Mathematics Toolbox for Machine Learning

Panos Parpas, April 2023

Introductions

- Panos Parpas
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Previously

- Research Fellow, Institute for Data, Systems, and Society, Massachusetts Institute of Technology (2009-2011)
- Global Model and Analytics Group, Credit Suisse (2007-2009)
- PhD in Stochastic Optimization (Imperial College London, 2005)
- CQF Alumni (2007)

Contents and Aims

Aims:

- Introduce a mathematical toolbox as used in ML
- Demonstrate mathematics with different ML models

A. Linear Algebra

1. Matrices and vectors
2. Measuring similarity
3. Eigenvectors/Eigenvalues
4. Matrix Factorisations

B. Calculus

C. Optimisation

1. Classes of Optimization Models/Algorithms
2. Gradient Descent (Stochastic, Acceleration, Momentum)
3. Optimality Conditions (constrained case)

Exercises with solutions available on the platform

Linear Algebra: Vectors, Matrices and Tensors

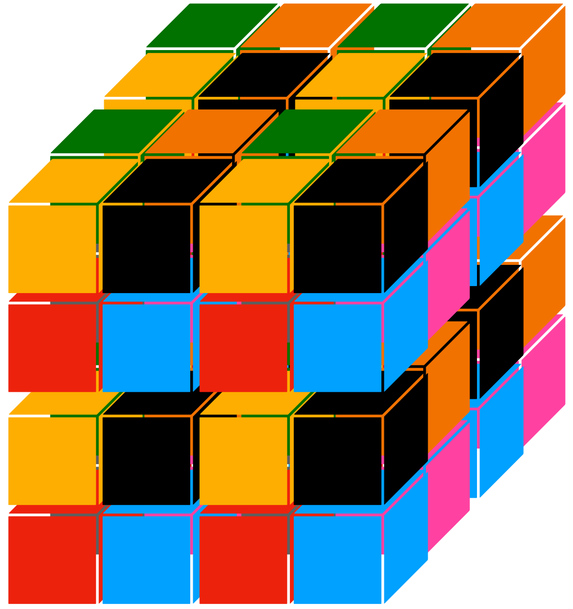
Vectors, matrices and tensors of real numbers can represent *most* of the objects encountered in ML

$\in \mathbb{R}^4$

Vector

$\in \mathbb{R}^{4\times4}$

Matrix



$\in \mathbb{R}^{4\times4\times4}$

Tensor

Vectors and Matrices as Functions

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Vector [0.1,-1.2,3.14] is also a function:

$$1 \mapsto 0.1$$
$$2 \mapsto -1.2$$
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Images as vectors:

$$\{1,...,...n\} \times \{1,...,...n\} \mapsto \mathbb{R}^3$$
$$[120,145] \mapsto [10,30,14]$$

Image Size (400,600)

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Bag of words model (Natural Language Processing)

```
John likes to watch movies. Mary likes movies too.
```

$$\text{John} \mapsto 1$$
$$\text{likes} \mapsto 2$$
$$\text{to} \mapsto 1$$
$$\text{watch} \mapsto 1$$
$$\text{movies} \mapsto 2$$
$$\text{Mary} \mapsto 1$$
$$\text{too} \mapsto 1$$

Inner Products Measure Distances

Inner (dot) product in $\mathbb{R}^d$: $\langle x, y \rangle = \sum_{i=1}^{d} x_i y_i = x^\top y$

Length (norm) in $\mathbb{R}^d$: $\|x\| = \sqrt{\langle x, x \rangle}$

Angle between vectors $\cos(\theta) = \dfrac{\langle x, y \rangle}{\|x\| \|y\|}$

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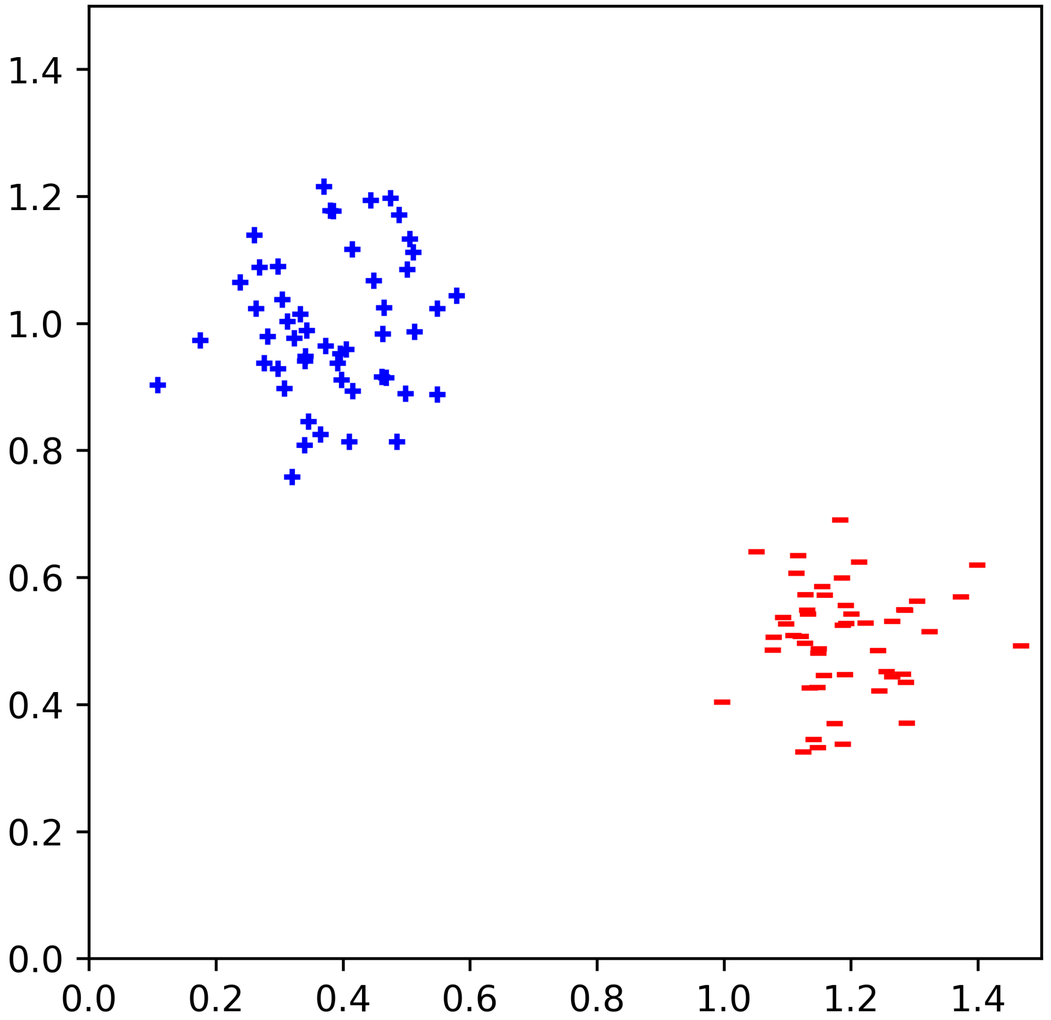
Data: $(x_1, y_1), \ldots, (x_m, y_m) \in \mathbb{R}^2 \times \pm 1$



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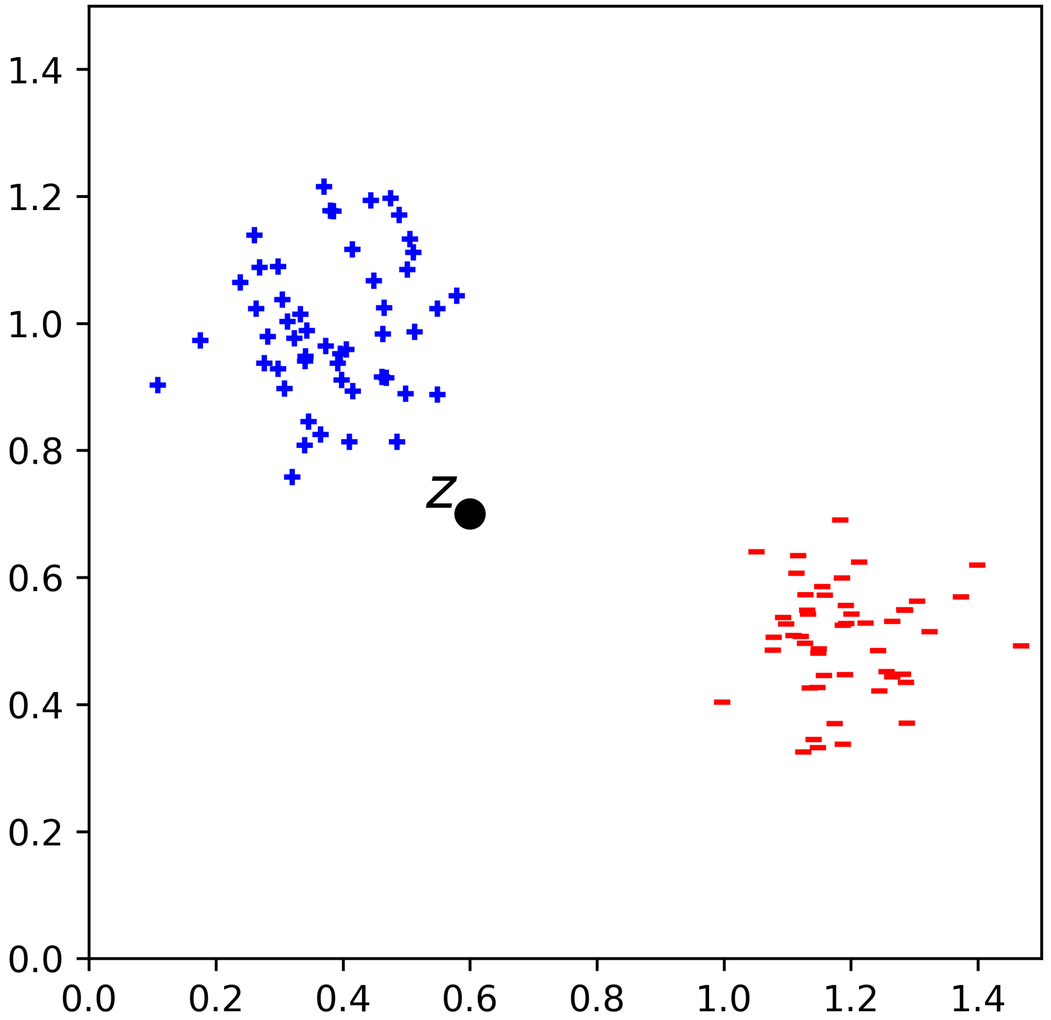

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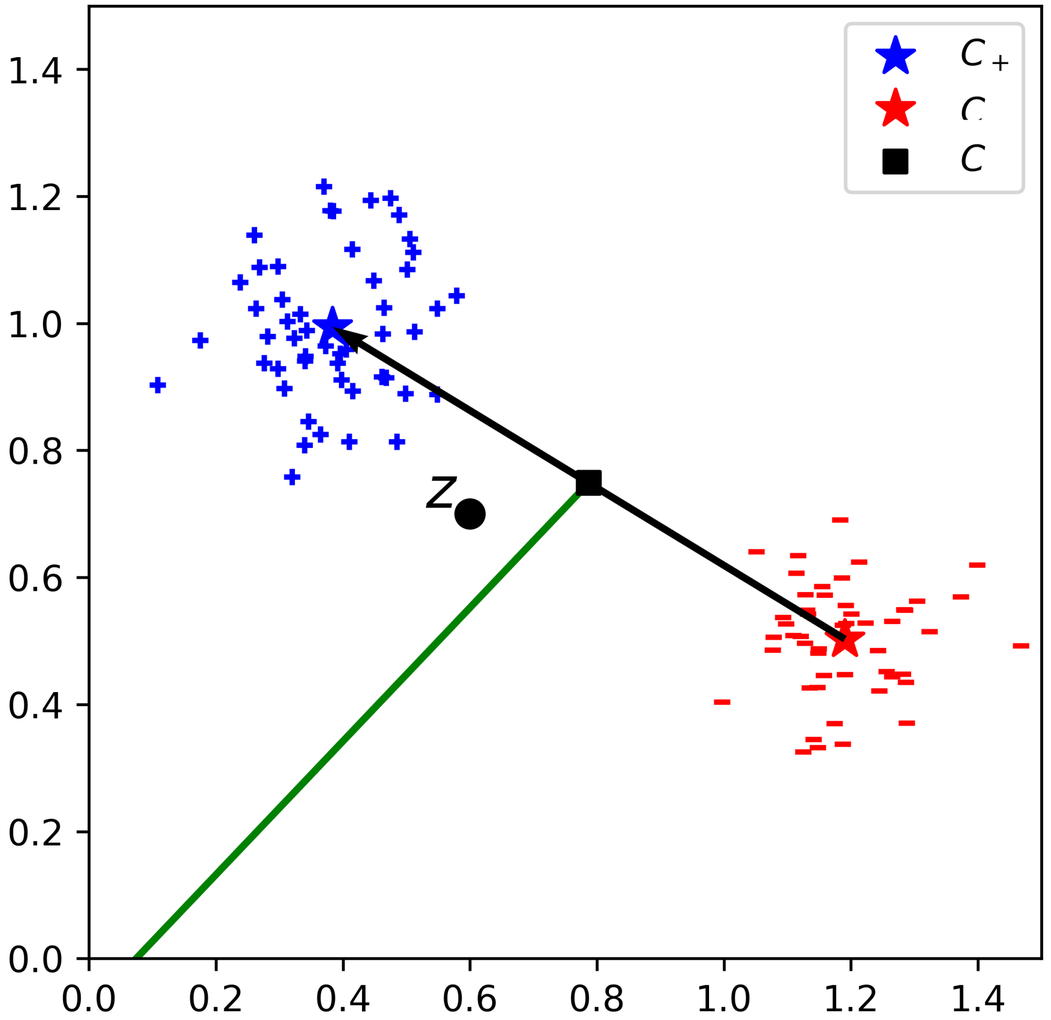
New point Z: Is it a + or a - ?

$$C_+ = \frac{1}{m_+} \sum_{i=1}^{m_+} x_i, C_- = \frac{1}{m_-} \sum_{i=1}^{m_-} x_i$$

$$C = \frac{1}{2}(C_+ + C_-), w = C_+ - C_-$$



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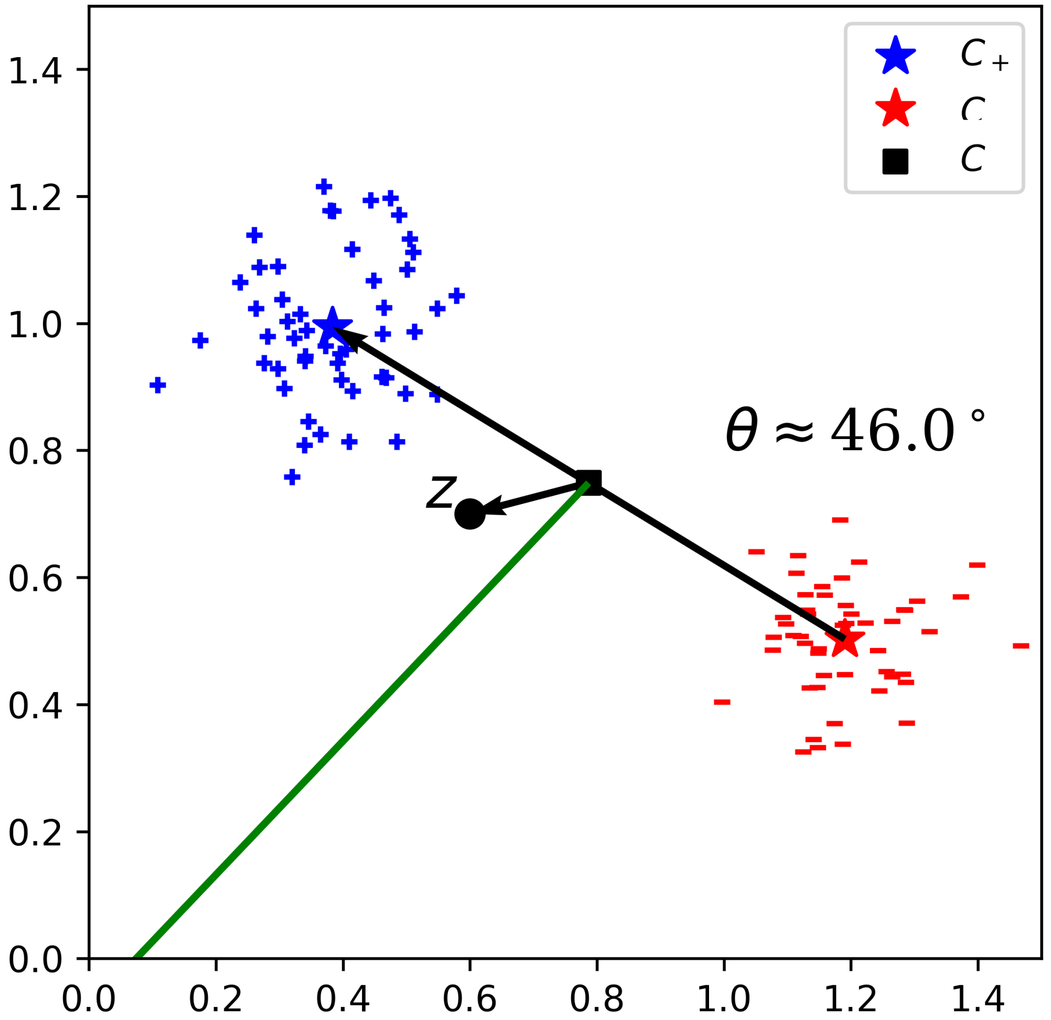

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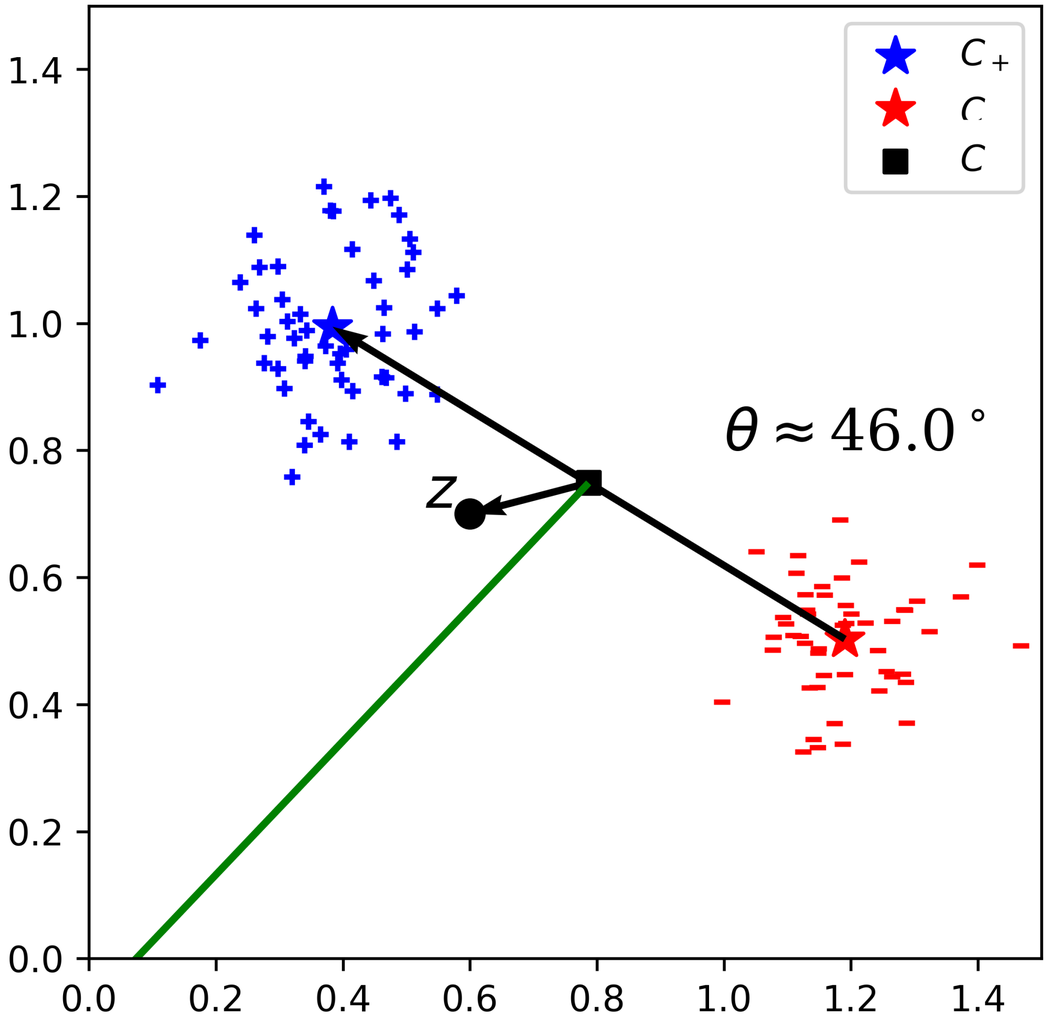

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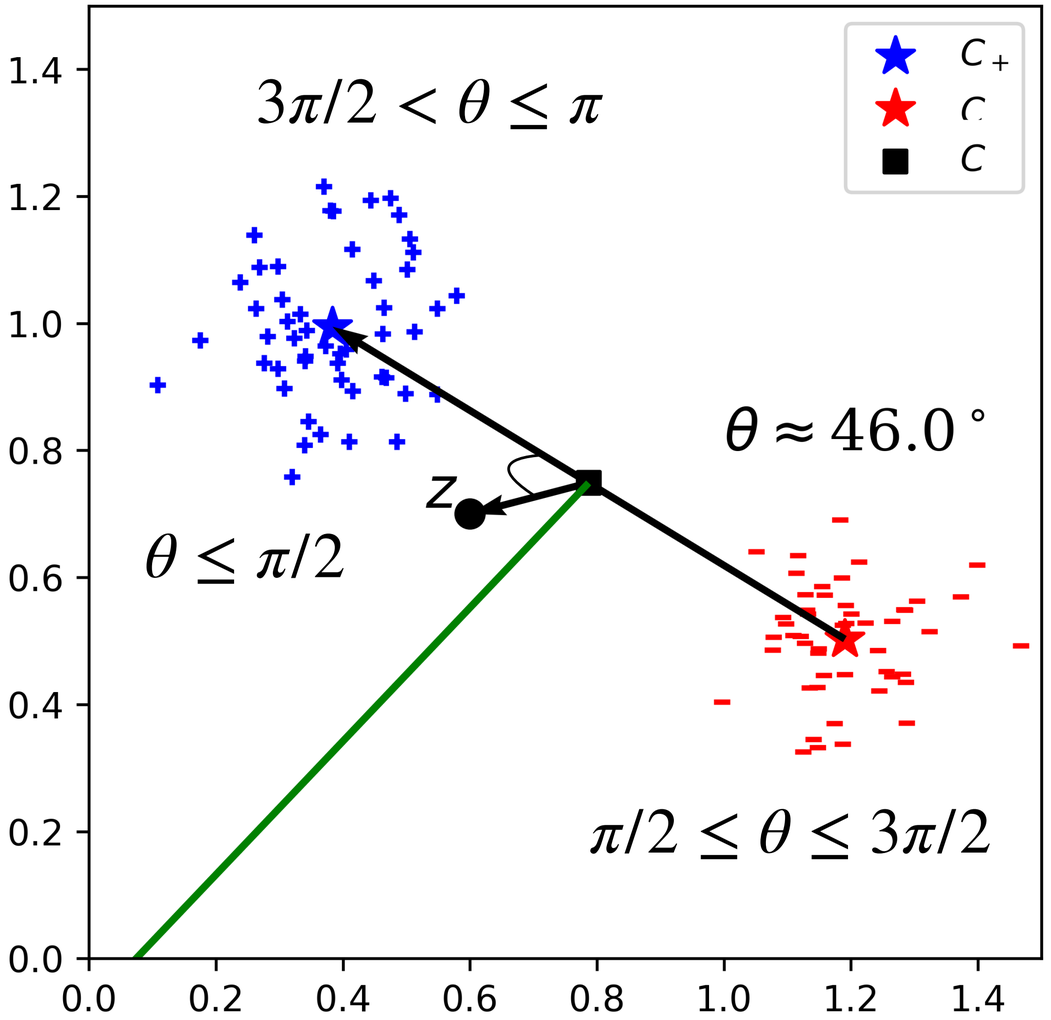

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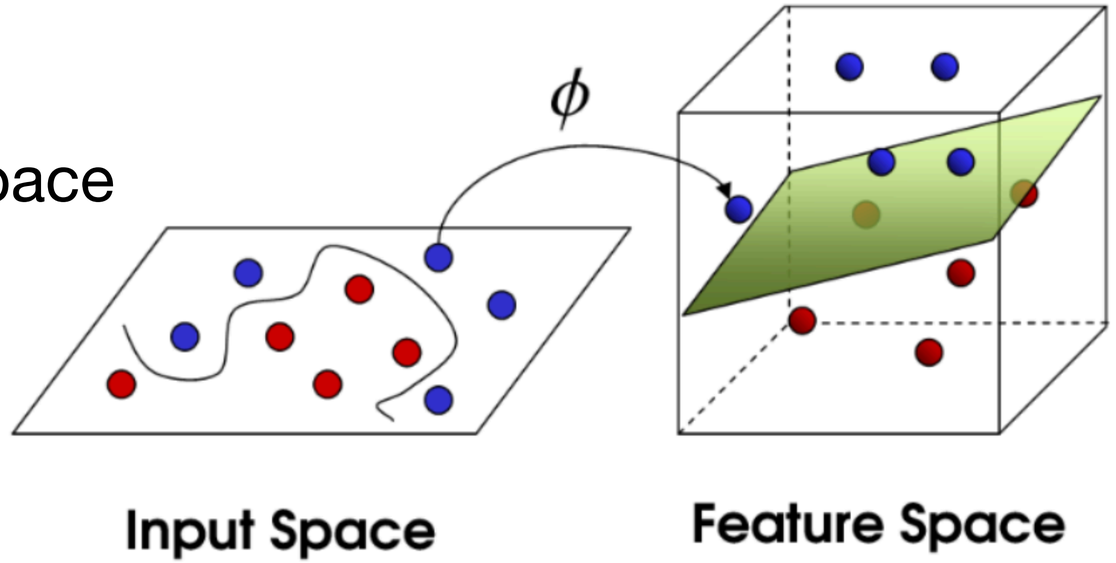
Inner product and non-linearities

Inner products can be generalised to deal with non-linearly separable data

1. Embed the data in an appropriate inner product space

non-linear map $\Phi : \mathcal{X} \mapsto \mathcal{H}$

Input Space Feature Space



2. Compute distances using inner products:

$$k(x, y) = \langle \Phi(x), \Phi(y) \rangle$$

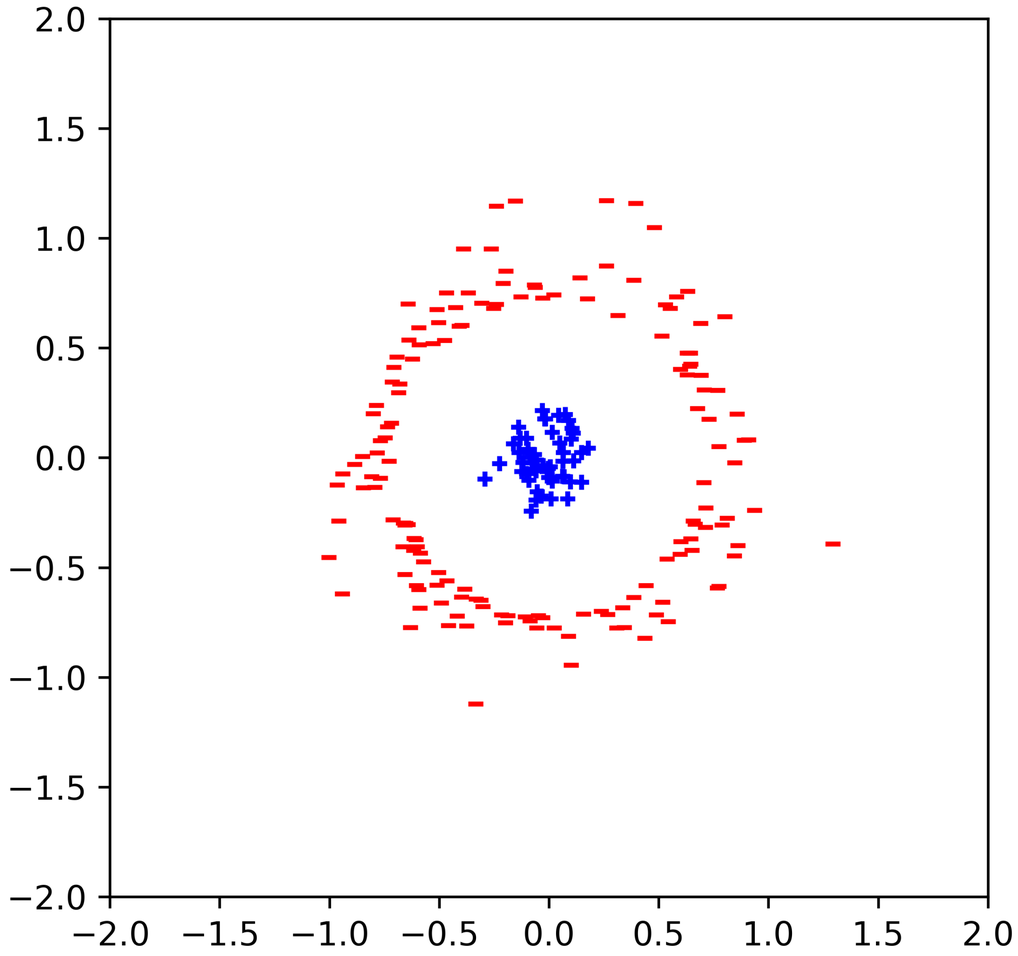
Kernel

Example: Data Lifting & Kernel Trick

Feature map:

$$\Phi : \mathbb{R}^2 \mapsto \mathbb{R}^3$$

$$\Phi(x) = [x_1^2 \; x_2^2 \; \sqrt{2}x_1x_2]^\top$$



Non-linearly separable data in hypothesis space

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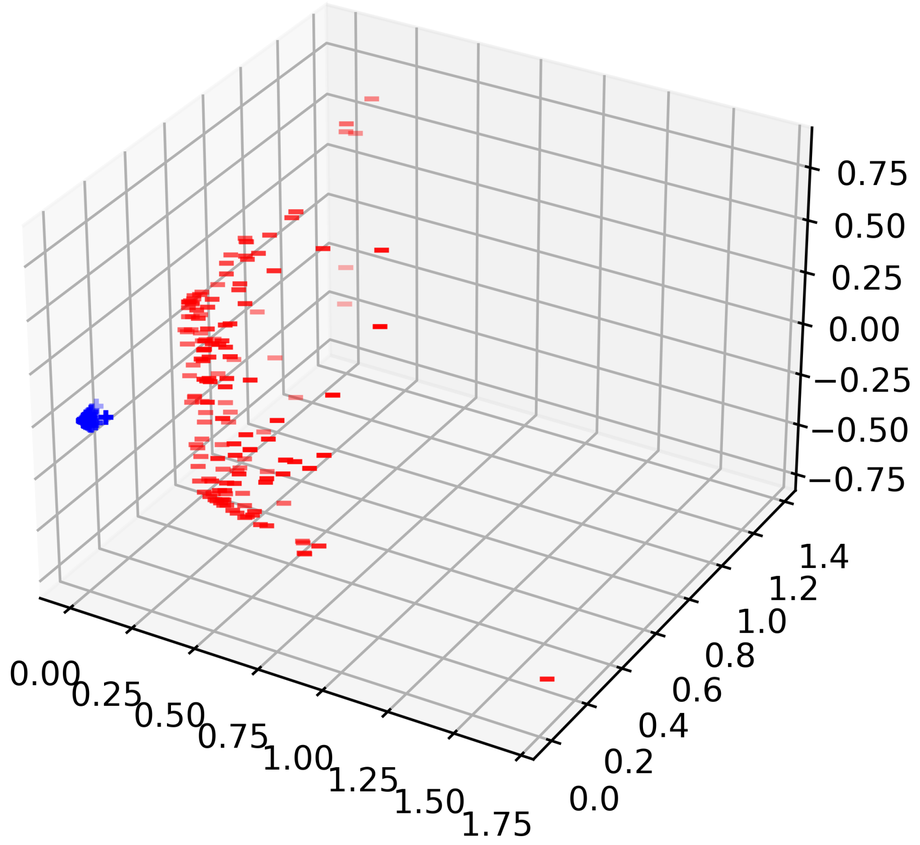

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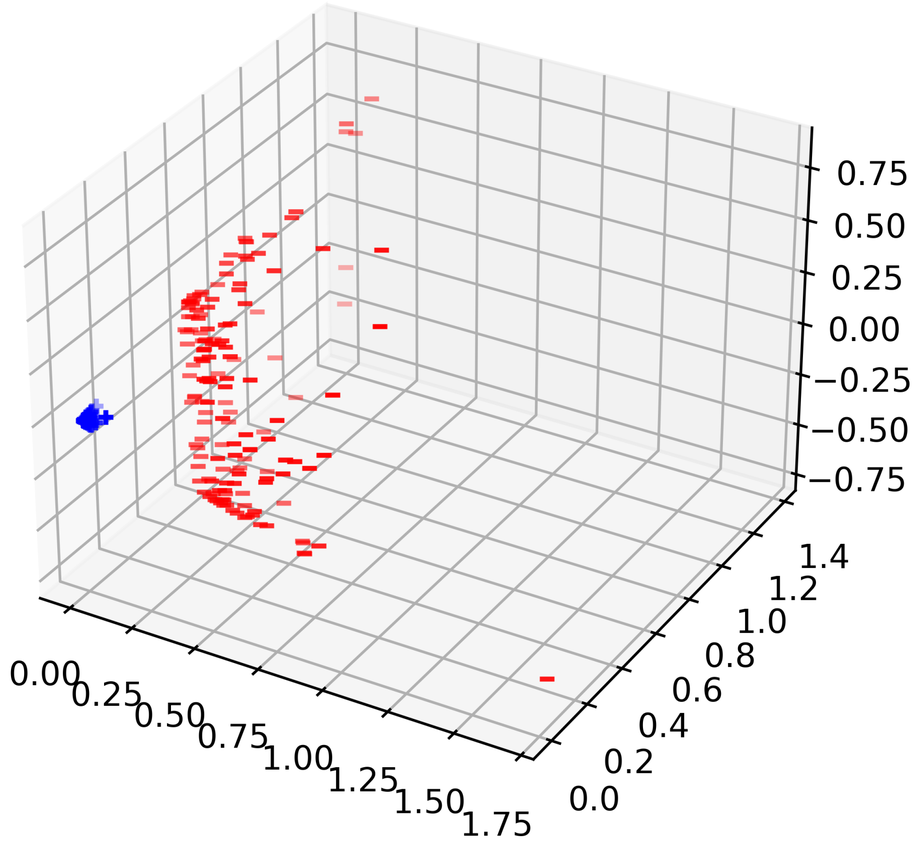

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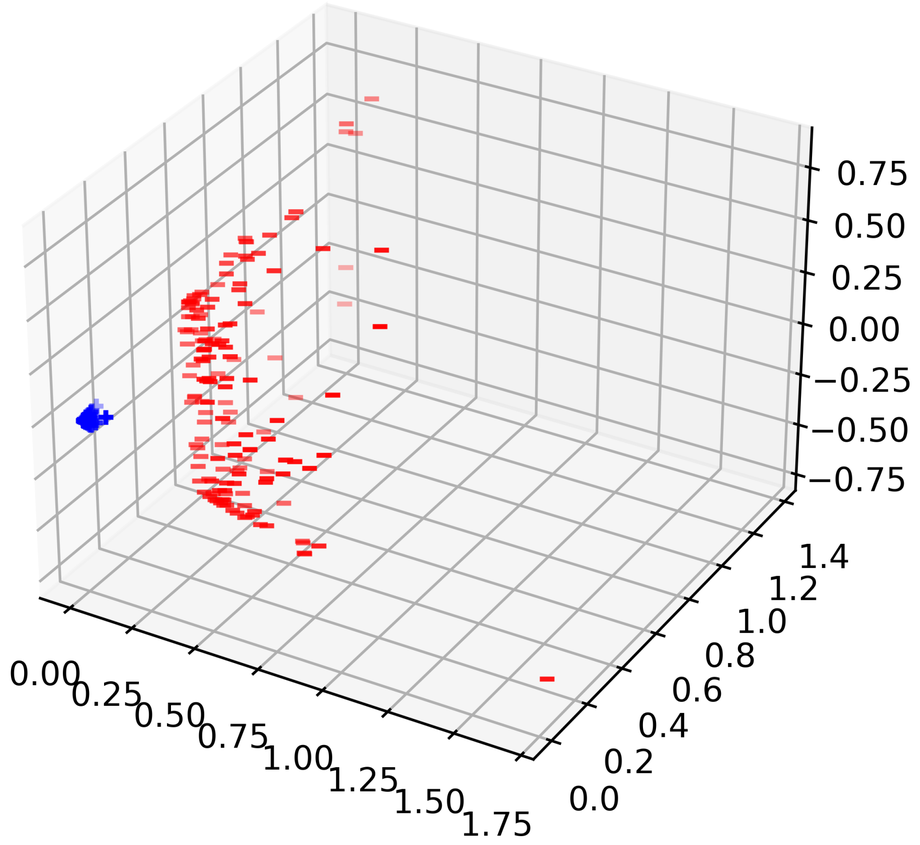

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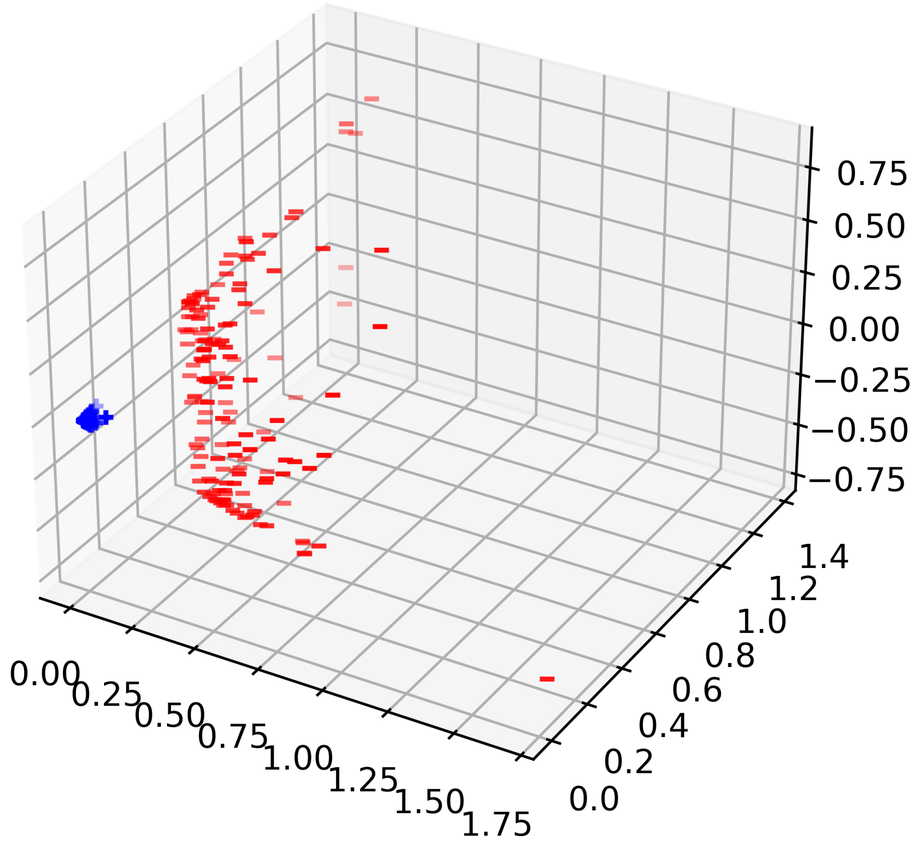
“Kernel trick”: avoid expensive operations in higher dimensions by finding an appropriate kernel



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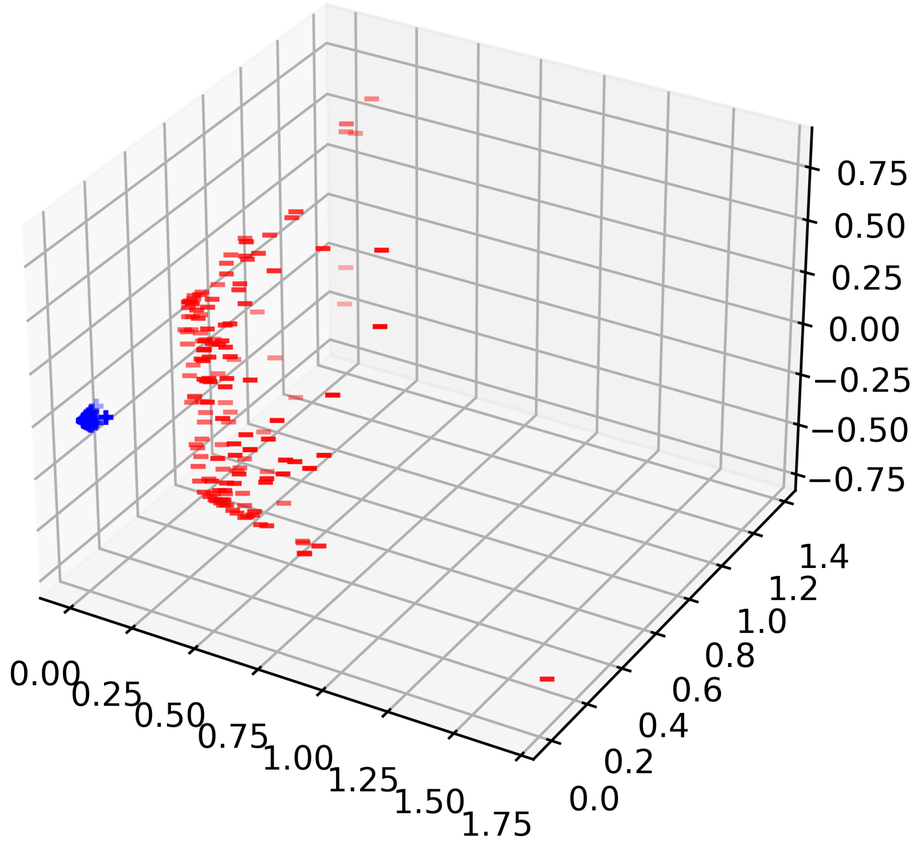
Is it always possible to do this?
Yes! (Mercer’s Theorem)



Data is linearly separable in feature space

Mercer’s and Cover’s Theorems

(Mercer's Theorem) A symmetric function can be written as the inner product

$$k(x, y) = \langle \Phi(x), \Phi(y) \rangle$$

if and only if k is positive semidefinite i.e.

$$\int k(x, y) g(x) g(y) dx dy \geq 0$$

Cover’s Theorem: As the dimension of the feature space increase, so does the probability of having linearly separable data.

Practical implication: increase the dimension of the feature space to make the data linearly separable and use the kernel trick to manage computation

Applications: support vector machines, kernel PCA, Bayesian Kernel Methods, Regularised Kernel Methods, and so much more!

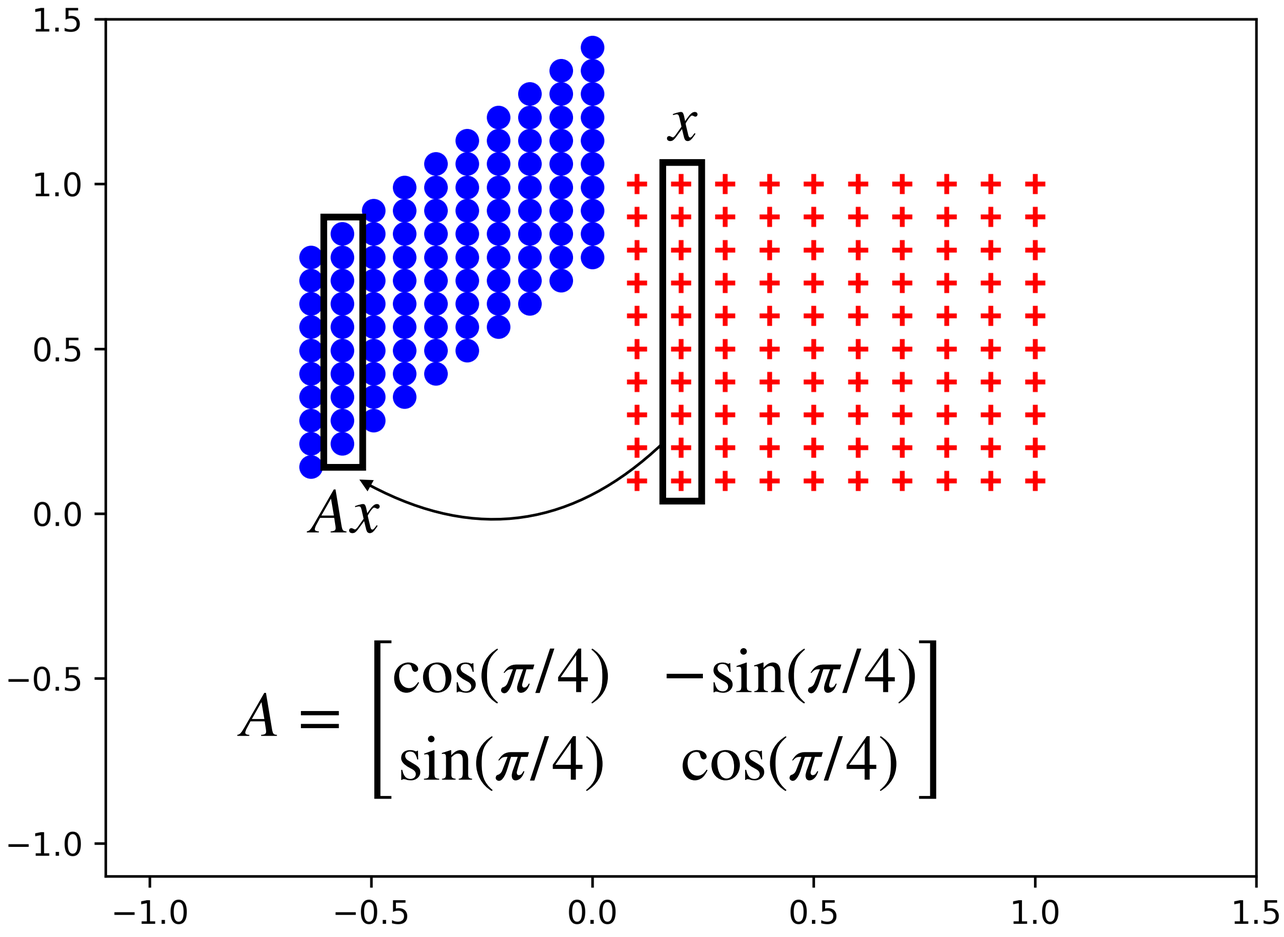
Matrix Decompositions/Factorisations

Tools:

- SVD (Singular Value Decomposition)
- Cholesky Decomposition
- Eigenvalue Decomposition

Applications:

- Dimensionality reduction
- Data scaling
- Simulation
- Preconditioning
- Recommender systems (netflix)
- Pagerank (Google)



$A \in \mathbb{R}^{N \times d}$ performs linear transformations on vectors in $\mathbb{R}^d$

Eigenvalues/Eigenvectors

Let $A \in \mathbb{R}^{n \times n}$ be a square matrix then $\lambda \in \mathbb{R}$ is an eigenvalue and $x \in \mathbb{R}^n \backslash 0$ the associated eigenvector:

$$Ax = \lambda x$$

Useful facts:

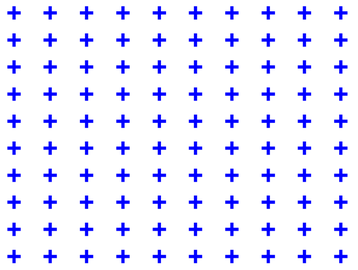
- The number of non-zero eigenvalues == number of linearly independent row/columns/rank
- Trace of matrix: $\text{trace}(A) = \sum_{i=1}^{n} A_{ii} = \sum_{i=1}^{n} \lambda_i$
- Determinant of matrix (measures volume)

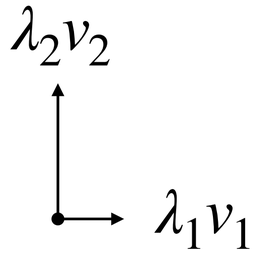
$$\det(A) = \prod_{i=1}^{n} A_{ii} = \prod_{i=1}^{n} \lambda_i$$

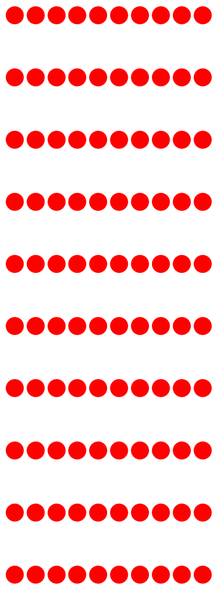
Intuition: Eigenvalues/Eigen Vectors

$$A_1 = \begin{bmatrix} \frac{1}{2} & 0 \\ 0 & 2 \end{bmatrix}$$

$$\lambda_1 = \frac{1}{2}, \lambda_2 = 2, v_1 = [1,0]^\top v_2 = [0,1]^\top .$$







Eigenvectors are canonical- i.e. mapping changes each direction

Area preserving. i.e determinant is the same

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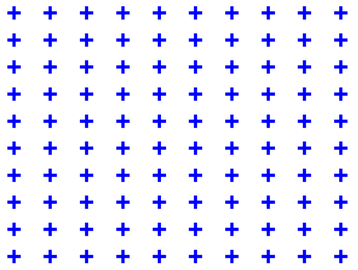

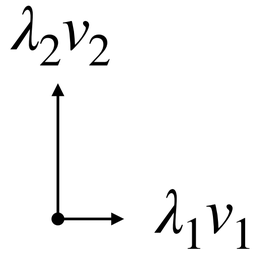

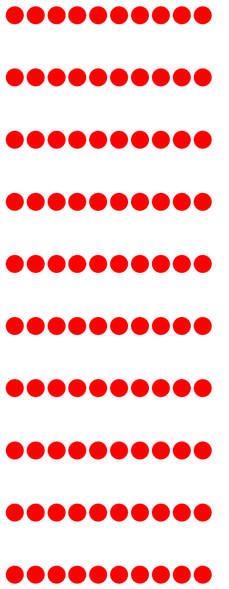

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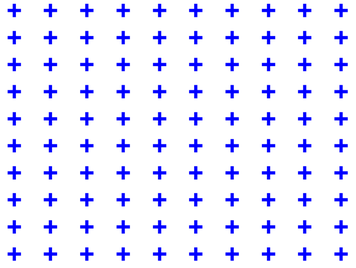
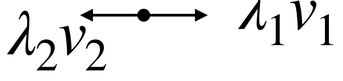
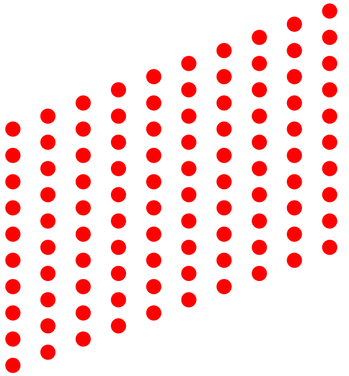
Area preserving. i.e determinant is the same

$$A_2 = \begin{bmatrix} 1 & \frac{1}{2} \\ 0 & 1 \end{bmatrix}$$

$$\lambda_1 = 1, \lambda_2 = 1, v_1 = [1,0]^\top v_2 = [-1,0]^\top .$$



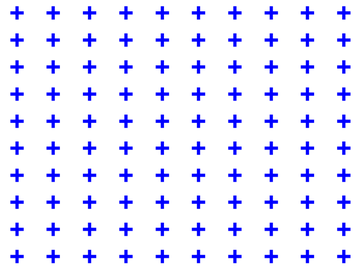


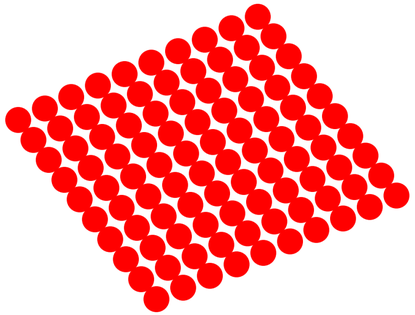


Eigenvectors are co-linear i.e. mapping changes only one direction
(Area preserving)

Intuition: Eigenvalues/Eigen Vectors

$$A_3 = \begin{bmatrix} \cos(\frac{\pi}{6}) & -\sin(\frac{\pi}{6}) \\ \sin(\frac{\pi}{6}) & \cos(\frac{\pi}{6}) \end{bmatrix}$$



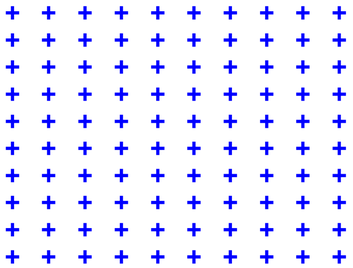


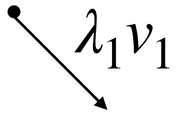
$\lambda_1 = 0.87 + 0.5j, \lambda_2 = 0.87 - 0.5j$

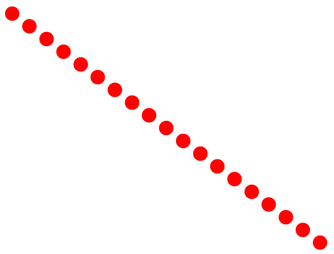
$v_1 = [0.71, -0.71j]^\top v_2 = [0.71, 0.7j]^\top .$

Eigenvalues are complex (rotation)

$$A_4 = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$





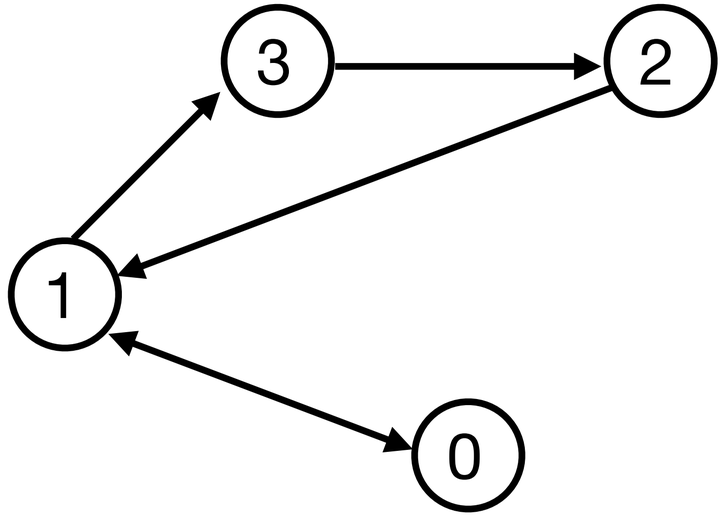


$\lambda_1 = 2, \lambda_2 = 0$

$v_1 = [0.71, -0.71]^\top v_2 = [0.71, 0.71]^\top .$

A zero eigenvalue means the direction in v_2 collapses (the matrix has linearly dependent rows). The determinant becomes 0, matrix/transformation is not invertible.

Computing Eigenvalues: Power Iteration



Graph view of the “web”

$$\begin{array}{c} \\ 0 \\ 1 \\ 2 \\ 3 \end{array}\begin{array}{c} \begin{array}{cccc} 0 & 1 & 2 & 3 \end{array} \\ \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{bmatrix} \end{array} = A$$

Columns of **adjacency matrix** are out-going edges from node

Link from node 3 to 2

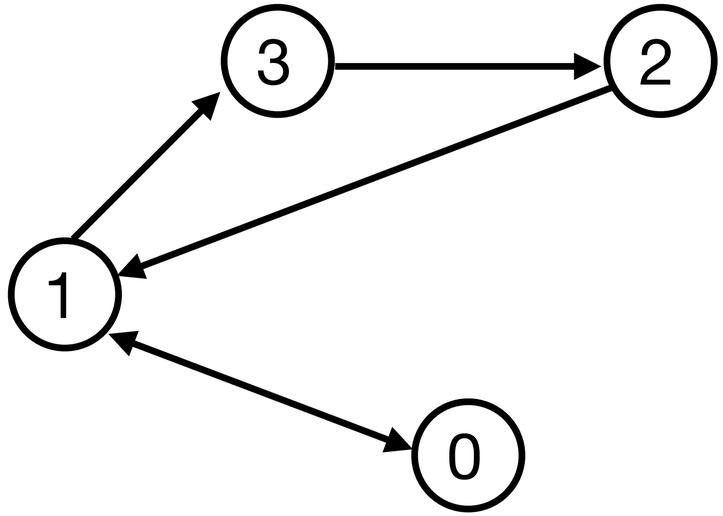
$$D = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

Degree matrix: diagonal matrix of sum of rows

$$M = AD^{-1} = \begin{bmatrix} 0 & 1/2 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1/2 & 0 & 0 \end{bmatrix}$$

Transition matrix: column stochastic matrix for a random surfer

Computing Eigenvalues: Power Iteration



Graph view of the “web”

$$M = \begin{bmatrix} 0 & 1/2 & 0 & 0 \\ 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1/2 & 0 & 0 \end{bmatrix}$$

Transition matrix: column stochastic matrix for a random surfer e.g. if on page 1 then 0.5 probability to go to 0 or 3

Power Iteration: $v_{t+1} = Mv_t$

After a few iterations v converges to:

$$[0.2, 0.4, 0.2, 0.2]^\top$$

Cholesky Decomposition*

A symmetric positive definite matrix can be factorized into a product $A = LL^{\top}$ where L is a lower triangular matrix with positive diagonal elements

$$A = \begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{bmatrix} = \begin{bmatrix} l_{11} & \cdots & 0 \\ \vdots & \ddots & \vdots \\ l_{n1} & \cdots & l_{nn} \end{bmatrix} \begin{bmatrix} l_{11} & \cdots & l_{n1} \\ \vdots & \ddots & \vdots \\ 0 & \cdots & l_{nn} \end{bmatrix}$$

L is called the Cholesky factor of A and is unique.

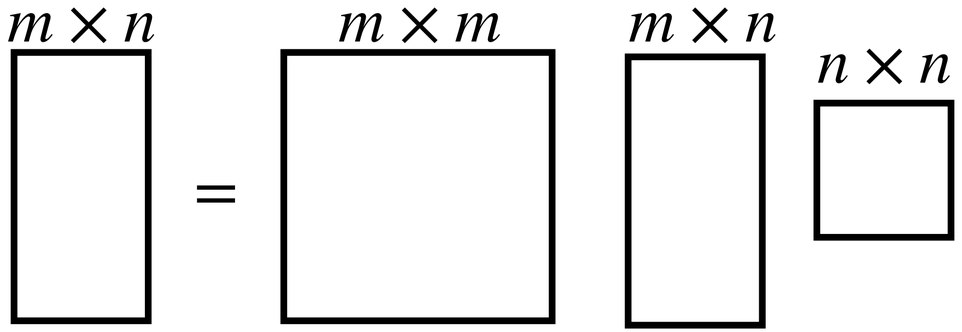
Applications:

Factorisation of Gaussian random variables
Solving linear systems of equations

* A square root for matrices. A special case of LU decomposition which applies to all square matrices

Singular Value Decomposition (SVD)

For a matrix $A \in \mathbb{R}^{m \times n}$ rank $r = \min\{m, n\}$ then SVD is of the form $A = USV^\top$



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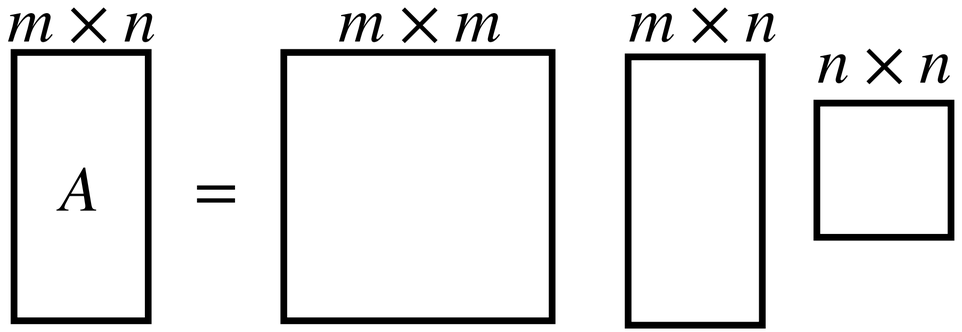

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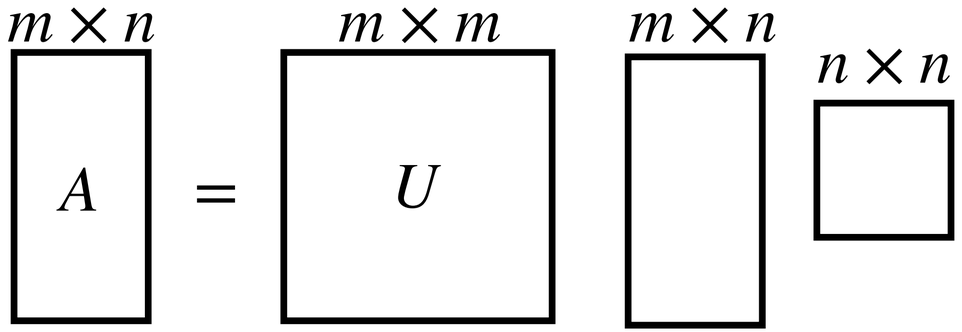

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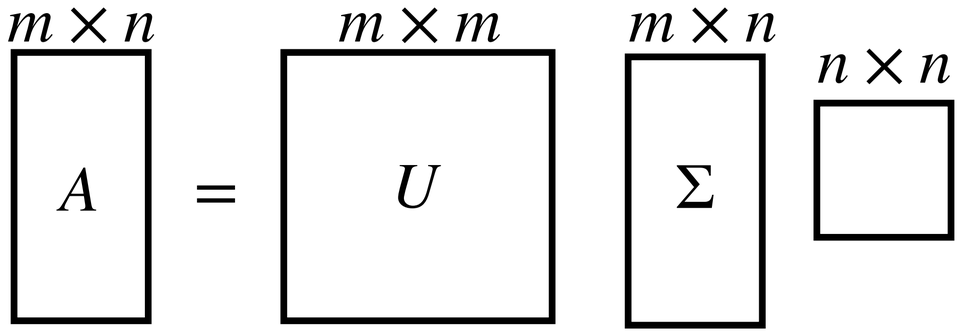

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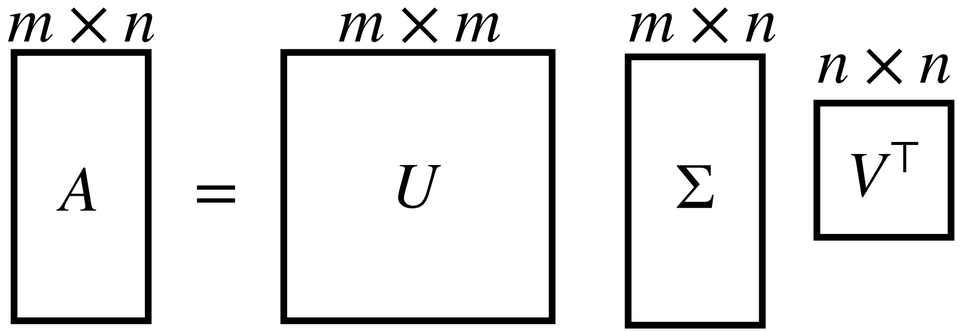

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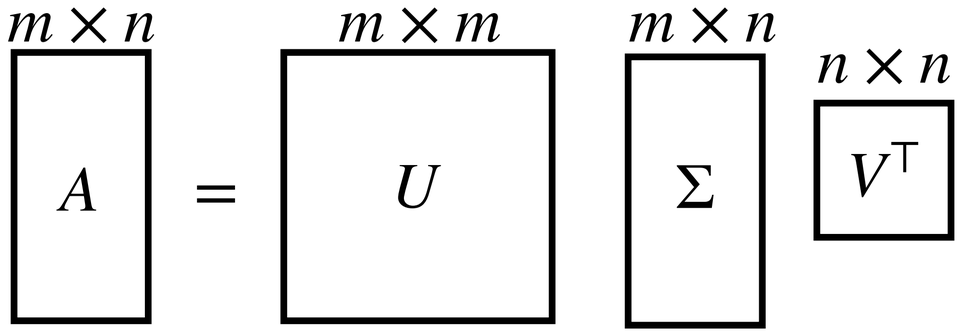

where $U \in \mathbb{R}^{m \times m}$, $V \in \mathbb{R}^{n \times n}$ are orthogonal matrices and

Σ has entries $\Sigma_{ii} = \sigma_i \geq 0$ and $\Sigma_{ij} = 0$ if $i \neq j$.

The columns of $U(V)$ are called the left (right) singular vectors of A.

The σ_i are called the singular values of A.

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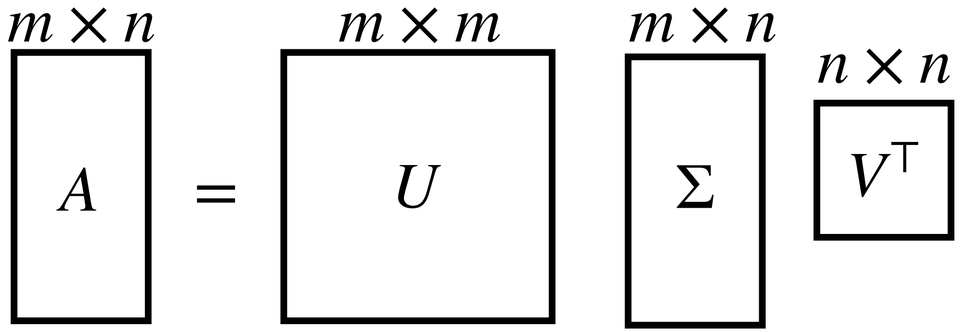

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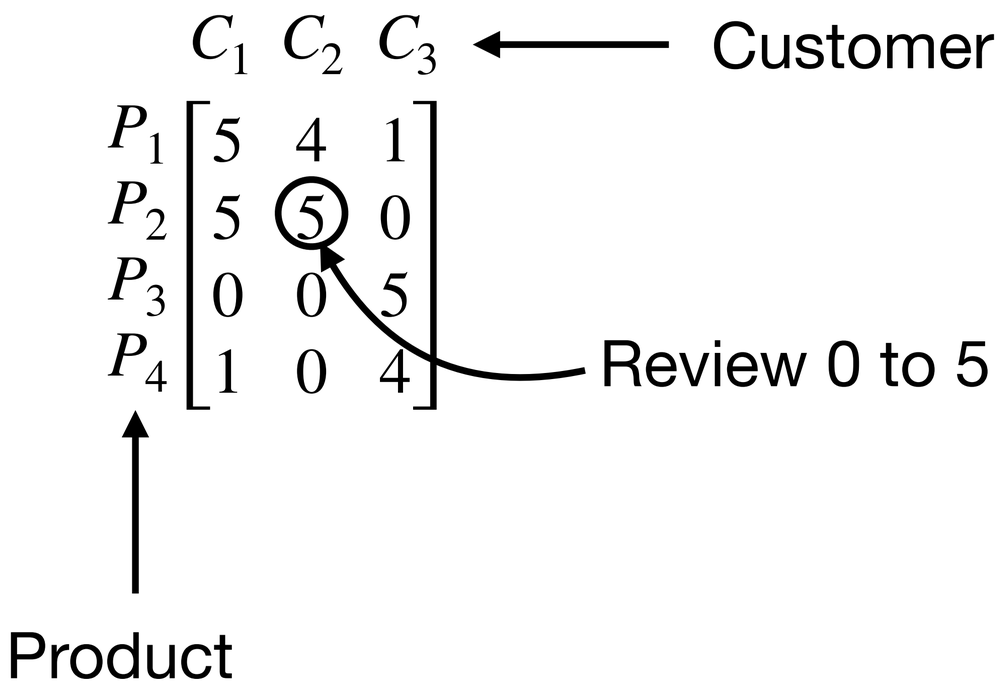
- SVD can be applied to **any** matrix (not just symmetric matrices), other definitions of SVD are sometimes used but equivalent to the one above
- **Extremely** useful in ML and is for dimensionality reduction (Principal Component Analysis), solving linear systems (linear regression), noise removal, outlier detection, feature engineering, etc…

SVD in Recommender Systems

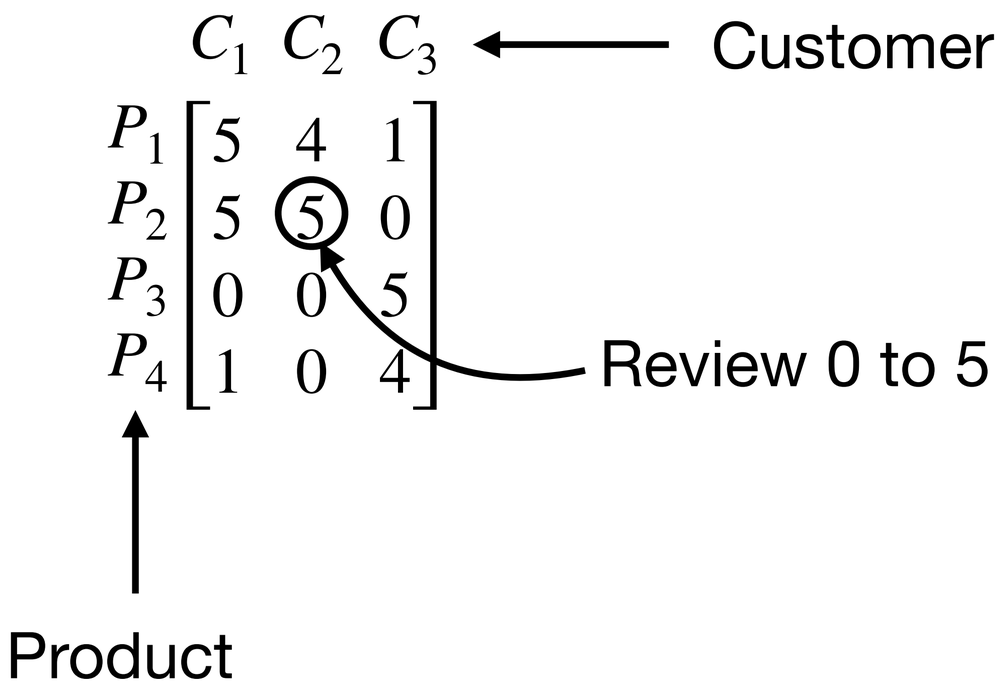


Some observations:

C_1 and C_2 appear to like similar products

P_3 and P_4 are liked by a single person

SVD in Recommender Systems



Some observations:

C_1 and C_2 appear to like similar products

P_3 and P_4 are liked by a single person

How do you automate these observations?

SVD captures the relationships between customers and products

SVD in Recommender Systems

$$\begin{array}{c} \\ P_1 \\ P_2 \\ P_3 \\ P_4 \end{array}\begin{array}{c} \begin{array}{ccc} C_1 & C_2 & C_3 \end{array} \\ \begin{bmatrix} 5 & 4 & 1 \\ 5 & 5 & 0 \\ 0 & 0 & 5 \\ 1 & 0 & 4 \end{bmatrix} \end{array} = \begin{bmatrix} -0.6710 & 0.0236 & 0.4647 & -0.5774 \\ -0.7197 & 0.2054 & -0.4759 & 0.4619 \\ -0.0939 & -0.7705 & -0.5268 & -0.3464 \\ -0.1515 & -0.6030 & 0.5293 & -0.5774 \end{bmatrix}$$

Stereotypical Products

$$\begin{bmatrix} 9.6438 & 0 & 0 \\ 0 & 6.3639 & 0 \\ 0 & 0 & 0.7056 \\ 0 & 0 & 0 \end{bmatrix}$$

Singular values ‘mix’ singular vectors to reproduce data

Stereotypical Customers

$$\begin{bmatrix} -0.7367 & -0.6516 & -0.1811 \\ 0.0852 & 0.1762 & -0.9807 \\ 0.6708 & -0.7379 & -0.0743 \end{bmatrix}$$

SVD in Recommender Systems

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Stereotypical Products

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$$\begin{bmatrix} 9.6438 & 0 & 0 \\ 0 & 6.3639 & 0 \\ 0 & 0 & 0.7056 \\ 0 & 0 & 0 \end{bmatrix} \Sigma$$

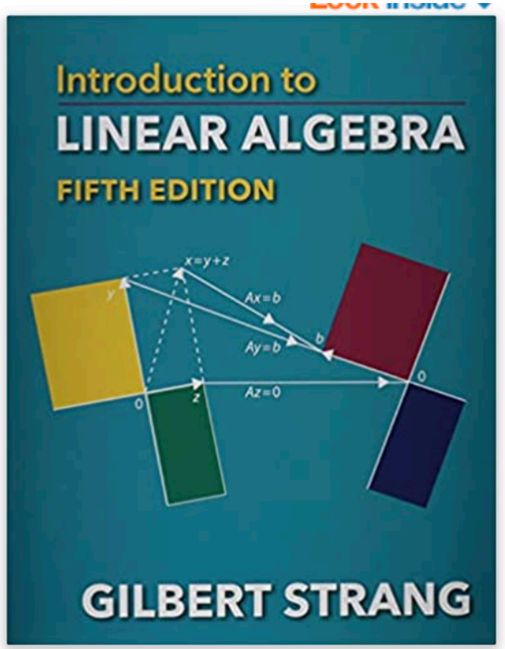
Singular values ‘mix’ singular vectors to reproduce data

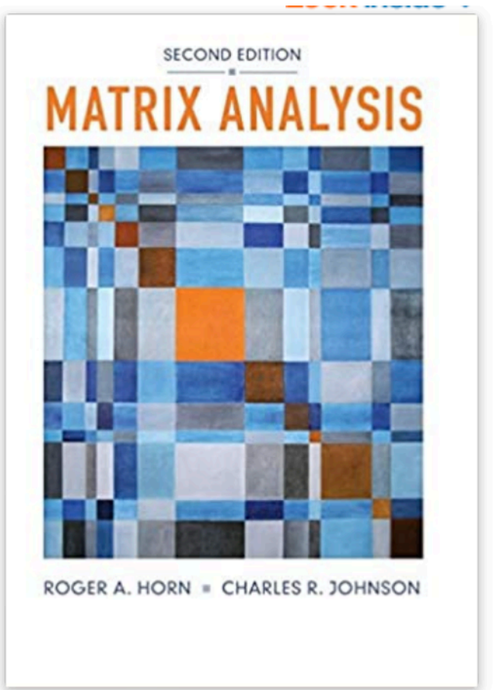
Stereotypical Customers

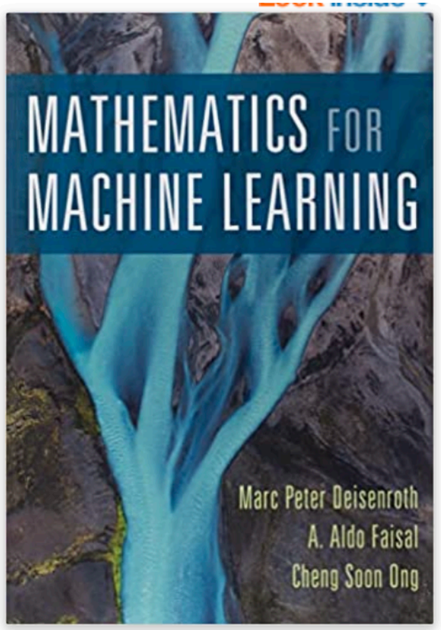
$$\begin{bmatrix} -0.7367 & -0.6516 & -0.1811 \\ 0.0852 & 0.1762 & -0.9807 \\ 0.6708 & -0.7379 & -0.0743 \end{bmatrix} V^\top$$

Linear Algebra Summary

- In ML we represent data as vectors
- Necessary to go beyond simple geometric vectors (but computation often reduces to this)
- Inner products measure distances
- If the space is “non-linear” kernels can help
- Matrix factorisations are used to give insights and reduce dimensions







Calculus Background

Gradient of $L : \mathbb{R}^d \mapsto \mathbb{R}$

$$\nabla L(w) = \begin{bmatrix} \frac{\partial L(w)}{\partial w_1} & \cdots & \frac{\partial L(w)}{\partial w_d} \end{bmatrix}$$

Hessian of $L : \mathbb{R}^d \mapsto \mathbb{R}$

$$\nabla^2 L(w) = \begin{bmatrix} \frac{\partial^2 L(w)}{\partial w_1^2} & \cdots & \frac{\partial^2 L(w)}{\partial w_1 \partial w_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 L(w)}{\partial w_1 \partial w_d} & \cdots & \frac{\partial^2 L(w)}{\partial w_d \partial w_d} \end{bmatrix}$$

We use the convention that the gradient is a column vector i.e $\nabla L \in \mathbb{R}^{1 \times d}$

Gradient of $f(\mathbf{x}) = x_1^2 + x_1x_2 + x_3x_2 + x_3^2$

$$\nabla f(\mathbf{x}) = \left[\frac{\partial f(\mathbf{x})}{\partial x1}\frac{\partial f(\mathbf{x})}{\partial x2}\frac{\partial f(\mathbf{x})}{\partial x3}\right] = \left[2x_1 + x_2x_1 + x_3x_2 + 2x_3\right]$$

Hessian of $f(\mathbf{x}) = x_1^2 + x_1x_2 + x_3x_2 + x_3^2$

$$\nabla^2 f(\mathbf{x}) = \begin{bmatrix} \frac{\partial^2 f(\mathbf{x})}{\partial x_1^2} & \frac{\partial^2 f(\mathbf{x}))}{\partial x_1 \partial x_2} & \frac{\partial^2 f(\mathbf{x}))}{\partial x_1 \partial x_3} \\ \frac{\partial^2 f(\mathbf{x})}{\partial x_1 x_2} & \frac{\partial^2 f(\mathbf{x}))}{\partial x_2^2} & \frac{\partial^2 f(\mathbf{x}))}{\partial x_2 \partial x_3} \\ \frac{\partial^2 f(\mathbf{x})}{\partial x_1 x_3} & \frac{\partial^2 f(\mathbf{x}))}{\partial x_2 x_3} & \frac{\partial^2 f(\mathbf{x}))}{\partial x_3^2} \end{bmatrix} = \begin{bmatrix} 2 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 2 \end{bmatrix}$$

Differentiation Rules (1d)

- Sum Rule

$$\big(f(x)+g(x)\big)' = f'(x)+g'(x) = \frac{df(x)}{dx} + \frac{dg(x)}{dx}$$

- Product Rule

$$\big(f(x)g(x)\big)' = f'(x)g(x)+f(x)g'(x) = \frac{df(x)}{dx}g(x) + f(x)\frac{dg(x)}{dx}$$

- Chain Rule

$$(g\circ f)'(x) = \big(g(f(x))\big)' = g'(f(x))f'(x) = \frac{dg(f(x))}{df}\frac{df(x)}{dx}$$

- Quotient Rule

$$\left(\frac{f(x)}{g(x)}\right)' = \frac{f(x)'g(x)-f(x)g(x)'}{(g(x))^2} = \frac{\frac{df}{dx}g(x)-f(x)\frac{dg}{dx}}{(g(x))^2}$$

Chain Rule Example

$$(g \circ f)'(x) = \big(g(f(x))\big)' = g'(f(x))f'(x) = \frac{dg}{df}\frac{df}{dx}$$

$$\begin{aligned} g(z) &= 6z + 3 \\ z = f(x) &= -2x + 5 \\ (g \circ f)'(x) &= \underbrace{(6)}_{dg/df}\underbrace{(-2)}_{df/dx} \\ &= -12 \end{aligned}$$

$$\begin{aligned} g(z) &= \tanh(z) \\ z = f(x) &= x^n \\ (g \circ f)'(x) &= \underbrace{(1 - \tanh^2(x^n))}_{dg/df}\underbrace{nx^{n-1}}_{df/dx} \end{aligned}$$

Vector Differentiation — Index Notation

Consider the multivariate Linear Regression problem

$$L(\boldsymbol{\theta}) = \sum_{n=1}^{N} (y_n - \boldsymbol{\phi}(x_n)^\top \boldsymbol{\theta})^2 = ||\mathbf{y} - \Phi(X)\boldsymbol{\theta}||^2$$

Suppose $\theta \in \mathbb{R}^d$, what is $\nabla L(\theta)$?

We could write all the expressions in index notation

Then *carefully* differentiate every term

Most ML algorithms/software rely on *multivariate* chain rule

But let's do the slow way first!

Index Notation — Examples

$$|\mathbf{x}|^2 = \sum_i x_i^2$$

$$\mathbf{x}^\mathsf{T}\mathbf{y} = \sum_i x_i y_i$$

$$\mathbf{y} = f(\mathbf{x})\mathbf{x} \implies y_i = f(\mathbf{x})x_i$$

$$\boldsymbol{A}\mathbf{x} = ?$$

$$[\boldsymbol{A}\mathbf{x}]_j = \sum_j A_{ij}x_j$$

$$\boldsymbol{A}\mathbf{x} = \left[\sum_j A_{ij}x_j\right]_i$$

Index Notation — Linear Regression

$$L(\boldsymbol{\theta}) = \sum_{n=1}^{N} (y_n - \boldsymbol{\phi}(x_n)^\top \boldsymbol{\theta})^2 = ||\mathbf{y} - \Phi(X)\boldsymbol{\theta}||^2$$

$$= \sum_{n=1}^{N} \left(y_n - \sum_{m=1}^{M} \phi_m(x_n)\theta_m \right)^2$$

$$[\nabla L]_i = \frac{\partial L}{\partial \theta_i} = \frac{\partial}{\partial \theta_i} \sum_{n=1}^{N} \left(y_n - \sum_{m=1}^{M} \phi_m(x_n)\theta_m \right)^2$$

$$= \sum_{n} 2 \left(y_n - \sum_{m=1}^{M} \phi_m(x_n)\theta_m \right) \frac{\partial}{\partial \theta_i} \left(y_n - \sum_{k=1}^{M} \phi_k(x_n)\theta_k \right)$$

Index Notation — Linear Regression

$$\frac{\partial L}{\partial \theta_i} = -2 \sum_n \left(y_n - \sum_{m=1}^{M} \phi_m(x_n)\theta_m \right) \sum_k \phi_k(x_n) \frac{\partial \theta_k}{\partial \theta_i}$$

$$\frac{\partial L}{\partial \theta_i} = -2 \sum_n \left(y_n - \sum_{m=1}^{M} \phi_m(x_n)\theta_m \right) \sum_k \phi_k(x_n) \delta_{ki}$$

$$= -2 \sum_n \left(y_n - \sum_{m=1}^{M} \phi_m(x_n)\theta_m \right) \phi_i(x_n)$$

That was a lot of work! But there is an easier way, which turns out to generalise well to other types of models e.g. deep neural networks

Linear Regression — Multivariate Chain Rule

$$L(\boldsymbol{\theta}) = \sum_{n=1}^{N} (y_n - \boldsymbol{\phi}(x_n)^\top \boldsymbol{\theta})^2 = ||\mathbf{y} - \Phi(X)\boldsymbol{\theta}||^2$$

Instead of seeing this as a multivariate function we could write it as the composition of a scalar function with a multivariate function:

$f(g(\boldsymbol{\theta}))$ with $f : \mathbb{R}^D \mapsto \mathbb{R}$ and $g : \mathbb{R}^E \mapsto \mathbb{R}^D$

If we have a chain rule like the one below, computations would simplify a lot!

$$\frac{\partial f(g(\boldsymbol{\theta}))}{\partial \boldsymbol{\theta}} = \frac{\partial f}{\partial g}\frac{\partial g}{\partial \boldsymbol{\theta}}$$

But how do we compute a derivative wrt another vector?

Differentiation wrt a scalar

Revisit the definition of derivative

$$x : \mathbb{R} \mapsto \mathbb{R}^d$$

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \lim_{\Delta t \to 0} \frac{\mathbf{x}(t + \Delta t) - \mathbf{x}(t)}{\Delta t}$$

Compute each element using index notation:

$$\left[\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t}\right]_i = \lim_{\Delta t \to 0} \frac{x_i(t + \Delta t) - x_i(t)}{\Delta t}$$

Using our convention: $\frac{d\mathbf{x}}{dt} \in \mathbb{R}^{d \times 1}$

Multivariate Chain Rule w.r.t. scalar

There is a multivariate chain rule and using our convention it looks like an inner product!

Index notation:

$$\frac{df(\mathbf{g}(t))}{dt} = \sum_{i=1}^{D} \frac{\partial f}{\partial g_i} \frac{\partial g_i}{\partial t}$$

Vector form:

$$\frac{df(\mathbf{g}(t))}{dt} = \frac{\partial f}{\partial \mathbf{g}} \frac{\partial \mathbf{g}}{\partial t}$$

Row

Column

Multivariate Chain Rule w.r.t. scalar — Example

Consider $f : \mathbb{R}^2 \to \mathbb{R}, \quad \boldsymbol{x} : \mathbb{R} \to \mathbb{R}^2$

$$f(\boldsymbol{x}) = f(x_1, x_2) = x_1^2 + 2x_2\,,$$

$$\boldsymbol{x}(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix} = \begin{bmatrix} \sin(t) \\ \cos(t) \end{bmatrix}$$

What are the dimensions of $\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{x}}$ and $\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t}$?

1×2 and 2×1

Compute the gradient $\frac{\mathrm{d}f}{\mathrm{d}t}$ using the chain rule:

$$\frac{\mathrm{d}f}{\mathrm{d}t} = \frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{x}}\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}t} = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} \end{bmatrix} \begin{bmatrix} \frac{\partial x_1}{\partial t} \\ \frac{\partial x_2}{\partial t} \end{bmatrix} = \begin{bmatrix} 2\sin t & 2 \end{bmatrix} \begin{bmatrix} \cos t \\ -\sin t \end{bmatrix}$$

$$= 2\sin t \cos t - 2\sin t = 2\sin t(\cos t - 1)$$

Derivative of a vector wrt vector

We saw the chain rule if we were differentiating w.r.t. a scalar:

$$\frac{\mathrm{d}f(\boldsymbol{g}(t))}{\mathrm{d}t} = \sum_{i=1}^{D} \frac{\partial f}{\partial g_i} \frac{\mathrm{d}g_i}{\mathrm{d}t} = \underbrace{\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{g}}}_{\text{row}} \cdot \underbrace{\frac{\mathrm{d}\boldsymbol{g}}{\mathrm{d}t}}_{\text{column}} \qquad \boldsymbol{g}(t) \in \mathbb{R}^D$$

What happens if we differentiate w.r.t. a vector?

$\implies$ As before, we just stack the derivatives w.r.t. each of the inputs.

$$\frac{\partial f(\boldsymbol{g}(\mathbf{x}))}{\partial x_j} = \sum_{i=1}^{D} \frac{\partial f}{\partial g_i} \frac{\partial g_i}{\partial x_j} \qquad \boldsymbol{g}(\mathbf{x}) \in \mathbb{R}^D$$

This is a matrix multiplication! Can write in vector form:

$$\frac{\mathrm{d}f(\boldsymbol{g}(\mathbf{x}))}{\mathrm{d}\mathbf{x}} = \underbrace{\frac{\mathrm{d}f}{\mathrm{d}\boldsymbol{g}}}_{\text{row}} \cdot \underbrace{\frac{\mathrm{d}\boldsymbol{g}}{\mathrm{d}\mathbf{x}}}_{\text{matrix}}$$

Derivative of a vector wrt vector

$\mathbf{f} : \mathbb{R}^N \mapsto \mathbb{R}^M$

$$\boldsymbol{y} = \boldsymbol{f}(\boldsymbol{x}) \in \mathbb{R}^M, \quad \boldsymbol{x} \in \mathbb{R}^N$$

$$\begin{bmatrix} y_1 \\ \vdots \\ y_M \end{bmatrix} = \begin{bmatrix} f_1(\boldsymbol{x}) \\ \vdots \\ f_M(\boldsymbol{x}) \end{bmatrix} = \begin{bmatrix} f_1(x_1, \ldots, x_N) \\ \vdots \\ f_M(x_1, \ldots, x_N) \end{bmatrix}$$

- Jacobian matrix (collection of all partial derivatives)

$$\begin{bmatrix} \frac{dy_1}{d\boldsymbol{x}} \\ \vdots \\ \frac{dy_M}{d\boldsymbol{x}} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \vdots & & \vdots \\ \frac{\partial f_M}{\partial x_1} & \cdots & \frac{\partial f_M}{\partial x_N} \end{bmatrix} \in \mathbb{R}^{M \times N}$$

Dimensions of Derivative of a vector wrt vector

In general: A function $\boldsymbol{f} : \mathbb{R}^{N} \rightarrow \mathbb{R}^{M}$ has a gradient that is an $M \times N$-matrix with

$$\frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{x}} \in \mathbb{R}^{M \times N}, \qquad \mathrm{d}\boldsymbol{f}[m,n] = \frac{\partial f_m}{\partial x_n}$$

Gradient dimension: # target dimensions $\times$ # input dimensions

Example

$$\boldsymbol{f}(\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x}, \qquad \boldsymbol{f}(\boldsymbol{x}) \in \mathbb{R}^M, \quad \boldsymbol{A} \in \mathbb{R}^{M\times N}, \quad \boldsymbol{x} \in \mathbb{R}^N$$

$$\begin{bmatrix} y_1 \\ \vdots \\ y_M \end{bmatrix} = \begin{bmatrix} f_1(\boldsymbol{x}) \\ \vdots \\ f_M(\boldsymbol{x}) \end{bmatrix} = \begin{bmatrix} A_{11}x_1 + A_{12}x_2 + & \cdots & + A_{1N}x_N \\ \vdots & \vdots & \vdots \\ A_{M1}x_1 + A_{M2}x_2 + & \cdots & + A_{MN}x_N \end{bmatrix}$$

- Compute the gradient $\frac{\mathrm{d}f}{\mathrm{d}x}$
  - Gradient:

$$f_i(\boldsymbol{x}) = \sum_{k=1}^{N} A_{ik}x_k \qquad \Longrightarrow \quad \frac{\partial f_i}{\partial x_j} = \sum_k A_{ik}\frac{\partial x_k}{\partial x_j} = \sum_k A_{ik}\delta_{kj} = A_{ij}$$

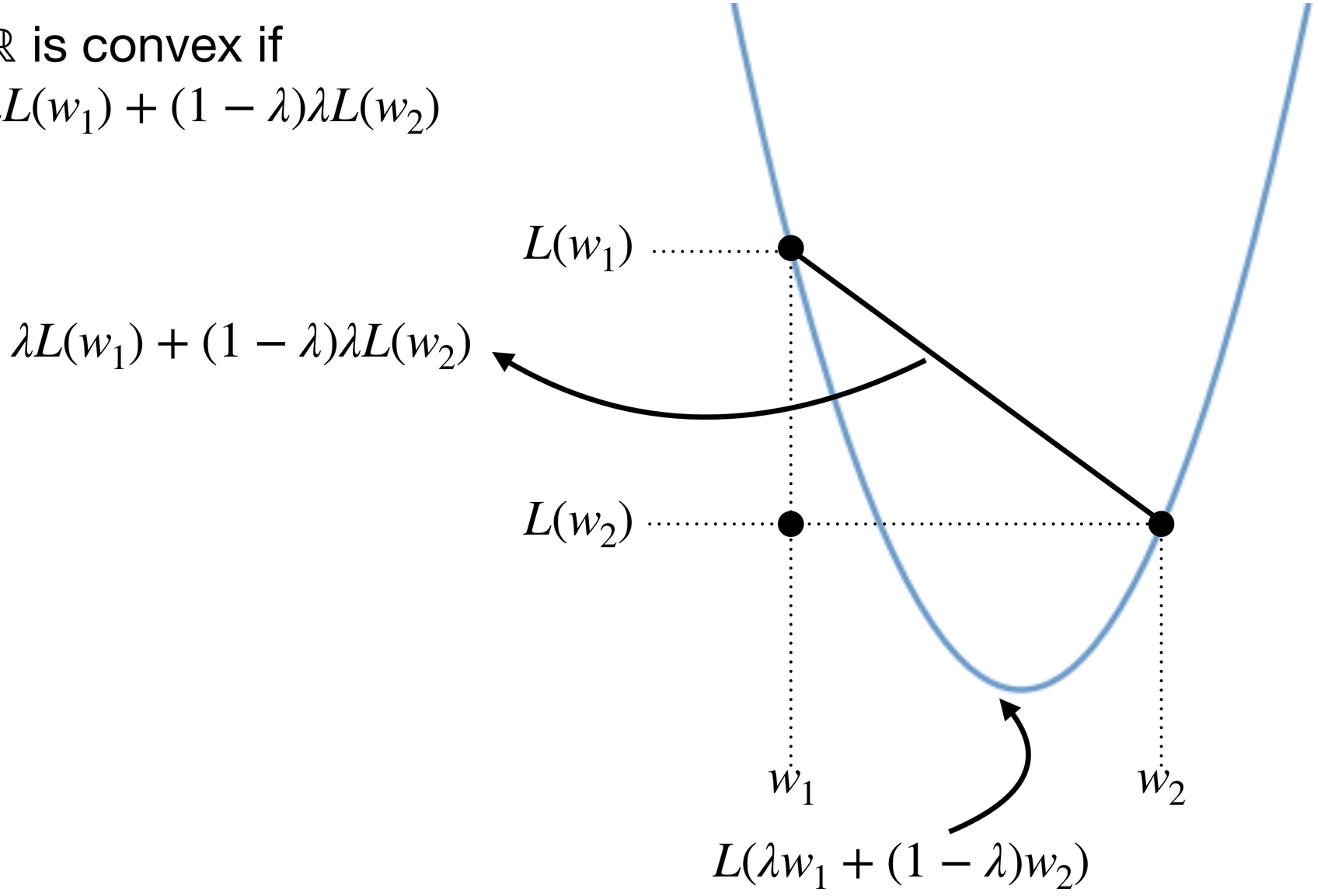
$$\Longrightarrow \quad \frac{\mathrm{d}\boldsymbol{f}}{\mathrm{d}\boldsymbol{x}} = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \cdots & \frac{\partial f_1}{\partial x_N} \\ \vdots & & \vdots \\ \frac{\partial f_M}{\partial x_1} & \cdots & \frac{\partial f_M}{\partial x_N} \end{bmatrix} = \begin{bmatrix} A_{11} & \cdots & A_{1N} \\ \vdots & & \vdots \\ A_{M1} & \cdots & A_{MN} \end{bmatrix} = \boldsymbol{A} \in \mathbb{R}^{M\times N}$$

Convex Functions

A function $L : \mathbb{R}^d \mapsto \mathbb{R}$ is convex if

$$L(\lambda w_1 + (1-\lambda)w_2) \leq \lambda L(w_1) + (1-\lambda)\lambda L(w_2)$$

$$0 \leq \lambda \leq 1$$



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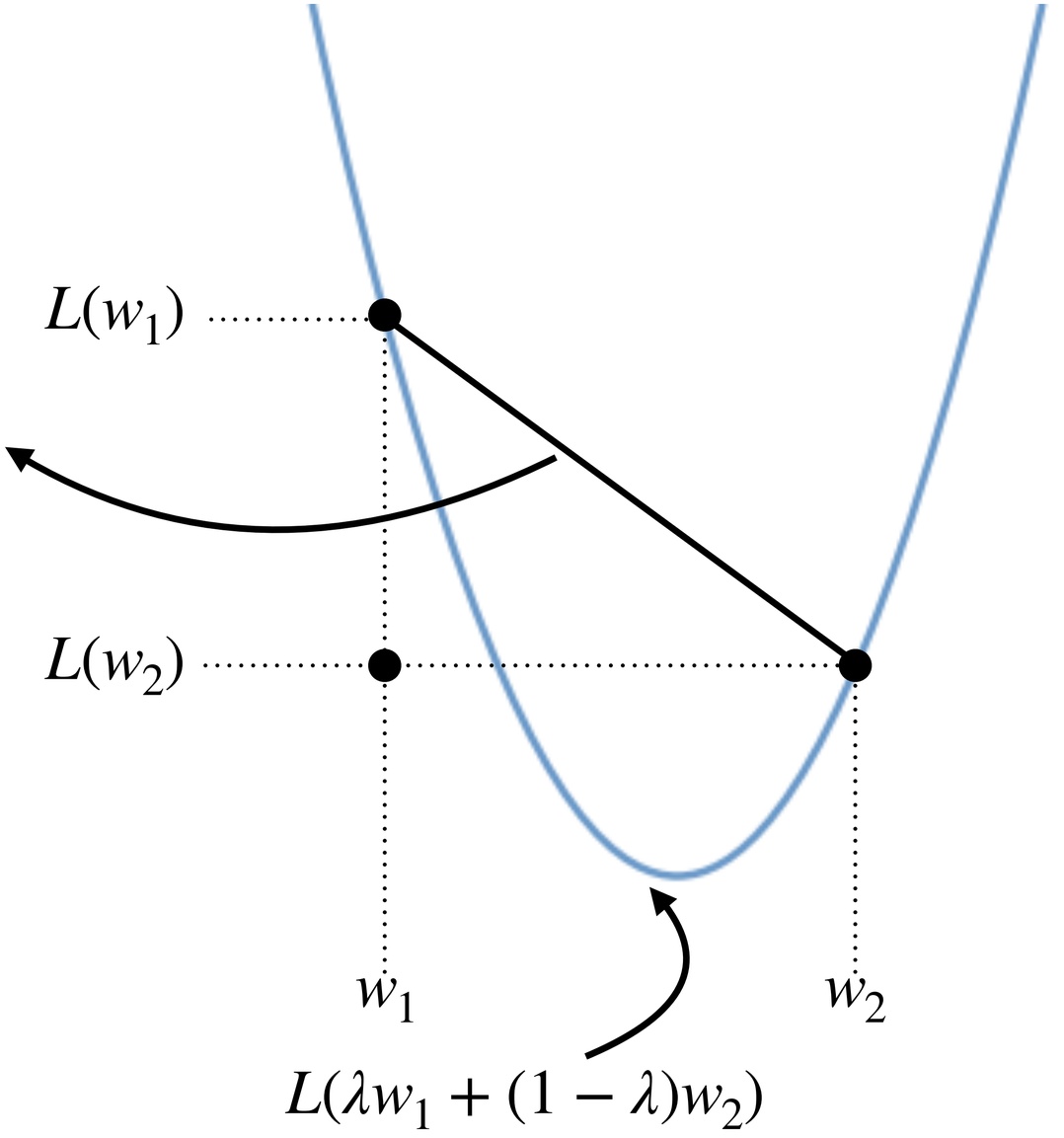


Useful test for convexity:

$\nabla^2 L(w)$ is positive definite

Convex functions have **unique** minimum

Examples in ML: regression, SVMs are convex, NNs typically are not

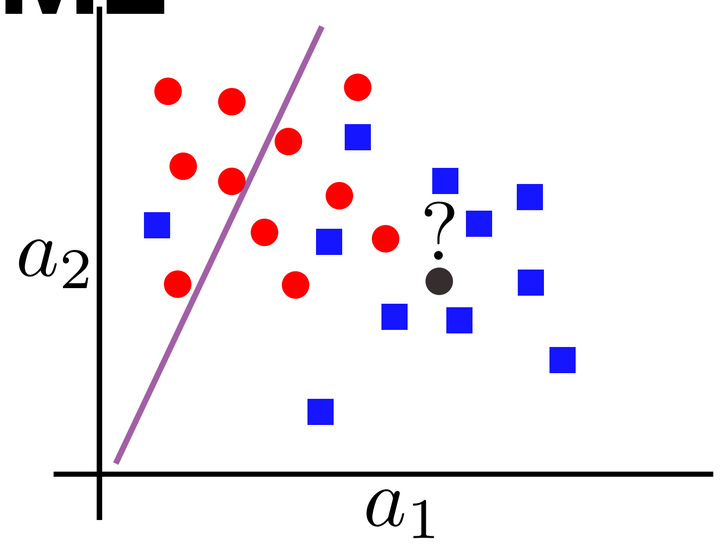
Optimization is everywhere in ML

Typical ML models have parameters to be tuned e.g.

$$\min_{w} \|Aw - b\|^2 + \|w\|_2^2$$

Data **fidelity** term

Regularisation term



Even complex ML models are an optimisation problem, e.g. (DNNs have a complicated objective function but are just a huge optimisation problem)

Other **applications** of optimisation:

- **Reinforcement learning** (branch of dynamic optimisation under uncertainty)
- **Variational Inference/Sampling** (e.g. Bayesian optimisation)
- Mathematical **foundations** of ML (e.g. decision trees, more on this in the next lecture!)

Optimization is everywhere in ML

ML projects “typical” steps :

- **Understand** the data (e.g. feature engineering, dimensionality reduction)
- Model **development** (e.g. choosing the architecture of a NN)
- **Optimising** the model

Fortunately, most ML libraries have state-of-the-art optimisation algorithms

Unlike linear algebra algorithms, they require more care to use

Knowledge of optimisation is necessary to **develop novel ML models and solve them**

Classes of Optimization Models

- **Unconstrained Optimization:** $\min_{w \in \mathbb{R}^d} L(w)$ ← Select parameters over all d-dim vectors

  (most ML models are unconstrained, e.g. linear regression, NNs)

- **Constrained Optimization** $\min_{w \in \mathscr{W}} L(w)$ ← Select parameters from a set

  (e.g. support vector machines)

  - **Convex Optimization** (convex constraints and loss function, easier to solve and interpret, unique solution, e.g. linear regression, SVMs)
  - **Non-convex Optimization** (hard to solve, multiple solutions, e.g. RL, NNs (e.g. neural nets)
  - **Discrete Optimization** (particular subclass of constrained non-convex optimisation where the set $\mathscr{W}$ is discrete, e.g.$w \in \{\pm 1\}$ (**very difficult** to solve, e.g. interpretable ML, verifiability of ML models)

Optimization Terminology

$$\min_{w \in \mathbb{R}^d} L(w)$$

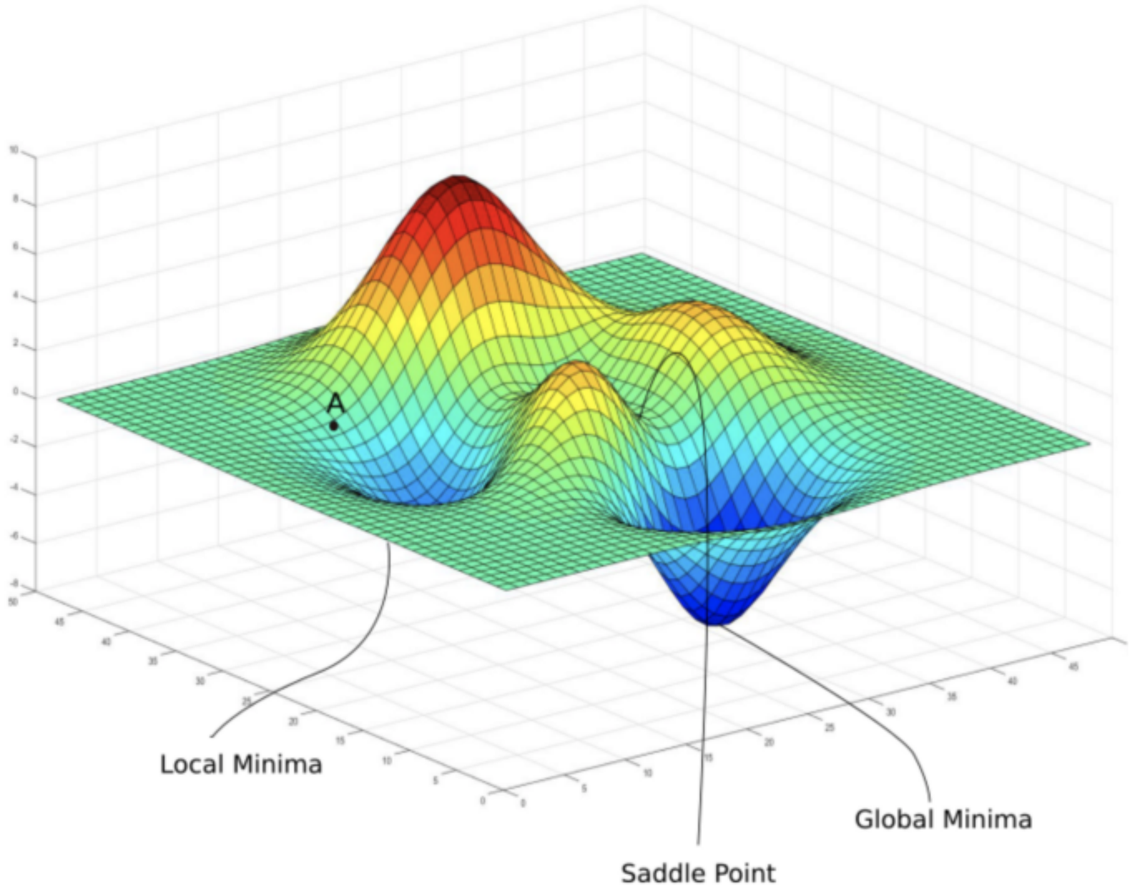
A point $w^\star \in \mathbb{R}^d$

Satisfies first order conditions: $\nabla L(w^\star) = 0$ (critical/stationary points)

If $\nabla^2 L(w^\star) \succ 0$ (local minimum)

If $\nabla^2 L(w^\star) \prec 0$ (local maximum)

otherwise a saddle point



Example Linear Regression in 1d

$$f(x) = a \cdot x \qquad L(a) = \sum_{n=1}^{N} (f(x_n) - y_n)^2$$

$$\frac{\mathrm{d}L}{\mathrm{d}a} = \sum_{n=1}^{N} 2(ax_n - y_n)x_n = \sum_{n=1}^{N} 2ax_n^2 - 2x_n y_n = 0$$

$$2a \sum_n x_n^2 = \sum_n 2x_n y_n$$

$$a = \frac{\sum_n x_n y_n}{\sum_n x_n^2}$$

$$\frac{\mathrm{d}^2 L}{\mathrm{d}a^2} = \sum_{n=1}^{N} 2x_n^2 \geqslant 0$$

Classes of Optimization Solvers

- **Zero Order** Methods (black-box, derivative-free optimization) (require function values only, **very slow** (e.g. Nelder-Mead)
- **First Order** Methods (require gradients, for smooth problems converge linearly, scales to very large problems (e.g. gradient descent)
- **Second Order** Methods (require gradients, Hessians, typically converge to minima, very fast, do not scale well (e.g. Newton method)

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- **Simplex** method (special algorithm for linear optimization)
- **Interior Point Method** (polynomial time algorithm for linear, quadratic and other convex problems).
- **Projection and proximal** methods (special algorithms for problems with certain constraint sets)
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In ML we typically use stochastic variants of all the above (more later)

Optimization Methods rely on local approximations

$$w^\star \in \arg\min_{w \in \mathbb{R}^d} L(w)$$

1. Given an initial point w

2. Select d (**direction**) to improve solution e.g.

$$L(w+d) < L(w) \text{ or } \|w^\star - (w+d)\| < \|w^\star - w\|$$

3. Update solution (**learning**) $w \leftarrow w + \tau\, d$

Positive scalar (step-size, learning rate)

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Positive scalar (step-size, learning rate)

Repeat the process until happy with the solution, **but how is d chosen?**

Local Approximations with Gradient Descent

How do we ensure that $L(w_{k+1}) < L(w_k)$?

GD makes a local quadratic approximation:

$$\hat{L}(w) \triangleq L(w_k) + \langle \nabla L(w_k), w - w_k \rangle + \frac{1}{2\tau}\|w - w_k\|_2^2$$

Approx. only uses first order information

$$w_{k+1} = \arg\min \hat{L}(w_k)$$

since $\nabla \hat{L}(w_{k+1}) = 0$ if $w_{k+1} = w_k - \tau \nabla L(w_k)$

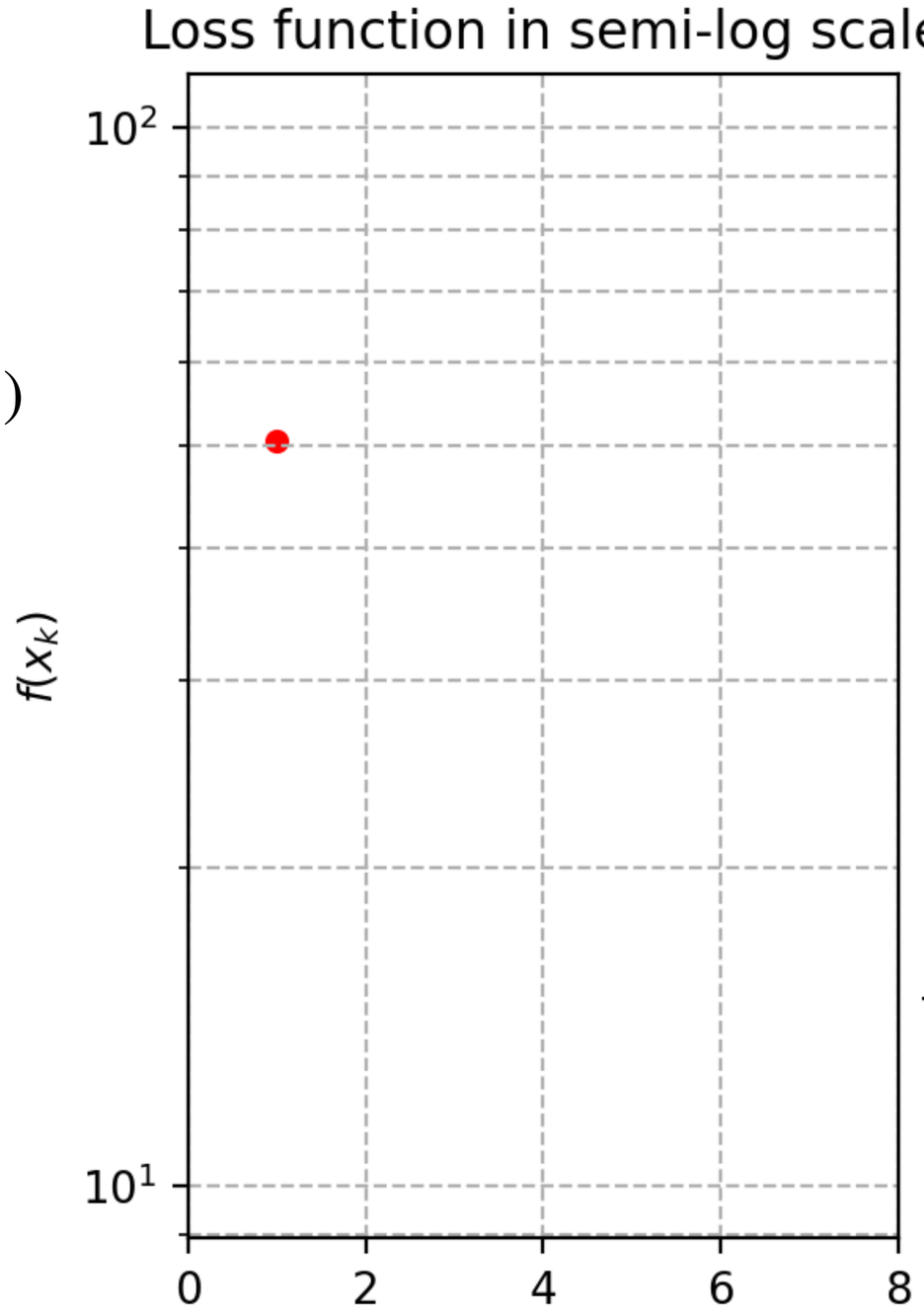
Can be shown that for τ small enough GD will converge to a stationary point

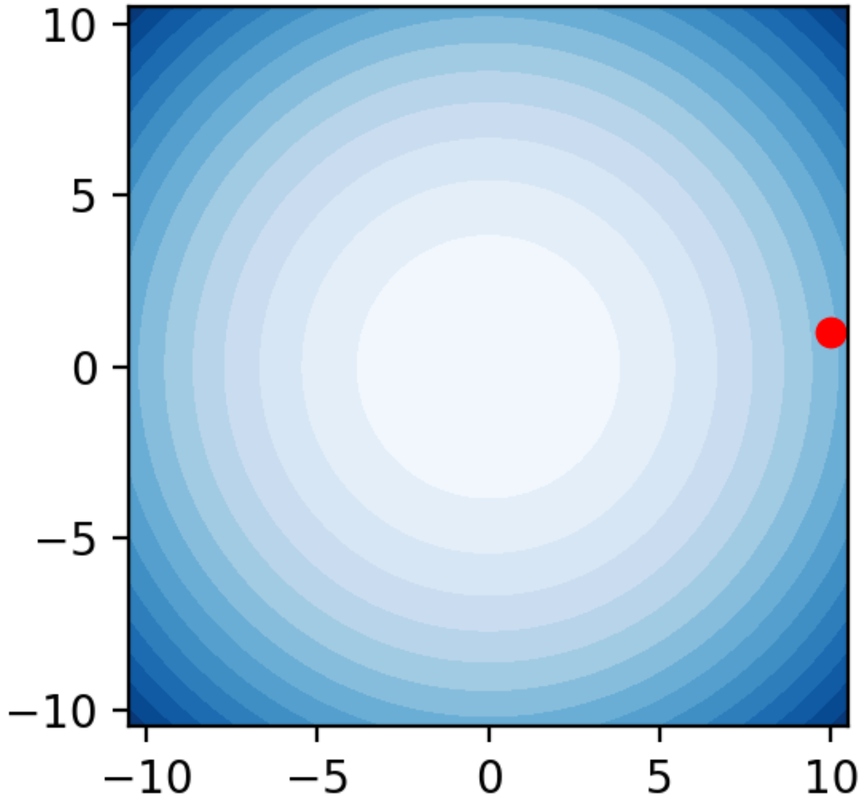
When GD works well

$$\min \frac{1}{2}(x_1^2 + \gamma x_2^2),$$

$\gamma = 1$, initial point $(10,1)$

G.D. with $\tau = 0.5$





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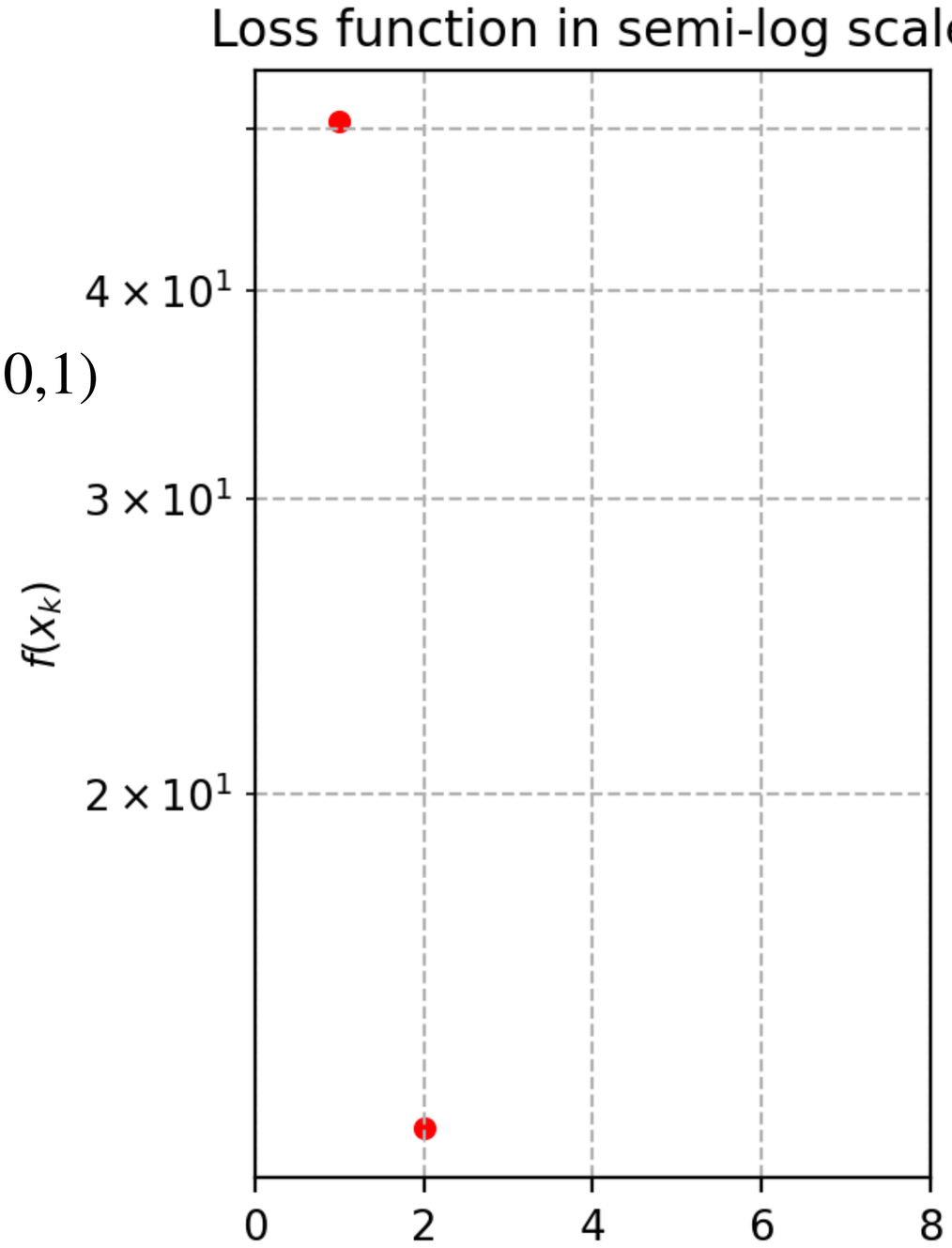

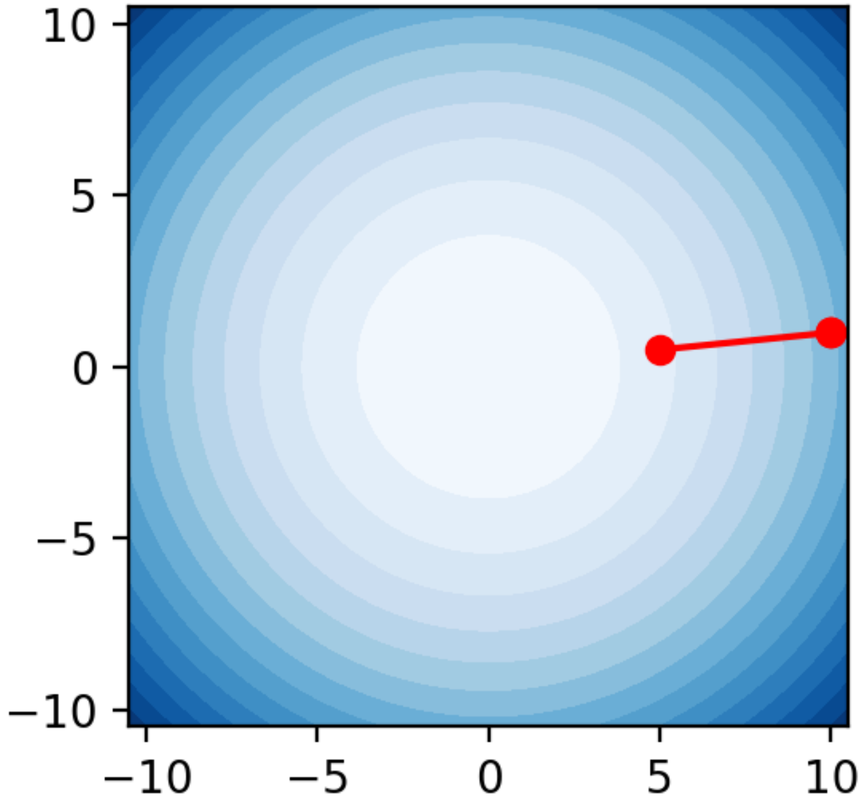

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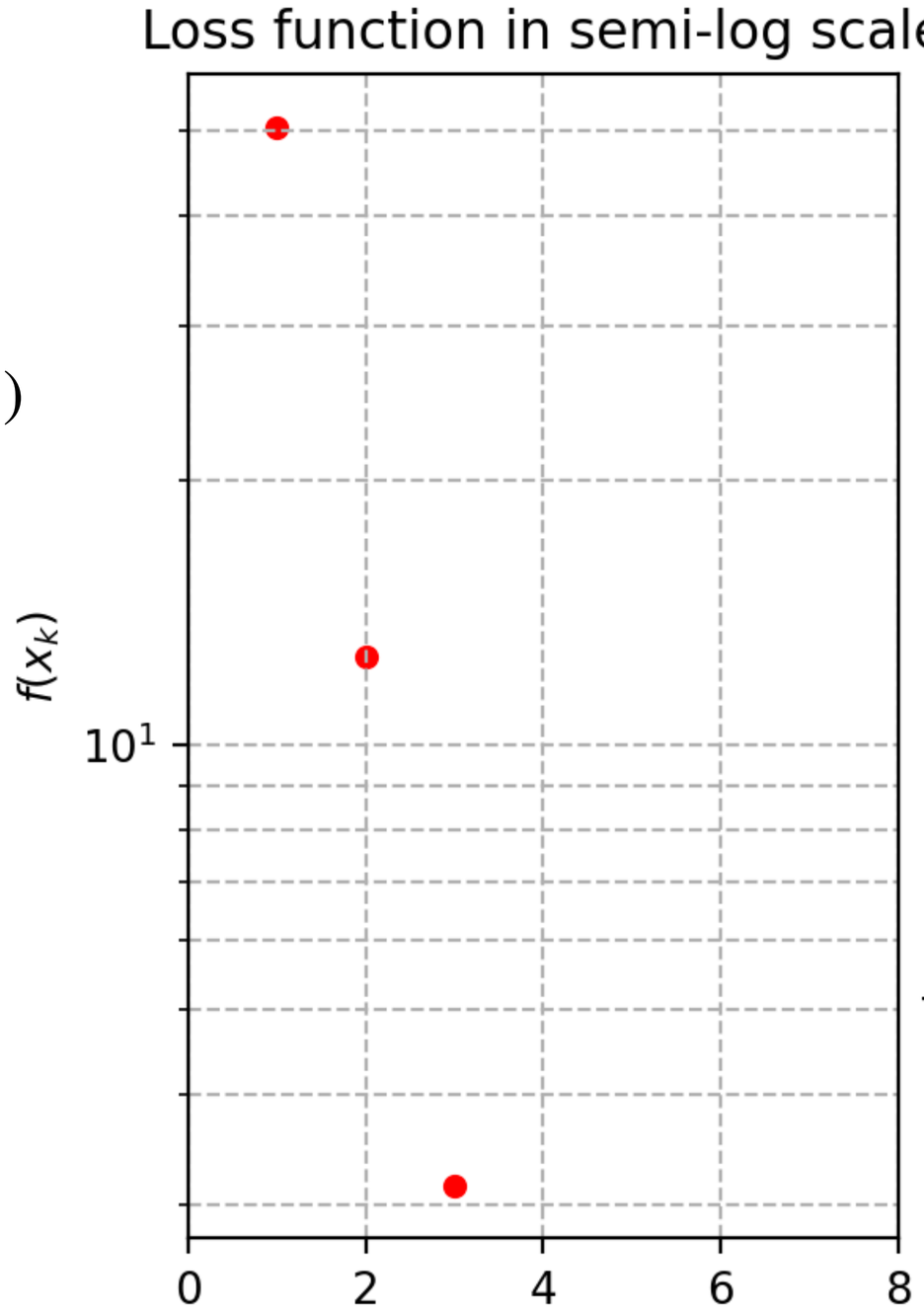

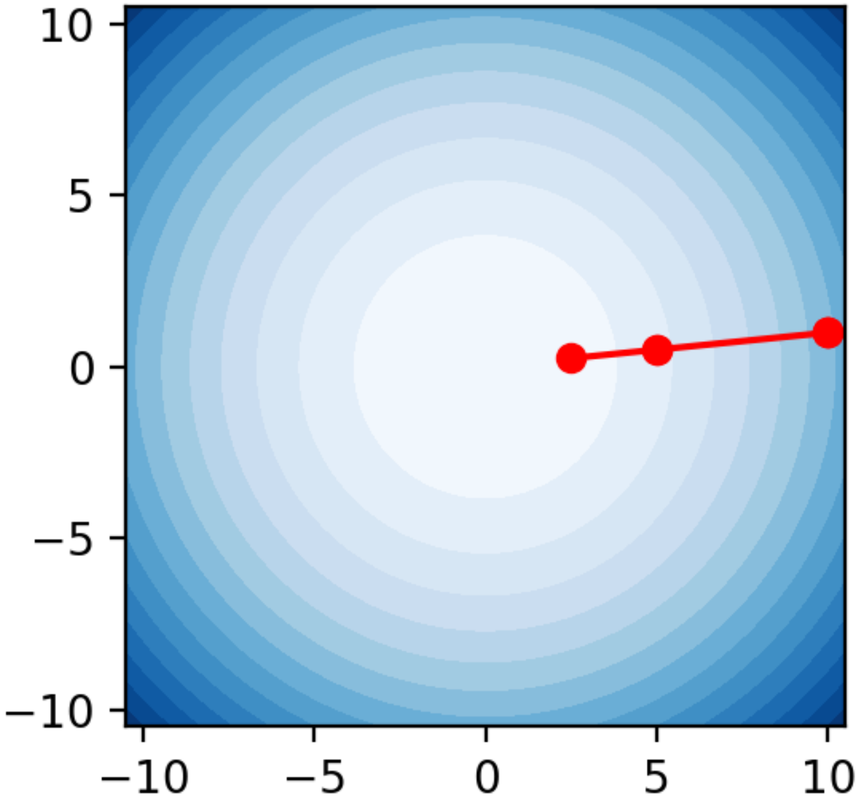

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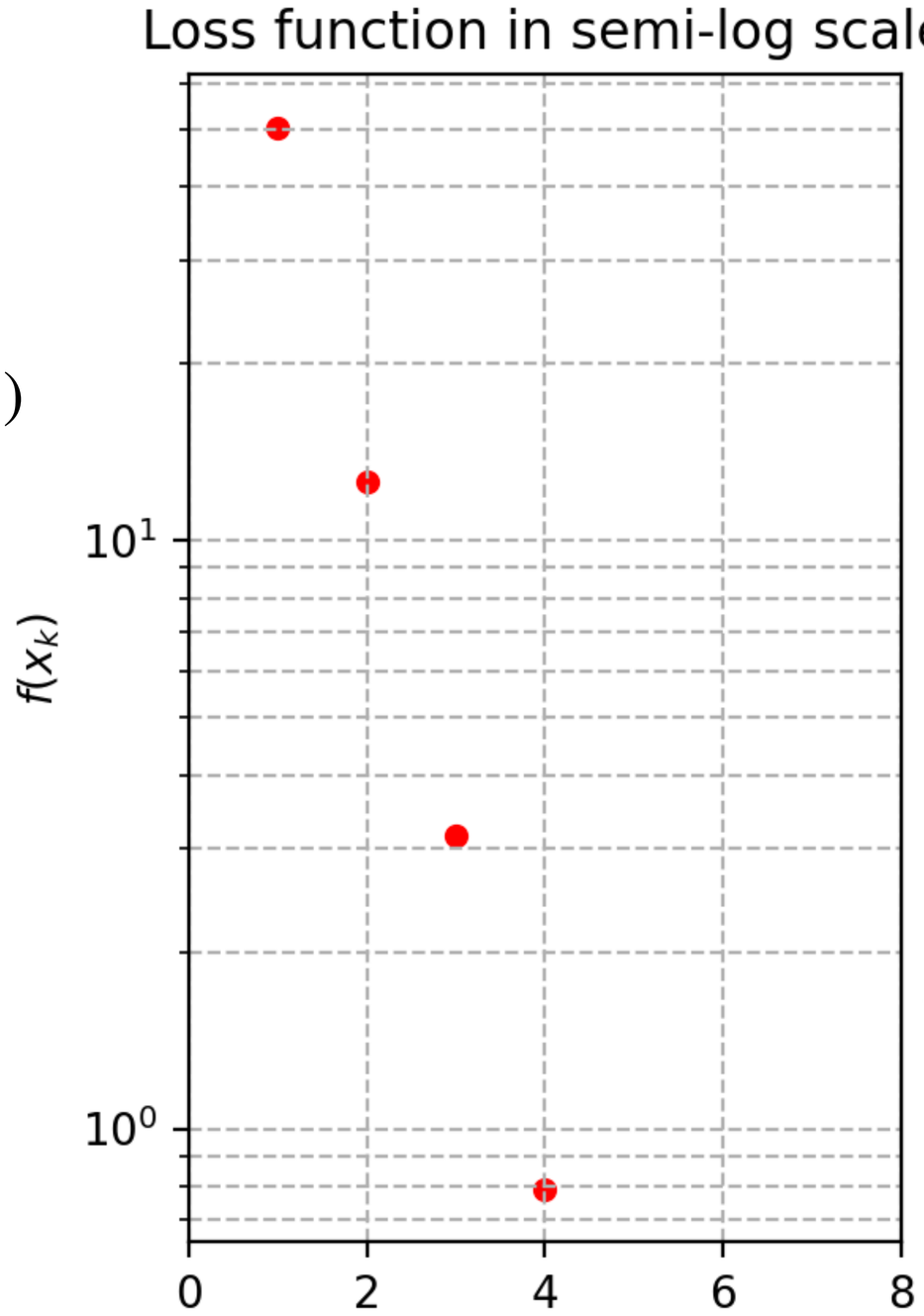

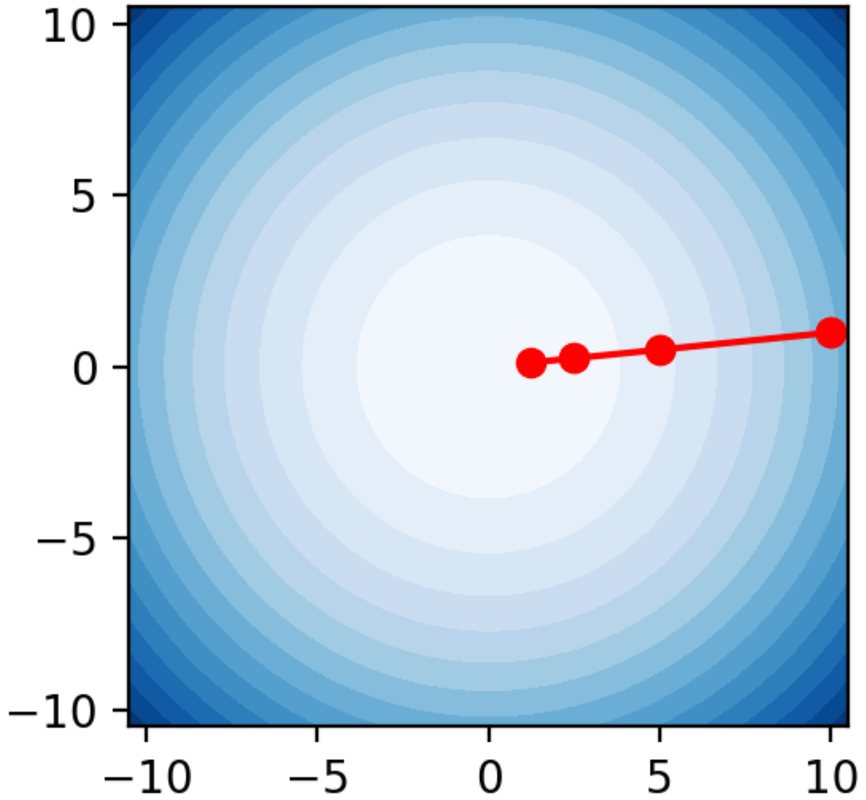

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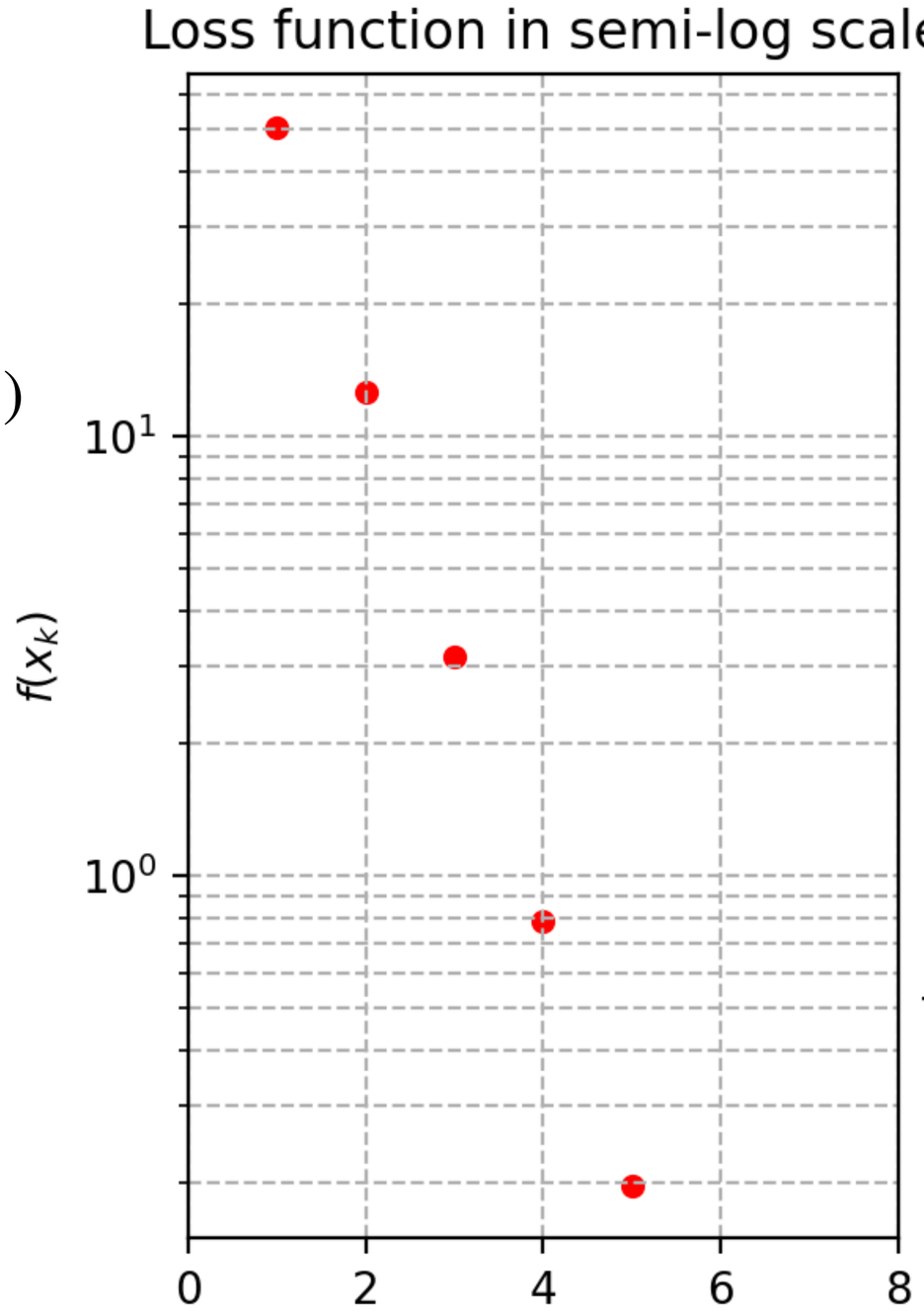

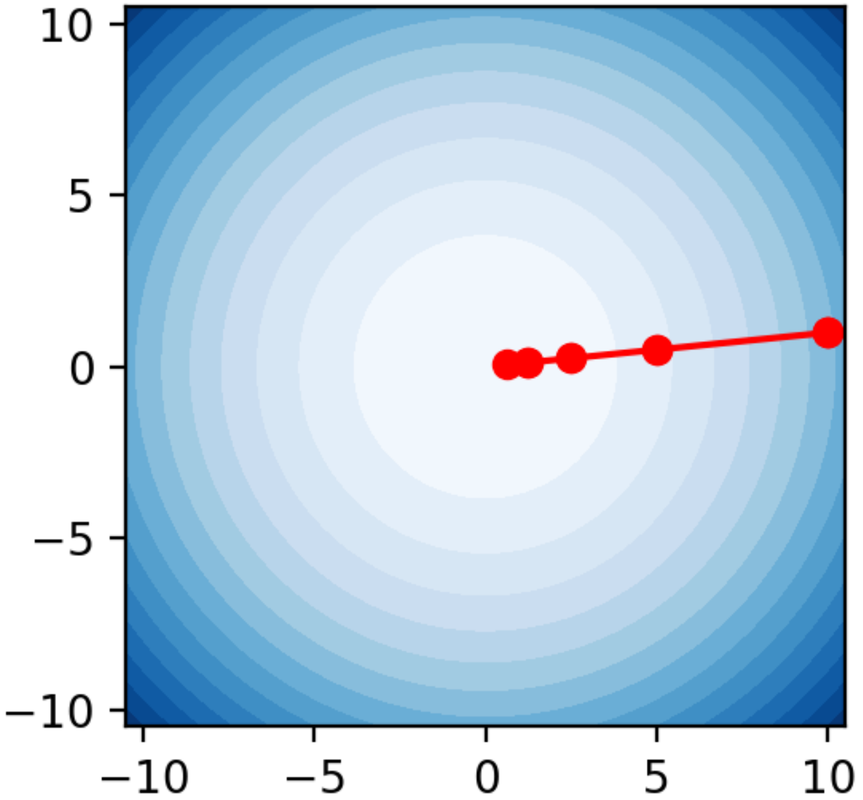

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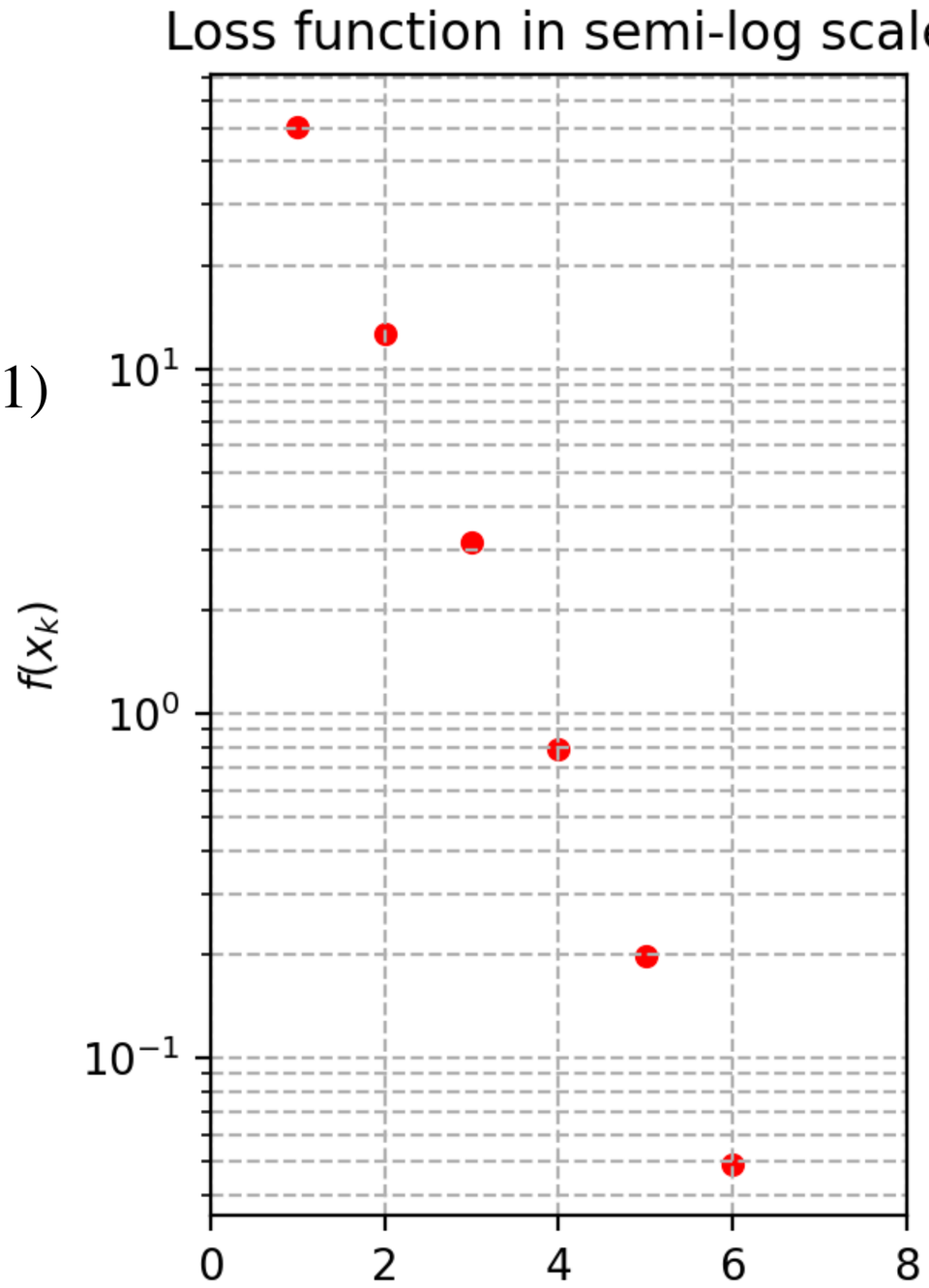

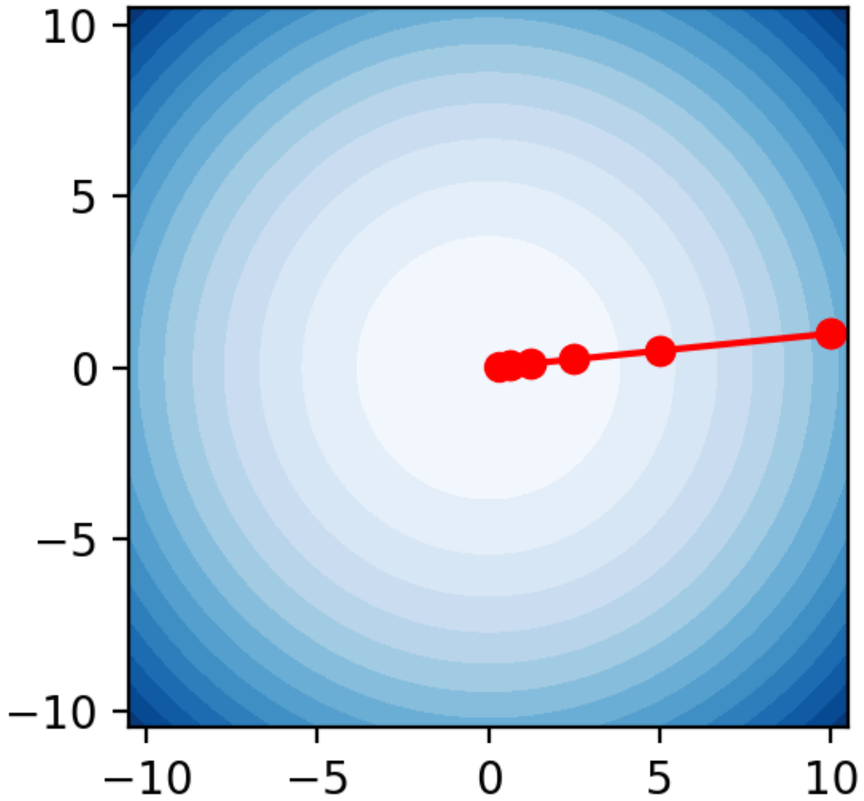

GD can fail for ill-conditioned problems

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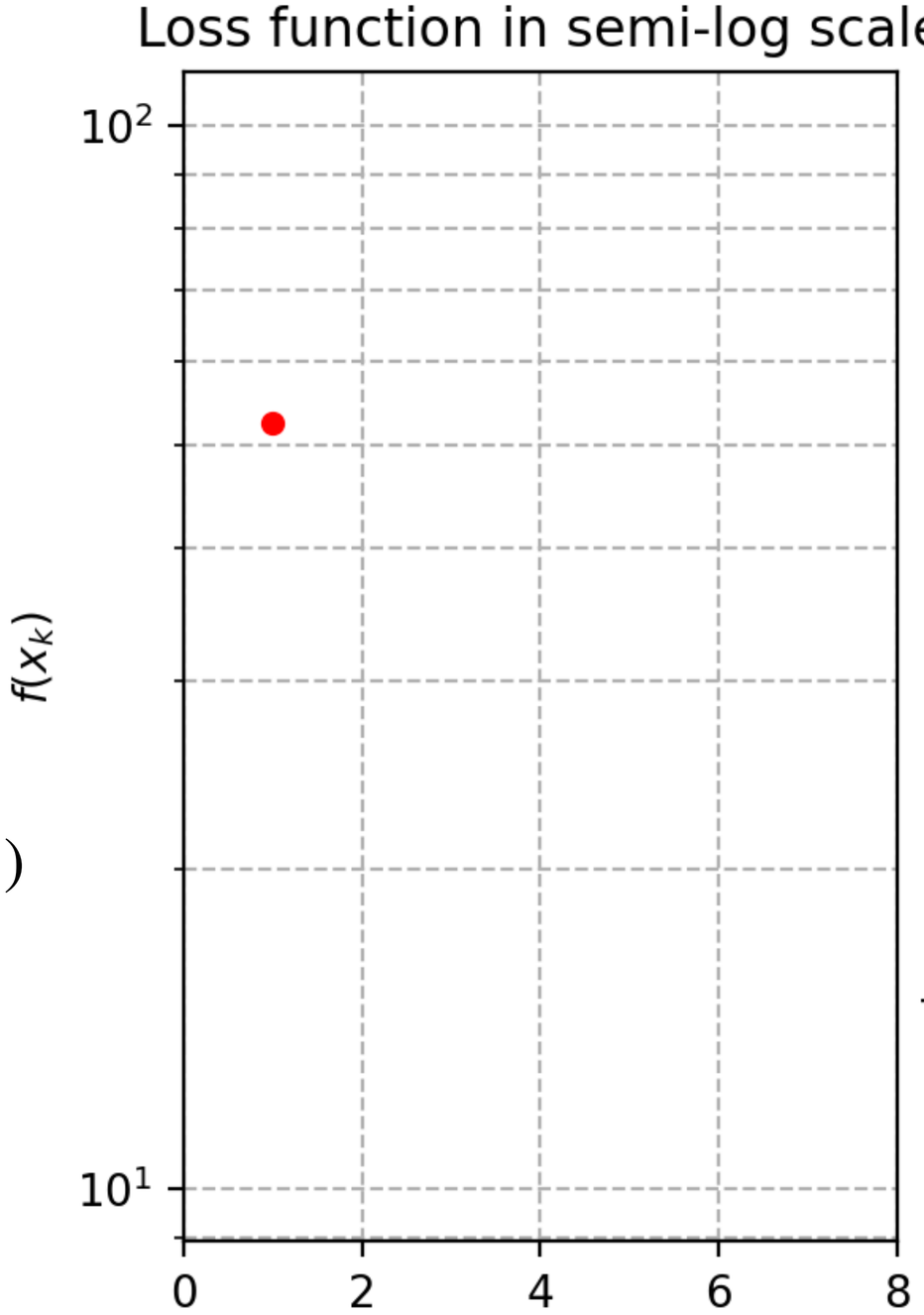

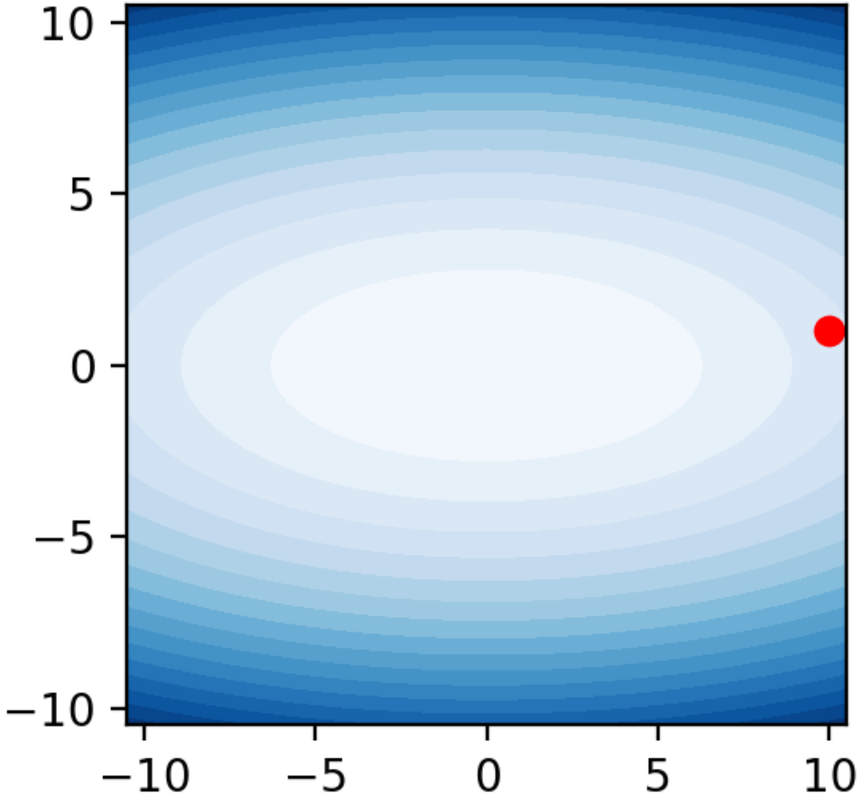

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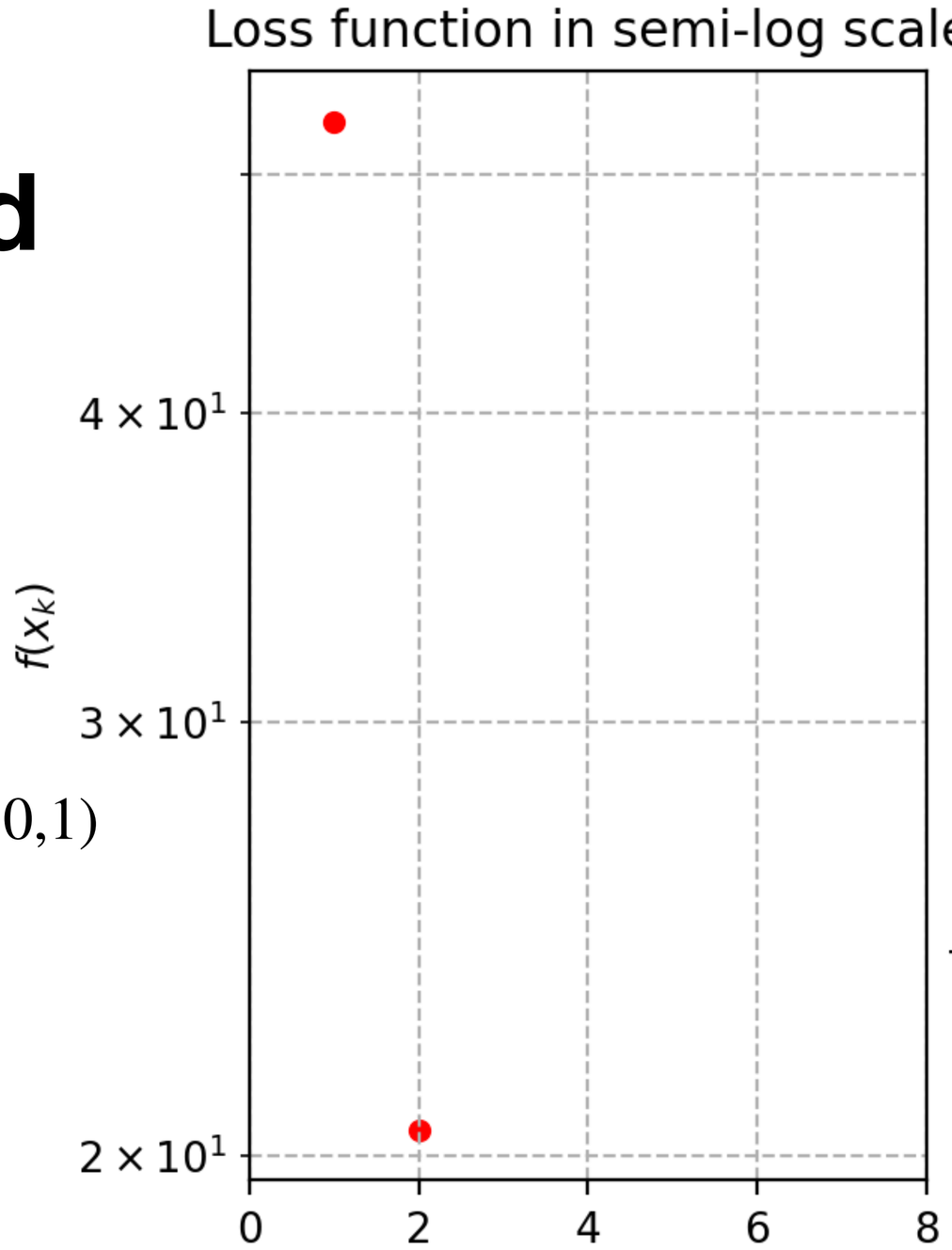

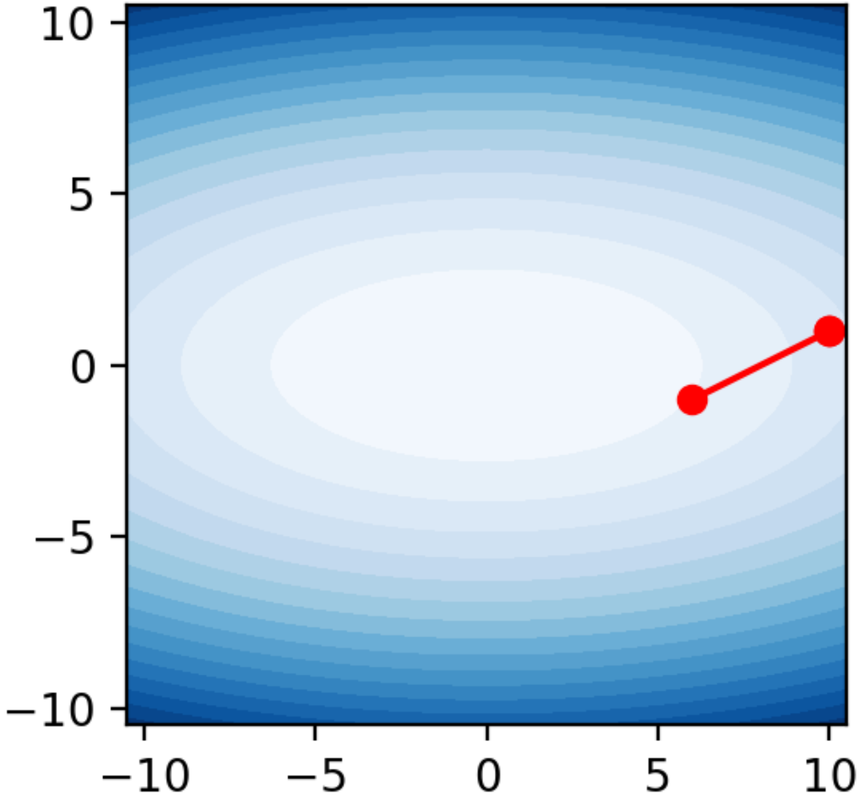

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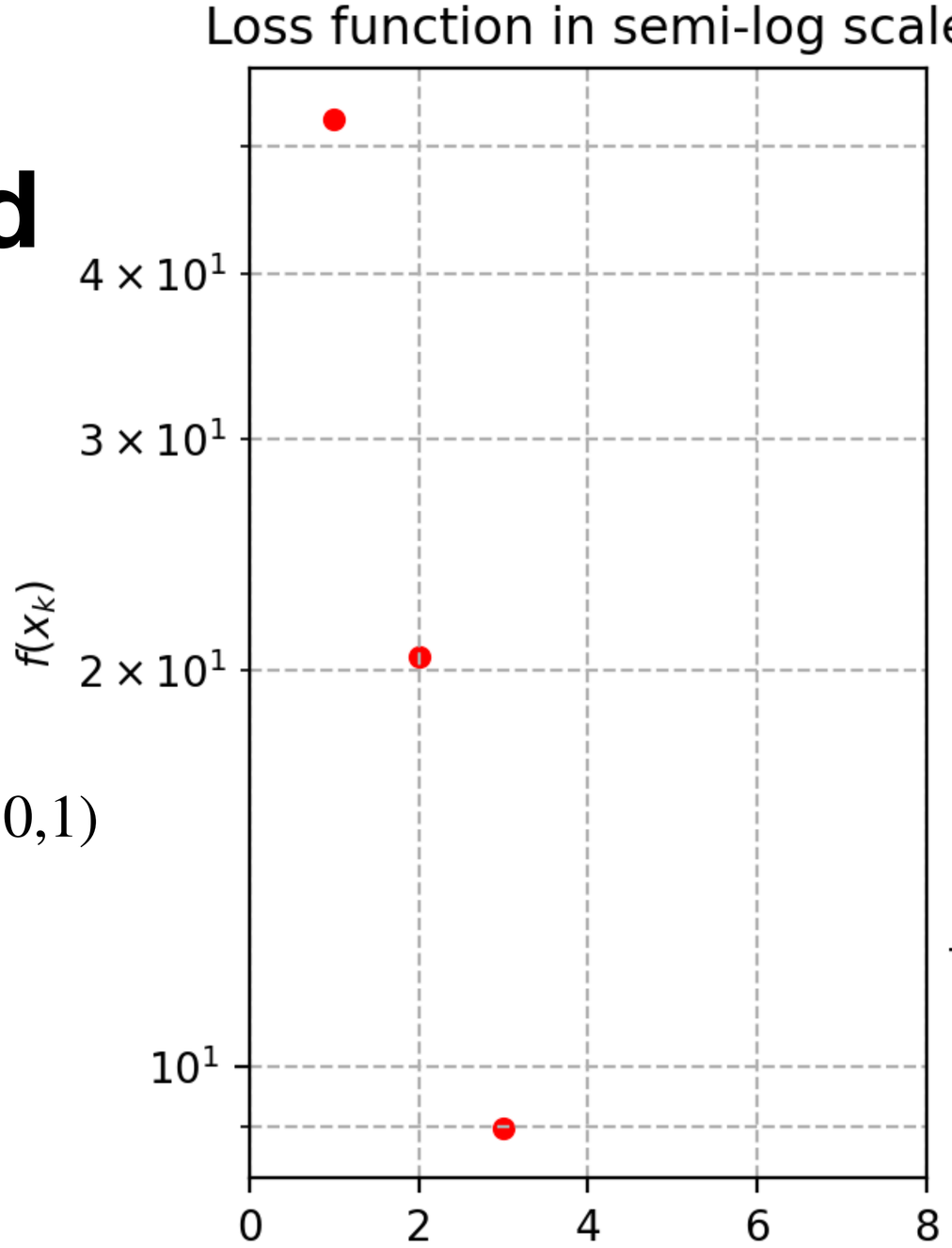

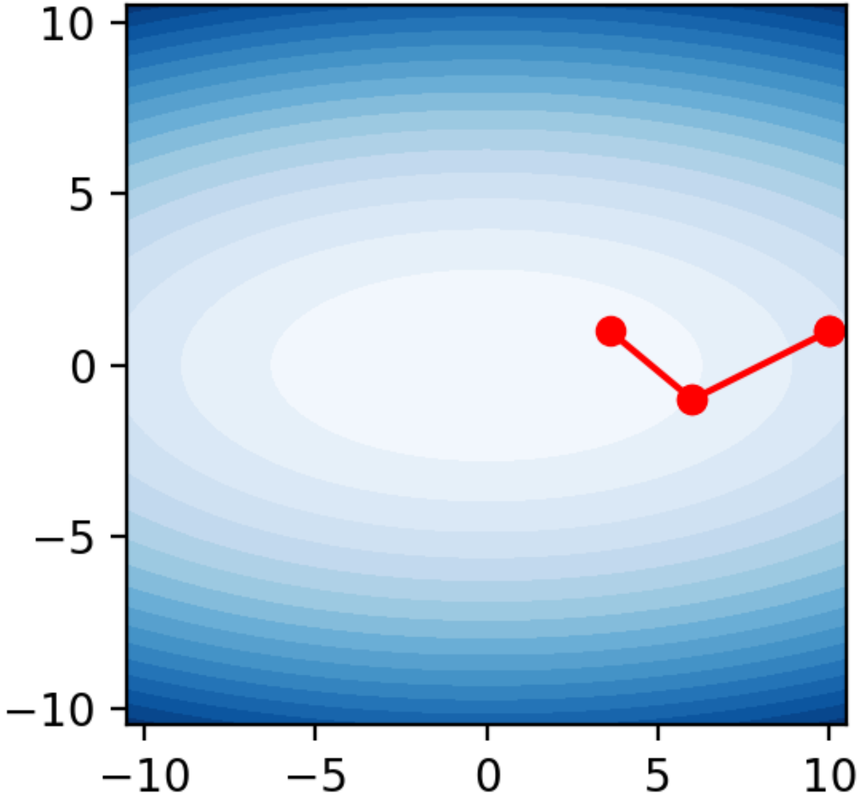

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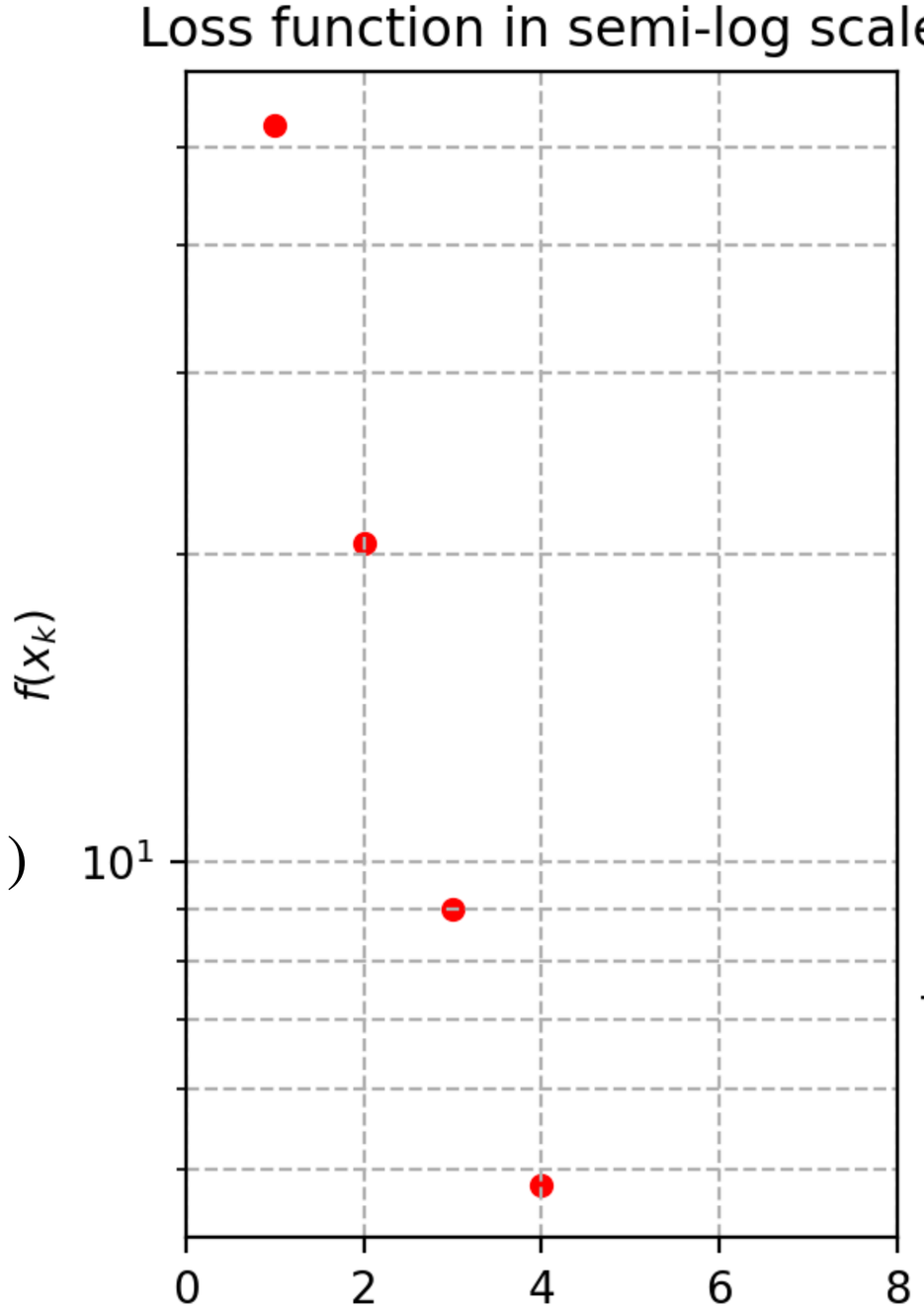

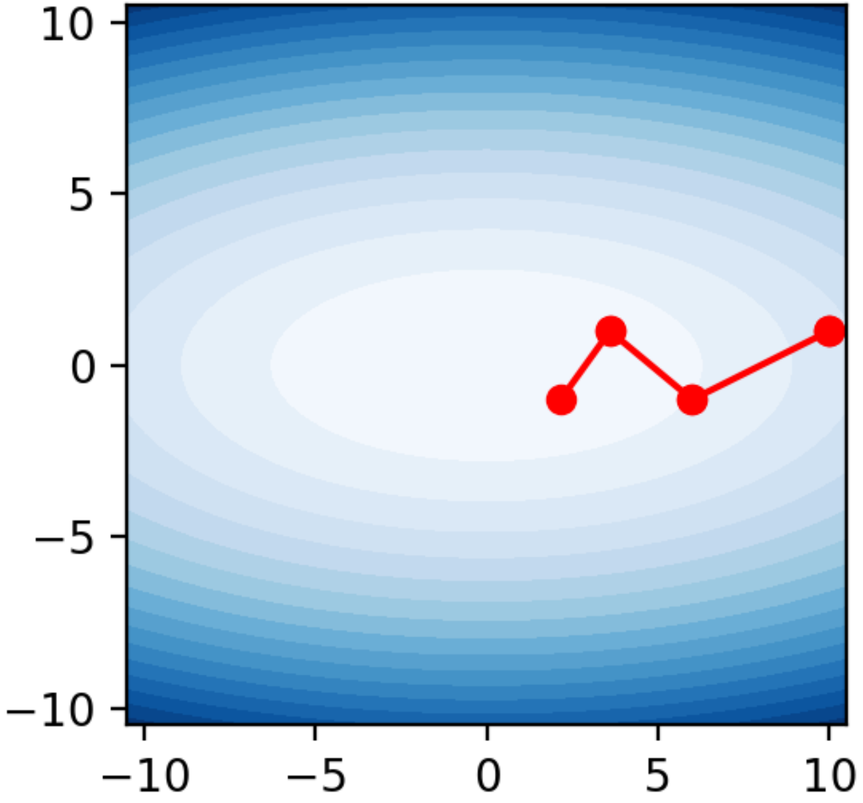

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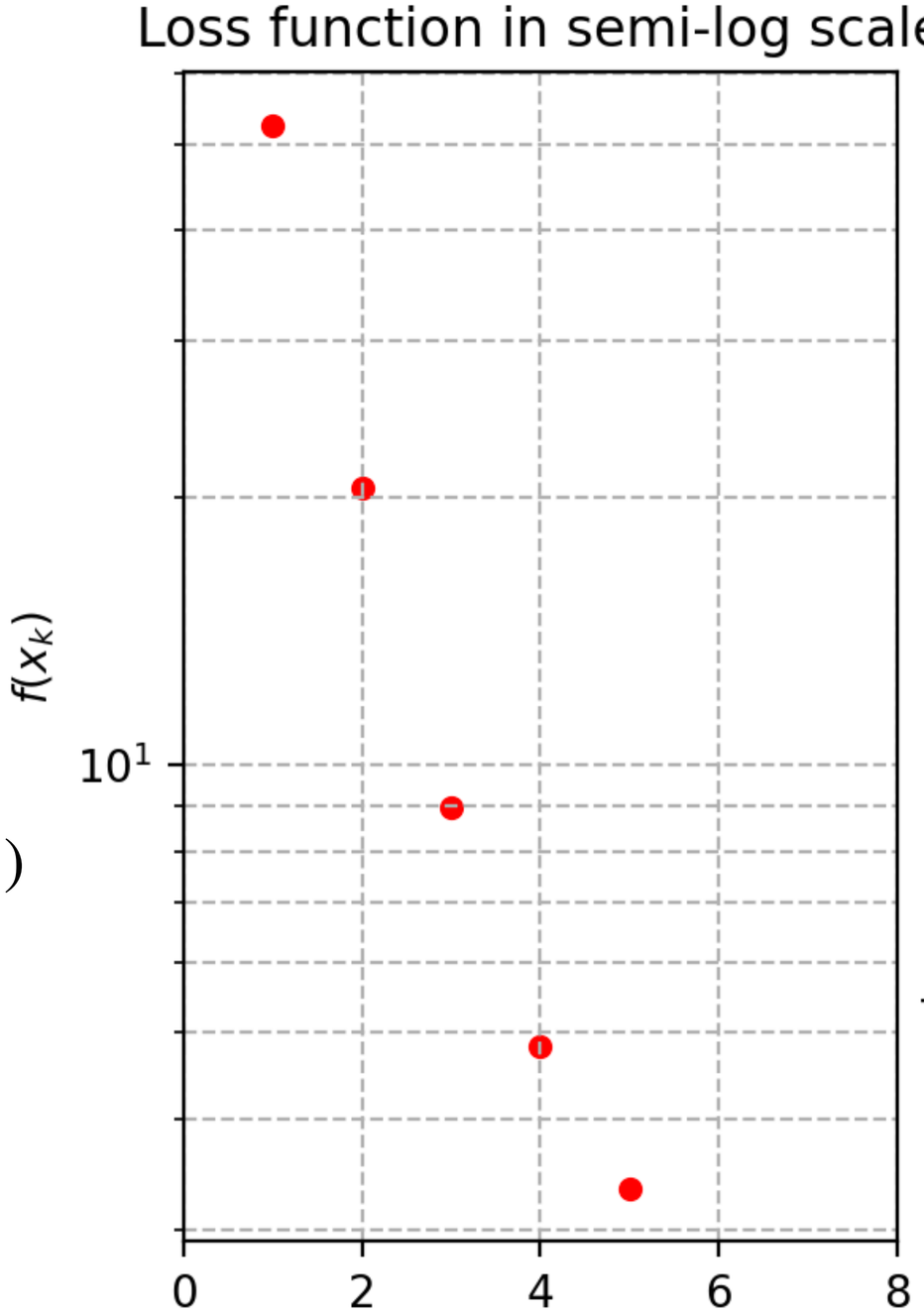

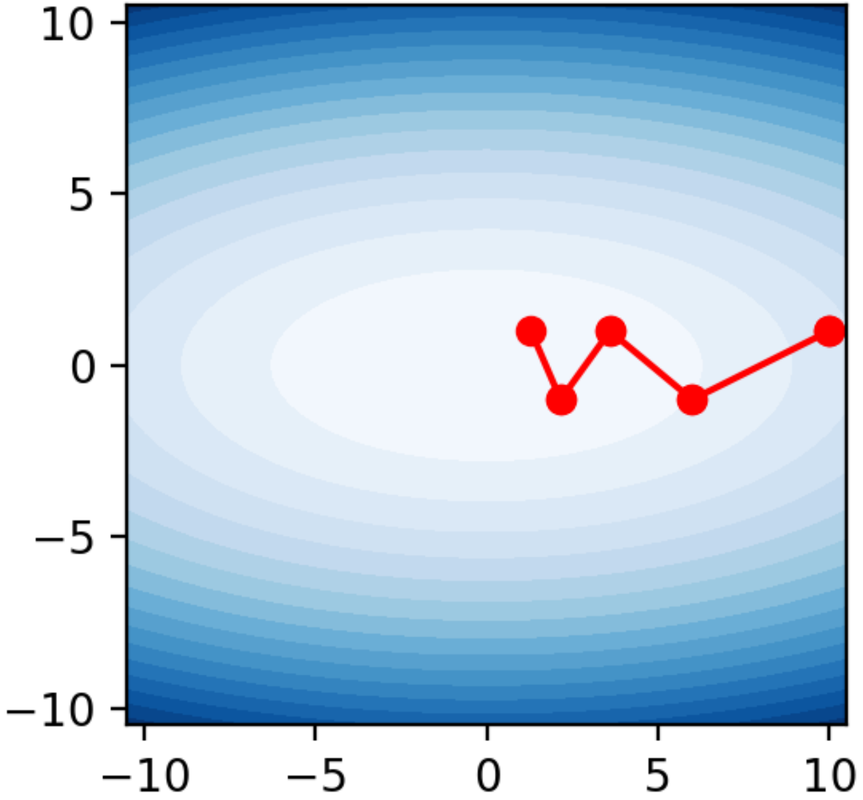

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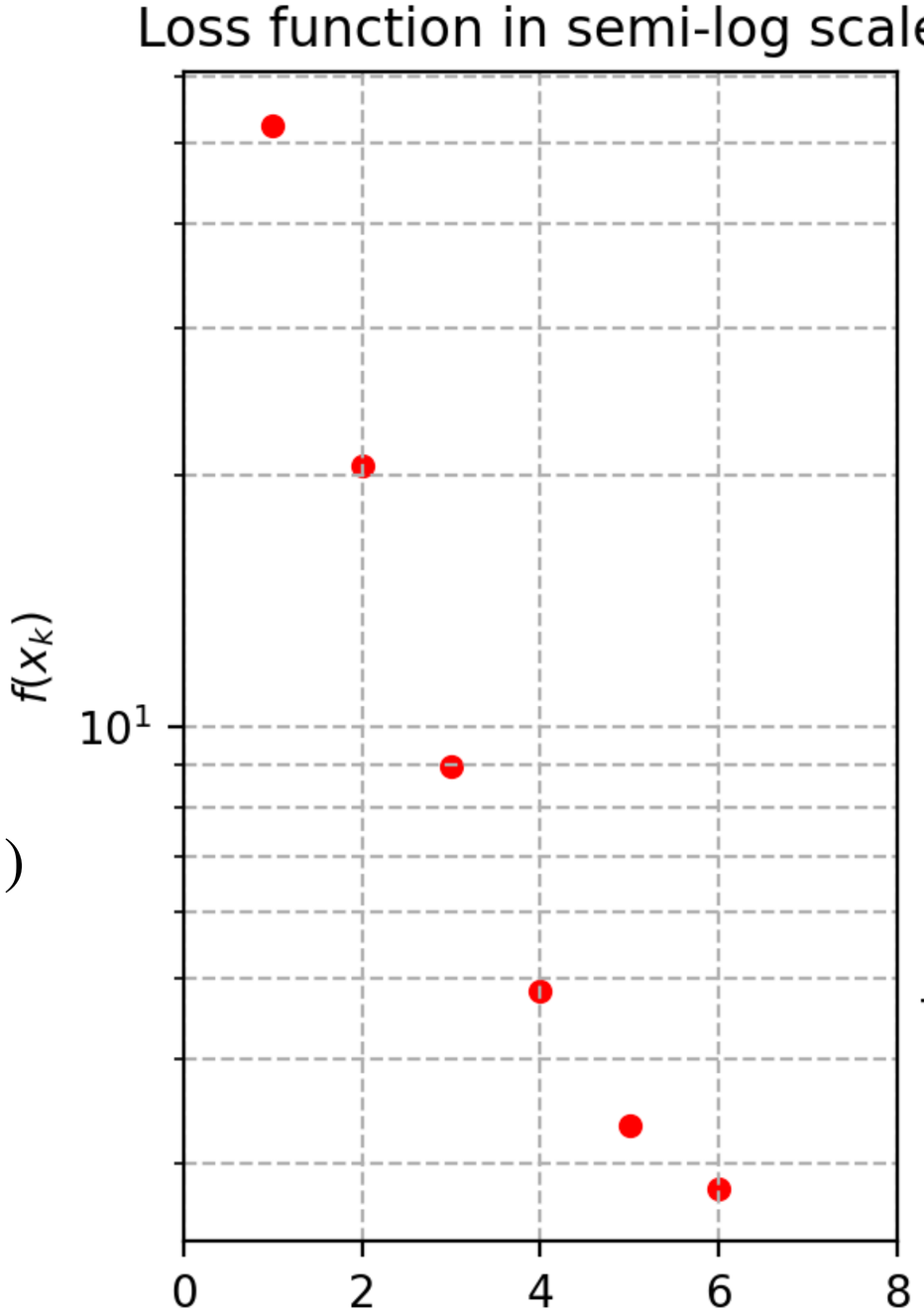
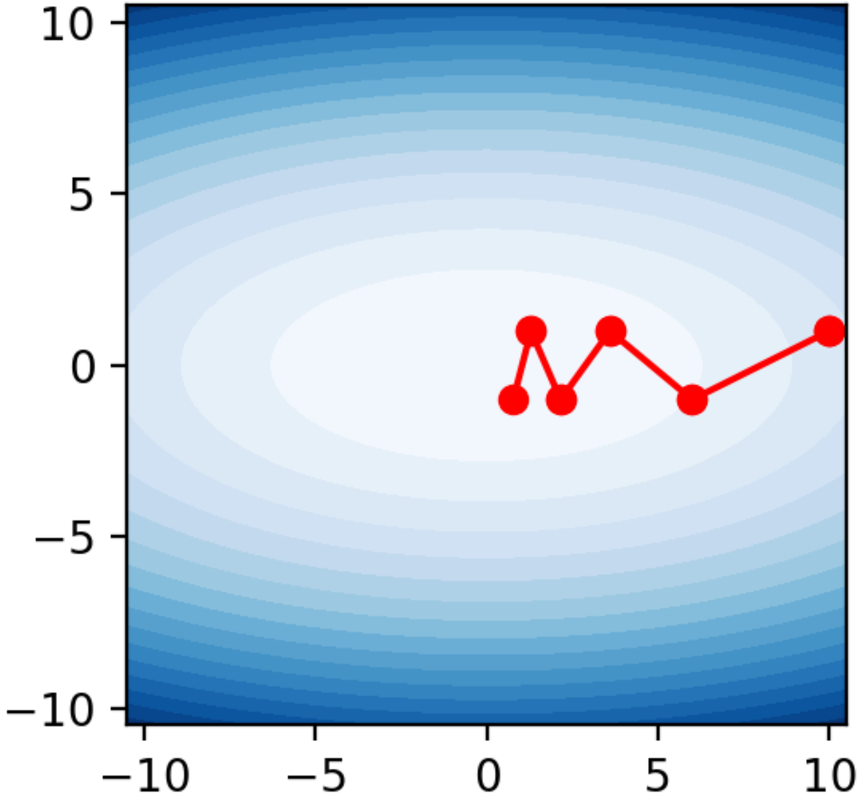




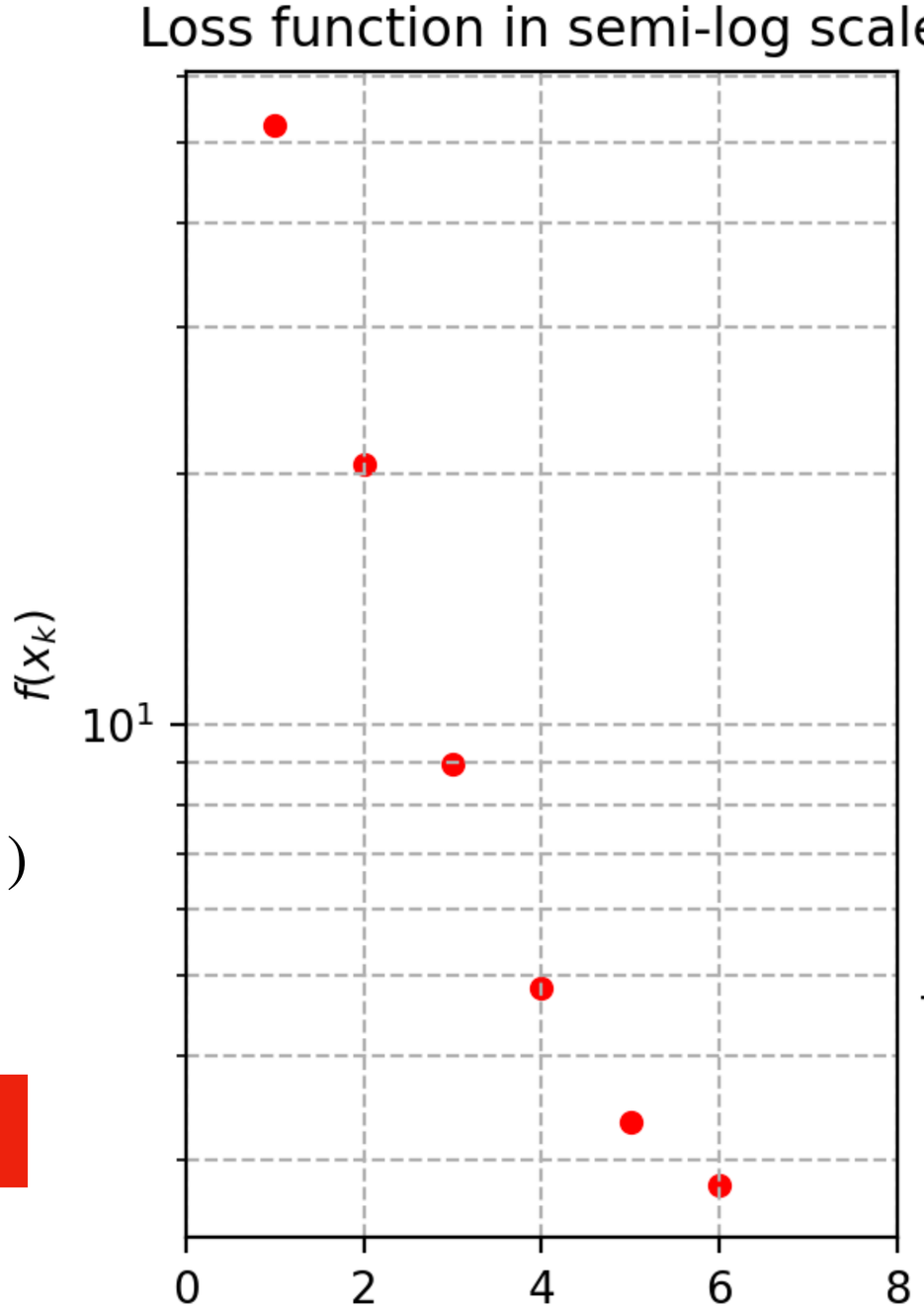
GD can fail for ill-conditioned problems

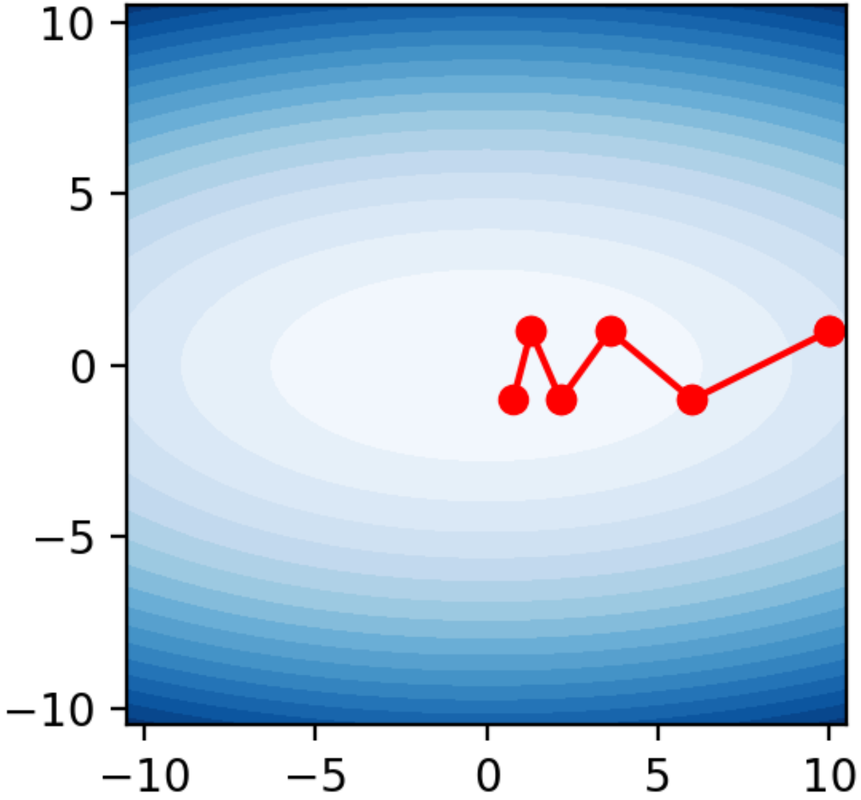
$$\min \frac{1}{2}(x_1^2 + \gamma x_2^2),$$

$\gamma = 5$, initial point $(10,1)$

G.D. with $\tau = 0.4$

Key insight for ML scale your data!

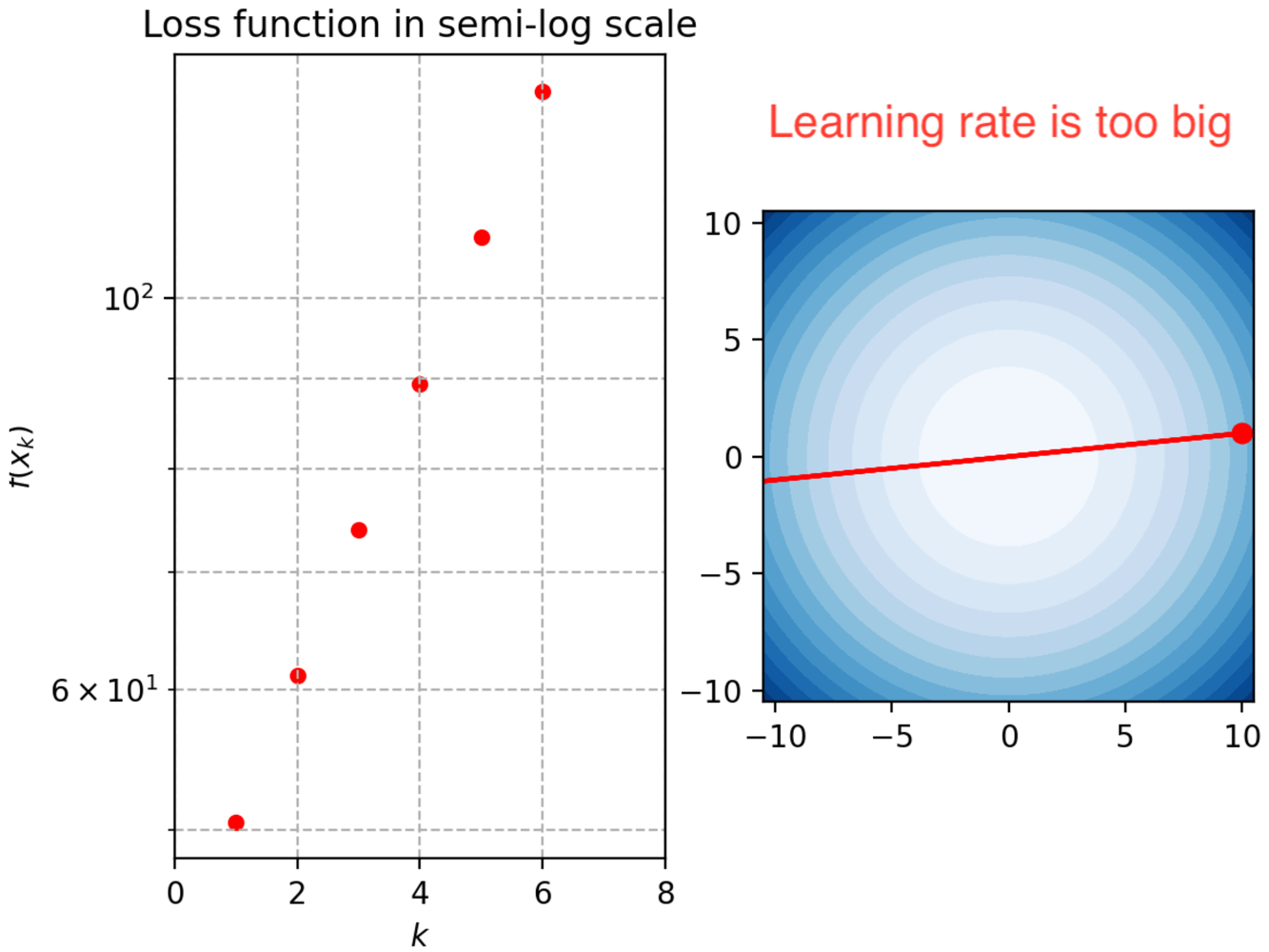




Selecting the learning rate

For deterministic problems the learning rate is chosen by **line-search**

In ML gradients are stochastic and choosing the learning rate is set by **trial and error**!



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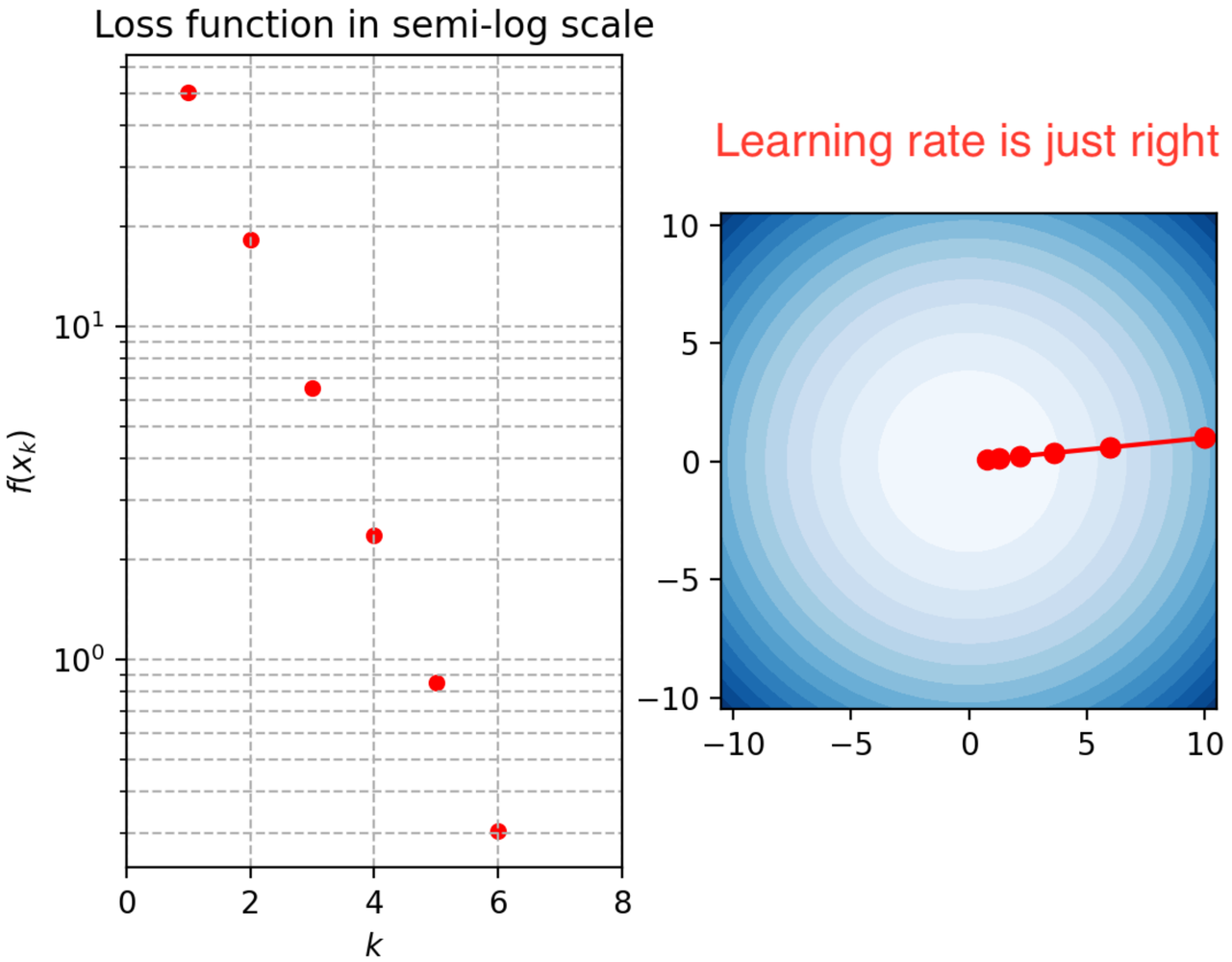

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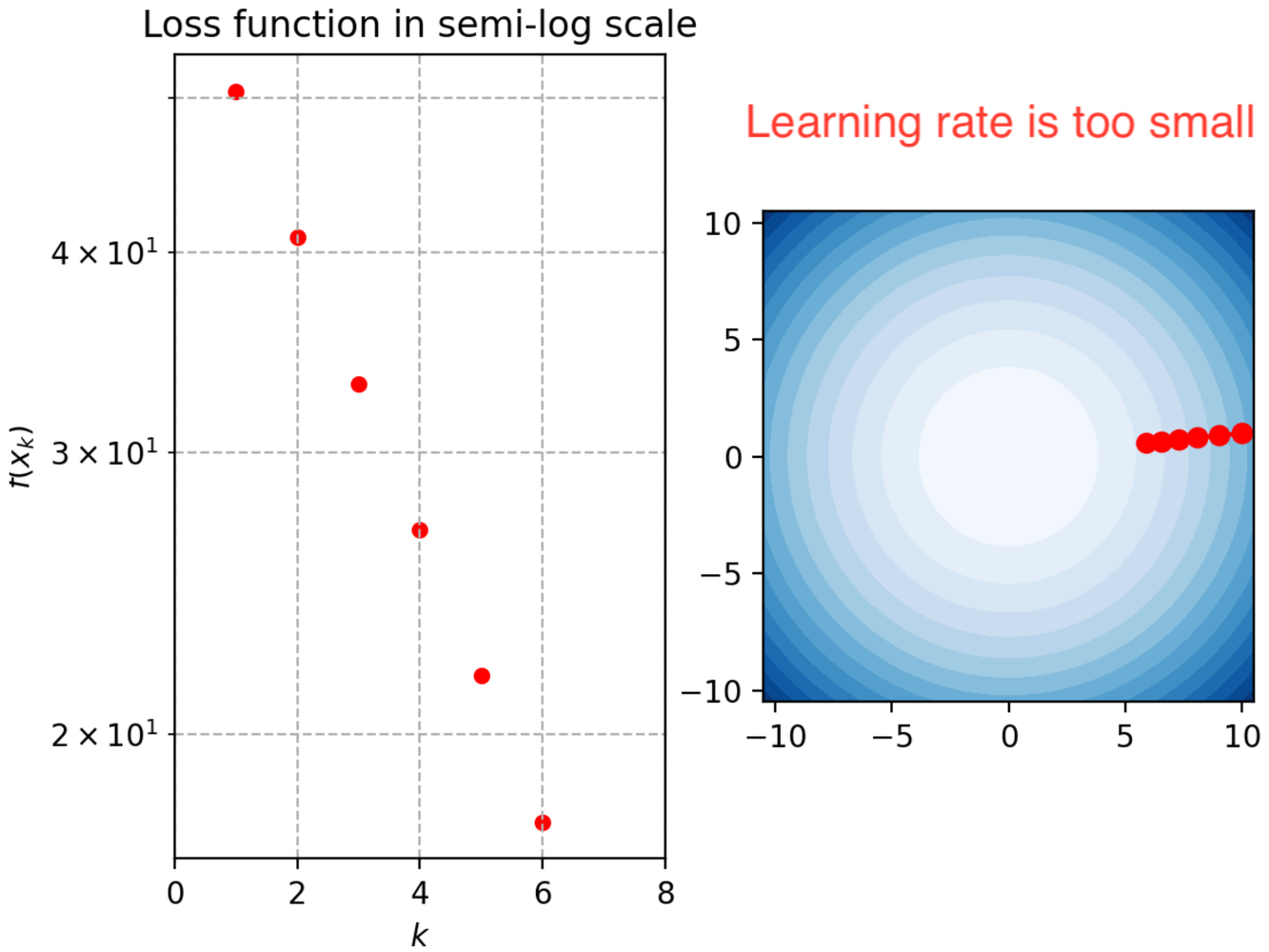
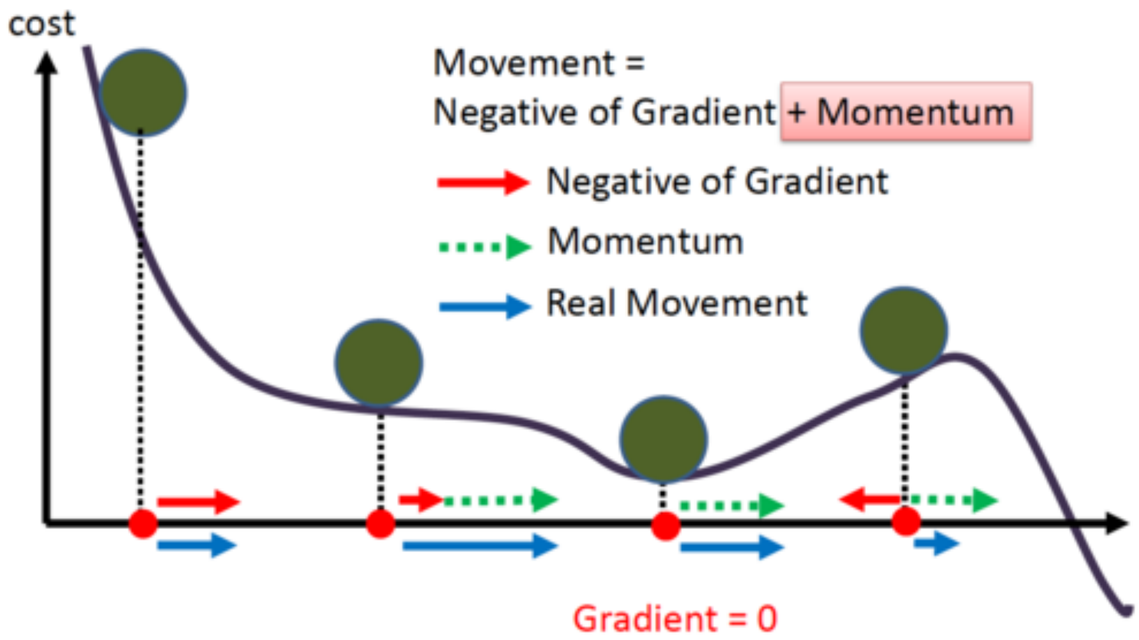


Gradient Descent with Momentum (Acceleration)

GD works by following the negative gradient (direction of steepest descent)



Possible issues:

- Ill conditioning (loss function changes more in some dimensions than others)
- Flat regions (gradient is small, but not zero)
- Shallow minima

Adding a **momentum term** to GD (may) help with these problems

Gradient Descent with Momentum Motivation

$$\boxed{\min_{x \in \mathbb{R}^d} f(x)} \tag{1}$$

The Gradient Descent (GD) algorithm:

$$\boxed{\dot{x} = -\nabla f(x),}$$

The fixed points of GD coincide with the stationary points of f (since $\nabla f(x^\star) = 0$

GD not the only dynamical system with this property.

Consider the second order dynamical system:

$$\mu \ddot{x} = -\nabla f(x) - b\dot{x}, \tag{2}$$

where $\mu \geq 0$ & $b \geq 0$

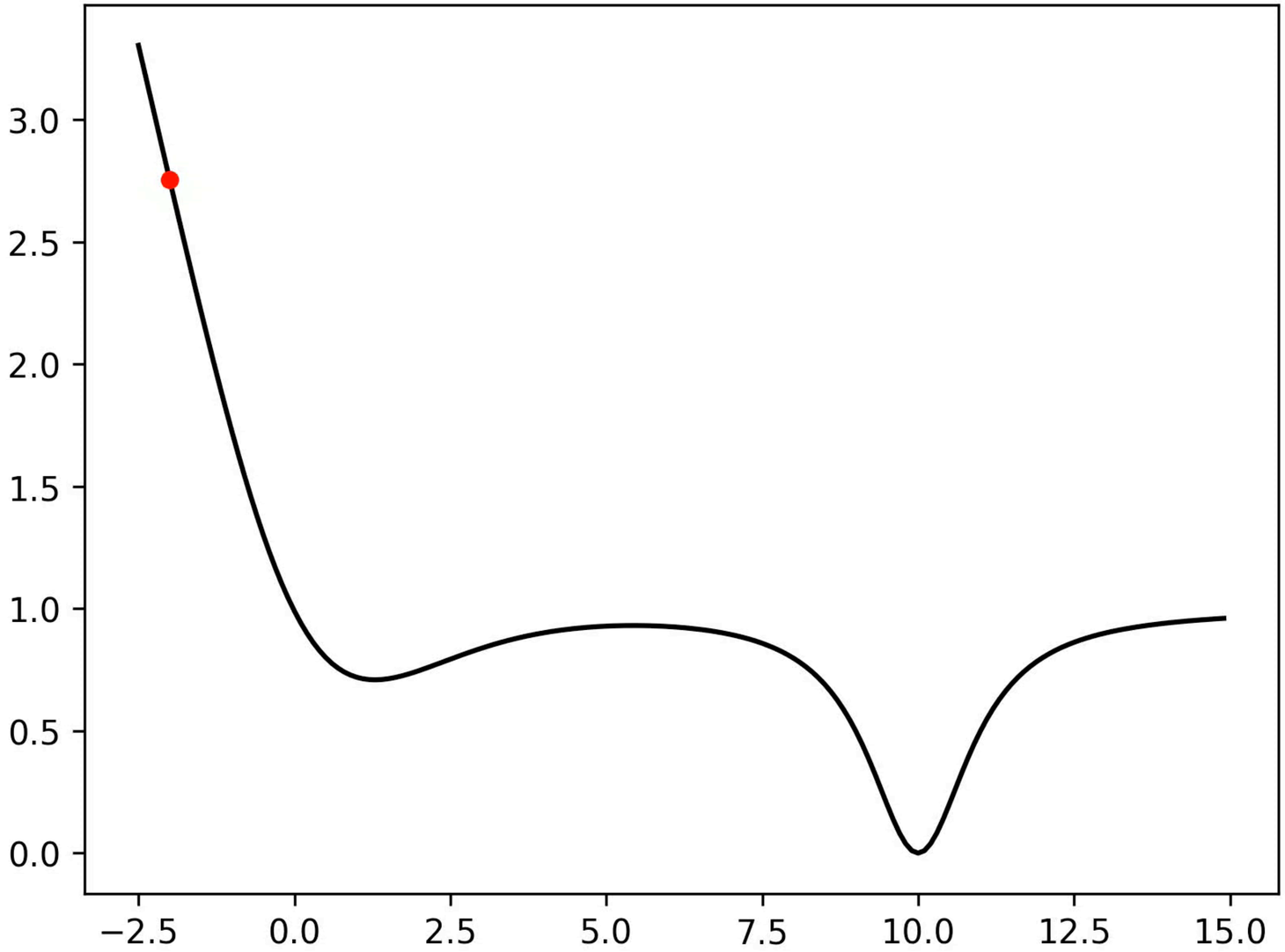
If we allow $\mu \to 0$ we have that the fixed points of (2) coincide with the stationary points of f.

Gradient Descent Near a local minimum

$$\dot{x} = -\nabla f(x)$$

Note how the algorithm slows down near the minimum

(The gradient is small)



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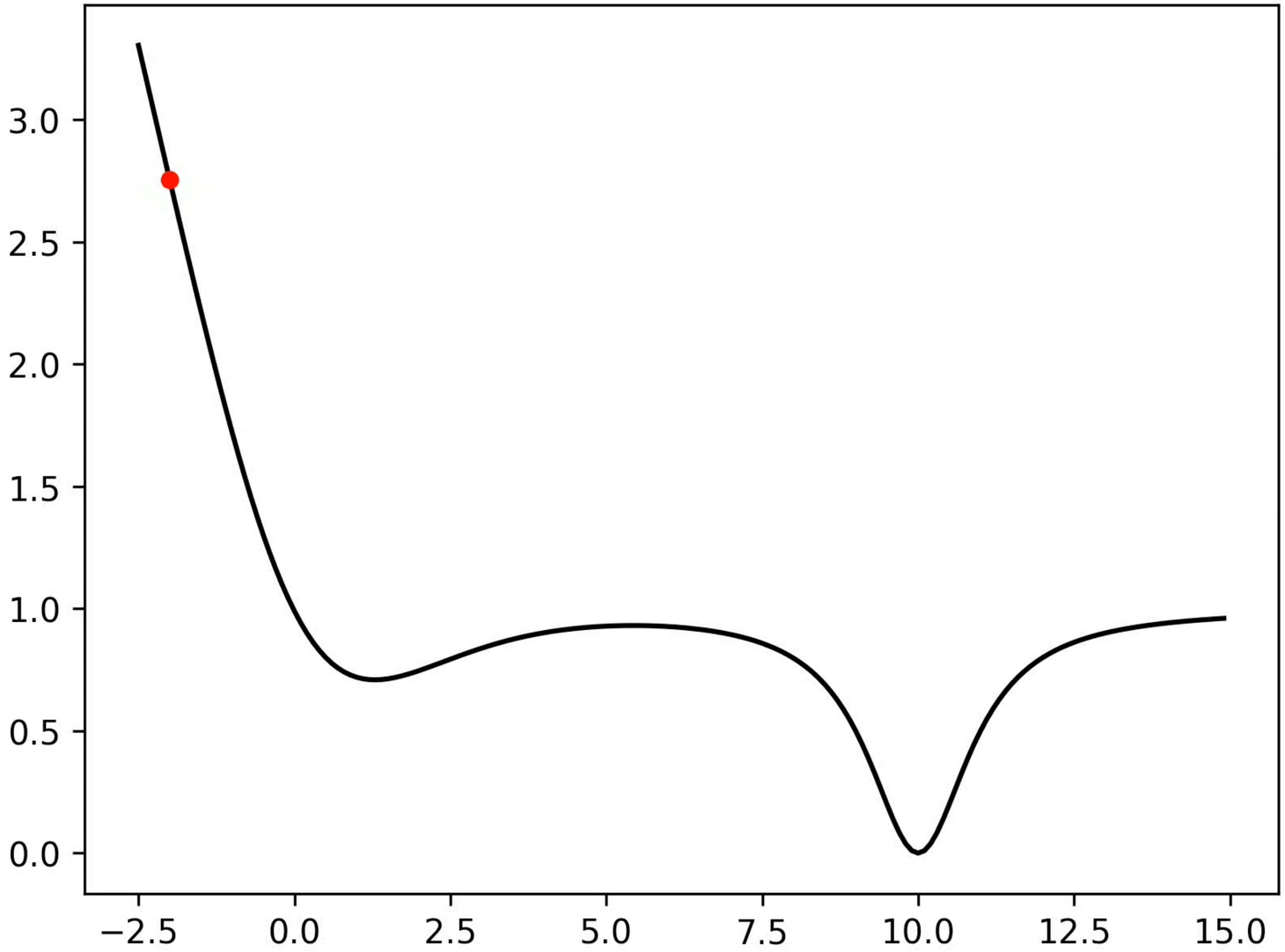
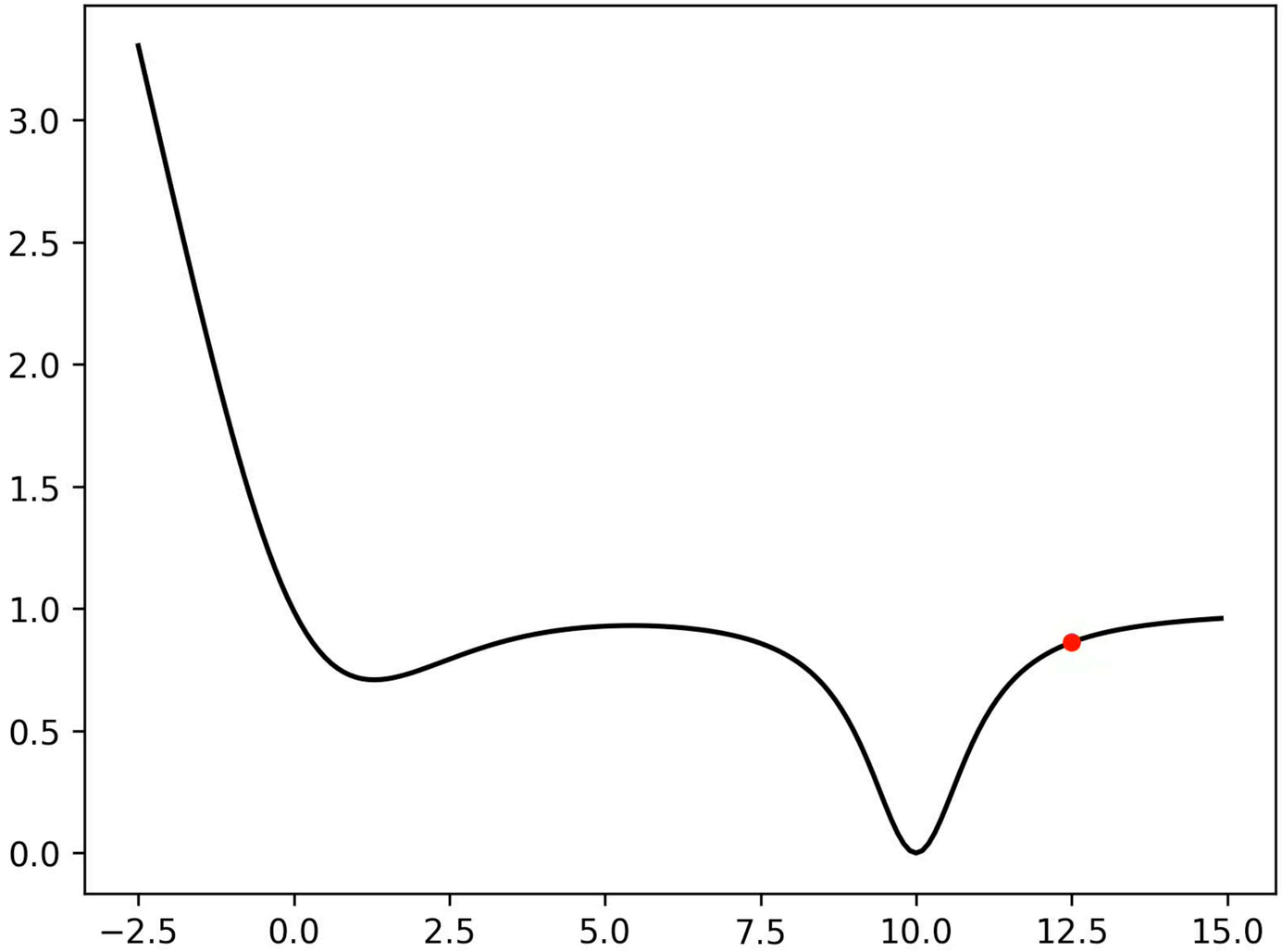


Gradient Descent Around Flat Regions

$$\dot{x} = -\nabla f(x)$$

Note how the algorithm slows because the function is flat (second derivative is small)



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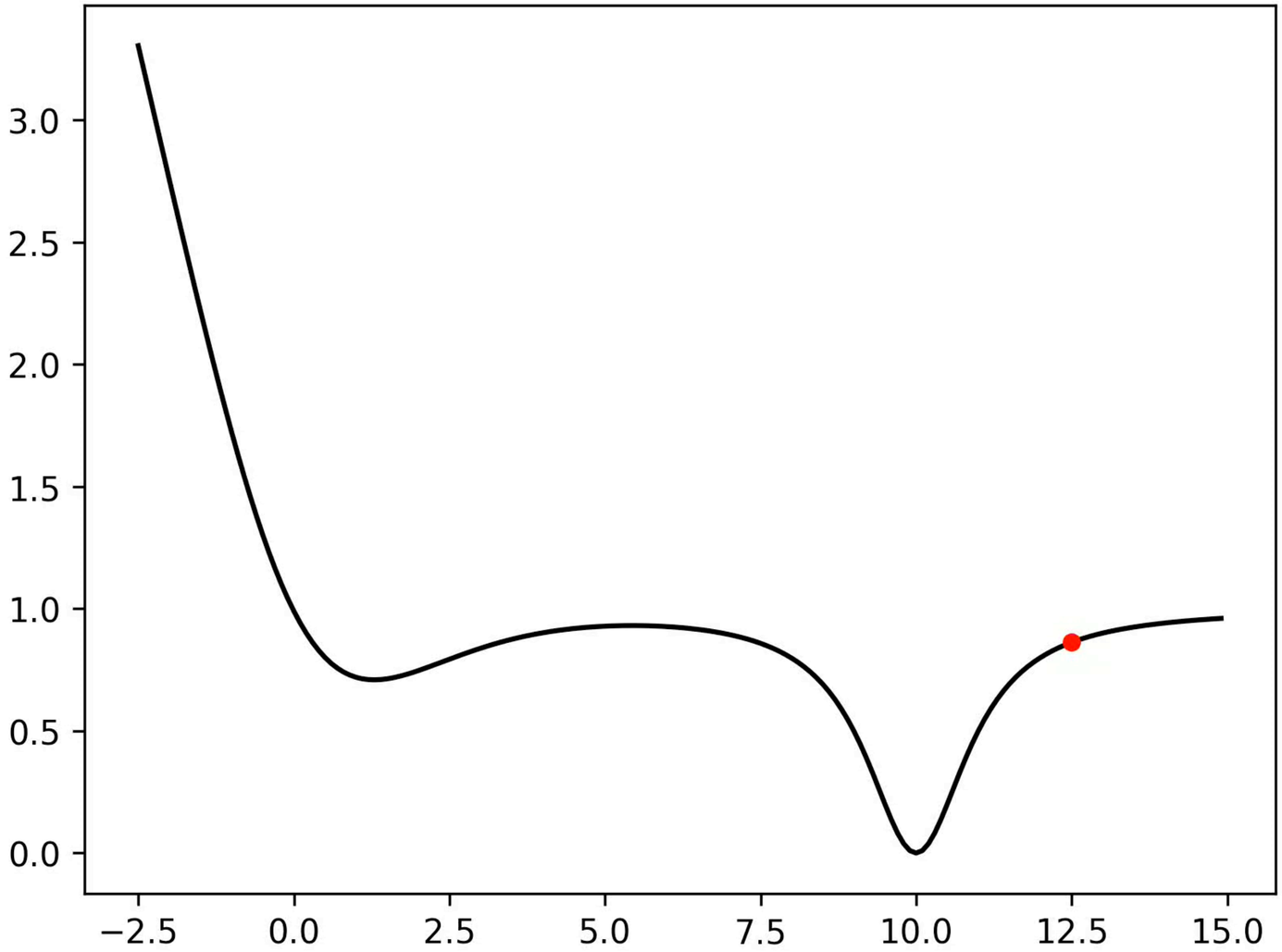
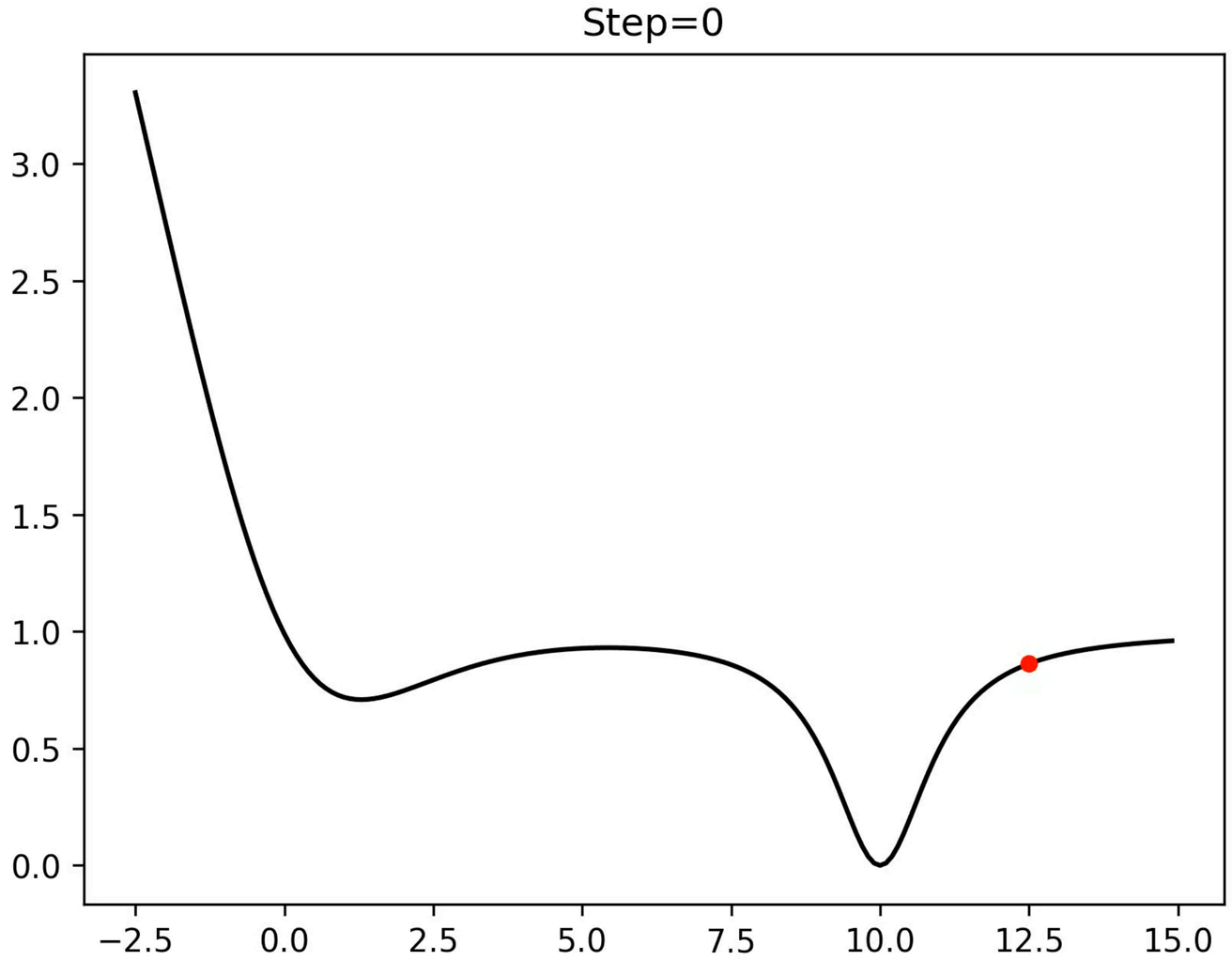


Gradient Descent with Momentum

$$\mu\ddot{x} + \dot{x} = -\nabla f(x)$$

Animation is with fixed momentum

(How most practitioners use it, but theory requires the momentum to decrease)



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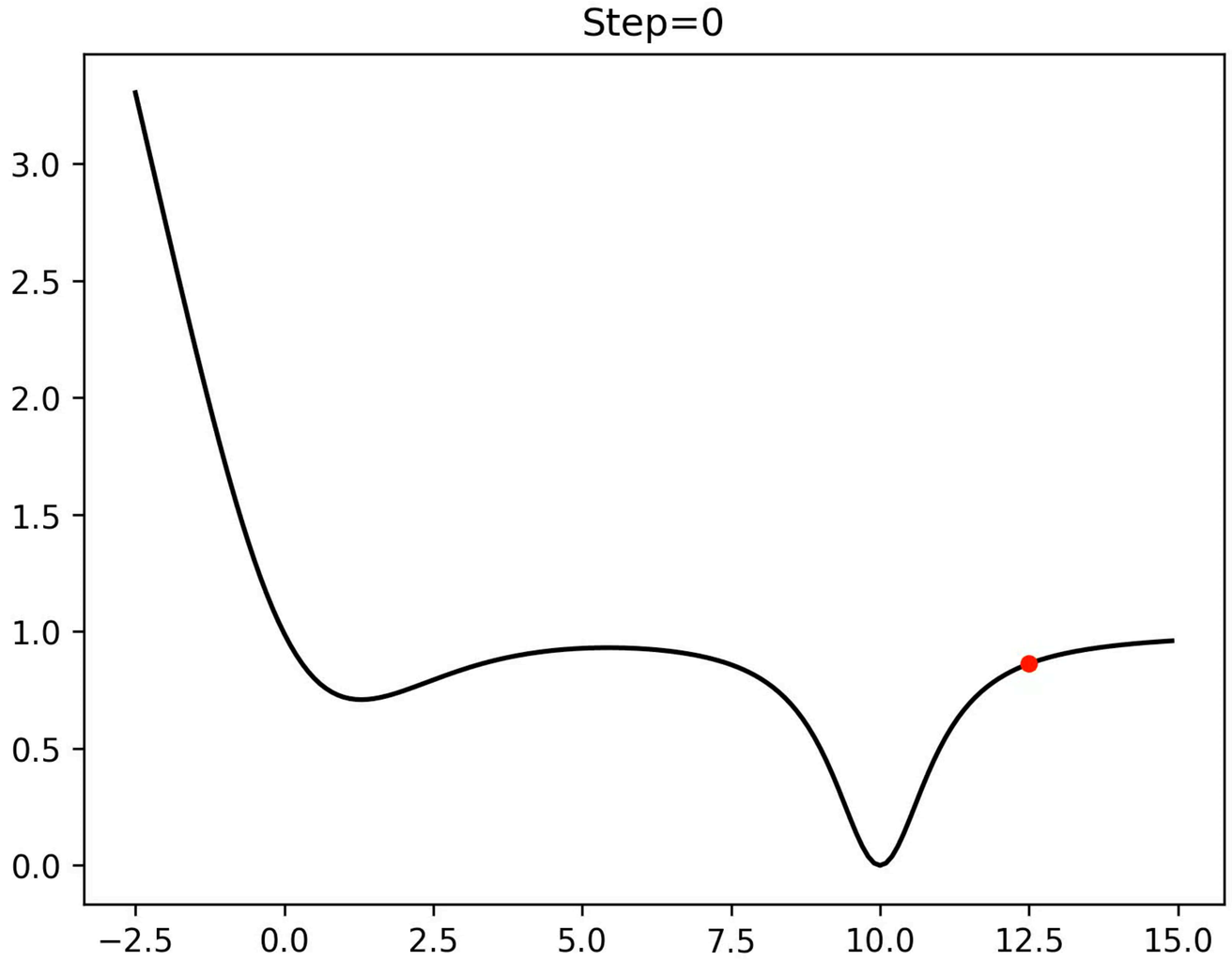


Gradient Descent with Momentum (Acceleration)

$$z_{k+1} = \beta z_k + \nabla L(w_k)$$
$$w_{k+1} = w_k - \tau z_{k+1}$$

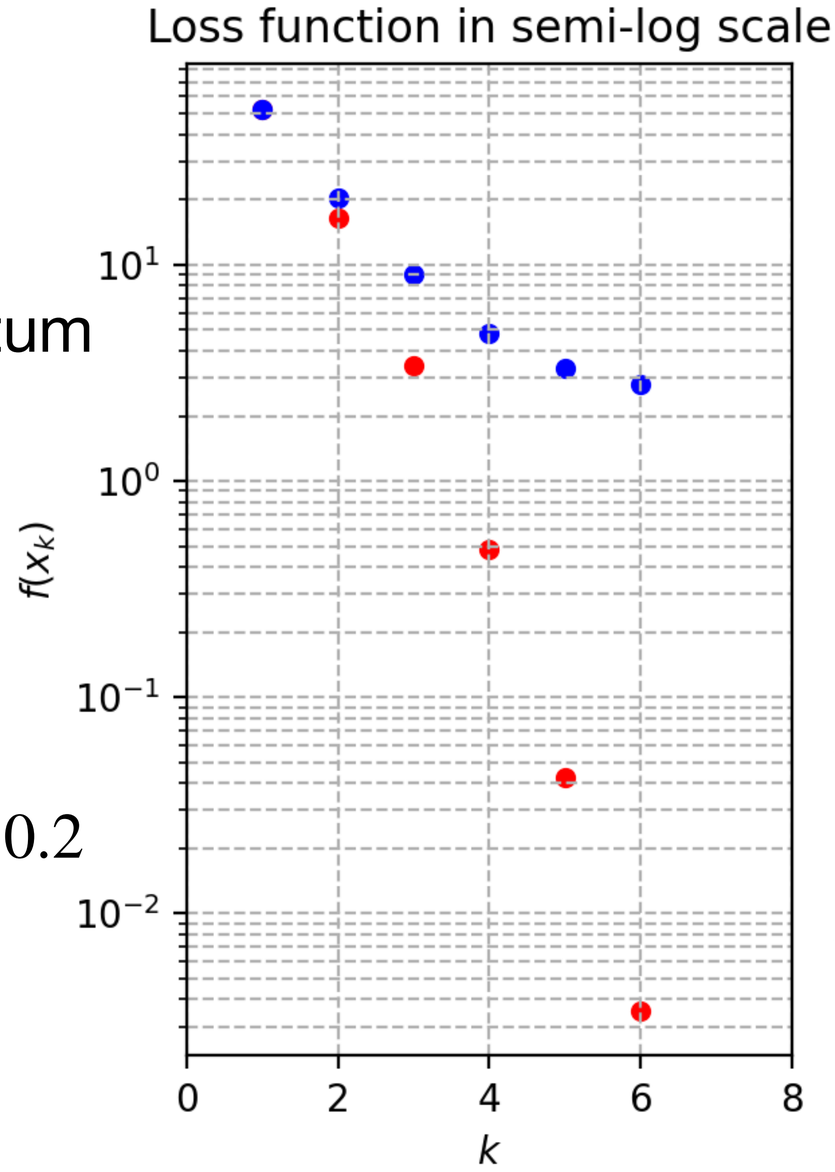
$\beta \geq 0$ controls momentum

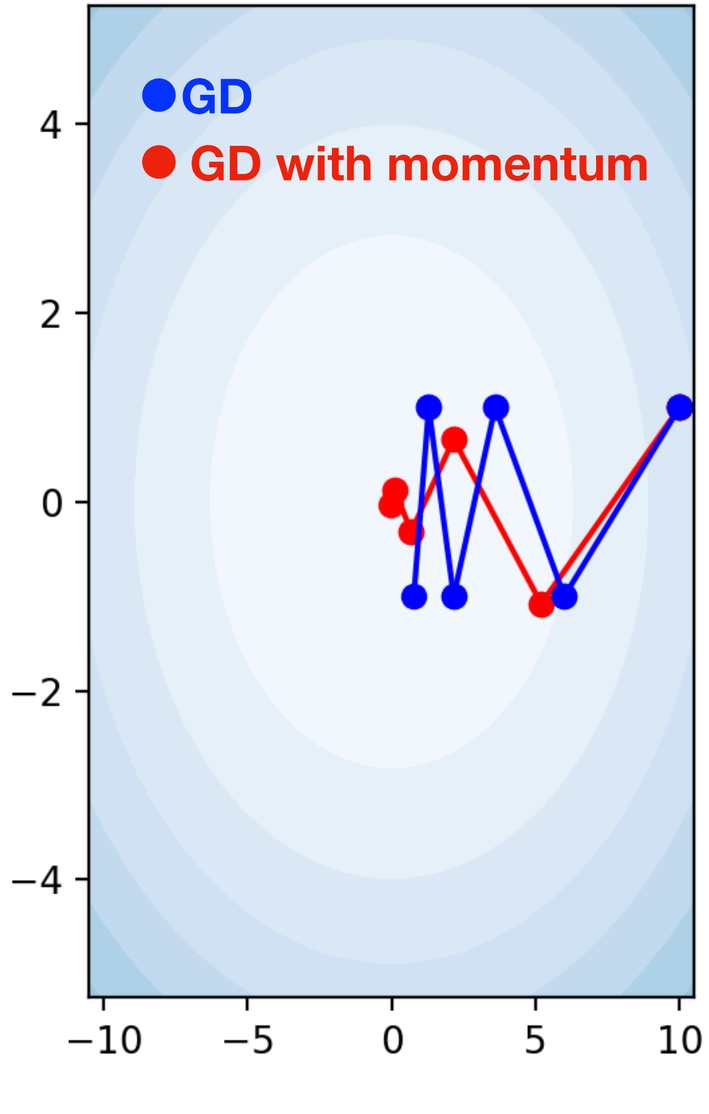
$$\min \frac{1}{2}(x_1^2 + \gamma x_2^2),$$

$\gamma = 5$, initial point $(10,1)$

G.D. with $\tau = 0.4$

G.D. with momentum $\tau = 0.4, \beta = 0.2$





Stochastic Gradient Descent

$$\min_{w \in \mathbb{R}^d} L(w) = \frac{1}{N} \sum_{i=1}^{N} l(w, \xi_i)$$

Loss functions in ML are a sum of functions

Loss associated with ith example ξ_i

''True" gradient: $\nabla L(w) = \frac{1}{N} \sum_{i=1}^{N} \nabla L(w, \xi_i)$

Stochastic gradient: $\nabla \hat{L}(w) = \frac{1}{|B|} \sum_{i \in B} \nabla L(w, \xi_i)$

Where B is a subset of $\{1, \ldots, N\}$ without replacement of size $M \leq N$

M is the size of the batch

$\mathbb{E} \nabla \hat{L}(w_i) = \nabla L(w_i)$ i.e. stochastic gradient is unbiased

Why use a Stochastic Gradient?

Typical Objective function in ML (logistic regression):

$$\min_{w \in \mathbb{R}^d} L(w) = \frac{1}{N} \sum_{i=1}^{N} \underbrace{(-y_i x_i^\top w + \log(1 + e^{x_i^\top w}))}_{L(w, \xi_i)}$$

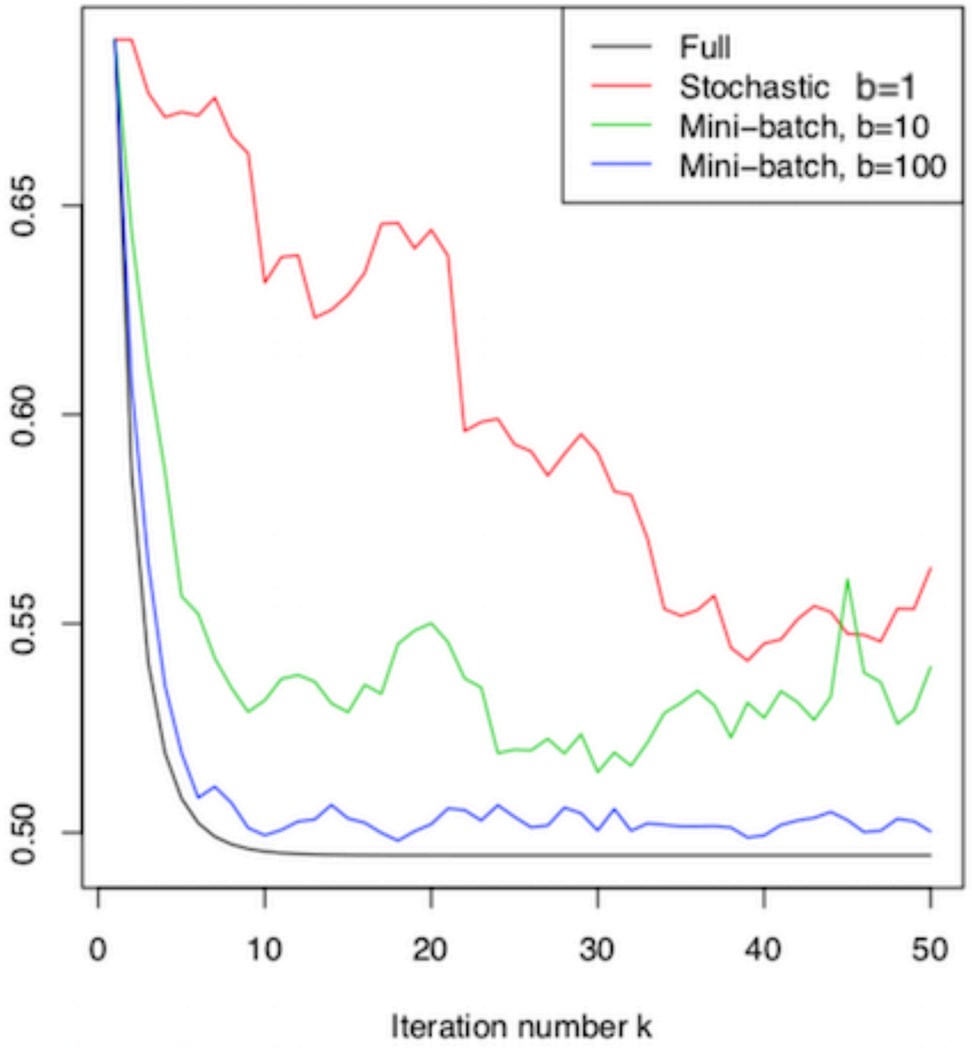
where $\xi_i = (y_i, x_i) \in \{\pm 1\} \times \mathbb{R}^d$ are labels and data respectively

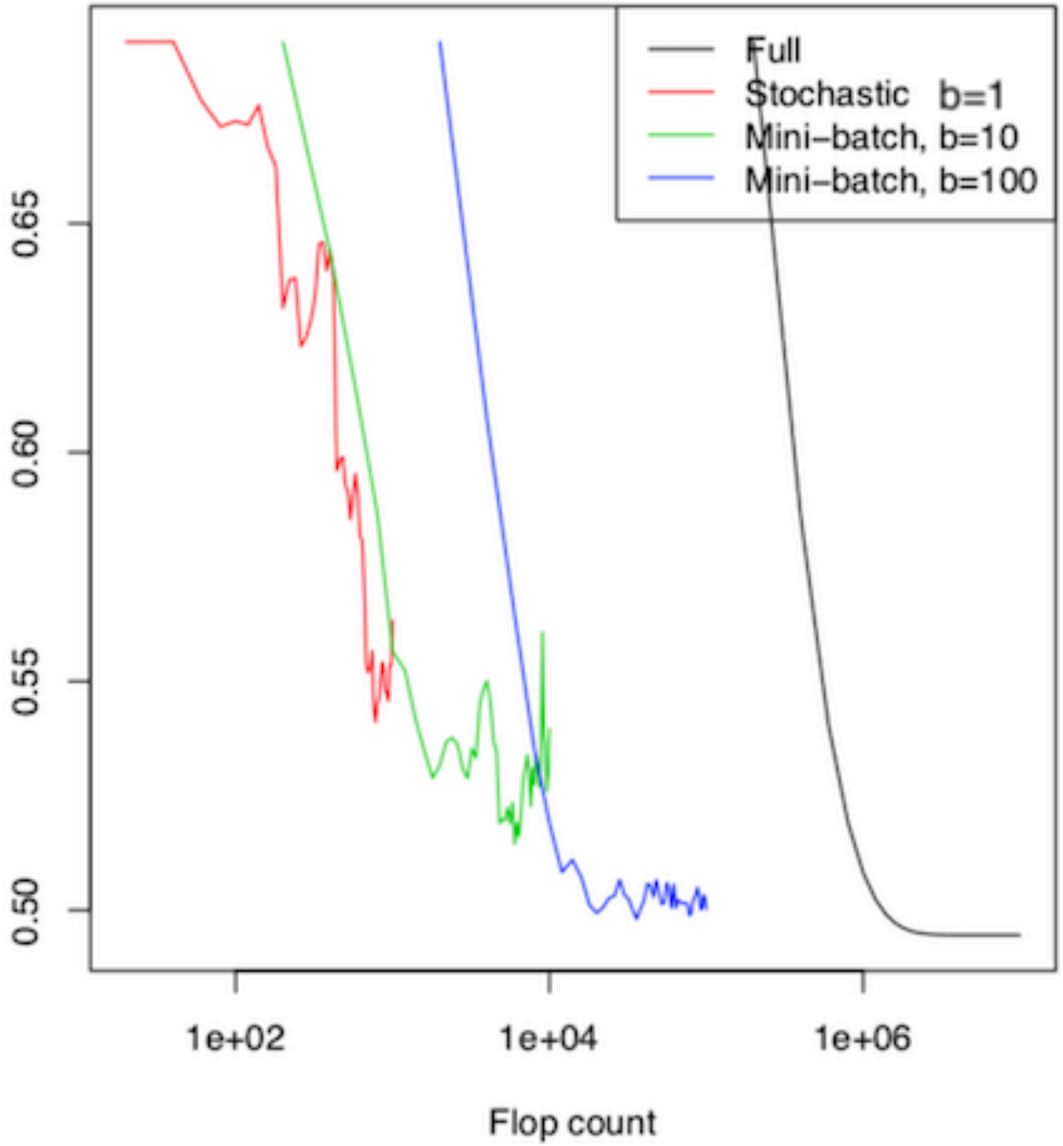
''True" gradient: $\nabla L(w) = \frac{1}{N} \sum_{i=1}^{N} \nabla L(w, \xi_i)$ comp. cost $\approx N \times d$

b-Batch Stochastic gradient: $\nabla \widehat{L}(w) = \frac{1}{b} \sum_{i \in B} \nabla L(w, \xi_i)$ comp. cost $\approx b \times d$

For huge problems each iteration is much cheaper.
But is the algorithm faster?

Why use a Stochastic Gradient?





Why use a Stochastic Gradient?

Advantages of SG:

- Can easily adjust b to ensure gradients fit in available CPU/GPU constraints
- Noise due to mini-batch may help escape shallow local minima (theory is weak but some numerical evidence to support this)
- Since the exact minimum is less relevant in ML mini-batching is popular

Disadvantages of SG:

- Possibly high variance
- Setting the learning rate can be difficult

Constrained Optimization

Constrained Optimization

$$L^\star = \min_w L(w) \qquad L : \mathbb{R}^d \mapsto \mathbb{R}$$

$$g_i(w) = 0, \quad i = 1, \ldots, M \qquad g_i : \mathbb{R}^d \mapsto \mathbb{R}$$

Equality Constrained Problem

Lagrangian function: $\mathscr{L}(w, \lambda) = L(w) + \sum_{i=1}^{M} \lambda_i g_i(w)$

where $\lambda_i \in \mathbb{R}$ are the Lagrange multipliers

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$$h_i(w) \le 0, \quad i = 1,\ldots,P \qquad h_i : \mathbb{R}^d \mapsto \mathbb{R}$$

General Constrained Problem

Lagrangian function:

$$\mathscr{L}(w,\lambda,\mu) = L(w) + \sum_{i=1}^{M} \lambda_i g_i(w) + \sum_{i=1}^{P} \mu_i h_i(w)$$

where $\lambda_i \in \mathbb{R}, \mu_i \ge 0$ are the Lagrange multipliers

Lagrangian Duality

$$\mathscr{L}(w, \lambda, \mu) = L(w) + \sum_{i=1}^{M} \lambda_i g_i(w) + \sum_{i=1}^{P} \mu_i h_i(w)$$

Lagrangian

$$Q(\lambda, \mu) = \min_{w} \mathscr{L}(w, \lambda, \mu)$$

Dual Function

$$Q^\star = \max_{\lambda_i \in \mathbb{R}, \mu_i \geq 0} Q(\lambda, \mu)$$

Dual Problem

Weak duality: $F^\star \geq Q^\star$

Holds even if the problem is non-convex, the dual problem is always concave

Strong duality: $F^\star = Q^\star$

Holds if the problem is convex, convex loss and constraints

Optimality Conditions (KKT)

$$L^\star = \min_w L(w)$$
$$g_i(w) = 0, \quad i = 1,\ldots,M$$
$$h_i(w) \leq 0, \quad i = 1,\ldots,P$$

First-order necessary conditions:

$$\nabla_w \mathscr{L}(w,\lambda) = \nabla_w L(w) + \sum_{i=1}^{M} \lambda_i \nabla_w g_i(w) = 0$$

$$g_i(w) = 0 \qquad i = 1,\ldots,M$$
$$h_i(w) \leq 0 \qquad i = 1,\ldots,P$$
$$\lambda_i h_i(w) = 0,\ \lambda_i \geq 0 \qquad i = 1,\ldots,P$$

Support Vector Machines

$$\min_w \frac{1}{2}||w||_2^2$$

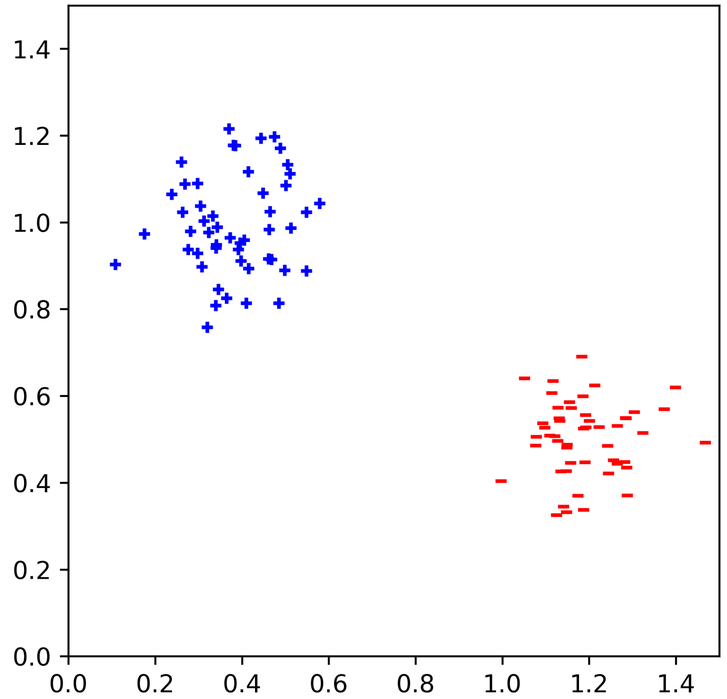
s.t. $y_i w^\top x_i \geq 1 \qquad i = 1,\ldots,N$

$\max_{\lambda_i \geq 0} L(\lambda)$:Dual Problem

$$L(\lambda) = \min_w \frac{1}{2}\|w\|_2^2 + \sum_{i=1}^{N} \lambda_i (1 - y_i w^\top x_i)$$

From Optimality conditions $w = \sum_{i=1}^{N} \lambda_i y_i x_i$ i.e $L(\lambda) = \sum_{i=1}^{N} -\frac{1}{2} \sum_{i,j}^{N} \lambda_i \lambda_j y_i y_j x_i^\top x_j$

$$\max_{\lambda_i \geq 0} L(\lambda) = \sum_{i=1}^{N} -\frac{1}{2} \sum_{i,j}^{N} \lambda_i \lambda_j y_i y_j x_i^\top x_j$$



Dual problem only contains inner products (use kernel trick to increase feature space without additional cost)

Optimisation in ML — Remarks

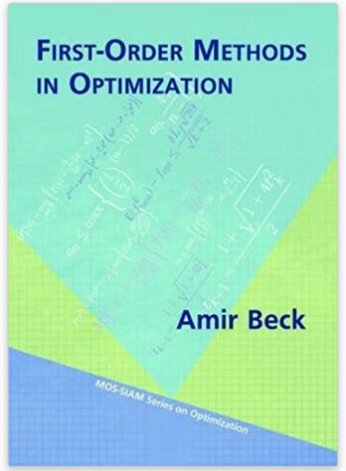
Optimisation is everywhere in ML.

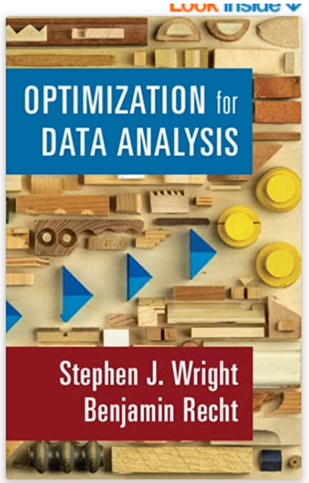
Both the model and the optimisation algorithm are critical to the success of ML projects, especially if the model is non-convex and has noise.

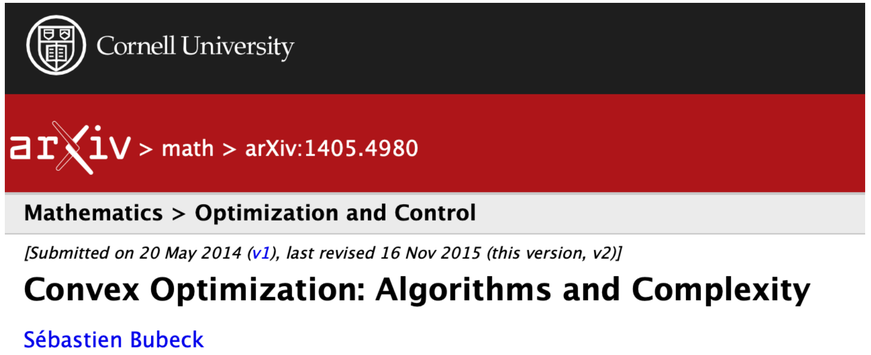
Acceleration may help, and choosing a learning rate can be time-consuming.

Scaling data is essential before calling an optimisation algorithm.

The **theory of optimisation is vital** for a deeper understanding of ML






Cornell University

arXiv > math > arXiv:1405.4980

Mathematics > Optimization and Control

[Submitted on 20 May 2014 (v1), last revised 16 Nov 2015 (this version, v2)]

Convex Optimization: Algorithms and Complexity

Sébastien Bubeck

Contents and Aims

Aims:

- Introduce a mathematical toolbox as used in ML
- Demonstrate mathematics with different ML models

A. **Linear Algebra**
    1. Matrices and vectors
    2. Measuring similarity
    3. Eigenvectors/Eigenvalues
    4. Matrix Factorisations
B. **Calculus**
C. **Optimisation**
    1. Classes of Optimization Models/Algorithms
    2. Gradient Descent (Stochastic, Acceleration, Momentum)
    3. Optimality Conditions (constrained case)