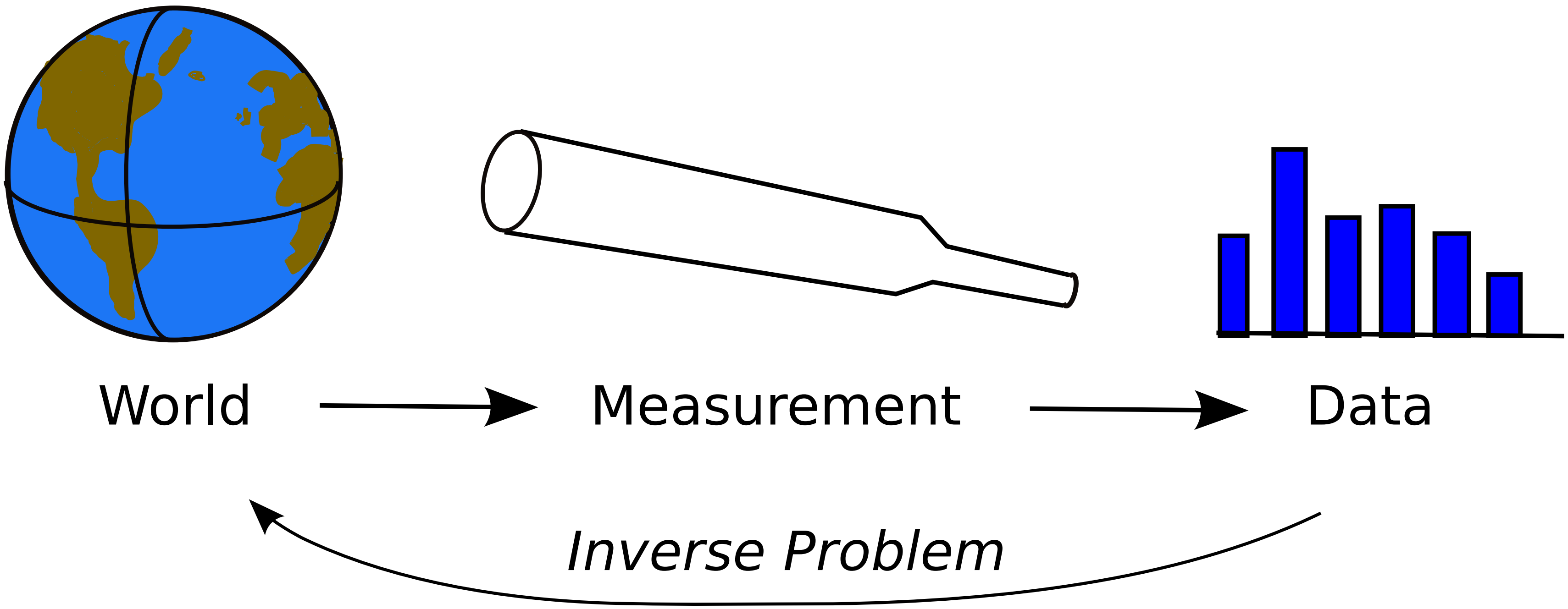
Advanced Machine Learning

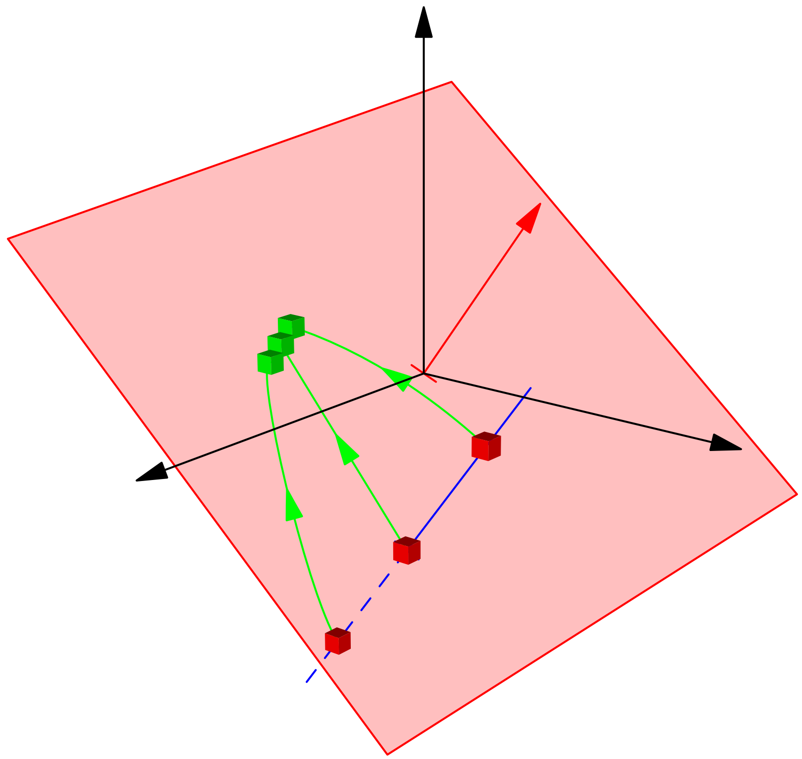
Understand Mappings



Mappings, Eigenvectors

Outline

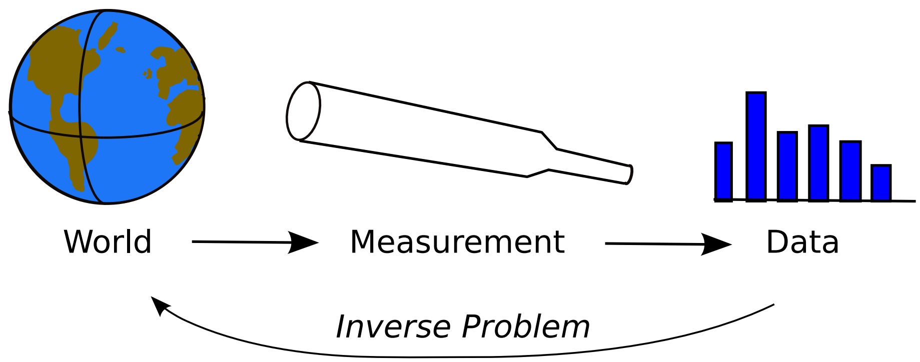
1. **Mappings**
2. Linear Maps
3. Eigenvectors



Transforming Data

- In the last lecture we spent time developing a sophisticate view of vector spaces and operators

- At a mathematical level machine learning can be viewed as performing an inverse mapping



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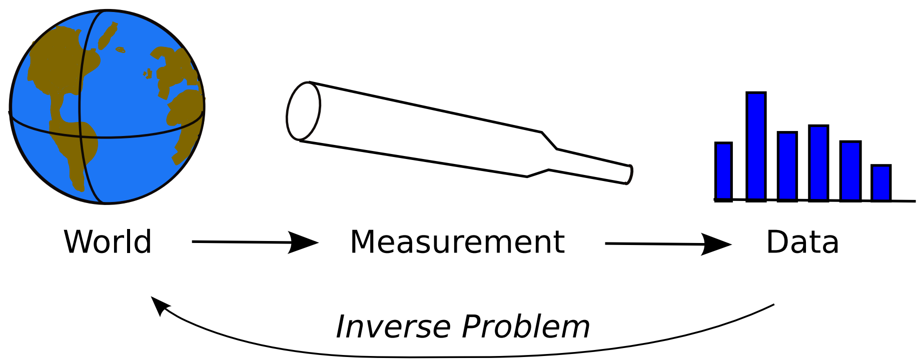

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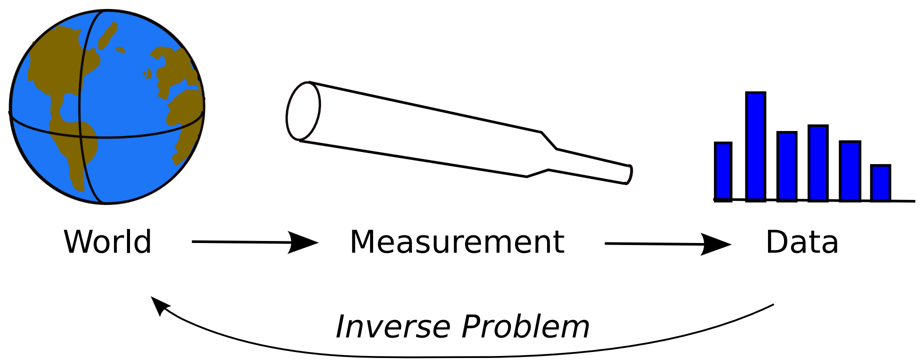

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Inverse Problems

- Given m observations $\{(\boldsymbol{x}_k, y_k) | k = 1, \ldots, m\}$ and p unknown $\boldsymbol{w} = (w_1, w_2, \ldots w_p)$ such that $\boldsymbol{x}_k^\mathsf{T} \boldsymbol{w} = y_k$ then to find $\boldsymbol{w}$
- Define the *design matrix* as the matrix of feature vectors

$$\mathbf{X} = \begin{pmatrix} \boldsymbol{x}_1^\mathsf{T} \\ \boldsymbol{x}_2^\mathsf{T} \\ \ldots \\ \boldsymbol{x}_m^\mathsf{T} \end{pmatrix} = \begin{pmatrix} x_{11} & x_{12} & \cdots & x_{1p} \\ x_{21} & x_{22} & \cdots & x_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m1} & x_{m2} & \cdots & x_{mp} \end{pmatrix}$$

- and the target vector $\boldsymbol{y} = (y_1, y_2, \cdots, y_m)^\mathsf{T}$
- Then if $m = p$ we have $\boldsymbol{y} = \mathbf{X}\boldsymbol{w}$ or $\boldsymbol{w} = \mathbf{X}^{-1}\boldsymbol{y}$

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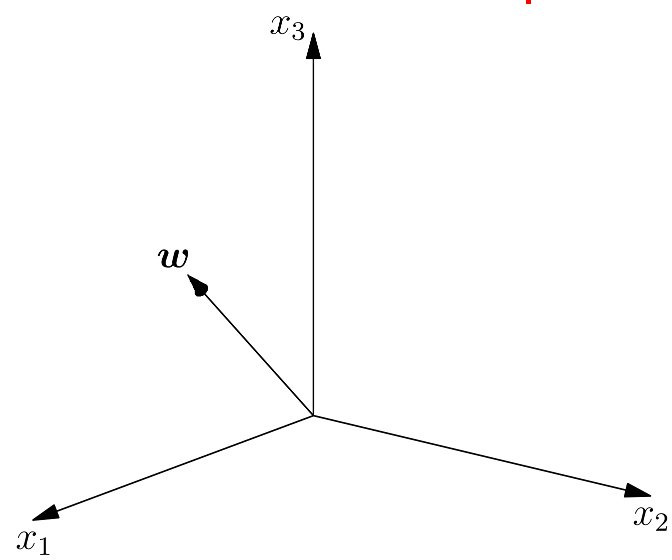
- $y_k = \boldsymbol{x}_k^\mathsf{T} \boldsymbol{w}$ depends on distance from separating plane



- If $m > p$ then $\mathbf{X}$ isn't square so doesn't have an inverse
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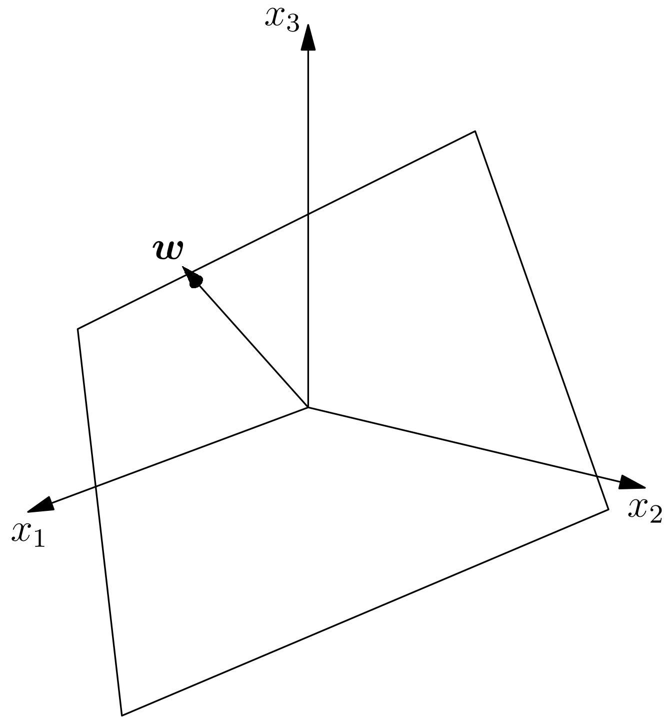

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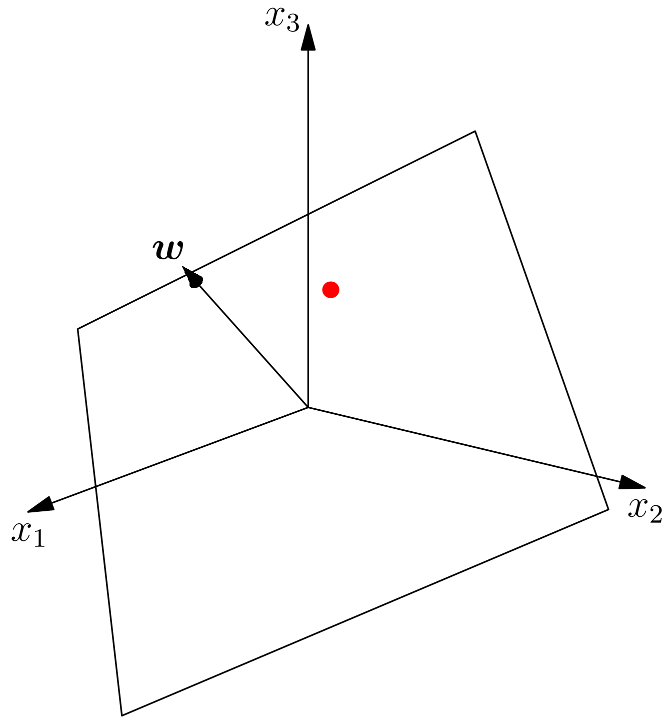

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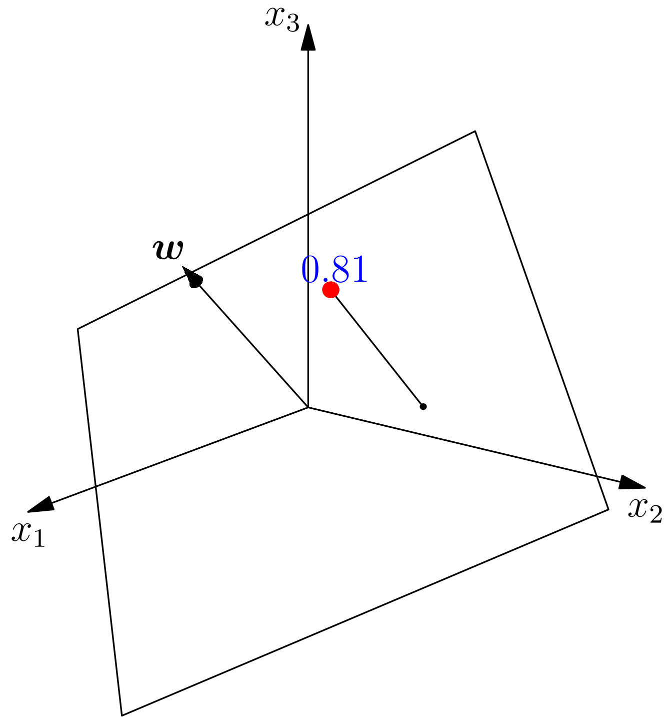

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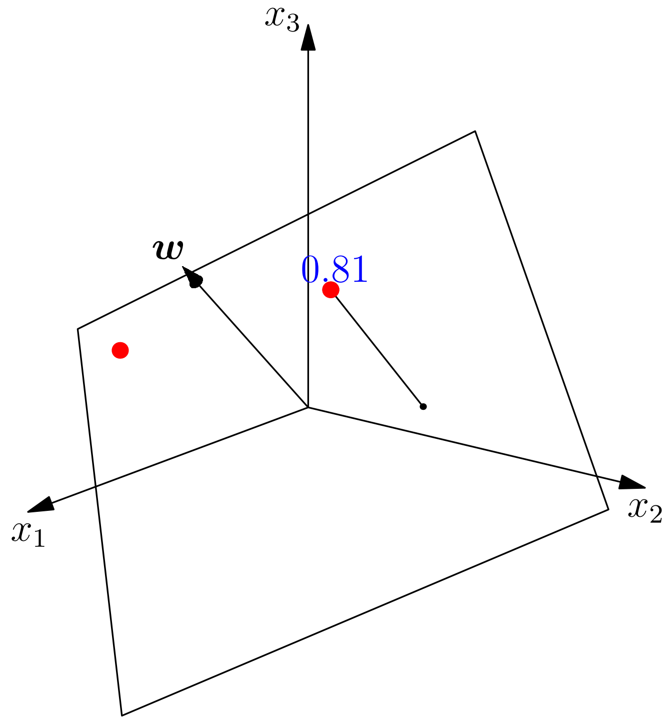

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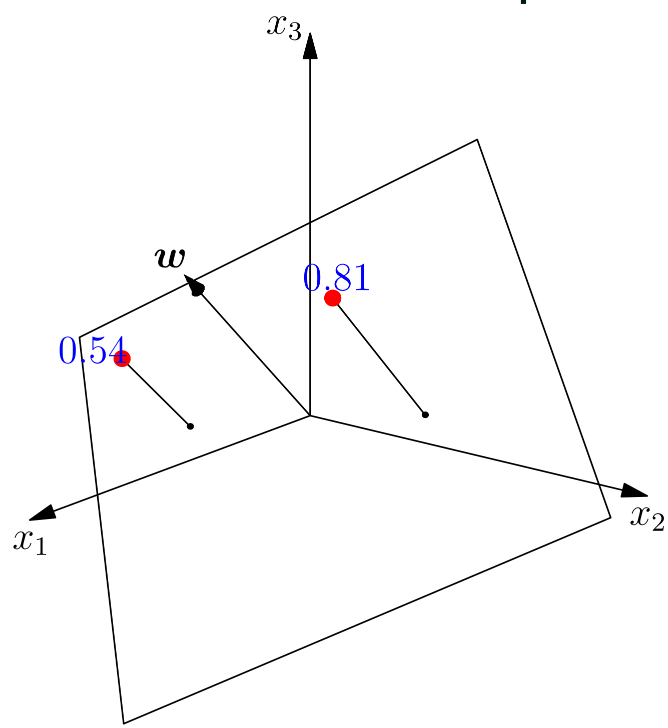

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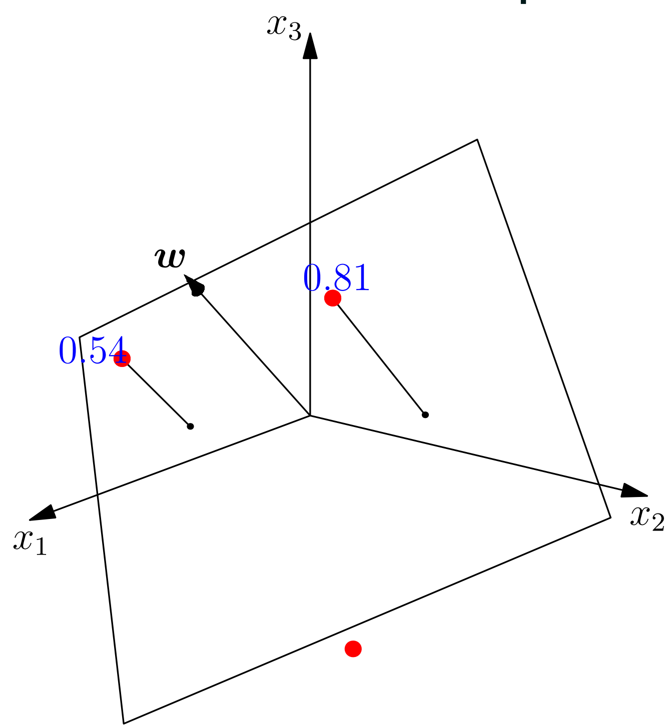

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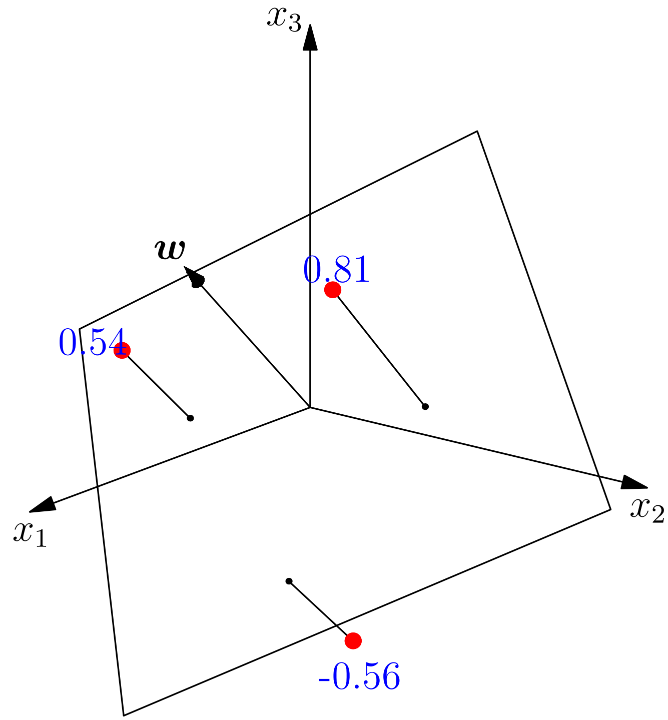

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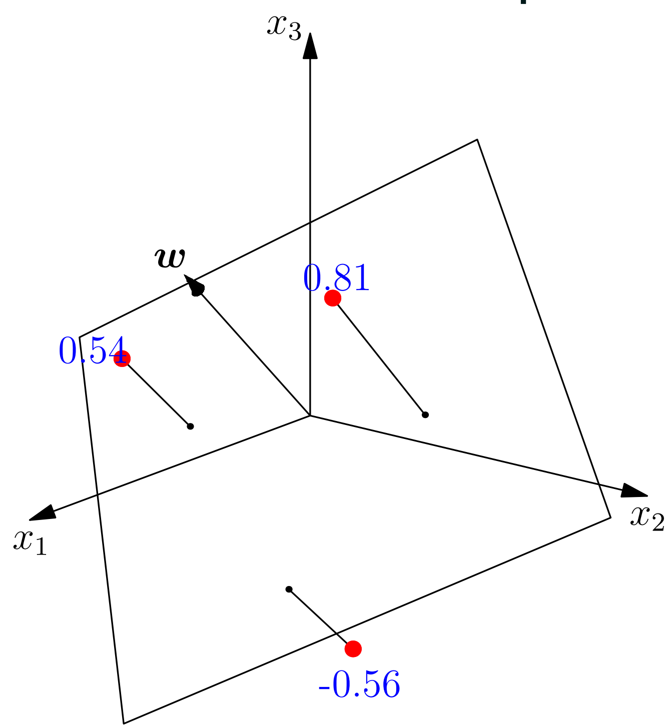

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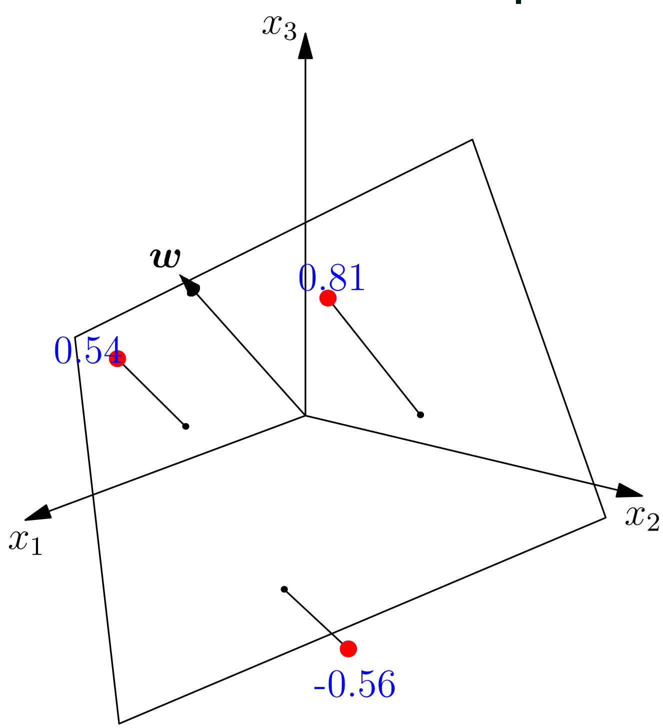

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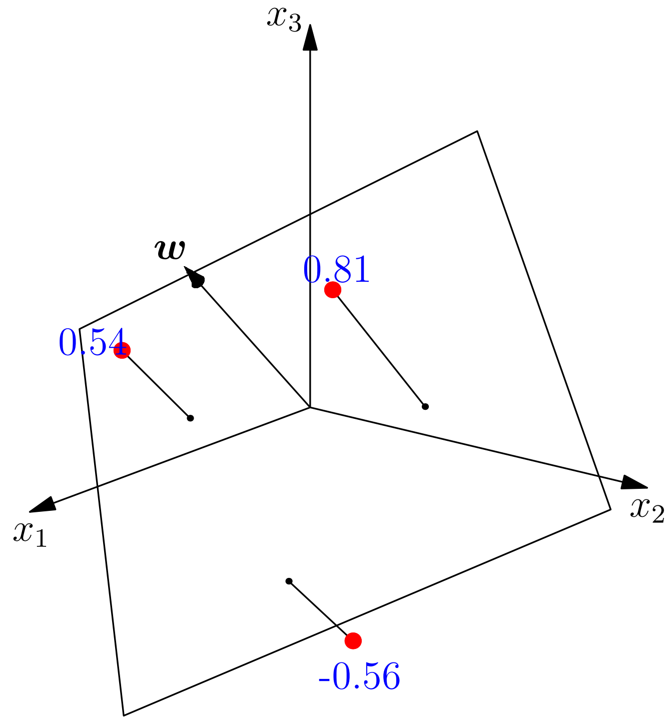

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Linear Least Squares

- The error of input pattern $\boldsymbol{x}_k$ is

$$\epsilon_k = \boldsymbol{x}_k^{\mathsf{T}} \boldsymbol{w} - y_k$$

- The squared error

$$E(\boldsymbol{w}|\mathcal{D}) = \sum_{k=1}^{P} \left(\boldsymbol{x}_k^{\mathsf{T}} \boldsymbol{w} - y_k\right)^2 = \sum_{k=1}^{P} \epsilon_k^2 = \|\boldsymbol{\epsilon}\|^2$$

- We can define the error vector

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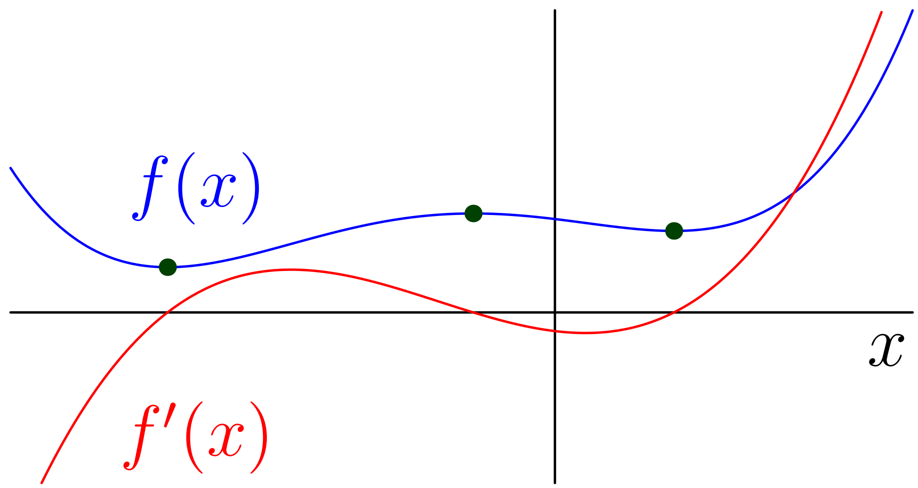
Finding a Minimum

- The minima of a one dimensional function, $f(x)$, are given by $f'(x) = 0$



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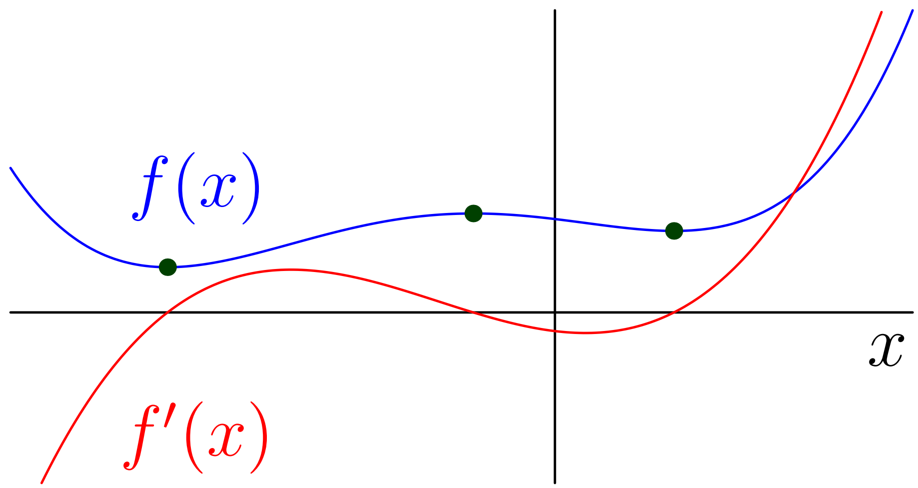

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Gradients

- The **grad** operator $\boldsymbol{\nabla}$ is the gradient operator in high dimensions

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Least Squares Solution

- The least squared solution is give by

$$\begin{aligned} \nabla E(\boldsymbol{w}|\mathcal{D}) = \nabla \|\boldsymbol{\epsilon}\|^2 &= \nabla \|\mathbf{X}\boldsymbol{w} - \boldsymbol{y}\|^2 \\ &= \nabla \left(\boldsymbol{w}^{\mathsf{T}}\mathbf{X}^{\mathsf{T}}\mathbf{X}\,\boldsymbol{w} - 2\boldsymbol{w}^{\mathsf{T}}\mathbf{X}^{\mathsf{T}}\boldsymbol{y} + \boldsymbol{y}^{\mathsf{T}}\boldsymbol{y} \right) \\ &= 2\left(\mathbf{X}^{\mathsf{T}}\mathbf{X}\,\boldsymbol{w} - \mathbf{X}^{\mathsf{T}}\boldsymbol{y} \right) = 0 \end{aligned}$$

- Or

$$\boldsymbol{w} = \left(\mathbf{X}^{\mathsf{T}}\mathbf{X}\right)^{-1}\mathbf{X}^{\mathsf{T}}\boldsymbol{y} = \mathbf{X}^{+}\boldsymbol{y}$$

- $\mathbf{X}^{+} = \left(\mathbf{X}^{\mathsf{T}}\mathbf{X}\right)^{-1}\mathbf{X}^{\mathsf{T}}$ is known as the pseudo inverse
- For non-square matrices Matlab uses the pseudo inverse so in Matlab we can write

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w = X\y
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w = X\y
```

Least Squares Solution

- The least squared solution is give by

$$\begin{aligned}\boldsymbol{\nabla} E(\boldsymbol{w}|\mathcal{D}) &= \boldsymbol{\nabla}\|\boldsymbol{\epsilon}\|^2 = \boldsymbol{\nabla}\|\mathbf{X}\boldsymbol{w} - \boldsymbol{y}\|^2 \\ &= \boldsymbol{\nabla}\left(\boldsymbol{w}^{\mathsf{T}}\mathbf{X}^{\mathsf{T}}\mathbf{X}\,\boldsymbol{w} - 2\boldsymbol{w}^{\mathsf{T}}\mathbf{X}^{\mathsf{T}}\boldsymbol{y} + \boldsymbol{y}^{\mathsf{T}}\boldsymbol{y}\right) \\ &= 2\left(\mathbf{X}^{\mathsf{T}}\mathbf{X}\,\boldsymbol{w} - \mathbf{X}^{\mathsf{T}}\boldsymbol{y}\right) = 0\end{aligned}$$

- Or

$$\boldsymbol{w} = \left(\mathbf{X}^{\mathsf{T}}\mathbf{X}\right)^{-1}\mathbf{X}^{\mathsf{T}}\boldsymbol{y} = \mathbf{X}^{+}\boldsymbol{y}$$

- $\mathbf{X}^{+} = \left(\mathbf{X}^{\mathsf{T}}\mathbf{X}\right)^{-1}\mathbf{X}^{\mathsf{T}}$ is known as the pseudo inverse
- For non-square matrices Matlab uses the pseudo inverse so in Matlab we can write

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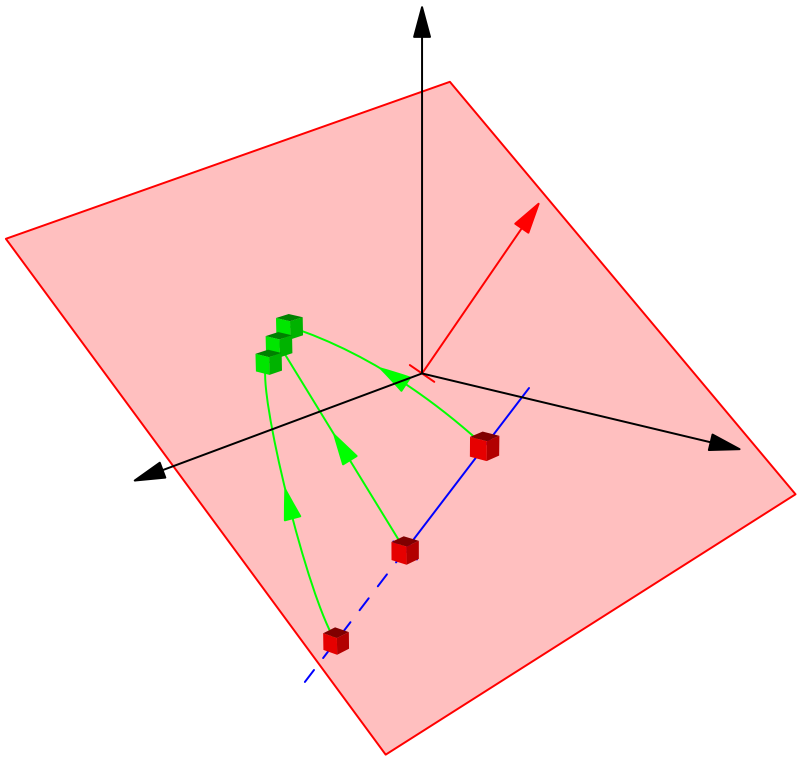
Outline

1. Mappings
2. **Linear Maps**
3. Eigenvectors



Solving Inverse Problems

- Gauss showed us how to solve **over-constrained** problems (we have more observations than parameters)
- We seek a solution which isn't necessarily exact but minimises an error
- But, what if we have more parameters than observations
- That is, we are **under-constrained**
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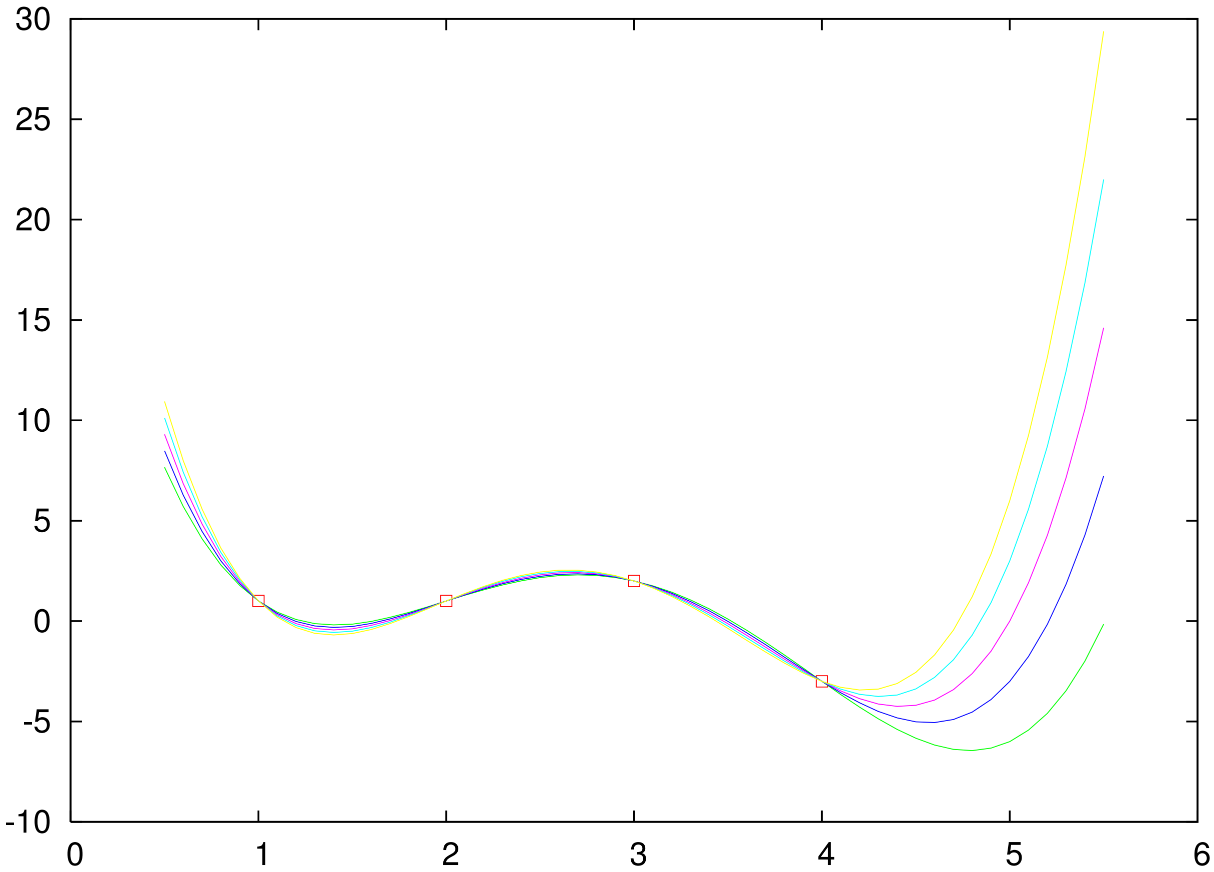
- This is very typical of most machine learning problems

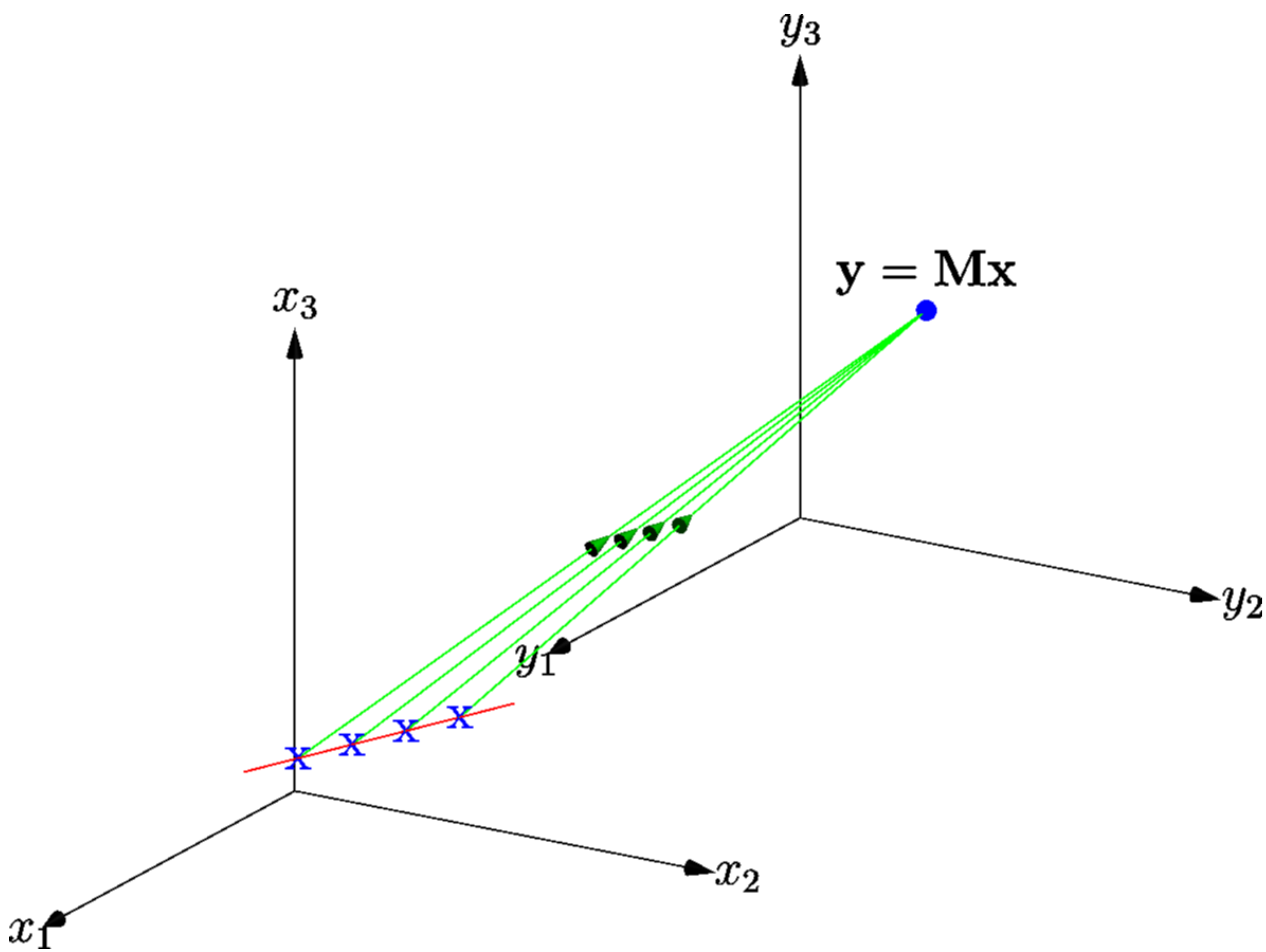
Under Constrained Systems

- If we have less data-points than parameters then there will be multiple solutions



What is the Inverse?

- Many points can map to the same points



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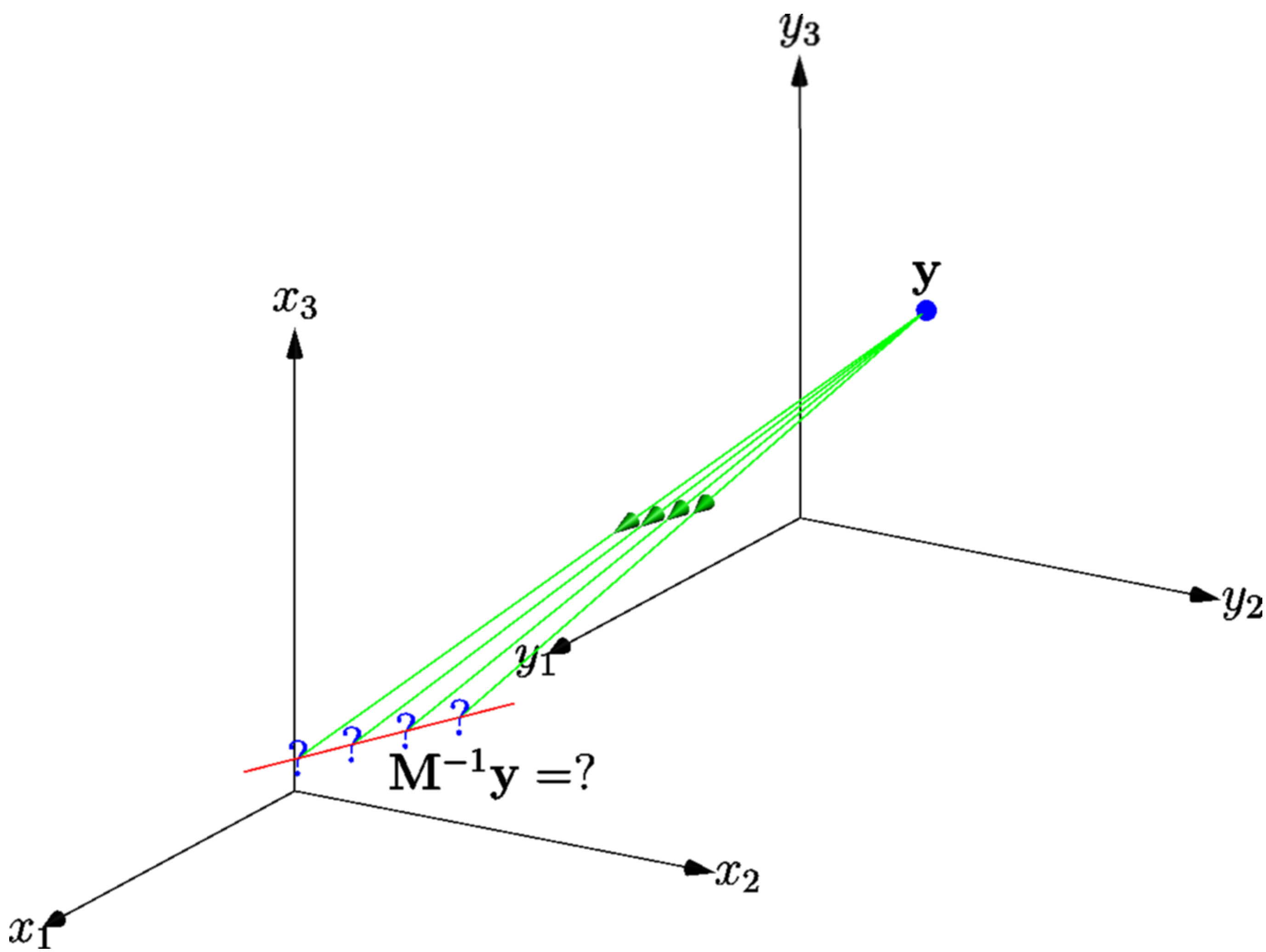

Under-constrained Systems

- The system is **under-constrained**
- We have more unknowns than equations
- The inverse is not unique
- Solving the inverse problem ($\boldsymbol{w} = \left(\mathbf{X}^{\mathsf{T}}\mathbf{X}\right)^{-1}\mathbf{X}^{\mathsf{T}}\boldsymbol{y}$) is said to be **ill-posed**
- The inverse $\left(\mathbf{X}^{\mathsf{T}}\mathbf{X}\right)^{-1}$ doesn't exist
- If we have a complicated learning machine and not sufficient data we often end with an ill-posed inverse problem (there are lots of sets of parameters that explain the data)

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Ill-Conditions

- Singular matrices are rare (although they occur when we don't have enough data), but matrices that are close to being singular are common
- If a matrix is close to singular it is ill-conditioned
- Ill-conditioned matrices have some small eigenvalues
- All points get contracted towards a plane
- Large matrices are very often ill conditioned

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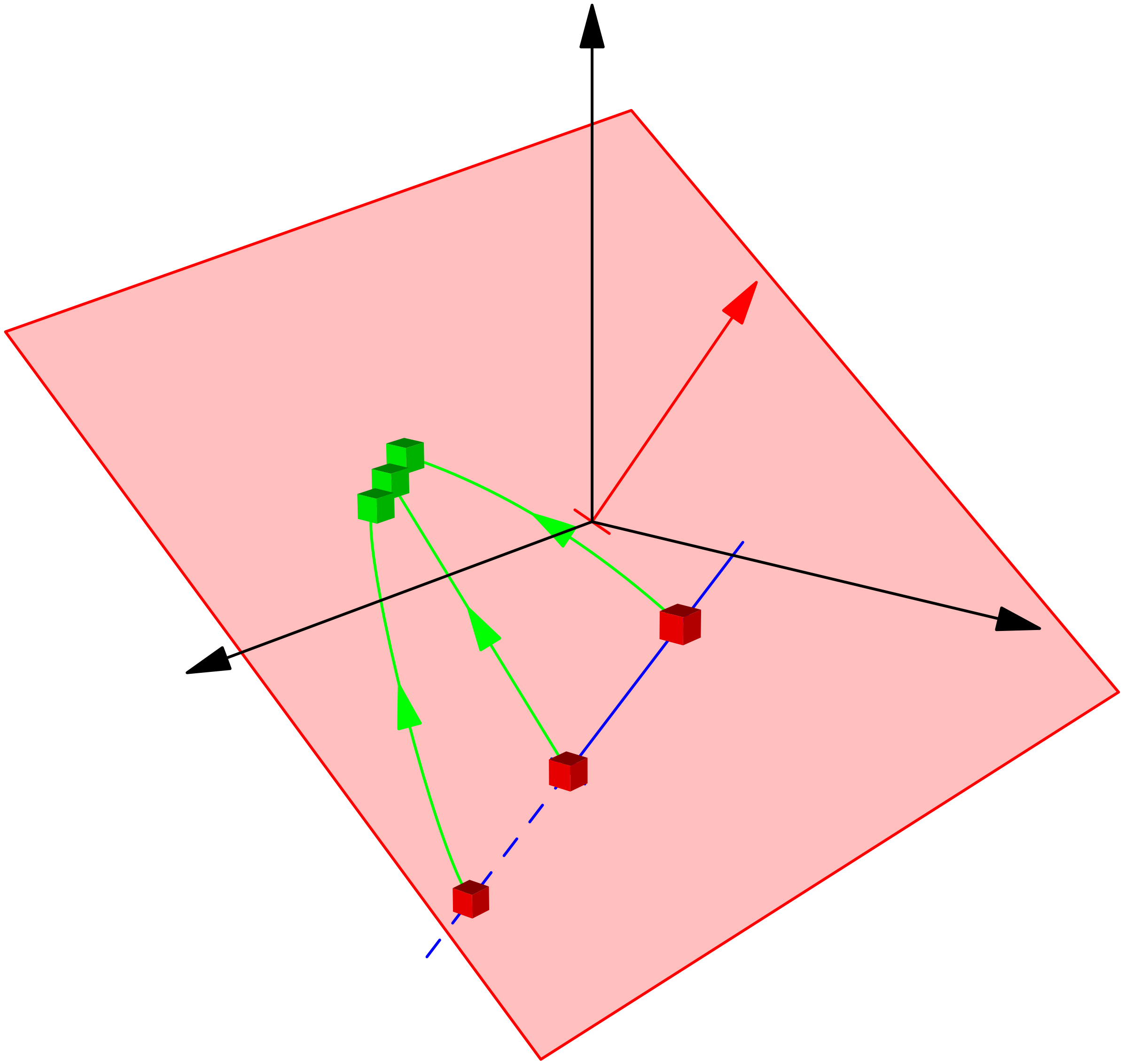

Ill-Conditioning in ML

- Ill-conditioning in machine learning occurs when a very small change in the learning data causes a large change in the predictions of the learning machine
- In linear regression the matrix $\mathbf{X}^\mathsf{T}\mathbf{X}$ is ill-conditioned when we have as many data points as parameters
- Much of machine learning is concerned with making learning machines better conditioned
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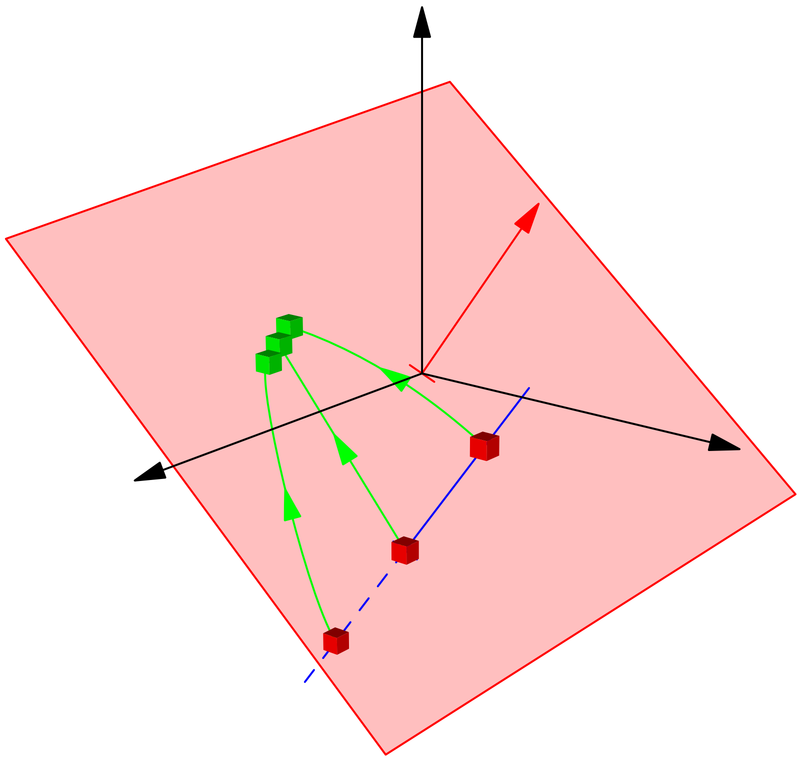

Eigenvalue equation

- Eigen-systems help us to understand mappings
- A vector $\boldsymbol{v}$ is said to be an **eigenvector** if

$$\mathbf{M}\boldsymbol{v} = \lambda\,\boldsymbol{v}$$

- $\mathbf{M}$ is square (i.e. $n \times n$)
- Where the number λ is the **eigenvalue**
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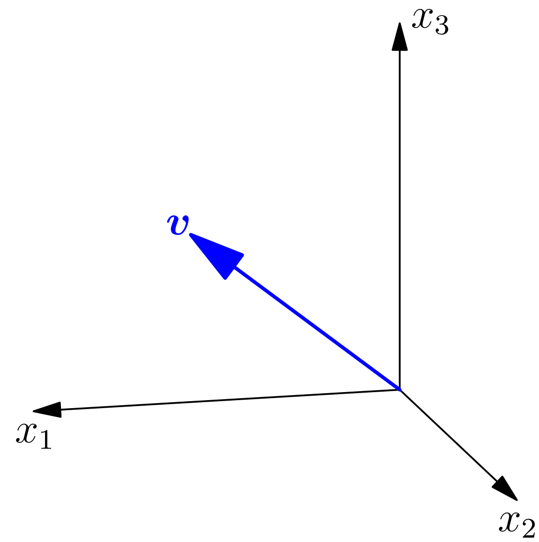

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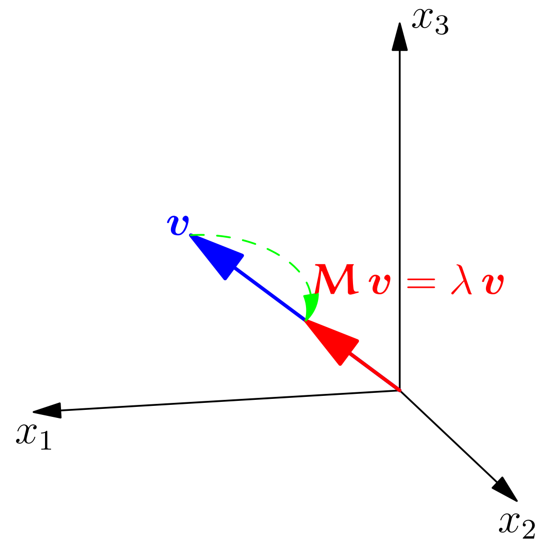

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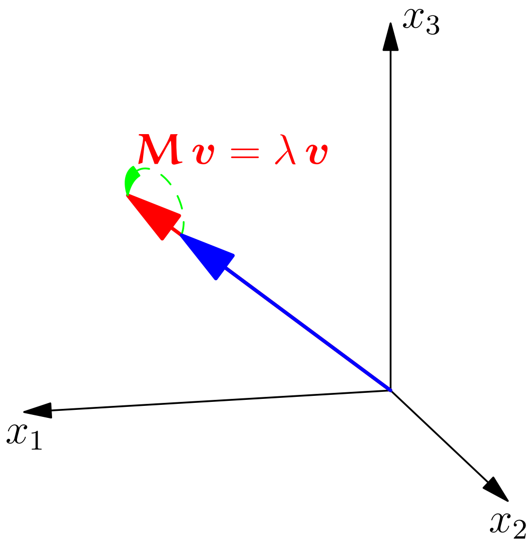

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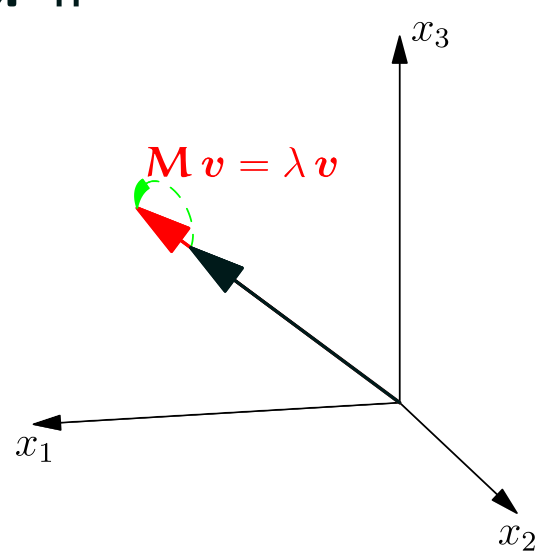

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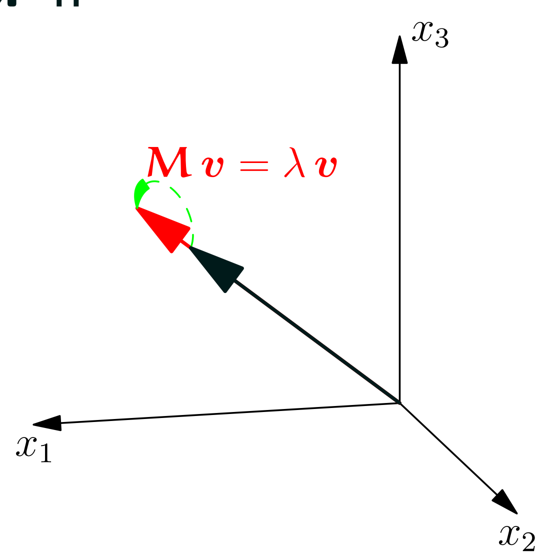

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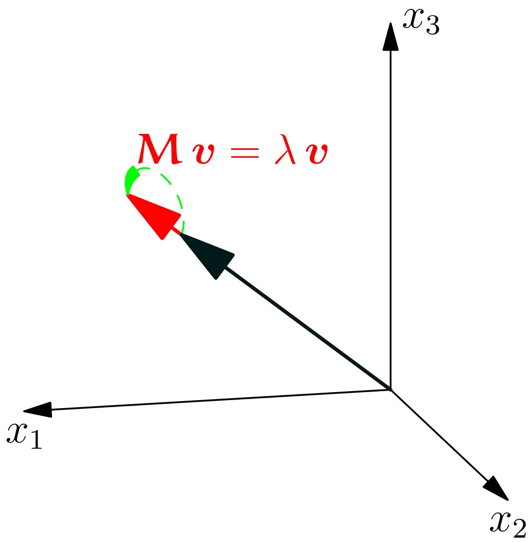

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Symmetric Matrices

- If $\boldsymbol{M}$ is an $n \times n$ **symmetric** matrix then it has n real orthogonal eigenvectors with real eigenvalues

- We denote the i^{th} eigenvector by $\boldsymbol{v}_i$ and the corresponding eigenvalue by λ_i so that

$$\boldsymbol{M}\boldsymbol{v}_i = \lambda_i \boldsymbol{v}_i$$

- Orthogonal means that if $i \neq j$ then

$$\boldsymbol{v}_i^{\mathsf{T}} \boldsymbol{v}_j = 0$$

- (We can always normalise eigenvectors if we want)

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Proof of Orthogonality

- $(\mathbf{M}\boldsymbol{v}_i = \lambda_i \boldsymbol{v}_i)^{\mathsf{T}}$ implies $\boldsymbol{v}_i^{\mathsf{T}} \mathbf{M}^{\mathsf{T}} = \lambda_i \boldsymbol{v}_i^{\mathsf{T}}$
- When $\mathbf{M}$ is symmetric then $\mathbf{M}\boldsymbol{v}_i = \lambda_i \boldsymbol{v}_i \Rightarrow \boldsymbol{v}_i^{\mathsf{T}} \mathbf{M} = \lambda_i \boldsymbol{v}_i^{\mathsf{T}}$
- Consider two eigenvectors $\boldsymbol{v}_i$ and $\boldsymbol{v}_j$ of $\mathbf{M}$

$$\begin{aligned} \boldsymbol{v}_i^{\mathsf{T}} \mathbf{M} \boldsymbol{v}_j &= (\boldsymbol{v}_i^{\mathsf{T}} \mathbf{M}) \boldsymbol{v}_j = \lambda_i \boldsymbol{v}_i^{\mathsf{T}} \boldsymbol{v}_j \\ &= \boldsymbol{v}_i^{\mathsf{T}} (\mathbf{M} \boldsymbol{v}_j) = \lambda_j \boldsymbol{v}_i^{\mathsf{T}} \boldsymbol{v}_j \end{aligned}$$

- So either $\lambda_i = \lambda_j$ or $\boldsymbol{v}_i^{\mathsf{T}} \boldsymbol{v}_j = 0$
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Orthogonal Matrices

- We can construct an **orthogonal** matrix $\mathbf{V}$ from the eigenvectors

$$\mathbf{V} = (\boldsymbol{v}_1, \boldsymbol{v}_2, \cdots, \boldsymbol{v}_n)$$

- Matrix $\mathbf{V}$ is an $n \times n$ matrix

- Because of the orthogonality of the vectors $\boldsymbol{v}_i$

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- We have shown that $\mathbf{V}^{\mathsf{T}}\mathbf{V} = \mathbf{I}$
- Thus multiply both sides on the left by $\mathbf{V}$

$$\mathbf{V}\mathbf{V}^{\mathsf{T}}\mathbf{V} = \mathbf{V}$$

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Invertible Matrices

- A matrix, $\mathbf{M}$, will be singular (uninvertible) if there exists a vector $\boldsymbol{x}$ $(\neq \mathbf{0})$ such that

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Rotations

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- As a consequent they define rotations (and possibly a reflection)

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Matrix Decomposition

- Taking the matrix of eigenvectors, $\boldsymbol{V}$, then

$$\mathbf{M}\,\mathbf{V} = \mathbf{M}(\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_n) = (\lambda_1\,\boldsymbol{v}_1, \lambda_2\,\boldsymbol{v}_2, \ldots, \lambda_n\,\boldsymbol{v}_n) = \mathbf{V}\,\boldsymbol{\Lambda}$$

- where $\boldsymbol{\Lambda} = \mathrm{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n) = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix}$

- Now

$$\mathbf{M} = \mathbf{M}\,\mathbf{V}\,\mathbf{V}^{\mathsf{T}} = \mathbf{V}\,\boldsymbol{\Lambda}\,\mathbf{V}^{\mathsf{T}}$$

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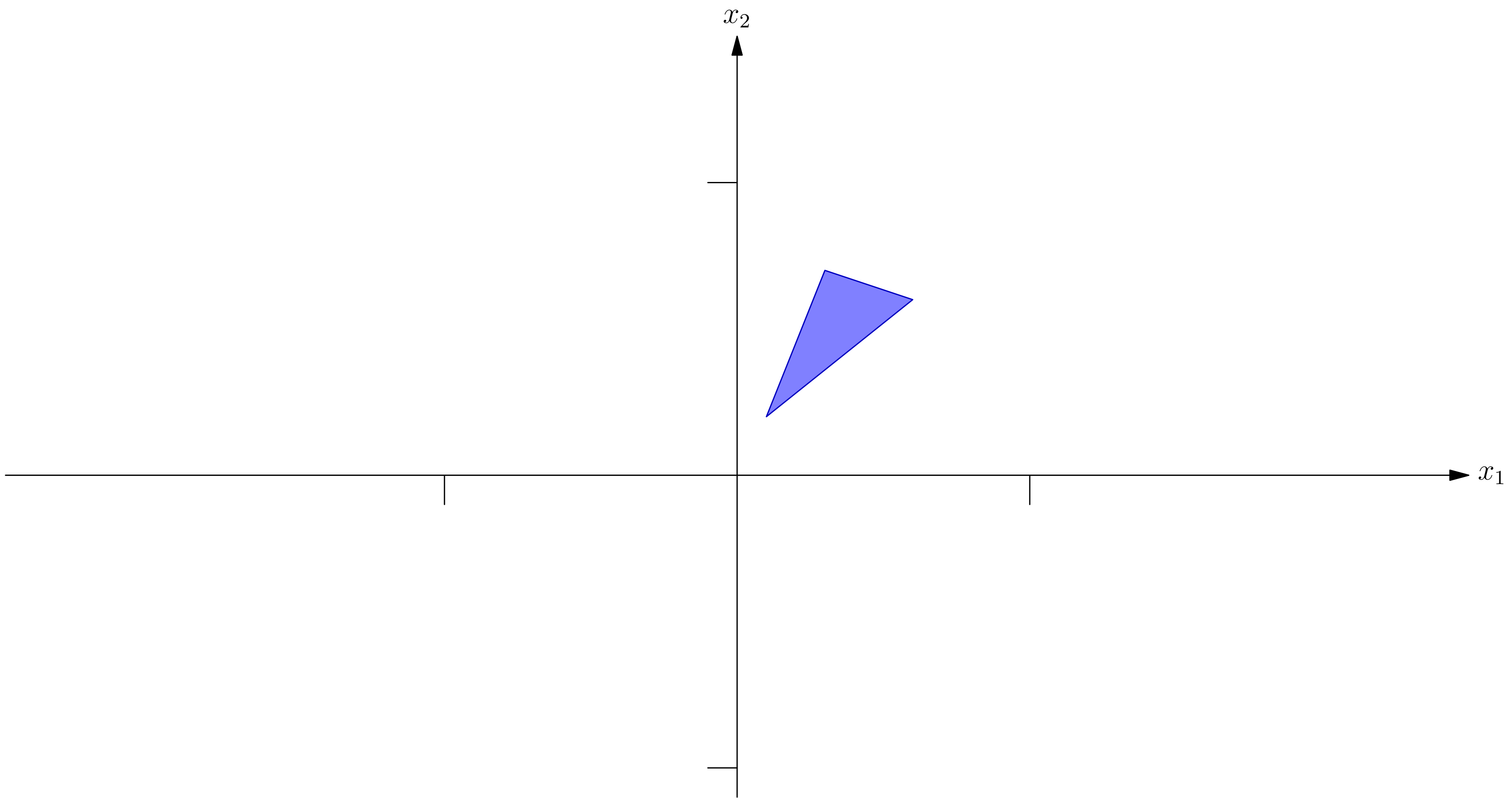
Mappings by Symmetric Matrices

$$\mathbf{M} = \begin{pmatrix} 0.83 & -0.31 \\ -0.31 & 1.9 \end{pmatrix} = \mathbf{V}\mathbf{S}\mathbf{V}^\mathsf{T} = \begin{pmatrix} \cos(-75) & \sin(-75) \\ -\sin(-75) & \cos(-75) \end{pmatrix} \begin{pmatrix} 2 & 0 \\ 0 & 0.75 \end{pmatrix} \begin{pmatrix} \cos(75) & \sin(75) \\ -\sin(75) & \cos(75) \end{pmatrix}$$



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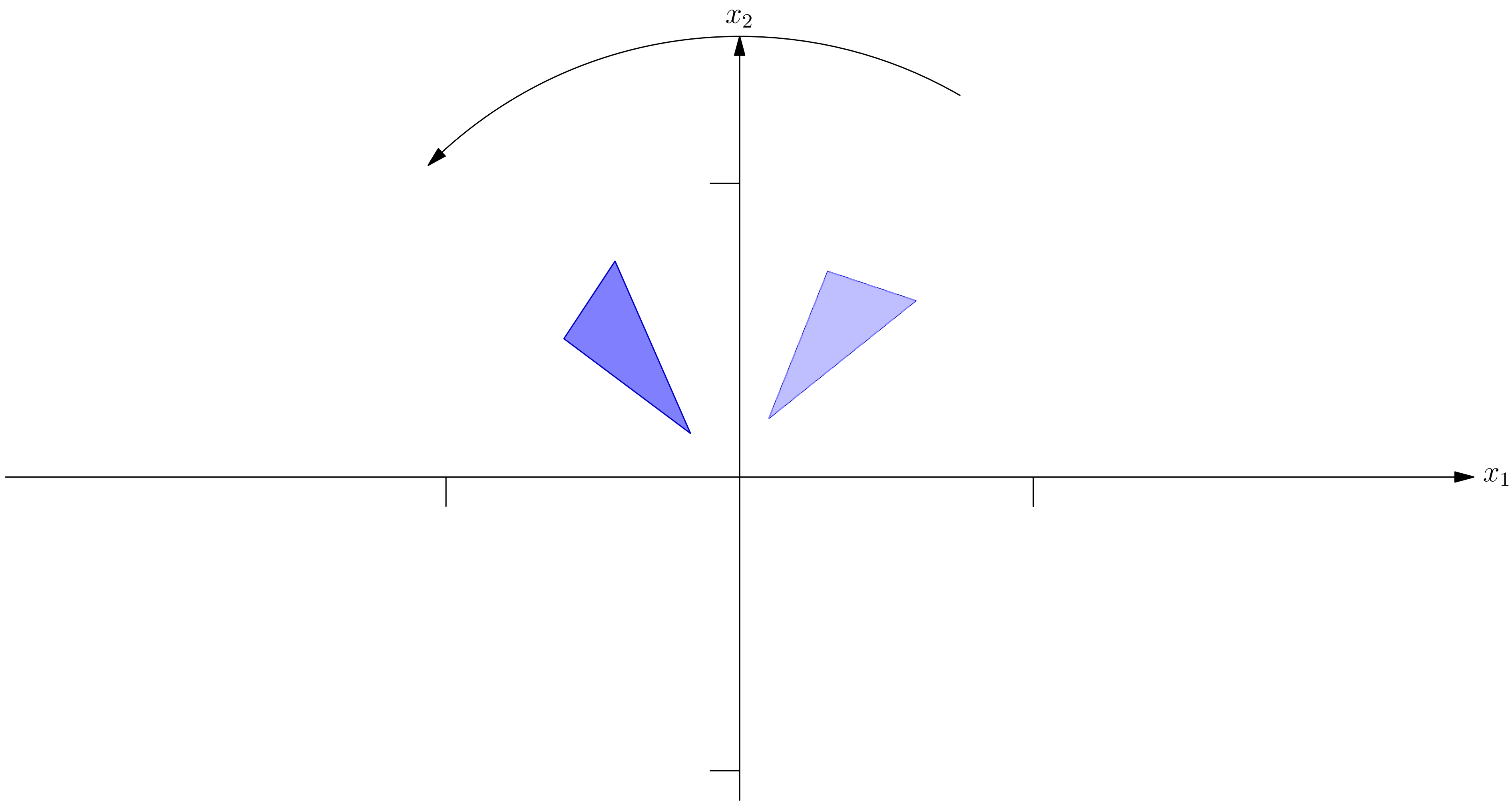

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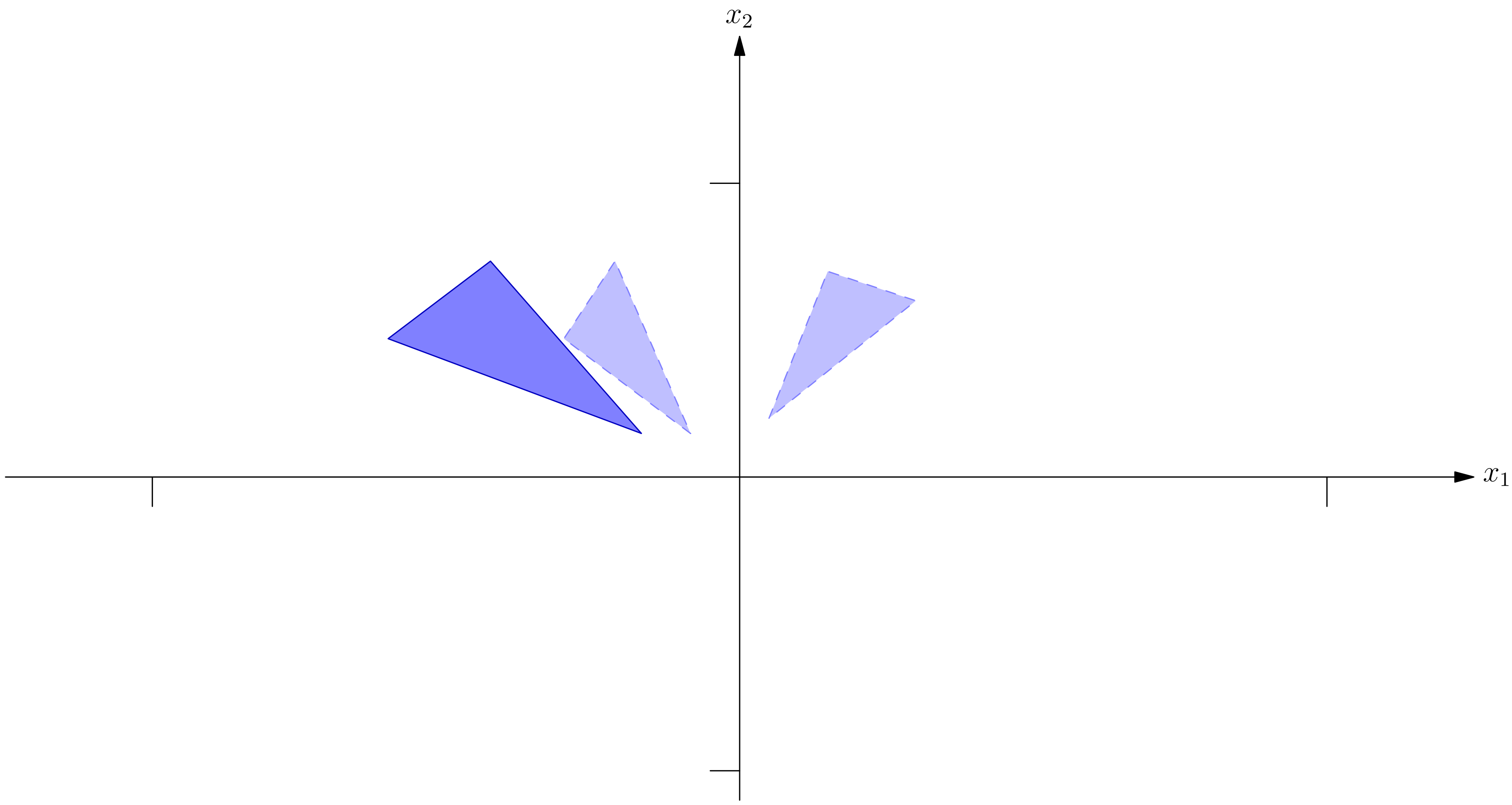

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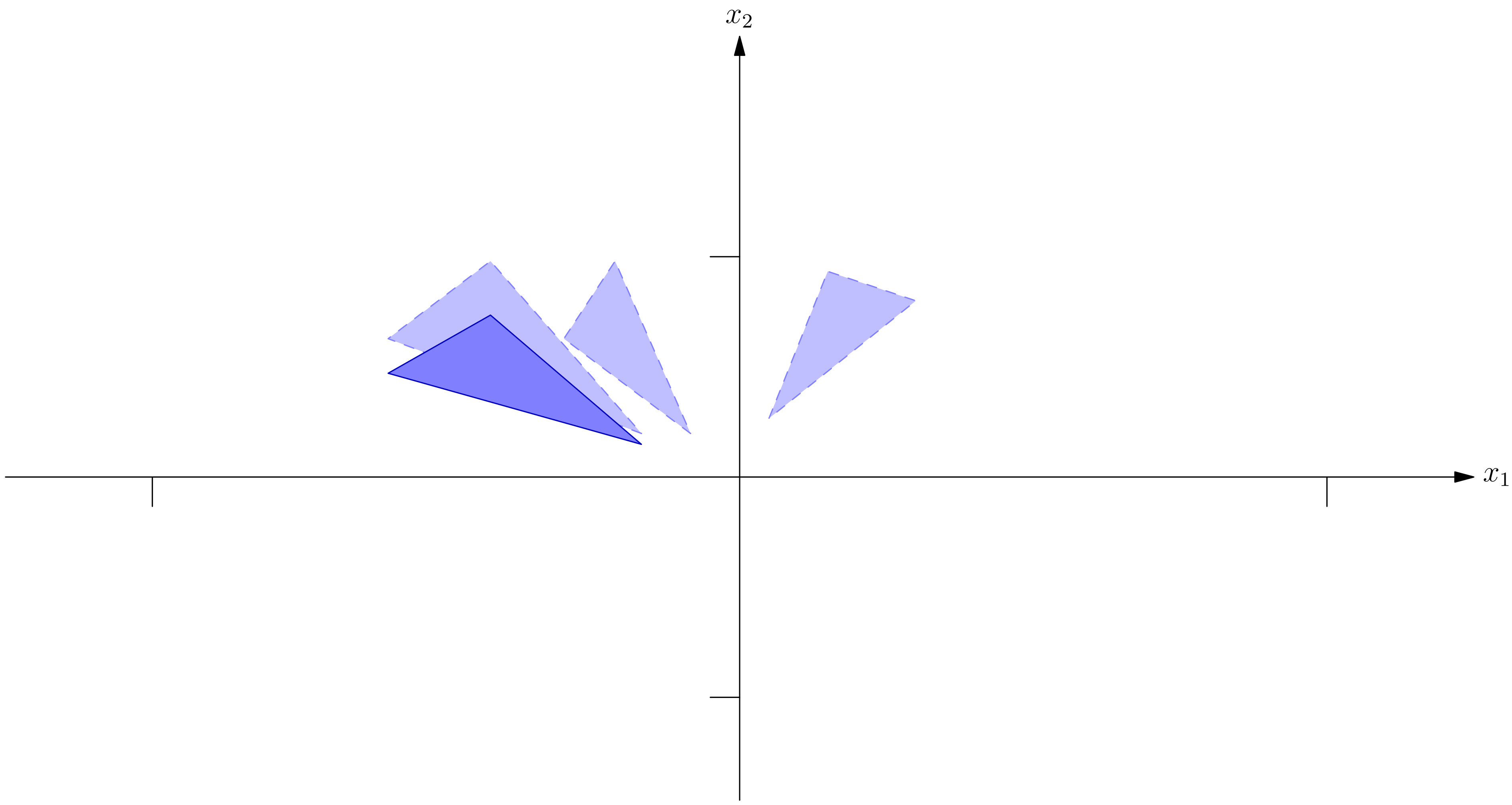

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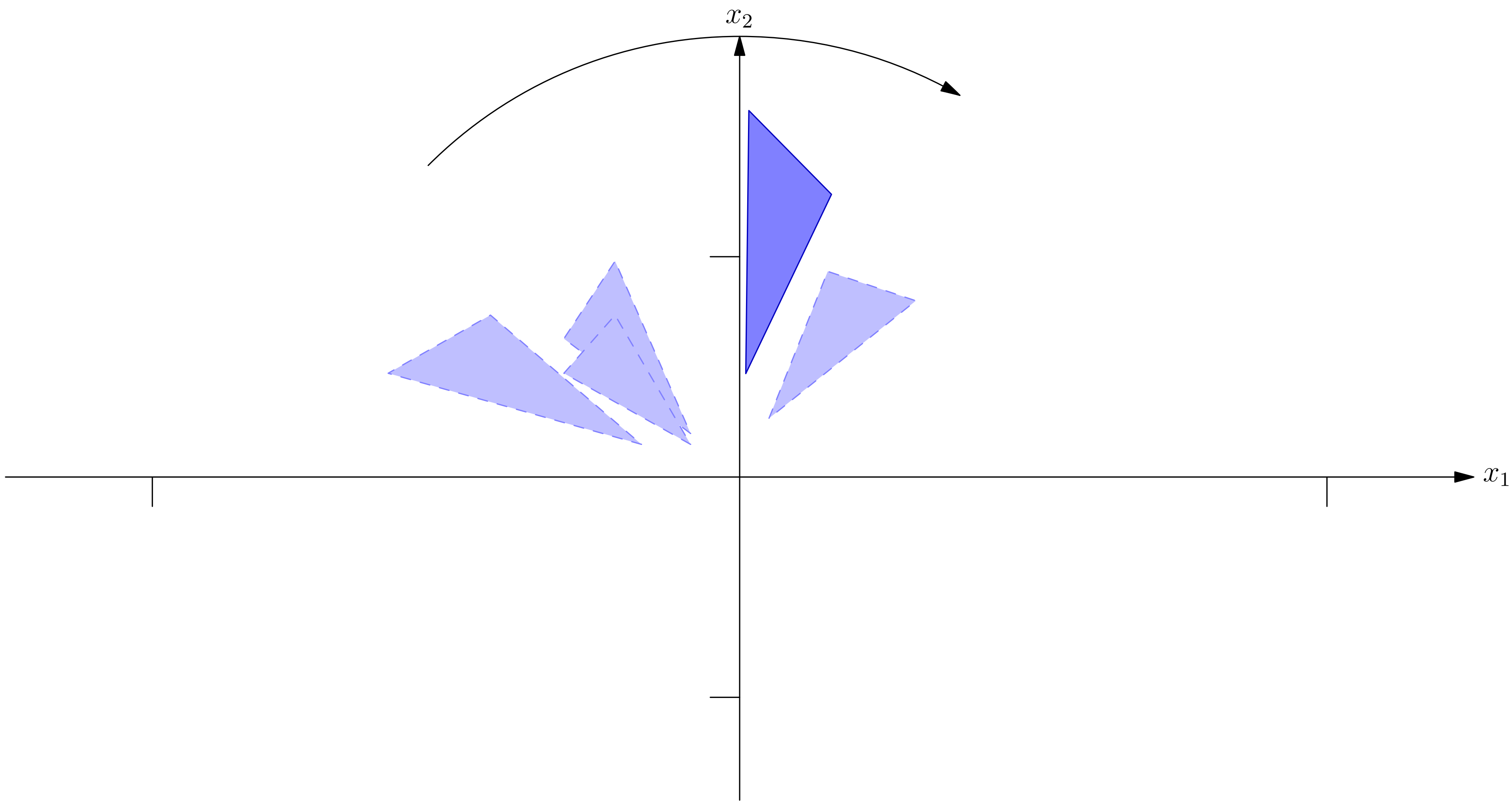

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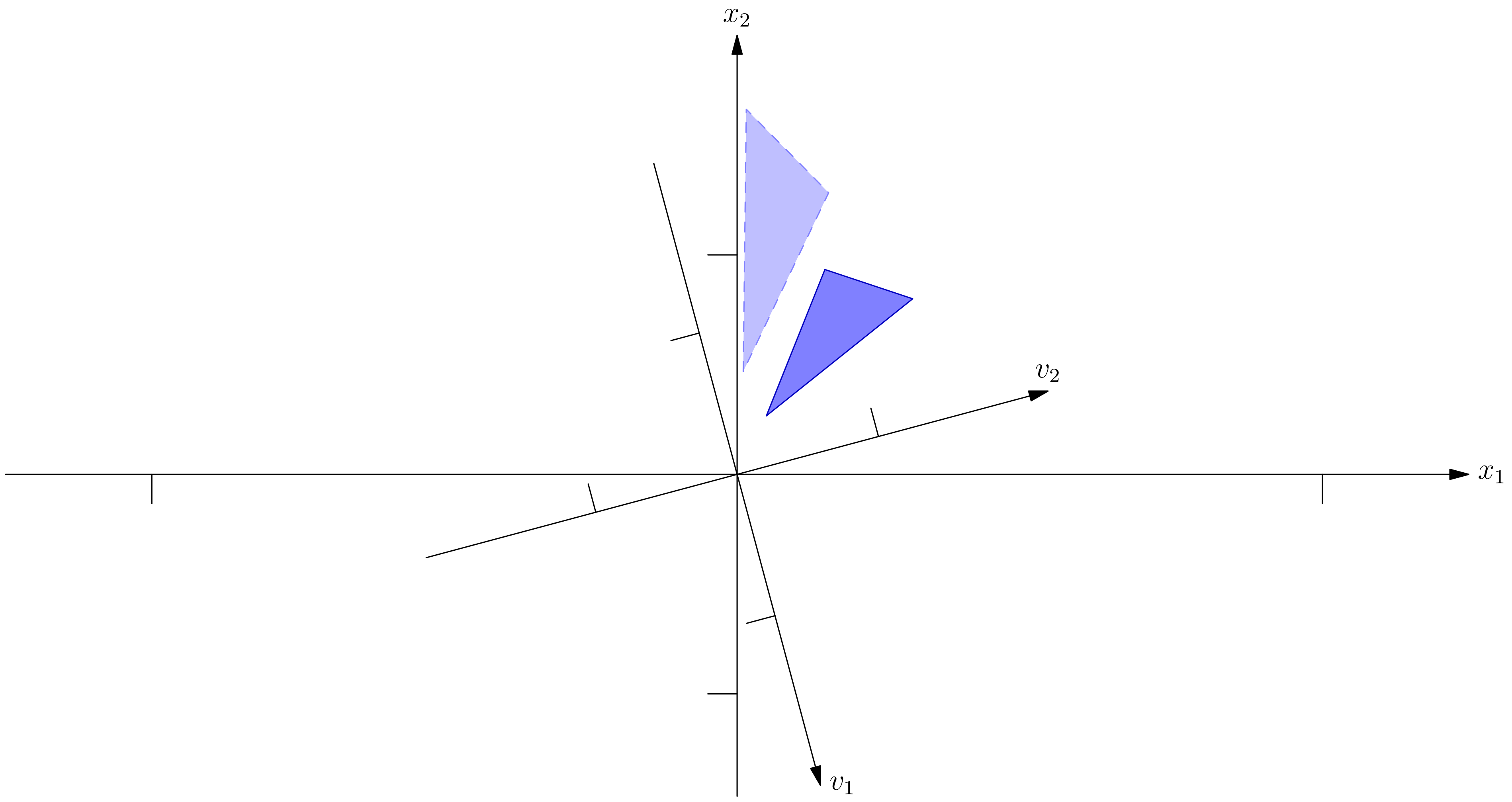

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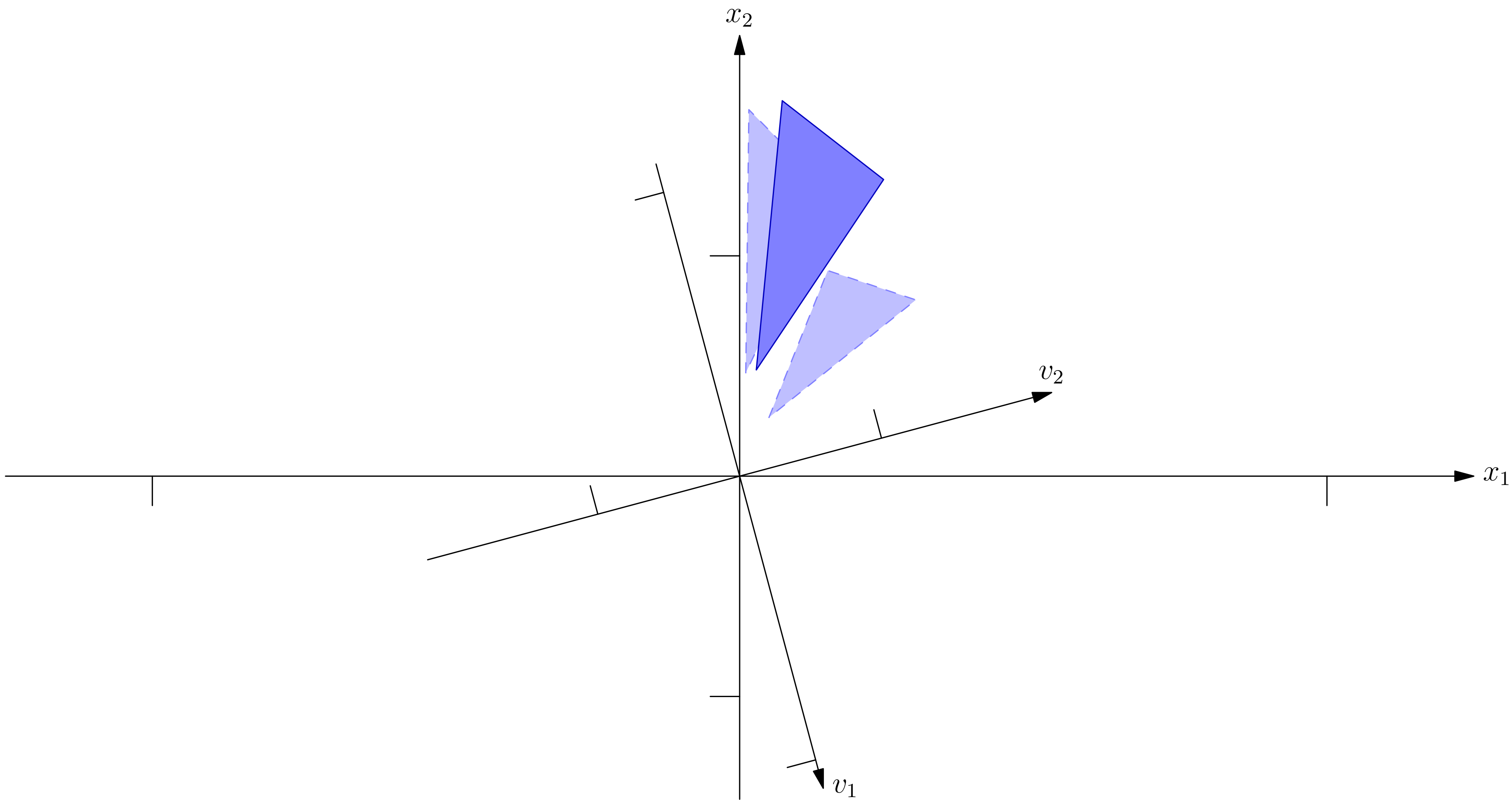

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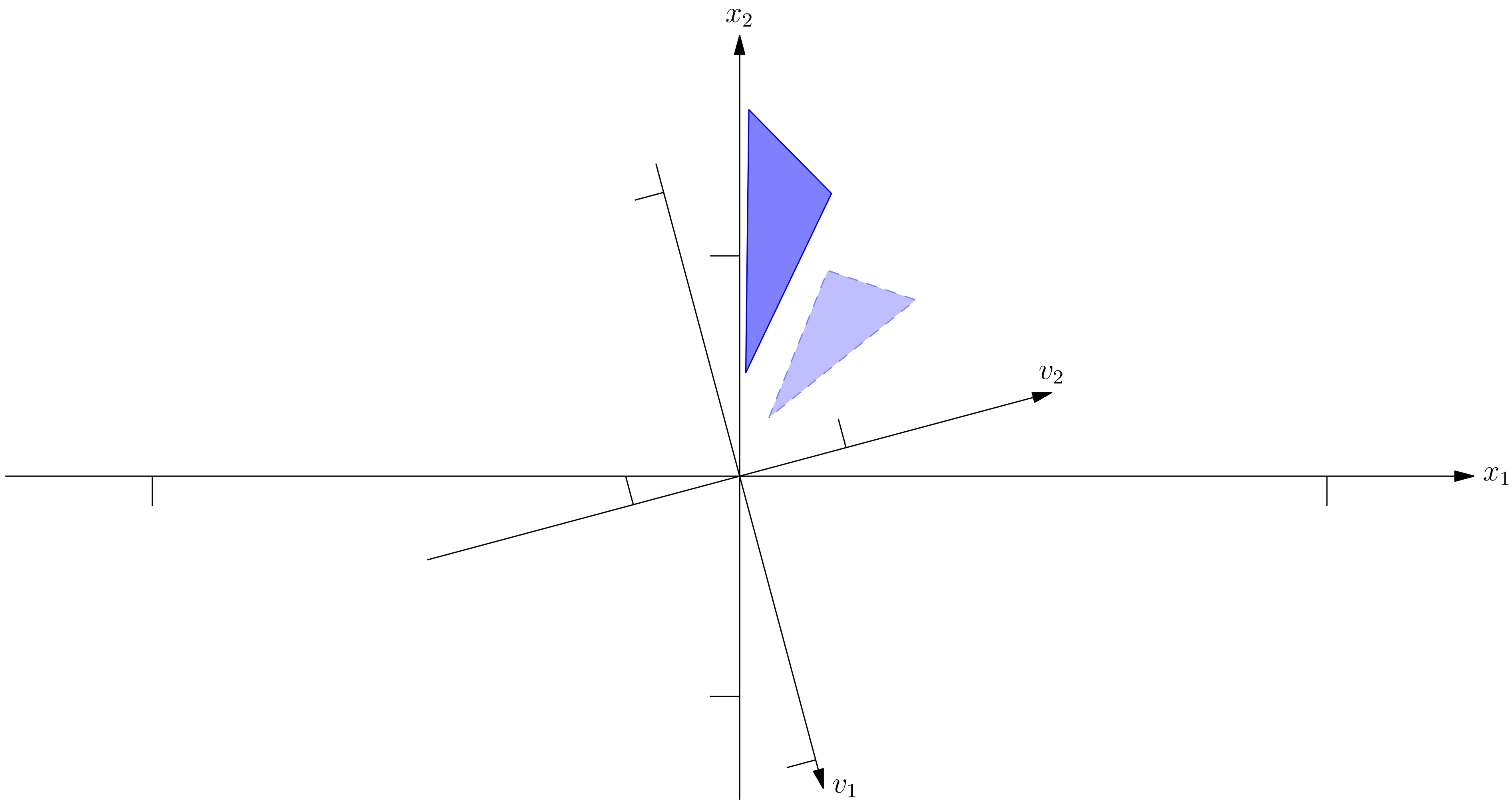

Inverses

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$$\mathbf{M} = \mathbf{V}\,\mathbf{\Lambda}\,\mathbf{V}^{\mathsf{T}} \qquad\qquad \mathbf{M}^{-1} = \mathbf{V}\,\mathbf{\Lambda}^{-1}\,\mathbf{V}^{\mathsf{T}}$$

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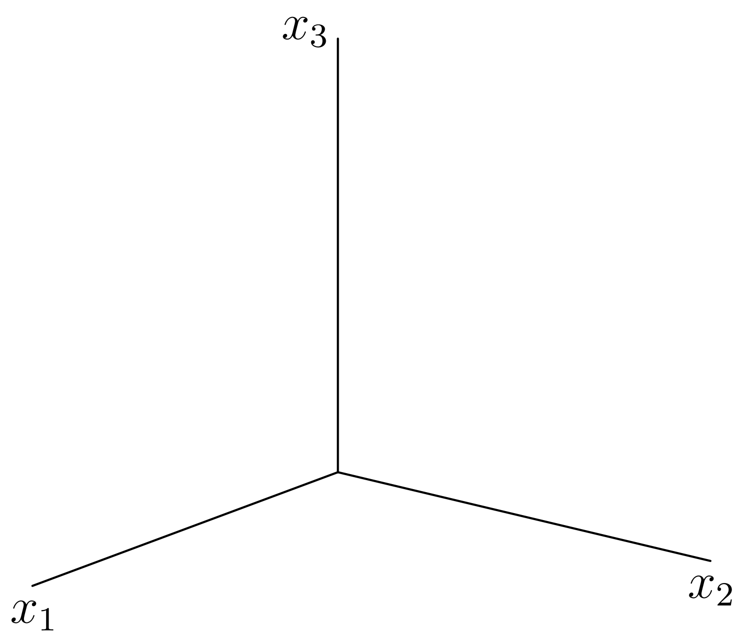

$$\boldsymbol{M} = \begin{pmatrix} 0.80 & 0.01 & 0.25 \\ 0.01 & 0.85 & 0.48 \\ 0.25 & 0.48 & 0.5 \end{pmatrix}$$
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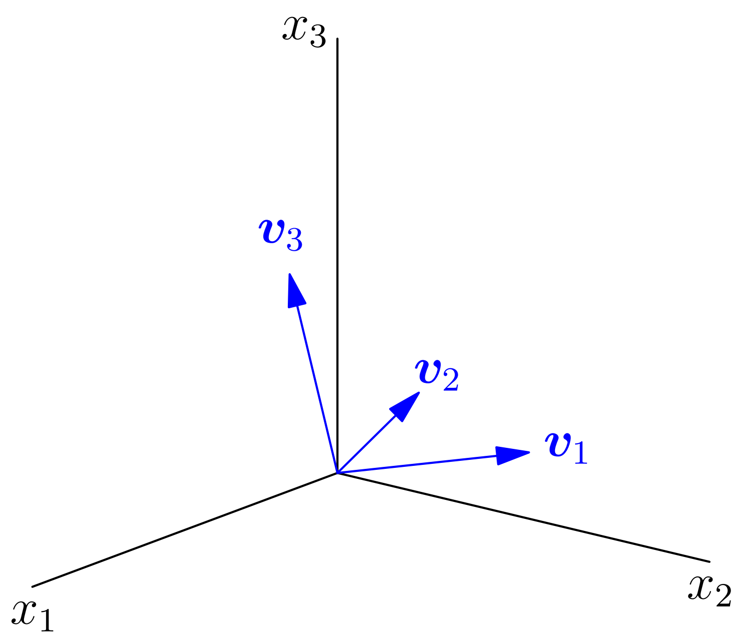

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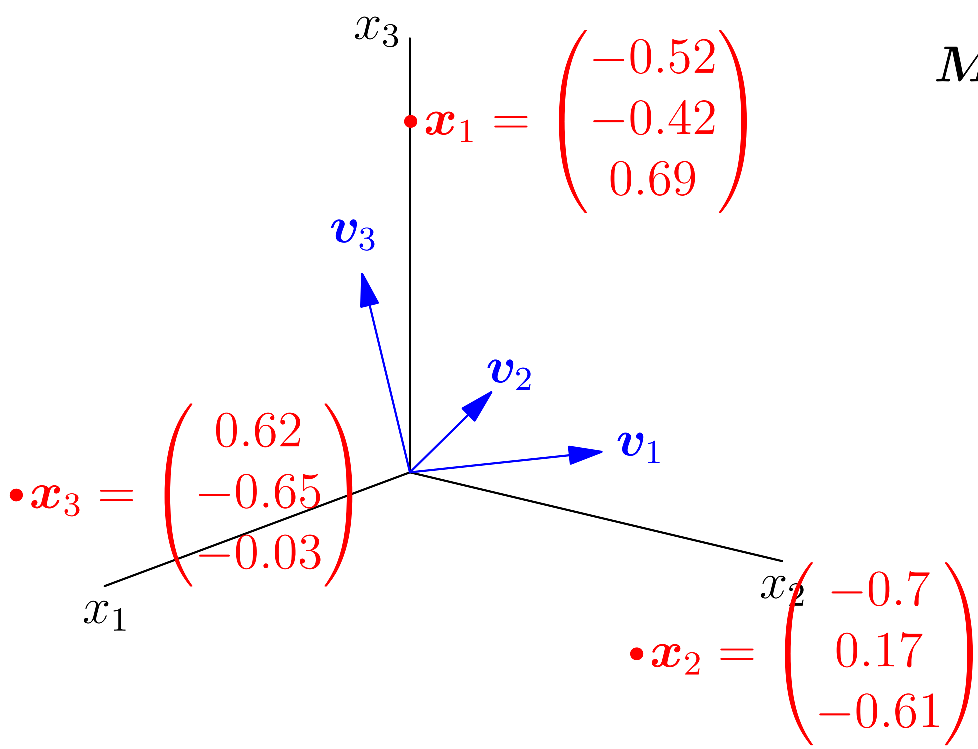

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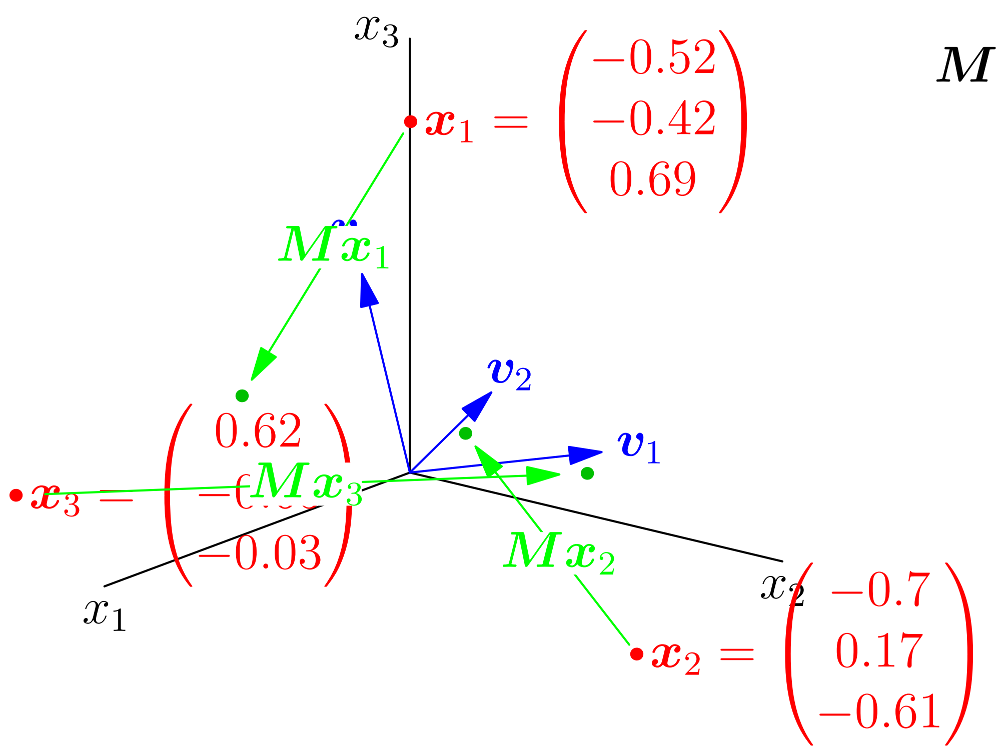

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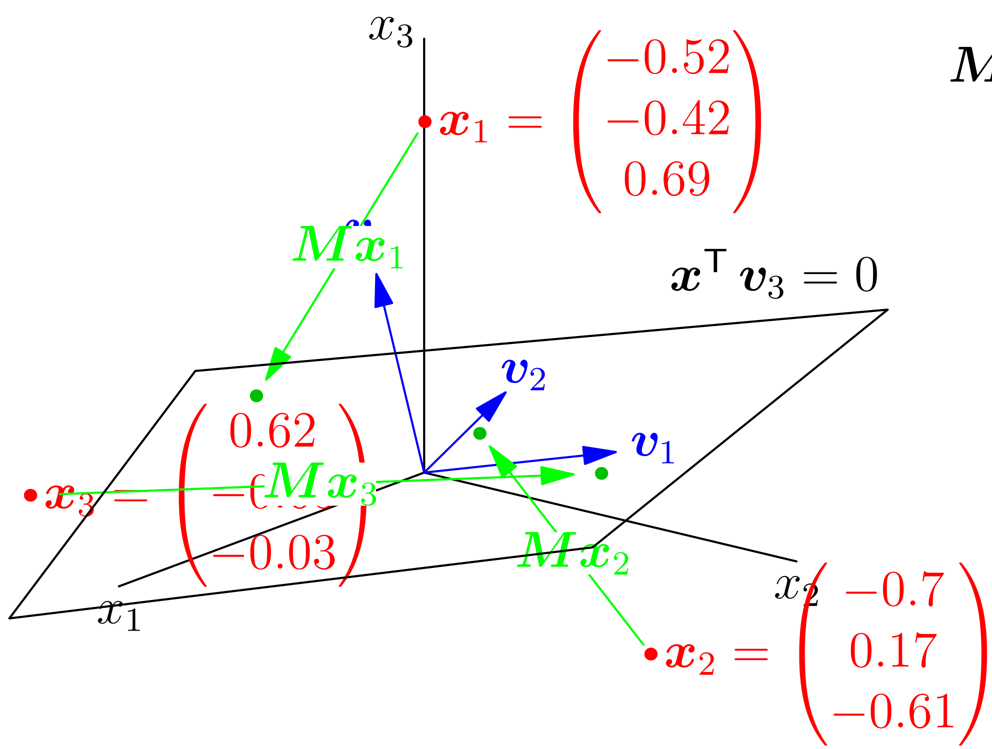

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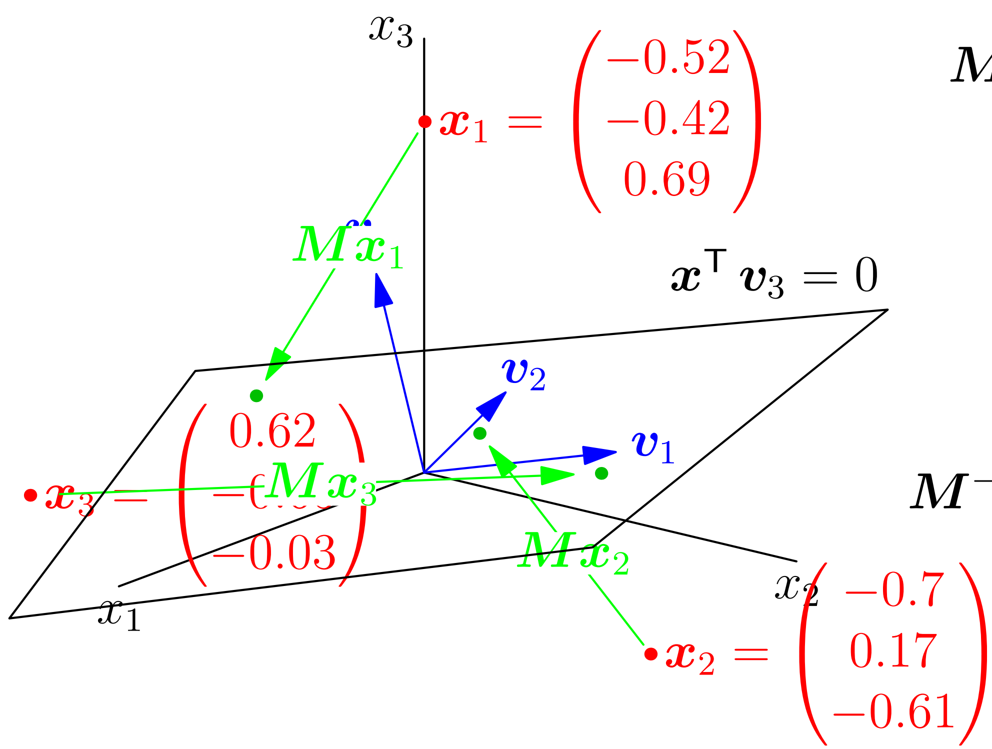

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$$\boldsymbol{M}^{-1} = \begin{pmatrix} 1.9 & 1.17 & -2.1 \\ 1.17 & 3.34 & -3.8 \\ -2.1 & -3.8 & 6.8 \end{pmatrix}$$

$$= \boldsymbol{V} \begin{pmatrix} 1.25 & 0 & 0 \\ 0 & 0.8 & 0 \\ 0 & 0 & 10 \end{pmatrix} \boldsymbol{V}^\mathsf{T}$$

Condition Number

- Taking matrix inverses can be inherently unstable
- Any small error can be amplified by taking the inverse
- The stability of the inverse depends on the ratio of smallest eigenvalue to the largest eigenvalue (i.e. the biggest possible amplification compared to the smallest)
- Note that the Hilbert-norm of a matrix is the absolute value of the largest eigenvalue
- The condition number is given by

$$\|\mathbf{M}\|_H \times \|\mathbf{M}^{-1}\|_H = \frac{|\lambda_{\mathsf{max}}|}{|\lambda_{\mathsf{min}}|}$$

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Summary

- Linear mappings are commonly used in machine learning algorithms such as regression
- We will often meet the pseudo-inverse involving inverting $\mathbf{X}^{\mathsf{T}}\mathbf{X}$
- They can be inherently unstable to noise in the inputs
- We can understand symmetric operators by looking at their eigenvectors
- Function spaces can similarly be understood in terms of eigenfunctions

Summary

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