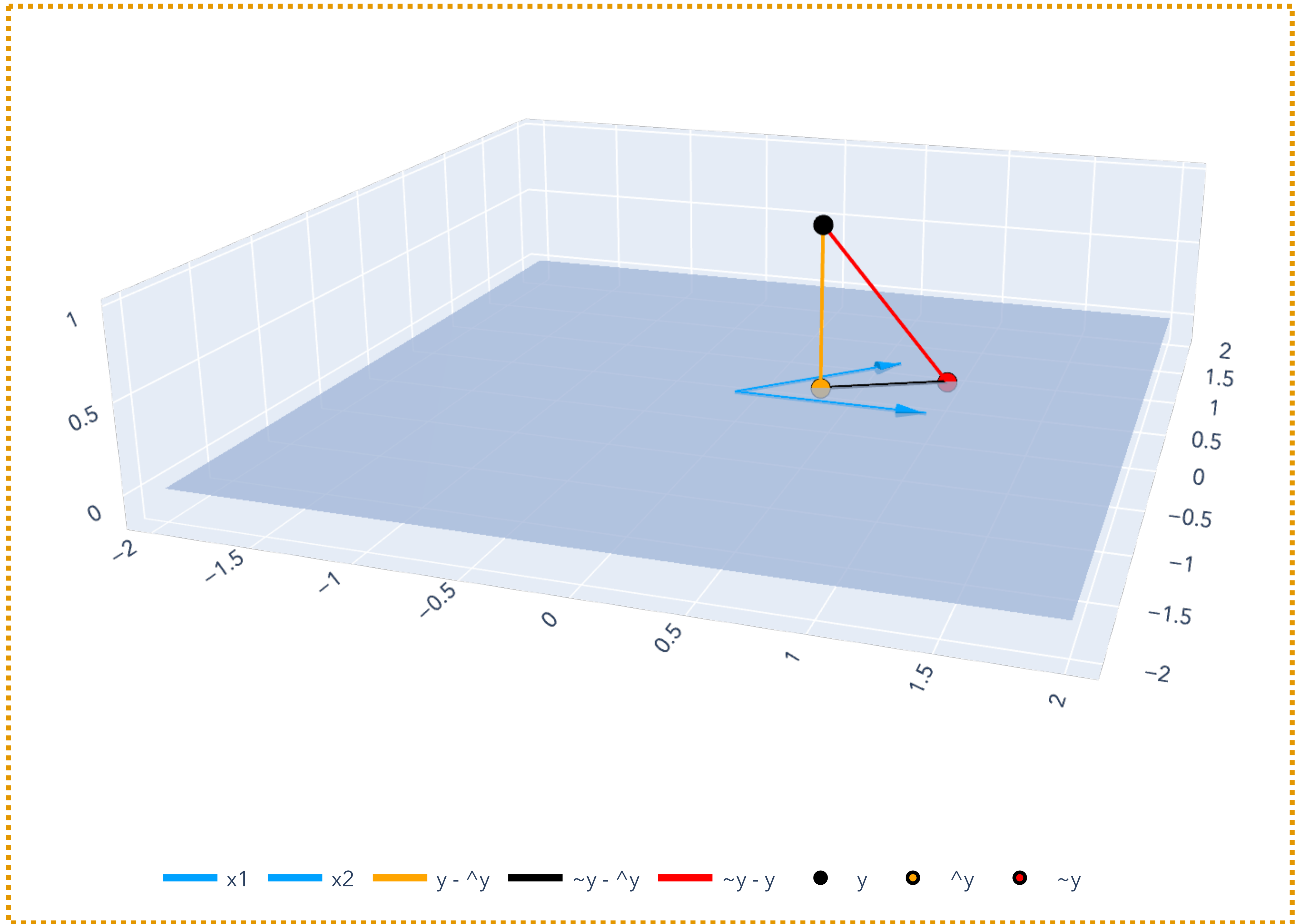
Ordinary Least Squares

Geometry of Least Squares

So, $\hat{\mathbf{y}} = \mathbf{X}\mathbf{w} = w_1\mathbf{x}_1 + w_2\mathbf{x}_2 \in \mathbb{R}^3$, which we can write as: $\hat{\mathbf{y}} \in \text{span}(\text{col}(\mathbf{X}))$.

The true labels $\mathbf{y} \in \mathbb{R}^n$ might not be in $\text{span}(\text{col}(\mathbf{X}))$.

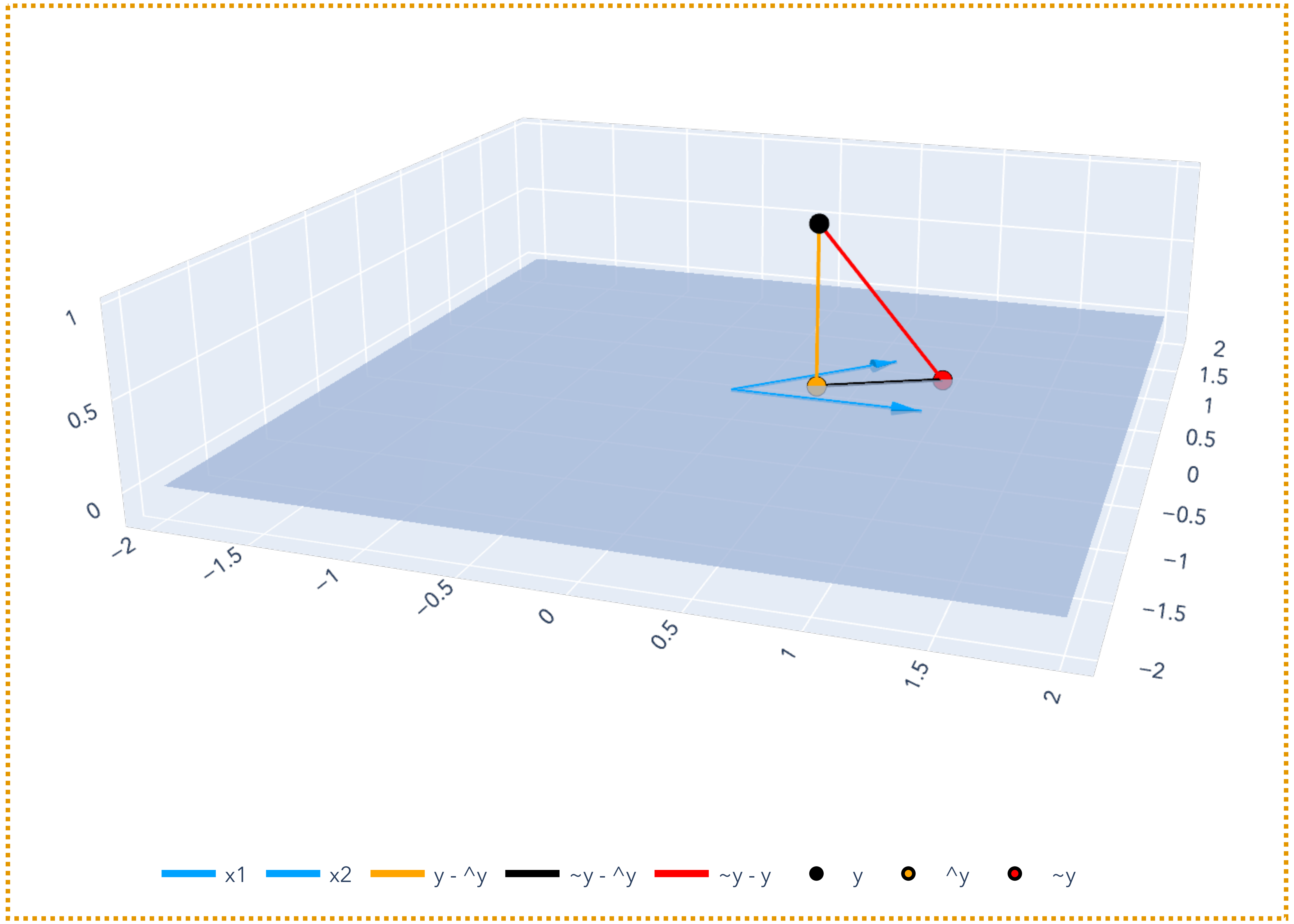
<u>Goal:</u> Find $\mathbf{w} \in \mathbb{R}^d$ that minimizes $\|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$.



Ordinary Least Squares

Geometry of Least Squares

<u>Goal:</u> Find $\mathbf{w} \in \mathbb{R}^d$ that minimizes $\|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$.

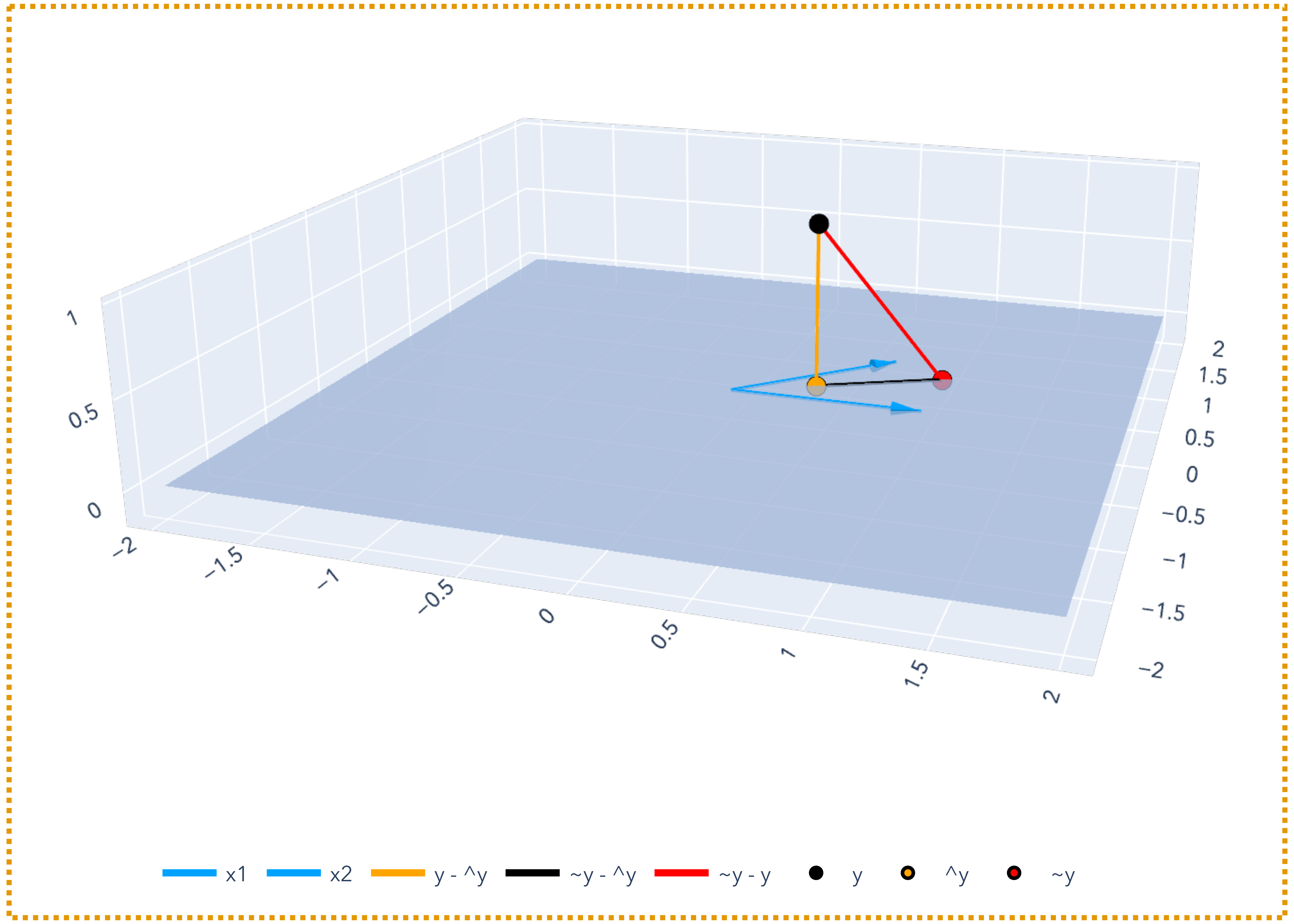


Ordinary Least Squares

Geometry of Least Squares

<u>Goal:</u> Find $\mathbf{w} \in \mathbb{R}^d$ that minimizes $\|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$.

Which point on $\mathrm{span}(\mathrm{col}(\mathbf{X}))$ *minimizes the distance from* $\mathbf{y}$ *to* $\mathrm{span}(\mathrm{col}(\mathbf{X}))$*?*



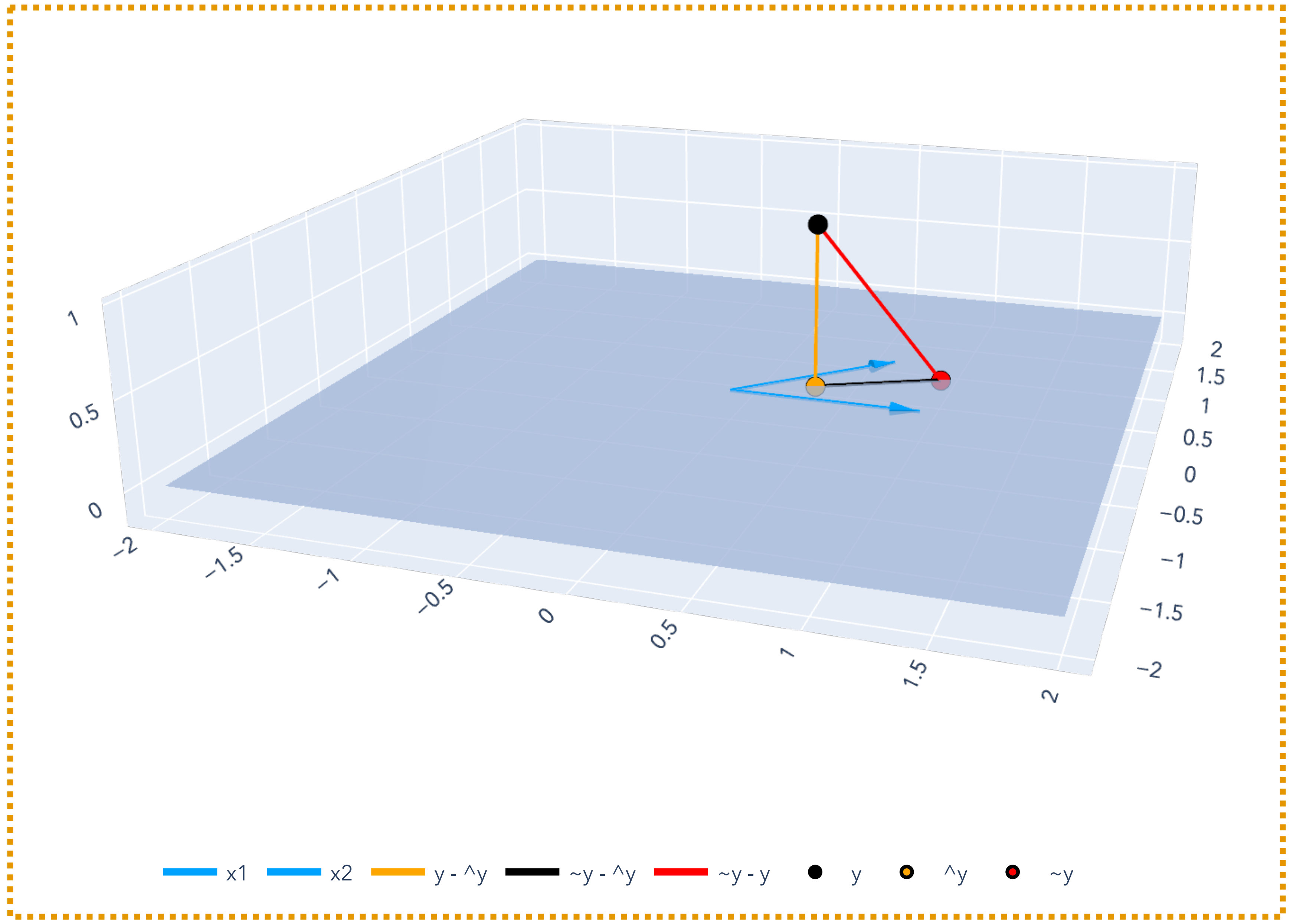
Ordinary Least Squares

Geometry of Least Squares

<u>Goal:</u> Find $\mathbf{w} \in \mathbb{R}^d$ that minimizes $\|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$.

Which point on $\operatorname{span}(\operatorname{col}(\mathbf{X}))$ *minimizes the distance from* $\mathbf{y}$ *to* $\operatorname{span}(\operatorname{col}(\mathbf{X}))$*?*

The point a perpendicular line down to $\operatorname{span}(\operatorname{col}(\mathbf{X}))$*!*

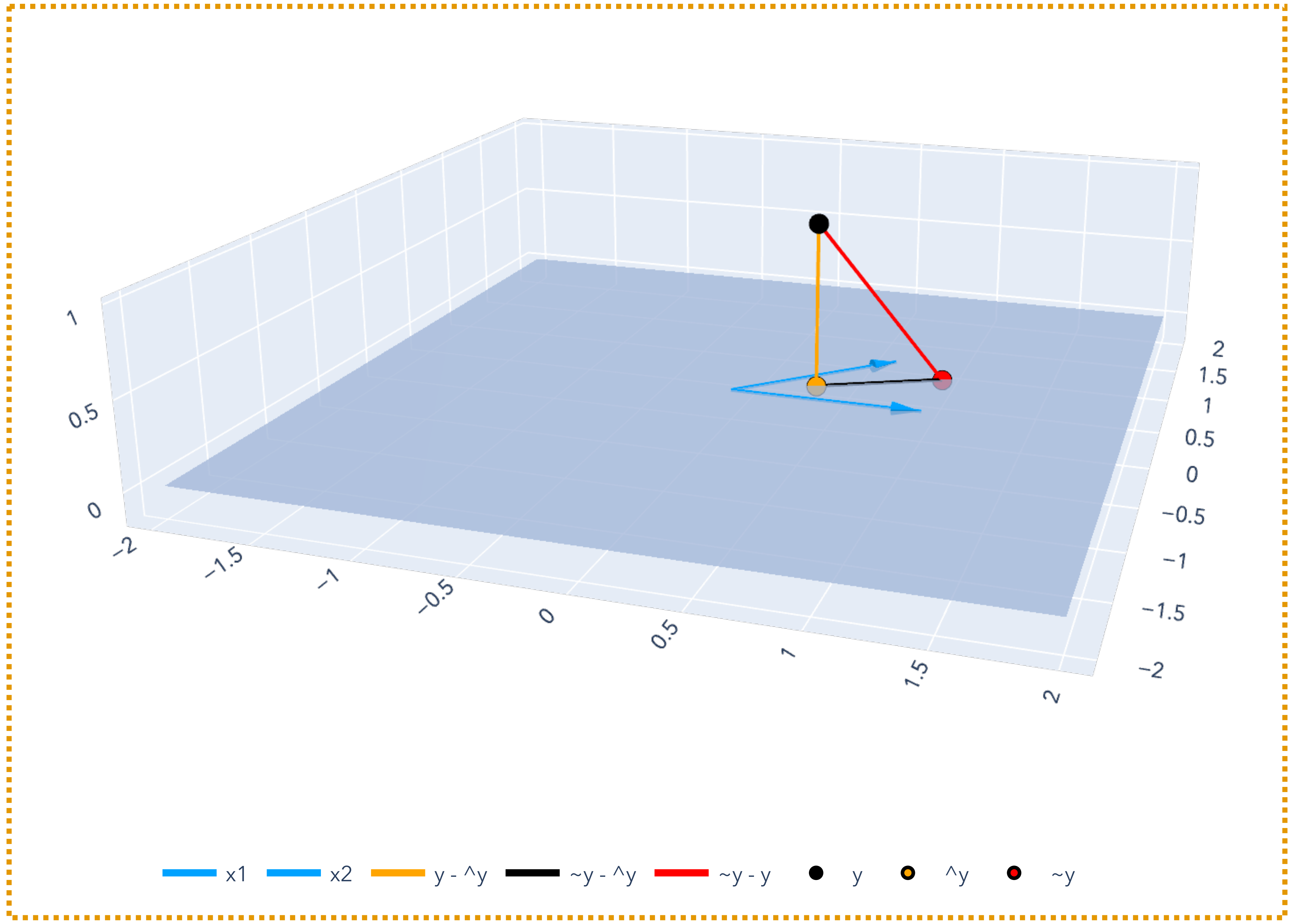


Ordinary Least Squares

Geometry of Least Squares

A *projection* of $\mathbf{y} \in \mathbb{R}^n$ onto $\mathrm{span}(\mathrm{col}(\mathbf{X}))$ gives us $\hat{\mathbf{y}} \in \mathbb{R}^n$, and $\mathbf{X}\hat{\mathbf{w}} = \hat{\mathbf{y}}$.

Let $\tilde{\mathbf{y}} \in \mathbb{R}^n$ be any other vector in $\mathrm{span}(\mathrm{col}(\mathbf{X}))$, written $\mathbf{X}\tilde{\mathbf{w}} = \tilde{\mathbf{y}}$.

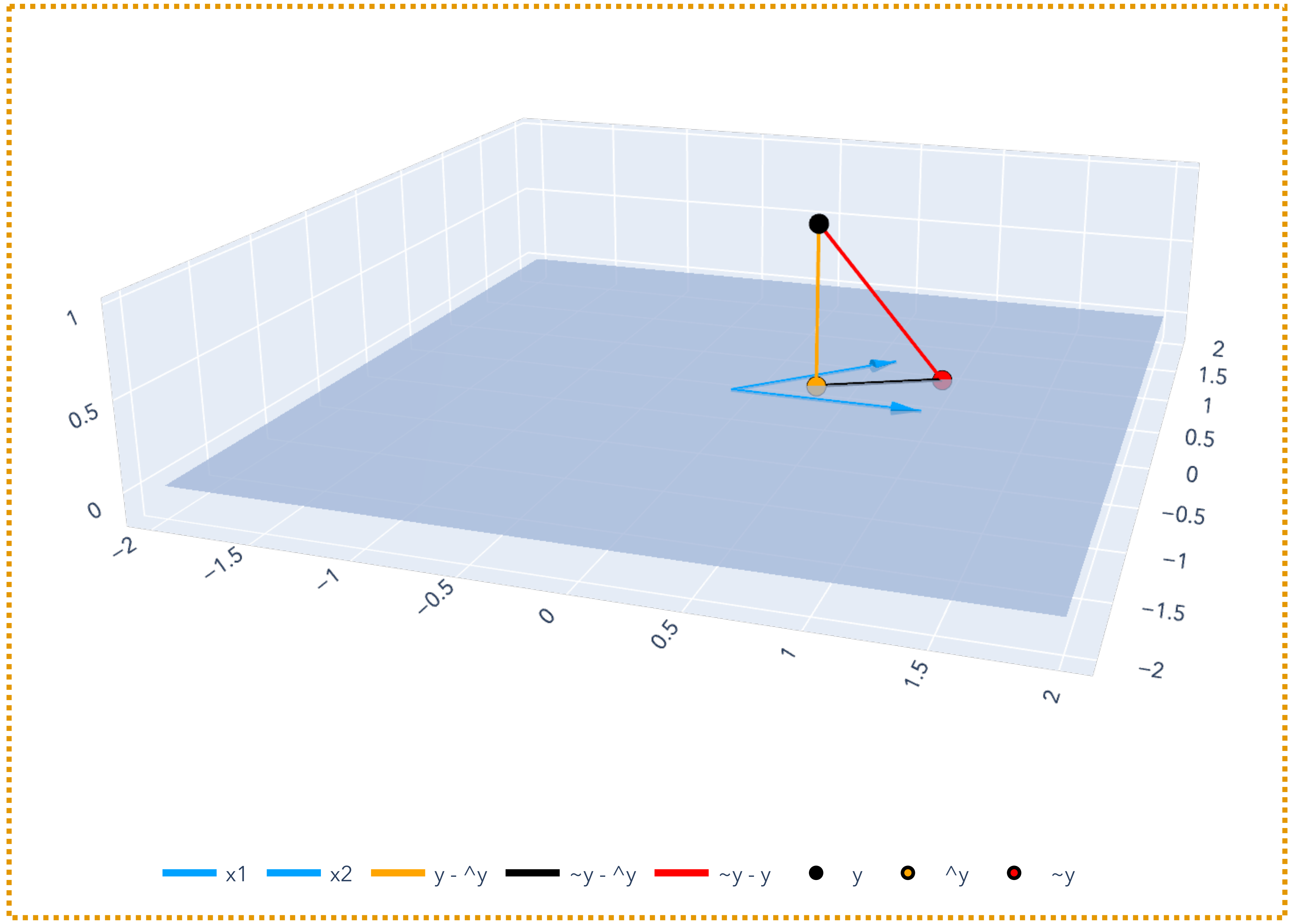


Ordinary Least Squares

Geometry of Least Squares

Let $\hat{\mathbf{y}} = \mathbf{X}\hat{\mathbf{w}}$ be the projection of $\mathbf{y}$. Let $\tilde{\mathbf{y}} = \mathbf{X}\tilde{\mathbf{w}}$ be any other $\tilde{\mathbf{y}}$.

The distances $\|\mathbf{y} - \hat{\mathbf{y}}\|$ and $\|\mathbf{y} - \tilde{\mathbf{y}}\|$ are the lengths of the residuals $\|\hat{\mathbf{r}}\|$ and $\|\tilde{\mathbf{r}}\|$.



Ordinary Least Squares

Geometry of Least Squares

Let $\tilde{\mathbf{y}} = \mathbf{X}\tilde{\mathbf{w}}$ be any other vector in $\mathrm{span}(\mathrm{col}(\mathbf{X}))$.

By the Pythagorean Theorem,

$||\hat{\mathbf{r}}||^2 + ||\tilde{\mathbf{y}} - \hat{\mathbf{y}}||^2 = ||\tilde{\mathbf{r}}||^2.$

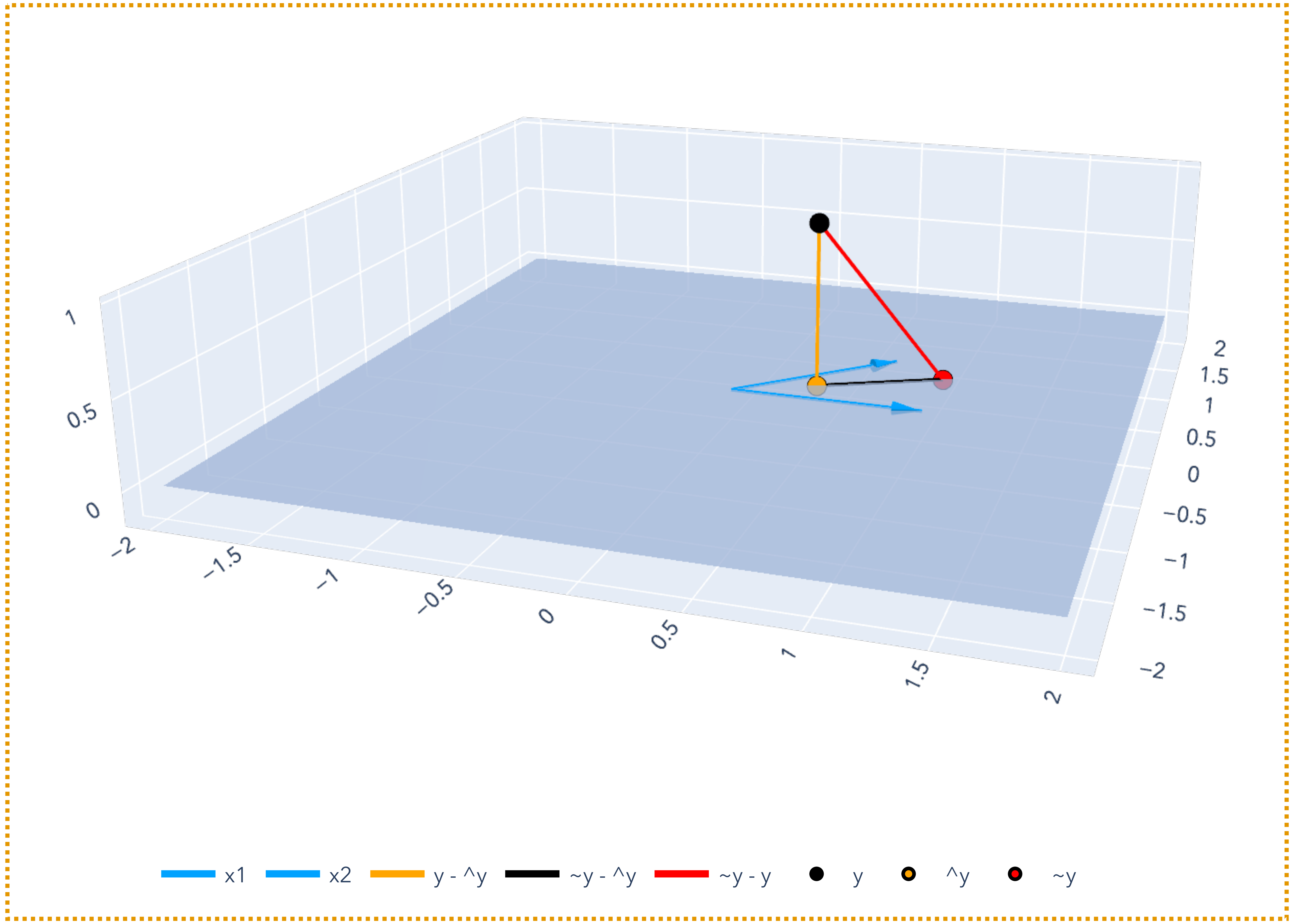
But $||\tilde{\mathbf{y}} - \hat{\mathbf{y}}||^2 \geq 0$, so:

$||\hat{\mathbf{r}}||^2 \leq ||\tilde{\mathbf{r}}||^2.$

By definition, $\hat{\mathbf{r}} = \mathbf{X}\hat{\mathbf{w}} - \mathbf{y}$ and $\tilde{\mathbf{r}} = \mathbf{X}\tilde{\mathbf{w}} - \mathbf{y}$.

Therefore,

$||\mathbf{X}\hat{\mathbf{w}} - \mathbf{y}||^2 \leq ||\mathbf{X}\tilde{\mathbf{w}} - \mathbf{y}||^2.$



Ordinary Least Squares

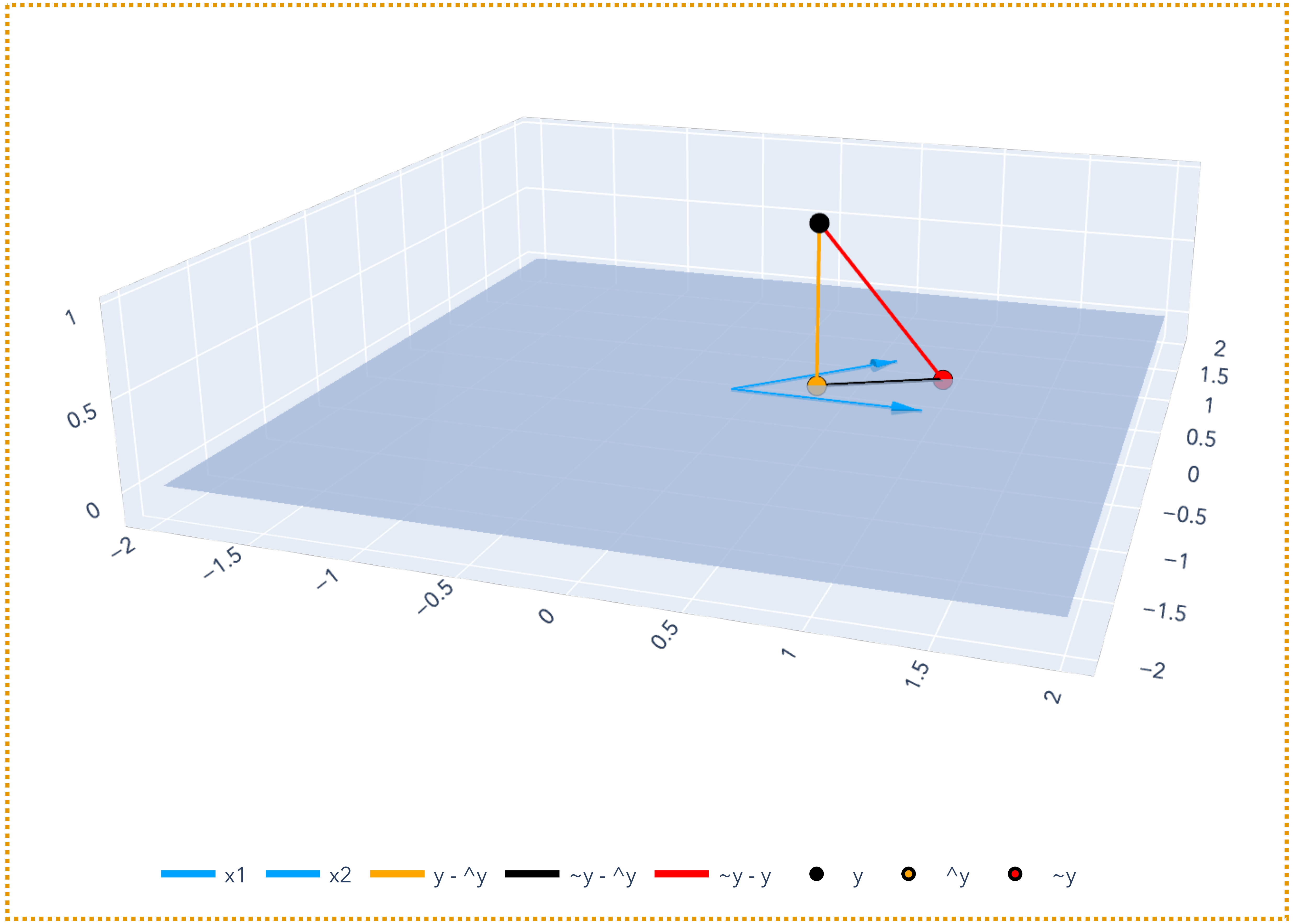
Geometry of Least Squares

Therefore:

$$\|\mathbf{X}\hat{\mathbf{w}} - \mathbf{y}\|^2 \leq \|\mathbf{X}\tilde{\mathbf{w}} - \mathbf{y}\|^2,$$

where $\hat{\mathbf{w}} \in \mathbb{R}^d$ is obtained from the *projection* $\hat{\mathbf{y}}$ of $\mathbf{y} \in \mathbb{R}^d$ onto $\mathrm{span}(\mathrm{col}(\mathbf{X}))$, and $\tilde{\mathbf{w}} \in \mathbb{R}^d$ is any other vector.

But what is $\hat{\mathbf{w}}$?



Orthogonality

Definition

Two vectors $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{y} \in \mathbb{R}^n$ are orthogonal if

$$\langle \mathbf{x}, \mathbf{y} \rangle = \mathbf{x}^\top \mathbf{y} = 0.$$

So, if a vector $\mathbf{v} \in \mathbb{R}^n$ is orthogonal to a whole set of vectors $\{\mathbf{x}_1, \ldots, \mathbf{x}_d\}$, we can write this in matrix form.

$$\mathbf{X} = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{x}_1 & \cdots & \mathbf{x}_d \\ \downarrow & & \downarrow \end{bmatrix}$$

$$\mathbf{X}^\top \mathbf{v} = \mathbf{0}.$$

Ordinary Least Squares

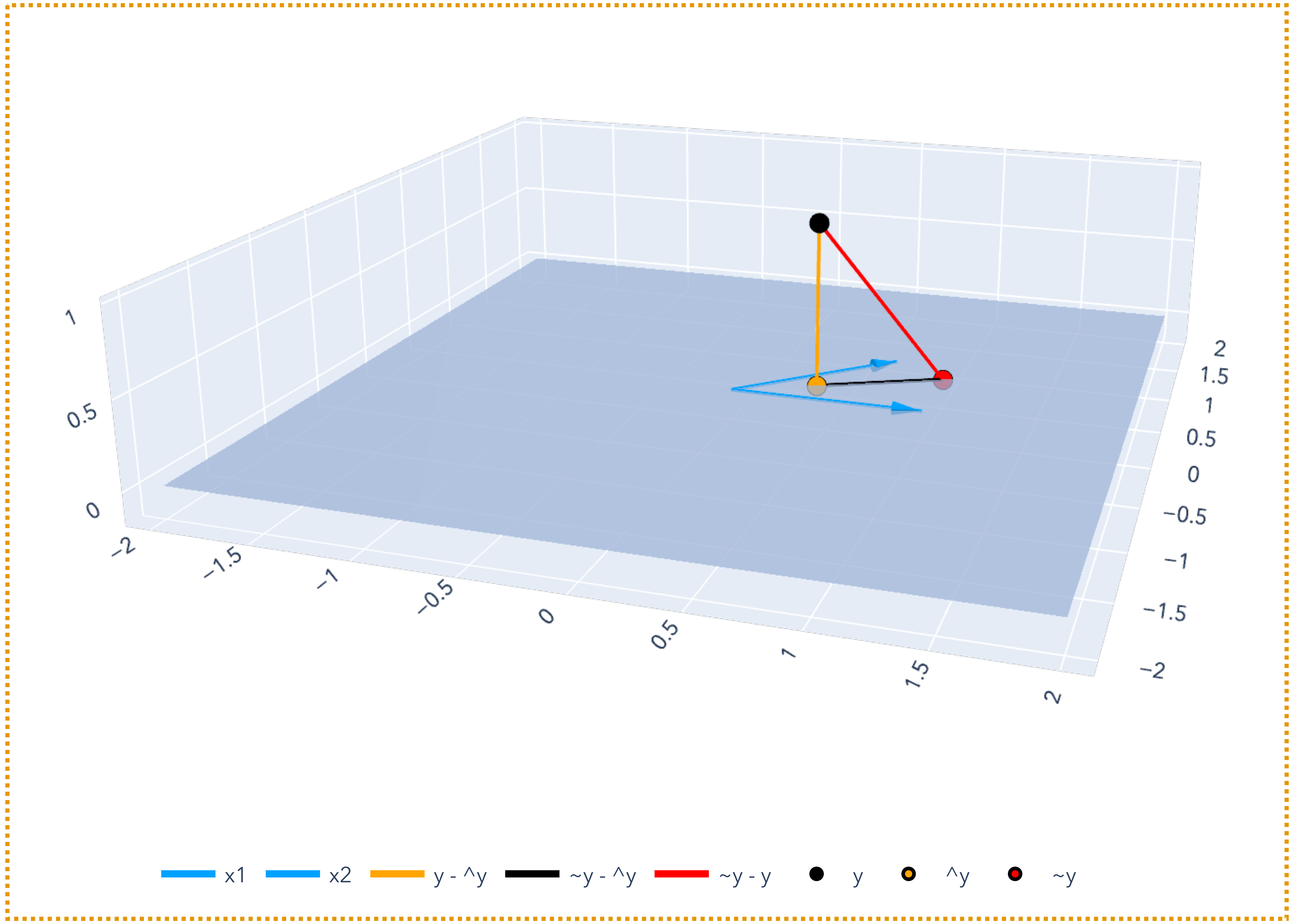
The Normal Equations

From the picture, $\hat{\mathbf{r}} = \mathbf{X}\hat{\mathbf{w}} - \mathbf{y}$ is *orthogonal* to $\mathrm{span}(\mathrm{col}(\mathbf{X}))$:

$$\mathbf{X}^\top \hat{\mathbf{r}} = \mathbf{0} \implies \mathbf{X}^\top \left(\mathbf{X}\hat{\mathbf{w}} - \mathbf{y}\right) = \mathbf{0}\,.$$

This gives us the normal equations:

$$\mathbf{X}^\top \mathbf{y} = \mathbf{X}^\top \mathbf{X}\hat{\mathbf{w}}.$$



Ordinary Least Squares

The Normal Equations

Finally, we need to solve the normal equations:

$$\underbrace{\mathbf{X}^\top \mathbf{y}}_{\mathbb{R}^d} = \underbrace{\mathbf{X}^\top \mathbf{X}}_{\mathbb{R}^{d \times d}} \underbrace{\hat{\mathbf{w}}}_{\mathbb{R}^d}.$$

Linear Independence

Idea

A collection of vectors $\mathbf{a}_1, \ldots, \mathbf{a}_d \in \mathbb{R}^n$ is linearly independent if there are no redundancies – no vector $\mathbf{a}_i$ can be written as a linear combination of the others.

Linear Independence

Definition

A collection of vectors $\mathbf{a}_1, \ldots, \mathbf{a}_d \in \mathbb{R}^n$ is linearly independent if $\alpha_1 \mathbf{a}_1 + \ldots + \alpha_d \mathbf{a}_d = \mathbf{0}$ if and only if $\alpha_i = 0$ for all $i \in [d]$.

Equivalently, there *does not* exist $\mathbf{a}_i$ that can be written in terms of the others:

$$\mathbf{a}_i = \alpha_1 \mathbf{a}_1 + \ldots + \alpha_{i-1} \mathbf{a}_{i-1} + \alpha_{i+1} \mathbf{a}_{i+1} + \ldots + \alpha_d \mathbf{a}_d.$$

If there *does* exist $\mathbf{a}_i$ that can be written in terms of the others, the collection is *linearly dependent*.

Linear Independence

Definition

A collection of vectors $\mathbf{a}_1, \ldots, \mathbf{a}_d \in \mathbb{R}^n$ is linearly independent if $\alpha_1\mathbf{a}_1 + \ldots + \alpha_d\mathbf{a}_d = \mathbf{0}$ if and only if $\alpha_i = 0$ for all $i \in [d]$.

Equivalently, this matrix-vector product (column view)

$$\mathbf{A}\alpha = \begin{bmatrix} \uparrow & \ldots & \uparrow \\ \mathbf{a}_1 & \ldots & \mathbf{a}_d \\ \downarrow & \ldots & \downarrow \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_d \end{bmatrix} = \alpha_1 \begin{bmatrix} \uparrow \\ \mathbf{a}_1 \\ \downarrow \end{bmatrix} + \ldots + \alpha_d \begin{bmatrix} \uparrow \\ \mathbf{a}_d \\ \downarrow \end{bmatrix}$$

is $\mathbf{0}$ if and only if $\alpha = \mathbf{0}$.

Multiplication

Matrix-vector multiplication (column view)

To multiply a matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ and a vector $\mathbf{w} \in \mathbb{R}^d$, we can think of the *column view*:

$$\mathbf{X}\mathbf{w} = \begin{bmatrix} \uparrow & & \uparrow \\ \mathbf{x}_1 & \cdots & \mathbf{x}_d \\ \downarrow & & \downarrow \end{bmatrix} \begin{bmatrix} w_1 \\ \vdots \\ w_d \end{bmatrix} = w_1 \begin{bmatrix} \uparrow \\ \mathbf{x}_1 \\ \downarrow \end{bmatrix} + \ldots + w_d \begin{bmatrix} \uparrow \\ \mathbf{x}_d \\ \downarrow \end{bmatrix}.$$

The result is $\mathbf{X}\mathbf{w} \in \mathbb{R}^n$.

Interpretation: $\mathbf{X}\mathbf{w}$ is a *linear combination* of the columns of $\mathbf{X}$.

Linear Independence

Examples

$$\left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 2 \\ 2 \\ 0 \end{bmatrix} \right\}$$ is *not* linearly independent.

$$\left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix} \right\}$$ is linearly independent.

$$\left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 2 \end{bmatrix} \right\}$$ is linearly independent.

Rank

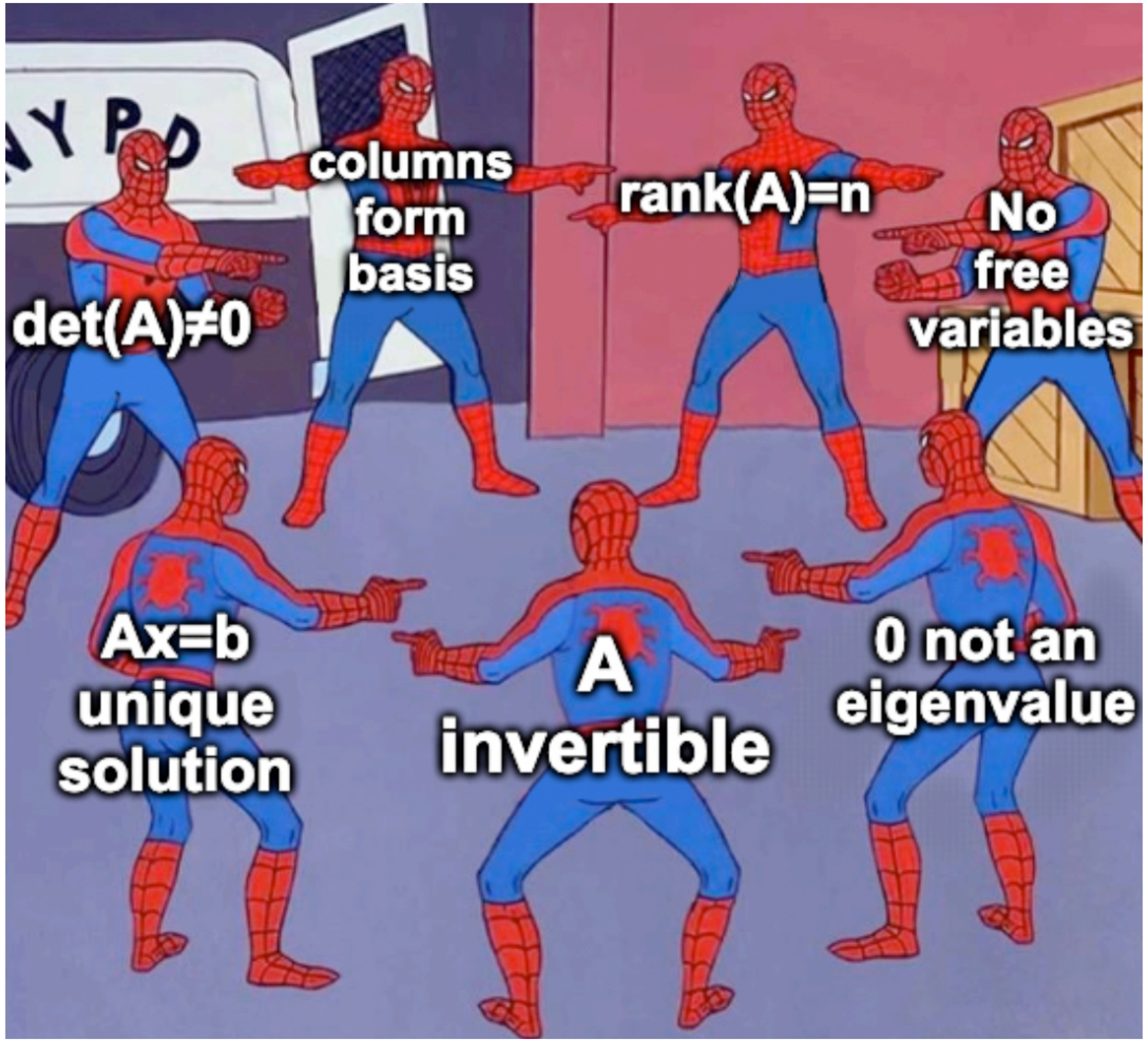
Definition

Rank is the number of linearly independent columns in a matrix. This is always the same as the number of linearly independent rows in a matrix.

For $\mathbf{A} \in \mathbb{R}^{n \times d}$, it is always the case that: $\mathrm{rank}(\mathbf{A}) \leq \min\{n, d\}$.

If $\mathrm{rank}(\mathbf{A}) = \min\{n, d\}$, then we say $\mathbf{A}$ is *full rank*.

Remember this?



Ordinary Least Squares

The Normal Equations

Finally, we need to solve the normal equations:

$$\underbrace{\mathbf{X}^\top \mathbf{y}}_{\mathbb{R}^d} = \underbrace{\mathbf{X}^\top \mathbf{X}}_{\mathbb{R}^{d\times d}} \underbrace{\hat{\mathbf{w}}}_{\mathbb{R}^d}.$$

For $\mathbf{X} \in \mathbb{R}^{n\times d}$, if $n \geq d$ and $\operatorname{rank}(\mathbf{X}) = d$, then: $\operatorname{rank}(\mathbf{X}^\top \mathbf{X}) = d \iff \mathbf{X}^\top \mathbf{X}$ has d linearly independent columns $\iff (\mathbf{X}^\top \mathbf{X})^{-1}$ exists.

Ordinary Least Squares

The Normal Equations

$$\underbrace{\mathbf{X}^\top \mathbf{y}}_{\mathbb{R}^d} = \underbrace{\mathbf{X}^\top \mathbf{X}}_{\mathbb{R}^{d\times d}} \underbrace{\hat{\mathbf{w}}}_{\mathbb{R}^d}.$$

Finally, solving the normal equations:

$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}$$

Ordinary Least Squares

Main Theorem

Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ with $n \geq d$ and $\mathrm{rank}(\mathbf{X}) = d$ (the columns of $\mathbf{X}$ are linearly independent).

Then, the solution $\hat{\mathbf{w}} \in \mathbb{R}^d$ that minimizes $\|\mathbf{X}\mathbf{w} - \mathbf{y}\|$, i.e.

$$\|\mathbf{X}\hat{\mathbf{w}} - \mathbf{y}\| \leq \|\mathbf{X}\mathbf{w} - \mathbf{y}\| \text{ for all } \mathbf{w} \in \mathbb{R}^d,$$

is given by:

$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

Recap

Lesson Overview

Takeaways

Regression. The basic problem in machine learning is regression. We have *training data* in the form of a data matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ and labels $\mathbf{y} \in \mathbb{R}^n$. We seek a model $\hat{\mathbf{w}} \in \mathbb{R}^d$ such that $\mathbf{X}\hat{\mathbf{w}} \approx \mathbf{y}$.

Least squares. One way to find a model for the data is through *least squares*: choose $\hat{\mathbf{w}}$ that minimizes$\|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$.

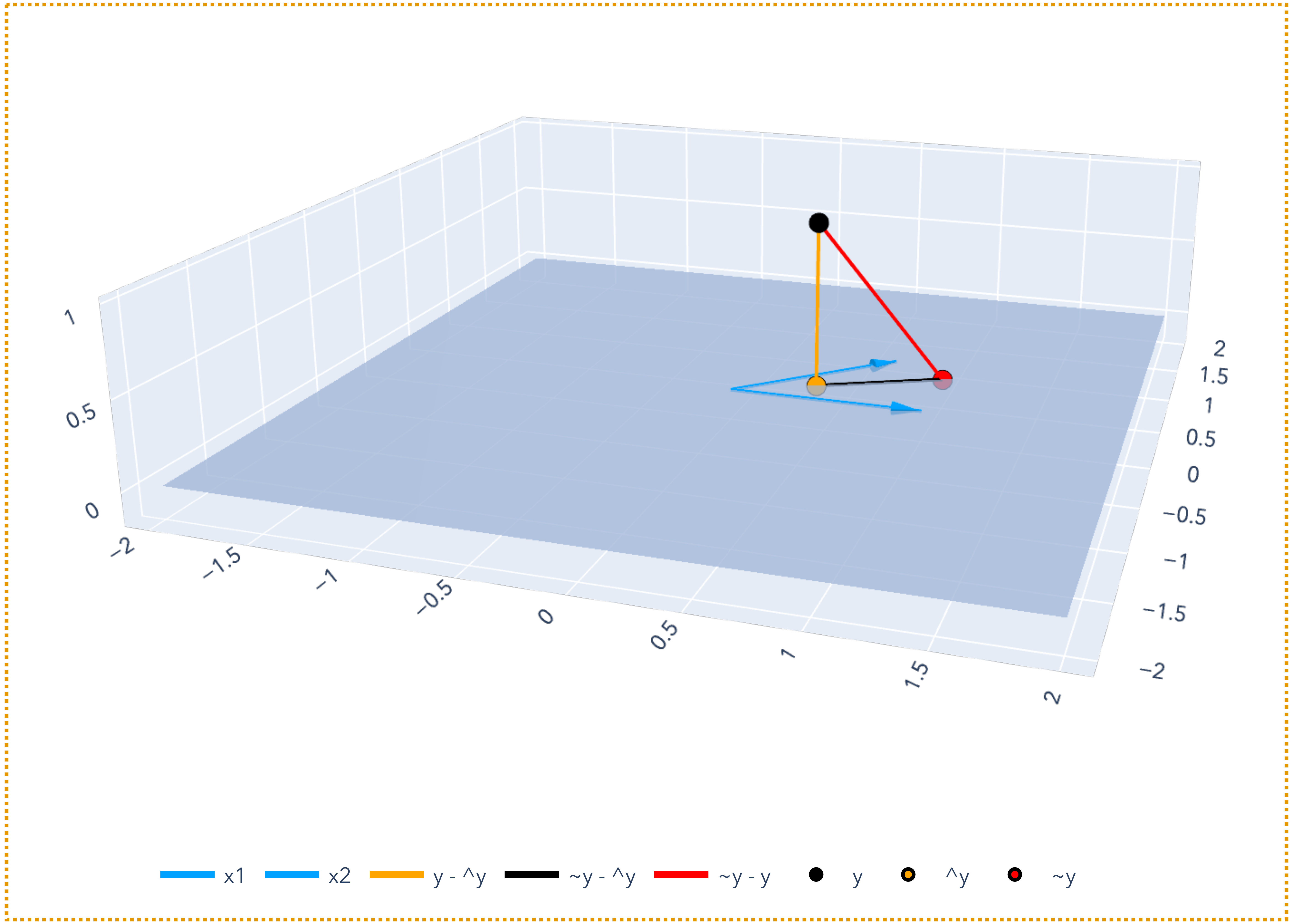
Span and orthogonality. We can solve least squares by noticing that $\mathbf{X}\hat{\mathbf{w}} - \mathbf{y}$ is *orthogonal* to $\mathrm{span}(\mathrm{cols}(\mathbf{X}))$. This gives us the normal equations: $\mathbf{X}^\top \mathbf{X}\hat{\mathbf{w}} = \mathbf{X}^\top \mathbf{y}$.

Linear independence. To solve the normal equations, we need $\mathbf{X}$ to be full *rank* (its d columns are *linearly independent*). Then, we can invert and solve the normal equations.

$$\hat{\mathbf{w}} = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

Lesson Overview

Big Picture: Least Squares



Lesson Overview

Big Picture: Gradient Descent