Linear Classification and Support Vector Machine and Stochastic Gradient Descent

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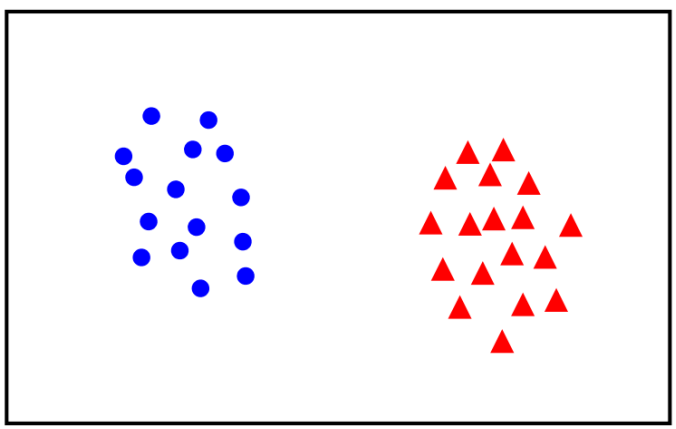
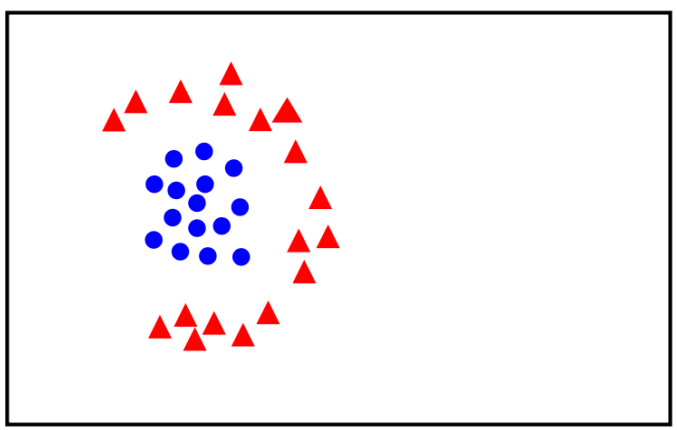
Binary Classification

Given training data $(\mathbf{x}_i, y_i)$ for $i = 1 \ldots n$, with $\mathbf{x}_i \in R^m$ and $y_i \in \{-1, 1\}$, learn a classfier $f(\mathbf{x})$ such that

$$f(\mathbf{x}_i) \begin{cases} \geq 0 & y_i = +1 \\ < 0 & y_i = -1 \end{cases}$$

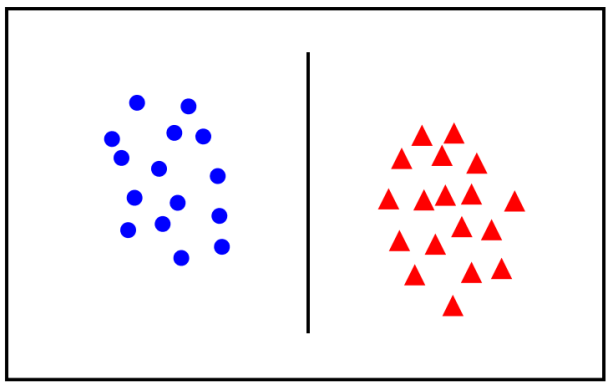
i.e. $y_i f(\mathbf{x}_i) > 0$ for a correct classification

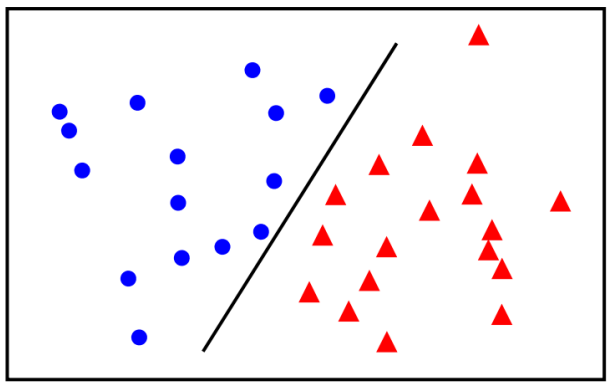




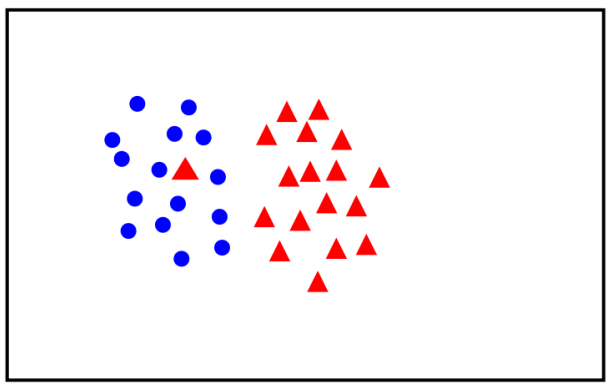
Linear Separability

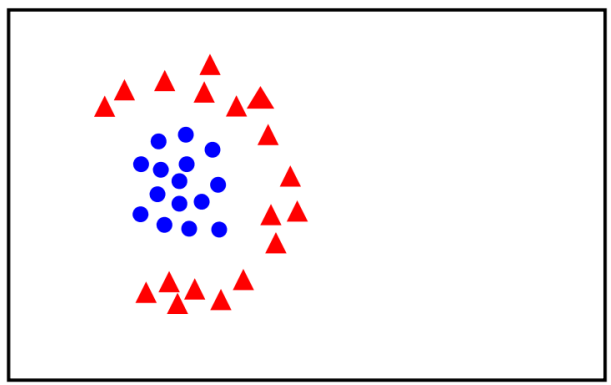
linearly separable





not linearly separable

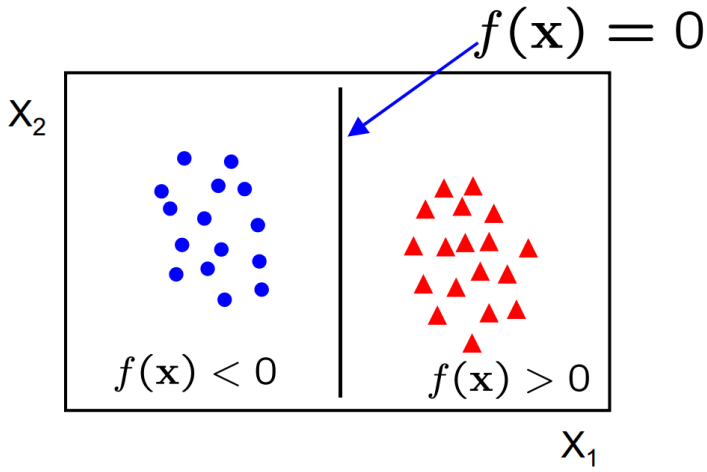




Linear Classifiers

A linear classifier has the form:

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

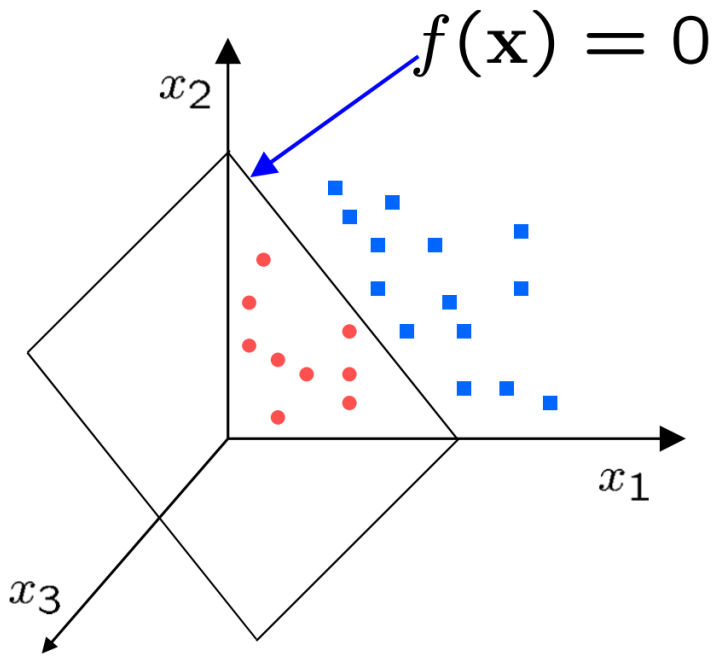


- In 2D the discriminant is a line
- $\mathbf{w}$ is the normal to the line, and b is the bias
- $\mathbf{w}$ is known as the weight vector

Linear Classifiers

A linear classifier has the form:

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



- In $3D$ the discriminant is a plane, and in mD it is a hyperplane

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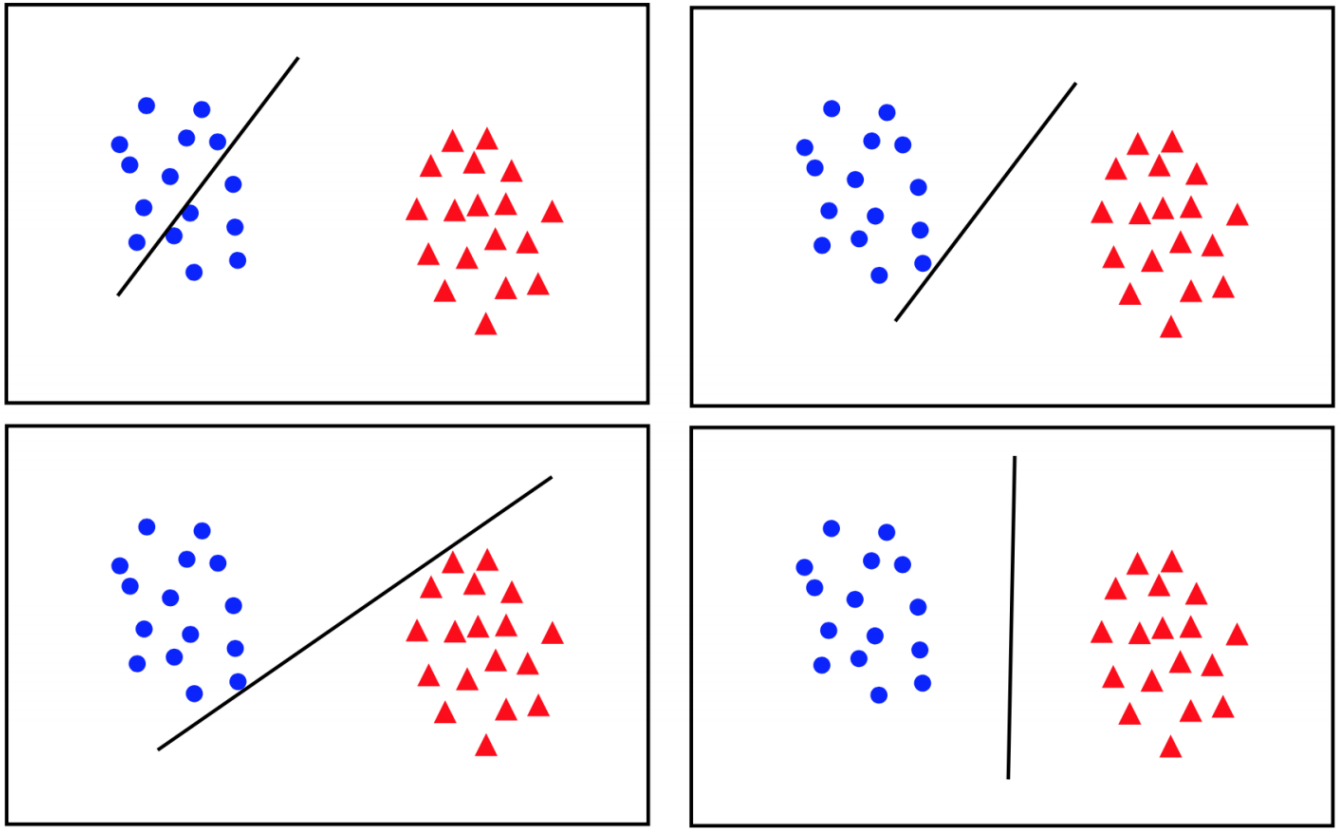
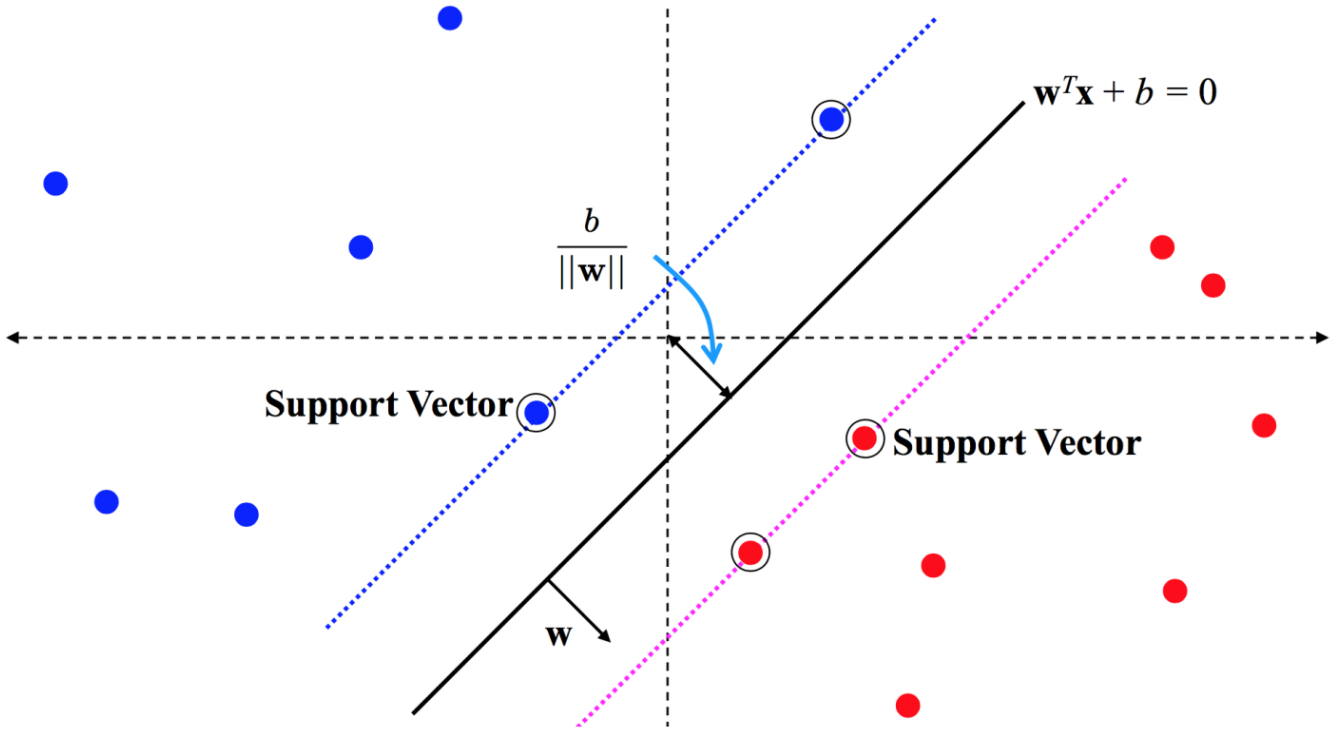
What's a Good Decision Boundary?



- Maximum margin solution: most stable under perturbations of the inputs

Max-margin Methods



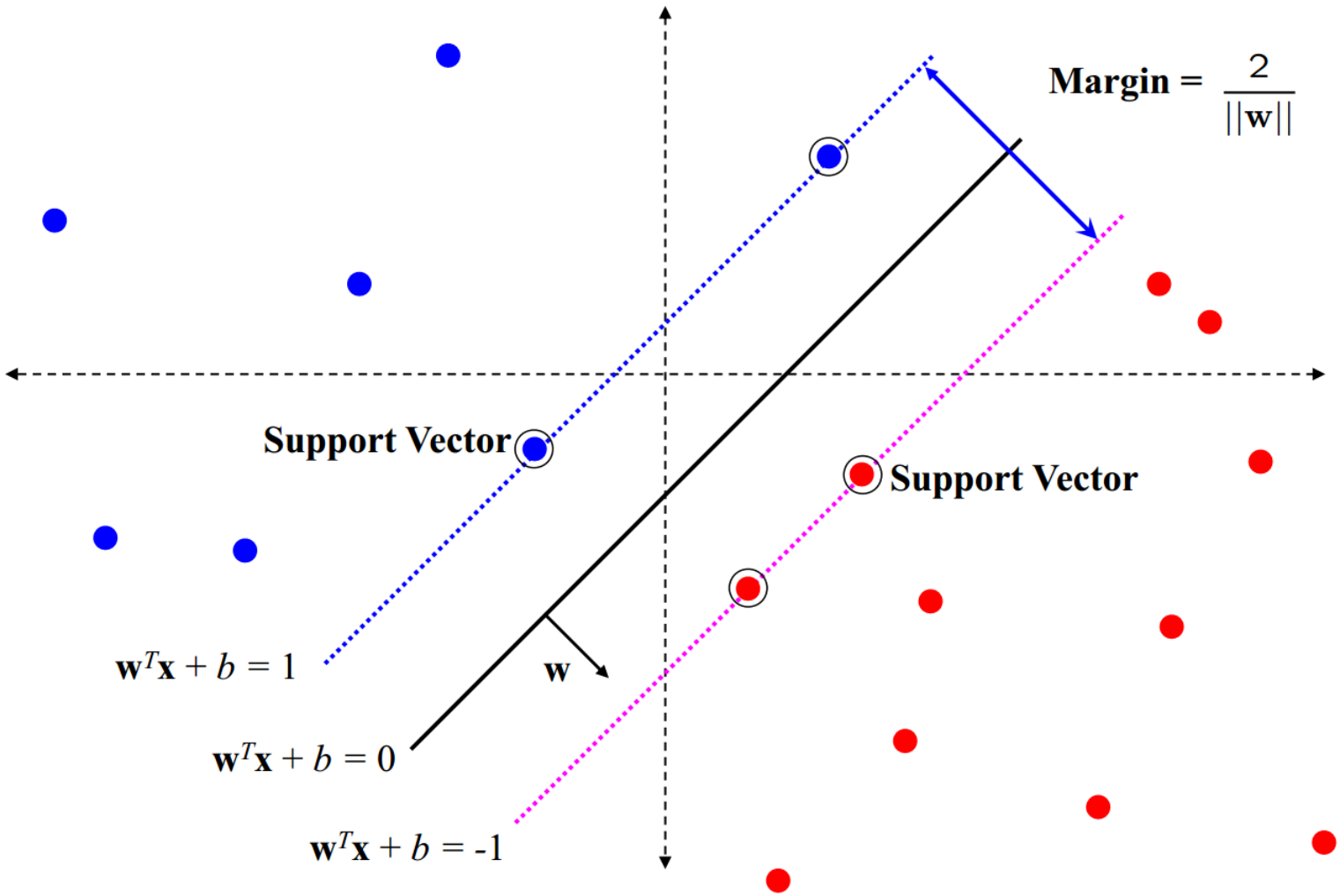
- Select two parallel hyperplanes that separate the two classes of data and let the distance between them as large as possible
- The region bounded by these two hyperplanes is called the "margin"

SVM-sketch Derivation

- Choose normalization such that $\mathbf{w}^\top \mathbf{x}_+ + b = +1$ and $\mathbf{w}^\top \mathbf{x}_- + b = -1$ for the positive and negative support vectors respectively
- Then the magin is given by

$$\frac{\mathbf{w}}{\|\mathbf{w}\|} \cdot (\mathbf{x}_+ - \mathbf{x}_-) = \frac{\mathbf{w}^\top (\mathbf{x}_+ - \mathbf{x}_-)}{\|\mathbf{w}\|} = \frac{2}{\|\mathbf{w}\|}$$

Support Vector Machine



Basic Support Vector Machine

- Learning the SVM can be formulated as an optimization:

$$\max_{\mathbf{w},b} \frac{2}{\|\mathbf{w}\|}$$

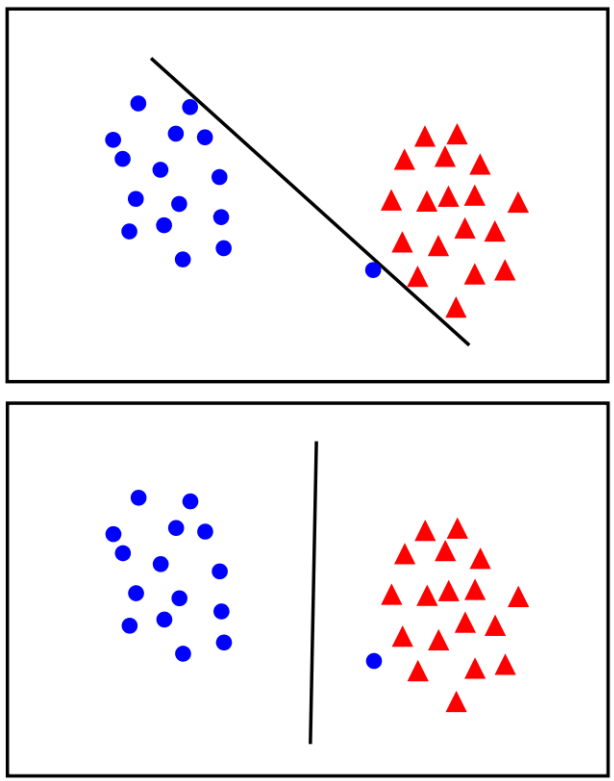
$$s.t. \quad \mathbf{w}^\top \mathbf{x}_i + b \begin{cases} \geqslant 1 & y_i = +1 \\ \leqslant -1 & y_i = -1 \end{cases}$$

- Or equivalently:

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

$$s.t. \quad y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geqslant 1, \qquad i = 1, 2, \ldots, n$$

Linear Separability Again: What is The Best **w**?



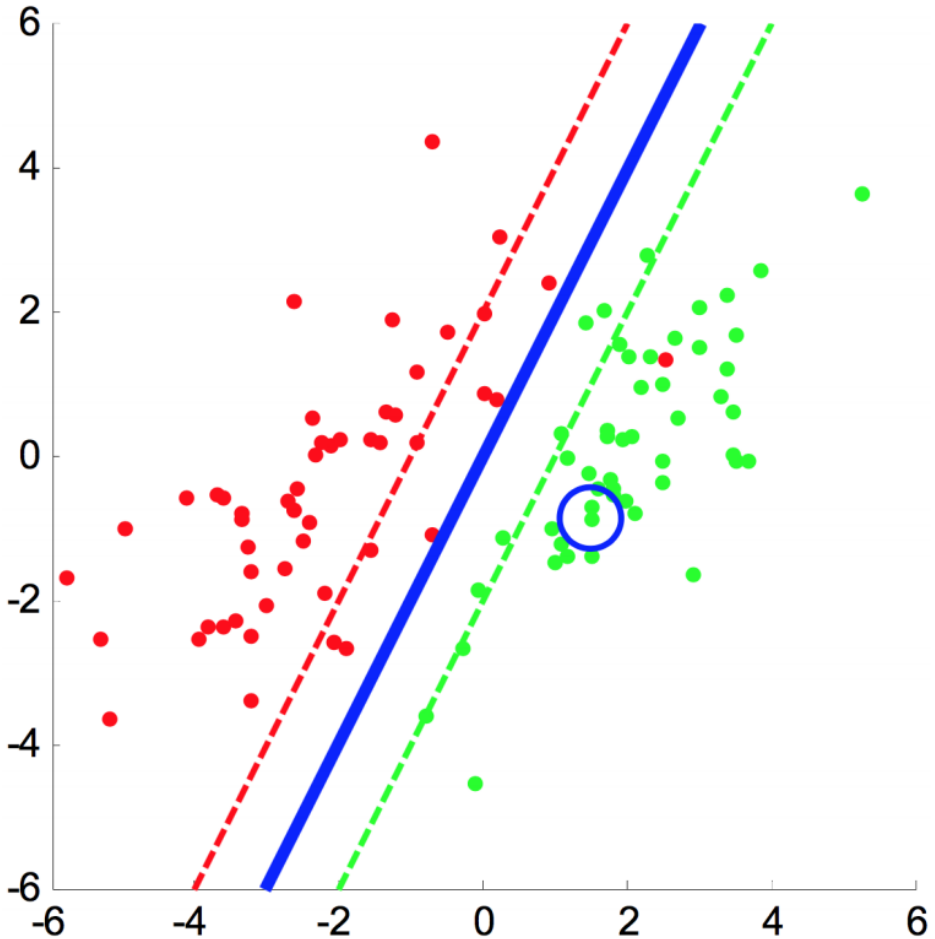
• the points can be linearly separated but there is a very narrow margin

• but possibly the large margin solution is better, even though one constraint is violated

In general there is a trade off between the margin and the number of mistakes on the training data

Linear Separability Again: What is The Best **w**?

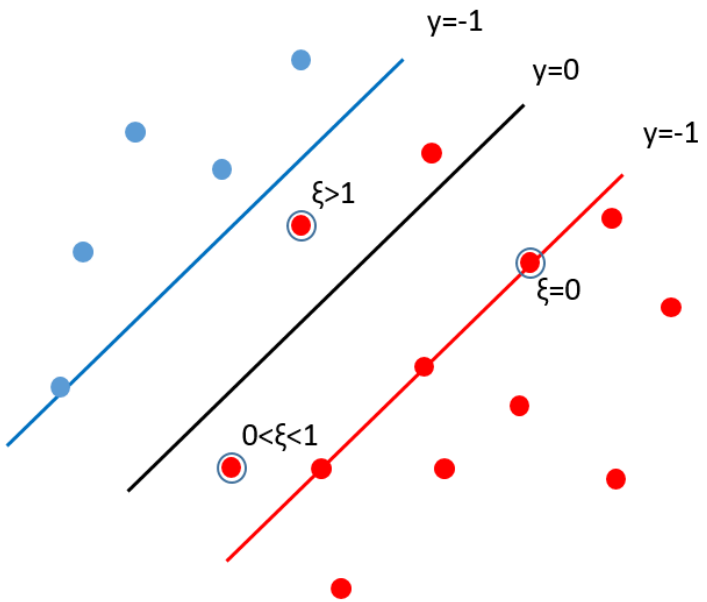
Moreover, training data may not be linearly separable!



A Relaxed Formulation

Introduce variable $\xi_i \geqslant 0$, for each i, which represents how much example i is on wrong side of margin boundary

- If $\xi_i = 0$ then it is ok
- If $0 < \xi_i < 1$ it is correctly classified, but with a smaller margin than $\frac{1}{\|\mathbf{w}\|}$
- If $\xi_i > 1$ then it is incorrectly classified



Soft Margin Formulation

The optimization problem becomes:

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

$$s.t. \quad y_i(\mathbf{w}^\top \mathbf{x}_i + b) \geqslant 1 - \boldsymbol{\xi}_i, \qquad i = 1, 2, \ldots, n$$

Hinge Loss

Hinge loss:

$$\text{Hinge loss} = \xi_i = \max(0, 1 - y_i(\mathbf{w}^\top \mathbf{x}_i + b))$$

The optimization problem becomes:

$$\min_{\mathbf{w},b} \quad \frac{\|\mathbf{w}\|^2}{2} + C \sum_{i=1}^{n} \max(0, 1 - y_i(\mathbf{w}^\top \mathbf{x}_i + b))$$

Dual Problem

An optimization problem can be considered in two ways, primal problem and dual problem

- for primal problem of basic SVM:

$$\min_{\mathbf{w},b} \frac{\|\mathbf{w}\|^2}{2}$$
$$s.t. \quad y_i(\mathbf{w}^T\mathbf{x}_i + b) \geqslant 1, \qquad i = 1, 2, \ldots, n$$

- its Lagrange function is:

$$\mathcal{L}(\mathbf{w}, b, \boldsymbol{\alpha}) = \frac{1}{2}\|\mathbf{w}\|^2 + \sum_{i=1}^{n} \alpha_i(1 - y_i(\mathbf{w}^T\mathbf{x}_i + b)) \qquad (1)$$

Dual Problem

- its Lagrange "dual function" is:

$$\mathbf{D}(\boldsymbol{\alpha}) = \inf \boldsymbol{\mathcal{L}}(\mathbf{w}, b, \boldsymbol{\alpha})$$

Dual function gives the lower bound of the optimal value of primal problem

- dual problem: the best lower bound dual function can get

$$\max_{\boldsymbol{\alpha}} \mathbf{D}(\boldsymbol{\alpha})$$

Dual Problem

- setting partial derivative of $\mathbf{D}$ with respect to $\mathbf{w}$ to 0:

$$\begin{aligned} \nabla_w \mathbf{D} &= \mathbf{w} - \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i = 0 \\ \rightarrow \mathbf{w} &= \sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i = 0 \end{aligned} \tag{2}$$

- setting partial derivative of $\mathcal{L}$ with respect to b to 0:

$$\nabla_b \mathbf{D} = \sum_{i=1}^{n} \alpha_i y_i = 0 \tag{3}$$

Dual Problem

- adding (2), (3) to (1):

$$\begin{aligned}
\mathcal{L}(\mathbf{w}, b, \boldsymbol{\alpha}) &= \frac{1}{2}\|\mathbf{w}\|^2 + \sum_{i=1}^{n} \alpha_i (1 - y_i(\mathbf{w}^T \mathbf{x}_i + b)) \\
&= \frac{1}{2}\mathbf{w}^\top \mathbf{w} + \sum_{i=1}^{n} \alpha_i - \sum_{i=1}^{n} \mathbf{w}^\top \alpha_i y_i \mathbf{x}_i - \sum_{i=1}^{n} \alpha_i y_i \\
&= \frac{1}{2}\mathbf{w}^\top \mathbf{w} + \sum_{i=1}^{n} \alpha_i - \mathbf{w}^\top \mathbf{w} - 0 \\
&= \sum_{i=1}^{n} \alpha_i - \frac{1}{2}[\sum_{i=1}^{n} \alpha_i y_i \mathbf{x}_i]^\top [\sum_{j=1}^{n} \alpha_i y_i \mathbf{x}_i] \\
&= \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^\top \mathbf{x}_j
\end{aligned}$$

Dual Problem

- finally, we can get the dual problem:

$$\max_{\boldsymbol{\alpha}} \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^\top \mathbf{x}_j$$

$$\text{s.t.} \quad \sum_{i=1}^{n} \alpha_i y_i = 0,$$

$$\alpha_i \geqslant 0, \quad i = 1, 2, \ldots, n$$

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Gradient Descent

- True gradient descent is a batch algorithm, slow but sure

$$\mathbf{w} := \mathbf{w} - \eta \nabla L(\mathbf{w}) = \mathbf{w} - \eta \frac{1}{n} \sum_{i=1}^{n} \nabla L_i(\mathbf{w})$$

Stochastic Optimization Motivation

- Information is redundant
- Sufficient samples means we can afford more frequent, noisy updates
- Never-ending stream means we should not wait for all data
- Tracking non-stationary data means that the target is moving

Stochastic Optimization

Idea: estimate function and gradient from a small, current subsample of your data and with enough iterations and data, you will converge to the true minimum

- Better for large datasets and often faster convergence
- Hard to reach high accuracy
- Best classical methods can not handle stochastic approximation
- Theoretical definitions for convergence not as well defined

Stochastic Gradient Descent (SGD)

- In SDG the true gradient of $L(w)$ is approximated by a gradient of a single example:

$$\mathbf{w} := \mathbf{w} - \eta \nabla L_i(\mathbf{w})$$

- Although random noise is introduced, it behaves like gradient descent in its expectation

Stochastic Gradient Descent

SGD works similar as GD, but more quickly by estimating gradient from a few examples at a time

Algorithm 1: GD

1 Initialize parameter $\mathbf{w}$ and learning rate η
2 **while** an approximate minimum is not obtained **do**
3 $\quad \mathbf{w} := \mathbf{w} - \eta \frac{1}{n} \sum_{i=1}^{n} \nabla L_i(\mathbf{w})$
4 **end**

Algorithm 2: SGD

1 Initialize parameter $\mathbf{w}$ and learning rate η
2 **while** an approximate minimum is not obtained **do**
3 $\quad$ Randomly select an example i in the training set
4 $\quad \mathbf{w} := \mathbf{w} - \eta \nabla L_i(\mathbf{w})$
5 **end**

The Benefits of SGD

- Gradient is easy to calculate (instantaneous)
- Less prone to local minima
- Small memory footprint
- Get to a reasonable solution quickly
- Works for non-stationary environments as well as online settings
- Can be used for more complex models and error surfaces

Importance of Learning Rate

- Learning rate has a large impact on convergence
  - Too small $\rightarrow$ too slow
  - Too large $\rightarrow$ oscillatory and may even diverge
- Should learning rate be fixed or adaptive?
- Is convergence necessary?
  - Non-stationary: convergence may not be required
  - Stationary: learning rate should decrease with time
  - Robbins-Monroe sequence is adequate $\eta_t = \frac{1}{t}$

Minibatch Stochastic Gradient Descent

- Rather than using a single point, use a random subset where the size is less than the original data size

$$\mathbf{w} := \mathbf{w} - \eta \frac{1}{|\mathcal{S}_k|} \sum_{i \in \mathcal{S}_k} \nabla_{\mathbf{w}} L_i(\mathbf{w}), \text{ where } \mathcal{S}_k \subseteq [n]$$

- Like the single random sample, the full gradient is approximated via an unbiased noisy estimate
- Random subset reduces the variance by a factor of $\frac{1}{|\mathcal{S}_k|}$, but is also $|\mathcal{S}_k|$ times more expensive

Minibatch Stochastic Gradient Descent

MSGD works identically to SGD, except that we use more than one training example to make each estimate of the gradient

Algorithm 3: MSGD

Initialize parameter $\mathbf{w}$ and learning rate η
while an approximate minimum is not obtained **do**
  Randomly select $|\boldsymbol{\mathcal{S}}_k|$ examples in the training set
  $\mathbf{w} := \mathbf{w} - \eta \frac{1}{|\boldsymbol{\mathcal{S}}_k|} \sum_{i \in \boldsymbol{\mathcal{S}}_k} \nabla_{\mathbf{w}} L_i(\mathbf{w})$
end

Algorithm 4: SGD

Initialize parameter $\mathbf{w}$ and learning rate η
while an approximate minimum is not obtained **do**
  Randomly select an example i in the training set
  $\mathbf{w} := \mathbf{w} - \eta \nabla L_i(\mathbf{w})$
end

Example

- Optimization problem:

$$\min_{\mathbf{w},b} \quad f : \frac{\|\mathbf{w}\|^2}{2} + C\sum_{i=1}^{N} \max(0, 1 - y_i(\mathbf{w}^\top x_i + b))$$

- Gradient computation:

$$\nabla f = \begin{bmatrix} \nabla_{\mathbf{w}} f(\mathbf{w}, b) \\ \nabla_b f(\mathbf{w}, b) \end{bmatrix}$$

- Update costs:
  Batch: $O(nm)$
  Stochastic: $O(m)$
  Mini-batch: $O(|\boldsymbol{\mathcal{S}}_k|m)$

Gradient Computation

$$\mathbf{w} = \begin{bmatrix} w_1 & \dots & w_n \end{bmatrix}^\top$$
$$\|\mathbf{w}\|^2 = \|\mathbf{w}\|_2^2 = w_1^2 + w_2^2 + \cdots + w_n^2$$

- Writting in the denominator-layout notation:

$$\begin{aligned} \frac{\partial(\|\mathbf{w}\|^2)}{\partial \mathbf{w}} &= \begin{bmatrix} \frac{\partial(w_1^2+w_2^2+\cdots+w_n^2)}{\partial w_1} & \dots & \frac{\partial(w_1^2+w_2^2+\cdots+w_n^2)}{\partial w_n} \end{bmatrix}^\top \\ &= \begin{bmatrix} 2w_1 & \dots & 2w_n \end{bmatrix}^\top \\ &= 2\mathbf{w} \end{aligned}$$

- so:

$$\frac{1}{2} \cdot \frac{\partial(\|\mathbf{w}\|^2)}{\partial \mathbf{w}} = \mathbf{w}$$

Gradient Computation

- Let $g_{\mathbf{w}}(\mathbf{x}_i) = \frac{\partial(\max(0, 1 - y_i(\mathbf{w}^\top \mathbf{x}_i + b)))}{\partial \mathbf{w}}$
- if $1 - y_i(\mathbf{w}^\top \mathbf{x}_i + b) >= 0$:

$$\begin{aligned} g_{\mathbf{w}}(\mathbf{x}_i) &= \frac{\partial(-y_i(\mathbf{w}^\top \mathbf{x}_i + b))}{\partial \mathbf{w}} \\ &= -\frac{\partial(y_i \mathbf{w}^\top \mathbf{x}_i)}{\partial \mathbf{w}} \\ &= -y_i \mathbf{x}_i \end{aligned}$$

- if $1 - y_i(\mathbf{w}^\top \mathbf{x}_i + b) < 0$:

$$g_{\mathbf{w}}(\mathbf{x}_i) = 0$$

Gradient Computation

- so:

$$g_{\mathbf{w}}(\mathbf{x}_i) = \begin{cases} -y_i \mathbf{x}_i & 1 - y_i(\mathbf{w}^\top \mathbf{x}_i + b) >= 0 \\ 0 & 1 - y_i(\mathbf{w}^\top \mathbf{x}_i + b) < 0 \end{cases}$$

- Let $g_b(\mathbf{x}_i) = \frac{\partial(\max(0, 1 - y_i(\mathbf{w}^\top \mathbf{x}_i + b)))}{\partial b}$

$$g_b(\mathbf{x}_i) = \begin{cases} -y_i & 1 - y_i(\mathbf{w}^\top \mathbf{x}_i + b) >= 0 \\ 0 & 1 - y_i(\mathbf{w}^\top \mathbf{x}_i + b) < 0 \end{cases}$$

Gradient Computation

- At last we have:

$$\frac{\partial f(\mathbf{w}, b)}{\mathbf{w}} = \mathbf{w} + C \sum_{i=1}^{N} g_{\mathbf{w}}(\mathbf{x}_i)$$

- and:

$$\frac{\partial f(\mathbf{w}, b)}{b} = C \sum_{i=1}^{N} g_b(\mathbf{x}_i)$$

Example

- n=10000,d=20

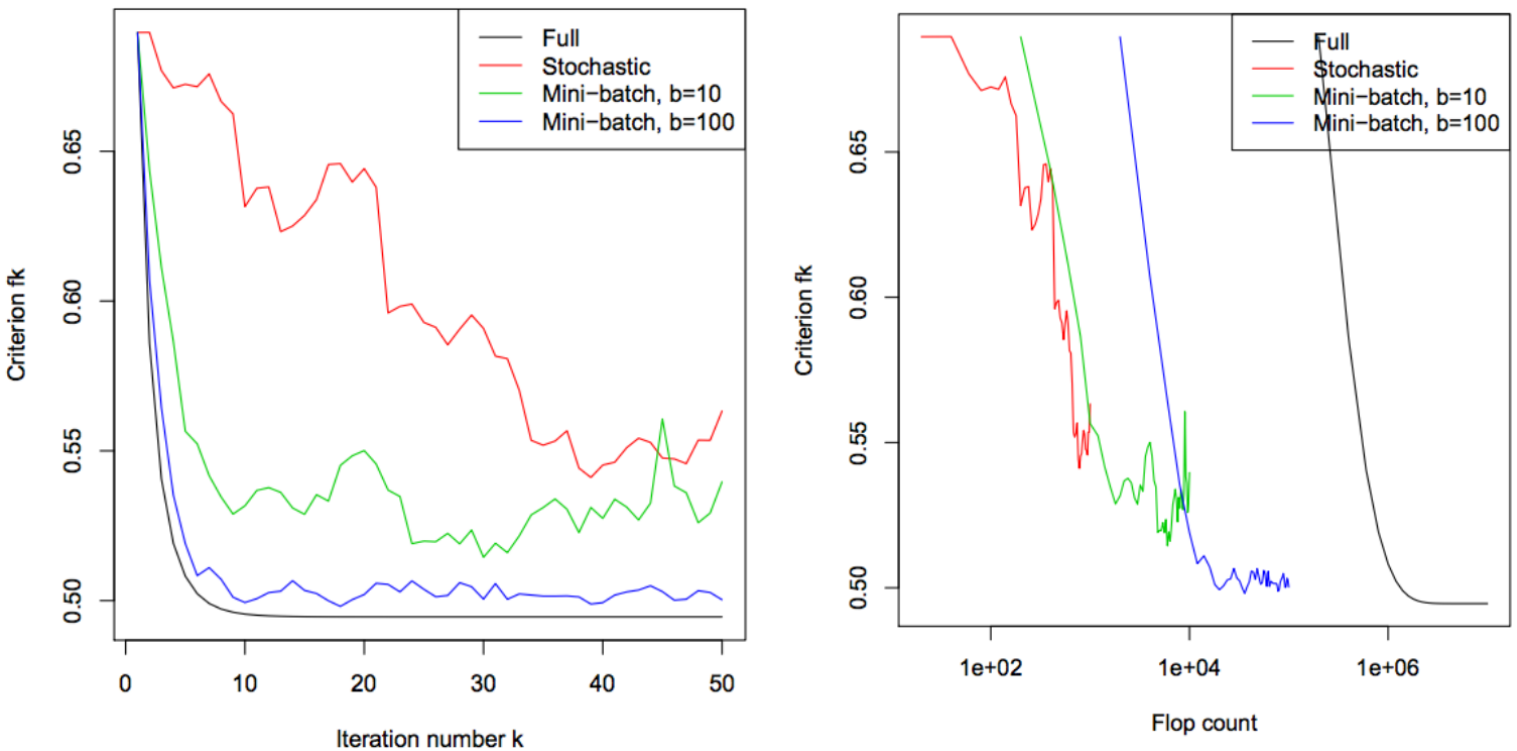

Figure: Iterations make better progress as mini-batch size is larger but also takes more computation time

SGD Recommendations

Randomly shuffle training examples

- Although theory says you should randomly pick examples, it is easier to make a pass through your training set sequentially
- Shuffling before each iteration eliminates the effect of order

Monitor both training cost and validation error

- Set aside samples for a decent validation set
- Compute the objective on the training set and validation set (expensive but better than overfitting or wasting computation)

SGD Recommendations

Check gradient using finite differences

- If computation is slightly incorrect can yield erratic and slow algorithm
- Verify your code by slightly perturbing the parameter and inspecting differences between the two gradients

Experiment with the learning rates using small sample of training set

- SGD convergence rates are independent from sample size
- Use traditional optimization algorithms as a reference point

SGD Recommendations

Leverage sparsity of the training examples

- For very high-dimensional vectors with few non zero coefficients, you only need to update the weight coefficients corresponding to nonzero pattern in $\mathbf{x}$

Use learning rates of the form $\eta_t = \eta_0(1 + \eta_0\lambda t)^{-1}$

- Allows you to start from reasonable learning rates determined by testing on a small sample
- Works well in most situations if the initial point is slightly smaller than best value observed in training sample

THANK YOU!