

Review of fundamentals

IFT 725 - Réseaux neuronaux

LINEAR ALGEBRA

Topics: matrix, vector, norms, products

- Vector: $\mathbf{x} = [x_1, \dots, x_d]^\top = \begin{bmatrix} x_1 \\ \vdots \\ x_d \end{bmatrix}$
 - product: $\langle \mathbf{x}^{(1)}, \mathbf{x}^{(2)} \rangle = \mathbf{x}^{(1)\top} \mathbf{x}^{(2)} = \sum_{i=1}^d x_i^{(1)} x_i^{(2)}$
 - norm: $\|\mathbf{x}\|_2 = \sqrt{\mathbf{x}^\top \mathbf{x}} = \sqrt{\sum_i x_i^2}$ (Euclidean)
- Matrix: $\mathbf{X} = \begin{bmatrix} X_{1,1} & \dots & X_{1,m} \\ \vdots & \vdots & \vdots \\ X_{n,1} & \dots & X_{n,m} \end{bmatrix}$
 - product: $(\mathbf{X}^{(1)} \mathbf{X}^{(2)})_{i,j} = \mathbf{X}_{i,\cdot}^{(1)} \mathbf{X}_{\cdot,j}^{(2)} = \sum_k \mathbf{X}_{i,k}^{(1)} \mathbf{X}_{k,j}^{(2)}$
 - norm: $\|\mathbf{X}\|_F = \sqrt{\text{trace}(\mathbf{X}^\top \mathbf{X})} = \sqrt{\sum_i \sum_j X_{i,j}^2}$ (Frobenius)

LINEAR ALGEBRA

Topics: special matrices

- Identity matrix \mathbf{I} :
$$\mathbf{I}_{i,j} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$
- Diagonal matrix \mathbf{X} : $X_{i,j} = 0$ if $i \neq j$
- Lower triangular matrix \mathbf{X} : $X_{i,j} = 0$ if $i < j$
- Symmetric matrix \mathbf{X} : $X_{i,j} = X_{j,i}$ (i.e. $\mathbf{X}^\top = \mathbf{X}$)
- Square matrix: matrix with same number of rows and columns

LINEAR ALGEBRA

Topics: operations on matrices

- Trace of matrix: $\text{trace}(\mathbf{X}) = \sum_i X_{i,i}$

- trace of products:

$$\text{trace}(\mathbf{X}^{(1)} \mathbf{X}^{(2)} \mathbf{X}^{(3)}) = \text{trace}(\mathbf{X}^{(3)} \mathbf{X}^{(1)} \mathbf{X}^{(2)}) = \text{trace}(\mathbf{X}^{(2)} \mathbf{X}^{(3)} \mathbf{X}^{(1)})$$

- Inverse of matrix: $\mathbf{X}^{-1} \mathbf{X} = \mathbf{X} \mathbf{X}^{-1} = \mathbf{I}$

- doesn't exist if determinant is 0

- inverse of product: $(\mathbf{X}^{(1)} \mathbf{X}^{(2)})^{-1} = \mathbf{X}^{(2)-1} \mathbf{X}^{(1)-1}$

- Transpose of matrix: $(\mathbf{X}^\top)_{i,j} = \mathbf{X}_{j,i}$

- transpose of product: $(\mathbf{X}^{(1)} \mathbf{X}^{(2)})^\top = \mathbf{X}^{(2)\top} \mathbf{X}^{(1)\top}$

LINEAR ALGEBRA

Topics: operations on matrices

- Determinant

- ▶ of triangular matrix: $\det(\mathbf{X}) = \prod_i \mathbf{X}_{i,i}$
- ▶ of transpose of matrix: $\det(\mathbf{X}^\top) = \det(\mathbf{X})$
- ▶ of inverse of matrix: $\det(\mathbf{X}^{-1}) = \det(\mathbf{X})^{-1}$
- ▶ of product of matrix: $\det(\mathbf{X}^{(1)}\mathbf{X}^{(2)}) = \det(\mathbf{X}^{(1)})\det(\mathbf{X}^{(2)})$

LINEAR ALGEBRA

Topics: properties of matrices

- Orthogonal matrix: $\mathbf{X}^\top = \mathbf{X}^{-1}$
- Positive definite matrix: $\mathbf{v}^\top \mathbf{X} \mathbf{v} > 0 \quad \forall \mathbf{v} \in \mathbb{R}$
 - if $\ll \geq \gg$, then positive semi-definite

LINEAR ALGEBRA

Topics: linear dependence, rank, range and nullspace

- Set of linearly dependent vectors $\{\mathbf{x}^{(t)}\}$:

$$\exists \mathbf{w}, t^* \text{ such that } \mathbf{x}^{(t^*)} = \sum_{t \neq t^*} w_t \mathbf{x}^{(t)}$$

- Rank of matrix: number of linear independent columns
- Range of a matrix:

$$\mathcal{R}(\mathbf{X}) = \{\mathbf{x} \in \mathbb{R}^n \mid \exists \mathbf{w} \text{ such that } \mathbf{x} = \sum_j w_j \mathbf{X}_{\cdot, j}\}$$

- Nullspace of a matrix:

$$\{\mathbf{x} \in \mathbb{R}^n \mid \mathbf{x} \notin \mathcal{R}(\mathbf{X})\}$$

LINEAR ALGEBRA

Topics: eigenvalues and eigenvectors of a matrix

- Eigenvalues and eigenvectors

$$\{ \lambda_i, \mathbf{u}_i \mid \mathbf{X}\mathbf{u}_i = \lambda_i \mathbf{u}_i \text{ and } \mathbf{u}_i^\top \mathbf{u}_j = 1_{i=j} \}$$

- Properties

- ▶ can write $\mathbf{X} = \sum_i \lambda_i \mathbf{u}_i \mathbf{u}_i^\top$
- ▶ determinant of **any** matrix: $\det(\mathbf{X}) = \prod_i \lambda_i$
- ▶ positive definite if $\lambda_i > 0 \quad \forall i$
- ▶ rank of matrix is the number of non-zero eigenvalues

DIFFERENTIAL CALCULUS

Topics: derivative, partial derivative

- Derivative:

$$\frac{d}{dx} f(x) = \lim_{\Delta \rightarrow 0} \frac{f(x + \Delta) - f(x)}{\Delta}$$

- ▶ direction and rate of increase of function

- Partial derivative:

$$\frac{\partial}{\partial x} f(x, y) = \lim_{\Delta \rightarrow 0} \frac{f(x + \Delta, y) - f(x, y)}{\Delta}$$

$$\frac{\partial}{\partial y} f(x, y) = \lim_{\Delta \rightarrow 0} \frac{f(x, y + \Delta) - f(x, y)}{\Delta}$$

- ▶ direction and rate of increase for variable assuming others are fixed

DIFFERENTIAL CALCULUS

Topics: derivative, partial derivative

- Example:

$$f(x, y) = \frac{x^2}{y}$$

$$\frac{\partial f(x, y)}{\partial x} = \underbrace{\frac{2x}{y}}$$

treat y
as constant

$$\frac{\partial f(x, y)}{\partial y} = \underbrace{\frac{-x^2}{y^2}}$$

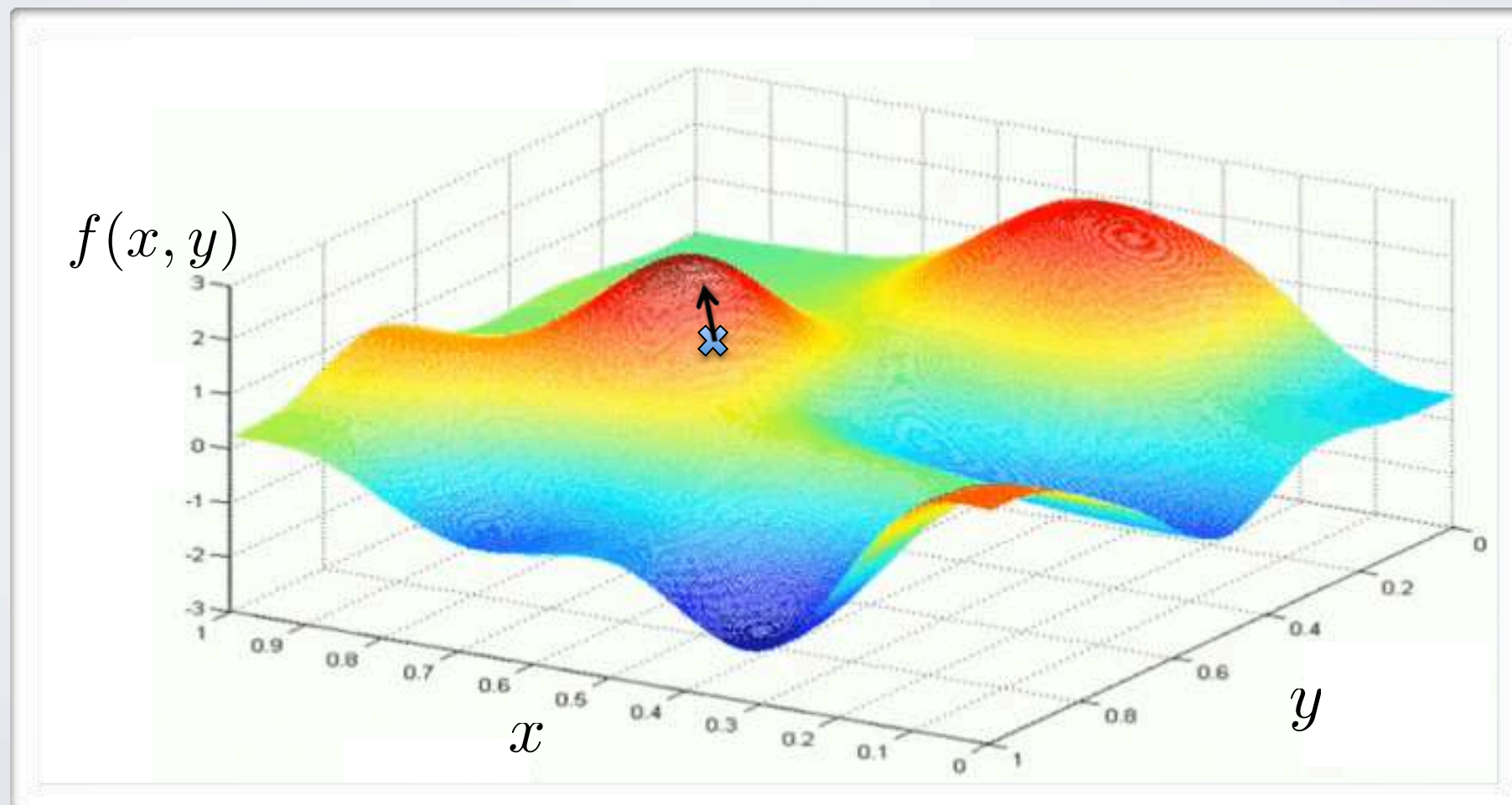
treat x
as constant

DIFFERENTIAL CALCULUS

Topics: gradient

- Gradient:

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = \left[\frac{\partial}{\partial x_1} f(\mathbf{x}), \dots, \frac{\partial}{\partial x_d} f(\mathbf{x}) \right]^\top = \begin{bmatrix} \frac{\partial}{\partial x_1} f(\mathbf{x}) \\ \vdots \\ \frac{\partial}{\partial x_d} f(\mathbf{x}) \end{bmatrix}$$



DIFFERENTIAL CALCULUS

Topics: Jacobian, Hessian

- Hessian:

$$\nabla_{\mathbf{x}}^2 f(\mathbf{x}) = \begin{bmatrix} \frac{\partial^2}{\partial x_1^2} f(\mathbf{x}) & \cdots & \frac{\partial^2}{\partial x_1 \partial x_d} f(\mathbf{x}) \\ \vdots & \cdots & \vdots \\ \frac{\partial^2}{\partial x_d \partial x_1} f(\mathbf{x}) & \cdots & \frac{\partial^2}{\partial x_d^2} f(\mathbf{x}) \end{bmatrix}$$

- If $\mathbf{f}(\mathbf{x}) = [f(\mathbf{x})_1, \dots, f(\mathbf{x})_k]^\top$ is a vector, the Jacobian is:

$$\nabla_{\mathbf{x}} \mathbf{f}(\mathbf{x}) = \begin{bmatrix} \frac{\partial}{\partial x_1} f(\mathbf{x})_1 & \cdots & \frac{\partial}{\partial x_d} f(\mathbf{x})_1 \\ \vdots & \cdots & \vdots \\ \frac{\partial}{\partial x_1} f(\mathbf{x})_k & \cdots & \frac{\partial}{\partial x_d} f(\mathbf{x})_k \end{bmatrix}$$

DIFFERENTIAL CALCULUS

Topics: gradient for matrices

- If scalar function $f(\mathbf{X})$ takes a matrix \mathbf{X} as input

$$\nabla_{\mathbf{X}} f(\mathbf{X}) = \begin{bmatrix} \frac{\partial}{\partial X_{1,1}} f(\mathbf{X}) & \cdots & \frac{\partial}{\partial X_{1,m}} f(\mathbf{X}) \\ \vdots & \cdots & \vdots \\ \frac{\partial}{\partial X_{n,1}} f(\mathbf{X}) & \cdots & \frac{\partial}{\partial X_{n,m}} f(\mathbf{X}) \end{bmatrix}$$

- For functions that output functions and take matrices as input, we organize into 3D tensors

PROBABILITY

Topics: probability space

- Probability space: triplet (Ω, \mathcal{F}, P)

- ▶ Ω is the space of possible outcomes
- ▶ \mathcal{F} is the space of possible events
- ▶ P is a probability measure mapping an outcome to its probability $[0, 1]$
- ▶ example: throwing a die
 - $\Omega = \{1, 2, 3, 4, 5, 6\}$
 - $e = \{1, 5\} \in \mathcal{F}$ (i.e. die is either 1 or 5)
 - $P(\{1, 5\}) = \frac{2}{6}$

- Properties:

$$1. P(\{\omega\}) \geq 0 \quad \forall \omega \in \Omega \qquad 2. \sum_{\omega \in \Omega} P(\{\omega\}) = 1$$

PROBABILITY

Topics: random variable

- Random variable: a function on outcomes
- Examples:
 - ▶ X is the value of the outcome
 - ▶ O is 1 if the outcome is 1, 3 or 5, otherwise it's 0
 - ▶ S is 1 if the outcome is smaller than 4, otherwise it's 0

PROBABILITY

Topics: distributions (joint, marginal, conditional)

- Joint distribution: $p(X = x, O = o, S = s)$ ($p(x, s, o)$ for short)
 - the probability of a complete assignment of all random variables
 - example: $p(X = 1, O = 1, S = 0) = 0$
- Marginal distribution: $p(o, s) = \sum_x p(x, o, s)$
 - the probability of a partial assignment
 - example: $p(O = 1, S = 0) = \frac{1}{6}$
- Conditional distribution: $p(S = s | O = o)$
 - the probability of some variables, assuming an assignment of other variables
 - example: $p(S = 1 | O = 1) = \frac{2}{3}$

PROBABILITY

Topics: probability chain rule, Bayes rule

- Probability chain rule: $p(s, o) = p(s|o)p(o) = p(o|s)p(s)$
 - in general:

$$p(\mathbf{x}) = \prod_i p(x_i | x_1, \dots, x_{i-1})$$

- Bayes rule:

$$p(O = o | S = s) = \frac{p(S=s|O=o)p(O=o)}{\sum_{o'} p(S=s|O=o')p(O=o')}$$

PROBABILITY

Topics: independence between variables

- Independence: variables X_1 and X_2 are independent if

$$p(x_1, x_2) = p(x_1)p(x_2)$$

$$\text{or } p(x_1|x_2) = p(x_1)$$

$$\text{or } p(x_2|x_1) = p(x_2)$$

- Conditional independence: variables X_1 and X_2 are independent given X_3 if

$$p(x_1, x_2|x_3) = p(x_1|x_3)p(x_2|x_3)$$

$$\text{or } p(x_1|x_2, x_3) = p(x_1|x_3)$$

$$\text{or } p(x_2|x_1, x_3) = p(x_2|x_3)$$

PROBABILITY

Topics: expectation, variance

- Expectation: $E[X] = \sum_x x p(X = x)$
 - properties:
 - $E[X + Y] = E[X] + E[Y]$
 - $E[f(X)] = \sum_x f(x) p(X = x)$
 - if independent, $E[XY] = E[X]E[Y]$
- Variance: $\text{Var}[X] = \sum_x (x - E(X))^2 p(X = x)$
 - properties:
 - $\text{Var}[X] = E[X^2] - E[X]^2$
 - if independent, $\text{Var}[X + Y] = \text{Var}[X] + \text{Var}[Y]$

PROBABILITY

Topics: covariance matrix

- Covariance:

$$\begin{aligned}\text{Cov}(X_1, X_2) &= \text{E}[(X_1 - \text{E}[X_1])(X_2 - \text{E}[X_2])] \\ &= \sum_{x_1} \sum_{x_2} (x_1 - \text{E}[X_1])(x_2 - \text{E}[X_2]) p(x_1, x_2)\end{aligned}$$

- ▶ if independent $\text{Cov}(X_1, X_2) = 0$
- ▶ $\text{Var}(X) = \text{Cov}(X, X)$

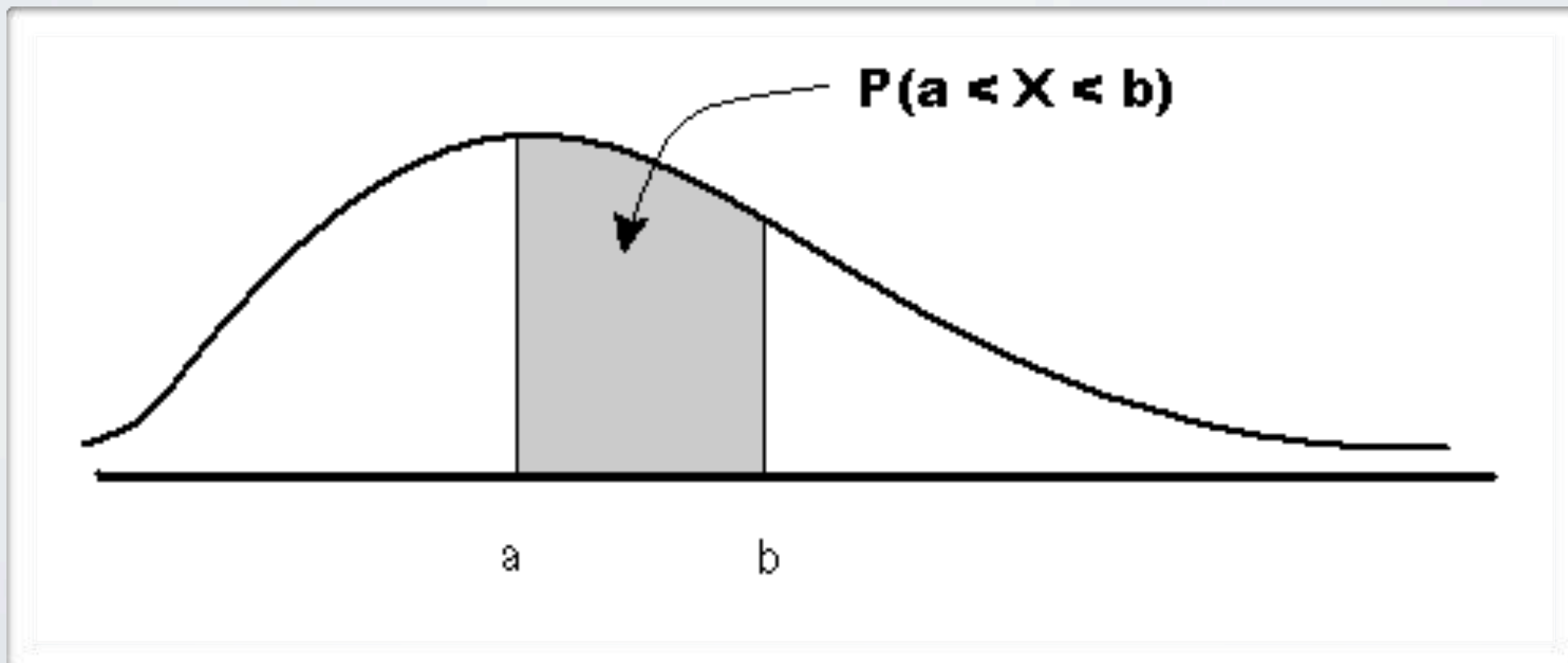
- Covariance matrix:

$$\text{Cov}(\mathbf{X}) = \begin{bmatrix} \text{Cov}(X_1, X_1) & \dots & \text{Cov}(X_1, X_d) \\ \vdots & \ddots & \vdots \\ \text{Cov}(X_d, X_1) & \dots & \text{Cov}(X_d, X_d) \end{bmatrix}$$

PROBABILITY

Topics: continuous variables

- for continuous variable X , $p(x)$ is a density function
 - $P(X \in A) = \int_{x \in A} p(x) dx$
 - the probability $P(X = x)$ is zero for continuous variables
 - in previous equations, summations would be replaced by integrals



PROBABILITY

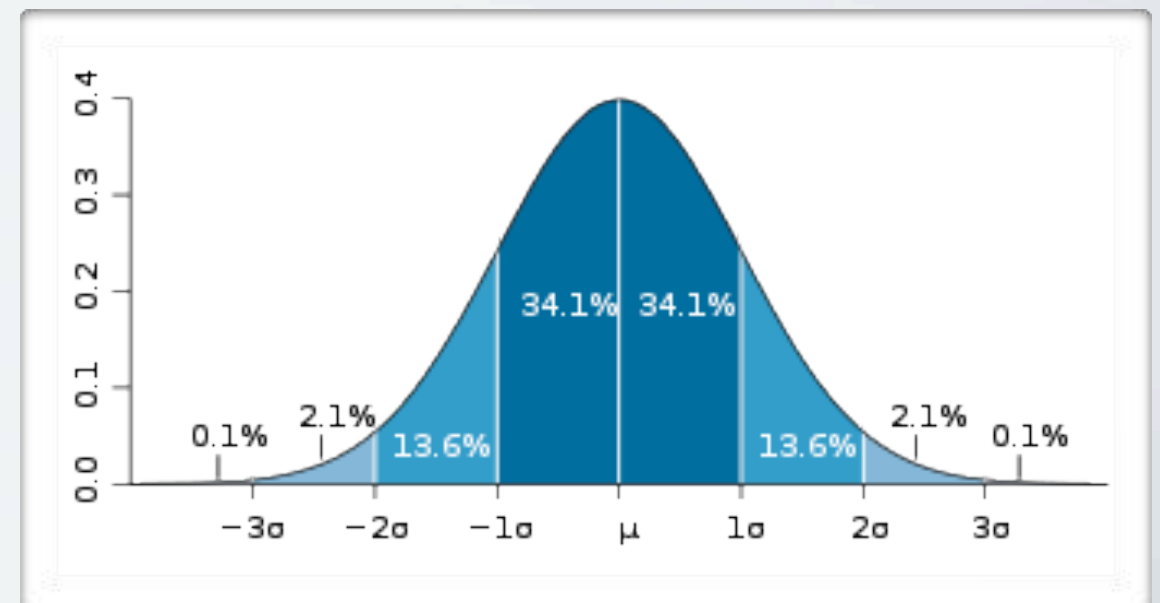
Topics: Bernoulli, Gaussian distributions

- Bernoulli variable: $X \in \{0, 1\}$

- $p(X = 1) = \mu$
- $p(X = 0) = 1 - \mu$
- $E[X] = \mu$
- $\text{Var}[X] = \mu(1 - \mu)$

- Gaussian variable: $X \in \mathbb{R}$

- $p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$
- $E[X] = \mu$
- $\text{Var}[X] = \sigma^2$



PROBABILITY

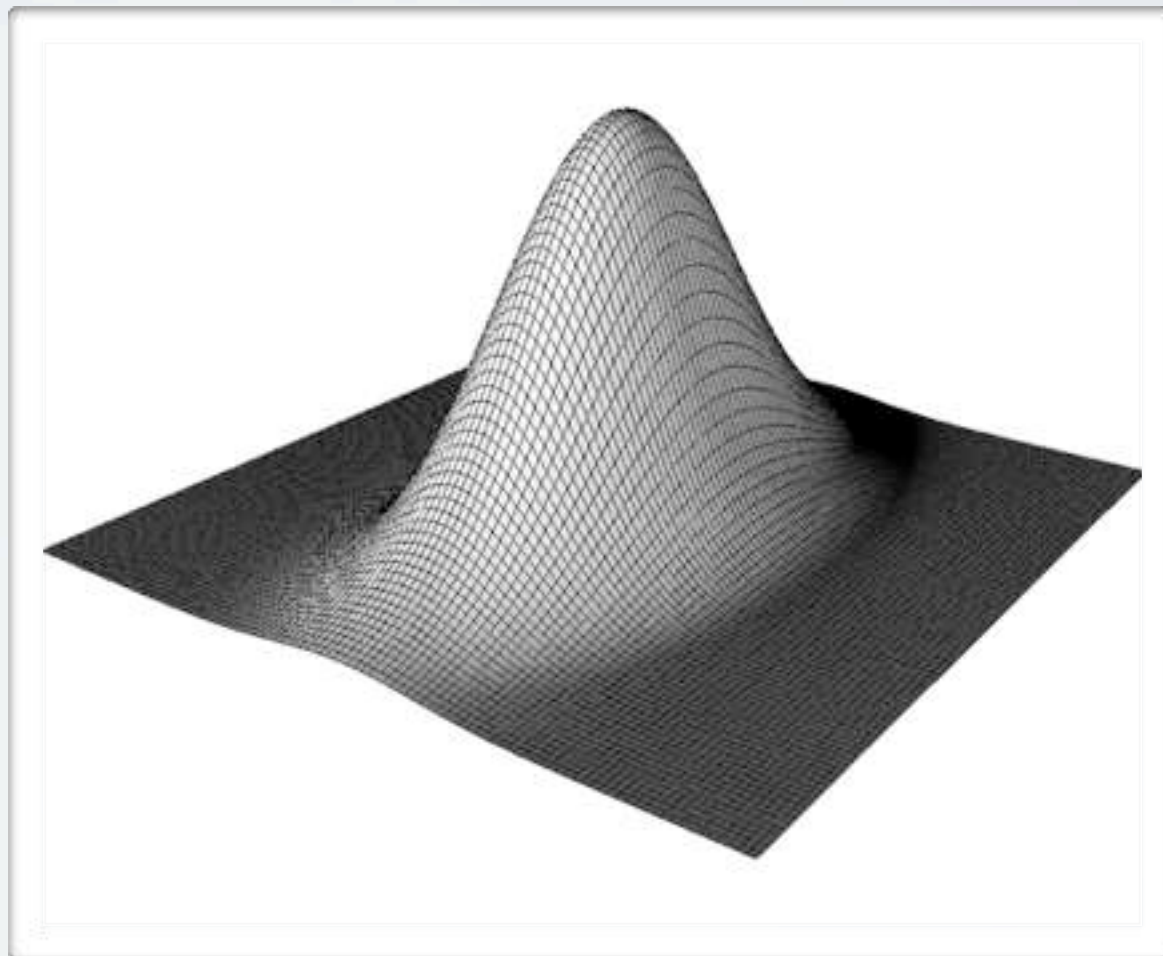
Topics: Multivariate Gaussian distributions

- Gaussian variable: $\mathbf{X} \in \mathbb{R}^d$

- $$p(\mathbf{x}) = \frac{1}{\sqrt{(2\pi)^d \det(\Sigma)}} \exp \left(-\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu})^\top \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}) \right)$$

- $$\mathbb{E}[\mathbf{X}] = \boldsymbol{\mu}$$

- $$\text{Cov}[\mathbf{X}] = \Sigma$$



STATISTICS

Topics: estimate of the expectation and covariance matrix

- Sample mean:

$$\hat{\boldsymbol{\mu}} = \frac{1}{T} \sum_t \mathbf{x}^{(t)}$$

- Sample variance:

$$\hat{\sigma}^2 = \frac{1}{T-1} \sum_t (\mathbf{x}^{(t)} - \hat{\boldsymbol{\mu}})^2$$

- Sample covariance matrix:

$$\hat{\boldsymbol{\Sigma}} = \frac{1}{T-1} \sum_t (\mathbf{x}^{(t)} - \hat{\boldsymbol{\mu}})(\mathbf{x}^{(t)} - \hat{\boldsymbol{\mu}})^\top$$

- These estimators are unbiased, i.e.:

$$\mathbb{E}[\hat{\boldsymbol{\mu}}] = \boldsymbol{\mu} \quad \mathbb{E}[\hat{\sigma}^2] = \sigma^2 \quad \mathbb{E}[\hat{\boldsymbol{\Sigma}}] = \boldsymbol{\Sigma}$$

STATISTICS

Topics: confidence interval

- Confidence interval of the sample mean (ID):
 - ▶ if T is big, the following estimator is approx. Gaussian with mean 0 and variance 1

$$\frac{\hat{\mu} - \mu}{\sqrt{\hat{\sigma}^2 / T}}$$

- ▶ then we have that, with 95% probability, that

$$\mu \in \hat{\mu} \pm 1.96 \sqrt{\hat{\sigma}^2 / T}$$

STATISTICS

Topics: maximum likelihood, I.I.D. hypothesis

- maximum likelihood estimator (MLE):

$$\hat{\theta} = \arg \max_{\theta} p(\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(T)})$$

- ▶ the sample mean is the MLE for a Gaussian distribution
- ▶ the sample covariance matrix isn't, but this is

$$\frac{T-1}{T} \hat{\Sigma} = \frac{1}{T} \sum_t (\mathbf{x}^{(t)} - \hat{\boldsymbol{\mu}})(\mathbf{x}^{(t)} - \hat{\boldsymbol{\mu}})^\top$$

- Independent and identically distributed variables

$$p(\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(T)}) = \prod_t p(\mathbf{x}^{(t)})$$

SAMPLING

Topics: Monte Carlo estimate

- Monte Carlo estimate:
 - a method to approximate an expensive expectation

$$\mathbb{E}[f(\mathbf{X})] = \sum_{\mathbf{x}} f(\mathbf{x}) p(\mathbf{x}) \approx \frac{1}{K} \sum_k f(\mathbf{x}^{(k)})$$

- the $\mathbf{x}^{(k)}$ must be sampled from $p(\mathbf{x})$

SAMPLING

Topics: importance sampling

- Importance sampling:

- ▶ a sampling method for when $p(\mathbf{x})$ is expensive to sample from

$$\mathbb{E}[f(\mathbf{X})] = \sum_{\mathbf{x}} f(\mathbf{x}) \frac{p(\mathbf{x})}{q(\mathbf{x})} q(\mathbf{x}) \approx \frac{1}{K} \sum_k f(\mathbf{x}^{(k)}) \frac{p(\mathbf{x})}{q(\mathbf{x})}$$

- ▶ $q(\mathbf{x})$ is easier to sample from and should be as similar as possible to $p(\mathbf{x})$
 - designing a good $q(\mathbf{x})$ is often hard to do

SAMPLING

Topics: Markov Chain Monte Carlo (MCMC)

- MCMC:

- ▶ iterative method to generate the sequence of $\mathbf{x}^{(k)}$
- ▶ the set of $\mathbf{x}^{(k)}$ will be dependent of each other $\mathbf{x}^{(k)}$

$$\mathbf{x}^{(1)} \xrightarrow{T(\mathbf{x}' \leftarrow \mathbf{x})} \mathbf{x}^{(2)} \xrightarrow{T(\mathbf{x}' \leftarrow \mathbf{x})} \mathbf{x}^{(3)} \xrightarrow{T(\mathbf{x}' \leftarrow \mathbf{x})} \dots \xrightarrow{T(\mathbf{x}' \leftarrow \mathbf{x})} \mathbf{x}^{(K)}$$

- ▶ $T(\mathbf{x}' \leftarrow \mathbf{x})$ is a transition operator, that must satisfy certain properties
- ▶ K must be big for the set of samples be representative of distribution
- ▶ usually, we drop the first samples, which are not reliable

SAMPLING

Topics: Gibbs sampling

- Gibbs sampling:

- ▶ MCMC method which uses the following transition operator $T(\mathbf{x}' \leftarrow \mathbf{x})$
 - pick a variable x_i
 - obtain \mathbf{x}' by only resampling this variable according to

$$p(x_i | x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_d)$$

- return \mathbf{x}'
- ▶ often, we simply cycle through the variables, in random order

MACHINE LEARNING

Topics: supervised learning

- Learning example: (\mathbf{x}, y)
- Task to solve: predict target y from input \mathbf{x}
 - classification: target is a class ID (from 0 to nb. of class - 1)
 - regression: target is a real number

MACHINE LEARNING

Topics: unsupervised learning

- Learning example: \mathbf{x}
- No explicit target to predict
 - clustering: partition data into groups
 - feature extraction: learn meaningful features automatically
 - dimensionality reduction: learning a lower-dimensional representation of input

MACHINE LEARNING

Topics: learning algorithm, model, training set

- Learning algorithm
 - takes as input a training set $\mathcal{D}^{\text{train}} = \{(\mathbf{x}^{(t)}, y^{(t)})\}$
 - outputs a model $f(\mathbf{x}; \boldsymbol{\theta})$
- We then say the model $f(\mathbf{x}; \boldsymbol{\theta})$ was trained on $\mathcal{D}^{\text{train}}$
 - the model has learned the information present in $\mathcal{D}^{\text{train}}$
- We can now use the model $f(\mathbf{x}; \boldsymbol{\theta})$ on new inputs

MACHINE LEARNING

Topics: training, validation and test sets, generalization

- Training set $\mathcal{D}^{\text{train}}$ serves to train a model
- Validation set $\mathcal{D}^{\text{valid}}$ serves to select hyper-parameters
- Test set $\mathcal{D}^{\text{test}}$ serves to estimate the generalization performance (error)
- Generalization is the behavior of the model on **unseen examples**
 - this is what we care about in machine learning!

MACHINE LEARNING

Topics: capacity of a model, underfitting, overfitting, hyper-parameter, model selection

- Capacity: flexibility of a model
- Hyper-parameter: a parameter of a model that is not trained (specified before training)
- Underfitting: state of model which could improve generalization with more training or capacity
- Overfitting: state of model which could improve generalization with more training or capacity
- Model selection: process of choosing the best hyper-parameters on validation set

MACHINE LEARNING

Topics: capacity of a model, underfitting, overfitting, hyperparameter, model selection



MACHINE LEARNING

Topics: interaction between training set size/capacity/training time and training error/generalization error

- If capacity increases:
 - training error will ?
 - generalization error will ?
- If training time increases:
 - training error will ?
 - generalization error will ?
- If training set size increases:
 - generalization error will ?
 - difference between the training and generalization error will ?

MACHINE LEARNING

Topics: interaction between training set size/capacity/training time and training error/generalization error

- If capacity increases:
 - ▶ training error will decrease
 - ▶ generalization error will ?
- If training time increases:
 - ▶ training error will ?
 - ▶ generalization error will ?
- If training set size increases:
 - ▶ generalization error will ?
 - ▶ difference between the training and generalization error will ?

MACHINE LEARNING

Topics: interaction between training set size/capacity/training time and training error/generalization error

- If capacity increases:
 - training error will decrease
 - generalization error will increase or decrease
- If training time increases:
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 - generalization error will ?
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 - generalization error will ?
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MACHINE LEARNING

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MACHINE LEARNING

Topics: empirical risk minimization, regularization

- Empirical risk minimization
 - framework to design learning algorithms

$$\arg \min_{\boldsymbol{\theta}} \frac{1}{T} \sum_t l(f(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)}) + \lambda \Omega(\boldsymbol{\theta})$$

- $l(f(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)})$ is a loss function
 - $\Omega(\boldsymbol{\theta})$ is a regularizer (penalizes certain values of $\boldsymbol{\theta}$)
- Learning is cast as optimization
 - ideally, we'd optimize classification error, but it's not smooth
 - loss function is a surrogate for what we truly should optimize (e.g. upper bound)

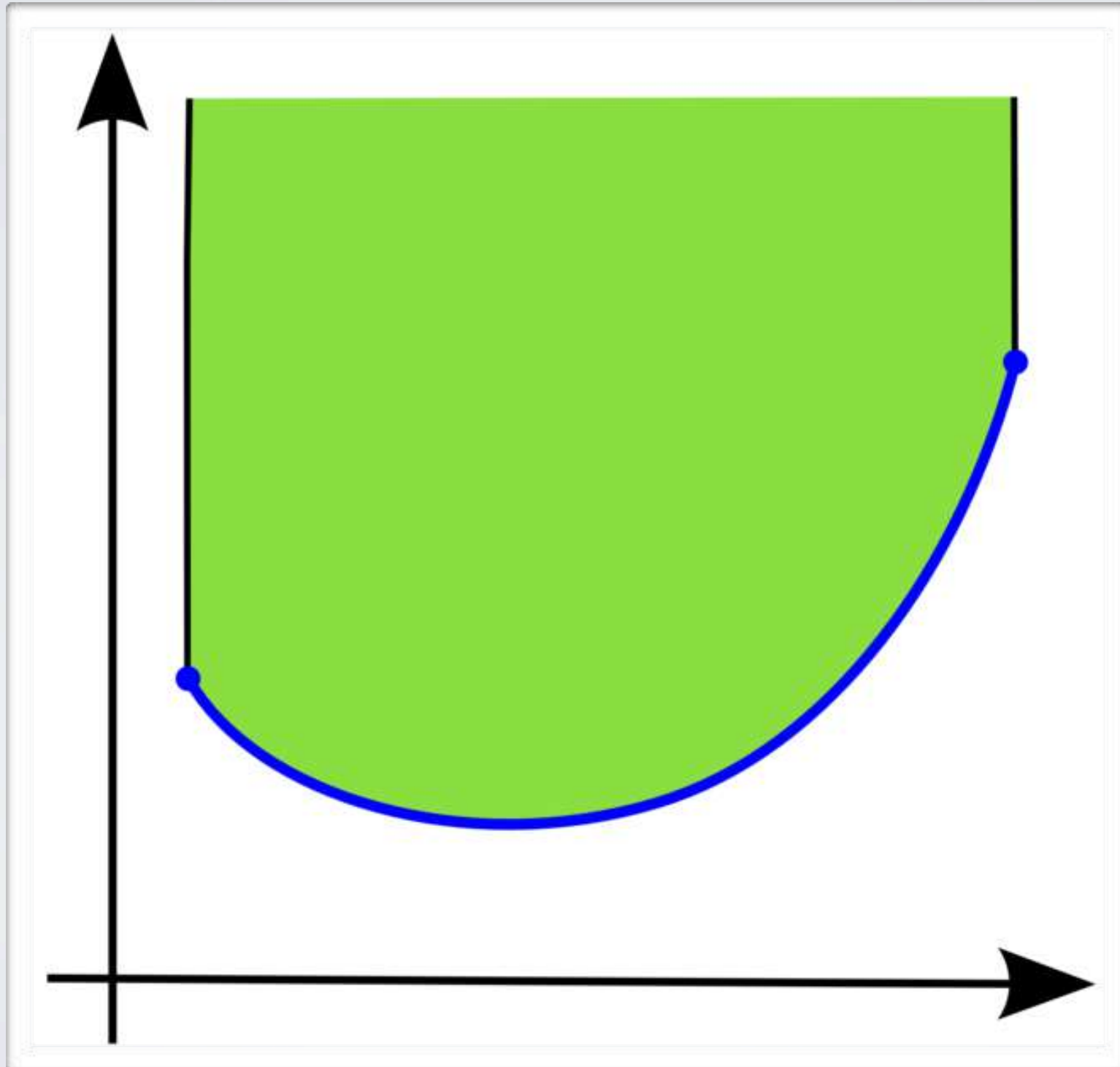
MACHINE LEARNING

Topics: gradient descent

- Gradient descent: procedure to minimize a function
 - compute gradient
 - take step in opposite direction

MACHINE LEARNING

Topics: gradient descent

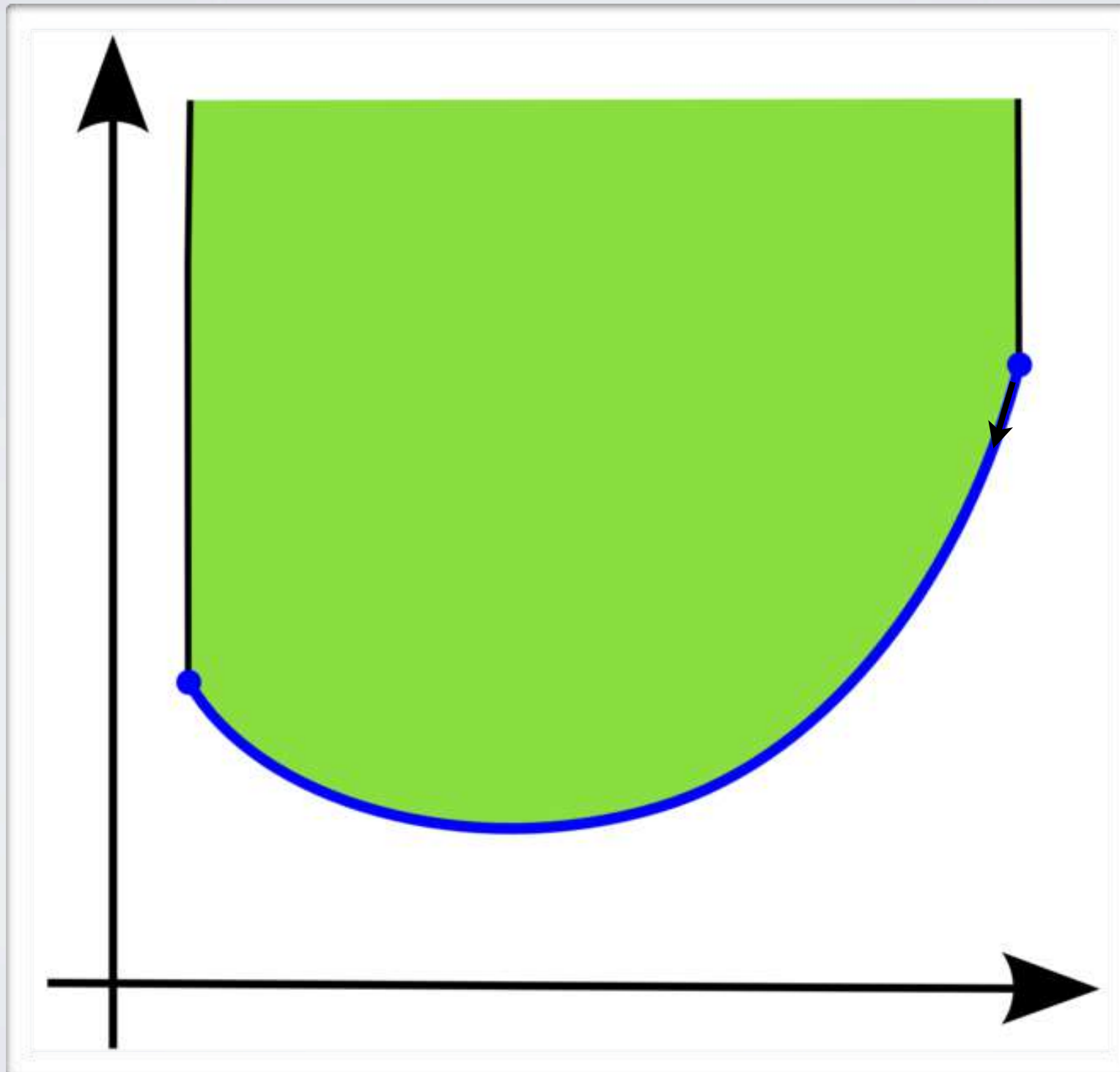


Descent
direction

$$-\frac{\partial f(x)}{\partial x}$$

MACHINE LEARNING

Topics: gradient descent

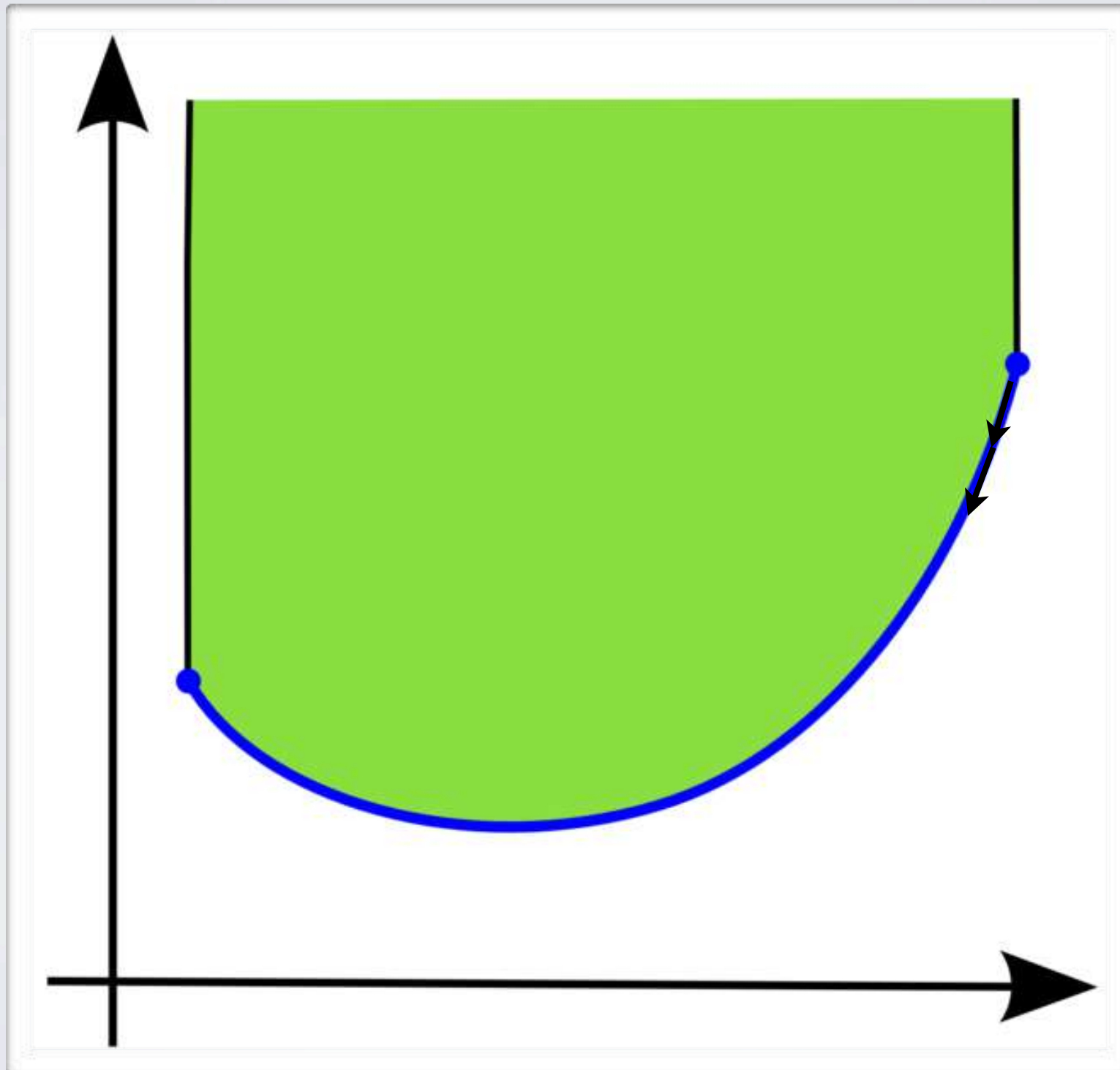


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MACHINE LEARNING

Topics: gradient descent

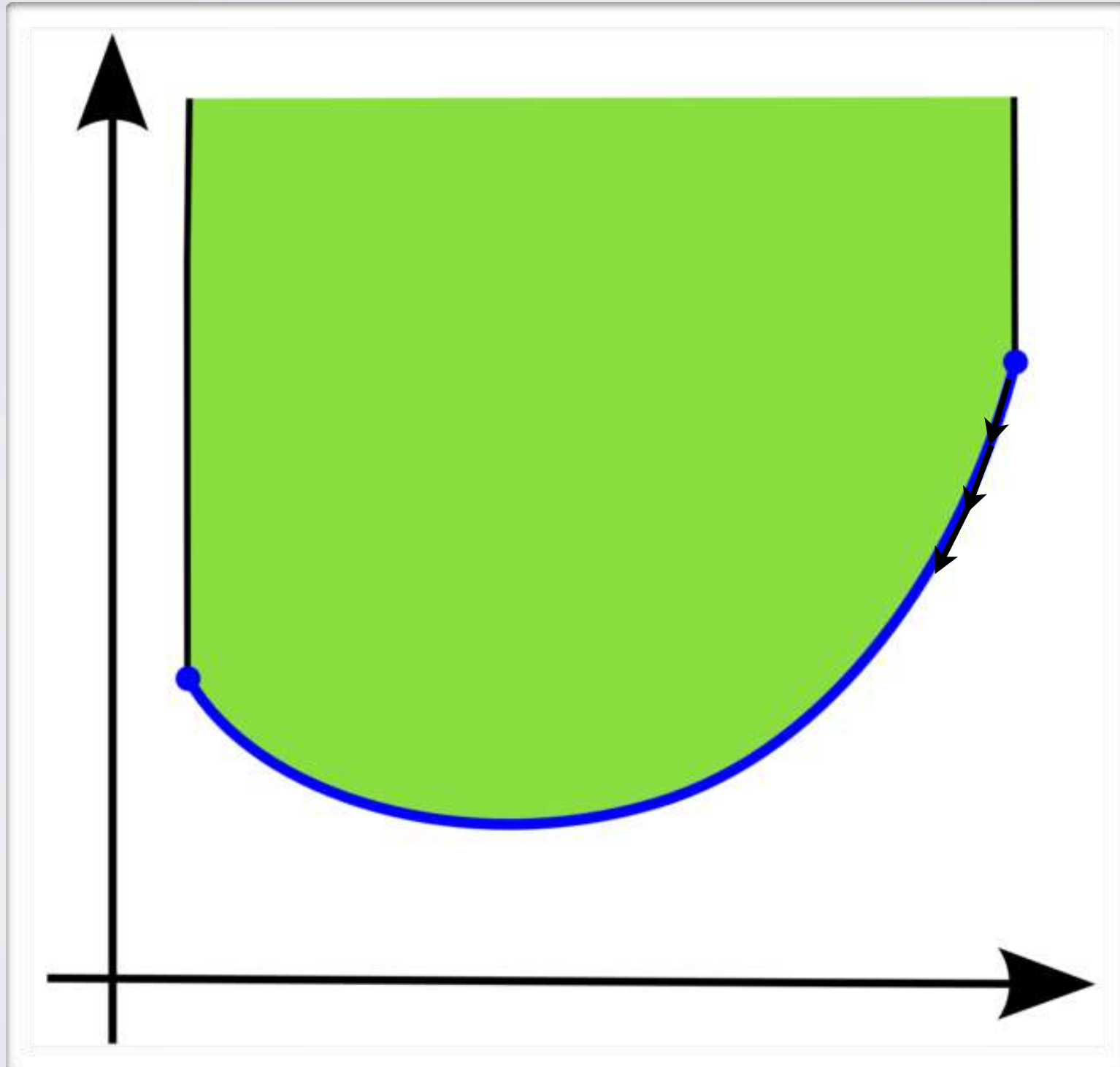


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MACHINE LEARNING

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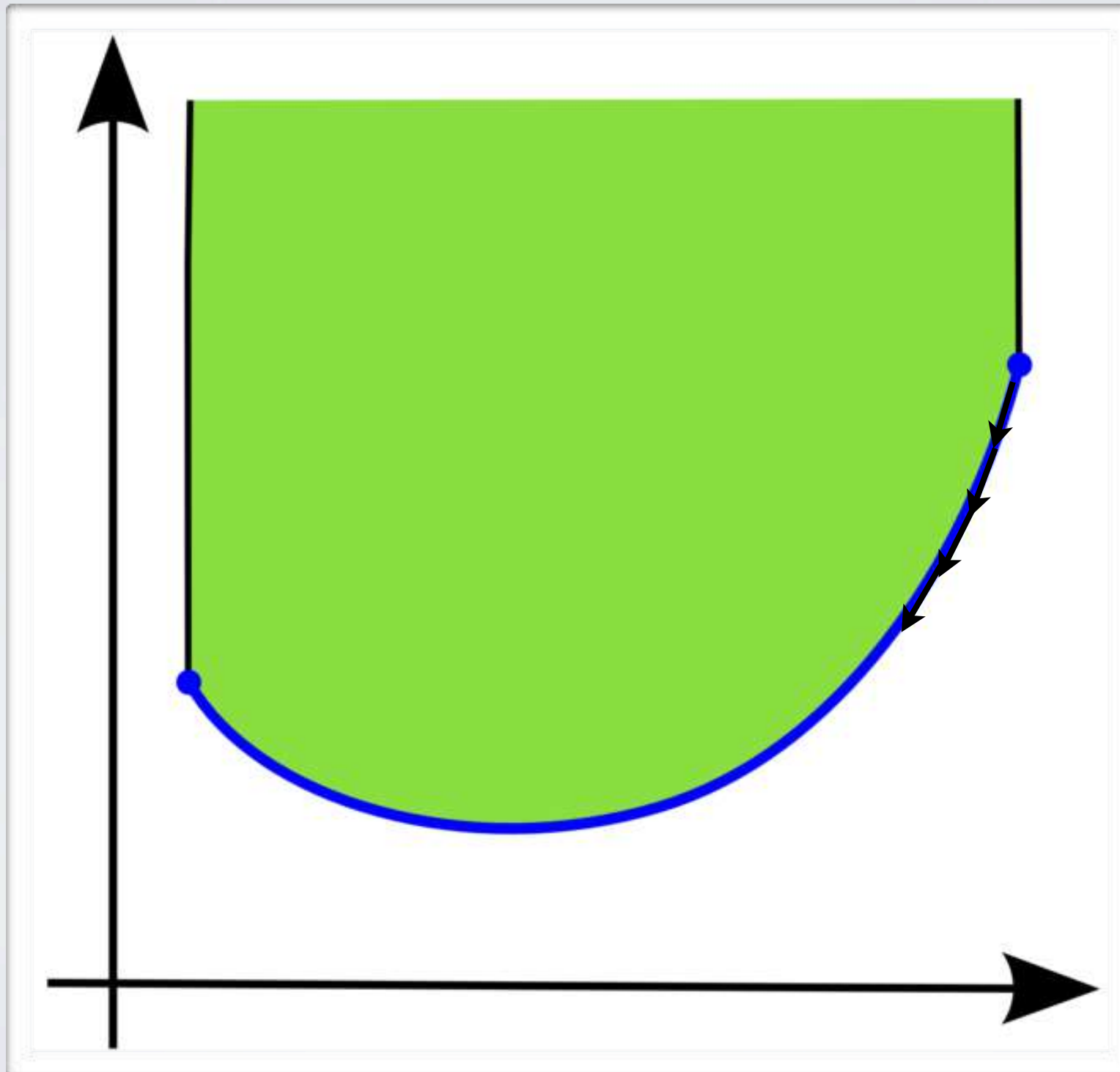


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MACHINE LEARNING

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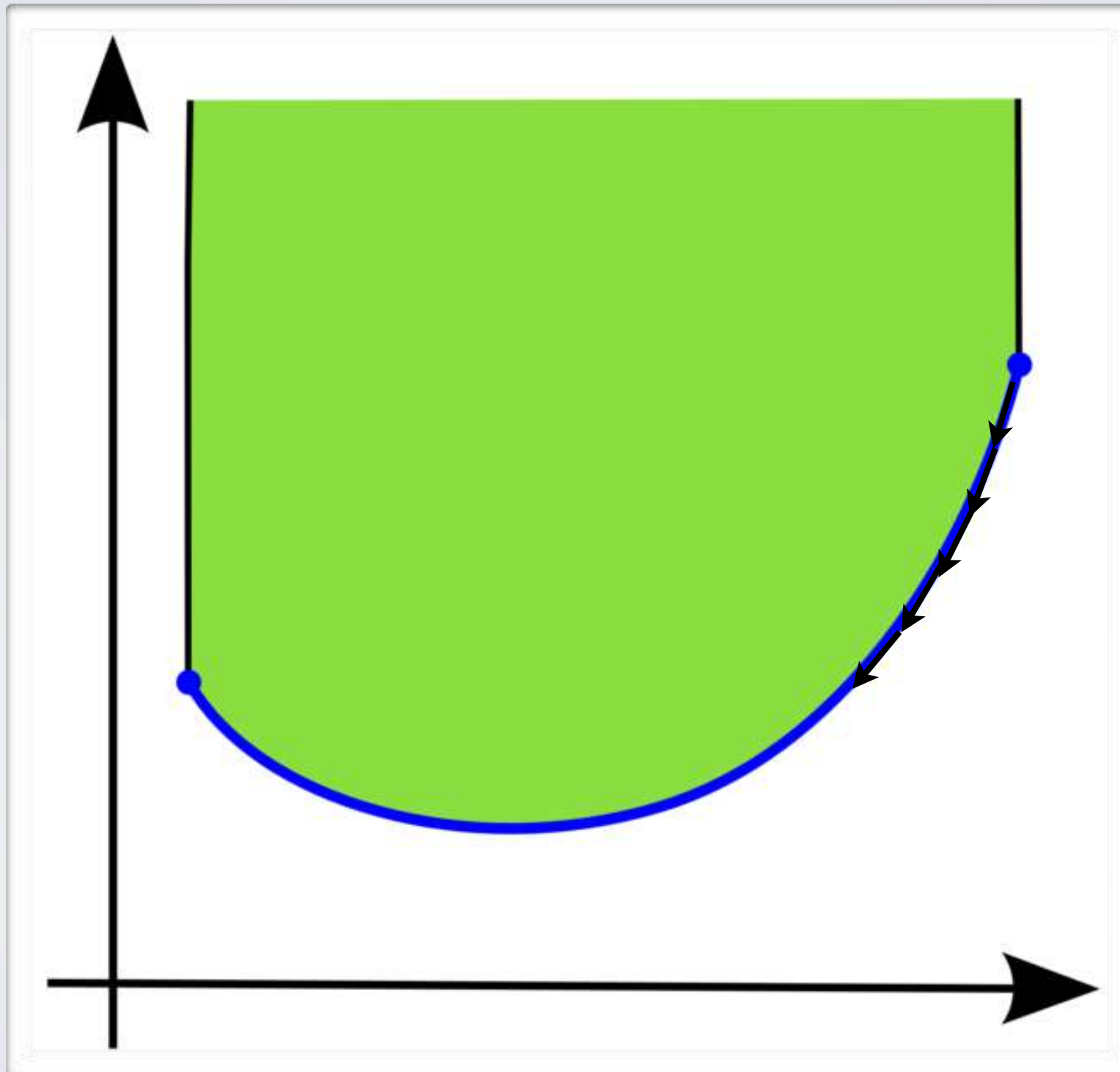


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MACHINE LEARNING

Topics: gradient descent

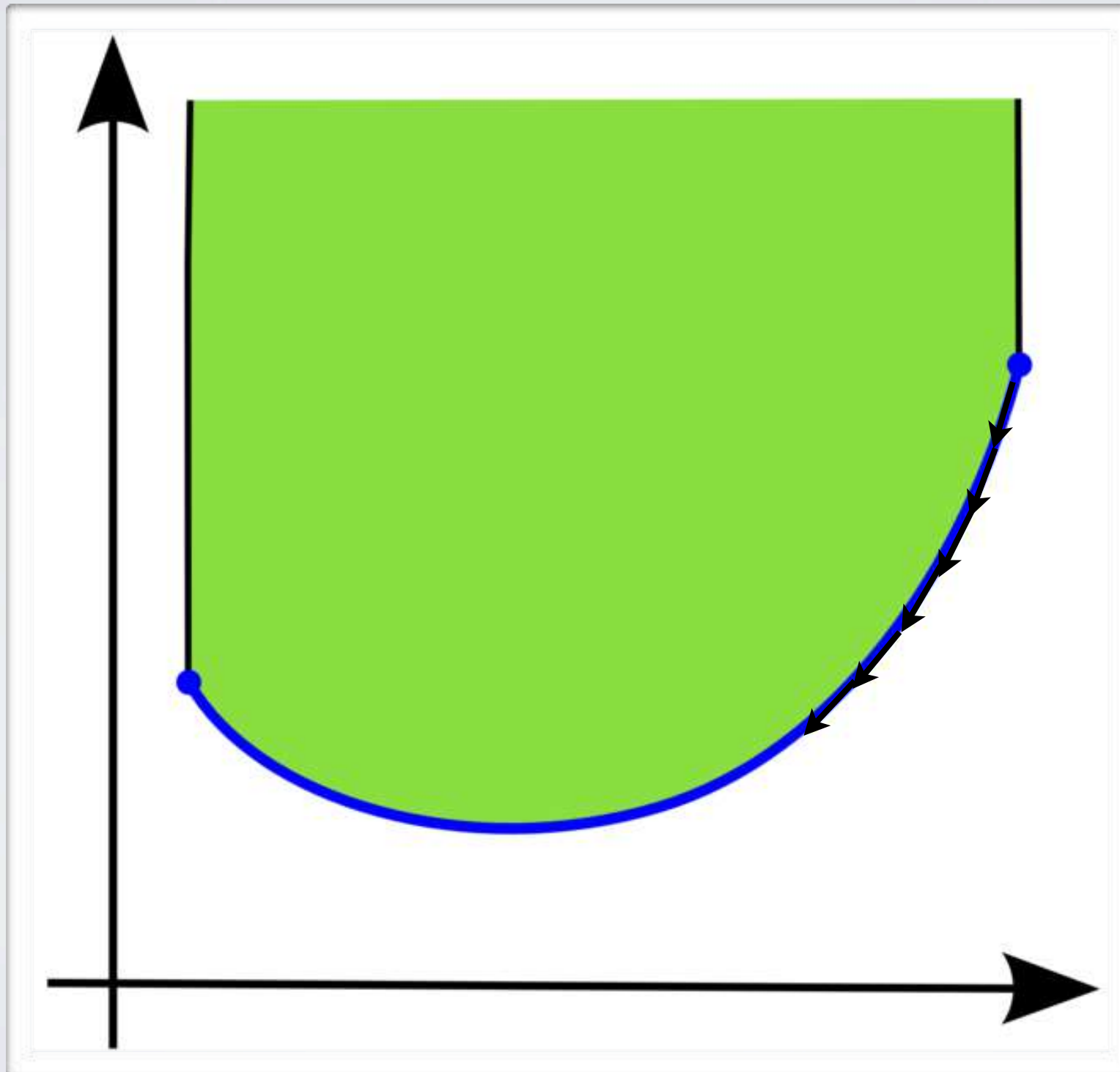


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MACHINE LEARNING

Topics: gradient descent



Descent
direction

$$-\frac{\partial f(x)}{\partial x}$$

MACHINE LEARNING

Topics: gradient descent

- Gradient descent for empirical risk minimization

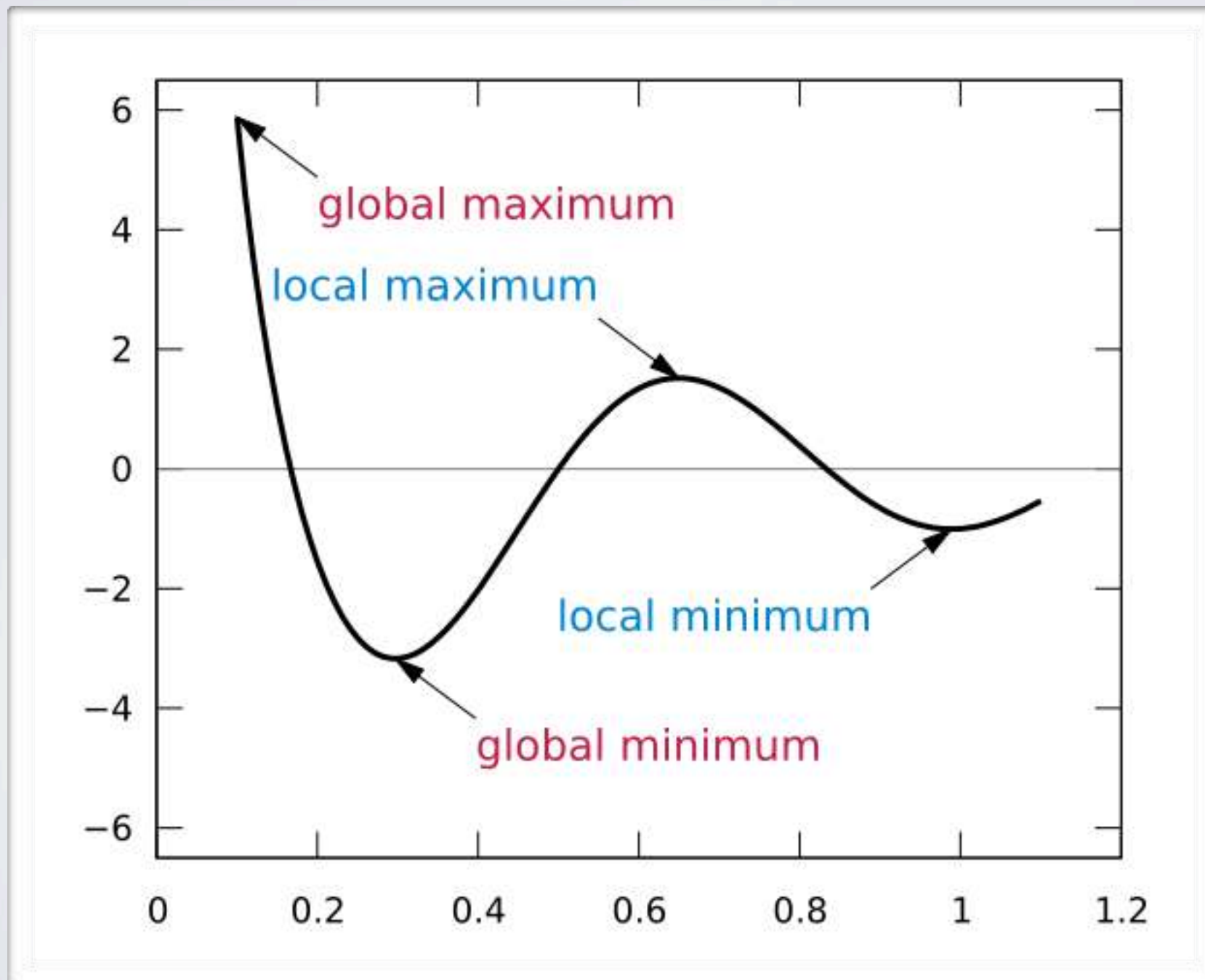
- ▶ initialize $\boldsymbol{\theta}$

- ▶ for N iterations

- $\Delta = -\frac{1}{T} \sum_t \nabla_{\boldsymbol{\theta}} l(f(\mathbf{x}^{(t)}; \boldsymbol{\theta}), y^{(t)}) - \lambda \nabla_{\boldsymbol{\theta}} \Omega(\boldsymbol{\theta})$
- $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha \Delta$

MACHINE LEARNING

Topics: local and global optima



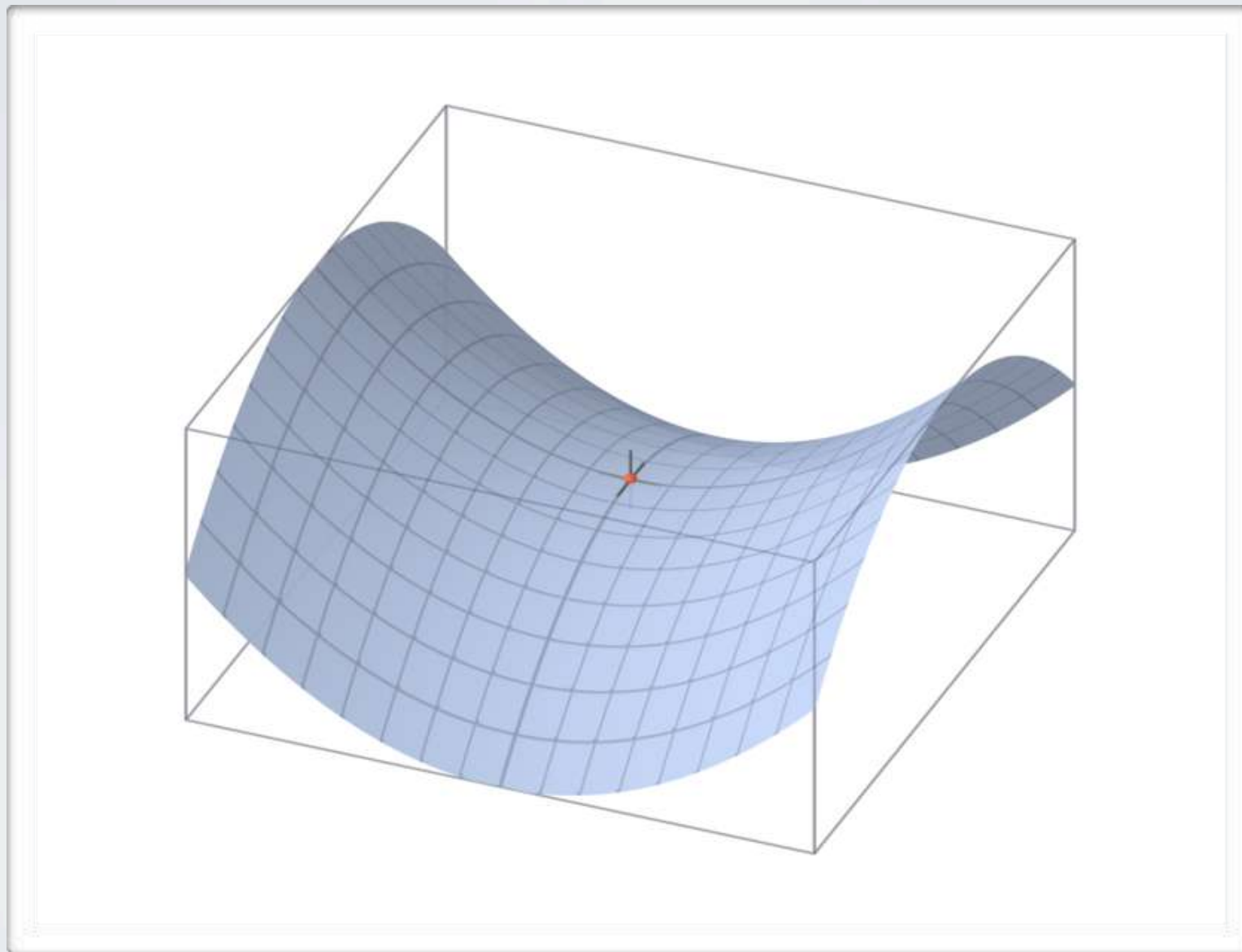
MACHINE LEARNING

Topics: critical points, local optima, saddle point, curvature

- Critical points: $\{\mathbf{x} \in \mathbb{R}^d \mid \nabla_{\mathbf{x}} f(\mathbf{x}) = 0\}$
- Curvature in direction \mathbf{v} : $\mathbf{v}^\top \nabla_{\mathbf{x}}^2 f(\mathbf{x}) \mathbf{v}$
- Types of critical points:
 - ▶ local minima: $\mathbf{v}^\top \nabla_{\mathbf{x}}^2 f(\mathbf{x}) \mathbf{v} > 0 \quad \forall \mathbf{v}$ (i.e. $\nabla_{\mathbf{x}}^2 f(\mathbf{x})$ positive definite)
 - ▶ local maxima: $\mathbf{v}^\top \nabla_{\mathbf{x}}^2 f(\mathbf{x}) \mathbf{v} < 0 \quad \forall \mathbf{v}$ (i.e. $\nabla_{\mathbf{x}}^2 f(\mathbf{x})$ negative definite)
 - ▶ saddle point: curvature is positive in certain directions and negative in others

MACHINE LEARNING

Topics: saddle point



MACHINE LEARNING

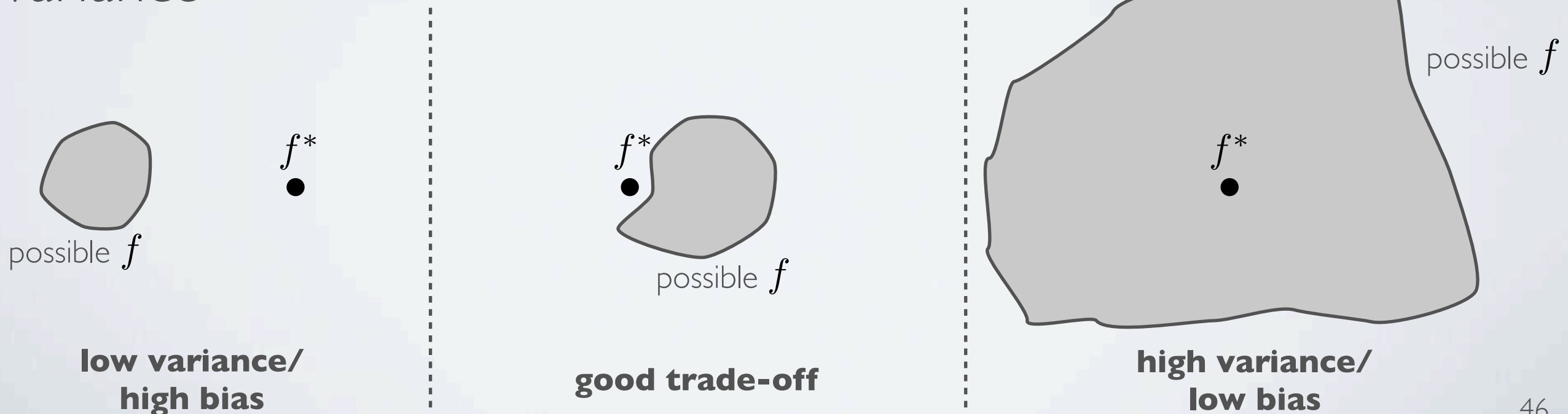
Topics: stochastic gradient descent

- Algorithm that performs updates after each example
 - initialize θ
 - for N iterations
 - for each training example $(\mathbf{x}^{(t)}, y^{(t)})$
 - ✓ $\Delta = -\nabla_{\theta} l(f(\mathbf{x}^{(t)}; \theta), y^{(t)}) - \lambda \nabla_{\theta} \Omega(\theta)$
 - ✓ $\theta \leftarrow \theta + \alpha \Delta$

MACHINE LEARNING

Topics: bias-variance trade-off

- Variance of trained model: does it vary a lot if the training set changes
- Bias of trained model: is the average model close to the true solution
- Generalization error can be seen as the sum of bias and the variance



MACHINE LEARNING

Topics: parametric vs. non-parametric

- Parametric model: its capacity is fixed and does not increase with the amount of training data
 - examples: linear classifier, neural network with fixed number of hidden units, etc.
- Non-parametric model: the capacity increases with the amount of training data
 - examples: k nearest neighbors classifier, neural network with adaptable hidden layer size, etc.