

lecture 5: learning

deep learning for vision

Yannis Avrithis

Inria Rennes-Bretagne Atlantique

Rennes, Nov. 2017 – Jan. 2018



outline

- machine learning
- binary classification
- binary classification, again
- multi-class classification
- regression
- multiple layers

machine learning

machine learning

supervised learning

- learn to map an input to a target output, which can be discrete (**classification**) or continuous (**regression**)

unsupervised learning

- learn a compact representation of the data that can be useful for other tasks, e.g. density estimation, clustering, sampling, dimension reduction, manifold learning
- but: in many cases, labels can be obtained automatically, transforming an unsupervised task to supervised
- also: semi-supervised, weakly supervised, ambiguous/noisy labels, self-supervised *etc.*

reinforcement learning

- learn to select actions, supervised by occasional rewards
- not studied here

machine learning

supervised learning

- learn to map an input to a target output, which can be discrete (**classification**) or continuous (**regression**)

unsupervised learning

- learn a compact representation of the data that can be useful for other tasks, e.g. density estimation, clustering, sampling, dimension reduction, manifold learning
- but: in many cases, labels can be obtained automatically, transforming an unsupervised task to supervised
- also: semi-supervised, weakly supervised, ambiguous/noisy labels, self-supervised *etc.*

reinforcement learning

- learn to select actions, supervised by occasional rewards
- not studied here

machine learning

supervised learning

- learn to map an input to a target output, which can be discrete (**classification**) or continuous (**regression**)

unsupervised learning

- learn a compact representation of the data that can be useful for other tasks, e.g. density estimation, clustering, sampling, dimension reduction, manifold learning
- but: in many cases, labels can be obtained automatically, transforming an unsupervised task to supervised
- also: semi-supervised, weakly supervised, ambiguous/noisy labels, self-supervised *etc.*

reinforcement learning

- learn to select actions, supervised by occasional rewards
- not studied here

machine learning

supervised learning

- learn to map an input to a target output, which can be discrete (**classification**) or continuous (**regression**)

unsupervised learning

- learn a compact representation of the data that can be useful for other tasks, e.g. density estimation, clustering, sampling, dimension reduction, manifold learning
- but: in many cases, labels can be obtained automatically, transforming an unsupervised task to supervised
- also: semi-supervised, weakly supervised, ambiguous/noisy labels, self-supervised *etc.*

reinforcement learning

- learn to select actions, supervised by occasional rewards
- not studied here

main objective

- through a learning task/objective that may be unimportant, we are primarily interested in learning good **representations** for computer vision tasks
- we are interested in **parametric** models where we learn a fixed set of parameters, rather than **non-parametric**, where training data are memorized
- we are interested in learning **explicit mappings** from raw input to representation, rather than constructing a representation of an entire dataset that is hard to extend to new samples
- we may occasionally use “**hand-crafted**” features or matching methods, but with the objective of learning better ones

main objective

- through a learning task/objective that may be unimportant, we are primarily interested in learning good **representations** for computer vision tasks
- we are interested in **parametric** models where we learn a fixed set of parameters, rather than **non-parametric**, where training data are memorized
- we are interested in learning **explicit mappings** from raw input to representation, rather than constructing a representation of an entire dataset that is hard to extend to new samples
- we may occasionally use “**hand-crafted**” features or matching methods, but with the objective of learning better ones

main objective

- through a learning task/objective that may be unimportant, we are primarily interested in learning good **representations** for computer vision tasks
- we are interested in **parametric** models where we learn a fixed set of parameters, rather than **non-parametric**, where training data are memorized
- we are interested in learning **explicit mappings** from raw input to representation, rather than constructing a representation of an entire dataset that is hard to extend to new samples
- we may occasionally use “**hand-crafted**” features or matching methods, but with the objective of learning better ones

main objective

- through a learning task/objective that may be unimportant, we are primarily interested in learning good **representations** for computer vision tasks
- we are interested in **parametric** models where we learn a fixed set of parameters, rather than **non-parametric**, where training data are memorized
- we are interested in learning **explicit mappings** from raw input to representation, rather than constructing a representation of an entire dataset that is hard to extend to new samples
- we may occasionally use “**hand-crafted**” features or matching methods, but with the objective of learning better ones

learning and optimization

- in a supervised setting, given a **distribution** p of input data \mathbf{x} and target outputs t we want to learn the parameters $\boldsymbol{\theta}$ of a **prediction model** $f(\mathbf{x}, \boldsymbol{\theta})$ by minimizing the **risk** (objective, cost, or error) function

$$E^*(\boldsymbol{\theta}) := \mathbb{E}_{(\mathbf{x}, t) \sim p} L(f(\mathbf{x}; \boldsymbol{\theta}), t)$$

where L is a per-sample **loss function** that compares predictions $f(\mathbf{x}; \boldsymbol{\theta})$ to targets t

- since the true distribution p is unknown, we use the empirical distribution \hat{p} of a training set $\mathbf{x}_1, \dots, \mathbf{x}_m$ with associated target outputs t_1, \dots, t_n and minimize instead the **empirical risk**

$$E(\boldsymbol{\theta}) := \mathbb{E}_{(\mathbf{x}, t) \sim \hat{p}} L(f(\mathbf{x}; \boldsymbol{\theta}), t) = \frac{1}{n} \sum_{i=1}^n L(f(\mathbf{x}_i; \boldsymbol{\theta}), t_i),$$

converting the learning problem to **optimization**

learning and optimization

- in a supervised setting, given a **distribution** p of input data \mathbf{x} and target outputs t we want to learn the parameters $\boldsymbol{\theta}$ of a **prediction model** $f(\mathbf{x}, \boldsymbol{\theta})$ by minimizing the **risk** (objective, cost, or error) function

$$E^*(\boldsymbol{\theta}) := \mathbb{E}_{(\mathbf{x}, t) \sim p} L(f(\mathbf{x}; \boldsymbol{\theta}), t)$$

where L is a per-sample **loss function** that compares predictions $f(\mathbf{x}; \boldsymbol{\theta})$ to targets t

- since the true distribution p is unknown, we use the empirical distribution \hat{p} of a training set $\mathbf{x}_1, \dots, \mathbf{x}_m$ with associated target outputs t_1, \dots, t_n and minimize instead the **empirical risk**

$$E(\boldsymbol{\theta}) := \mathbb{E}_{(\mathbf{x}, t) \sim \hat{p}} L(f(\mathbf{x}; \boldsymbol{\theta}), t) = \frac{1}{n} \sum_{i=1}^n L(f(\mathbf{x}_i; \boldsymbol{\theta}), t_i),$$

converting the learning problem to **optimization**

however

- the empirical risk is prone to **overfitting** the training set (even memorizing it), if non-parametric
- we need to balance our model's **capacity** with the amount of training data, find ways to **regularize** the objective function and use a **validation** set to select **hyperparameters** so that our model **generalizes** on new samples
- the ideal loss function may be hard to optimize, so we have to use a **surrogate** loss function that may as well improve generalization
- still, all functions encountered are **non-convex** so we can only hope for local minima

however

- the empirical risk is prone to **overfitting** the training set (even memorizing it), if non-parametric
- we need to balance our model's **capacity** with the amount of training data, find ways to **regularize** the objective function and use a **validation** set to select **hyperparameters** so that our model **generalizes** on new samples
- the ideal loss function may be hard to optimize, so we have to use a **surrogate** loss function that may as well improve generalization
- still, all functions encountered are **non-convex** so we can only hope for local minima

however

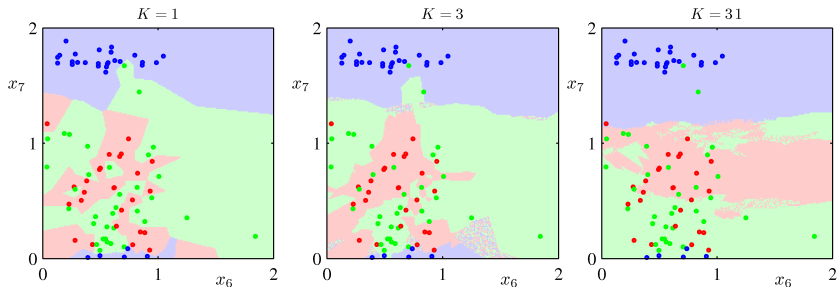
- the empirical risk is prone to **overfitting** the training set (even memorizing it), if non-parametric
- we need to balance our model's **capacity** with the amount of training data, find ways to **regularize** the objective function and use a **validation** set to select **hyperparameters** so that our model **generalizes** on new samples
- the ideal loss function may be hard to optimize, so we have to use a **surrogate** loss function that may as well improve generalization
- still, all functions encountered are **non-convex** so we can only hope for local minima

however

- the empirical risk is prone to **overfitting** the training set (even memorizing it), if non-parametric
- we need to balance our model's **capacity** with the amount of training data, find ways to **regularize** the objective function and use a **validation** set to select **hyperparameters** so that our model **generalizes** on new samples
- the ideal loss function may be hard to optimize, so we have to use a **surrogate** loss function that may as well improve generalization
- still, all functions encountered are **non-convex** so we can only hope for local minima

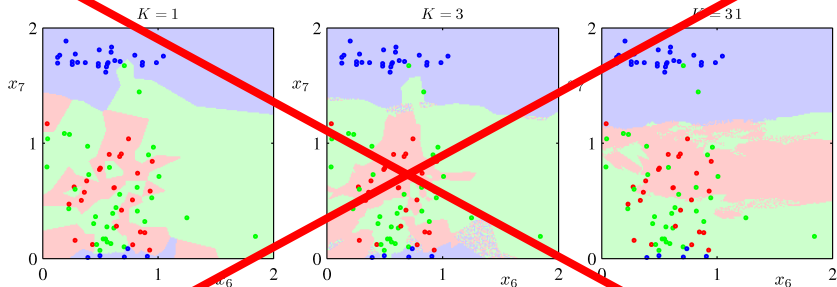
binary classification

k -nearest neighbor classifier



- an input sample is classified by majority voting (ties broken at random) over the class labels of its k -nearest neighbors in the training set
- no training needed, but prediction can be slow
- we are **not interested** in such an approach (**for now**) because it gives us no opportunity to learn a representation

k -nearest neighbor classifier



- an input sample is classified by majority voting (ties broken at random) over the class labels of its k -nearest neighbors in the training set
- no training needed, but prediction can be slow
- we are **not interested** in such an approach (**for now**) because it gives us no opportunity to learn a representation

perceptron

[Rosenblatt 1962]



- perceptron, as introduced by Rosenblatt, refers to a wide range of network architectures, learning algorithms and hardware implementations
- due to Minsky and Papert, perceptron now refers to a binary linear classifier and an algorithm
- let's have a closer look at that

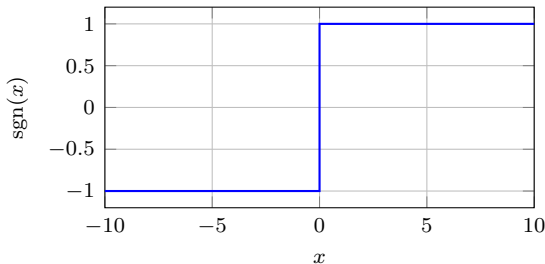
perceptron model

- given input $\mathbf{x} \in \mathbb{R}^d$, the perceptron is a generalized linear model

$$y = f(\mathbf{x}; \mathbf{w}) := \text{sgn}(\mathbf{w}^\top \mathbf{x})$$

where $\mathbf{w} \in \mathbb{R}^d$ is a **weight (parameter)** vector to be learned, and

$$\text{sgn}(x) := \begin{cases} +1, & x \geq 0 \\ -1, & x < 0 \end{cases}$$



perceptron algorithm

- an input \mathbf{x} with output $y = f(\mathbf{x}; \mathbf{w})$ is **classified** to class C_1 if $y = 1$ and to C_2 if $y = -1$
- given a training sample $\mathbf{x} \in \mathbb{R}^d$ and a target variable $s \in \{-1, 1\}$, \mathbf{x} is **correctly** classified iff output $y = f(\mathbf{x}; \mathbf{w})$ equals s , i.e. $sy > 0$
- we are given **training samples** $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$ and **target variables** $s_1, \dots, s_n \in \{-1, 1\}$
- starting from an initial parameter vector $\mathbf{w}^{(0)}$, the algorithm learns by iteratively choosing a random sample \mathbf{x}_i that is misclassified and updating

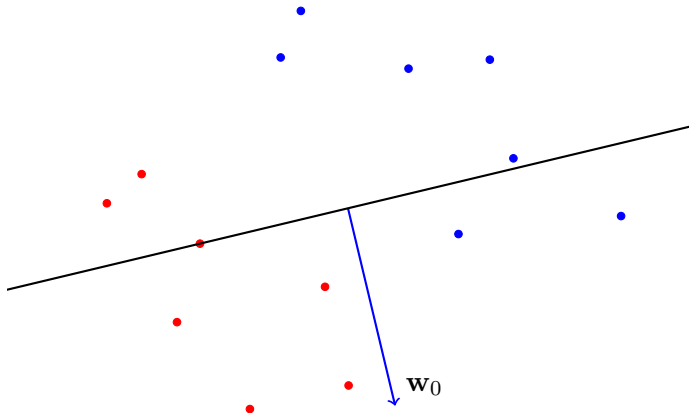
$$\mathbf{w}^{(\tau+1)} \leftarrow \mathbf{w}^{(\tau)} + \epsilon s_i \mathbf{x}_i$$

perceptron algorithm

- an input \mathbf{x} with output $y = f(\mathbf{x}; \mathbf{w})$ is **classified** to class C_1 if $y = 1$ and to C_2 if $y = -1$
- given a training sample $\mathbf{x} \in \mathbb{R}^d$ and a target variable $s \in \{-1, 1\}$, \mathbf{x} is **correctly** classified iff output $y = f(\mathbf{x}; \mathbf{w})$ equals s , i.e. $sy > 0$
- we are given **training samples** $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$ and **target variables** $s_1, \dots, s_n \in \{-1, 1\}$
- starting from an initial parameter vector $\mathbf{w}^{(0)}$, the algorithm learns by iteratively choosing a random sample \mathbf{x}_i that is misclassified and updating

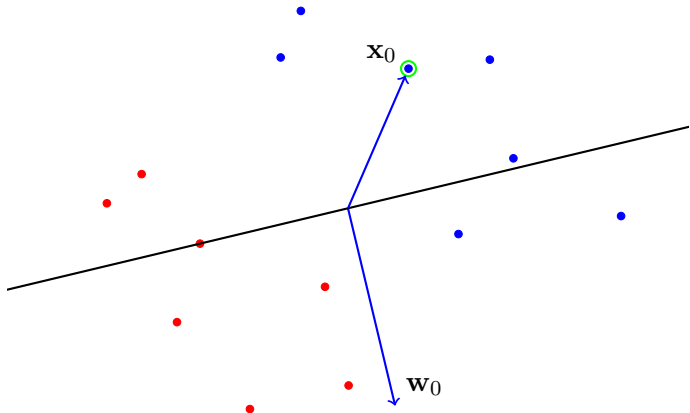
$$\mathbf{w}^{(\tau+1)} \leftarrow \mathbf{w}^{(\tau)} + \epsilon s_i \mathbf{x}_i$$

perceptron algorithm



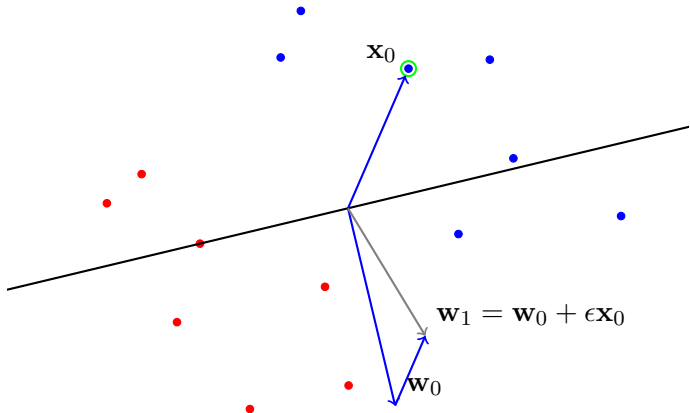
- initial parameter vector w_0 , normal to the decision boundary and pointing to the region to be classified as blue (+)

perceptron algorithm



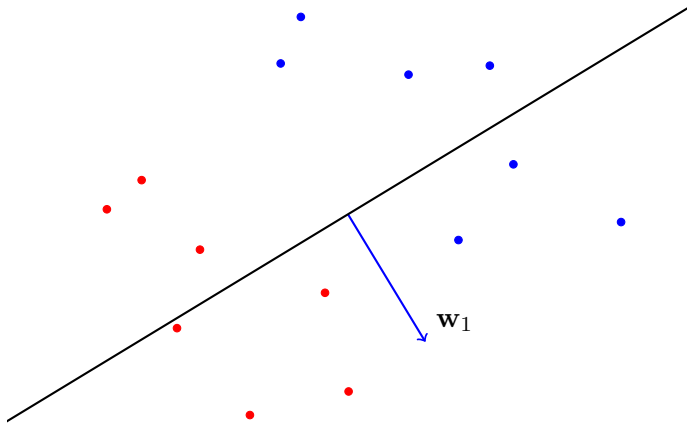
- pick a random point x_0 that is misclassified: blue (+) in red (-) region

perceptron algorithm



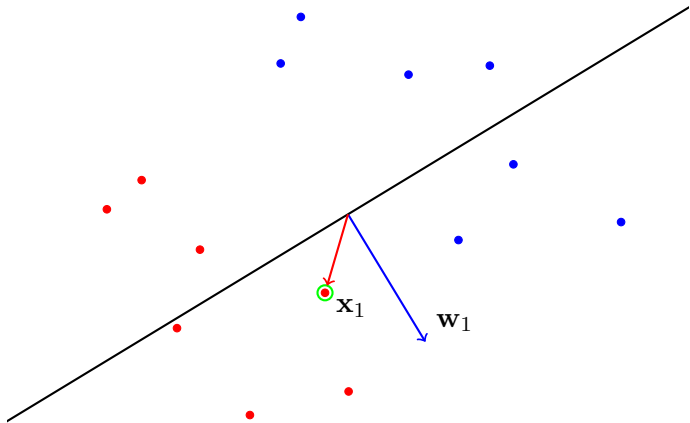
- because x_0 is blue and w is pointing at blue, we **add** ϵx_0 to w_0

perceptron algorithm



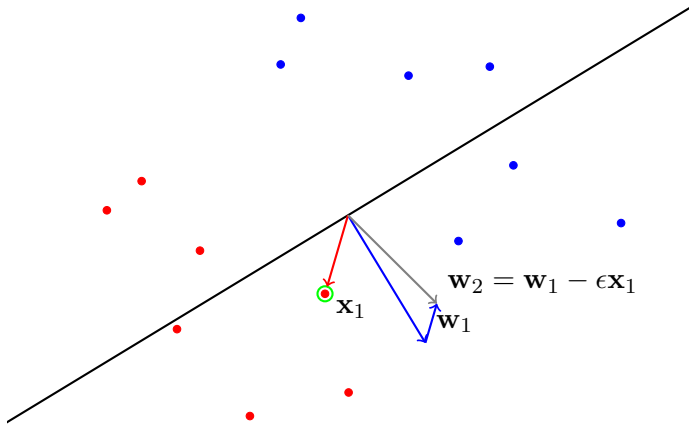
- with the new parameter vector w_1 , the decision boundary is updated

perceptron algorithm



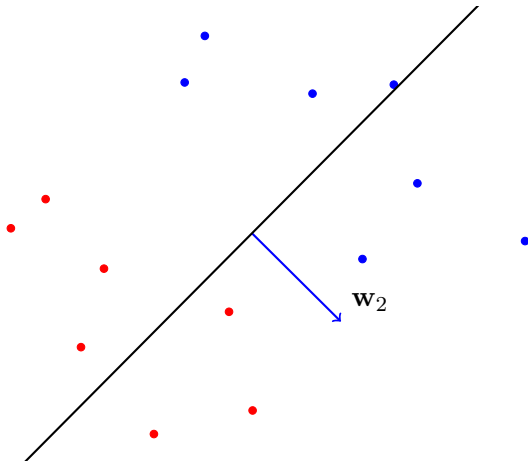
- pick a new random point x_1 that is misclassified: red in blue region

perceptron algorithm



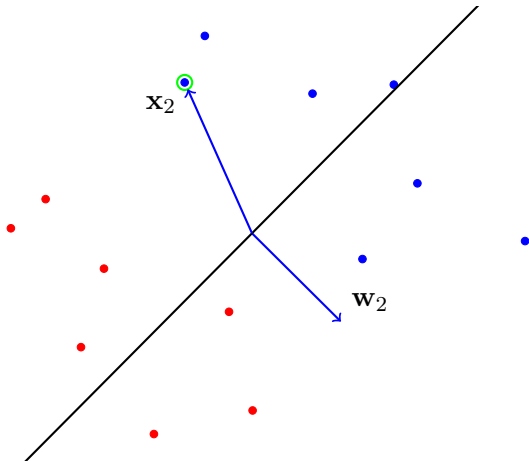
- because x_1 is red and w is pointing at blue, we **subtract** ϵx_1 from w_1

perceptron algorithm



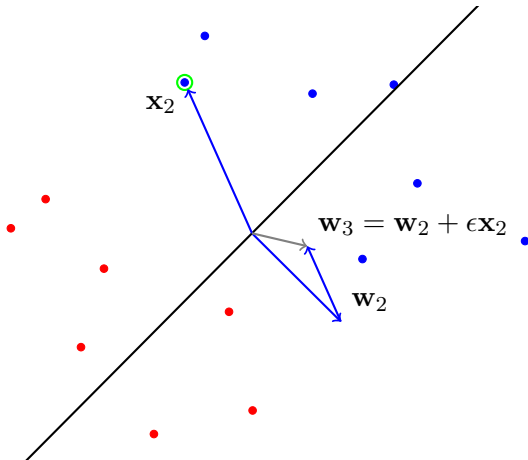
- with the new w_2 , the decision boundary is updated again

perceptron algorithm



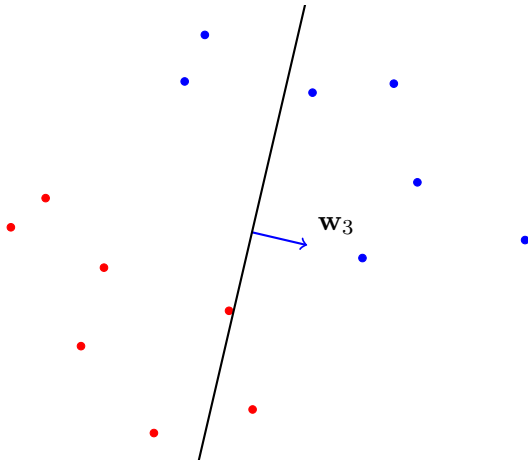
- again, random point x_2 , blue misclassified in red region

perceptron algorithm



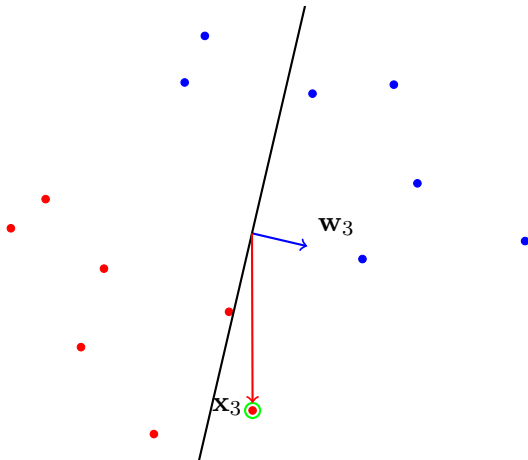
- and we add ϵx_2 to w_2

perceptron algorithm



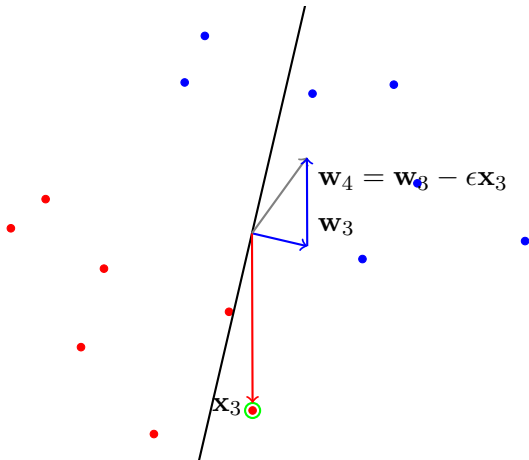
● now at w_3

perceptron algorithm



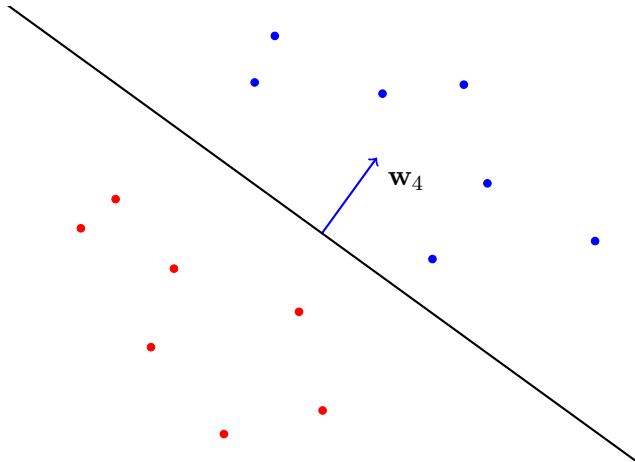
- one last random point x_3 , red in blue region

perceptron algorithm



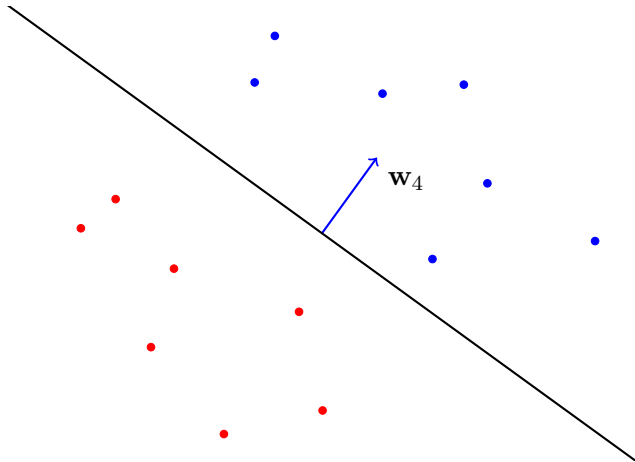
- and we subtract

perceptron algorithm



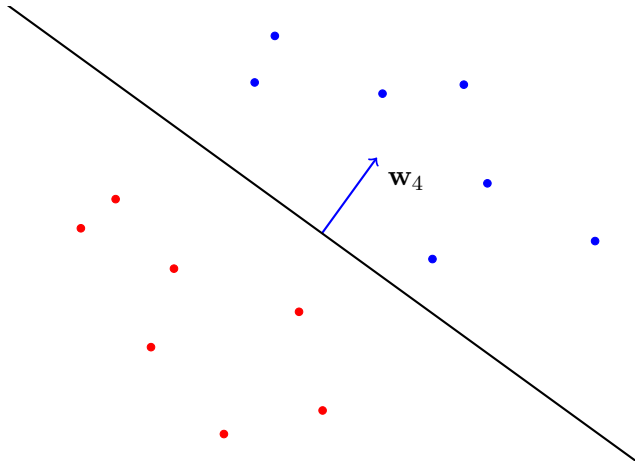
- finally at w_4 , all points are classified correctly

perceptron algorithm



- finally at w_4 , all points are classified correctly

perceptron algorithm



- finally at w_4 , all points are classified correctly

“details”

- we do not say anything about **convergence** now; we will discuss later
- there is one more parameter to be learned: a more general linear model would be

$$y = f(\mathbf{x}; \mathbf{w}, b) := \text{sgn}(\mathbf{w}^\top \mathbf{x} + b)$$

where $\mathbf{w} \in \mathbb{R}^d$ is a **weight** vector, and b is a **bias**

- this is often omitted because we can just add an extra dimension $d+1$ to \mathbf{x} and \mathbf{w} and always set $x_{d+1} = 1$; then w_{d+1} plays the role of bias
- but in many cases weights and bias need separate treatment
- it is common to use a (fixed) set of **basis functions** on the raw input and write $\phi(\mathbf{x})$ instead of \mathbf{x}
- the linear model itself is not affected by this choice, but the classifier is; again, we discuss this later

“details”

- we do not say anything about **convergence** now; we will discuss later
- there is one more parameter to be learned: a more general linear model would be

$$y = f(\mathbf{x}; \mathbf{w}, b) := \text{sgn}(\mathbf{w}^\top \mathbf{x} + b)$$

where $\mathbf{w} \in \mathbb{R}^d$ is a **weight** vector, and b is a **bias**

- this is often omitted because we can just add an extra dimension $d+1$ to \mathbf{x} and \mathbf{w} and always set $x_{d+1} = 1$; then w_{d+1} plays the role of bias
- but in many cases weights and bias need separate treatment
- it is common to use a (fixed) set of **basis functions** on the raw input and write $\phi(\mathbf{x})$ instead of \mathbf{x}
- the linear model itself is not affected by this choice, but the classifier is; again, we discuss this later

“details”

- we do not say anything about **convergence** now; we will discuss later
- there is one more parameter to be learned: a more general linear model would be

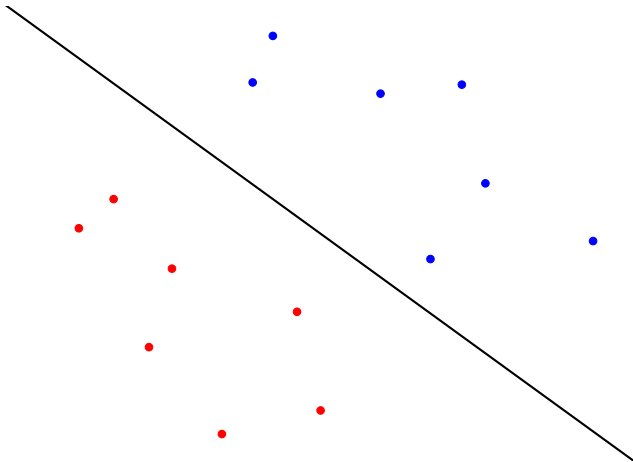
$$y = f(\mathbf{x}; \mathbf{w}, b) := \text{sgn}(\mathbf{w}^\top \mathbf{x} + b)$$

where $\mathbf{w} \in \mathbb{R}^d$ is a **weight** vector, and b is a **bias**

- this is often omitted because we can just add an extra dimension $d+1$ to \mathbf{x} and \mathbf{w} and always set $x_{d+1} = 1$; then w_{d+1} plays the role of bias
- but in many cases weights and bias need separate treatment
- it is common to use a (fixed) set of **basis functions** on the raw input and write $\phi(\mathbf{x})$ instead of \mathbf{x}
- the linear model itself is not affected by this choice, but the classifier is; again, we discuss this later

support vector machine (SVM)

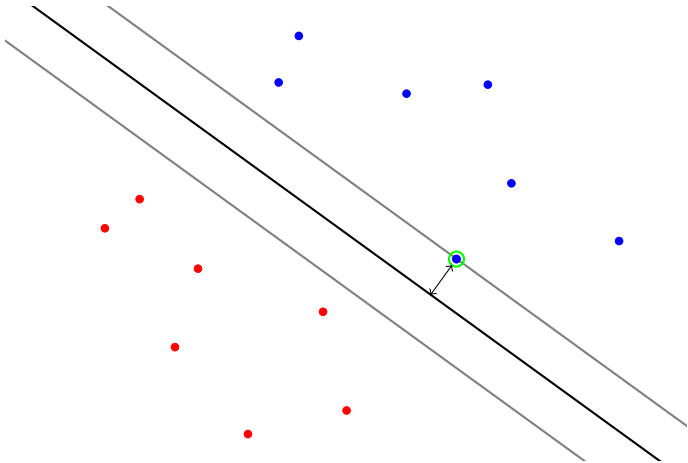
[Boser et al. 1992]



- given a decision boundary that classifies all points correctly, define the **margin** as its distance to the nearest point

support vector machine (SVM)

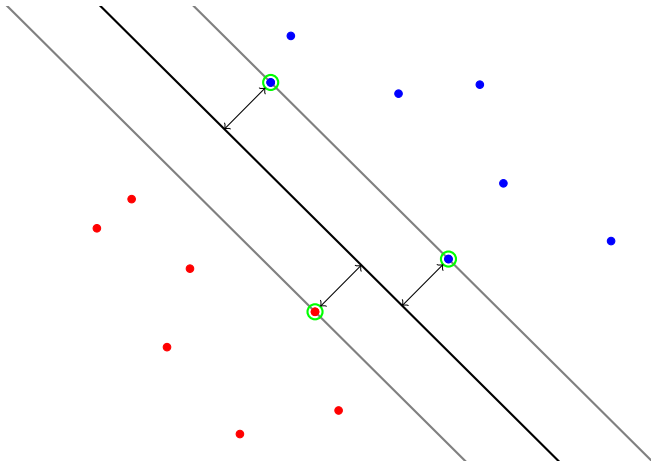
[Boser et al. 1992]



- this was not optimal in the case of perceptron

support vector machine (SVM)

[Boser et al. 1992]



- there is another decision boundary for which the margin is maximum; the vectors at this distance are the **support vectors**

SVM model

- there is now an explicit bias parameter b , but otherwise the SVM model is the same: **activation**

$$a := \mathbf{w}^\top \mathbf{x} + b$$

and **output**

$$y = f(\mathbf{x}; \mathbf{w}, b) := \text{sgn}(\mathbf{w}^\top \mathbf{x} + b) = \text{sgn}(a)$$

- again, an input \mathbf{x} with $a = \mathbf{w}^\top \mathbf{x} + b$ and output $y = \text{sgn}(a)$ is **classified** to class C_1 if $y = 1$ ($a \geq 0$) and to C_2 if $y = -1$ ($a < 0$)
- again, given a training sample \mathbf{x} and a target variable s , \mathbf{x} is **correctly** classified iff $sy > 0$, i.e. $sa = s(\mathbf{w}^\top \mathbf{x} + b) \geq 0$
- we are given **training samples** $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$ and **target variables** $s_1, \dots, s_n \in \{-1, 1\}$

SVM model

- there is now an explicit bias parameter b , but otherwise the SVM model is the same: **activation**

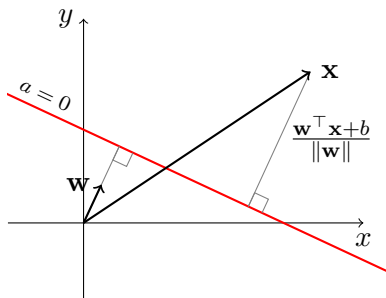
$$a := \mathbf{w}^\top \mathbf{x} + b$$

and **output**

$$y = f(\mathbf{x}; \mathbf{w}, b) := \text{sgn}(\mathbf{w}^\top \mathbf{x} + b) = \text{sgn}(a)$$

- again, an input \mathbf{x} with $a = \mathbf{w}^\top \mathbf{x} + b$ and output $y = \text{sgn}(a)$ is **classified** to class C_1 if $y = 1$ ($a \geq 0$) and to C_2 if $y = -1$ ($a < 0$)
- again, given a training sample \mathbf{x} and a target variable s , \mathbf{x} is **correctly** classified iff $sy > 0$, i.e. $sa = s(\mathbf{w}^\top \mathbf{x} + b) \geq 0$
- we are given **training samples** $\mathbf{x}_1, \dots, \mathbf{x}_n \in \mathbb{R}^d$ and **target variables** $s_1, \dots, s_n \in \{-1, 1\}$

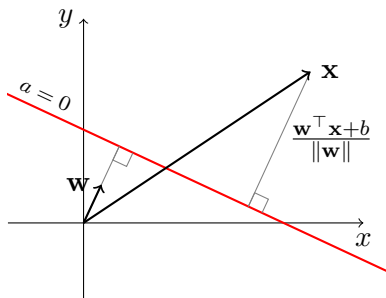
margin



- the distance of \mathbf{x} to the boundary is $|\mathbf{w}^\top \mathbf{x} + b|/\|\mathbf{w}\|$
- this is $s(\mathbf{w}^\top \mathbf{x} + b)/\|\mathbf{w}\|$ if it is classified correctly
- if all points are classified correctly, then the margin is

$$\frac{1}{\|\mathbf{w}\|} \min_i (s_i(\mathbf{w}^\top \mathbf{x}_i + b))$$

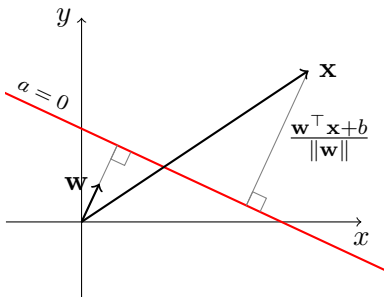
margin



- the distance of \mathbf{x} to the boundary is $|\mathbf{w}^\top \mathbf{x} + b|/\|\mathbf{w}\|$
- this is $s(\mathbf{w}^\top \mathbf{x} + b)/\|\mathbf{w}\|$ if it is classified correctly
- if all points are classified correctly, then the margin is

$$\frac{1}{\|\mathbf{w}\|} \min_i (s_i(\mathbf{w}^\top \mathbf{x}_i + b))$$

margin



- the distance of \mathbf{x} to the boundary is $|\mathbf{w}^\top \mathbf{x} + b|/\|\mathbf{w}\|$
- this is $s(\mathbf{w}^\top \mathbf{x} + b)/\|\mathbf{w}\|$ if it is classified correctly
- if all points are classified correctly, then the margin is

$$\frac{1}{\|\mathbf{w}\|} \min_i (s_i(\mathbf{w}^\top \mathbf{x}_i + b))$$

maximum margin

- the margin is **invariant** to scaling of \mathbf{w} and b , so we choose $s_i a_i = s_i(\mathbf{w}^\top \mathbf{x}_i + b) = 1$ for the point that is nearest to the boundary
- then, the margin is maximized by

$$\arg \min_{\mathbf{w}, b} \frac{1}{2} \|\mathbf{w}\|^2$$

subject to

$$s_i a_i \geq 1$$

for all training samples i , where $a_i := \mathbf{w}^\top \mathbf{x}_i + b$

- this is a **quadratic programming** problem

maximum margin

- the margin is **invariant** to scaling of \mathbf{w} and b , so we choose $s_i a_i = s_i(\mathbf{w}^\top \mathbf{x}_i + b) = 1$ for the point that is nearest to the boundary
- then, the margin is maximized by

$$\arg \min_{\mathbf{w}, b} \frac{1}{2} \|\mathbf{w}\|^2$$

subject to

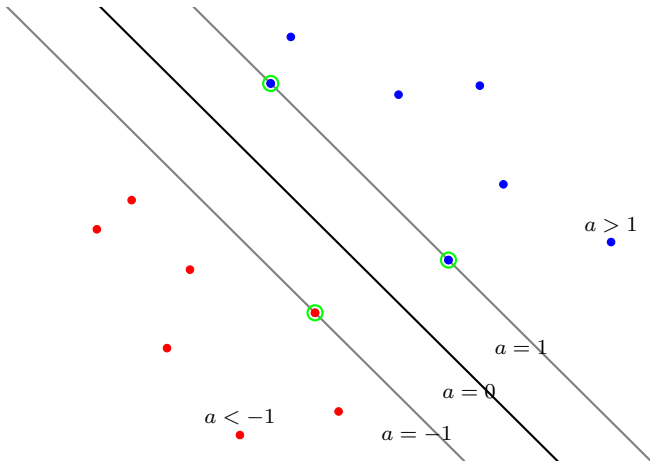
$$s_i a_i \geq 1$$

for all training samples i , where $a_i := \mathbf{w}^\top \mathbf{x}_i + b$

- this is a **quadratic programming** problem

overlapping class distributions

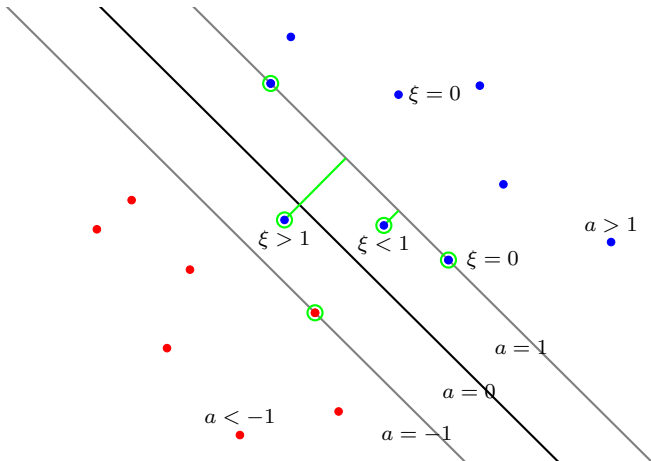
[Cortes and Vapnik 1995]



- assuming that all training samples can be correctly classified is unrealistic

overlapping class distributions

[Cortes and Vapnik 1995]



- introduce **slack variables** $\xi_i \geq 0$ that should be minimized; $\xi_i \leq 1$ for correctly classified samples, $\xi_i = 0$ beyond the margin

overlapping class distributions

- the constraints $s_i a_i \geq 1$ are now replaced by

$$s_i a_i \geq 1 - \xi_i$$

$$\xi_i \geq 0$$

where $a_i := \mathbf{w}^\top \mathbf{x}_i + b$

- and the objective $\arg \min_{\mathbf{w}, b} \frac{1}{2} \|\mathbf{w}\|^2$ is replaced by

$$\arg \min_{\mathbf{w}, b} \frac{C}{n} \sum_{i=1}^n \xi_i + \frac{1}{2} \|\mathbf{w}\|^2$$

where hyperparameter C controls the trade-off between slack variables and margin

overlapping class distributions

- the constraints $s_i a_i \geq 1$ are now replaced by

$$s_i a_i \geq 1 - \xi_i$$

$$\xi_i \geq 0$$

where $a_i := \mathbf{w}^\top \mathbf{x}_i + b$

- and the objective $\arg \min_{\mathbf{w}, b} \frac{1}{2} \|\mathbf{w}\|^2$ is replaced by

$$\arg \min_{\mathbf{w}, b} \frac{C}{n} \sum_{i=1}^n \xi_i + \frac{1}{2} \|\mathbf{w}\|^2$$

where hyperparameter C controls the trade-off between slack variables and margin

“details”

- we do not say anything about how to solve this problem yet
- the standard treatment of SVM introduces Lagrange multipliers for the constraints and results in the **dual** formulation where coordinates only appear in dot products
- at this point, writing $\phi(\mathbf{x})$ instead of \mathbf{x} , gives rise to

$$\kappa(\mathbf{x}, \mathbf{y}) = \phi(\mathbf{x})^\top \phi(\mathbf{y})$$

- this **kernel trick** can make the classifier nonlinear assuming an appropriate positive-definite kernel function κ for the problem at hand
- we are **not interested** in this approach here because
 - we want to learn a parametric model and discard the training data after learning
 - we do not want to design a matching function κ any more than designing the representation ϕ ; we want to learn from raw data

“details”

- we do not say anything about how to solve this problem yet
- the standard treatment of SVM introduces Lagrange multipliers for the constraints and results in the **dual** formulation where coordinates only appear in dot products
- at this point, writing $\phi(\mathbf{x})$ instead of \mathbf{x} , gives rise to

$$\kappa(\mathbf{x}, \mathbf{y}) = \phi(\mathbf{x})^\top \phi(\mathbf{y})$$

- this **kernel trick** can make the classifier nonlinear assuming an appropriate positive-definite kernel function κ for the problem at hand
- we are **not interested** in this approach here because
 - we want to learn a parametric model and discard the training data after learning
 - we do not want to design a matching function κ any more than designing the representation ϕ ; we want to learn from raw data

“details”

- we do not say anything about how to solve this problem yet
- the standard treatment of SVM introduces Lagrange multipliers for the constraints and results in the **dual** formulation where coordinates only appear in dot products
- at this point, writing $\phi(\mathbf{x})$ instead of \mathbf{x} , gives rise to

$$k(\mathbf{x}, \mathbf{y}) = \phi(\mathbf{x})^T \phi(\mathbf{y})$$

- this **kernel trick** can make the classifier nonlinear assuming an appropriate positive-definite kernel function κ for the problem at hand
- we are **not interested** in this approach here because
 - we want to learn a parametric model and discard the training data after learning
 - we do not want to design a matching function κ any more than designing the representation ϕ ; we want to learn from raw data

(binary) logistic regression

[Cox 1958]

- again, activation (but here we omit the bias)

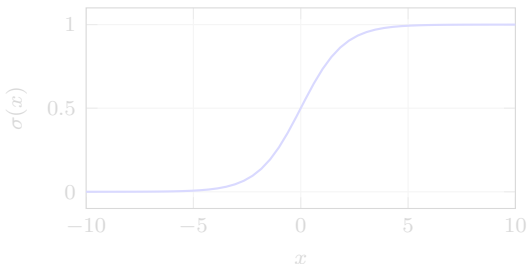
$$a = \mathbf{w}^\top \mathbf{x}$$

and output

$$y = f(\mathbf{x}; \mathbf{w}) := \sigma(\mathbf{w}^\top \mathbf{x}) = \sigma(a)$$

- but now we have a different nonlinearity: σ is the **sigmoid** function

$$\sigma(x) := \frac{1}{1 + e^{-x}}$$



(binary) logistic regression

[Cox 1958]

- again, activation (but here we omit the bias)

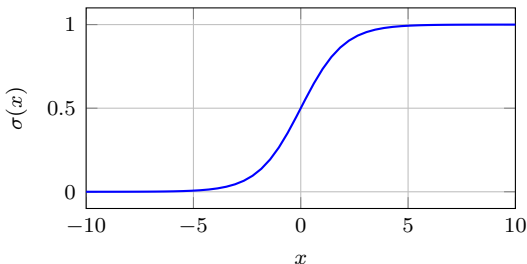
$$a = \mathbf{w}^\top \mathbf{x}$$

and output

$$y = f(\mathbf{x}; \mathbf{w}) := \sigma(\mathbf{w}^\top \mathbf{x}) = \sigma(a)$$

- but now we have a different nonlinearity: σ is the **sigmoid** function

$$\sigma(x) := \frac{1}{1 + e^{-x}}$$



probabilistic interpretation

- the output y represents the **posterior probability** of class C_1 given input \mathbf{x} , which by Bayes rule is

$$\begin{aligned} y = p(C_1|\mathbf{x}) &= \frac{p(\mathbf{x}|C_1)p(C_1)}{p(\mathbf{x}|C_1)p(C_1) + p(\mathbf{x}|C_2)p(C_2)} \\ &= \frac{1}{1 + e^{-a}} = \sigma(a) \end{aligned}$$

- here the activation a is defined to represent the **log-odds**

$$a = \ln \frac{p(C_1|\mathbf{x})}{p(C_2|\mathbf{x})} = \ln \frac{p(\mathbf{x}|C_1)p(C_1)}{p(\mathbf{x}|C_2)p(C_2)}$$

maximum likelihood

- we are given **training samples** $X = (\mathbf{x}_1, \dots, \mathbf{x}_n)$ with $\mathbf{x}_i \in \mathbb{R}^d$ and **target variables** $T = (t_1, \dots, t_n)$ with $t_i \in \{0, 1\}$
- **watch out:** target variables are in $\{0, 1\}$ here, not $\{-1, 1\}$
- the probabilistic interpretation allows us to define the learning objective: maximize the **likelihood** function

$$p(T|X, \mathbf{w}) = \prod_{i=1}^n y_i^{t_i} (1 - y_i)^{1-t_i}$$

- or, minimize the (average) **cross-entropy** error function

$$E(\mathbf{w}) := -\frac{1}{n} \sum_{i=1}^n (t_i \ln y_i + (1 - t_i) \ln(1 - y_i))$$

where $y_i = \sigma(a_i) = \sigma(\mathbf{w}^\top \mathbf{x}_i)$

maximum likelihood

- we are given **training samples** $X = (\mathbf{x}_1, \dots, \mathbf{x}_n)$ with $\mathbf{x}_i \in \mathbb{R}^d$ and **target variables** $T = (t_1, \dots, t_n)$ with $t_i \in \{0, 1\}$
- **watch out**: target variables are in $\{0, 1\}$ here, not $\{-1, 1\}$
- the probabilistic interpretation allows us to define the learning objective: maximize the **likelihood** function

$$p(T|X, \mathbf{w}) = \prod_{i=1}^n y_i^{t_i} (1 - y_i)^{1-t_i}$$

- or, minimize the (average) **cross-entropy** error function

$$E(\mathbf{w}) := -\frac{1}{n} \sum_{i=1}^n (t_i \ln y_i + (1 - t_i) \ln(1 - y_i))$$

where $y_i = \sigma(a_i) = \sigma(\mathbf{w}^\top \mathbf{x}_i)$

maximum likelihood

- we are given **training samples** $X = (\mathbf{x}_1, \dots, \mathbf{x}_n)$ with $\mathbf{x}_i \in \mathbb{R}^d$ and **target variables** $T = (t_1, \dots, t_n)$ with $t_i \in \{0, 1\}$
- **watch out**: target variables are in $\{0, 1\}$ here, not $\{-1, 1\}$
- the probabilistic interpretation allows us to define the learning objective: maximize the **likelihood** function

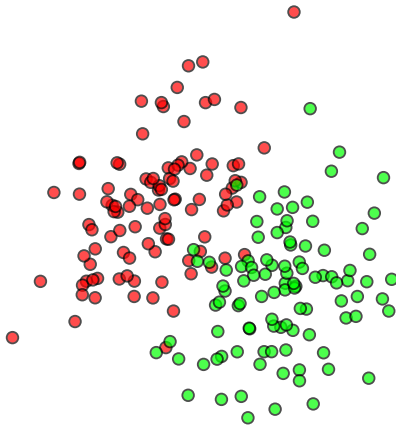
$$p(T|X, \mathbf{w}) = \prod_{i=1}^n y_i^{t_i} (1 - y_i)^{1-t_i}$$

- or, minimize the (average) **cross-entropy** error function

$$E(\mathbf{w}) := -\frac{1}{n} \sum_{i=1}^n (t_i \ln y_i + (1 - t_i) \ln(1 - y_i))$$

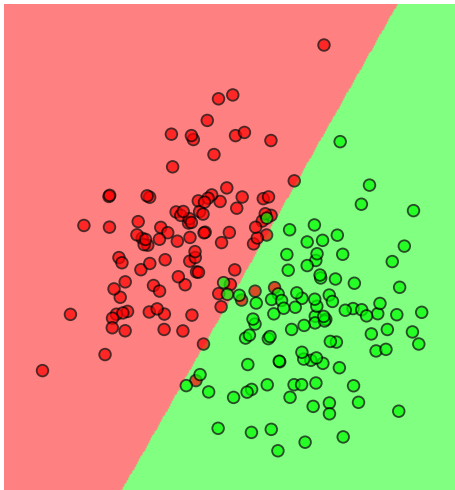
where $y_i = \sigma(a_i) = \sigma(\mathbf{w}^\top \mathbf{x}_i)$

binary classifiers



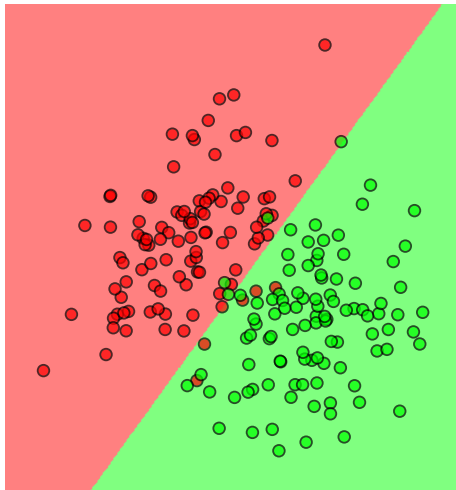
raw data

binary classifiers



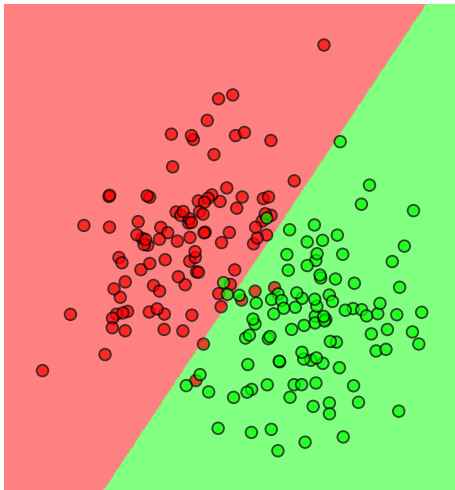
perceptron

binary classifiers



SVM

binary classifiers



logistic regression

binary classification, again

three solutions so far

	perceptron	SVM	logistic
objective	—	yes	yes
constraints	—	yes	—
regularizer	—	yes	—
algorithm	yes	—	—
probabilistic	—	—	yes

perceptron, again

- “choose a random sample i that is misclassified and update”

$$\mathbf{w}^{(\tau+1)} \leftarrow \mathbf{w}^{(\tau)} + \epsilon s_i \mathbf{x}_i$$

- given sample \mathbf{x}_i , if $s_i y_i > 0$ (i.e. $s_i a_i \geq 0$) the sample is correctly classified and there is no action; otherwise, we attempt to minimize $-s_i a_i = -s_i \mathbf{w}^\top \mathbf{x}_i$: the error function is

$$E(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n E_i(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n [-s_i a_i]_+ = \frac{1}{n} \sum_{i=1}^n [-s_i \mathbf{w}^\top \mathbf{x}_i]_+$$

- indeed, given any random sample \mathbf{x}_i (correctly classified or not), the update is

$$\mathbf{w}^{(\tau+1)} \leftarrow \mathbf{w}^{(\tau)} - \epsilon \nabla_{\mathbf{w}} E_i(\mathbf{w}^{(\tau)})$$

perceptron, again

- “choose a random sample i that is misclassified and update”

$$\mathbf{w}^{(\tau+1)} \leftarrow \mathbf{w}^{(\tau)} + \epsilon s_i \mathbf{x}_i$$

- given sample \mathbf{x}_i , if $s_i y_i > 0$ (i.e. $s_i a_i \geq 0$) the sample is correctly classified and there is no action; otherwise, we attempt to minimize $-s_i a_i = -s_i \mathbf{w}^\top \mathbf{x}_i$: the **error function** is

$$E(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n E_i(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n [-s_i a_i]_+ = \frac{1}{n} \sum_{i=1}^n [-s_i \mathbf{w}^\top \mathbf{x}_i]_+$$

- indeed, given any random sample \mathbf{x}_i (correctly classified or not), the update is

$$\mathbf{w}^{(\tau+1)} \leftarrow \mathbf{w}^{(\tau)} - \epsilon \nabla_{\mathbf{w}} E_i(\mathbf{w}^{(\tau)})$$

perceptron, again

- “choose a random sample i that is misclassified and update”

$$\mathbf{w}^{(\tau+1)} \leftarrow \mathbf{w}^{(\tau)} + \epsilon s_i \mathbf{x}_i$$

- given sample \mathbf{x}_i , if $s_i y_i > 0$ (i.e. $s_i a_i \geq 0$) the sample is correctly classified and there is no action; otherwise, we attempt to minimize $-s_i a_i = -s_i \mathbf{w}^\top \mathbf{x}_i$: the **error function** is

$$E(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n E_i(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^n [-s_i a_i]_+ = \frac{1}{n} \sum_{i=1}^n [-s_i \mathbf{w}^\top \mathbf{x}_i]_+$$

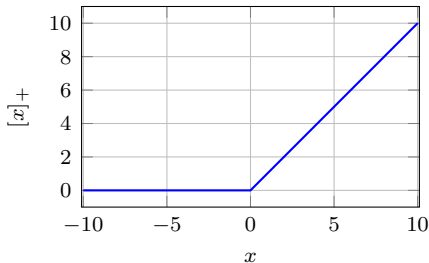
- indeed, given any random sample \mathbf{x}_i (correctly classified or not), the update is

$$\mathbf{w}^{(\tau+1)} \leftarrow \mathbf{w}^{(\tau)} - \epsilon \nabla_{\mathbf{w}} E_i(\mathbf{w}^{(\tau)})$$

positive part

- quantity $[x]_+$ is the positive part of x ; this function also known as **rectified linear unit** (ReLU):

$$\text{relu}(x) := [x]_+ := \max(0, x)$$



gradient descent

- in general, given an error function in parameters θ of the additive form

$$E(\theta) = \frac{1}{n} \sum_{i=1}^n E_i(\theta),$$

- online** (or stochastic) gradient descent updates the parameters after seeing one random sample i , according to

$$\theta^{(\tau+1)} \leftarrow \theta^{(\tau)} - \epsilon \nabla_{\theta} E_i(\theta^{(\tau)})$$

- batch** gradient descent updates the parameters once after seeing the entire dataset, according to

$$\theta^{(\tau+1)} \leftarrow \theta^{(\tau)} - \epsilon \nabla_{\theta} E(\theta^{(\tau)})$$

gradient descent

- in general, given an error function in parameters θ of the additive form

$$E(\theta) = \frac{1}{n} \sum_{i=1}^n E_i(\theta),$$

- online** (or stochastic) gradient descent updates the parameters after seeing one random sample i , according to

$$\theta^{(\tau+1)} \leftarrow \theta^{(\tau)} - \epsilon \nabla_{\theta} E_i(\theta^{(\tau)})$$

- batch** gradient descent updates the parameters once after seeing the entire dataset, according to

$$\theta^{(\tau+1)} \leftarrow \theta^{(\tau)} - \epsilon \nabla_{\theta} E(\theta^{(\tau)})$$

gradient descent

- in general, given an error function in parameters θ of the additive form

$$E(\theta) = \frac{1}{n} \sum_{i=1}^n E_i(\theta),$$

- online** (or stochastic) gradient descent updates the parameters after seeing one random sample i , according to

$$\theta^{(\tau+1)} \leftarrow \theta^{(\tau)} - \epsilon \nabla_{\theta} E_i(\theta^{(\tau)})$$

- batch** gradient descent updates the parameters once after seeing the entire dataset, according to

$$\theta^{(\tau+1)} \leftarrow \theta^{(\tau)} - \epsilon \nabla_{\theta} E(\theta^{(\tau)})$$

gradient descent

- **mini-batch** (or **stochastic**) gradient descent (SGD) is the most common option and updates the parameters after seeing a random subset $I \subset \{1, \dots, n\}$ of samples of fixed size $m = |I|$ according to

$$\boldsymbol{\theta}^{(\tau+1)} \leftarrow \boldsymbol{\theta}^{(\tau)} - \epsilon \frac{1}{m} \sum_{i \in I} \nabla_{\boldsymbol{\theta}} E_i(\boldsymbol{\theta}^{(\tau)})$$

- ϵ is the **learning rate** and is a **hyperparameter**; we will discuss later the convergence to a local minimum of E and conditions on ϵ
- whatever the choice, an iteration over the entire dataset is called an **epoch**
- stochastic versions make more sense when dataset is redundant
- it is important to take **random** samples

gradient descent

- **mini-batch** (or **stochastic**) gradient descent (SGD) is the most common option and updates the parameters after seeing a random subset $I \subset \{1, \dots, n\}$ of samples of fixed size $m = |I|$ according to

$$\boldsymbol{\theta}^{(\tau+1)} \leftarrow \boldsymbol{\theta}^{(\tau)} - \epsilon \frac{1}{m} \sum_{i \in I} \nabla_{\boldsymbol{\theta}} E_i(\boldsymbol{\theta}^{(\tau)})$$

- ϵ is the **learning rate** and is a **hyperparameter**; we will discuss later the convergence to a local minimum of E and conditions on ϵ
- whatever the choice, an iteration over the entire dataset is called an **epoch**
- stochastic versions make more sense when dataset is redundant
- it is important to take **random** samples

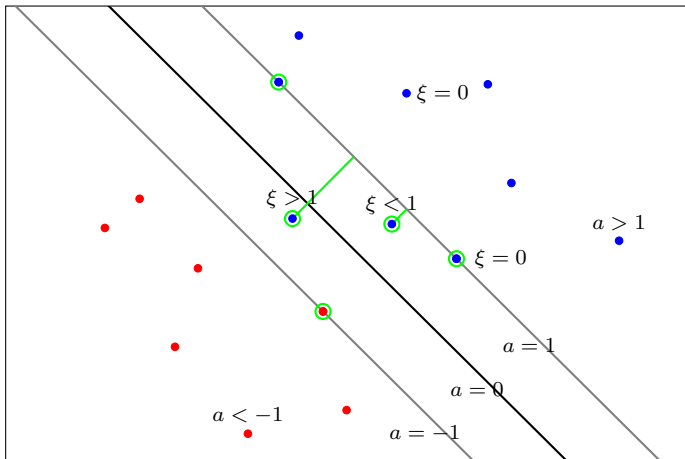
gradient descent

- **mini-batch** (or **stochastic**) gradient descent (SGD) is the most common option and updates the parameters after seeing a random subset $I \subset \{1, \dots, n\}$ of samples of fixed size $m = |I|$ according to

$$\boldsymbol{\theta}^{(\tau+1)} \leftarrow \boldsymbol{\theta}^{(\tau)} - \epsilon \frac{1}{m} \sum_{i \in I} \nabla_{\boldsymbol{\theta}} E_i(\boldsymbol{\theta}^{(\tau)})$$

- ϵ is the **learning rate** and is a **hyperparameter**; we will discuss later the convergence to a local minimum of E and conditions on ϵ
- whatever the choice, an iteration over the entire dataset is called an **epoch**
- stochastic versions make more sense when dataset is redundant
- it is important to take **random** samples

SVM, again



- either $s_i a_i \geq 1$ and $\xi_i = 0$ (correct side of margin) or $\xi_i = 1 - s_i a_i$

SVM, again

- the constraints

$$s_i a_i \geq 1 - \xi_i$$

$$\xi_i \geq 0$$

do not tell the whole truth

- either $s_i a_i \geq 1$ and $\xi_i = 0$ (correct side of margin) or $\xi_i = 1 - s_i a_i$, that is, $\xi_i = [1 - s_i a_i]_+$
- the error function becomes

$$E(\mathbf{w}, b) = \frac{1}{n} \sum_{i=1}^n [1 - s_i a_i]_+ + \frac{\lambda}{2} \|\mathbf{w}\|^2$$

without ξ_i and **without constraints**, where $\lambda = 1/C$

SVM, again

- the constraints

$$s_i a_i \geq 1 - \xi_i$$

$$\xi_i \geq 0$$

do not tell the whole truth

- either $s_i a_i \geq 1$ and $\xi_i = 0$ (correct side of margin) or $\xi_i = 1 - s_i a_i$, that is, $\xi_i = [1 - s_i a_i]_+$
- the error function becomes

$$E(\mathbf{w}, b) = \frac{1}{n} \sum_{i=1}^n [1 - s_i a_i]_+ + \frac{\lambda}{2} \|\mathbf{w}\|^2$$

without ξ_i and **without constraints**, where $\lambda = 1/C$

SVM, again

- the constraints

$$s_i a_i \geq 1 - \xi_i$$

$$\xi_i \geq 0$$

do not tell the whole truth

- either $s_i a_i \geq 1$ and $\xi_i = 0$ (correct side of margin) or $\xi_i = 1 - s_i a_i$, that is, $\xi_i = [1 - s_i a_i]_+$
- the error function becomes

$$E(\mathbf{w}, b) = \frac{1}{n} \sum_{i=1}^n [1 - s_i a_i]_+ + \frac{\lambda}{2} \|\mathbf{w}\|^2$$

without ξ_i and **without constraints**, where $\lambda = 1/C$

weight decay

- recall that the margin in SVM is invariant to scaling \mathbf{w} and b
- same for perceptron error function
- in logistic regression, the sigmoid tends to a non-smooth step function as $\|\mathbf{w}\|$ becomes larger
- as $\|\mathbf{w}\|$ increases, the classifier function becomes more sensitive to perturbations in the input and is harder to generalize to new data
- the term

$$\frac{\lambda}{2} \|\mathbf{w}\|^2$$

helps to keep $\|\mathbf{w}\|$ low because its gradient is $-\lambda\mathbf{w}$; it is a standard **regularization** method and we can add it to any method including perceptron and logistic regression

- λ is another **hyperparameter**
- weight decay is only applied to weights, not to bias

weight decay

- recall that the margin in SVM is invariant to scaling \mathbf{w} and b
- same for perceptron error function
- in logistic regression, the sigmoid tends to a non-smooth step function as $\|\mathbf{w}\|$ becomes larger
- as $\|\mathbf{w}\|$ increases, the classifier function becomes more sensitive to perturbations in the input and is harder to generalize to new data
- the term

$$\frac{\lambda}{2} \|\mathbf{w}\|^2$$

helps to keep $\|\mathbf{w}\|$ low because its gradient is $-\lambda\mathbf{w}$; it is a standard **regularization** method and we can add it to any method including perceptron and logistic regression

- λ is another **hyperparameter**
- weight decay is only applied to weights, not to bias

weight decay

- recall that the margin in SVM is invariant to scaling \mathbf{w} and b
- same for perceptron error function
- in logistic regression, the sigmoid tends to a non-smooth step function as $\|\mathbf{w}\|$ becomes larger
- as $\|\mathbf{w}\|$ increases, the classifier function becomes more sensitive to perturbations in the input and is harder to generalize to new data
- the term

$$\frac{\lambda}{2} \|\mathbf{w}\|^2$$

helps to keep $\|\mathbf{w}\|$ low because its gradient is $-\lambda\mathbf{w}$; it is a standard **regularization** method and we can add it to any method including perceptron and logistic regression

- λ is another **hyperparameter**
- weight decay is only applied to weights, not to bias

weight decay

- recall that the margin in SVM is invariant to scaling \mathbf{w} and b
- same for perceptron error function
- in logistic regression, the sigmoid tends to a non-smooth step function as $\|\mathbf{w}\|$ becomes larger
- as $\|\mathbf{w}\|$ increases, the classifier function becomes more sensitive to perturbations in the input and is harder to generalize to new data
- the term

$$\frac{\lambda}{2} \|\mathbf{w}\|^2$$

helps to keep $\|\mathbf{w}\|$ low because its gradient is $-\lambda\mathbf{w}$; it is a standard **regularization** method and we can add it to any method including perceptron and logistic regression

- λ is another **hyperparameter**
- weight decay is only applied to weights, not to bias

logistic regression, again

- recall that

$$E(\mathbf{w}) := -\frac{1}{n} \sum_{i=1}^n (t_i \ln y_i + (1 - t_i) \ln(1 - y_i))$$

where $y_i = \sigma(a_i) = \sigma(\mathbf{w}^\top \mathbf{x}_i)$

- using variables $s_i = 2t_i - 1$ in $\{-1, 1\}$, each term is

if $t_i = 1$ ($s_i = 1$)	$\ln \sigma(a_i)$
if $t_i = 0$ ($s_i = -1$)	$\ln(1 - \sigma(a_i)) = \ln \sigma(-a_i)$
in either case	$\ln \sigma(s_i a_i)$

- the error function becomes

$$E(\mathbf{w}) = -\frac{1}{n} \sum_{i=1}^n \ln \sigma(s_i a_i) = \frac{1}{n} \sum_{i=1}^n \ln(1 + e^{-s_i a_i})$$

logistic regression, again

- recall that

$$E(\mathbf{w}) := -\frac{1}{n} \sum_{i=1}^n (t_i \ln y_i + (1 - t_i) \ln(1 - y_i))$$

where $y_i = \sigma(a_i) = \sigma(\mathbf{w}^\top \mathbf{x}_i)$

- using variables $s_i = 2t_i - 1$ in $\{-1, 1\}$, each term is

if $t_i = 1$ ($s_i = 1$)	$\ln \sigma(a_i)$
if $t_i = 0$ ($s_i = -1$)	$\ln(1 - \sigma(a_i)) = \ln \sigma(-a_i)$
in either case	$\ln \sigma(s_i a_i)$

- the error function becomes

$$E(\mathbf{w}) = -\frac{1}{n} \sum_{i=1}^n \ln \sigma(s_i a_i) = \frac{1}{n} \sum_{i=1}^n \ln(1 + e^{-s_i a_i})$$

logistic regression, again

- recall that

$$E(\mathbf{w}) := -\frac{1}{n} \sum_{i=1}^n (t_i \ln y_i + (1 - t_i) \ln(1 - y_i))$$

where $y_i = \sigma(a_i) = \sigma(\mathbf{w}^\top \mathbf{x}_i)$

- using variables $s_i = 2t_i - 1$ in $\{-1, 1\}$, each term is

if $t_i = 1$ ($s_i = 1$)	$\ln \sigma(a_i)$
if $t_i = 0$ ($s_i = -1$)	$\ln(1 - \sigma(a_i)) = \ln \sigma(-a_i)$
in either case	$\ln \sigma(s_i a_i)$

- the error function becomes

$$E(\mathbf{w}) = -\frac{1}{n} \sum_{i=1}^n \ln \sigma(s_i a_i) = \frac{1}{n} \sum_{i=1}^n \ln(1 + e^{-s_i a_i})$$

maximum posterior

- weight decay also appears in probabilistic formulations by considering the weight vector a random variable and incorporating a Gaussian prior for \mathbf{w}

$$p(\mathbf{w}|\lambda) = \exp\left(-\frac{\lambda}{2}\|\mathbf{w}\|^2\right)$$

- the posterior distribution given the dataset X, T is

$$p(\mathbf{w}|X, T) \propto p(T|X, \mathbf{w})p(\mathbf{w}|\lambda)$$

- taking negative logarithm, the error function to minimize is

$$E(\mathbf{w}) = -\ln p(T|X, \mathbf{w}) + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

maximum posterior

- weight decay also appears in probabilistic formulations by considering the weight vector a random variable and incorporating a Gaussian prior for \mathbf{w}

$$p(\mathbf{w}|\lambda) = \exp\left(-\frac{\lambda}{2}\|\mathbf{w}\|^2\right)$$

- the posterior distribution given the dataset X, T is

$$p(\mathbf{w}|X, T) \propto p(T|X, \mathbf{w})p(\mathbf{w}|\lambda)$$

- taking negative logarithm, the error function to minimize is

$$E(\mathbf{w}) = -\ln p(T|X, \mathbf{w}) + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

maximum posterior

- weight decay also appears in probabilistic formulations by considering the weight vector a random variable and incorporating a Gaussian prior for \mathbf{w}

$$p(\mathbf{w}|\lambda) = \exp\left(-\frac{\lambda}{2}\|\mathbf{w}\|^2\right)$$

- the posterior distribution given the dataset X, T is

$$p(\mathbf{w}|X, T) \propto p(T|X, \mathbf{w})p(\mathbf{w}|\lambda)$$

- taking negative logarithm, the error function to minimize is

$$E(\mathbf{w}) = -\ln p(T|X, \mathbf{w}) + \frac{\lambda}{2}\|\mathbf{w}\|^2$$

error function and optimization

- in all three cases, we can define the **error function** (or cost function)

$$E(\boldsymbol{\theta}) := \frac{1}{n} \sum_{i=1}^n L(\hat{f}(\mathbf{x}_i; \boldsymbol{\theta}), s_i) + \frac{\lambda}{2} \|\mathbf{w}\|^2$$

- there are **no constraints**: in all three cases, we can use (stochastic) gradient descent to minimize the error function with respect to parameters $\boldsymbol{\theta}$

error function and optimization

- in all three cases, we can define the **error function** (or cost function)

$$E(\boldsymbol{\theta}) := \underbrace{\frac{1}{n} \sum_{i=1}^n L(\hat{f}(\mathbf{x}_i; \boldsymbol{\theta}), s_i)}_{\text{data term}} + \frac{\lambda}{2} \|\mathbf{w}\|^2$$

data term

- there are **no constraints**: in all three cases, we can use (stochastic) gradient descent to minimize the error function with respect to parameters $\boldsymbol{\theta}$

error function and optimization

- in all three cases, we can define the **error function** (or cost function)

$$E(\boldsymbol{\theta}) := \frac{1}{n} \sum_{i=1}^n L(\hat{f}(\mathbf{x}_i; \boldsymbol{\theta}), s_i) + \frac{\lambda}{2} \|\mathbf{w}\|^2$$

data term

regularization term

- there are **no constraints**: in all three cases, we can use (stochastic) gradient descent to minimize the error function with respect to parameters $\boldsymbol{\theta}$

error function and optimization

- in all three cases, we can define the **error function** (or cost function)

$$E(\boldsymbol{\theta}) := \frac{1}{n} \sum_{i=1}^n L(\hat{f}(\mathbf{x}_i; \boldsymbol{\theta}), s_i) + \frac{\lambda}{2} \|\mathbf{w}\|^2$$

data term

regularization term

- there are **no constraints**: in all three cases, we can use (stochastic) gradient descent to minimize the error function with respect to parameters $\boldsymbol{\theta}$

prediction function

- in all three cases, we can use parameters $\theta = (\mathbf{w}, b)$ and

$$\hat{f}(\mathbf{x}; \mathbf{w}, b) = \mathbf{w}^\top \mathbf{x} + b$$

to make predictions during **learning (training)**; this is the activation, without the nonlinearity

- in all three cases, when the optimal parameters $\theta^* = \arg \min_{\theta} E(\theta)$ are found, use the **prediction function**

$$f(\mathbf{x}; \mathbf{w}^*, b^*) = \text{sgn}(\mathbf{w}^{*\top} \mathbf{x} + b^*) = \begin{cases} +1, & \mathbf{w}^{*\top} \mathbf{x} + b^* \geq 0 \\ -1, & \mathbf{w}^{*\top} \mathbf{x} + b^* < 0 \end{cases}$$

to classify new samples during **inference (testing)**

prediction function

- in all three cases, we can use parameters $\theta = (\mathbf{w}, b)$ and

$$\hat{f}(\mathbf{x}; \mathbf{w}, b) = \mathbf{w}^\top \mathbf{x} + b$$

to make predictions during **learning (training)**; this is the activation, without the nonlinearity

- in all three cases, when the optimal parameters $\theta^* = \arg \min_{\theta} E(\theta)$ are found, use the **prediction function**

$$f(\mathbf{x}; \mathbf{w}^*, b^*) = \text{sgn}(\mathbf{w}^{*\top} \mathbf{x} + b^*) = \begin{cases} +1, & \mathbf{w}^{*\top} \mathbf{x} + b^* \geq 0 \\ -1, & \mathbf{w}^{*\top} \mathbf{x} + b^* < 0 \end{cases}$$

to classify new samples during **inference (testing)**

loss function

- in all cases, we can use **loss function**

$$L(a, s) = \ell(sa)$$

where a is the activation and s the target variable in $\{-1, 1\}$ (“sign”)

- the only difference is

	$\ell(x)$
perceptron	$[-x]_+$
SVM (hinge)	$[1 - x]_+$
logistic	$\ln(1 + e^{-x})$

loss function

- in all cases, we can use **loss function**

$$L(a, s) = \ell(sa)$$

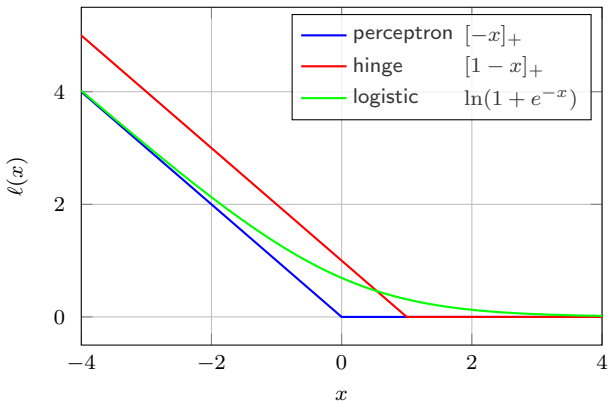
where a is the activation and s the target variable in $\{-1, 1\}$ (“sign”)

- the only difference is

	$\ell(x)$
perceptron	$[-x]_+$
SVM (hinge)	$[1 - x]_+$
logistic	$\ln(1 + e^{-x})$

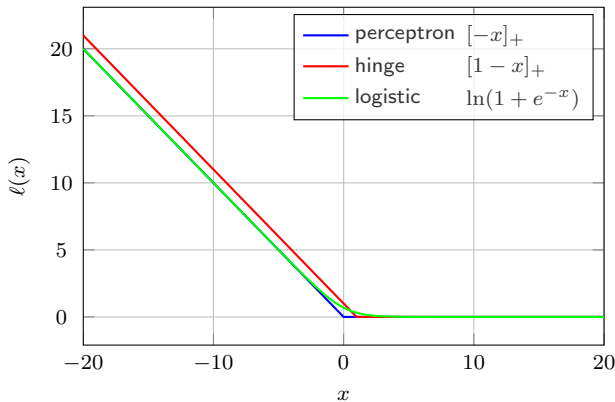
loss function

- perceptron and logistic are asymptotically equivalent
- both SVM and logistic penalize small positive errors



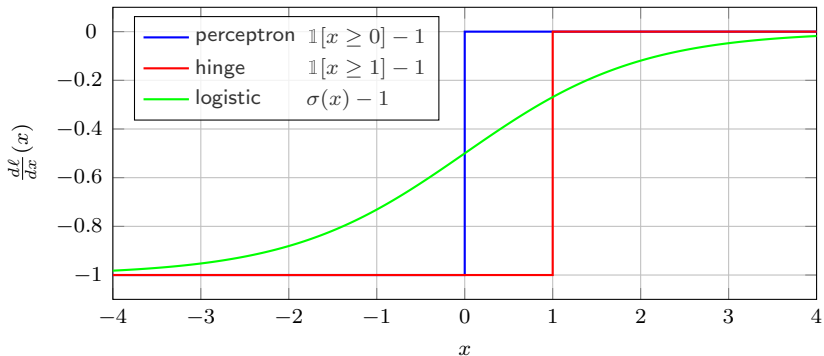
loss function

- perceptron and logistic are asymptotically equivalent
- both SVM and logistic penalize small positive errors



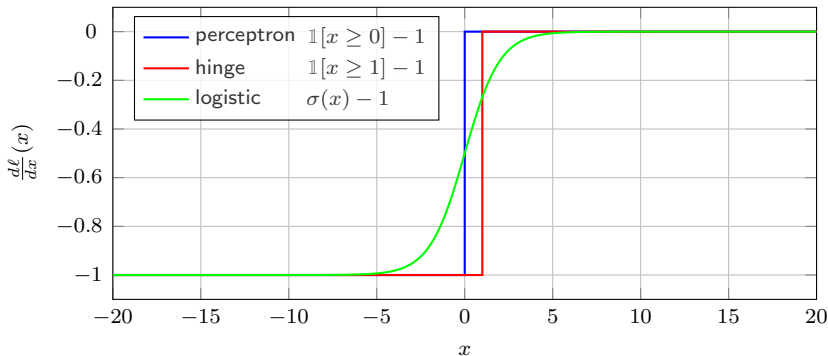
derivatives

- the actual value of the loss is never used; all that matters is its derivative



derivatives

- the actual value of the loss is never used; all that matters is its derivative



derivatives

- in all cases, a sample that is correctly classified with an activation well above some margin **does not contribute** at all to the error function: the loss derivative is zero
- in all cases, a sample that is correctly classified with an activation well below some margin has a **fixed negative contribution**: the loss derivative is -1
- the same holds for logistic regression, which is unexpected if one looks at the **saturating** form of the sigmoid ($\frac{d\sigma}{dx}(x)$ tends to zero for $|x| \rightarrow \infty$)
- this is because the log of cross-entropy **cancels** the effect of the exp of the sigmoid and is a good reason the treat these two as one function operating directly on the activation

derivatives

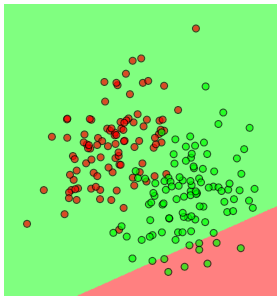
- in all cases, a sample that is correctly classified with an activation well above some margin **does not contribute** at all to the error function: the loss derivative is zero
- in all cases, a sample that is correctly classified with an activation well below some margin has a **fixed negative contribution**: the loss derivative is -1
- the same holds for logistic regression, which is unexpected if one looks at the **saturating** form of the sigmoid ($\frac{d\sigma}{dx}(x)$ tends to zero for $|x| \rightarrow \infty$)
- this is because the log of cross-entropy **cancels** the effect of the exp of the sigmoid and is a good reason to treat these two as one function operating directly on the activation

question

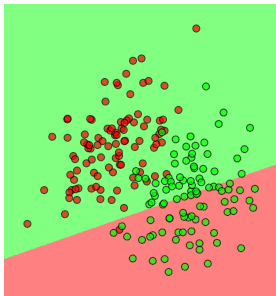
- perceptron and hinge loss differ only by a shift; once the bias is learned, aren't they equivalent?

training

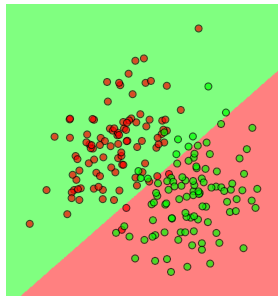
epoch 0



perceptron



hinge

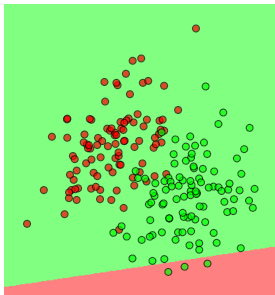


logistic

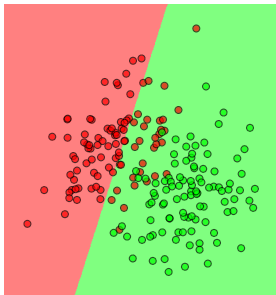
- $k = 2, n = 200, m = 10, \epsilon = 10^{-3}, \lambda = 10^{-3}$

training

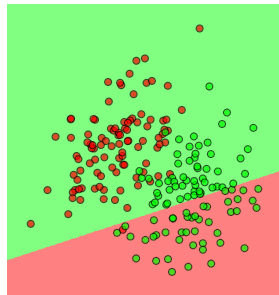
epoch 1



perceptron



hinge

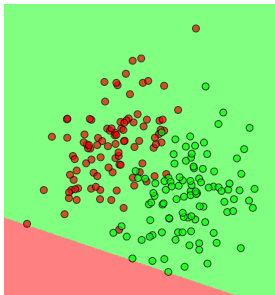


logistic

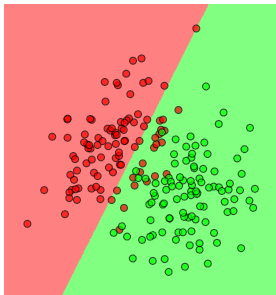
- $k = 2, n = 200, m = 10, \epsilon = 10^{-3}, \lambda = 10^{-3}$

training

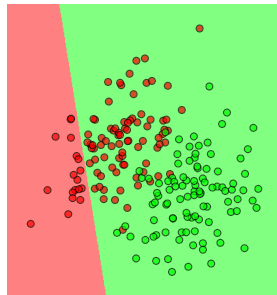
epoch 2



perceptron



hinge

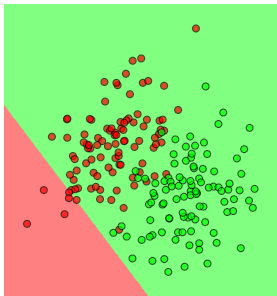


logistic

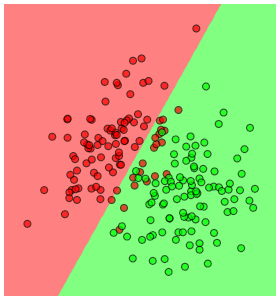
- $k = 2, n = 200, m = 10, \epsilon = 10^{-3}, \lambda = 10^{-3}$

training

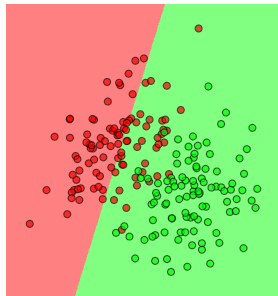
epoch 3



perceptron



hinge

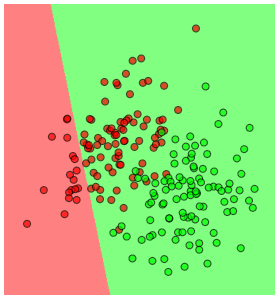


logistic

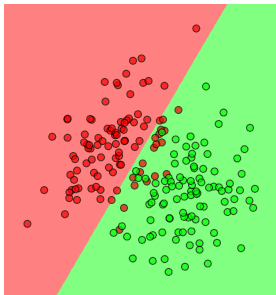
- $k = 2, n = 200, m = 10, \epsilon = 10^{-3}, \lambda = 10^{-3}$

training

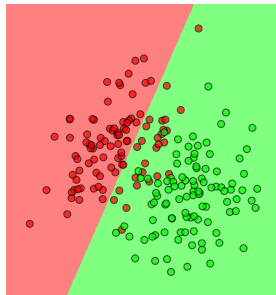
epoch 4



perceptron



hinge

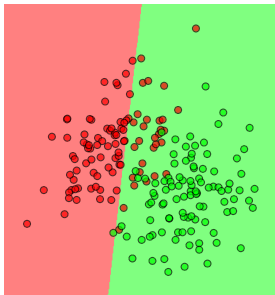


logistic

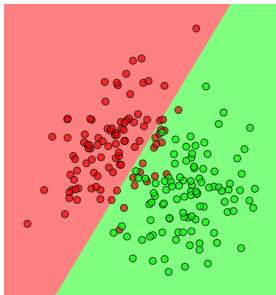
- $k = 2, n = 200, m = 10, \epsilon = 10^{-3}, \lambda = 10^{-3}$

training

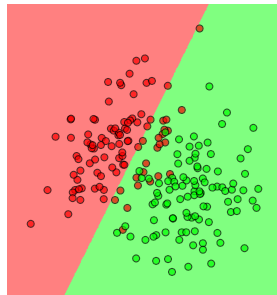
epoch 5



perceptron



hinge

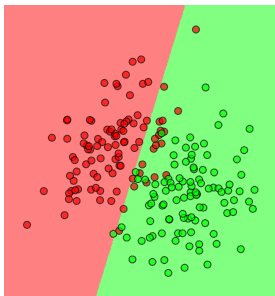


logistic

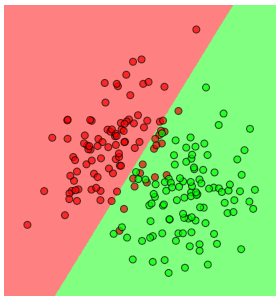
- $k = 2, n = 200, m = 10, \epsilon = 10^{-3}, \lambda = 10^{-3}$

training

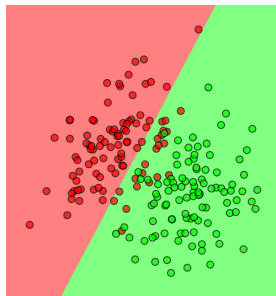
epoch 6



perceptron



hinge

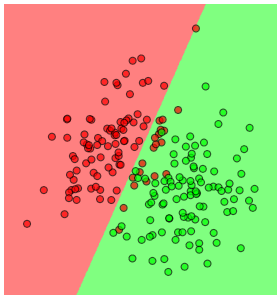


logistic

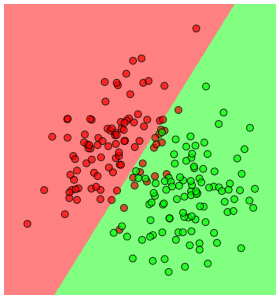
- $k = 2, n = 200, m = 10, \epsilon = 10^{-3}, \lambda = 10^{-3}$

training

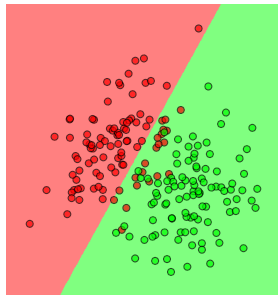
epoch 7



perceptron



hinge

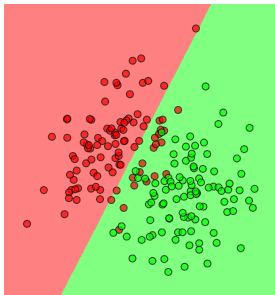


logistic

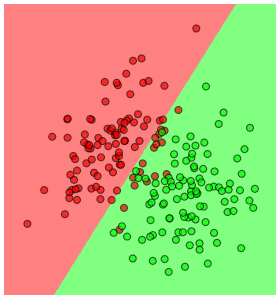
- $k = 2, n = 200, m = 10, \epsilon = 10^{-3}, \lambda = 10^{-3}$

training

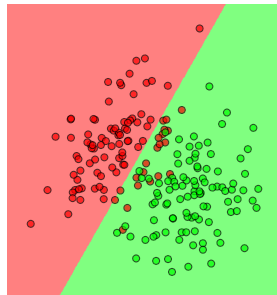
epoch 8



perceptron



hinge

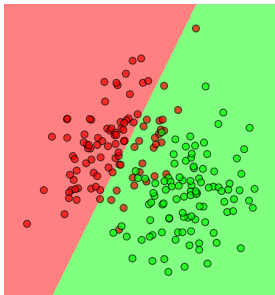


logistic

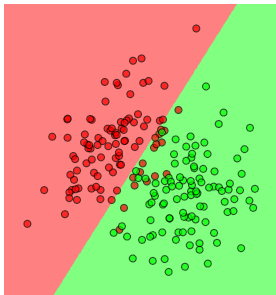
- $k = 2, n = 200, m = 10, \epsilon = 10^{-3}, \lambda = 10^{-3}$

training

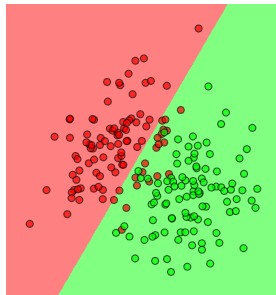
epoch 9



perceptron



hinge



logistic

- $k = 2, n = 200, m = 10, \epsilon = 10^{-3}, \lambda = 10^{-3}$

multi-class classification

multi-class logistic regression

- there are now k classes C_1, \dots, C_k and, given input $\mathbf{x} \in \mathbb{R}^d$, one activation per class for $j = 1, \dots, k$

$$a_j = \mathbf{w}_j^\top \mathbf{x} + b_j$$

or, in matrix form

$$\mathbf{a} = (a_1, \dots, a_k) = W^\top \mathbf{x} + \mathbf{b}$$

where $W = (\mathbf{w}_1, \dots, \mathbf{w}_k)$ is a $d \times k$ weight matrix and $\mathbf{b} = (b_1, \dots, b_k)$ a bias vector

- and one output $y_j \in [0, 1]$ per class for $j = 1, \dots, k$

$$y_j = f_j(\mathbf{x}; W, \mathbf{b}) := \sigma_j(W^\top \mathbf{x} + \mathbf{b}) = \sigma_j(\mathbf{a})$$

or output vector $\mathbf{y} \in [0, 1]^k$

$$\mathbf{y} = (y_1, \dots, y_k) = f(\mathbf{x}; W, \mathbf{b}) := \sigma(W^\top \mathbf{x} + \mathbf{b})$$

multi-class logistic regression

- there are now k classes C_1, \dots, C_k and, given input $\mathbf{x} \in \mathbb{R}^d$, one activation per class for $j = 1, \dots, k$

$$a_j = \mathbf{w}_j^\top \mathbf{x} + b_j$$

or, in matrix form

$$\mathbf{a} = (a_1, \dots, a_k) = W^\top \mathbf{x} + \mathbf{b}$$

where $W = (\mathbf{w}_1, \dots, \mathbf{w}_k)$ is a $d \times k$ weight matrix and $\mathbf{b} = (b_1, \dots, b_k)$ a bias vector

- and one output $y_j \in [0, 1]$ per class for $j = 1, \dots, k$

$$y_j = f_j(\mathbf{x}; W, \mathbf{b}) := \sigma_j(W^\top \mathbf{x} + \mathbf{b}) = \sigma_j(\mathbf{a})$$

or output vector $\mathbf{y} \in [0, 1]^k$

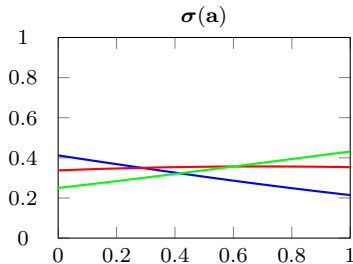
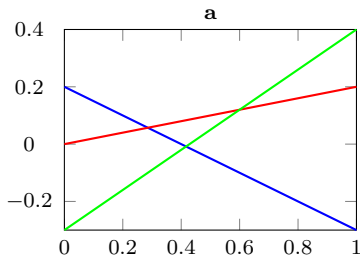
$$\mathbf{y} = (y_1, \dots, y_k) = f(\mathbf{x}; W, \mathbf{b}) := \sigma(W^\top \mathbf{x} + \mathbf{b})$$

softmax

- the softmax function generalizes the sigmoid function and yields a vector of k values in $[0, 1]$ by exponentiating and then normalizing

$$\sigma(\mathbf{a}) := \text{softmax}(\mathbf{a}) := \frac{1}{\sum_j e^{a_j}} (e^{a_1}, \dots, e^{a_k})$$

- as activation values increase, softmax tends to focus on the maximum

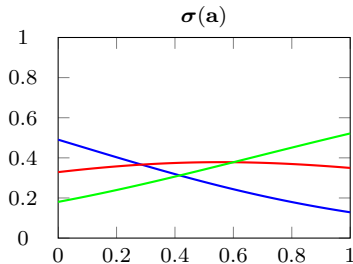
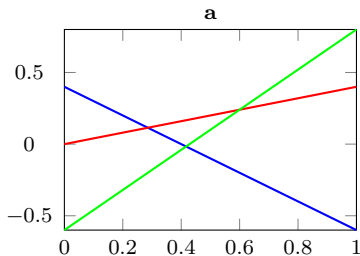


softmax

- the softmax function generalizes the sigmoid function and yields a vector of k values in $[0, 1]$ by exponentiating and then normalizing

$$\sigma(\mathbf{a}) := \text{softmax}(\mathbf{a}) := \frac{1}{\sum_j e^{a_j}} (e^{a_1}, \dots, e^{a_k})$$

- as activation values increase, softmax tends to focus on the maximum

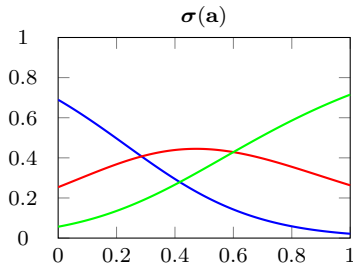
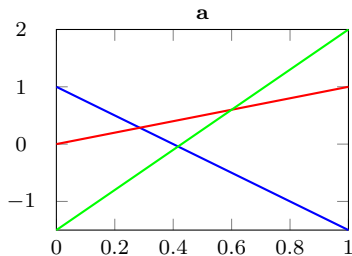


softmax

- the softmax function generalizes the sigmoid function and yields a vector of k values in $[0, 1]$ by exponentiating and then normalizing

$$\sigma(\mathbf{a}) := \text{softmax}(\mathbf{a}) := \frac{1}{\sum_j e^{a_j}} (e^{a_1}, \dots, e^{a_k})$$

- as activation values increase, softmax tends to focus on the maximum

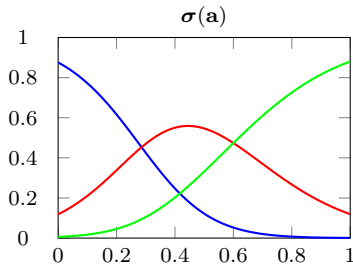
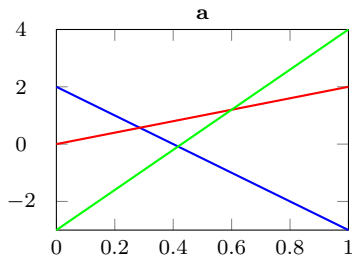


softmax

- the softmax function generalizes the sigmoid function and yields a vector of k values in $[0, 1]$ by exponentiating and then normalizing

$$\sigma(\mathbf{a}) := \text{softmax}(\mathbf{a}) := \frac{1}{\sum_j e^{a_j}} (e^{a_1}, \dots, e^{a_k})$$

- as activation values increase, softmax tends to focus on the maximum

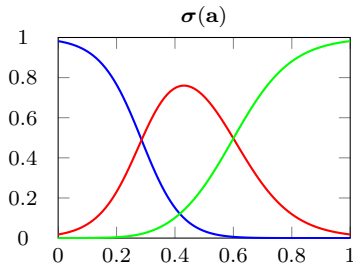
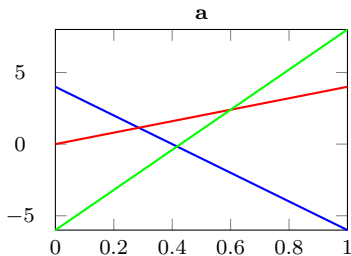


softmax

- the softmax function generalizes the sigmoid function and yields a vector of k values in $[0, 1]$ by exponentiating and then normalizing

$$\sigma(\mathbf{a}) := \text{softmax}(\mathbf{a}) := \frac{1}{\sum_j e^{a_j}} (e^{a_1}, \dots, e^{a_k})$$

- as activation values increase, softmax tends to focus on the maximum

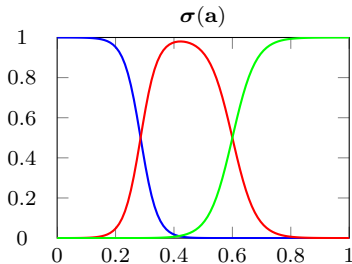
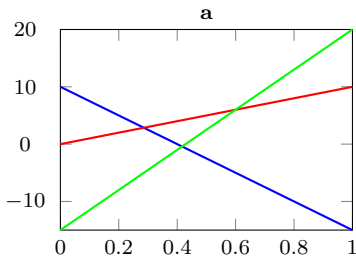


softmax

- the softmax function generalizes the sigmoid function and yields a vector of k values in $[0, 1]$ by exponentiating and then normalizing

$$\sigma(\mathbf{a}) := \text{softmax}(\mathbf{a}) := \frac{1}{\sum_j e^{a_j}} (e^{a_1}, \dots, e^{a_k})$$

- as activation values increase, softmax tends to focus on the maximum

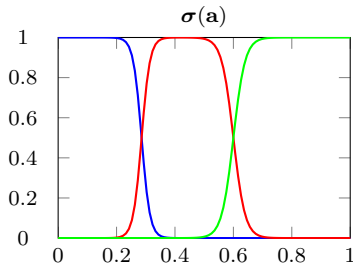
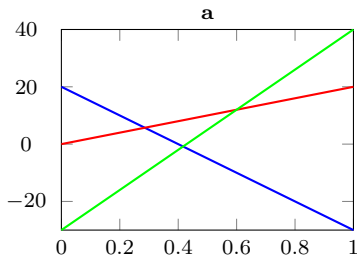


softmax

- the softmax function generalizes the sigmoid function and yields a vector of k values in $[0, 1]$ by exponentiating and then normalizing

$$\sigma(\mathbf{a}) := \text{softmax}(\mathbf{a}) := \frac{1}{\sum_j e^{a_j}} (e^{a_1}, \dots, e^{a_k})$$

- as activation values increase, softmax tends to focus on the maximum

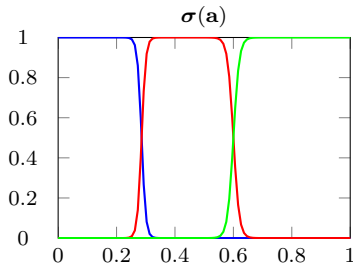
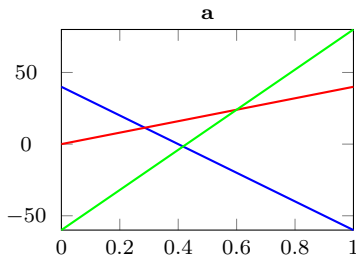


softmax

- the softmax function generalizes the sigmoid function and yields a vector of k values in $[0, 1]$ by exponentiating and then normalizing

$$\sigma(\mathbf{a}) := \text{softmax}(\mathbf{a}) := \frac{1}{\sum_j e^{a_j}} (e^{a_1}, \dots, e^{a_k})$$

- as activation values increase, softmax tends to focus on the maximum



cross-entropy error

- we are given **training samples** $X = (\mathbf{x}_1, \dots, \mathbf{x}_n) \in \mathbb{R}^{d \times n}$ and **target variables** $T = (\mathbf{t}_1, \dots, \mathbf{t}_n) \in \{0, 1\}^{k \times n}$
- this is an **1-of- k** or **one-hot** encoding scheme: $t_{ji} = \mathbb{1}[\mathbf{x}_i \in C_j]$
- there is a similar **probabilistic** interpretation: output y_{ji} represents the posterior class probability $p(C_j | \mathbf{x}_i)$
- again, maximizing the likelihood function yields the average **cross-entropy** error function

$$E(W, \mathbf{b}) = \frac{1}{n} \sum_{i=1}^n L(\mathbf{a}_i, \mathbf{t}_i) = -\frac{1}{n} \sum_{i=1}^n \sum_{j=1}^k t_{ji} \ln y_{ji}$$

where $Y = (\mathbf{y}_1, \dots, \mathbf{y}_n)$ and $\mathbf{y}_i = \sigma(\mathbf{a}_i) = \sigma(W^\top \mathbf{x}_i + \mathbf{b})$

cross-entropy error

- we are given **training samples** $X = (\mathbf{x}_1, \dots, \mathbf{x}_n) \in \mathbb{R}^{d \times n}$ and **target variables** $T = (\mathbf{t}_1, \dots, \mathbf{t}_n) \in \{0, 1\}^{k \times n}$
- this is an **1-of- k** or **one-hot** encoding scheme: $t_{ji} = \mathbb{1}[\mathbf{x}_i \in C_j]$
- there is a similar **probabilistic** interpretation: output y_{ji} represents the posterior class probability $p(C_j | \mathbf{x}_i)$
- again, maximizing the likelihood function yields the average **cross-entropy** error function

$$E(W, \mathbf{b}) = \frac{1}{n} \sum_{i=1}^n L(\mathbf{a}_i, \mathbf{t}_i) = -\frac{1}{n} \sum_{i=1}^n \sum_{j=1}^k t_{ji} \ln y_{ji}$$

where $Y = (\mathbf{y}_1, \dots, \mathbf{y}_n)$ and $\mathbf{y}_i = \boldsymbol{\sigma}(\mathbf{a}_i) = \boldsymbol{\sigma}(W^\top \mathbf{x}_i + \mathbf{b})$

cross-entropy loss

- given a single sample \mathbf{x} and target variable \mathbf{t} , and corresponding producing activation $\mathbf{a} = W^\top \mathbf{x} + \mathbf{b}$, the loss function is

$$\begin{aligned} L(\mathbf{a}, \mathbf{t}) &= -\mathbf{t}^\top \ln \boldsymbol{\sigma}(\mathbf{a}) \\ &= -\mathbf{t}^\top \left(\mathbf{a} - \ln \left(\sum_{j=1}^k e^{a_j} \right) \right) \end{aligned}$$

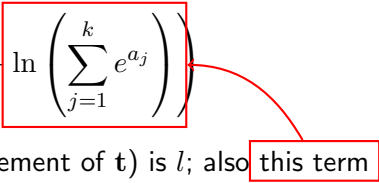
- suppose the **correct label** (nonzero element of \mathbf{t}) is l ; also this term can be approximated by the maximum element of \mathbf{a} :

$$L(\mathbf{a}, \mathbf{t}) \simeq \max \mathbf{a} - a_l$$

so there is loss if the activation of the correct class is not maximum

cross-entropy loss

- given a single sample \mathbf{x} and target variable \mathbf{t} , and corresponding producing activation $\mathbf{a} = W^\top \mathbf{x} + \mathbf{b}$, the loss function is

$$L(\mathbf{a}, \mathbf{t}) = -\mathbf{t}^\top \ln \sigma(\mathbf{a})$$
$$= -\mathbf{t}^\top \left(\mathbf{a} - \ln \left(\sum_{j=1}^k e^{a_j} \right) \right)$$


- suppose the **correct label** (nonzero element of \mathbf{t}) is l ; also **this term** can be approximated by the maximum element of \mathbf{a} :

$$L(\mathbf{a}, \mathbf{t}) \simeq \max \mathbf{a} - a_l$$

so **there is loss if the activation of the correct class is not maximum**

cross-entropy loss derivative

- remember, **it's only derivatives that matter**
- the derivative of the cross-entropy loss with respect to the activation is particularly simple, no approximation needed:

$$\frac{\partial L}{\partial \mathbf{a}}(\mathbf{a}, \mathbf{t}) = \boldsymbol{\sigma}(\mathbf{a}) - \mathbf{t} = \mathbf{y} - \mathbf{t}$$

- again, **exp and log cancel**, and that's a reason to keep softmax followed by cross-entropy as one function
- example (correct label $l = 3$):

\mathbf{t}	0	0	1	0	0	0
\mathbf{a}	0.3	0.1	0.8	0.4	0.0	0.2
$\frac{dL}{da}$	0.3	0.1	-0.2	0.4	0.0	0.2

- by increasing a class activation, the loss decreases if the class is correct, and increases otherwise

cross-entropy loss derivative

- remember, **it's only derivatives that matter**
- the derivative of the cross-entropy loss with respect to the activation is particularly simple, no approximation needed:

$$\frac{\partial L}{\partial \mathbf{a}}(\mathbf{a}, \mathbf{t}) = \boldsymbol{\sigma}(\mathbf{a}) - \mathbf{t} = \mathbf{y} - \mathbf{t}$$

- again, **exp and log cancel**, and that's a reason to keep softmax followed by cross-entropy as one function
- example (correct label $l = 3$):

\mathbf{t}	0	0	1	0	0	0
\mathbf{a}	0.3	0.1	0.8	0.4	0.0	0.2
$\frac{dL}{d\mathbf{a}}$	0.3	0.1	-0.2	0.4	0.0	0.2

- by increasing a class activation, the loss decreases if the class is correct, and increases otherwise

cross-entropy loss derivative

- remember, **it's only derivatives that matter**
- the derivative of the cross-entropy loss with respect to the activation is particularly simple, no approximation needed:

$$\frac{\partial L}{\partial \mathbf{a}}(\mathbf{a}, \mathbf{t}) = \boldsymbol{\sigma}(\mathbf{a}) - \mathbf{t} = \mathbf{y} - \mathbf{t}$$

- again, **exp and log cancel**, and that's a reason to keep softmax followed by cross-entropy as one function
- example (correct label $l = 3$):

\mathbf{t}	0	0	1	0	0	0
\mathbf{a}	0.3	0.1	0.8	0.4	0.0	0.2
$\frac{dL}{d\mathbf{a}}$	0.3	0.1	-0.2	0.4	0.0	0.2

- by increasing a class activation, the loss decreases if the class is correct, and increases otherwise

multiclass SVM

- following the representation of **correct label** $l \in \{1, \dots, k\}$
- several extensions, e.g. Weston and Watkins

$$L(\mathbf{a}, l) := \left[1 + \max_{j \neq l} a_j - a_l \right]_+$$

similar to the previous approximation of cross-entropy, plus margin

- Crammer and Singer

$$L(\mathbf{a}, l) := \sum_{j \neq l} [1 + a_j - a_l]_+$$

penalizes **all** labels that have better activation than the correct one

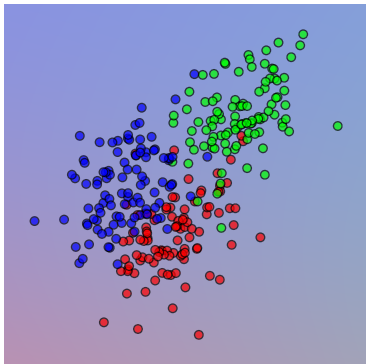
- both interpretable with simple derivatives

multiclass SVM

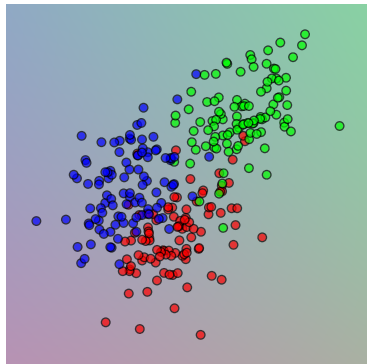
- we now apply logistic regression and SVM (W&W) to classify three classes in 2d
- **soft assignment**: to visualize the class confidences, we apply `softmax` to activations in each case, even if SVM is not probabilistic
- **hard assignment**: now we threshold activations with `sgn` instead, as we do in testing
- we repeat at different epochs during training

prediction: soft assignment

epoch 00



hinge (W&W)

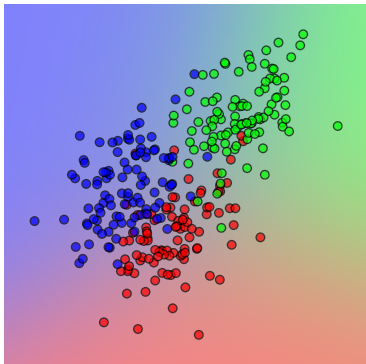


logistic

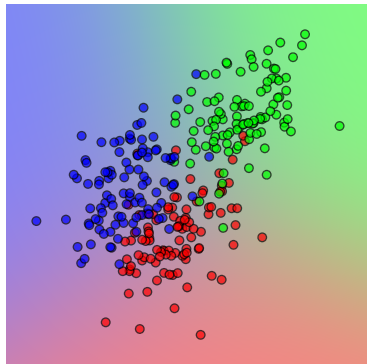
- $k = 3, n = 300, m = 10, \epsilon = 10^{-1}, \lambda = 10^{-3}$

prediction: soft assignment

epoch 05



hinge (W&W)

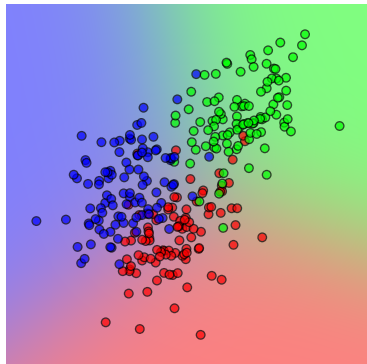
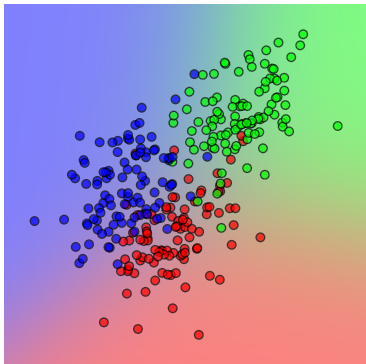


logistic

- $k = 3, n = 300, m = 10, \epsilon = 10^{-1}, \lambda = 10^{-3}$

prediction: soft assignment

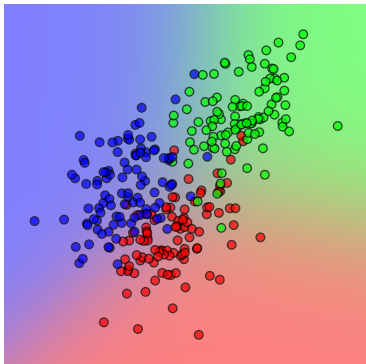
epoch 10



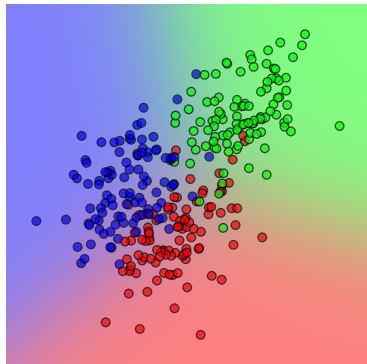
- $k = 3, n = 300, m = 10, \epsilon = 10^{-1}, \lambda = 10^{-3}$

prediction: soft assignment

epoch 15



hinge (W&W)

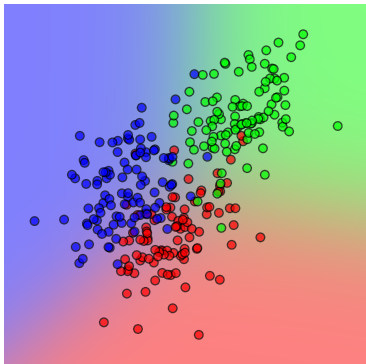


logistic

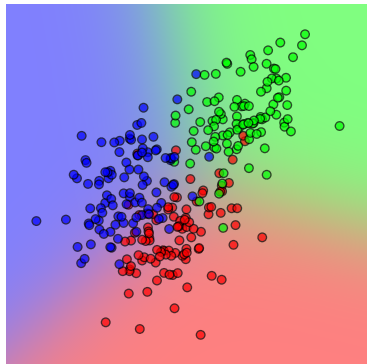
- $k = 3, n = 300, m = 10, \epsilon = 10^{-1}, \lambda = 10^{-3}$

prediction: soft assignment

epoch 20



hinge (W&W)

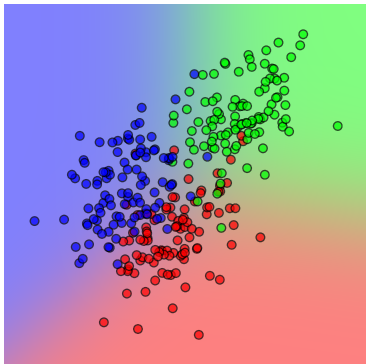


logistic

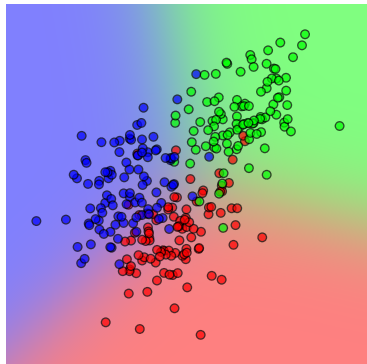
- $k = 3, n = 300, m = 10, \epsilon = 10^{-1}, \lambda = 10^{-3}$

prediction: soft assignment

epoch 25



hinge (W&W)

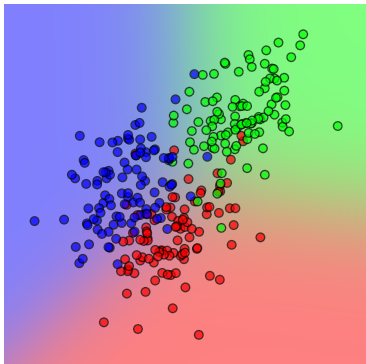


logistic

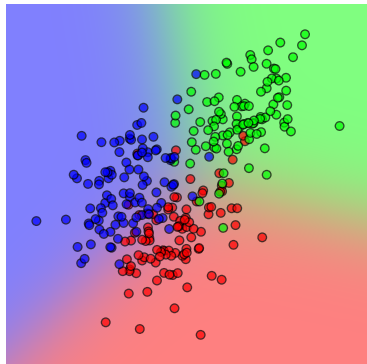
- $k = 3, n = 300, m = 10, \epsilon = 10^{-1}, \lambda = 10^{-3}$

prediction: soft assignment

epoch 30



hinge (W&W)

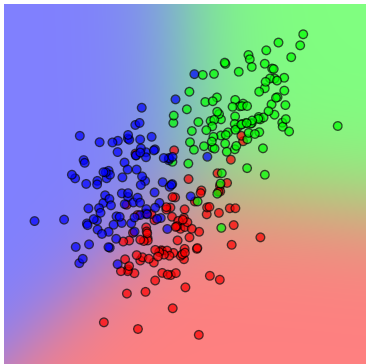


logistic

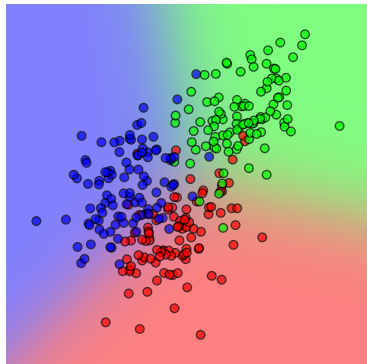
- $k = 3, n = 300, m = 10, \epsilon = 10^{-1}, \lambda = 10^{-3}$

prediction: soft assignment

epoch 35



hinge (W&W)

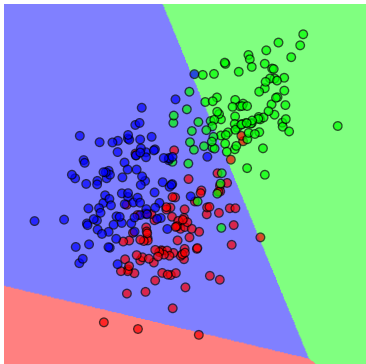


logistic

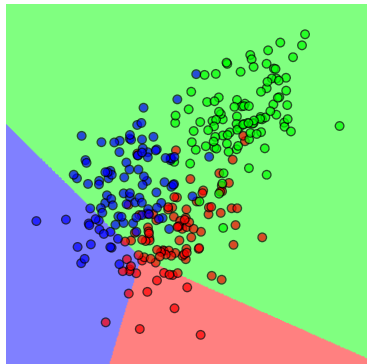
- $k = 3, n = 300, m = 10, \epsilon = 10^{-1}, \lambda = 10^{-3}$

prediction: hard assignment

epoch 00



hinge (W & W)

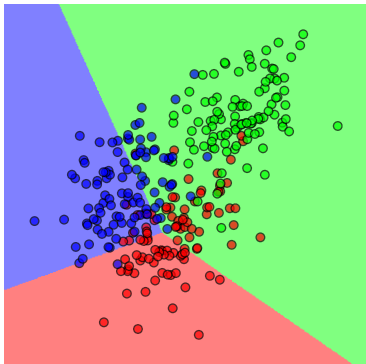


logistic

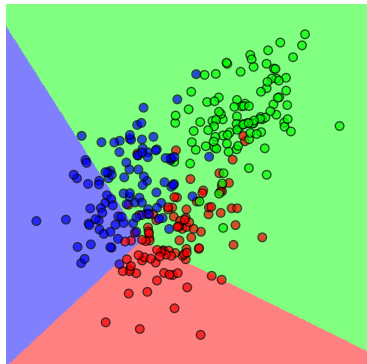
- $k = 3, n = 300, m = 10, \epsilon = 10^{-2}, \lambda = 10^{-3}$

prediction: hard assignment

epoch 04



hinge (W & W)

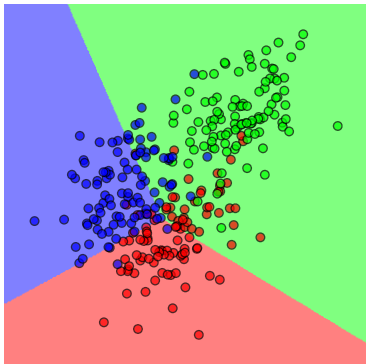


logistic

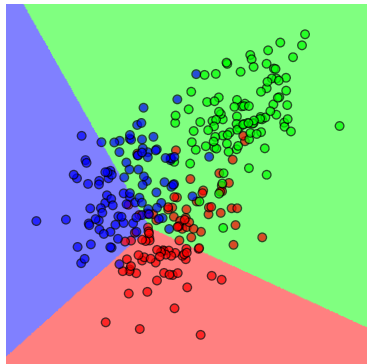
- $k = 3, n = 300, m = 10, \epsilon = 10^{-2}, \lambda = 10^{-3}$

prediction: hard assignment

epoch 08



hinge (W & W)

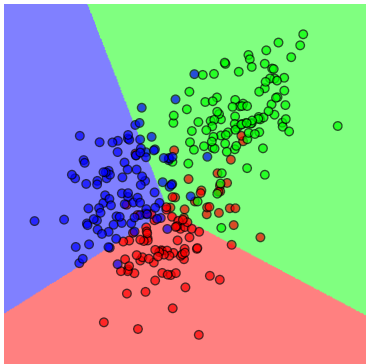


logistic

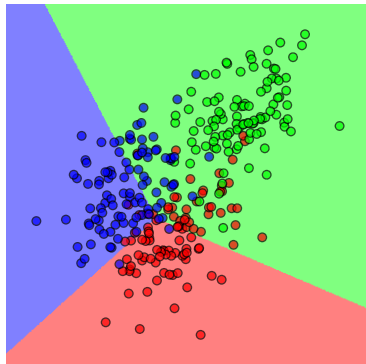
- $k = 3, n = 300, m = 10, \epsilon = 10^{-2}, \lambda = 10^{-3}$

prediction: hard assignment

epoch 12



hinge (W & W)

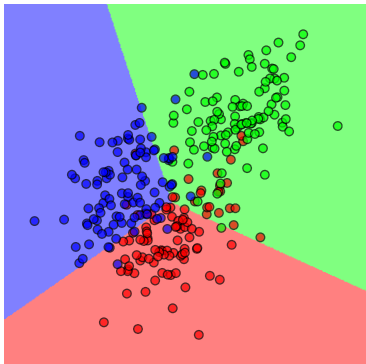


logistic

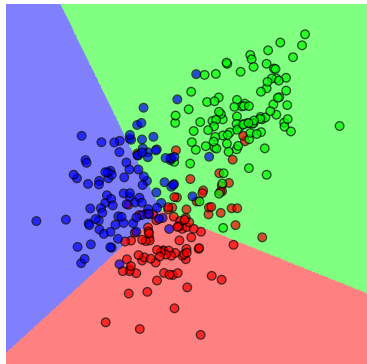
- $k = 3, n = 300, m = 10, \epsilon = 10^{-2}, \lambda = 10^{-3}$

prediction: hard assignment

epoch 16



hinge (W & W)

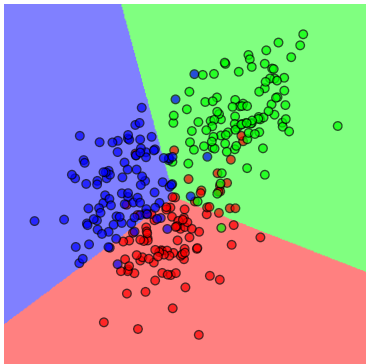


logistic

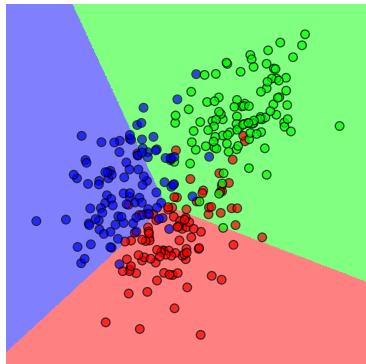
- $k = 3, n = 300, m = 10, \epsilon = 10^{-2}, \lambda = 10^{-3}$

prediction: hard assignment

epoch 20



hinge (W & W)

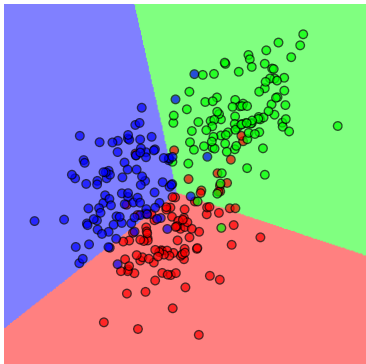


logistic

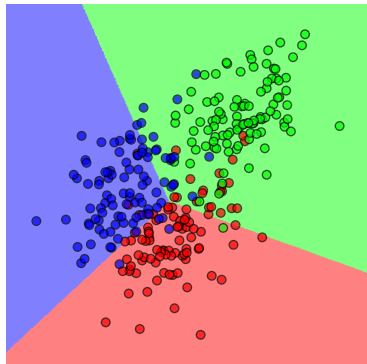
- $k = 3, n = 300, m = 10, \epsilon = 10^{-2}, \lambda = 10^{-3}$

prediction: hard assignment

epoch 24



hinge (W & W)

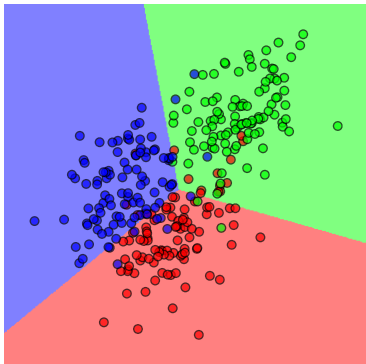


logistic

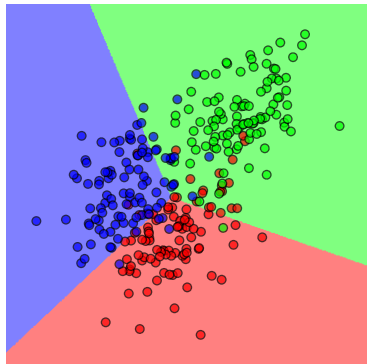
- $k = 3, n = 300, m = 10, \epsilon = 10^{-2}, \lambda = 10^{-3}$

prediction: hard assignment

epoch 28



hinge (W & W)



logistic

- $k = 3, n = 300, m = 10, \epsilon = 10^{-2}, \lambda = 10^{-3}$

MNIST digits dataset

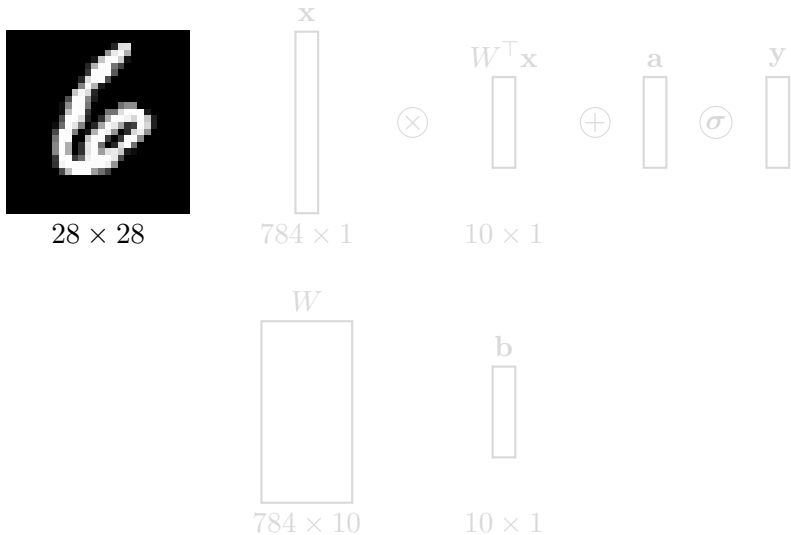


- 10 classes, 60k training images, 10k test images, 28×28 images

from images to vectors

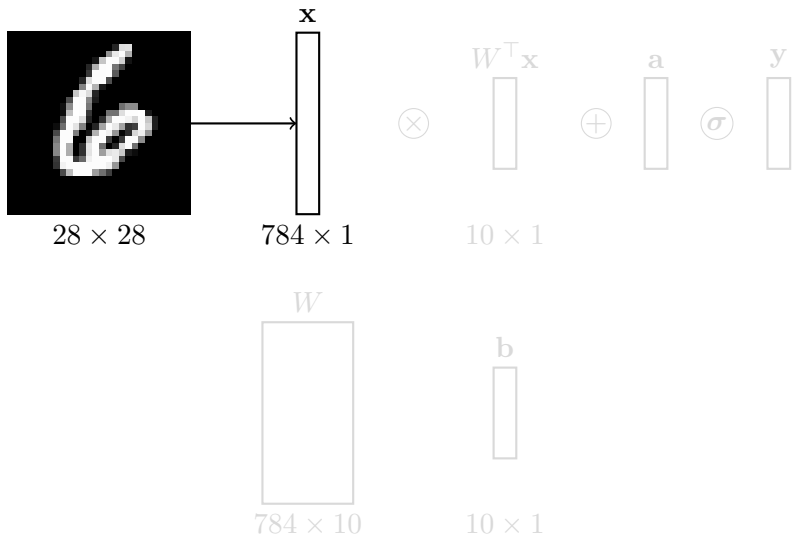
- all classifiers considered so far work with vectors
- we have seen how to extract a descriptor—a vector—from an image
- however, the point now is how to **learn** to extract a descriptor
- so we start from raw pixels: a gray-scale input image is just a 28×28 matrix, and we vectorize it into 784×1

linear classifier on raw pixels



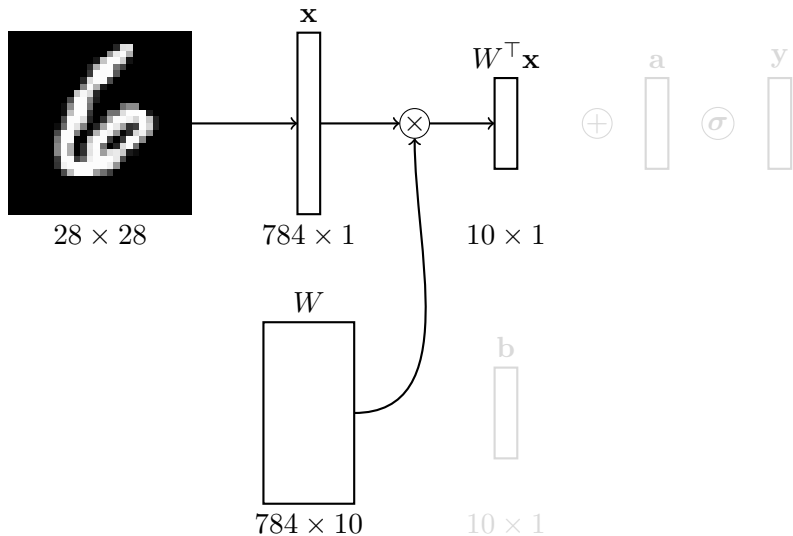
- input - weights - bias - softmax - parameters to be learned

linear classifier on raw pixels



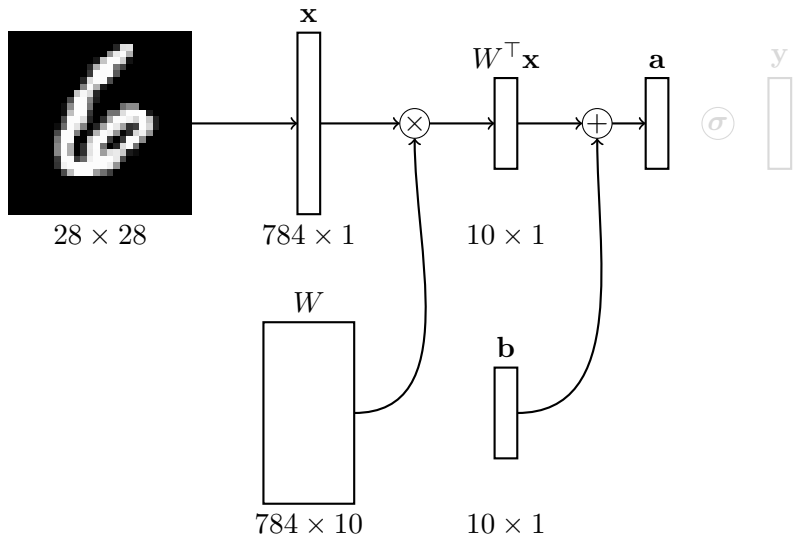
- input - weights - bias - softmax - parameters to be learned

linear classifier on raw pixels



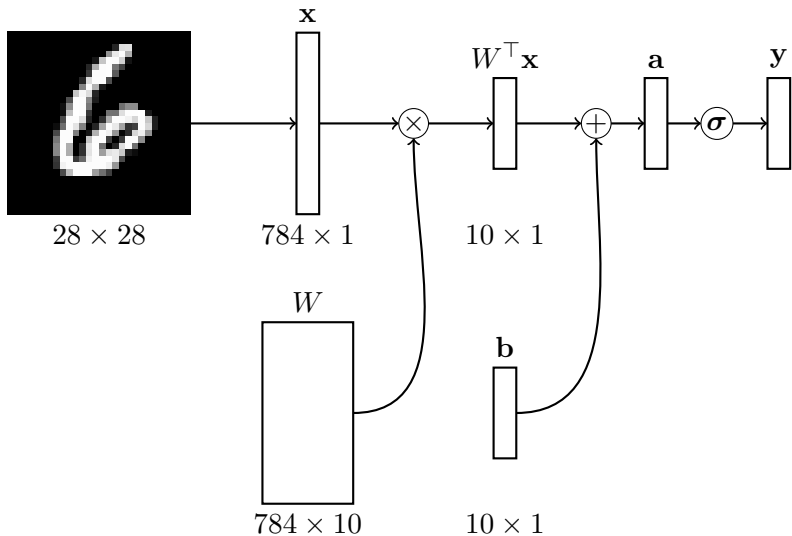
- input - weights - bias - softmax - parameters to be learned

linear classifier on raw pixels



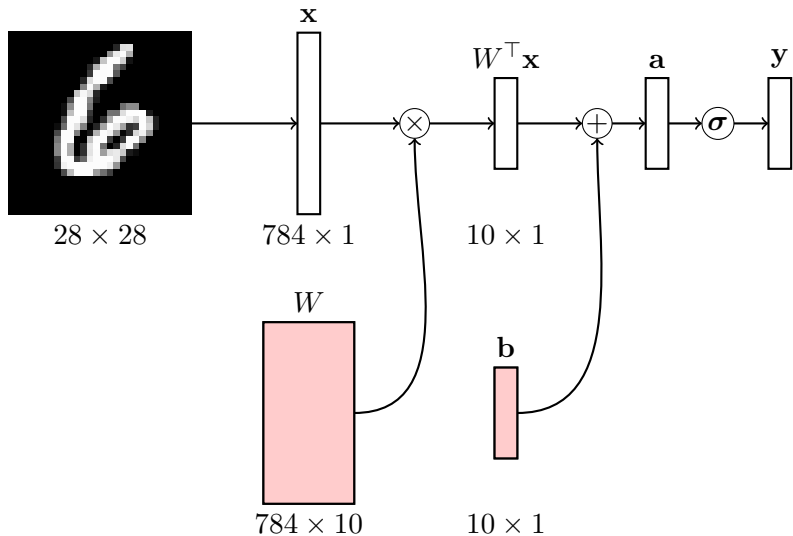
- input - weights - bias - softmax - parameters to be learned

linear classifier on raw pixels



- input - weights - bias - softmax - parameters to be learned

linear classifier on raw pixels

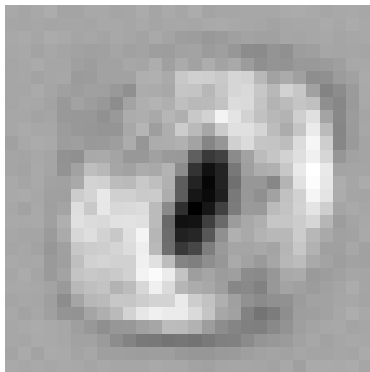


- input - weights - bias - softmax - parameters to be learned

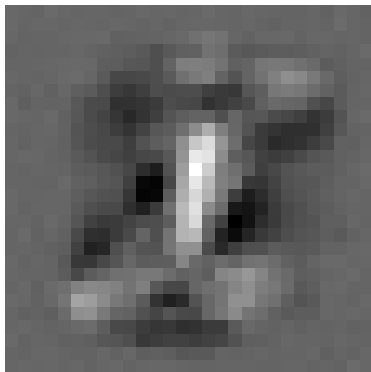
what is being learned?

- the columns of W are multiplied with \mathbf{x} ; they live in the same space
- we can reshape each one back from 784×1 to 28×28 : it should look like a digit

linear classifier on MNIST: patterns



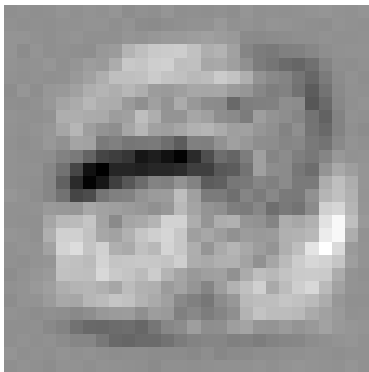
0



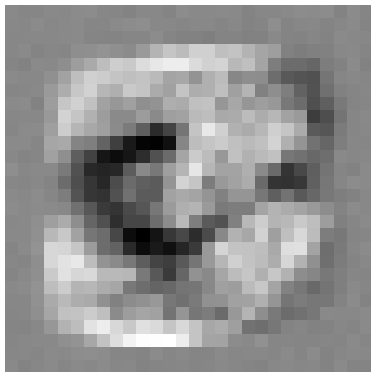
1

- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- test error 7.67%

linear classifier on MNIST: patterns



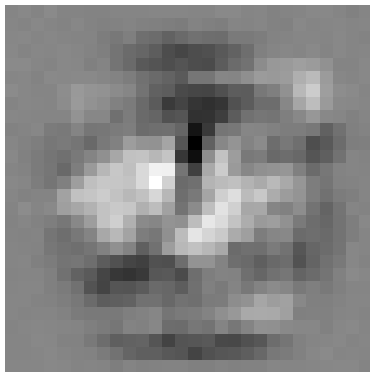
2



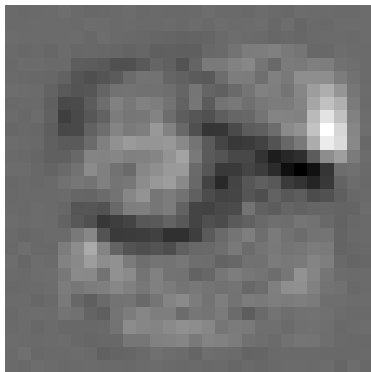
3

- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- test error 7.67%

linear classifier on MNIST: patterns



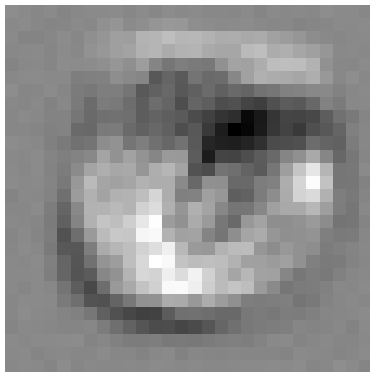
4



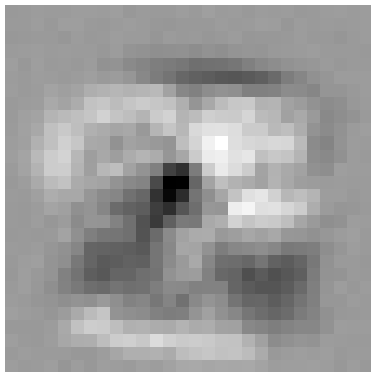
5

- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- test error 7.67%

linear classifier on MNIST: patterns



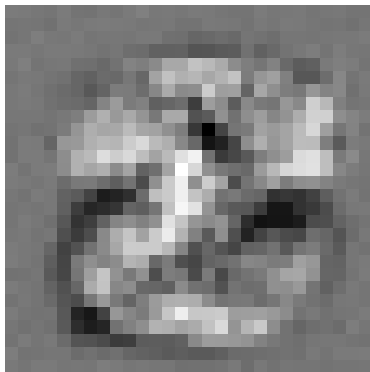
6



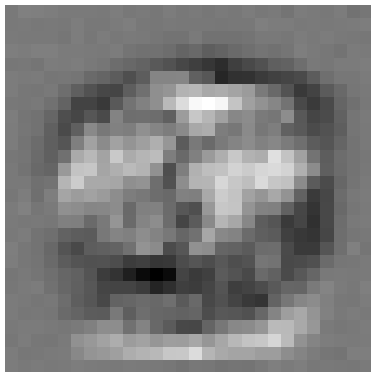
7

- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- test error 7.67%

linear classifier on MNIST: patterns



8

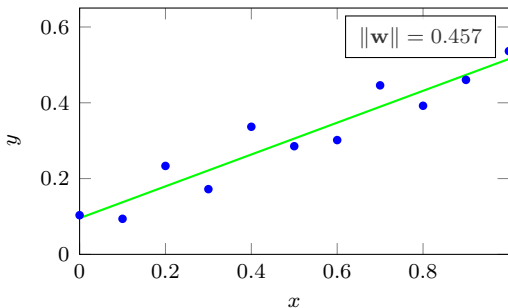


9

- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- test error 7.67%

regression

line fitting



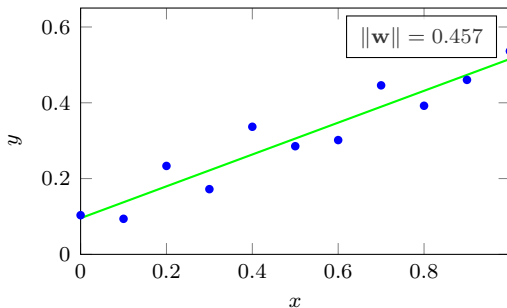
- linear model with parameters $\mathbf{w} = (a, b)$

$$y = ax + b = (a, b)^\top (x, 1) = \mathbf{w}^\top \phi(x)$$

- least squares error given samples (x_1, \dots, x_n) , targets $\mathbf{t} = (t_1, \dots, t_n)$

$$E(\mathbf{w}) = \sum_{i=1}^n (\mathbf{w}^\top \phi(x_i) - t_i)^2$$

line fitting



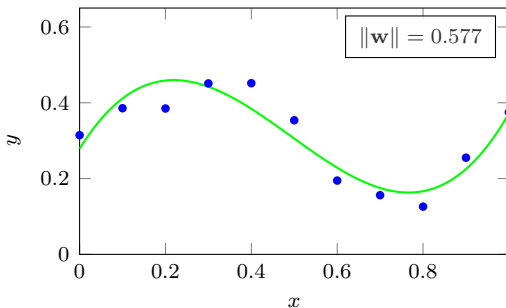
- linear model with parameters $\mathbf{w} = (a, b)$

$$y = ax + b = (a, b)^\top (x, 1) = \mathbf{w}^\top \phi(x)$$

- least squares solution, where $\Phi = (\phi(x_1); \dots; \phi(x_n)) \in \mathbb{R}^{n \times 2}$

$$\mathbf{w}^* = (\Phi^\top \Phi)^{-1} \Phi^\top \mathbf{t}$$

polynomial curve fitting



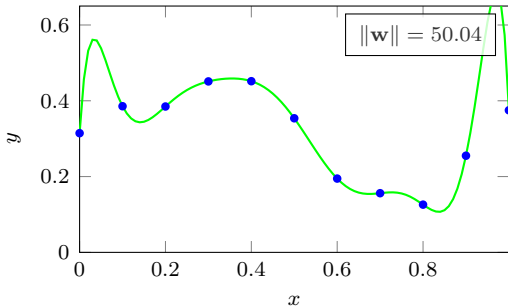
- linear model with parameters $\mathbf{w} \in \mathbb{R}^4$

$$y = \mathbf{w}^\top \phi(x) = \mathbf{w}^\top (1, x, x^2, x^3)$$

- least squares solution, where $\Phi = (\phi(x_1); \dots; \phi(x_n)) \in \mathbb{R}^{n \times 4}$

$$\mathbf{w}^* = (\Phi^\top \Phi)^{-1} \Phi^\top \mathbf{t}$$

overfitting



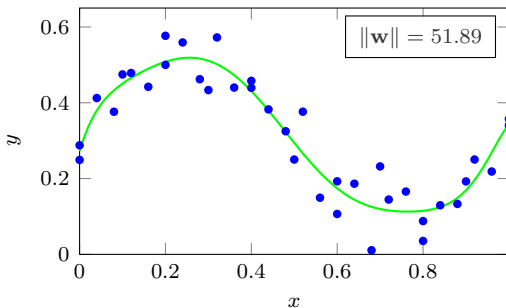
- linear model with parameters $\mathbf{w} \in \mathbb{R}^{11}$

$$y = \mathbf{w}^\top \phi(x) = \mathbf{w}^\top (1, x, x^2, \dots, x^{10})$$

- least squares solution, where $\Phi = (\phi(x_1); \dots; \phi(x_n)) \in \mathbb{R}^{n \times 11}$

$$\mathbf{w}^* = (\Phi^\top \Phi)^{-1} \Phi^\top \mathbf{t}$$

more data



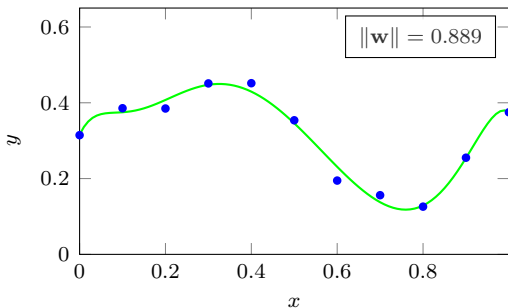
- linear model with parameters $\mathbf{w} \in \mathbb{R}^{11}$

$$y = \mathbf{w}^\top \phi(x) = \mathbf{w}^\top (1, x, x^2, \dots, x^{10})$$

- least squares solution, where $\Phi = (\phi(x_1); \dots; \phi(x_n)) \in \mathbb{R}^{n \times 11}$

$$\mathbf{w}^* = (\Phi^\top \Phi)^{-1} \Phi^\top \mathbf{t}$$

regularization



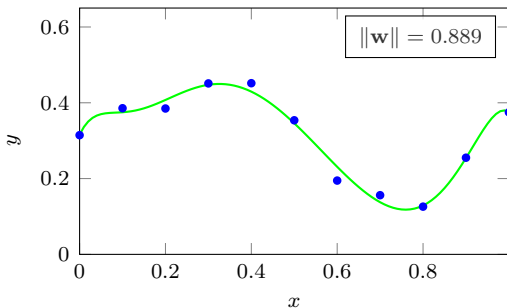
- linear model with parameters $\mathbf{w} \in \mathbb{R}^{11}$

$$y = \mathbf{w}^\top \phi(x) = \mathbf{w}^\top (1, x, x^2, \dots, x^{10})$$

- regularized least squares error with parameter λ

$$E(\mathbf{w}) = \sum_{i=1}^n (\mathbf{w}^\top \phi(x_i) - t_i)^2 + \frac{\lambda}{2} \|\mathbf{w}\|^2$$

regularization



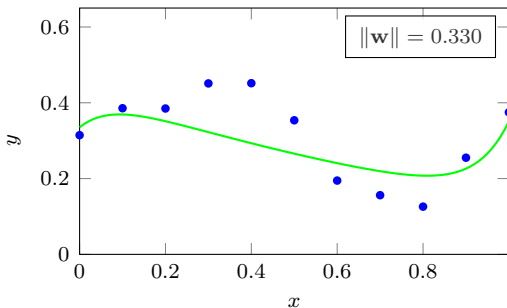
- linear model with parameters $\mathbf{w} \in \mathbb{R}^{11}$

$$y = \mathbf{w}^\top \phi(x) = \mathbf{w}^\top (1, x, x^2, \dots, x^{10})$$

- regularized least squares solution with parameter $\lambda = 10^{-3}$

$$\mathbf{w}^* = (\lambda I + \Phi^\top \Phi)^{-1} \Phi^\top \mathbf{t}$$

severe regularization



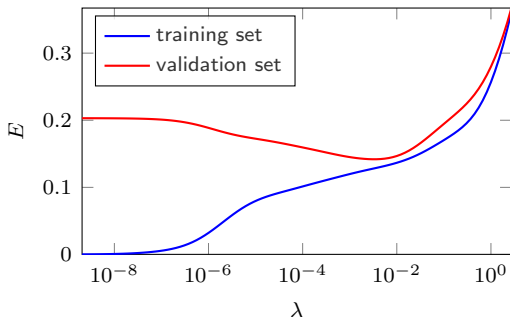
- linear model with parameters $\mathbf{w} \in \mathbb{R}^{11}$

$$y = \mathbf{w}^\top \phi(x) = \mathbf{w}^\top (1, x, x^2, \dots, x^{10})$$

- regularized least squares solution with parameter $\lambda = 1$

$$\mathbf{w}^* = (\lambda I + \Phi^\top \Phi)^{-1} \Phi^\top \mathbf{t}$$

generalization error



- linear model with parameters $\mathbf{w} \in \mathbb{R}^{11}$

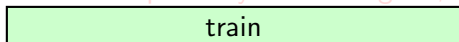
$$y = \mathbf{w}^\top \phi(x) = \mathbf{w}^\top (1, x, x^2, \dots, x^{10})$$

- regularized least squares solution with parameter $\lambda \in [10^{-8}, 10^0]$

$$\mathbf{w}^* = (\lambda I + \Phi^\top \Phi)^{-1} \Phi^\top \mathbf{t}$$

setting hyperparameters

- optimize both parameters and hyperparameters on the training set:
could work perfectly on training set, no idea how it works on test set



- train parameters on training set, hyperparameters on test set: no idea how it works no new data; the test set represents new data and should never be touched but for evaluation at the very end

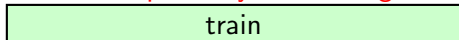


- train parameters on training set, hyperparameters on validation set: great, validation data are new so we test our model's generalization; test data are also new and are only used for evaluation



setting hyperparameters

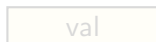
- optimize both parameters and hyperparameters on the training set:
could work perfectly on training set, no idea how it works on test set



- train parameters on training set, hyperparameters on test set: no idea how it works no new data; the test set represents new data and should never be touched but for evaluation at the very end

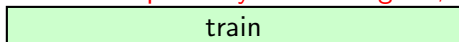


- train parameters on training set, hyperparameters on validation set: great, validation data are new so we test our model's generalization; test data are also new and are only used for evaluation

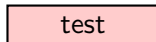
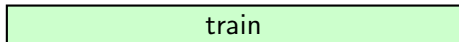


setting hyperparameters

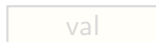
- optimize both parameters and hyperparameters on the training set:
could work perfectly on training set, no idea how it works on test set



- train parameters on training set, hyperparameters on test set: no idea how it works no new data; the test set represents new data and should never be touched but for evaluation at the very end

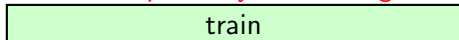


- train parameters on training set, hyperparameters on validation set: great, validation data are new so we test our model's generalization; test data are also new and are only used for evaluation

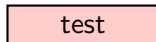
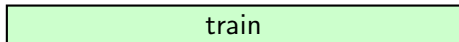


setting hyperparameters

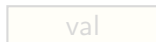
- optimize both parameters and hyperparameters on the training set:
could work perfectly on training set, no idea how it works on test set



- train parameters on training set, hyperparameters on test set: no idea how it works no new data; the test set represents new data and should never be touched but for evaluation at the very end

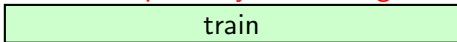


- train parameters on training set, hyperparameters on validation set:
great, validation data are new so we test our model's generalization;
test data are also new and are only used for evaluation

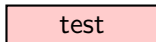
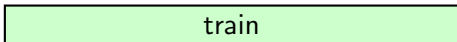


setting hyperparameters

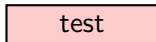
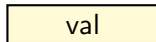
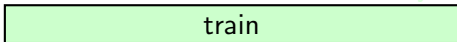
- optimize both parameters and hyperparameters on the training set:
could work perfectly on training set, no idea how it works on test set



- train parameters on training set, hyperparameters on test set: no idea how it works no new data; the test set represents new data and should never be touched but for evaluation at the very end

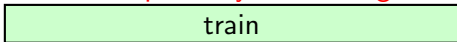


- train parameters on training set, hyperparameters on validation set:
great, validation data are new so we test our model's generalization;
test data are also new and are only used for evaluation

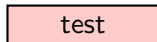
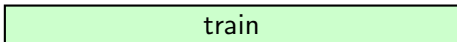


setting hyperparameters

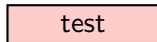
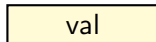
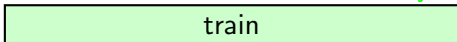
- optimize both parameters and hyperparameters on the training set:
could work perfectly on training set, no idea how it works on test set



- train parameters on training set, hyperparameters on test set: no idea how it works no new data; the test set represents new data and should never be touched but for evaluation at the very end



- train parameters on training set, hyperparameters on validation set: great, validation data are new so we test our model's generalization; test data are also new and are only used for evaluation



k -fold cross-validation

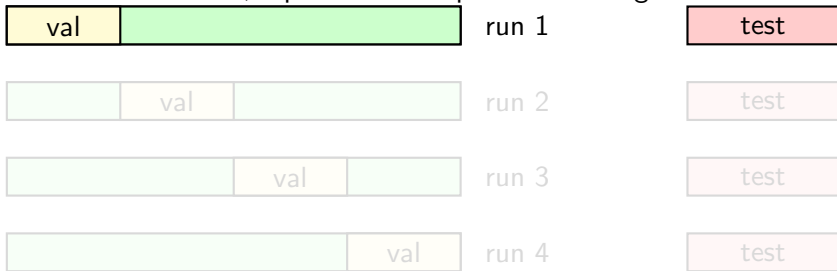
- split data into k groups; treat $k - 1$ as training and 1 as validation, measure on test set; repeat over all splits and average the results



- too expensive for large datasets:** better use only one split; even better, each dataset has an official validation set so results are comparable

k -fold cross-validation

- split data into k groups; treat $k - 1$ as training and 1 as validation, measure on test set; repeat over all splits and average the results



- too expensive for large datasets: better use only one split; even better, each dataset has an official validation set so results are comparable

k -fold cross-validation

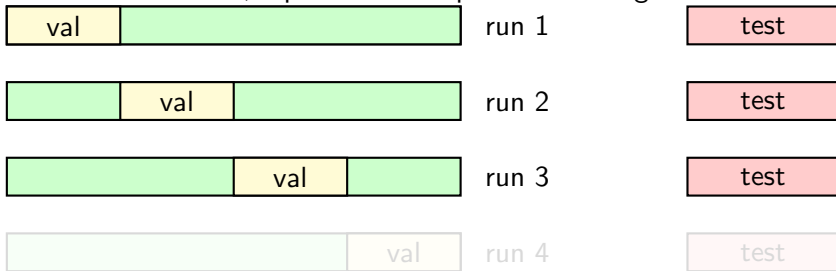
- split data into k groups; treat $k - 1$ as training and 1 as validation, measure on test set; repeat over all splits and average the results



- too expensive for large datasets:** better use only one split; even better, each dataset has an official validation set so results are comparable

k -fold cross-validation

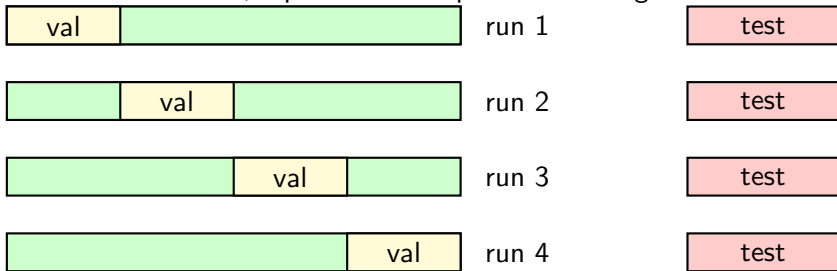
- split data into k groups; treat $k - 1$ as training and 1 as validation, measure on test set; repeat over all splits and average the results



- too expensive for large datasets:** better use only one split; even better, each dataset has an official validation set so results are comparable

k -fold cross-validation

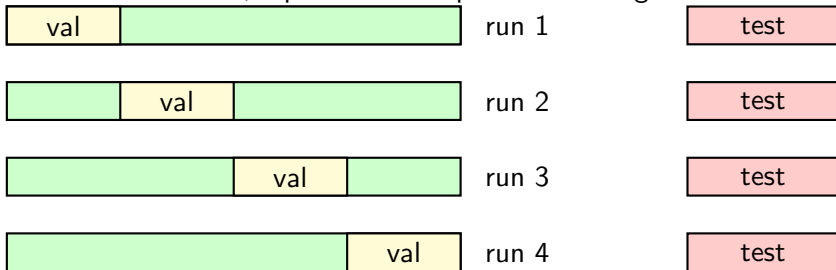
- split data into k groups; treat $k - 1$ as training and 1 as validation, measure on test set; repeat over all splits and average the results



- too expensive for large datasets: better use only one split; even better, each dataset has an official validation set so results are comparable

k -fold cross-validation

- split data into k groups; treat $k - 1$ as training and 1 as validation, measure on test set; repeat over all splits and average the results



- too expensive for large datasets:** better use only one split; even better, each dataset has an official validation set so results are comparable

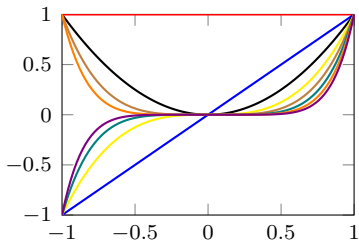
“basis” functions

- the most interesting idea discussed here is that the model becomes **nonlinear** in the raw input by expressing the unknown function as a linear combination (with unknown weights) of a number of fixed nonlinear “**basis**” functions
- we can re-use this idea in classification because classification is really regression followed by thresholding (or comparison)

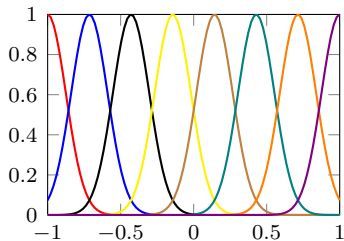
“basis” functions

- the most interesting idea discussed here is that the model becomes **nonlinear** in the raw input by expressing the unknown function as a linear combination (with unknown weights) of a number of fixed nonlinear “**basis**” functions
- we can re-use this idea in classification because classification is really regression followed by thresholding (or comparison)

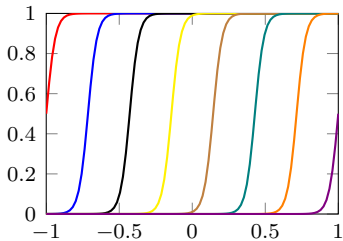
basis functions



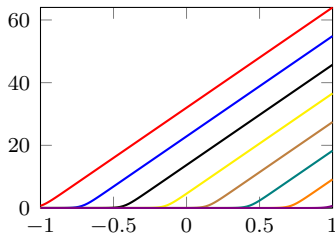
polynomial



Gaussian

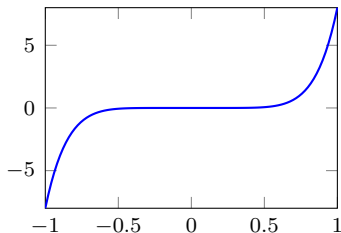


sigmoid

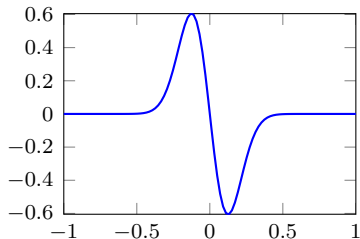


softplus

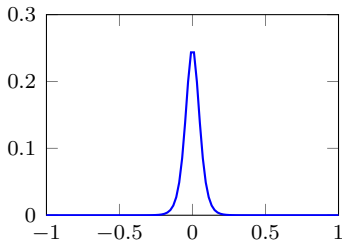
basis function derivatives



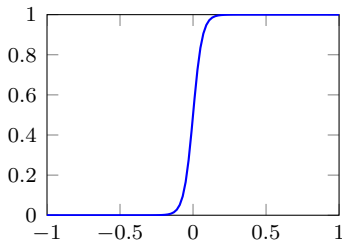
polynomial



Gaussian



sigmoid



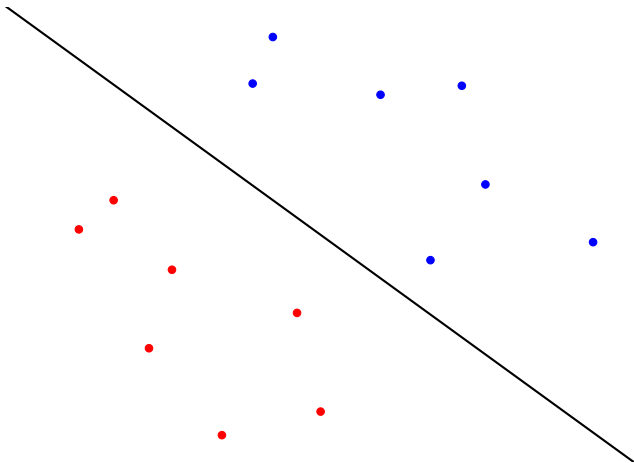
softplus

basis functions

- we want basis functions to cover the entire space so that any arbitrary input can be expressed as a linear combination of such functions
- the Gaussian is localized, the others have larger support
- polynomials and their derivatives can get extremely large; the range of all the others can be easily controlled
- the derivatives of the Gaussian and sigmoid are localized; the derivative of softplus is nonzero over half of the space

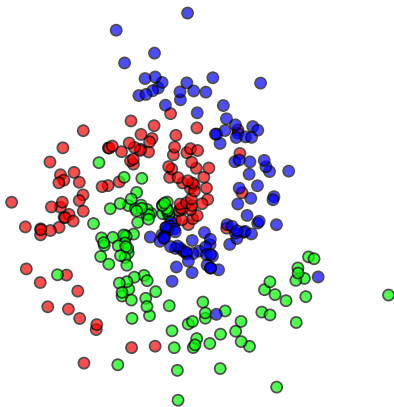
multiple layers

linear separability



- two point sets $X_1, X_2 \subset \mathbb{R}^d$ are linearly separable iff there is \mathbf{w}, b such that $\mathbf{w}^\top \mathbf{x}_1 < b < \mathbf{w}^\top \mathbf{x}_2$ for $\mathbf{x}_1 \in X_1, \mathbf{x}_2 \in X_2$
- or, they can be separated by a perceptron

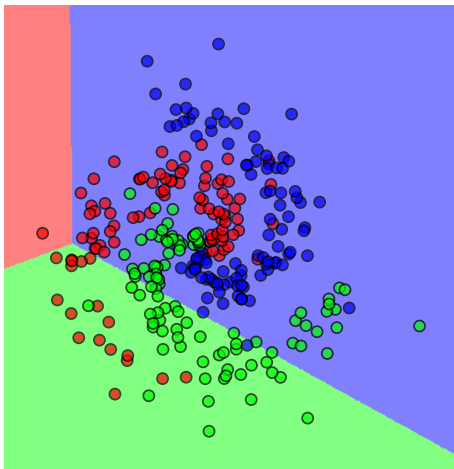
non-linearly separable classes



credit: dataset adapted from Andrej Karpathy

linear classifier

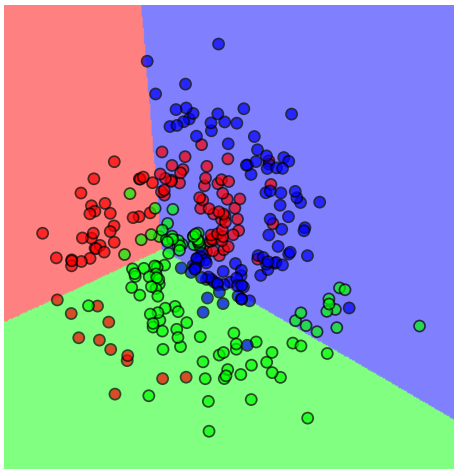
epoch 00



- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

linear classifier

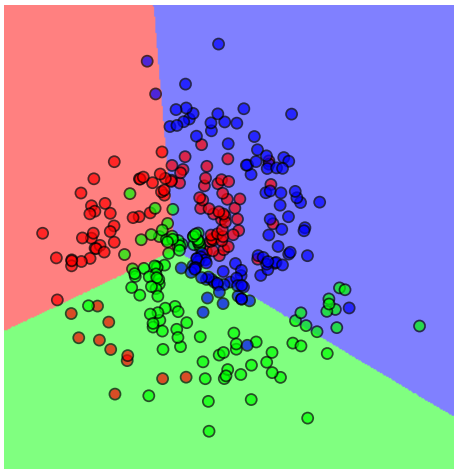
epoch 05



- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

linear classifier

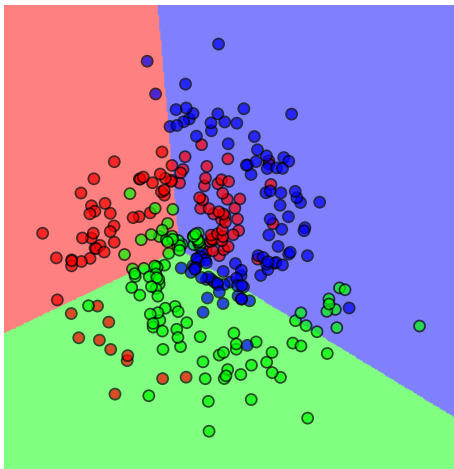
epoch 10



- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

linear classifier

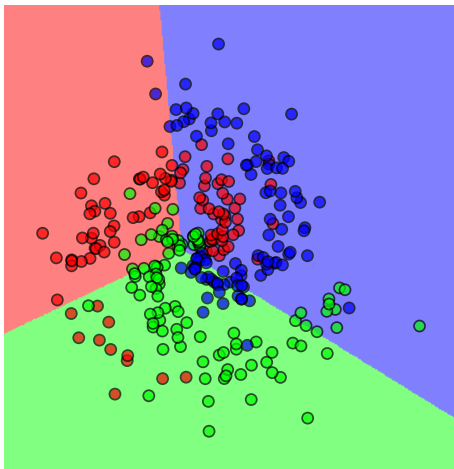
epoch 15



- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

linear classifier

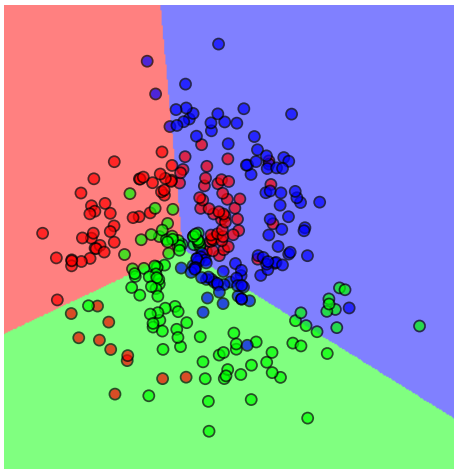
epoch 20



- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

linear classifier

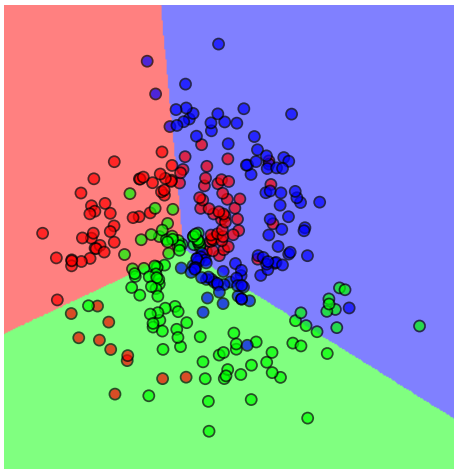
epoch 25



- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

linear classifier

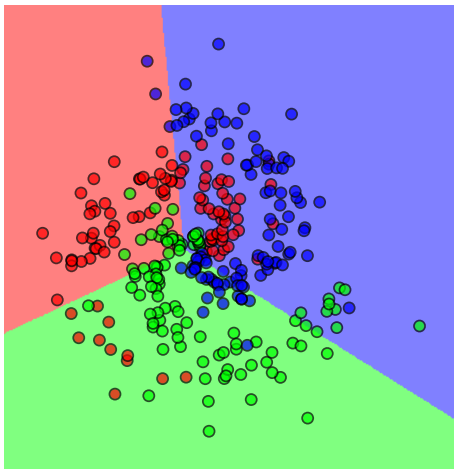
epoch 30



- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

linear classifier

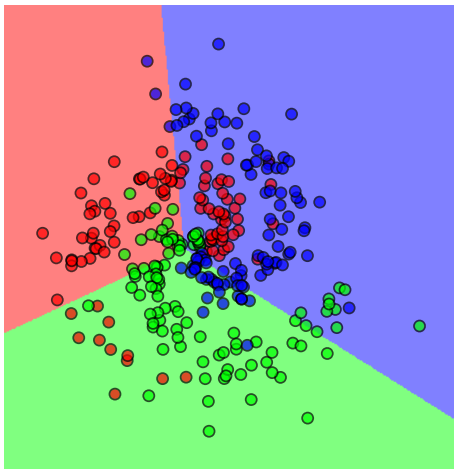
epoch 35



- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

linear classifier

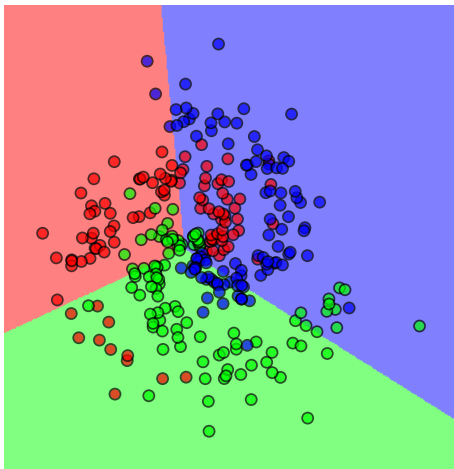
epoch 40



- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

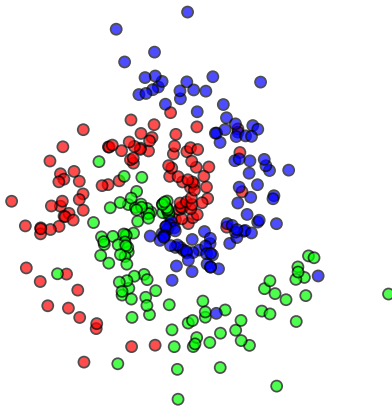
linear classifier

epoch 45



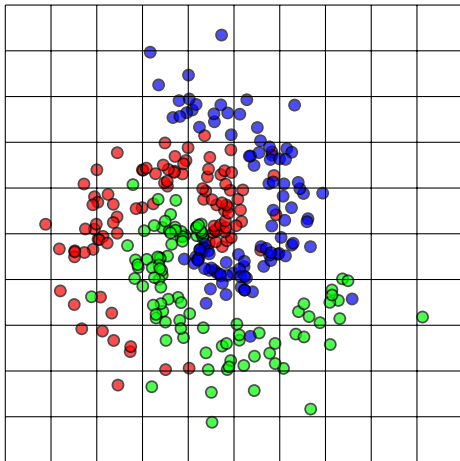
- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

nonlinear?



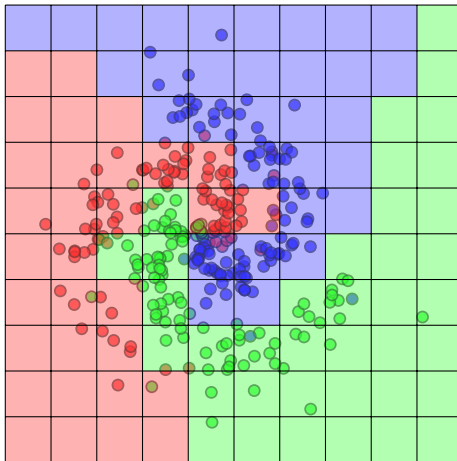
- so how do we make our classifier nonlinear?

nonlinear?



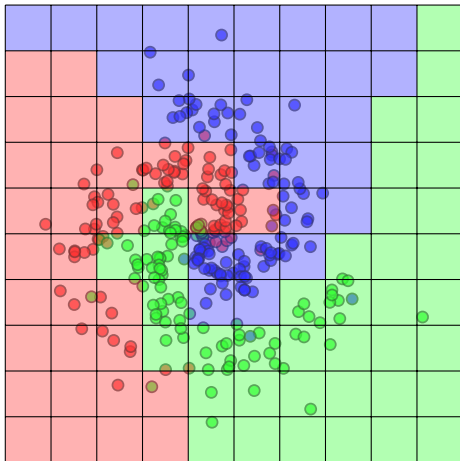
- define a 10×10 grid over the entire space

nonlinear?



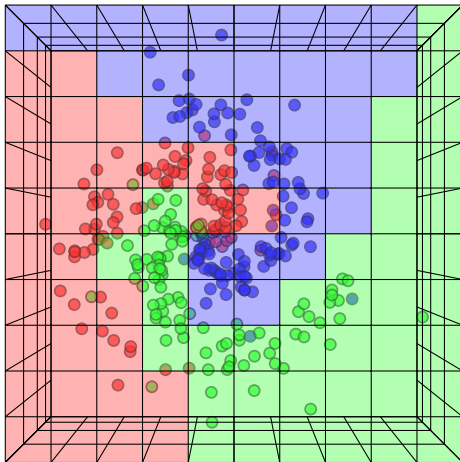
- and a (Gaussian?) basis function centered at every cell

nonlinear?



- then, a linear classifier can separate the 3 classes in 100 dimensions!

the curse of dimensionality



- but, in 3 dimensions we would need 1000 basis functions; and remember, a 320×200 image is a vector in $\mathbb{R}^{64,000}$

basis functions

- we need a small set of basis functions to cover the entire space, or at least the regions where our data live
- we did use fixed basis functions before: the **Gabor filters** discretized the 2d space of scales and orientations in uniform bins and their responses were used as vectors
- but right in the next layer, the dimensions increase and we cannot afford to have fixed basis functions everywhere: we have to **learn from the data**, as we did with the **codebooks**
- codebooks were trained by clustering the features of the observed data, in an unsupervised fashion; but, now, we have the opportunity to learn them **jointly** with the classifier, in a **supervised** fashion
- so, each basis function will have itself some parameters to learn, but what form should the function have?
- **why not just like a classifier?**

basis functions

- we need a small set of basis functions to cover the entire space, or at least the regions where our data live
- we did use fixed basis functions before: the **Gabor filters** discretized the 2d space of scales and orientations in uniform bins and their responses were used as vectors
- but right in the next layer, the dimensions increase and we cannot afford to have fixed basis functions everywhere: we have to **learn from the data**, as we did with the **codebooks**
- codebooks were trained by clustering the features of the observed data, in an unsupervised fashion; but, now, we have the opportunity to learn them **jointly** with the classifier, in a **supervised** fashion
- so, each basis function will have itself some parameters to learn, but what form should the function have?
- why not just like a classifier?

basis functions

- we need a small set of basis functions to cover the entire space, or at least the regions where our data live
- we did use fixed basis functions before: the **Gabor filters** discretized the 2d space of scales and orientations in uniform bins and their responses were used as vectors
- but right in the next layer, the dimensions increase and we cannot afford to have fixed basis functions everywhere: we have to **learn from the data**, as we did with the **codebooks**
- codebooks were trained by clustering the features of the observed data, in an unsupervised fashion; but, now, we have the opportunity to learn them **jointly** with the classifier, in a **supervised** fashion
- so, each basis function will have itself some parameters to learn, but what form should the function have?
- **why not just like a classifier?**

two-layer network

- we describe each sample with a **feature** vector obtained by a **nonlinear** function
- we model this function after a (binary) **logistic regression unit**: much like this unit can act as a classifier, it might also “detect” features that can be useful in the final classification
- layer 1 \rightarrow “features”

$$\mathbf{a}_1 = W_1^\top \mathbf{x} + \mathbf{b}_1, \quad \mathbf{z} = h(\mathbf{a}_1) = h(W_1^\top \mathbf{x} + \mathbf{b}_1)$$

where h is a nonlinear **activation function**

- layer 2 \rightarrow class probabilities

$$\mathbf{a}_2 = W_2^\top \mathbf{z} + \mathbf{b}_2, \quad \mathbf{y} = \sigma(\mathbf{a}_2) = \sigma(W_2^\top \mathbf{z} + \mathbf{b}_2)$$

- $\theta := (W_1, \mathbf{b}_1, W_2, \mathbf{b}_2)$ is the set of parameters to learn

two-layer network

- we describe each sample with a **feature** vector obtained by a **nonlinear** function
- we model this function after a (binary) **logistic regression unit**: much like this unit can act as a classifier, it might also “detect” features that can be useful in the final classification
- layer 1 \rightarrow “features”

$$\mathbf{a}_1 = W_1^\top \mathbf{x} + \mathbf{b}_1, \quad \mathbf{z} = h(\mathbf{a}_1) = h(W_1^\top \mathbf{x} + \mathbf{b}_1)$$

where h is a nonlinear **activation function**

- layer 2 \rightarrow class probabilities

$$\mathbf{a}_2 = W_2^\top \mathbf{z} + \mathbf{b}_2, \quad \mathbf{y} = \sigma(\mathbf{a}_2) = \sigma(W_2^\top \mathbf{z} + \mathbf{b}_2)$$

- $\theta := (W_1, \mathbf{b}_1, W_2, \mathbf{b}_2)$ is the set of parameters to learn

two-layer network

- we describe each sample with a **feature** vector obtained by a **nonlinear** function
- we model this function after a (binary) **logistic regression unit**: much like this unit can act as a classifier, it might also “detect” features that can be useful in the final classification
- layer 1 \rightarrow “features”

$$\mathbf{a}_1 = W_1^\top \mathbf{x} + \mathbf{b}_1, \quad \mathbf{z} = h(\mathbf{a}_1) = h(W_1^\top \mathbf{x} + \mathbf{b}_1)$$

where h is a nonlinear **activation function**

- layer 2 \rightarrow class probabilities

$$\mathbf{a}_2 = W_2^\top \mathbf{z} + \mathbf{b}_2, \quad \mathbf{y} = \sigma(\mathbf{a}_2) = \sigma(W_2^\top \mathbf{z} + \mathbf{b}_2)$$

- $\theta := (W_1, \mathbf{b}_1, W_2, \mathbf{b}_2)$ is the set of parameters to learn

two-layer network

- we describe each sample with a **feature** vector obtained by a **nonlinear** function
- we model this function after a (binary) **logistic regression unit**: much like this unit can act as a classifier, it might also “detect” features that can be useful in the final classification
- layer 1 \rightarrow “features”

$$\mathbf{a}_1 = W_1^\top \mathbf{x} + \mathbf{b}_1, \quad \mathbf{z} = h(\mathbf{a}_1) = h(W_1^\top \mathbf{x} + \mathbf{b}_1)$$

where h is a nonlinear **activation function**

- layer 2 \rightarrow class probabilities

$$\mathbf{a}_2 = W_2^\top \mathbf{z} + \mathbf{b}_2, \quad \mathbf{y} = \sigma(\mathbf{a}_2) = \sigma(W_2^\top \mathbf{z} + \mathbf{b}_2)$$

- $\theta := (W_1, \mathbf{b}_1, W_2, \mathbf{b}_2)$ is the set of parameters to learn

activation function h

- this should be nonlinear, otherwise the whole network will be linear and we don't gain much by the hierarchy (but: linear layers **can be** useful sometimes)
- it shouldn't have any more parameters, at least for now: all the parameters in a layer are W, \mathbf{b}
- it is a vector-to-vector function and there are still endless choices of nonlinear functions
- so we make the simplest choice for now: an **element-wise** function
- from the functions we saw previously, we leave polynomials and Gaussians out, and bring a couple more

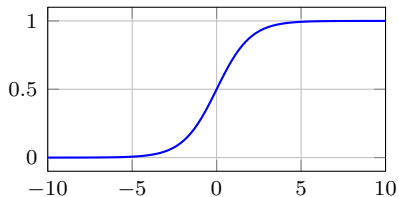
activation function h

- this should be nonlinear, otherwise the whole network will be linear and we don't gain much by the hierarchy (but: linear layers **can be** useful sometimes)
- it shouldn't have any more parameters, at least for now: all the parameters in a layer are W, \mathbf{b}
- it is a vector-to-vector function and there are still endless choices of nonlinear functions
- so we make the simplest choice for now: an **element-wise** function
- from the functions we saw previously, we leave polynomials and Gaussians out, and bring a couple more

activation function h

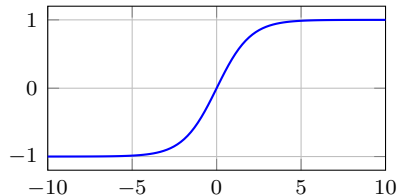
- this should be nonlinear, otherwise the whole network will be linear and we don't gain much by the hierarchy (but: linear layers **can be** useful sometimes)
- it shouldn't have any more parameters, at least for now: all the parameters in a layer are W, \mathbf{b}
- it is a vector-to-vector function and there are still endless choices of nonlinear functions
- so we make the simplest choice for now: an **element-wise** function
- from the functions we saw previously, we leave polynomials and Gaussians out, and bring a couple more

activation functions



$$\sigma(x) = \frac{1}{1+e^{-x}}$$

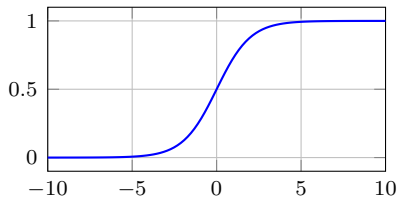
sigmoid



$$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} = 2\sigma(x) - 1$$

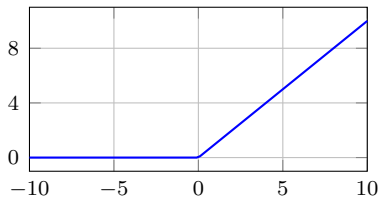
hyperbolic tangent

activation functions



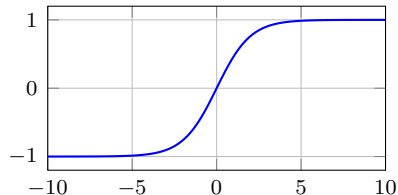
$$\sigma(x) = \frac{1}{1+e^{-x}}$$

sigmoid



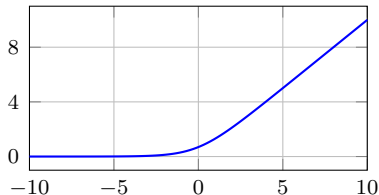
$$\text{relu}(x) = [x]_+ = \max(0, x)$$

rectified linear unit (ReLU)



$$\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} = 2\sigma(x) - 1$$

hyperbolic tangent



$$\zeta(x) = \log(1 + e^x)$$

softplus

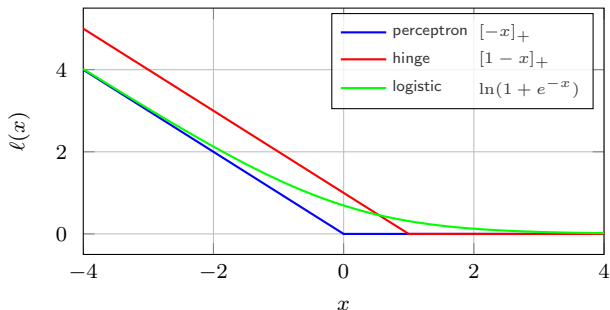
activation functions

- \tanh and sigmoid model exactly what a classifier makes (a decision), but they are smooth unlike sgn whose derivative is zero everywhere: indeed, they have been standard choices for decades.
- relu and its “soft” version softplus are like which functions we have seen?

activation functions

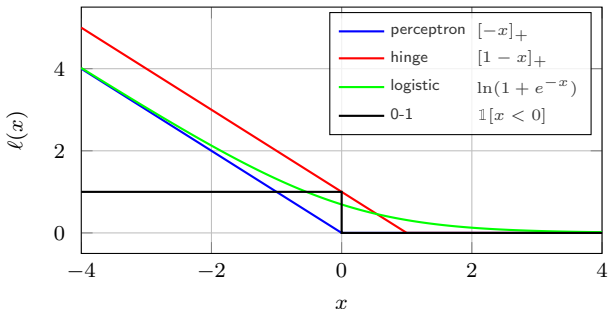
- \tanh and sigmoid model exactly what a classifier makes (a decision), but they are smooth unlike sgn whose derivative is zero everywhere: indeed, they have been standard choices for decades.
- relu and its “soft” version softplus are like which functions we have seen?

back to loss functions



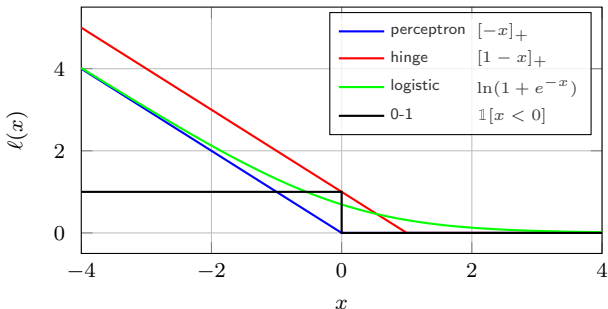
- $\text{relu}(x) = [x]_+$ and $\zeta(x) = \log(1 + e^x)$ are the flipped versions of the perceptron and logistic loss functions, respectively
- also shown is the 0-1 misclassification loss, which is what we actually evaluate during testing and why don't we optimize that instead?
- because it's difficult: its derivative is zero everywhere

back to loss functions



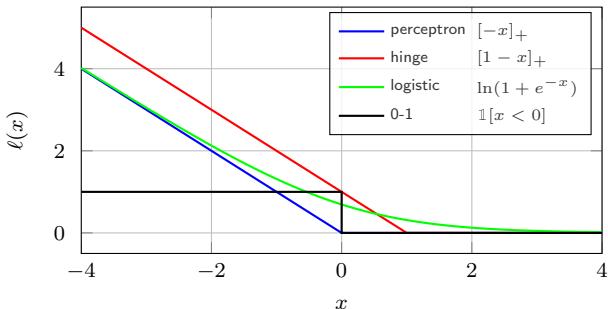
- $\text{relu}(x) = [x]_+$ and $\zeta(x) = \log(1 + e^x)$ are the flipped versions of the perceptron and logistic loss functions, respectively
- also shown is the 0-1 misclassification loss, which is what we actually evaluate during testing: and why don't we optimize that instead?
- because it's difficult: its derivative is zero everywhere

back to loss functions



- $\text{relu}(x) = [x]_+$ and $\zeta(x) = \log(1 + e^x)$ are the flipped versions of the perceptron and logistic loss functions, respectively
- also shown is the 0-1 misclassification loss, which is what we actually evaluate during testing: **and why don't we optimize that instead?**
- because it's difficult: its derivative is zero everywhere

back to loss functions



- $\text{relu}(x) = [x]_+$ and $\zeta(x) = \log(1 + e^x)$ are the flipped versions of the perceptron and logistic loss functions, respectively
- also shown is the 0-1 misclassification loss, which is what we actually evaluate during testing: **and why don't we optimize that instead?**
- because it's difficult: its derivative is zero everywhere

surrogate loss functions

- all three loss functions we have seen are **surrogate** (proxy) for the 0-1 loss: their derivative is constant for $x \rightarrow -\infty$
- they also often work better because even if the 0-1 loss is low (or zero) on the training set, they improve on the **test set**
- even so, we could have used a sigmoid instead, which is the smooth version of the 0-1 loss, but we didn't: its derivative tends to zero for $x \rightarrow -\infty$
- so if **just one** sigmoid is harder than relu, softplus etc. in a linear classifier, **why use 100 of those in the hidden units of a two-layer network?**

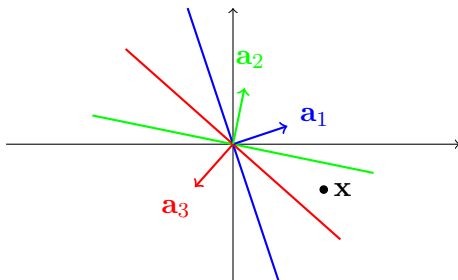
surrogate loss functions

- all three loss functions we have seen are **surrogate** (proxy) for the 0-1 loss: their derivative is constant for $x \rightarrow -\infty$
- they also often work better because even if the 0-1 loss is low (or zero) on the training set, they improve on the **test set**
- even so, we could have used a sigmoid instead, which is the smooth version of the 0-1 loss, but we didn't: its derivative tends to zero for $x \rightarrow -\infty$
- so if **just one** sigmoid is harder than relu, softplus etc. in a linear classifier, **why use 100 of those in the hidden units of a two-layer network?**

surrogate loss functions

- all three loss functions we have seen are **surrogate** (proxy) for the 0-1 loss: their derivative is constant for $x \rightarrow -\infty$
- they also often work better because even if the 0-1 loss is low (or zero) on the training set, they improve on the **test set**
- even so, we could have used a sigmoid instead, which is the smooth version of the 0-1 loss, but we didn't: its derivative tends to zero for $x \rightarrow -\infty$
- so if **just one** sigmoid is harder than relu, softplus etc. in a linear classifier, **why use 100 of those in the hidden units of a two-layer network?**

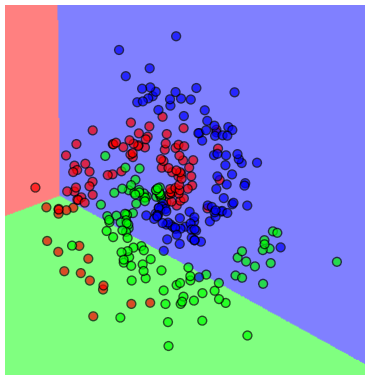
remember LSH?



- in LSH, we used a number of random projections followed by sgn to produce a **binary code** as a description of x
- here, we use again a number of (initially) random projections followed by relu instead, acting like a switch: half space is zeroed out, the other half passes through
- in the nonzero part, gradients are also nonzero and we can use them to adapt the projections themselves

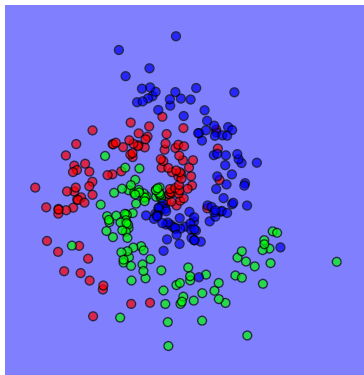
two-layer classifier

epoch 00



linear

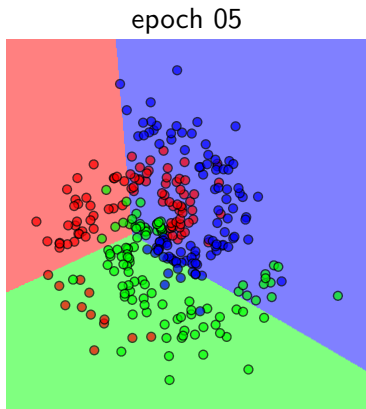
epoch 000



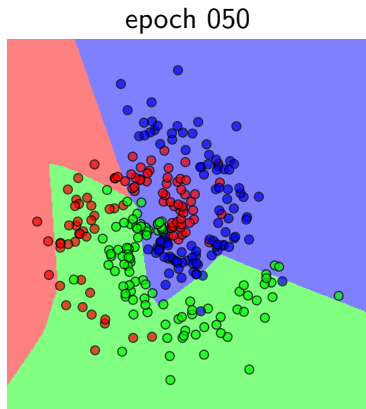
two-layer

- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

two-layer classifier



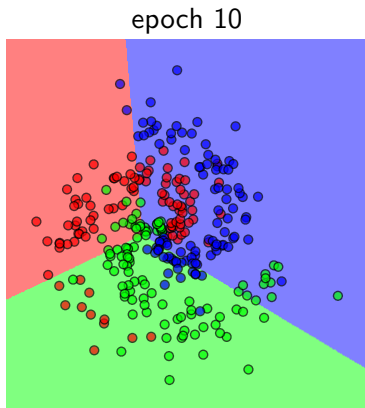
linear



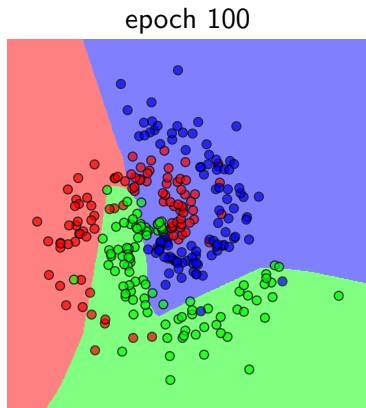
two-layer

- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

two-layer classifier



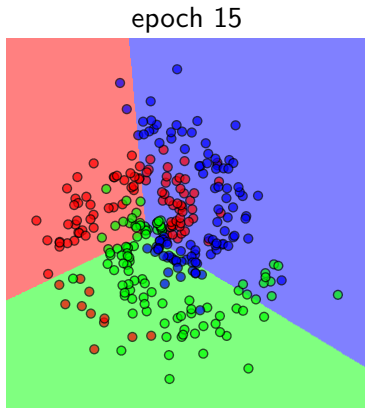
linear



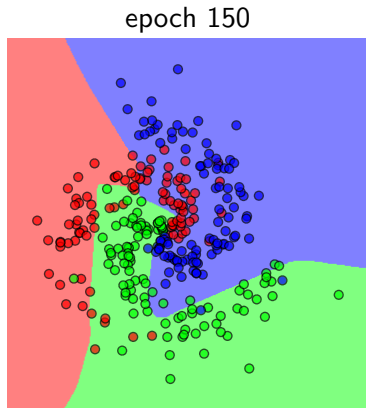
two-layer

- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

two-layer classifier



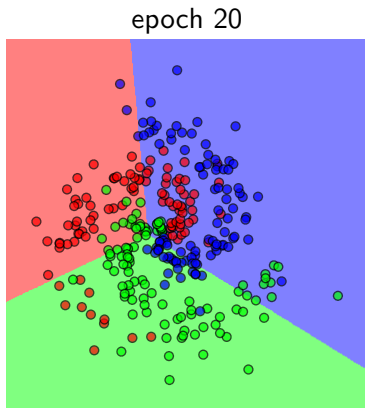
linear



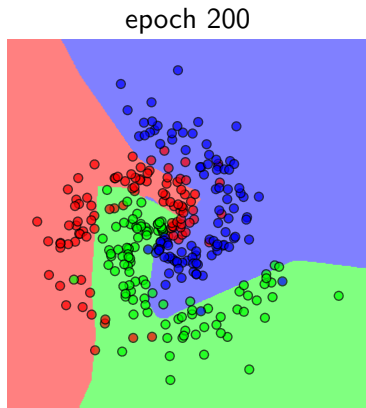
two-layer

- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

two-layer classifier



linear

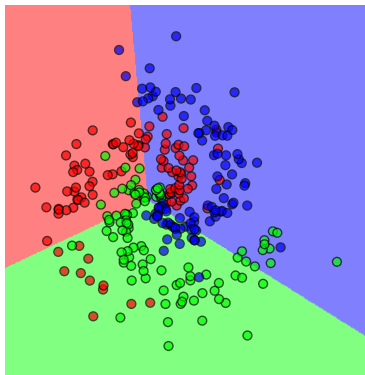


two-layer

- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

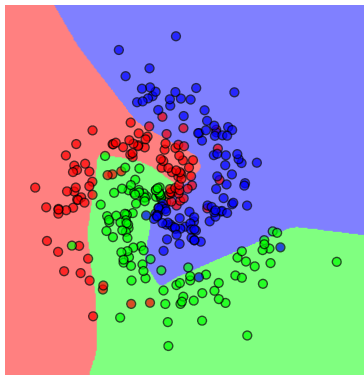
two-layer classifier

epoch 25



linear

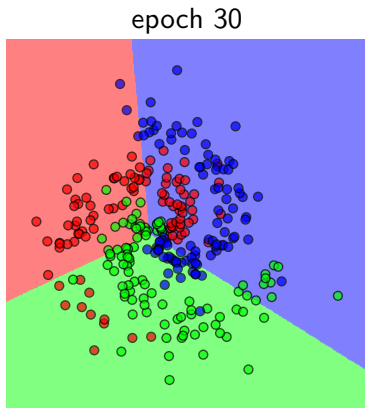
epoch 250



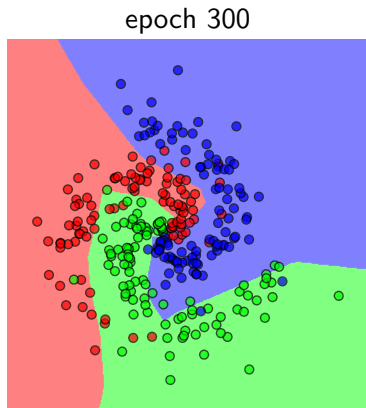
two-layer

- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

two-layer classifier



linear

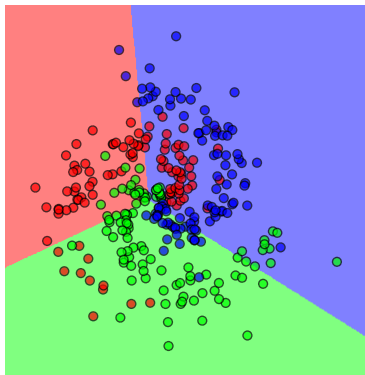


two-layer

- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

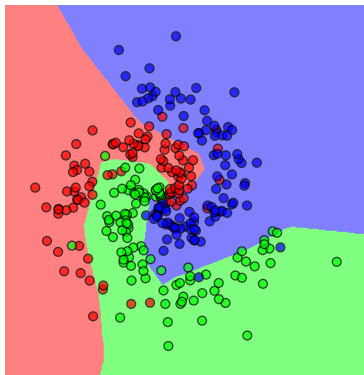
two-layer classifier

epoch 35



linear

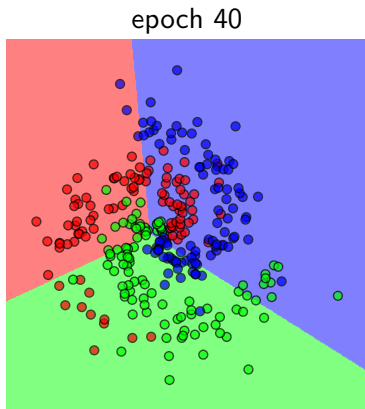
epoch 350



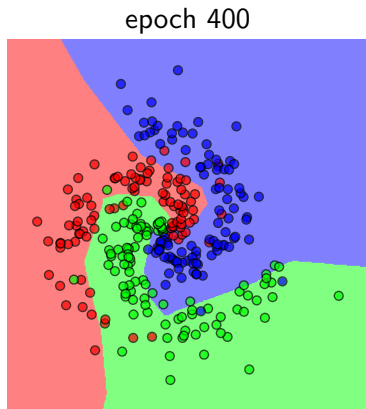
two-layer

- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

two-layer classifier



linear

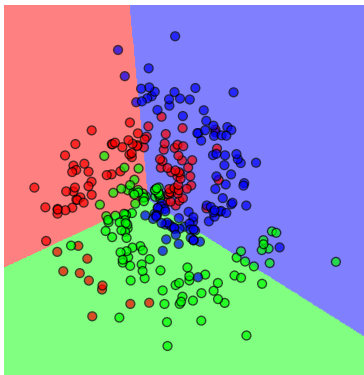


two-layer

- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

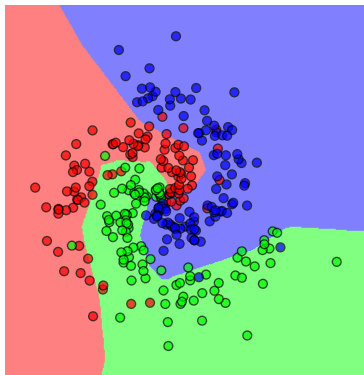
two-layer classifier

epoch 45



linear

epoch 450



two-layer

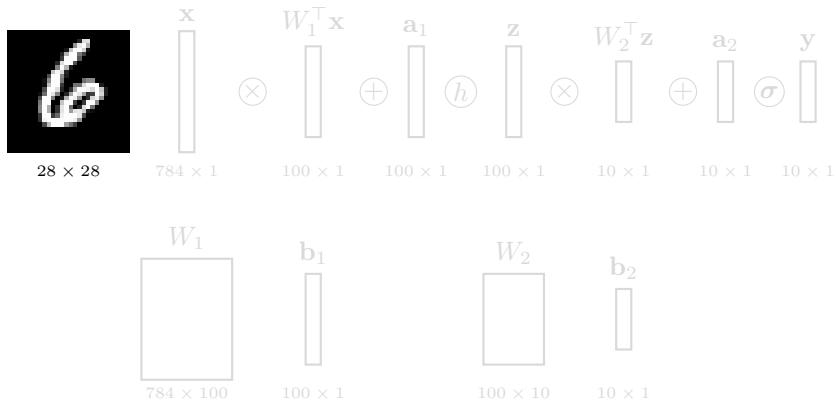
- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

MNIST digits dataset



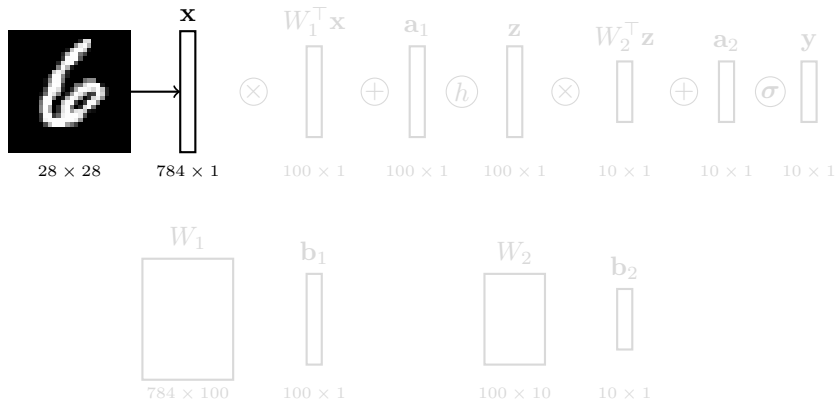
- 10 classes, 60k training images, 10k test images, 28×28 images

two-layer classifier on raw pixels



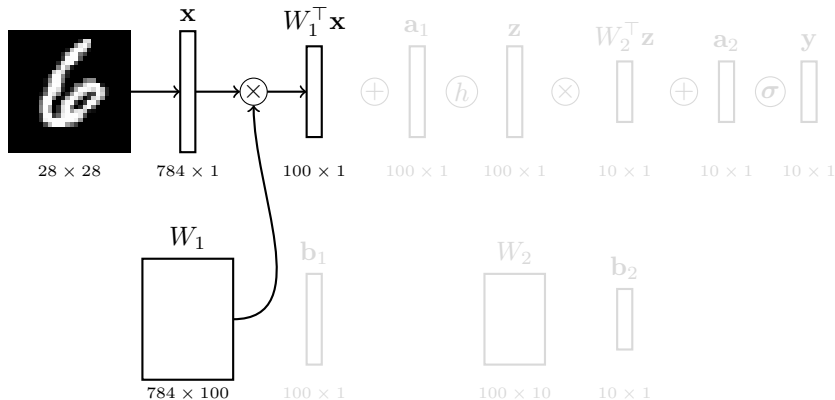
- input - layer 1 weights and bias - relu activation function - layer 2 weights and bias - softmax
- parameter learning using cross-entropy on y (or rather, directly on a_2)

two-layer classifier on raw pixels



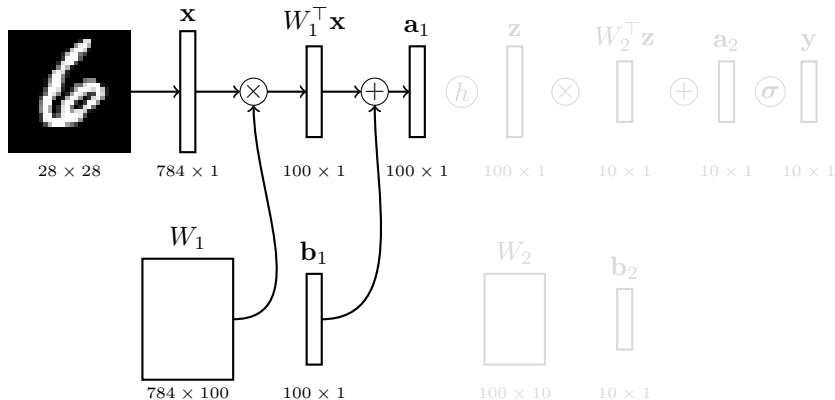
- input - layer 1 weights and bias - relu activation function - layer 2 weights and bias - softmax
- parameter learning using cross-entropy on y (or rather, directly on a_2)

two-layer classifier on raw pixels



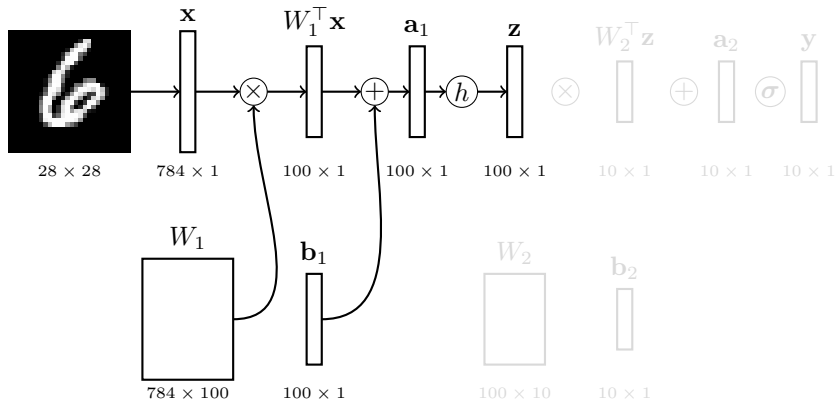
- input - layer 1 weights and bias - relu activation function - layer 2 weights and bias - softmax
- parameter learning using cross-entropy on y (or rather, directly on a_2)

two-layer classifier on raw pixels



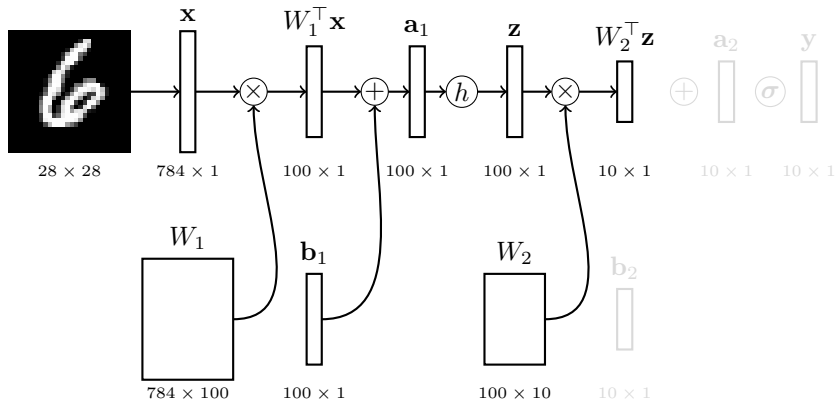
- input - layer 1 weights and bias - relu activation function - layer 2 weights and bias - softmax
- parameter learning using cross-entropy on y (or rather, directly on a_2)

two-layer classifier on raw pixels



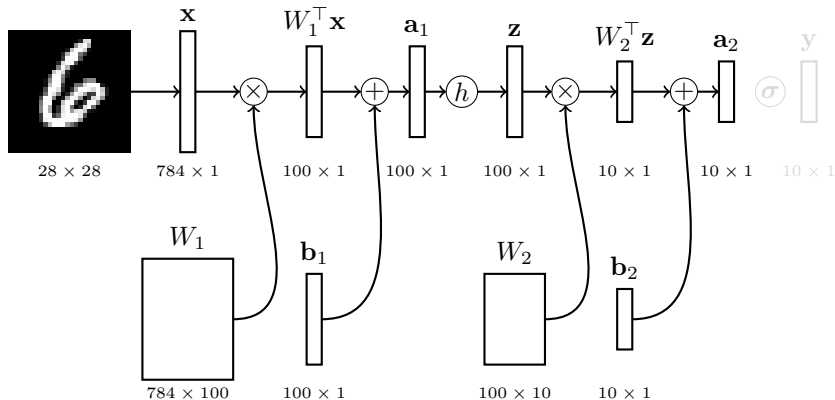
- input - layer 1 weights and bias - relu activation function - layer 2 weights and bias - softmax
- parameter learning using cross-entropy on y (or rather, directly on a_2)

two-layer classifier on raw pixels



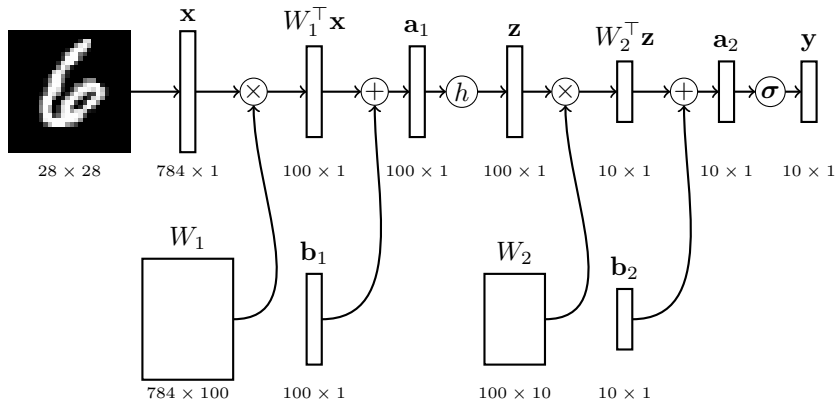
- input - layer 1 weights and bias - relu activation function - layer 2 weights and bias - softmax
- parameter learning using cross-entropy on y (or rather, directly on a_2)

two-layer classifier on raw pixels



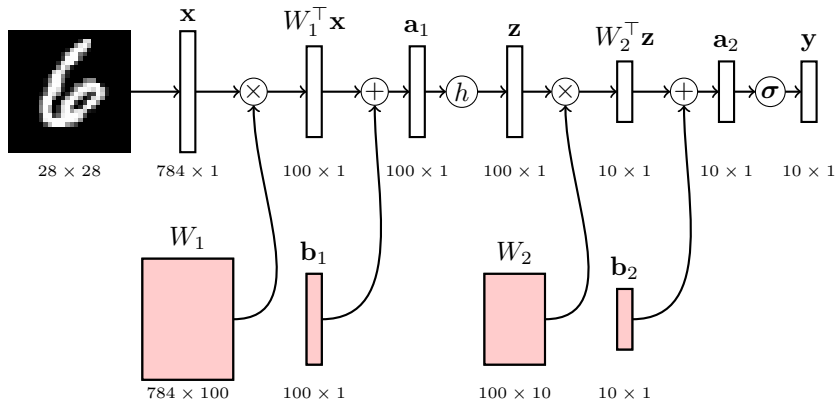
- input - layer 1 weights and bias - relu activation function - layer 2 weights and bias - softmax
- parameter learning using cross-entropy on y (or rather, directly on a_2)

two-layer classifier on raw pixels



- input - layer 1 weights and bias - relu activation function - layer 2 weights and bias - softmax
- parameter learning using cross-entropy on y (or rather, directly on a_2)

two-layer classifier on raw pixels



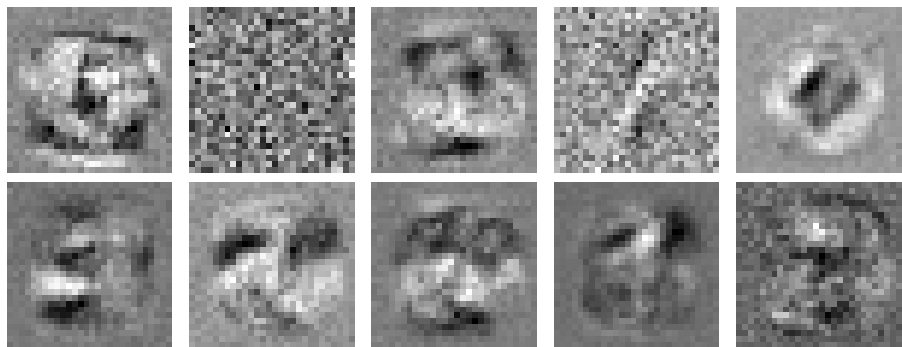
- input - layer 1 weights and bias - relu activation function - layer 2 weights and bias - softmax
- parameter learning using cross-entropy on y (or rather, directly on a_2)

what is being learned?

- the columns of W_1 are multiplied with \mathbf{x} ; they live in the same space, as in the linear classifier
- we can reshape each one back from 784×1 to 28×28 : but now it shouldn't look like a digit; rather, like a pattern that might help in recognizing digits
- these patterns are **shared**: once the activations are computed, they can be used in the next layer to score any of the digits
- the columns of W_2 are in an 100-dimensional space that we can't make much sense of now; but we'll revisit this later

MNIST: two-layer classifier

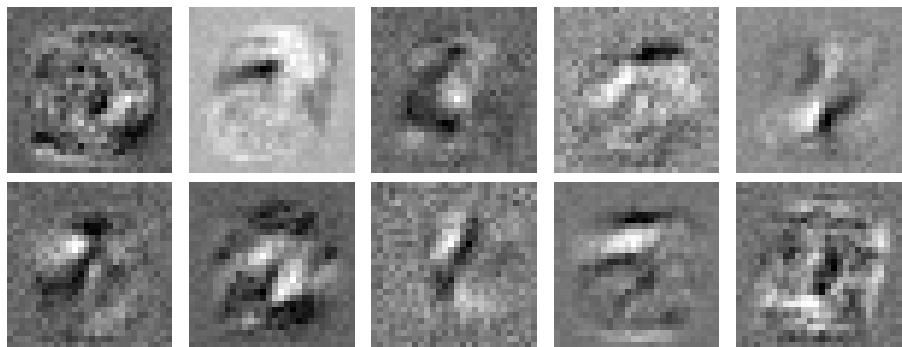
filters 00-09



- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- hidden layer width: 100; test error 2.54%

MNIST: two-layer classifier

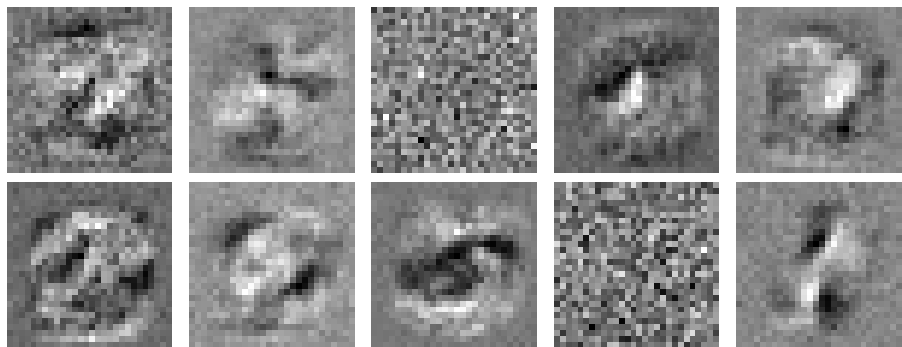
filters 10-19



- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- hidden layer width: 100; test error 2.54%

MNIST: two-layer classifier

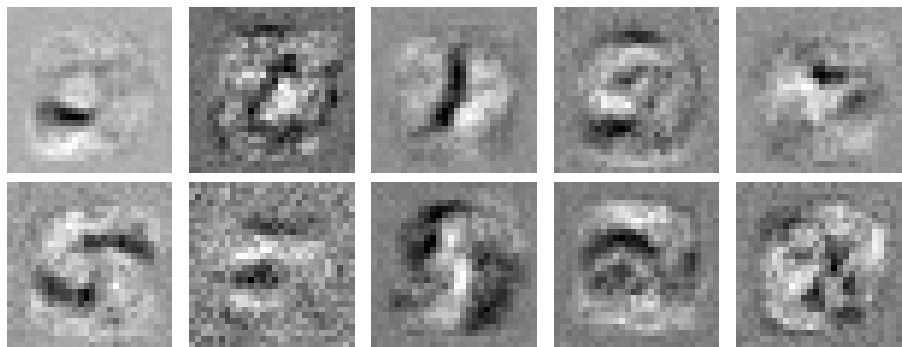
filters 20-29



- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- hidden layer width: 100; test error 2.54%

MNIST: two-layer classifier

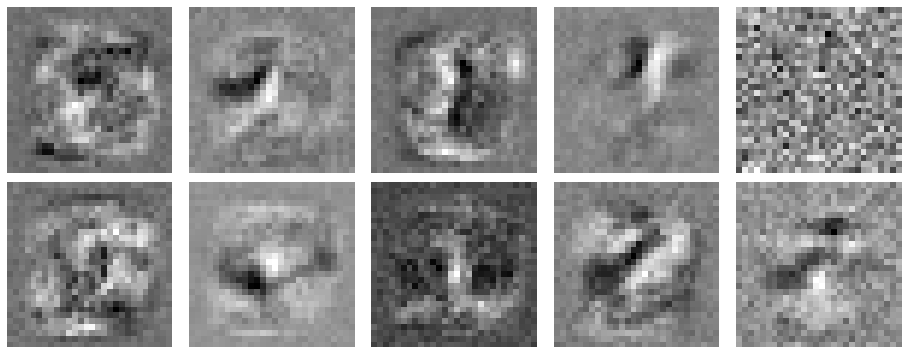
filters 30-39



- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- hidden layer width: 100; test error 2.54%

MNIST: two-layer classifier

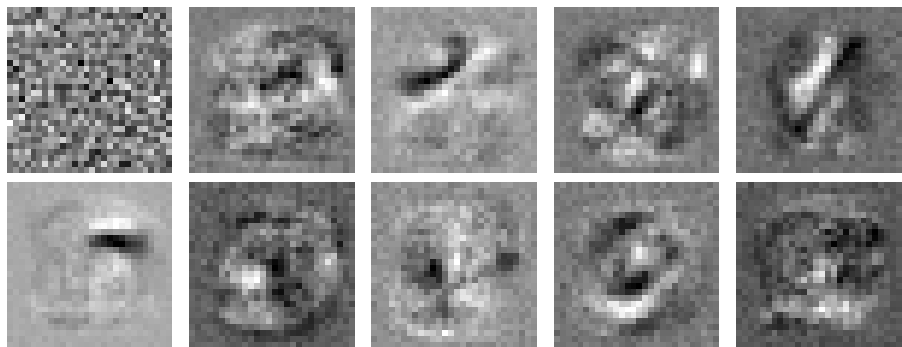
filters 40-49



- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- hidden layer width: 100; test error 2.54%

MNIST: two-layer classifier

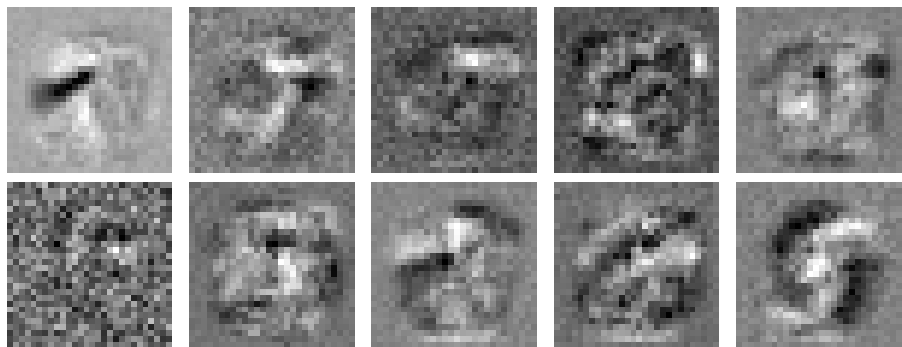
filters 50-59



- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- hidden layer width: 100; test error 2.54%

MNIST: two-layer classifier

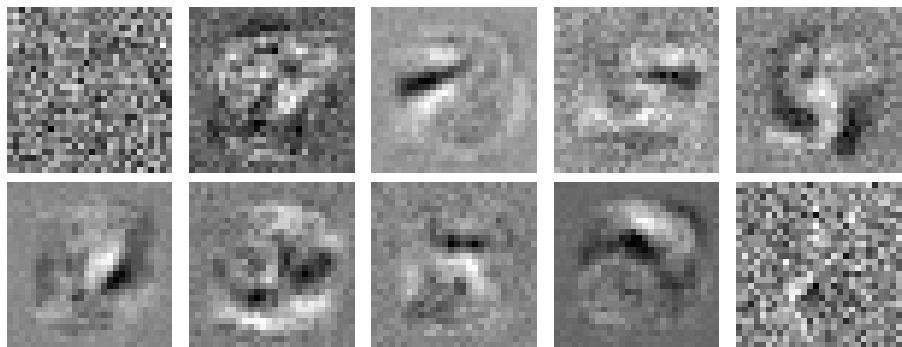
filters 60-69



- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- hidden layer width: 100; test error 2.54%

MNIST: two-layer classifier

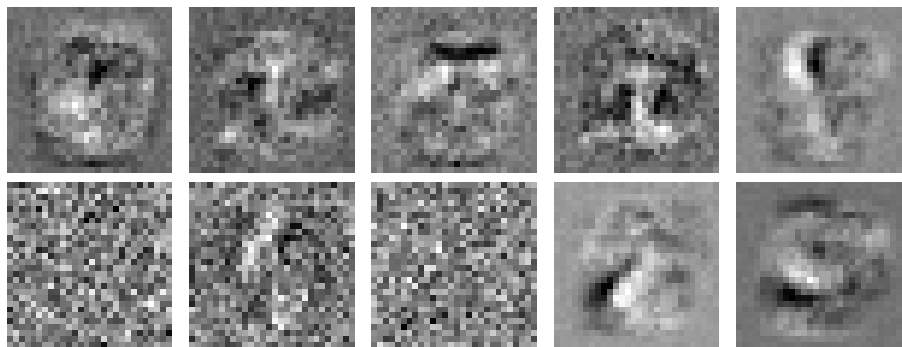
filters 70-79



- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- hidden layer width: 100; test error 2.54%

MNIST: two-layer classifier

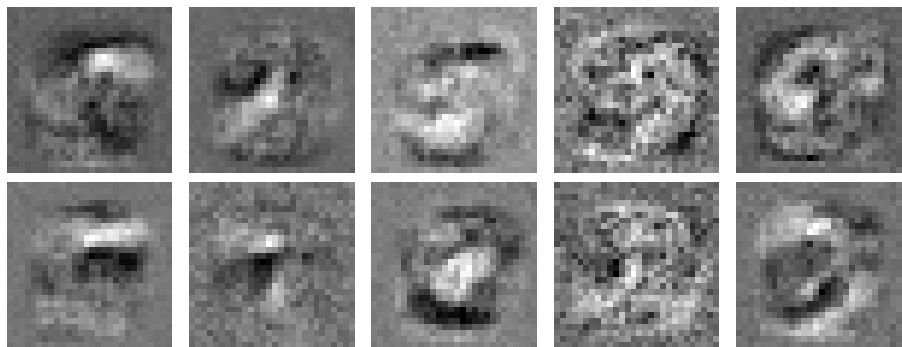
filters 80-89



- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- hidden layer width: 100; test error 2.54%

MNIST: two-layer classifier

filters 90-99



- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- hidden layer width: 100; test error 2.54%

summary

- only care about learning features: so, not interested e.g. in nearest neighbor search or dual SVM formulation
- three different linear classifiers, perceptron, SVM and logistic regression, only differ slightly in their loss function, which is similar to relu in all cases
- stochastic gradient descent optimization
- multi-class classification, softmax and MNIST
- linear regression, basis functions, overfitting, validation, hyperparameter optimization
- learning basis functions, two-layer networks, activation functions, connection to classifier loss functions
- why relu makes sense