Linear Regression

Analytical solution, gradient descent, feature expansion

Machine Learning and Data Mining, 2022

Artem Maevskiy

National Research University Higher School of Economics

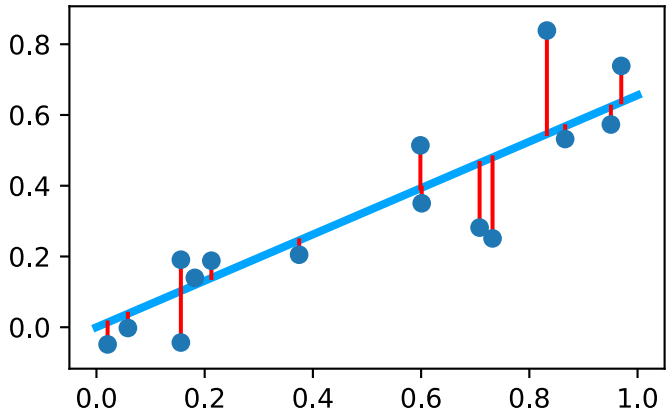
September 10, 2022

Why study linear models?

Linear models in a nutshell

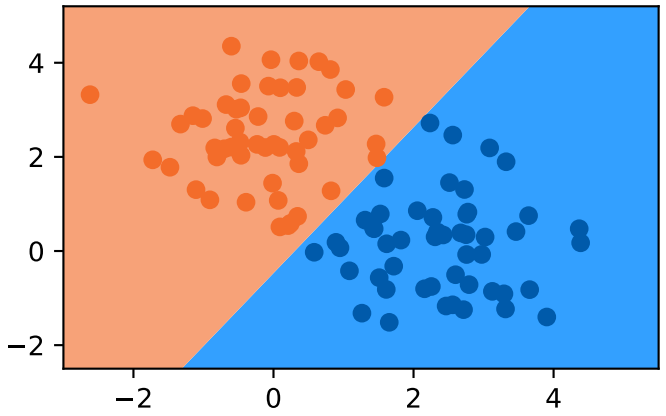
Regression:

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



Classification:

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

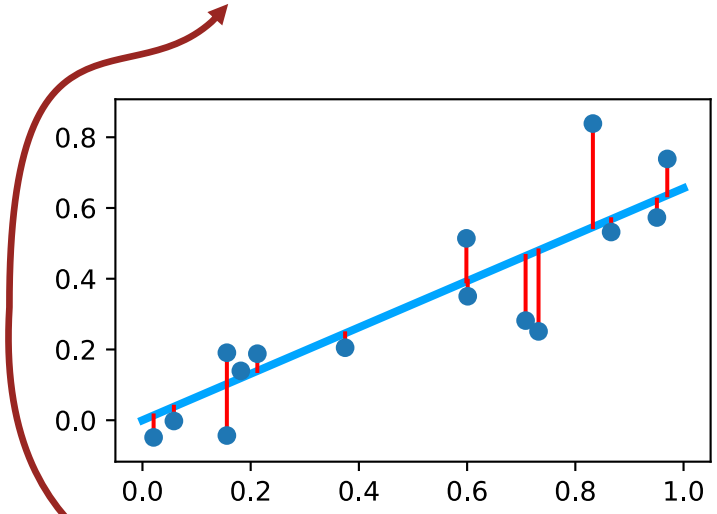


Outputs linear in inputs

Linear models in a nutshell

Regression:

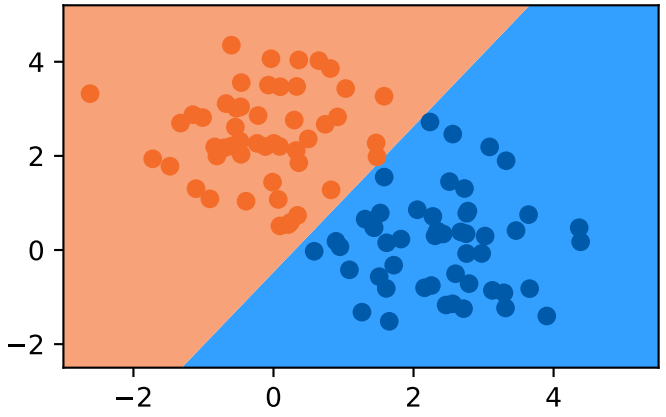
$$\hat{f}(x) = \theta^{\mathrm{T}} x$$



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

Classification:

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

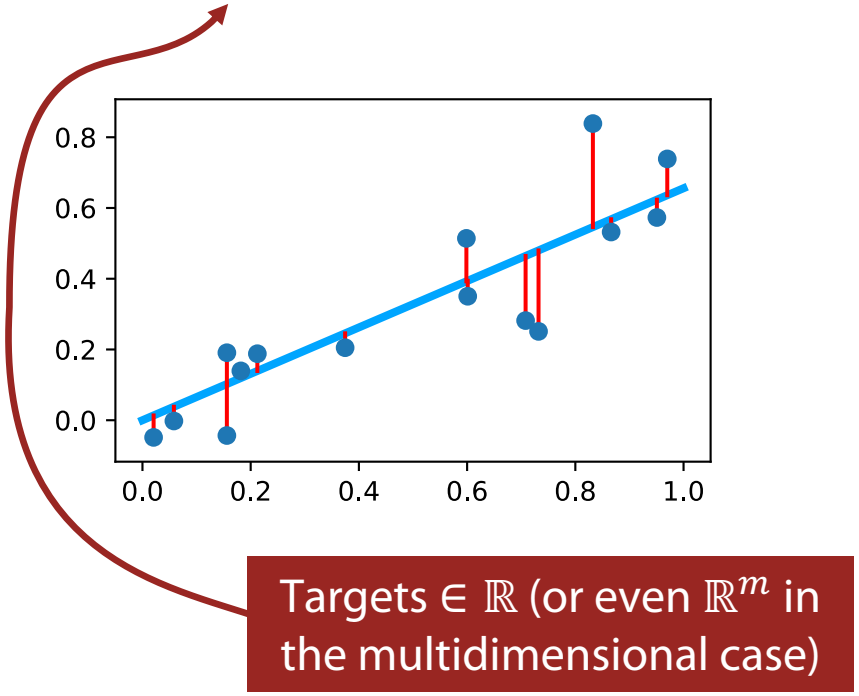


Outputs linear in inputs

Linear models in a nutshell

Regression:

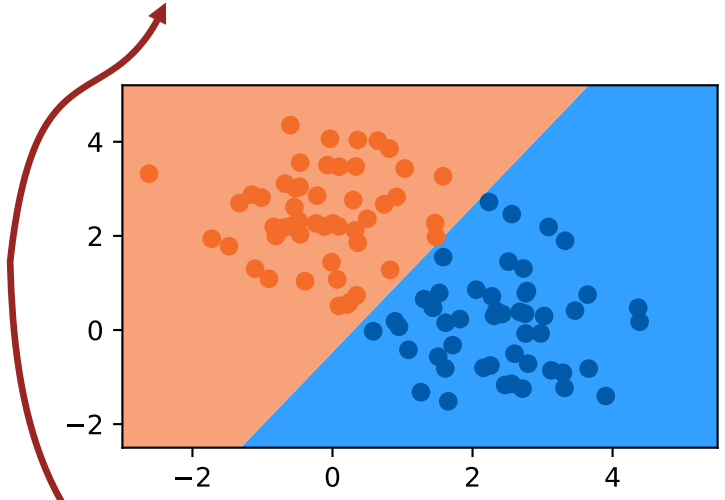
$$\hat{f}(x) = \theta^{\mathrm{T}} x$$



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

Classification:

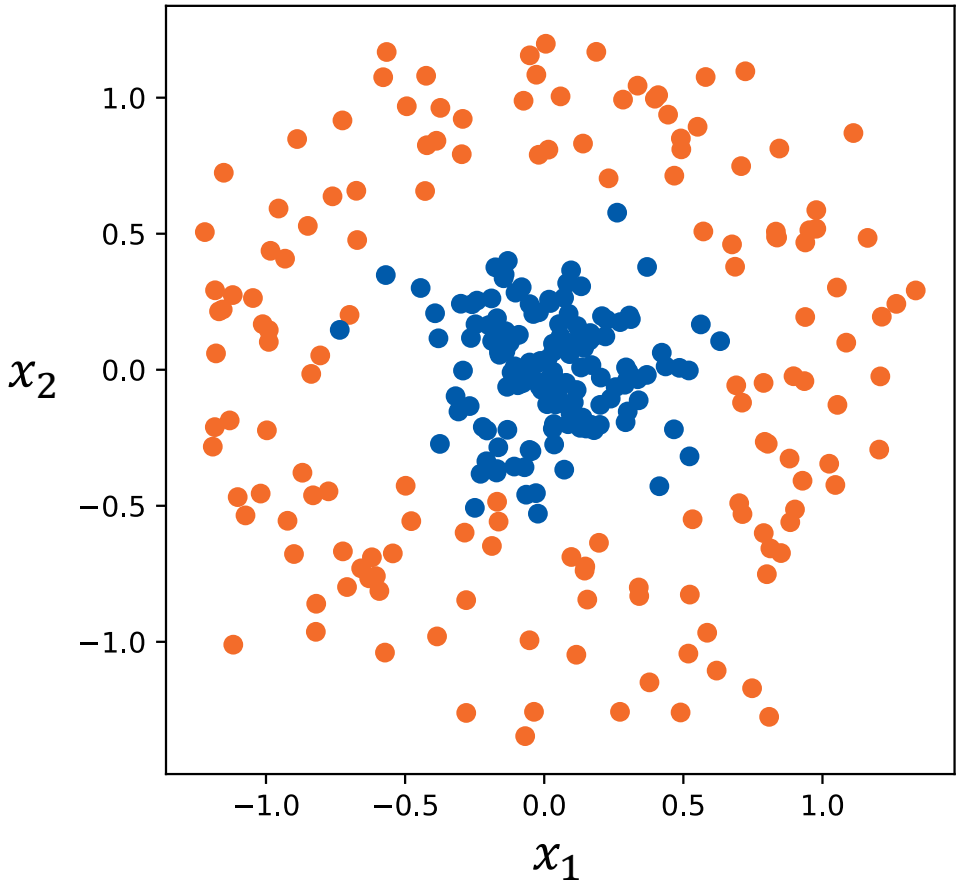
$$\hat{f}(x) = \mathbb{I}[\theta^{\mathrm{T}} x > 0]$$

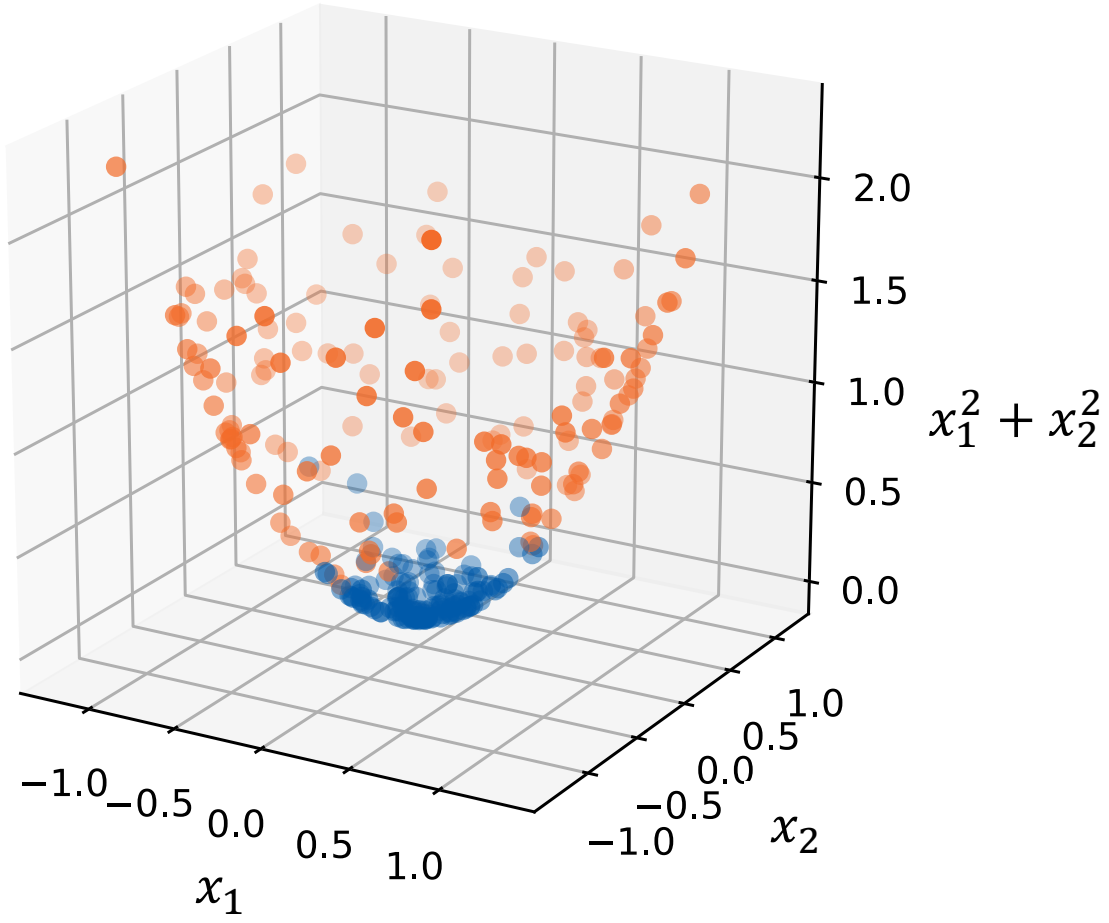


Targets $\in$ some finite set

Outputs linear in inputs

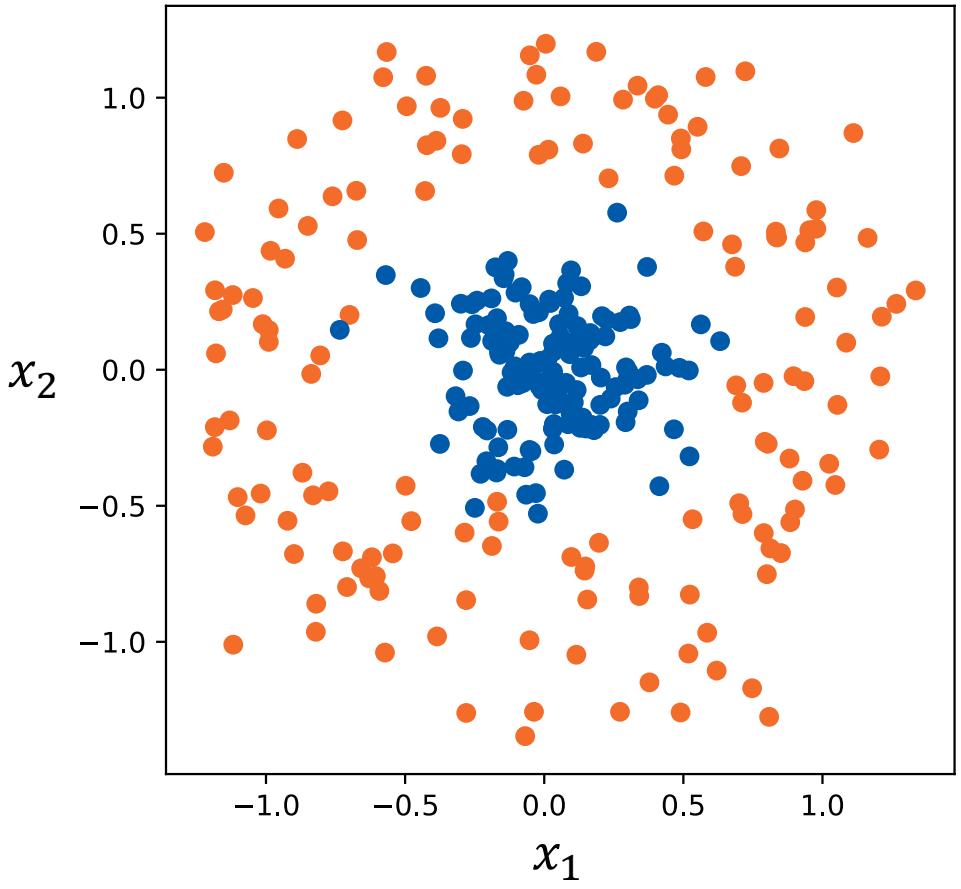
The hidden power

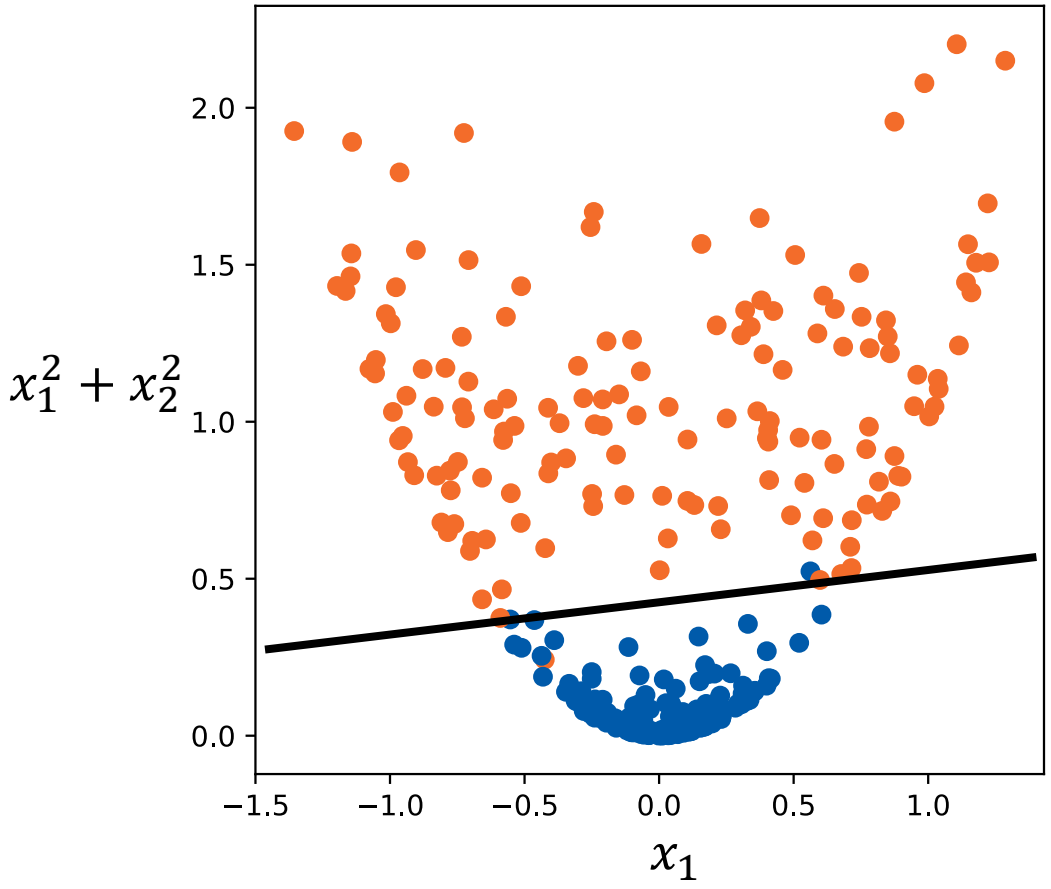




- Linearly **inseparable** ⟶ **separable** by **transforming the features**

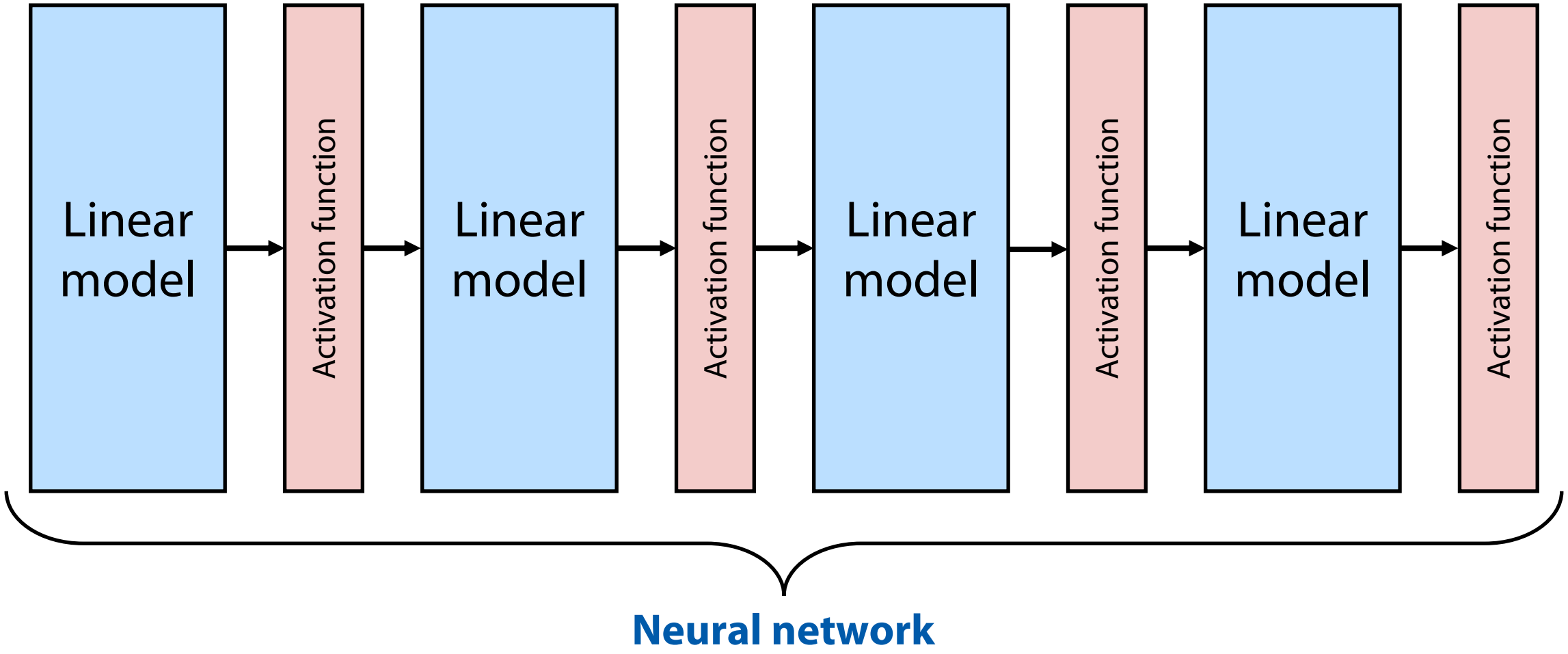
The hidden power





- Linearly **inseparable** ⟶ **separable** by **transforming the features**

Building block for deep models



- Better intuition for deep neural networks training

Interpretability

- One can take a look at the weights corresponding to each of the features separately, e.g.:

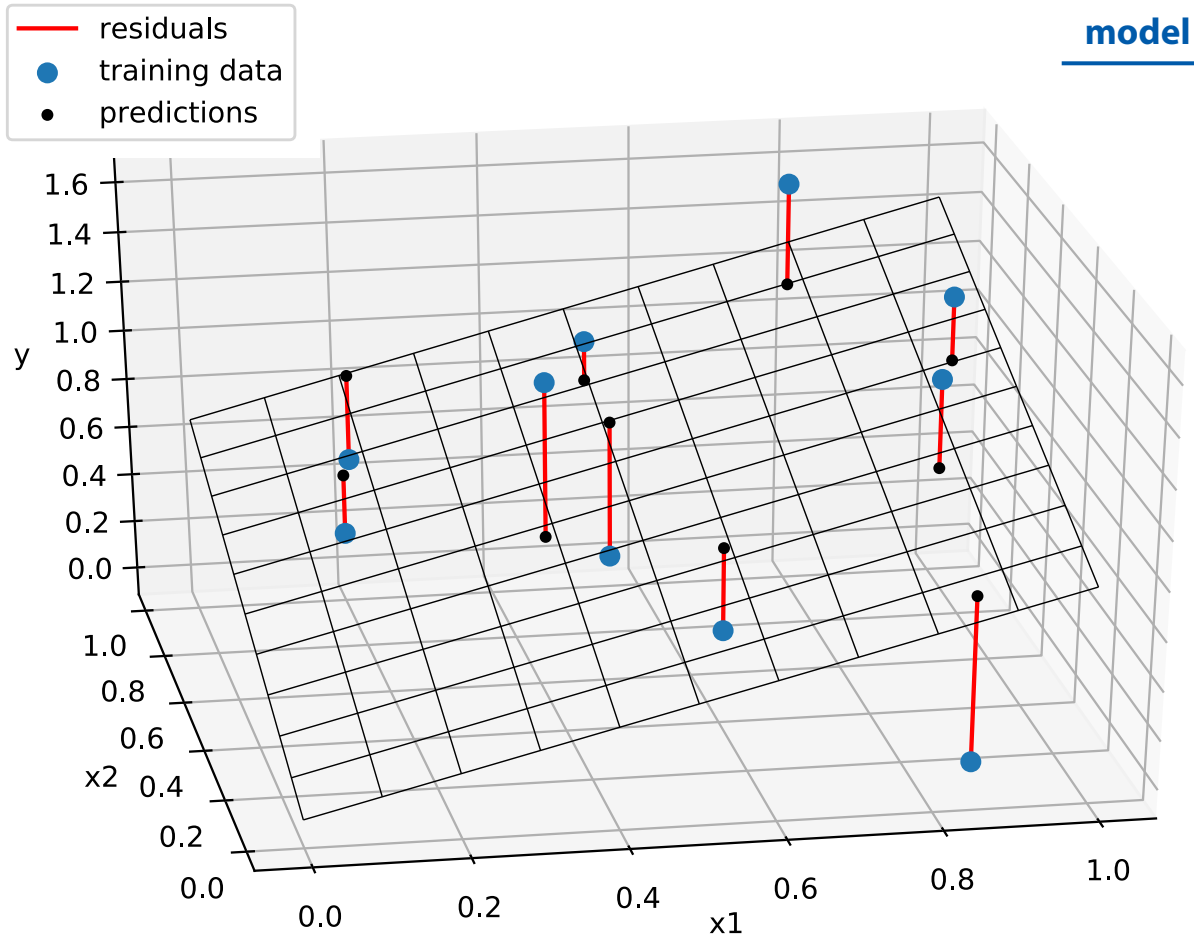
Note: this example is not based on real data, but rather taken from the lecturer's imagination

$$\textbf{PredictedIncome} = 1000 + 10 \times \textbf{Age} + 1000 \times \textbf{HasHigherEducation} - 0.1 \times \textbf{DistanceFromCapital}$$

- Higher weight means more impact on the prediction
  - Note: features need to be of same scale if you want to compare their weights

Linear Regression

Linear Regression model



model prediction

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

parameters vector

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

features vector

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

$$\frac{1}{N} \sum_{i=1 \ldots N} \left(y_i - \hat{f}_\theta(x_i) \right)^2 \longrightarrow \min_\theta$$

Mean Squared Error (MSE loss)

Common loss functions

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

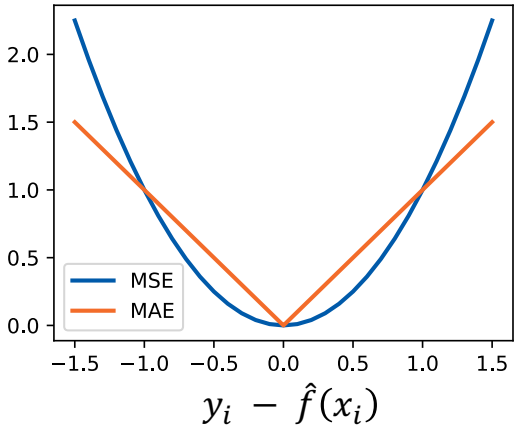
Common loss functions

Mean squared error (MSE):

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

Mean absolute error (MAE):

$$\frac{1}{N}\sum_{i=1\dots N}\left|y_i - \hat{f}_\theta(x_i)\right|$$



Common loss functions

Mean squared error (MSE):

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

Mean absolute error (MAE):

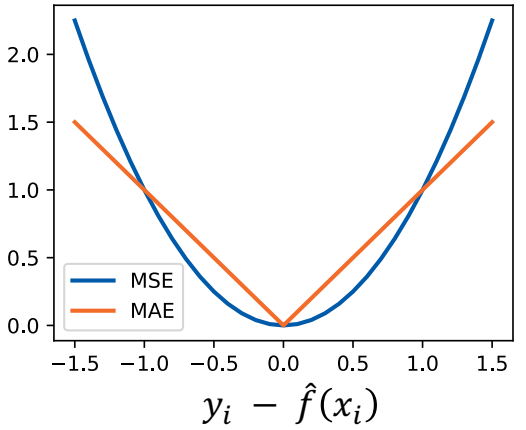
$$\frac{1}{N}\sum_{i=1\dots N}\left|y_i - \hat{f}_\theta(x_i)\right|$$

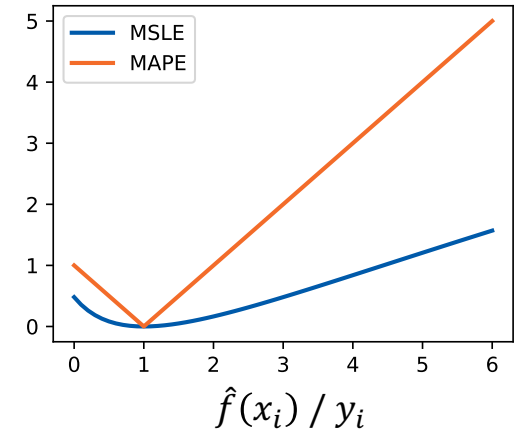
Mean absolute percentage error (MAPE):

$$\frac{1}{N}\sum_{i=1\dots N}\left|\frac{y_i - \hat{f}_\theta(x_i)}{y_i}\right|$$

Mean squared logarithmic error (MSLE):

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





Common loss functions

Mean squared error (MSE):

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

Mean absolute error (MAE):

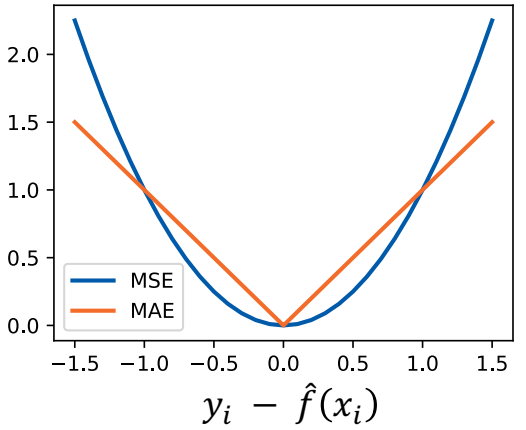
$$\frac{1}{N}\sum_{i=1\dots N}\left|y_i - \hat{f}_\theta(x_i)\right|$$

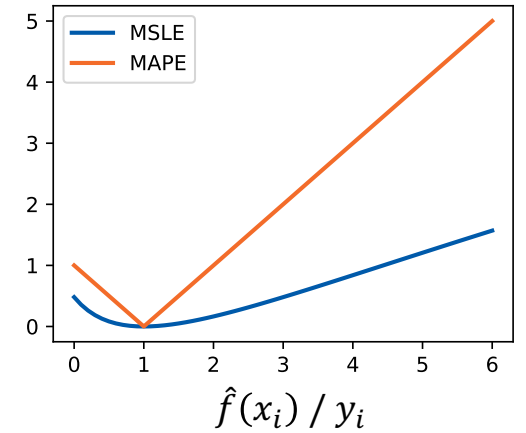
Mean absolute percentage error (MAPE):

$$\frac{1}{N}\sum_{i=1\dots N}\left|\frac{y_i - \hat{f}_\theta(x_i)}{y_i}\right|$$

Mean squared logarithmic error (MSLE):

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

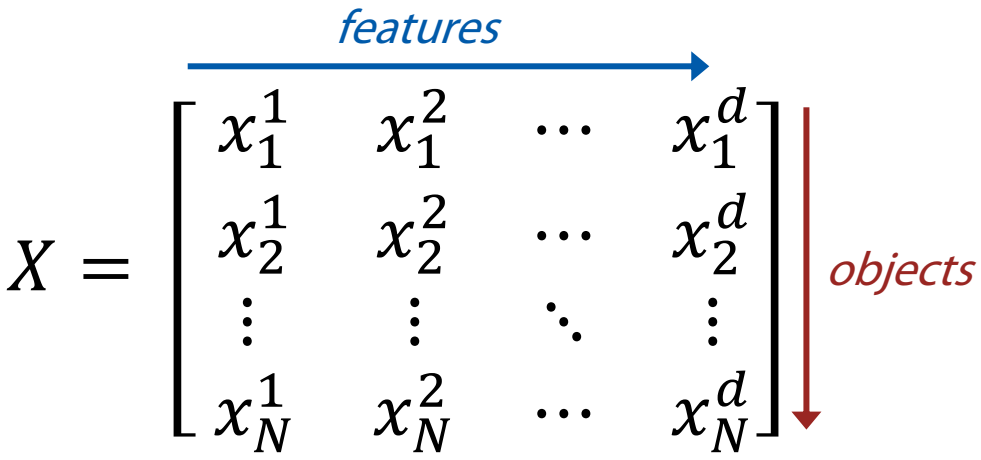




- Different **loss functions** also are related to different **assumptions about the data**

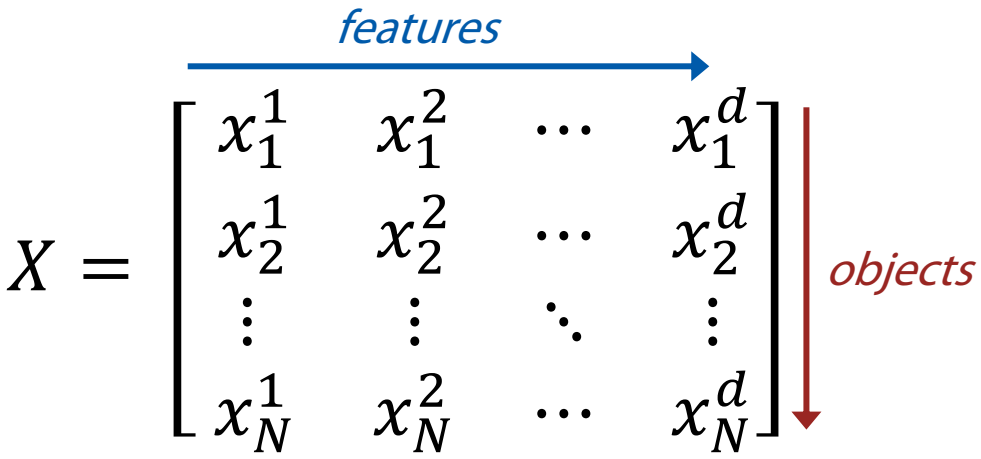
Analytical solution

- Recall the design matrix:



Analytical solution

- Recall the design matrix:



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

- We can use it to rewrite the MSE loss:

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

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

Analytical solution

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

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

Analytical solution

- Working on the 1st derivative*:

$$\frac{\partial}{\partial \theta} \mathcal{L}_{\text{MSE}} \sim \frac{\partial}{\partial \theta} (y - X\theta)^{\text{T}} (y - X\theta)$$

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

Analytical solution

- Working on the 1st derivative*:

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

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

Analytical solution

- Working on the 1st derivative*:

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

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

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

Analytical solution

- Working on the 1st derivative*:

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

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

- Solution:

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

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

Analytical solution

- Working on the 1st derivative*:

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

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

- Solution:

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

Note that this matrix needs to be invertible

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

Analytical solution

- 2nd derivative:

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

Analytical solution

- 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**

Analytical solution

For some non-zero vector v:

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

- 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**

Analytical solution

- 2nd derivative:

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

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

- This needs to be **positive definite**

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**

Analytical solution

For some non-zero vector v:

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

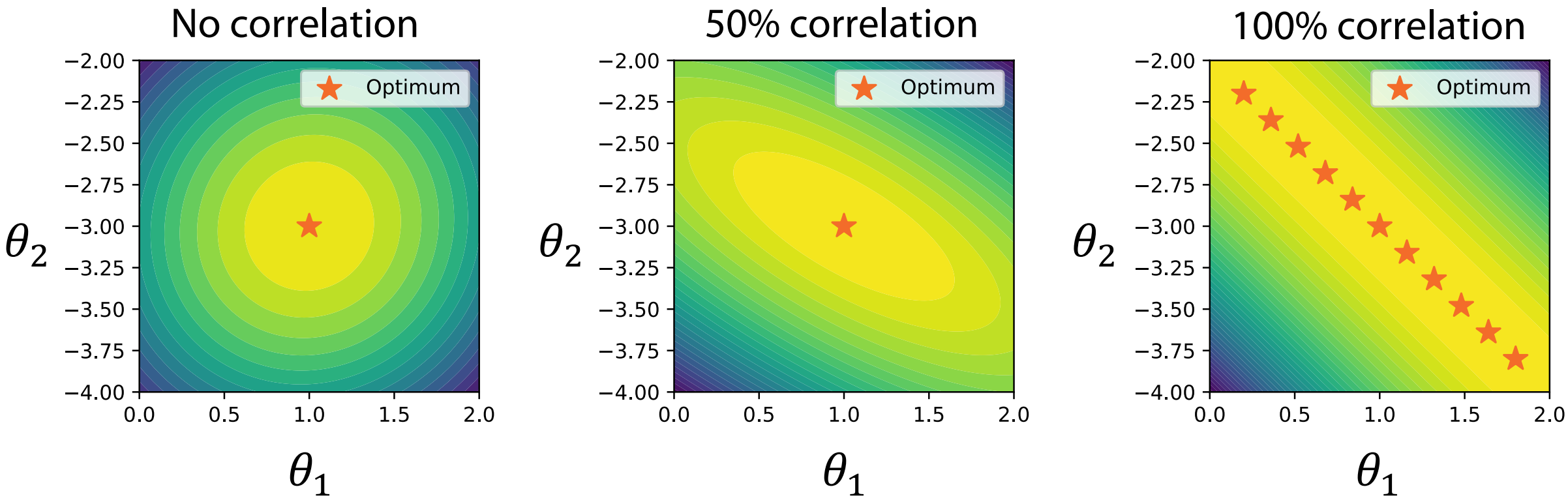
when columns of X are linearly independent

- 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!



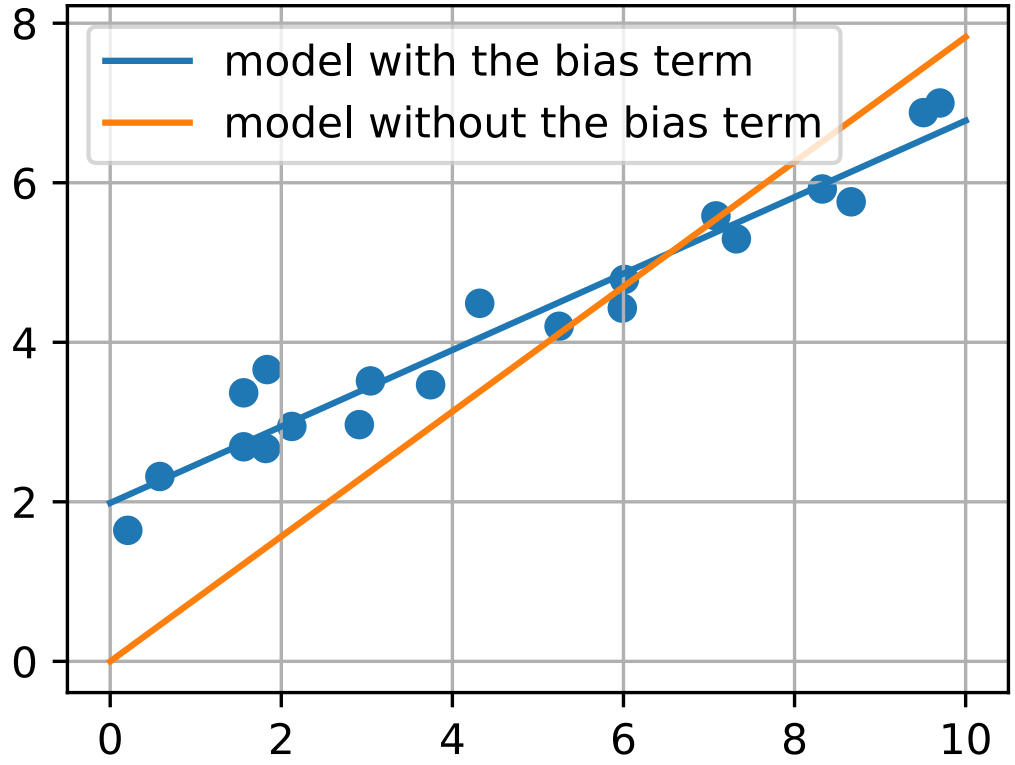
MSE level maps

Bias term

a.k.a. intercept term

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

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



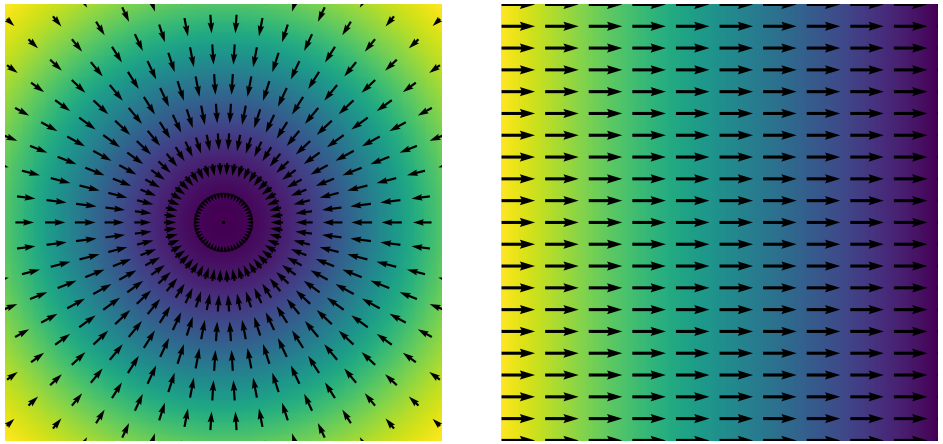
- No need to redo the math – just add a **constant feature** to the design matrix:

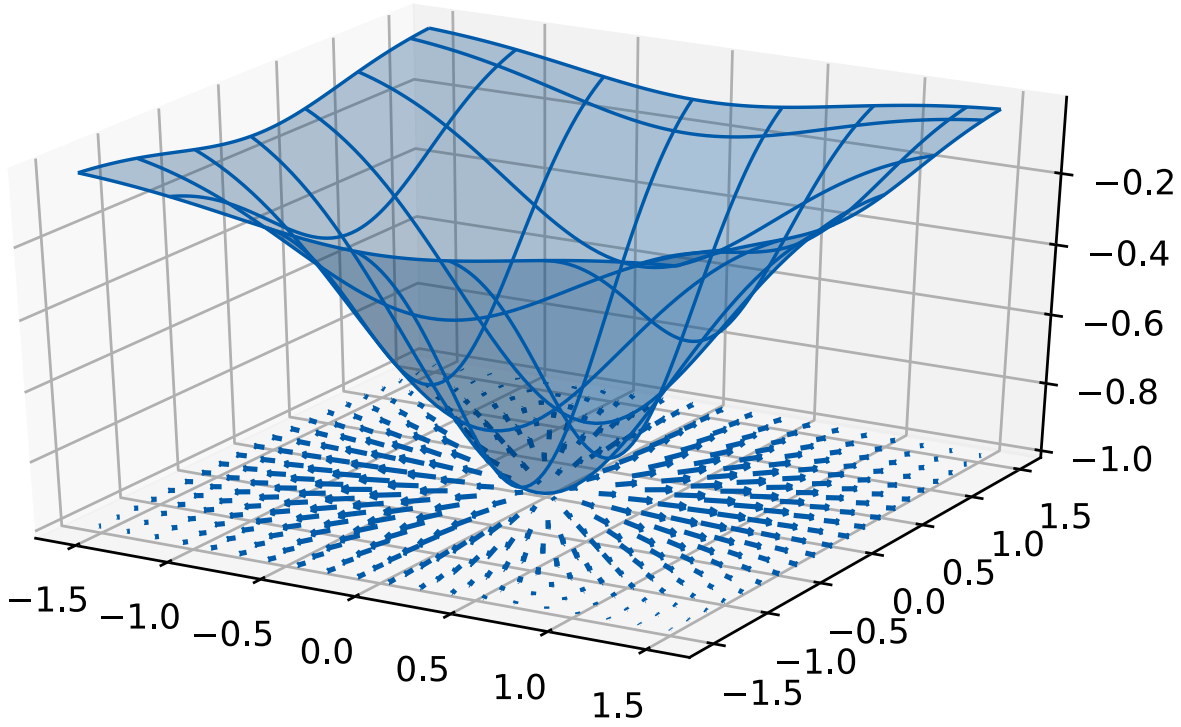
$$X = \begin{bmatrix} x_1^1 & x_1^2 & \cdots & x_1^d \\ x_2^1 & x_2^2 & \cdots & x_2^d \\ \vdots & \vdots & \ddots & \vdots \\ x_N^1 & x_N^2 & \cdots & x_N^d \end{bmatrix} \longrightarrow X = \begin{bmatrix} 1 & x_1^1 & x_1^2 & \cdots & x_1^d \\ 1 & x_2^1 & x_2^2 & \cdots & x_2^d \\ \vdots & \vdots &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

Numerical & Stochastic Optimization

Gradient

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





Gradient Descent Optimization

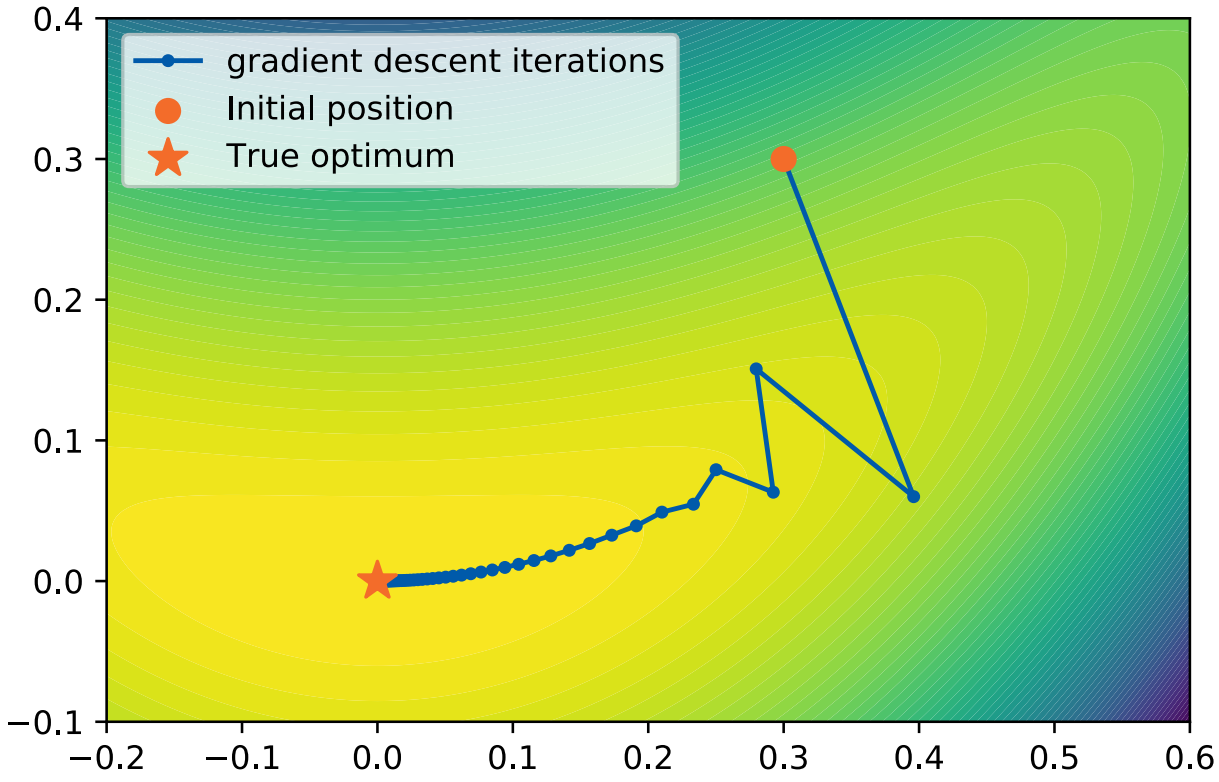
- Can optimize functions starting at some initial point $x^{(0)}$ and moving opposite to the gradient:

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

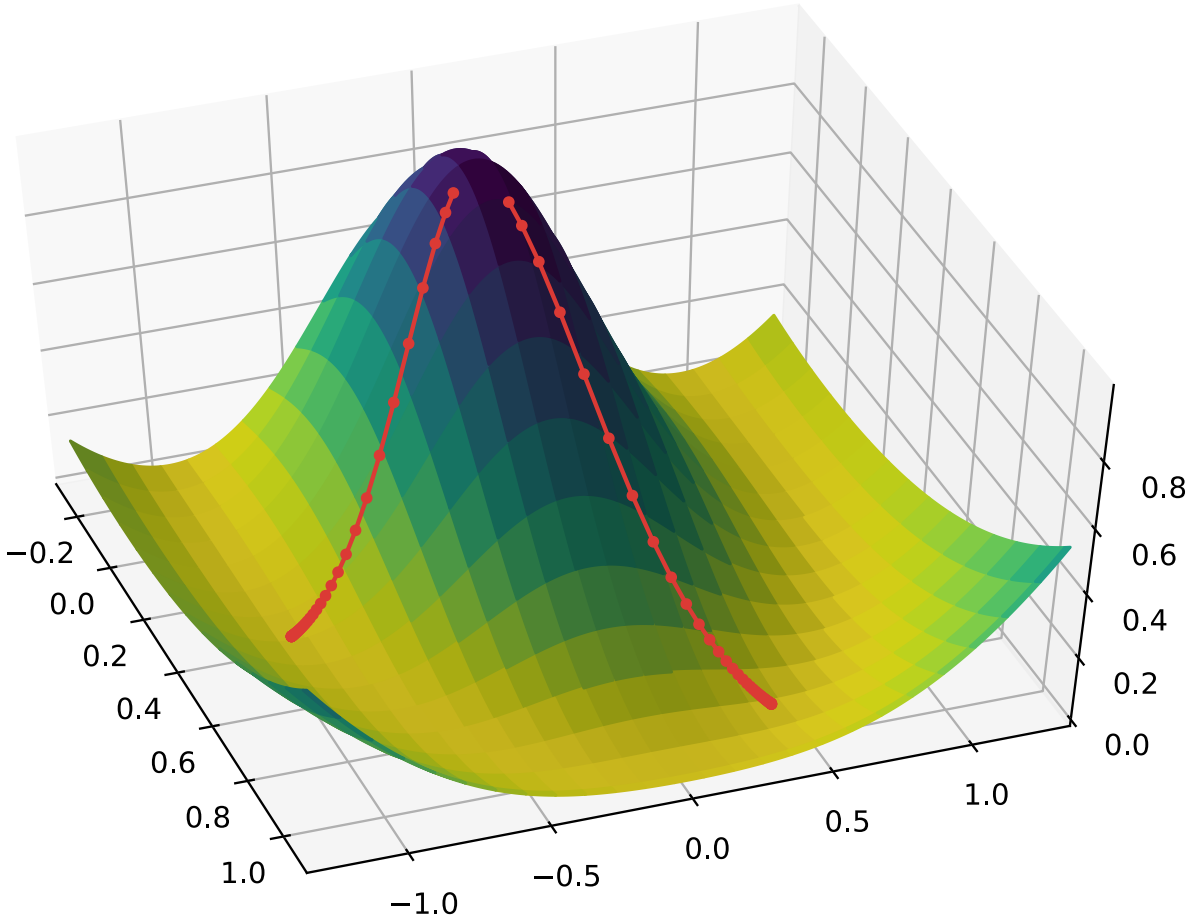
with $\alpha \in \mathbb{R},\ \alpha > 0$ – learning rate.

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

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

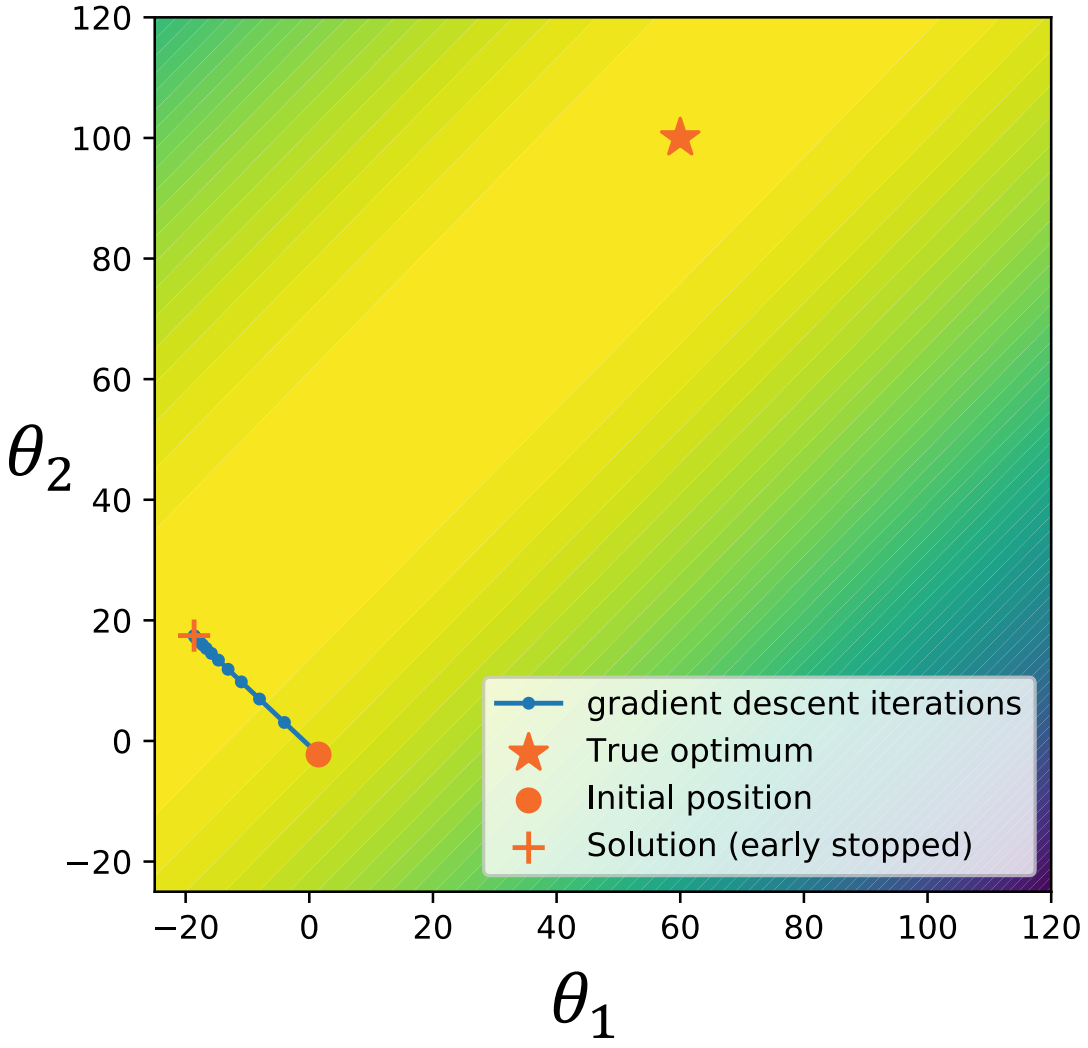


Gradient descent for non-convex functions



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

Gradient descent as means for regularisation



- Large parameter values typically mean overfitting
- You may avoid this problem by initializing parameters with **small values** and **early stopping** the gradient descent

Stochastic Gradient Descent (SGD)

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

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

Stochastic Gradient Descent (SGD)

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

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

- For large N, gradient descent is computationally inefficient and may be unfeasible in terms of memory consumption

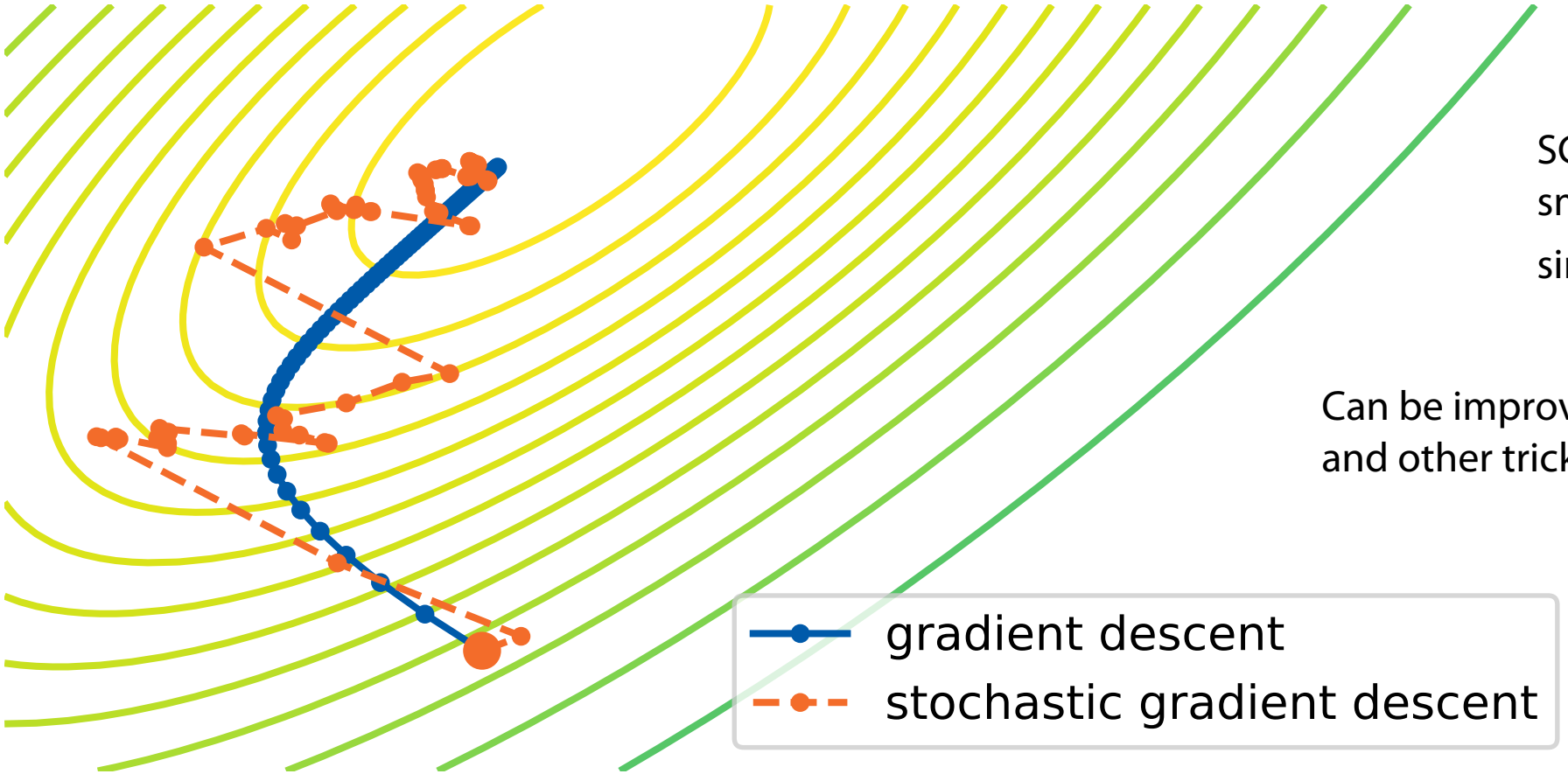
Stochastic Gradient Descent (SGD)

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

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

- 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 Φ: $\mathbb{R}^d \to \mathbb{R}^{d'}$

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

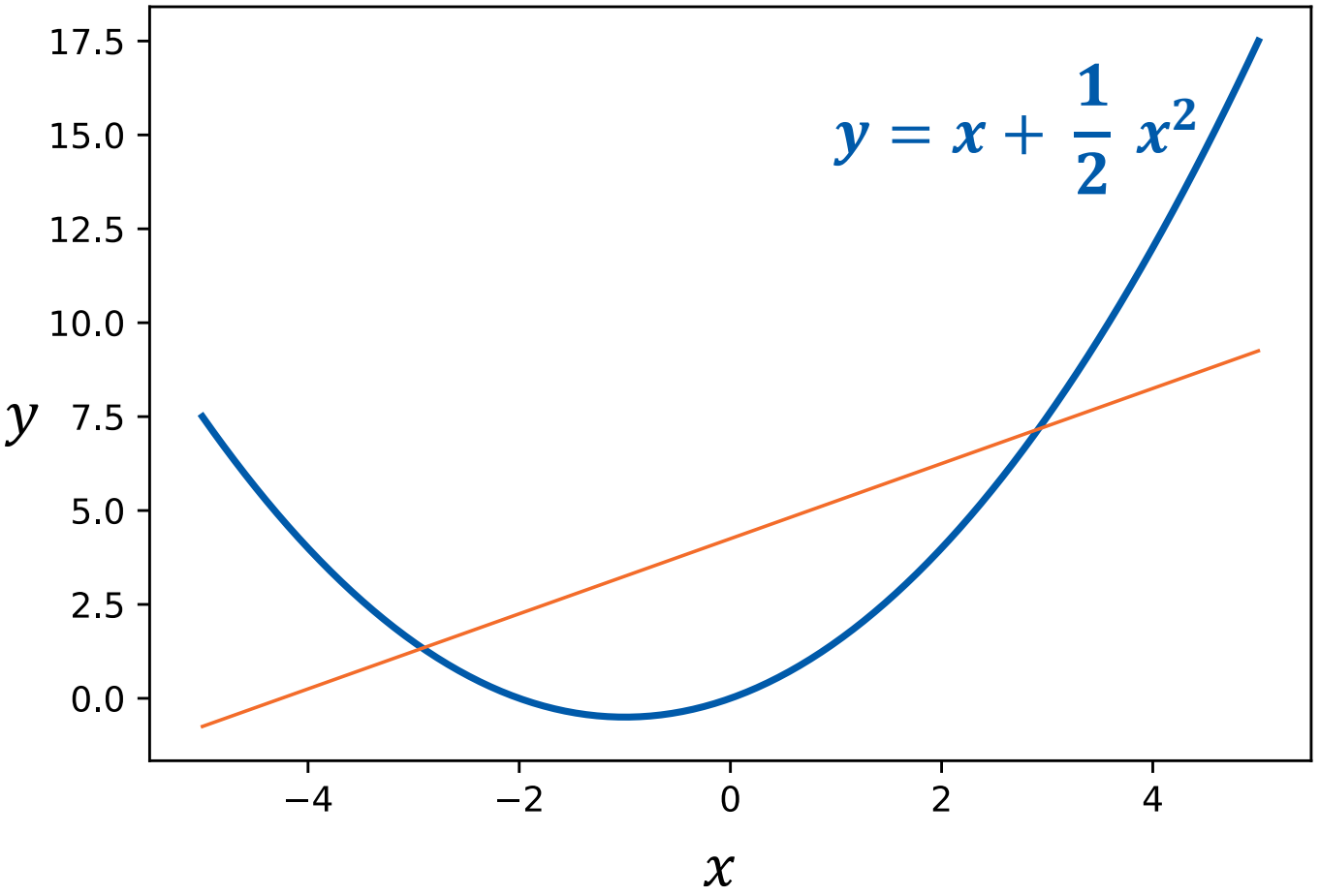
Feature expansion

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

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

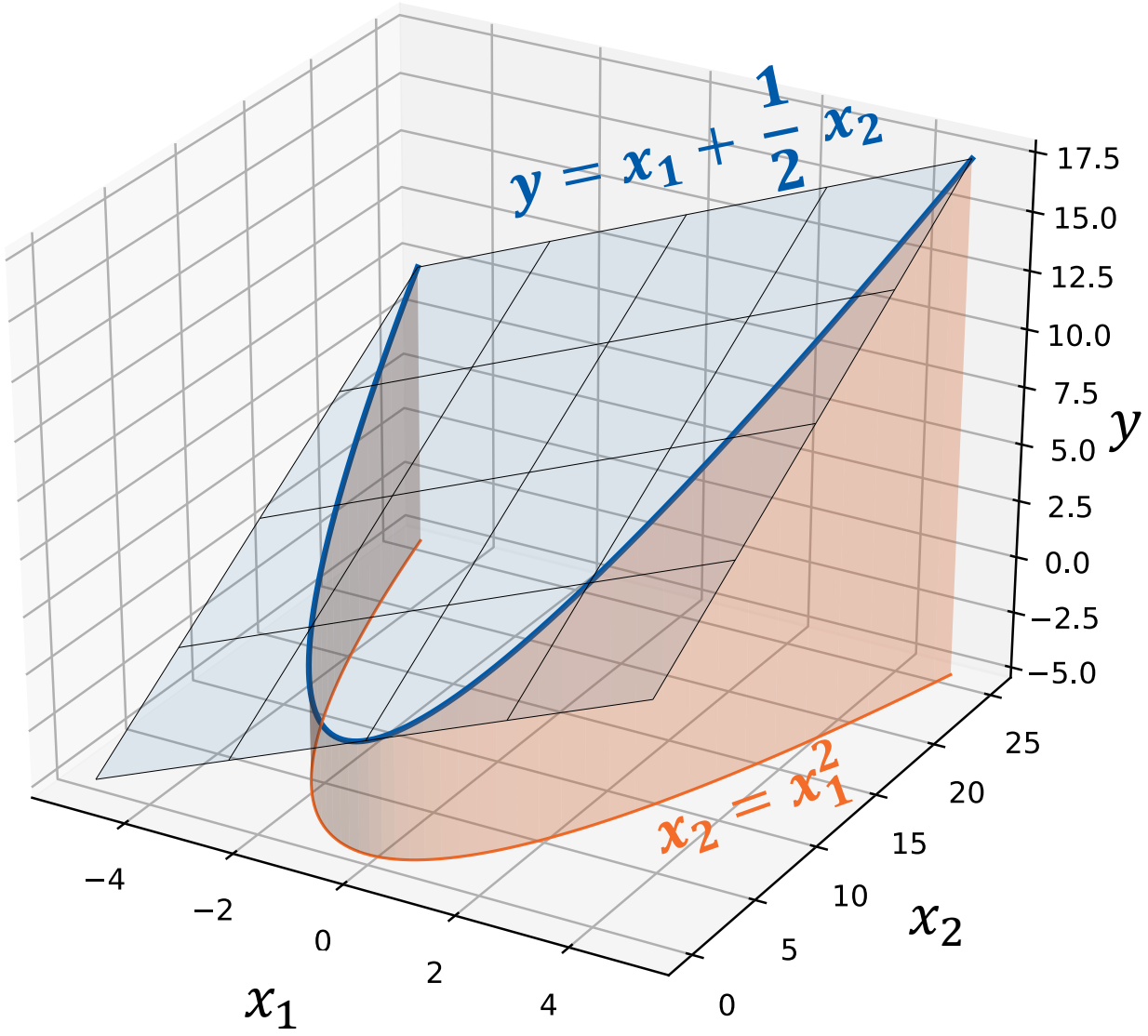
- Finding the best function Φ is called **feature engineering**
  - It is an important part of machine learning and requires deep understanding of the underlying problem and the data

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

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

Summary

- Understanding linear models gives **useful insights** into more complicated machine learning algorithms and optimization
- Linear Regression with MSE loss allows for **analytical solution**

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**

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

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

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?

Thank you!


amaevskij@hse.ru


SiLiKhon

Artem Maevskiy