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

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.

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



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- 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
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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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converting the learning problem to optimization



- 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

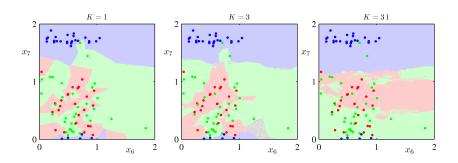
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binary classification

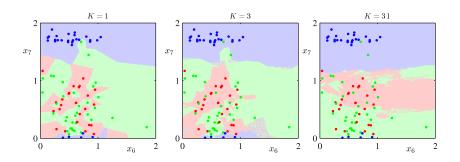
k-nearest neighbor classifier



- 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 because it gives us no opportunity to learn a representation



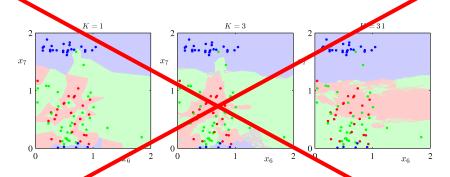
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perceptron

[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

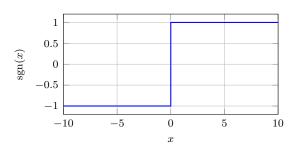
perceptron model

ullet 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

$$\operatorname{sgn}(x) := \left\{ \begin{array}{ll} +1, & x \ge 0 \\ -1, & x < 0 \end{array} \right.$$



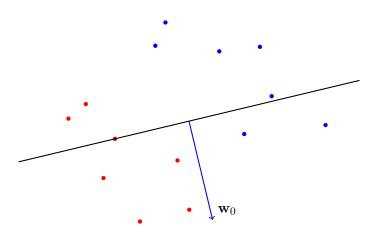
- an input ${\bf x}$ with output $y=f({\bf x};{\bf w})$ is classified to class C_1 if y=1 and to C_2 if y=-1
- given a training sample $\mathbf{x} \in \mathbb{R}^d$ and a target variable $s \in \{-1, 1\}$, \mathbf{x} is correctly classified iff output $y = f(\mathbf{x}; \mathbf{w})$ equals s, i.e. sy > 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

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

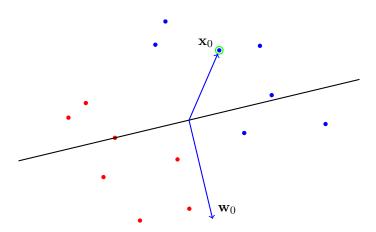
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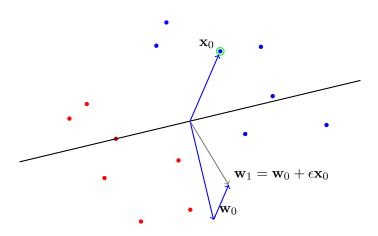




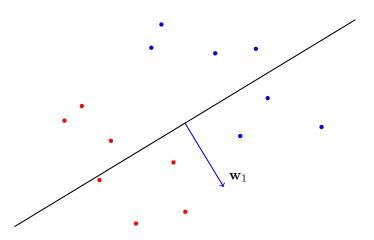
• initial parameter vector \mathbf{w}_0 , normal to the decision boundary and pointing to the region to be classified as blue (+)



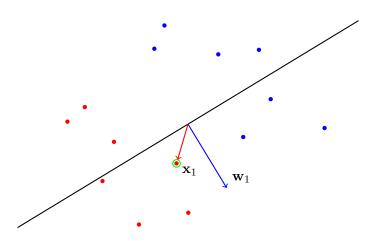
• pick a random point \mathbf{x}_0 that is misclassified: blue (+) in red (-) region



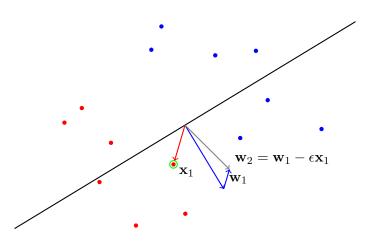
ullet because ${f x}_0$ is blue and ${f w}$ is pointing at blue, we add $\epsilon {f x}_0$ to ${f w}_0$



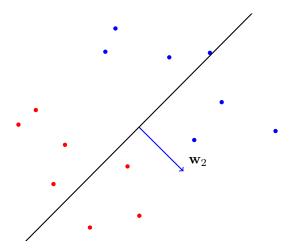
ullet with the new parameter vector \mathbf{w}_1 , the decision boundary is updated



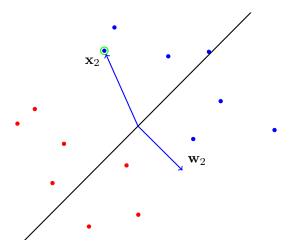
ullet pick a new random point ${f x}_1$ that is misclassified: red in blue region



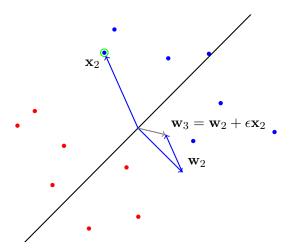
ullet because \mathbf{x}_1 is red and \mathbf{w} is pointing at blue, we subtract $\epsilon \mathbf{x}_1$ from \mathbf{w}_1



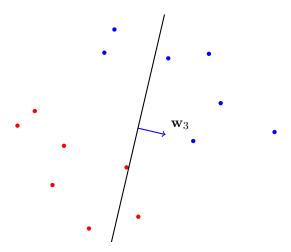
ullet with the new \mathbf{w}_2 , the decision boundary is updated again



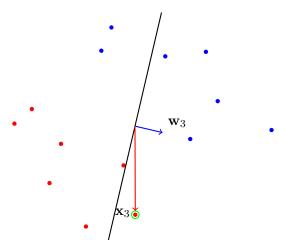
ullet again, random point \mathbf{x}_2 , blue misclassified in red region



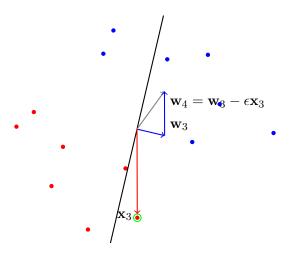
ullet and we add $\epsilon \mathbf{x}_2$ to \mathbf{w}_2



• now at \mathbf{w}_3



ullet one last random point ${f x}_3$, red in blue region



• and we subtract



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



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- 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





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

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



SVM model

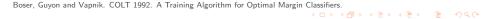
 there is now an explicit bias parameter b, but otherwise the SVM model is the same: activation

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

and output

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

- again, an input ${\bf x}$ with $a={\bf w}^{\top}{\bf x}+b$ and output $y={\rm sgn}(a)$ 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 $s_1, \dots, s_n \in \{-1, 1\}$



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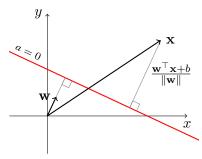
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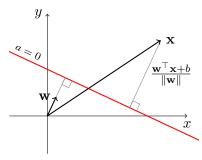
margin



- the distance of ${\bf x}$ to the boundary is $|{\bf w}^{\top}{\bf x} + b|/\|{\bf w}\|$
- 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

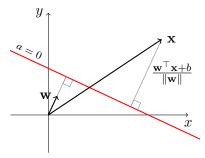


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maximum margin

- 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

$$s_i a_i \ge 1$$

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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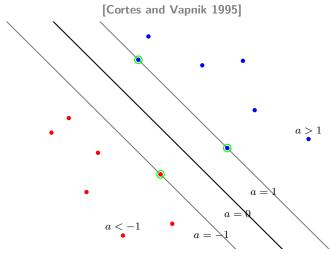
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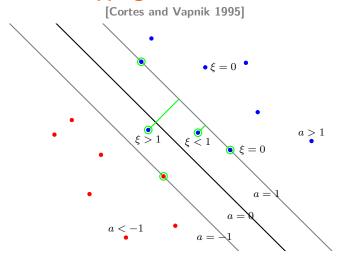
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 assuming that all training samples can be correctly classified is unrealistic





• 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

• the constraints $s_i a_i \ge 1$ are now replaced by

$$s_i a_i \ge 1 - \xi_i$$
$$\xi_i \ge 0$$

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

• and the objective $rg \min_{\mathbf{w},b} rac{1}{2} \|\mathbf{w}\|^2$ 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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where hyperparameter ${\cal C}$ controls the trade-off between slack variables and margin

- 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)

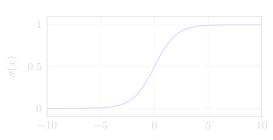
$$a = \mathbf{w}^{\top} \mathbf{x}$$

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

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





(binary) logistic regression

[Cox 1958]

again, activation (but here we omit the bias)

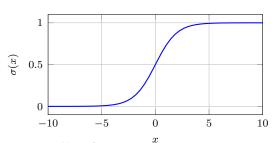
$$a = \mathbf{w}^{\mathsf{T}} \mathbf{x}$$

and output

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

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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

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

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 $X=(\mathbf{x}_1,\ldots,\mathbf{x}_n)$ with $\mathbf{x}_i\in\mathbb{R}^d$ and target variables $T=(t_1,\ldots,t_n)$ 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

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

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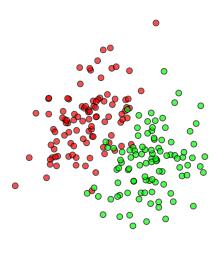
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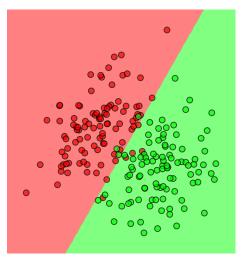
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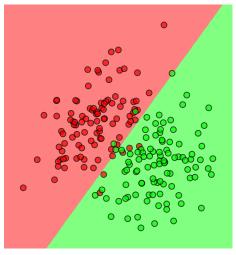




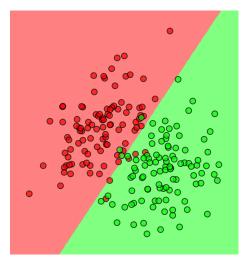
raw data



perceptron



SVM



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

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

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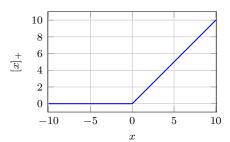
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positive part

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

$$relu(x) := [x]_+ := max(0, x)$$



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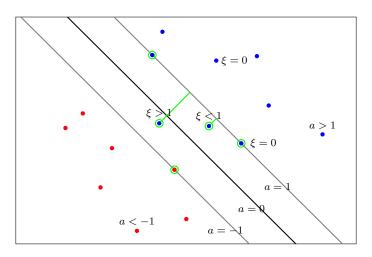
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• either $s_i a_i \geq 1$ and $\xi_i = 0$ (correct side of margin) or $\xi_i = 1 - s_i a_i$

the constraints

$$s_i a_i \ge 1 - \xi_i$$

$$\xi_i \ge 0$$

do not tell the whole truth

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

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- ullet recall that the margin in SVM is invariant to scaling ${f w}$ and b
- same for perceptron error function
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maximum posterior

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

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prediction function

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

to make predictions during training; this is the activation, without the nonlinearity

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

the only difference is

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SVM (hinge)	$[1-x]_{+}$
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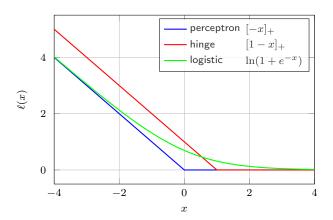
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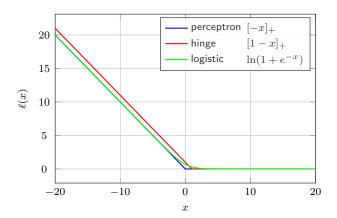
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	$\ell(x)$
perceptron	$[-x]_+$
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- perceptron and logistic are asymptotically equivalent
- both SVM and logistic penalize small positive errors

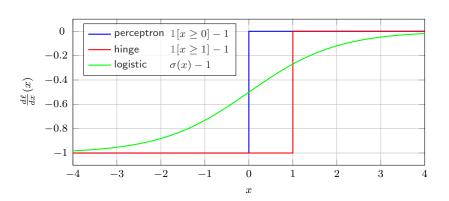


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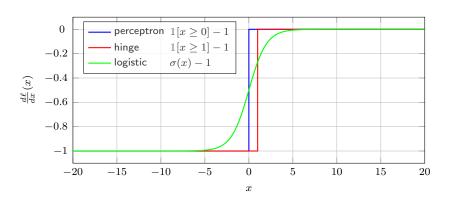
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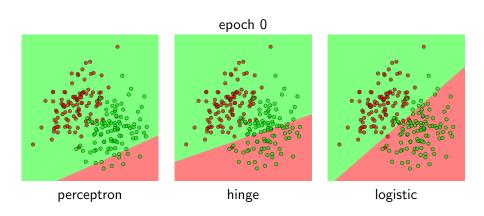
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- in all cases, a sample that is correctly classified with an activation well below some margin has a fixed negative contribution: the loss derivative is -1
- the same holds for logistic regression, which is unexpected if one looks at the saturating 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

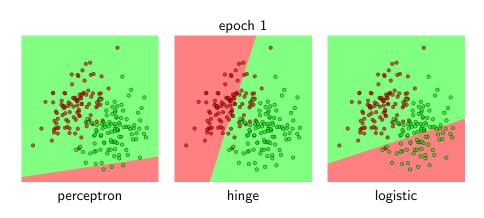
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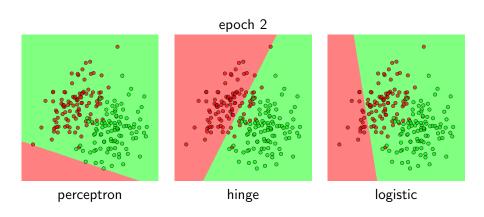
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- the same holds for logistic regression, which is unexpected if one looks at the saturating form of the sigmoid $(\frac{d\sigma}{dx}(x)$ tends to zero for $|x|\to\infty)$
- this is because the \log of cross-entropy cancels the effect of the \exp of the sigmoid and is a good reason the treat these two as one function operating directly on the activation

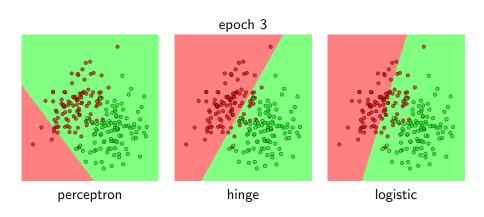
question

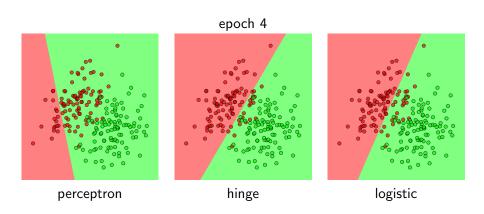
• perceptron and hinge loss differ only by a shift; once the bias is learned, aren't they equivalent?

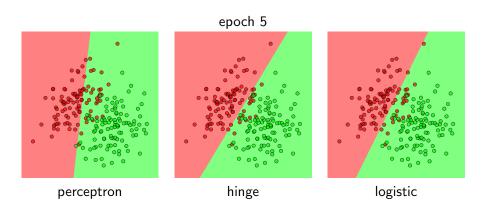


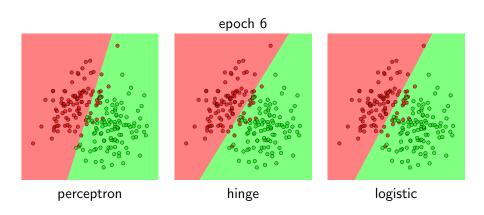


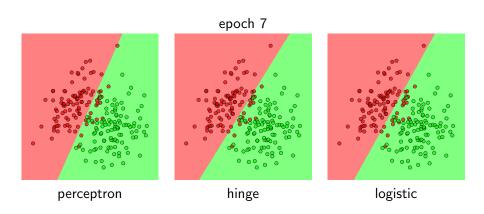


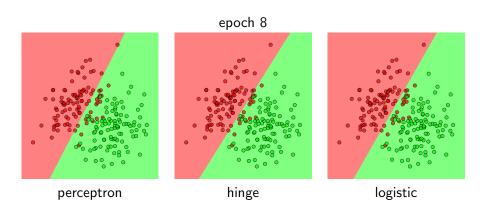


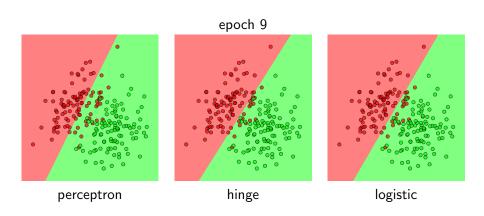












multi-class classification

multi-class logistic regression

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

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

or, in matrix form

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

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

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

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

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

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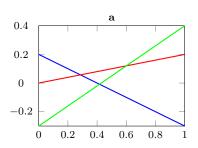
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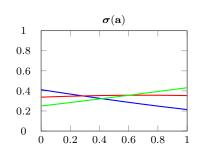
$$\mathbf{y} = (y_1, \dots, y_k) = f(\mathbf{x}; W, \mathbf{b}) := \boldsymbol{\sigma}(W^{\top}\mathbf{x} + \mathbf{b})$$



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

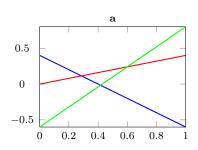
$$\sigma(\mathbf{a}) := \operatorname{softmax}(\mathbf{a}) := \frac{1}{\sum_{j} e^{a_j}} (e^{a_1}, \dots, e^{a_k})$$

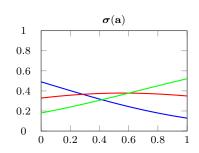




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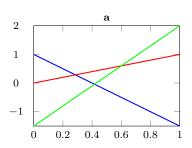
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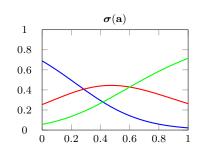




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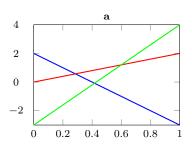
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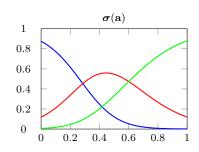




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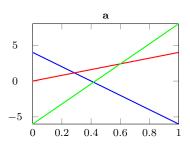
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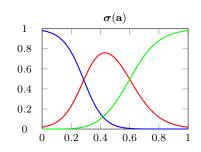




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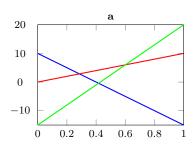
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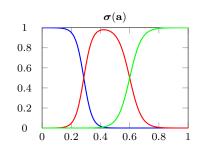




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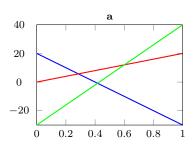
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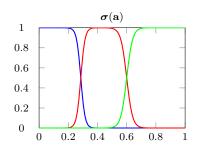




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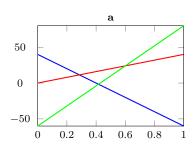
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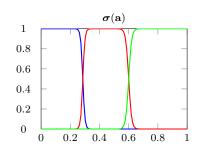




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cross-entropy error

- we are given training samples $X=(\mathbf{x}_1,\ldots,\mathbf{x}_n)\in\mathbb{R}^{d\times n}$ and target variables $T=(\mathbf{t}_1,\ldots,\mathbf{t}_n)\in\{0,1\}^{k\times n}$
- 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

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

• suppose the correct label (nonzero element of t) is l; also this term can be approximated by the maximum element of 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



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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):

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



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multiclass SVM

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

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

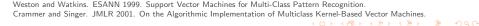
similar to the previous approximation of cross-entropy, plus margin

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

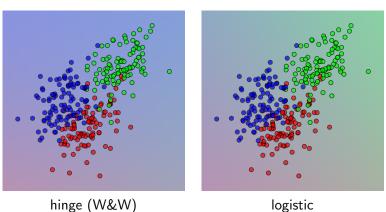


multiclass SVM

- 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
- \bullet hard assignment: now we threshold activations with ${\rm sgn}$ instead, as we do in testing
- · we repeat at different epochs during training

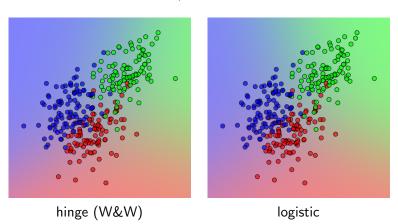
prediction: soft assignment

epoch 00



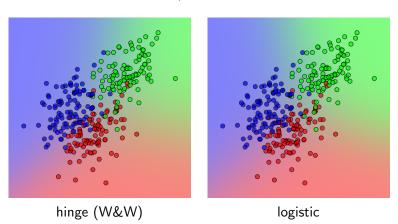
prediction: soft assignment

epoch 05

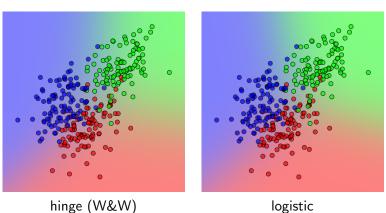


prediction: soft assignment

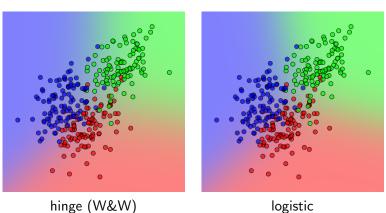
epoch 10



epoch 15

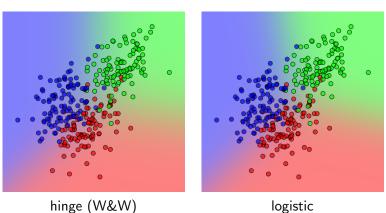


epoch 20

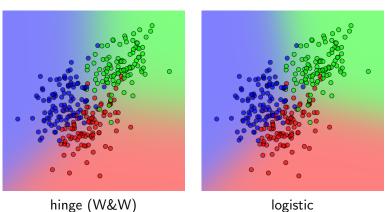


hinge (W&W)

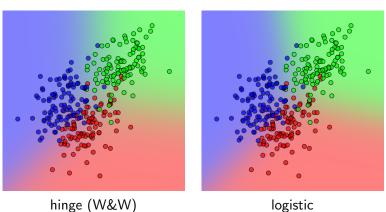
epoch 25



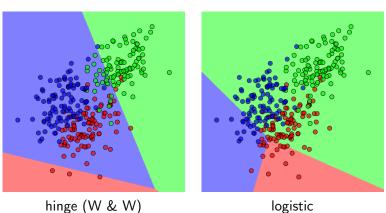
epoch 30



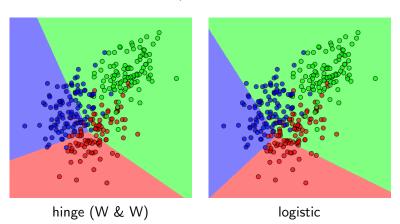
epoch 35



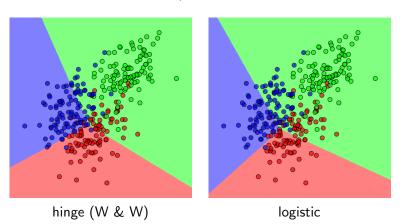
epoch 00



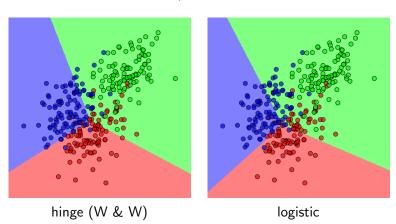
epoch 04



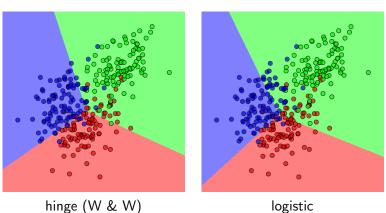
epoch 08



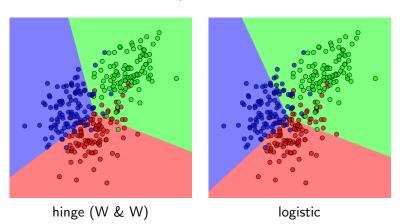
epoch 12



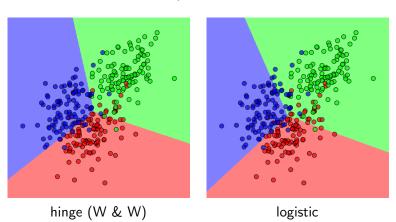
epoch 16



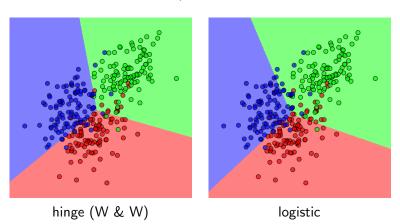
epoch 20



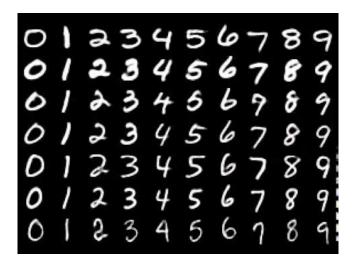
epoch 24



epoch 28



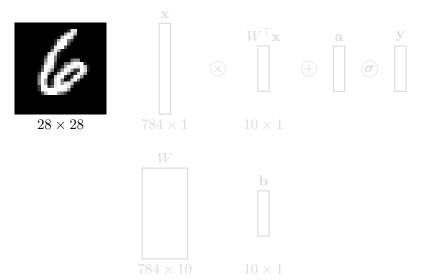
MNIST digits dataset

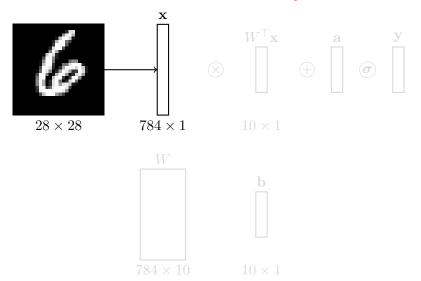


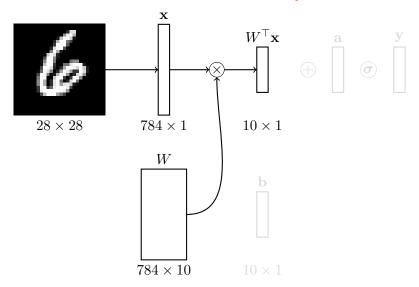
ullet 10 classes, 60k training images, 10k test images, 28 imes 28 images

from images to vectors

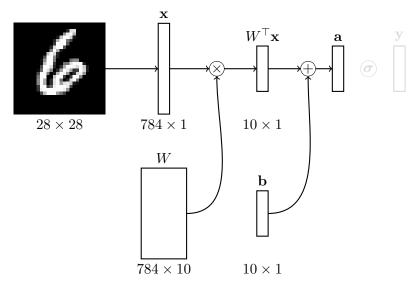
- all classifiers considered so far work with vectors
- we have seen how to extract a descriptor—a vector—from an image
- however, the point now is how to learn to extract a descriptor
- so we start from raw pixels: a gray-scale input image is just a 28×28 matrix, and we vectorize it into 784×1



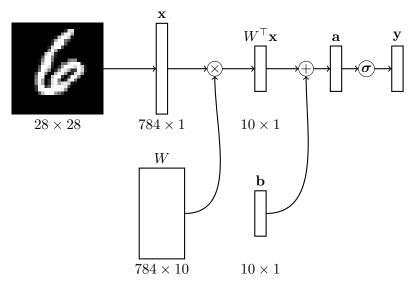




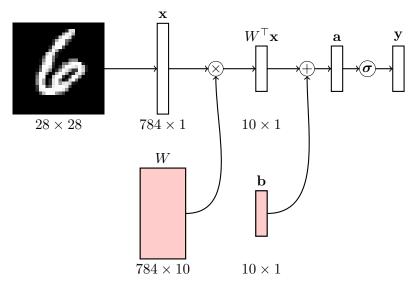








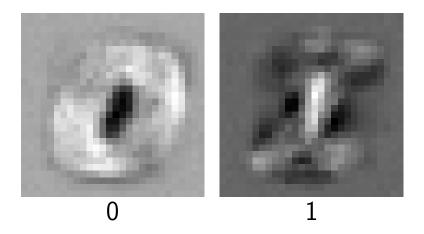




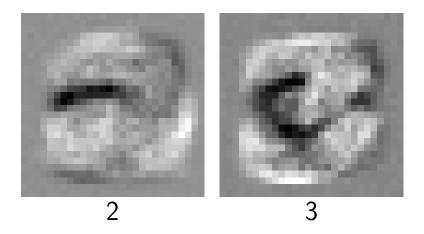


what is being learned?

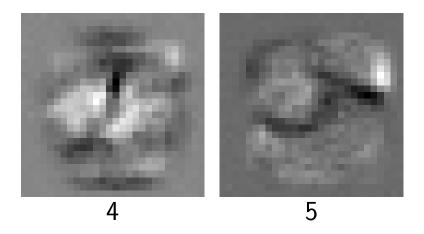
- ullet the columns of W are multiplied with ${f x}$; they live in the same space
- we can reshape each one back from 784×1 to $28\times 28:$ it should look like a digit



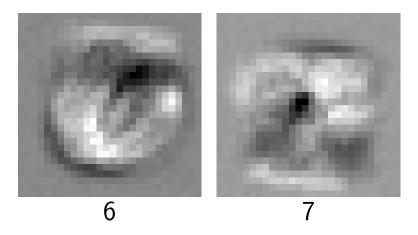
- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- test error 7.67%



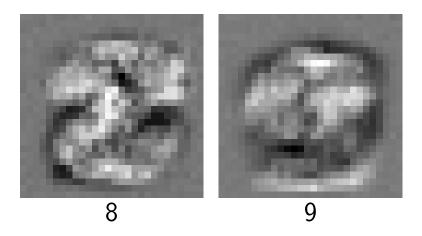
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regression

0.6 0.4 0.6 0.8 0.8

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

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

x

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

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

0.6 0.4 0.2 0.0 0.2 0.2 0.4 0.6 0.8

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

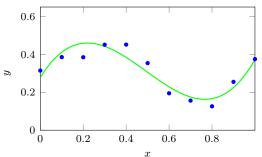
$$y = ax + b = (a, b)^{\top}(x, 1) = \mathbf{w}^{\top}\phi(x)$$

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



ullet 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 $\Phi = (\phi(x_1); \ldots; \phi(x_n)) \in \mathbb{R}^{n \times 4}$

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

0.6 0.4 0.2 0.2 0.2 0.3 0.4 0.5 0.2 0.6 0.8

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

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

x

• 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 0.6 0.4 0.2 0.0 0.2 0.4 0.6 0.8

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

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

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

regularization 0.6 0.4 0.2 0.0 0.2 0.4 0.6 0.8

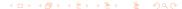
ullet linear model with parameters $\mathbf{w} \in \mathbb{R}^{11}$

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

x

ullet 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 0.6 0.4 0.2 0.0 0.2 0.4 0.6 0.8

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

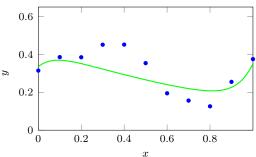
$$y = \mathbf{w}^{\mathsf{T}} \phi(x) = \mathbf{w}^{\mathsf{T}} (1, x, x^2, \dots, x^{10})$$

x

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

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

severe regularization



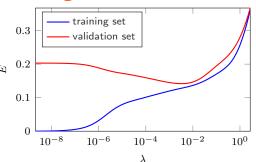
ullet linear model with parameters $\mathbf{w} \in \mathbb{R}^{11}$

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

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

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

generalization error



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

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

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

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

•	optimize both parameters and hyperparameters on the training 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 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

train

val

test

•	optimize both parameters and hyperp	aramet	ers on	the trai	nin	g se	t:
	could work perfectly on training set, r	no idea	how it	works	on	test	set
	train						

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 test

•	 optimize both parameters and hyperparameters on the training se 					t:
	could work perfectly on training set, n	no idea	how it	works or	n test	set
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train test

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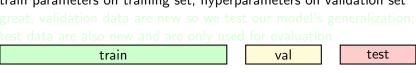
train test

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train parameters on training set, hyperparameters on validation set



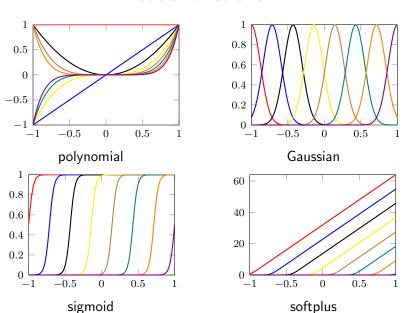
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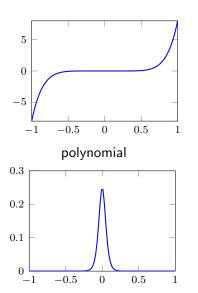
• split data into k groups; treat k-1 as training and 1 as validation, measure on test set; repeat over all splits and average the results

measure on test set; repeat over all splits and average the results							
val		run 1	test				
val		run 2	test				
	val		test				
		_					
	val		test				

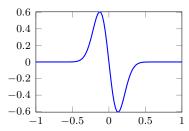
basis functions

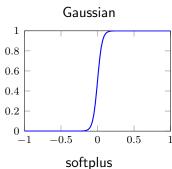


basis function derivatives



sigmoid





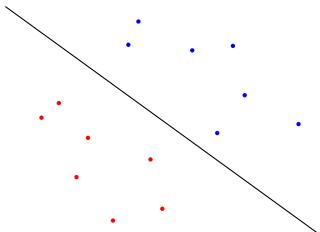


basis functions

- 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 softplus is nonzero over half of the space

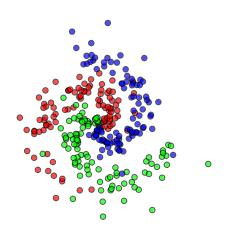
multiple layers

linear separability

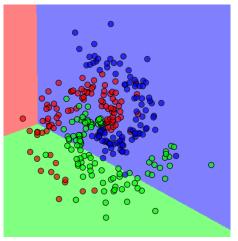


- two point sets $X_1, X_2 \subset \mathbb{R}^d$ are linearly separable iff there is \mathbf{w}, b such that $\mathbf{w}^\top x_1 < b < \mathbf{w}^\top x_2$ for $\mathbf{x}_1 \in X_1, \mathbf{x}_2 \in X_2$
- or, they can be separated by a perceptron

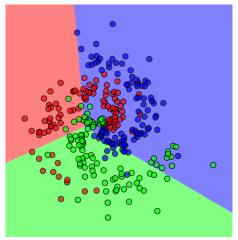
non-linearly separable classes



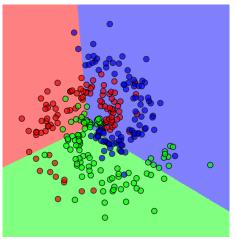
epoch 00



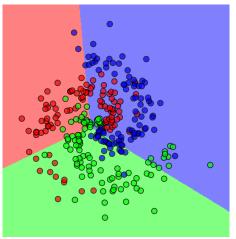
epoch 05



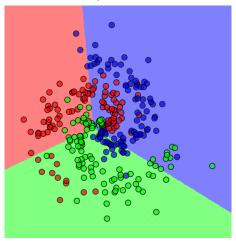
epoch 10



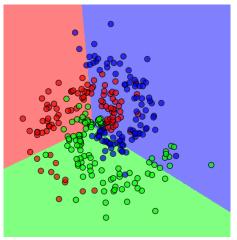
epoch 15



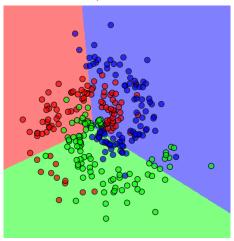
epoch 20



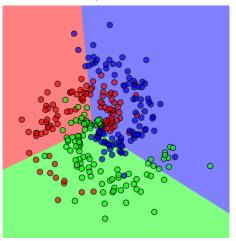
epoch 25



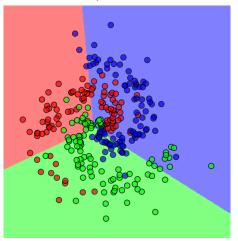
epoch 30



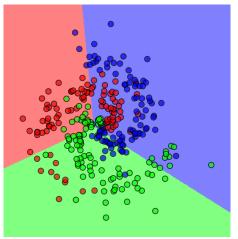
epoch 35

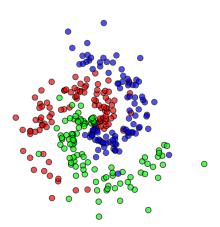


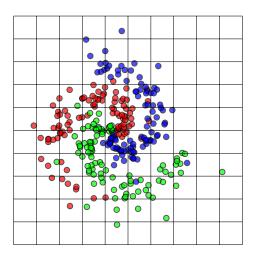
epoch 40



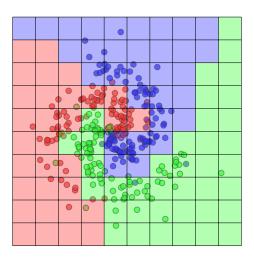
epoch 45



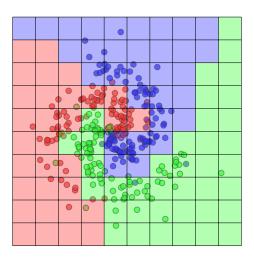




• define a 10×10 grid over the entire space

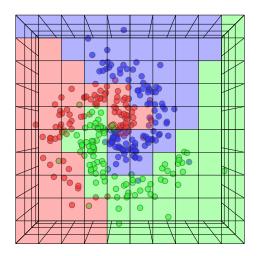


• and a (Gaussian?) basis function centered at every cell



ullet 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?

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- 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 o "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 → class probabilities

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

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



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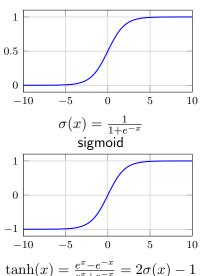
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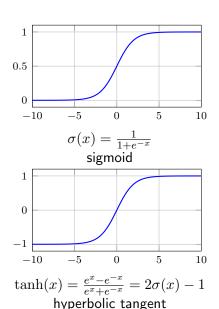
- this should be nonlinear, otherwise the whole network will be linear and we don't gain much by the hierarchy (but: linear layers can be useful sometimes)
- it shouldn't have any more parameters, at least for now: all the parameters in a layer are W, \mathbf{b}
- it is a vector-to-vector function and 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

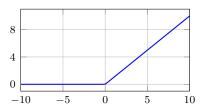
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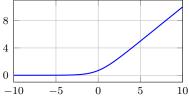
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$$anh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}} = 2\sigma(x) - 1$$
 hyperbolic tangent



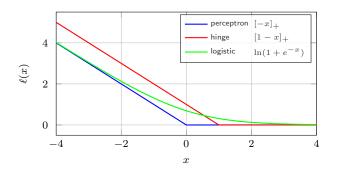




$$\zeta(x) = \log(1 + e^x)$$
 softplus

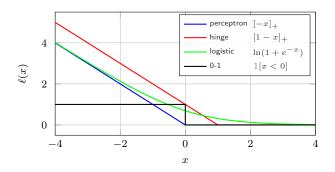
- tanh and sigmoid model exactly what a classifier makes (a decision), but they are smooth unlike sgn whose derivative is zero everywhere: indeed, they have been standard choices for decades.
- relu and its "soft" version softplus are like which functions we have seen?

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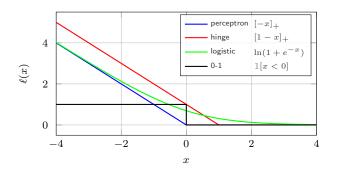
- $\mathrm{relu}(x) = [x]_+$ and $\zeta(x) = \log(1+e^x)$ are the flipped versions of the perceptron and logistic loss functions, respectively
- also shown is the 0-1 misclassification loss, which is what we actually evaluate during testing; and why don't we optimize that instead?
- because it's difficult: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





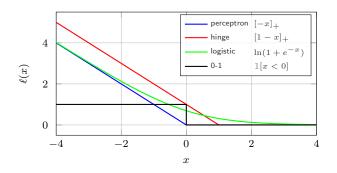
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surrogate loss functions

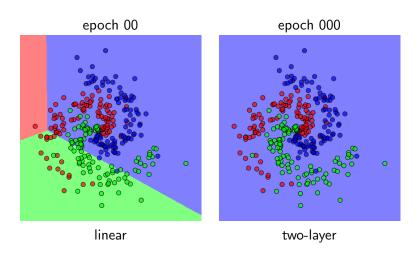
- all three loss functions we have seen are surrogate (proxy) for the 0-1 loss: their derivative is constant for $x \to -\infty$
- they also often work better because even if the 0-1 loss is low (or zero) on the training set, they improve on the test set
- even so, we could have used a sigmoid instead, 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?

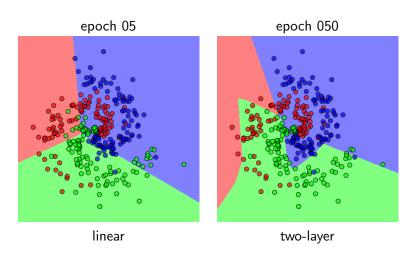
surrogate loss functions

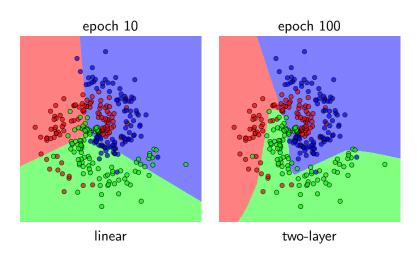
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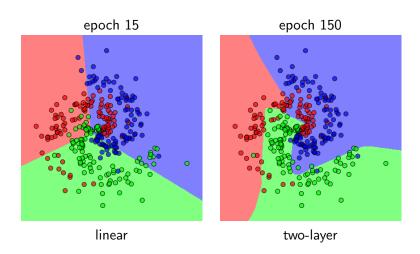
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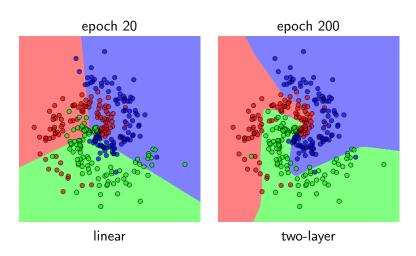
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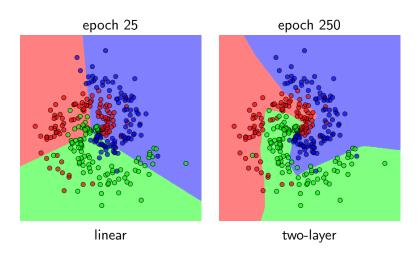


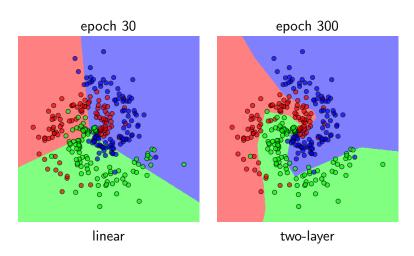


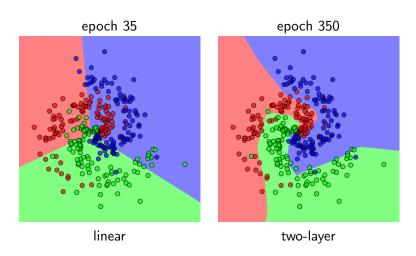


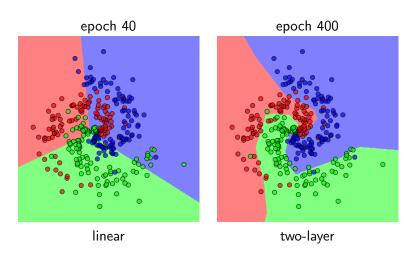


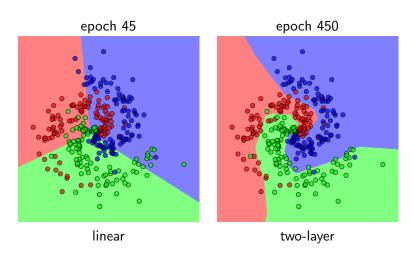




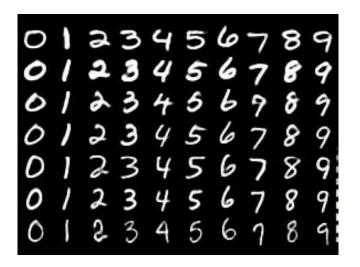




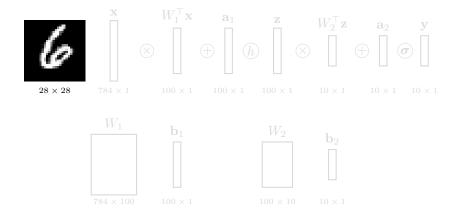




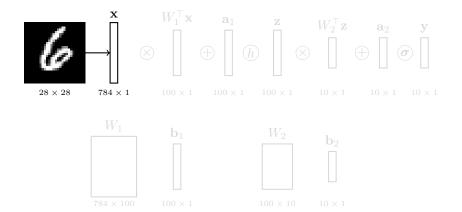
MNIST digits dataset



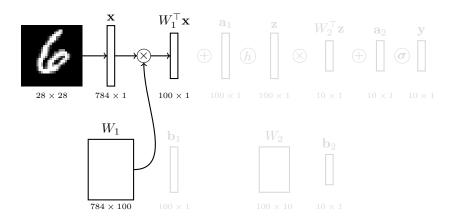
 \bullet 10 classes, 60k training images, 10k test images, 28 \times 28 images



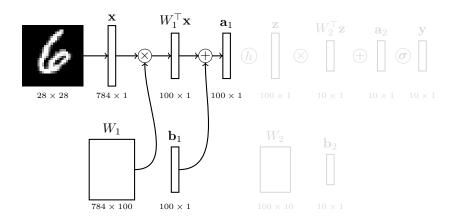
- input layer 1 weights and bias activation layer 2 weights and bias softmax
- \bullet parameter learning using cross-entropy on y (or rather, directly on $a_2)$



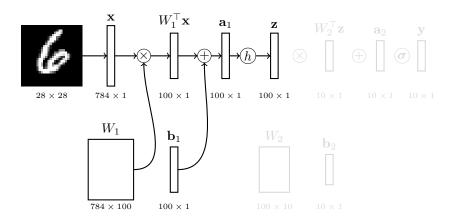
- input layer 1 weights and bias activation layer 2 weights and bias
 softmax
- ullet parameter learning using cross-entropy on y (or rather, directly on a_2)



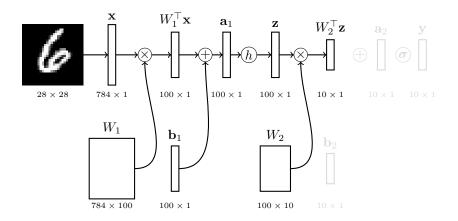
- input layer 1 weights and bias activation layer 2 weights and bias
 softmax
- ullet parameter learning using cross-entropy on ${f y}$ (or rather, directly on ${f a}_2)$



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

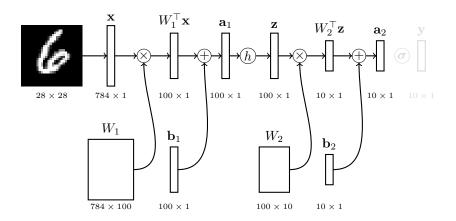


- input layer 1 weights and bias activation layer 2 weights and bias
 softmax
- ullet parameter learning using cross-entropy on ${f y}$ (or rather, directly on ${f a}_2)$



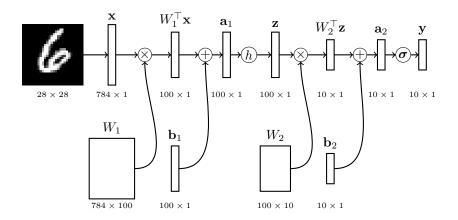
- input layer 1 weights and bias activation layer 2 weights and bias
 softmax
- ullet parameter learning using cross-entropy on ${f y}$ (or rather, directly on ${f a}_2)$

two-layer classifier on raw pixels



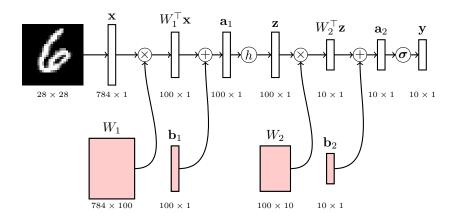
- input layer 1 weights and bias activation layer 2 weights and bias
 softmax
- ullet parameter learning using cross-entropy on ${f y}$ (or rather, directly on ${f a}_2)$

two-layer classifier on raw pixels



- input layer 1 weights and bias activation layer 2 weights and bias
 softmax
- ullet parameter learning using cross-entropy on ${f y}$ (or rather, directly on ${f a}_2$)

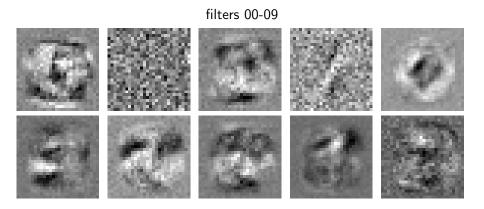
two-layer classifier on raw pixels



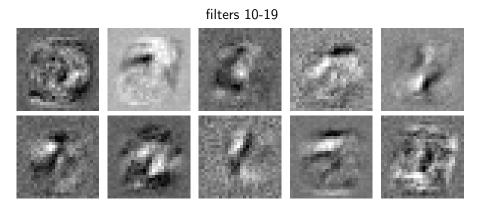
- input layer 1 weights and bias activation layer 2 weights and bias
 softmax
- ullet parameter learning using cross-entropy on ${f y}$ (or rather, directly on ${f a}_2)$

what is being learned?

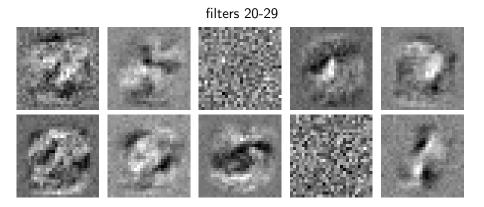
- the columns of W_1 are multiplied with \mathbf{x} ; they live in the same space, as in the linear classifier
- we can reshape each one back from 784×1 to 28×28 : but now it shouldn't look like a digit; rather, like a pattern that might help in recognizing digits
- these patterns are shared: once the 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



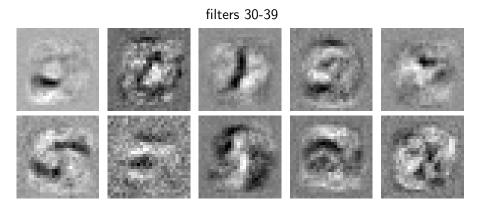
- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- hidden layer width: 100; test error 2.54%



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- hidden layer width: 100; test error 2.54%



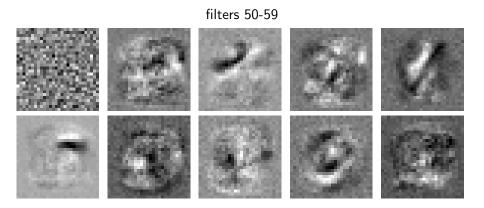
- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- hidden layer width: 100; test error 2.54%



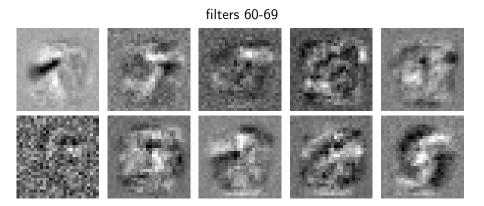
- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- hidden layer width: 100; test error 2.54%

filters 40-49

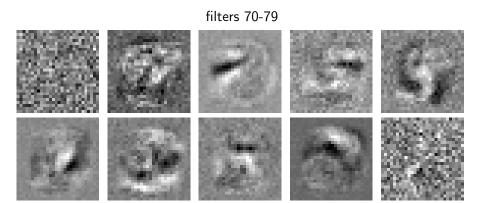
- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- hidden layer width: 100; test error 2.54%



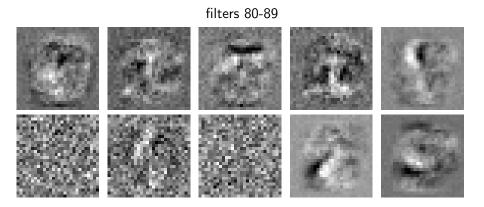
- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
- hidden layer width: 100; test error 2.54%



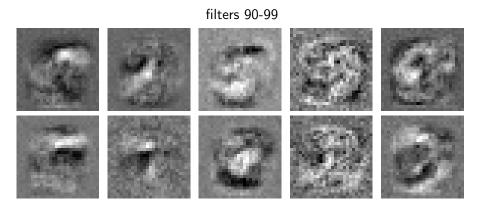
- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
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- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda = 10^{-4}$
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- $k = 3, n = 60000, m = 6000, \epsilon = 10^{-1}, \lambda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