

Machine Learning with Python

MTH786U/P 2022/23

Lecture 5: From ridge regression to the LASSO

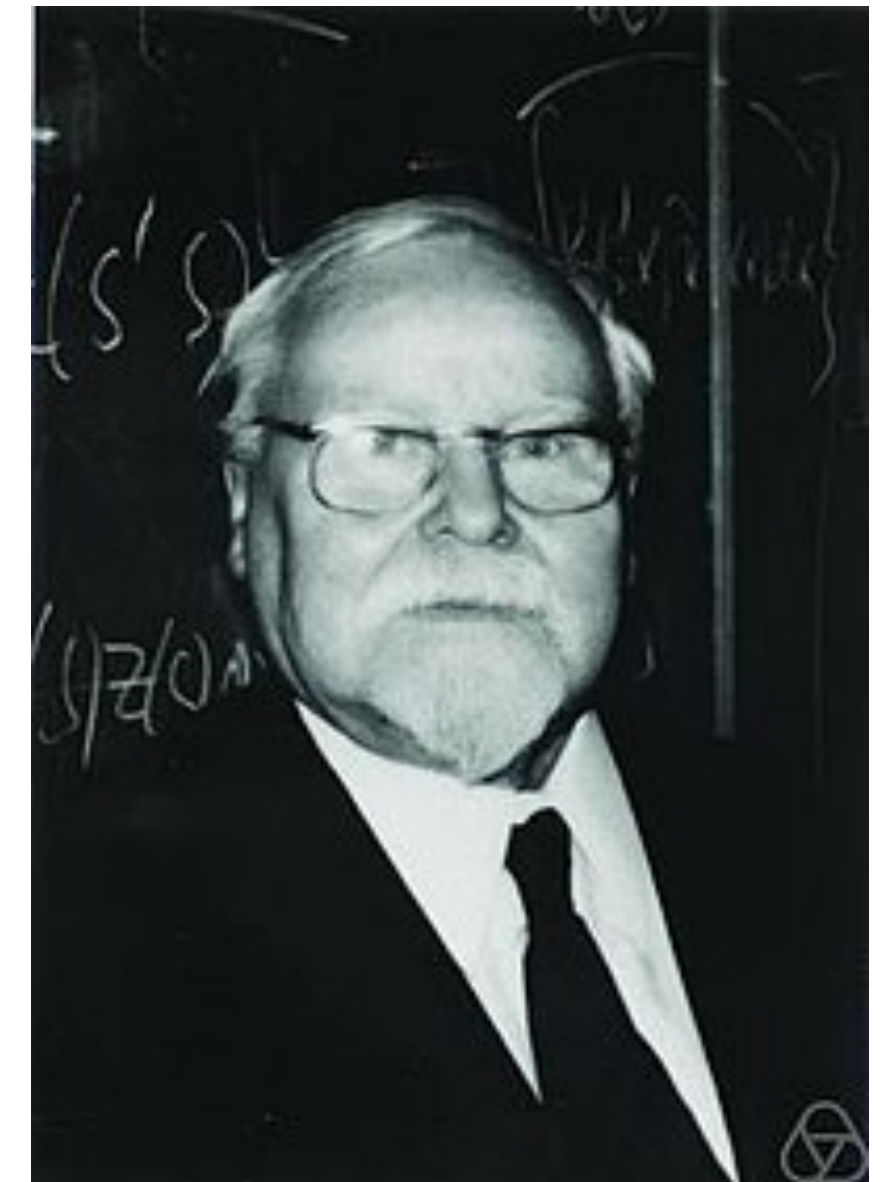
Nicola Perrà, Queen Mary University of London (QMUL)

Recap: Ridge regression

Two weeks ago we learned about the minimisation problem

$$\hat{\mathbf{w}} = \arg \min_{\mathbf{w}} \left\{ \frac{1}{2} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \frac{\alpha}{2} \|\mathbf{w}\|^2 \right\}$$

that is known as *Tikhonov regularisation*
or *ridge regression*



Andrey Tikhonov, 1906 - 1993



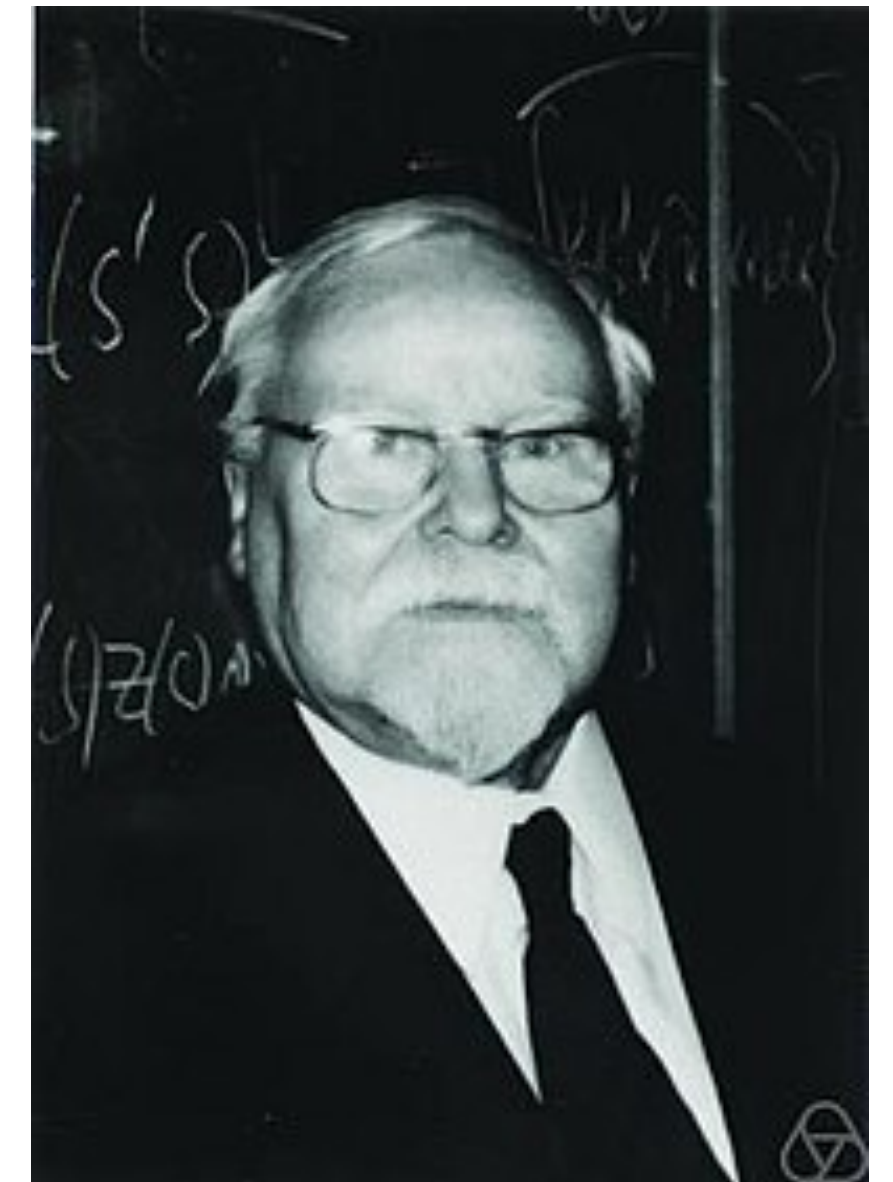
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Standard regression term

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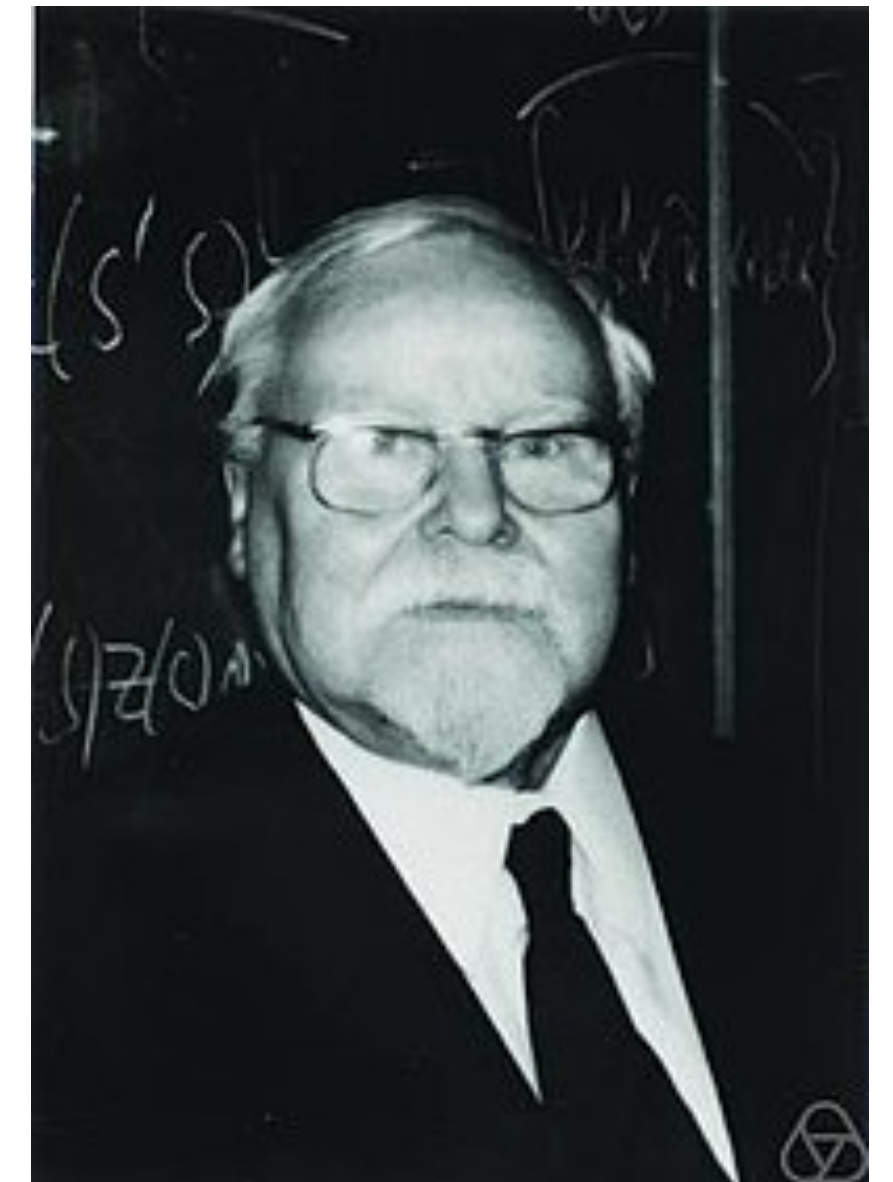
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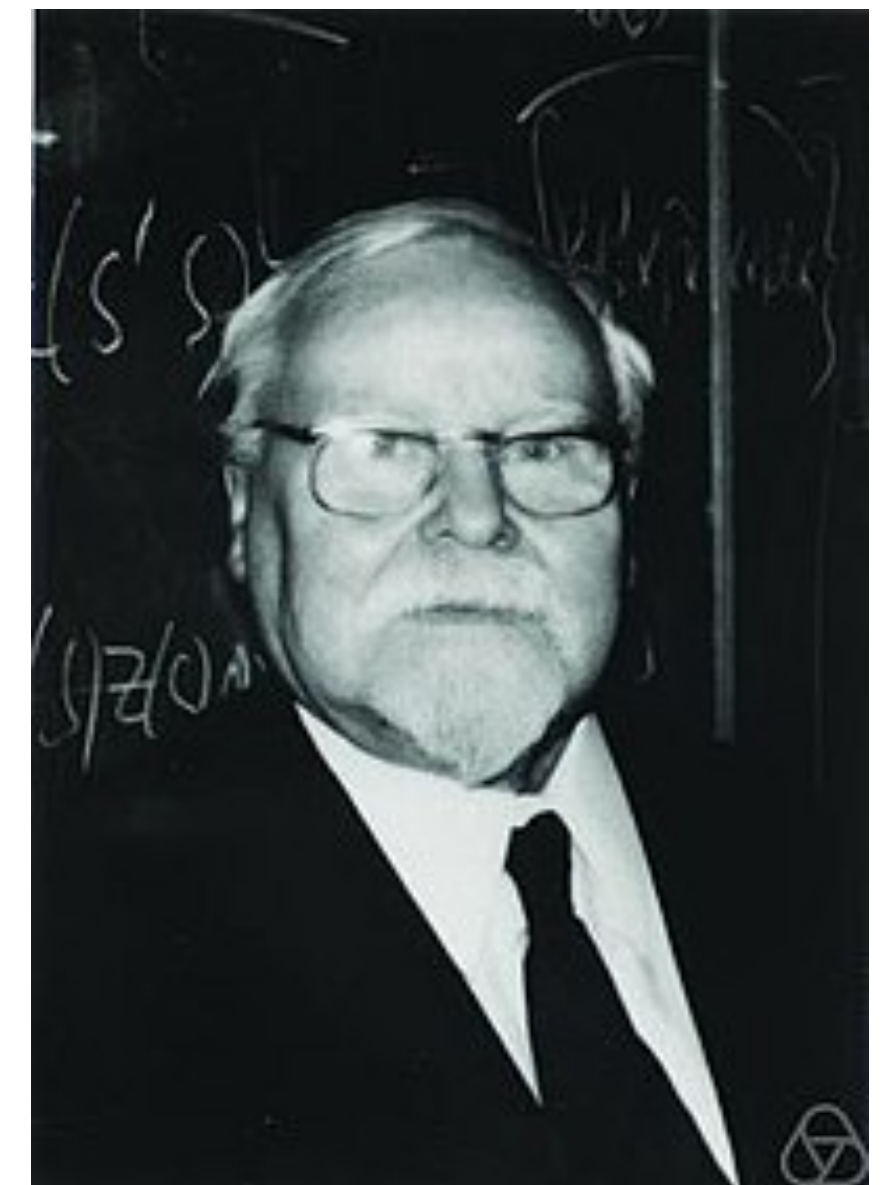
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Standard regression term

Regularisation term

Regularisation parameter

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Variational regularisation

A more general form of the previous problem is variational regularisation

$$\hat{\mathbf{w}} = \arg \min_{\mathbf{w}} \{L(\mathbf{w}) + R(\mathbf{w})\}$$



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Data term/
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Previous example:

$$L(\mathbf{w}) = \frac{1}{2} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$$

$$R(\mathbf{w}) = \frac{\alpha}{2} \|\mathbf{w}\|^2$$



ℓ_1 regularisation / the lasso

Variational regularisation: $\hat{\mathbf{w}} = \arg \min_{\mathbf{w}} \{L(\mathbf{w}) + R(\mathbf{w})\}$



ℓ_1 regularisation / the lasso

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Choose $R(\mathbf{w}) = \alpha \|\mathbf{w}\|_1 := \alpha \sum_{k=1}^n |w_k|$ and $L(\mathbf{w}) = \frac{1}{2} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$



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What is the advantage of using the one-norm over the two-norm?



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Sparsity!



ℓ_1 regularisation / the lasso

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Implicit reduction of parameters



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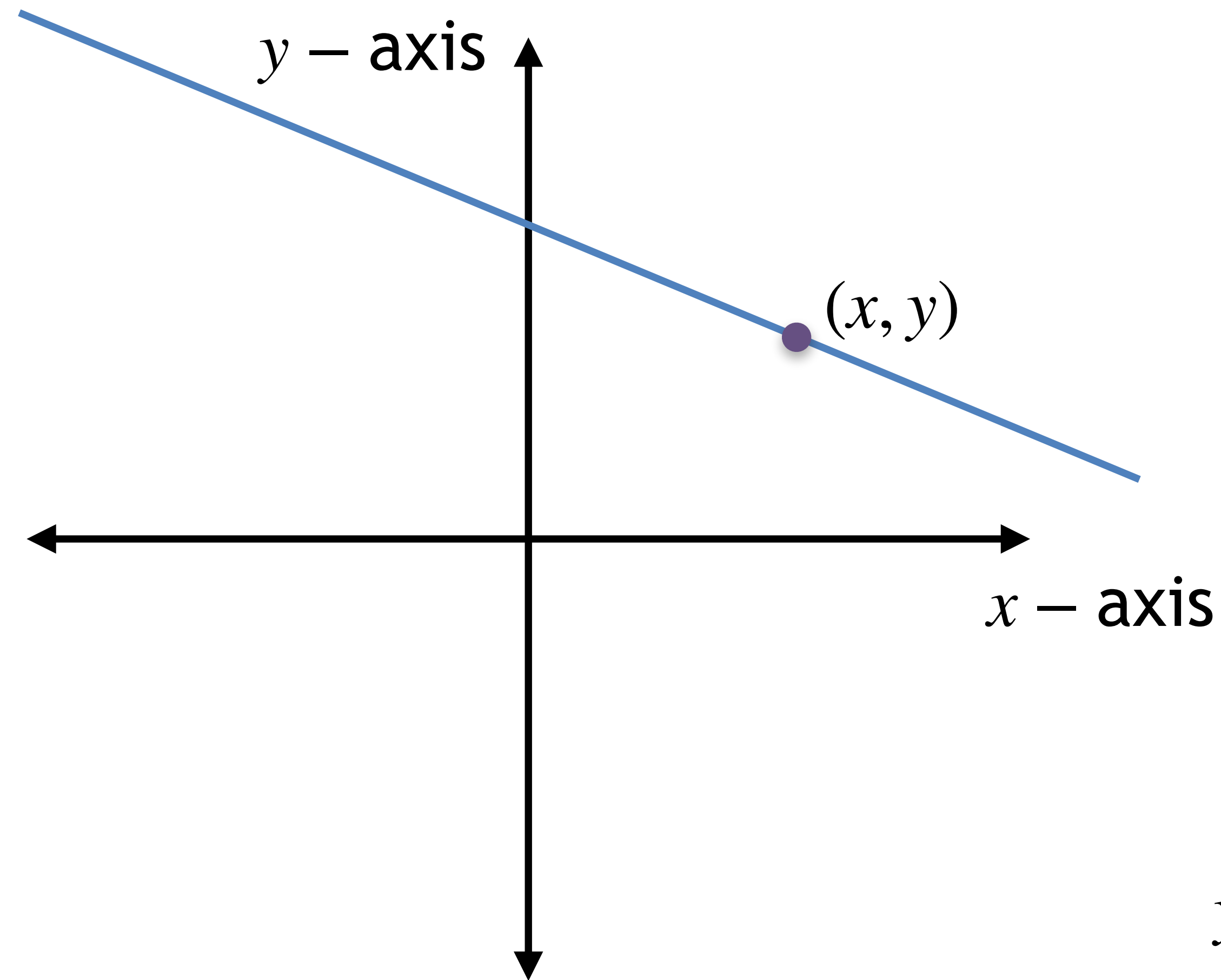
Implicit reduction of parameters

LASSO = Least Absolute Shrinkage and Selection Operator



ℓ_1 regularisation / the lasso

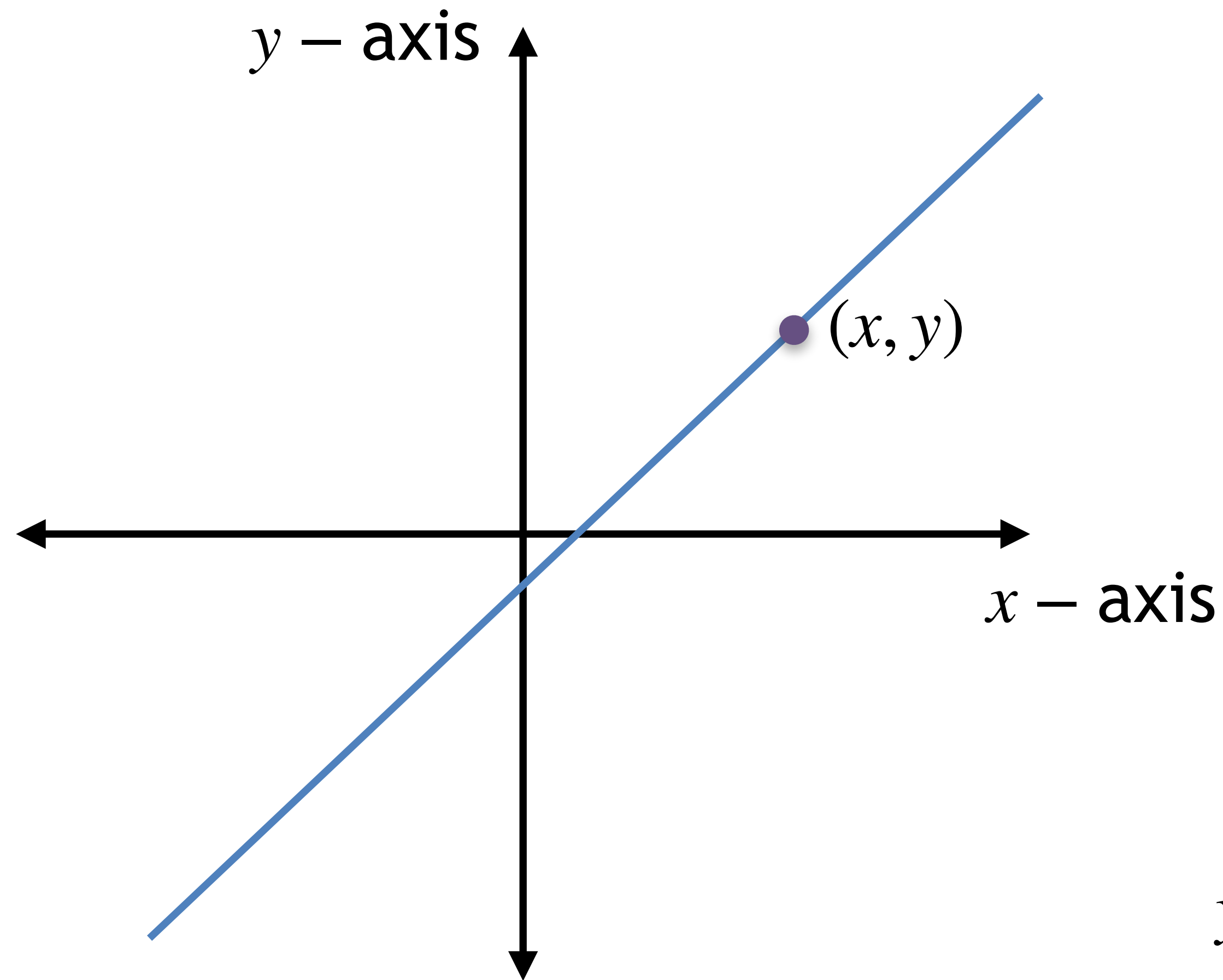
Example: fit line with just one input/output data sample (x, y)



$$y = w_1x + w_0$$

ℓ_1 regularisation / the lasso

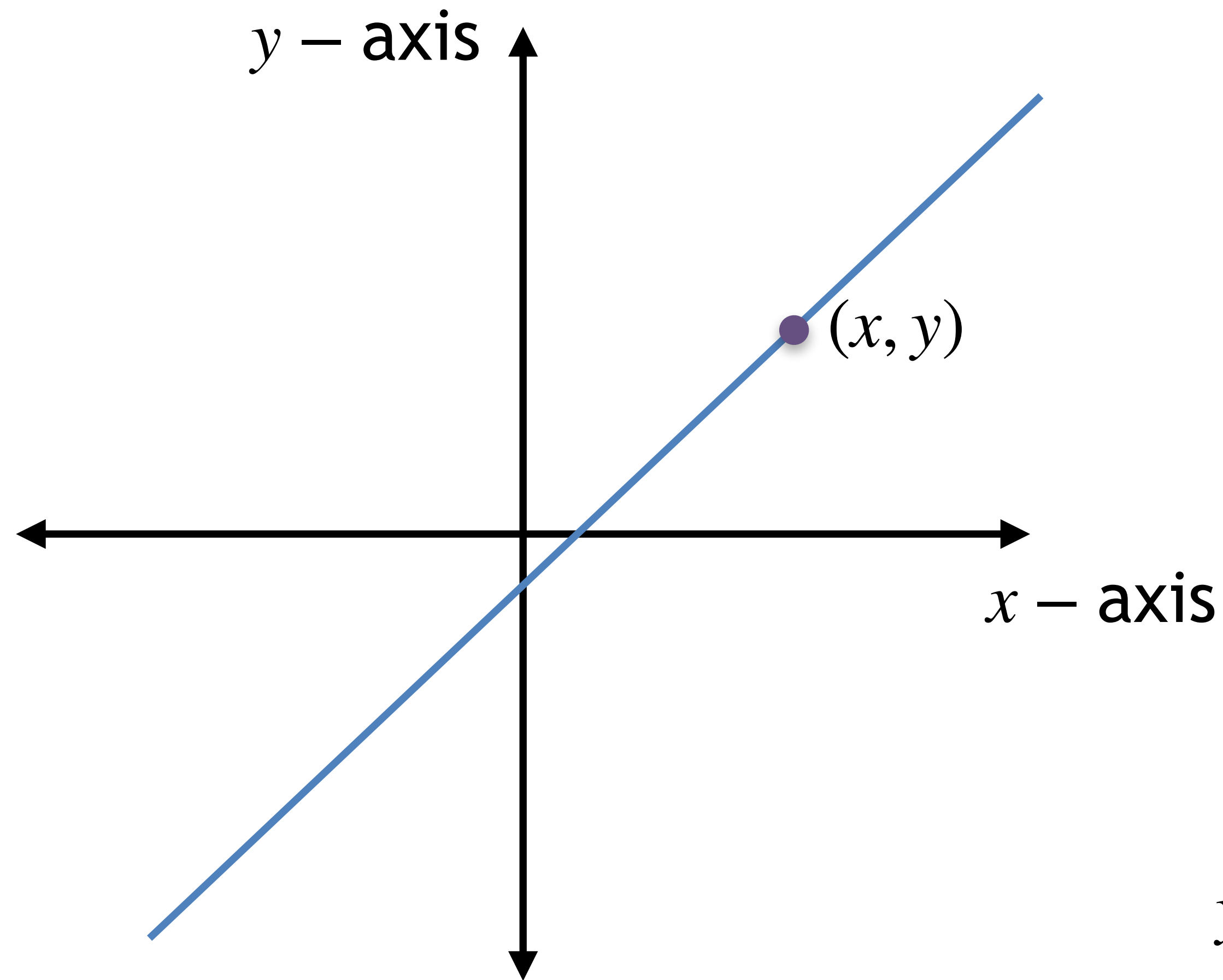
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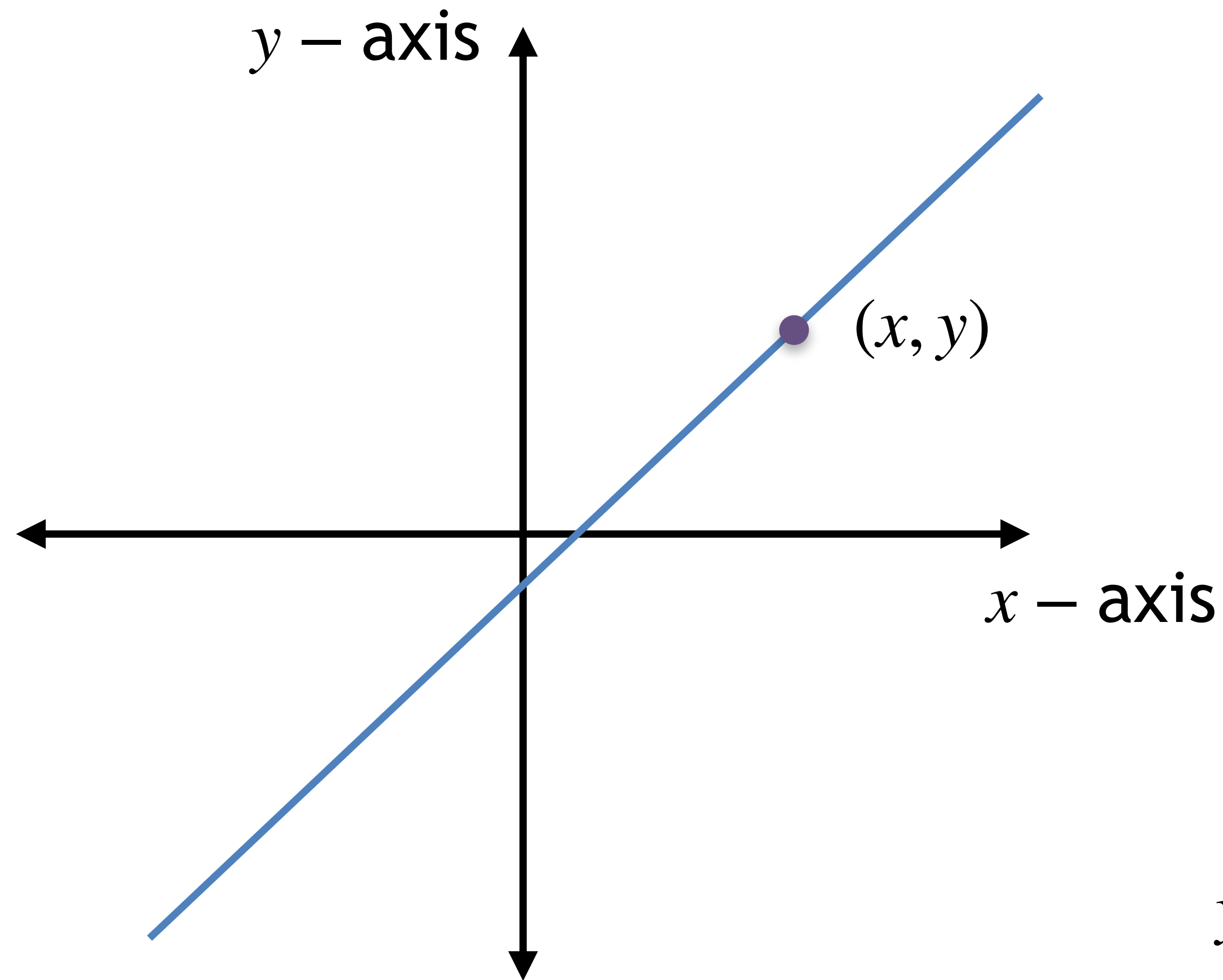


Which solution do we pick?

$$y = w_1x + w_0$$

ℓ_1 regularisation / the lasso

Example: fit line with just one input/output data sample (x, y)

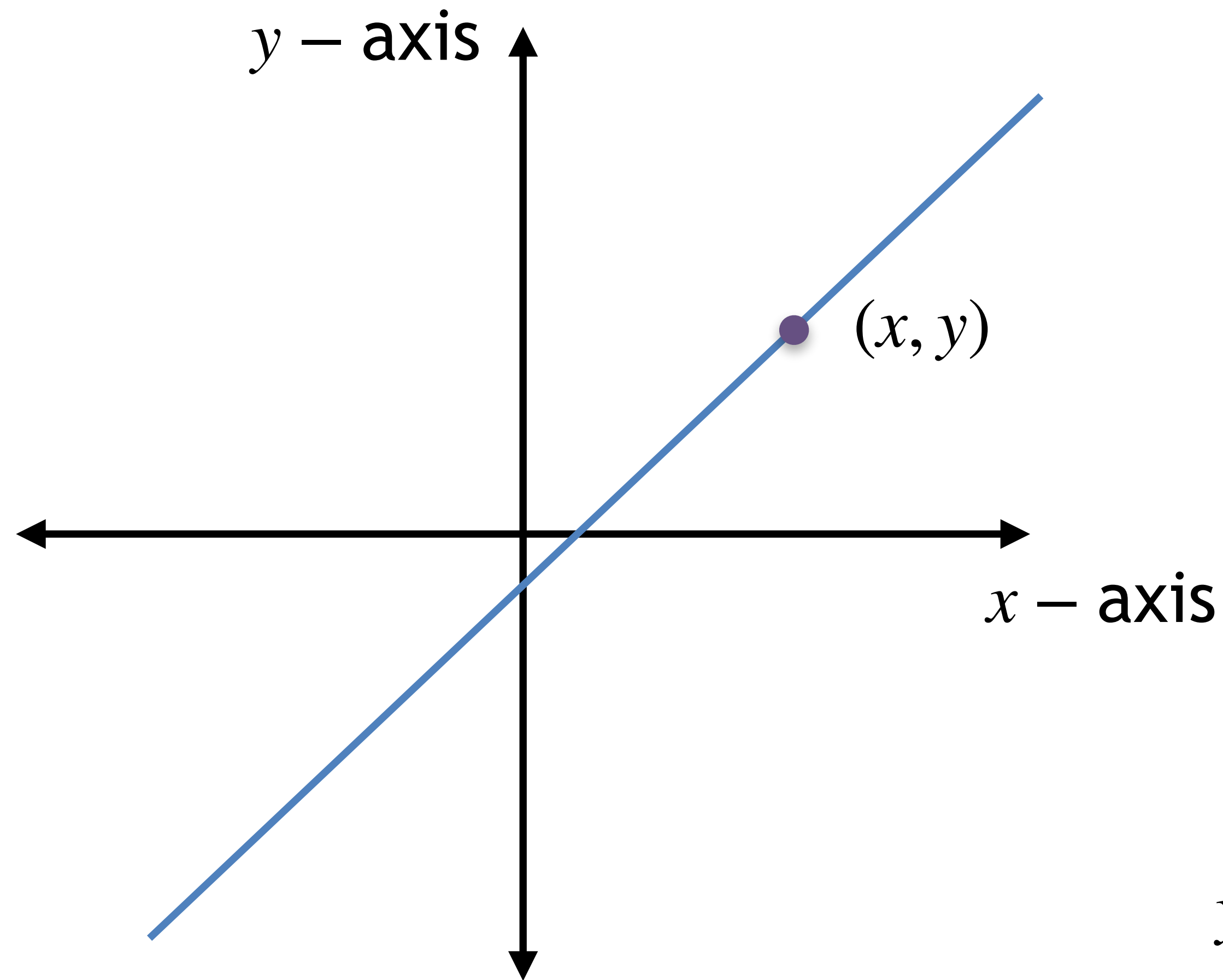


Simplicity idea:

$$y = w_1x + w_0$$

ℓ_1 regularisation / the lasso

Example: fit line with just one input/output data sample (x, y)



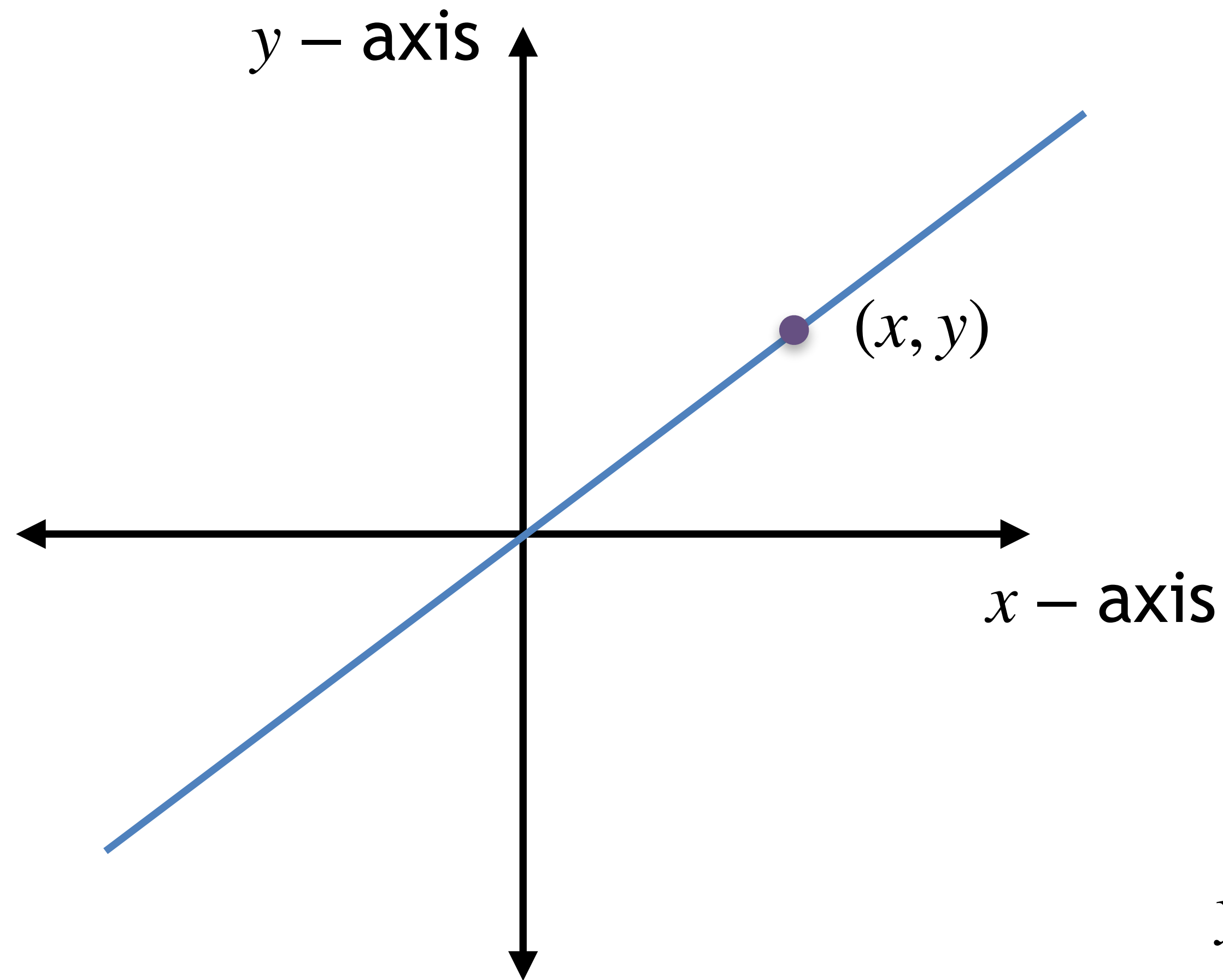
Simplicity idea:

Let either w_0 or w_1 be zero!

$$y = w_1x + w_0$$

ℓ_1 regularisation / the lasso

Example: fit line with just one input/output data sample (x, y)



Simplicity idea:

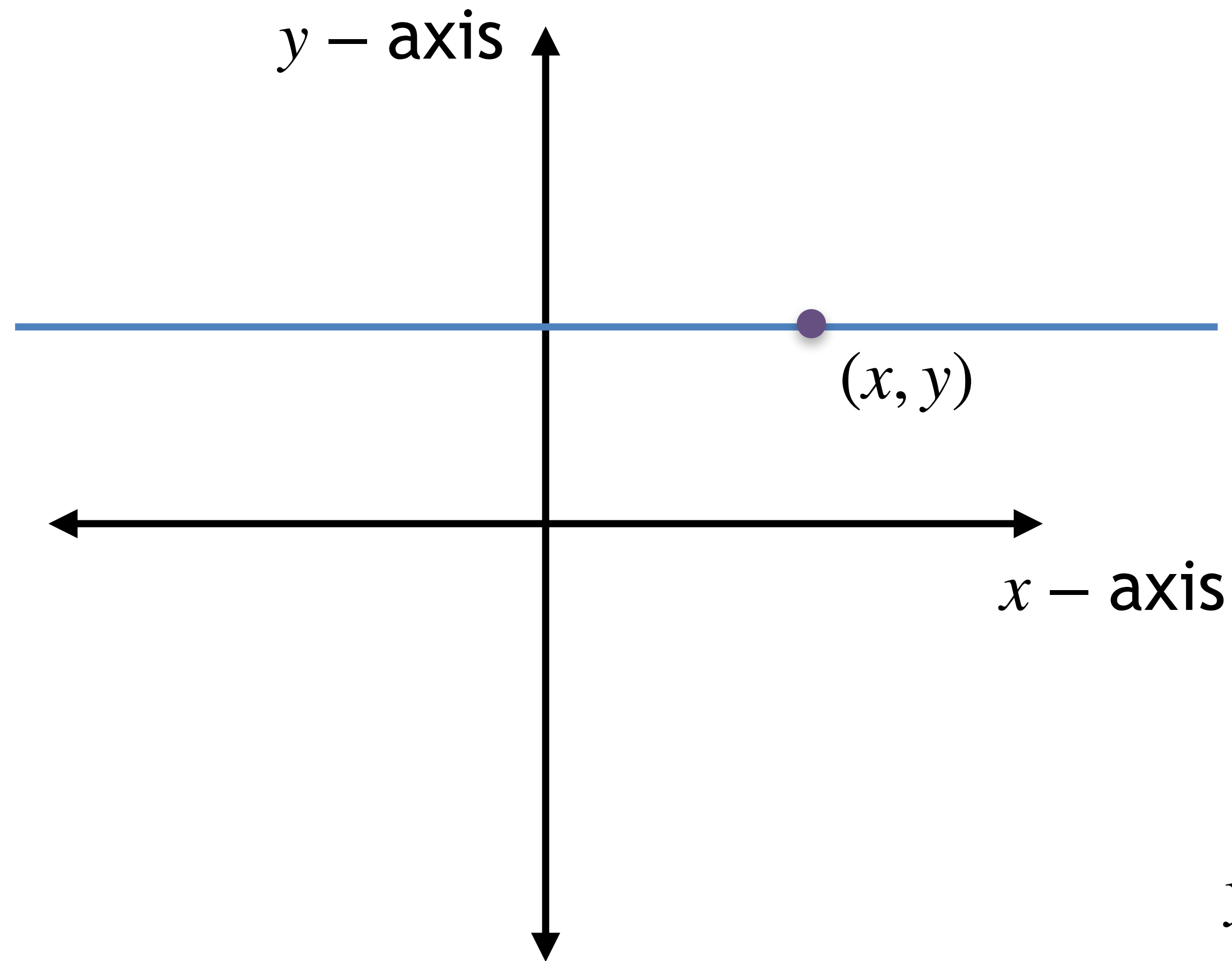
$$w_0 = 0$$

$$y = xw_1$$

$$y = w_1x + w_0$$

ℓ_1 regularisation / the lasso

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Simplicity idea:

$$w_1 = 0$$

$$y = w_0$$

$$y = w_1x + w_0$$

ℓ_1 regularisation / the lasso



ℓ^1 regularisation / the lasso

In general, why (or how) does the ℓ^1 norm make \hat{w} sparse?



ℓ_1 regularisation / the lasso

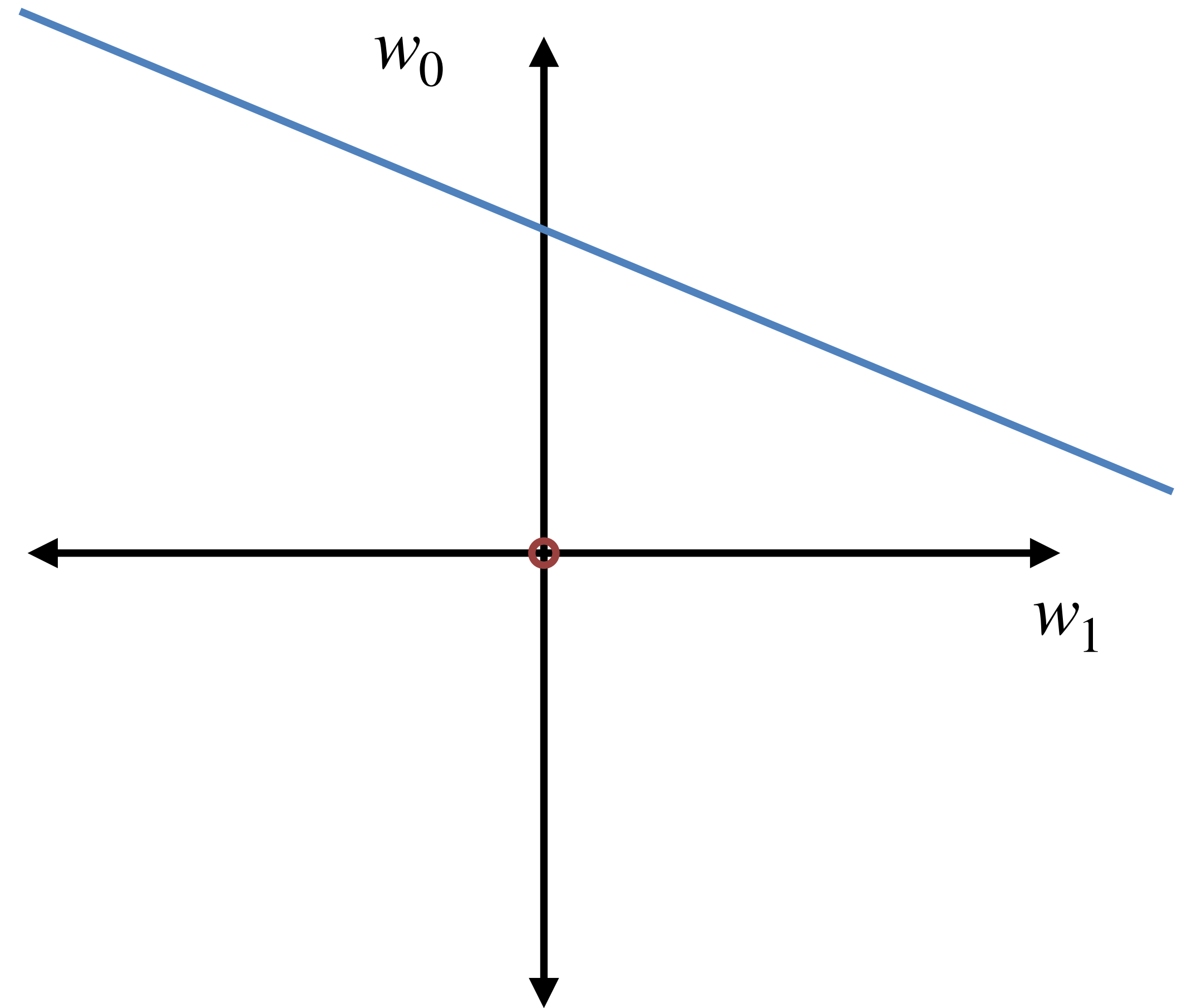
The solution of the problem

$$y = w_0 + w_1 x$$

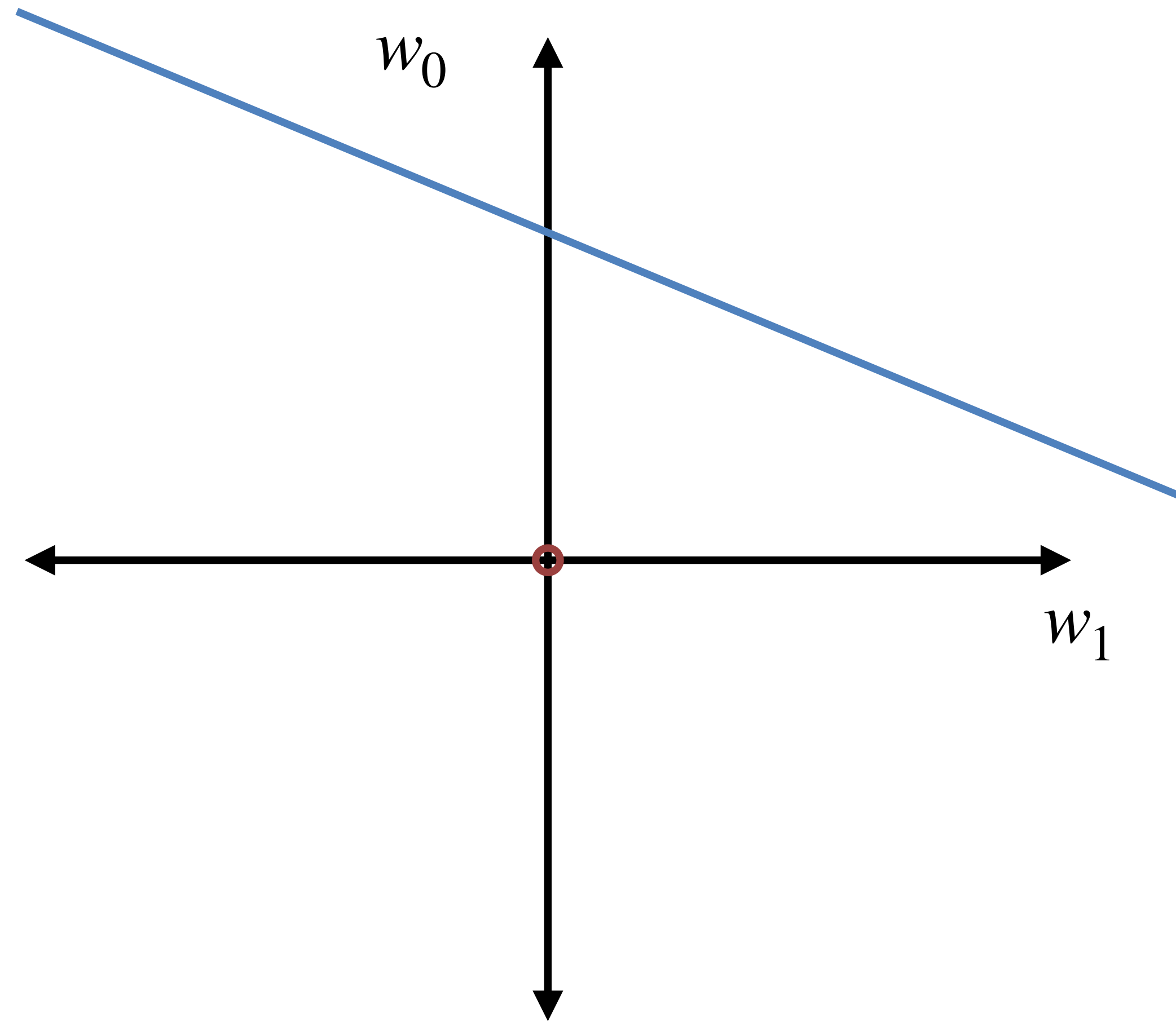
is a point in this space

We can indeed write

$$w_0 = y - w_1 x$$



ℓ_1 regularisation / the lasso



Minimise

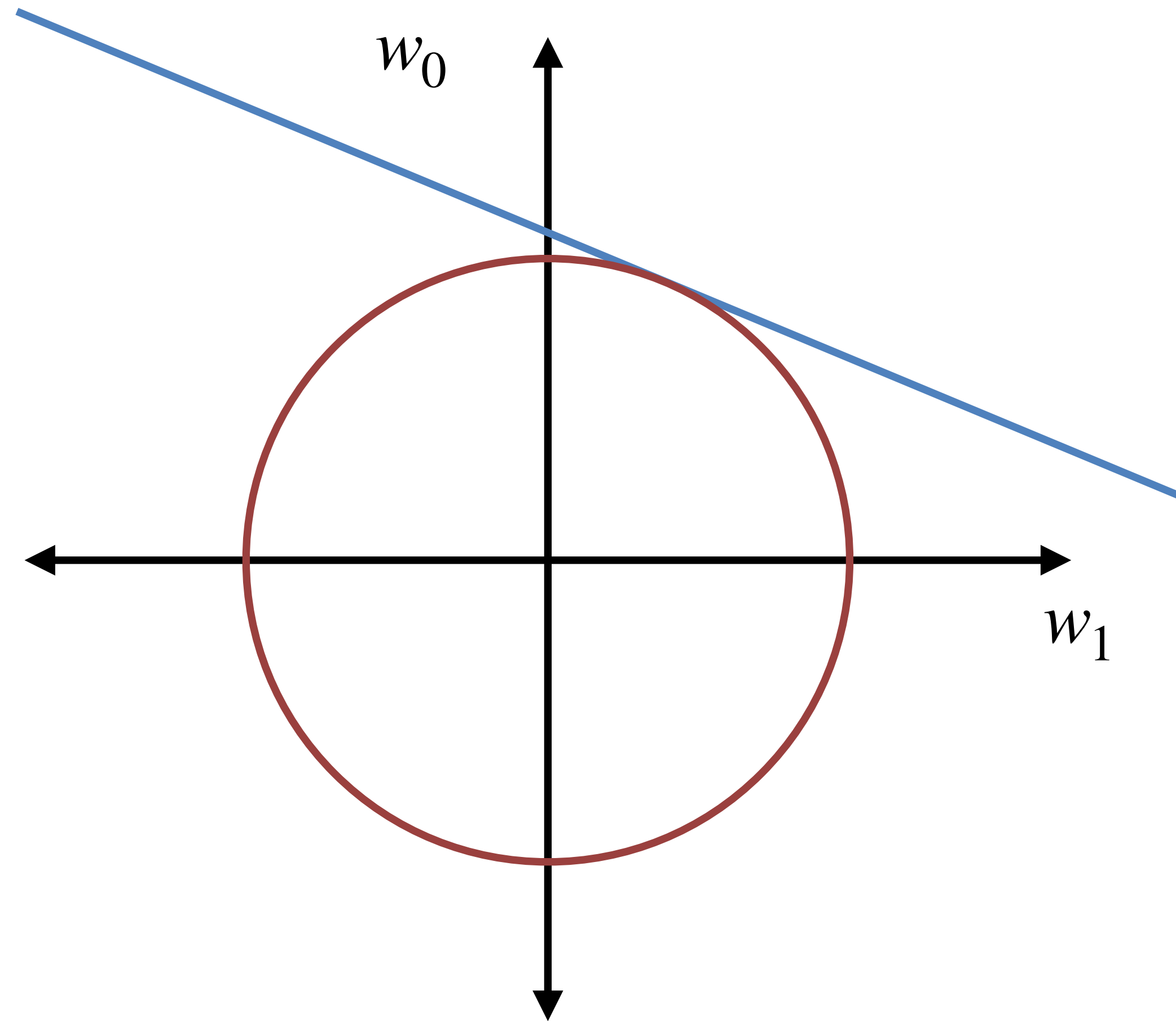
$$\sqrt{w_0^2 + w_1^2}$$

subject to

$$w_0 = -w_1x + y$$



ℓ_1 regularisation / the lasso



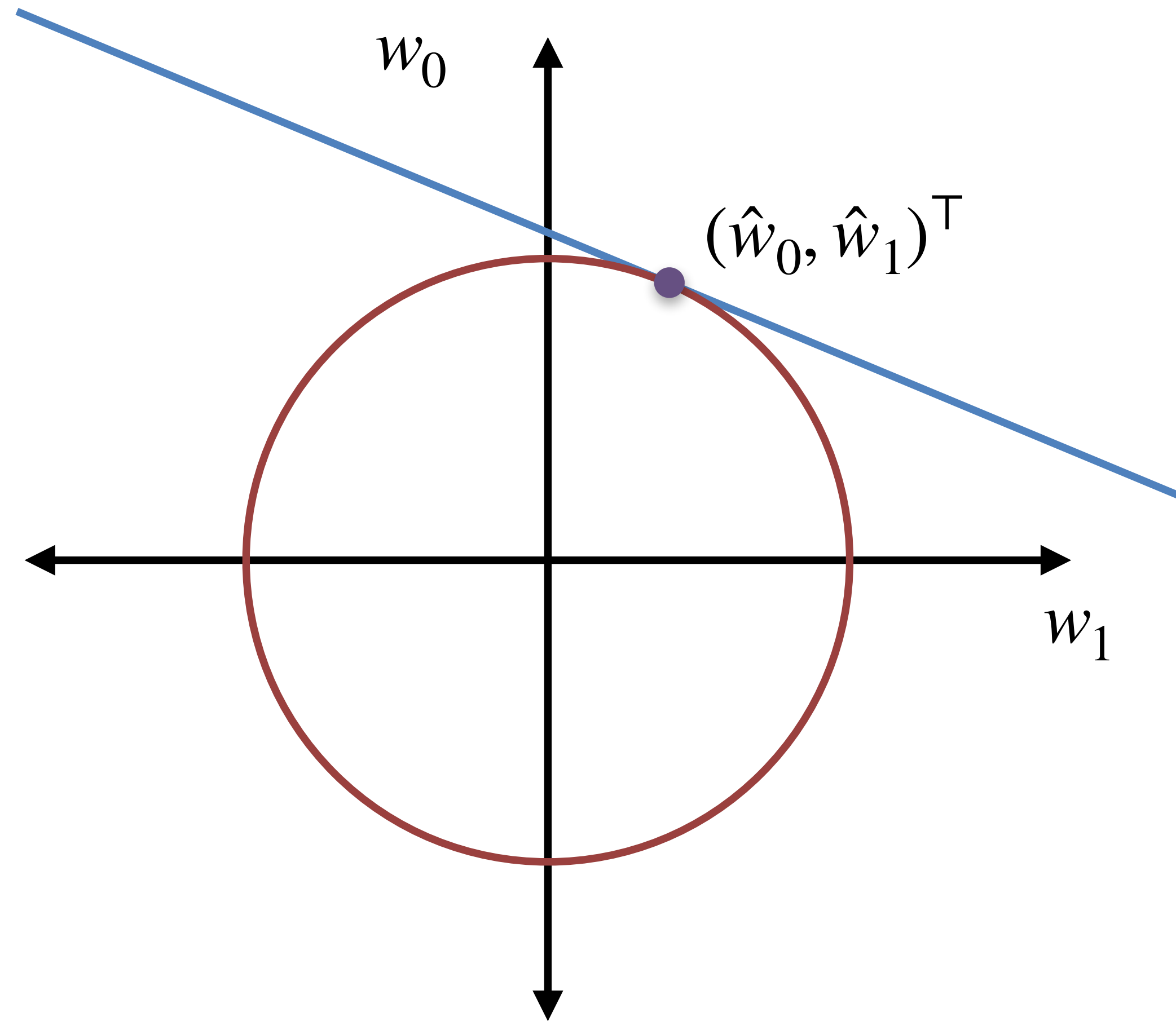
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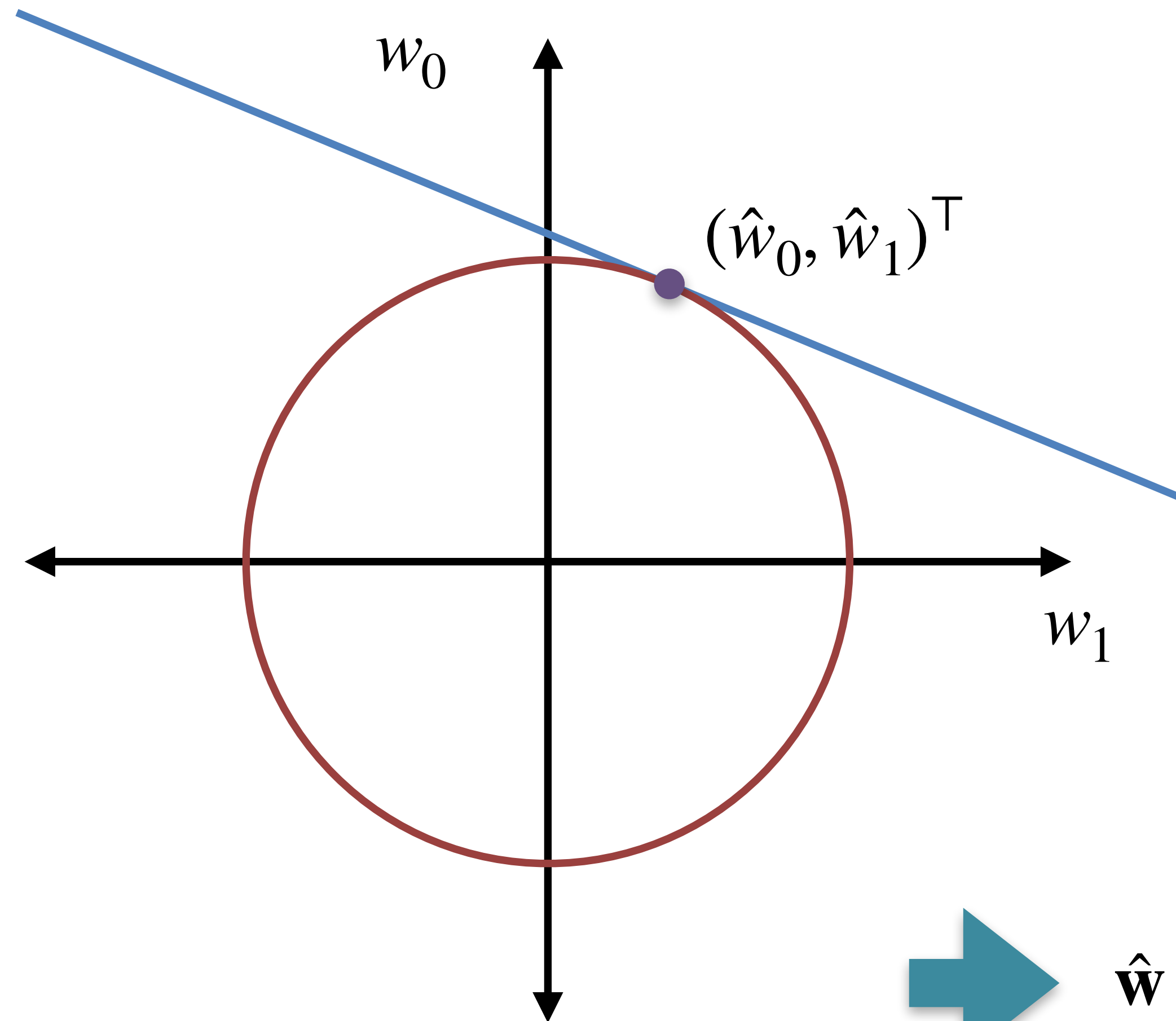
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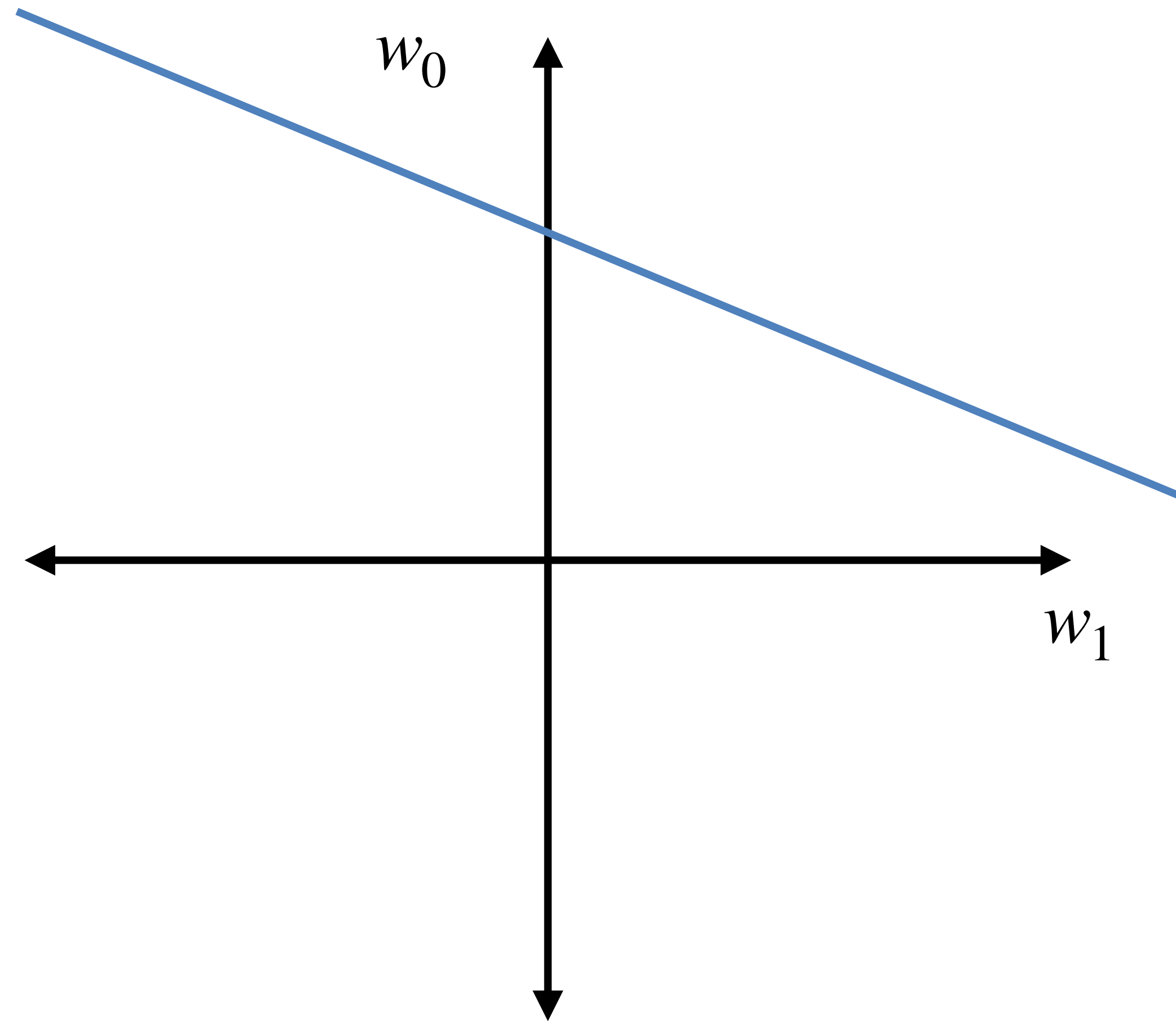
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$\hat{\mathbf{w}} = (\hat{w}_0, \hat{w}_1)^T$ most likely **not** sparse

ℓ_1 regularisation / the lasso



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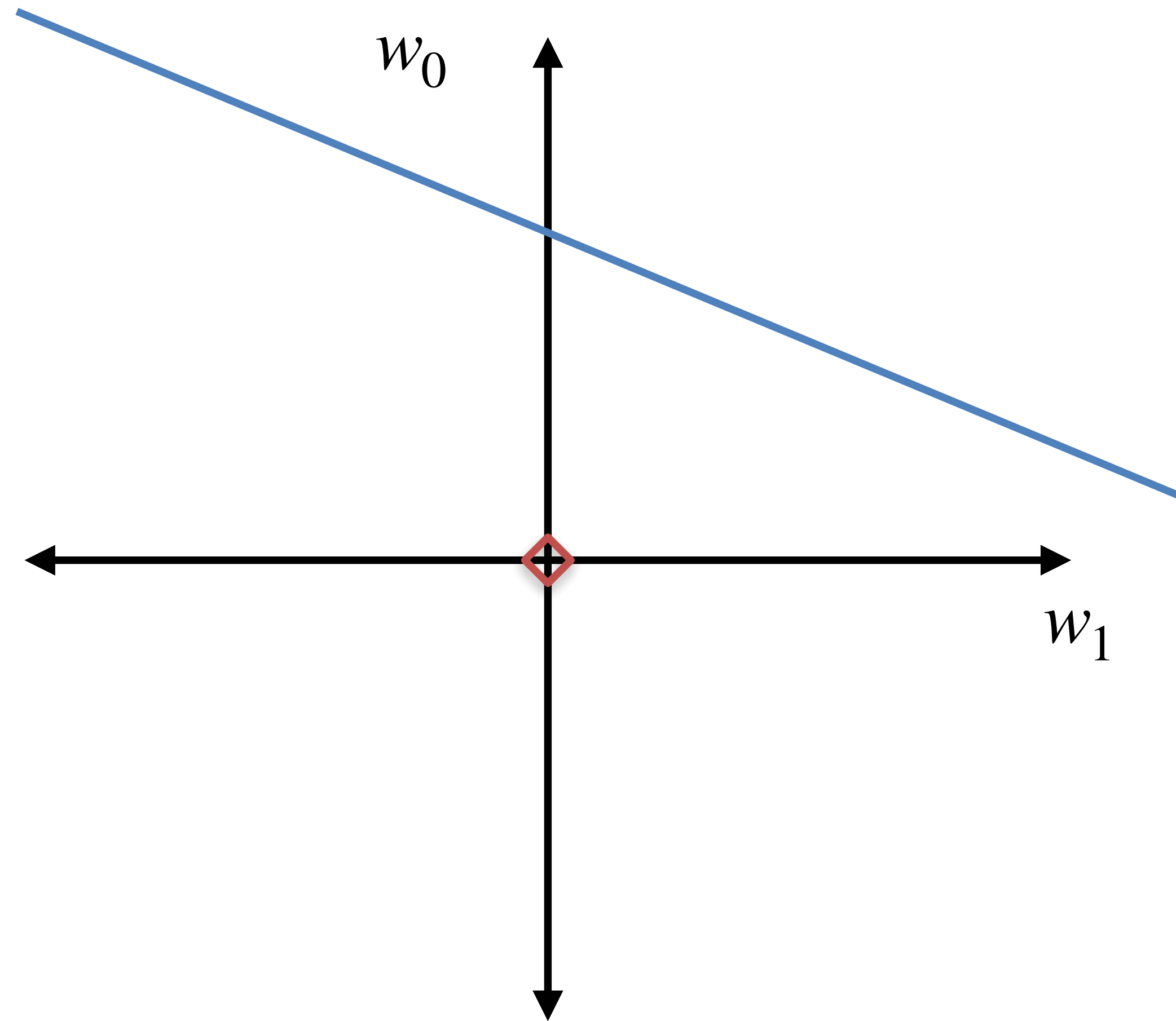
$$|w_0| + |w_1|$$

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ℓ_1 regularisation / the lasso



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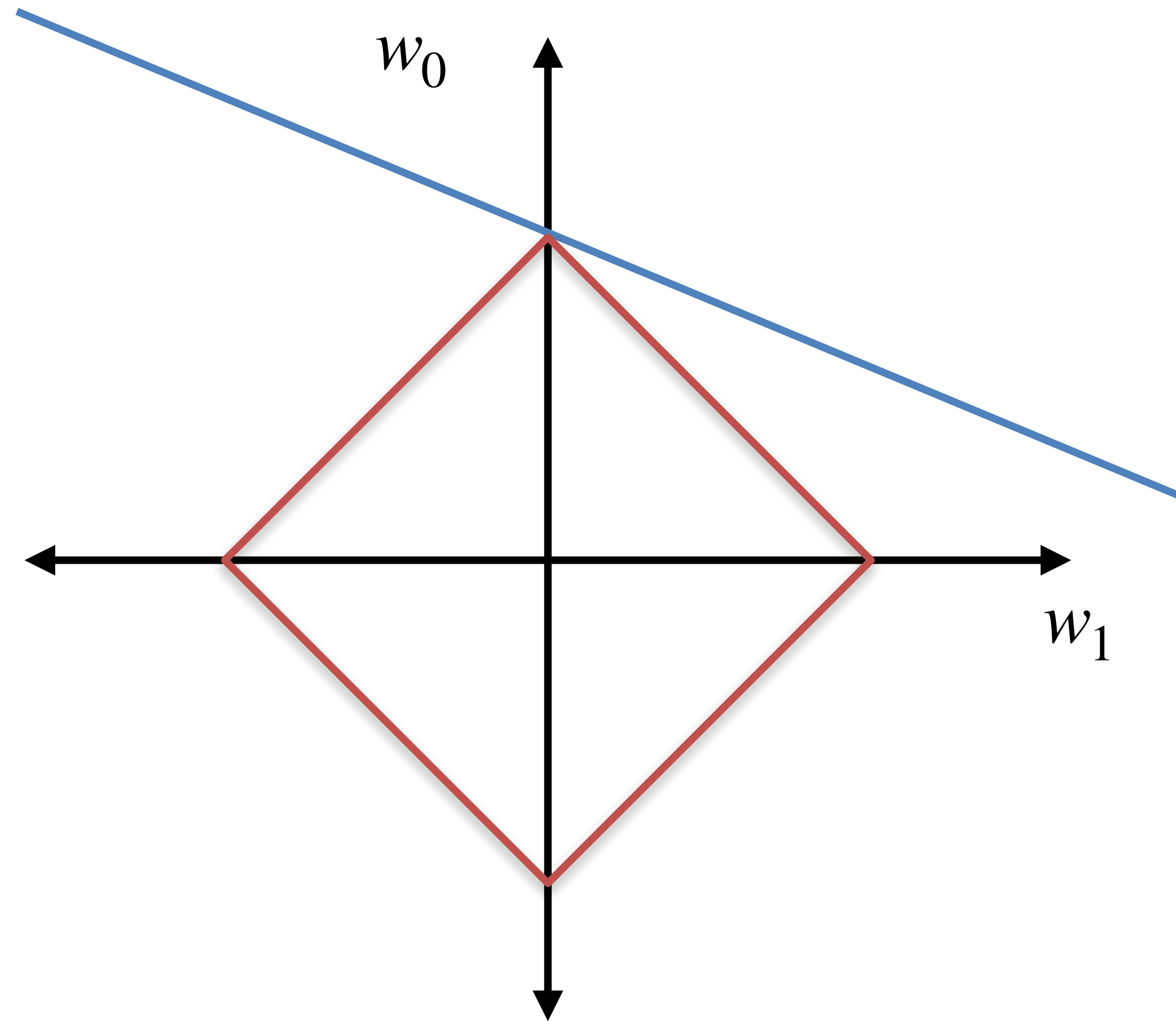
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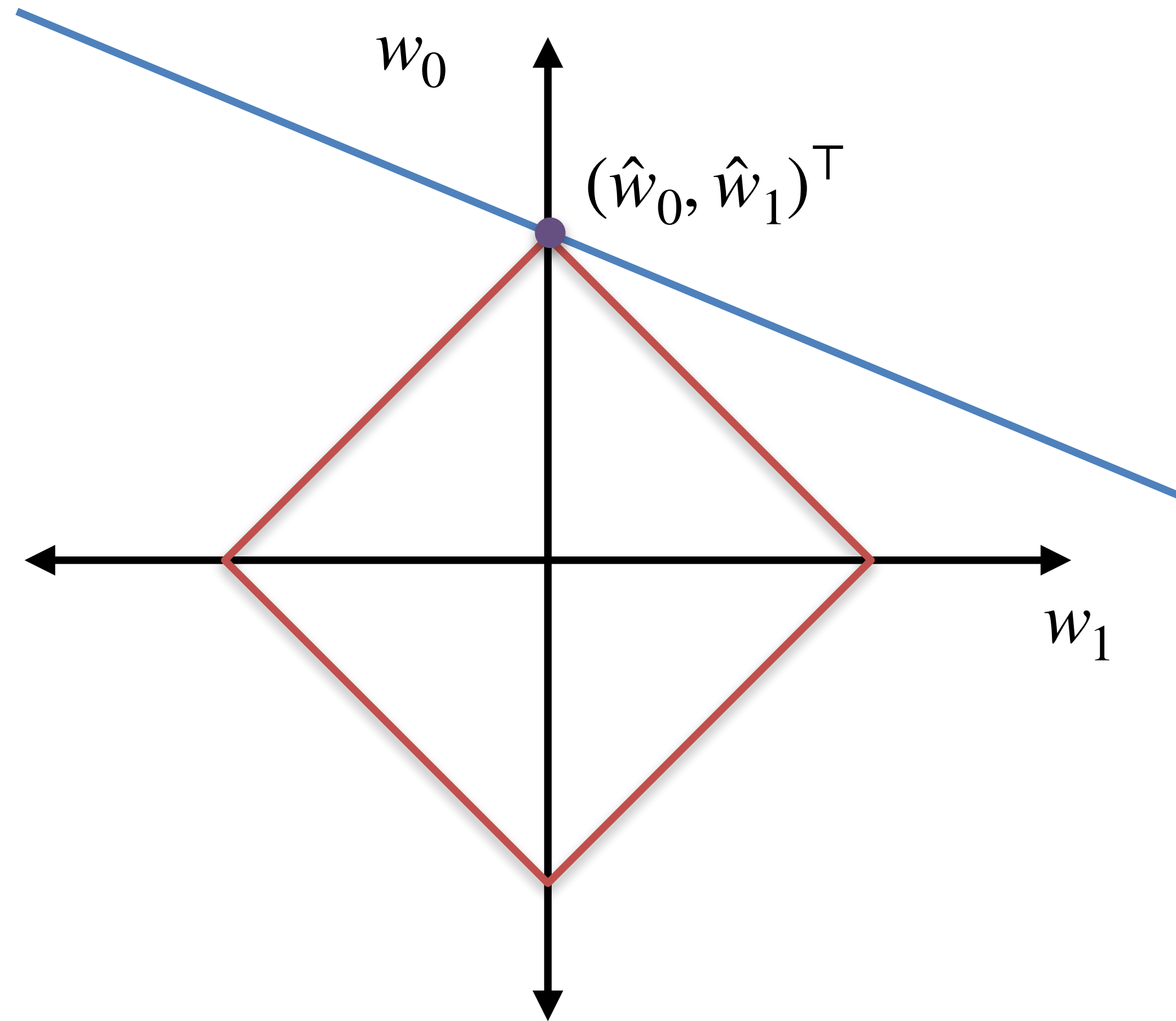
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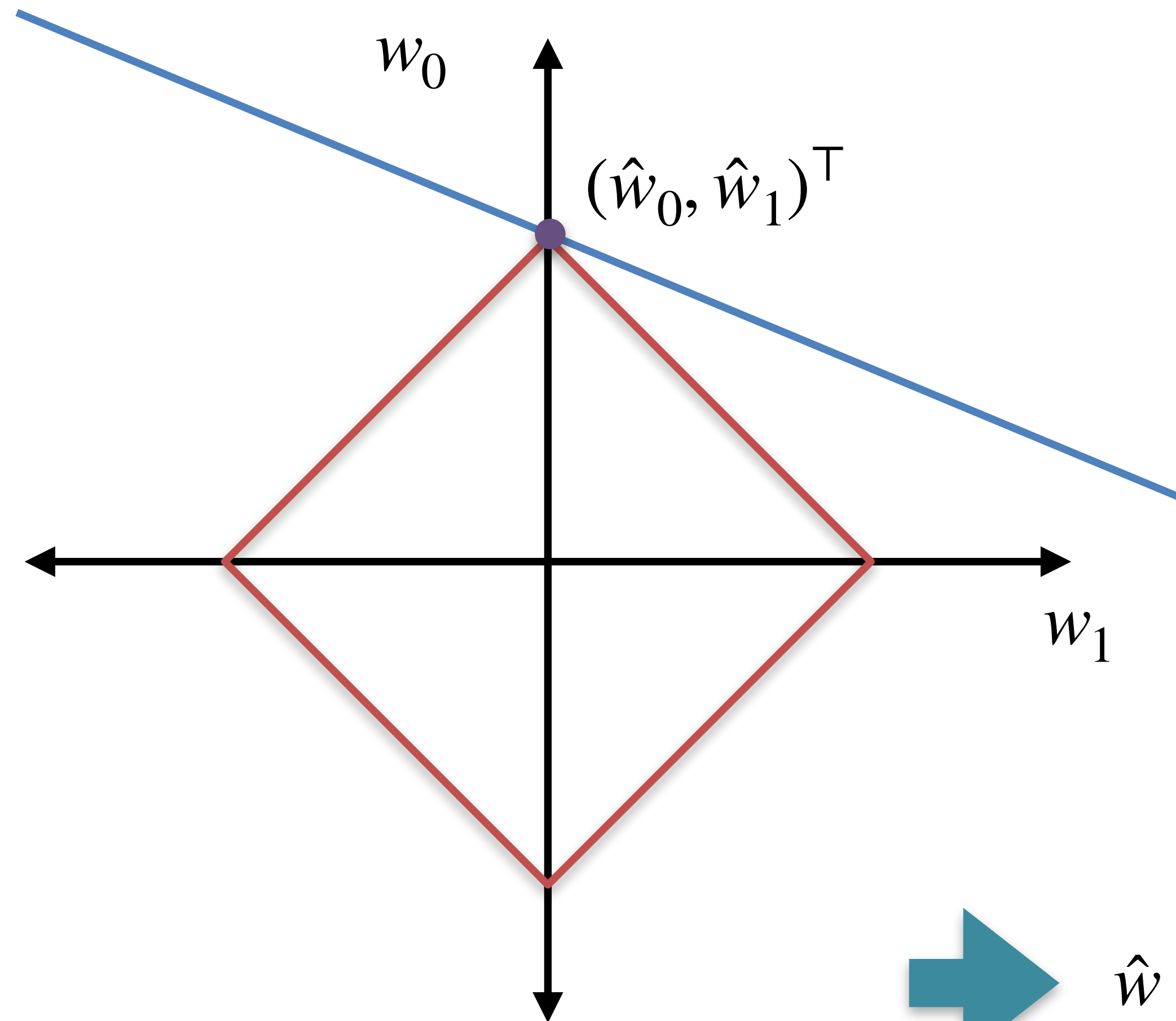
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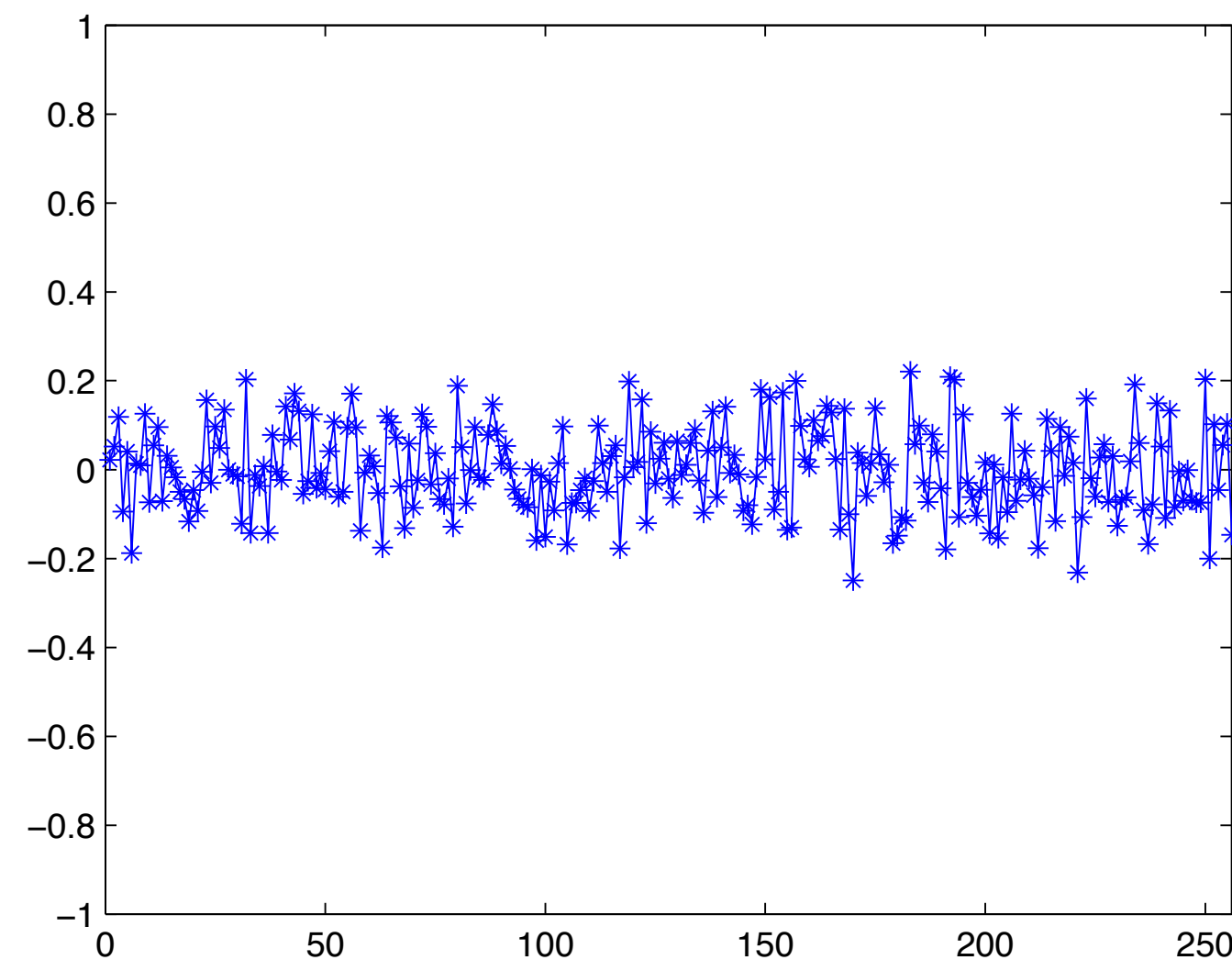
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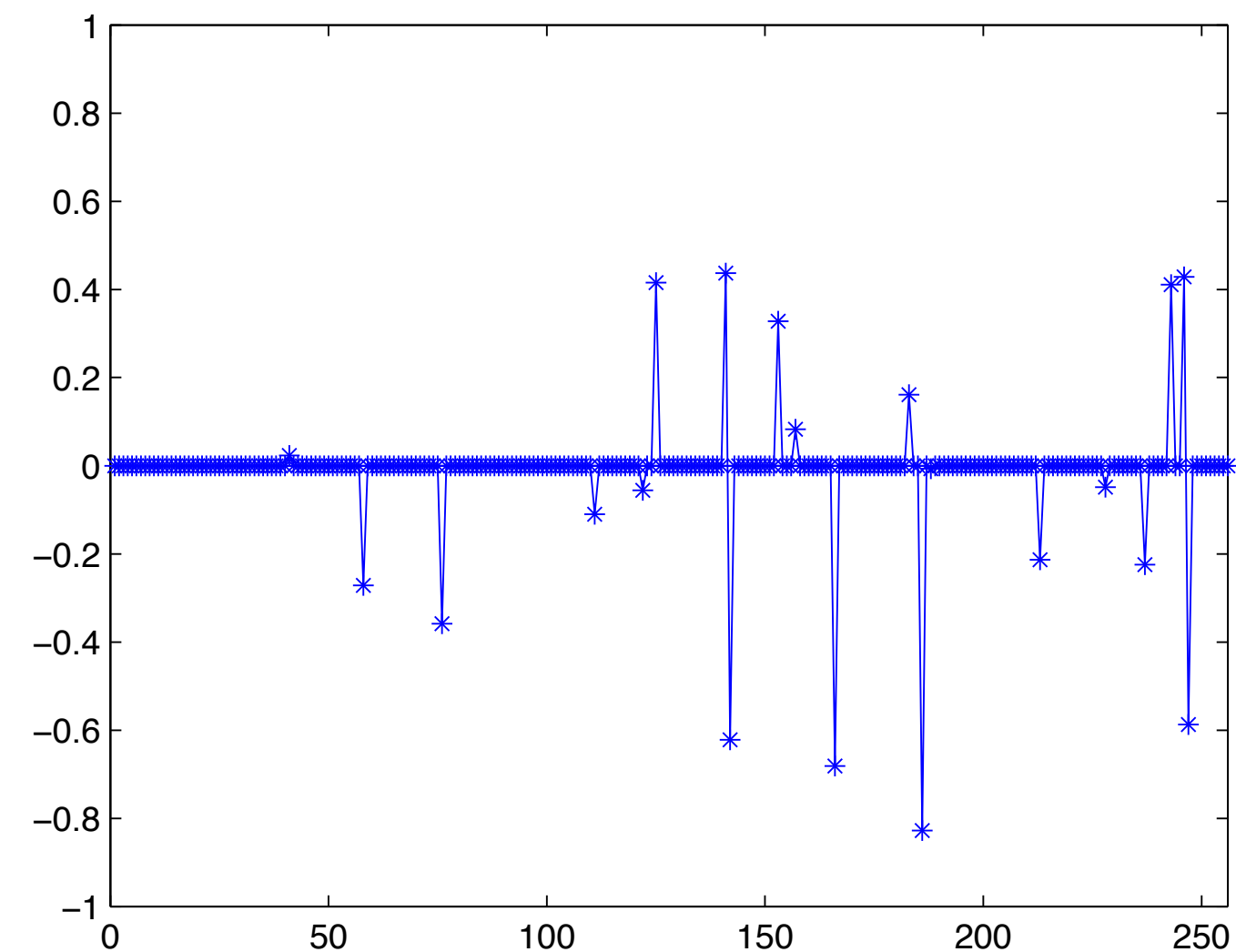
most likely sparse!

One of the coordinates
must be zero

ℓ_1 regularisation / the lasso



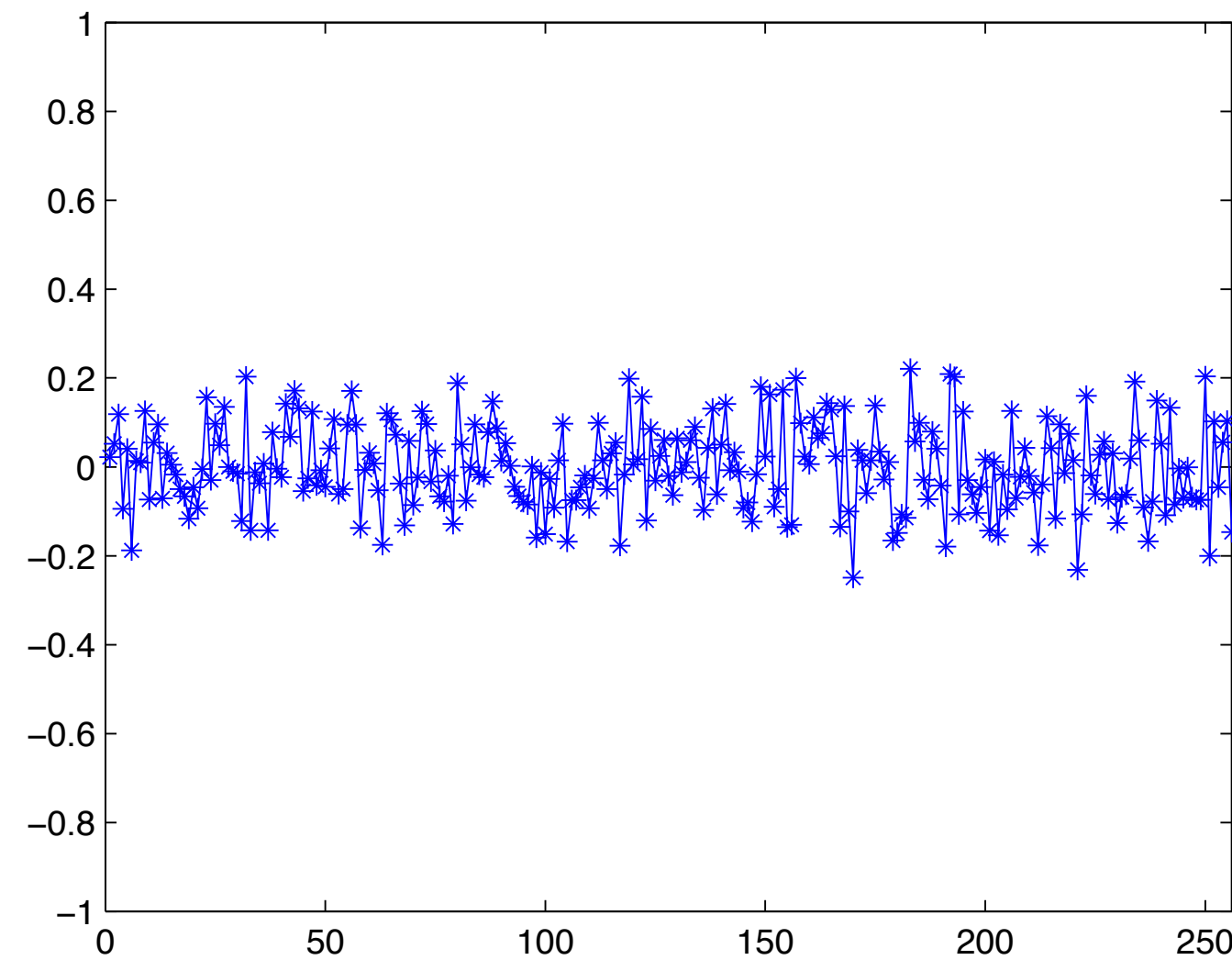
(a) Dense



(b) Sparse

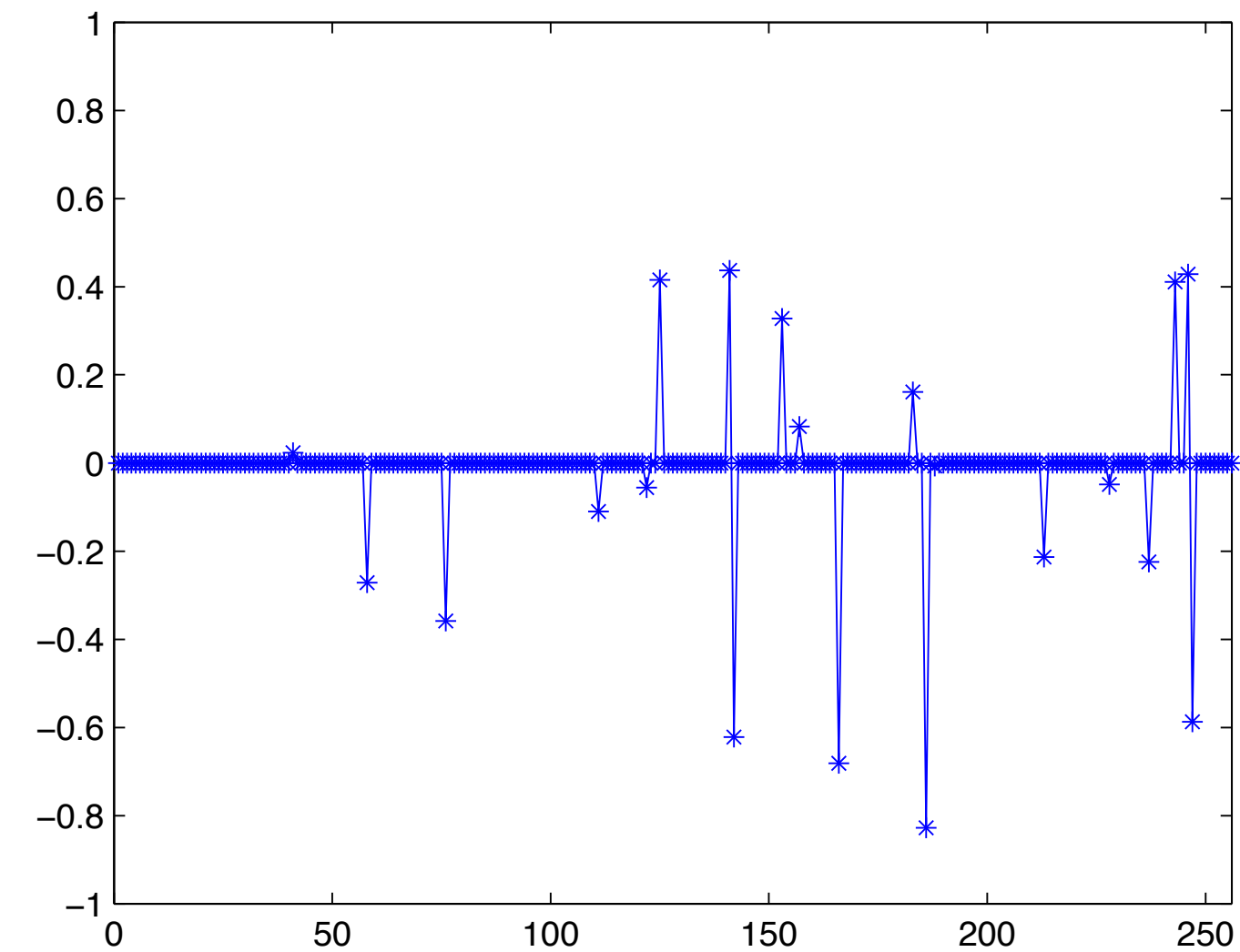


ℓ_1 regularisation / the lasso



(a) Dense

$$\|\text{signal in a)}\|_2 \approx 1.5431$$

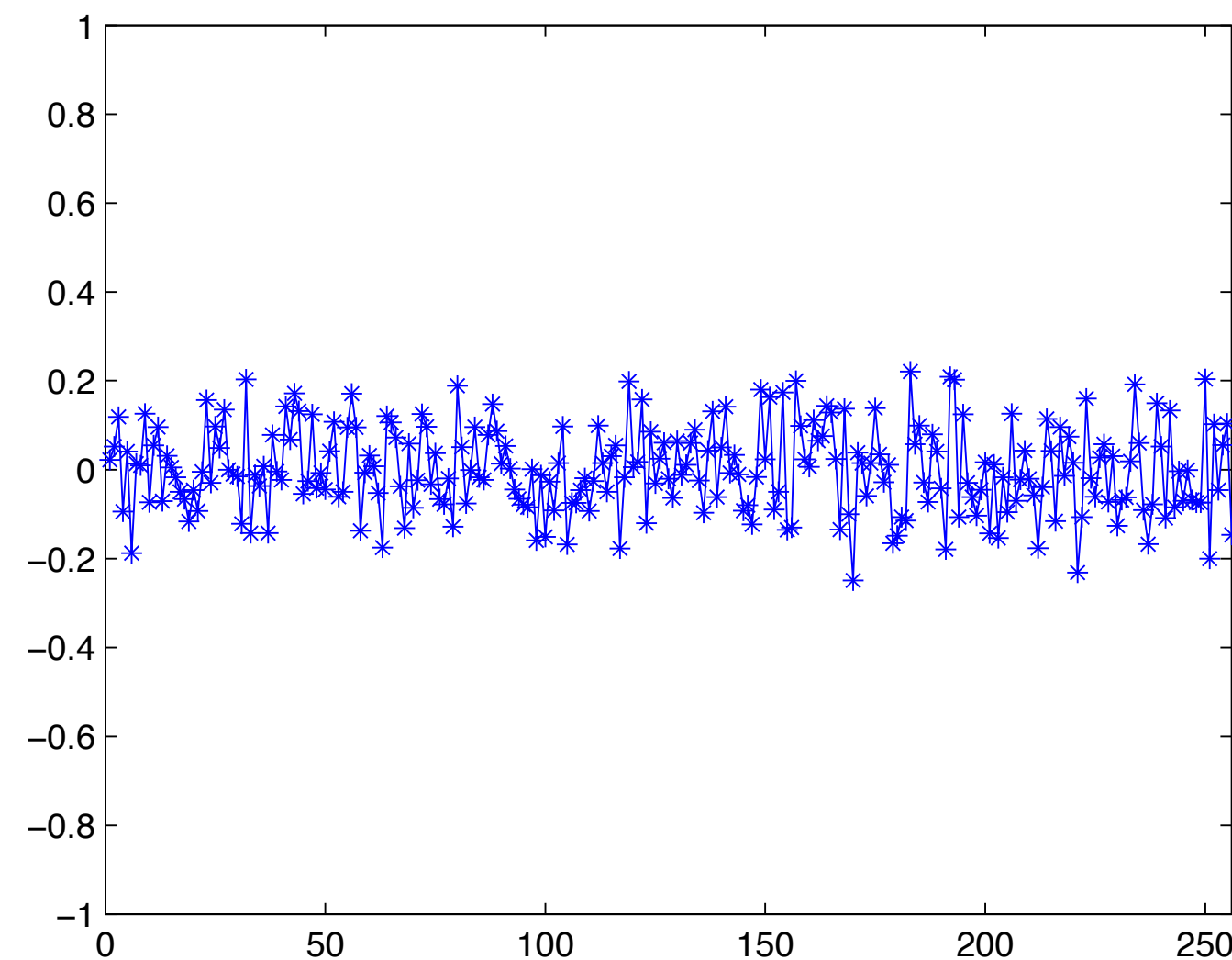


(b) Sparse

$$\|\text{signal in a)}\|_1 \approx 20.061$$



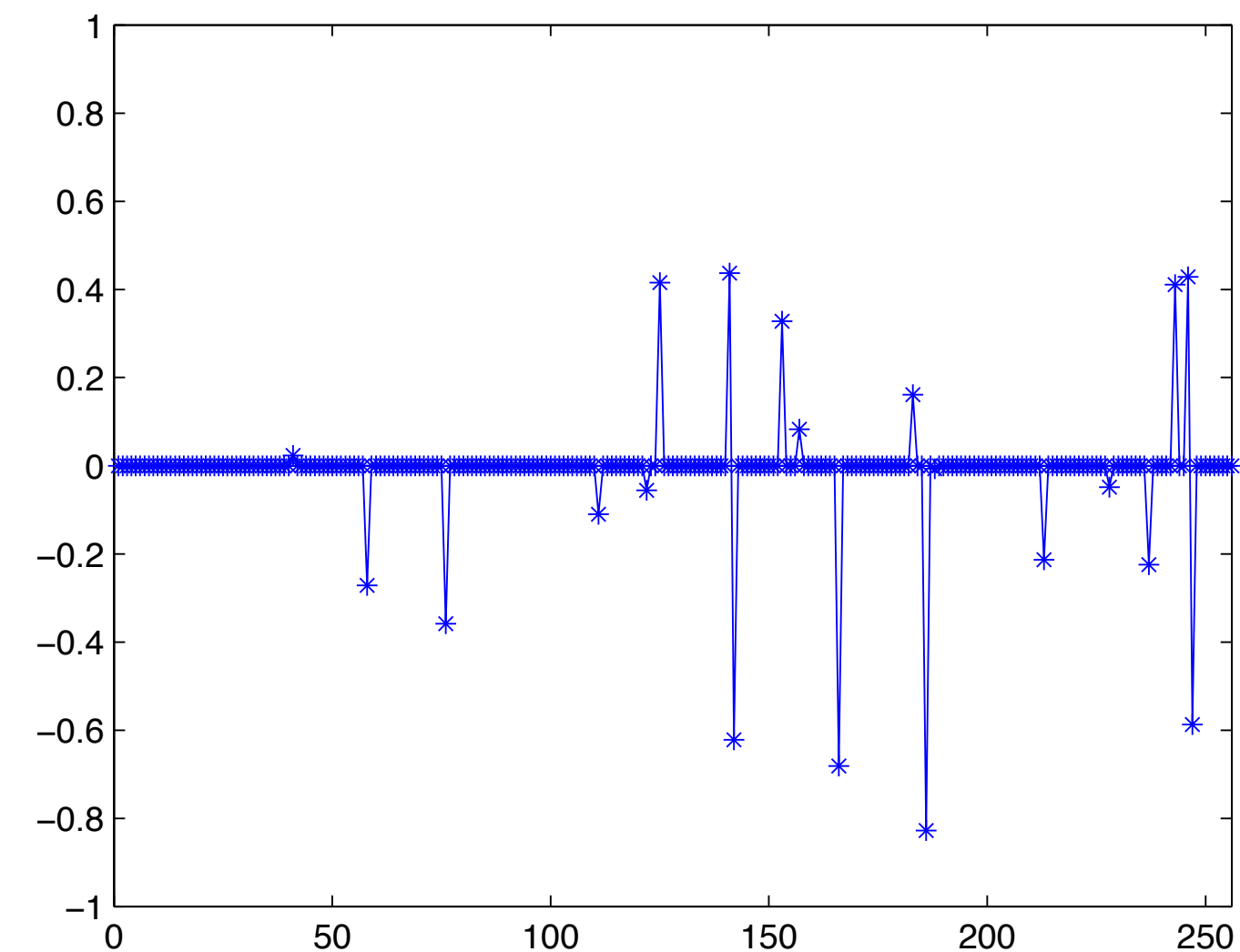
ℓ_1 regularisation / the lasso



(a) Dense

$$\|\text{signal in a})\|_2 \approx 1.5431$$

$$\|\text{signal in b})\|_2 \approx 1.7472$$

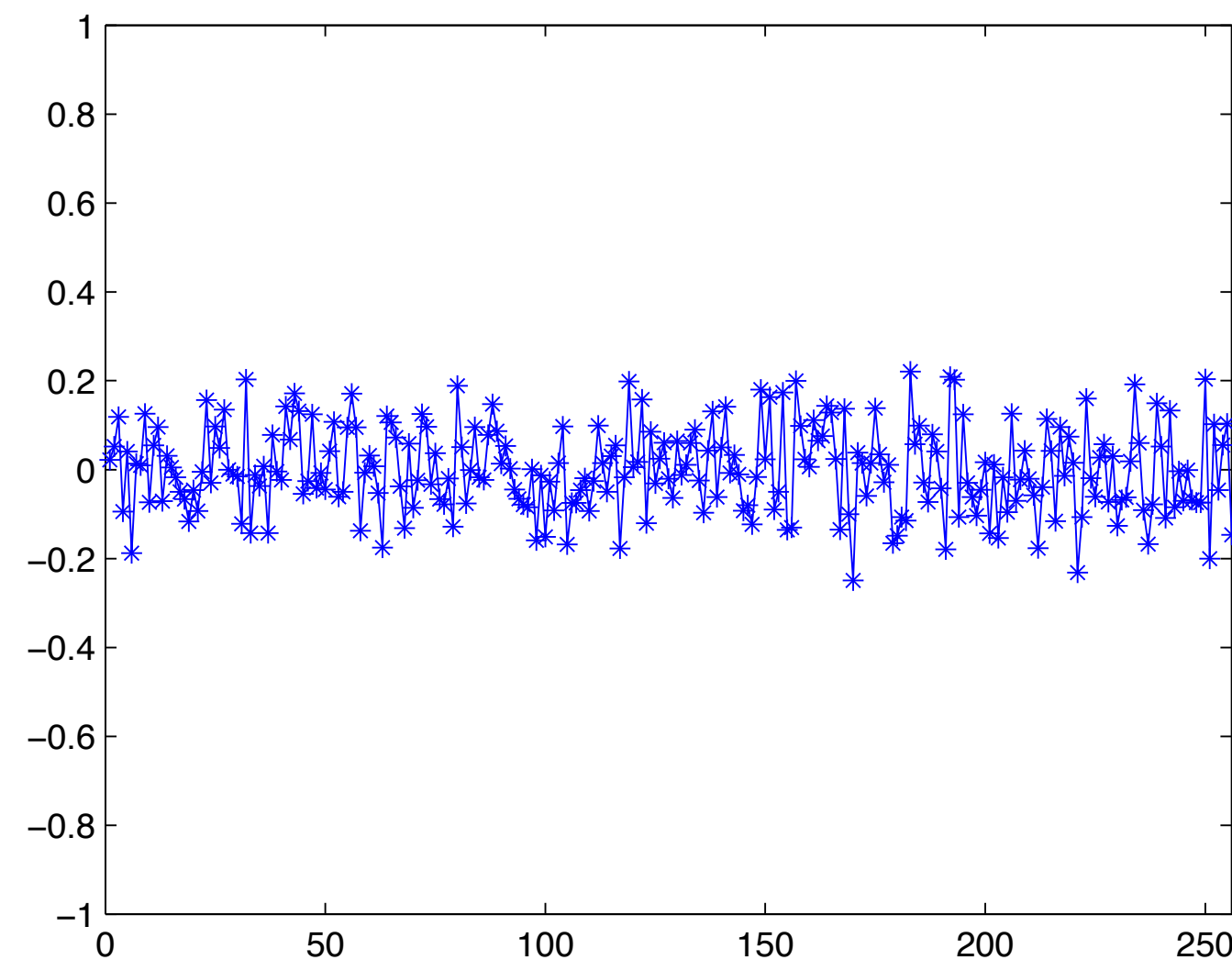


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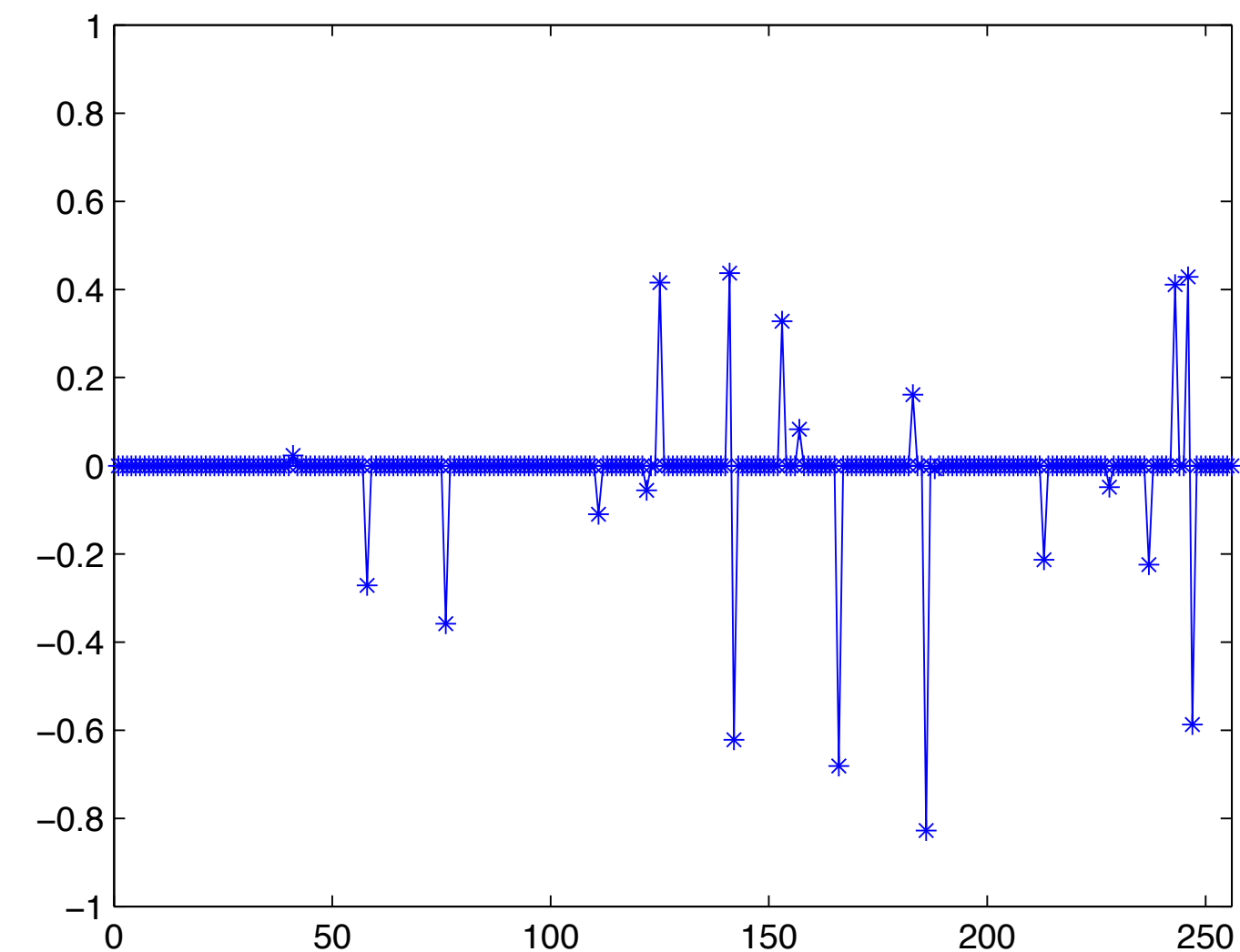
ℓ_1 regularisation / the lasso



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Lasso would select the sparse solution!



HOW TO SOLVE LASSO OR MORE IN GENERAL OPTIMIZATION PROBLEMS?

Why optimisation?

In the previous lectures, we have studied regression problems of the form

$$\hat{\mathbf{w}} = \arg \min_{\mathbf{w} \in \mathbb{R}^{d+1}} E(\mathbf{w})$$



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For

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where f is linear in w , we have seen that we can compute $\hat{\mathbf{w}}$ by solving a linear system of equations



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But: how do we minimise E in general?



Grid search?

How about using grid search?

Evaluate a function E at points on a grid and record smallest value



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Disadvantages:

- computationally infeasible for large no. of parameters
- no guarantee that we compute a minimum



Smooth optimisation

Smooth functions (continuously differentiable) allow the application of more systematic searches compared to grid search

$$E \in C^1(\mathbb{R}^{d+1}) \quad \Rightarrow \quad \nabla E \text{ exists and is continuous}$$



Smooth optimisation

Example for smooth optimisation: gradient descent

$$\mathbf{w}^{k+1} = \mathbf{w}^k - \tau \nabla E(\mathbf{w}^k)$$

for some $\mathbf{w}^0 \in \mathbb{R}^n$ and a constant $\tau > 0$.

Procedure to find a minimum of w !



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⋮

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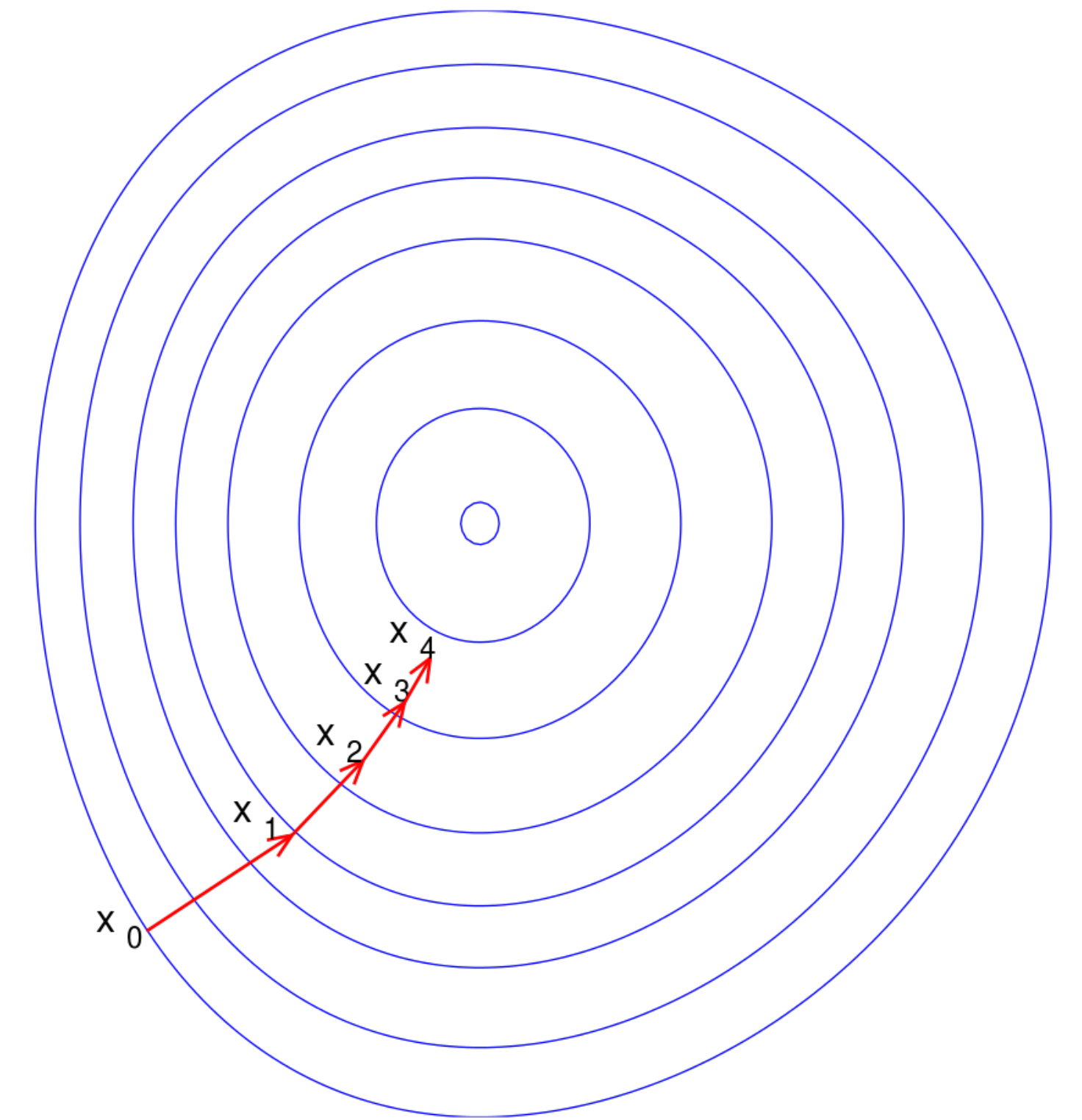
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$$\mathbf{w}^k = \mathbf{w}^{k-1} - \tau \nabla E(\mathbf{w}^{k-1})$$

Every step of the procedure is also known as an iterate or update

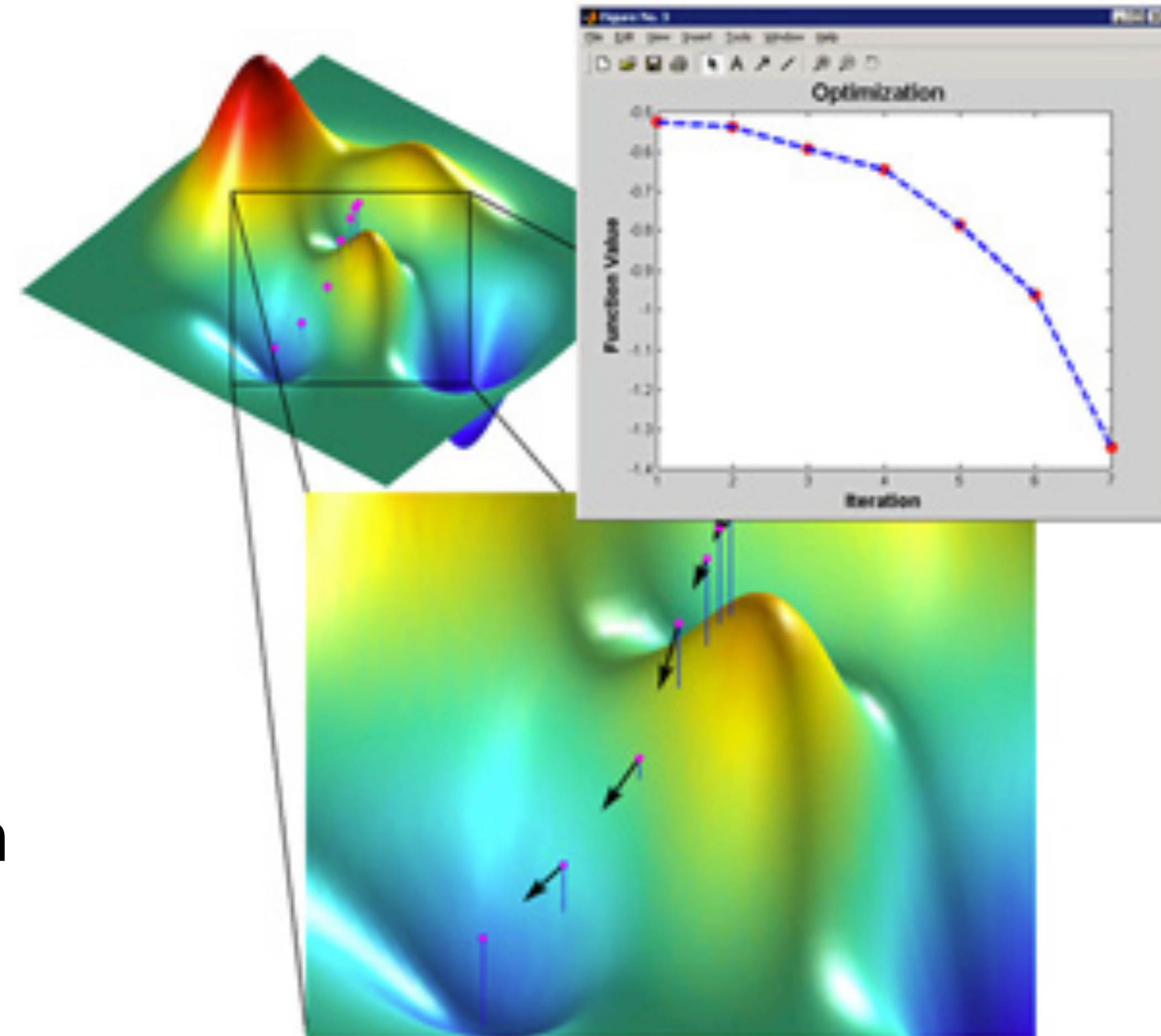


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Gradient descent

Gradient descent is an iterative procedure

Every step of the procedure is also known as an iterate or update



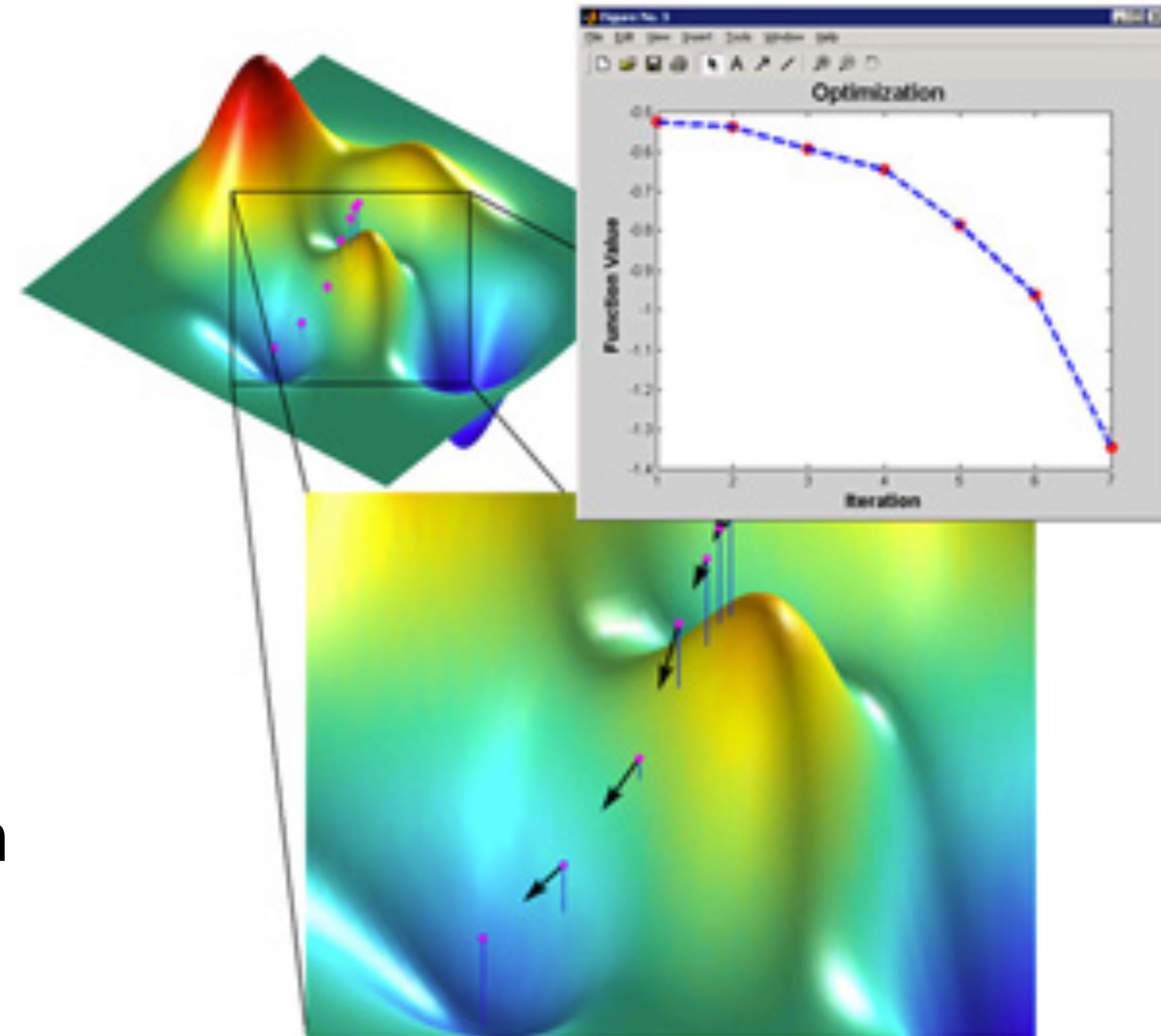
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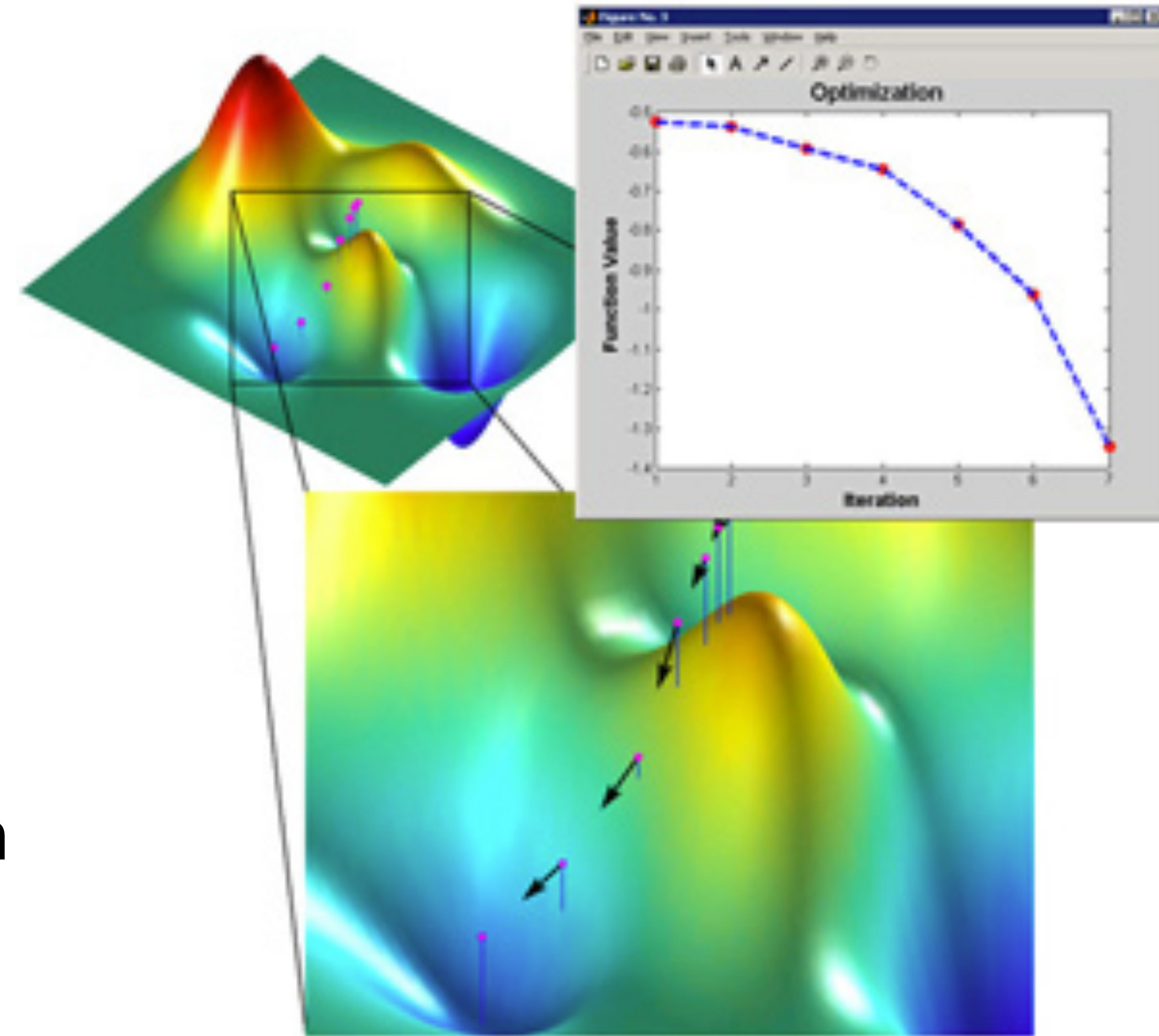
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Gradient descent

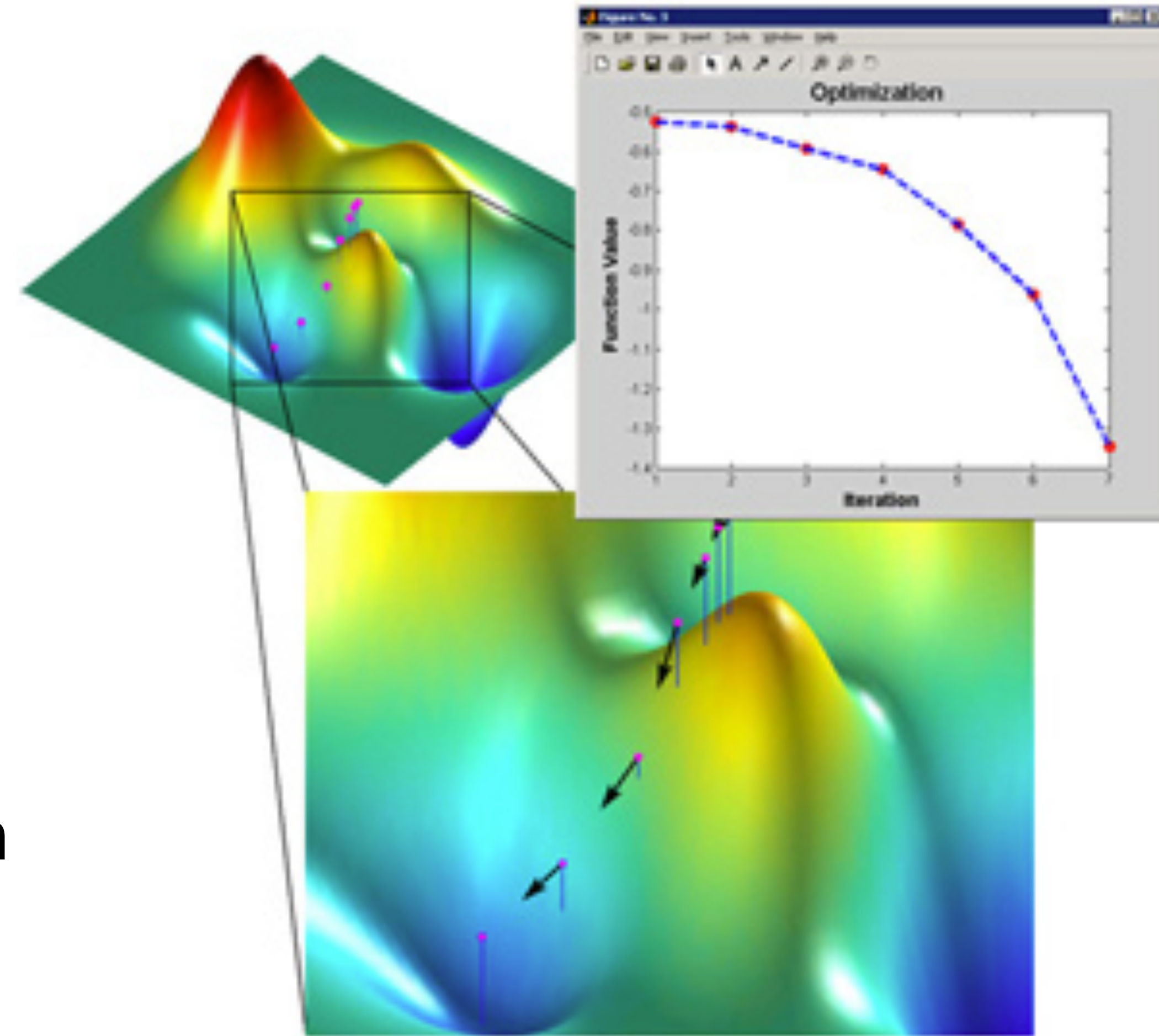
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Gradient descent

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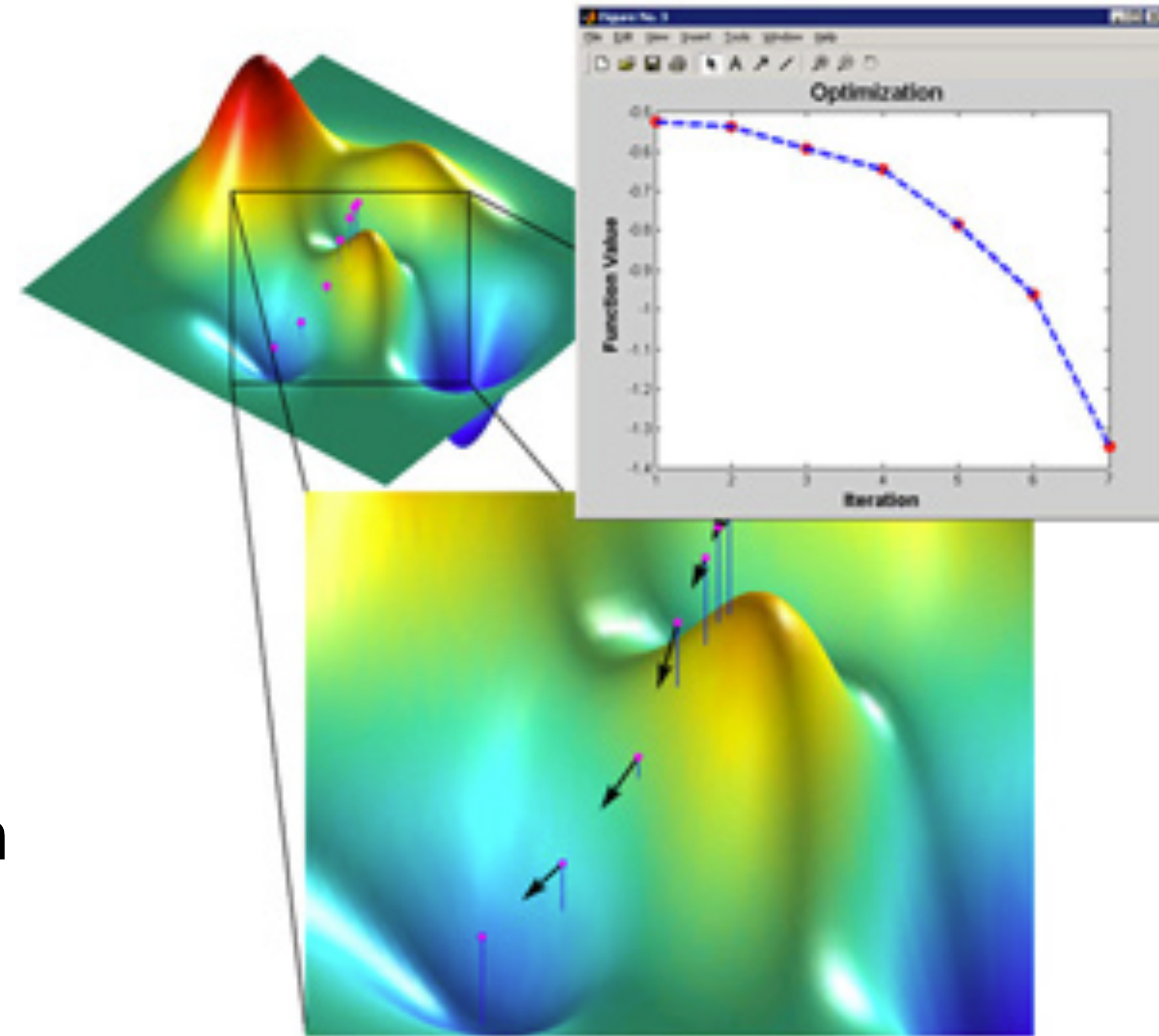
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Gradient descent

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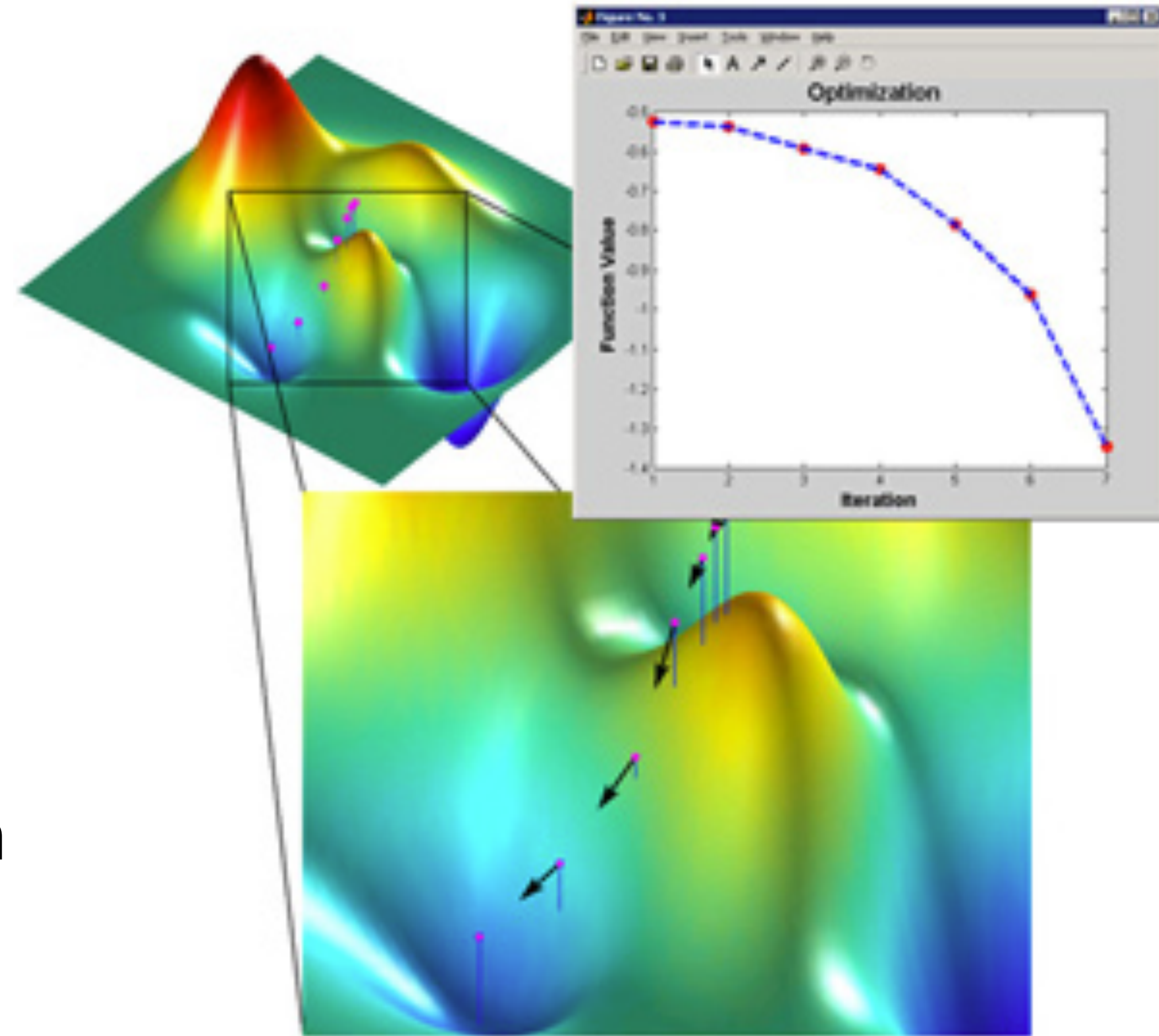
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⋮

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Gradient descent

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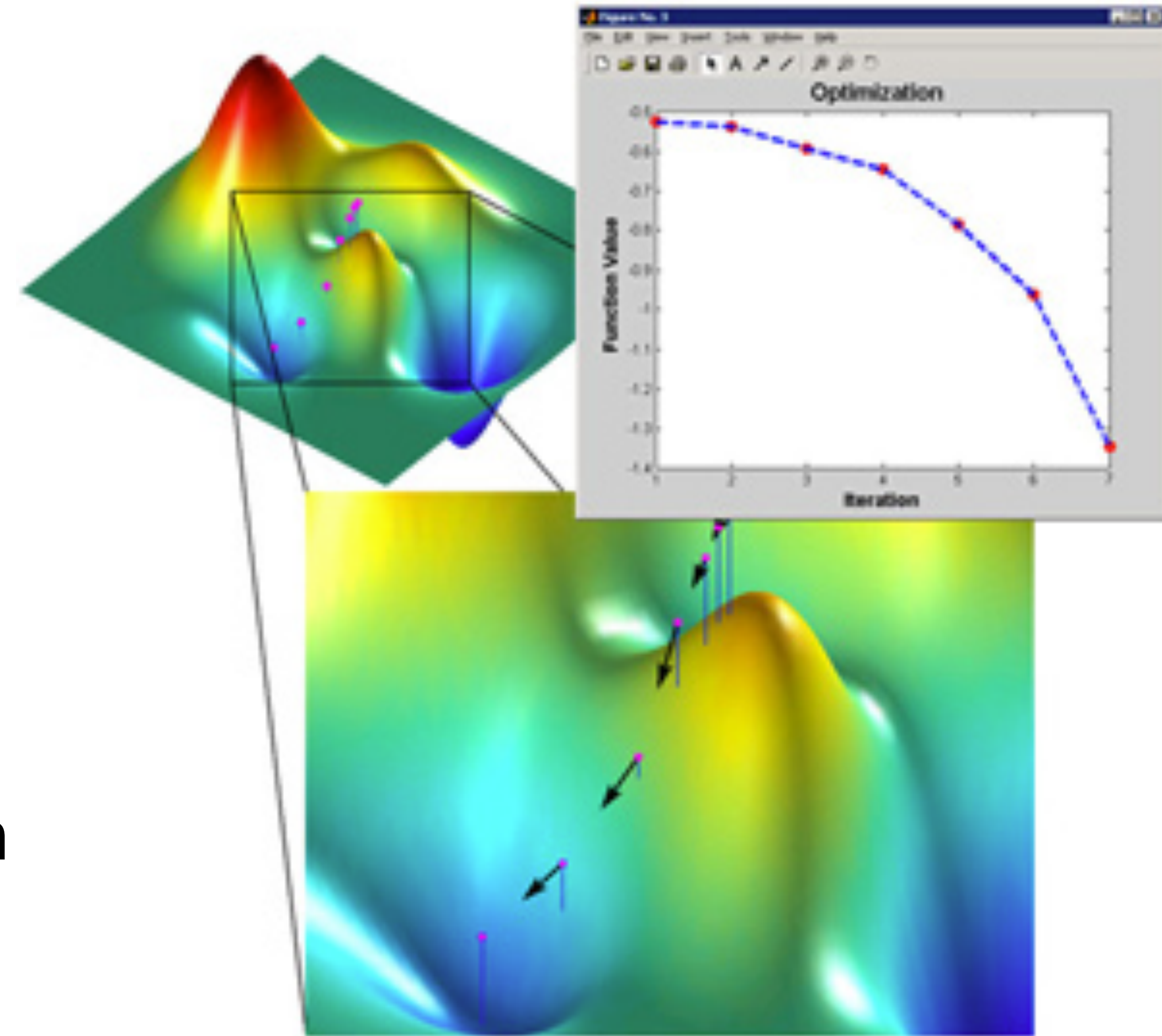
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⋮

$$\mathbf{w}^k = \mathbf{w}^{k-1} - \tau \nabla E(\mathbf{w}^{k-1})$$

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Gradient descent: examples

One parameter MSE-model:

$$\text{MSE}(w) = \frac{1}{2s} \sum_{i=1}^s |w - y_i|^2$$



Gradient descent: examples

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Gradient:

$$\nabla \text{MSE}(w) = w - \frac{1}{s} \sum_{i=1}^s y_i$$



Gradient descent: examples

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Gradient:

$$\nabla \text{MSE}(w) = w - \frac{1}{s} \sum_{i=1}^s y_i$$

We have learnt that

$$\nabla \text{MSE}(w) = w - \frac{1}{s} \sum_{i=1}^s y_i = 0 \rightarrow \hat{w} = \bar{y}$$



Gradient descent: examples



Gradient descent: examples

Gradient descent:

$$w^{k+1} = w^k - \tau \left(w^k - \frac{1}{s} \sum_{i=1}^s y_i \right) = (1 - \tau)w^k + \frac{\tau}{s} \sum_{i=1}^s y_i$$



Gradient descent: examples

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For $\tau = 1$

$$w^{k+1} = \frac{1}{s} \sum_{i=1}^s y_i$$



Gradient descent: examples

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For $\tau = 1$

$$w^{k+1} = \frac{1}{s} \sum_{i=1}^s y_i$$

For a general value of τ ?



Gradient descent: examples

General linear MSE-model:
$$\text{MSE}(\mathbf{w}) = \frac{1}{2s} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$$



Gradient descent: examples

General linear MSE-model: $MSE(\mathbf{w}) = \frac{1}{2s} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$

Recall: $\nabla MSE(\mathbf{w}) = \frac{1}{s} \mathbf{X}^T (\mathbf{X}\mathbf{w} - \mathbf{y})$



Gradient descent: examples

General linear MSE-model:
$$\text{MSE}(\mathbf{w}) = \frac{1}{2s} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$$

Recall:
$$\nabla \text{MSE}(\mathbf{w}) = \frac{1}{s} \mathbf{X}^\top (\mathbf{X}\mathbf{w} - \mathbf{y})$$

Gradient descent:
$$\mathbf{w}^{k+1} = \mathbf{w}^k + \frac{\tau}{s} \mathbf{X}^\top (\mathbf{y} - \mathbf{X}\mathbf{w}^k)$$



Gradient descent: examples

General linear MSE-model:
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Gradient descent:
$$\begin{aligned} \mathbf{w}^{k+1} &= \mathbf{w}^k + \frac{\tau}{s} \mathbf{X}^\top (\mathbf{y} - \mathbf{X}\mathbf{w}^k) \\ &= \left(I - \frac{\tau}{s} \mathbf{X}^\top \mathbf{X} \right) \mathbf{w}^k + \frac{\tau}{s} \mathbf{X}^\top \mathbf{y} \end{aligned}$$



Gradient descent: examples

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$$\text{MSE}(\mathbf{w}) = \frac{1}{2s} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2$$

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Gradient descent: examples

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Does this work for any τ ?

Gradient descent

Why (and when) does it work?



Gradient descent

Why (and when) does it work?

Assumption: E is Lipschitz-continuous with constant L (or L -smooth), i.e.

$$\|\nabla E(\mathbf{x}) - \nabla E(\mathbf{y})\| \leq L\|\mathbf{x} - \mathbf{y}\| \quad \forall x, y \in \mathbb{R}^n$$



Gradient descent

Why (and when) does it work?

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$$\|\nabla E(\mathbf{x}) - \nabla E(\mathbf{y})\| \leq L\|\mathbf{x} - \mathbf{y}\| \quad \forall \mathbf{x}, \mathbf{y} \in \mathbb{R}^n$$

Then the function

$$G(x) := \frac{L}{2}\|\mathbf{x}\|^2 - E(\mathbf{x})$$

is convex for all $\mathbf{x} \in \mathbb{R}^n$.



Gradient descent

Why (and when) does it work?

Assumptions: • the function E is τ^{-1} smooth

• the function $G(\mathbf{w}) := \frac{1}{2\tau} \|\mathbf{w}\|^2 - E(\mathbf{w})$ is convex

for all $\mathbf{w} \in \mathbb{R}^n$



Gradient descent

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for all $\mathbf{w} \in \mathbb{R}^n$

Then (converge theorem) we can show

1. that $E(\mathbf{w}^{k+1}) \leq E(\mathbf{w}^k)$

2. as well as $\lim_{k \rightarrow \infty} E(\mathbf{w}^k) = E(\hat{\mathbf{w}})$ with rate $1/k$



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Proof:



Gradient descent

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Proof: in the lecture notes, but not examinable! 😊

Gradient descent: examples

What is the value of τ that allows convergence?



Gradient descent: examples

What is the value of τ that allows convergence?

$$E(\mathbf{w}) = \frac{1}{2s} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 \rightarrow \nabla E(\mathbf{w}) = \frac{1}{s} \mathbf{X}^\top (\mathbf{X}\mathbf{w} - \mathbf{y})$$



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$$\|\nabla E(\mathbf{w}) - \nabla E(\mathbf{v})\| = \frac{1}{s} \|\mathbf{X}^\top \mathbf{X}(\mathbf{w} - \mathbf{v})\|$$



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Gradient descent: examples

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Hence the function is τ^{-1} smooth and converge is guaranteed for $\frac{1}{\tau} = \frac{\|\mathbf{X}^\top \mathbf{X}\|}{s}$



Gradient descent: examples

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Hence the function is τ^{-1} smooth and convergence is guaranteed for $\frac{1}{\tau} = \frac{\|\mathbf{X}^\top \mathbf{X}\|}{s}$

This implies convergence for any $\tau \leq \frac{s}{\|\mathbf{X}^\top \mathbf{X}\|}$

Gradient descent

- Assumptions:
- the function E is τ^{-1} smooth
 - the function $G(\mathbf{w}) := \frac{1}{2\tau} \|\mathbf{w}\|^2 - E(\mathbf{w})$ is convex
- for all $\mathbf{w} \in \mathbb{R}^n$

What can we do if the assumptions are not met?



Gradient descent

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Backtracking:



Gradient descent

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- for all $\mathbf{w} \in \mathbb{R}^n$

What can we do if the assumptions are not met?

Backtracking: compute \mathbf{w}^{k+1} and check $E(\mathbf{w}^{k+1}) \leq E(\mathbf{w}^k)$

$$\begin{cases} \text{keep } \tau \text{ as it is} & \text{if } E(\mathbf{w}^{k+1}) \leq E(\mathbf{w}^k) \\ \text{decrease } \tau & \text{if } E(\mathbf{w}^{k+1}) > E(\mathbf{w}^k) \end{cases}$$

Gradient descent

Remark: in the (modern) machine learning literature...



Gradient descent

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...gradient descent is also known as **batch** gradient descent



Gradient descent

Remark: in the (modern) machine learning literature...

...gradient descent is also known as **batch** gradient descent

...the stepsize τ is also known as the **learning rate** (bad name)





SOLVING LASSO

LASSO

How can we solve the LASSO computationally?

$$\mathbf{w}_\alpha = \arg \min_{\mathbf{w}} \left\{ \frac{1}{2} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \alpha \|\mathbf{w}\|_1 \right\}$$



LASSO

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Can we just compute $\nabla E(\mathbf{w}_\alpha) = 0$ for $E(\mathbf{w}) := \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2/2 + \alpha \|\mathbf{w}\|_1$?



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We cannot do this, since E is not differentiable!



LASSO

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Can we use the same machinery we developed for the other problems?



LASSO

No!

$$\mathbf{w}_\alpha = \arg \min_{\mathbf{w}} \left\{ \frac{1}{2} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \alpha \|\mathbf{w}\|_1 \right\}$$

The l1 norm is not differentiable in zero



LASSO

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The l1 norm is not differentiable in zero

We can smooth the one-norm to make this problem differentiable!



LASSO

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We can smooth the one-norm to make this problem differentiable!

Note that we can write

$$|\mathbf{w}| = \max_{p \in [-1, 1]} \mathbf{w}p$$



LASSO

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We can smooth the one-norm to make this problem differentiable!

We can modify slightly the l1 norm to smooth the function

$$|\mathbf{w}|_\tau = \max_{p \in [-1, 1]} wp - \frac{\tau}{2} |p|^2$$



LASSO

Note that we can write

$$|\mathbf{w}|_{\tau} = \max_{p \in [-1, 1]} wp - \frac{\tau}{2} |p|^2$$



LASSO

Note that we can write

$$|\mathbf{w}|_{\tau} = \max_{p \in [-1,1]} wp - \frac{\tau}{2} |p|^2$$

This problem has a closed form solution

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$$\hat{p} = \arg \max_{p \in [-1,1]} wp - \frac{\tau}{2} |p|^2$$

$$\Leftrightarrow \hat{p} = \begin{cases} 1 & w > \tau \\ \frac{w}{\tau} & |w| \leq \tau \\ -1 & w < -\tau \end{cases}$$



LASSO

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Why?



LASSO

We need to solve

$$|\mathbf{w}|_{\tau} = \max_{p \in [-1, 1]} wp - \frac{\tau}{2} |p|^2$$



LASSO

We need to solve

$$|\mathbf{w}|_{\tau} = \max_{p \in [-1, 1]} wp - \frac{\tau}{2} |p|^2$$

The function we are trying to maximize is a parabola of this type

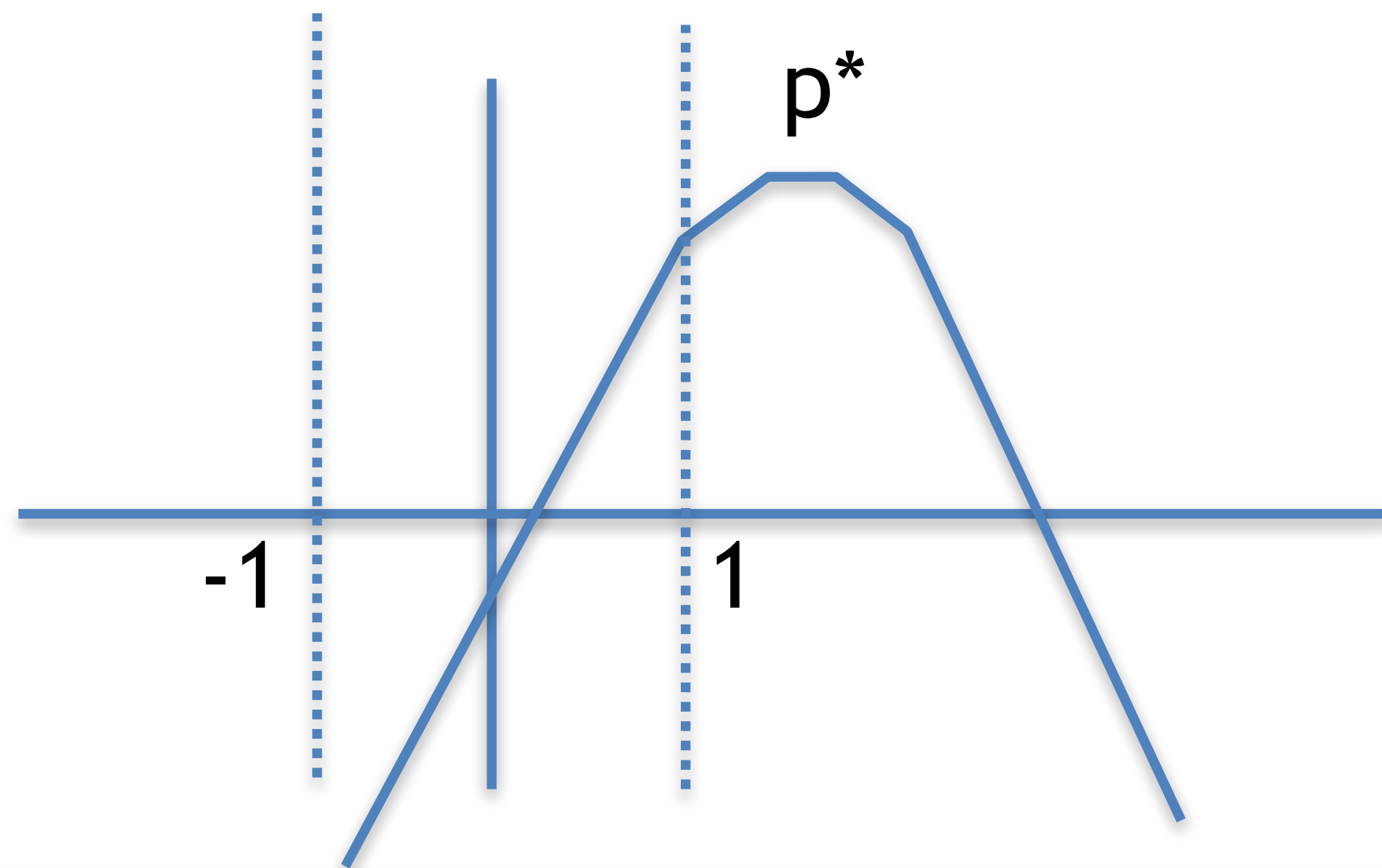


LASSO

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The function we are trying to maximize is a parabola of this type



p is bounded by -1 and 1

LASSO

How do we get the max?

$$|\mathbf{w}|_{\tau} = \max_{p \in [-1, 1]} wp - \frac{\tau}{2} |p|^2$$



LASSO

How do we get the max?

$$|w|_{\tau} = \max_{p \in [-1, 1]} wp - \frac{\tau}{2} |p|^2$$

Compute the gradient!



LASSO

How do we get the max?

$$|\mathbf{w}|_{\tau} = \max_{p \in [-1, 1]} wp - \frac{\tau}{2} |p|^2$$

Compute the gradient!

$$\nabla |\mathbf{w}|_{\tau} = w - \tau p \quad \rightarrow \hat{p} = \frac{w}{\tau}$$



LASSO

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$$\nabla |\mathbf{w}|_{\tau} = w - \tau p \quad \rightarrow \quad \hat{p} = \frac{w}{\tau}$$

$$-1 \leq \hat{p} \leq 1 \rightarrow -\tau \leq w \leq \tau$$



LASSO

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Compute the gradient!

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$$|w| \leq \tau$$



LASSO

Hence, for $|w| \leq \tau$ the max is obtained substituting \hat{p} in the expression

Hence

$$|w|_{\tau} = \frac{w^2}{2\tau}$$



LASSO

Hence, for $|w| \leq \tau$ the max is obtained substituting \hat{p} in the expression

$$|w| = \max_{p \in [-1,1]} wp - \frac{\tau}{2} |p|^2$$

Hence

$$|w|_{\tau} = \frac{w^2}{2\tau}$$



LASSO

Hence, for $|w| \leq \tau$ the max is obtained substituting \hat{p} in the expression

$$|\mathbf{w}| = \max_{p \in [-1,1]} wp - \frac{\tau}{2} |p|^2 = w \frac{w}{\tau} - \frac{\tau}{2} \frac{w^2}{\tau^2} = \frac{w^2}{2\tau}$$

Hence

$$|\mathbf{w}|_{\tau} = \frac{w^2}{2\tau}$$



LASSO

For $w > \tau$ instead $\hat{p} > 1$



LASSO

For $w > \tau$ instead $\hat{p} > 1$

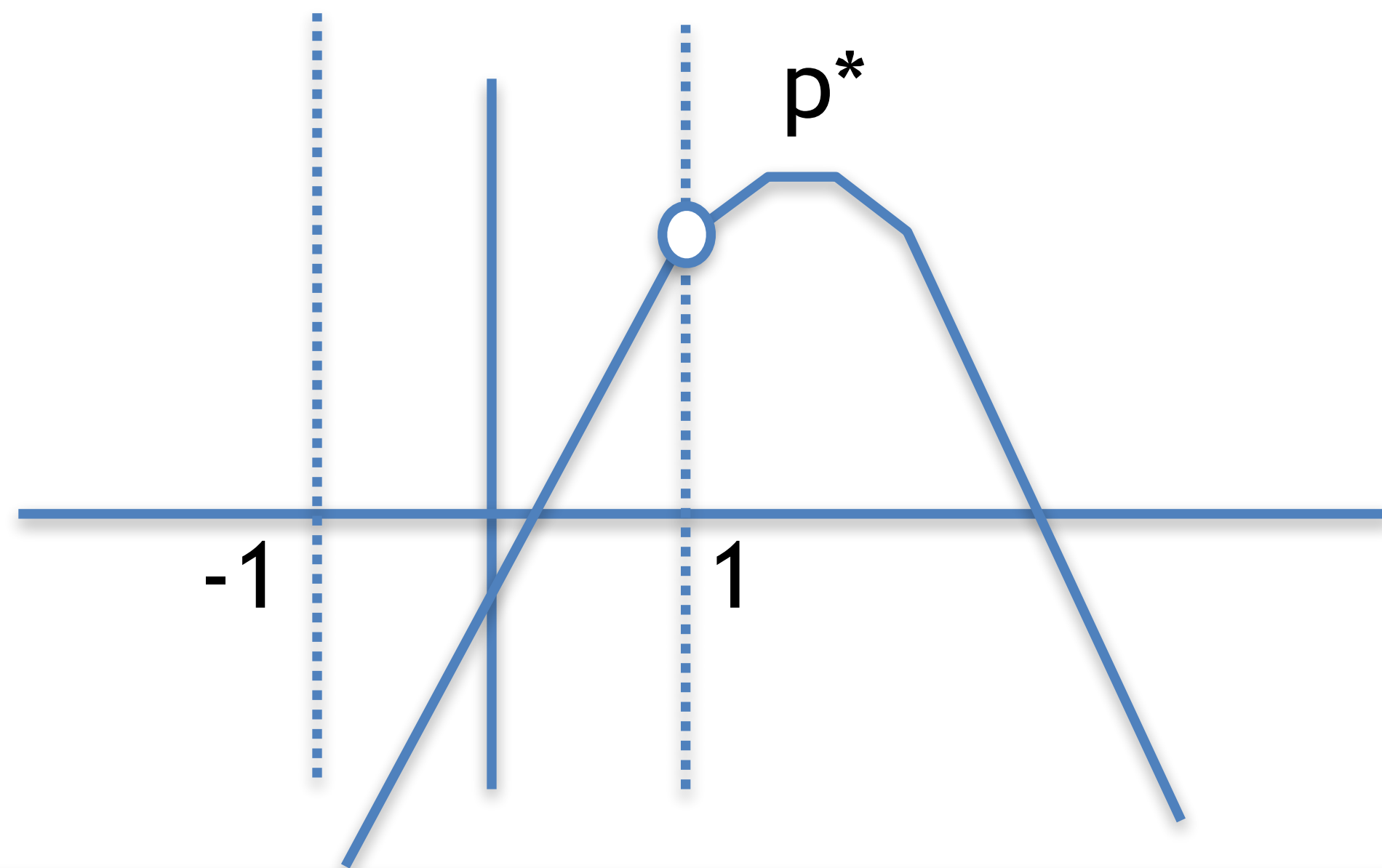
If the max is larger than one than the parabola is indeed like this



LASSO

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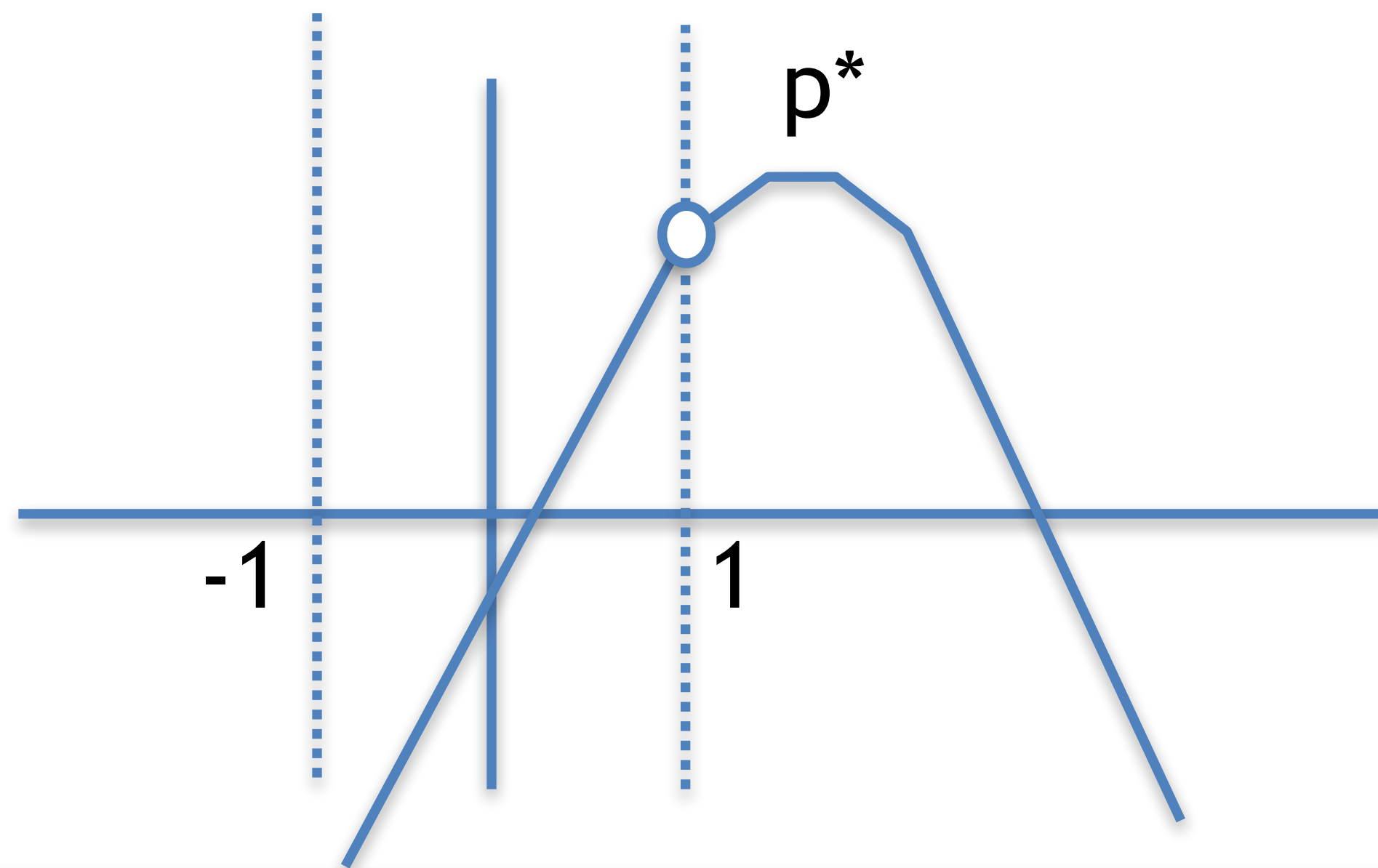
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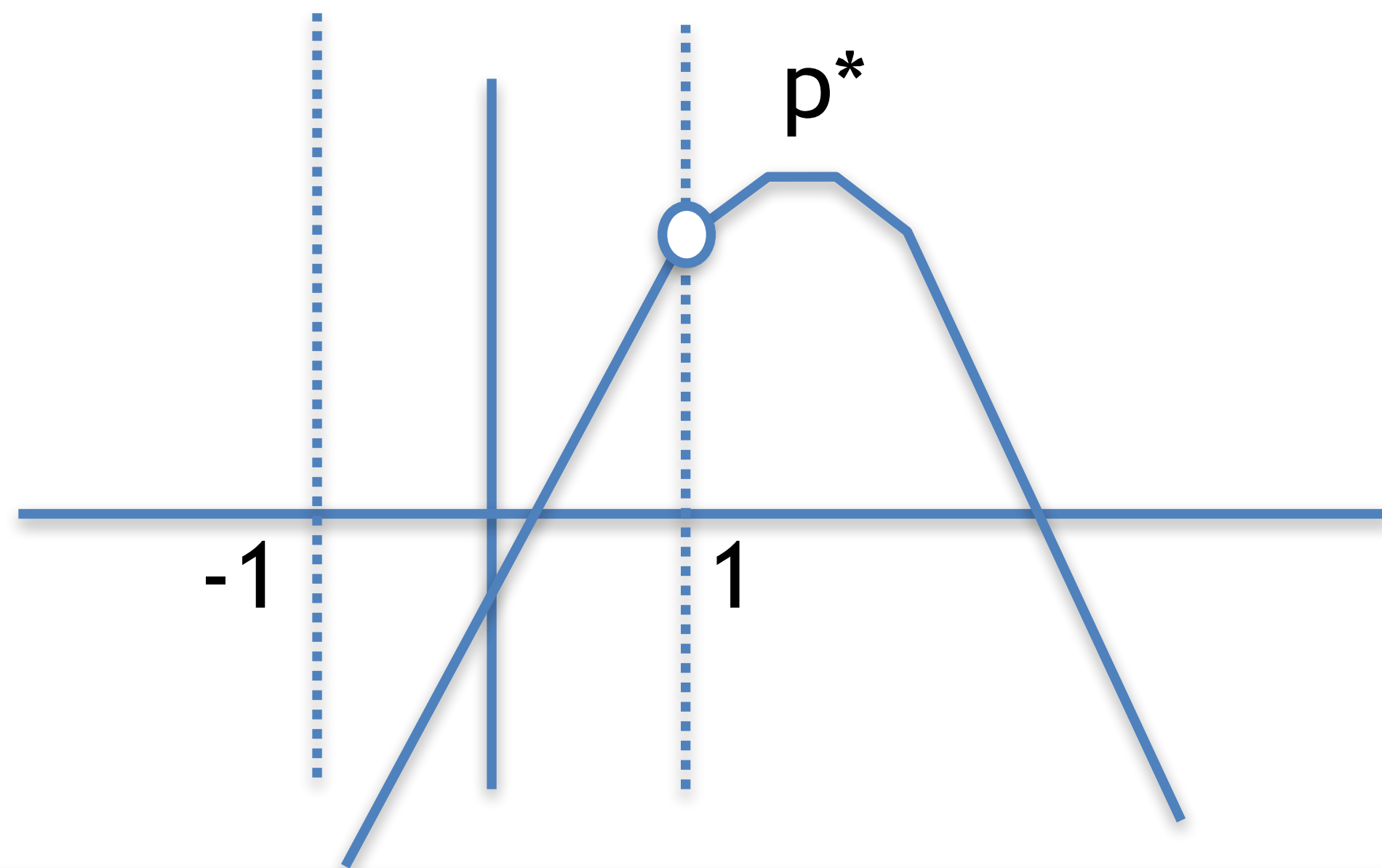


And the max is for $p=1$

LASSO

For $w > \tau$ instead $\hat{p} > 1$

If the max is larger than one than the parabola is indeed like this



And the max is for $p=1$

$$\text{This implies } |w|_{\tau} = w - \frac{\tau}{2}$$

LASSO

For $w < -\tau$ instead $\hat{p} < -1$



LASSO

For $w < -\tau$ instead $\hat{p} < -1$

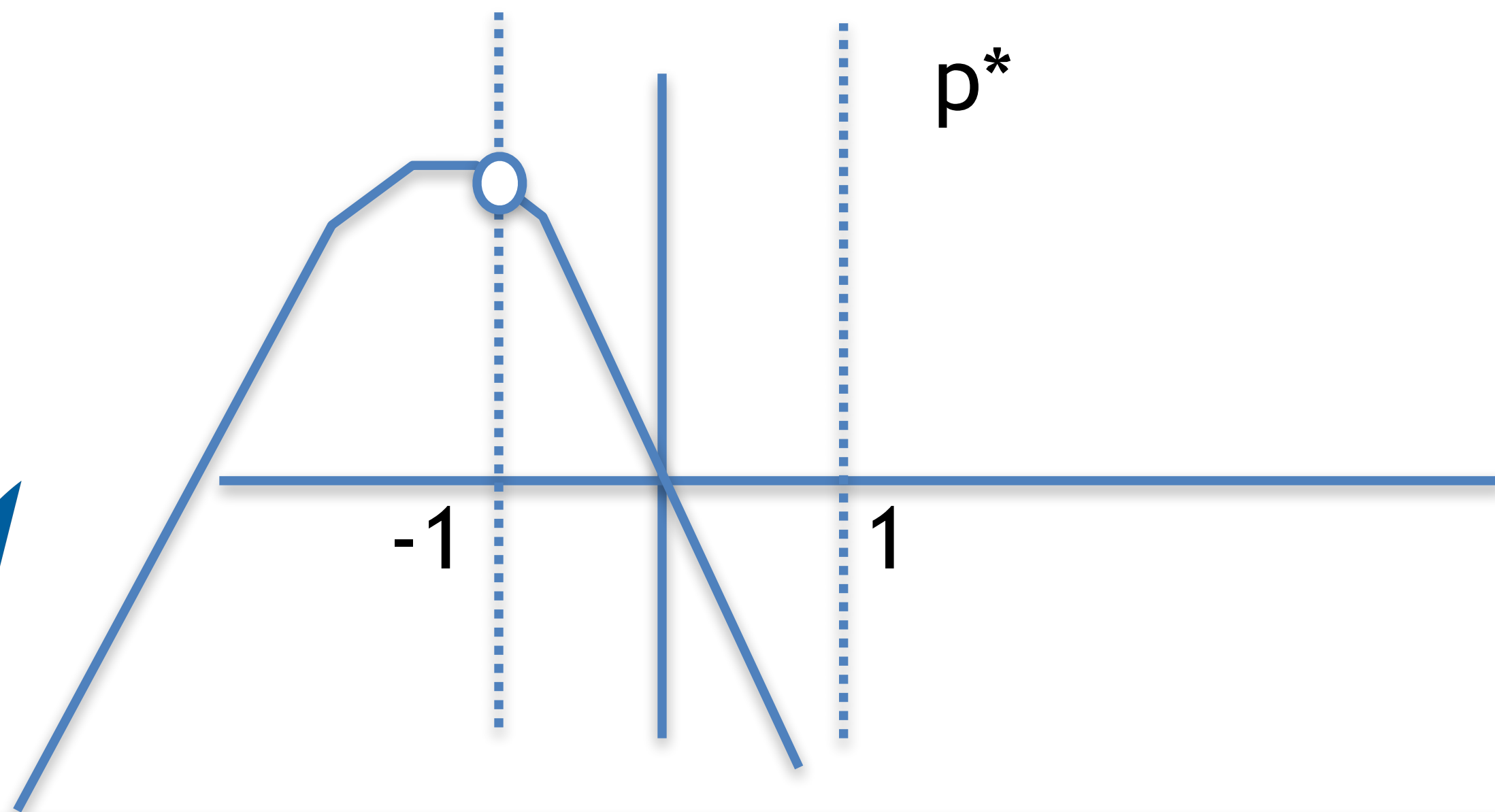
If the max is smaller than one than the parabola is instead like this



LASSO

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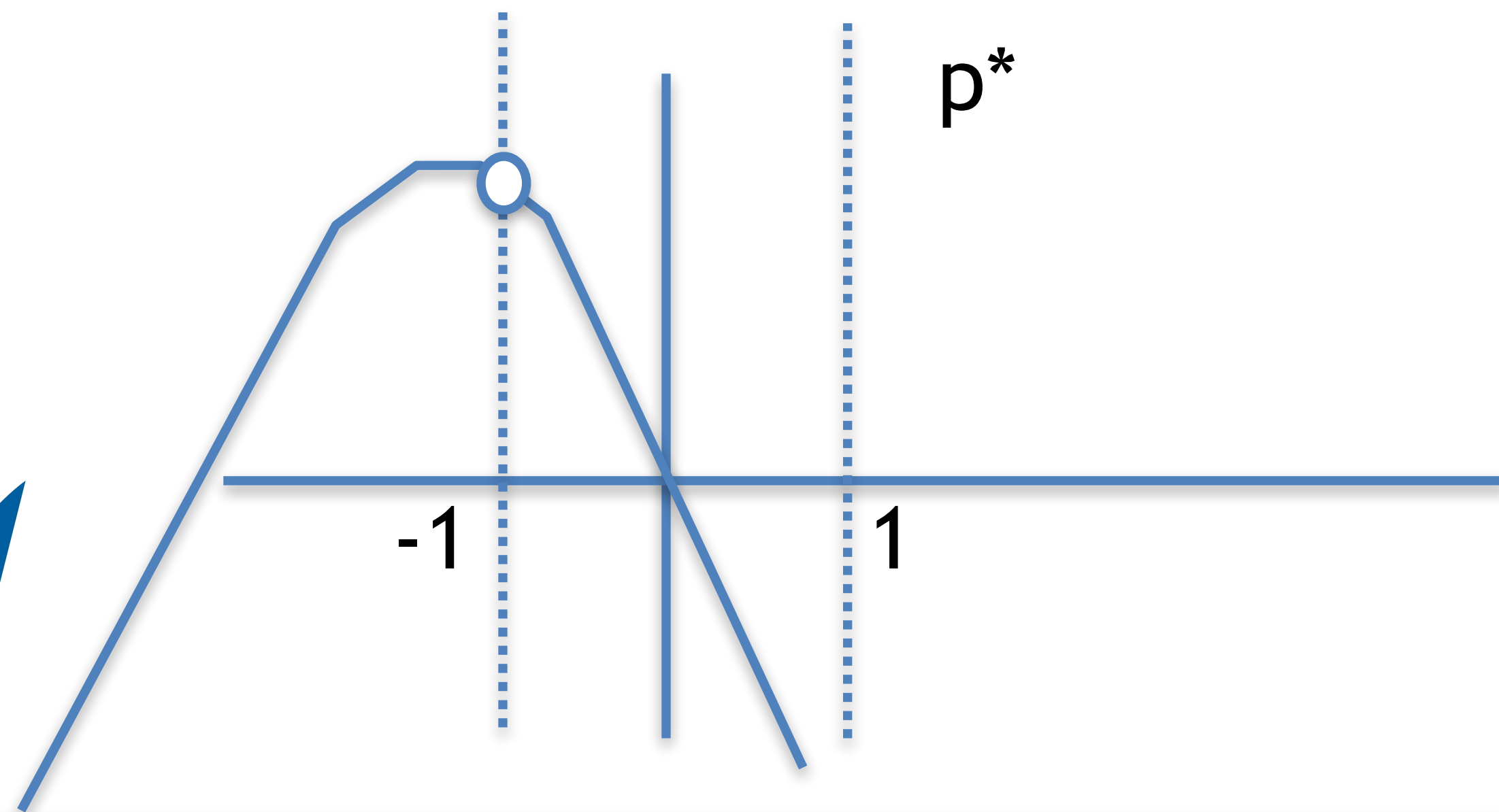
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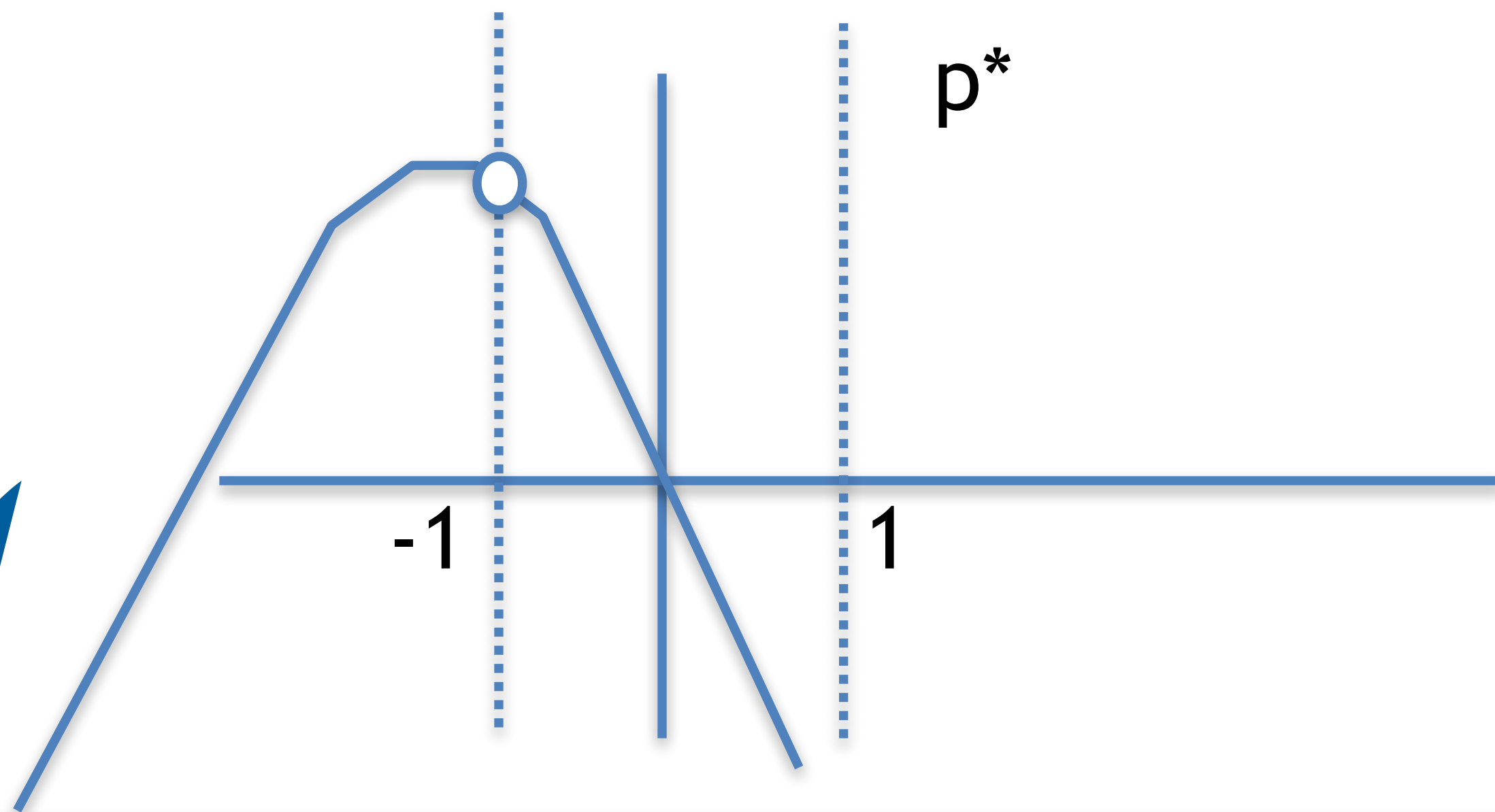


And the max is for $p = -1$

LASSO

For $w < -\tau$ instead $\hat{p} < -1$

If the max is smaller than one than the parabola is instead like this



And the max is for $p = -1$

$$\text{This implies } |w|_{\tau} = -w - \frac{\tau}{2}$$

LASSO

Hence

$$|\mathbf{w}|_{\tau} = \max_{p \in [-1,1]} wp - \frac{\tau}{2} |p|^2$$

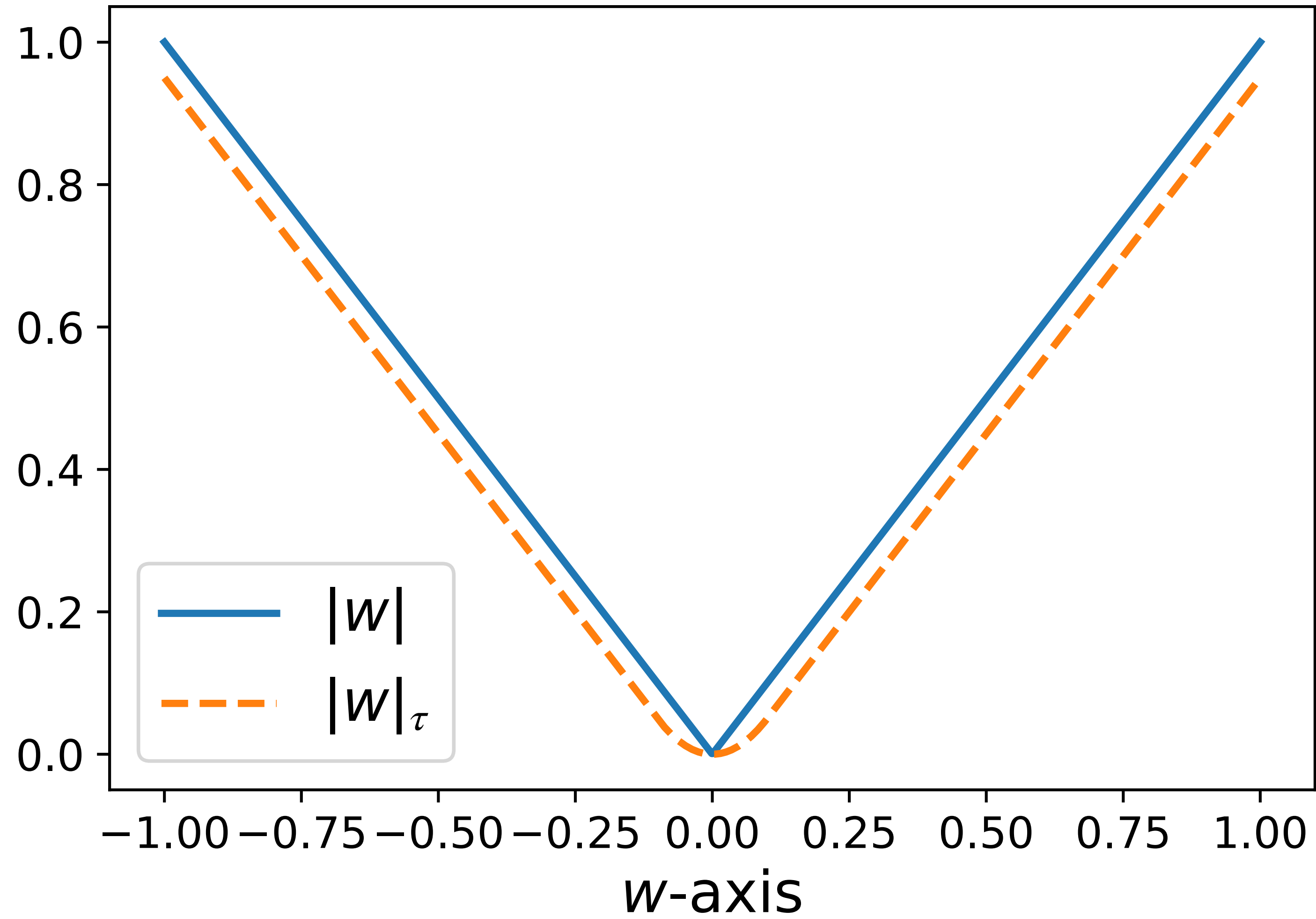
has a closed form solution

$$\hat{p} = \arg \max_{p \in [-1,1]} wp - \frac{\tau}{2} |p|^2$$

$$\Rightarrow \hat{p} = \begin{cases} 1 & w > \tau \\ \frac{w}{\tau} & |w| \leq \tau \\ -1 & w < -\tau \end{cases} \Rightarrow |\mathbf{w}|_{\tau} = \begin{cases} |w| - \frac{\tau}{2} & |w| > \tau \\ \frac{1}{2\tau} |w|^2 & |w| \leq \tau \end{cases}$$



LASSO



$$\tau = \frac{1}{10}$$

LASSO

The change in the l1 norm allows us to write

$$|\mathbf{w}|_{\tau} = \begin{cases} |w| - \frac{\tau}{2} & |w| > \tau \\ \frac{1}{2\tau} |w|^2 & |w| \leq \tau \end{cases}$$

for which we observe

$$\nabla |\mathbf{w}|_{\tau} = \begin{cases} 1 & w > \tau \\ \frac{1}{\tau} w & |w| \leq \tau \\ -1 & w < -\tau \end{cases}$$



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as well as

$$|\mathbf{w}|_{\tau} \leq |w| \leq |\mathbf{w}|_{\tau} + \frac{\tau}{2}$$



LASSO

We can therefore get a differentiable problem by replacing

$$\|\mathbf{w}\|_1 = \sum_{j=0}^d |w_j|$$

with

$$H_\tau(\mathbf{w}) = \sum_{j=0}^d |w_j|_\tau$$

Huber loss
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Smoothed LASSO:

$$\mathbf{w}_\alpha = \arg \min_{\mathbf{w} \in \mathbb{R}^{d+1}} \left\{ \frac{1}{2} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \alpha H_\tau(\mathbf{w}) \right\}$$



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LASSO

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One variant:



LASSO

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One variant: gradient descent for $E_\tau(\mathbf{w}) := \frac{1}{2} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + \alpha H_\tau(\mathbf{w})$:



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LASSO

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We have two competing terms due to the structure of E



LASSO

Alternative: forward-forward splitting for $E_\tau(\mathbf{w}) := \frac{1}{2\alpha} \|\mathbf{X}\mathbf{w} - \mathbf{y}\|^2 + H_\tau(\mathbf{w})$



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$$\mathbf{w}^{k+\frac{1}{2}} = \mathbf{w}^k - \frac{\tau}{\alpha} \mathbf{X}^\top (\mathbf{X}\mathbf{w}^k - \mathbf{y})$$

We move first towards the opposite of the max variation of MSE



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$$\mathbf{w}^{k+1} = \mathbf{w}^{k+\frac{1}{2}} - \tau \nabla H_\tau(\mathbf{w}^{k+\frac{1}{2}})$$

We move then towards the opposite of the max variation of the Huber loss function



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Converge for $\frac{\tau}{\alpha} \leq \|\mathbf{X}^\top \mathbf{X}\|^{-1}$

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Converge for any τ

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LASSO

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Hence we select $\frac{\tau}{\alpha} \leq \|\mathbf{X}^\top \mathbf{X}\|^{-1}$



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Note the following:

$$w - \tau \nabla |w|_\tau = w - \begin{cases} \tau & w > \tau \\ w & |w| \leq \tau \\ -\tau & w < -\tau \end{cases}$$



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The last term can be written as



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Hence, the soft-thresholding of the previous expression



LASSO

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This algorithm is also known as *ISTA* (= *iterative soft-thresholding algorithm*)



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Special case of *proximal gradient descent*

$$\mathbf{w}^{k+1} = (I + \tau \partial R)^{-1} (\mathbf{w}^k - \tau \nabla L(\mathbf{w}^k))$$

Proximal gradient method

Suppose we want to minimise $E(\mathbf{w}) = L(\mathbf{w}) + R(\mathbf{w})$



Proximal gradient method

Suppose we want to minimise $E(\mathbf{w}) = L(\mathbf{w}) + R(\mathbf{w})$

Assumptions: 1. L is differentiable, i.e., $\nabla L(\mathbf{w})$ exists

2. R has a simple proximal map, i.e.,

$$\text{prox}_{\tau R}(\mathbf{z}) := \arg \min_{\mathbf{x}} \left\{ \frac{1}{2} \|\mathbf{x} - \mathbf{z}\|^2 + \tau R(\mathbf{x}) \right\}$$

is easy to compute



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Then:

$$\mathbf{w}^{k+1} = \text{prox}_{\tau R} \left(\mathbf{w}^k - \tau \nabla L(\mathbf{w}^k) \right)$$



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Then: $\mathbf{w}^{k+1} = \text{prox}_{\tau R}(\mathbf{w}^k - \tau \nabla L(\mathbf{w}^k))$ Proximal gradient method



Proximal gradient method

For the choice $R(x) = \frac{1}{2}\|x\|^2$ this reads as

$$\text{prox}_{\frac{\tau}{2}\|\cdot\|^2}(z) = \arg \min_x \left\{ \frac{1}{2}\|x - z\|^2 + \frac{\tau}{2}\|x\|^2 \right\}$$



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Forget for a second the proximal map, we know how to solve that problem!



Proximal gradient method

$$\text{prox}_{\frac{\tau}{2}\|\cdot\|^2}(z) = \arg \min_x \left\{ \frac{1}{2}\|x - z\|^2 + \frac{\tau}{2}\|x\|^2 \right\}$$

This is a simple convex optimisation problem. If we define $E(x) := \frac{1}{2}\|x - z\|^2 + \frac{\tau}{2}\|x\|^2$, we obtain $\nabla E(x) = x - z + \tau x$. The global minimiser satisfies

$$\nabla E(\hat{x}) = 0 \quad \Leftrightarrow \quad \hat{x} = \frac{z}{1 + \tau}$$



Proximal gradient method

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$$\Rightarrow \quad \text{prox}_{\frac{\tau}{2}\|\cdot\|^2}(z) = \frac{z}{1 + \tau}$$



Proximal gradient method

Example for a proximal map

$$\text{prox}_{\tau R}(\mathbf{z}) := \arg \min_{\mathbf{x}} \left\{ \frac{1}{2} \|\mathbf{x} - \mathbf{z}\|^2 + \tau R(\mathbf{x}) \right\} \quad :$$



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For the choice $R(\mathbf{x}) = \begin{cases} 0 & \mathbf{x} \in C \\ \infty & \mathbf{x} \notin C \end{cases}$ this reads as

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Proximal gradient method

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Projection onto convex set C !



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This might be important in some real applications where we have some constraints on the x !

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Projection onto convex set C !

This might be important in some real applications where we have some constraints on the x !

$$\text{Example: } C = \{x \in \mathbb{R} \mid x \in [0,1]\}$$

Constrained optimisation

Special case:

$$R(w) = \begin{cases} 0 & w \in C \\ \infty & w \notin C \end{cases}$$

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Constrained optimisation

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$$\begin{aligned} \Rightarrow \text{prox}_{\tau R}(z) &= \arg \min_{w \in \mathbb{R}^n} \|w - z\|^2 + R(w) \\ &= \arg \min_{w \in C} \|w - z\|^2 = \text{proj}_C(z) \end{aligned}$$



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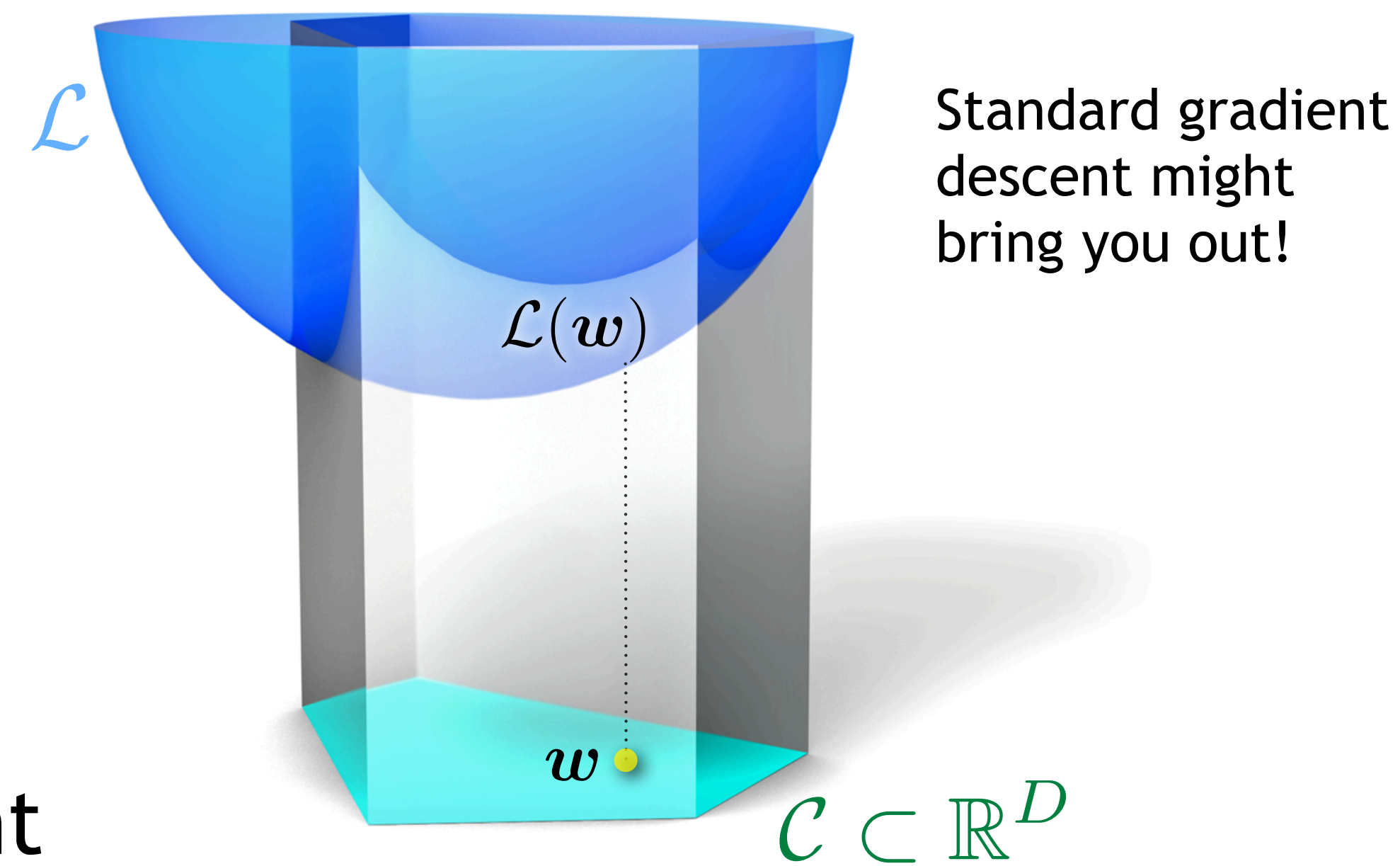
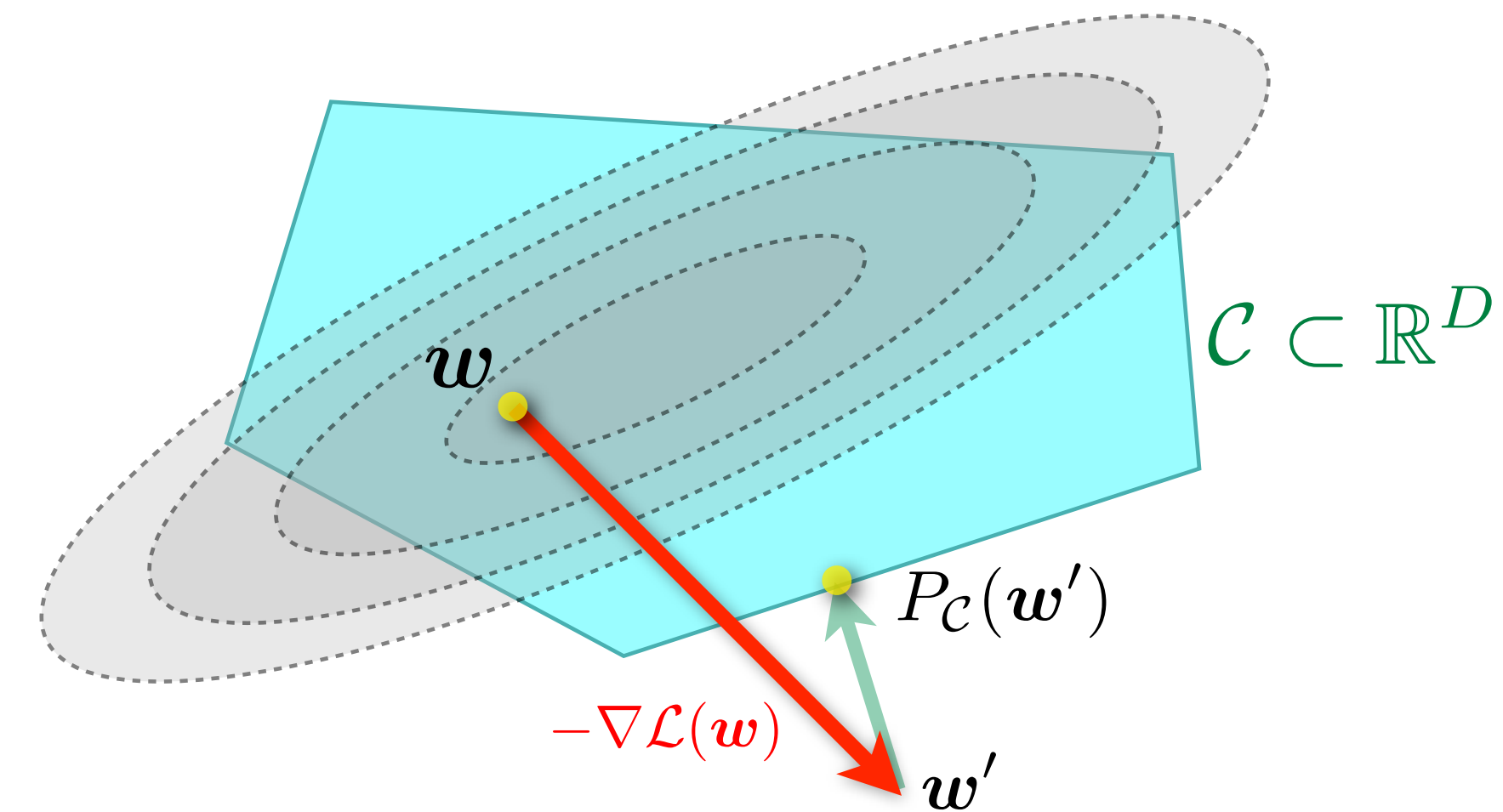
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$$= \arg \min_{w \in C} \|w - z\|^2 = \text{proj}_C(z)$$

$$\Rightarrow w^{k+1} = \text{proj}_C(w^k - \tau \nabla L(w^k))$$

Projected gradient descent



Proximal gradient method

Suppose we want to minimise $E(\mathbf{w}) = L(\mathbf{w}) + R(\mathbf{w})$

Assumptions: 1. L is differentiable, i.e. $\nabla L(\mathbf{w})$ exists

2. R has a simple proximal map, i.e.

$$\text{prox}_{\tau R}(\mathbf{z}) := \arg \min_{\mathbf{x}} \left\{ \frac{1}{2} \|\mathbf{x} - \mathbf{z}\|^2 + \tau R(\mathbf{x}) \right\}$$

is easy to compute

Proximal gradient method: $\mathbf{w}^{k+1} = \text{prox}_{\tau R}(\mathbf{w}^k - \tau \nabla L(\mathbf{w}^k))$



Proximal gradient descent

Minimise variational regularisation $L(\mathbf{w}) + R(\mathbf{w})$ iteratively via

$$\mathbf{w}^{k+1} = (I + \tau \partial R)^{-1} (\mathbf{w}^k - \tau \nabla L(\mathbf{w}^k))$$

where the *proximal map* is defined as

$$(I + \tau \partial R)^{-1}(\mathbf{z}) := \arg \min_{\mathbf{w} \in \mathbb{R}^{d+1}} \left\{ \frac{1}{2} \|\mathbf{w} - \mathbf{z}\|^2 + \tau R(\mathbf{w}) \right\}$$

