Linear Regression

Analytical solution, gradient descent, feature expansion

MISiS Mega Science, Spring Semester

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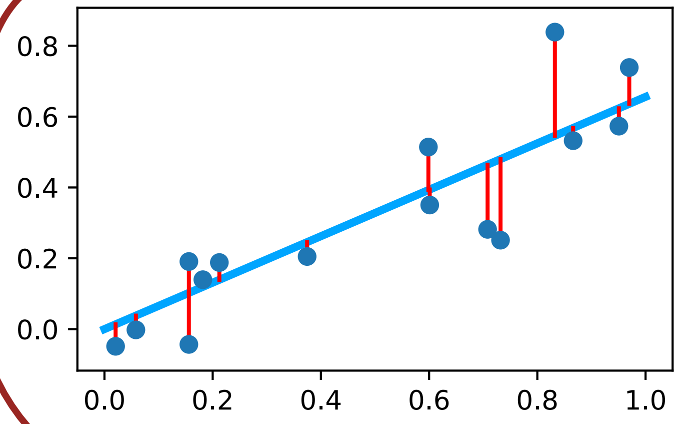
Why study linear models?

Linear models in a nutshell

Regression:

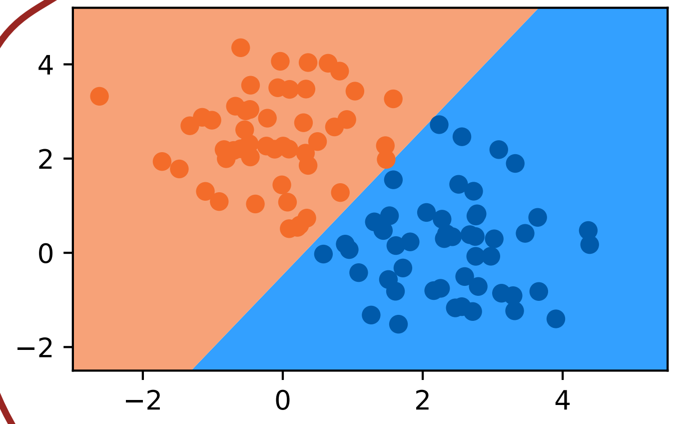
$$\hat{f}(x) = \theta^{\mathrm{T}} x$$



Targets $\in \mathbb{R}$ (or even $\mathbb{R}^m$ in the multidimensional case)

Classification:

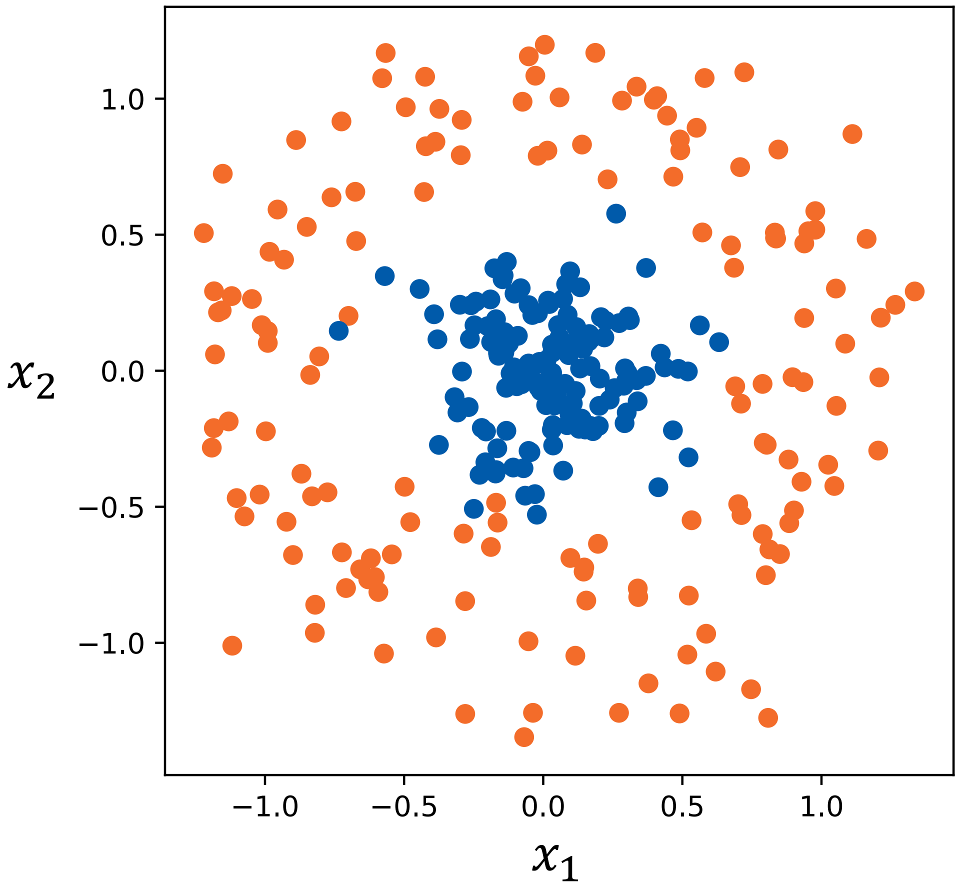
$$\hat{f}(x) = \mathbb{I}[\theta^{\mathrm{T}} x > 0]$$

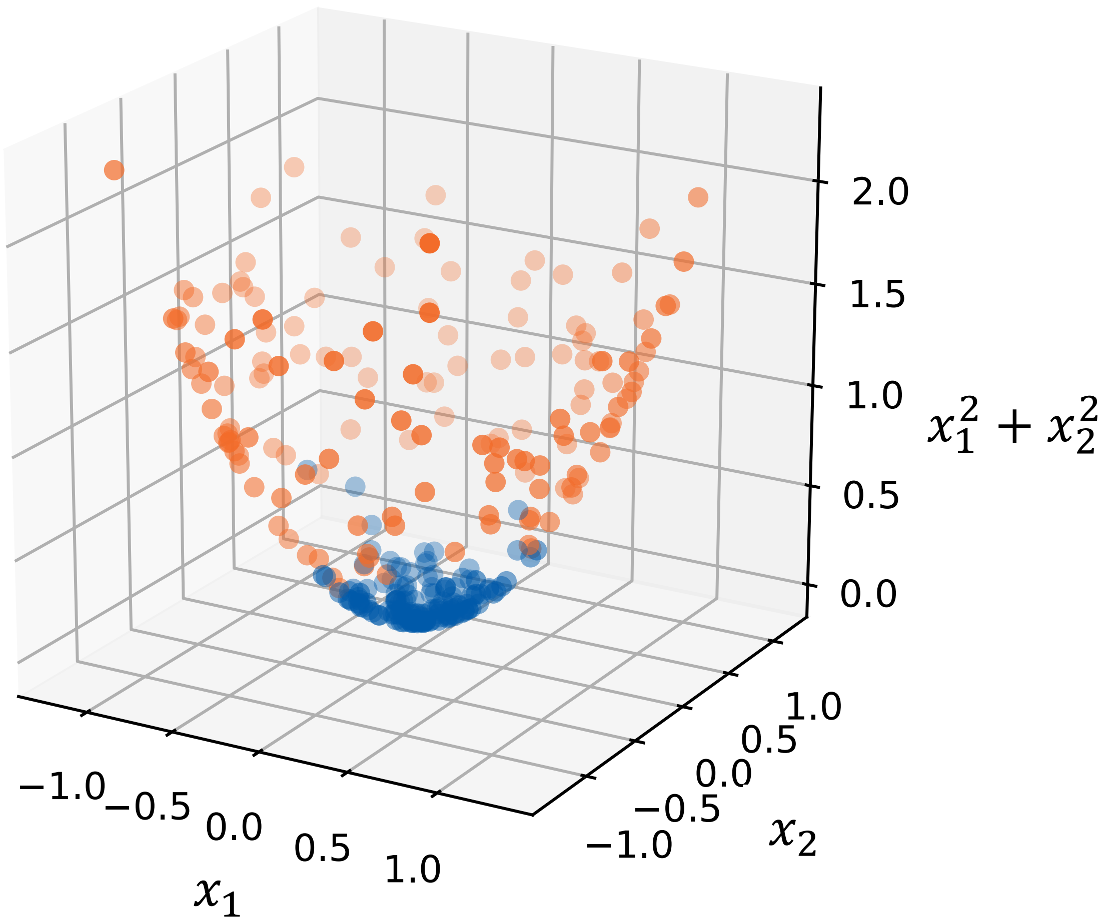


Targets $\in$ some finite set

Outputs linear in inputs

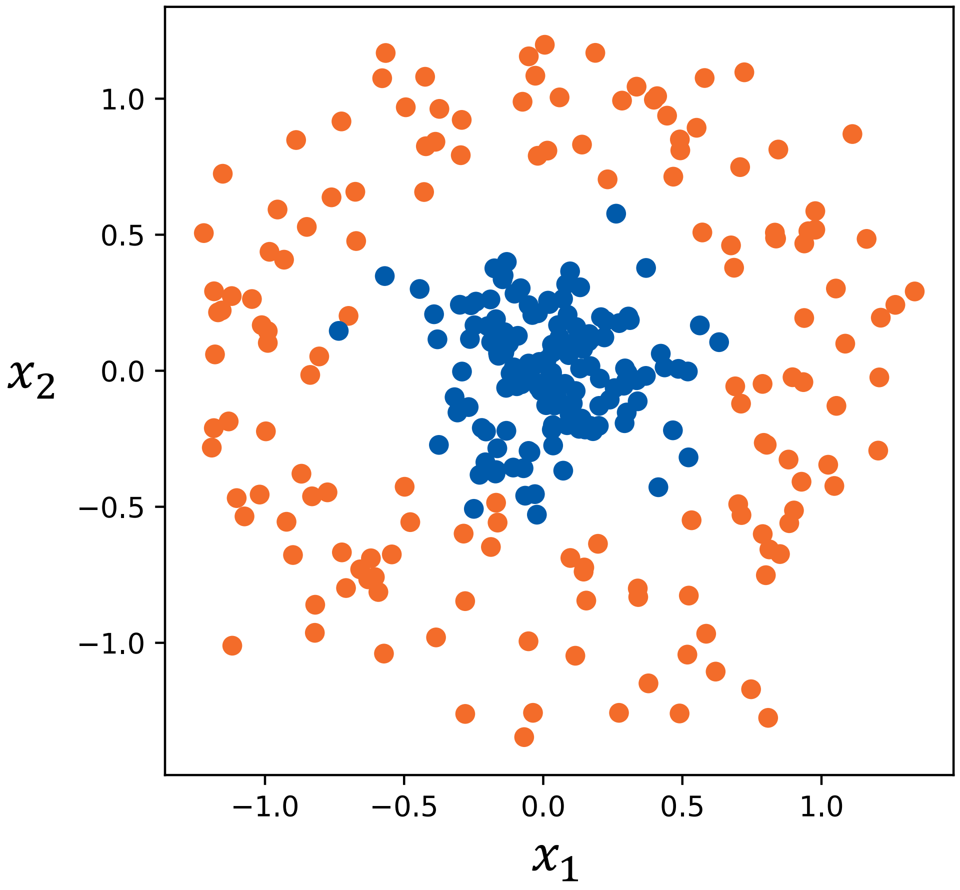
The hidden power

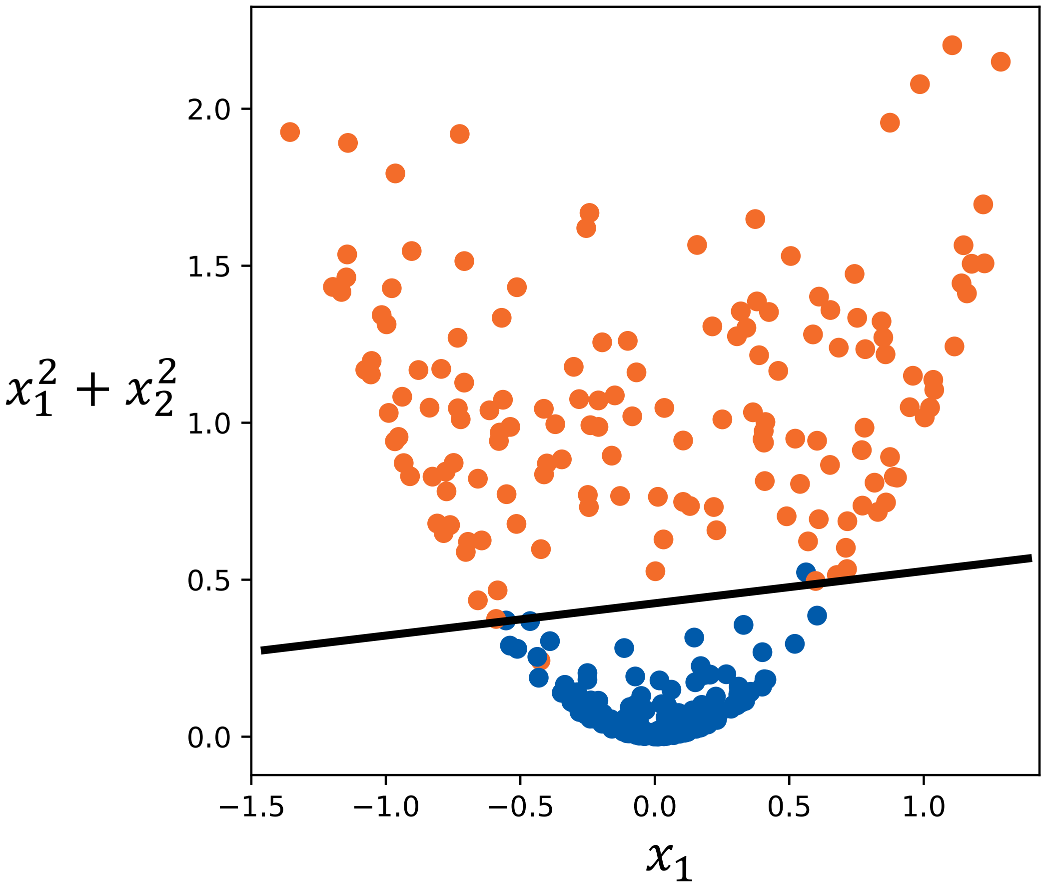




- Linearly **inseparable** $\longrightarrow$ **separable** by **transforming the features**

The hidden power





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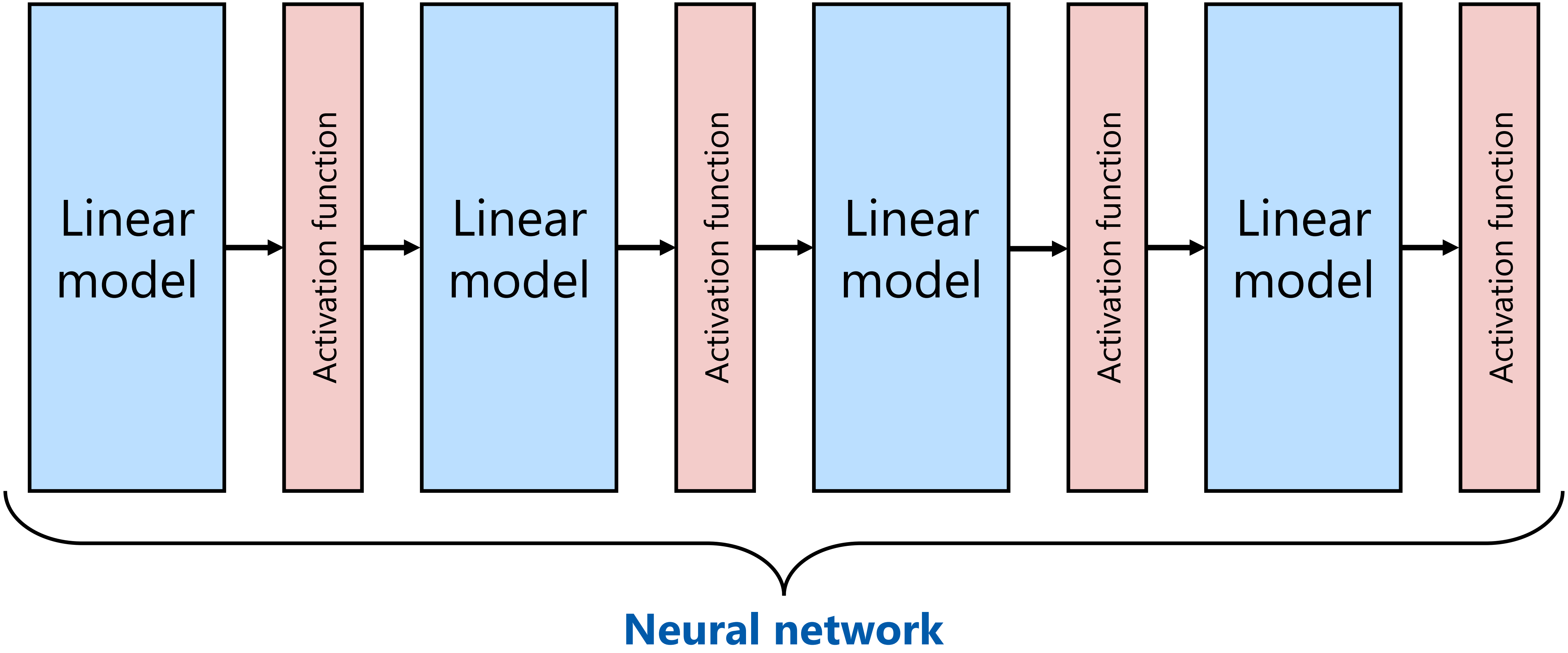
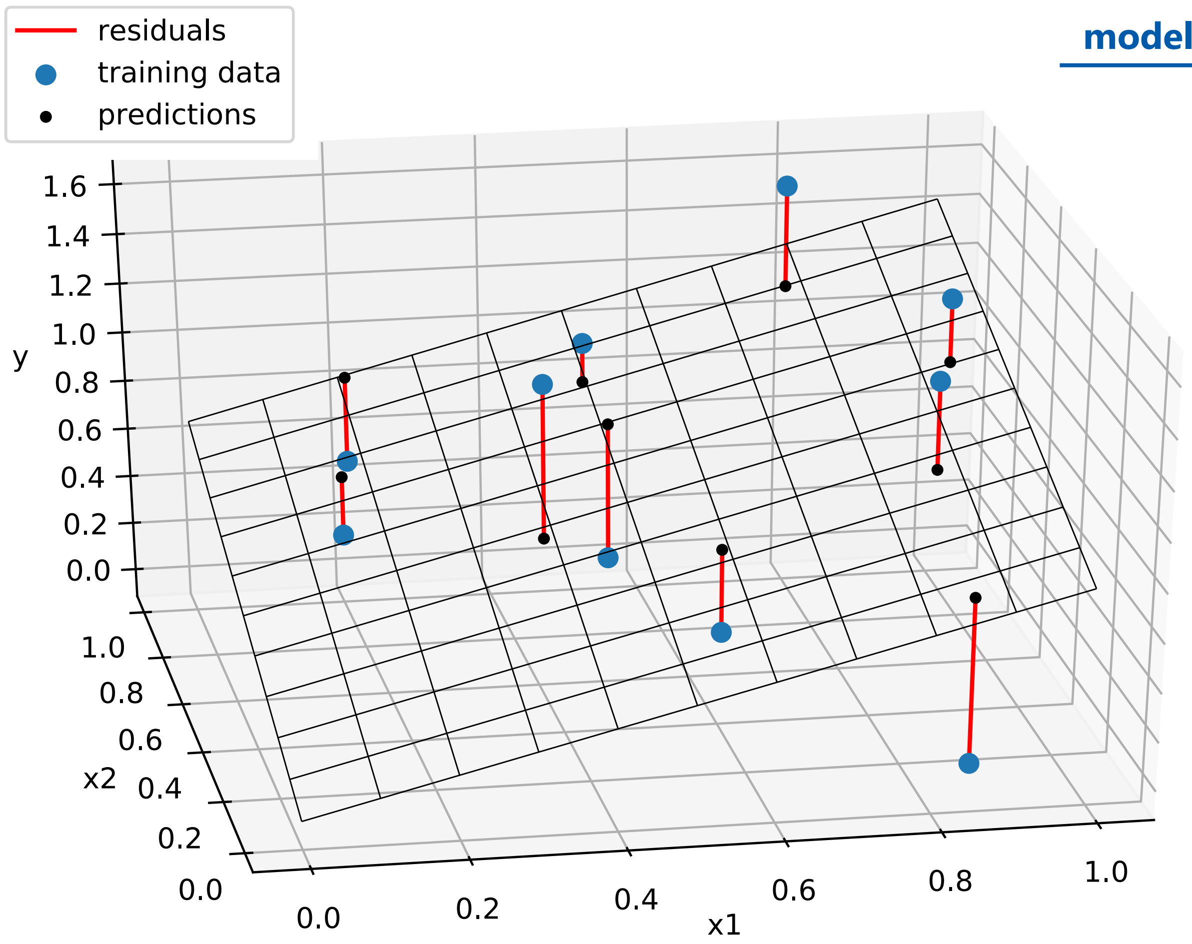
Building block for deep models



- Better intuition for deep neural networks training

Linear Regression

Linear Regression model



model prediction

$$\hat{f}_\theta(x) = \theta^T x$$

parameters vector

$$\theta \in \mathbb{R}^d$$

features vector

$$x \in \mathcal{X} \subset \mathbb{R}^d$$

$$\frac{1}{N} \sum_{i=1 \dots N} \left(y_i - \hat{f}_\theta(x_i)\right)^2 \xrightarrow[\theta]{} \min$$

Mean Squared Error (MSE loss)

Andrey Ustyuzhanin

Common loss functions

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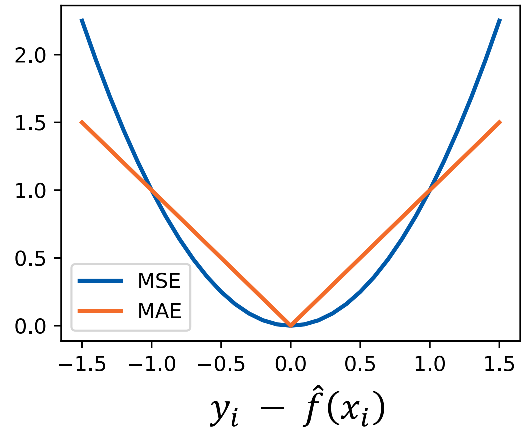


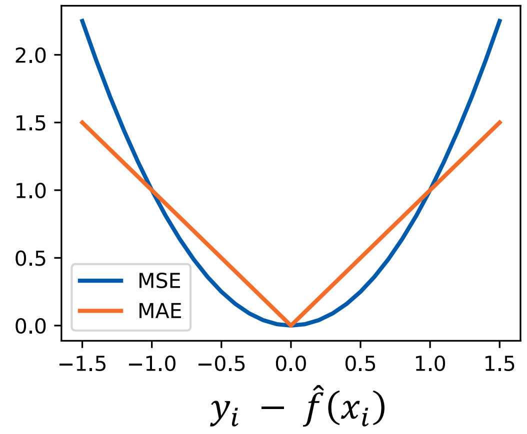
Common loss functions

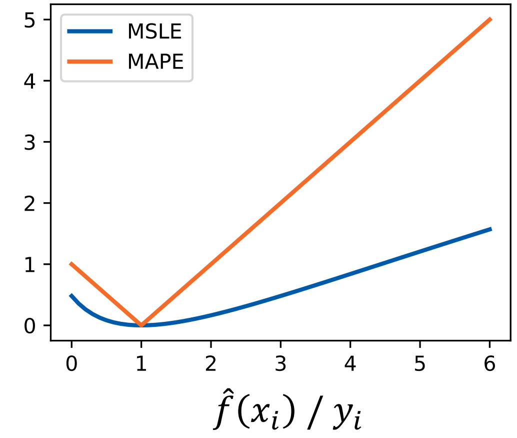
Mean squared error (MSE): $\frac{1}{N}\sum_{i=1...N}\left(y_i - \hat{f}_\theta(x_i)\right)^2$

Mean absolute error (MAE): $\frac{1}{N}\sum_{i=1...N}\left|y_i - \hat{f}_\theta(x_i)\right|$

Mean absolute percentage error (MAPE): $\frac{1}{N}\sum_{i=1...N}\left|\frac{y_i - \hat{f}_\theta(x_i)}{y_i}\right|$

Mean squared logarithmic error (MSLE): $\frac{1}{N}\sum_{i=1...N}\left(\log(y_i + 1) - \log\left(\hat{f}_\theta(x_i) + 1\right)\right)^2$





Common loss functions

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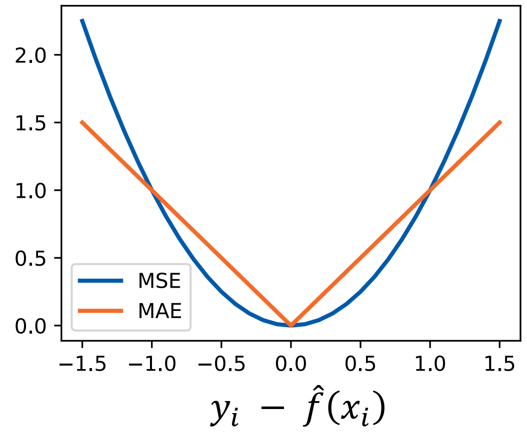

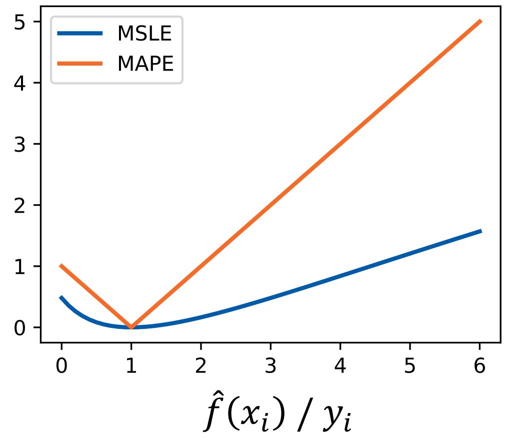

- Different **loss functions** also are related to different **assumptions about the data**

Analytical solution

- Recall the design matrix:

features →

$$X = \begin{bmatrix} x_1^1 & x_1^2 & \cdots & x_1^d \\ x_2^1 & x_2^2 & \cdots & x_2^d \\ \vdots & \vdots & \ddots & \vdots \\ x_N^1 & x_N^2 & \cdots & x_N^d \end{bmatrix}$$

↓ *objects*

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- We can use it to rewrite the MSE loss:

$$\mathcal{L}_{\text{MSE}} = \frac{1}{N} \sum_{i=1 \dots N} \left(y_i - \theta^{\mathrm{T}} x_i\right)^2 = \frac{1}{N} \|y - X\theta\|^2$$

$$y = (y_1, y_2, \dots, y_N)^{\mathrm{T}}$$ – vector of targets

Analytical solution

$$\mathcal{L}_{\mathrm{MSE}} \sim \|y - X\theta\|^2 \rightarrow \min_\theta$$

$$\begin{cases} \dfrac{\partial}{\partial\theta}\mathcal{L}_{\mathrm{MSE}} = 0 \\ \dfrac{\partial^2}{\partial\theta\partial\theta^{\mathrm{T}}}\mathcal{L}_{\mathrm{MSE}} > 0 \text{ (pos. def.)} \end{cases}$$

Analytical solution

- Working on the 1st derivative*:

$$\frac{\partial}{\partial\theta}\mathcal{L}_{\mathrm{MSE}} \sim \frac{\partial}{\partial\theta}(y - X\theta)^{\mathrm{T}}(y - X\theta) = -2X^{\mathrm{T}}(y - X\theta) = 0$$

$$X^{\mathrm{T}}y - X^{\mathrm{T}}X\theta = 0$$

- Solution:

$$\theta = \left(X^{\mathrm{T}}X\right)^{-1}X^{\mathrm{T}}y$$

Note that this matrix needs to be invertible

*some useful info about matrix calculus: https://en.wikipedia.org/wiki/Matrix_calculus#Identities

Analytical solution

For some non-zero vector v:

$$v^{\mathrm{T}}X^{\mathrm{T}}Xv = (Xv)^{\mathrm{T}}(Xv) = \|Xv\|^2 \geq 0$$

$$\neq 0$$

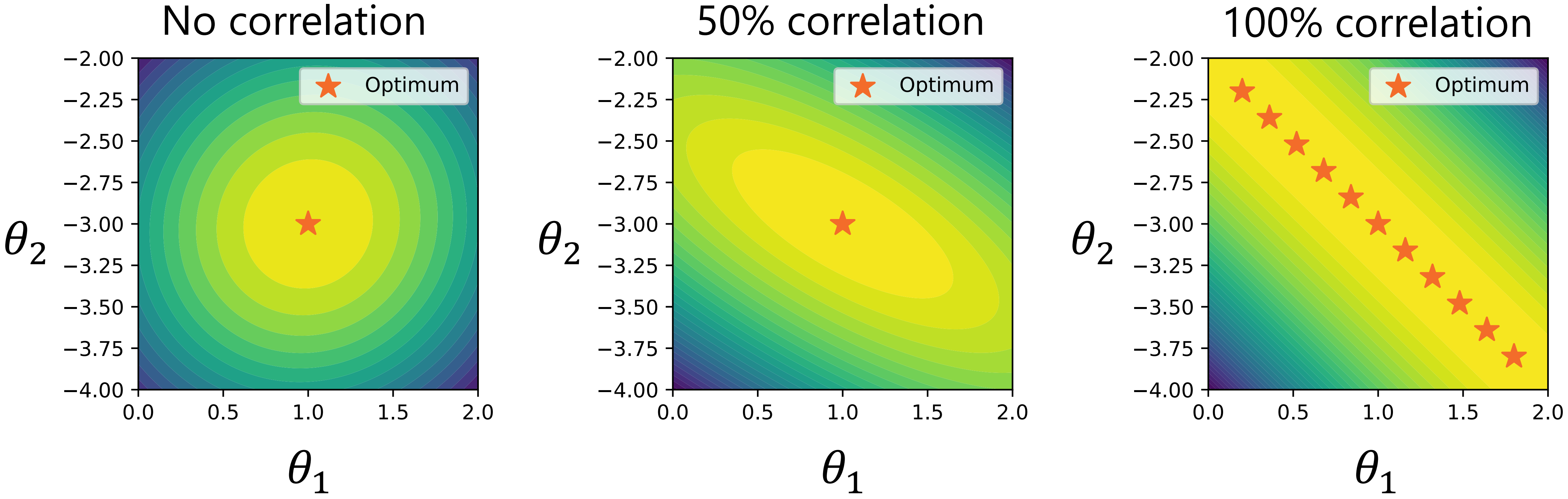
when columns of X are linearly independent

- 2nd derivative:

$$\frac{\partial^2}{\partial\theta\partial\theta^{\mathrm{T}}}\mathcal{L}_{\mathrm{MSE}} \sim 2X^{\mathrm{T}}X$$

- This needs to be **positive definite**
- True when all the features (columns of the design matrix) are **linearly independent**
- This also makes $X^T X$ invertible

Feature correlations matter!



MSE level maps

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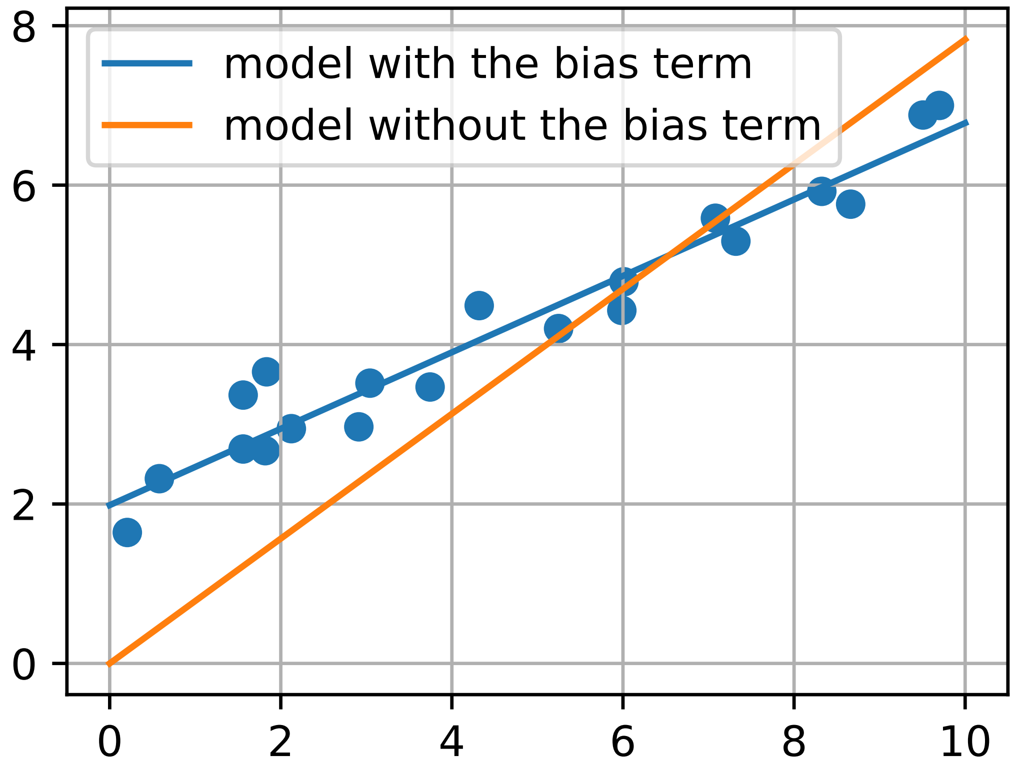
Bias term

a.k.a. intercept term

$$\hat{f}_\theta(x) = \theta^{\mathrm{T}} x + \theta_0$$

$$\theta \in \mathbb{R}^d$$
$$\theta_0 \in \mathbb{R}$$
$$x \in \mathcal{X} \subset \mathbb{R}^d$$

- No need to redo the math – just add a **constant feature** to the design matrix:

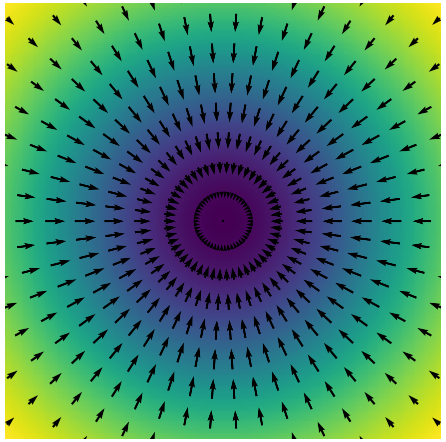


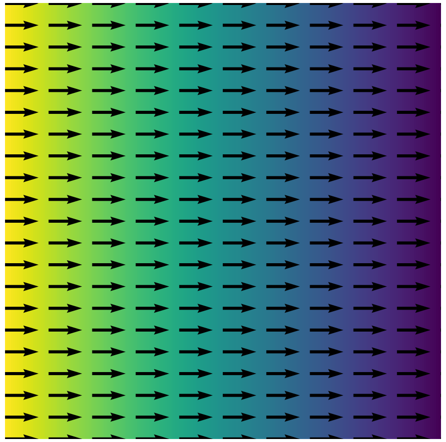
$$X = \begin{bmatrix} x_1^1 & x_1^2 & \cdots & x_1^d \\ x_2^1 & x_2^2 & \cdots & x_2^d \\ \vdots & \vdots & \ddots & \vdots \\ x_N^1 & x_N^2 & \cdots & x_N^d \end{bmatrix} \longrightarrow X = \begin{bmatrix} 1 & x_1^1 & x_1^2 & \cdots & x_1^d \\ 1 & x_2^1 & x_2^2 & \cdots & x_2^d \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_N^1 & x_N^2 & \cdots & x_N^d \end{bmatrix}$$

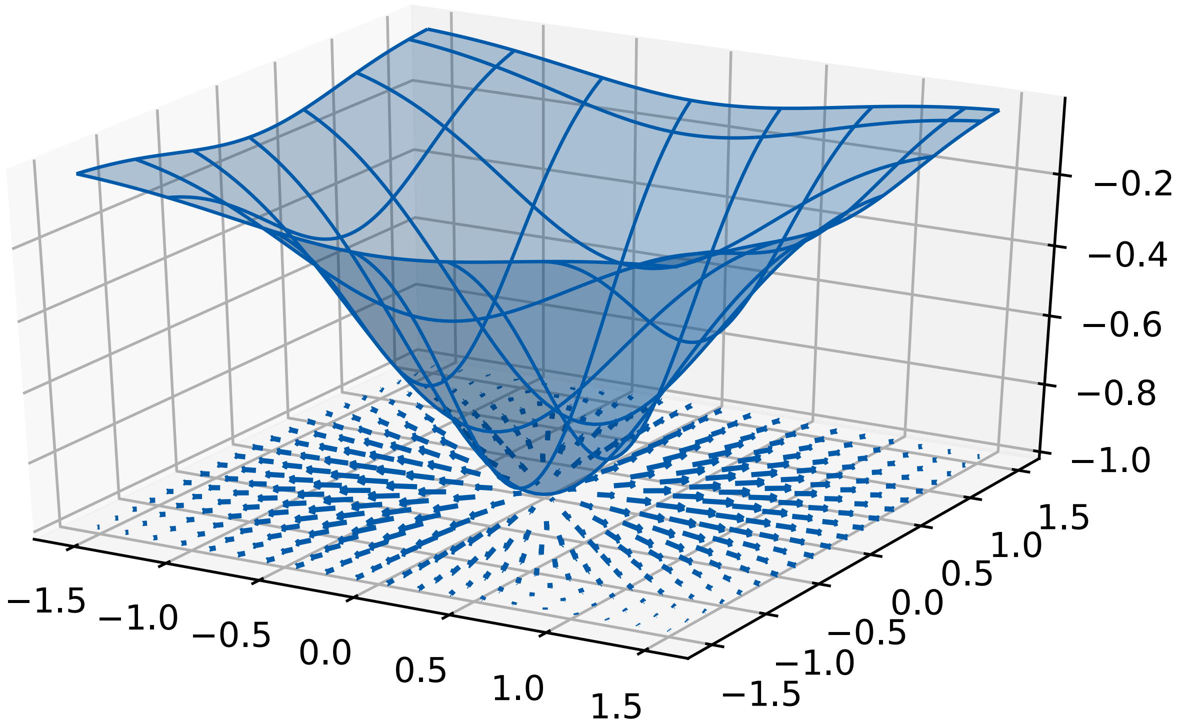
Numerical & Stochasic Optimization

Gradient

- Gradient: $\nabla_x f(x) \equiv \left(\frac{\partial f(x)}{\partial x_1}, \dots, \frac{\partial f(x)}{\partial x_d}\right)$
- Points towards **steepest function increase**







Gradient Descent Optimization

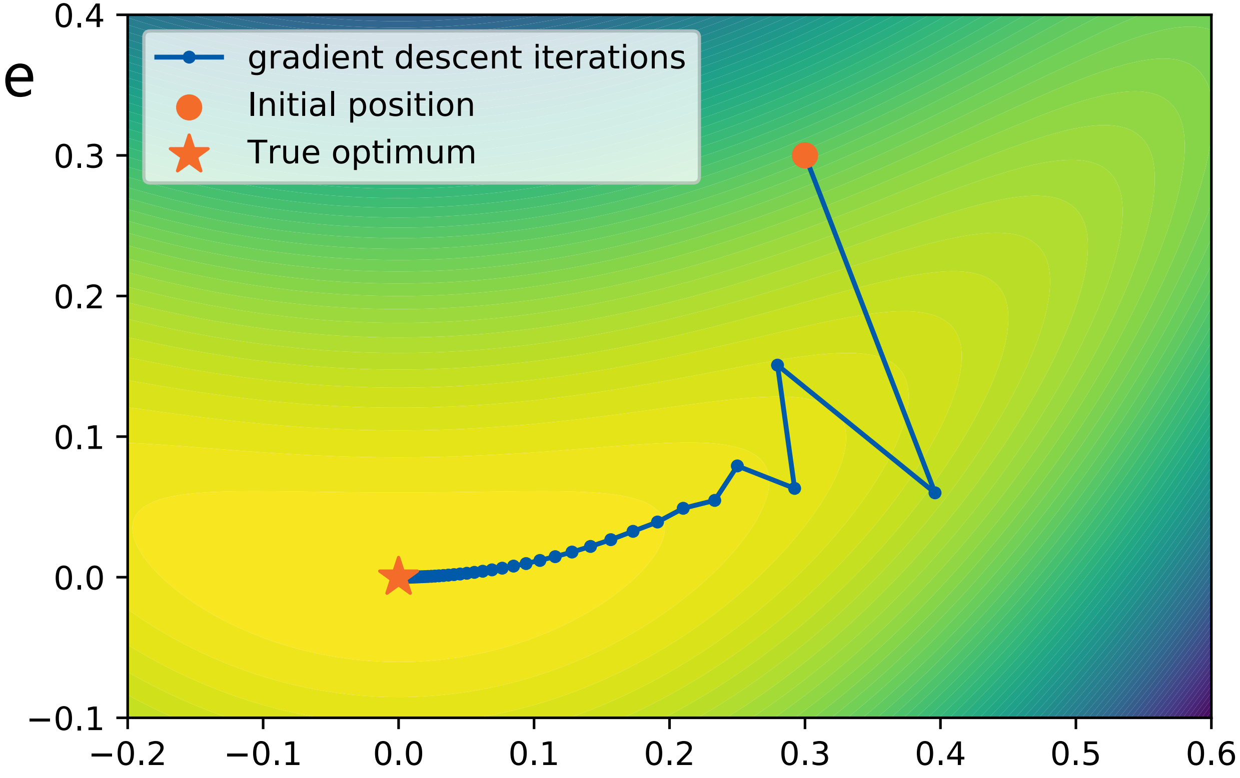
- Can optimize functions starting at some initial point $x^{(0)}$ and moving opposite to the gradient:

$$x^{(k)} \longleftarrow x^{(k-1)} - \alpha \nabla_x f\left(x^{(k-1)}\right)$$

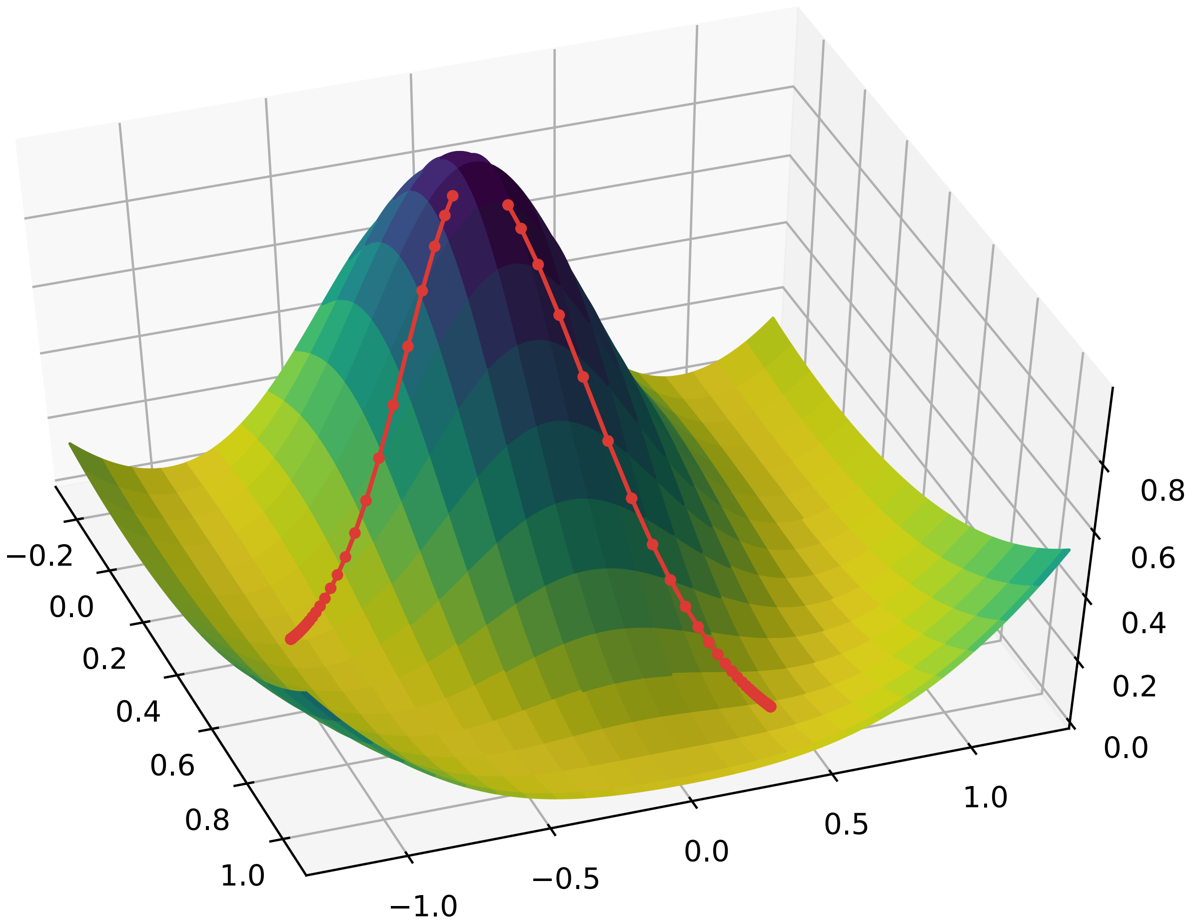
with $\alpha \in \mathbb{R},\ \alpha > 0$ – learning rate.

- For smooth **convex** functions with a single minimum x^*:

$$f\left(x^{(k)}\right) - f(x^*) = \mathcal{O}\left(\frac{1}{k}\right)$$



Gradient descent for non-convex functions



- May get to a minimum which is not global
- Result depends on the starting point

Stochastic Gradient Descent (SGD)

- In machine learning we optimize loss functions which are typically averages over objects:

$$L = \frac{1}{N} \sum_{i=1 \dots N} \mathcal{L}\left(y_i, \widehat{f_\theta}(x_i)\right)$$

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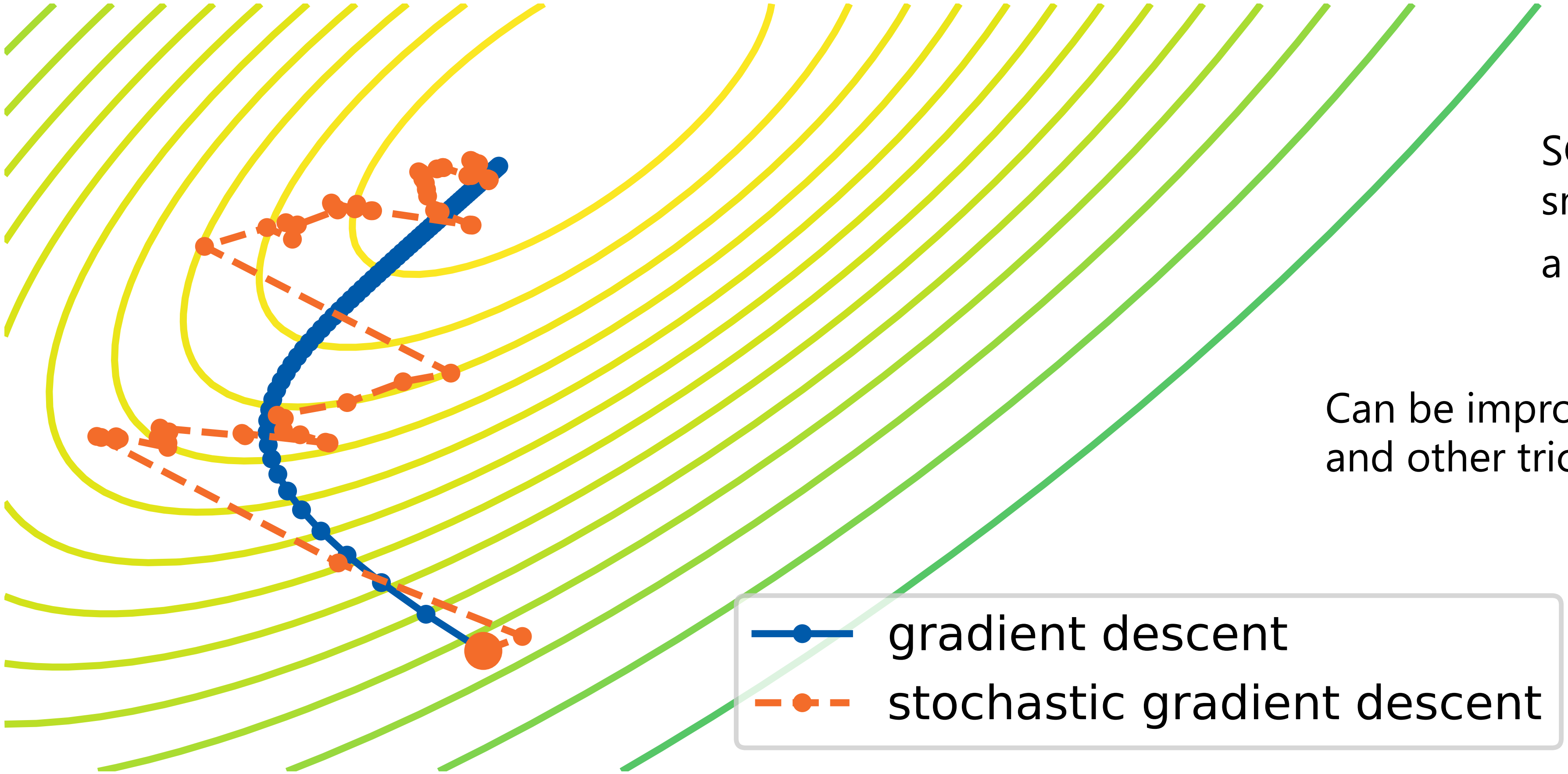
- For large N, gradient descent is computationally inefficient and may be unfeasible in terms of memory consumption
- Aternative:
  - At each step k pick $l_k \in \{1, \ldots, N\}$ at random
  - Optimize: $\theta^{(k)} \leftarrow \theta^{(k-1)} - \alpha \nabla_\theta \mathcal{L}\left(y_{l_k}, \widehat{f_\theta}(x_{l_k})\right)\Big|_{\theta = \theta^{(k-1)}}$

Stochastic Gradient Descent (SGD)



SGD convergence rate for smooth **convex** functions with a single minimum: $\mathcal{O}\left(\frac{1}{\sqrt{k}}\right)$

Can be improved by batching and other tricks

Feature Expansion

Feature expansion

- One can perform **feature transformations** with any function $\Phi\colon \mathbb{R}^d \to \mathbb{R}^{d'}$

$$X = \begin{bmatrix} x_1^1 & x_1^2 & \cdots & x_1^d \\ x_2^1 & x_2^2 & \cdots & x_2^d \\ \vdots & \vdots & \ddots & \vdots \\ x_N^1 & x_N^2 & \cdots & x_N^d \end{bmatrix} \longrightarrow \Phi(X) = \begin{bmatrix} \Phi^1(x_1^1, \dots, x_1^d) & \cdots & \Phi^{d'}(x_1^1, \dots, x_1^d) \\ \Phi^1(x_2^1, \dots, x_2^d) & \cdots & \Phi^{d'}(x_2^1, \dots, x_2^d) \\ \vdots & \ddots & \vdots \\ \Phi^1(x_N^1, \dots, x_N^d) & \cdots & \Phi^{d'}(x_N^1, \dots, x_N^d) \end{bmatrix}$$

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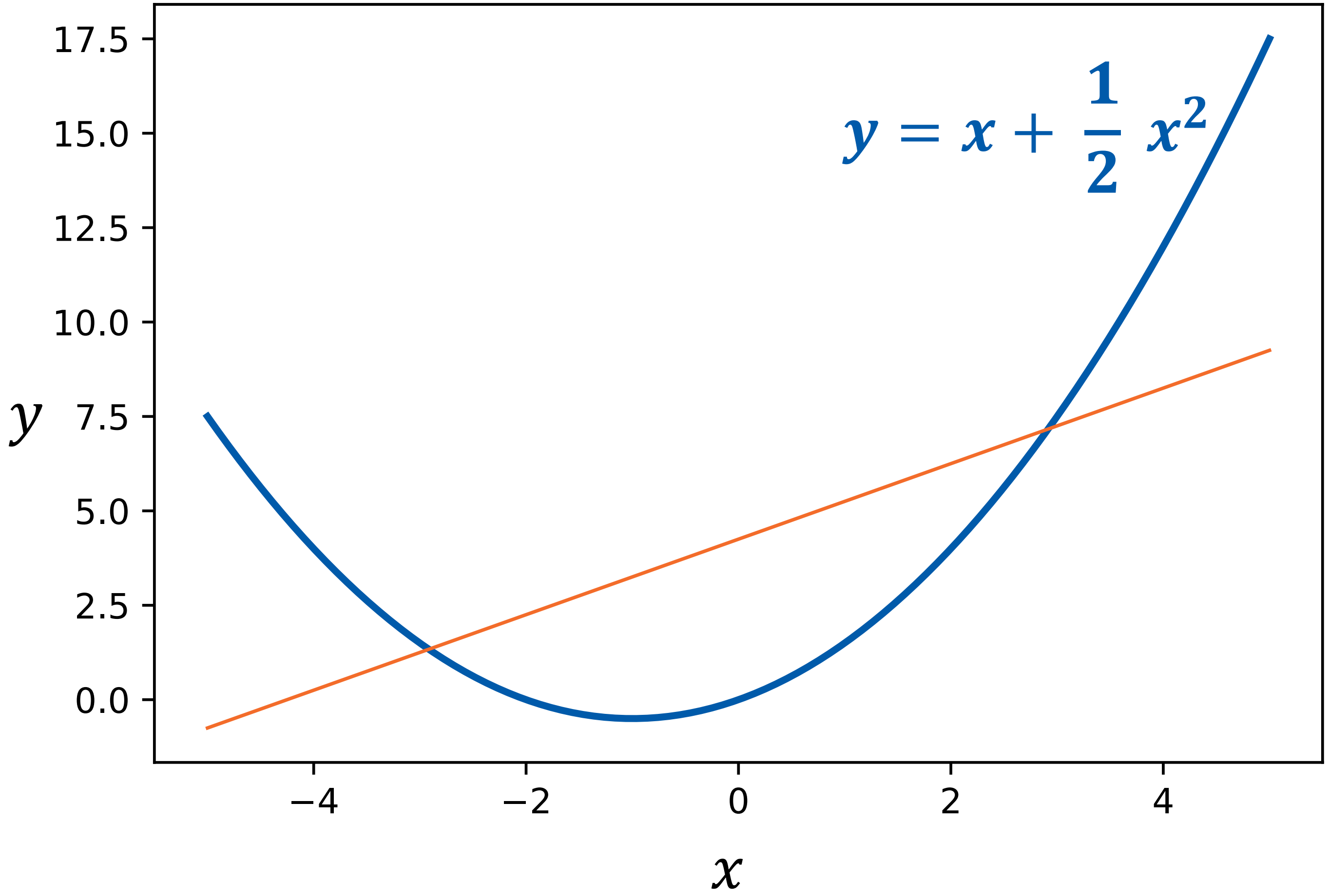
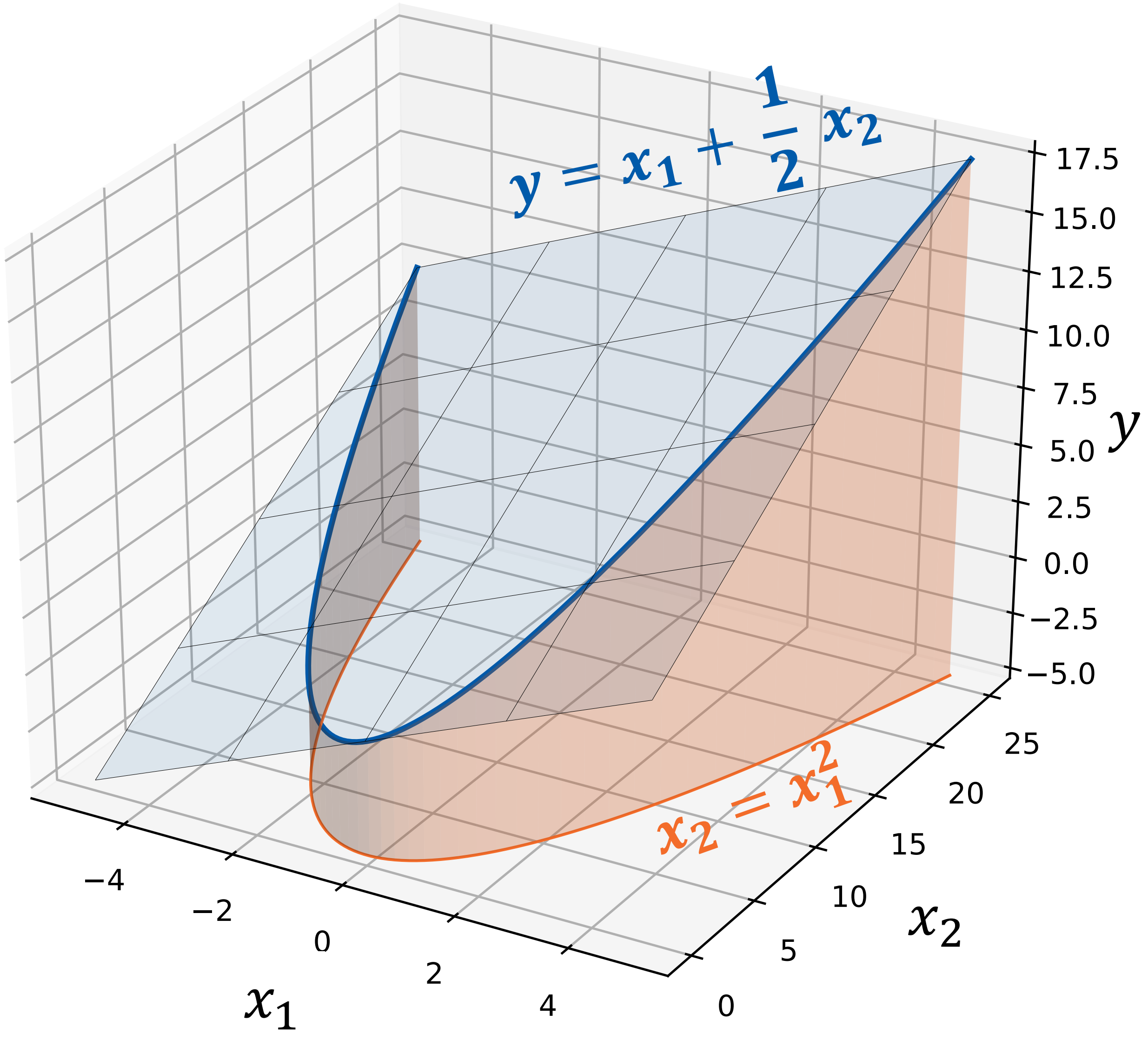
- Finding the best function Φ is called **feature engineering**
  - It is an important part of machine learning and requires deep understanding of the underlying problem and the data

Example: polynomial features



- Can't be solved with the only linear feature (x)

Example: polynomial features



- Introducing another feature does the job:

$$(x_1, x_2) \equiv (x, x^2)$$

- Now our estimate is:

$$\hat{f}(x) = \theta_1 x + \theta_2 x^2$$

Polynomial features of degree p (general case)

For the original features:

$$\left(x_i^1, x_i^2, \ldots, x_i^d \right)$$

introduce all unique multiplicative combinations of the form:

$$\left(x_i^{k_1}\right)^{p_1} \cdot \left(x_i^{k_2}\right)^{p_2} \cdot \ldots \cdot \left(x_i^{k_m}\right)^{p_m}$$

with $p_1 + p_2 + \ \ldots + p_m \leq p$

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Example: degree 3 polynomial features

For the original features (a, b, c):

$$(1, a, b, c, a^2, ab, ac, b^2, bc, c^2, a^3, a^2b, a^2c, ab^2, abc, ac^2, b^3, b^2c, bc^2, c^3)$$

Summary

- Understanding linear models gives **useful insights** into more complicated machine learning algorithms and optimization
- Linear Regression with MSE loss allows for **analytical solution**
- The stability of the solution depends on the **feature correlations**
- Linear models can be optimized with gradient descent and stochastic gradient descent
  - In some cases this can **regularize** the solution
- **Feature transformations** allow for very powerful use of the linear models
- Food for thought: how does polynomial feature expansion affect the complexity of the model?

Quiz / Questions

How many features do we totally end up with after applying degree-2 polynomial expansion (including the bias term) to a pair of features?

Image by: pixabay.com/users/alexas_fotos-686414/

A. four

B. five

C. six

D. seven

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Thank you!

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