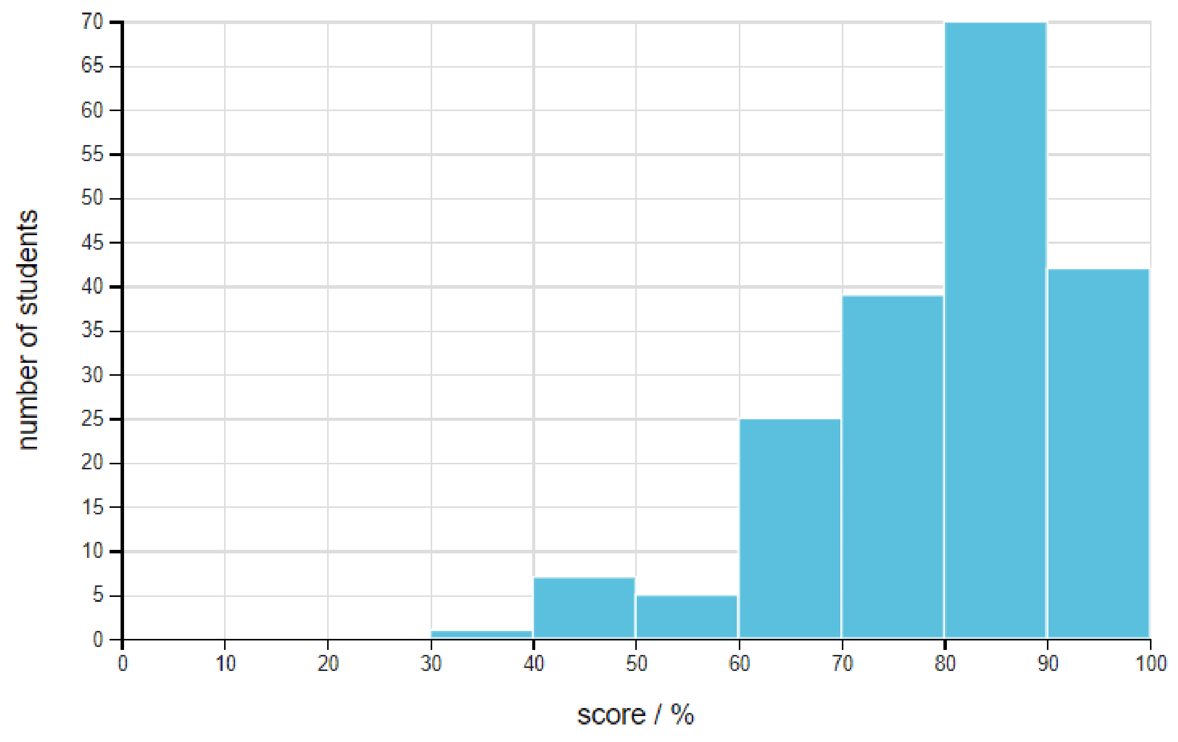
Optimization and Stochastic Gradient Descent

Applied Machine Learning
Derek Hoiem

Dall-E

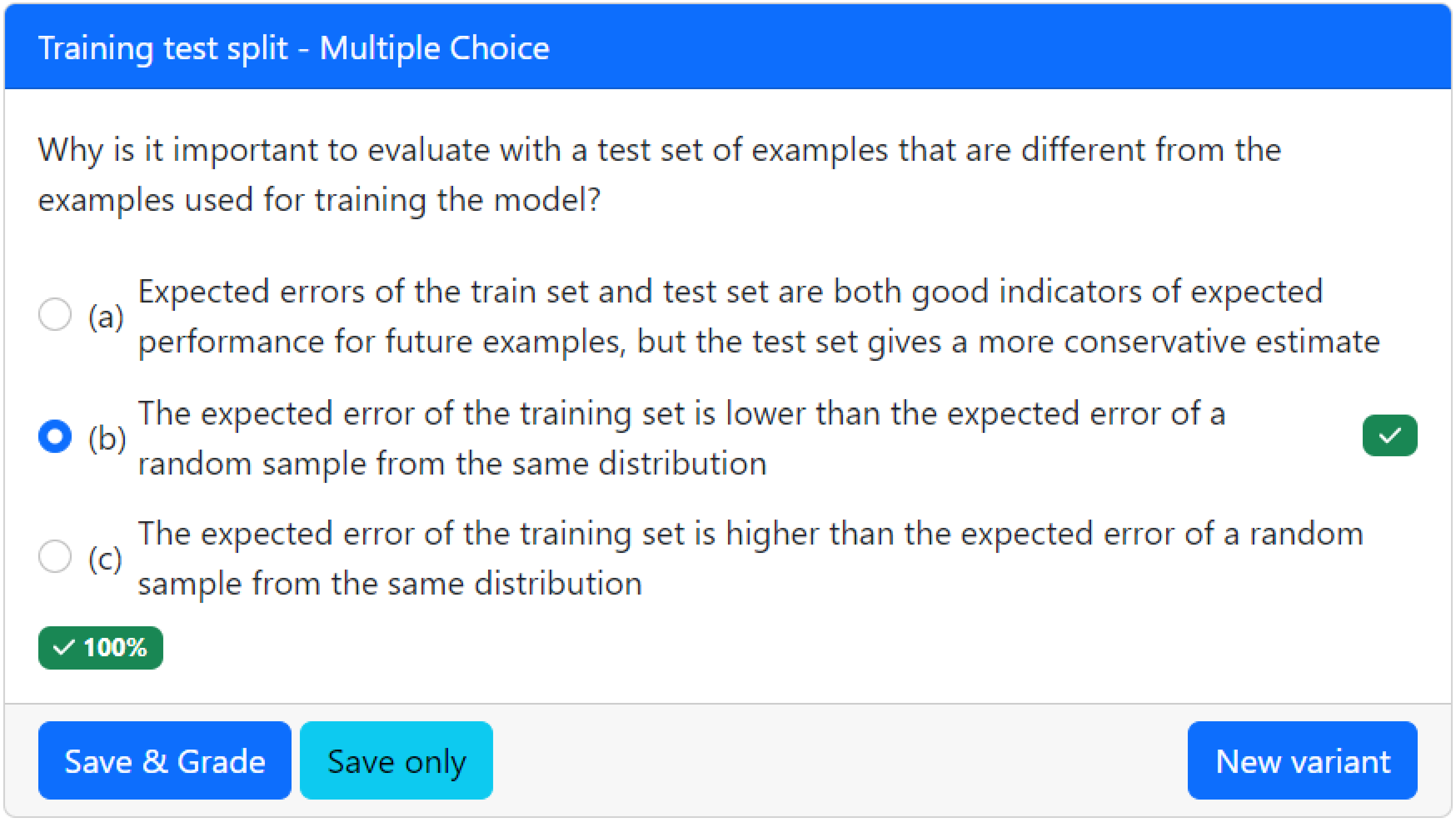
Exam 1

Exam 1: Score statistics



Number of students	189
Mean score	80%
Standard deviation	13%
Median score	83%
Minimum score	38%
Maximum score	100%
Number of 0%	0 (0% of class)
Number of 100%	2 (1% of class)

Questions with < 65% mean score



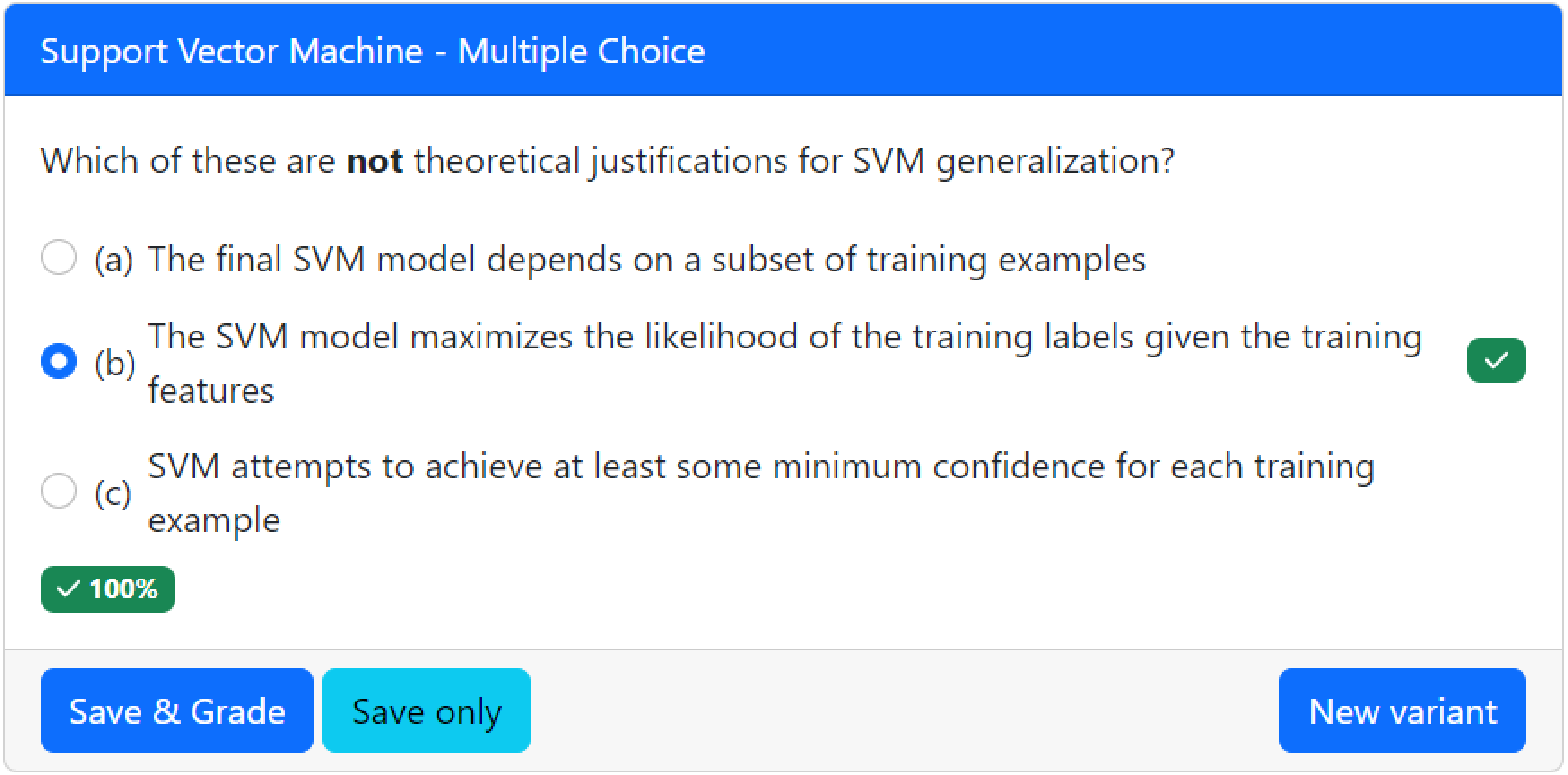
Training test split - Multiple Choice

Why is it important to evaluate with a test set of examples that are different from the examples used for training the model?

- ○ (a) Expected errors of the train set and test set are both good indicators of expected performance for future examples, but the test set gives a more conservative estimate
- ● (b) The expected error of the training set is lower than the expected error of a random sample from the same distribution ✓
- ○ (c) The expected error of the training set is higher than the expected error of a random sample from the same distribution

✓ 100%

Questions with < 65% mean score



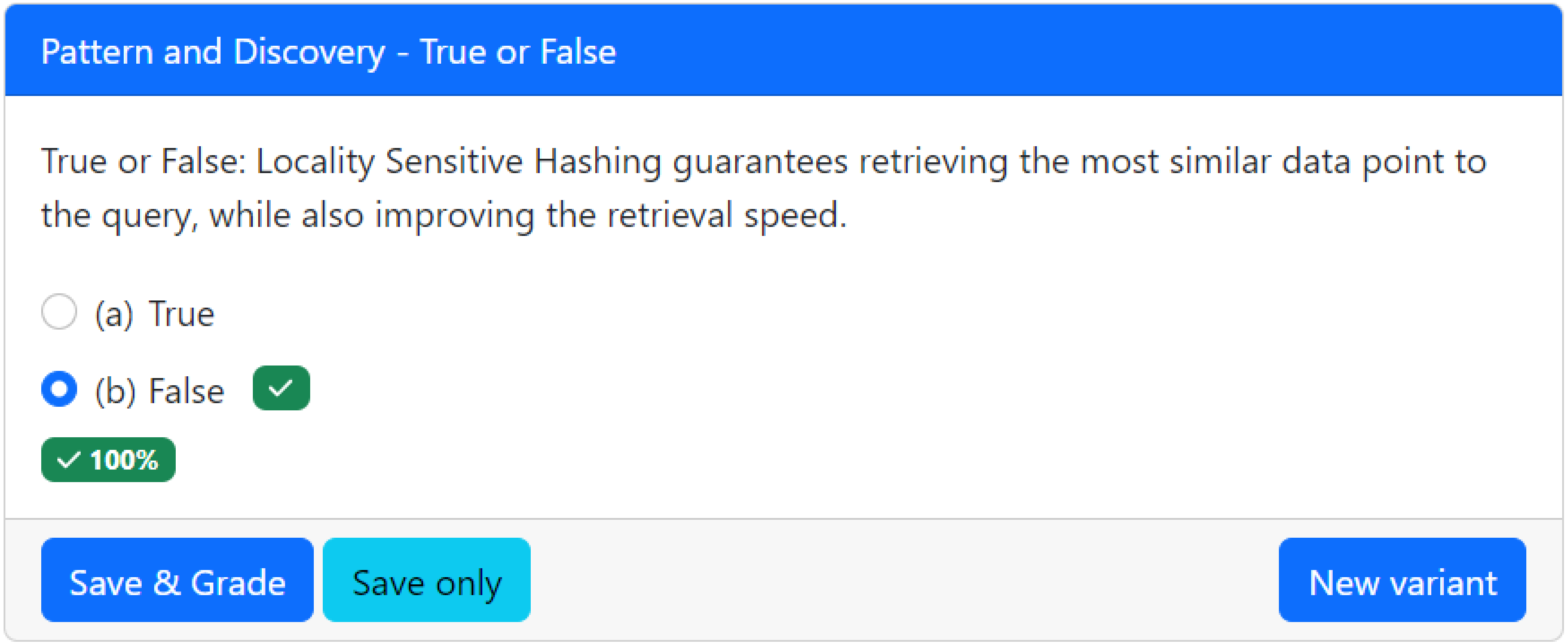
Support Vector Machine - Multiple Choice

Which of these are **not** theoretical justifications for SVM generalization?

- ( ) (a) The final SVM model depends on a subset of training examples
- [✓ (b)] The SVM model maximizes the likelihood of the training labels given the training features ✓
- ( ) (c) SVM attempts to achieve at least some minimum confidence for each training example

✓ 100%

Questions with < 65% mean score



Pattern and Discovery - True or False

True or False: Locality Sensitive Hashing guarantees retrieving the most similar data point to the query, while also improving the retrieval speed.

(a) True [✓ (b) False] ✓

✓ 100%

Reminder about grading

- Lowest exam score dropped
- 3 credit: $score = \dfrac{exam1 + exam2 + EP}{200 + \max(EP, 500)}$
- 4 credit: $score = \dfrac{exam1 + exam2 + EP}{200 + \max(EP, 625)}$

Example for 3 credit version:

- Exam scores: 70, 75, 85
- HW scores: 90, 120, 100, 130, 90
- Final project: 0
- Late days: 13 (-15 points)
- Participation points: 30
- EP = 90+120+100+130+90-15+30=545
- Grade = (75+85+545) / (200+545)=94.6%

Example for 4 credit version:

- Exam scores: 90, 75, 85
- HW scores: 120, 0, 120, 130, 110
- Final project: 100
- Late days: 10
- Participation points: 16
- EP = 120+0+120+130+110+125+16=596
- Grade = (90+85+596) / (200+625)=93.4%

Deep Learning

Deep learning is a way of learning effective representations, most effective when the inputs have important structures, such as images, audio, text

- Today: Stochastic Gradient Descent (SGD)
- Thurs: MLPs and backpropagation
- Oct 22: Convolutional networks, residual blocks, advanced SGD
- Oct 24: Training and adapting deep networks, computer vision
- Oct 29: Representing words, transformer blocks
- Oct 31: More transformers, use in vision and language
- Nov 5: Foundation models: CLIP and GPT

Machine learning optimization

	Optimization	Solution Depends on Initialization or Randomized Optimization?	Optimization Strategy is Important to Effectiveness?
KNN	N/A	No	No
K-means	Coordinate Descent	Yes	No
Linear Regression	Iterative	No	No
Logistic Regression	Iterative	No	No
Linear SVM	Iterative	No	No
Kernelized SVM	Iterative	No	No
EM Algorithm	Coordinate Descent	Yes	No
Decision Tree	Greedy selection	No	No

- For methods we learned so far, one optimizer may be faster or more memory efficient than other, but they will generally be able to achieve similar solutions.

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MLPs, Deep Networks	**Iterative**	**Yes**	**Yes**

- For methods we learned so far, one optimizer may be faster or more memory efficient than other, but they will generally be able to achieve similar solutions.
- For MLPs and deep networks, optimization is an important part of design.

This lecture

1. Batch gradient descent

2. PEGASOS: Stochastic Gradient Descent for SVM

3. Perceptrons

Gradient descent

```
gradient_descent(f'(x), x0, lr, niter)
  x = x0
  for t in range(niter):
    x = x - lr*f'(x)
  return x
```

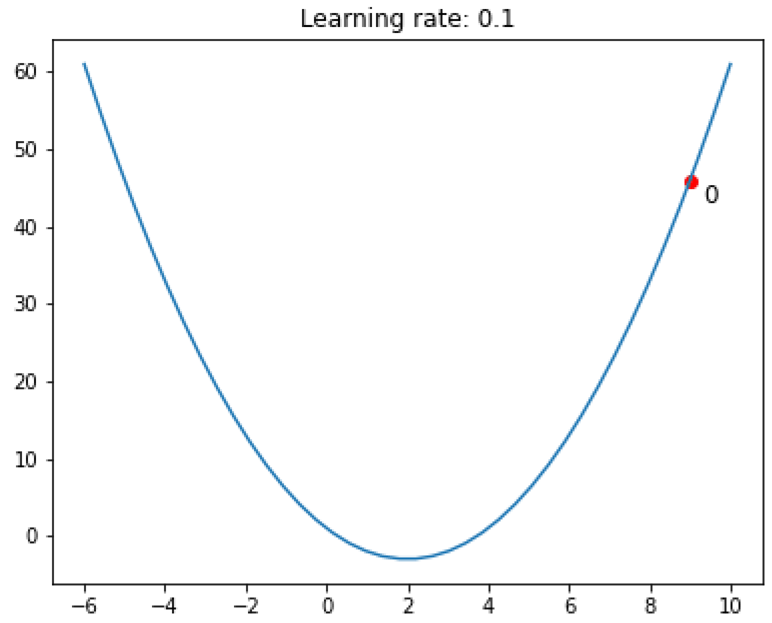
Gradient descent

```
gradient_descent(f′(x), x0, lr, niter)
  x = x0
  for t in range(niter):
    x = x - lr*f′(x)
  return x
```

Example:

$$f(x) = x^2 - 4x + 1$$

$$f'(x) = 2x - 4$$



Example: https://towardsdatascience.com/gradient-descent-algorithm-a-deep-dive-cf04e8115f21

Gradient descent

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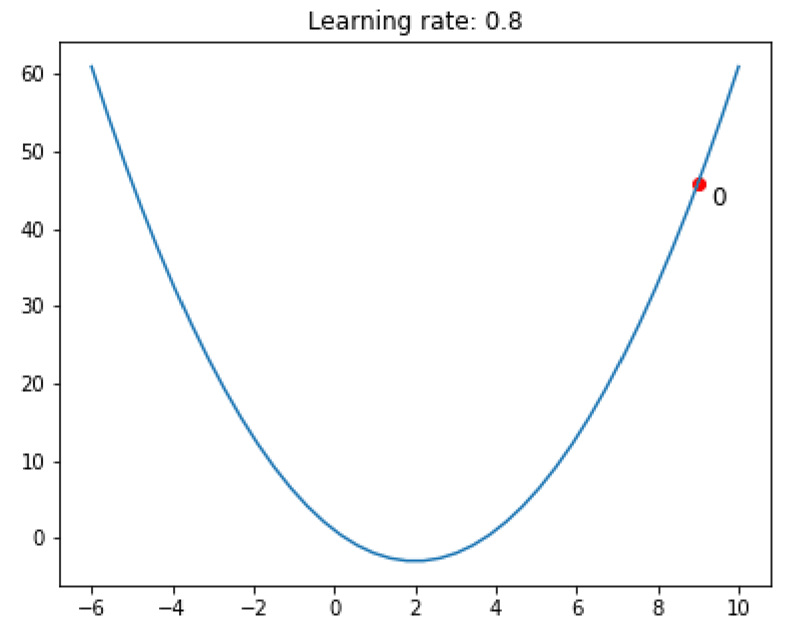
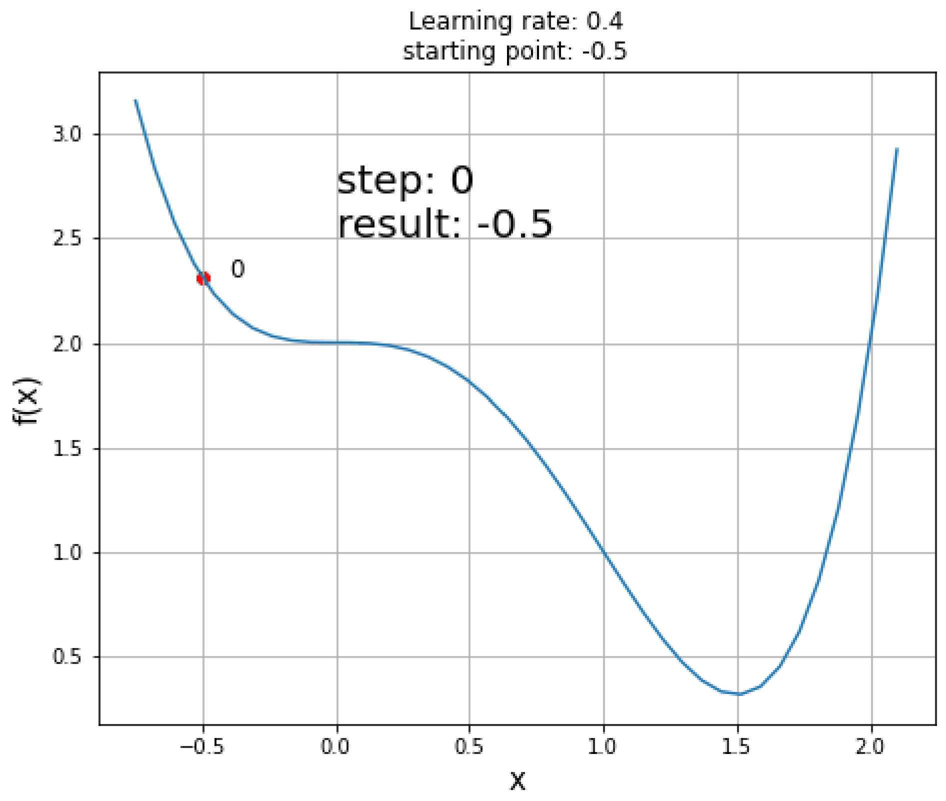
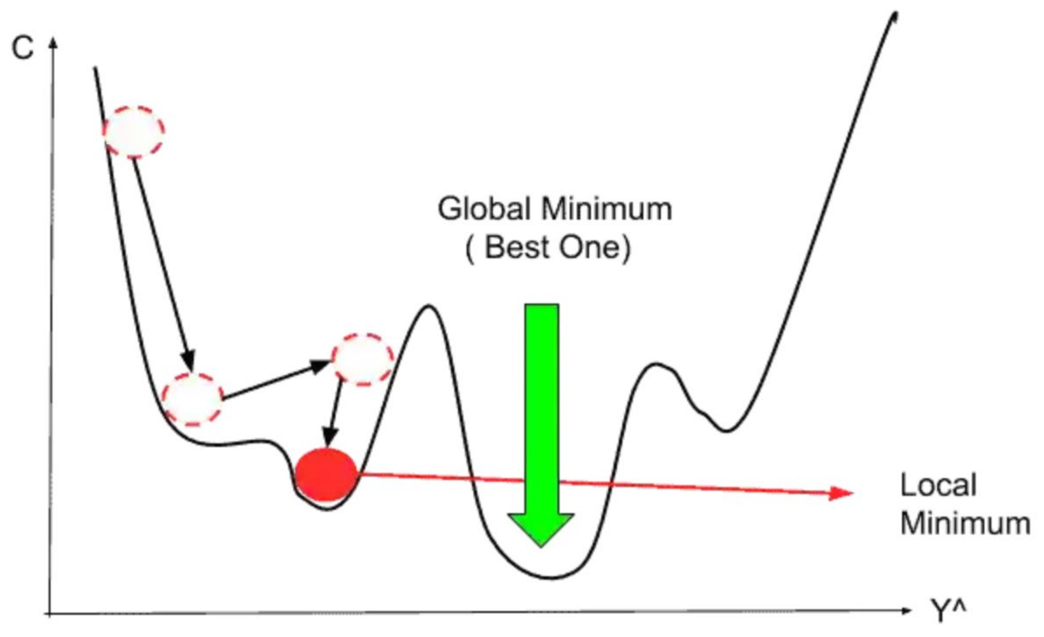


Example: https://towardsdatascience.com/gradient-descent-algorithm-a-deep-dive-cf04e8115f21

Gradient descent challenge cases



Saddle points (gradient = 0 in some parts of solution space)



Multiple local minima

Many models we've learned so far (e.g., SVM, logistic regression, linear regression) are convex, so they don't have these challenges.

Example: https://towardsdatascience.com/gradient-descent-algorithm-a-deep-dive-cf04e8115f21 Fig: https://www.mltut.com/stochastic-gradient-descent-a-super-easy-complete-guide/

Gradient Descent Visualization with Local Minima

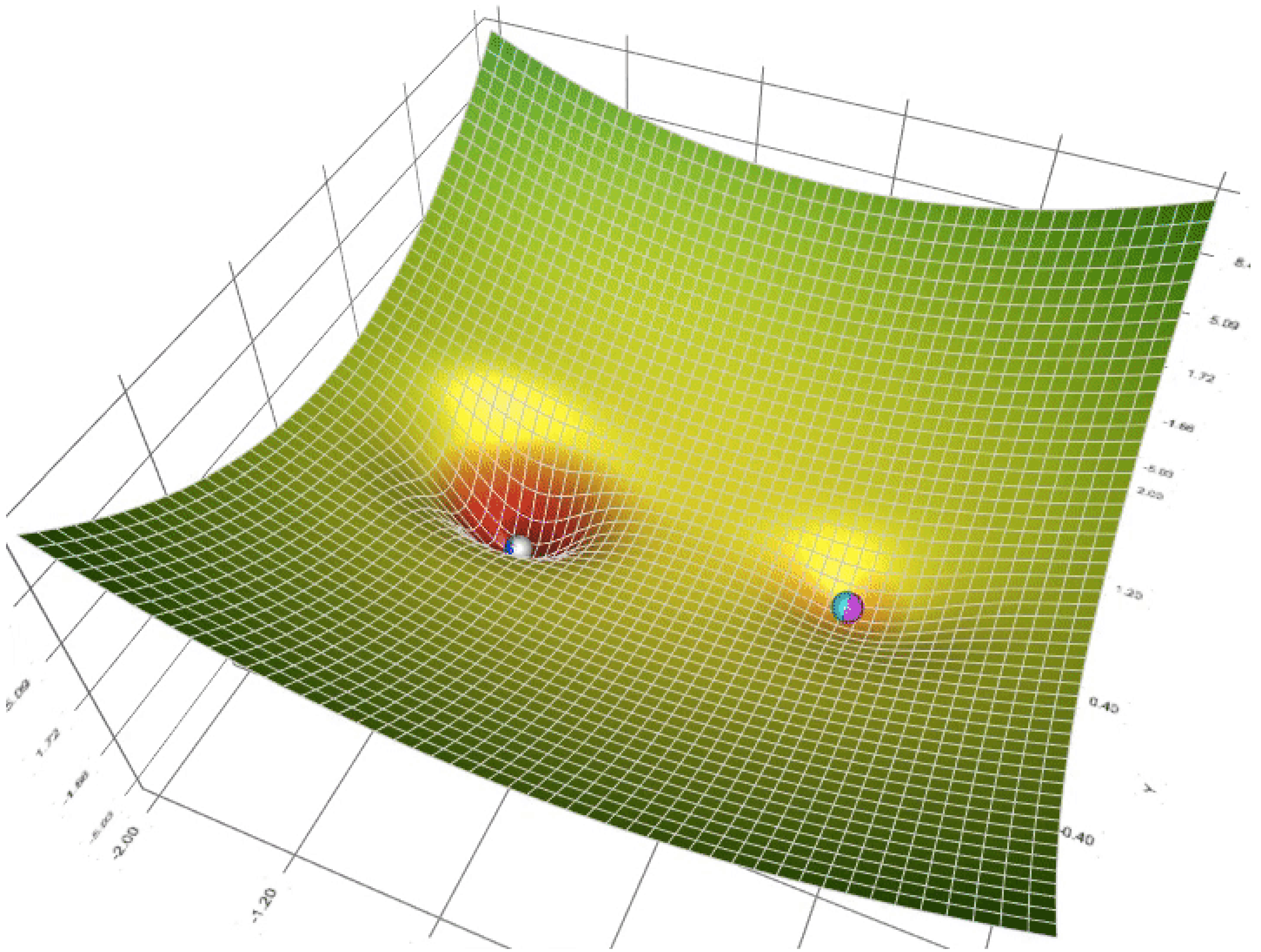


Figure source

Learning rates and learning schedules

- Learning rate = step size that is multiplied by gradient direction/magnitude
  - Large rate allows big movements toward optimum but might over-step
  - Small rate is less likely to over-step but could take longer

- Learning schedule: change learning rate over time
  - Constant
  - Exponential decay, e.g. lr = lr * 0.95
  - Linear, e.g. lr = lr0 *(1 – iter / max_iter)

SVM Formulation

Prediction

$$y_n = \text{sign}\left(\boldsymbol{w}^T x_n + b\right)$$

Optimization

Known as "hinge loss"
Penalty is paid if margin is less than 1

$$w^* = \underset{\boldsymbol{w}}{\text{argmin}} \left[\frac{1}{2}\lambda \|w\|^2 + \frac{1}{N}\sum_{n}^{N} \max(0, 1 - y_n\left(\boldsymbol{w}^T x_n + b\right)) \right]$$

Here, $y \in \{-1,1\}$ which is a common convention that simplifies notation for binary classifiers

Gradient descent with SVM

```
gradient_descent(f′(w,i,x,y), lr, niter)
  w = zeros(x.shape[1],)
  for t in range(niter):
    for i in range(len(w)):
      w[i] = w[i] – lr*f′(w,i,x,y)
  return x
```

$$f(\boldsymbol{w},\boldsymbol{x},\boldsymbol{y}) = \frac{1}{2}\lambda\|\boldsymbol{w}\|^2 + \frac{1}{N}\sum_{n}^{N}\max(0, 1 - y_n(\boldsymbol{w}^T\boldsymbol{x}_n))$$

$$f'(\boldsymbol{w},i,\boldsymbol{x},\boldsymbol{y}) = \lambda w_i + \frac{1}{N}\sum_{n} -\delta(y_n(\boldsymbol{w}^T\boldsymbol{x}_n) < 1)y_n x_{ni}$$

Only examples with score of correct answer less than 1 contribute to the gradient

Slow with large datasets, because need to compute scores for all examples in each step

Pegasos: Primal Estimated sub-GrAdient SOlver for SVM (2011)

$$\min_{\mathbf{w}} \frac{\lambda}{2}\|\mathbf{w}\|^2 + \frac{1}{m}\sum_{(\mathbf{x},y)\in S} \ell(\mathbf{w};(\mathbf{x},y))$$

$$\ell(\mathbf{w};(\mathbf{x},y)) = \max\{0, 1 - y\langle \mathbf{w},\mathbf{x}\rangle\}$$

SVM problem that we want to solve (Minimize weights square + sum of hinge losses on all samples)

$$f(\mathbf{w};i_t) = \frac{\lambda}{2}\|\mathbf{w}\|^2 + \ell(\mathbf{w};(\mathbf{x}_{i_t},y_{i_t}))$$

Problem in terms of **one** sample

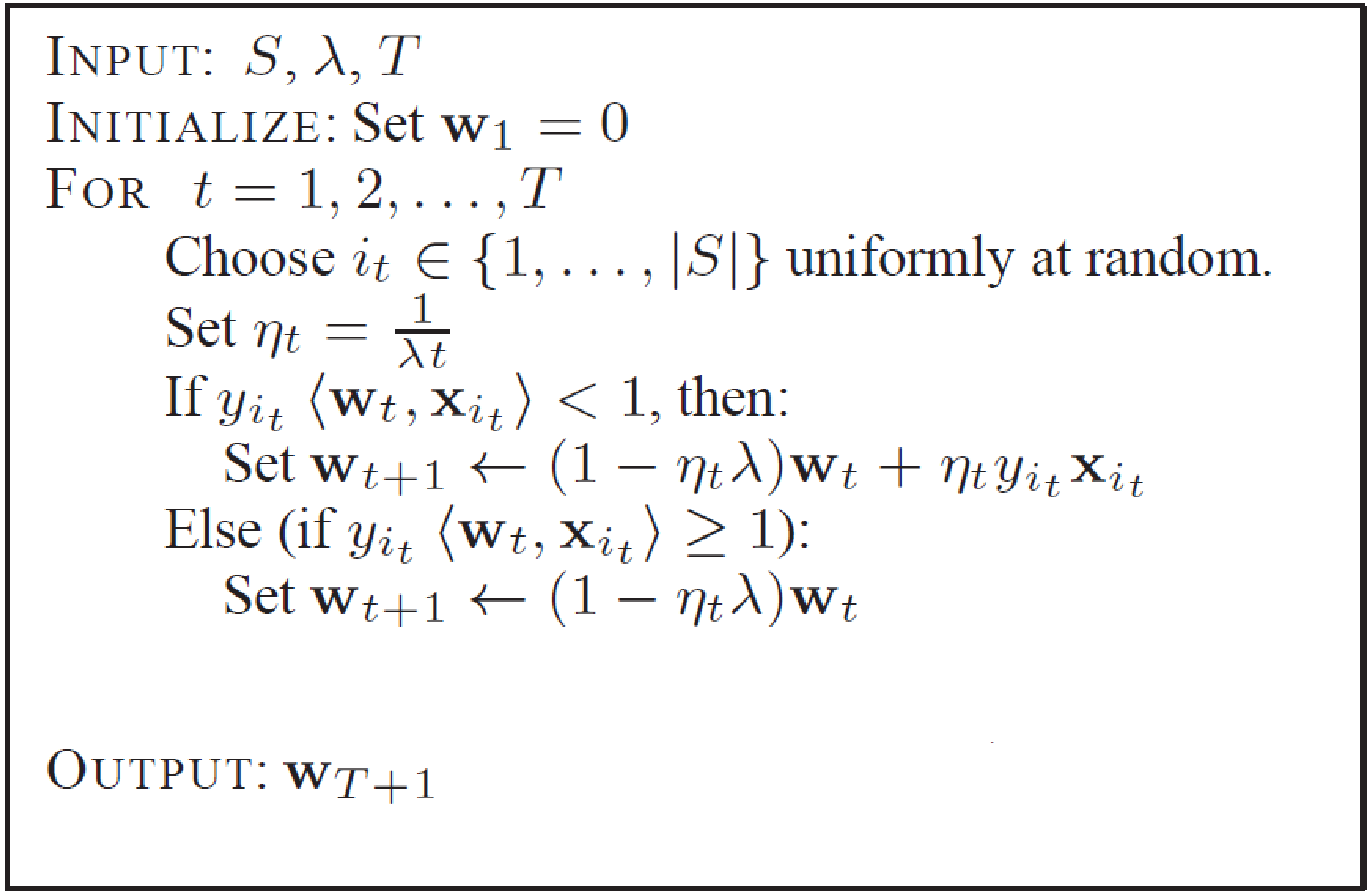
$$\nabla_t = \lambda\,\mathbf{w}_t - \mathbb{1}[y_{i_t}\langle \mathbf{w}_t,\mathbf{x}_{i_t}\rangle < 1]\,y_{i_t}\mathbf{x}_{i_t}$$

Gradient in terms of one sample

- Direction to move to improve solution

https://home.ttic.edu/~nati/Publications/PegasosMPB.pdf

Pegasos algorithm: Stochastic Gradient Descent (SGD)



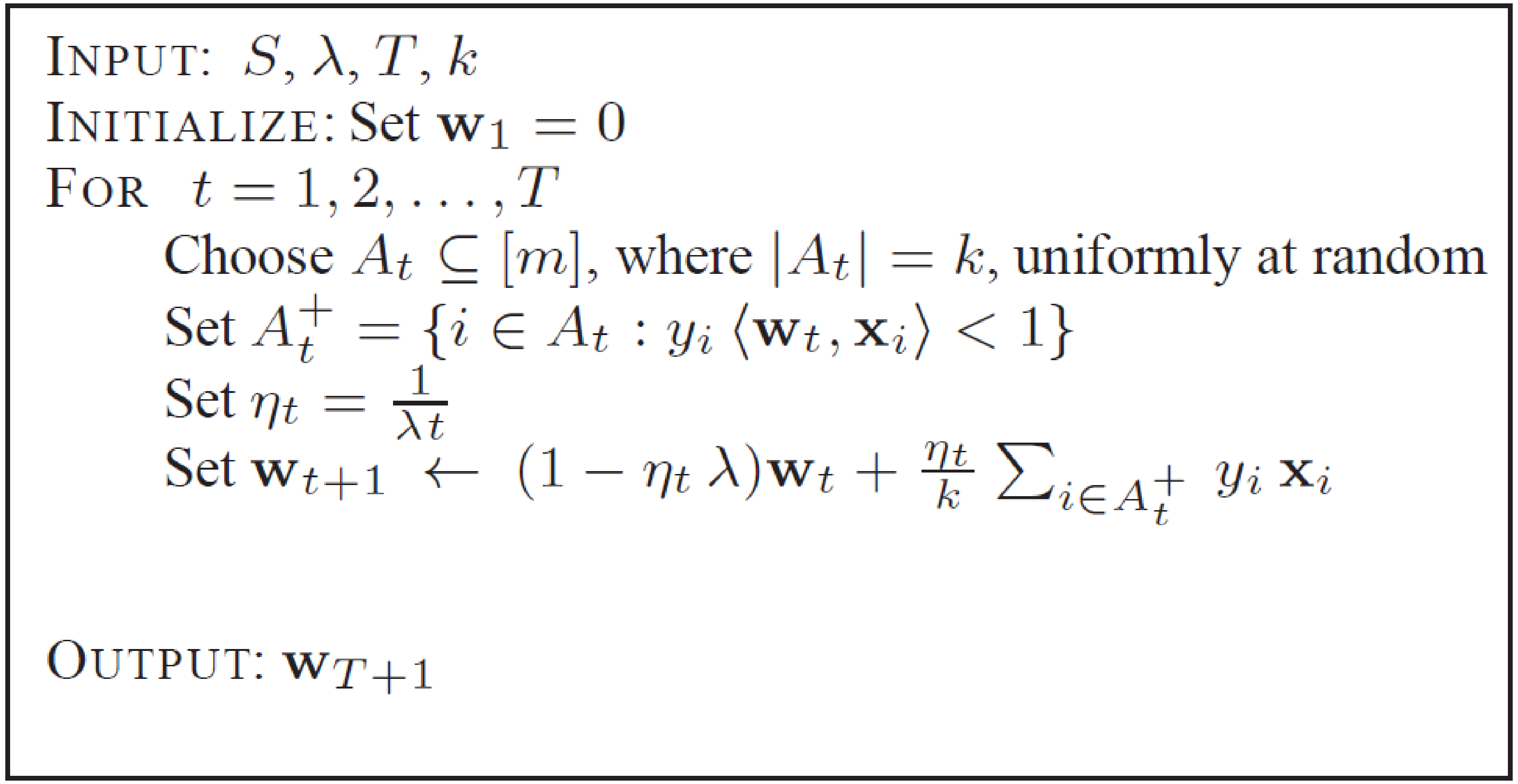
```
INPUT: $S, \lambda, T$
INITIALIZE: Set $\mathbf{w}_1 = 0$
FOR $t = 1, 2, \ldots, T$
    Choose $i_t \in \{1, \ldots, |S|\}$ uniformly at random.
    Set $\eta_t = \frac{1}{\lambda t}$
    If $y_{i_t} \langle \mathbf{w}_t, \mathbf{x}_{i_t} \rangle < 1$, then:
        Set $\mathbf{w}_{t+1} \leftarrow (1 - \eta_t \lambda)\mathbf{w}_t + \eta_t y_{i_t} \mathbf{x}_{i_t}$
    Else (if $y_{i_t} \langle \mathbf{w}_t, \mathbf{x}_{i_t} \rangle \geq 1$):
        Set $\mathbf{w}_{t+1} \leftarrow (1 - \eta_t \lambda)\mathbf{w}_t$

OUTPUT: $\mathbf{w}_{T+1}$
```

Notation

S:	training set
λ:	regularization weight
T:	number iterations
$\boldsymbol{w}_t$:	model weights
$\boldsymbol{x}_{i_t}$:	features for example i_t
y_{i_t}:	label for example i_t
η_t:	step size (“learning rate”)

Pegasos with **mini-batch**

- Calculating gradient based on multiple examples reduces variance of gradient estimate



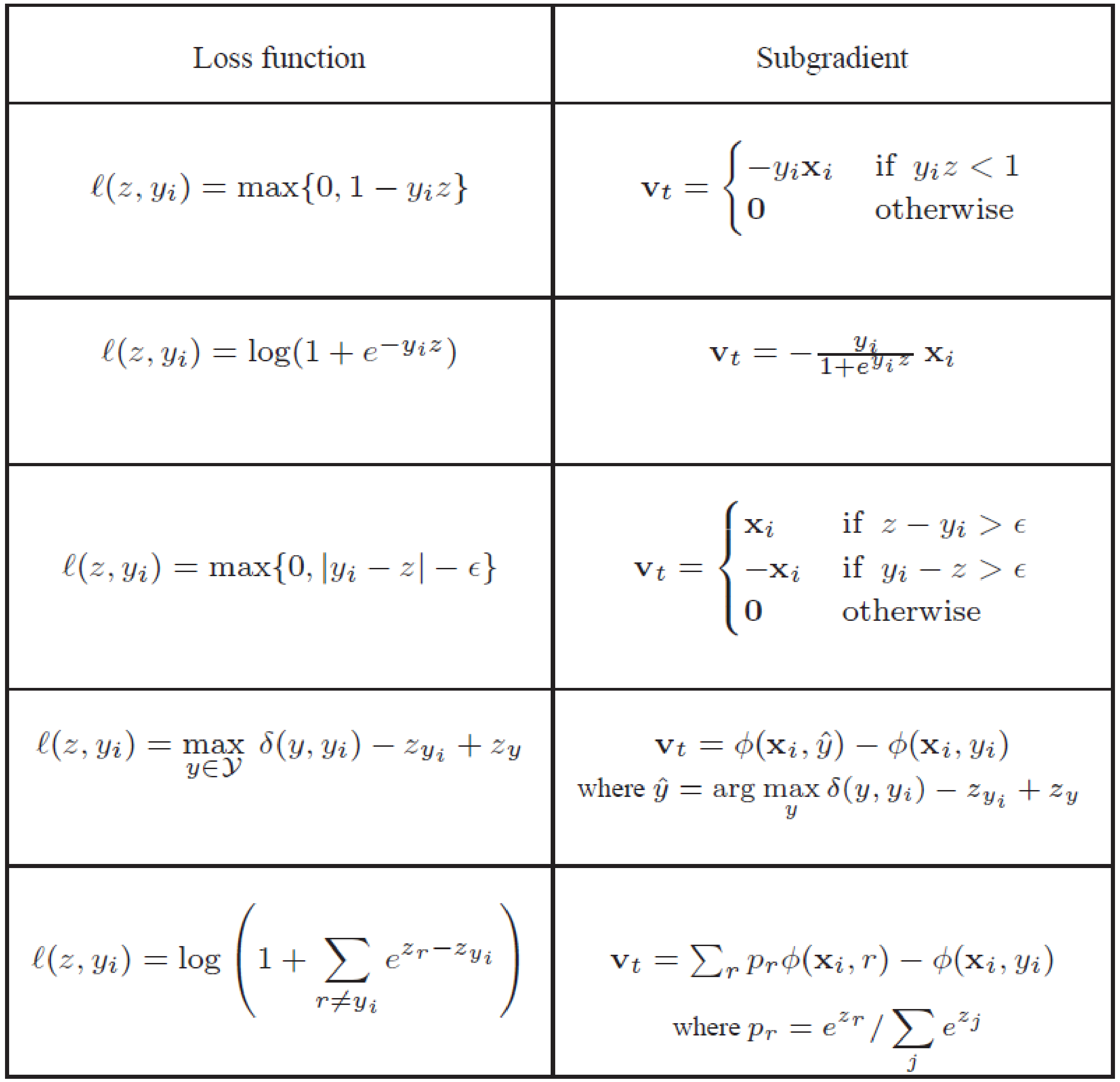
```
INPUT: $S, \lambda, T, k$
INITIALIZE: Set $\mathbf{w}_1 = 0$
FOR $t = 1, 2, \ldots, T$
    Choose $A_t \subseteq [m]$, where $|A_t| = k$, uniformly at random
    Set $A_t^+ = \{i \in A_t : y_i \langle \mathbf{w}_t, \mathbf{x}_i \rangle < 1\}$
    Set $\eta_t = \frac{1}{\lambda t}$
    Set $\mathbf{w}_{t+1} \leftarrow (1 - \eta_t \lambda)\mathbf{w}_t + \frac{\eta_t}{k} \sum_{i \in A_t^+} y_i \mathbf{x}_i$

OUTPUT: $\mathbf{w}_{T+1}$
```

k: batch size
m: number of training samples
A_t: batch of examples
A_t^+: examples within margin

S: training set
λ: regularization weight
T: number iterations
$\boldsymbol{w}_t$: model weights
$\boldsymbol{x}_i$: features for example i
y_i: label for example i
η_t: step size ("learning rate")

SGD applies to many losses

z is the score for y=1



	Loss function	Subgradient
SVM (hinge loss)	$\ell(z, y_i) = \max\{0, 1 - y_i z\}$	$\mathbf{v}_t = \begin{cases} -y_i \mathbf{x}_i & \text{if } y_i z < 1 \\ \mathbf{0} & \text{otherwise} \end{cases}$
Logistic regression / sigmoid loss	$\ell(z, y_i) = \log(1 + e^{-y_i z})$	$\mathbf{v}_t = -\frac{y_i}{1+e^{y_i z}} \mathbf{x}_i$
Hinge L1 regression	$\ell(z, y_i) = \max\{0, \lvert y_i - z\rvert - \epsilon\}$	$\mathbf{v}_t = \begin{cases} \mathbf{x}_i & \text{if } z - y_i > \epsilon \\ -\mathbf{x}_i & \text{if } y_i - z > \epsilon \\ \mathbf{0} & \text{otherwise} \end{cases}$
Margin loss between scores of most likely and correct label	$\ell(z, y_i) = \max_{y \in \mathcal{Y}} \delta(y, y_i) - z_{y_i} + z_y$	$\mathbf{v}_t = \phi(\mathbf{x}_i, \hat{y}) - \phi(\mathbf{x}_i, y_i)$ where $\hat{y} = \arg\max_y \delta(y, y_i) - z_{y_i} + z_y$
Variant of a logistic loss	$\ell(z, y_i) = \log\left(1 + \sum_{r \neq y_i} e^{z_r - z_{y_i}}\right)$	$\mathbf{v}_t = \sum_r p_r \phi(\mathbf{x}_i, r) - \phi(\mathbf{x}_i, y_i)$ where $p_r = e^{z_r} / \sum_j e^{z_j}$

SGD is fast compared to other optimization approaches

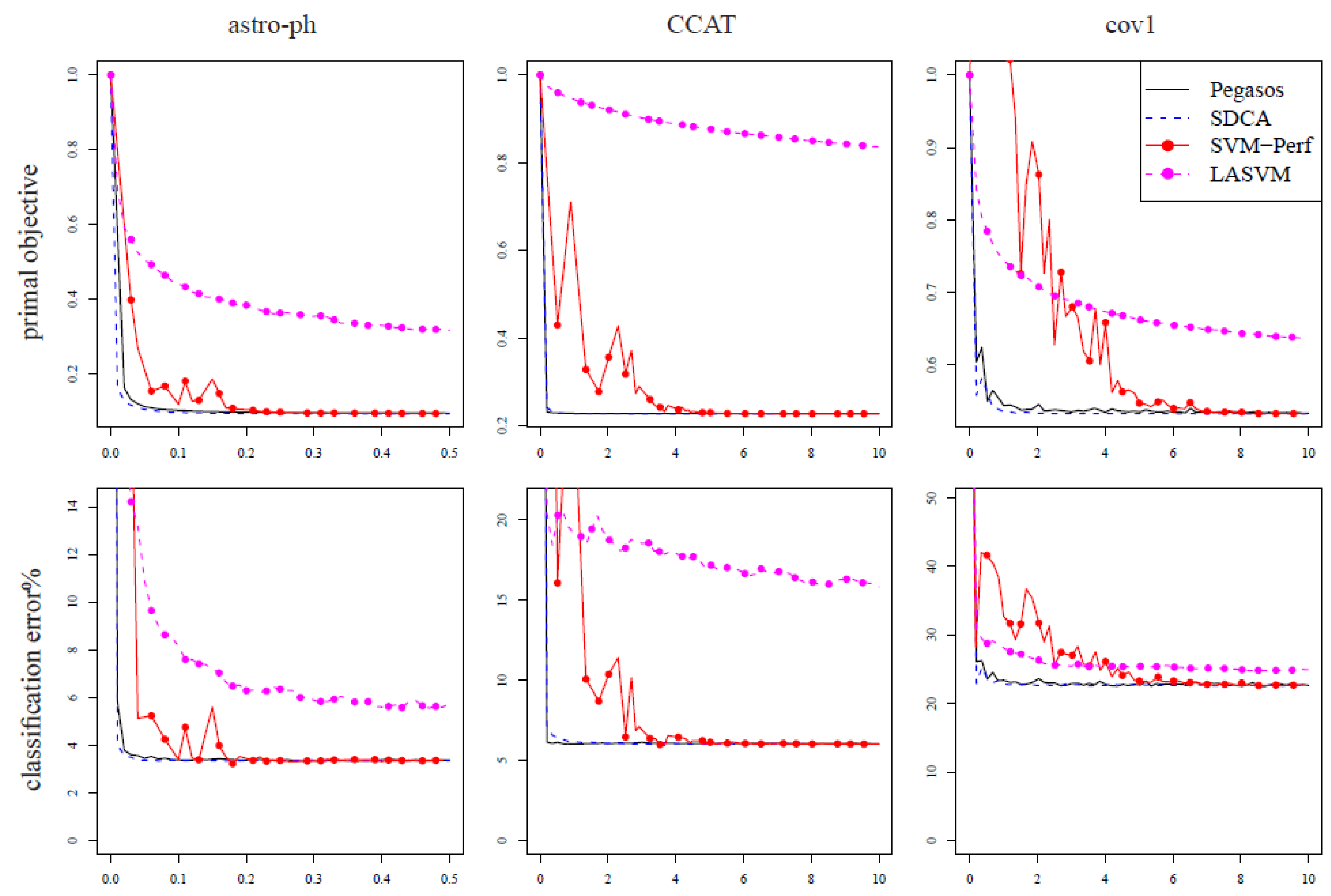
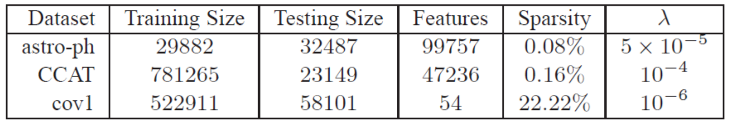


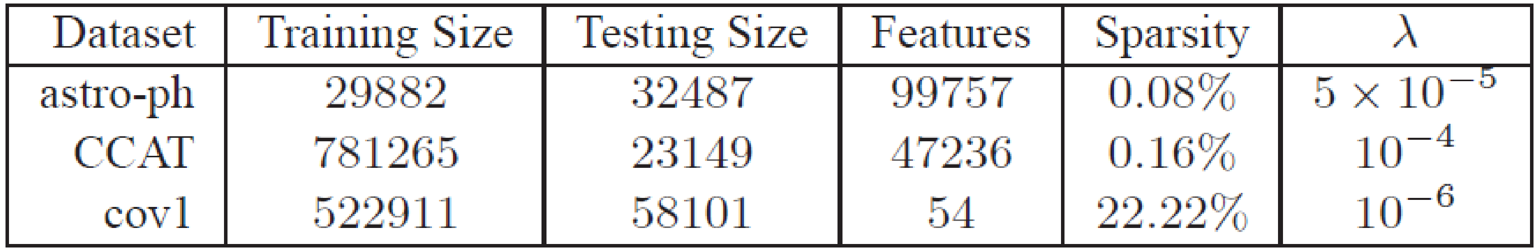
Fig. 4 Comparison of linear SVM optimizers. Primal suboptimality (top row) and testing classification error (bottom row), for one run each of Pegasos, stochastic DCA, SVM-Perf, and LASVM, on the astro-ph (left), CCAT (center) and cov1 (right) datasets. In all plots the horizontal axis measures runtime in seconds.



Dataset	Training Size	Testing Size	Features	Sparsity	λ
astro-ph	29882	32487	99757	0.08%	5×10^{-5}
CCAT	781265	23149	47236	0.16%	10^{-4}
cov1	522911	58101	54	22.22%	10^{-6}

SDCA = stochastic dual coordinate descent, another form of stochastic gradient optimization that chooses learning rate dynamically

Experiments with Linear SVM



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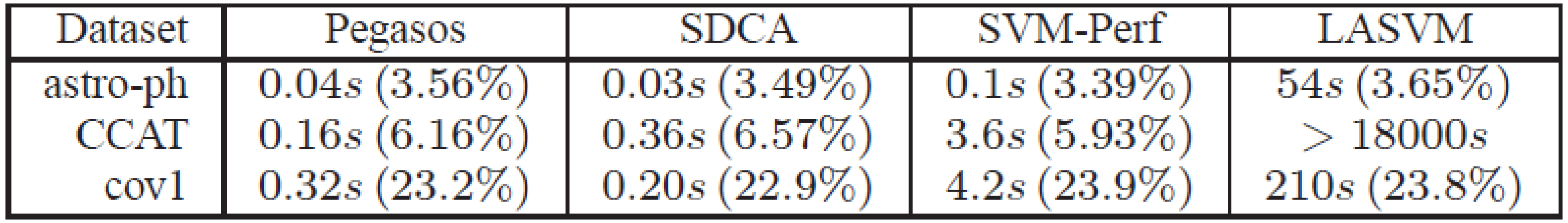
Training time and test error



Dataset	Pegasos	SDCA	SVM-Perf	LASVM
astro-ph	$0.04s$ (3.56%)	$0.03s$ (3.49%)	$0.1s$ (3.39%)	$54s$ (3.65%)
CCAT	$0.16s$ (6.16%)	$0.36s$ (6.57%)	$3.6s$ (5.93%)	$> 18000s$
cov1	$0.32s$ (23.2%)	$0.20s$ (22.9%)	$4.2s$ (23.9%)	$210s$ (23.8%)

Effect of mini-batch size

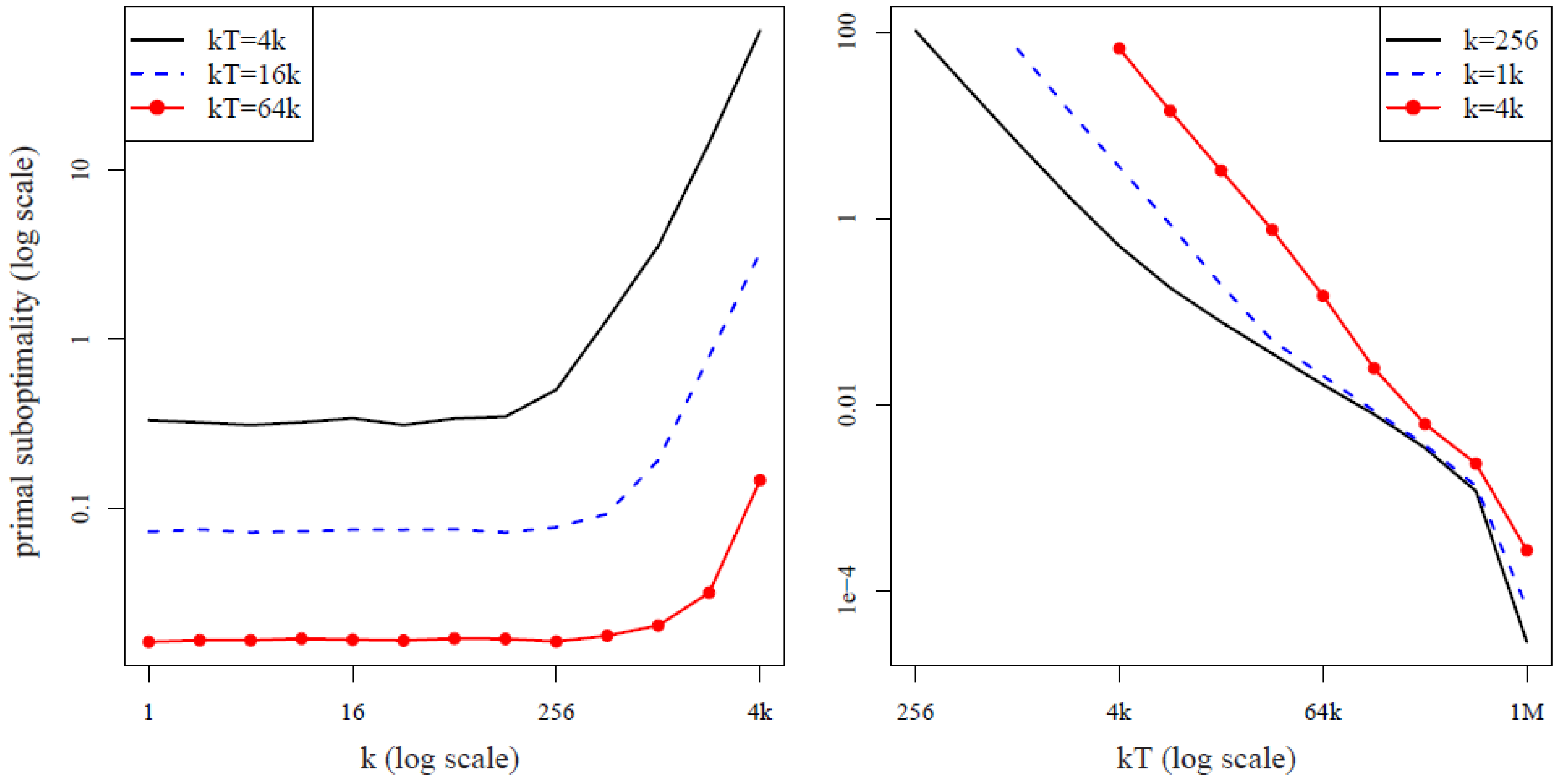
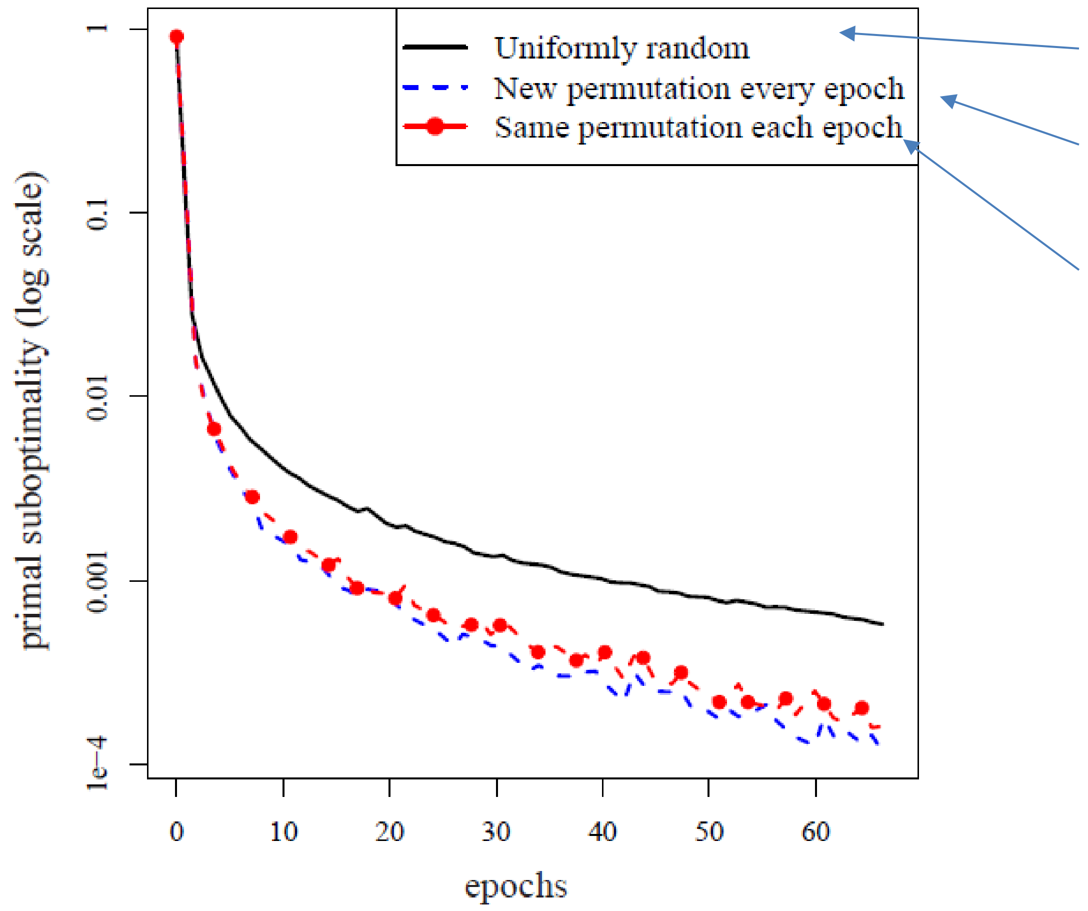


Fig. 7 The effect of the mini-batch size on the runtime of Pegasos for the astro-ph dataset. The first plot shows the primal suboptimality achieved for certain fixed values of overall runtime kT, for various values of the mini-batch size k. The second plot shows the primal suboptimality achieved for certain fixed values of k, for various values of kT. Very similar results were achieved for the CCAT dataset.

Effect of sampling procedure: randomly ordered epochs is best



Sampling with replacement

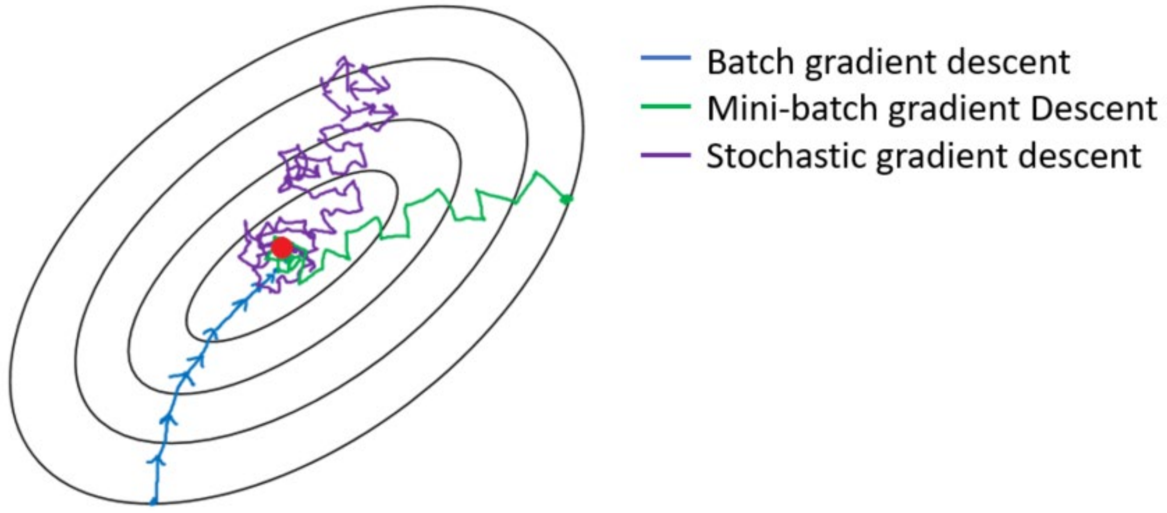
Use different random order for each “epoch”

Use same order for each epoch

Epoch: one run through the training set

Mini-Batch SGD vs. Full Batch Gradient Descent

- Mini-batch is faster
  - Time to compute gradient is $O(B)$ for batch size B, but standard error of gradient direction is $O\left(1/\sqrt{B}\right)$
  - E.g. batch size of 10000 vs 100 will take 100 times longer but reduce standard deviation by factor of 10
- Full batch is more stable, but the instability of SGD can help escape local minima
- We'll discuss enhancements to SGD, such as momentum later
- SGD training is highly parallelizable (good for GPU processing)



https://medium.com/analytics-vidhya/gradient-descent-vs-stochastic-gd-vs-mini-batch-sgd-fbd3a2cb4ba4

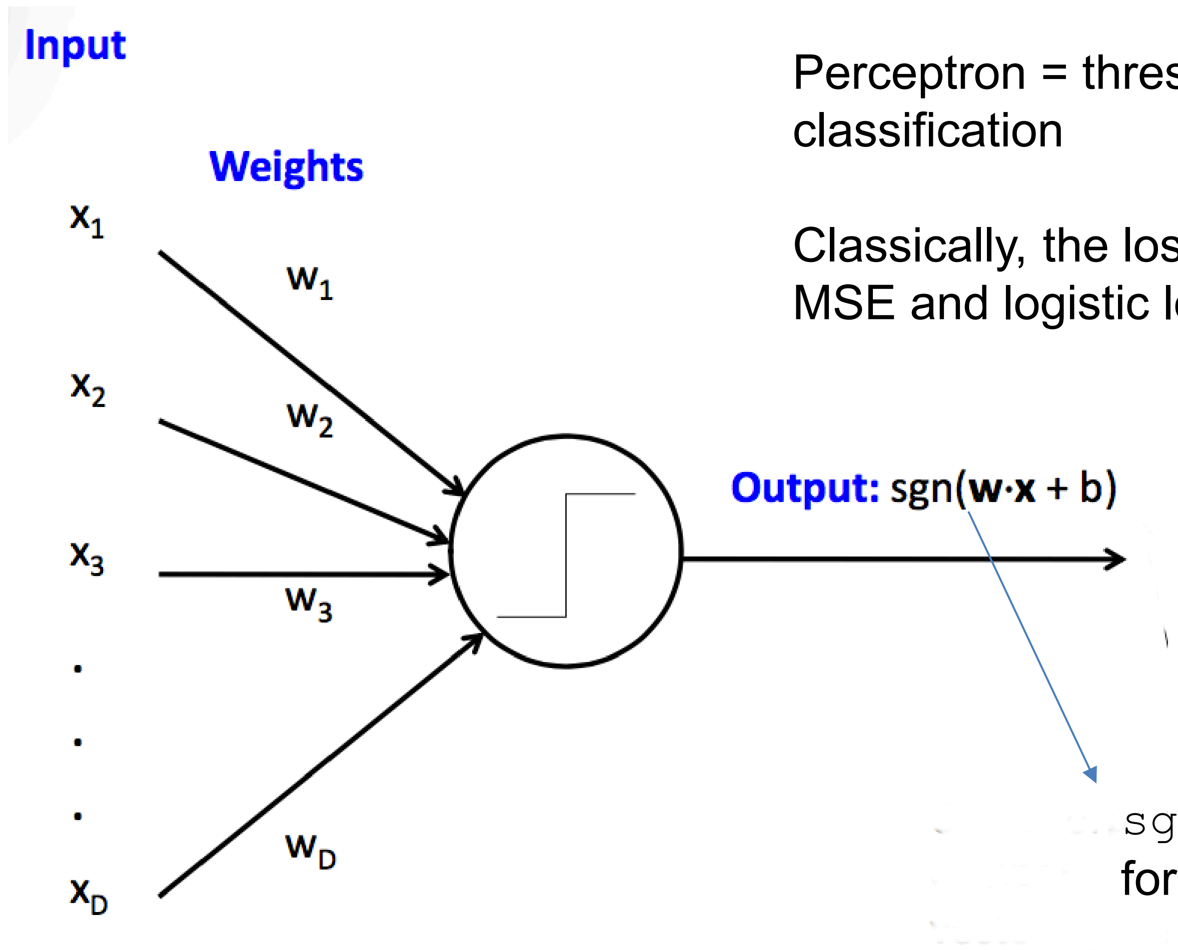
Pegasos: take-ways and surprising facts

- SGD is very simple and effective optimization algorithm – step toward better solution based on a small sample of training data
- Not very sensitive to mini-batch size (but larger batches can be much faster with GPU parallel processing)
- The same learning schedule is effective across several problems
- A *larger training set* makes it *faster* to obtain the same test performance

Q1-Q2

https://tinyurl.com/441-fa24-L14

Perceptron



Perceptron = thresholded linear prediction model for classification

Classically, the loss is a hinge loss (like SVM), but we'll consider MSE and logistic losses

`sgn` returns -1 for negative inputs and +1 for positive inputs

Fig source: CS 440

Perceptron Update Rule with MSE Loss

Prediction: $f(\boldsymbol{x}) = w_0 x_0 + w_1 x_1 + \ldots w_m x_m + b$

Error: $E(\boldsymbol{x}) = (\underset{\text{prediction}}{f(\boldsymbol{x})} - \underset{\text{target}}{y})^2$

Update w_i: take a step to decrease $E(\boldsymbol{x})$

$$\frac{\partial E(\boldsymbol{x})}{\partial w_i} = 2(f(\boldsymbol{x}) - y)[\frac{\partial (f(\boldsymbol{x}) - y)}{\partial w_i}]$$

$$\frac{\partial E(\boldsymbol{x})}{\partial w_i} = 2(f(\boldsymbol{x}) - y)x_i$$

Chain Rule:
$h(x) = f(g(x))$, then
$h'(x) = f'(g(x))g'(x)$

$$w_i = w_i \underset{\text{Make error } lower}{-} \underset{\text{Learning rate}}{\eta}(f(\boldsymbol{x}) - y)x_i$$

(the 2 is folded into the learning rate)

Perceptron Optimization by SGD (MSE Loss)

```
Randomly initialize weights, e.g. w ~ Gaus(mu=0, std=0.05)
For each iteration $t$:
    Split data into batches
    $\eta = 0.1/t$
    For each batch $X_b$:
        For each weight $w_i$:
            $w_i = w_i - \eta \frac{1}{|X_b|} \sum_{\boldsymbol{x}_n \in X_b} (f(\boldsymbol{x}_n) - y_n) x_{ni}$
```

With different loss, the update changes accordingly

Logistic loss:

$$f(\boldsymbol{x}) = w_0 x_0 + w_1 x_1 + \ldots w_m x_m + b$$

$$P(y|\boldsymbol{x}) = \frac{1}{1+\exp(-yf(x))}, y \in \{-1,1\}$$

$$E(\boldsymbol{x}) = -\log P(y|\boldsymbol{x})$$

$$w_i = w_i + \eta \frac{1}{|X_b|} \sum_{\boldsymbol{x}_n \in X_b} y_n x_{ni} (1 - P(y = y_n | x_n))$$

decrease –logP(y|x) → increase logP(y|x)

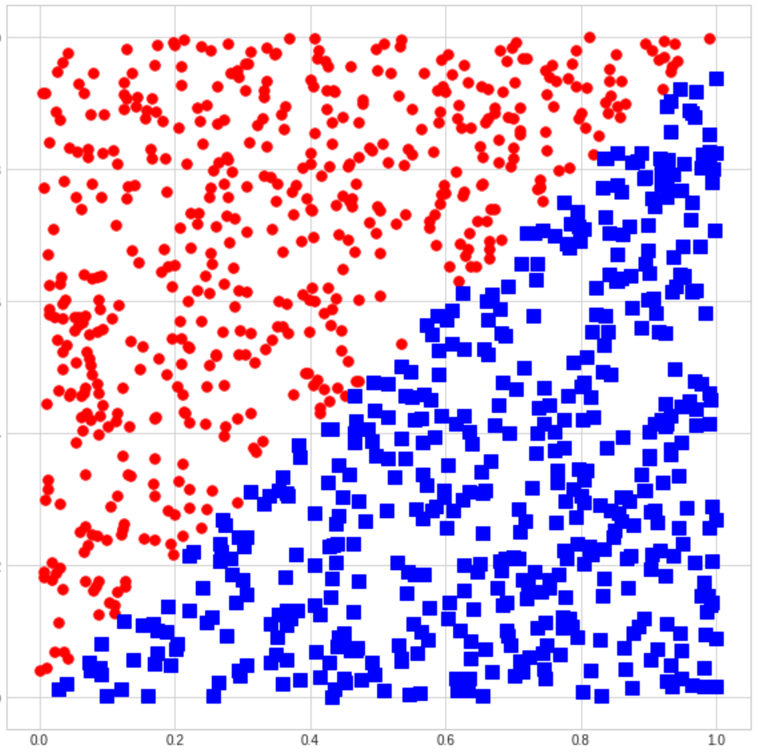
Q3

https://tinyurl.com/441-fa24-L14

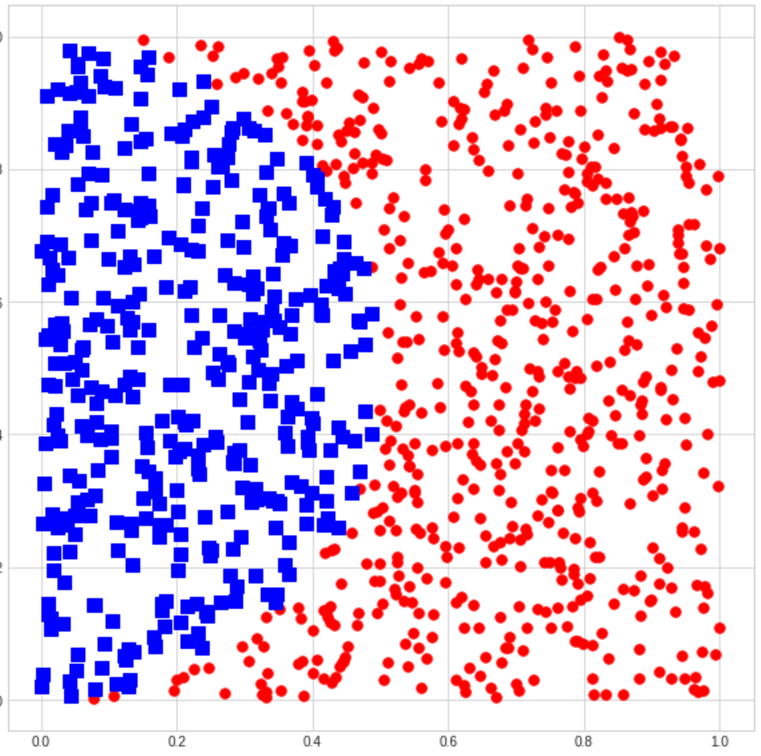
Demo

https://colab.research.google.com/drive/1nKNJyolqgzW53Rz59M2BZtyQM8bbrExb?usp=sharing

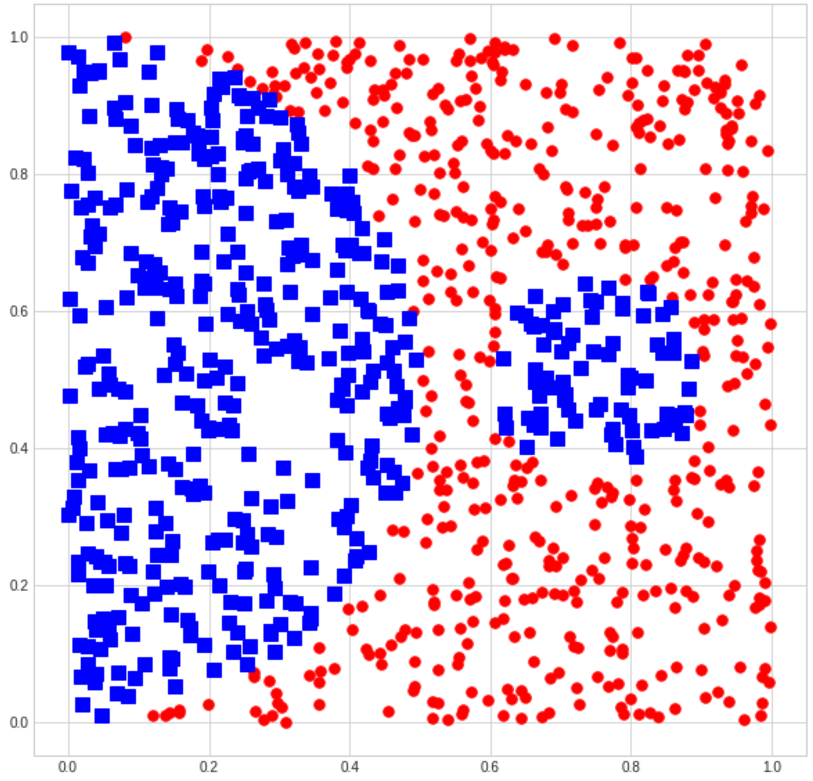
Which of these can a perceptron solve (fit with zero training error)?



(a)



(b)

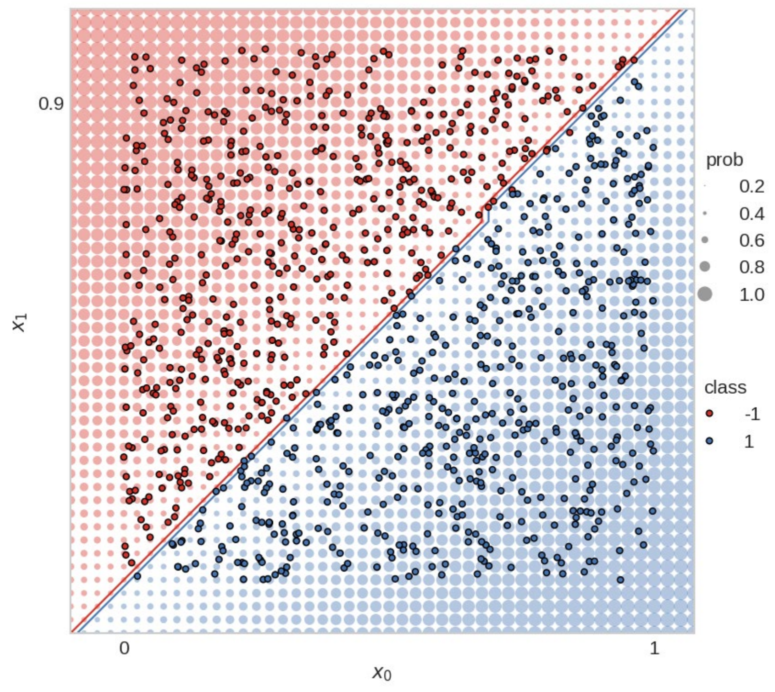


(c)

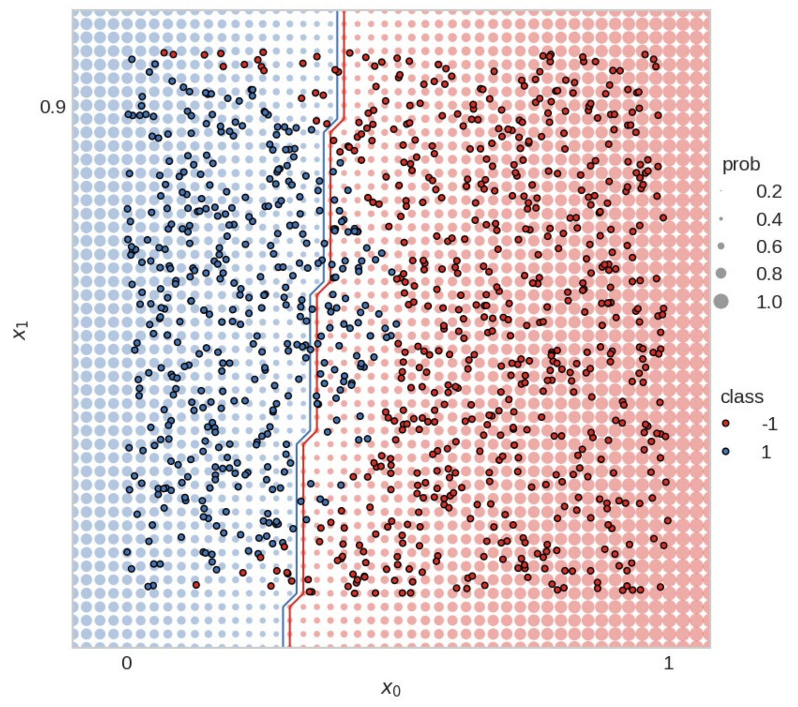
Perceptron is often not enough

- Perceptron is linear, but we often need a non-linear prediction function

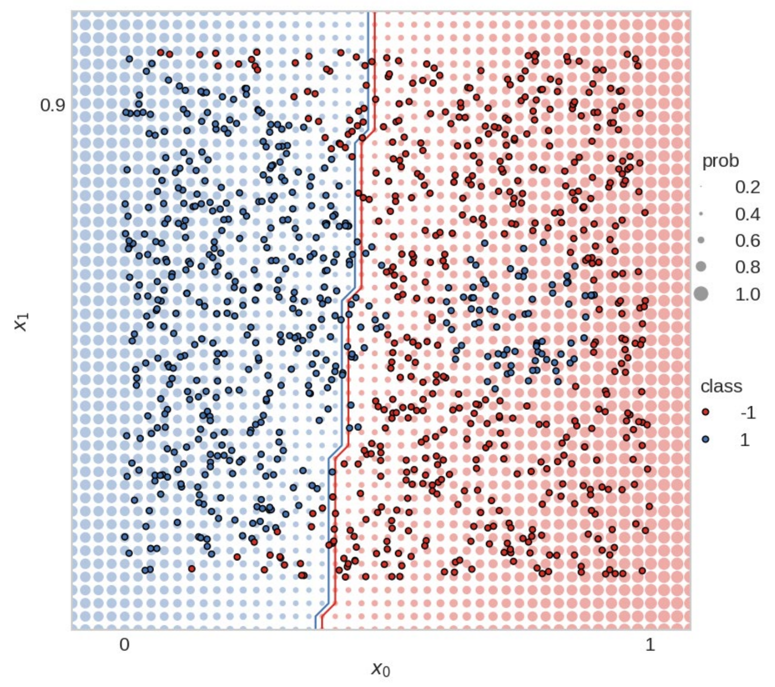
Which of these can a perceptron solve (fit with zero training error)?



Yes



No



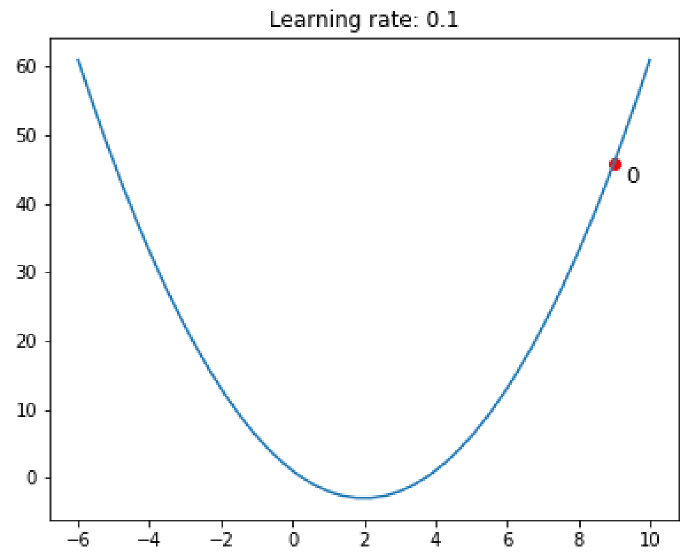
Not even close

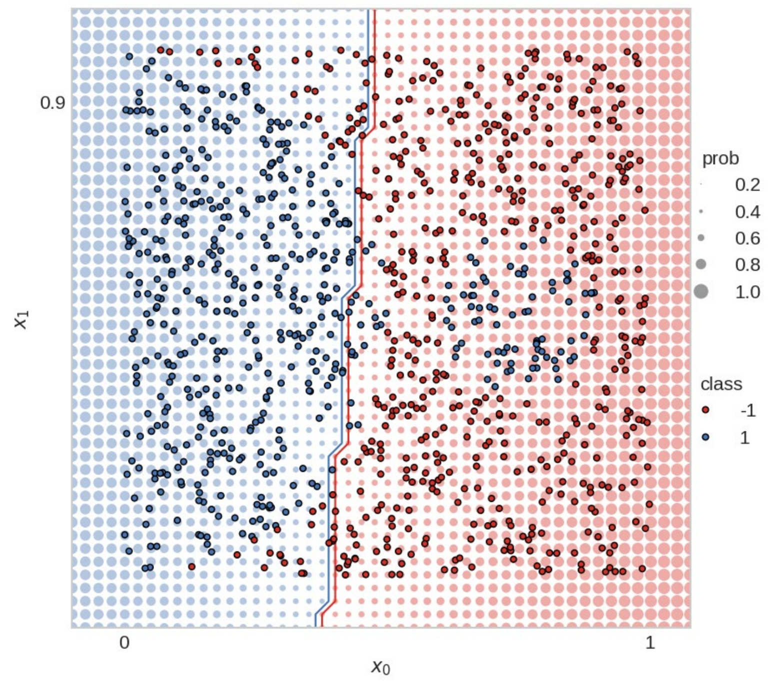
Q4

https://tinyurl.com/441-fa24-L14

Things to Remember

- Gradient descent iteratively steps in direction of negative gradient of loss
- Stochastic gradient descent estimates gradient using small batches of samples
  - Faster than full gradient descent
- Linear models have limited ability to fit the data – often need non-linear models like multilayer networks





Coming up

- Thursday: MLPs