lecture 5: learning

deep learning for vision

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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

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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

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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

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

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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

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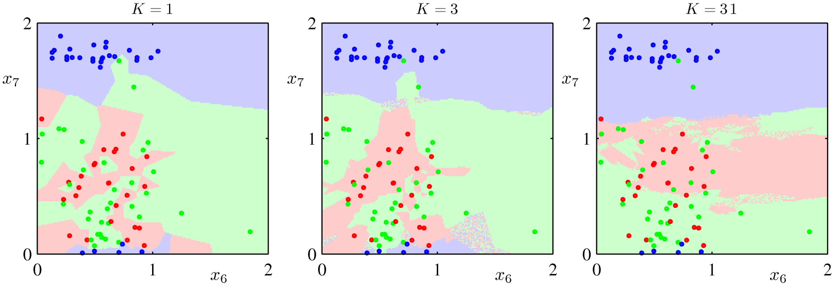
binary classification

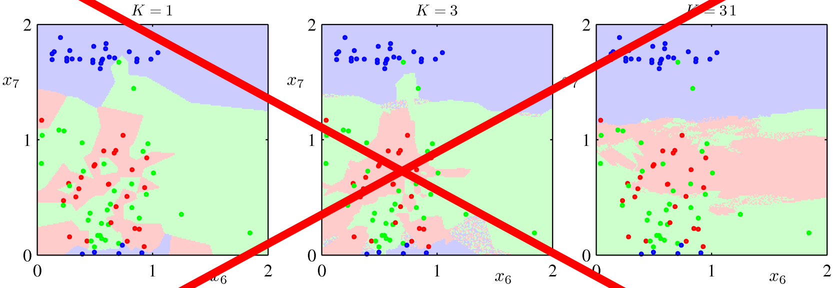
k-nearest neighbor classifier



- 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

Image credit: Bishop 2006. Pattern Recognition and Machine Learning.

k-nearest neighbor classifier



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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

Rosenblatt 1962. Principles of Neurodynamics

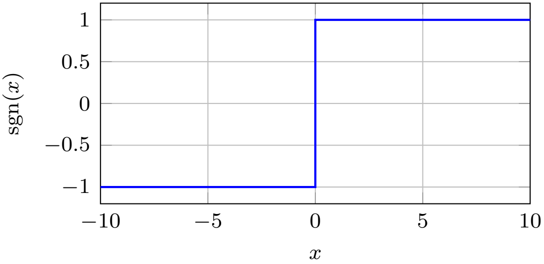
perceptron model

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

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

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

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



Rosenblatt 1962. Principles of Neurodynamics

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 $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$ and target variables $s_1, \ldots, s_n \in \{-1, 1\}$
- 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

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

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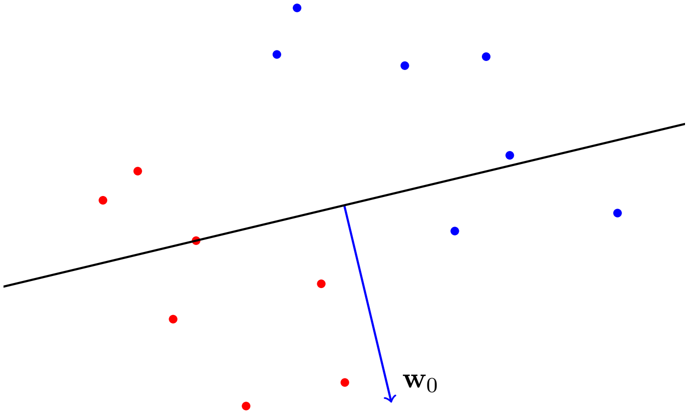
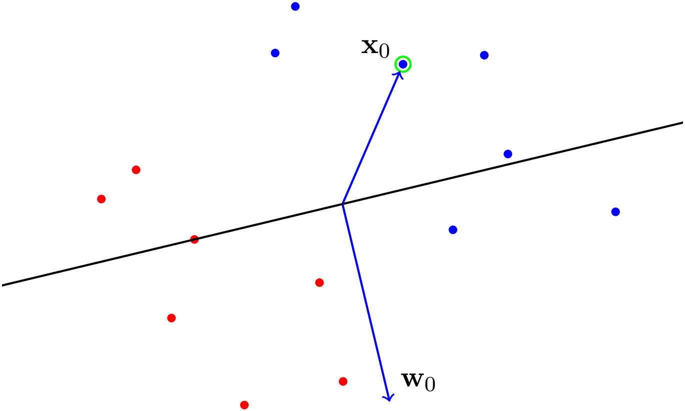


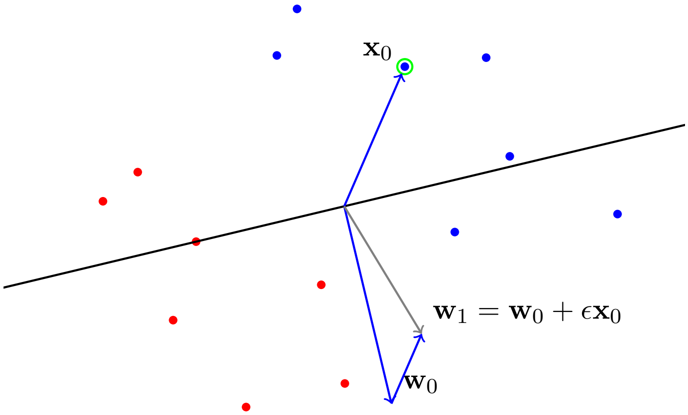
- initial parameter vector $\mathbf{w}_0$, normal to the decision boundary and pointing to the region to be classified as blue $(+)$

perceptron algorithm



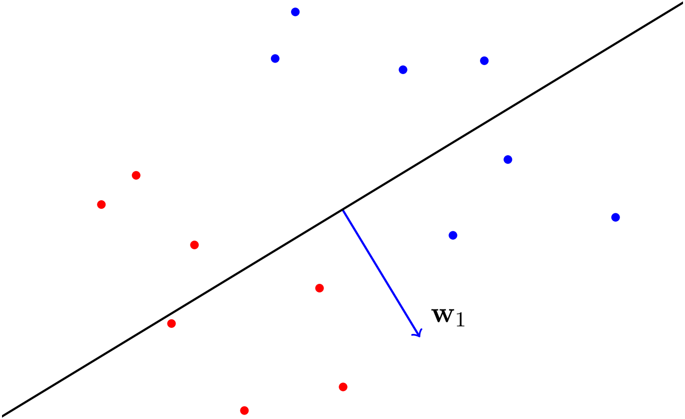
- pick a random point $\mathbf{x}_0$ that is misclassified: blue $(+)$ in red $(-)$ region

perceptron algorithm



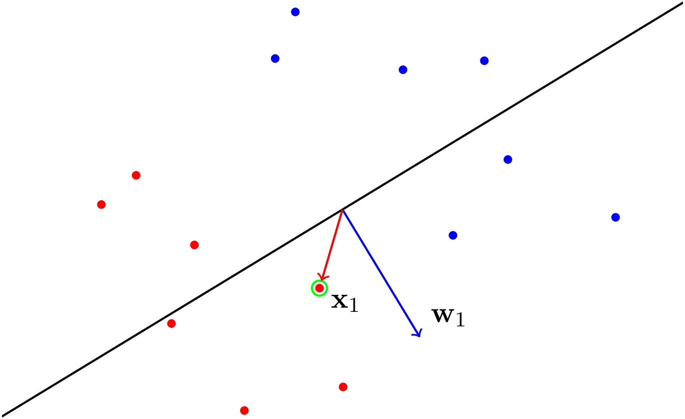
- because $\mathbf{x}_0$ is blue and $\mathbf{w}$ is pointing at blue, we add $\epsilon\mathbf{x}_0$ to $\mathbf{w}_0$

perceptron algorithm



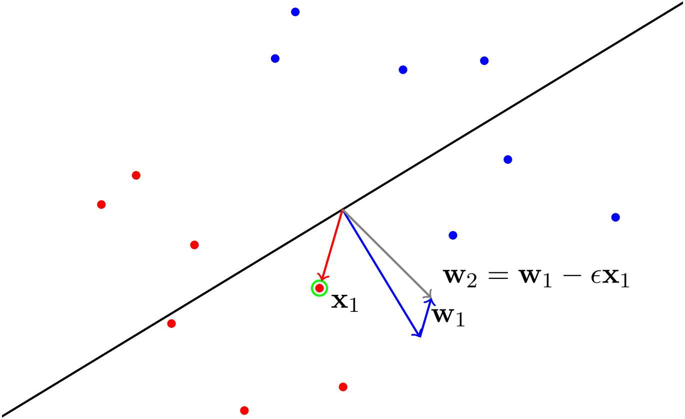
- with the new parameter vector $\mathbf{w}_1$, the decision boundary is updated

perceptron algorithm



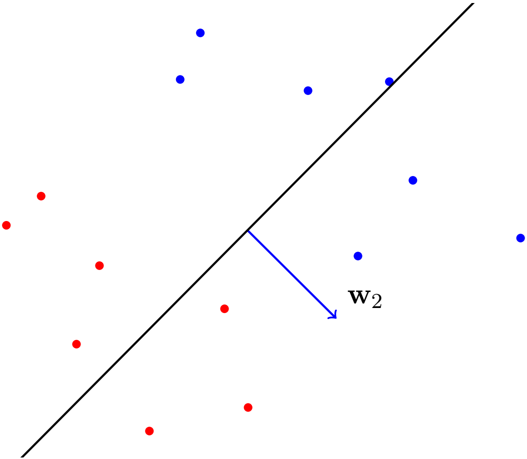
- pick a new random point $\mathbf{x}_1$ that is misclassified: red in blue region

perceptron algorithm



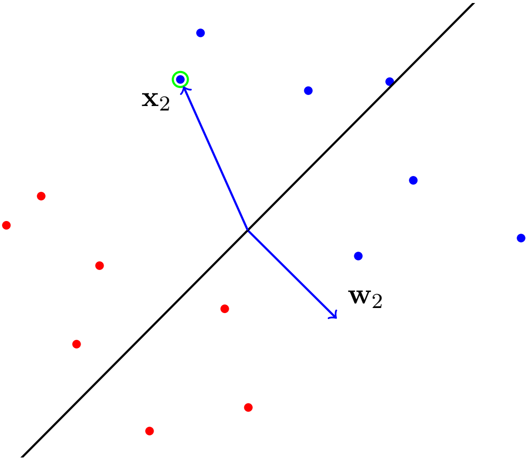
- because $\mathbf{x}_1$ is red and $\mathbf{w}$ is pointing at blue, we subtract $\epsilon\mathbf{x}_1$ from $\mathbf{w}_1$

perceptron algorithm



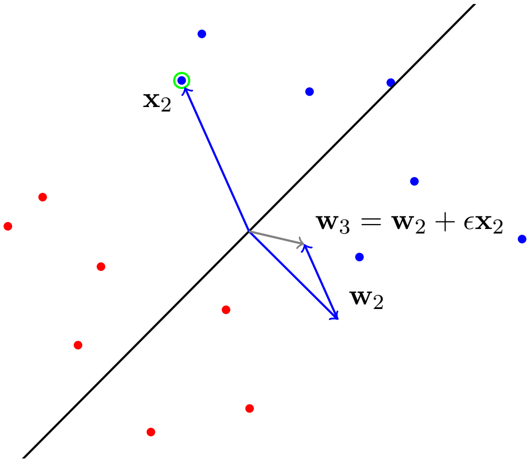
- with the new $\mathbf{w}_2$, the decision boundary is updated again

perceptron algorithm



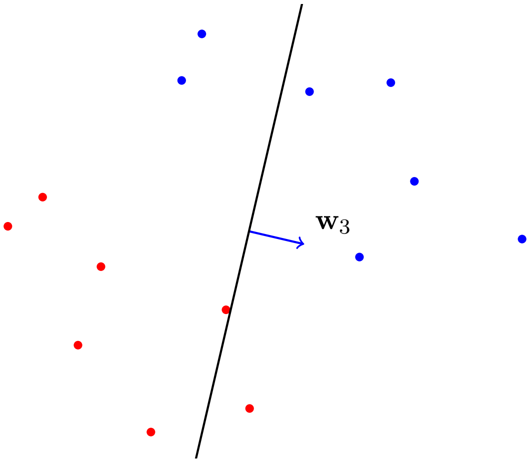
- again, random point $\mathbf{x}_2$, blue misclassified in red region

perceptron algorithm



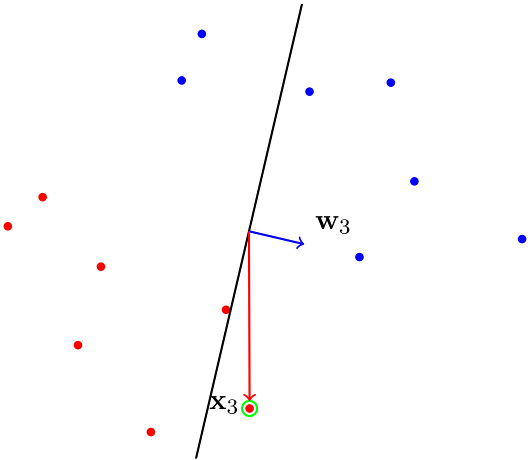
- and we add $\epsilon \mathbf{x}_2$ to $\mathbf{w}_2$

perceptron algorithm



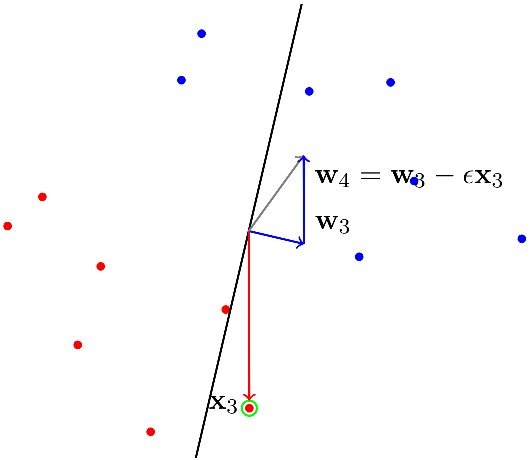
- now at $\mathbf{w}_3$

perceptron algorithm



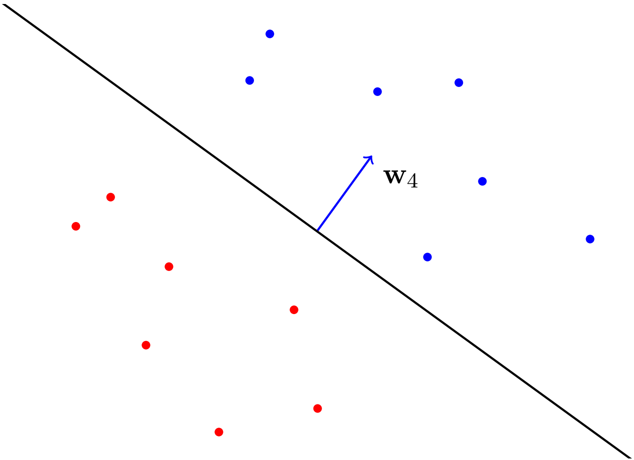
- one last random point $\mathbf{x}_3$, red in blue region

perceptron algorithm



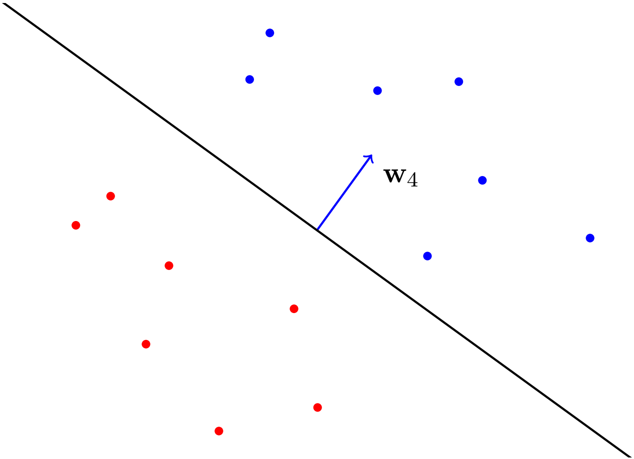
- and we subtract

perceptron algorithm



- finally at $\mathbf{w}_4$, all points are classified correctly

perceptron algorithm



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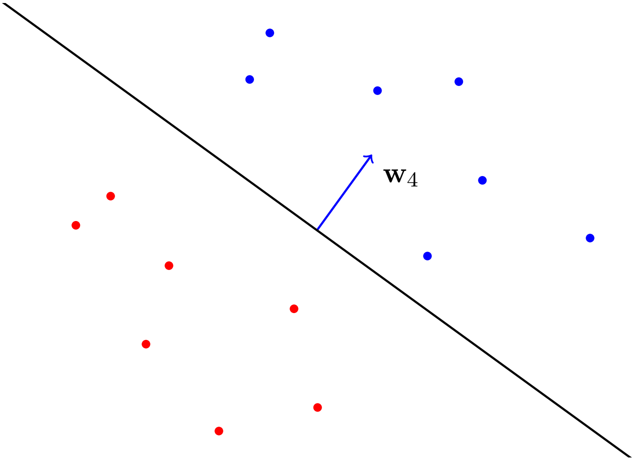

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“details”

- 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

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

  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

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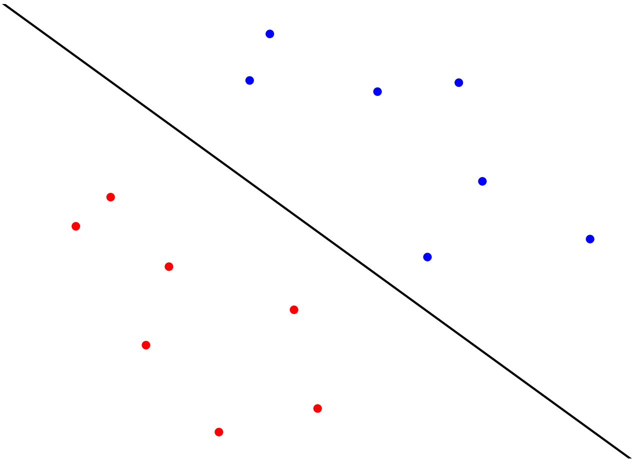
support vector machine (SVM)

[Boser et al. 1992]

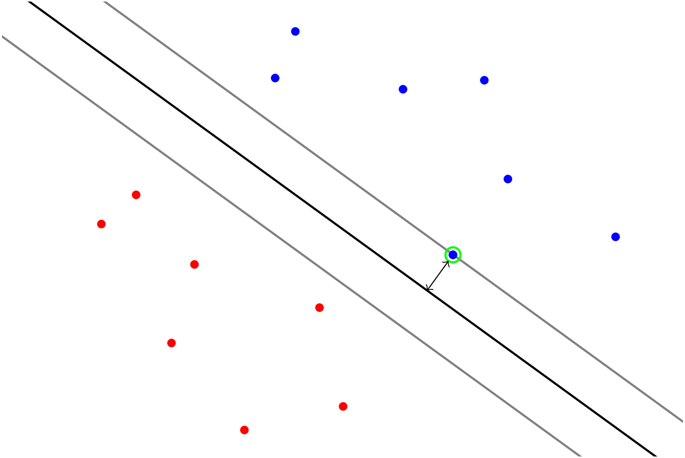


- given a decision boundary that classifies all points correctly, define the margin as its distance to the nearest point

Boser, Guyon and Vapnik. COLT 1992. A Training Algorithm for Optimal Margin Classifiers.

support vector machine (SVM)

[Boser et al. 1992]



- this was not optimal in the case of perceptron

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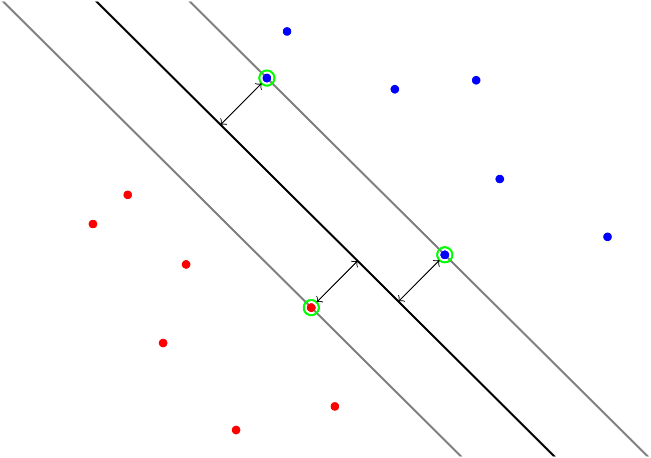

- there is another decision boundary for which the margin is maximum; the vectors at this distance are the support vectors

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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

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

- again, an input $\mathbf{x}$ with $a = \mathbf{w}^\top \mathbf{x} + b$ and output $y = \operatorname{sgn}(a)$ is classified to class C_1 if $y = 1$ ($a \geq 0$) and to C_2 if $y = -1$ ($a < 0$)
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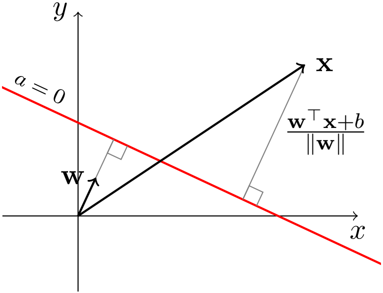
margin



- 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

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

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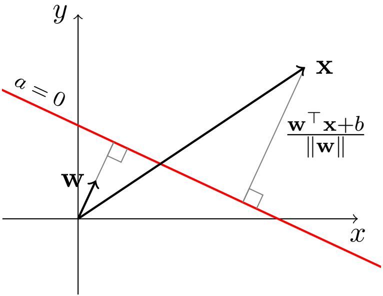

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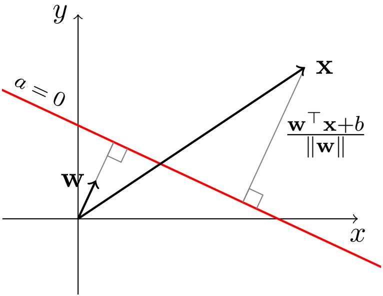

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maximum margin

- 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

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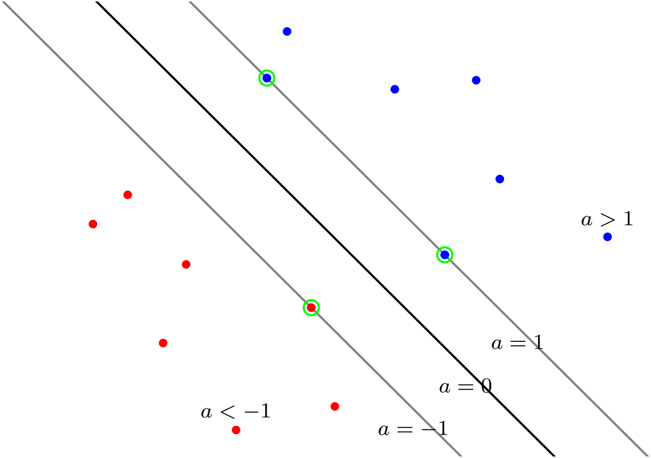
overlapping class distributions

[Cortes and Vapnik 1995]

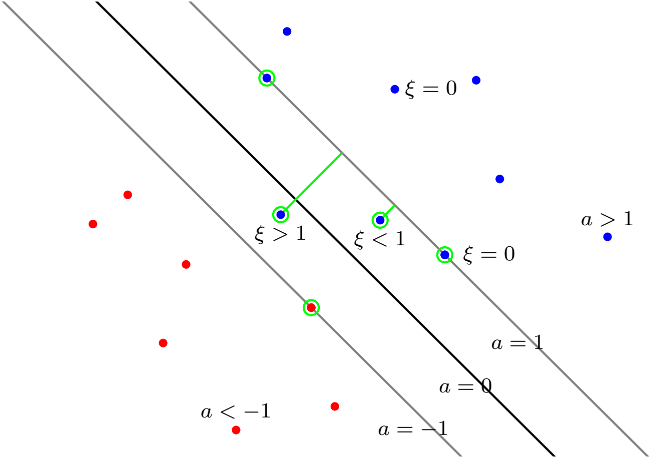


- assuming that all training samples can be correctly classified is unrealistic

Cortes and Vapnik. ML 1995. Support-Vector Networks.

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

Cortes and Vapnik. ML 1995. Support-Vector Networks.

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

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"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

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(binary) logistic regression

[Cox 1958]

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

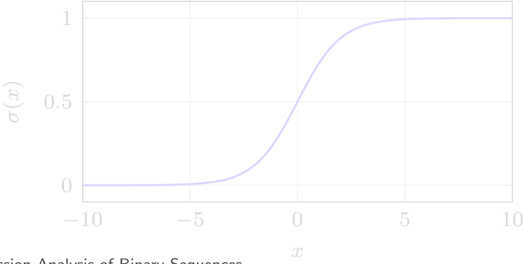
$$a = \mathbf{w}^\top \mathbf{x}$$

  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

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



Cox. JSTOR 1958. The Regression Analysis of Binary Sequences.

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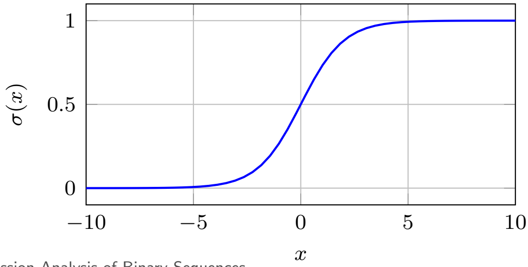

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probabilistic interpretation

- 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

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

Cox. JSTOR 1958. The Regression Analysis of Binary Sequences.

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

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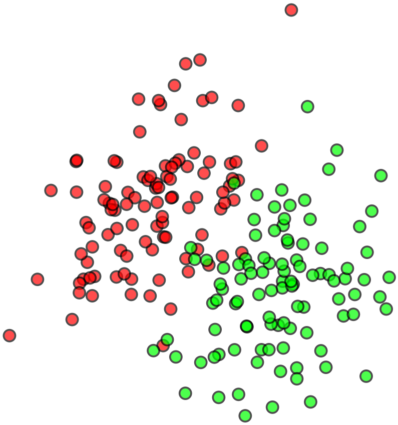
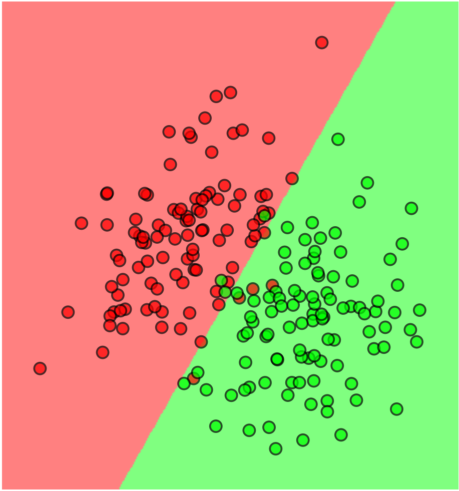
binary classifiers



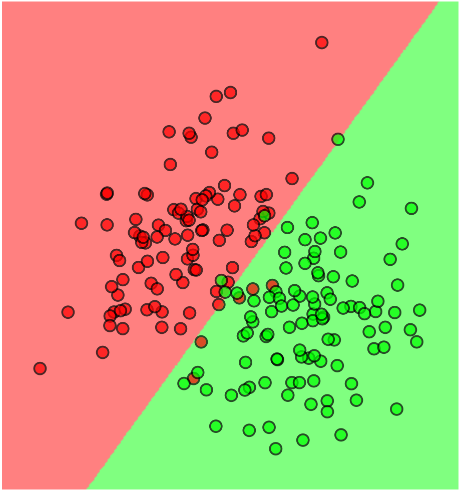
raw data

binary classifiers



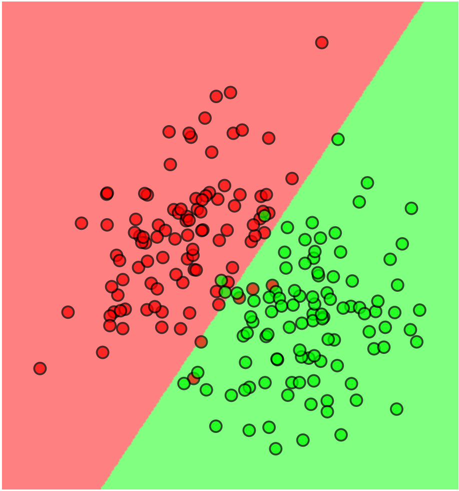
perceptron

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

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

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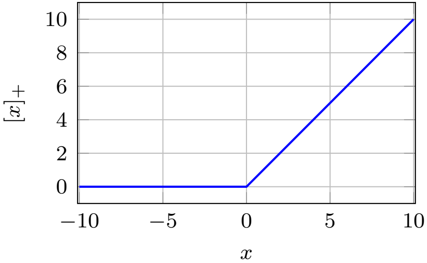
positive part

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

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



gradient descent

- in general, given an error function in parameters $\boldsymbol{\theta}$ of the additive form

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

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

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

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

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- 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

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- 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

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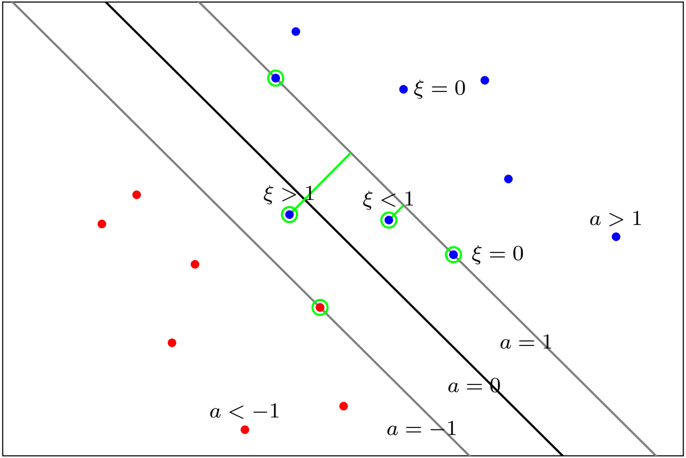
SVM, again



- 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

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  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 $\lambda = 1/C$

Cortes and Vapnik. ML 1995. Support-Vector Networks.

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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
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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 $\mathbf{w}$

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

- 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

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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 $\boldsymbol{\theta}$

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prediction function

- in all three cases, we can use parameters $\boldsymbol{\theta} = (\mathbf{w}, b)$ 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 $\boldsymbol{\theta}^* = \arg\min_{\boldsymbol{\theta}} E(\boldsymbol{\theta})$ are found, use the prediction function

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

  to classify new samples during inference (testing)

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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	$\ln(1 + e^{-x})$

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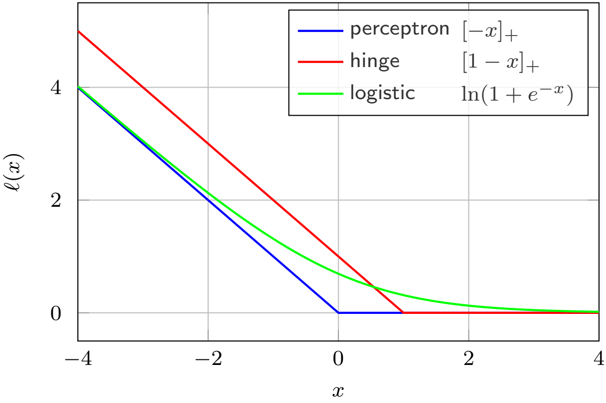
loss function

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



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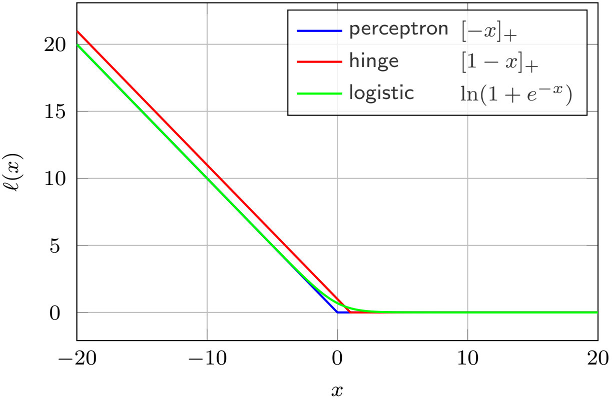

derivatives

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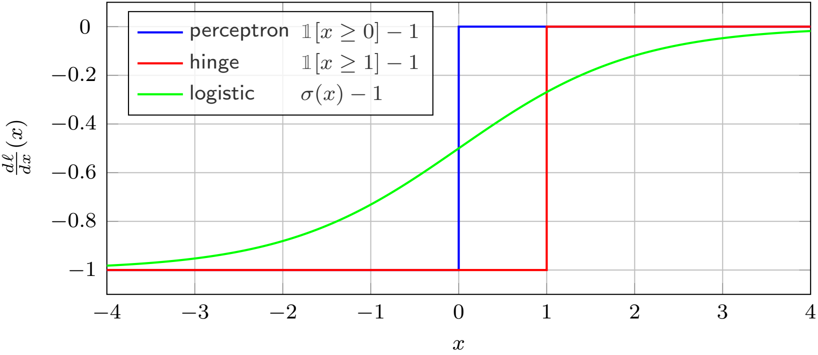

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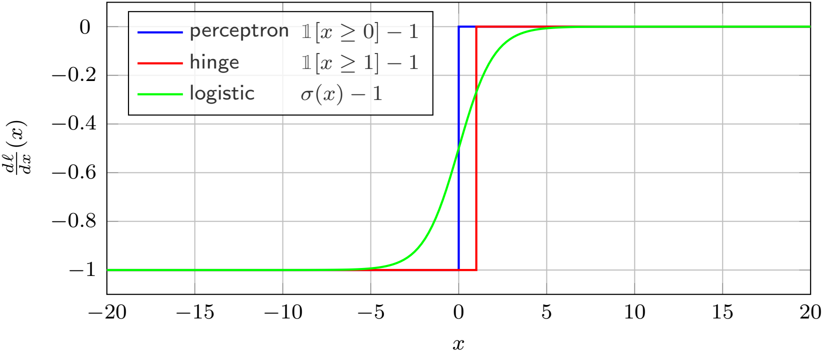

derivatives

- 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 $|x| \to \infty$)
- 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

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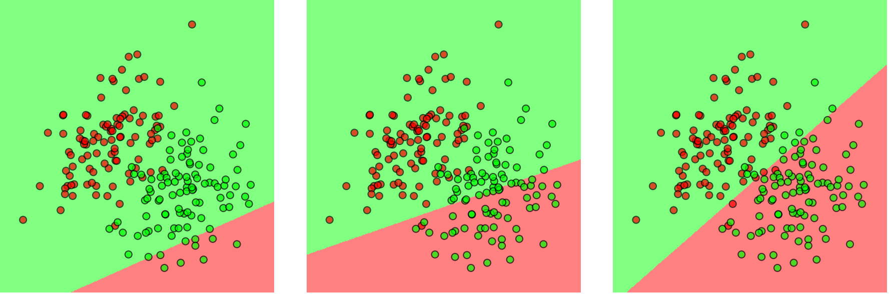
question

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

training

epoch 0



perceptron

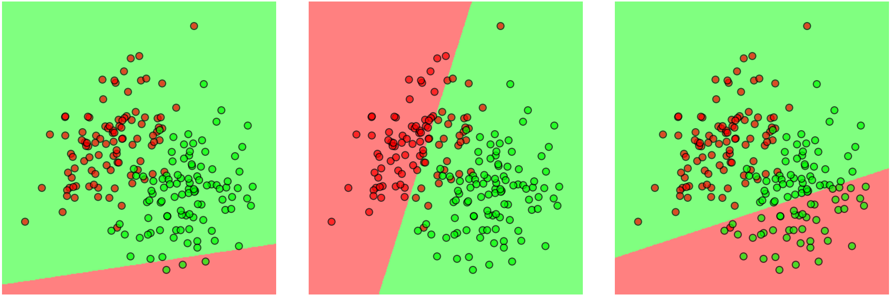
hinge

logistic

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

training

epoch 1



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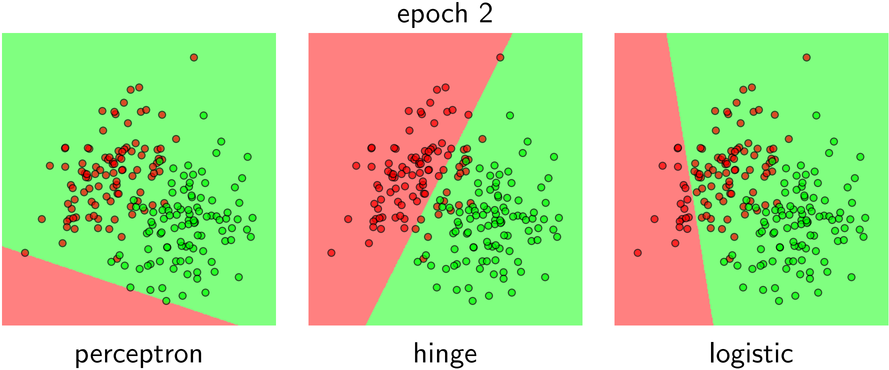

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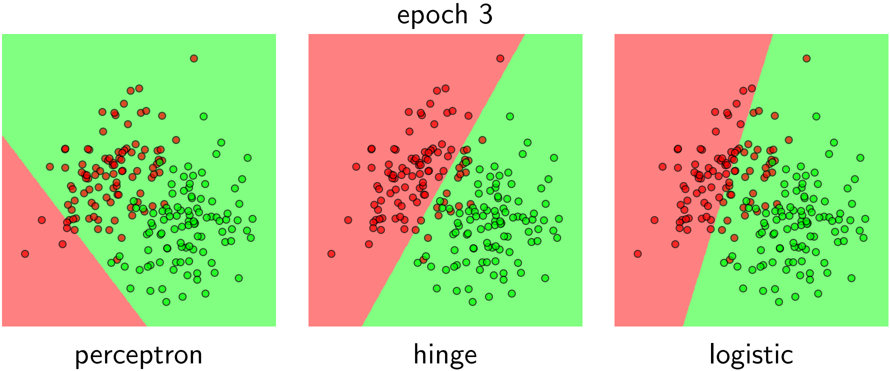


epoch 3

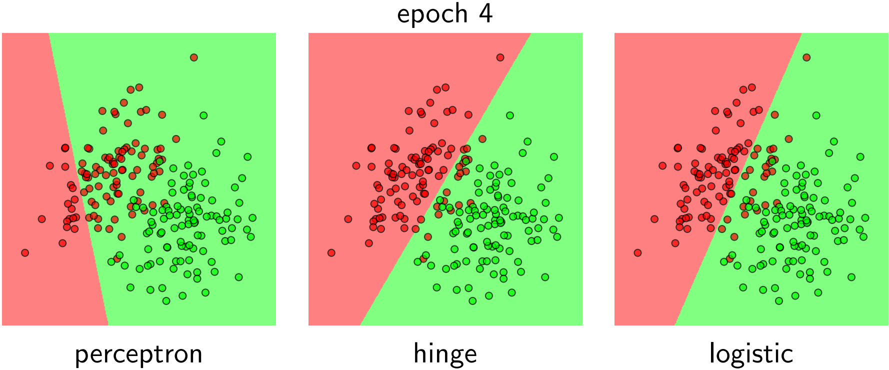
perceptron

hinge

logistic

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

training



epoch 4

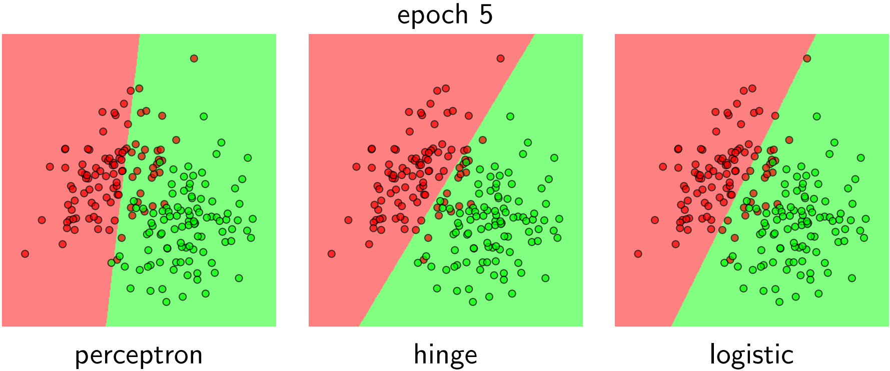
perceptron

hinge

logistic

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

training



epoch 5

perceptron

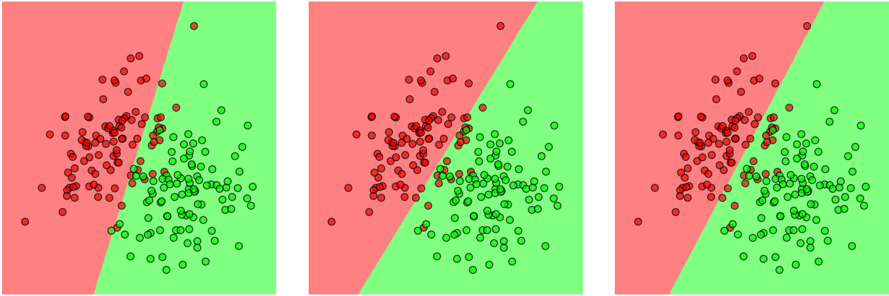
hinge

logistic

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

training

epoch 6



perceptron

hinge

logistic

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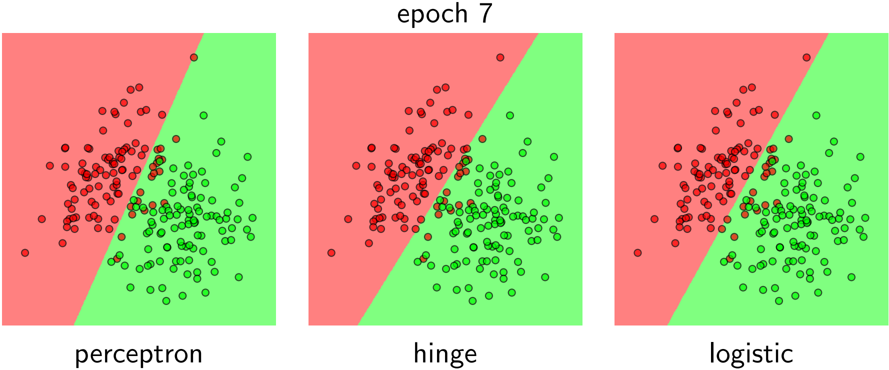
training



epoch 7

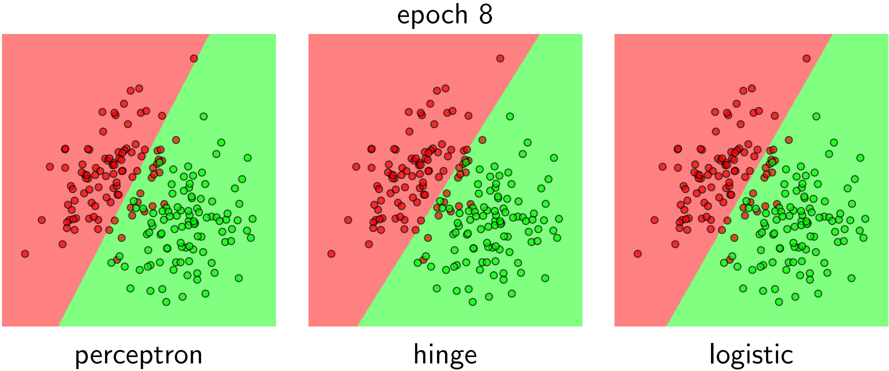
perceptron

hinge

logistic

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

training



epoch 8

perceptron

hinge

logistic

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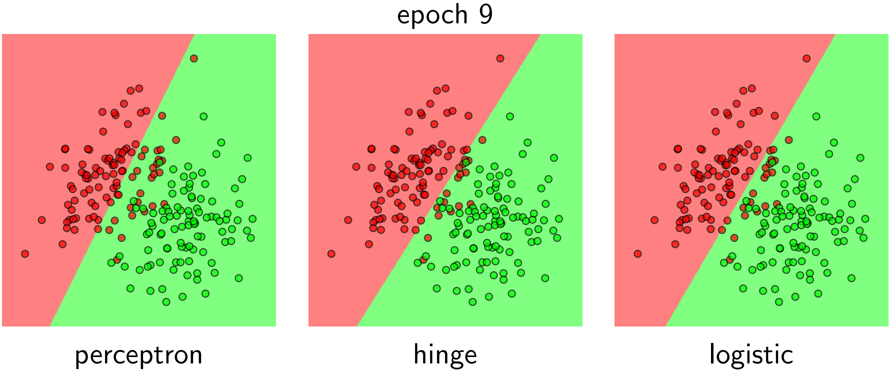
training


epoch 9

perceptron

hinge

logistic

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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 $j = 1, \dots, k$

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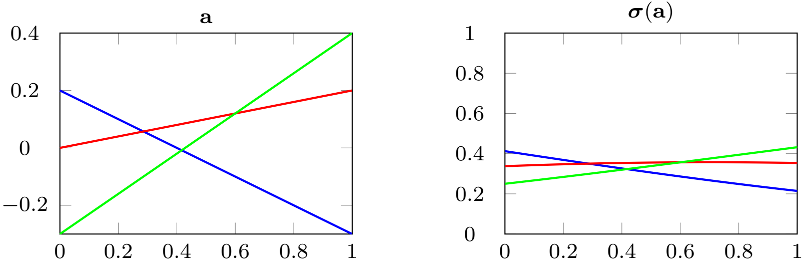
softmax

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

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

- as activation values increase, $\mathrm{softmax}$ tends to focus on the maximum



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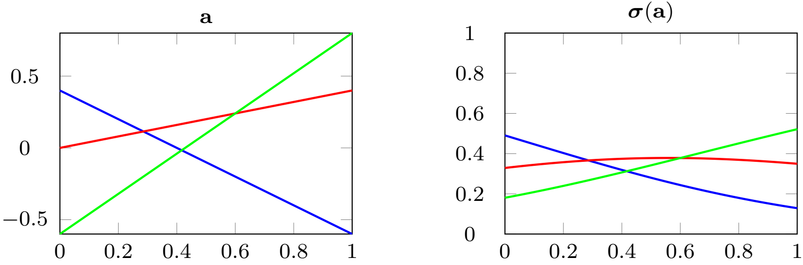

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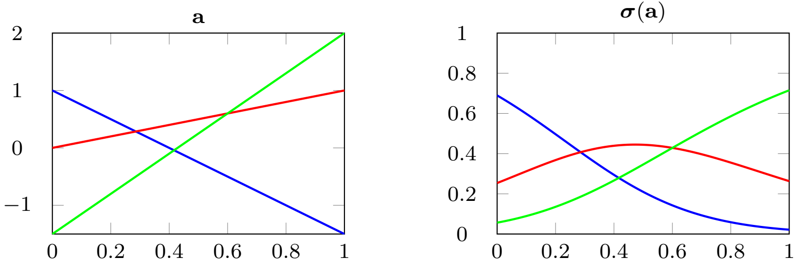

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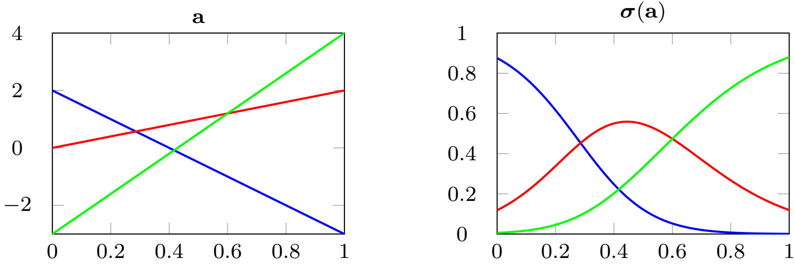

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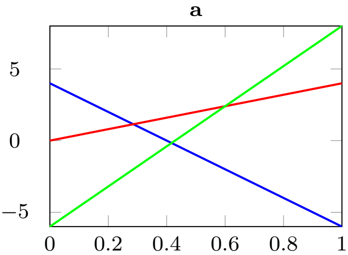

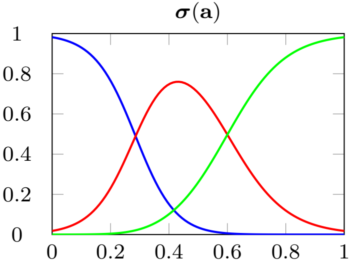

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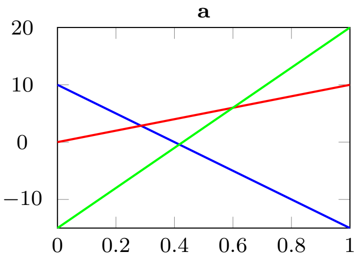

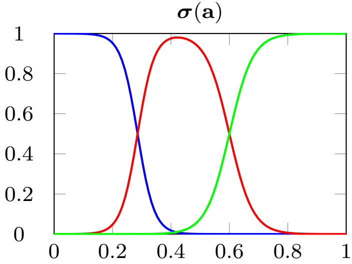

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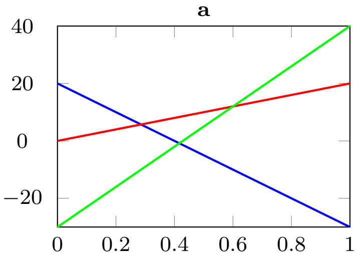

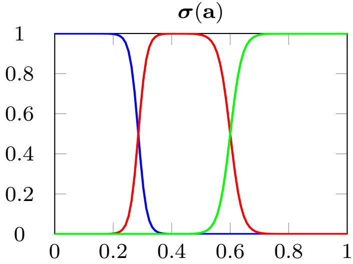

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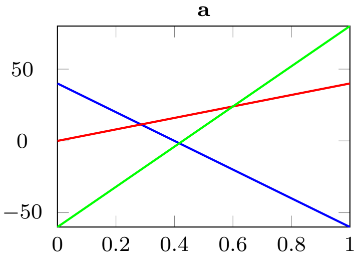

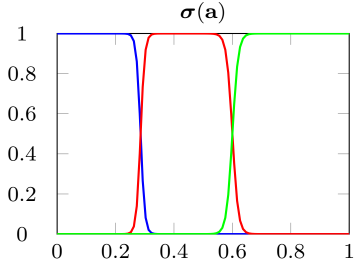

cross-entropy error

- 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

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

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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, *i.e.* $\mathbf{t} = \mathbf{e}_l$
- also this term can be approximated by the maximum element of $\mathbf{a}$:

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

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

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

- suppose the correct label (nonzero element of $\mathbf{t}$) is l, *i.e.* $\mathbf{t} = \mathbf{e}_l$
- also this term can be approximated by the maximum element of $\mathbf{a}$:

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

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:

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

- again, $\exp$ and $\log$ cancel, and that's a reason to keep $\mathrm{softmax}$ 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

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- 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

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

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

- Crammer and Singer

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

  penalizes all labels that have better activation than the correct one

- both interpretable with simple derivatives

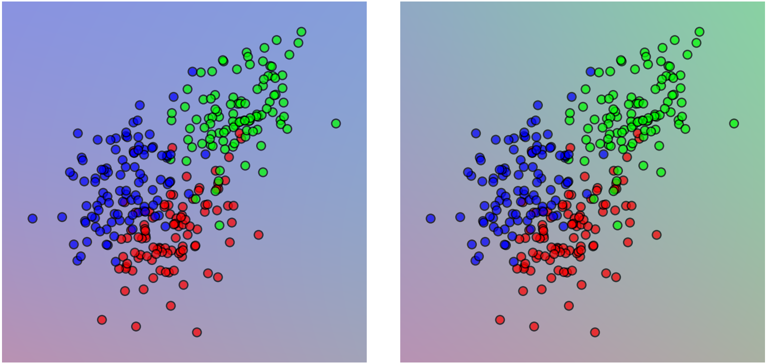
Weston and Watkins. ESANN 1999. Support Vector Machines for Multi-Class Pattern Recognition.
Crammer and Singer. JMLR 2001. On the Algorithmic Implementation of Multiclass Kernel-Based Vector Machines.

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 $\mathrm{softmax}$ 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



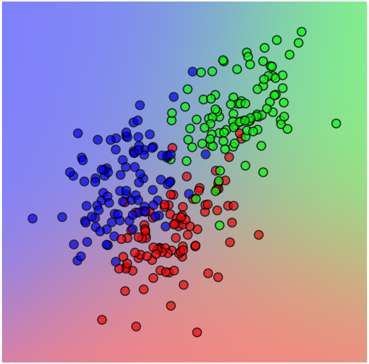
hinge (W&W)

logistic

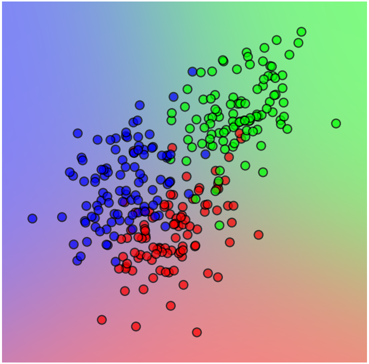
- $k = 3, n = 300, m = 10, \epsilon = 10^{-1}, \lambda = 10^{-3}$

prediction: soft assignment

epoch 05



hinge (W&W)

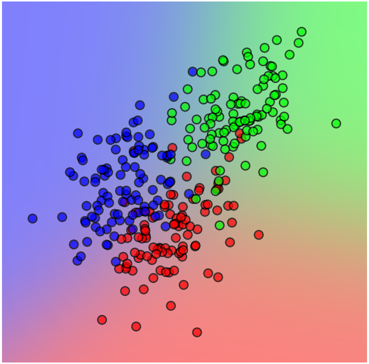


logistic

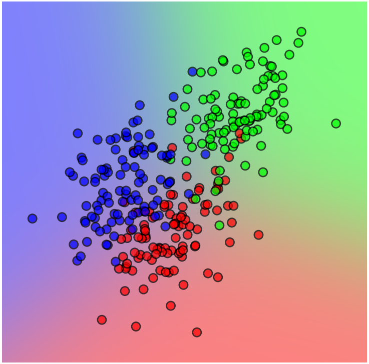
- $k = 3, n = 300, m = 10, \epsilon = 10^{-1}, \lambda = 10^{-3}$

prediction: soft assignment

epoch 10



hinge (W&W)

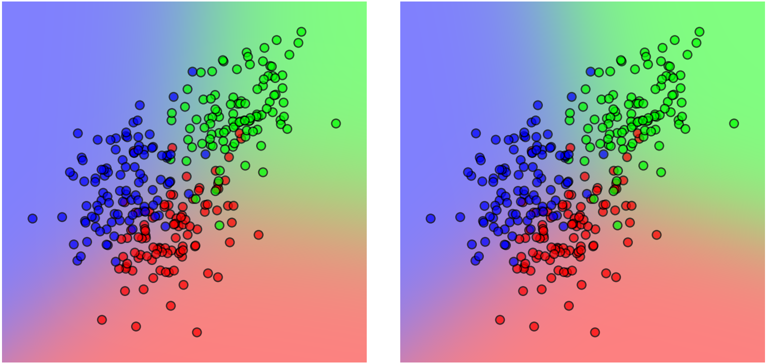


logistic

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

prediction: soft assignment

epoch 15



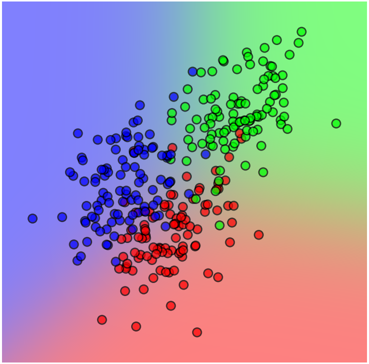
hinge (W&W)

logistic

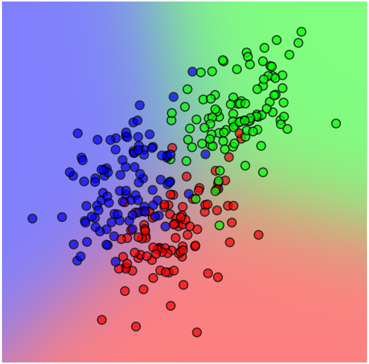
- $k = 3, n = 300, m = 10, \epsilon = 10^{-1}, \lambda = 10^{-3}$

prediction: soft assignment

epoch 20



hinge (W&W)

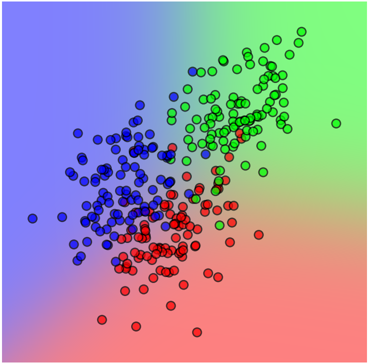


logistic

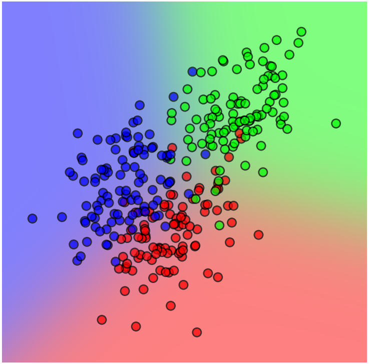
- $k = 3, n = 300, m = 10, \epsilon = 10^{-1}, \lambda = 10^{-3}$

prediction: soft assignment

epoch 25



hinge (W&W)

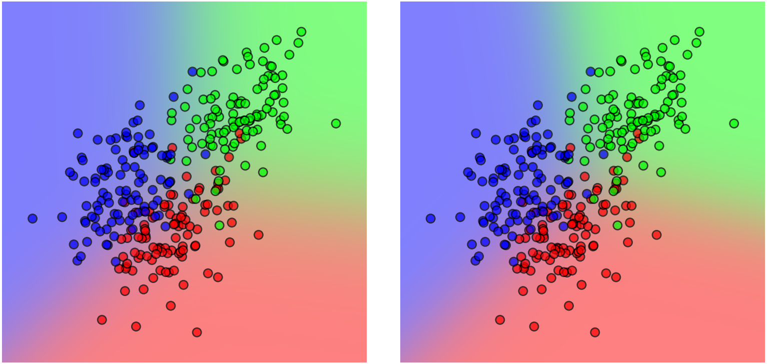


logistic

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

prediction: soft assignment

epoch 30



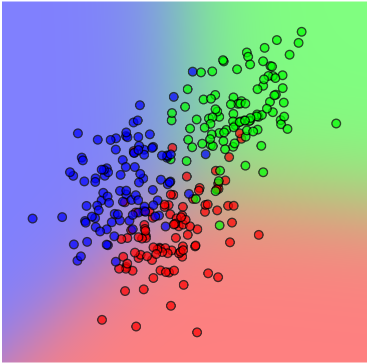
hinge (W&W)

logistic

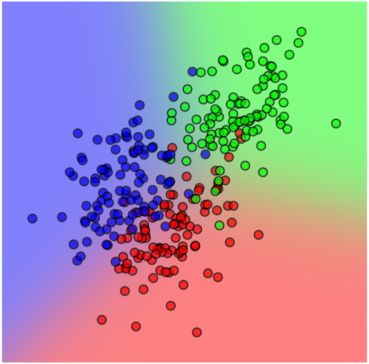
- $k = 3, n = 300, m = 10, \epsilon = 10^{-1}, \lambda = 10^{-3}$

prediction: soft assignment

epoch 35



hinge (W&W)

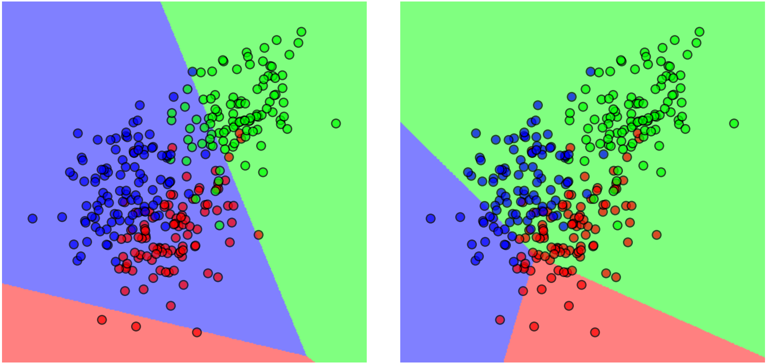


logistic

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

prediction: hard assignment

epoch 00



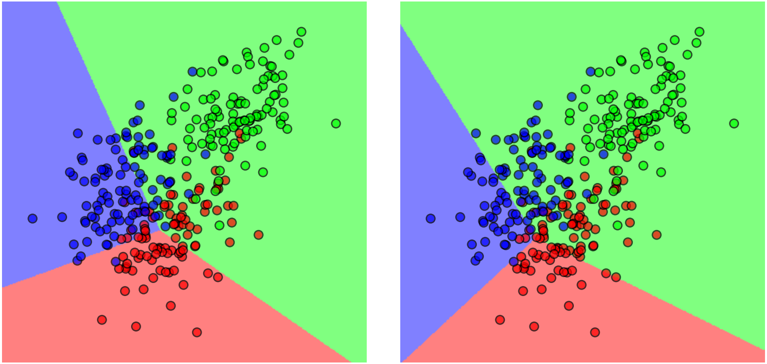
hinge (W & W)

logistic

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

prediction: hard assignment

epoch 04



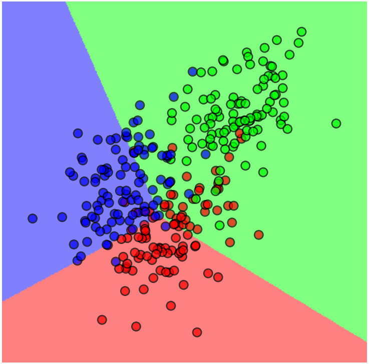
hinge (W & W)

logistic

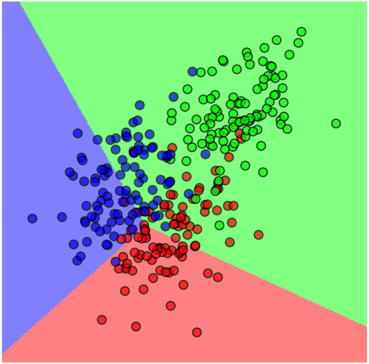
- $k = 3, n = 300, m = 10, \epsilon = 10^{-2}, \lambda = 10^{-3}$

prediction: hard assignment

epoch 08



hinge (W & W)

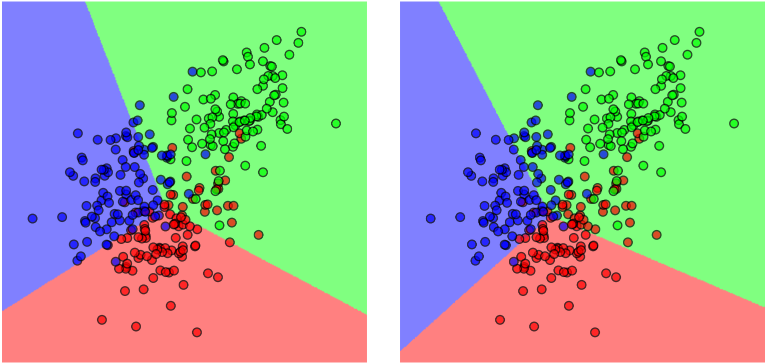


logistic

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

prediction: hard assignment

epoch 12



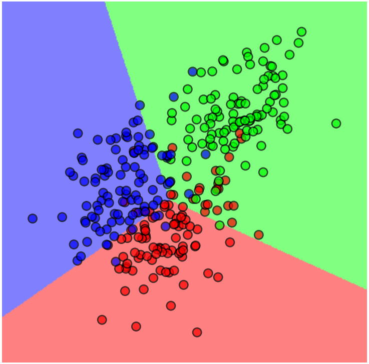
hinge (W & W)

logistic

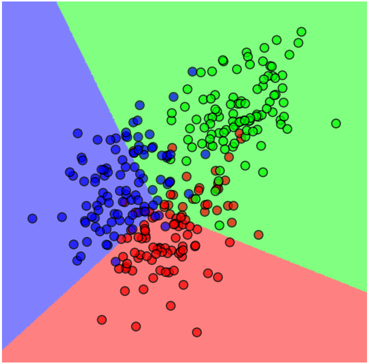
- $k = 3, n = 300, m = 10, \epsilon = 10^{-2}, \lambda = 10^{-3}$

prediction: hard assignment

epoch 16



hinge (W & W)

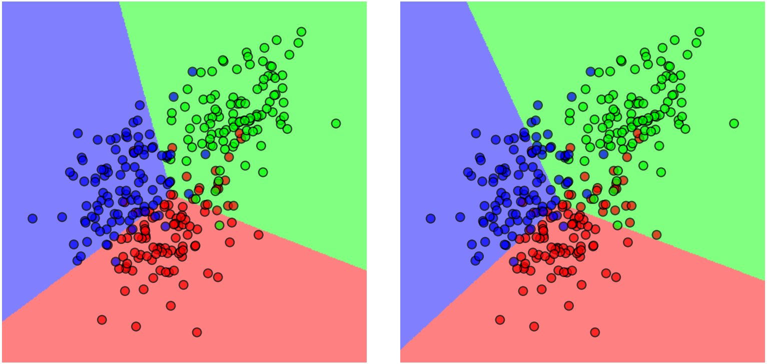


logistic

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

prediction: hard assignment

epoch 20

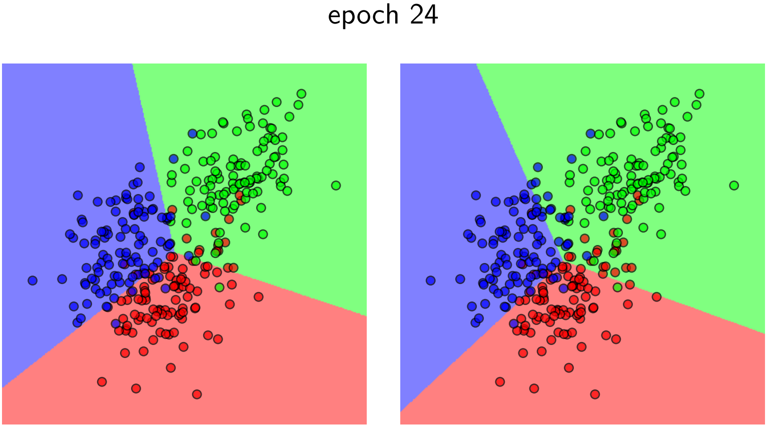


hinge (W & W)

logistic

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

prediction: hard assignment



epoch 24

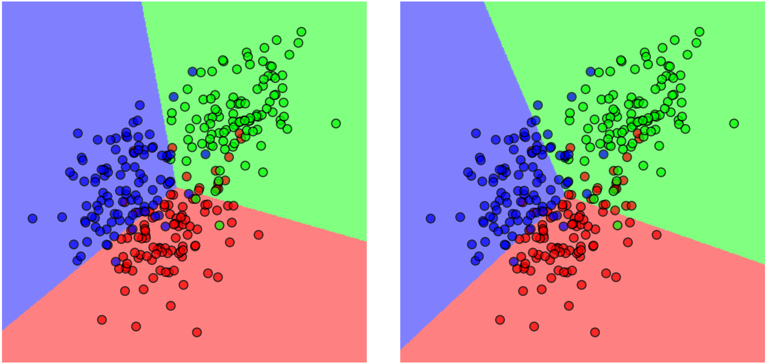
hinge (W & W)

logistic

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

prediction: hard assignment

epoch 28

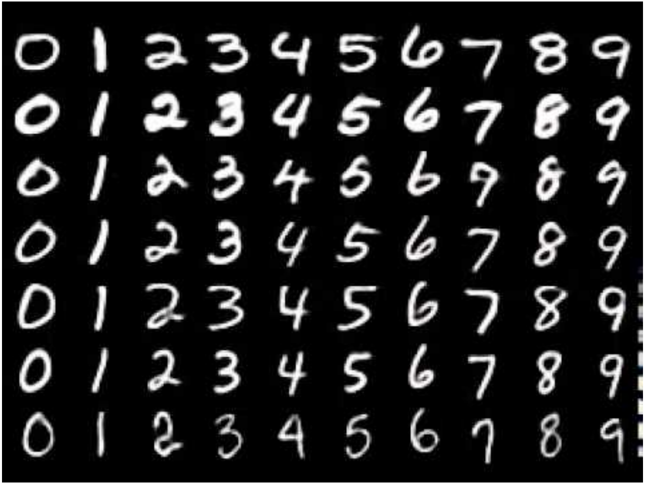


hinge (W & W)

logistic

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

MNIST digits dataset



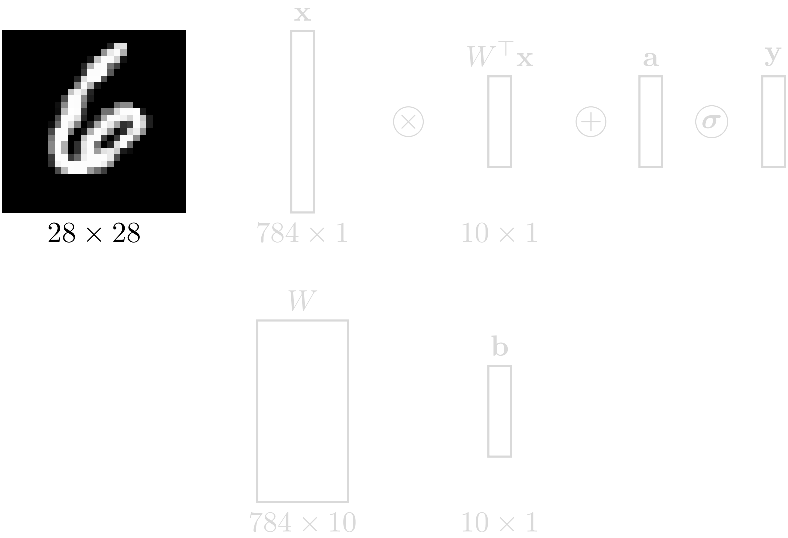
- 10 classes, 60k training images, 10k test images, 28 × 28 images

LeCun, Bottou, Bengio and Haffner IEEE Proc. 1998. Gradient-Based Learning Applied to Document Recognition.

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



28×28

$\mathbf{x}$

784×1

$\otimes$

$W^{\top}\mathbf{x}$

10×1

$\oplus$

$\mathbf{a}$

σ

$\mathbf{y}$

W

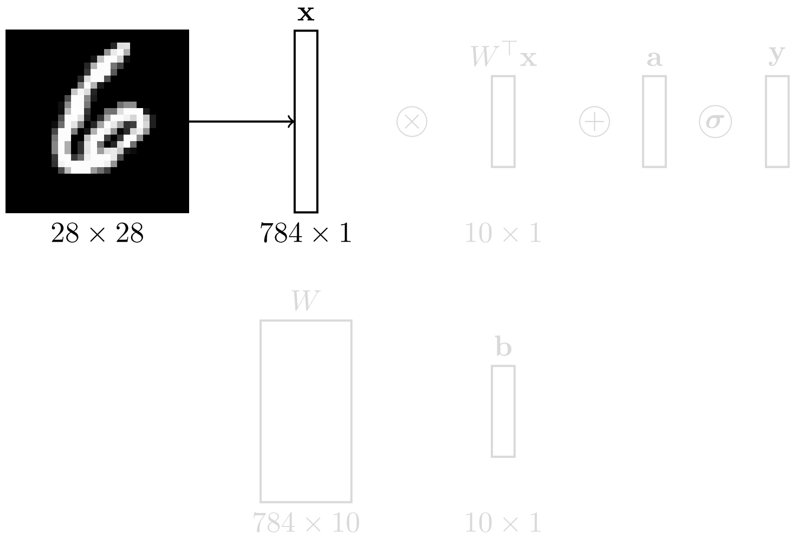
784×10

$\mathbf{b}$

10×1

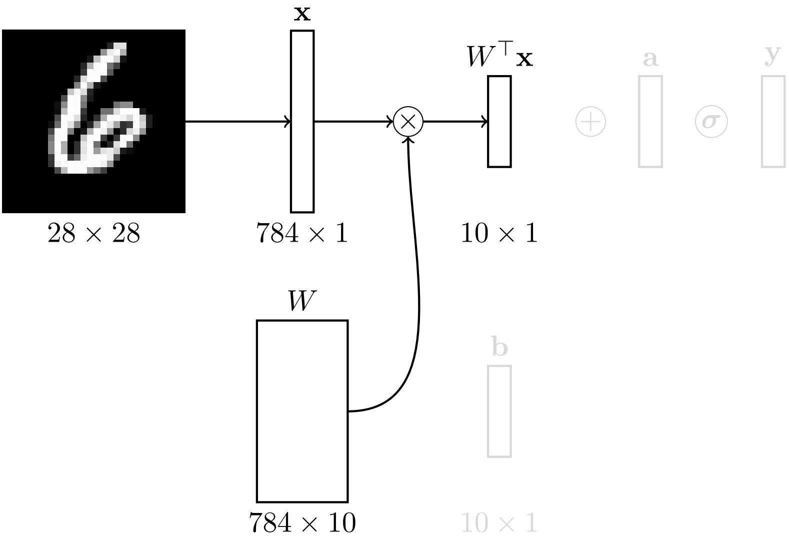
- input - weights - bias - softmax - parameters to be learned

linear classifier on raw pixels



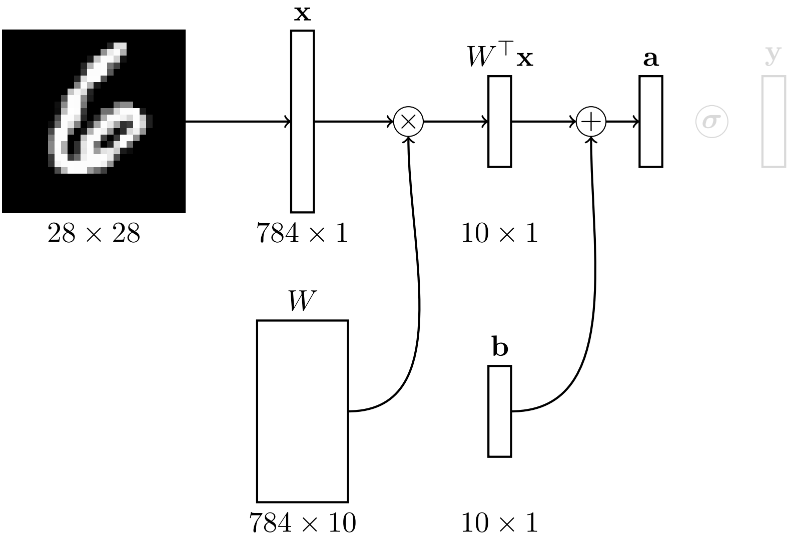
- input - weights - bias - softmax - parameters to be learned

linear classifier on raw pixels



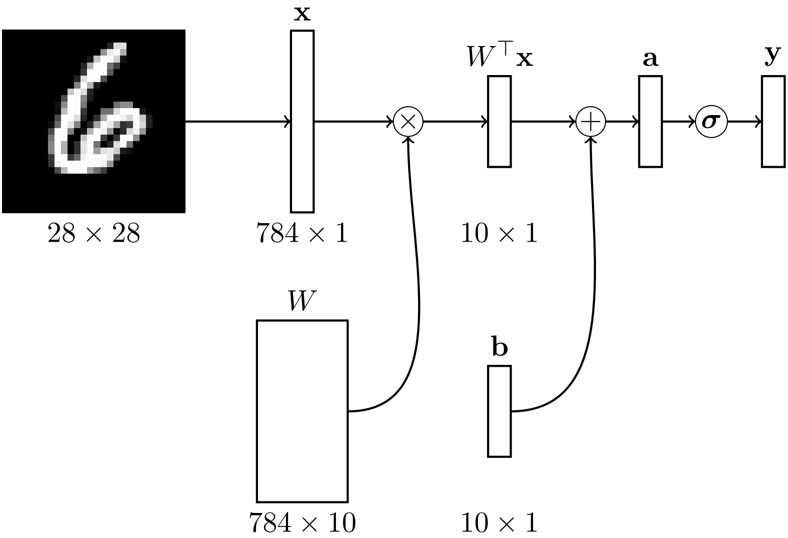
- input - weights - bias - softmax - parameters to be learned

linear classifier on raw pixels



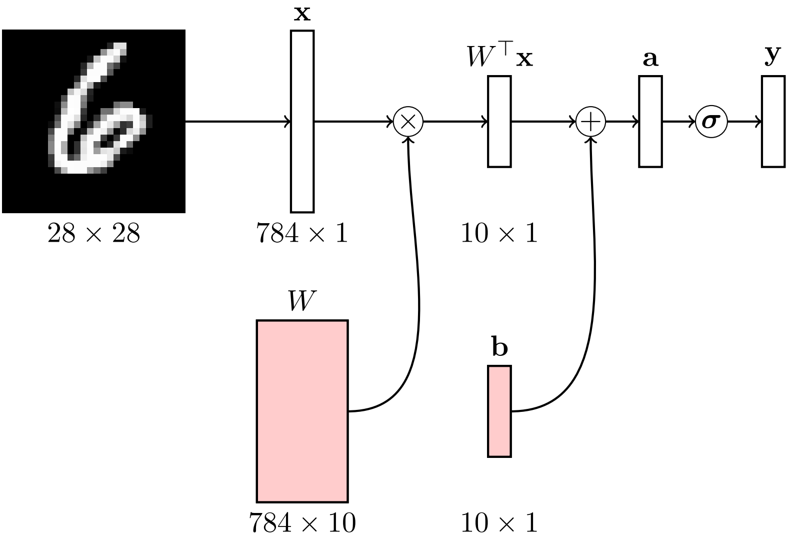
- input - weights - bias - softmax - parameters to be learned

linear classifier on raw pixels



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

linear classifier on raw pixels

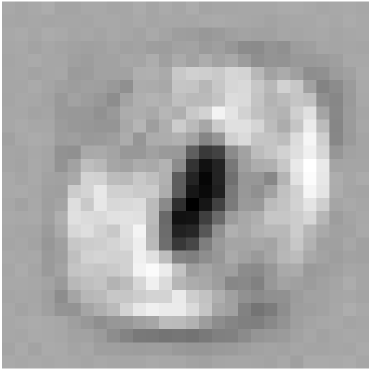


- input - weights - bias - softmax - parameters to be learned

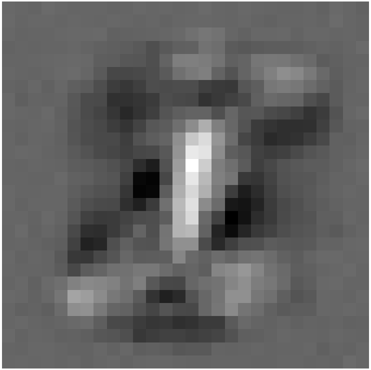
what is being learned?

- 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



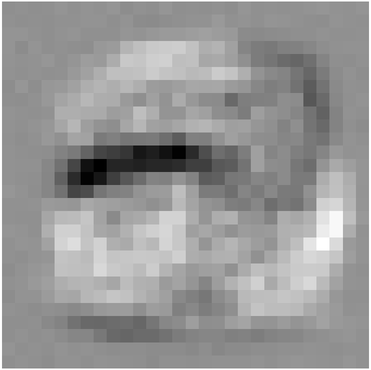
0



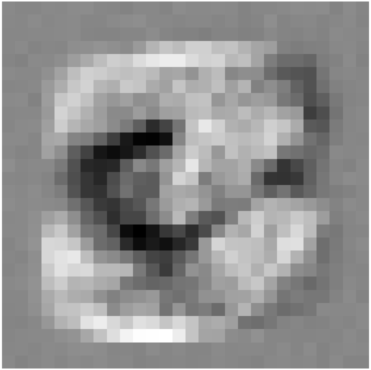
1

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

linear classifier on MNIST: patterns



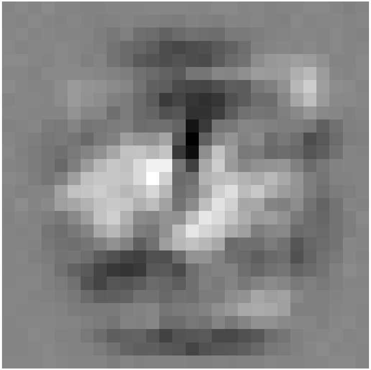
2



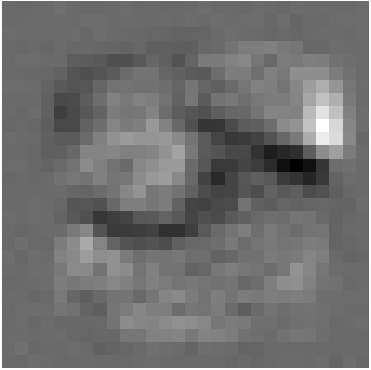
3

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

linear classifier on MNIST: patterns



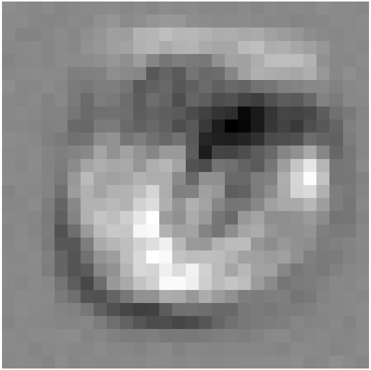
4



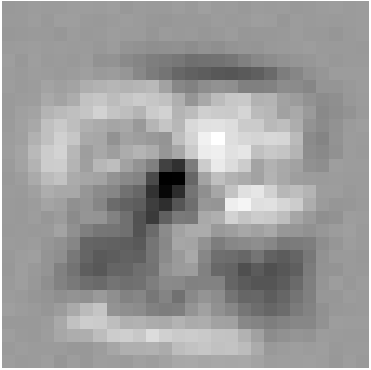
5

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

linear classifier on MNIST: patterns



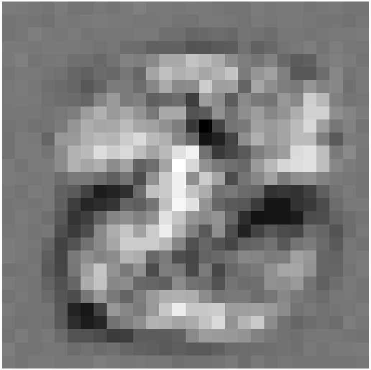
6



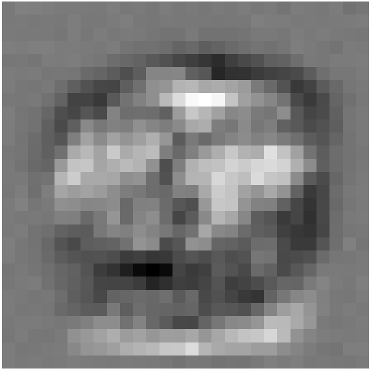
7

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

linear classifier on MNIST: patterns



8

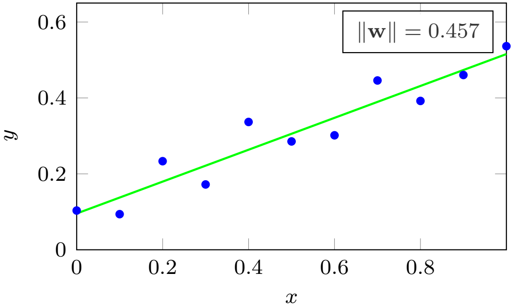


9

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

regression

line fitting



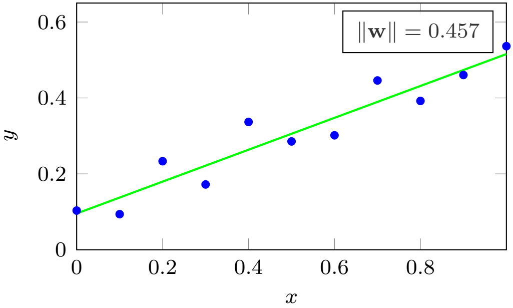
- linear model with parameters $\mathbf{w} = (a, b)$

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

- 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



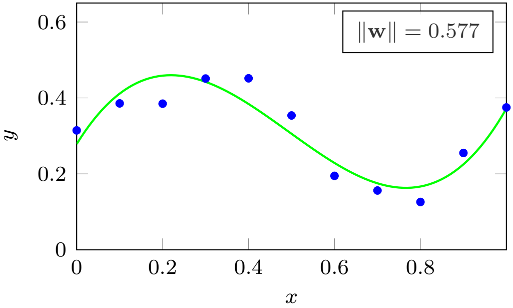
- linear model with parameters $\mathbf{w} = (a, b)$

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

- 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



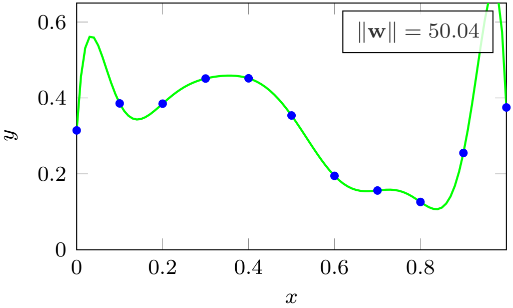
- linear model with parameters $\mathbf{w} \in \mathbb{R}^4$

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

- 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



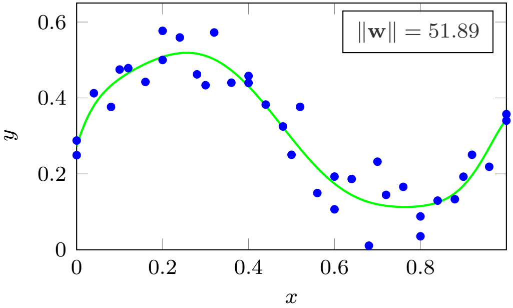
- linear model with parameters $\mathbf{w} \in \mathbb{R}^{11}$

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

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

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

more data



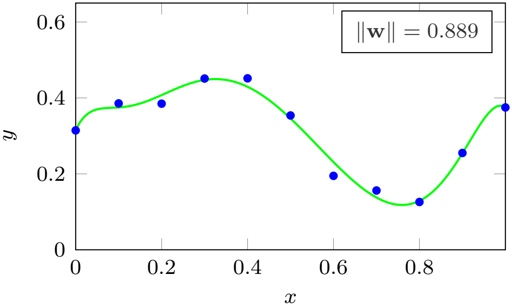
- linear model with parameters $\mathbf{w} \in \mathbb{R}^{11}$

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

- 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



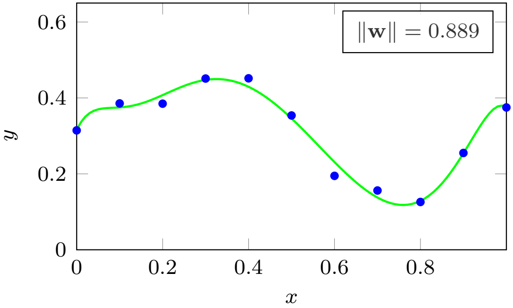
- linear model with parameters $\mathbf{w} \in \mathbb{R}^{11}$

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

- 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



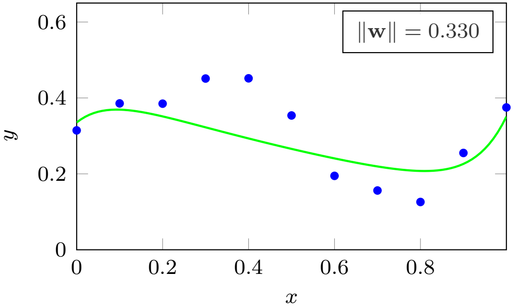
- linear model with parameters $\mathbf{w} \in \mathbb{R}^{11}$

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

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

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

severe regularization



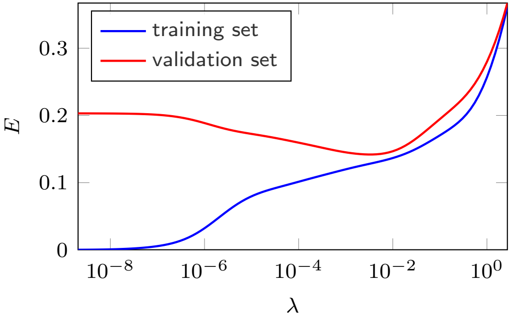
- linear model with parameters $\mathbf{w} \in \mathbb{R}^{11}$

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

- 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 $\mathbf{w} \in \mathbb{R}^{11}$

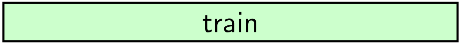
$$y = \mathbf{w}^\top \phi(x) = \mathbf{w}^\top (1, x, x^2, \dots, x^{10})$$

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

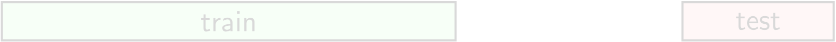
$$\mathbf{w}^* = (\lambda I + \Phi^\top \Phi)^{-1} \Phi^\top \mathbf{t}$$

setting hyperparameters

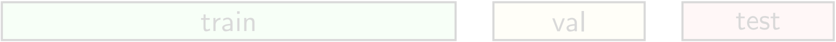
- optimize both parameters and hyperparameters on the training set: could work perfectly on training set, no idea how it works on test set



- 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

- 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 | test

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  train | val | test

setting hyperparameters

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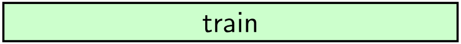

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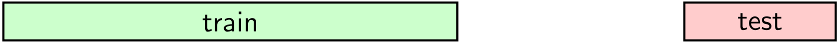

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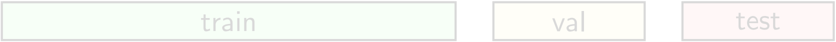

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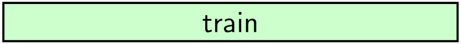

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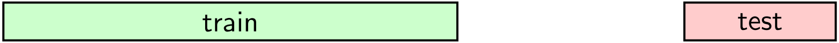

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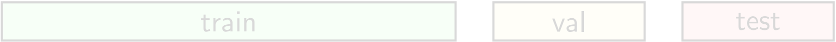

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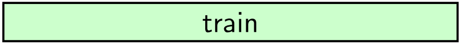

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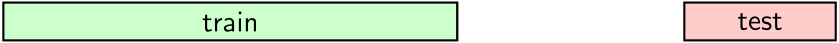

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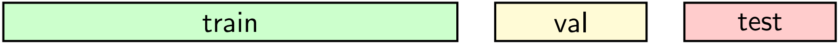

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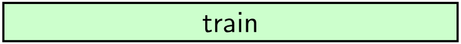

train

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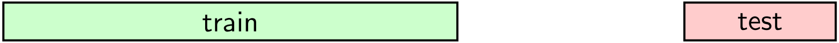

train

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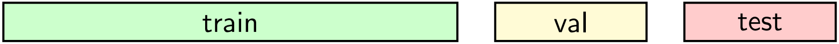


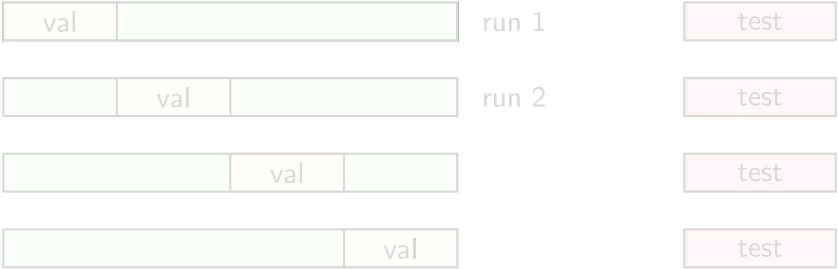
train

val

test

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



val run 1 test

val run 2 test

val test

val test

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

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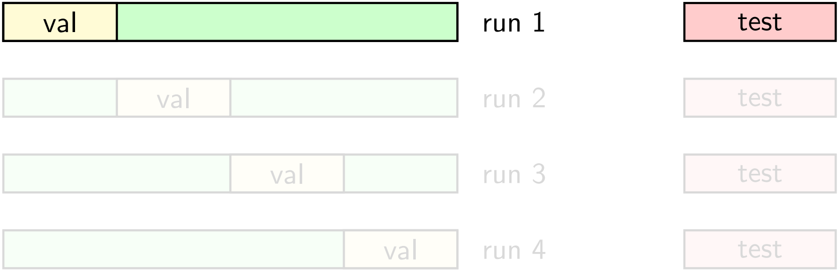

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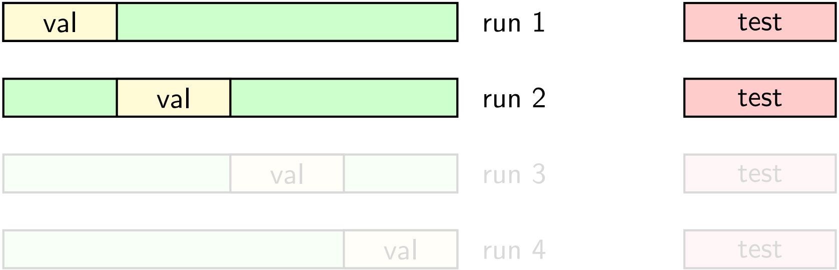

val run 1 test

val run 2 test

val run 3 test

val run 4 test

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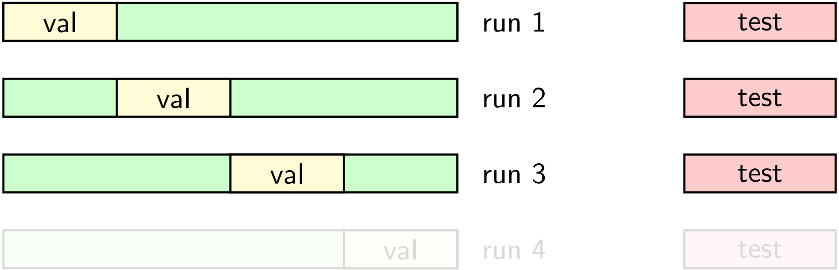

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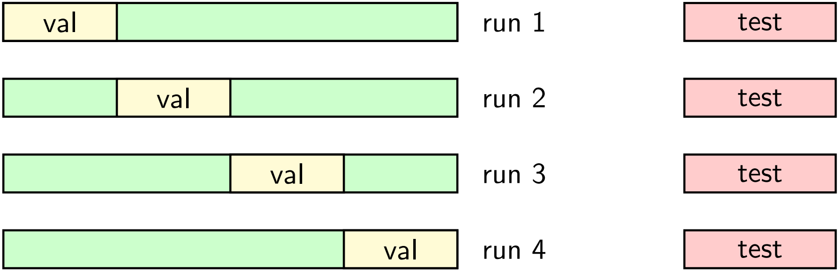

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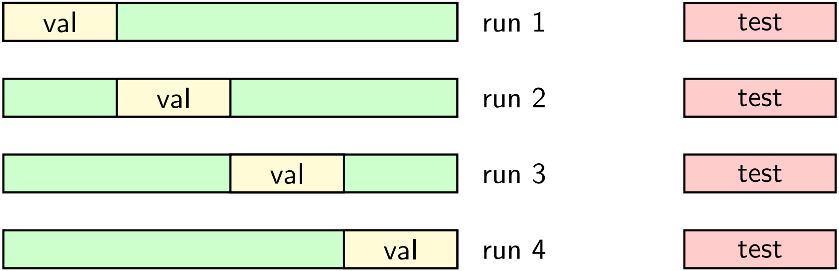

val run 1 test

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- 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
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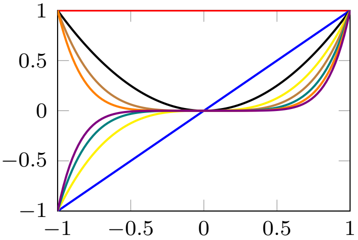
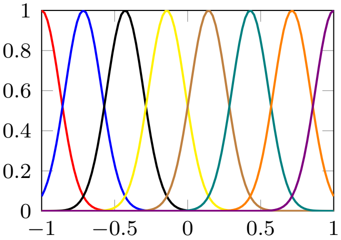
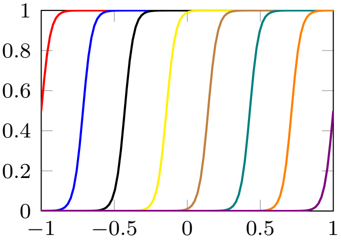
basis functions



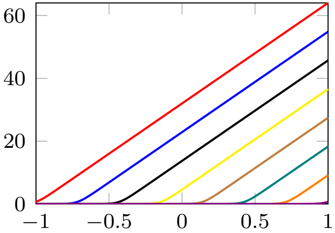
polynomial



Gaussian

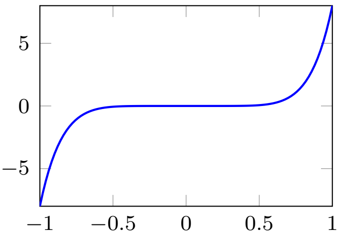


sigmoid

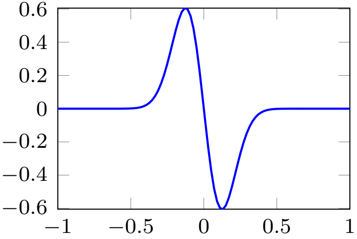


softplus

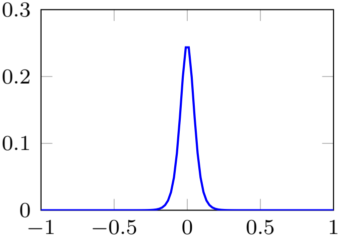
basis function derivatives



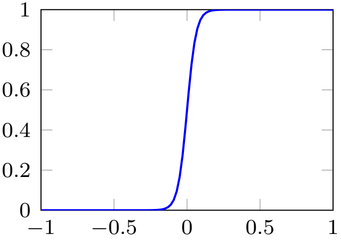
polynomial



Gaussian



sigmoid



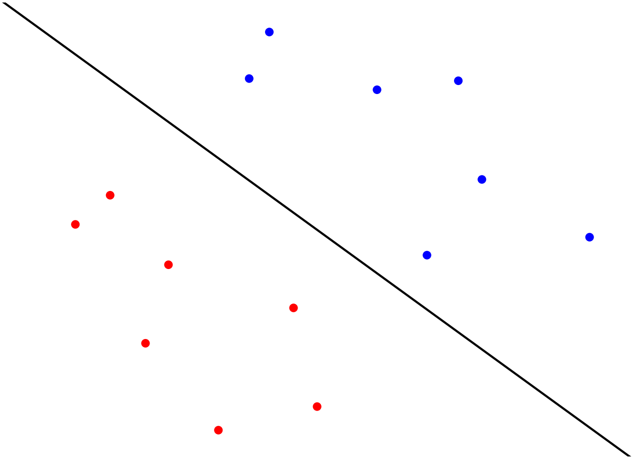
softplus

basis functions

- we want basis functions to cover the entire space so that any arbitrary input can be expressed as a linear of 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

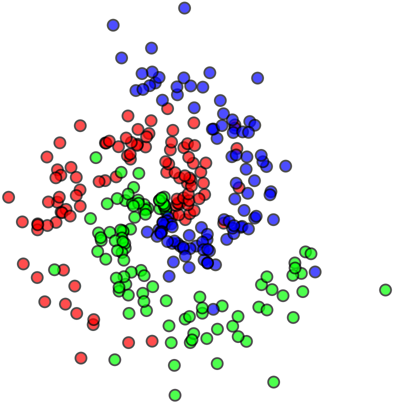
multiple layers

linear separability



- two point sets $X_1, X_2 \subset \mathbb{R}^d$ are linearly separable iff there is $\mathbf{w}, b$ such that $\mathbf{w}^\top x_1 < b < \mathbf{w}^\top x_2$ for $\mathbf{x}_1 \in X_1, \mathbf{x}_2 \in X_2$
- or, they can be separated by a perceptron

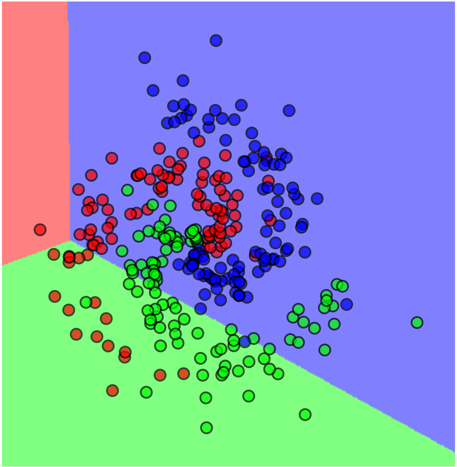
non-linearly separable classes



credit: dataset adapted from Andrej Karpathy

linear classifier

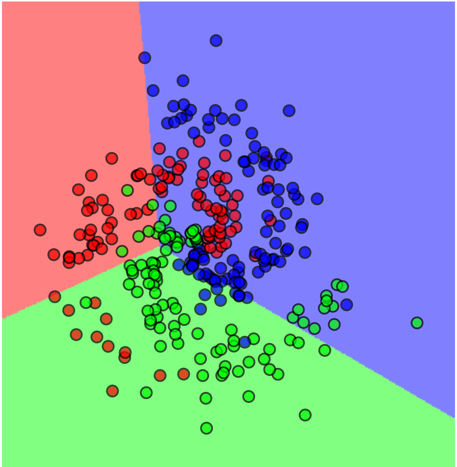
epoch 00



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

linear classifier

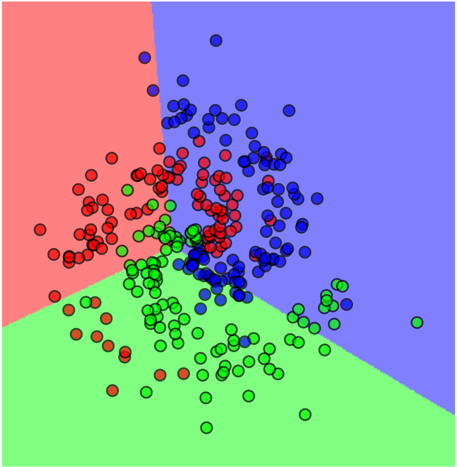
epoch 05



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

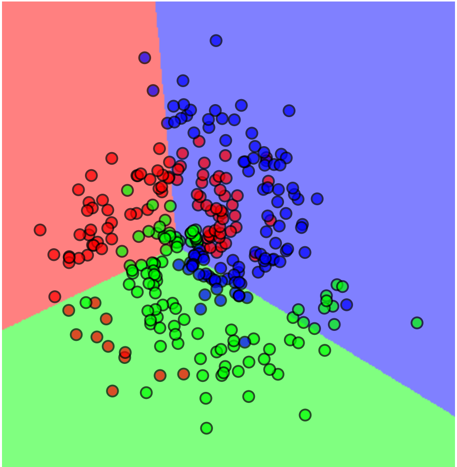
linear classifier

epoch 10



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

linear classifier

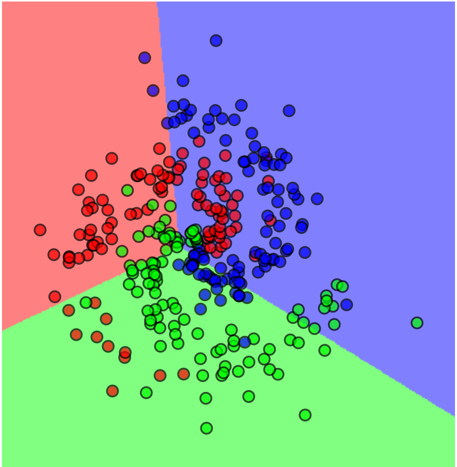


epoch 15

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

linear classifier

epoch 20



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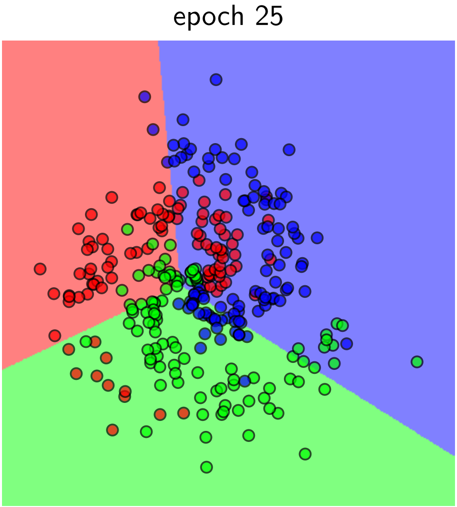
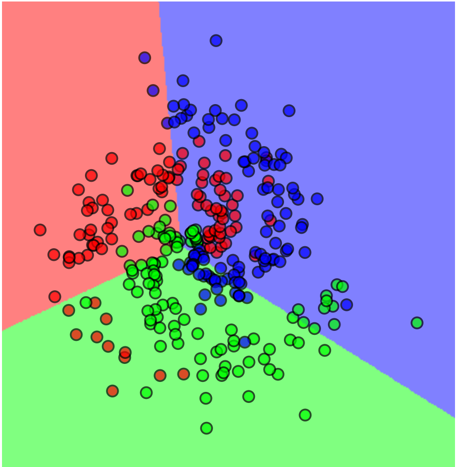
linear classifier



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

linear classifier

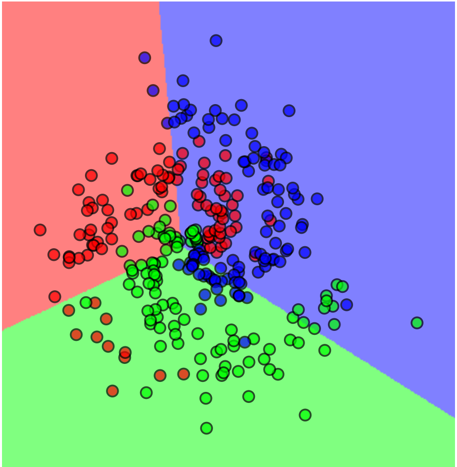
epoch 30



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

linear classifier

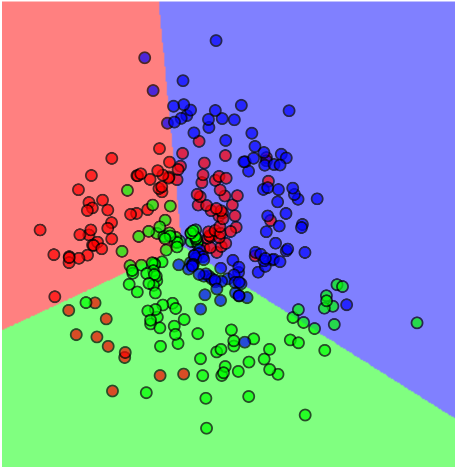
epoch 35



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

linear classifier

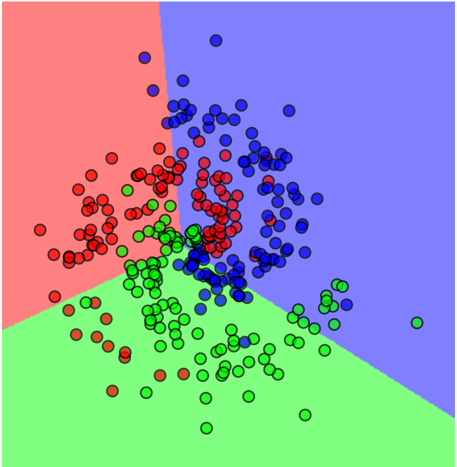
epoch 40



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

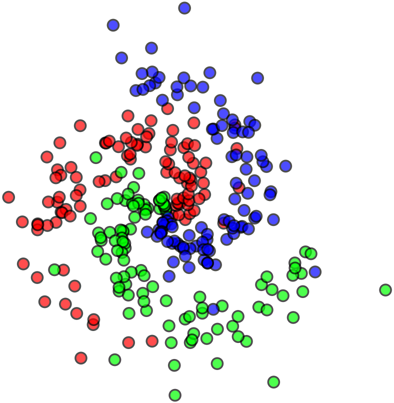
linear classifier

epoch 45



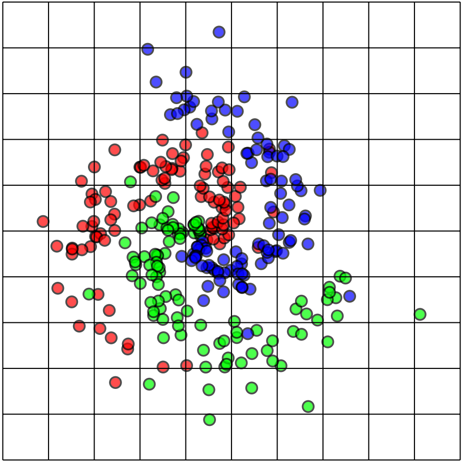
- $k = 3, n = 300, m = 100, \epsilon = 10^0, \lambda = 10^{-3}$

nonlinear?



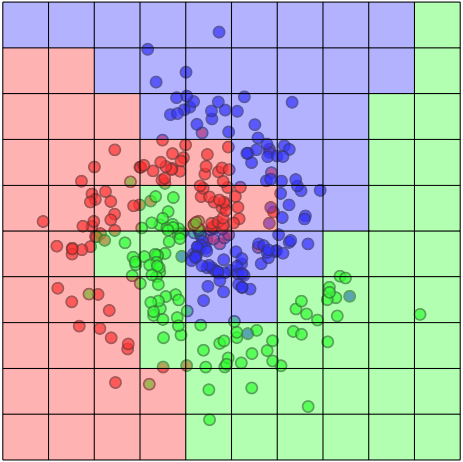
- so how do we make our classifier nonlinear?

nonlinear?



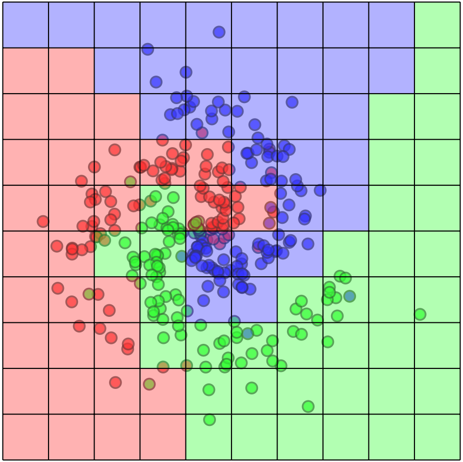
- define a 10×10 grid over the entire space

nonlinear?



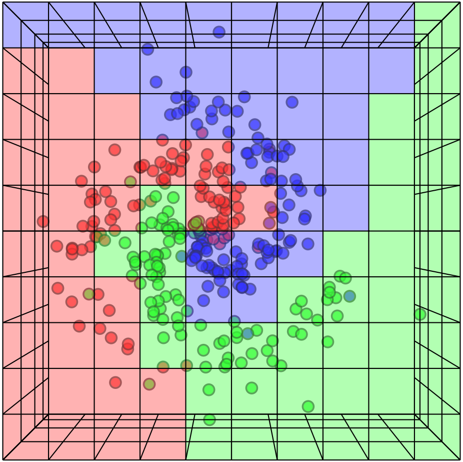
- and a (Gaussian?) basis function centered at every cell

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
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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 → “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
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- 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
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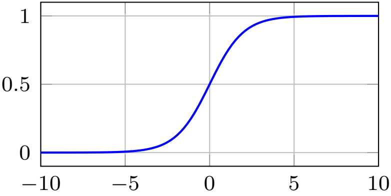
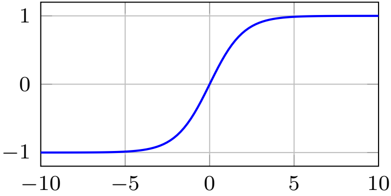


$\sigma(x) = \frac{1}{1+e^{-x}}$

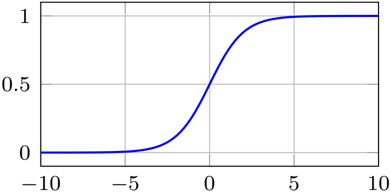
sigmoid



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

hyperbolic tangent

activation functions



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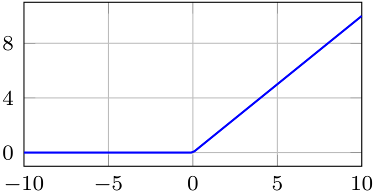
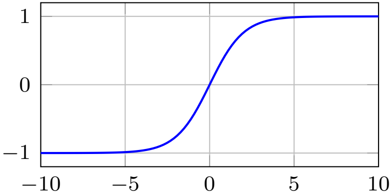


$$\mathrm{relu}(x) = [x]_+ = \max(0, x)$$

rectified linear unit (ReLU)



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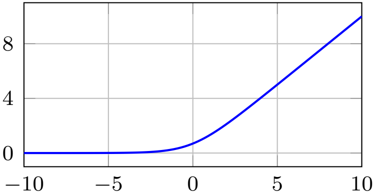

$$\zeta(x) = \log(1 + e^x)$$

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.
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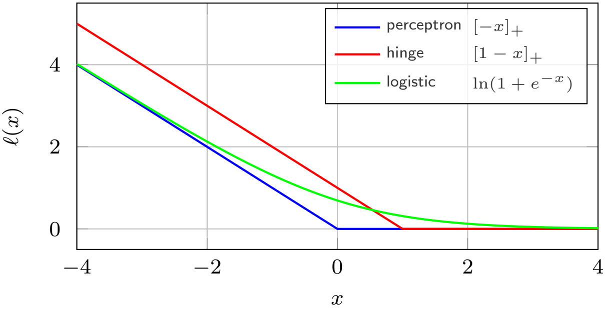
back to loss functions



- $\mathrm{relu}(x) = [x]_+$ 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

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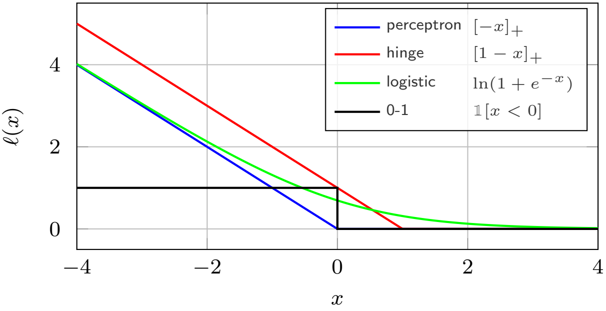

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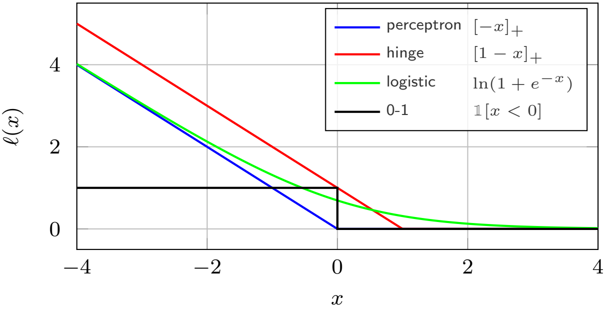

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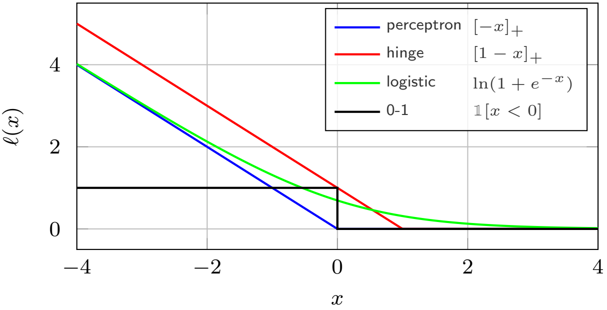

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surrogate loss functions

- all three loss functions we have seen are surrogate (proxy) for the 0-1 loss: their derivative is constant for $x \to -\infty$
- 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 $x \to -\infty$
- 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?

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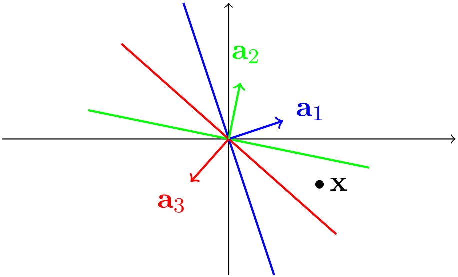
remember LSH?

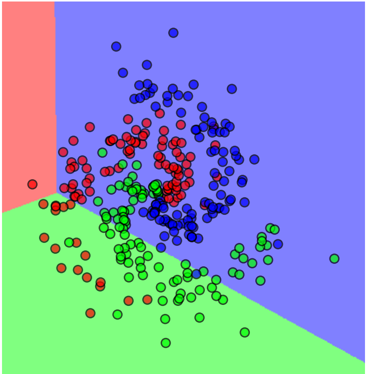


- in LSH, we used a number of random projections followed by sgn to produce a binary code as a description of $\mathbf{x}$
- here, we use again a number of (initially) random projections followed by relu instead, acting like a switch: half space is zeroed out, the other half passes through
- in the nonzero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

Charikar. STOC 2002. Similarity Estimation Techniques From Rounding Algorithms.

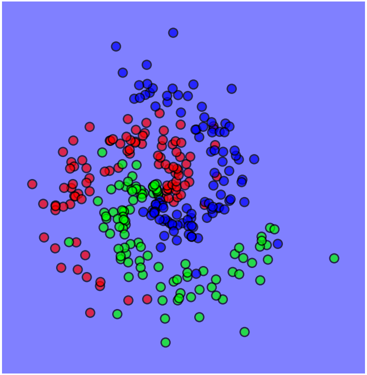
two-layer classifier

epoch 00



linear

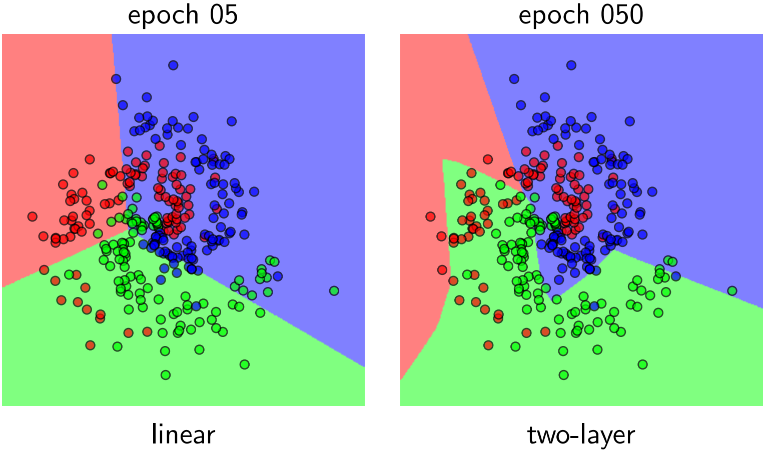
epoch 000



two-layer

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

two-layer classifier



epoch 05

epoch 050

linear

two-layer

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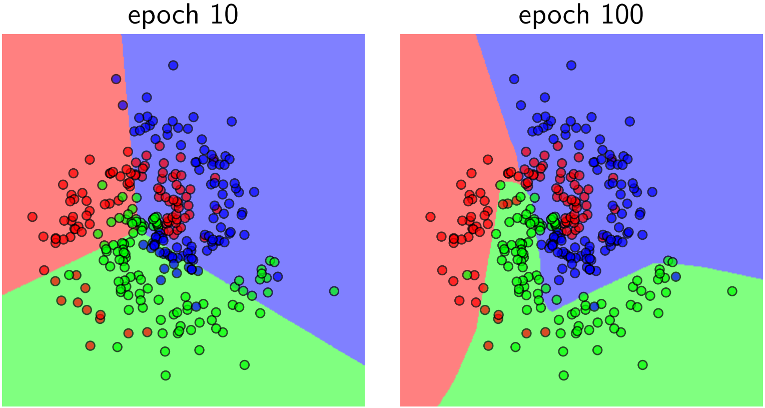
two-layer classifier



epoch 10

epoch 100

linear

two-layer

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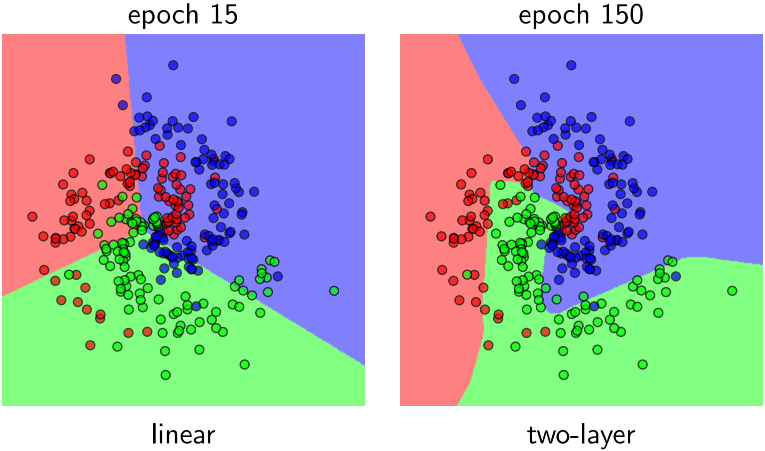
two-layer classifier



epoch 15

epoch 150

linear

two-layer

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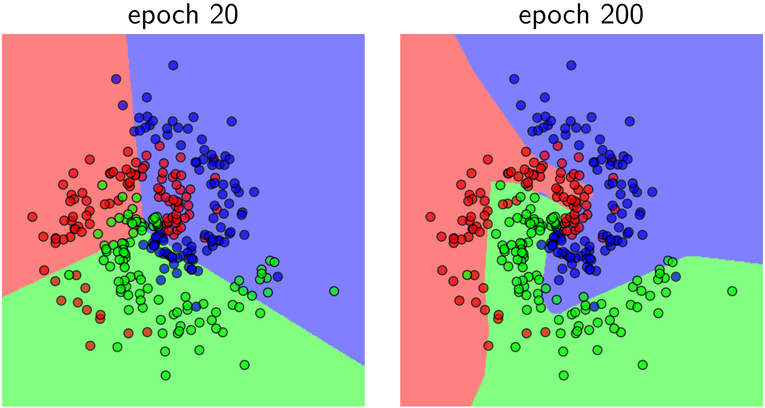
two-layer classifier


epoch 20

epoch 200

linear

two-layer

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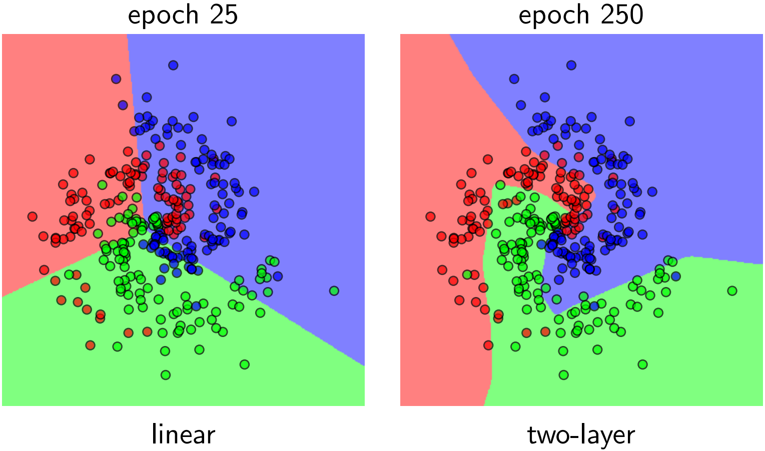
two-layer classifier



epoch 25

epoch 250

linear

two-layer

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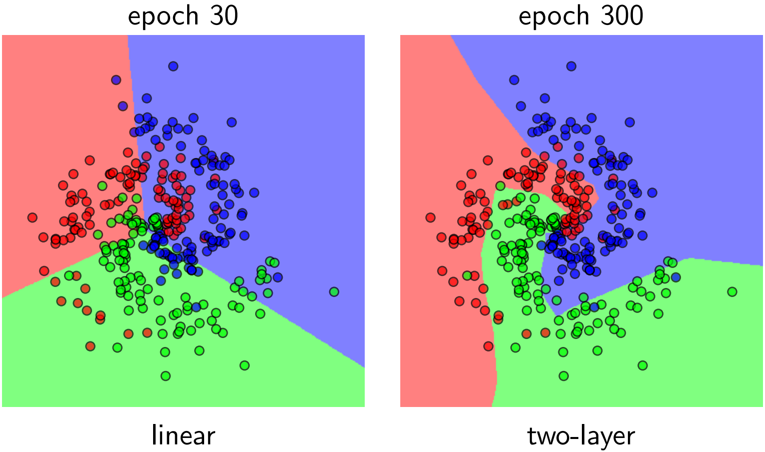
two-layer classifier



epoch 30

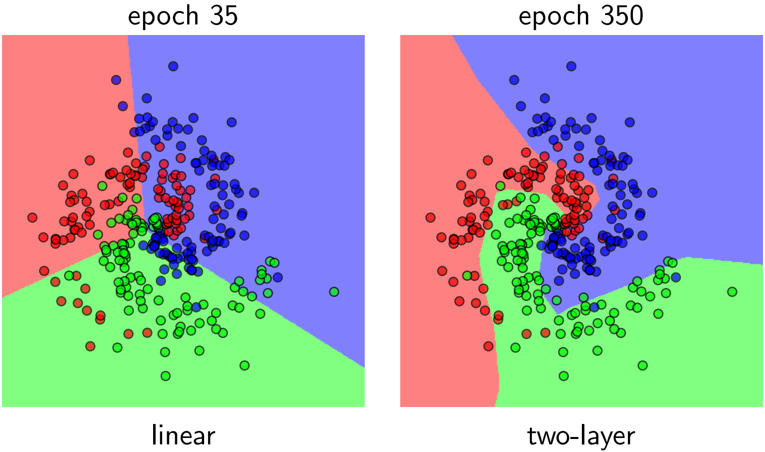
epoch 300

linear

two-layer

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

two-layer classifier



epoch 35

epoch 350

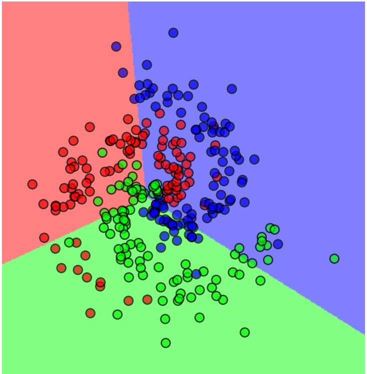
linear

two-layer

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

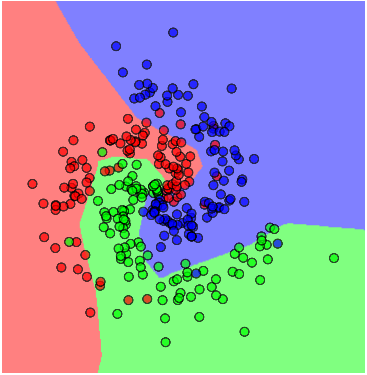
two-layer classifier

epoch 40



linear

epoch 400

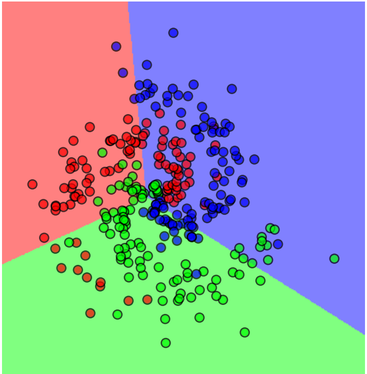


two-layer

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

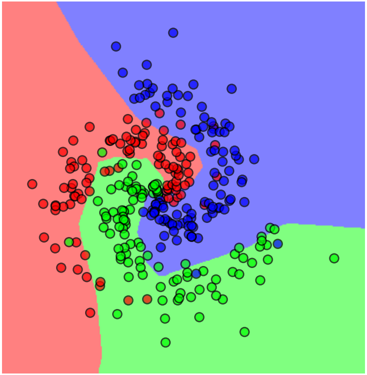
two-layer classifier

epoch 45



linear

epoch 450



two-layer

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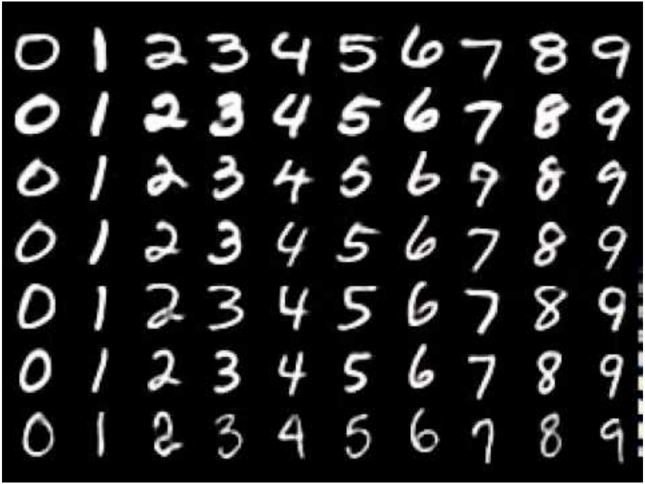
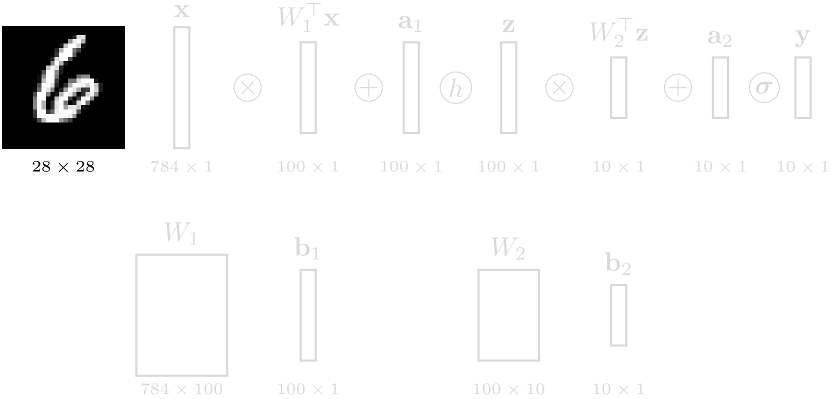
MNIST digits dataset



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

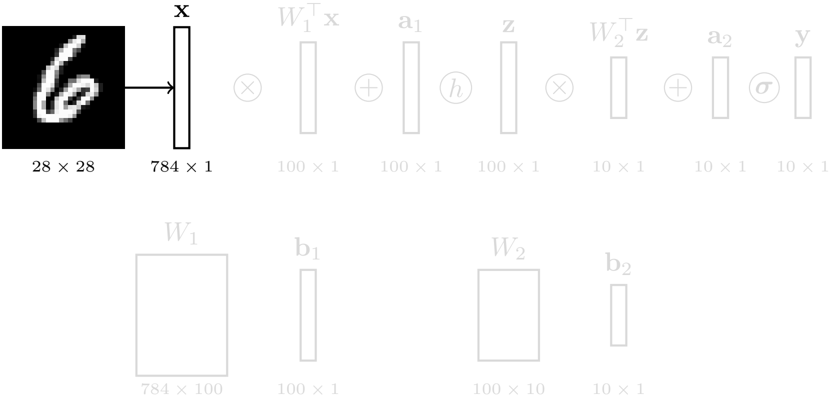
LeCun, Bottou, Bengio and Haffner IEEE Proc. 1998. Gradient-Based Learning Applied to Document Recognition.

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 $\mathbf{y}$ (or rather, directly on $\mathbf{a}_2$)

two-layer classifier on raw pixels



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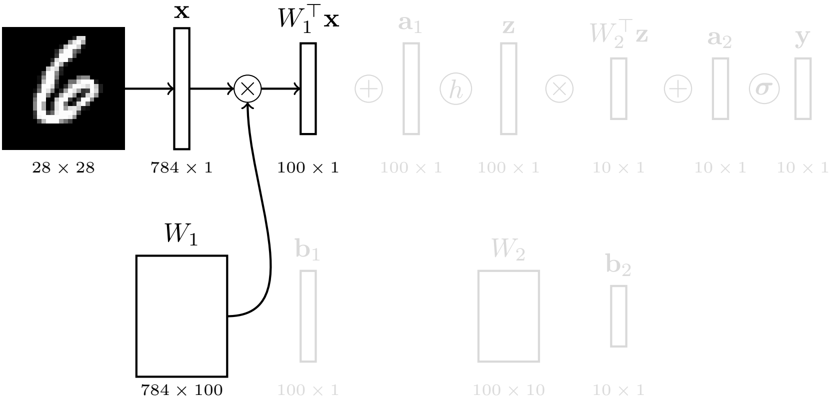

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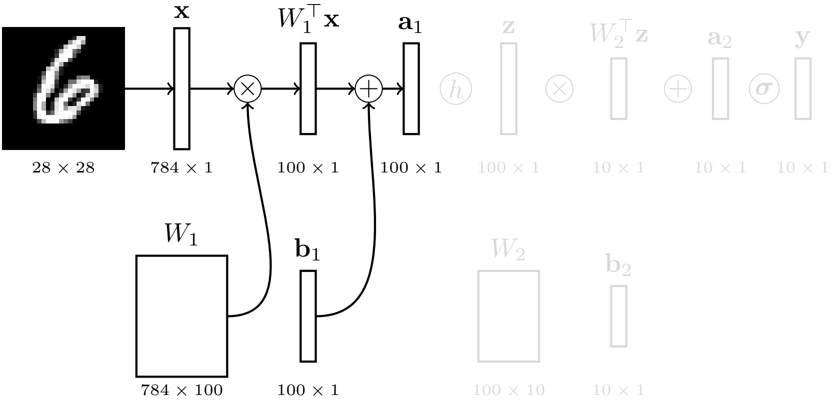

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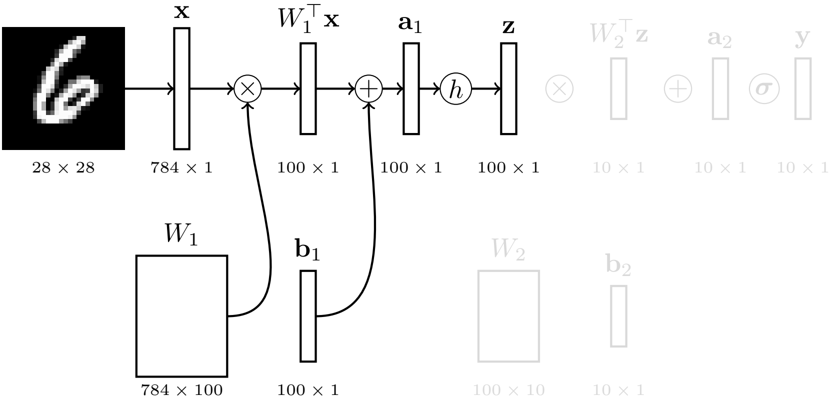

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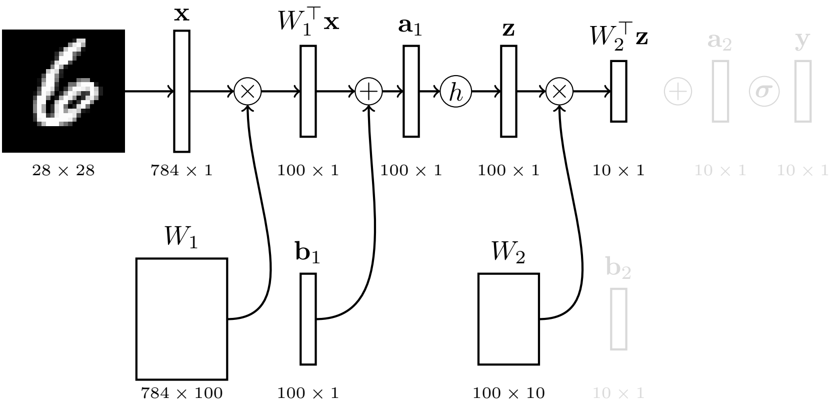

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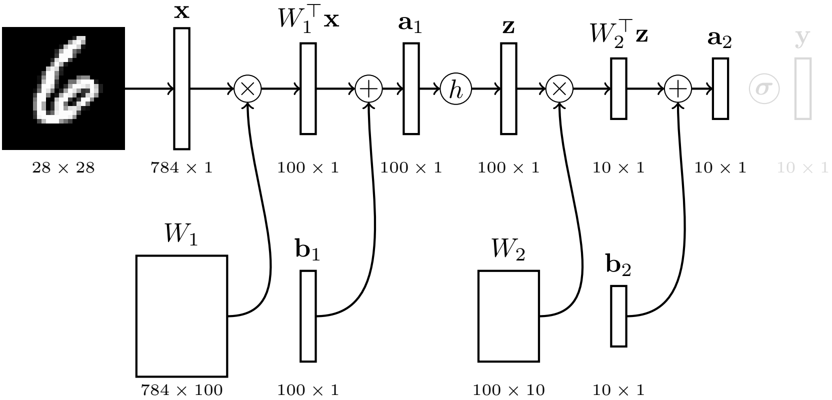

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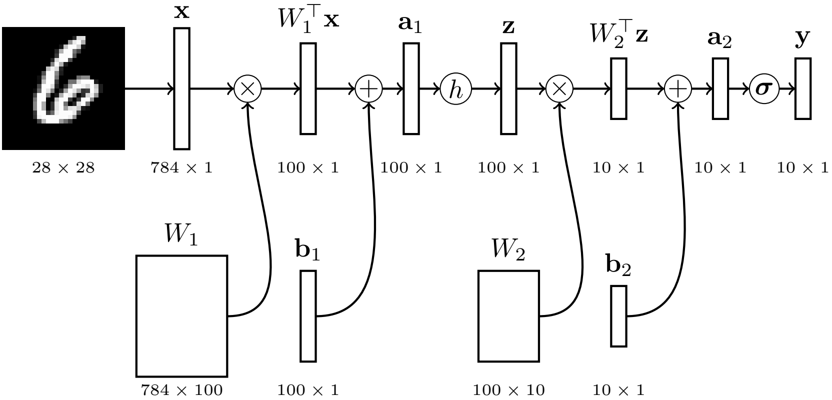

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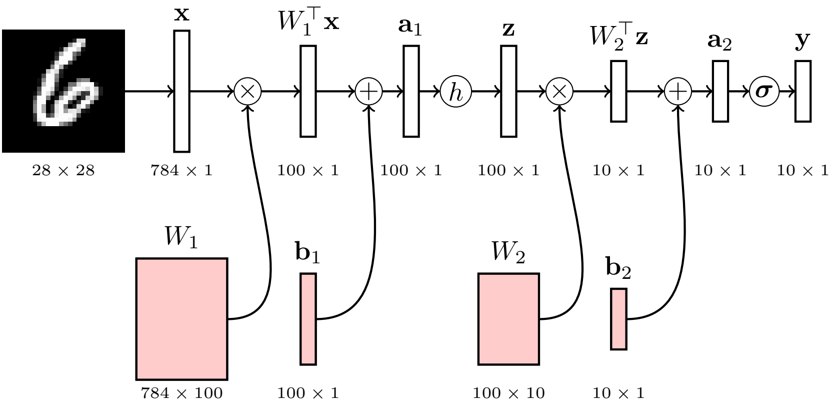

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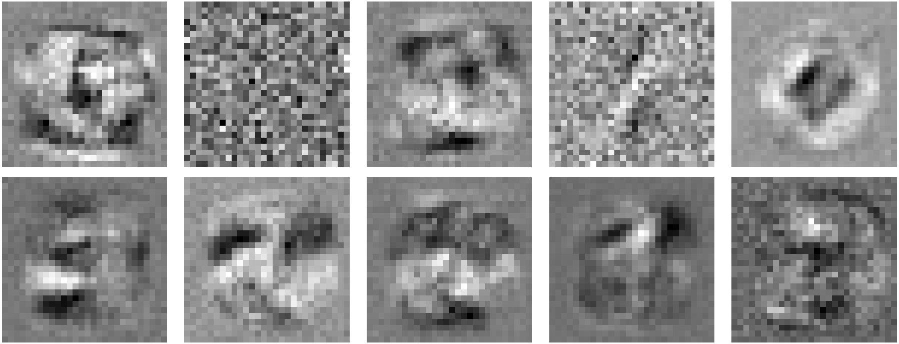
what is being learned?

- 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

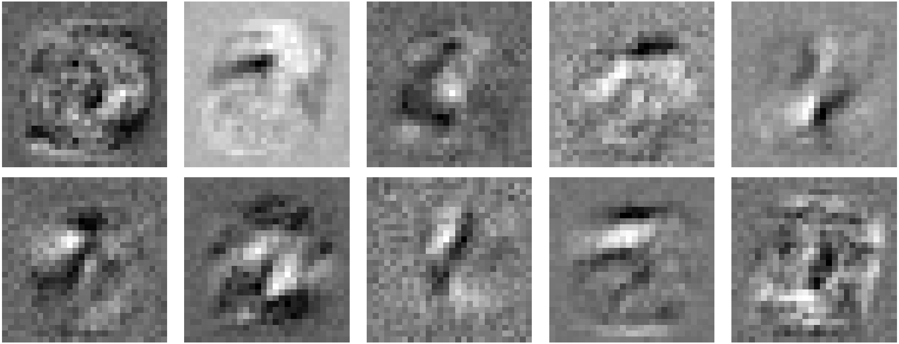
layer 1 weights 00-09



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

MNIST: two-layer classifier

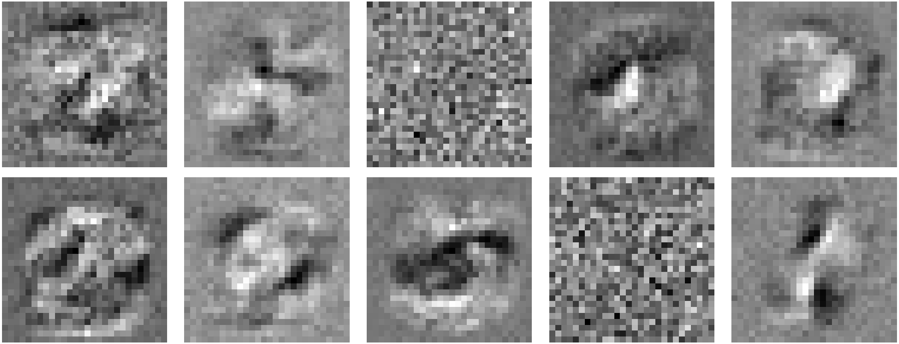
layer 1 weights 10-19



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

MNIST: two-layer classifier

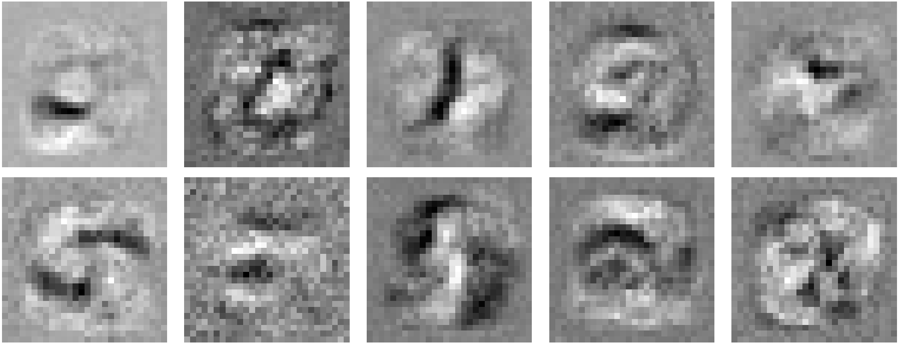
layer 1 weights 20-29



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

MNIST: two-layer classifier

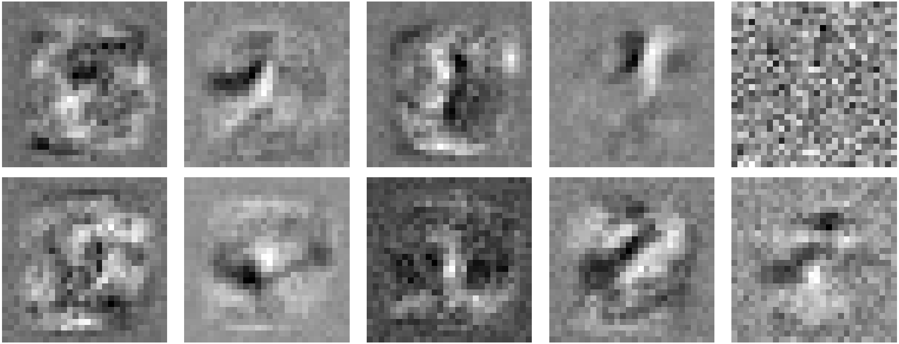
layer 1 weights 30-39



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

MNIST: two-layer classifier

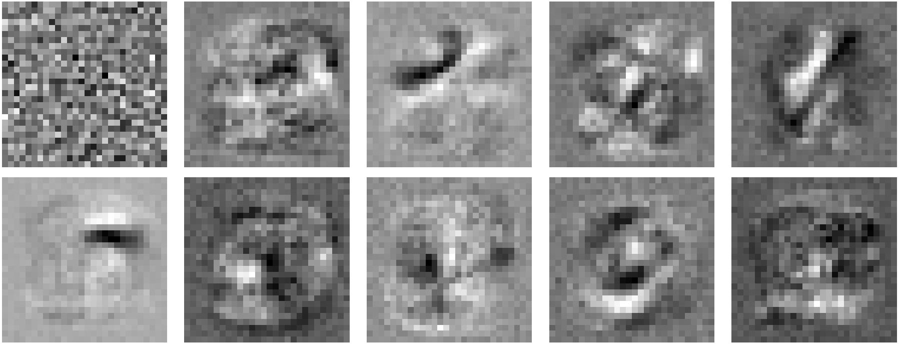
layer 1 weights 40-49



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

MNIST: two-layer classifier

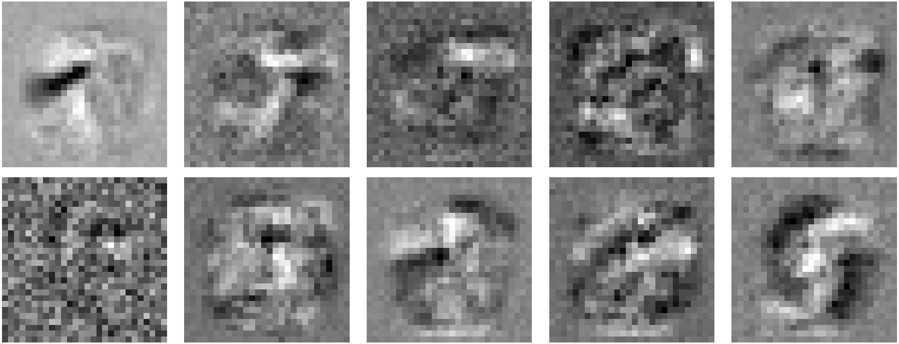
layer 1 weights 50-59



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

MNIST: two-layer classifier

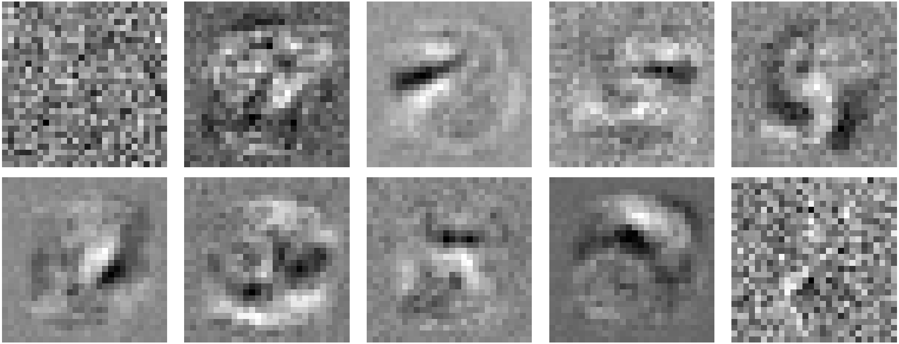
layer 1 weights 60-69



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

MNIST: two-layer classifier

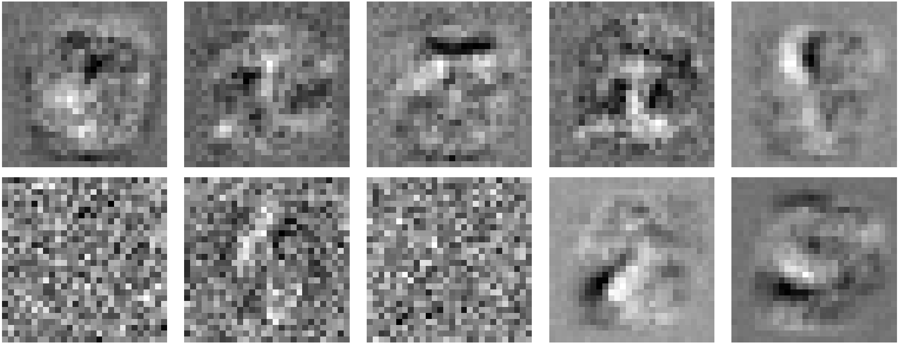
layer 1 weights 70-79



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

MNIST: two-layer classifier

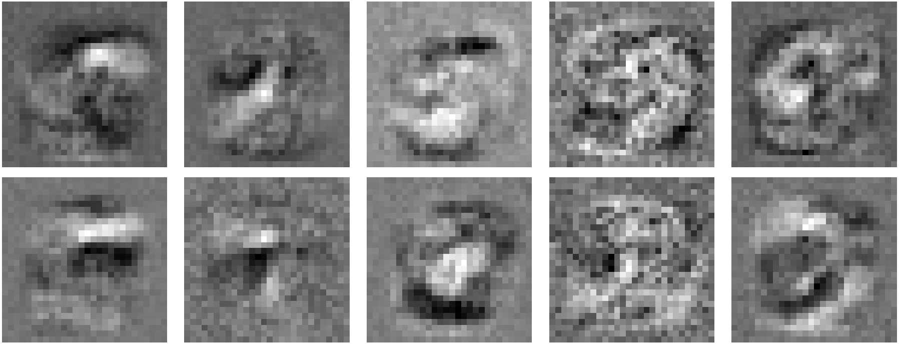
layer 1 weights 80-89



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

MNIST: two-layer classifier

layer 1 weights 90-99



- $k = 10, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- 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, $\mathrm{softmax}$ 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