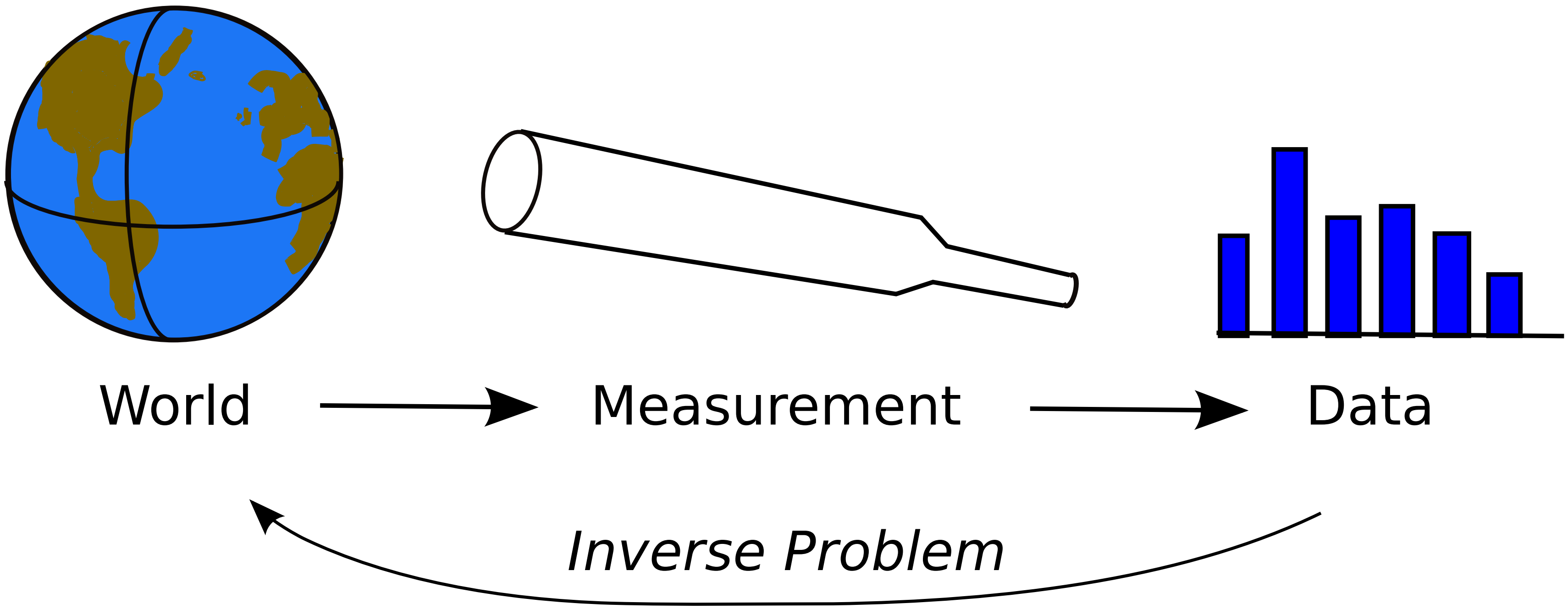
Advanced Machine Learning

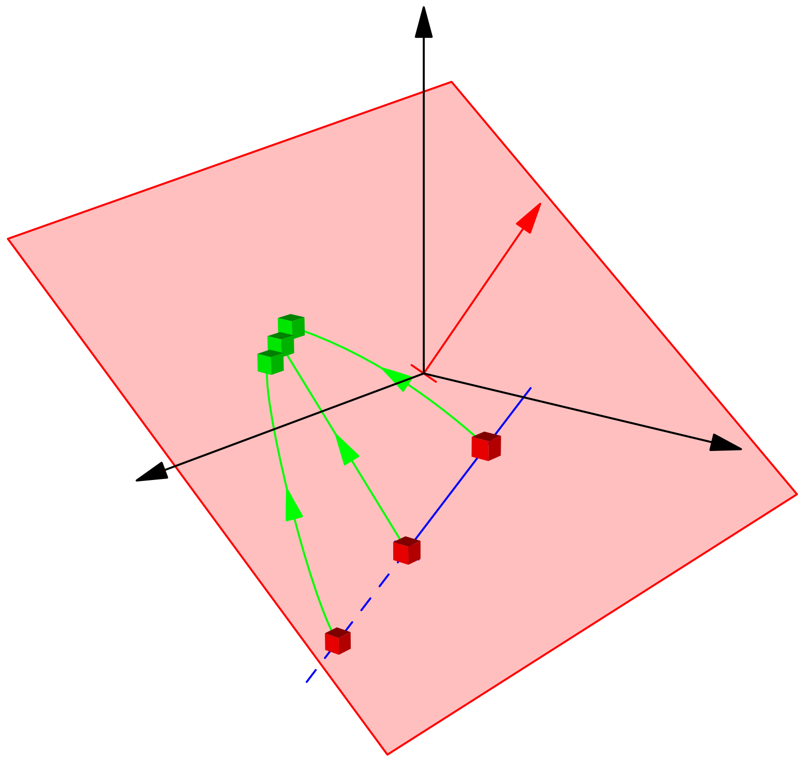
Understand Mappings



Mappings, Linear Maps, Solving Linear Systems

Outline

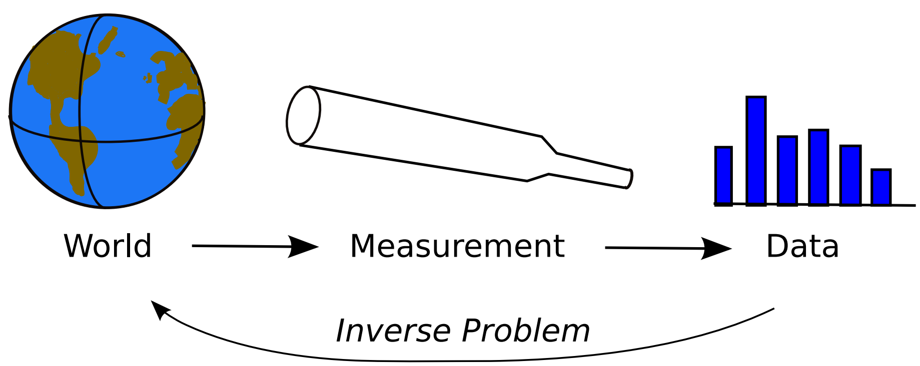
1. **Mappings**
2. Linear Maps



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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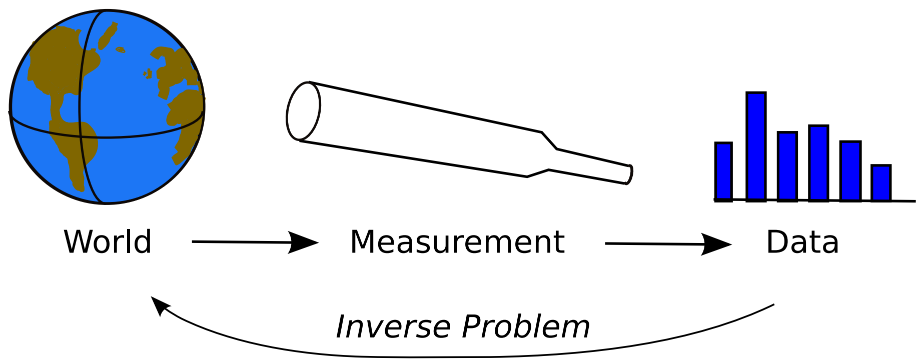

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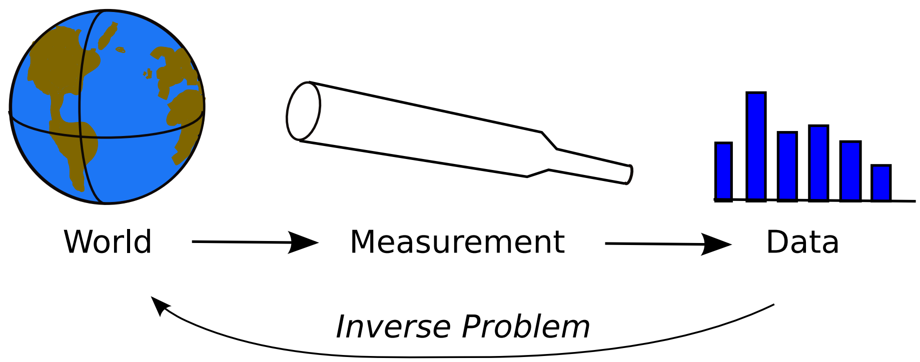

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Inverse Problems

- 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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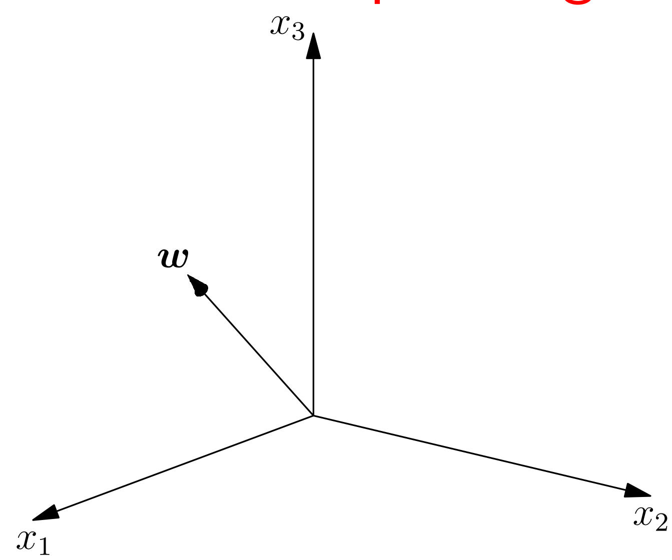
Linear Regression

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



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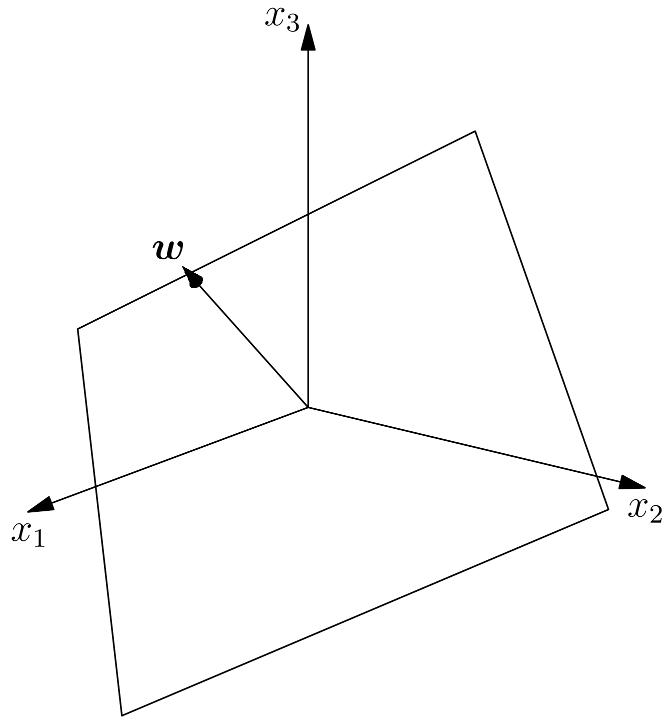

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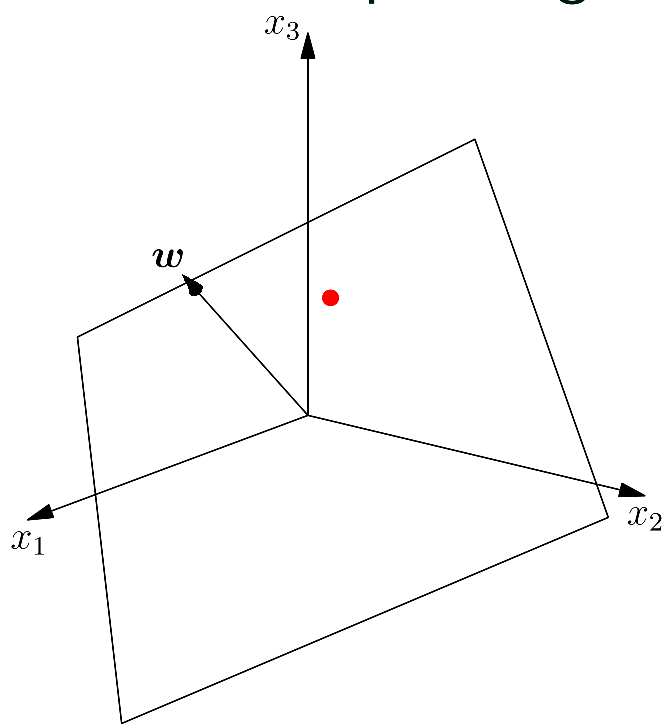

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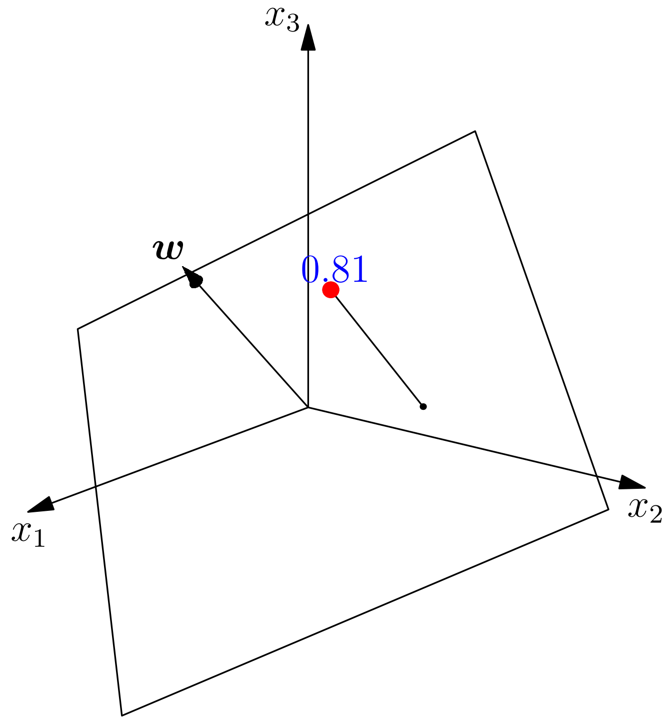

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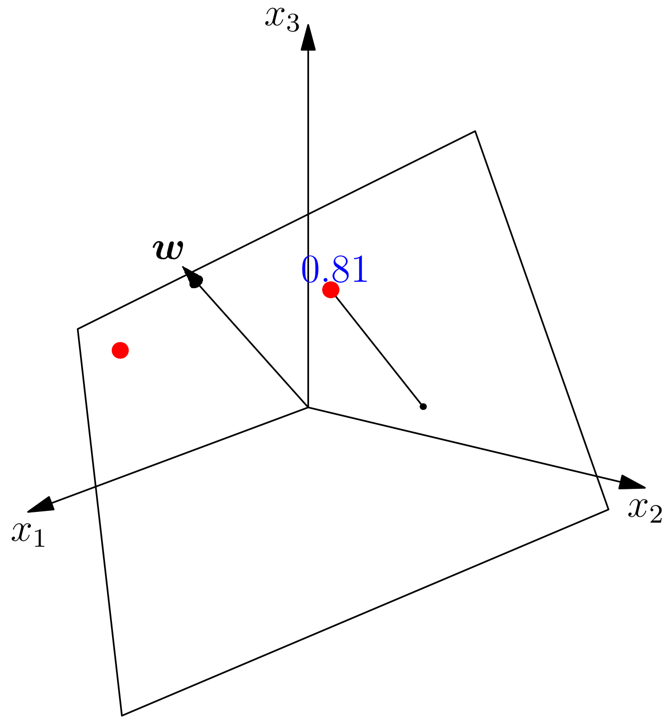

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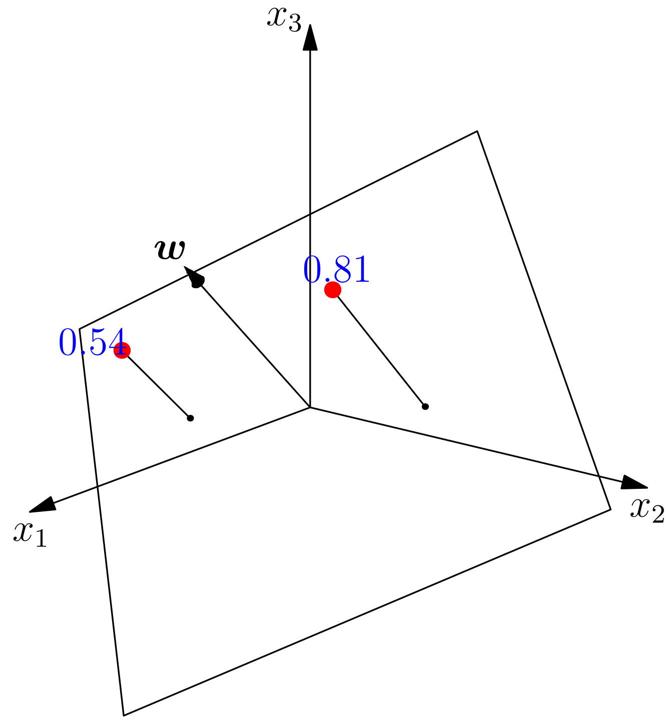

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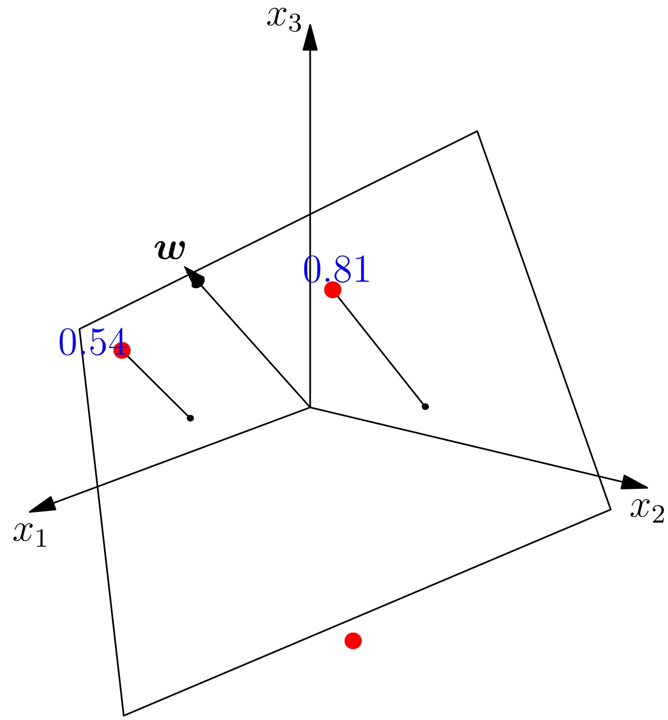

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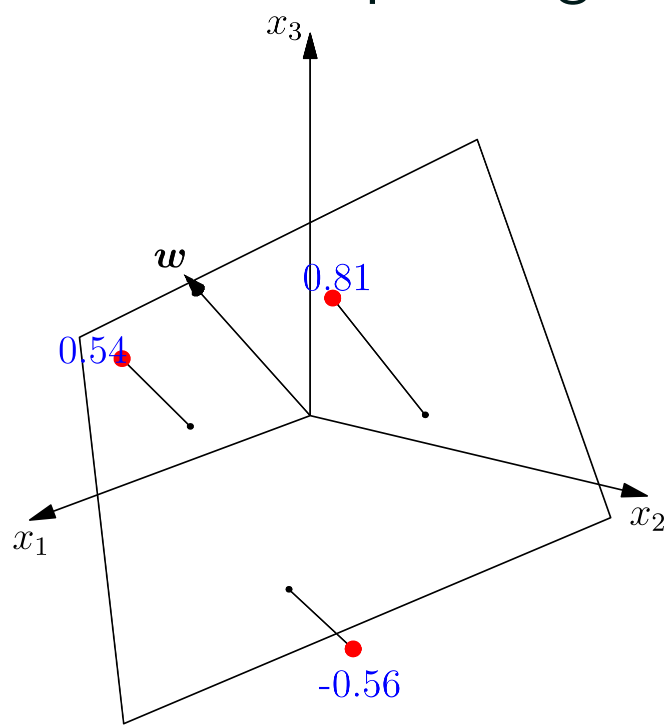

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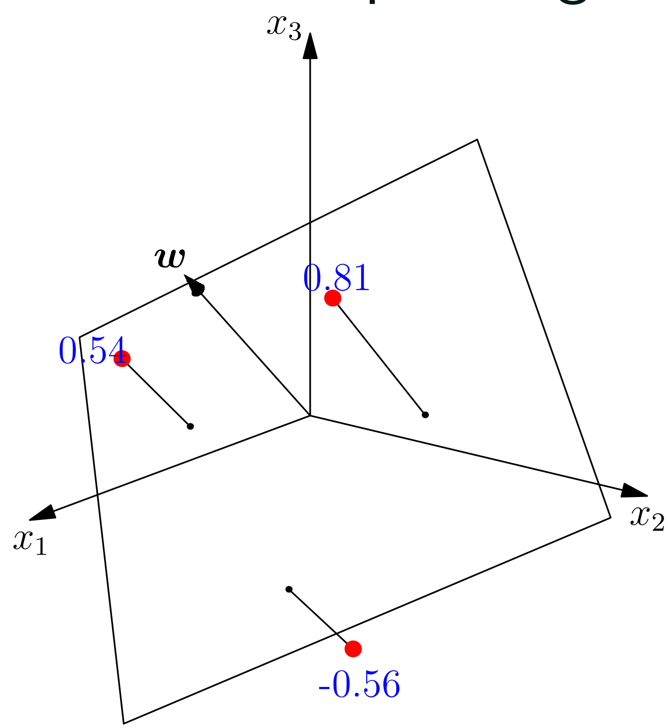

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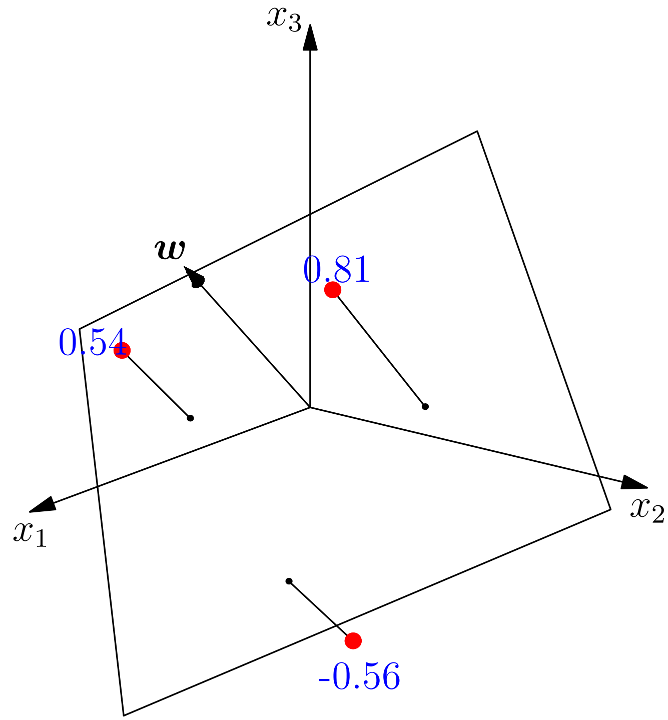

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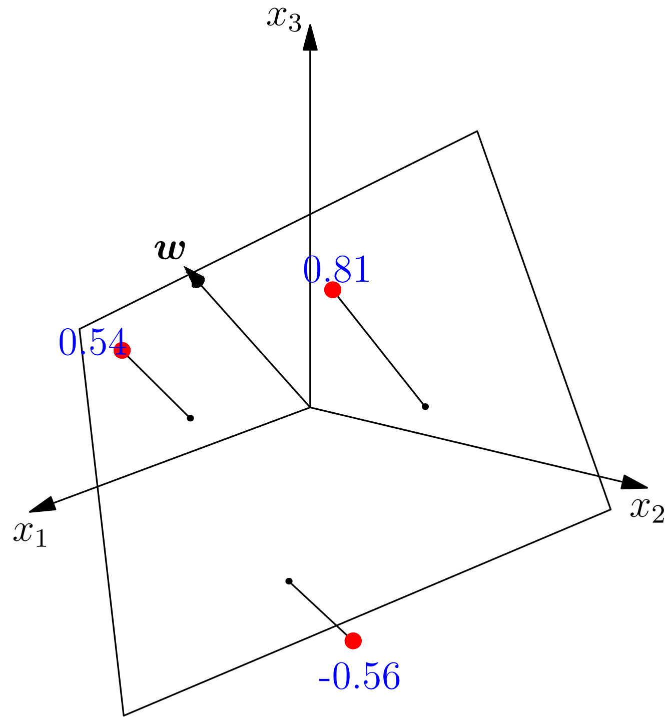

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Linear Least Squares

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

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

- The squared error

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

- We can define the error vector

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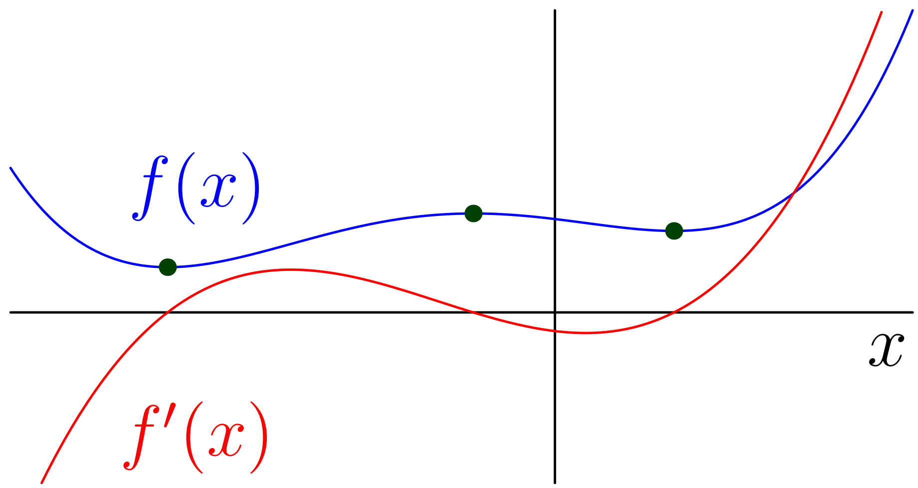
Finding a Minimum

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



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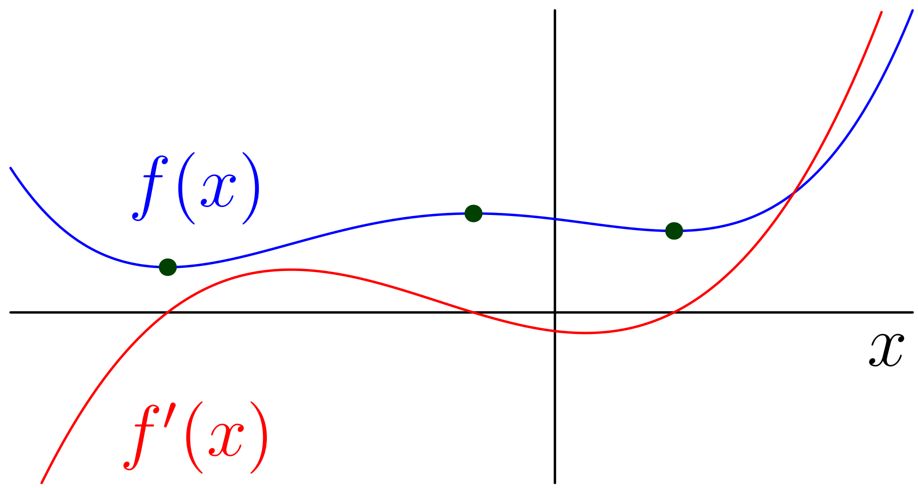

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Gradients

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

- 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

```
w = X\y
```

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Computing Gradients

- To understand gradients we sometimes need to go back to components

$$\nabla \boldsymbol{w}^{\mathsf{T}} \mathbf{M} \boldsymbol{w}$$

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$$\nabla \boldsymbol{w}^{\mathsf{T}} \mathbf{M} \boldsymbol{w} = \begin{pmatrix} \frac{\partial}{\partial w_1} \\ \frac{\partial}{\partial w_2} \\ \frac{\partial}{\partial w_3} \\ \vdots \end{pmatrix} \sum_{i,j} w_i M_{ij} w_j$$

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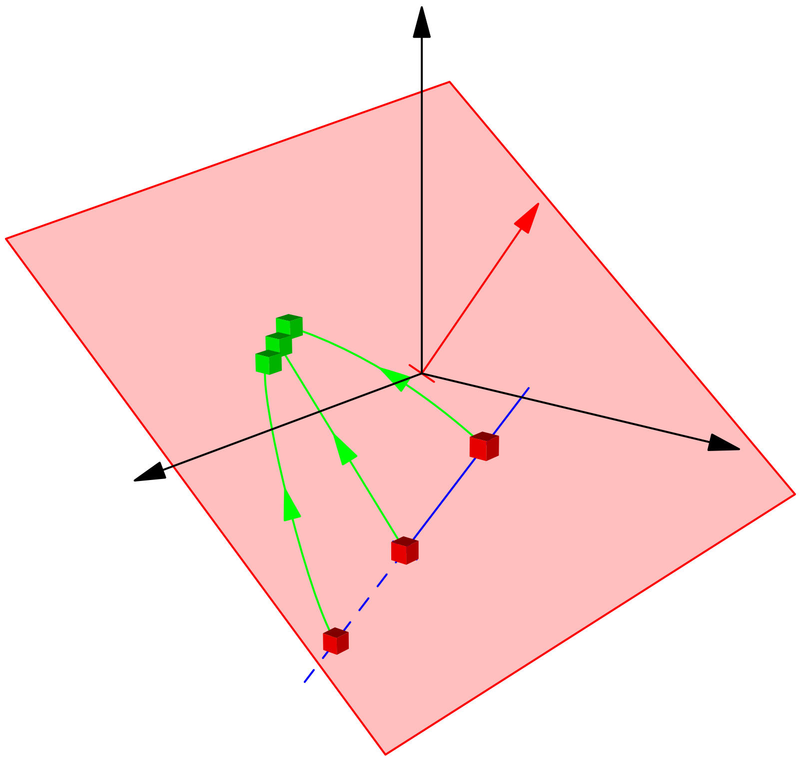
\end{aligned}
$$

- It is tedious to compute these things component-wise, but when you need to understand what is going on then go back to the basics

Outline

1. Mappings
2. **Linear Maps**



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**
- Note that in some directions you might be over-constrained and in other directions under-constrained

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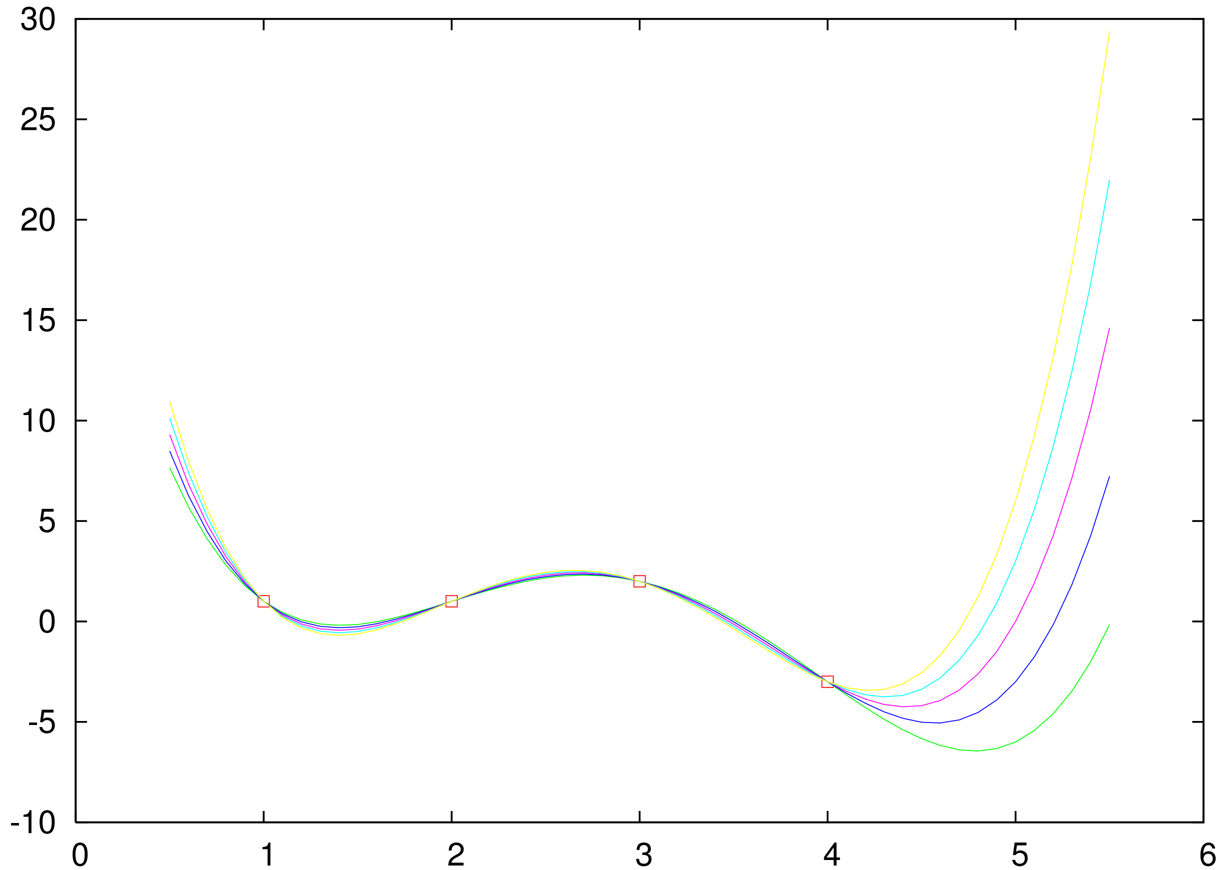
- This is very typical of most machine learning problems

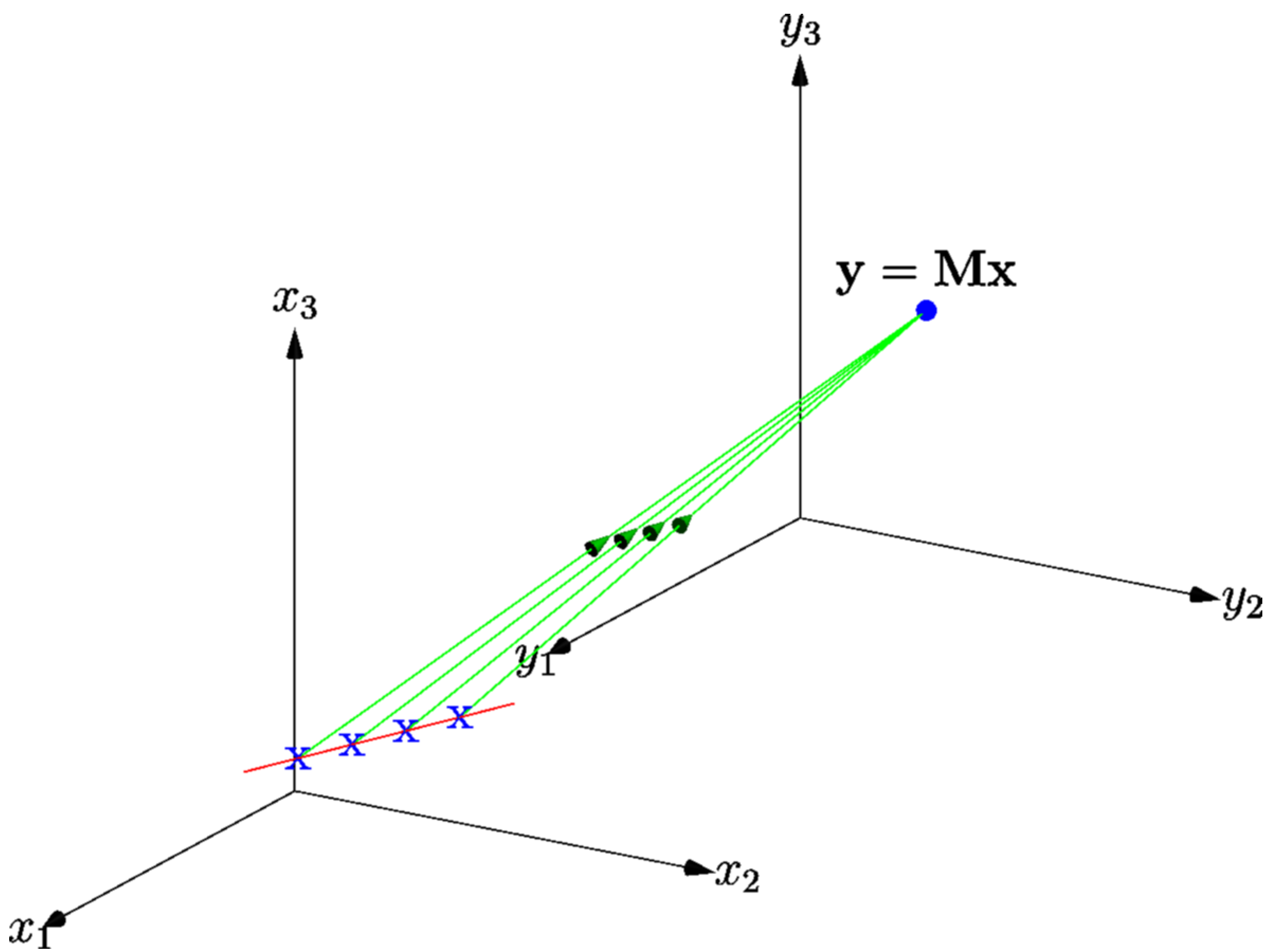
Under Constrained Systems

- 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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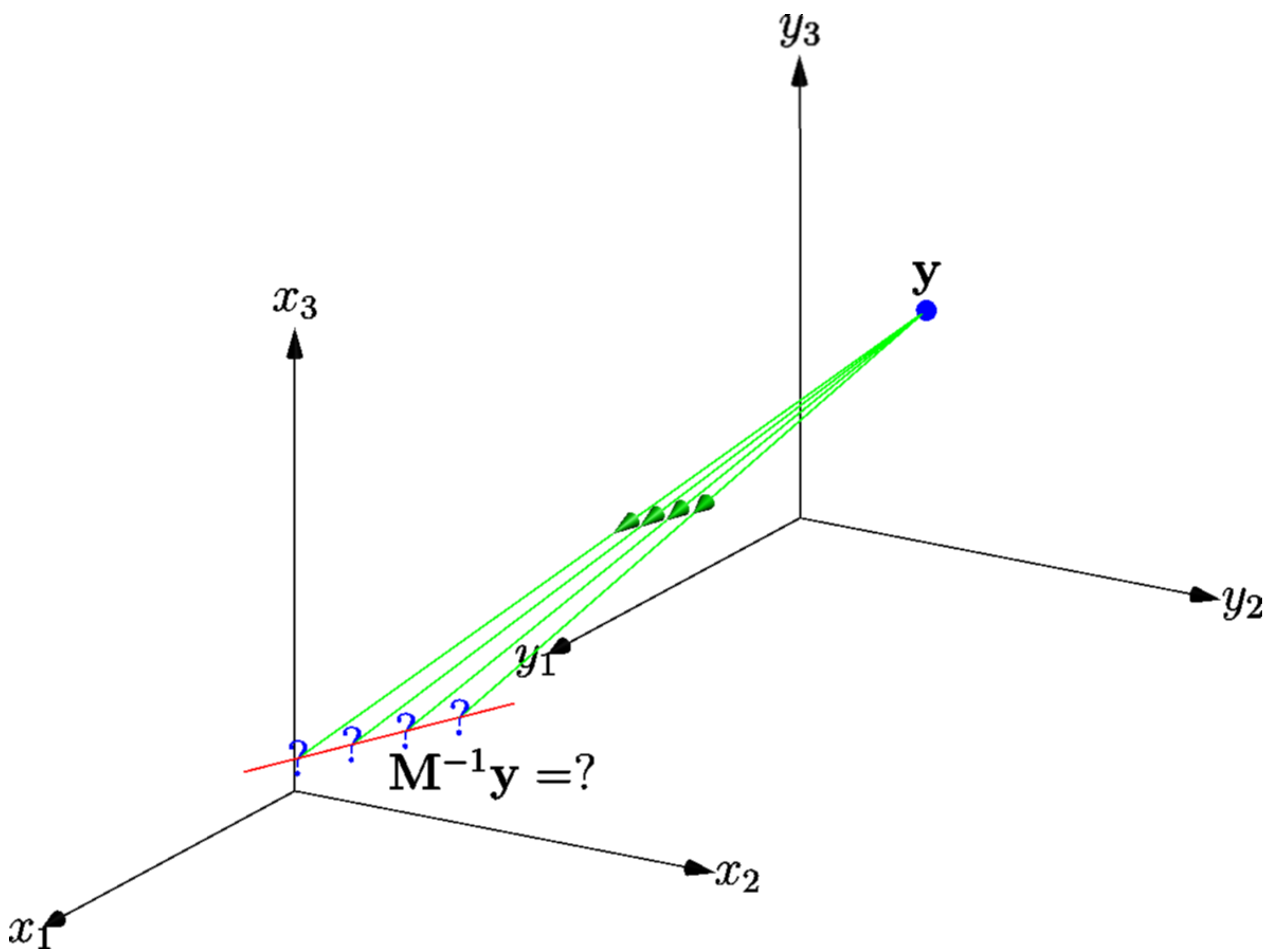

Under-constrained Systems

- 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**
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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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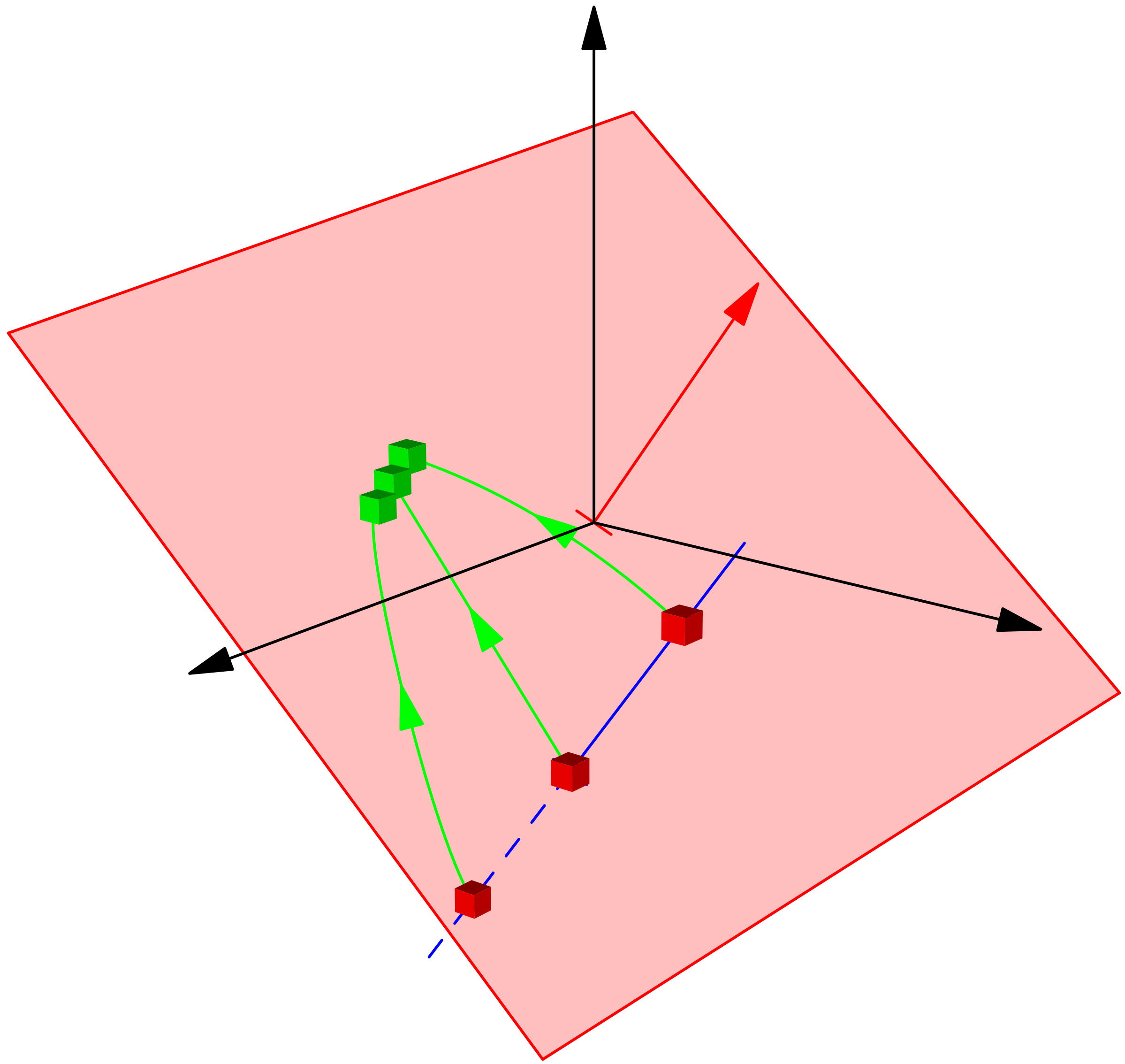
Ill-Conditioned Matrices



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

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