Math for Machine Learning

Week 1.2: Subspaces, Bases, and Orthogonality

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Logistics and Announcements

Lesson Overview

Regression. Fill in gaps from last time: invertibility and Pythagorean theorem.

Subspaces. Subsets of $\mathcal{S} \subseteq \mathbb{R}^n$ where we "stay inside" when performing linear combinations of vectors.

Bases. A "language" to describe all vectors in a subspace.

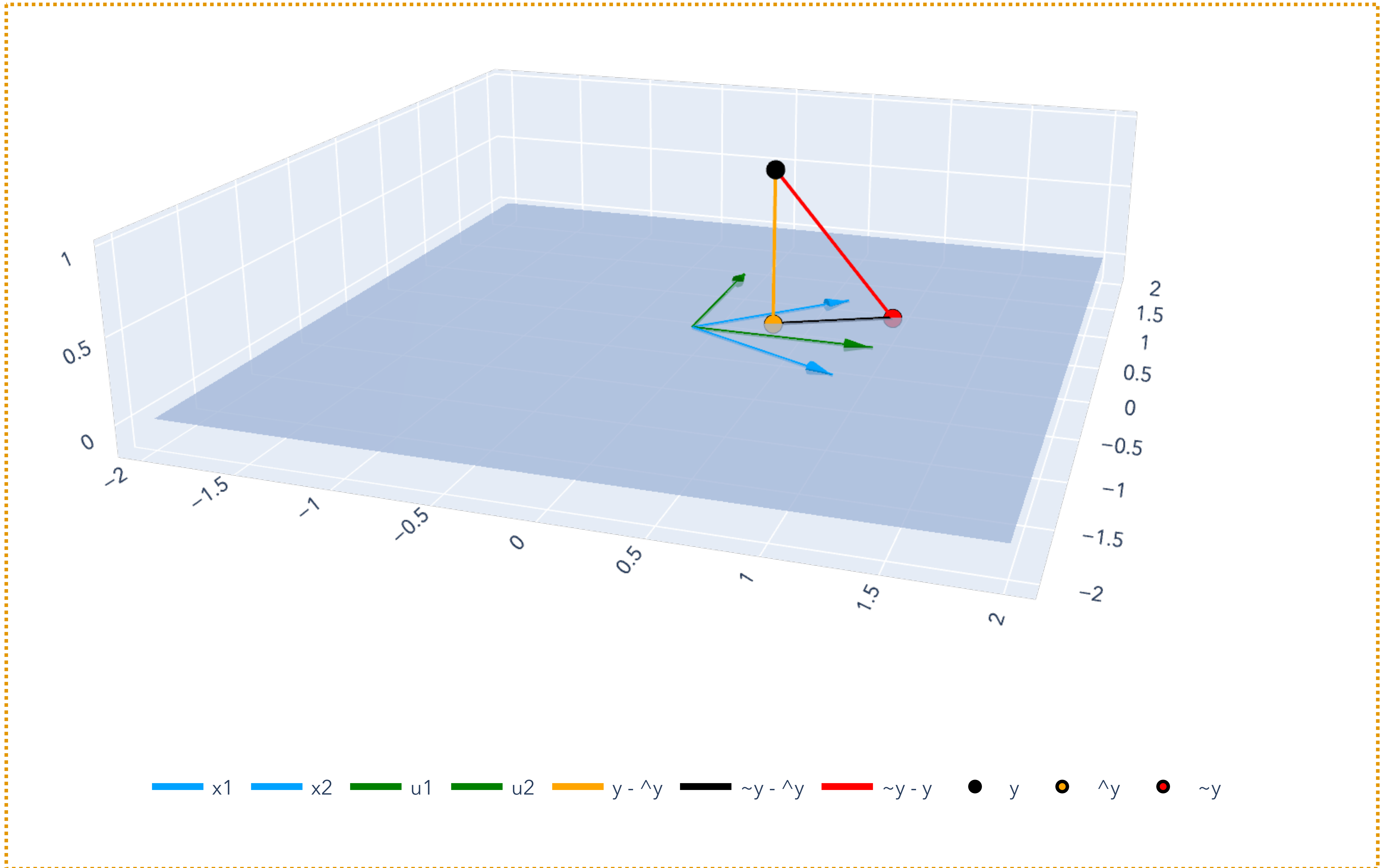
Orthogonality. Orthonormal bases are "good" bases to work with.

Projection. Formal definition of projection and the relationship between projection and least squares.

Least squares with orthonormal bases. If we have an orthonormal basis for $\text{span}(\text{col}(\mathbf{X}))$, least squares becomes much simpler.

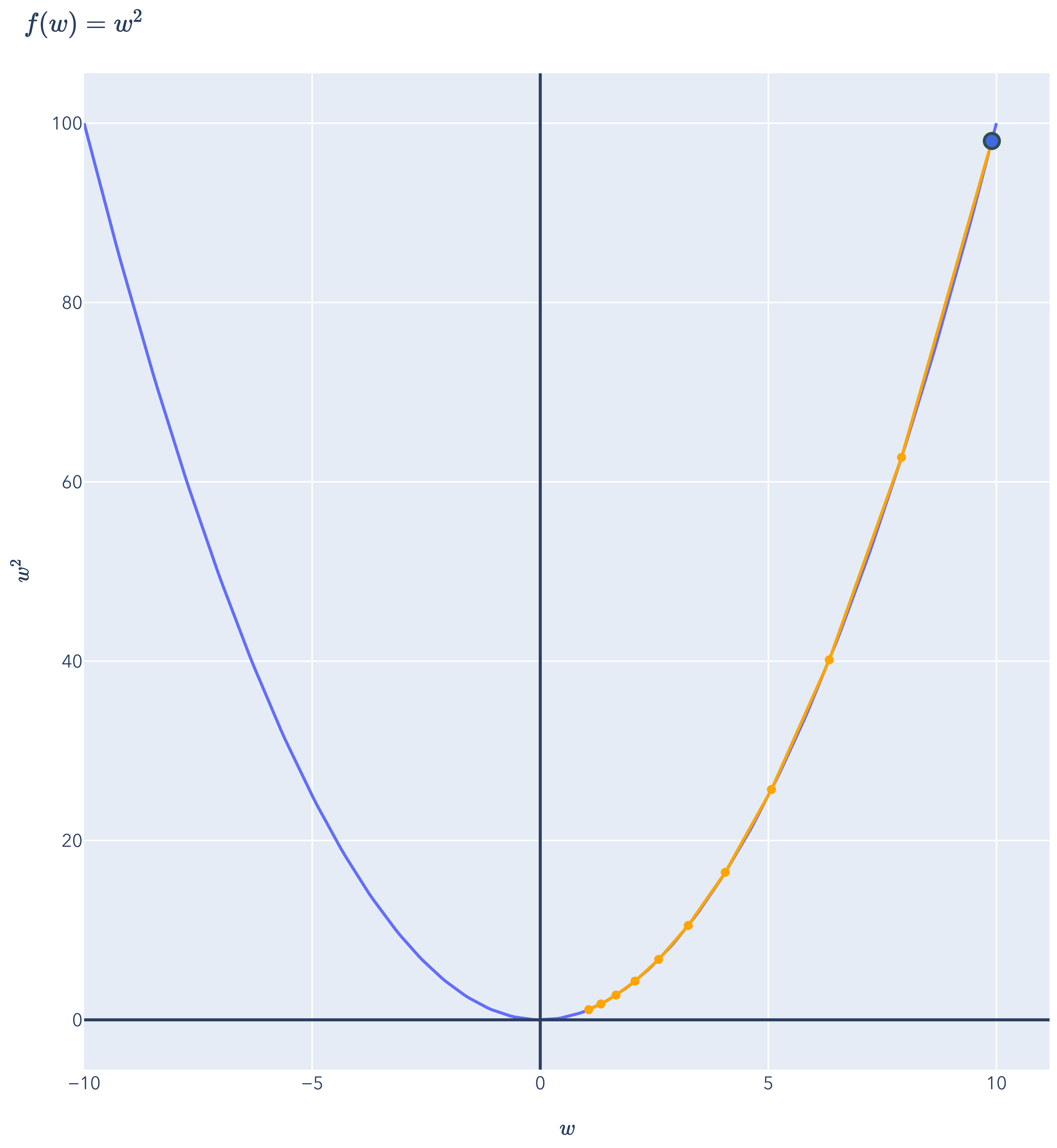
Lesson Overview

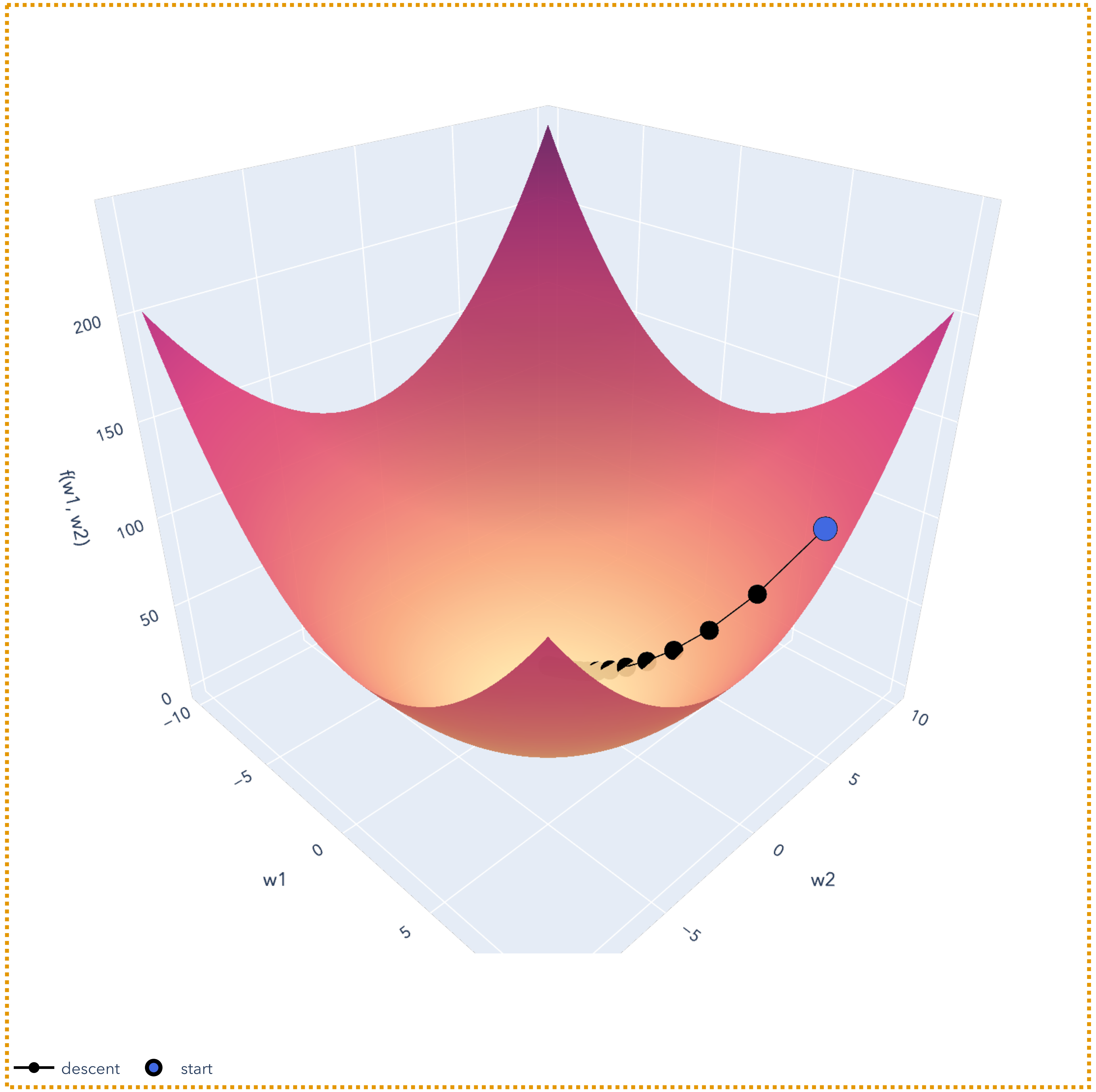
Big Picture: Least Squares



Lesson Overview

Big Picture: Gradient Descent





Least Squares

A Quick Review

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.

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*:

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

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*.

Regression

Setup (Example View)

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

$$\mathbf{X} = \begin{bmatrix} \leftarrow & \mathbf{x}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_n^\top & \rightarrow \end{bmatrix} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$, 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:

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

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

A note on intercepts

<u>Goal:</u> For each $i \in [n]$, what if we want to predict: $\hat{y}_i = \mathbf{w}^\top \mathbf{x}_i + w_0 = w_1 x_{i1} + \ldots + w_d x_{id} + w_0$?

<u>Solution:</u> We modify add a "dummy" 1 to each example:

$$\mathbf{x}_i^\top = \begin{bmatrix} x_{i1} & \ldots & x_{id} & 1 \end{bmatrix}.$$

Same as transforming the data matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ into $\mathbf{X}' \in \mathbb{R}^{n \times (d+1)}$:

$$\mathbf{X} = \begin{bmatrix} \leftarrow & \mathbf{x}_1^\top & \rightarrow \\ & \vdots & \\ \leftarrow & \mathbf{x}_n^\top & \rightarrow \end{bmatrix} \implies \mathbf{X}' = \begin{bmatrix} \leftarrow & \mathbf{x}_1^\top & \rightarrow & 1 \\ & \vdots & & \vdots \\ \leftarrow & \mathbf{x}_n^\top & \rightarrow & 1 \end{bmatrix}$$

Choose a weight vector that fits $\mathbf{X}'$: $\mathbf{w} \in \mathbb{R}^{d+1}$ such that $y_i \approx \hat{y}_i$ for $i \in [n]$, or:

$\mathbf{X}'\mathbf{w} = \hat{\mathbf{y}} \approx \mathbf{y}$. The last $(d+1)$ entry of $\mathbf{w}$ is the intercept, w_0.

We can always do this WLOG, so we'll focus on the "homogeneous" case.

Least Squares

Summary

Use the principle of *least squares* to find the $\hat{\mathbf{w}} \in \mathbb{R}^d$ that minimizes

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

Using geometric intuition: $\hat{\mathbf{y}}$ *is the vector for which* $\hat{\mathbf{y}} - \mathbf{y}$ *is perpendicular to* $\mathrm{span}(\mathrm{col}(\mathbf{X}))$.

By Pythagorean Theorem, any other vector $\tilde{\mathbf{y}} \in \mathrm{span}(\mathrm{col}(\mathbf{X}))$ gives a larger error:

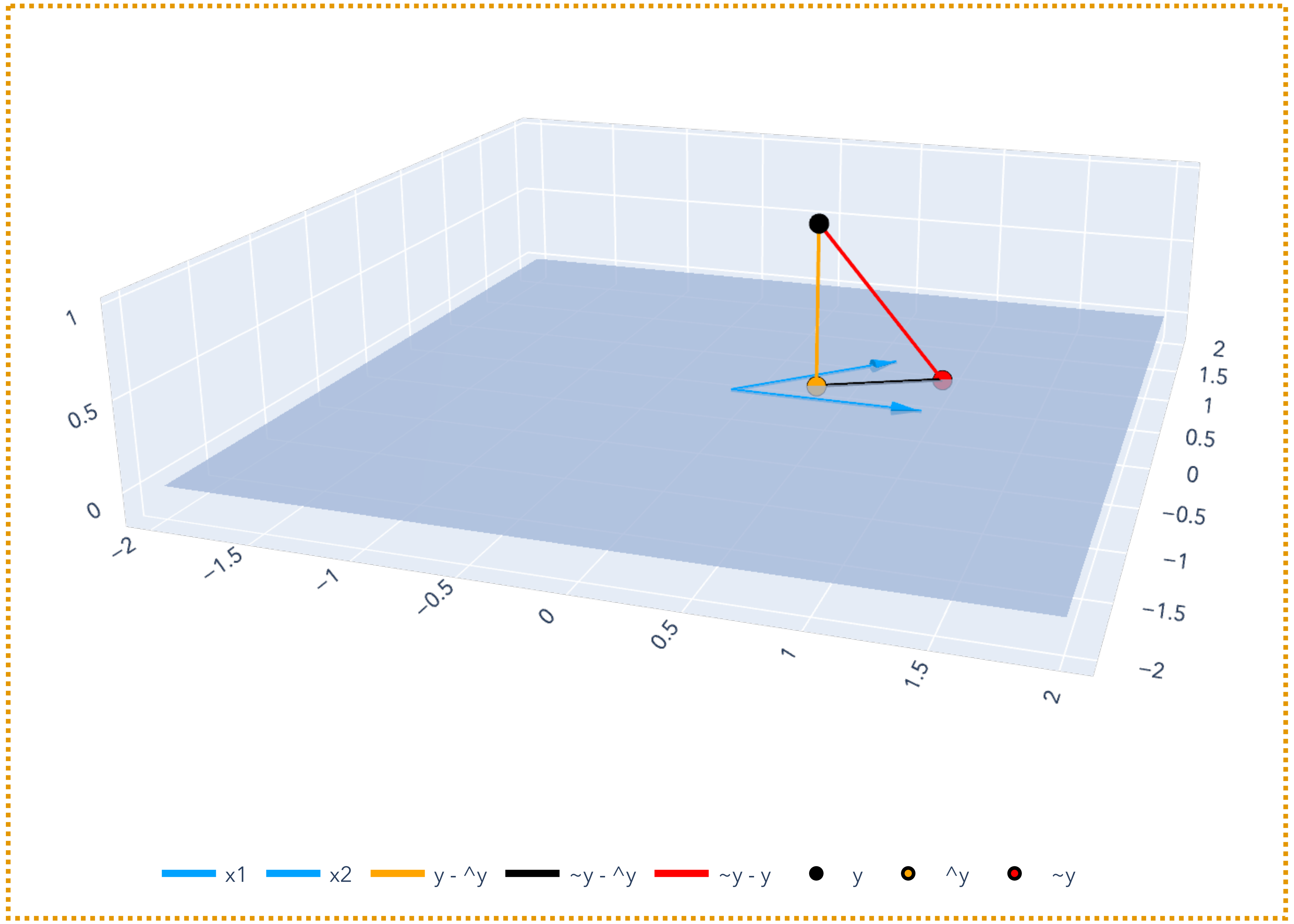
$$\|\hat{\mathbf{y}} - \mathbf{y}\|^2 \leq \|\tilde{\mathbf{y}} - \mathbf{y}\|^2.$$

Because $\hat{\mathbf{y}} - \mathbf{y}$ is perpendicular to $\mathrm{span}(\mathrm{col}(\mathbf{X}))$, we obtain the *normal equations:*

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

If $n \geq d$ and $\mathrm{rank}(\mathbf{X}) = d$, then $\mathbf{X}^\top \mathbf{X}$ *is invertible*, and

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



Least Squares

First missing item: invertibility of $\mathbf{X}^\top \mathbf{X}$

If $n \geq d$ and $\operatorname{rank}(\mathbf{X}) = d$, then $\mathbf{X}^\top \mathbf{X}$ is invertible.

"If there are no redundant features, then we can invert the normal equations"

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:

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

Subspaces

Subspaces

Idea

A subspace is a set of vectors that “stays within” the set under all linear combinations of the vectors.

Subspaces

Definition

A subspace $\mathcal{S} \subseteq \mathbb{R}^n$ is a subset of vectors that satisfies the property: if $\mathbf{v}, \mathbf{w} \in \mathcal{S}$, then $\alpha\mathbf{v} + \beta\mathbf{w} \in \mathcal{S}$ for any $\alpha, \beta \in \mathbb{R}$.

Any subspace $\mathcal{S}$ contains the zero vector: $\mathbf{0} \in \mathcal{S}$.

Subspaces

Examples

Example: $\mathscr{S}_0 := \mathbb{R}^2$

Subspaces

Examples

<u>Example</u>: $\mathcal{S}_1 := \{\mathbf{v} \in \mathbb{R}^2 : v_1 = 0\}$

Subspaces
Examples

<u>Example</u>: $\mathcal{S}_2 := \{\mathbf{v} \in \mathbb{R}^3 : v_1 = v_2\}$

Span
Review

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

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

Recall that this is equivalent to all the $\mathbf{y} \in \mathbb{R}^{n \times d}$ we obtain from matrix vector multiplication!

$$\mathbf{y} = \mathbf{A}\alpha, \text{ i.e. } \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} \uparrow & \uparrow & \uparrow \\ \mathbf{a}_1 & \ldots & \mathbf{a}_d \\ \downarrow & \downarrow & \downarrow \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_d \end{bmatrix}$$

Subspaces

Examples

<u>Example:</u> $\mathscr{S}_3 := \operatorname{span}\left(\begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \right)$

Subspaces

Examples

(Non)Example: $\mathcal{S}_4 := \{\mathbf{v} \in \mathbb{R}^3 : v_3 = 5\}$

Subspaces

Specific example: $\mathrm{span}(\mathrm{col}(\mathbf{X}))$

Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ with columns $\mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n$.

$$\mathrm{span}(\mathrm{col}(\mathbf{X})) = \{\mathbf{y} \in \mathbb{R}^n : \mathbf{y} = w_1\mathbf{x}_1 + \ldots + w_d\mathbf{x}_d\}$$

We will refer to this, later, as $\mathrm{CS}(\mathbf{X})$, the columnspace of $\mathbf{X}$.

Bases & Dimension

Basis

Idea

For a subspace $\mathcal{S}$, a basis is a *minimal* set of vectors that can "linearly describe" *any* vector in $\mathcal{S}$. A "language" for vectors in $\mathcal{S}$.

Basis

Linear Independence and Span

Recall the following two notions.

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 $i \in [d]$.

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

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

Basis
Definition

For a subspace $\mathcal{S} \subseteq \mathbb{R}^n$, a set of vectors $\mathbf{a}_1, \ldots, \mathbf{a}_d \in \mathcal{S}$ is a basis for $\mathcal{S}$ if:

$$\mathcal{S} = \mathrm{span}(\mathbf{a}_1, \ldots, \mathbf{a}_d) \text{ and } \mathbf{a}_1, \ldots, \mathbf{a}_d \text{ are linearly independent.}$$

Bases are not unique – there are infinitely many bases for any subspace.

However, all bases have the same number of elements.

Basis

Examples

Example: $\mathcal{S}_0 := \mathbb{R}^2$

Basis

Examples

Example: $\mathcal{S}_1 := \{\mathbf{v} \in \mathbb{R}^2 : v_1 = 0\}$

Basis

Examples

<u>Example</u>: $\mathcal{S}_2 := \{\mathbf{v} \in \mathbb{R}^3 : v_1 = v_2\}$

Dimension of a Subspace

Definition

The dimension of a subspace is the size of any of its bases.

For a subspace $\mathscr{S}$, write this as $\dim(\mathscr{S})$.

Matrices & Subspaces

Every matrix comes with four subspaces

Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be a matrix.

Its columnspace is $\mathrm{CS}(\mathbf{X}) = \{\mathbf{y} \in \mathbb{R}^n : \mathbf{y} = \mathbf{X}\mathbf{w},$ for any $\mathbf{w} \in \mathbb{R}^d\}$ (this was $\mathrm{span}(\mathrm{col}(\mathbf{X}))$).

Its nullspace/kernel is $\mathrm{NS}(\mathbf{X}) := \{\mathbf{w} \in \mathbb{R}^d : \mathbf{X}\mathbf{w} = \mathbf{0}\}$.

Its rowspace is $\mathrm{CS}(\mathbf{X}^\top) = \{\mathbf{y} \in \mathbb{R}^d : \mathbf{y} = \mathbf{X}^\top\mathbf{v},$ for any $\mathbf{v} \in \mathbb{R}^n\}$.

Its *left nullspace* is $\mathrm{NS}(\mathbf{X}^\top) := \{\mathbf{v} \in \mathbb{R}^n : \mathbf{X}^\top\mathbf{v} = \mathbf{0}\}$.

Rank-nullity theorem: $n = \dim(\mathrm{CS}(\mathbf{X})) + \dim(\mathrm{NS}(\mathbf{X}))$.

Matrices & Subspaces

Columnspace of a matrix

Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be a matrix, with columns $\mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n$.

We can think of its columnspace as:

$$\begin{aligned}
\mathrm{CS}(\mathbf{X}) := &\{\mathbf{y} \in \mathbb{R}^n : \mathbf{y} = \mathbf{X}\mathbf{w}, \text{ for any } \mathbf{w} \in \mathbb{R}^d\} \\
= &\{\mathbf{y} \in \mathbb{R}^n : \mathbf{y} = w_1\mathbf{x}_1 + \ldots + w_d\mathbf{x}_d, \text{ for any } w_i \in \mathbb{R}\} \\
= &\operatorname{span}(\mathbf{x}_1, \ldots, \mathbf{x}_d) = \operatorname{span}(\operatorname{col}(\mathbf{x}_1, \ldots, \mathbf{x}_d))
\end{aligned}$$

This is a subspace that “comes with” any matrix.

Matrices & Subspaces

Rank of a matrix

Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be a matrix, with columns $\mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n$.

The rank of $\mathbf{X}$ is the number of linearly independent columns (which is the same as the number of linearly independent rows).

It is always the case that: $\mathrm{rank}(\mathbf{X}) \leq \min\{n, d\}$. If $\mathrm{rank}(\mathbf{X}) = \min\{n, d\}$, then we say $\mathbf{X}$ is *full rank*.

Matrices & Subspaces

Rank & Invertibility

Let $\mathbf{X} \in \mathbb{R}^{d \times d}$ be a square matrix.

It is always the case that: $\operatorname{rank}(\mathbf{X}) \leq d$. If $\operatorname{rank}(\mathbf{X}) = d$, then we say $\mathbf{X}$ is *full rank*.

Basic fact from linear algebra:

$\mathbf{X}$ *is invertible if and only if it is full rank.*

Matrices & Subspaces

Dimension of the columnspace

Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be a matrix, with columns $\mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n$.

$$\mathrm{CS}(\mathbf{X}) = \mathrm{span}(\mathbf{x}_1, \ldots, \mathbf{x}_d)$$

$\mathrm{rank}(\mathbf{X})$ = how many of $\mathbf{x}_1, \ldots, \mathbf{x}_d$ are linearly independent

So, if $\mathrm{rank}(\mathbf{X}) = d$, then $\mathbf{x}_1, \ldots, \mathbf{x}_d$ form a *basis for the columnspace*!

Least Squares

First missing item: invertibility of $\mathbf{X}^\top \mathbf{X}$

If $n \geq d$ and $\mathrm{rank}(\mathbf{X}) = d$, then $\mathbf{X}^\top \mathbf{X}$ is invertible.

"If there are no redundant features, then we can invert the normal equations"

Least Squares

First missing item: invertibility of $\mathbf{X}^\top \mathbf{X}$

Theorem (Invertibility of $\mathbf{X}^\top \mathbf{X}$). Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be a matrix, with columns $\mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n$. If $n \geq d$ and $\mathrm{rank}(\mathbf{X}) = d$, then $\mathbf{X}^\top \mathbf{X}$ *is invertible.*

Proof. To show that $\mathbf{X}^\top \mathbf{X}$ is invertible, show $\mathrm{rank}(\mathbf{X}^\top \mathbf{X}) = d$.

Least Squares

First missing item: invertibility of $\mathbf{X}^\top \mathbf{X}$

Theorem (Invertibility of $\mathbf{X}^\top \mathbf{X}$). Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be a matrix, with columns $\mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n$. If $n \geq d$ and $\operatorname{rank}(\mathbf{X}) = d$, then $\mathbf{X}^\top \mathbf{X}$ *is invertible.*

Proof. To show that $\mathbf{X}^\top \mathbf{X}$ is invertible, show $\mathbf{X}^\top \mathbf{X}$ has d linearly independent columns.

$$\mathbf{X}^\top \mathbf{X} \mathbf{w} = \mathbf{0} \iff \mathbf{w} = \mathbf{0}.$$

Least Squares

First missing item: invertibility of $\mathbf{X}^\top\mathbf{X}$

Theorem (Invertibility of $\mathbf{X}^\top\mathbf{X}$). Let $\mathbf{X} \in \mathbb{R}^{n\times d}$ be a matrix, with columns $\mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n$. If $n \geq d$ and $\mathrm{rank}(\mathbf{X}) = d$, then $\mathbf{X}^\top\mathbf{X}$ *is invertible.*

Proof. To show that $\mathbf{X}^\top\mathbf{X}$ is invertible, show $\mathbf{X}^\top\mathbf{X}$ has d linearly independent columns.

$$\mathbf{X}^\top\mathbf{X}\mathbf{w} = \mathbf{0} \implies \mathbf{w} = \mathbf{0}.$$

Suppose $\mathbf{X}^\top\mathbf{X}\mathbf{w} = \mathbf{0}$. Let $\mathbf{w} \in \mathbb{R}^d$ be any vector.

Least Squares

First missing item: invertibility of $\mathbf{X}^\top \mathbf{X}$

Theorem (Invertibility of $\mathbf{X}^\top \mathbf{X}$). Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be a matrix, with columns $\mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n$. If $n \geq d$ and $\operatorname{rank}(\mathbf{X}) = d$, then $\mathbf{X}^\top \mathbf{X}$ *is invertible.*

Proof. To show that $\mathbf{X}^\top \mathbf{X}$ is invertible, show $\mathbf{X}^\top \mathbf{X}$ has d linearly independent columns.

$$\mathbf{X}^\top \mathbf{X} \mathbf{w} = \mathbf{0} \implies \mathbf{w} = \mathbf{0}.$$

Suppose $\mathbf{X}^\top \mathbf{X} \mathbf{w} = \mathbf{0}$. Let $\mathbf{w} \in \mathbb{R}^d$ be any vector. Take a dot product of both sides with $\mathbf{w}$:

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

$$\mathbf{w}^\top \mathbf{X}^\top \mathbf{X} \mathbf{w} = \|\mathbf{X} \mathbf{w}\|^2 = 0$$

Least Squares

First missing item: invertibility of $\mathbf{X}^\top \mathbf{X}$

Theorem (Invertibility of $\mathbf{X}^\top \mathbf{X}$). Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be a matrix, with columns $\mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n$. If $n \geq d$ and $\operatorname{rank}(\mathbf{X}) = d$, then $\mathbf{X}^\top \mathbf{X}$ *is invertible.*

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Suppose $\mathbf{X}^\top \mathbf{X} \mathbf{w} = \mathbf{0}$. Let $\mathbf{w} \in \mathbb{R}^d$ be any vector. Take a dot product of both sides with $\mathbf{w}$:

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

$$\mathbf{w}^\top \mathbf{X}^\top \mathbf{X} \mathbf{w} = \|\mathbf{X}\mathbf{w}\|^2 = 0 \implies \mathbf{X}\mathbf{w} = \mathbf{0}\,.$$

But $\operatorname{rank}(\mathbf{X}) = d$, so $\mathbf{X}$ has d linearly independent columns. Therefore, $\mathbf{w} = \mathbf{0}$.

Least Squares

First missing item: invertibility of $\mathbf{X}^\top \mathbf{X}$

Theorem (Invertibility of $\mathbf{X}^\top \mathbf{X}$). Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be a matrix, with columns $\mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n$. If $n \geq d$ and $\operatorname{rank}(\mathbf{X}) = d$, then $\mathbf{X}^\top \mathbf{X}$ *is invertible.*

Least Squares

Summary

Use the principle of *least squares* to find the $\hat{\mathbf{w}} \in \mathbb{R}^d$ that minimizes

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

Using geometric intuition: $\hat{\mathbf{y}}$ *is the vector for which* $\hat{\mathbf{y}} - \mathbf{y}$ *is perpendicular to* $\mathrm{span}(\mathrm{col}(\mathbf{X}))$.

By Pythagorean Theorem, any other vector $\tilde{\mathbf{y}} \in \mathrm{span}(\mathrm{col}(\mathbf{X}))$ gives a larger error:

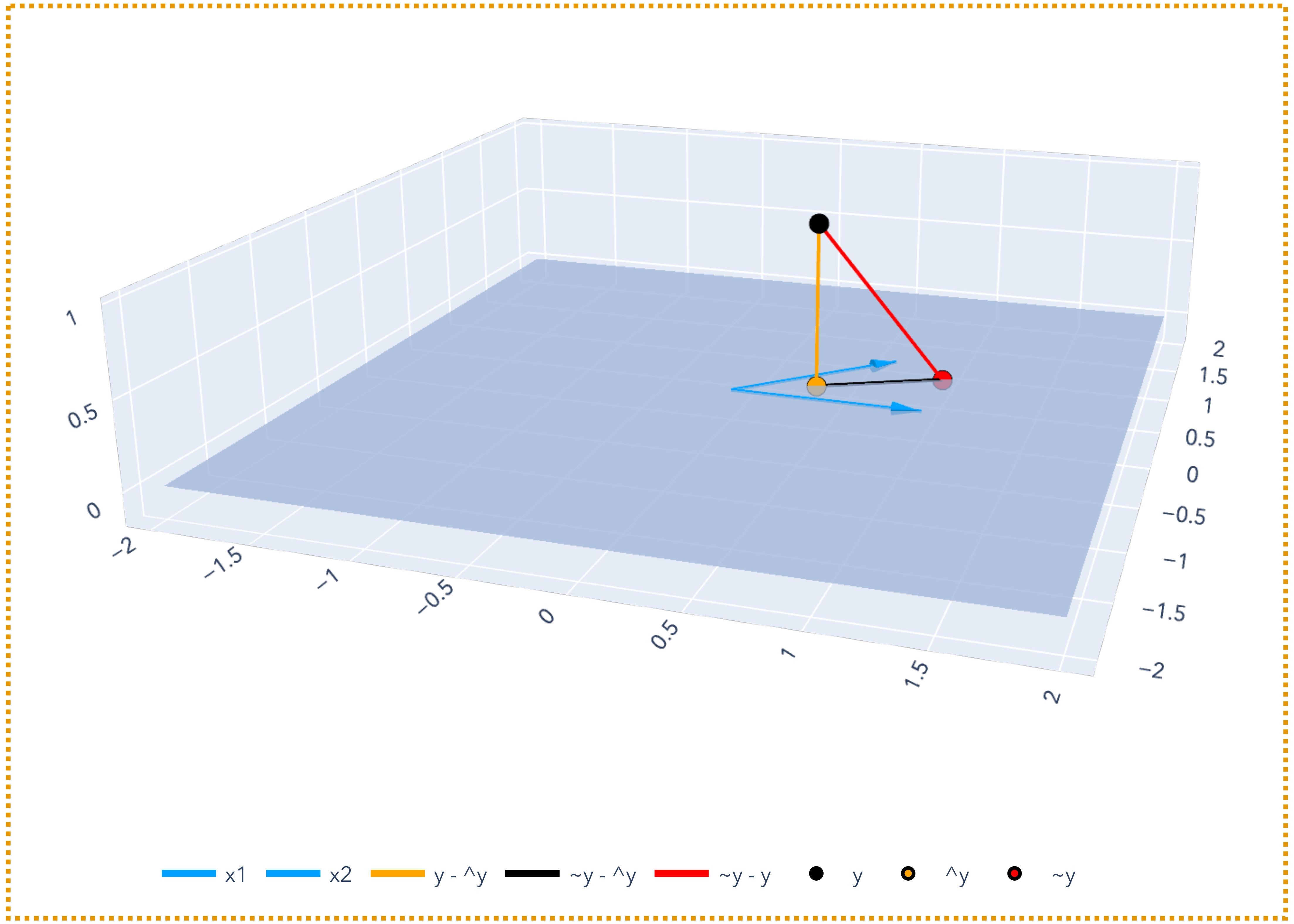
$$\|\hat{\mathbf{y}} - \mathbf{y}\|^2 \leq \|\tilde{\mathbf{y}} - \mathbf{y}\|^2.$$

Because $\hat{\mathbf{y}} - \mathbf{y}$ is perpendicular to $\mathrm{span}(\mathrm{col}(\mathbf{X}))$, we obtain the *normal equations:*

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

If $n \geq d$ and $\mathrm{rank}(\mathbf{X}) = d$, then $\mathbf{X}^\top \mathbf{X}$ *is invertible*, and

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



Least Squares

Summary

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

Using geometric intuition: $\hat{\mathbf{y}}$ *is the vector for which* $\hat{\mathbf{y}} - \mathbf{y}$ *is perpendicular to* $\mathrm{CS}(\mathbf{X})$.

By Pythagorean Theorem, any other vector $\tilde{\mathbf{y}} \in \mathrm{CS}(\mathbf{X})$ gives a larger error:

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

Because $\hat{\mathbf{y}} - \mathbf{y}$ is perpendicular to $\mathrm{CS}(\mathbf{X})$, we obtain the *normal equations:*

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

If $n \geq d$ and $\mathrm{rank}(\mathbf{X}) = d$, then $\mathbf{X}^\top \mathbf{X}$ *is invertible*, and

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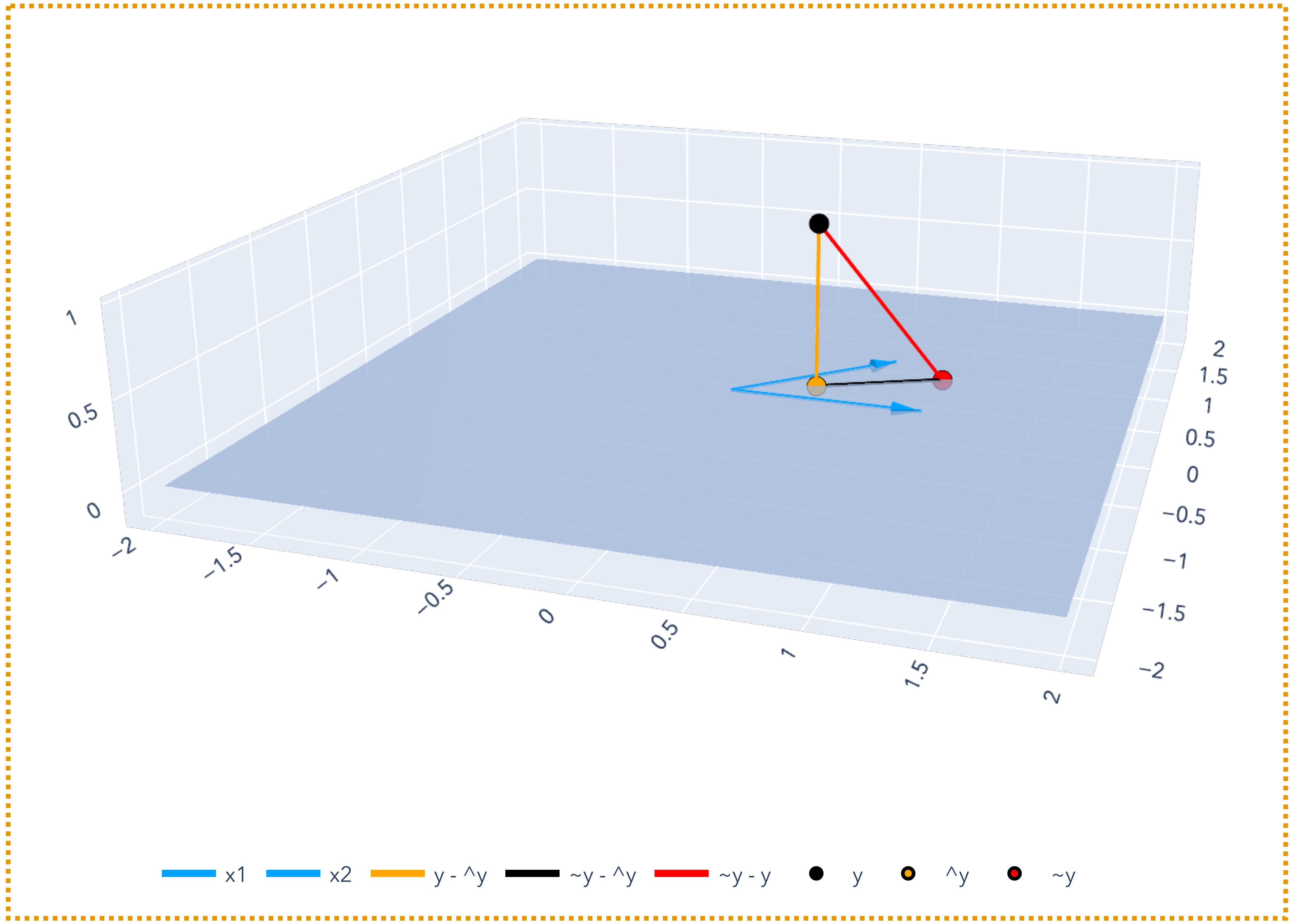


Least Squares

Second missing item: Pythagorean Theorem

By Pythagorean Theorem, any other vector $\tilde{\mathbf{y}} \in \mathrm{CS}(\mathbf{X})$ gives a larger error:

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

"The vector closest to $\mathbf{y}$ in the subspace is perpendicular."

Orthogonality

Definition and Orthonormal Bases

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:

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

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

In this course, dropping the "2" and just writing $\|\mathbf{x}\|$ denotes the Euclidean norm.

Orthogonality

Definition

Two vectors $\mathbf{v}, \mathbf{w} \in \mathbb{R}^n$ are orthogonal if $\langle \mathbf{v}, \mathbf{w} \rangle = \mathbf{v}^\top \mathbf{w} = 0$. In $\mathbb{R}^2$ and $\mathbb{R}^3$, this corresponds to our geometric notion of "perpendicular."

A set of vectors is orthogonal if every pair of distinct vectors in the set is orthogonal.

Orthogonality

Pythagorean Theorem

<u>Theorem (Pythagorean Theorem).</u> If vectors $\mathbf{v}, \mathbf{w} \in \mathbb{R}^n$ are orthogonal, then

$$\|\mathbf{v} + \mathbf{w}\|^2 = \|\mathbf{v}\|^2 + \|\mathbf{w}\|^2.$$

Proof. Let $\mathbf{v}, \mathbf{w} \in \mathbb{R}^n$ be orthogonal vectors. Expand the square $\|\mathbf{v} + \mathbf{w}\|^2$.

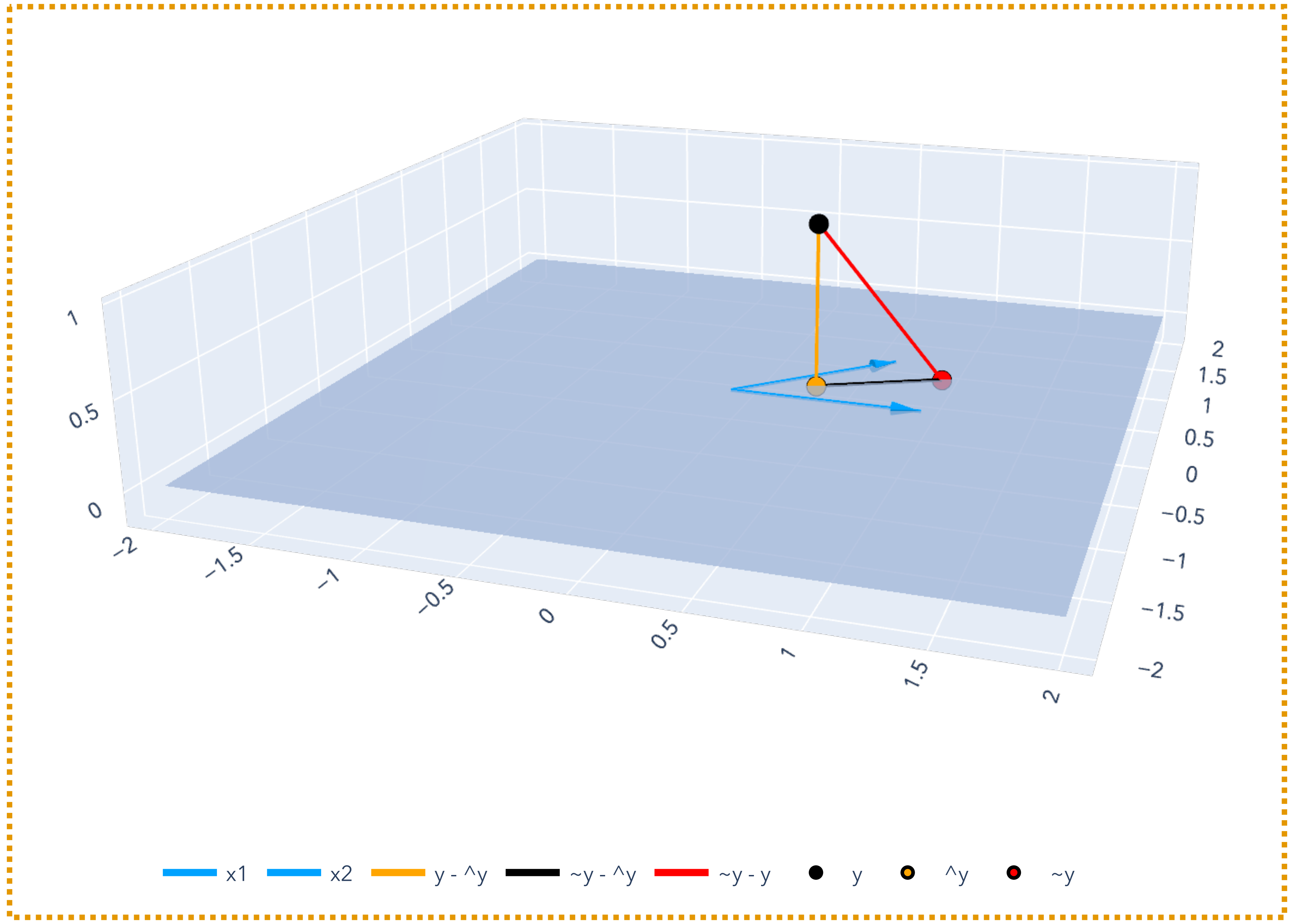
$$\begin{aligned}
\|\mathbf{v} + \mathbf{w}\|^2 &= \langle \mathbf{v} + \mathbf{w}, \mathbf{v} + \mathbf{w} \rangle \\
&= \langle \mathbf{v}, \mathbf{v} \rangle + \langle \mathbf{v}, \mathbf{w} \rangle + \langle \mathbf{w}, \mathbf{v} \rangle + \langle \mathbf{w}, \mathbf{w} \rangle \\
&= \langle \mathbf{v}, \mathbf{v} \rangle + 2\langle \mathbf{v}, \mathbf{w} \rangle + \langle \mathbf{w}, \mathbf{w} \rangle \\
&= \|\mathbf{v}\|^2 + \|\mathbf{w}\|^2
\end{aligned}$$

Least Squares

Second missing item: Pythagorean Theorem

By Pythagorean Theorem, any other vector $\tilde{\mathbf{y}} \in \mathrm{CS}(\mathbf{X})$ gives a larger error:

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

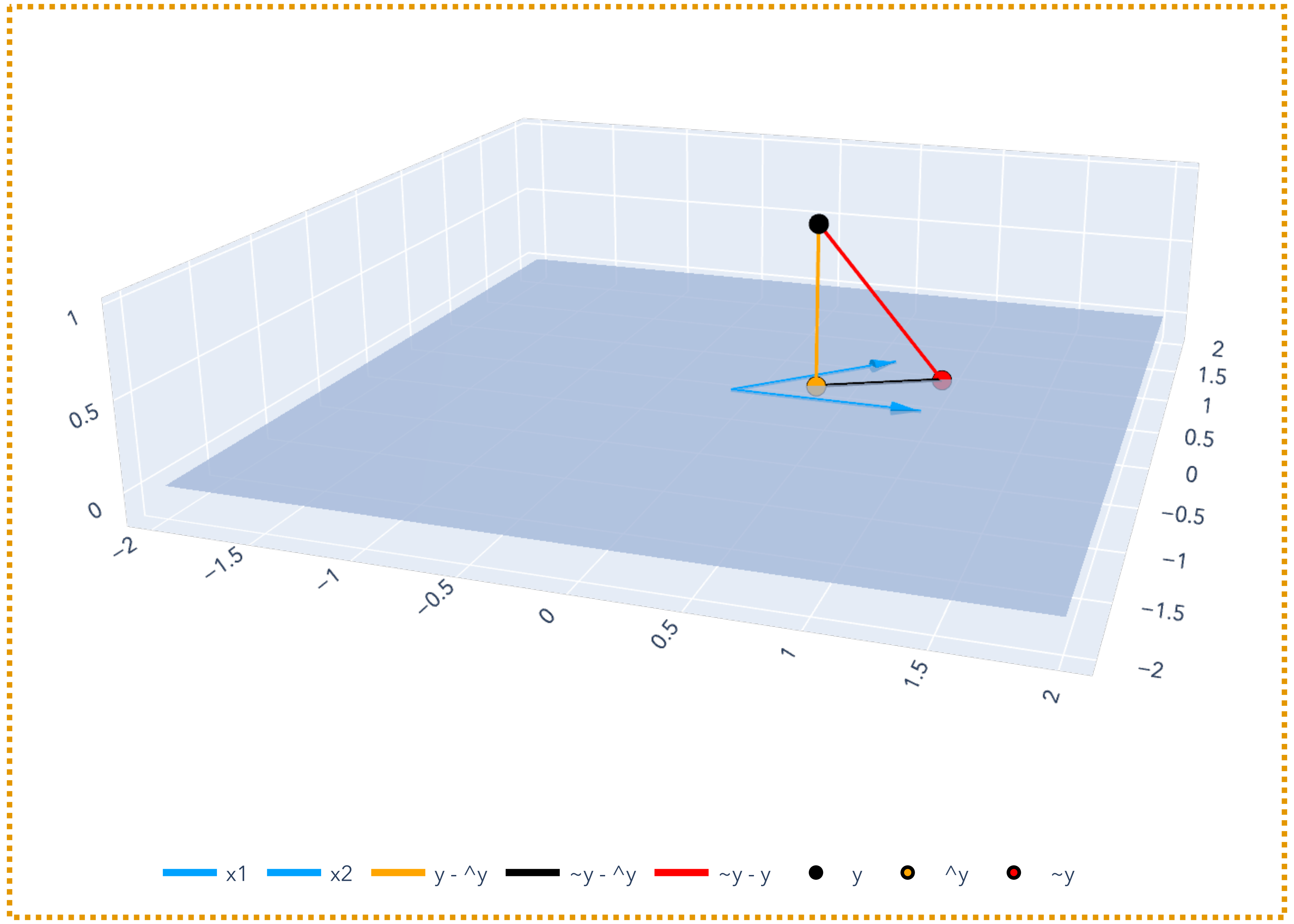


Least Squares

Second missing item: Pythagorean Theorem

Theorem (Projection minimizes distance). Let $\hat{\mathbf{y}} \in \mathrm{CS}(\mathbf{X})$ be the vector where $\hat{\mathbf{y}} - \mathbf{y}$ is orthogonal to any vector in $\mathrm{CS}(\mathbf{X})$ and let $\tilde{\mathbf{y}} \in \mathrm{CS}(\mathbf{X})$ be any other vector. Then

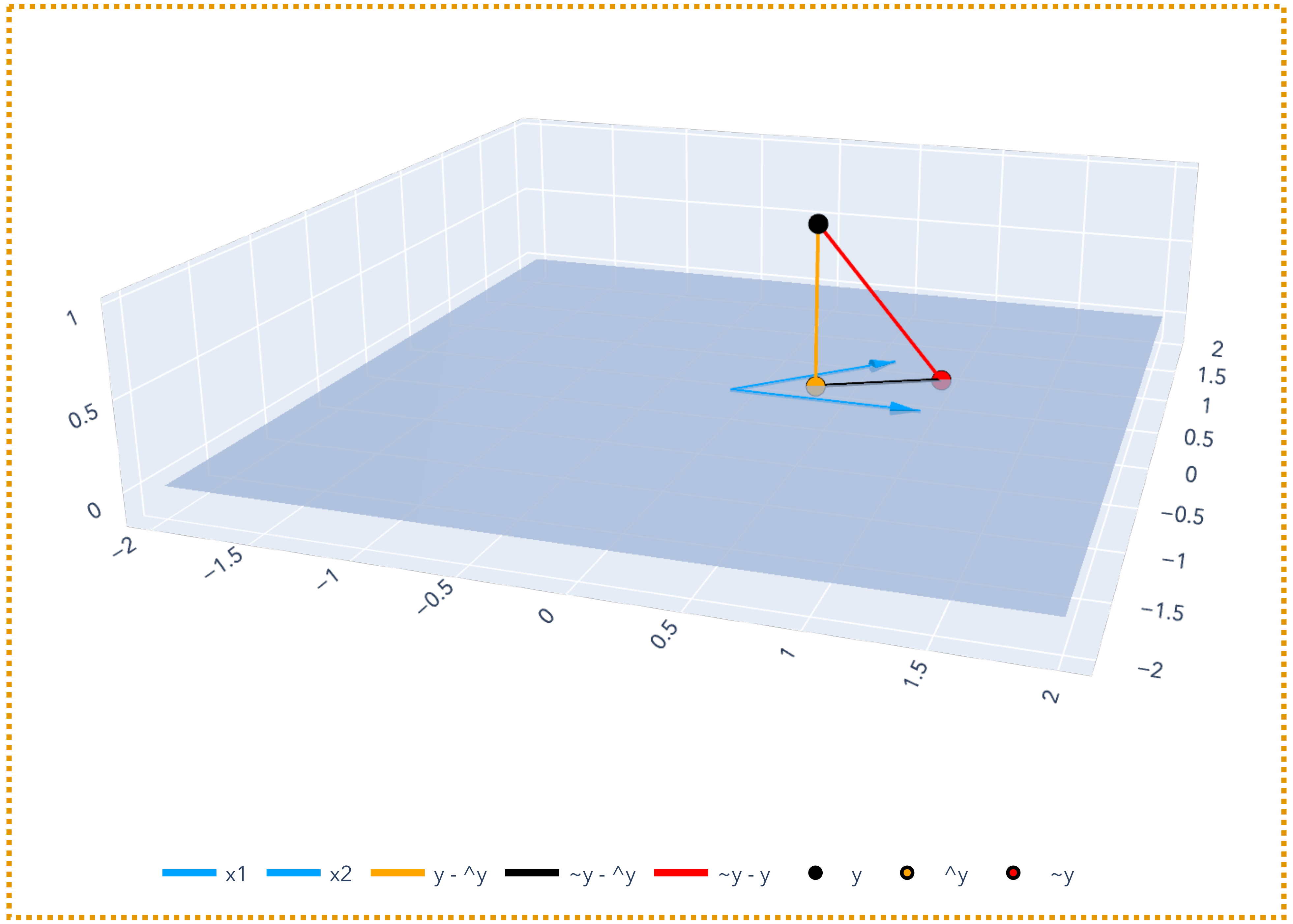
$$\|\hat{\mathbf{y}} - \mathbf{y}\|^2 \leq \|\tilde{\mathbf{y}} - \mathbf{y}\|^2.$$



Least Squares

Second missing item: Pythagorean Theorem

Theorem (Projection minimizes distance). Let $\hat{\mathbf{y}} \in \mathrm{CS}(\mathbf{X})$ be the vector where $\hat{\mathbf{y}} - \mathbf{y}$ is orthogonal to any vector in $\mathrm{CS}(\mathbf{X})$ and let $\tilde{\mathbf{y}} \in \mathrm{CS}(\mathbf{X})$ be any other vector. Then $||\hat{\mathbf{y}} - \mathbf{y}||^2 \leq ||\tilde{\mathbf{y}} - \mathbf{y}||^2$.



Proof. Because $\hat{\mathbf{y}} \in \mathrm{CS}(\mathbf{X})$ and $\tilde{\mathbf{y}} \in \mathrm{CS}(\mathbf{X})$ and $\mathrm{CS}(\mathbf{X})$ is a subspace, $\tilde{\mathbf{y}} - \hat{\mathbf{y}} \in \mathrm{CS}(\mathbf{X})$.

The vector $\hat{\mathbf{y}} - \mathbf{y}$ is orthogonal to any vector in $\mathrm{span}(\mathrm{col}(\mathbf{X}))$, so $\hat{\mathbf{y}} - \mathbf{y}$ is orthogonal to $\tilde{\mathbf{y}} - \hat{\mathbf{y}}$.

By the Pythagorean Theorem:

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

But because norms are always nonnegative,

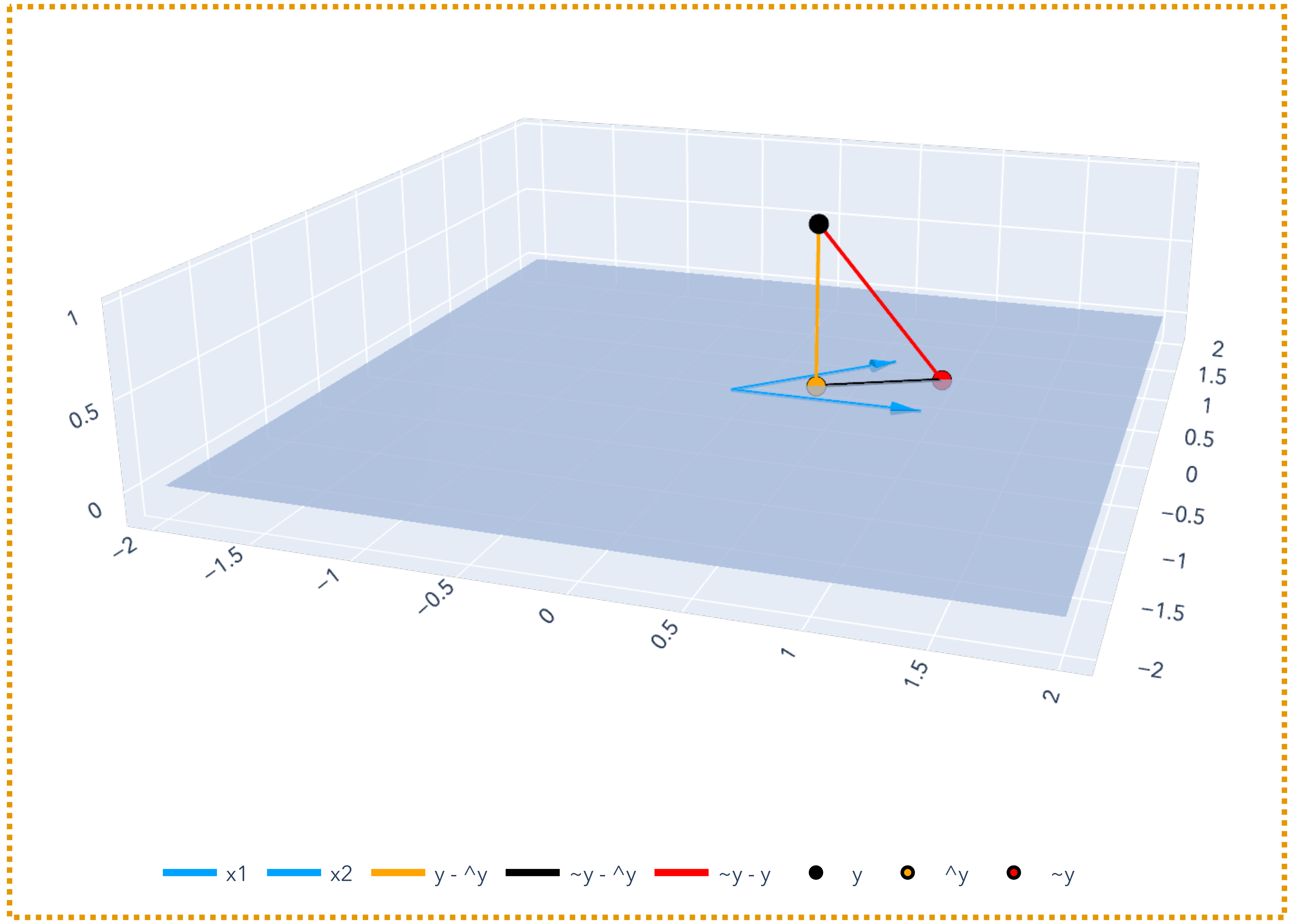
$$||\hat{\mathbf{y}} - \mathbf{y}||^2 \leq ||\tilde{\mathbf{y}} - \mathbf{y}||^2.$$

Least Squares

Second missing item: Pythagorean Theorem

Theorem (Projection minimizes distance). Let $\hat{\mathbf{y}} \in \mathrm{CS}(\mathbf{X})$ be the vector where $\hat{\mathbf{y}} - \mathbf{y}$ is orthogonal to any vector in $\mathrm{CS}(\mathbf{X})$ and let $\tilde{\mathbf{y}} \in \mathrm{CS}(\mathbf{X})$ be any other vector. Then

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



Least Squares

Summary

Use the principle of *least squares* to find the $\hat{\mathbf{w}} \in \mathbb{R}^d$ that minimizes

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

Using geometric intuition: $\hat{\mathbf{y}}$ *is the vector for which* $\hat{\mathbf{y}} - \mathbf{y}$ *is perpendicular to* $\mathrm{CS}(\mathbf{X})$.

By Pythagorean Theorem, any other vector $\tilde{\mathbf{y}} \in \mathrm{CS}(\mathbf{X})$ gives a larger error:

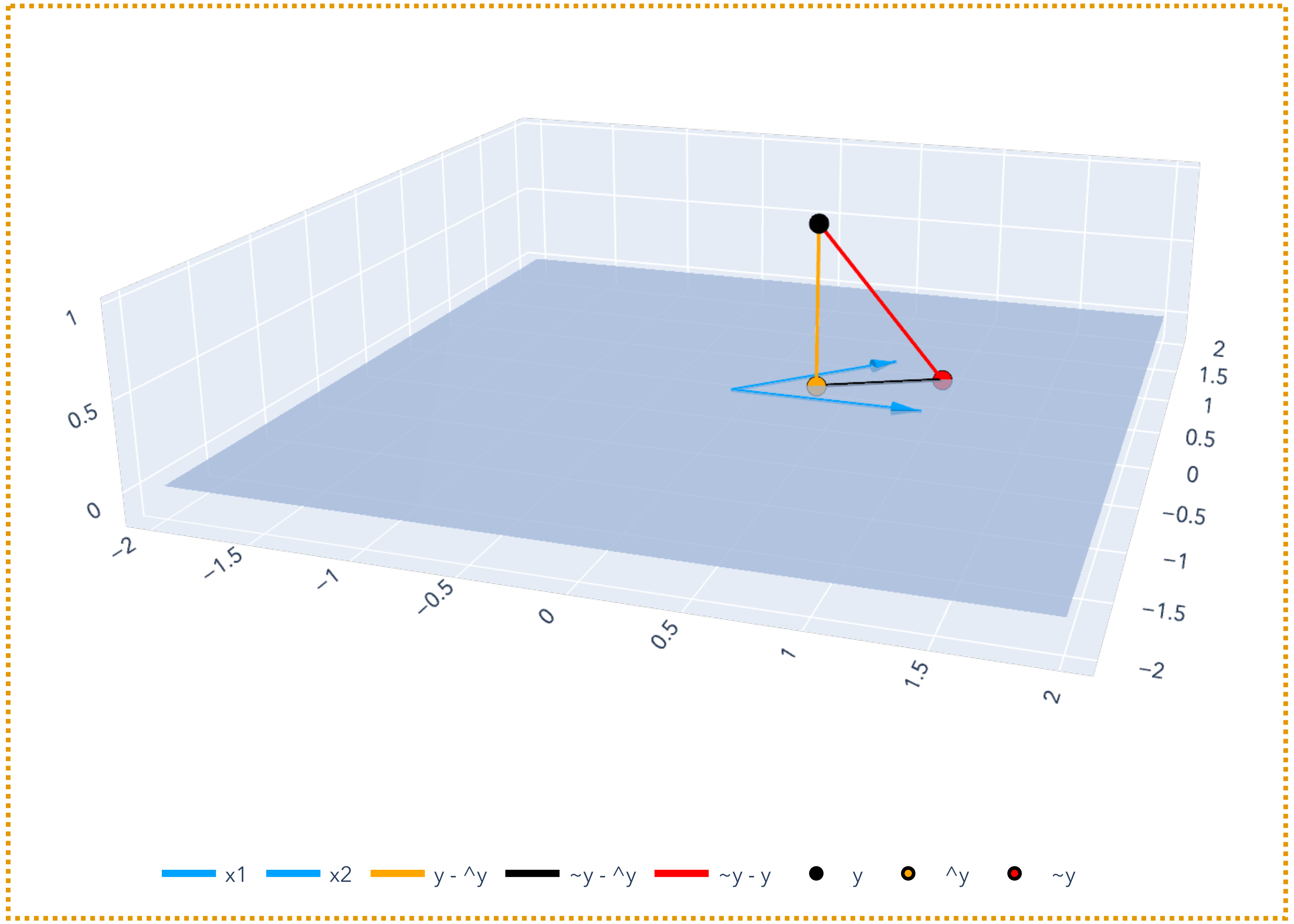
$$\|\hat{\mathbf{y}} - \mathbf{y}\|^2 \leq \|\tilde{\mathbf{y}} - \mathbf{y}\|^2.$$

Because $\hat{\mathbf{y}} - \mathbf{y}$ is perpendicular to $\mathrm{CS}(\mathbf{X})$, we obtain the *normal equations:*

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

If $n \geq d$ and $\mathrm{rank}(\mathbf{X}) = d$, then $\mathbf{X}^\top\mathbf{X}$ *is invertible*, and

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



Least Squares

Summary

Goal: Find the $\hat{\mathbf{w}} \in \mathbb{R}^d$ that minimizes

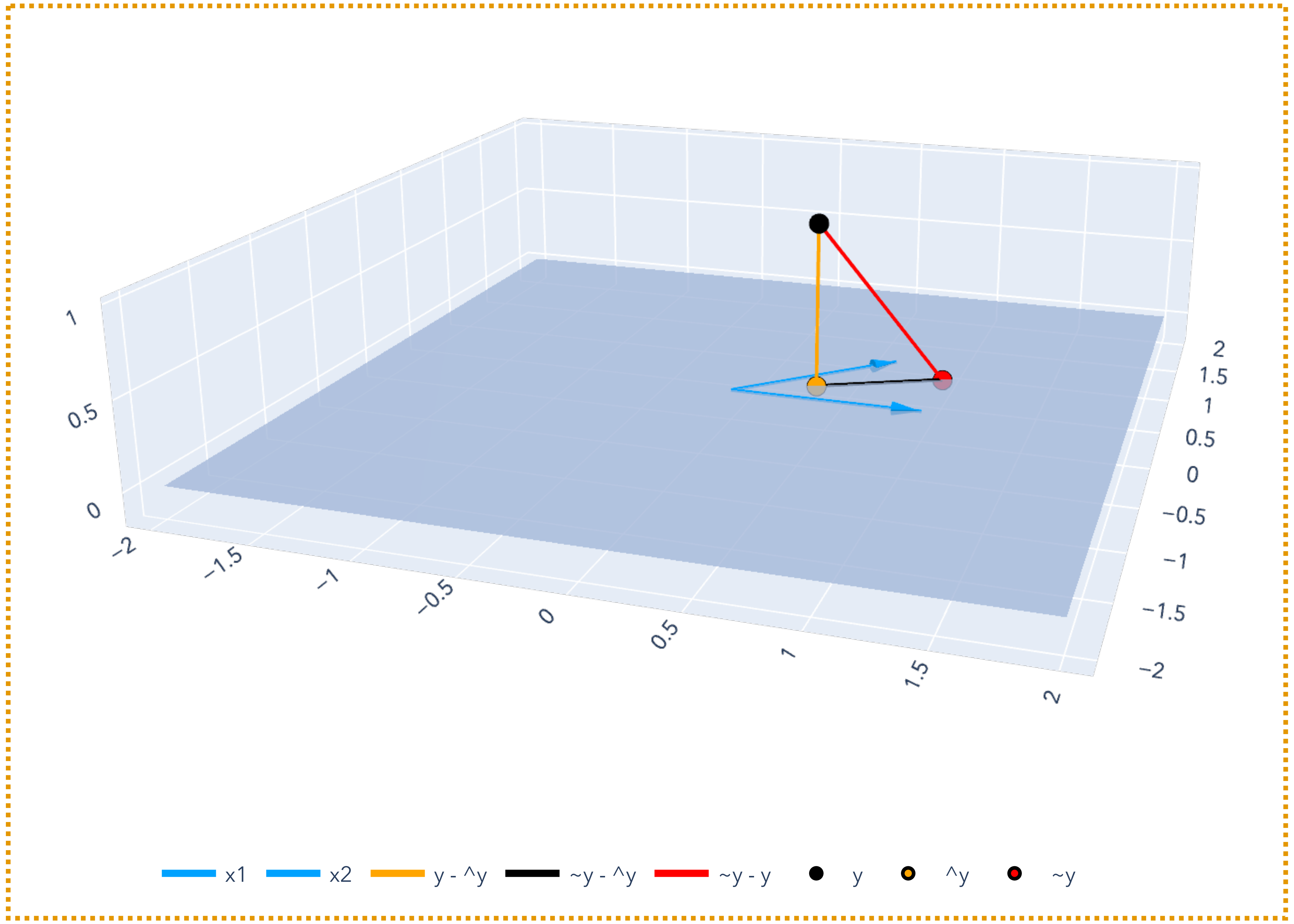
$$\|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2.$$

<u>Theorem (OLS).</u> If $n \geq d$ and $\text{rank}(\mathbf{X}) = d$, then:

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

To get predictions $\hat{\mathbf{y}} \in \mathbb{R}^n$:

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



Orthogonality

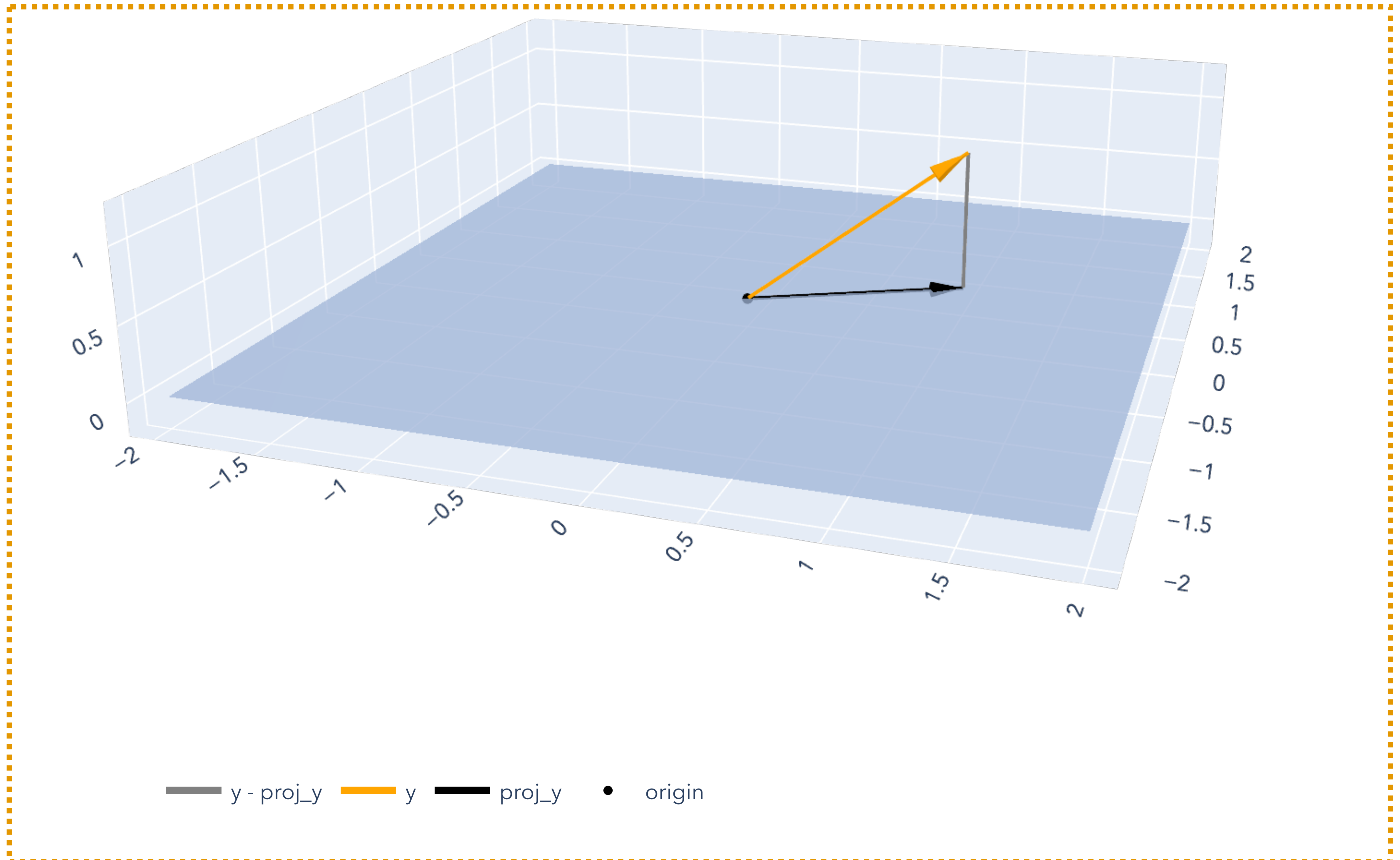
Projections

Projection

Idea: A vector's "shadow" on another set

For an arbitrary set $S \subseteq \mathbb{R}^n$, the projection of a vector $\mathbf{y} \in \mathbb{R}^n$ onto the set S is the closest vector $\hat{\mathbf{y}}$ in S to $\mathbf{y}$.

Denote this vector $\Pi_S(\mathbf{y}) := \hat{\mathbf{y}}$.



Projection

Projection of a vector onto an arbitrary set

For an arbitrary set $S \subseteq \mathbb{R}^n$, the projection of a vector $\mathbf{y} \in \mathbb{R}^n$ onto the set S is the closest vector $\hat{\mathbf{y}}$ in S to $\mathbf{y}$.

Denote this vector $\Pi_S(\mathbf{y}) := \hat{\mathbf{y}}$.

"Closest" in a Euclidean ("least squares") distance sense:

$$\Pi_S(\mathbf{y}) = \arg\min_{\hat{\mathbf{y}} \in S} \|\hat{\mathbf{y}} - \mathbf{y}\| = \|\hat{\mathbf{y}} - \mathbf{y}\|^2.$$

Projection

Projection of a vector onto a subspace

Let $\mathcal{X} \subseteq \mathbb{R}^n$ be a *subspace*, with the basis $\mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n$. Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be the matrix with $\mathbf{x}_1, \ldots, \mathbf{x}_d$ as its columns. *Any* point $\hat{\mathbf{y}} \in \mathcal{X}$ is a linear combination:

$$\begin{aligned} \hat{\mathbf{y}} &= w_1 \mathbf{x}_1 + \ldots + w_d \mathbf{x}_d \\ &= \mathbf{X}\mathbf{w} \end{aligned}$$

The projection of $\mathbf{y}$ onto $\mathcal{X}$ is:

$$\Pi_{\mathcal{X}}(\mathbf{y}) = \arg\min_{\hat{\mathbf{y}} \in \mathcal{X}} \|\hat{\mathbf{y}} - \mathbf{y}\|^2$$

Projection

Projection of a vector onto a subspace

Let $\mathscr{X} \subseteq \mathbb{R}^n$ be a *subspace*, with the basis $\mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n$. Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be the matrix with $\mathbf{x}_1, \ldots, \mathbf{x}_d$ as its columns. *Any* point $\hat{\mathbf{y}} \in \mathscr{X}$ is a linear combination:

$$
\begin{aligned}
\hat{\mathbf{y}} &= w_1 \mathbf{x}_1 + \ldots + w_d \mathbf{x}_d \\
&= \mathbf{X}\mathbf{w}
\end{aligned}
$$

This is equivalent to finding:

$$\hat{\mathbf{w}} = \underset{\hat{\mathbf{w}} \in \mathbb{R}^d}{\arg\min} \; \|\mathbf{X}\hat{\mathbf{w}} - \mathbf{y}\|^2$$

Least Squares as Projection

Projection Matrix

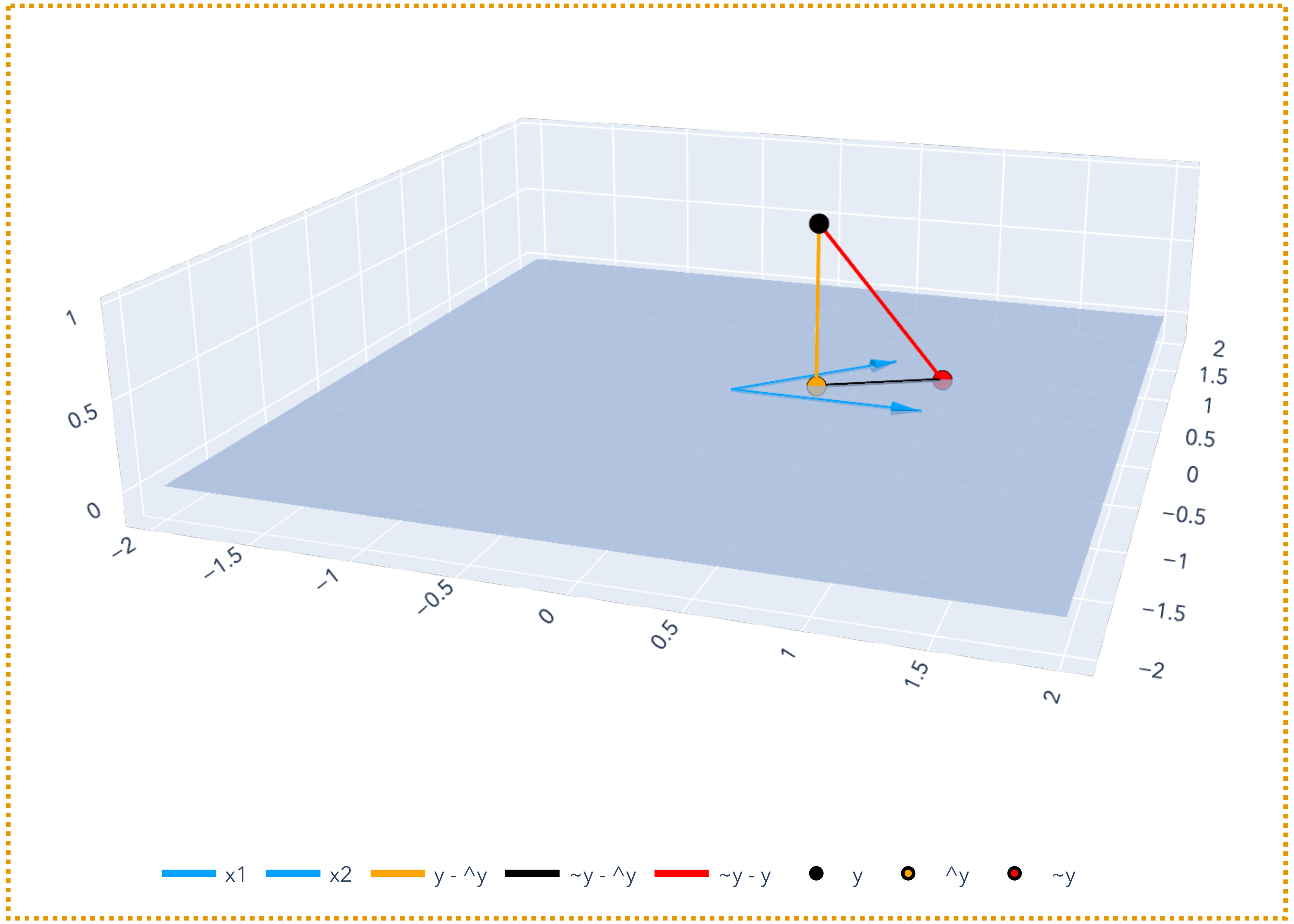
$$\hat{\mathbf{w}} = \arg\min_{\hat{\mathbf{w}} \in \mathbb{R}^d} \|\mathbf{X}\hat{\mathbf{w}} - \mathbf{y}\|^2$$

This is just least squares! By what we've learned…

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

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

Let $P_{\mathbf{X}} := \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \in \mathbb{R}^{n \times n}$ be the projection matrix for $\mathrm{span}(\mathrm{col}(\mathbf{X}))$.



Linearity

Review from linear algebra

Linearity is the central property in linear algebra. Cooking is typically linear.

Bacon, egg, cheese (on roll)	*Bacon, egg, cheese (on bagel)*	*Lox sandwich*
1 egg	1 egg	0 egg
1 slice of cheese	1 slice of cheese	0 slice of cheese
1 slice bacon	1 slice bacon	0 slice bacon
1 Kaiser roll	0 Kaiser roll	0 Kaiser roll
0 cream cheese	0 cream cheese	1 cream cheese
0 slices of lox	0 slices of lox	2 slices of lox
0 bagel	1 bagel	1 bagel

Linearity

Review from linear algebra

Linearity is the central property in linear algebra.

A function ("transformation") $T : \mathbb{R}^d \to \mathbb{R}^n$ is linear if T satisfies these two properties for any two vectors $\mathbf{a}, \mathbf{b} \in \mathbb{R}^d$:

$$T(\mathbf{a} + \mathbf{b}) = T(\mathbf{a}) + T(\mathbf{b})$$

$$T(c\mathbf{a}) = cT(\mathbf{a}) \text{ for any } c \in \mathbb{R}.$$

Linearity

Review from linear algebra

<u>**Example.**</u> Consider the function $T : \mathbb{R}^3 \to \mathbb{R}$, defined by:

$$T(\mathbf{x}) = 2x_1 + 3x_3.$$

Linearity

Review from linear algebra

Matrices also play by these rules. Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be a matrix and let $\mathbf{w}, \mathbf{v} \in \mathbb{R}^d$ be vectors.

$$\mathbf{X}(\mathbf{w} + \mathbf{v}) = \mathbf{X}\mathbf{w} + \mathbf{X}\mathbf{v}$$

$\mathbf{X}(c\mathbf{w}) = c(\mathbf{X}\mathbf{w})$ for any $c \in \mathbb{R}$.

Linearity

Review from linear algebra

<u>Theorem (Equivalence of linear transformations and matrices).</u>

Any linear transformation $T : \mathbb{R}^d \to \mathbb{R}^n$ has a corresponding matrix $\mathbf{A}_T \in \mathbb{R}^{n \times d}$ such that:

$$T(\mathbf{x}) = \mathbf{A}_T \mathbf{x}.$$

Any matrix $\mathbf{A} \in \mathbb{R}^{n \times d}$ has a corresponding linear transformation $T_{\mathbf{A}} : \mathbb{R}^d \to \mathbb{R}^n$ such that:

$$T_{\mathbf{A}}(\mathbf{x}) = \mathbf{A}\mathbf{x}.$$

Linearity

Review from linear algebra

$$T(\mathbf{x}) = \mathbf{A}_T\mathbf{x} \text{ and } T_{\mathbf{A}}(\mathbf{x}) = \mathbf{A}\mathbf{x}$$

This means that *matrix-vector multiplication is the same as applying a linear transformation*.

So one way of thinking of a matrix is an "action" applied to vectors.

Least Squares as Projection

Projection Matrix

Let $\mathscr{X} \subseteq \mathbb{R}^d$ be a *subspace* with basis $\mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n$. If $\mathbf{x}_1, \ldots, \mathbf{x}_d$ are linearly independent, making up the matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$,

$$\boxed{P_{\mathbf{X}} := \mathbf{X}(\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top} \in \mathbb{R}^{n \times n}$$

Encodes an *action* on vectors!

is the projection matrix onto $\mathscr{X}$.

To project a vector $\mathbf{y} \in \mathbb{R}^n$ onto $\mathscr{X}$, compute:

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

Least Squares

Orthonormal Bases and Projection

Norms and Inner Products

Unit Vectors

A vector $\mathbf{v} \in \mathbb{R}^d$ is a unit vector if $\|\mathbf{v}\| = 1$.

We can convert any vector into a unit vector by dividing itself by its norm:

$$\frac{\mathbf{v}}{\|\mathbf{v}\|}$$

Orthonormal Basis

“Good” Bases

How should we represent a subspace?

Take, for example, the subspace $\mathcal{S} = \{\mathbf{v} \in \mathbb{R}^3 : v_3 = 0\}$.

Orthonormal Basis

"Good" Bases

$$\mathcal{S} = \{\mathbf{v} \in \mathbb{R}^3 : v_3 = 0\}$$

Attempt 1: Use the span of a set of vectors: $\operatorname{span}\left(\begin{bmatrix}2\\1\\0\end{bmatrix}, \begin{bmatrix}0\\1\\0\end{bmatrix}, \begin{bmatrix}2\\3\\0\end{bmatrix}\right).$

Attempt 2: Use the span of a set of linearly independent vectors (a basis):

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

Attempt 3: Use the span of an orthonormal set of vectors (an orthonormal basis):

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

Orthonormal Basis

"Good" Bases

$$\mathcal{S} = \{\mathbf{v} \in \mathbb{R}^3 : v_3 = 0\}$$

$$\operatorname{span}\left(\begin{bmatrix}2\\1\\0\end{bmatrix}, \begin{bmatrix}0\\1\\0\end{bmatrix}, \begin{bmatrix}2\\3\\0\end{bmatrix}\right) \qquad \operatorname{span}\left(\begin{bmatrix}2\\1\\0\end{bmatrix}, \begin{bmatrix}0\\1\\0\end{bmatrix}\right) \qquad \operatorname{span}\left(\begin{bmatrix}1\\0\\0\end{bmatrix}, \begin{bmatrix}0\\1\\0\end{bmatrix}\right)$$

Orthonormal Basis

Definition

A set of vectors $\mathbf{u}_1, \ldots, \mathbf{u}_n \in \mathcal{S}$ is an orthonormal basis for the subspace $\mathcal{S}$ if they are a basis for $\mathcal{S}$ and, additionally:

$$\langle \mathbf{u}_i, \mathbf{u}_j \rangle = 0 \text{ for } i \neq j.$$

$$\|\mathbf{u}_i\| = 1 \text{ for } i \in [n].$$

Orthonormal Basis

Orthogonal Matrices

A square matrix $\mathbf{U} \in \mathbb{R}^{d \times d}$ is an orthogonal matrix if its columns $\mathbf{u}_1, \ldots, \mathbf{u}_d \in \mathbb{R}^d$ are orthogonal unit vectors:

$$\langle \mathbf{u}_i, \mathbf{u}_j \rangle = 0 \text{ for } i \neq j.$$

$$\|\mathbf{u}_i\| = 1 \text{ for } i \in [d].$$

These form an orthonormal basis for $\mathrm{span}(\mathrm{col}(\mathbf{U}))$.

Its rows are also orthogonal.

Orthonormal Basis

Orthogonal Matrices

A matrix $\mathbf{U} \in \mathbb{R}^{n \times d}$ is an semi-orthogonal matrix if its columns $\mathbf{u}_1, \ldots, \mathbf{u}_d \in \mathbb{R}^n$ are orthogonal unit vectors:

$$\langle \mathbf{u}_i, \mathbf{u}_j \rangle = 0 \text{ for } i \neq j.$$

$$\|\mathbf{u}_i\| = 1 \text{ for } i \in [d].$$

These form an orthonormal basis for $\text{span}(\text{col}(\mathbf{U}))$.

Orthonormal Basis

Properties of Orthogonal Matrices

Let a square matrix $\mathbf{U} \in \mathbb{R}^{d \times d}$ be an orthogonal matrix. Then:

$\mathbf{U}$ is its own inverse: $\mathbf{U}^\top \mathbf{U} = \mathbf{U}\mathbf{U}^\top = \mathbf{I}$.

$\mathbf{U}$ is length-preserving: $\|\mathbf{U}\mathbf{v}\| = \|\mathbf{v}\|$.

Orthonormal Basis

Properties of Orthogonal Matrices

Let matrix $\mathbf{U} \in \mathbb{R}^{n \times d}$ be an semi-orthogonal matrix. Then:

$\mathbf{U}$ is its own left inverse: $\mathbf{U}^\top \mathbf{U} = \mathbf{I}$.

$\mathbf{U}$ is length-preserving: $\|\mathbf{U}\mathbf{v}\| = \|\mathbf{v}\|$.

Orthogonal Bases in Least Squares

What if we had an orthogonal basis?

A basis is just a “language” for representing vectors in a subspace. For example, consider the subspace $\mathcal{S} = \{\mathbf{v} \in \mathbb{R}^3 : v_3 = 0\}$ and the vector

$$\hat{\mathbf{y}} = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$$

Basis 1: $\left\{ \begin{bmatrix} 2 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \right\}$

Orthogonal Bases in Least Squares

What if we had an orthogonal basis?

A basis is just a "language" for representing vectors in a subspace. For example, consider the subspace $\mathcal{S} = \{\mathbf{v} \in \mathbb{R}^3 : v_3 = 0\}$ and the vector

$$\hat{\mathbf{y}} = \begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}$$

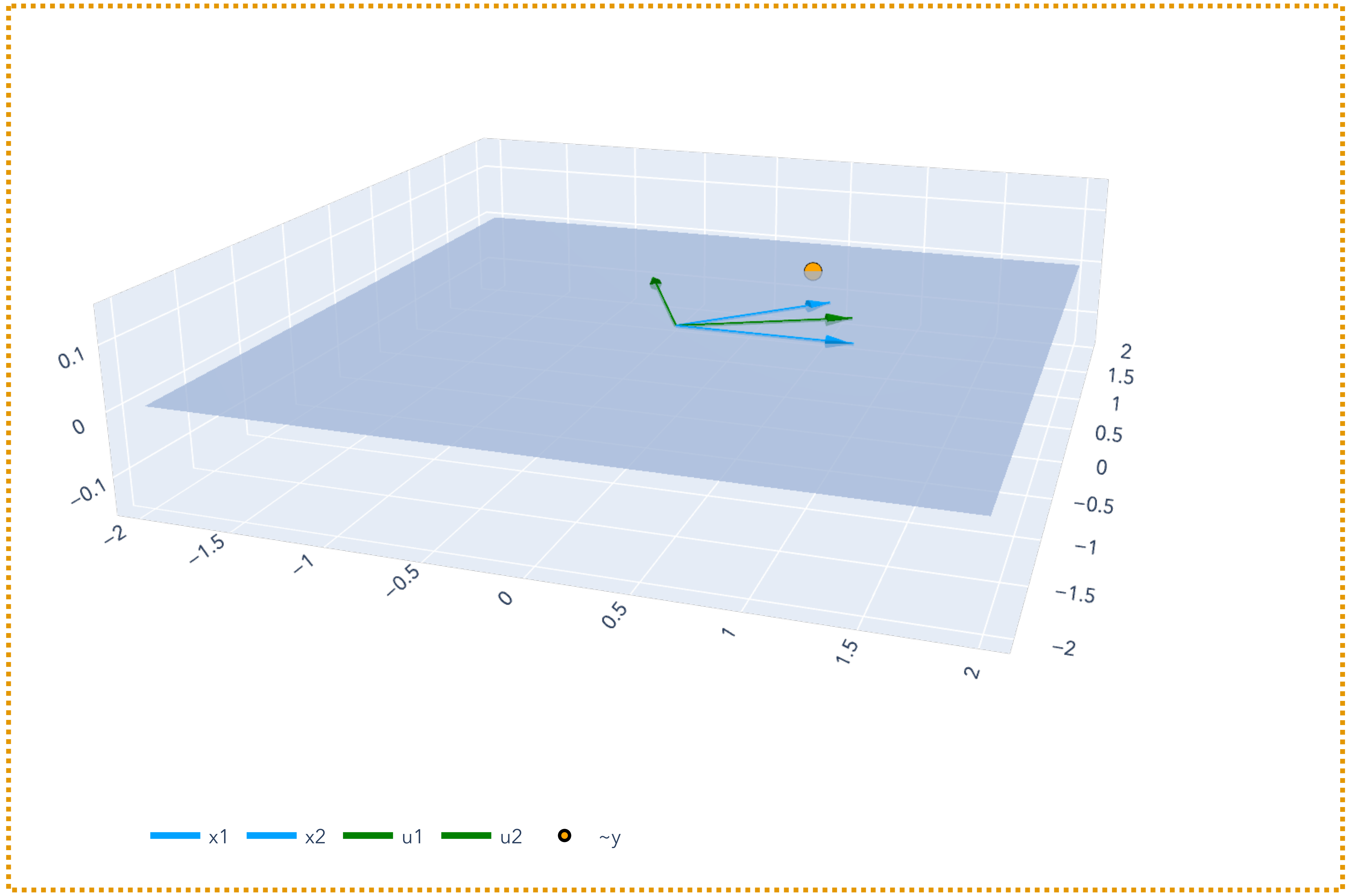
Basis 2: $\left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \right\}$

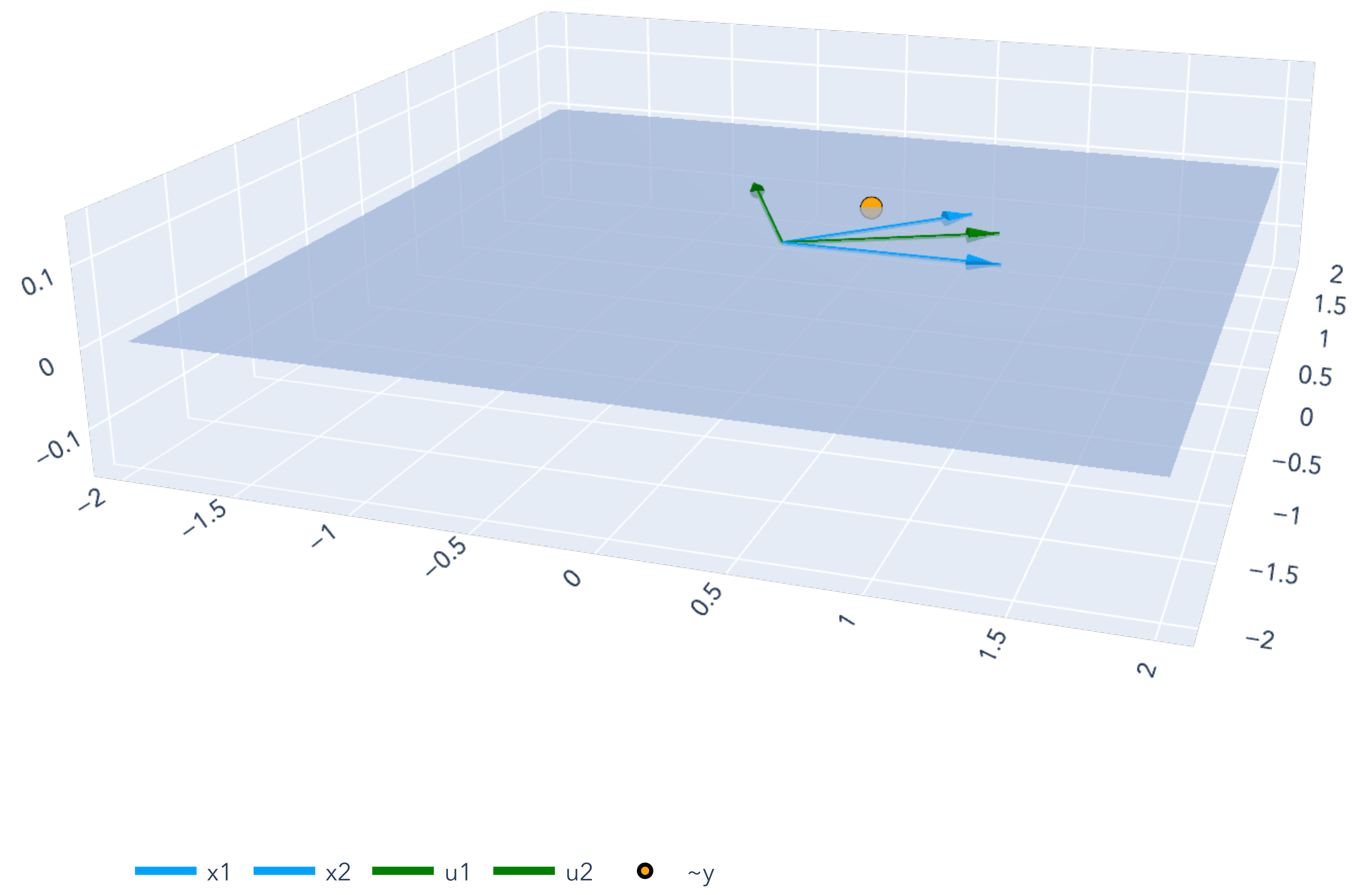
Orthogonal Bases in Least Squares

What if we had an orthogonal basis?

Every subspace $\mathscr{X} \subseteq \mathbb{R}^n$ has many choices of bases.

Some are better than others.





Orthogonal Bases in Least Squares

What if we had an orthogonal basis?

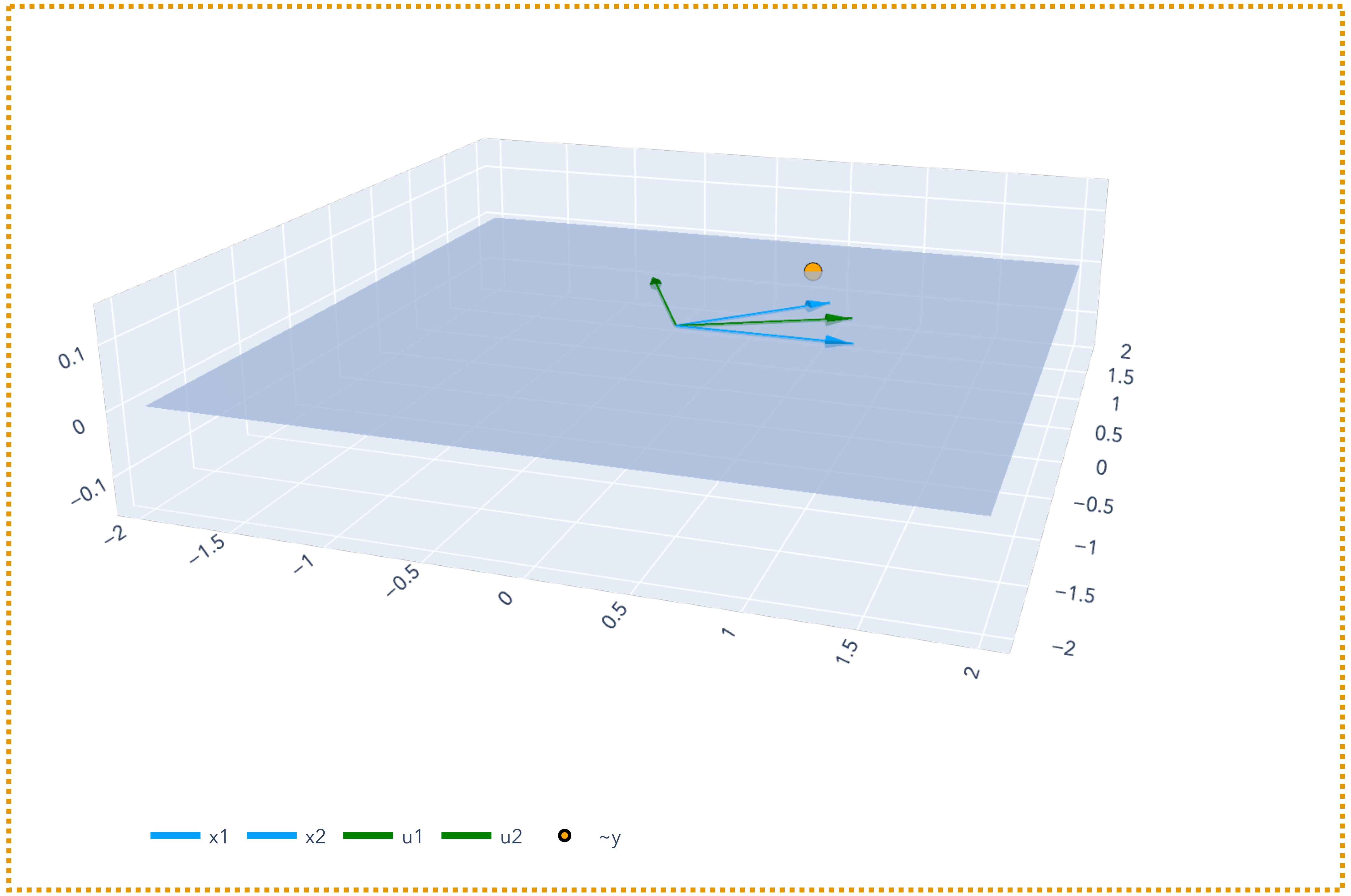
Let $\mathscr{X} \subseteq \mathbb{R}^n$ be a subspace, with $\dim(\mathscr{X}) = d$.

One basis: $\mathbf{x}_1, \ldots, \mathbf{x}_d \in \mathbb{R}^n$, with matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$.

Another basis: $\mathbf{u}_1, \ldots, \mathbf{u}_d \in \mathbb{R}^n$, with matrix $\mathbf{U} \in \mathbb{R}^{n \times d}$.

Then,

$$\mathscr{X} = \mathrm{CS}(\mathbf{U}) = \mathrm{CS}(\mathbf{X}).$$



Orthogonal Bases in Least Squares

What if we had an orthogonal basis?

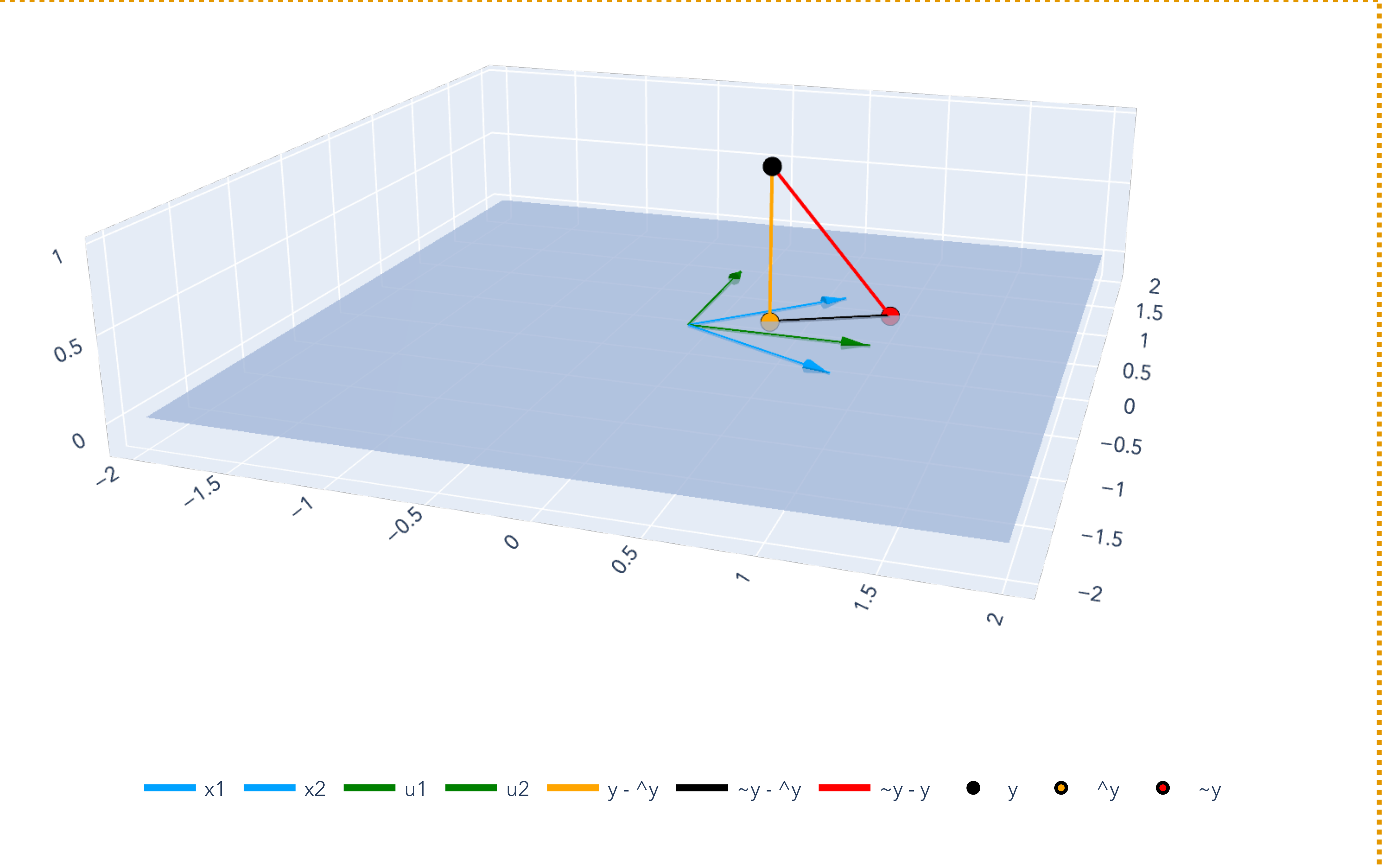
Let $\mathscr{X} \subseteq \mathbb{R}^n$ be a subspace, with $\dim(\mathscr{X}) = d$.

$$\mathscr{X} = \mathrm{CS}(\mathbf{U}) = \mathrm{CS}(\mathbf{X}).$$

Therefore, for any $\hat{\mathbf{y}} \in \mathscr{X}$, we can write:

$$\hat{\mathbf{y}} = \mathbf{X}\hat{\mathbf{w}} = \mathbf{U}\hat{\mathbf{w}}_{onb}.$$

Both $\hat{\mathbf{w}}, \hat{\mathbf{w}}_{onb} \in \mathbb{R}^d$ are valid ways to "represent" $\hat{\mathbf{y}}$.



Orthogonal Bases in Least Squares

What if we had an orthogonal basis?

How do we find $\hat{\mathbf{w}}_{onb} \in \mathbb{R}^d$ in $\hat{\mathbf{y}} = \mathbf{U}\hat{\mathbf{w}}_{onb}$?

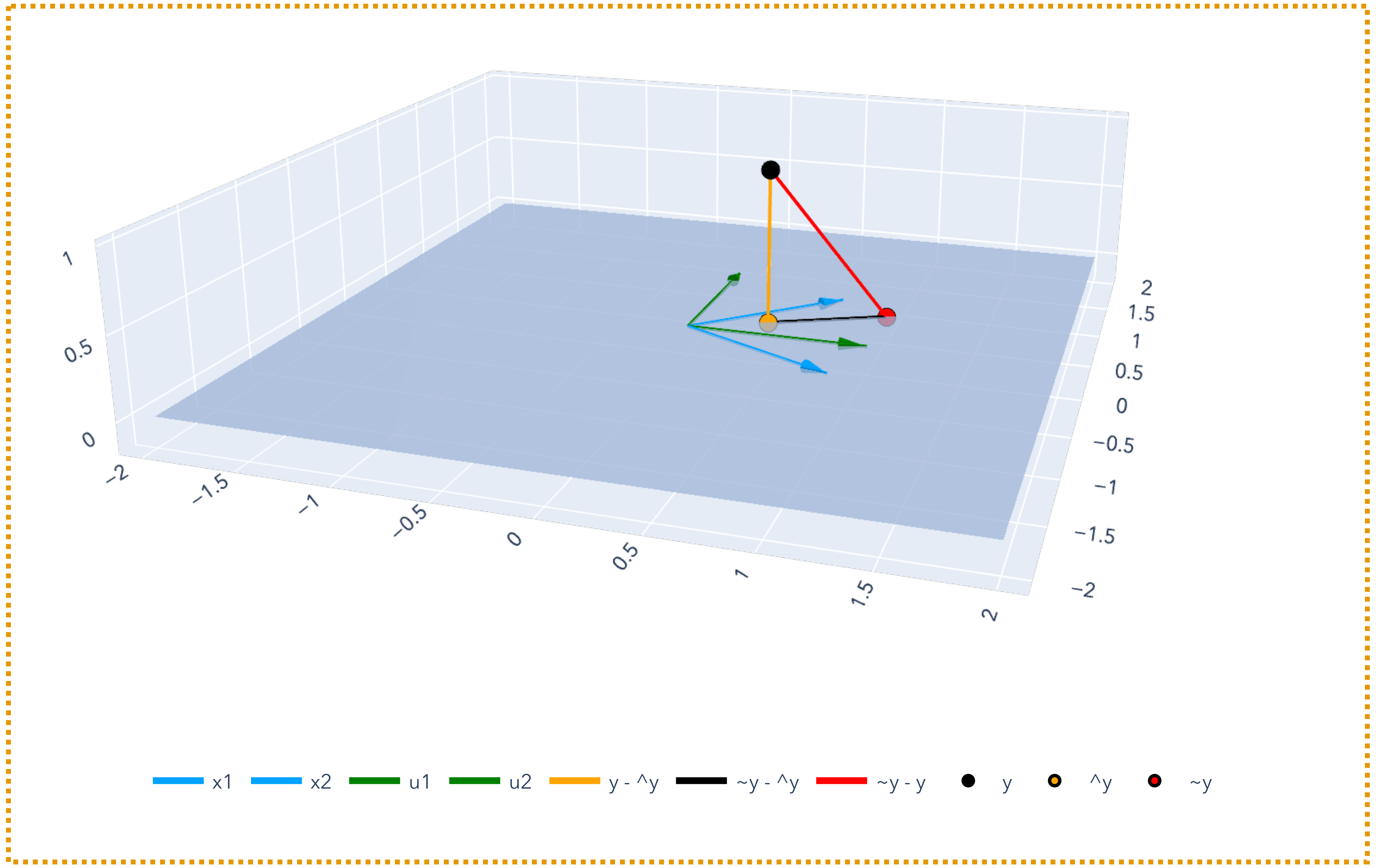
Least squares!

$$\hat{\mathbf{w}}_{onb} = \underset{\hat{\mathbf{w}}_{onb} \in \mathbb{R}^d}{\arg\min} \; \|\mathbf{y} - \mathbf{U}\hat{\mathbf{w}}_{onb}\|^2$$

The columns of $\mathbf{U}$ give an ONB for $\mathscr{X}$…

$$\hat{\mathbf{w}}_{onb} = (\mathbf{U}^\top\mathbf{U})^{-1}\mathbf{U}^\top\mathbf{y}$$

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



Orthonormal Basis

Why do we like an orthogonal basis?

Let $\mathscr{X}$ be a subspace. Let $\Pi_{\mathscr{X}}(\mathbf{y}) = \arg\min_{\hat{\mathbf{y}} \in \mathscr{X}} \|\hat{\mathbf{y}} - \mathbf{y}\|^2$ be the projection of $\mathbf{y}$ onto $\mathscr{X}$.

For an arbitrary matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ with $\mathrm{CS}(\mathbf{X}) = \mathscr{X}$,

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

For a *semi-orthogonal matrix* $\mathbf{U} \in \mathbb{R}^{n \times d}$ with $\mathrm{CS}(\mathbf{U}) = \mathscr{X}$,

$$\hat{\mathbf{w}}_{onb} = \mathbf{U}^\top \mathbf{y} \text{ and } \hat{\mathbf{y}} = \mathbf{U}\mathbf{U}^\top \mathbf{y}.$$

Much simpler – no inverse operations!

Orthonormal Basis

Why do we like an orthogonal basis?

Theorem (Projection with orthogonal matrices). Let $\mathscr{X} \subseteq \mathbb{R}^n$ be a subspace and let $\mathbf{u}_1, \ldots, \mathbf{u}_d \in \mathbb{R}^n$ be an orthonormal basis for $\mathscr{X}$, with semi-orthogonal matrix $\mathbf{U} \in \mathbb{R}^{n \times d}$. For any $\mathbf{y} \in \mathbb{R}^n$, the projection of $\mathbf{y}$ onto $\mathscr{X}$, i.e.

$$\Pi_{\mathscr{X}}(\mathbf{y}) = \arg\min_{\hat{\mathbf{y}} \in \mathscr{X}} \|\hat{\mathbf{y}} - \mathbf{y}\|^2$$

is given by

$$\Pi_{\mathscr{X}}(\mathbf{y}) = \mathbf{U}\mathbf{U}^\top \mathbf{y}.$$

Recap

Lesson Overview

Regression. Fill in gaps from last time: invertibility and Pythagorean theorem.

Subspaces. Subsets of $\mathcal{S} \subseteq \mathbb{R}^n$ where we "stay inside" when performing linear combinations of vectors.

Bases. A "language" to describe all vectors in a subspace.

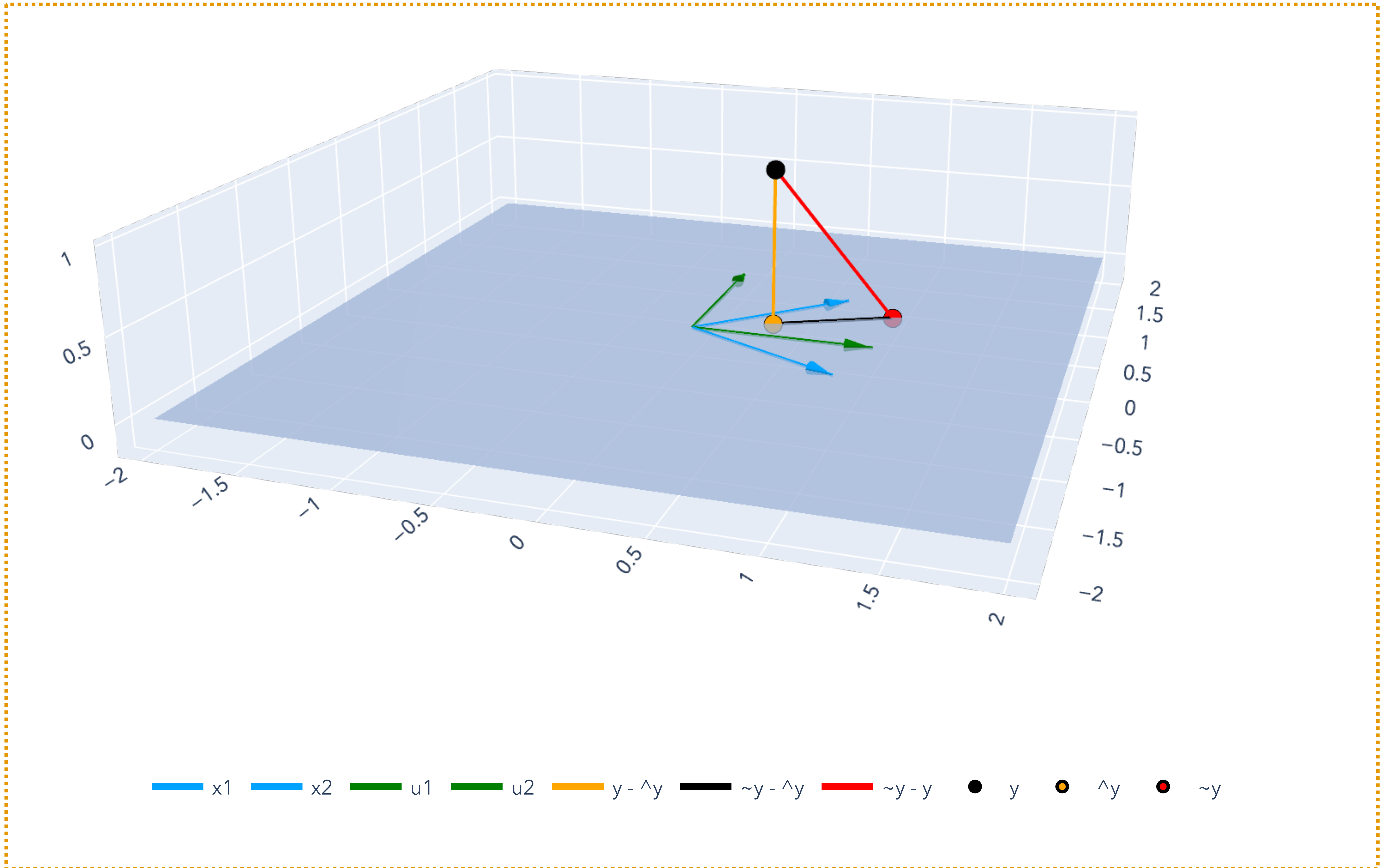
Orthogonality. Orthonormal bases are "good" bases to work with.

Projection. Formal definition of projection and the relationship between projection and least squares.

Least squares with orthonormal bases. If we have an orthonormal basis for $\mathbf{CS}(\mathbf{X})$, least squares becomes much simpler.

Lesson Overview

Big Picture: Least Squares



Lesson Overview

Big Picture: Gradient Descent