Elements of Linear Discriminant Functions

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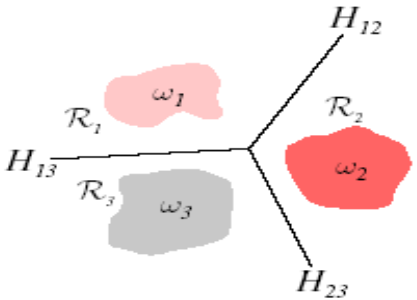
Introduction

- We assume here that the form of the discriminant functions $f_k(\boldsymbol{x};\boldsymbol{\theta}),\ k = 1,\dots,K$ is given, and that we can use the training data to estimate their parameters $\boldsymbol{\theta}$
  - In Part 4, instead, we assumed that the underlying probability densities were known

- These methods are known as *nonparametric*
  - No assumption on the form of the underlying data probability distributions is made

- We focus here on functions that are *linear* in $\boldsymbol{x}$, i.e., $f(\boldsymbol{x};\boldsymbol{\theta}) = \boldsymbol{w}^T\boldsymbol{x} + b$, with $\boldsymbol{\theta} = (\boldsymbol{w}, b)$

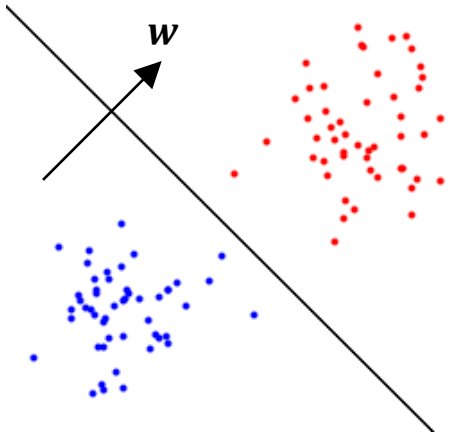


Example of linear discriminant functions on a 3-class classification problem

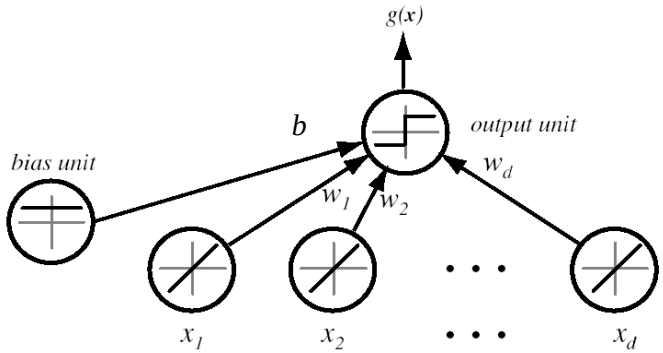
Linear Discriminant Functions

- **Linear function**: $f(\boldsymbol{x}) = \boldsymbol{w}^T\boldsymbol{x} + b = \sum_{j=1}^{d} w_j x_j + b$
  - $\boldsymbol{w}$ is the weight vector, and b the bias

- Two-class classification
  - Positive ($y = +1$) vs negative ($y = -1$) class
  - Decision rule: $y = \begin{cases} +1 & \text{if } f(\boldsymbol{x}) \geq 0 \\ -1, & \text{otherwise} \end{cases}$

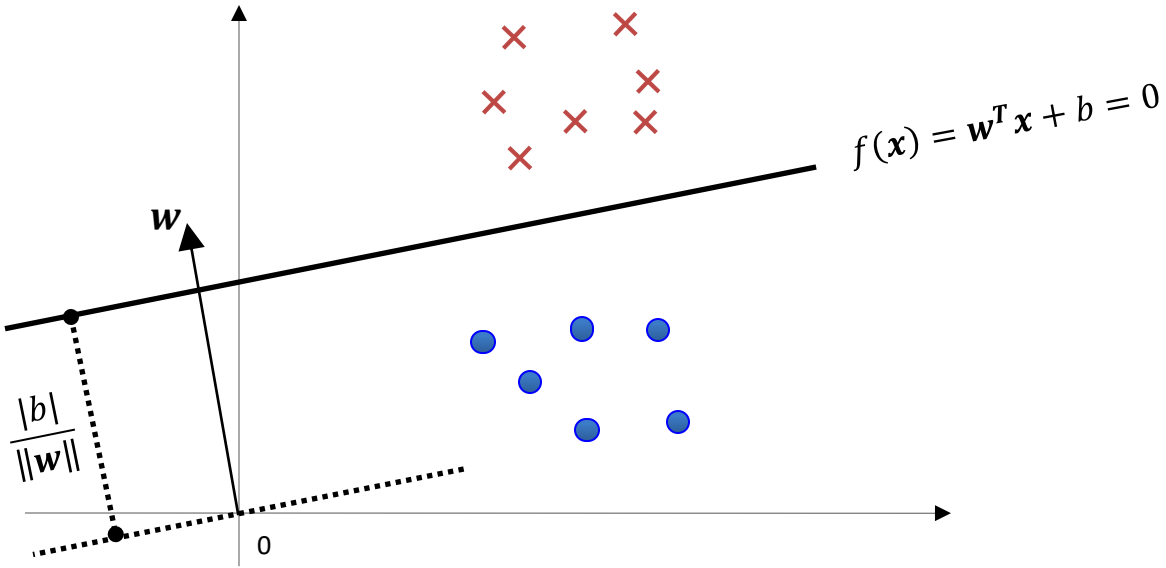


- **Graphical representation**
  - Each input feature value x_j is multiplied by the corresponding weight value w_j
  - Bias is multiplied by 1
  - The output unit sums all its inputs, computing $f(\boldsymbol{x})$ and thresholds it to estimate y (+1 or -1)



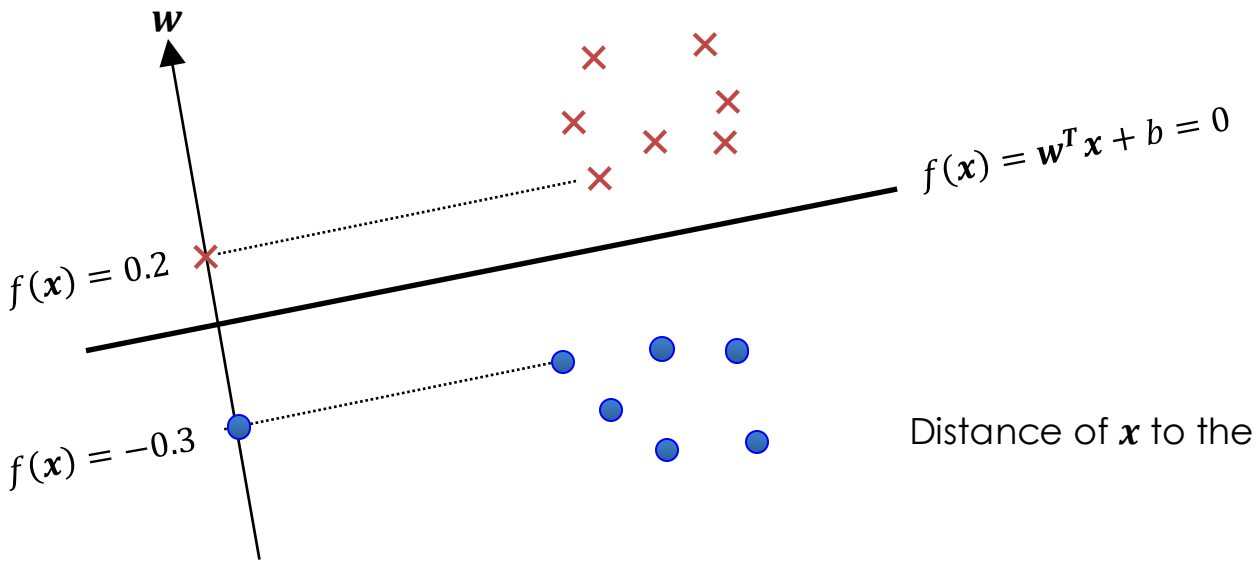
Linear Discriminant Functions

$\mathrm{D} = \{\boldsymbol{x}_i, y_i\}_{i=1}^{n}$
$\boldsymbol{x} \in \mathbb{R}^d$
$y \in \{-1, +1\}$



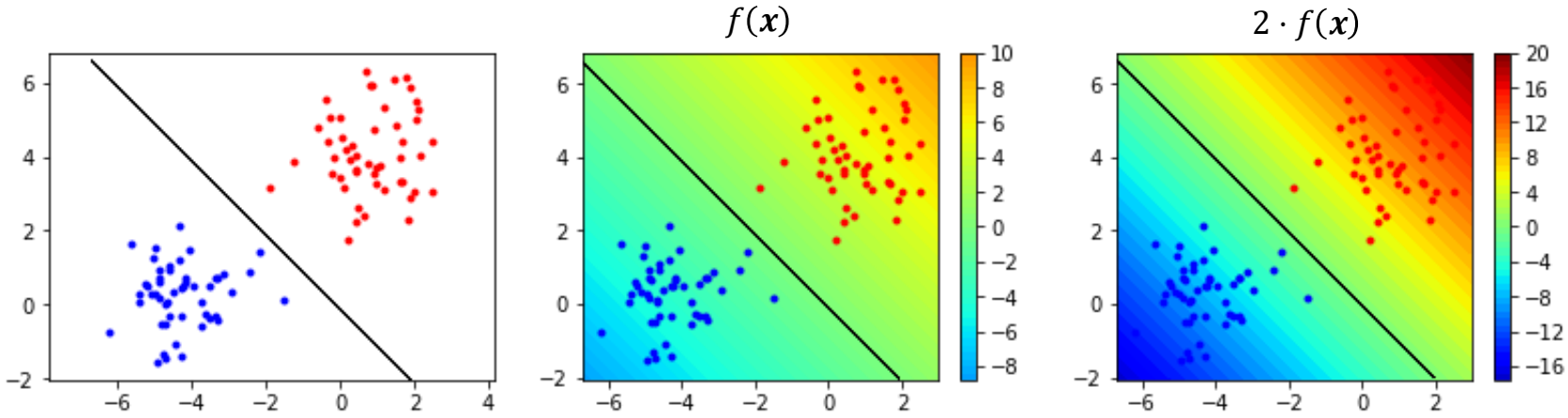
Linear Discriminant Functions

- The function $f(\boldsymbol{x}) = \boldsymbol{w}^T\boldsymbol{x} + b$ projects $\boldsymbol{x}$ onto the hyperplane normal
  - Its value is proportional to the distance of $\boldsymbol{x}$ to the hyperplane



Distance of $\boldsymbol{x}$ to the hyperplane: $\frac{|f(\boldsymbol{x})|}{\|\boldsymbol{w}\|}$

Linear Discriminant Functions



- By linearity, it is easy to see that multiplying $f(\boldsymbol{x})$ by a constant factor amounts to multiplying its parameters by the same factor
  - For example: $2 \cdot f(\boldsymbol{x}) = 2\,\boldsymbol{w}^T\boldsymbol{x} + 2b = \hat{\boldsymbol{w}}^T\boldsymbol{x} + \hat{b}$, with $\hat{\boldsymbol{w}} = 2\boldsymbol{w}$ and $\hat{b} = 2b$

- While the boundary at $f(\boldsymbol{x}) = 0$ does not change, the slope of the function changes!

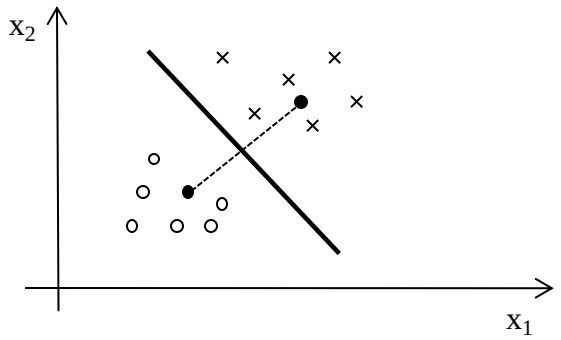
A Simple Example: The Nearest Mean Classifier (NMC)

- This classifier estimates the mean values $\boldsymbol{\mu_1}$ and $\boldsymbol{\mu_2}$ of the two classes from the training set and assigns unknown samples $\boldsymbol{x}^\star$ to the class with the smallest Euclidean distance:

$$d(\mathbf{x}^*, \boldsymbol{\mu}_2) \underset{\omega_2}{\overset{\omega_1}{\lessgtr}} d(\mathbf{x}^*, \boldsymbol{\mu}_1)$$

- It is easy to see that the decision boundary is the hyperplane perpendicular to the vector $(\boldsymbol{\mu_1} - \boldsymbol{\mu_2})$ and passing through the mean point $(\boldsymbol{\mu_1} + \boldsymbol{\mu_2})/2$

- Accordingly, the NMC is a linear classifier
  - Try to find its $\boldsymbol{w}$ and b parameter values!



Learning as an Optimization Problem

Learning as an Optimization Problem

- How do we estimate the classifier parameters $\boldsymbol{w}$ and b?

- Modern approaches formulate the learning problem as an **optimization problem**
  - This is generally true also for nonlinear classification functions $f(\boldsymbol{x}; \boldsymbol{\theta})$, including modern deep-learning approaches and neural networks

$$\boldsymbol{w}^\star, b^\star = \underset{\boldsymbol{w},b}{\operatorname{argmin}} \underbrace{\frac{1}{n}\sum_{i=1}^{n} \ell(y_i, f(\boldsymbol{x}_i))}_{\text{loss term } L(D,\boldsymbol{\theta})} + \underbrace{\lambda\, \Omega(\boldsymbol{w})}_{\text{regularization term } \Omega(\boldsymbol{w})}$$

λ: regularization hyperparameter

Learning as an Optimization Problem

- The loss function $\ell(y_i, f(\boldsymbol{x}_i))$ measures how much a prediction is wrong
  - e.g., the zero-one loss is 0 if points are correctly predicted, and 1 if they are not

- The regularization term $\Omega(\boldsymbol{\theta})$ imposes a penalty on the magnitude of the classifier parameters to avoid overfitting and promote smoother functions, i.e., functions that change more gradually as we move across the feature space

- The hyperparameter λ tunes the trade-off between the training loss and regularization
  - Larger values tend to promote more regularized functions but with a larger training error
  - Smaller values tend to reduce the training error but learn more complex functions

Learning as an Optimization Problem

- We start by considering a simplified setting in which we aim to find the best parameters $\boldsymbol{\theta} = (\boldsymbol{w}, b)$ that minimize the loss function $L(D, \boldsymbol{\theta})$, being $D = (\boldsymbol{x}_i, y_i)_{i=1}^{n}$ the training dataset:

$$\boldsymbol{\theta}^* = \text{argmin}_{\boldsymbol{\theta}} \, L(D, \boldsymbol{\theta}) = \frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f(\boldsymbol{x}_i; \boldsymbol{\theta}))$$

- The loss function quantifies the error that the classifier, parameterized by $\boldsymbol{\theta}$, is making on its predictions on the training data D
  - This is also known as the principle of **Empirical Risk Minimization (ERM)**

- How do we select the loss function $L(D, \boldsymbol{\theta})$ and solve the above problem?

Learning as an Optimization Problem

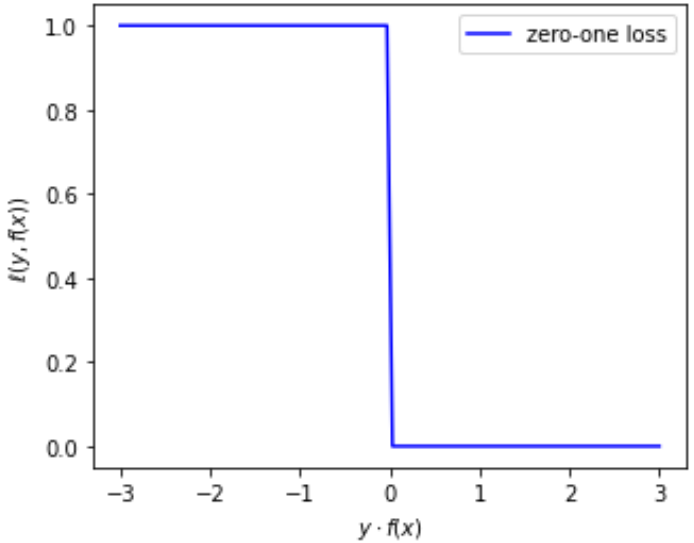
- In principle, we would like to minimize

$$L(D, \boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, f(\boldsymbol{x}_i; \boldsymbol{\theta}))$$

- where $\ell(y_i, f(\boldsymbol{x}_i; \boldsymbol{\theta}))$ is the zero-one loss
  - equal to 0 for correct predictions and 1 otherwise

$$\ell\big(y_i, f(\boldsymbol{x}_i; \boldsymbol{\theta})\big) = \begin{cases} 1, & \text{if } \; y \cdot f(\boldsymbol{x}) < 0 \\ 0, & \text{if } \; y \cdot f(\boldsymbol{x}) \geq 0 \end{cases}$$

- However, solving this problem directly is NP-hard and computationally inefficient
  - https://en.wikipedia.org/wiki/NP-hardness

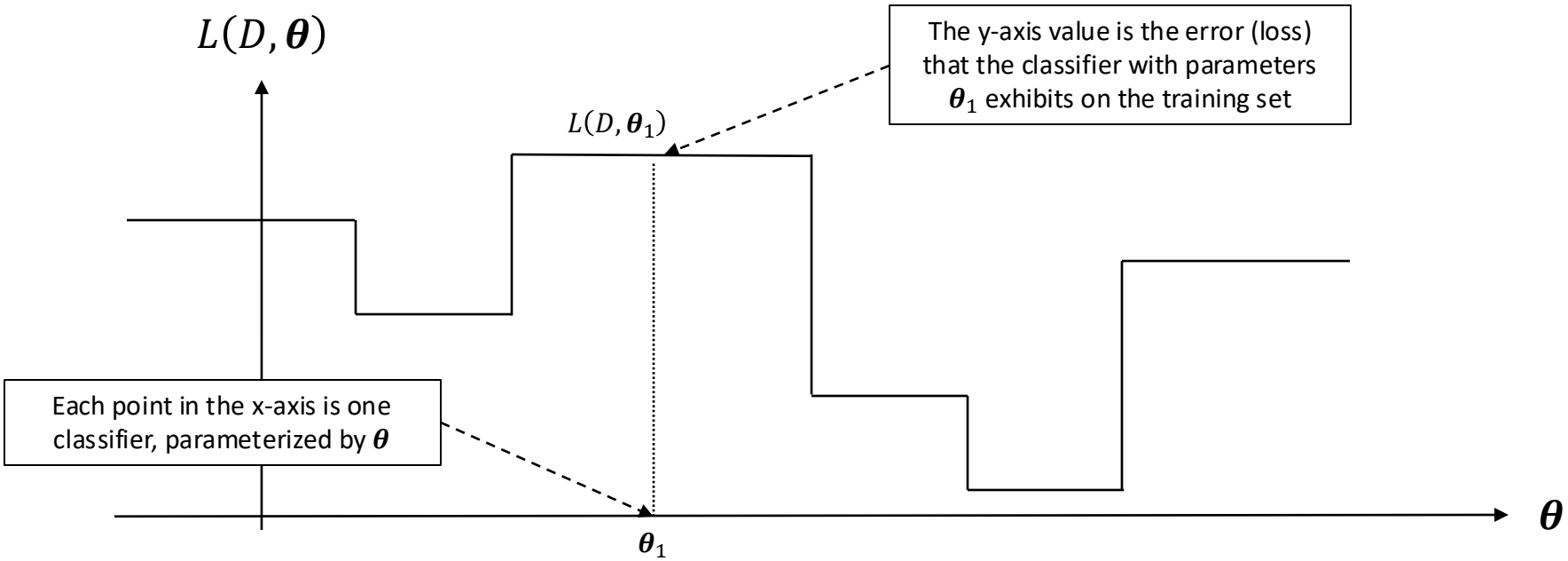


Note that $yf(\boldsymbol{x})$ is positive for correct predictions and negative for wrong ones.

For correct (wrong) predictions, y and $f(\boldsymbol{x})$ agree (disagree) in sign.

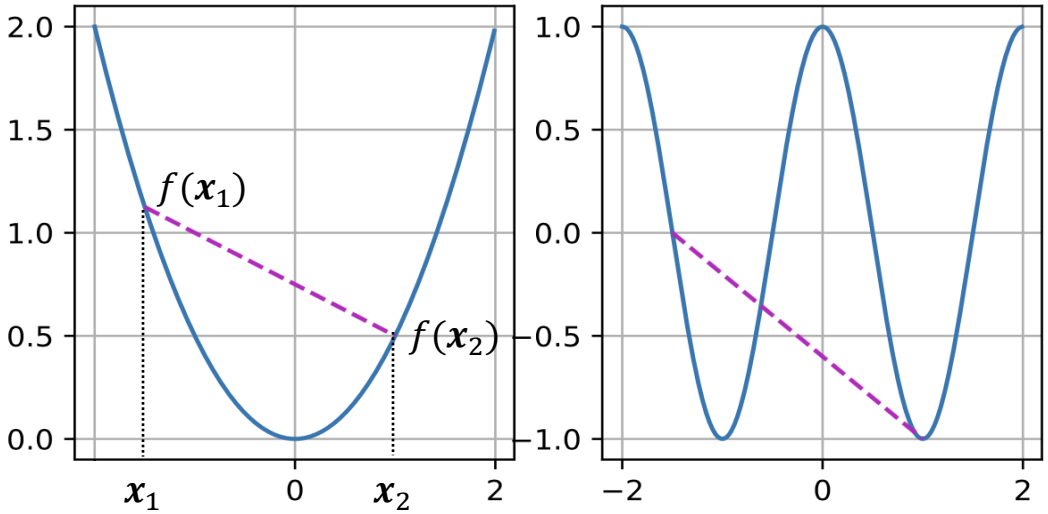
The Zero-One Loss Landscape

- Non convex, hard to optimize (flat regions, bad local minima)



Why Is Convexity Important for Optimization?

- **Convexity**: $f(\lambda \boldsymbol{x}_1 + (1-\lambda)\boldsymbol{x}_2) \leq \lambda f(\boldsymbol{x}_1) + (1-\lambda) f(\boldsymbol{x}_2), \quad \forall \boldsymbol{x}_1, \boldsymbol{x}_2, \quad \lambda \in [0,1]$



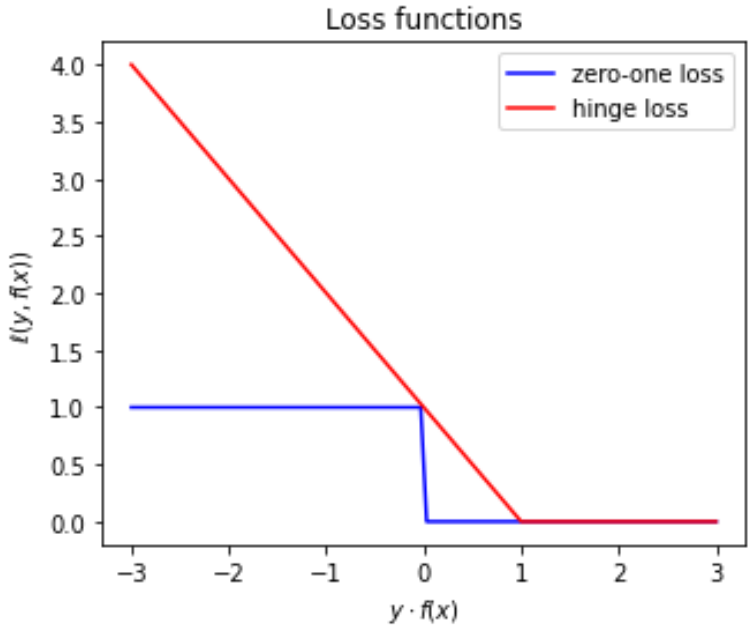
- **Desirable properties for optimization:** no local minima, convergence guarantees, etc.

Loss Functions

- Now, recall that we aim to minimize:

$$L(D, \boldsymbol{\theta}) = \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, f(\boldsymbol{x}_i; \boldsymbol{\theta}))$$

- being $\ell(y_i, f(\boldsymbol{x}_i; \boldsymbol{\theta}))$ the zero-one loss
- However, we know that minimizing this non-convex function is particularly difficult (NP hard)
- For this reason, convex (surrogate) loss functions are typically preferred
  - The tighter convex upper bound on the zero-one loss is called the **hinge loss**



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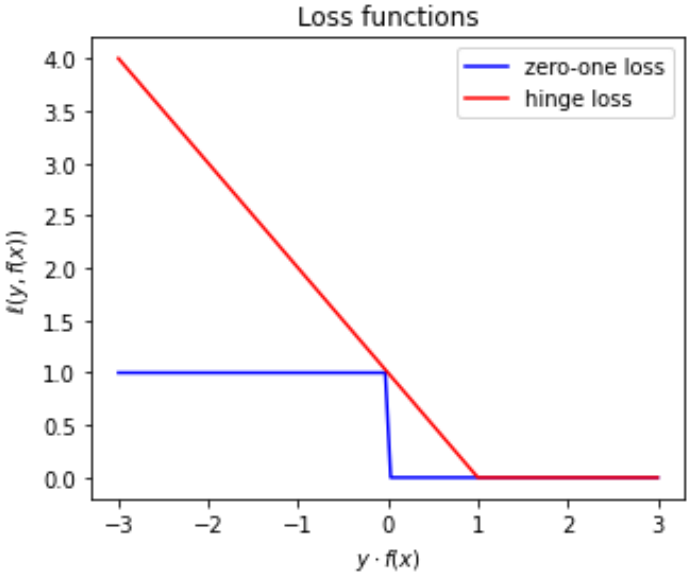
Hinge Loss

- The hinge loss is computed as:

$$\ell\big(y, f(\boldsymbol{x};\theta)\big) = \max(0, 1 - yf)$$

- It is the closest convex upper bound on the 0-1 loss
- Why are we interested in an upper bound?
  - since minimizing it, we also minimize the 0-1 loss
- Convexity helps find solutions efficiently while also providing guarantees on the optimality of the solution (global optima), algorithmic convergence, etc.
  - This is why convex surrogate functions are typically preferred in optimization



Note that $yf(\boldsymbol{x})$ is positive for correct predictions and negative for wrong ones

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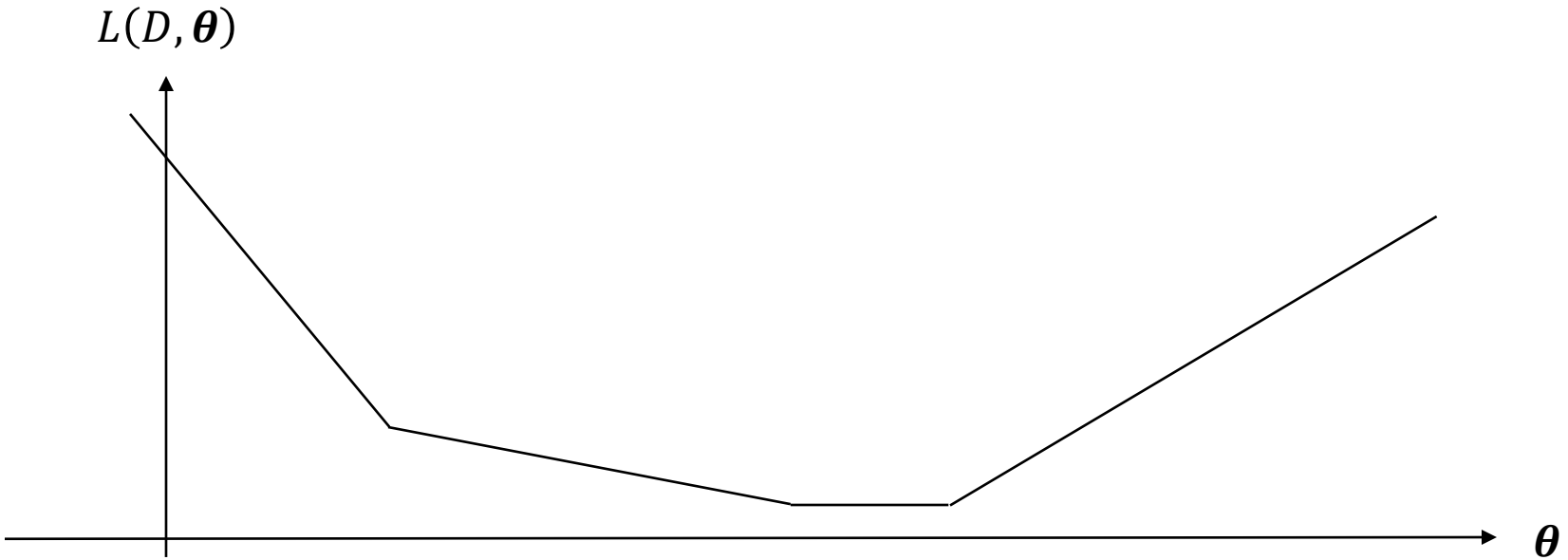
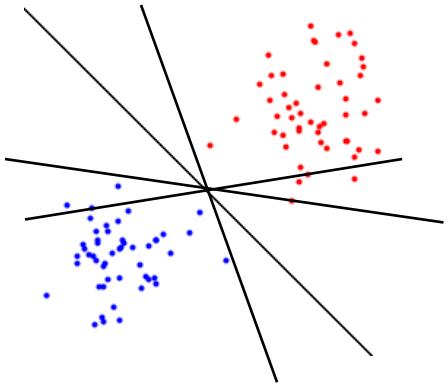
The Hinge Loss Landscape

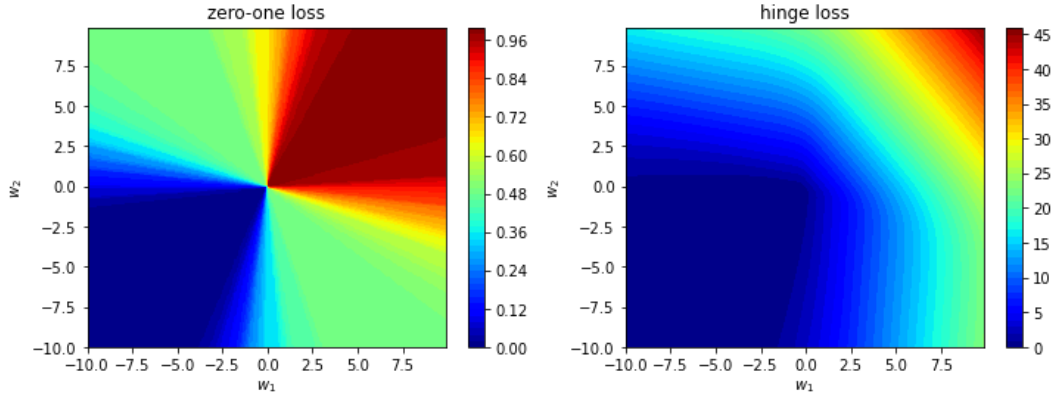
- Piecewise linear and convex, easier to optimize



A Closer Look at the Loss Minimization Problem

- Let's assume we fix $b = 0$ and aim to minimize the training loss only w.r.t. w_1, w_2
- Each pair w_1, w_2 thus represents a different linear classifier (passing through the origin)
- For each of these classifiers, we report the corresponding training loss in a colored plot
  - this will show us the optimization *landscape*, i.e., the surface of the function we aim to minimize





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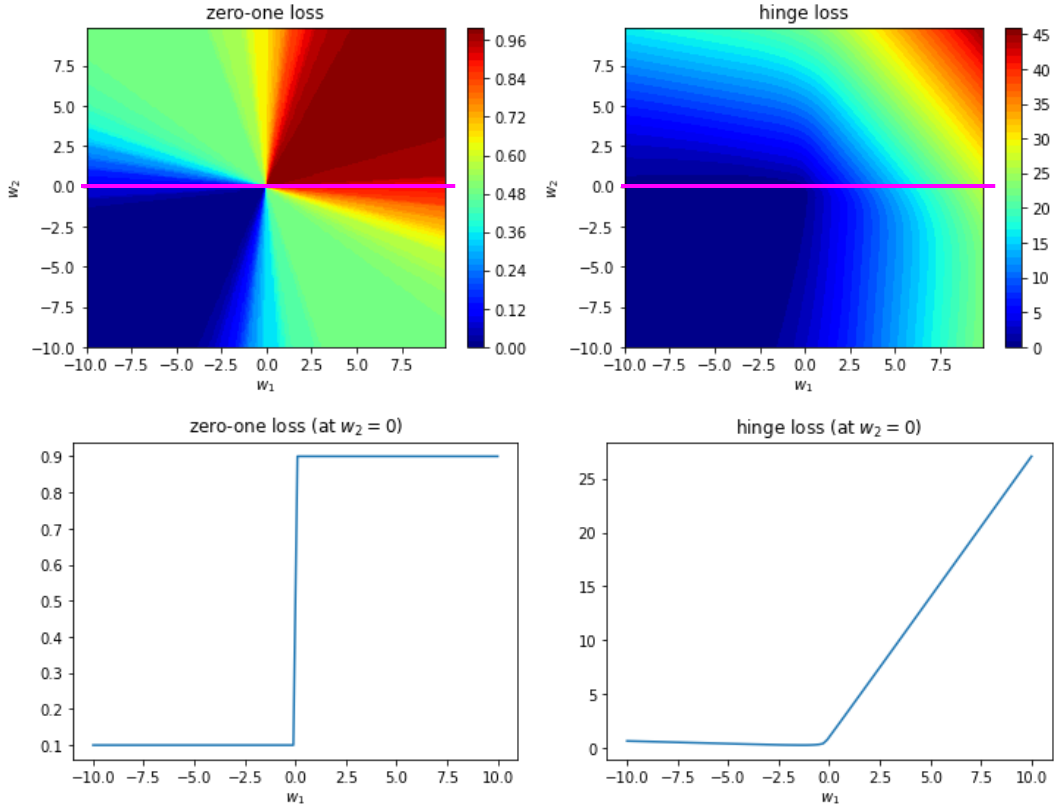
A Closer Look at the Loss Minimization Problem

- If we also fix $w_2 = 0$, and consider only optimizing w_1, we can also look at the profile of the loss along the line $w_2 = 0$
- Note how the zero-one loss again reports a sharp profile (behaving like a step function)
- The hinge loss instead decreases more gracefully towards one direction
- We can thus say that the hinge loss provides a **smooth** approximation to the 0-1 loss



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Loss Minimization with Gradient Descent

Gradient-based Optimization

- Optimizing *smooth* functions is much easier and efficient, as we can exploit **gradients**
  - This is not possible for the 0-1 loss (it is flat almost everywhere with gradients equal to zero)

- The key idea of gradient-based optimization is to start from a random point in the parameter space (*random initialization*) and then iteratively update the parameters along the gradient direction

- The gradient is the derivative of the loss function w.r.t. the classifier parameters:

$$L(D,\theta) = \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, f(\boldsymbol{x}_i;\theta)), \qquad \nabla_\theta L = \frac{1}{n}\sum_{i=1}^{n} \nabla_\theta \ell(y_i, f(\boldsymbol{x}_i;\theta))$$

- It is the direction in the parameter space along which the objective maximally increases
  - Following the negative gradient will thus minimize our training loss!

Gradient Descent (a.k.a. Steepest Descent)

- The simplest gradient-based optimizer is the **steepest-descent** method

```
1.  initialize θ, η, K, ε
2.  for k in {0, 1, ... , K − 1}:
3.      θ_{k+1} = θ_k − η∇L(θ_k)
4.      if |L(θ_k) − L(θ_{k+1})| < ε:
5.          break
```

- The parameters $\boldsymbol{\theta}$ are updated at each iteration, until
  - a maximum of K iterations are reached, or
  - the convergence/stop condition is met (lines 4-5 above)

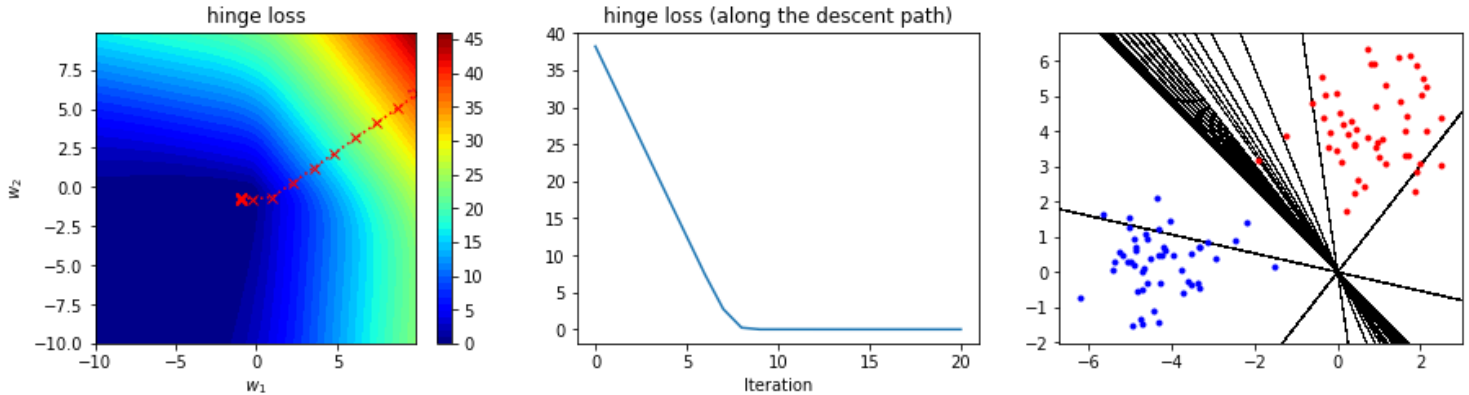
- The stop condition checks that the last update has not significantly modified the objective function (i.e., the training loss is almost constant, as ε is a small number)

- The learning rate (or gradient step size) η affects convergence. If it is too small, convergence is too slow; if it is too large, the gradient algorithm may not even converge at all. Usually η is reduced across iterations to ensure convergence

Steepest Descent on the Hinge Loss

- Consider again our running example. We start optimization from $w = (10, 6)$ and fix $b = 0$
  - See the notebook for details on the computation of the gradient of the hinge loss w.r.t. w, b

- Here's what the plots show:
  1. how weights change along the path until the local minimum (blue region) is reached
  2. how the hinge loss decreases along the path (convergence is reached when it becomes flat)
  3. how the linear classifier changes across iterations, converging to a solution that splits the training points achieving zero loss



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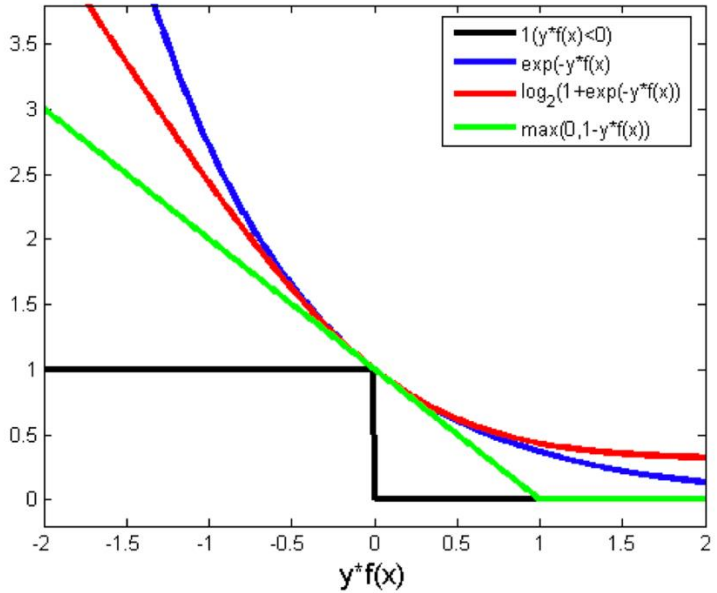
Other Convex Losses

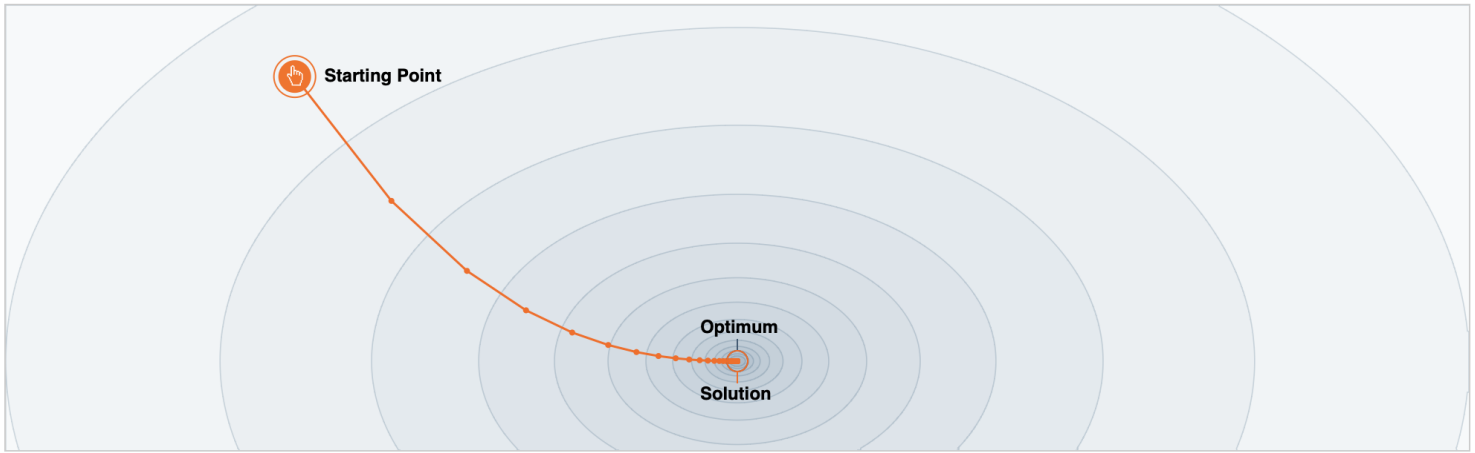
- Other convex upper bounds on the zero-one loss:
  - Hinge loss: $\ell\big(y, f(\boldsymbol{x})\big) = \max(0, 1 - yf)$
  - Exponential loss: $\ell\big(y, f(\boldsymbol{x})\big) = e^{-yf}$
  - Logistic loss: $\ell\big(y, f(\boldsymbol{x})\big) = \log_2(1 + e^{-yf})$



Gradient Descent: Step Size and Convergence

Example: Steepest Descent on Quadratic Objective

- Well-conditioned quadratic objective, small step size



Step-size α = 0.22

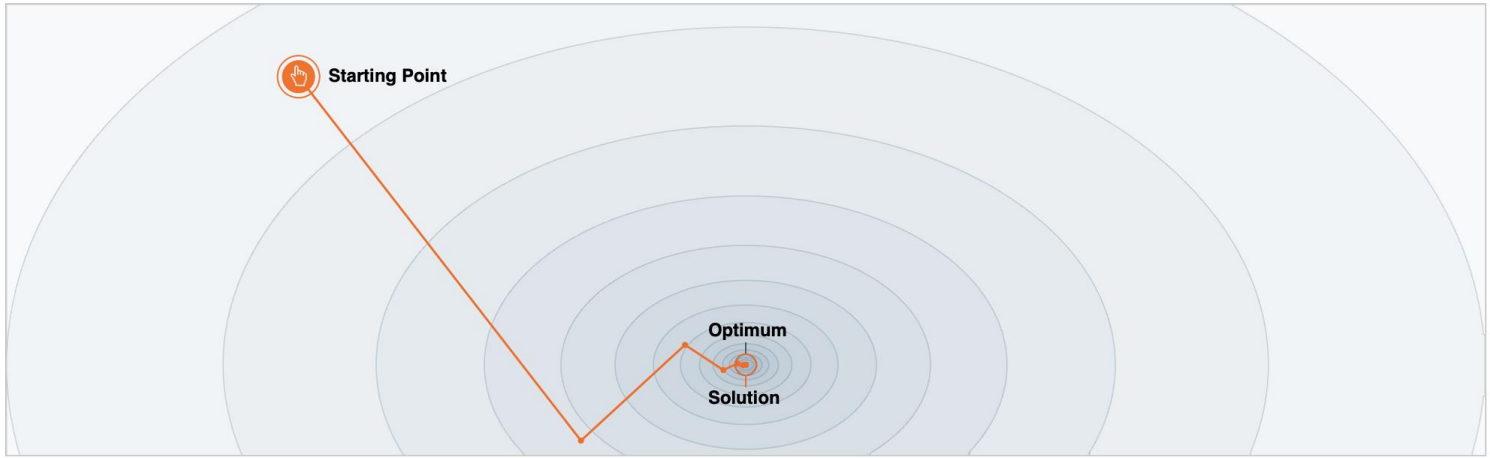
0 0.5 1.0

On a well-conditioned quadratic function, the gradient descent converges on few iterations to the optimum.

Examples from: http://fa.bianp.net/teaching/2018/eecs227at/gradient_descent.html

Example: Steepest Descent on Quadratic Objective

- Well-conditioned quadratic objective, large step size



Step-size α = 0.63

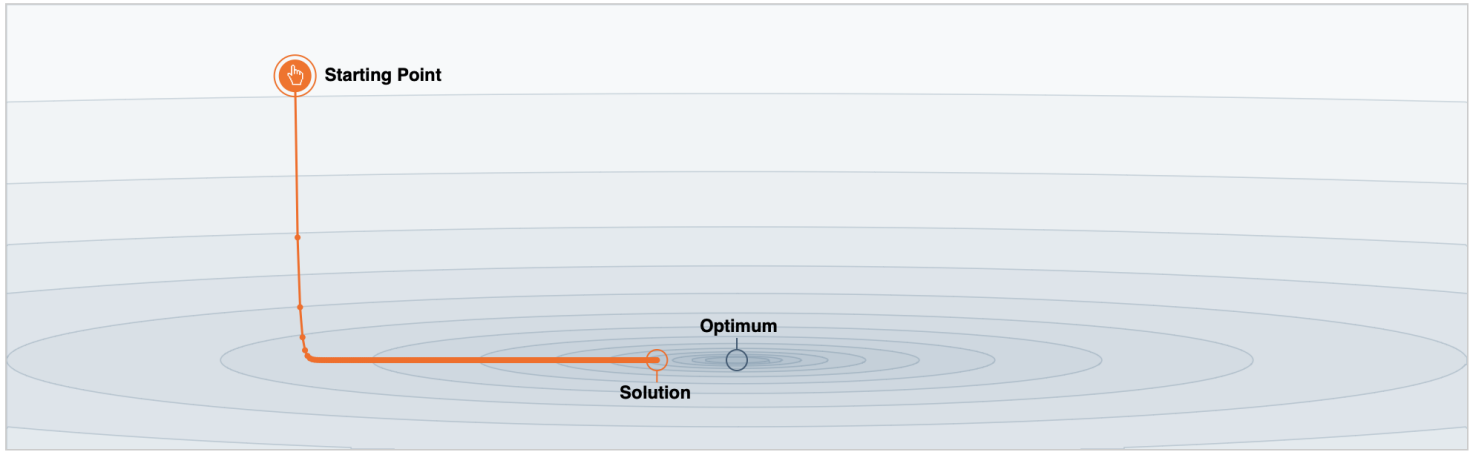
0 0.5 1.0

On a well-conditioned quadratic function, the gradient descent converges on few iterations to the optimum.

Examples from: http://fa.bianp.net/teaching/2018/eecs227at/gradient_descent.html

Example: Steepest Descent on Quadratic Objective

- Badly-conditioned quadratic objective, slow convergence



Step-size α = 0.63

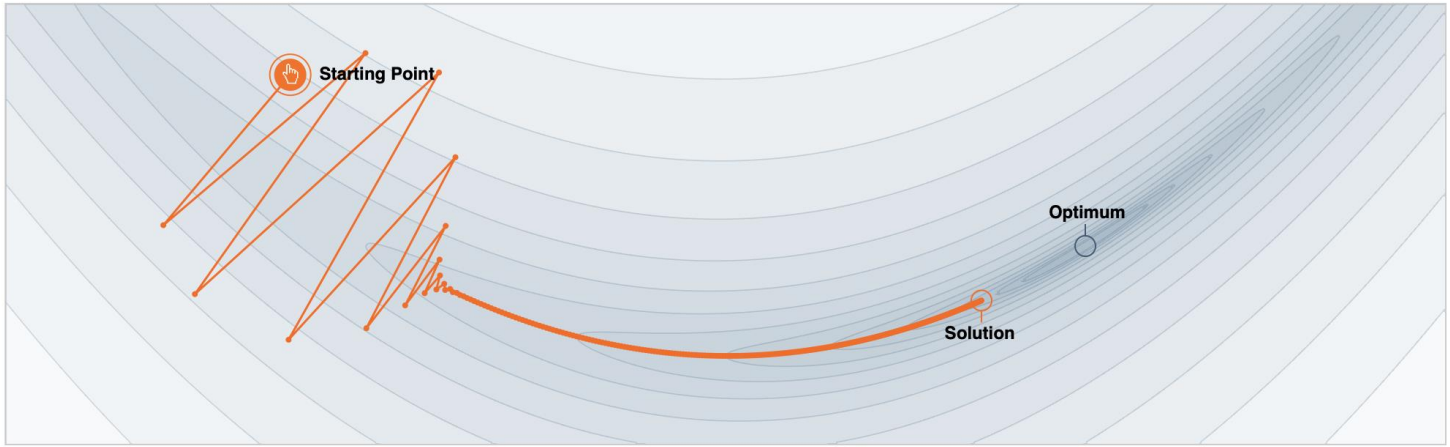
0 0.01 0.02

On a badly-conditioned quadratic function, the gradient descent converges takes many more iterations to converge than on the above well-conditioned problem. This is because gradient descent requires a much smaller step size on this problem to converge.

Examples from: http://fa.bianp.net/teaching/2018/eecs227at/gradient_descent.html

Example: Steepest Descent on Non-convex Objective

- Badly-conditioned non-convex objective, slow convergence and initial instability



Step-size α = 0.63

0 0.01 0.02

Gradient descent also converges on a badly-conditioned non-convex problem. Convergence is slow in this case.

Examples from: http://fa.bianp.net/teaching/2018/eecs227at/gradient_descent.html

Gradient Descent on Quadratic Objectives

Gradient Descent on Quadratic Objectives

- The steepest descent algorithm linearizes the function $L(D, \boldsymbol{\theta})$ around $\boldsymbol{\theta}$
  - It's a first-order Taylor expansion!
- If the function is quadratic or even non-convex, convergence may be too slow
- Alternatively, we can use a quadratic expansion for $L(D, \boldsymbol{\theta})$ around $\boldsymbol{\theta}$:

$$L(\boldsymbol{\theta}_{k+1}) \cong L(\boldsymbol{\theta}_k) + \nabla L(\boldsymbol{\theta}_k)(\boldsymbol{\theta}_{k+1} - \boldsymbol{\theta}_k) + \frac{1}{2}(\boldsymbol{\theta}_{k+1} - \boldsymbol{\theta}_k)^T \mathbf{H}_k (\boldsymbol{\theta}_{k+1} - \boldsymbol{\theta}_k)$$

- Note that $\mathbf{H}_k = \nabla^2_{\boldsymbol{\theta},\boldsymbol{\theta}} L(\boldsymbol{\theta}_k)$ is the Hessian matrix (containing the second derivatives)

Steepest Descent with Exact Step

- The quadratic expansion can be used to find the optimal step size η_k at each iteration
- If we plug-in the update rule: $\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \eta_k \nabla L(\boldsymbol{\theta}_k)$ in the previous expression, we obtain:

$$L(\boldsymbol{\theta}_{k+1}) \cong L(\boldsymbol{\theta}_k) - \eta_k \|\nabla L(\boldsymbol{\theta}_k)\|^2 + \frac{1}{2}\eta_k^2 \nabla L(\boldsymbol{\theta}_k)^T \mathbf{H}_k \nabla L(\boldsymbol{\theta}_k)$$

- The minimization of the quadratic form of $L(\boldsymbol{\theta}_{k+1})$ derived before can be solved in closed form, by setting the derivate with respect to η_k equal to zero, and solving for η_k
- The solution provides the optimal step size to be set at each iteration:

$$\eta_k = \frac{\|\nabla L(\boldsymbol{\theta}_k)\|^2}{\nabla L(\boldsymbol{\theta}_k)^T \mathbf{H}_k \nabla L(\boldsymbol{\theta}_k)}$$

Newton-Raphson Method

- The quadratic expansion below can be directly minimized via a closed-form solution

$$L(\boldsymbol{\theta}_{k+1}) \cong L(\boldsymbol{\theta}_k) + \nabla L(\boldsymbol{\theta}_k)(\boldsymbol{\theta}_{k+1} - \boldsymbol{\theta}_k) + \frac{1}{2}(\boldsymbol{\theta}_{k+1} - \boldsymbol{\theta}_k)^T \mathbf{H}_k(\boldsymbol{\theta}_{k+1} - \boldsymbol{\theta}_k)$$

- By setting the derivative of L w.r.t. $\boldsymbol{\theta}_k$ equal to 0, we obtain: $\nabla L(\boldsymbol{\theta}_k) + \mathbf{H}_k(\boldsymbol{\theta}_{k+1} - \boldsymbol{\theta}_k) = \mathbf{0}$
- The solution is the update rule for Newton-Raphson: $\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \mathbf{H}_k^{-1} \nabla L(\boldsymbol{\theta}_k)$

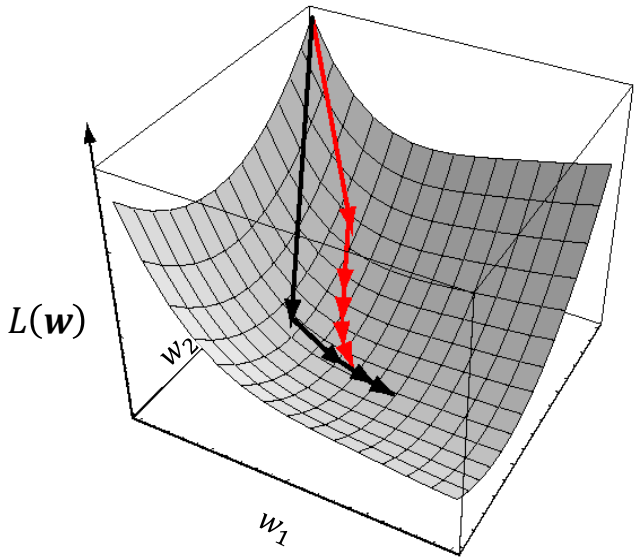
Newton-Raphson method

1. initialize θ, K, ε
2. for k in {0, 1, ... , $K-1$}:
3. $\boldsymbol{\theta}_{k+1} = \boldsymbol{\theta}_k - \mathbf{H}_k^{-1} \nabla L(\boldsymbol{\theta}_k)$
4. if $|L(\boldsymbol{\theta}_k) - L(\boldsymbol{\theta}_{k+1})| < \varepsilon$:
5. break

Example: Newton-Raphson vs Steepest Descent

- **Steepest descent** in red
- **Newton-Raphson** in black

- **Newton-Raphson**
  - **Pros.** Faster convergence
  - **Cons.** Hessian inversion is computationally expensive. If Hessian is badly conditioned, convergence may be problematic



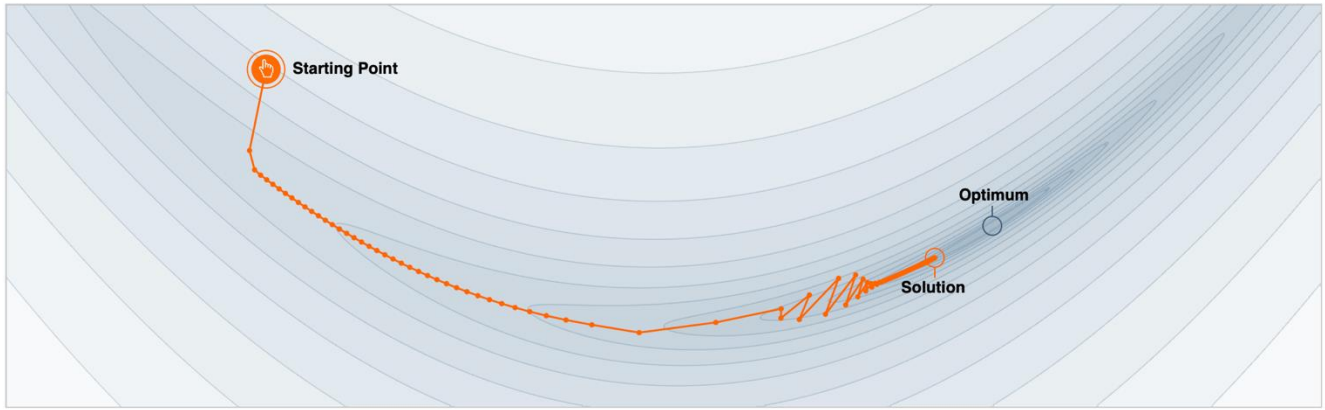
Example: Newton-Raphson on Quadratic Objective

- Exact solution in one iteration

Examples from: http://fa.bianp.net/teaching/2018/eecs227at/newton.html

Example: Newton-Raphson on Non-convex Objective

- Badly-conditioned non-convex objective, numerical instabilities in Hessian inversion



Examples from: http://fa.bianp.net/teaching/2018/eecs227at/newton.html

Tuning the Step Size

- In general, these quadratic approximations are computationally expensive, as they involve Hessian computation/inversion

- Lightweight **line-search methods** are thus preferred to find an approximate good step size at each iteration. See, e.g., *backtracking* line search:
  - http://fa.bianp.net/teaching/2018/eecs227at/gradient_descent.html

- Other strategies instead just decrease η_k at each iteration, with different decaying rates. See, e.g., *cosine annealing*:
  - https://towardsdatascience.com/https-medium-com-reina-wang-tw-stochastic-gradient-descent-with-restarts-5f511975163

Summary

- Linear classification functions for binary (2-class) classification
- Loss minimization principle (*learning the classifier parameters*)
  - Convex optimization / loss functions
- Gradient-based optimizers
  - Steepest descent
  - Newton-Raphson method
- Tuning the step size (*line-search and decay strategies*)

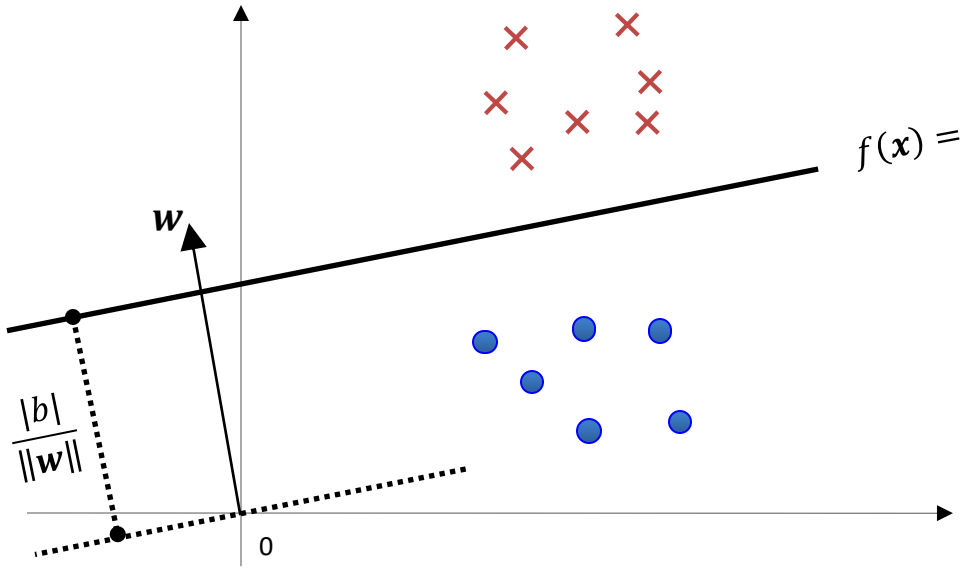
Support Vector Machines

Support Vector Machines (SVMs)

- State-of-the-art model with strong mathematical interpretation and significant practical relevance in many applications
- Invented by Russian mathematician Vladmir Vapnik in mid 1960s, and ideas much extended in 1990s
- Uses a specific type of loss function and learning algorithm
  - convex optimization / quadratic programming
- Can solve non-linearly separable problems

A Short Recap on Linear Discriminant Functions

$\mathrm{D} = \{\boldsymbol{x}_i, y_i\}_{i=1}^{n}$
$\boldsymbol{x} \in \mathbb{R}^d$
$y \in \{-1, +1\}$



$f(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x} + b = 0$

Distance of $\boldsymbol{x}$ to the hyperplane: $\frac{|f(\boldsymbol{x})|}{\|\boldsymbol{w}\|}$

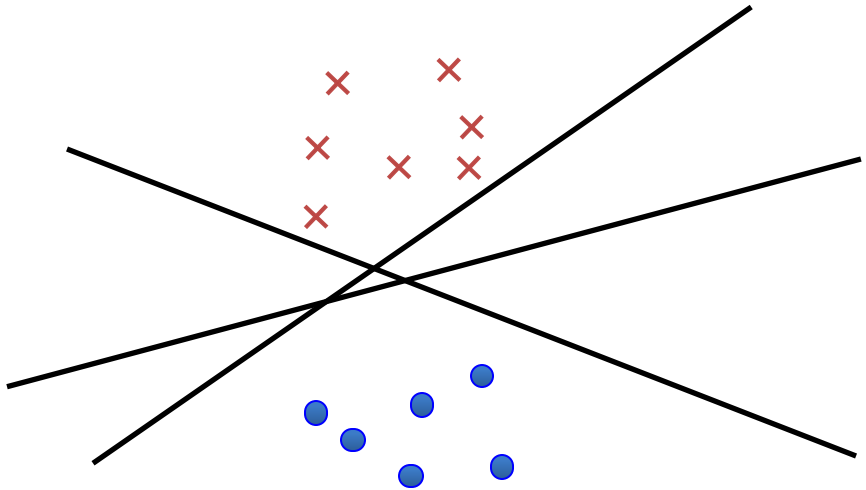
Support Vector Machines

The *“no maths”* version

Underlying Idea

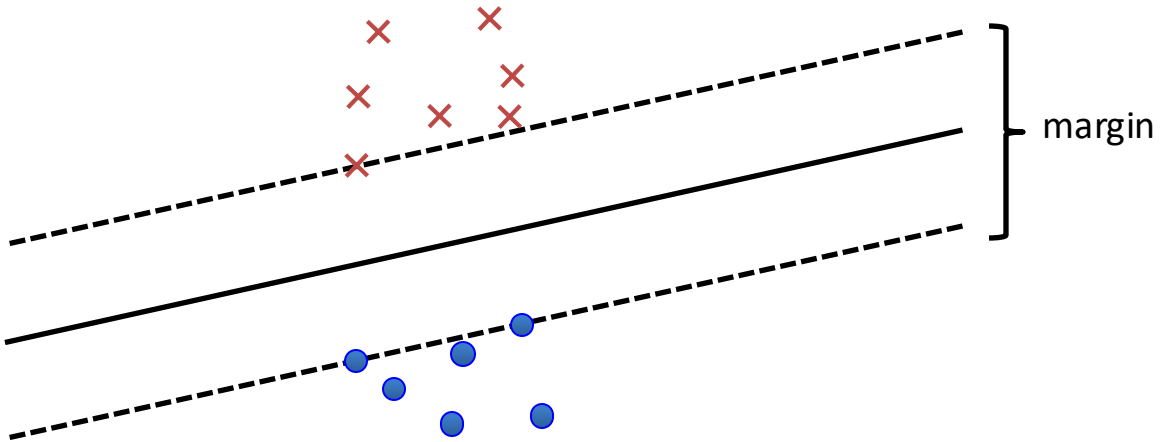
- Several possible decision boundaries
  - All get 100% accuracy on this training data

- Which one would you pick? Why?



Underlying Idea: Margin Maximization

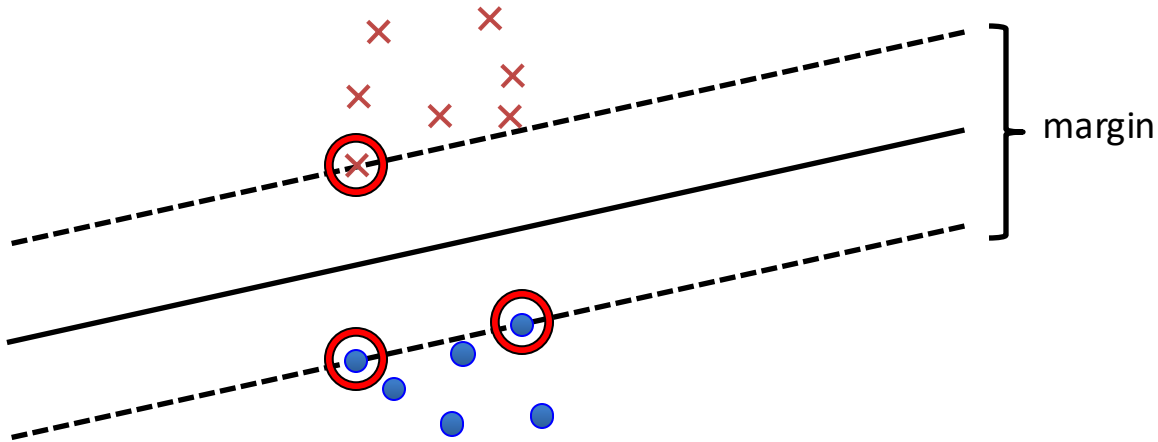
- The SVM finds this one – the furthest boundary from the two clusters



- Distance to the closest training points is called "margin"
  - equal on both sides of the boundary

Margin Maximization and Support Vectors

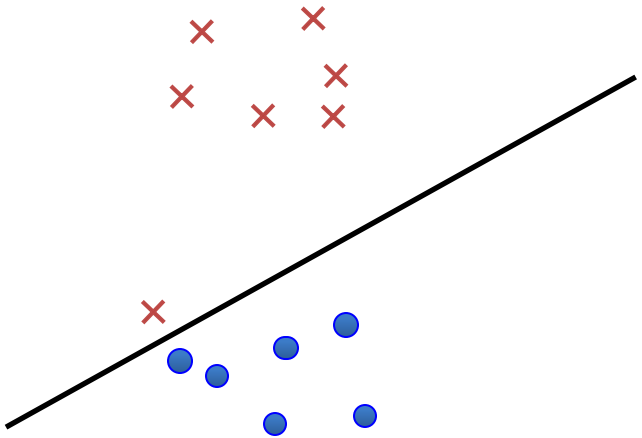
- The circled points are called ***support vectors***



- The decision hyperplane only depends on the SVs
  - the other points can move freely without violating the margin

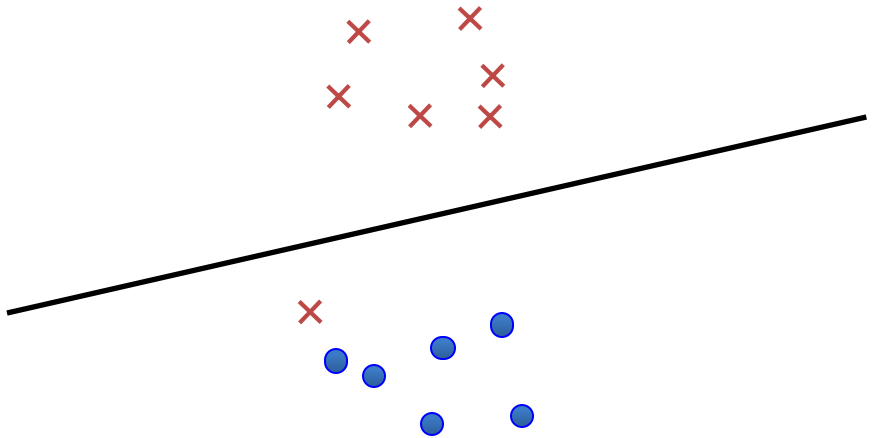
What About Outliers?

- This is the "optimal" boundary – doesn't seem so clever though

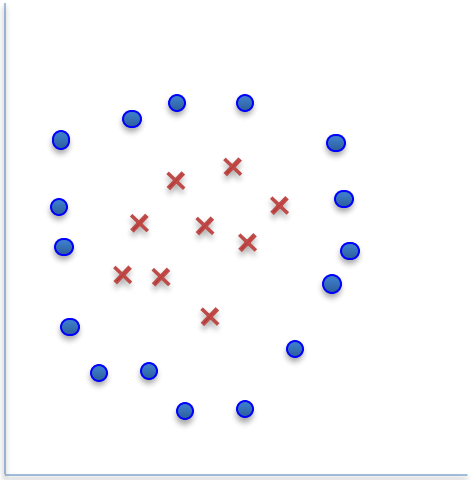


What About Outliers?

- SVM can selectively ignore certain data points (e.g., outliers)
  - soft-margin maximization

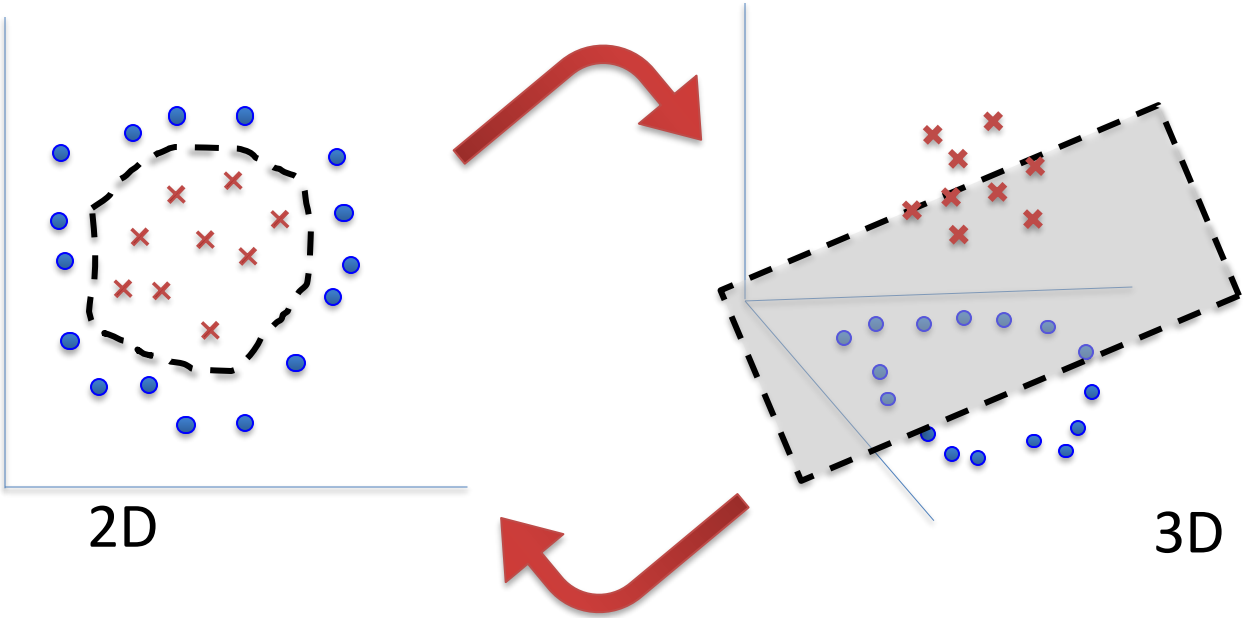


What If Data Is More Complex?



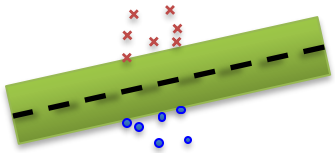
What If Data Is More Complex? Use Kernels!

- Project it onto a higher-dimensional space, and optimize a linear model
  - This amounts to learning a non-linear model in the input space

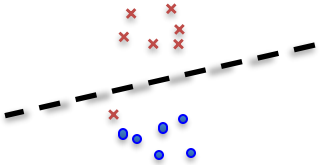


SVMs – Slightly More Technical Terms

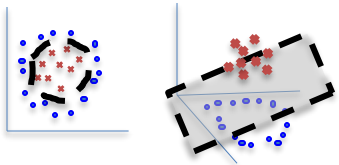
- Find the boundary with **maximum margin**



- Allow **soft-margin** violations to deal with outliers



- Use **kernels**, and the **kernel trick,** to solve nonlinear problems



Support Vector Machines

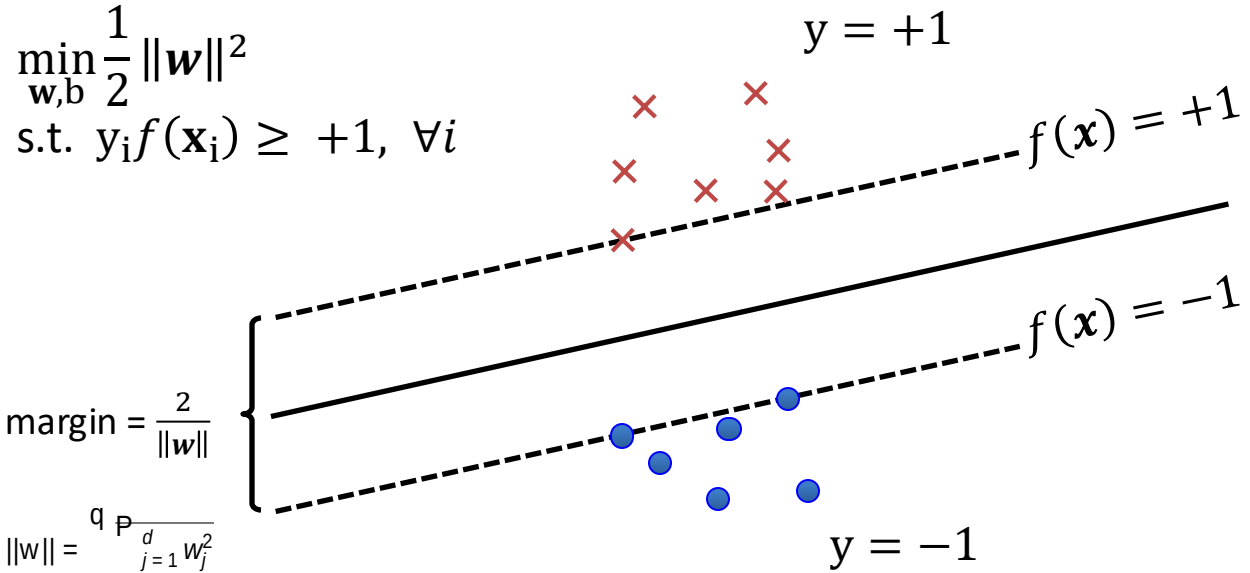
The *"some maths"* version

Hard-margin SVM (linearly-separable data)

- All points should be correctly classified (within the margin)

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

$$\text{s.t. } y_i f(\mathbf{x}_i) \geq +1, \ \forall i$$



The Problem of Margin Maximization

$$\text{minimise} \quad \frac{1}{2}\|\mathbf{w}\|^2$$

$$\text{subject to} \quad y_i f(\mathbf{x}_i) \geq 1, \quad i = 1, \ldots, N$$

- The above problem can be solved with the classical Lagrange optimization technique

$$L = \frac{1}{2}\|\mathbf{w}\|^2 - \sum_{i=1}^{\ell} \alpha_i \left[y_i \left(\mathbf{w} \cdot \mathbf{x}_i + b \right) - 1 \right]$$

$$\max_{\alpha_1, \ldots, \alpha_\ell} \min_{\mathbf{w}, b} L\left(\alpha_1, \ldots, \alpha_\ell, \mathbf{w}, b\right)$$

$$\text{s.t.} \quad \alpha_i \geq 0, \quad i = 1, \ldots, N$$

Deriving the Dual Form

- At the optimum, the derivatives of L w.r.t. **w** and b vanish, which gives:

$$\mathbf{w} = \sum_i \alpha_i y_i \mathbf{x}_i \qquad \sum_i \alpha_i y_i = 0.$$

- Substituting into L, we obtain the **dual problem for the hard-margin SVM**:

$$\begin{aligned} \max_{\boldsymbol{\alpha}} \ & \textstyle\sum_i \alpha_i - \frac{1}{2} \sum_{i,j} y_i \alpha_i \, \boldsymbol{x}_i^T \boldsymbol{x}_j \alpha_j y_j \\ \text{s.t.} \quad & \alpha_i \geq 0, \ \forall i \\ & \textstyle\sum_i \alpha_i y_i = 0 \, , \forall i \end{aligned}$$

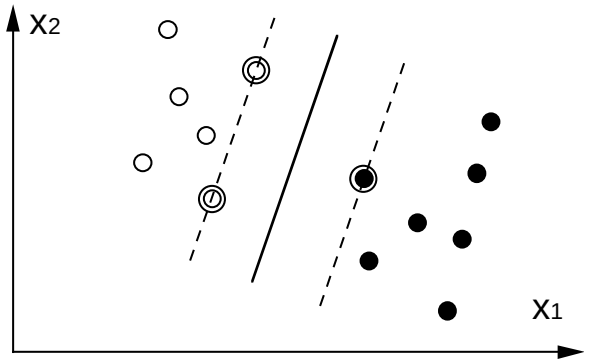
Support Vectors

- Lagrangian of the dual problem: $L_D(\alpha) = \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} y_i \alpha_i \, \boldsymbol{x}_i^T \boldsymbol{x}_j \alpha_j y_j$

- The optimal solution is the hyperplane:

$$\sum_{i=1}^{\ell} y_i \alpha_i \left(\mathbf{x}_i \cdot \mathbf{x}\right) + b = 0$$

- The samples for which $\alpha_i \neq 0$ are called the **support vectors**

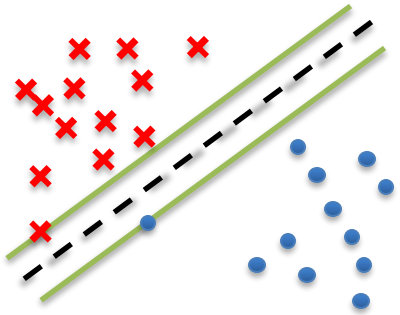


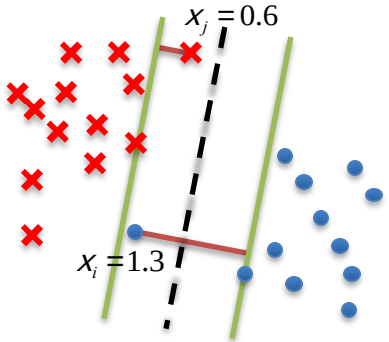
Soft-margin SVM

- What if data is not linearly separable / outliers? We allow points to violate the margin
- Trade-off between margin and loss on training data, tuned via the hyperparameter C

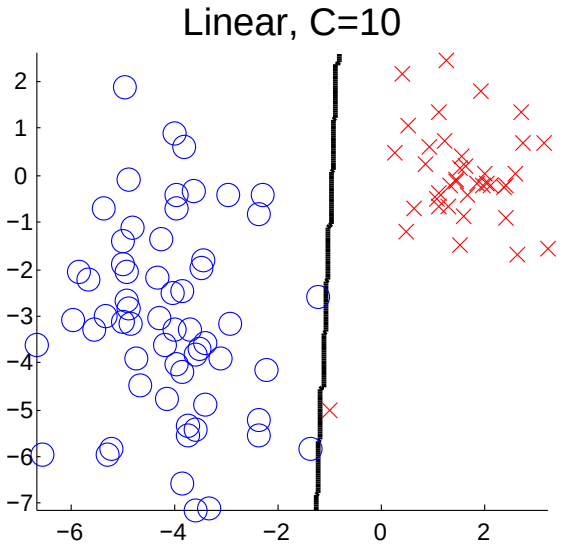
$$\min_{\mathbf{w},b,\xi_i} \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_i \xi_i$$
$$\text{s.t. } y_i f(\mathbf{x}_i) \geq 1 - \xi_i, \ \forall i$$
$$\xi_i \geq 0, \ \forall i$$

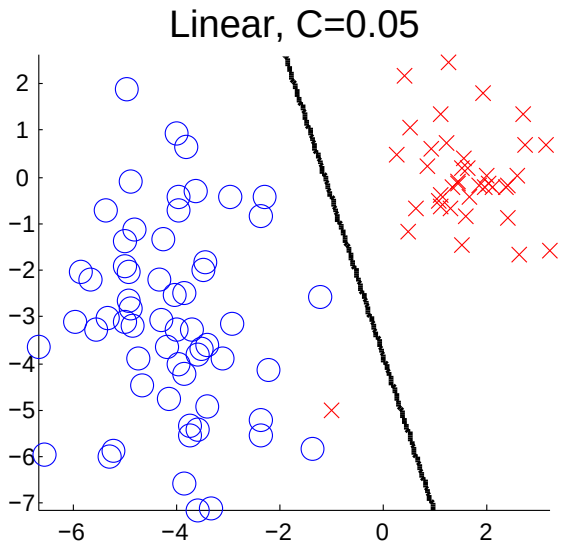
ξ_i: slack variables





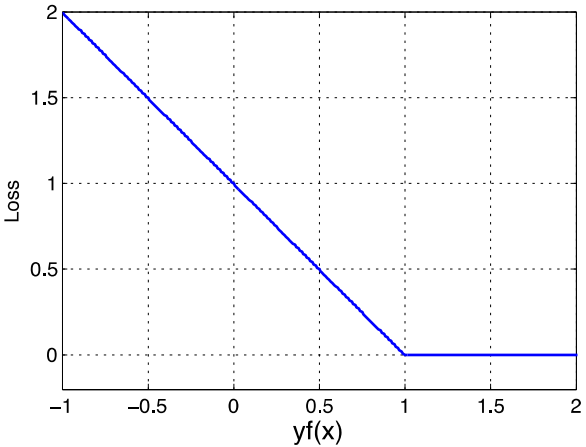
Effect of the Hyperparameter C





Slack Variables and the Hinge Loss

- The constraints $\xi_i \geq 1 - \mathrm{y_i} f(\mathbf{x_i})$, $\xi_i \geq 0$ are equivalent to $\xi_i = \max\left(0, 1 - \mathrm{y_i} f(\mathbf{x_i})\right)$
- That's exactly the **hinge loss**!
- We can use it to derive an unconstrained version of the primal problem:



$$\min_{\boldsymbol{w},b} \underbrace{\frac{1}{2}\|\boldsymbol{w}\|^2}_{\text{margin term}} + C \underbrace{\sum_i \max(0, 1 - y_i f(\boldsymbol{x}_i))}_{\text{hinge loss (summed over training points)}}$$

Dual form of the Soft-margin SVM

- Replacing the optimality conditions

$$\frac{\partial L_P}{\partial w_\nu} = w_\nu - \sum_i \alpha_i y_i x_{i\nu} = 0 \qquad \frac{\partial L_P}{\partial b} = -\sum_i \alpha_i y_i = 0 \qquad \frac{\partial L_P}{\partial \xi_i} = C - \alpha_i - \mu_i = 0$$

- ... into the Lagrangian of the primal problem,

$$L_P = \frac{1}{2}\|\mathbf{w}\|^2 + C\sum_i \xi_i - \sum_i \alpha_i\{y_i(\mathbf{x}_i \cdot \mathbf{w} + b) - 1 + \xi_i\} - \sum_i \mu_i \xi_i$$

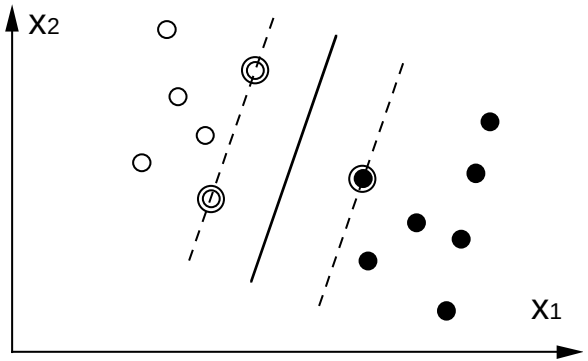
- we obtain:

$$\max_{\boldsymbol{\alpha}} \ \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} y_i \alpha_i \, \boldsymbol{x}_i^T \boldsymbol{x}_j \alpha_j y_j$$
$$\text{s.t.} \quad 0 \le \alpha_i \le C, \ \forall i$$
$$\sum_i \alpha_i y_i = 0 \, , \forall i$$

Sparsity of Support Vectors in SVMs

- Why do SVMs find only few support vectors?

$$\max_{\boldsymbol{\alpha}} \ \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} y_i \alpha_i \, \boldsymbol{x}_i^T \boldsymbol{x}_j \alpha_j y_j$$
$$\text{s.t.} \quad 0 \le \alpha_i \le C, \ \forall i$$
$$\sum_i \alpha_i y_i = 0 \, , \forall i$$



- The dual problem has a sparse solution
  - Many of the α values will be zero (*complementary slackness*)

- Karush-Kuhn-Tucker (equilibrium) conditions:

$$g_i = \frac{\partial W}{\partial \alpha_i} = \sum_j Q_{ij}\alpha_j + y_i b - 1 = y_i f(\mathbf{x}_i) - 1 \quad \begin{cases} \geq 0; & \alpha_i = 0 \\ = 0; & 0 < \alpha_i < C \\ \leq 0; & \alpha_i = C \end{cases}$$

Reserve vectors
Margin SVs
Error SVs

$$\frac{\partial W}{\partial b} = \sum_j y_j \alpha_j = 0$$

How to Solve Primal and Dual SVM learning?

- These are both Quadratic Programming (QP) problems

$$\min_{\mathbf{w},\mathrm{b},\xi_i} \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_i \xi_i$$
$$\text{s.t. } \mathrm{y_i} f(\mathbf{x_i}) \geq 1 - \xi_i, \ \forall i$$
$$\xi_i \geq 0, \ \forall i$$

$$\max_{\boldsymbol{\alpha}} \ \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} y_i \alpha_i \, \boldsymbol{x}_i^T \boldsymbol{x}_j \alpha_j y_j$$
$$\text{s.t. } 0 \leq \alpha_i \leq C, \ \forall i$$
$$\sum_i \alpha_i y_i = 0 \, , \forall i$$

- State-of-the-art QP solvers are standard and efficient

- However, dedicated (and much more efficient) solvers have been developed specifically for SVMs
  - **Sequential Minimal Optimization (SMO)** is one of them, used also in the popular LibSVM library

How to Solve Primal and Dual SVM learning?

- SMO however does not scale efficiently with the training set size
- Not appropriate to deal with modern, large data sets
- Modern techniques optimize directly the primal (unconstrained) form using Stochastic Gradient Descent (SGD) and subgradients
- Subgradients overcome the non-differentiability of the hinge loss when $yf(\boldsymbol{x}) = 1$

$$\min_{\boldsymbol{w},b} \frac{1}{2}\|\boldsymbol{w}\|^2 + C\sum_i \max(0,1 - y_i f(\boldsymbol{x}_i))$$

Stochastic Gradient Descent (SGD)

- Set the learning rate η (using decay if needed)

- Repeat until an approximate minimum is obtained:
  - Randomly select K samples from the training data (i.e., one batch)
  - Update parameters $w' = w - \eta \nabla L$ using the K samples

- **Pros**: several variants of this algorithm have been proposed
  - They are very efficient – and incremental
  - Data loading in batches avoids keeping the full dataset in memory
  - Convergence is well studied and often satisfied in practice

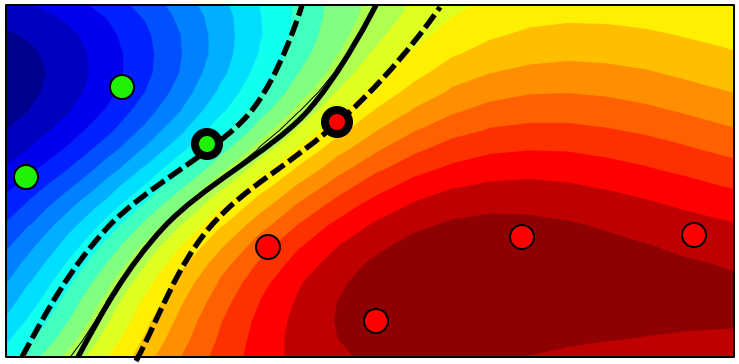
- **Cons**: parameters (e.g., learning rate) can be difficult to tune

The Kernel Trick

- Soft-margin SVM deals with non-linearly separable data but it is still a linear classifier
  - It exhibits poor performance if data is not properly shaped or "mostly" linearly separable

- The *kernel trick* overcomes this limitation by allowing us to learn an **SVM with a nonlinear decision function in input space!**

How?



The Kernel Trick

- The dual SVM formulation reveals that both the learning problem and classification can be expressed only in terms of **scalar products** between samples!

$$\max_{\boldsymbol{\alpha}} \ \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} y_i \alpha_i \, \boldsymbol{x}_i^T \boldsymbol{x}_j \alpha_j y_j$$
$$\text{s.t.} \quad 0 \leq \alpha_i \leq C, \ \forall i$$
$$\sum_i \alpha_i y_i = 0 \, , \forall i$$

$$f(\boldsymbol{x}) = \boldsymbol{w}^T \boldsymbol{x} + b = \sum_i y_i \alpha_i \, \boldsymbol{x}_i^T \boldsymbol{x}$$

- It also holds for the primal form, thanks to this property:
  - see the *Representer Theorem* for further details

$$\mathbf{w} = \sum_i \alpha_i y_i \mathbf{x}_i$$

The Kernel Trick

- We are not required to compute the scalar product in the input space
- We can use any function $k(\boldsymbol{x}_i, \boldsymbol{x}_j) = \boldsymbol{\phi}(\boldsymbol{x}_i)^T \boldsymbol{\phi}(\boldsymbol{x}_j)$ given that it implicitly corresponds to a scalar product in some other space (Mercer's condition)

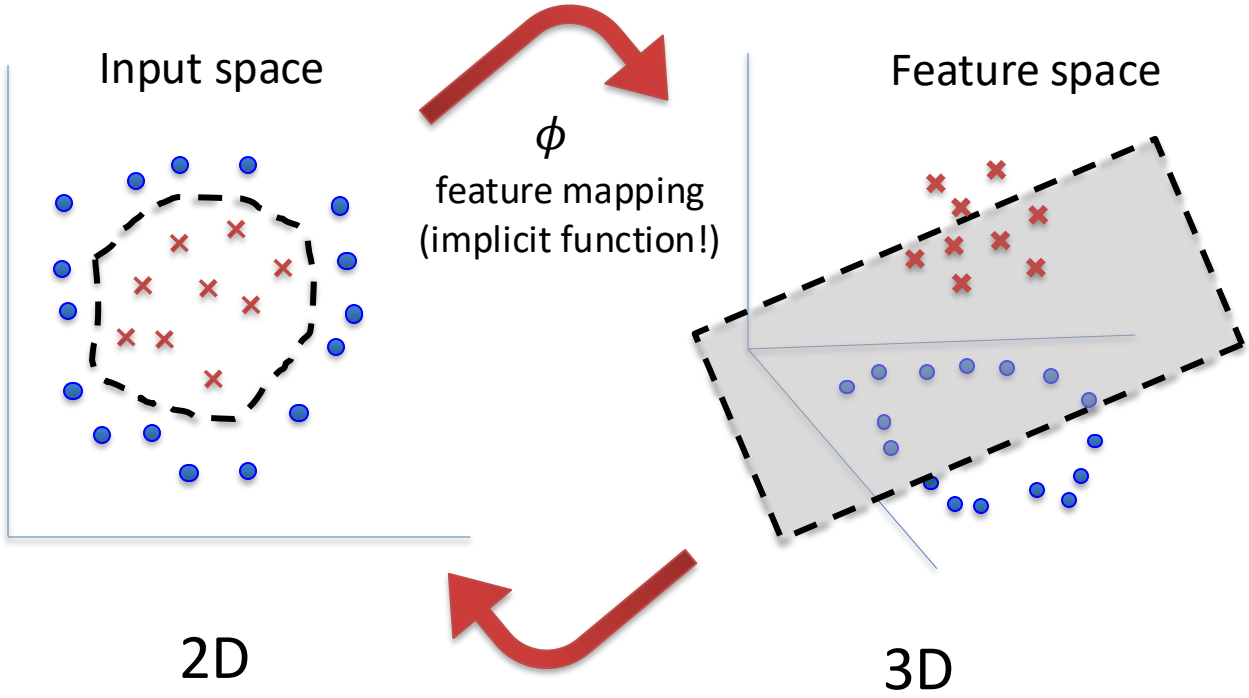
- Kernel functions are symmetric and positive semi-definite (PSD) if

$$\sum_{i,j=1}^{n} c_i c_j K(x_i, x_j) \geq 0 \qquad (1.1)$$

holds for any $n \in \mathbb{N}, x_1, \ldots, x_n \in \mathcal{X}, c_1, \ldots, c_n \in \mathbb{R}$.

- **Note**: SVMs also converge when using symmetric non-PSD kernels (although the learning problem is no longer convex)

The Kernel Trick



Cover's Theorem on Separability of Patterns

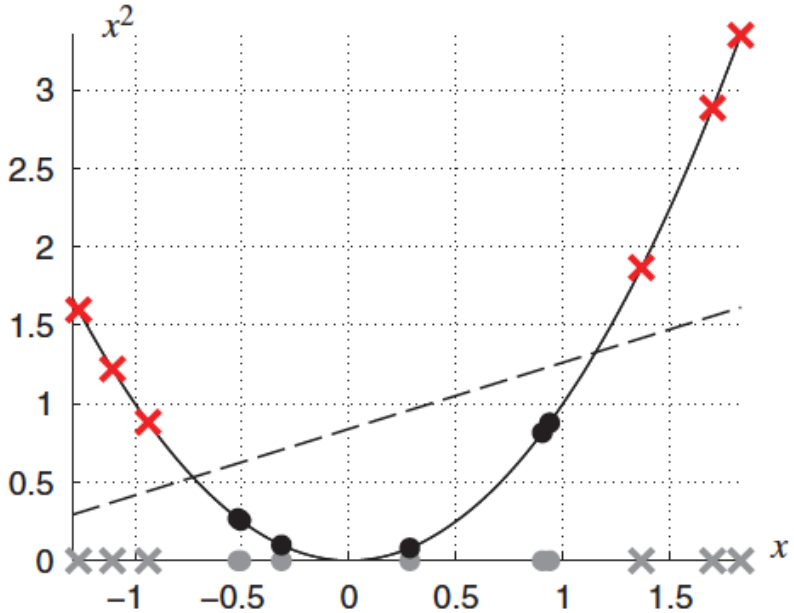
- "*A complex pattern-classification problem cast in a high-dimensional space non-linearly is more likely to be linearly separable than in a low-dimensional space*"

- The power of SVMs resides in the fact that they represent a robust and efficient implementation of Cover's theorem

- SVMs operate in two stages
  - Perform a non-linear mapping of the input vector x onto a high-dimensional space that is hidden from the inputs or the outputs
  - Construct an optimal separating hyperplane in the high-dimensional feature space

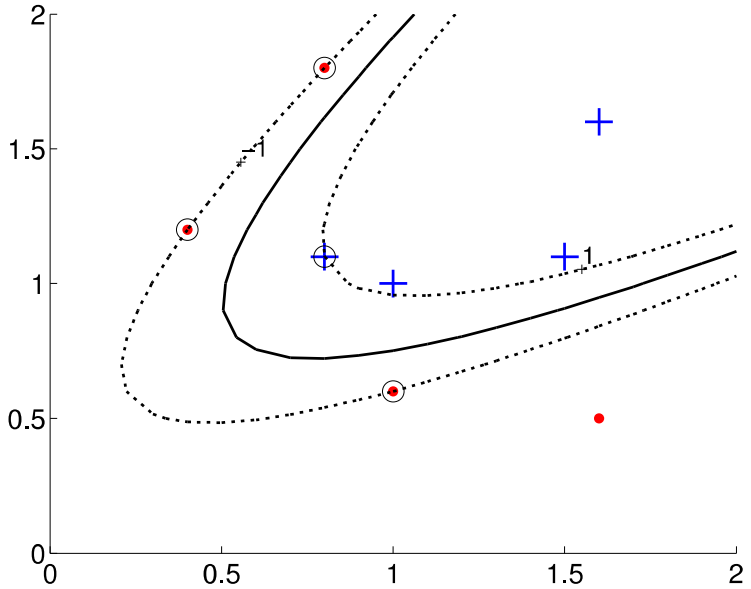
Cover's Theorem on Separability of Patterns

- *"A complex pattern-classification problem cast in a high-dimensional space non-linearly is more likely to be linearly separable than in a low-dimensional space"*



Polynomial Kernel, with d=2

$$K(\mathbf{x}_i, \mathbf{x}') = (1 + \mathbf{x}_i^T \mathbf{x}')^d$$



The Polynomial Kernel

$$K(\mathbf{x}_i, \mathbf{x}') = (1 + \mathbf{x}_i^T \mathbf{x}')^d$$

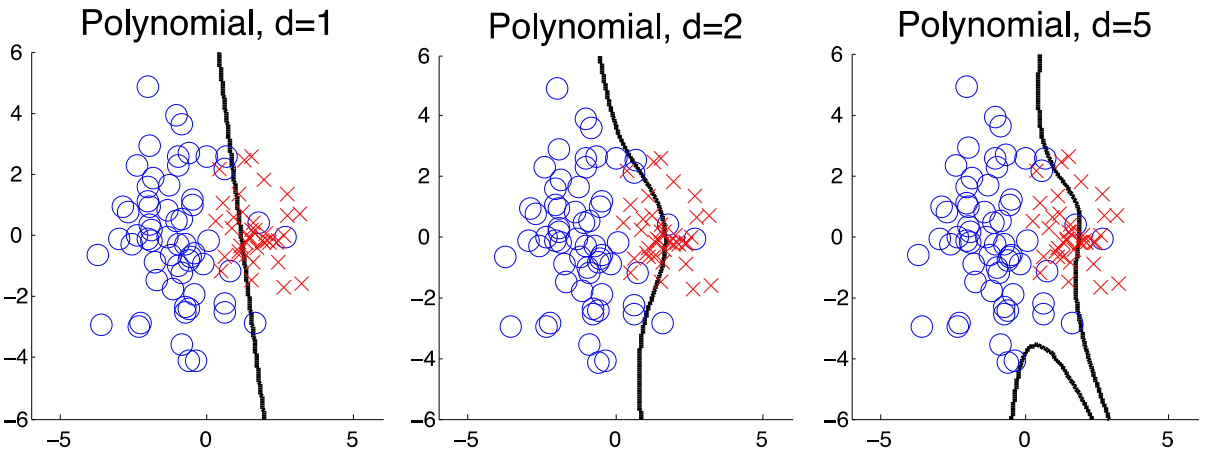
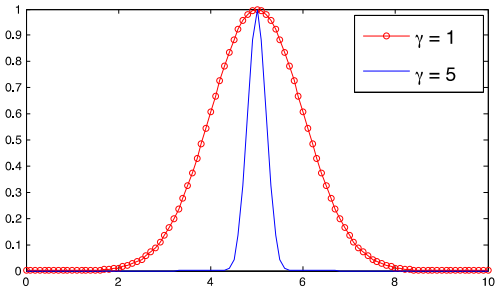
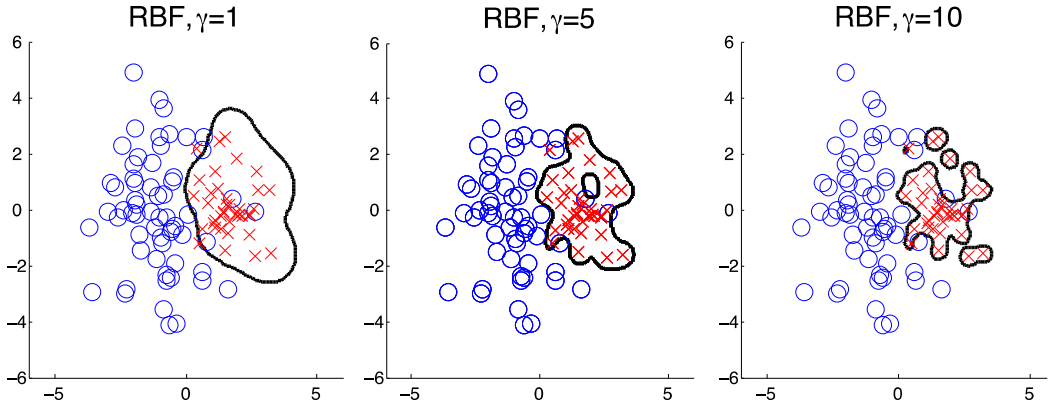


Figure 4.6: The effect of the degree parameter when using a polynomial kernel.

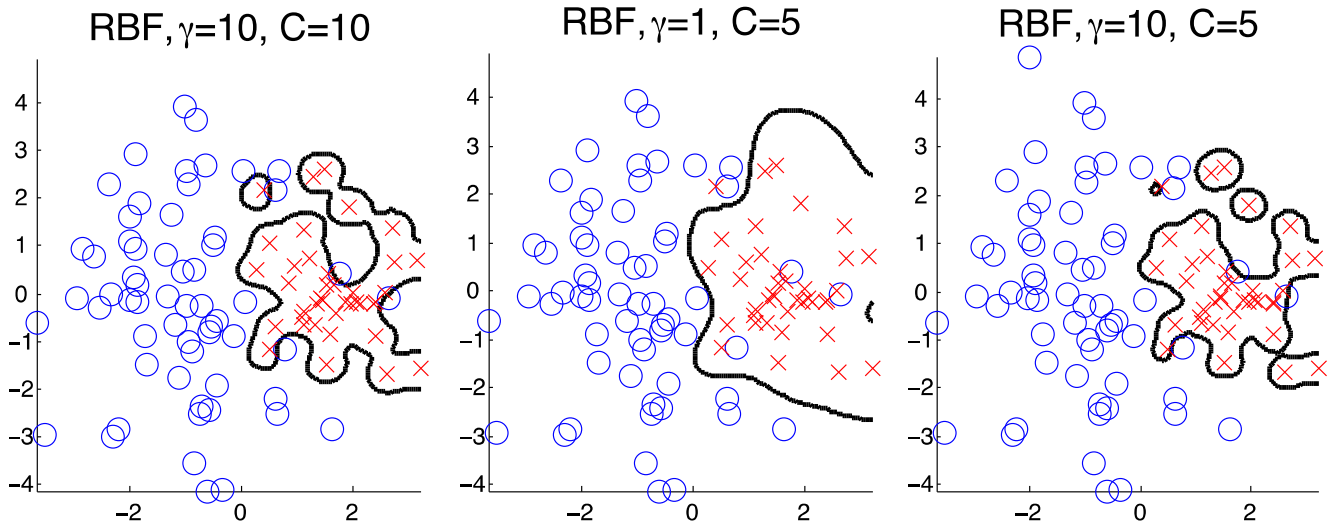
The Gaussian Kernel (Radial Basis Function, RBF)

$$K(\mathbf{x_i}, \mathbf{x}') = e^{-\gamma(\mathbf{x}_i - \mathbf{x}')^2}$$





Playing with the Hyperparameters



Suggested Readings

A Tutorial on Support Vector Machines for Pattern Recognition

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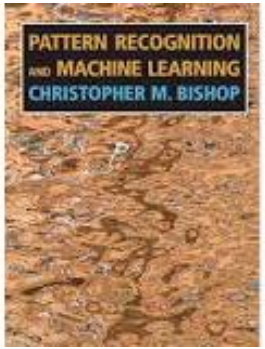


Pattern Recognition and Machine Learning
Book by Christopher Bishop

Chapter 7

Convex Optimization
Stephen Boyd and Lieven Vandenberghe

Cambridge University Press

More on Linear Classifiers

More on Linear Classifiers

- The unconstrained version of the SVM primal problem...

$$\min_{\boldsymbol{w},b} C \sum_i \max(0, 1 - y_i f(\boldsymbol{x}_i)) + \frac{1}{2} \|\boldsymbol{w}\|^2$$

- ... can be seen as an instance of a more general problem

$$\min_{\boldsymbol{w},b} \underbrace{\frac{1}{n} \sum_{i=1}^{n} \ell(y_i, f(\boldsymbol{x}_i))}_{\text{loss term}} + \underbrace{\lambda \Omega(\boldsymbol{w})}_{\text{regularization term}}$$

λ : trade-off parameter

loss term (empirical loss on training data)

regularization term (controls overfitting / classifier capacity)

More on Linear Classifiers

- This objective function amounts to minimizing the generalization error on test data
  - see C. Burges' tutorial and Statistical Learning Theory by V. Vapnik

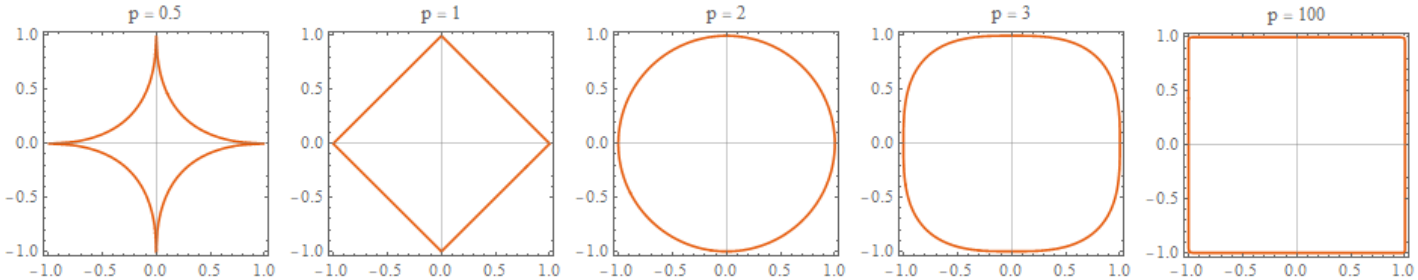
$$\min_{\boldsymbol{w},b} \frac{1}{n}\sum_{i=1}^{n} \ell(y_i, f(\boldsymbol{x}_i)) + \lambda\Omega(\boldsymbol{w})$$

- Different choices of loss and regularization yield different learning algorithms for linear classifiers – all trainable with SGD (and scikit-learn). Some examples are:
  - Hinge + l2: SVM
  - Hinge + l1: 1-norm SVM
  - Squared loss + l2: Ridge Regression
  - Squared loss + l1: LASSO
  - Logistic loss + l2: Logistic Regression

Regularizers

- $\Omega(\boldsymbol{w})$: typically convex penalties on the classifier parameters are used
  - ℓ_p norms with $p \geq 1$, $\ell_p(\boldsymbol{w}) = \left(\sum_j |w_j|^p\right)^{1/p}$

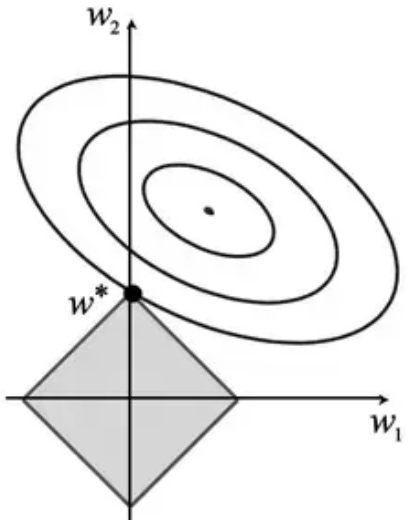
- Most popular examples
  - ℓ_0 is not convex, and amounts to counting non-zero elements in $\boldsymbol{w}$
  - $\ell_1 = |w_1| + |w_2| + \cdots + |w_d|$
  - $\ell_2 = w_1^2 + w_2^2 + \ldots + w_d^2$
  - $\ell_\infty = \max_j |w_j|$



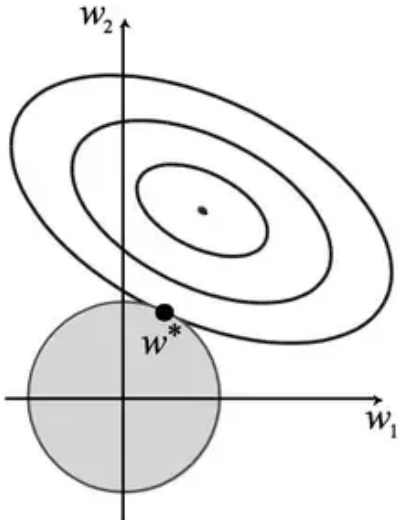
Sparsity

- ℓ_0 and ℓ_1 regularization enforce *sparsity*, i.e., many values in $\boldsymbol{w}$ will be set to zero
  - Why? The optimum is often found at one of the vertices!

- Sparsity helps automatically perform feature selection
- Features assigned $w_j = 0$ can be disregarded



ℓ_1



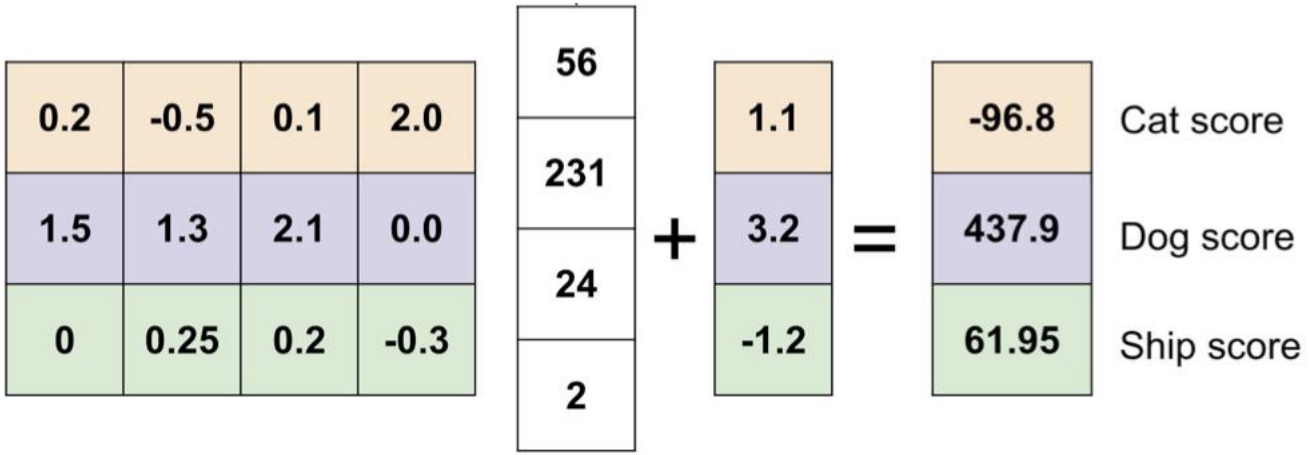
ℓ_2

Multiclass Classification with Linear Classifiers

Multiclass Linear Classifiers

- Linear functions can be also naturally extended to multiclass problems

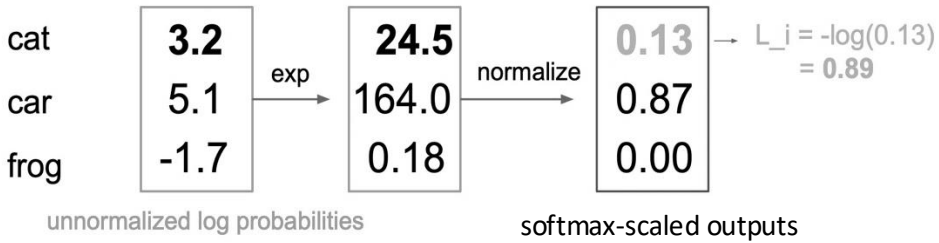
$$f(\boldsymbol{x}) = \mathbf{W}^{\mathrm{T}}\boldsymbol{x} + \boldsymbol{b}$$

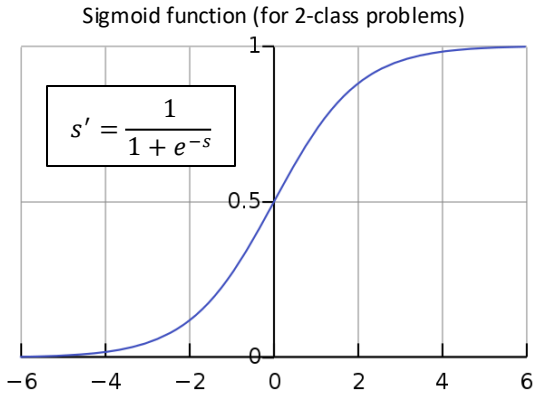


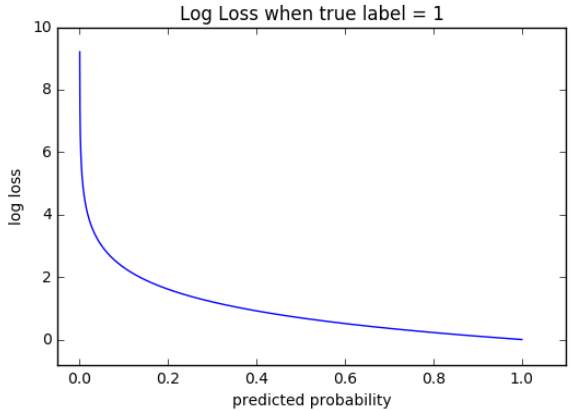
Logistic/Softmax Classifier

- Multiclass loss used to learn $\mathbf{W}, \boldsymbol{b}$

- Softmax scaling and cross-entropy (or log) loss
  - The classifier outputs one score per class $f(\boldsymbol{x}) = (s_1, \dots, s_k)$
  - Outputs are softmax scaled: $s'_l = \frac{e^{s_l}}{\sum_j e^{s_j}}$
  - Cross-entropy loss: $L(y_i, f(\boldsymbol{x}_i)) = -\log(s'_{y_i})$







Multiclass Classification with Binary Classifiers

Multiclass Classification with Binary (two-class) Classifiers

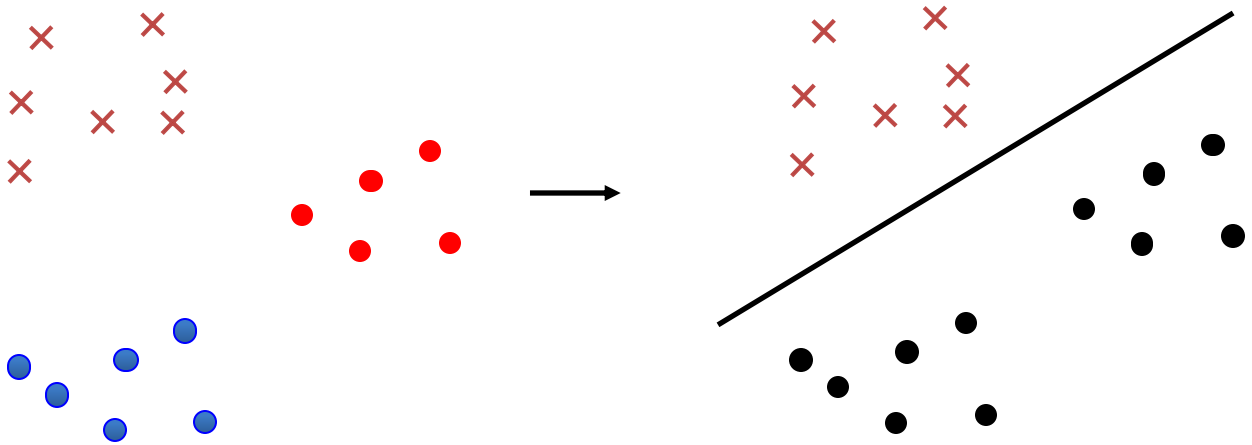
- How to use binary classifiers (not necessarily linear) for multi-class classification (c>2)?

- Recall that one object belongs only to one class!
  - y is in the set {0, 1, ..., c-1}

- Two common schemes:
  - One-vs-all (or one-vs-rest) classification (OVA / OVR)
  - One-vs-one classification (OVO)

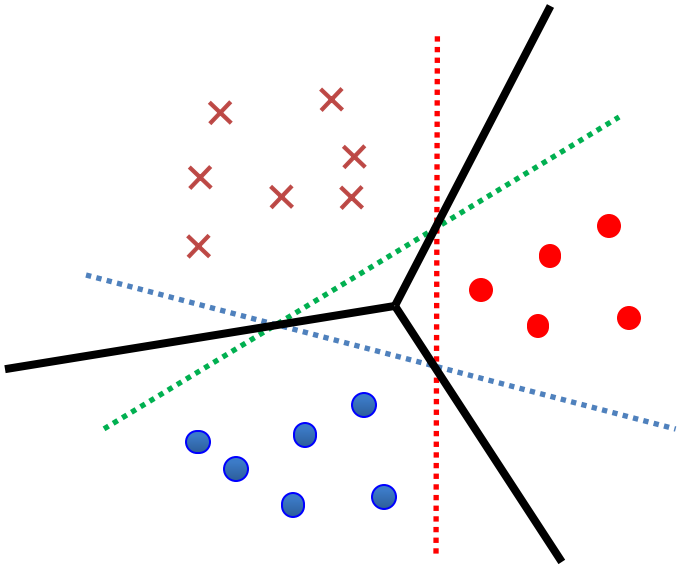
One-vs-all Multiclass Classification

- Train one binary classifier for each class k
- Samples for which y=k are labeled as +1
- The remaining classes are all labeled as -1



One-vs-all Multiclass Classification

- Combine with $y = \text{argmax}_k\ f_k(\mathbf{x})$



One-vs-one Multiclass Classification

- Train one binary classifier for class i vs class j
- All possible pairs are considered
  - c(c-1)/2 total number of binary classifiers
- Combined as:

$$f(\mathbf{x}) = \arg\max_i \left(\sum_j f_{ij}(\mathbf{x}) \right)$$

Note that $f_{ij} = -f_{ji}$ and that the sum is for j=0,...,c-1

Pros and Cons

- One-vs-all classification
  - One classifier per class, trained using all data
- One-vs-one classification
  - combinatorial number of classifiers (all possible pairs, c(c-1)/2), trained using much smaller data subsets
- Trade-off between number of classifiers and complexity of the learning algorithm
- In practice, rather equivalent classification accuracies
  - No free lunch

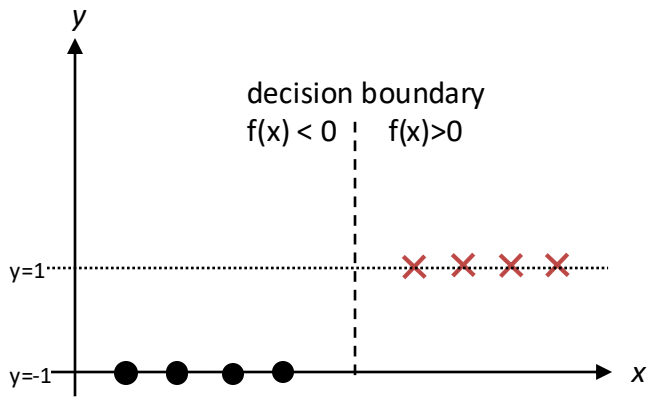
Classification vs Regression (with linear estimators)

Classification vs Regression

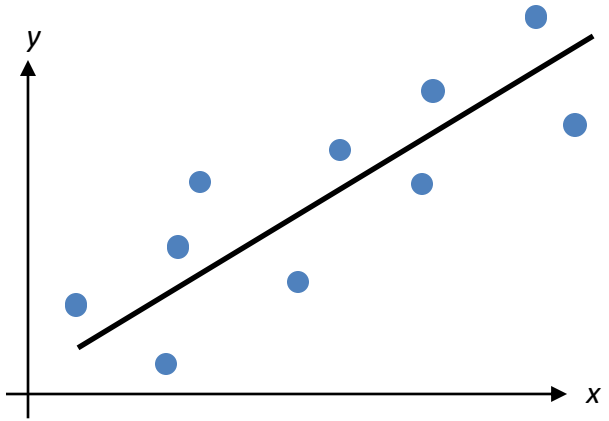
- In both classification and regression, the goal is to estimate a function f(**x**) that estimates the truth value y for each given sample **x**
- **In this chapter we've discussed linear functions**
- In classification problems, the set of labels is discretized
  - $y \in \{0, \dots, c-1\}$
- In regression problems, the set of labels (or better, target values) is typically a continuous value
  - $y \in \mathrm{R}$ (e.g., the set of real numbers)

Classification vs Regression

Classification (estimates y in a discrete set, e.g., {-1,1})

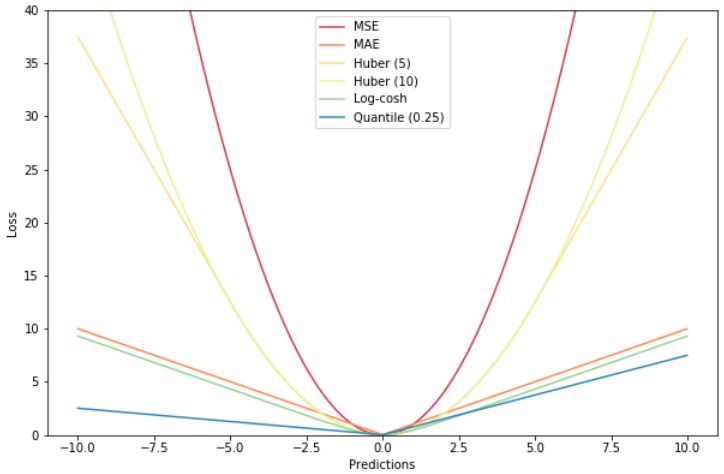


Regression estimates continuous-valued *y*



Classification vs Regression

- The loss functions used in the two problems reflect this behavior
- For classification problems, correctly-classified points are assigned a loss equal to zero
  - e.g., the hinge loss gives zero penalty to points for which $yf(\boldsymbol{x}) \geq 1$
- For regression problems, the loss is zero only if $f(\boldsymbol{x})$ is exactly equal to y
  - e.g., the mean squared error (MSE) is given as the average of $\left(\mathrm{y} - f(\boldsymbol{x})\right)^2$ over all points



Ridge Regression

- It uses the mean squared error (MSE) as the error function and l2 regularization on the feature weights:

$$L(\boldsymbol{w}) = \frac{1}{2n} \|\mathbf{X}\boldsymbol{w} - \boldsymbol{y}\|^2 + \lambda \|\boldsymbol{w}\|^2$$

- Minimizing $L(\boldsymbol{w})$ provides the following closed-form solution:

$$\boldsymbol{w} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\boldsymbol{y} \ ,$$

- being **I** the identity matrix, and $\lambda > 0$ a trade-off parameter.

- In this case, adding a small diagonal (ridge) to the (positive semi-definite) matrix $\mathbf{X}^T\mathbf{X}$ makes it more stable for pseudo-inversion (as it increases its minimum eigenvalue)

Ridge Regression

- Ridge regression can be solved in closed form, through matrix pseudo-inversion
  - Too computationally demanding for large feature sets and datasets

- It is also possible to solve it using gradient-descent procedures, including SGD, which is much faster and better suited to large, high-dimensional training sets

LASSO and Elastic Net

- Least Absolute Shrinkage and Selection Operator (LASSO) uses sparse penalty on $\boldsymbol{w}$ for embedded feature selection

$$L(\boldsymbol{w}) = \frac{1}{2n}\|\mathbf{X}\boldsymbol{w} - \boldsymbol{y}\|^2 + \lambda\|\boldsymbol{w}\|_1$$

- The Elastic Net overcomes some issues arising when learning LASSO on badly-conditioned problems, by combining l1 and l2 regularization

$$L(\boldsymbol{w}) = \frac{1}{2n}\|\mathbf{X}\boldsymbol{w} - \boldsymbol{y}\|^2 + \lambda_1\|\boldsymbol{w}\|_1 + \lambda_2\|\boldsymbol{w}\|_2^2$$

References

- Pattern Classification, R. O. Duda, P. E. Hart, and D. G. Stork, John Wiley & Sons, 2000
- L. Kuncheva, Combining pattern classifiers, Wiley, 2004.
- C. Bishop, Pattern Recognition and Machine Learning, Springer, 2007.
- S. Boyd and L. Vandenberghe, Convex Optimization, Cambridge University Press, 2004.

- **Acknowledgments:** I would like to thank Prof. Gavin Brown for the permission to use the material on SVMs from his course on ML at the University of Manchester, UK.

Exercises

Exercise 1

- Consider the data

$$\mathbf{X} = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ -1 & -2 \\ -2 & -1 \end{bmatrix}, \qquad \mathbf{y} = \begin{bmatrix} 1 \\ 1 \\ -1 \\ -1 \end{bmatrix}$$

- and the linear classification function $f(\boldsymbol{x}) = \boldsymbol{w}^T\boldsymbol{x} + b$, with $\boldsymbol{w} = [1\ 1]^T$ and $b = 0$.

- Points are classified as positive if $f(\boldsymbol{x}) \geq 0$

- Classify the data points in $\mathbf{X}$ and compute the overall classification error

Exercise 1: Solution

- Samples in $\mathbf{X}$ are stored as rows, hence it is not difficult to compute the values of the discriminant function as

$$f(\mathbf{X}) = \boldsymbol{X}\boldsymbol{w} + b = \begin{bmatrix} 1 & 2 \\ 2 & 1 \\ -1 & -2 \\ -2 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \end{bmatrix} = \begin{bmatrix} 3 \\ 3 \\ -3 \\ -3 \end{bmatrix}$$

- which, compared against 0, gives the classification labels

$$\boldsymbol{y}_c = \begin{bmatrix} 1 \\ 1 \\ -1 \\ -1 \end{bmatrix}$$

- Since they are exactly equal to the true labels $\boldsymbol{y}$, the classification error is zero

Exercise 2

- Given the following data samples

$$\mathbf{X} = \begin{bmatrix} -1 & 0 \\ 0 & -1 \\ 0 & 0 \\ 0 & 2 \\ 1 & 2 \\ 2 & 1 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 1 \\ 1 \\ 1 \\ -1 \\ -1 \\ -1 \end{bmatrix},$$

- find the linear discriminant function using the criterion function (perceptron loss):

$$L_p(\boldsymbol{w}, b) = \sum_i \ \max(0, -y_i(\boldsymbol{w}^T \boldsymbol{x}_i + b))$$

- Initialize $\boldsymbol{w} = [0.1, 0.1]^T,\ b = 0.1,\ \eta = 1,\ \theta = 0$
- Use the termination condition: $\eta(|\ \nabla_{\boldsymbol{w}} L_p(\boldsymbol{w}, b)| + |\nabla_b L_p(\boldsymbol{w}, b)|) \leq \theta$

Exercise 2: Solution

begin initialize $\boldsymbol{w}, b, \eta, \theta$
  do
    select samples for which $y_i f(\boldsymbol{x}_i) < 0$
    update $\boldsymbol{w} \leftarrow \boldsymbol{w} - \eta \nabla_{\boldsymbol{w}} L_p(\boldsymbol{w}, b)$ and $b \leftarrow b - \eta \nabla_b L_p(\boldsymbol{w}, b)$
      (using the selected samples)
  until $\eta(|\nabla_{\boldsymbol{w}} L_p(\boldsymbol{w}, b)| + |\nabla_b L_p(\boldsymbol{w}, b)|) < \theta$
end

- Here we have to compute the derivatives w.r.t $\boldsymbol{w}$ and b:

$$\nabla_{\boldsymbol{w}} L_p(\boldsymbol{w}, b) = -\sum_{i:y_i f(\boldsymbol{x}_i)<0} y_i \boldsymbol{x}_i$$

$$\nabla_b L_p(\boldsymbol{w}, b) = -\sum_{i:y_i f(\boldsymbol{x}_i)<0} y_i$$

Exercise 2: Solution

Iteration 1

- We first have to classify the data points with the current $\boldsymbol{w}$ and b

$$f(\mathbf{X}) = \boldsymbol{X}\boldsymbol{w} + b = \begin{bmatrix} -1 & 0 \\ 0 & -1 \\ 0 & 0 \\ 0 & 2 \\ 1 & 2 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} 0.1 \\ 0.1 \end{bmatrix} + 0.1 = \begin{bmatrix} 0 \\ 0 \\ 0.1 \\ 0.3 \\ 0.4 \\ 0.4 \end{bmatrix}$$

Exercise 2: Solution

- Then, consider the classification errors for which $y_i f(\boldsymbol{x}_i) < 0$

$$\boldsymbol{y} f(\mathbf{X}) = \begin{bmatrix} 1 \\ 1 \\ 1 \\ -1 \\ -1 \\ -1 \end{bmatrix} \circ \begin{bmatrix} 0 \\ 0 \\ 0.1 \\ 0.3 \\ 0.4 \\ 0.4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0.1 \\ -0.3 \\ -0.4 \\ -0.4 \end{bmatrix}$$

- The three last patterns are wrongly classified, so they will be used to update $\boldsymbol{w}$ and b

$$\nabla_{\boldsymbol{w}} L_p(\boldsymbol{w}, b) = -\sum_{i:y_i f(\boldsymbol{x}_i)<0} y_i \boldsymbol{x}_i = +1 \begin{bmatrix} 0 \\ 2 \end{bmatrix} + 1 \begin{bmatrix} 1 \\ 2 \end{bmatrix} + 1 \begin{bmatrix} 2 \\ 1 \end{bmatrix} = \begin{bmatrix} 3 \\ 5 \end{bmatrix}$$

$$\nabla_b L_p(\boldsymbol{w}, b) = -\sum_{i:y_i f(\boldsymbol{x}_i)<0} y_i = 3$$

Exercise 2: Solution

- **Parameter updates**
  $\boldsymbol{w} \leftarrow \boldsymbol{w} - \eta \nabla_{\boldsymbol{w}} L_p(\boldsymbol{w}, b)$ and $b \leftarrow b - \eta \nabla_b L_p(\boldsymbol{w}, b)$

$$\boldsymbol{w} = \begin{bmatrix} 0.1 \\ 0.1 \end{bmatrix} - 1 \begin{bmatrix} 3 \\ 5 \end{bmatrix} = \begin{bmatrix} -2.9 \\ -4.9 \end{bmatrix}$$

$$b = 0.1 - 1 * 3 = -2.9$$

- **Termination condition** $\eta(|\nabla_{\boldsymbol{w}} L_p(\boldsymbol{w}, b)| + |\nabla_b L_p(\boldsymbol{w}, b)|) \leq \theta$

$$t = 1 * (|3| + |5| + |3|) \leq \theta = 0$$

- Termination condition is *False* (then, loop continues)

Exercise 2: Solution

iter	$\boldsymbol{y}f(\boldsymbol{x})$	L_p	$\nabla_{\boldsymbol{w}}L_p, \nabla_b L_p$	$\boldsymbol{w}, b$	t	θ
1.	[0. 0. 0.1 -0.3 -0.4 -0.4]	1.1	[3 5] 3	[-2.9 -4.9] -2.9	11.0	0
2.	[0. 2. -2.9 12.7 15.6 13.6]	2.9	[0 0] -1	[-2.9 -4.9] -1.9	1.0	0
3.	[1. 3. -1.9 11.7 14.6 12.6]	1.9	[0 0] -1	[-2.9 -4.9] -0.9	1.0	0
4.	[2. 4. -0.9 10.7 13.6 11.6]	0.9	[0 0] -1	[-2.9 -4.9] 0.1	1.0	0
5.	[3. 5. 0.1 9.7 12.6 10.6]	0.0	[0 0] 0	[-2.9 -4.9] 0.1	0.0	0

Homework: Plot the data points and the decision function at each iteration

Exercise 3

- Given a regression problem and the following data samples

$$\mathbf{X} = \begin{bmatrix} -1 & 0 \\ 0 & -1 \\ 0 & 0 \\ 0 & 2 \\ 1 & 2 \\ 2 & 1 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 0.1 \\ 0.1 \\ 0.1 \\ 0.1 \\ 0.1 \\ 0.1 \end{bmatrix},$$

- find the linear discriminant function via ordinary least squares (OLS), i.e., by minimizing:

$$L_r(\boldsymbol{w}) = \frac{1}{2}\sum_{i=1}^{N}(\boldsymbol{w}^T\boldsymbol{x}_i + b - y_i)^2$$

- Initialize $\boldsymbol{w} = [0.1, 0.1]^T,\ b = 0.1,\ \eta = 0.1,\ \theta = 0.06$

Exercise 3: Solution

- The solution (a.k.a. Widrow-Hoff or least-mean-squares) algorithm is

begin initialize w, θ, η, $k=0$
  repeat
    $\boldsymbol{w}=\boldsymbol{w} - \eta \nabla_{\boldsymbol{w}} L_r(\boldsymbol{w}, b)$
    $b=b - \eta \nabla_b L_r(\boldsymbol{w}, b)$
  until $\eta\ (|\nabla_w L_r(\boldsymbol{w}, b)| + |\nabla_b L_r(\boldsymbol{w}, b)|) <= \theta$

- The derivatives w.r.t $\boldsymbol{w}$ and b:

$$\nabla_{\boldsymbol{w}} L_r(\boldsymbol{w}, b) = \sum_{i=1}^{N} (\boldsymbol{w}^T \boldsymbol{x}_i + b - y_i)\, \boldsymbol{x}_i$$
$$\nabla_b L_r(\boldsymbol{w}, b) = \sum_{i=1}^{N} (\boldsymbol{w}^T \boldsymbol{x}_i + b - y_i)$$

Exercise 3: Solution

iter	$f(\boldsymbol{x})$	L_r	$\nabla_{\boldsymbol{w}} L_{\mathrm{r}}, \nabla_b L_r$	$\boldsymbol{w}, b$	t	θ=0.06
1.	0.1*[0 0 1 3 4 4]	0.240	[1. 1.4], 0.6	[0. -0.04], 0.04	0.3	
2.	0.01*[4 8 4 -4 -4 0]	0.057	[-0.28 -0.64], -0.52	[0.028 0.024], 0.092	0.14	
3.	0.01*[6 7 9 14 17 17]	0.014	[0.25 0.32], 0.104	[0.0032 -0.008], 0.0816	0.07	
4.	0.01*[8 9 8 7 7 8]	0.003	[-0.05 -0.14], -0.136	[0.008 0.006], 0.09	0.03	

Homework: Plot the data points and the decision function at each iteration