Lecture 15: Coordinate Descent (continued)

- How to solve non-smooth optimization like Lasso?

$$\hat{w}_{\text{Lasso}} = \arg\min_{w \in \mathbb{R}^d} \underbrace{\|\mathbf{y} - \mathbf{X}w\|_2^2 + \lambda \|w\|_1}_{f(w)}$$

Coordinate descent for Lasso

- let us apply coordinate descent on Lasso, which minimizes
$$\text{minimize}_w \mathscr{L}(w) + \lambda \|w\|_1 = \|\mathbf{X}w - \mathbf{y}\|_2^2 + \lambda\, \|w\|_1$$

- the goal is to derive an **analytical rule** for updating $w_j^{(t)}$'s

- let us first write the update rule explicitly for $w_1^{(t)}$
    - first step is to write the loss in terms of w_1

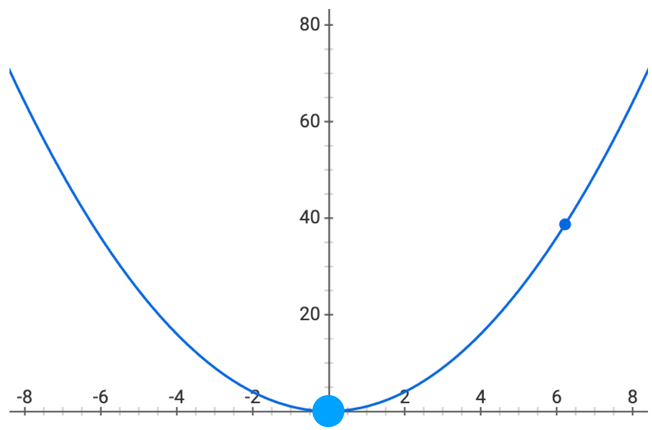
$$\left\| \mathbf{X}[:,1]w_1 \;-\; \left(\mathbf{y} - \mathbf{X}[:,2:d]w_{2:d}\right) \right\|_2^2 + \lambda\Big(\, |\, w_1\,| + \underbrace{\|w_{2:d}\|_1}_{\text{constant}}\,\Big)$$

- hence, the coordinate descent update boils down to

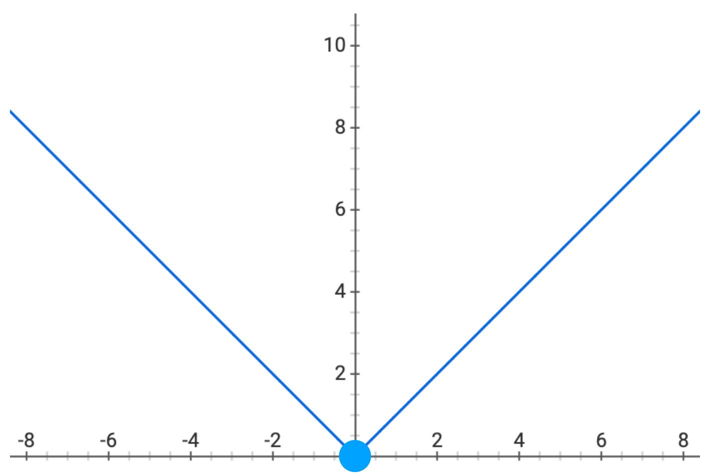
$$w_1^{(t)} \leftarrow \arg\min_{w_1} \underbrace{\left\| \mathbf{X}[:,1]w_1 \;-\; \left(\mathbf{y} - \mathbf{X}[:,2:d]w_{2:d}^{(t-1)}\right) \right\|_2^2 + \lambda\, |\, w_1\,|}_{f(w_1)}$$

How do we find the minima?

- for **convex differentiable** functions, the minimum is achieved at points where gradient is zero



- for **convex non-differentiable** functions, the minimum is achieved at points where sub-gradient includes zero



Finding the minima for $(aw_1 - b)^2 + \lambda |w_1|$

- the minimizer $w_1^{(t)}$ is when zero is included in the sub-gradient

$$\partial f(w_1) = \begin{cases} 2a(aw_1 - b) + \lambda & \text{for } w_1 > 0 \\ [-2ab - \lambda, -2ab + \lambda] & \text{for } w_1 = 0 \\ 2a(aw_1 - b) - \lambda & \text{for } w_1 < 0 \end{cases}$$

Finding the minima for $(aw_1 - b)^2 + \lambda |w_1|$

- the minimizer $w_1^{(t)}$ is when zero is included in the sub-gradient

$$\partial f(w_1) = \begin{cases} 2a(aw_1 - b) + \lambda & \text{for } w_1 > 0 \\ [-2ab - \lambda, -2ab + \lambda] & \text{for } w_1 = 0 \\ 2a(aw_1 - b) - \lambda & \text{for } w_1 < 0 \end{cases}$$

Finding the minima for $(aw_1 - b)^2 + \lambda |w_1|$

- the minimizer $w_1^{(t)}$ is when zero is included in the sub-gradient

$$\partial f(w_1) = \begin{cases} 2a(aw_1 - b) + \lambda & \text{for } w_1 > 0 \\ [-2ab - \lambda, -2ab + \lambda] & \text{for } w_1 = 0 \\ 2a(aw_1 - b) - \lambda & \text{for } w_1 < 0 \end{cases}$$

Finding the minima for $(aw_1 - b)^2 + \lambda |w_1|$

- considering all three cases, we get the following update rule by setting the sub-gradient to zero

$$w_1^{(t)} \leftarrow \begin{cases} \frac{b}{a} - \frac{\lambda}{2a^2} & \text{for } 2ab > \lambda \\ 0 & \text{for } -\lambda \leq 2ab \leq \lambda \\ \frac{b}{a} + \frac{\lambda}{2a^2} & \text{for } \lambda < -2ab \end{cases} \iff \frac{-\lambda}{2a^2} \leq \frac{b}{a} \leq \frac{\lambda}{2a^2}$$

How do we find the minimizer?

- the minimizer $w_1^{(t)}$ is when zero is included in the sub-gradient

$$\partial f(w_1) = \begin{cases} 2a(aw_1 - b) + \lambda & \text{for } w_1 > 0 \\ [-2ab - \lambda, -2ab + \lambda] & \text{for } w_1 = 0 \\ 2a(aw_1 - b) - \lambda & \text{for } w_1 < 0 \end{cases}$$

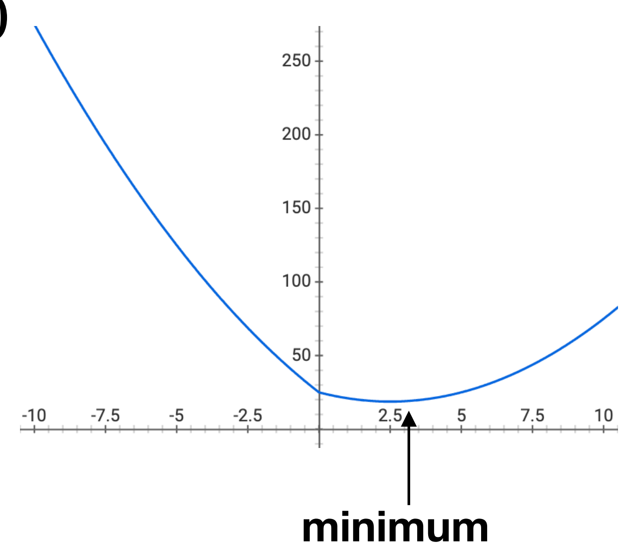
- case 1:
  - $2a(aw_1 - b) + \lambda = 0$ for some $w_1 > 0$
  - this happens when

$$w_1 = \frac{-\lambda + 2ab}{2a^2} > 0$$

  - hence,

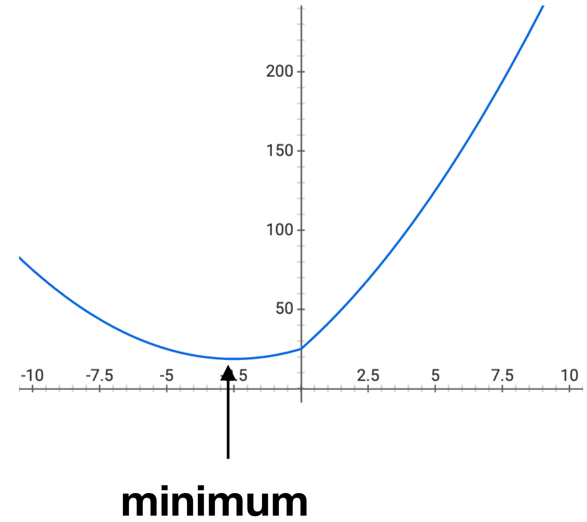
$$w_1^{(t)} \leftarrow \frac{b}{a} - \frac{\lambda}{2a^2},$$

if $\lambda < 2ab$



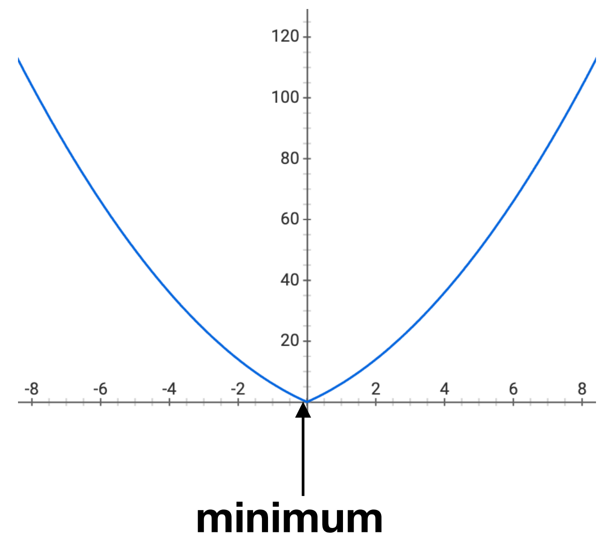
- case 2:
  - $2a(aw_1 - b) - \lambda = 0$ for some $w_1 < 0$
  - this happens when
    $$w_1 = \frac{\lambda + 2ab}{2a^2} < 0$$
  - hence,
    $$w_1^{(t)} \leftarrow \frac{b}{a} + \frac{\lambda}{2a^2},$$

    if $\lambda < -2ab$



- case 3:
  - $0 \in [-2ab - \lambda, -2ab + \lambda]$
  - and $w_1 = 0$
  - hence,
    $$w_1^{(t)} \leftarrow 0,$$

    if $-\lambda \leq 2ab \leq \lambda$

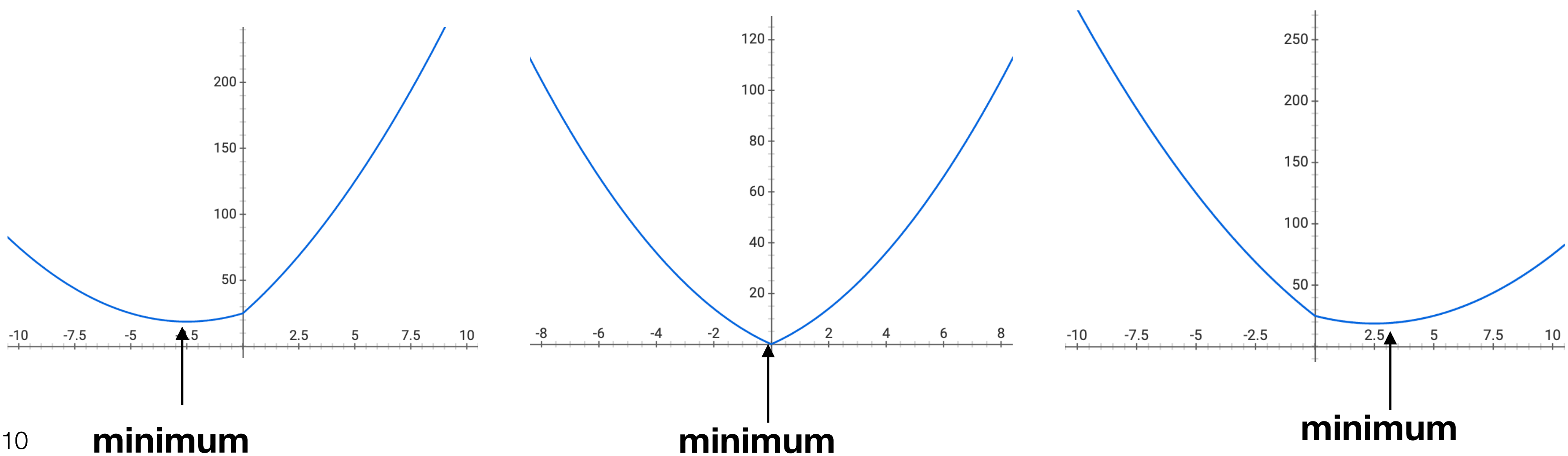


Coordinate descent on Lasso

- considering all three cases, we get the following update rule by setting the sub-gradient to zero

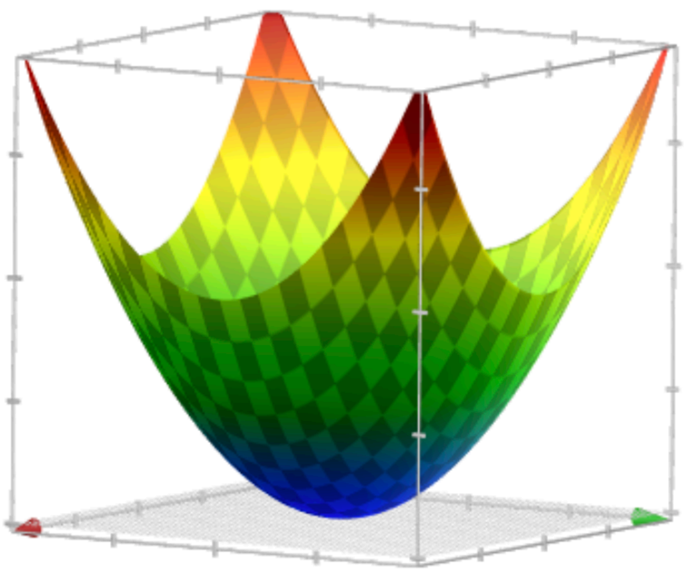
$$w_1^{(t)} \leftarrow \begin{cases} \frac{b}{a} - \frac{\lambda}{2a^2} & \text{for } 2ab > \lambda \\ 0 & \text{for } -\lambda \leq 2ab \leq \lambda \\ \frac{b}{a} + \frac{\lambda}{2a^2} & \text{for } \lambda < -2ab \end{cases}$$

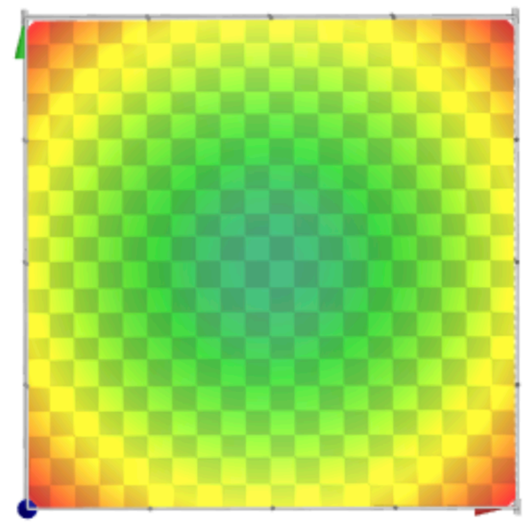
- where $a = \sqrt{\mathbf{X}[:,1]^T\mathbf{X}[:,1]}$, and $b = \dfrac{\mathbf{X}[:,1]^T\left(\mathbf{y} - \mathbf{X}[:,2:d]w_{-1}\right)}{\sqrt{\mathbf{X}[:,1]^T\mathbf{X}[:,1]}}$



When does coordinate descent work?

- Consider minimizing a **differentiable convex** function $f(x)$, then coordinate descent converges to the global minima

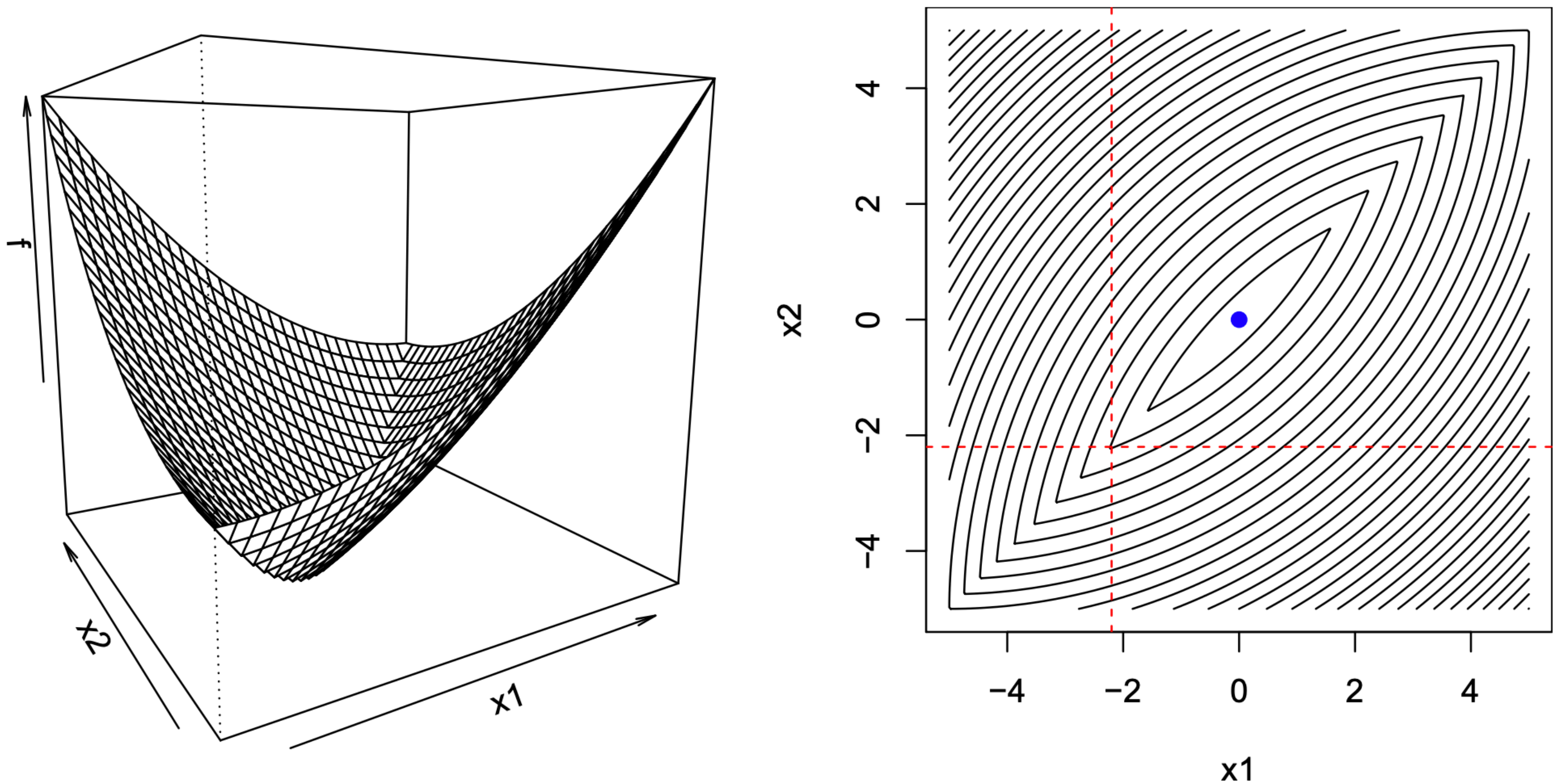




- when coordinate descent has stopped, that means $\dfrac{\partial f(x)}{\partial x_j} = 0$ for all $j \in \{1, \ldots, d\}$
- this implies that the gradient $\nabla_x f(x) = 0$, which happens only at minimum

When does coordinate descent work?

- Consider minimizing a **non-differentiable convex** function $f(x)$, then coordinate descent can get stuck

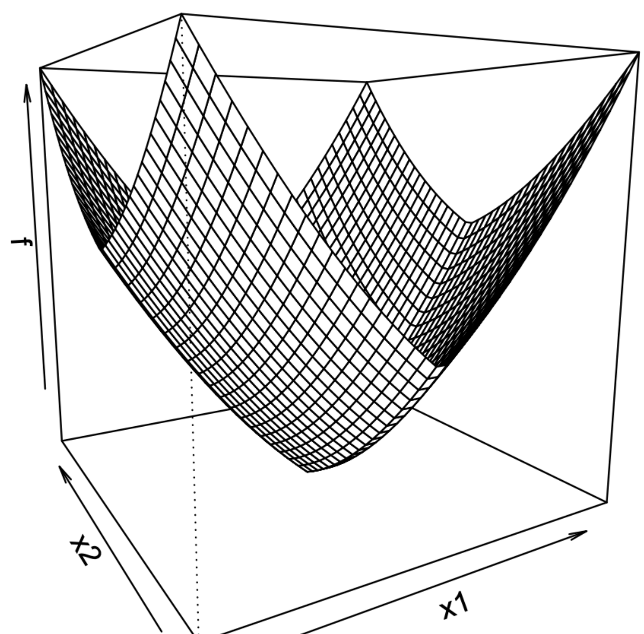


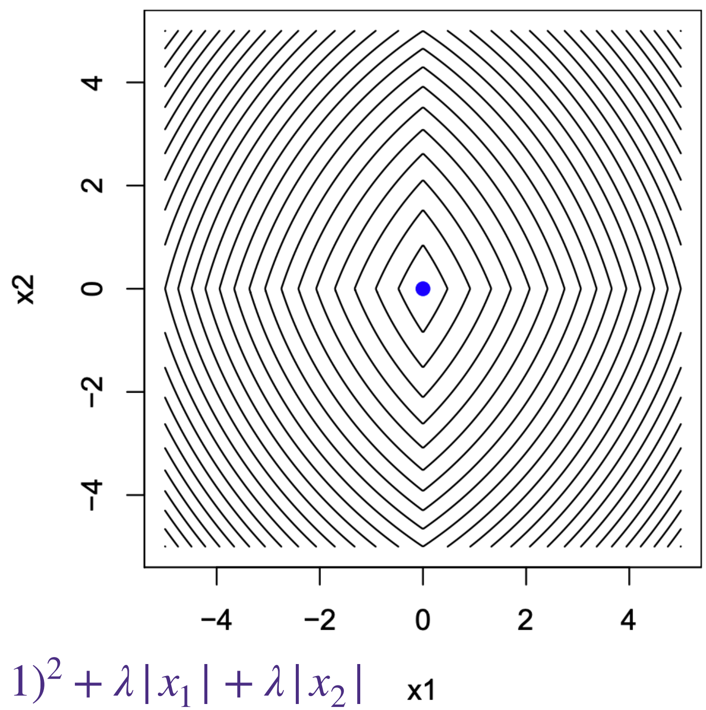
-

$$f(x_1, x_2) = (3x_1 + 4x_2 + 1)^2 + \lambda |x_1 - x_2|$$

When does coordinate descent work?

- then how can coordinate descent find optimal solution for Lasso?
- consider minimizing a **non-differentiable convex** function but has a structure of $f(x) = g(x) + \sum_{j=1}^{d} h_j(x_j)$, with differentiable convex function $g(x)$ and coordinate-wise non-differentiable convex functions $h_j(x_j)$'s, then coordinate descent converges to the global minima





-

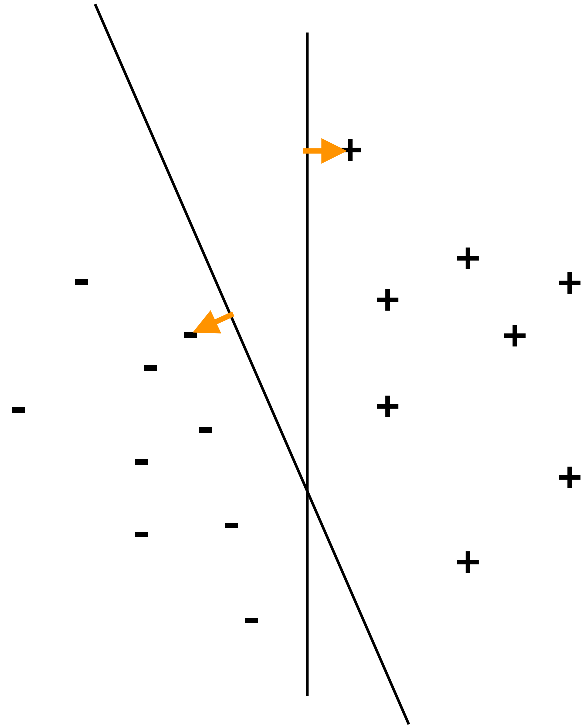
$f(x_1, x_2) = (3x_1 + 4x_2 + 1)^2 + \lambda |x_1| + \lambda |x_2|$

Questions?

Lecture 16:
Support Vector Machines

How do we choose the best linear classifier?

- informally, **margin** of a set of examples to a decision boundary is the distance to the closest point to the decision boundary
- for linearly separable datasets, **maximum margin** classifier is a natural choice
- large margin implies that the decision boundary can change without losing accuracy, so the learned model is more robust against new data points

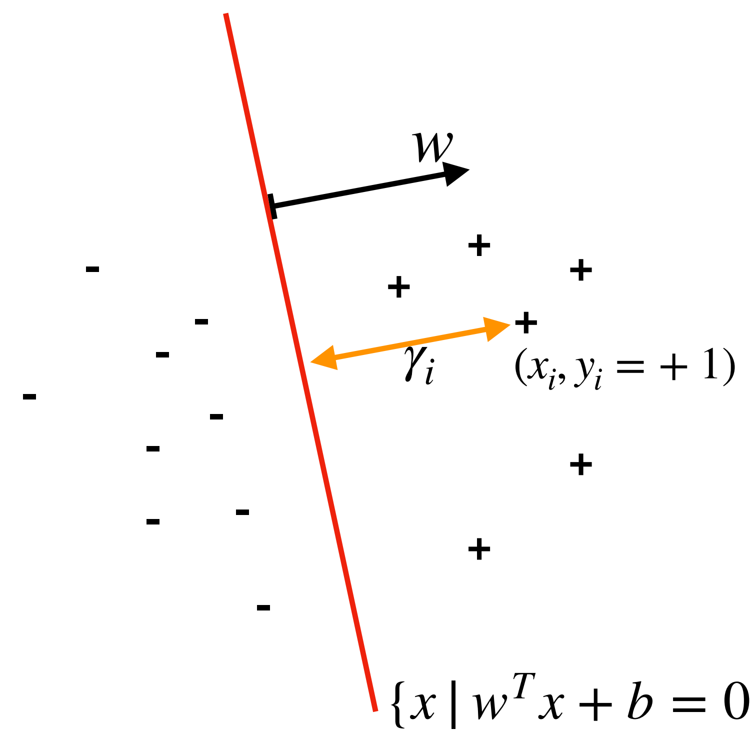


Geometric margin

- given a set of training examples $\{(x_i, y_i)\}_{i=1}^n$
- and a linear classifier $(w, b) \in \mathbb{R}^d \times \mathbb{R}$
- such that the decision boundary is
  a separating hyperplane $\{x \mid \underbrace{b + w_1 x[1] + w_2 x[2] + \cdots + w_d x[d]}_{w^T x + b} = 0\}$,
  which is the set of points that are orthogonal to w with a shift of b
- we define **functional margin** of (b, w) with respect to a training example (x_i, y_i) as the distance from the point (x_i, y_i) to the decision boundary, which is

$$\gamma_i = y_i \frac{(w^T x_i + b)}{\|w\|_2}$$

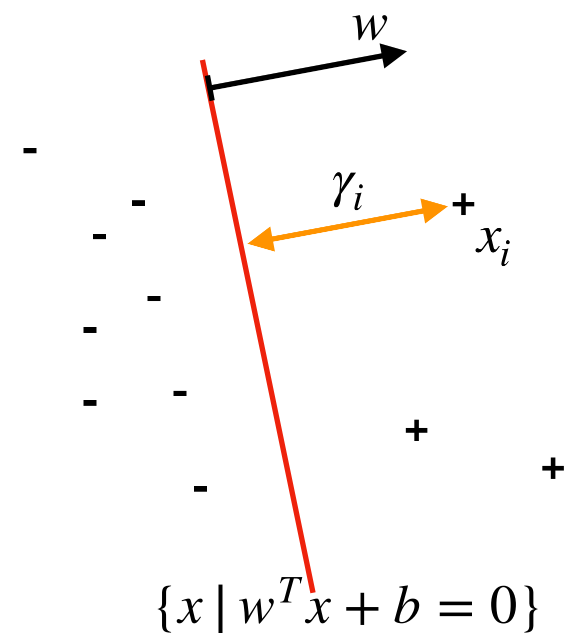
(The proof is on the next slide)



Geometric margin

- the distance γ_i from a hyperplane $\{x \mid w^T x + b = 0\}$ to a point x_i can be computed geometrically as follows
- We know that if you move from x_i in the negative direction of w by length γ_i, you arrive at the line, which can be written as

$$\left(x_i - \frac{w}{\|w\|_2} \gamma_i \right) \text{ is in } \{x \mid w^T x + b = 0\}$$



- so we can plug the point in the formula:

$$w^T \left(x_i - \frac{w}{\|w\|_2} \gamma_i \right) + b \;=\; 0$$

which is

$$w^T x_i - \frac{\|w\|_2^2}{\|w\|_2} \gamma_i + b \;=\; 0$$

and hence

$$\gamma_i \;=\; \frac{w^T x_i + b}{\|w\|_2},$$

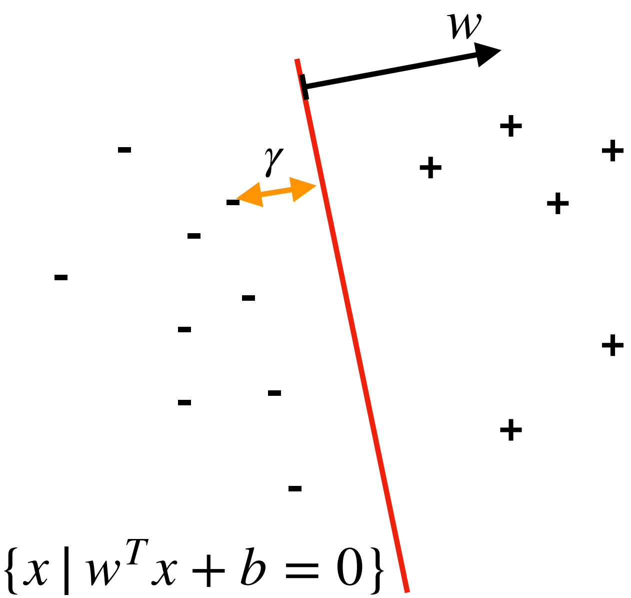
and we multiply it by y_i so that for negative samples we use the opposite direction of $-w$ instead of w

Geometric margin

- the **margin** with respect to a set is defined as

$$\gamma = \min_{i=1}^{n} \gamma_i$$

- among all linear classifiers, we would like to find one that has the **maximum margin**



Maximum margin classifier

- we propose the following optimization problem:

$$\text{maximize}_{w\in\mathbb{R}^d, b\in\mathbb{R}, \gamma\in\mathbb{R}} \quad \gamma$$

(maximize the margin)

$$\text{subject to} \quad \frac{y_i(w^T x_i + b)}{\|w\|_2} \geq \gamma \quad \text{for all } i \in \{1,\ldots,n\}$$

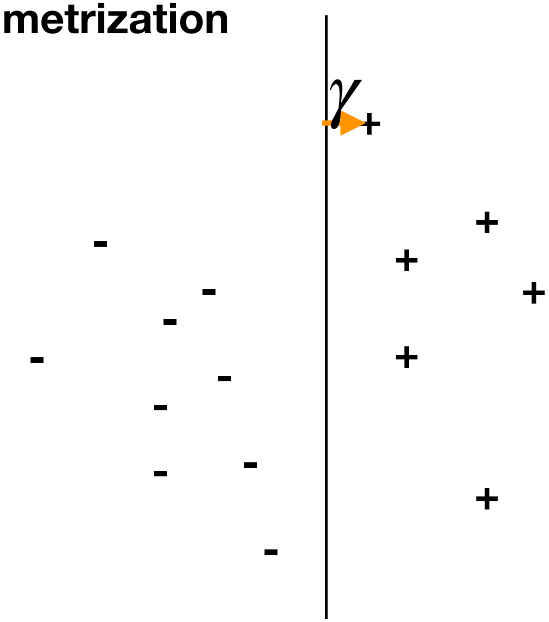
(s.t. γ is a lower bound on the margin)

- if we fix (w, b), the optimal solution of the optimization is the margin
- together with (w, b), this finds the classifier with the maximum margin
- note that this problem is **scale invariant** in (w, b), i.e. changing a (w, b) to $(2w, 2b)$ does not change either the feasibility or the objective value, hence the following reparametrization is valid
- the above optimization looks difficult, so we transform it using **reparametrization**

$$\text{maximize}_{w\in\mathbb{R}^d, b\in\mathbb{R}, \gamma\in\mathbb{R}} \quad \gamma$$

$$\text{subject to} \quad \frac{y_i(w^T x_i + b)}{\|w\|_2} \geq \gamma \quad \text{for all } i \in \{1,\ldots,n\}$$

$$\|w\|_2 = \frac{1}{\gamma}$$



- Because of scale invariance, the optimal solution does not change, as the solutions to the original problem did not depend on $\|w\|_2$, and only depends on the direction of w

- $\text{maximize}_{w\in\mathbb{R}^d, b\in\mathbb{R}, \gamma\in\mathbb{R}} \quad \gamma$

  subject to $\quad \dfrac{y_i(w^T x_i + b)}{\|w\|_2} \geq \gamma$ for all $i \in \{1,\ldots,n\}$

  $\|w\|_2 = \dfrac{1}{\gamma}$

- the above optimization still looks difficult, but can be transformed into

  $\text{maximize}_{w\in\mathbb{R}^d, b\in\mathbb{R}} \quad \dfrac{1}{\|w\|_2}$ **(maximize the margin)**

  subject to $\quad \dfrac{y_i(w^T x_i + b)}{\|w\|_2} \geq \dfrac{1}{\|w\|_2}$ for all $i \in \{1,\ldots,n\}$ **(now $\dfrac{1}{\|w\|_2}$ plays the role of a lower bound on the margin)**

  which simplifies to

  $\text{minimize}_{w\in\mathbb{R}^d, b\in\mathbb{R}} \quad \|w\|_2^2$

  subject to $\quad y_i(w^T x_i + b) \geq 1$ for all $i \in \{1,\ldots,n\}$

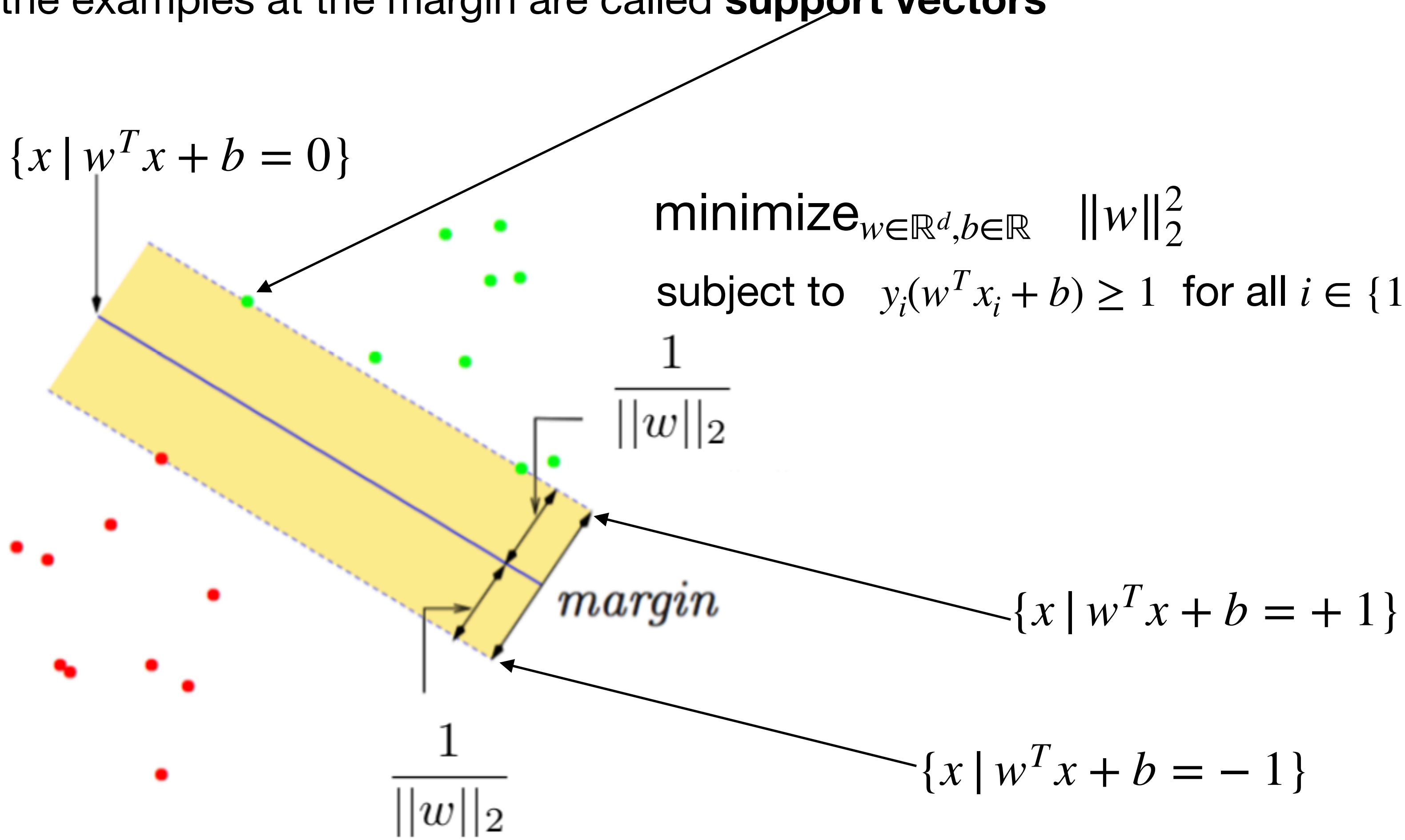
- this is a **quadratic program with linear constraints**, which can be easily solved
- once the optimal solution is found, the margin of that classifier (w, b) is $\dfrac{1}{\|w\|_2}$

What if the data is not separable?

- we cheated a little in the sense that the reparametrization of $\|w\|_2 = \dfrac{1}{\gamma}$ is possible only if the the margins are positive,
  i.e. the data is linearly separable with a positive margin
- otherwise, there is no feasible solution
- the examples at the margin are called **support vectors**

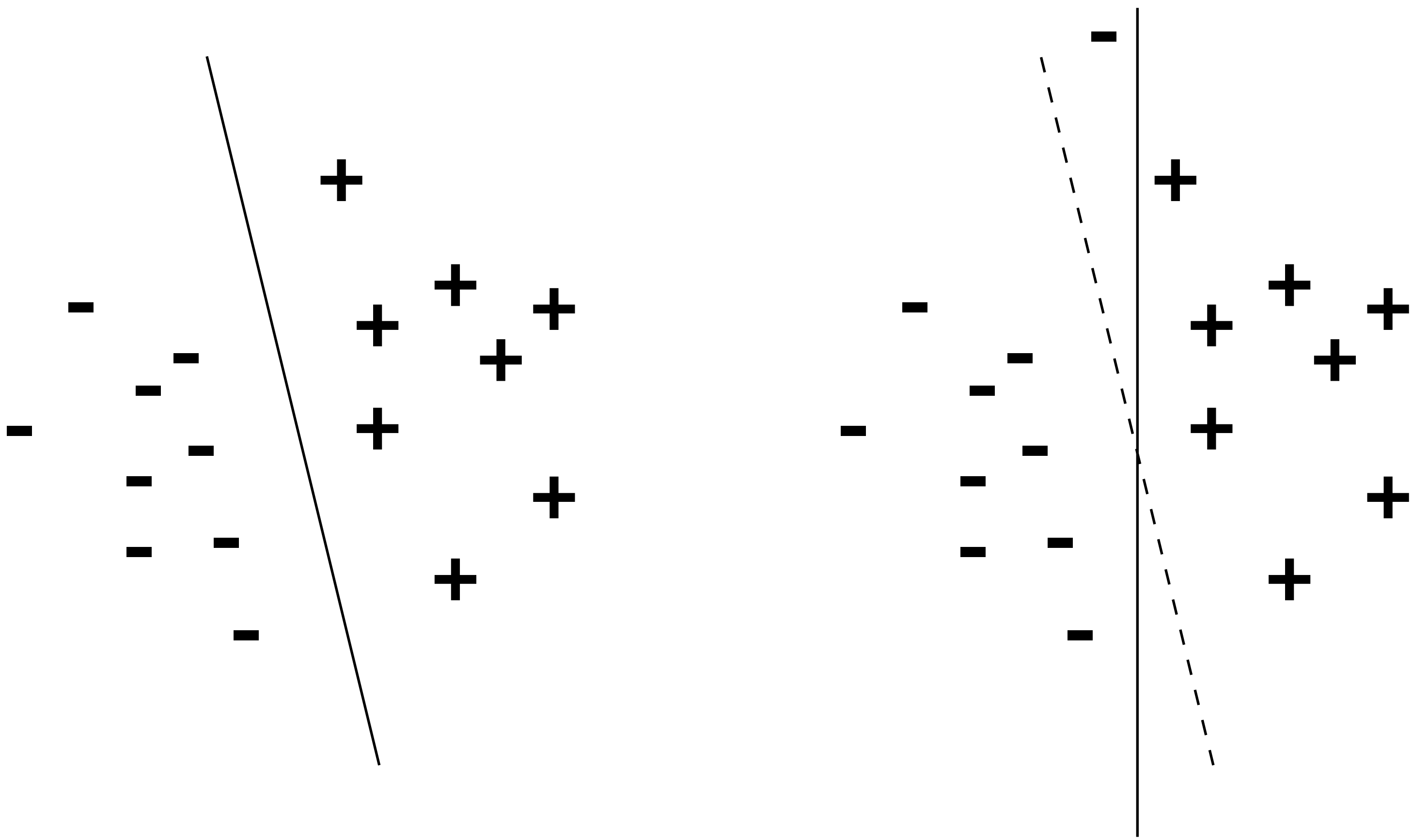
$$\text{minimize}_{w \in \mathbb{R}^d, b \in \mathbb{R}} \quad \|w\|_2^2$$

subject to $\quad y_i(w^T x_i + b) \geq 1 \quad$ for all $i \in \{1, \ldots, n\}$



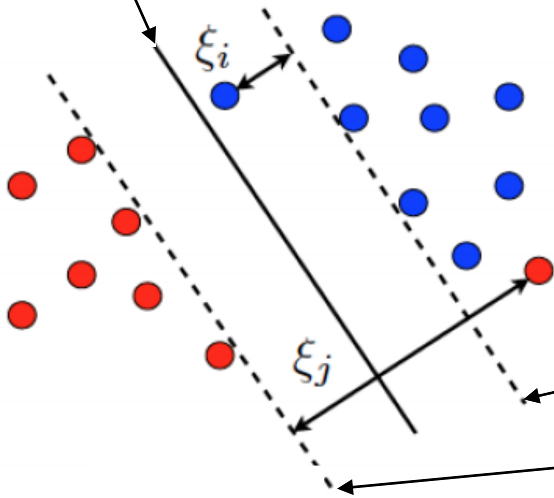
Two issues

- max-margin formulation we proposed is sensitive to outliers



- it does not generalize to non-separable datasets

What if the data is not separable?



- we introduce slack so that some points can violate the margin condition
  $$y_i(w^T x_i + b) \;\geq\; 1 - \xi_i$$

- this gives a new optimization problem with some positive constant $c \in \mathbb{R}$

$$\text{minimize}_{w \in \mathbb{R}^d, b \in \mathbb{R}, \xi \in \mathbb{R}^n} \quad \|w\|_2^2 + c \sum_{i=1}^{n} \xi_i$$

$$\text{subject to} \quad y_i(w^T x_i + b) \geq 1 - \xi_i \quad \text{for all } i \in \{1, \ldots, n\}$$

$$\xi_i \;\geq 0 \quad \text{for all } i \in \{1, \ldots, n\}$$

the (re-scaled) margin (for each sample) is allowed to be less than one,
but you pay $c\xi_i$ in the cost, and c balances the two goals:
maximizing the margin for most examples vs. having small number of violations

Support Vector Machine

- for the optimization problem

$$\text{minimize}_{w\in\mathbb{R}^d, b\in\mathbb{R}, \xi\in\mathbb{R}^n} \quad \|w\|_2^2 + c\sum_{i=1}^{n}\xi_i$$

$$\text{subject to} \quad y_i(w^Tx_i + b) \geq 1 - \xi_i \quad \text{for all } i \in \{1,\ldots,n\}$$

$$\xi_i \geq 0 \quad \text{for all } i \in \{1,\ldots,n\}$$

notice that at optimal solution, ξ_i's satisfy

- $\xi_i = 0$ if margin is big enough $y_i(w^Tx_i + b) \geq 1$, or
- $\xi_i = 1 - y_i(w^Tx_i + b)$, if the example is within the margin $y_i(w^Tx_i + b) < 1$

- so one can write
  - $\xi_i = \max\{0, 1 - y_i(w^Tx_i + b)\}$, which gives

$$\text{minimize}_{w\in\mathbb{R}^d, b\in\mathbb{R}} \quad \frac{1}{c}\|w\|_2^2 + \sum_{i=1}^{n}\max\{0, 1 - y_i(w^Tx_i + b)\}$$

Sub-gradient descent for SVM

- SVM is the solution of

$$\text{minimize}_{w\in\mathbb{R}^d, b\in\mathbb{R}} \quad \frac{1}{c}\|w\|_2^2 + \sum_{i=1}^{n} \max\{0, 1 - y_i(w^T x_i + b)\}$$

- as it is non-differentiable, we solve it using sub-gradient descent
- which is exactly the same as gradient descent, except when we are at a non-differentiable point, we take one of the sub-gradients instead of the gradient (recall sub-gradient is a set)
- this means that we can take (a generic form derived from previous page)

$$\partial_w \ell(w^T x_i + b, y_i) \;=\; \mathbf{I}\{y_i(w^T x_i + b) \le 1\}(-y_i x_i)$$

and apply

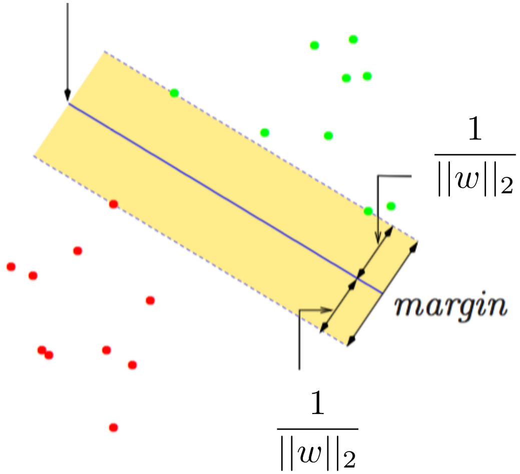
$$w^{(t+1)} \;\leftarrow\; w^{(t)} - \eta \left(\sum_{i=1}^{n} \mathbf{I}\{y_i((w^{(t)})^T x_i + b^{(t)}) \le 1\}(-y_i x_i) \;+\; \frac{2}{c} w^{(t)} \right)$$

$$b^{(t+1)} \;\leftarrow\; b^{(t)} - \eta \sum_{i=1}^{n} \mathbf{I}\{y_i((w^{(t)})^T x_i + b^{(t)}) \le 1)\}(-y_i)$$

Lecture 17:
Kernels

What if the data is not linearly separable?

- $x^T w + b = 0$



some points don't satisfy margin constraint:

$$\min_{w,b} ||w||_2^2$$

$$y_i(x_i^T w + b) \geq 1 \quad \forall i$$

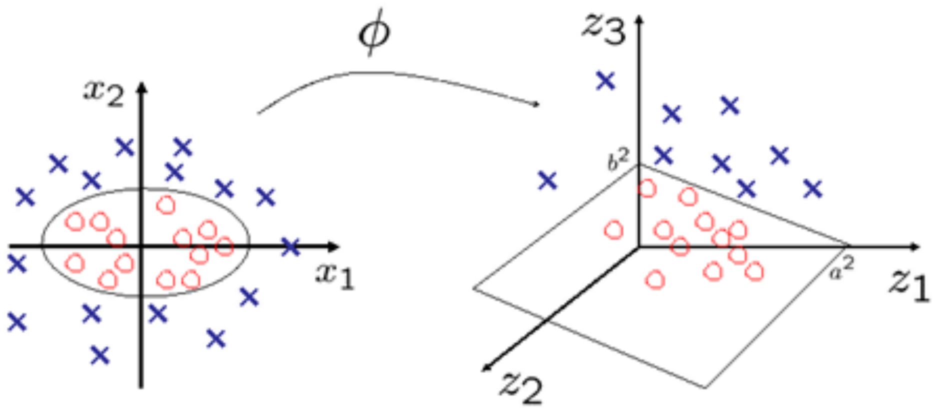
Two options:

1. Introduce slack to this optimization problem (Support Vector Machine)
2. **Lift to higher dimensional space (Kernels)**

What if the data is not linearly separable?

- Use features, for example,

$x = (x_1, x_2) \in \mathbb{R}^2$ $\qquad$ $z = \left(x_1, x_2, \sqrt{x_1^2 + x_2^2} \right) \in \mathbb{R}^3$



- In high dimensional feature space, it is easier to linearly separate different classes

Creating Features

- Feature mapping $h : \mathbb{R}^d \to \mathbb{R}^p$ maps original data into a rich and high-dimensional feature space (usually $d \ll p$)

For example, in d=1, one can use

$$h(x) = \begin{bmatrix} h_1(x) \\ h_2(x) \\ \vdots \\ h_p(x) \end{bmatrix} = \begin{bmatrix} x \\ x^2 \\ \vdots \\ x^p \end{bmatrix}$$

For example, for d>1,
one can generate vectors $\{u_j\}_{j=1}^p \subset \mathbb{R}^d$

and define features:

$$h_j(x) = (u_j^T x)^2$$

$$h_j(x) = \frac{1}{1 + \exp(u_j^T x)}$$

$$h_j(x) = \cos(u_j^T x)$$

Feature space can get really large really quickly!

Degree-d Polynomials

How do we deal with high-dimensional lifts/data?

A fundamental trick in ML: use kernels

A function $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ is a *kernel* for a map ϕ if $K(x, x') = \phi(x) \cdot \phi(x')$ for all x, x'.

This notation is for dot product (which is the same as inner product)

- So, if we can represent our
  - training algorithms and
  - decision rules for prediction
- as functions of dot products of feature maps (i.e. $\{\phi(x) \cdot \phi(x')\}$)

  and if we can find a kernel for our feature map such that

  $$K(x \,.\, x') = \phi(x) \cdot \phi(x')$$

then we can avoid explicitly copmuting (high-dimensional) $\{\phi(x)\}$

Linear Regression as Kernels

- Consider Ridge regression: $\hat{w} = \arg\min_{w \in \mathbb{R}^d} \|\mathbf{y} - \mathbf{X}w\|_2^2 + \lambda \|w\|_2^2$

Dot-product of polynomials

$$\Phi(\mathbf{u}) \cdot \Phi(\mathbf{v}) = \text{polynomials of degree exactly } d$$

$$d = 1 : \phi(u) = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \qquad \langle \phi(u), \phi(v) \rangle = u_1 v_1 + u_2 v_2$$

$$d = 2 : \phi(u) = \begin{bmatrix} u_1^2 \\ u_2^2 \\ u_1 u_2 \\ u_2 u_1 \end{bmatrix} \qquad \langle \phi(u), \phi(v) \rangle = u_1^2 v_1^2 + u_2^2 v_2^2 + 2 u_1 u_2 v_1 v_2$$

Dot-product of polynomials

$$\Phi(\mathbf{u}) \cdot \Phi(\mathbf{v}) = \text{polynomials of degree exactly } d$$

$$d = 1 : \phi(u) = \begin{bmatrix} u_1 \\ u_2 \end{bmatrix} \qquad \langle \phi(u), \phi(v) \rangle = u_1 v_1 + u_2 v_2$$

$$d = 2 : \phi(u) = \begin{bmatrix} u_1^2 \\ u_2^2 \\ u_1 u_2 \\ u_2 u_1 \end{bmatrix} \qquad \langle \phi(u), \phi(v) \rangle = u_1^2 v_1^2 + u_2^2 v_2^2 + 2 u_1 u_2 v_1 v_2$$

Feature space can get really large really quickly!

General d : Dimension of $\phi(u)$ is roughly p^d if $u \in \mathbb{R}^p$

Feature expansion can be written **implicitly** $K(\mathbf{u}, \mathbf{v}) = (\mathbf{u} \cdot \mathbf{v})^p$

Examples of Kernels

- **Polynomials of degree exactly d**

$$K(\mathbf{u}, \mathbf{v}) = (\mathbf{u} \cdot \mathbf{v})^p$$

- **Polynomials of degree up to d**

$$K(\mathbf{u}, \mathbf{v}) = (\mathbf{u} \cdot \mathbf{v} + 1)^p$$

- **Gaussian (squared exponential) kernel**

$$K(\mathbf{u}, \mathbf{v}) = \exp\left(-\frac{||\mathbf{u} - \mathbf{v}||^2}{2\sigma^2}\right)$$

- **Sigmoid**

$$K(u, v) = \tanh(\gamma \cdot u^T v + r)$$

The Kernel Trick

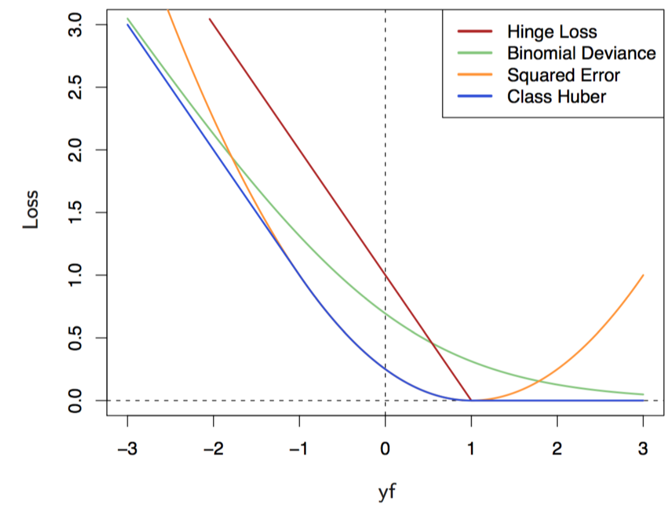
Pick a kernel K

For a linear predictor, show $w = \sum_i \alpha_i x_i$

Change loss function/decision rule to only access data through dot products

Substitute $K(x_i, x_j)$ for $x_i^T x_j$

Loss Functions



$$\{(x_i, y_i)\}_{i=1}^n \qquad x_i \in \mathbb{R}^d \qquad y_i \in \mathbb{R}$$

- Loss functions: $\displaystyle\sum_{i=1}^n \ell_i(w)$

Squared error Loss: $\ell_i(w) = (y_i - x_i^T w)^2$

Logistic Loss: $\ell_i(w) = \log(1 + \exp(-y_i\, x_i^T w))$

0/1 loss: $\ell_i(w) = \mathbb{I}[\text{sign}(y_i) \neq \text{sign}(x_i^T w)]$

Hinge Loss: $\ell_i(w) = \max\{0, 1 - y_i x_i^T w\}$

The Kernel Trick for regularized least squares

$$\widehat{w} = \arg\min_{w} \sum_{i=1}^{n} (y_i - x_i^T w)^2 + \lambda ||w||_w^2$$

There exists an $\alpha \in \mathbb{R}^n$: $\widehat{w} = \sum_{i=1}^{n} \alpha_i x_i$

The Kernel Trick for regularized least squares

$$\widehat{w} = \arg\min_{w} \sum_{i=1}^{n} (y_i - x_i^T w)^2 + \lambda ||w||_w^2$$

There exists an $\alpha \in \mathbb{R}^n$: $\widehat{w} = \sum_{i=1}^{n} \alpha_i x_i$

$$\widehat{\alpha} = \arg\min_{\alpha} \sum_{i=1}^{n} (y_i - \sum_{j=1}^{n} \alpha_j \langle x_j, x_i \rangle)^2 + \lambda \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j \langle x_i, x_j \rangle$$

$$= \arg\min_{\alpha} \sum_{i=1}^{n} (y_i - \sum_{j=1}^{n} \alpha_j K(x_i, x_j))^2 + \lambda \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j K(x_i, x_j)$$

$$= \arg\min_{\alpha} ||\mathbf{y} - \mathbf{K}\alpha||_2^2 + \lambda \alpha^T \mathbf{K} \alpha$$

$$K(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle$$

Why regularization?

Typically, $\mathbf{K} \succ 0$. What if $\lambda = 0$?

$$\widehat{\alpha} = \arg\min_{\alpha} ||\mathbf{y} - \mathbf{K}\alpha||_2^2 + \lambda \alpha^T \mathbf{K} \alpha$$

Why regularization?

Typically, $\mathbf{K} \succ 0$. What if $\lambda = 0$?

$$\widehat{\alpha} = \arg\min_{\alpha} ||\mathbf{y} - \mathbf{K}\alpha||_2^2 + \lambda\alpha^T\mathbf{K}\alpha$$

Unregularized kernel least squares can (over) fit **any data**!

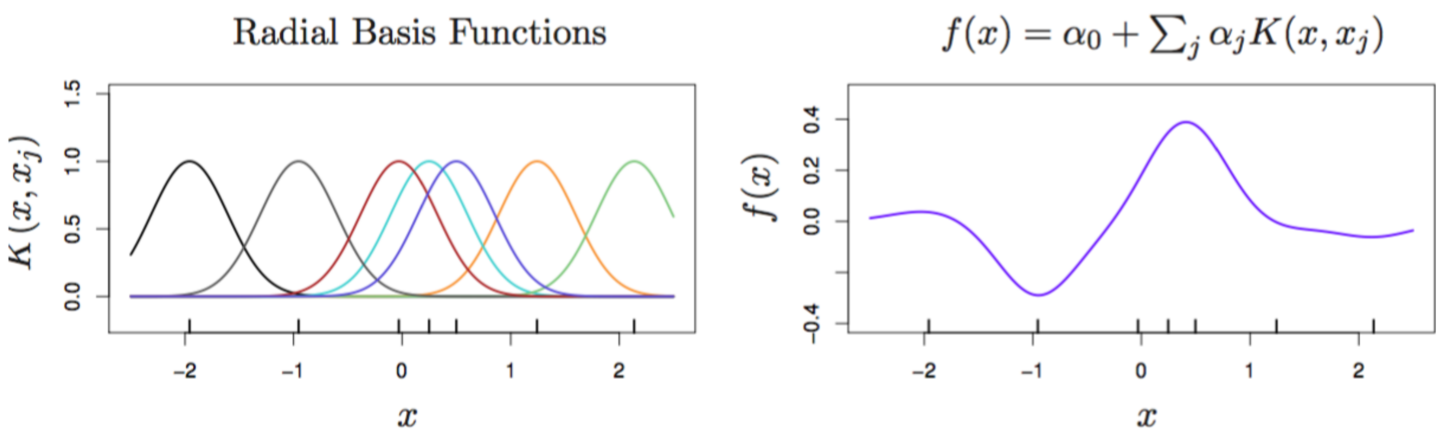
$$\widehat{\alpha} = \mathbf{K}^{-1}\mathbf{y}$$

The Kernel Trick for SVMs

RBF Kernel

$$K(\mathbf{u}, \mathbf{v}) = \exp\left(-\frac{||\mathbf{u} - \mathbf{v}||_2^2}{2\sigma^2}\right)$$

This is like weighting "bumps" on each point

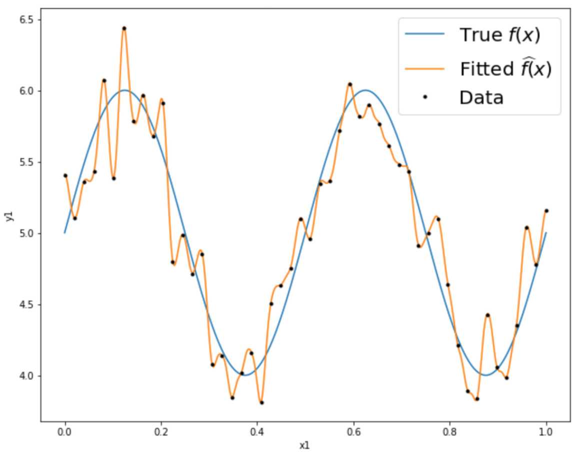


RBF Kernel

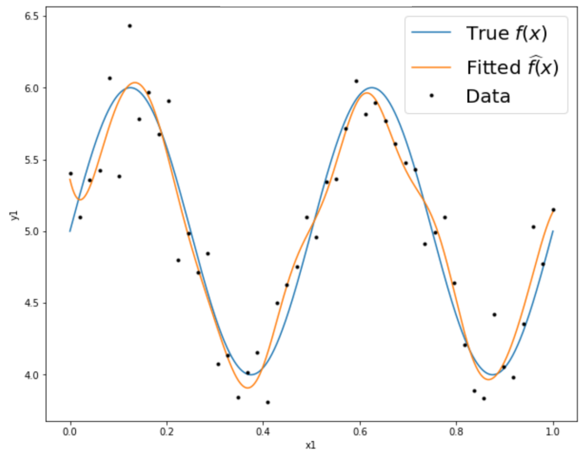
$$K(\mathbf{u},\mathbf{v}) = \exp\left(-\frac{||\mathbf{u}-\mathbf{v}||_2^2}{2\sigma^2}\right)$$

The bandwidth sigma has an enormous effect on fit:

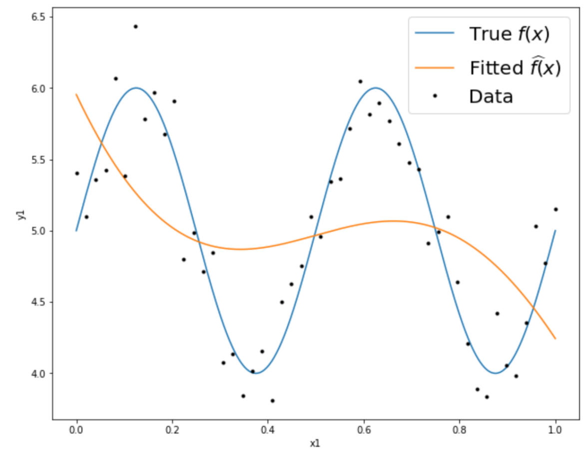
$\sigma = 10^{-2}$ $\lambda = 10^{-4}$



$\sigma = 10^{-1}$ $\lambda = 10^{-4}$



$\sigma = 10^{-0}$ $\lambda = 10^{-4}$



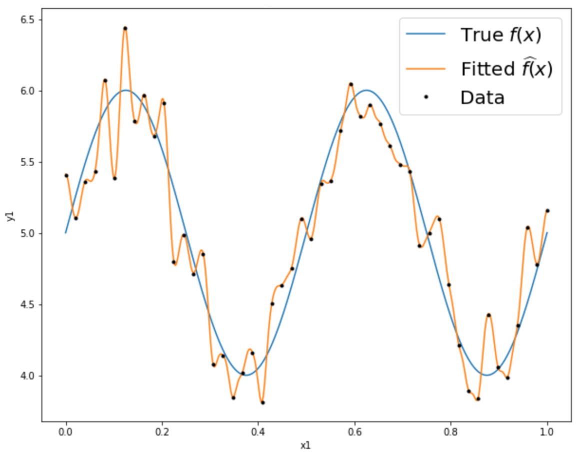
$$\widehat{f}(x) = \sum_{i=1}^{n} \widehat{\alpha}_i K(x_i, x)$$

RBF Kernel

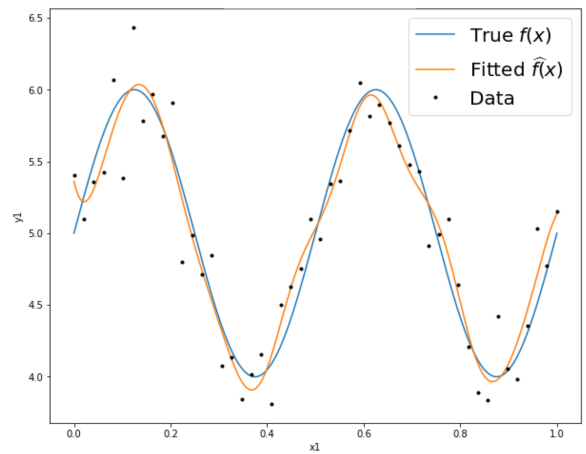
$$K(\mathbf{u}, \mathbf{v}) = \exp\left(-\frac{||\mathbf{u} - \mathbf{v}||_2^2}{2\sigma^2}\right)$$

The bandwidth sigma has an enormous effect on fit:

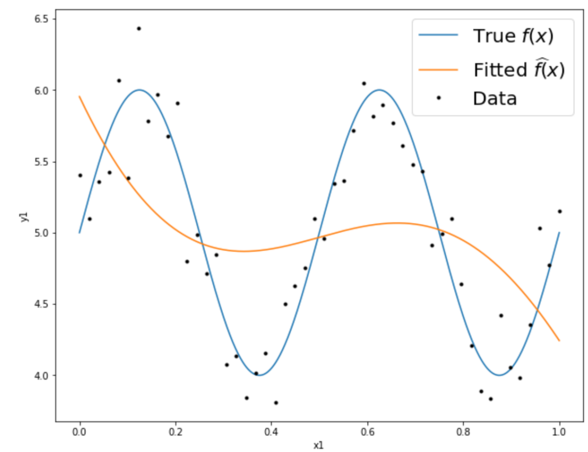
$\sigma = 10^{-2} \quad \lambda = 10^{-4}$



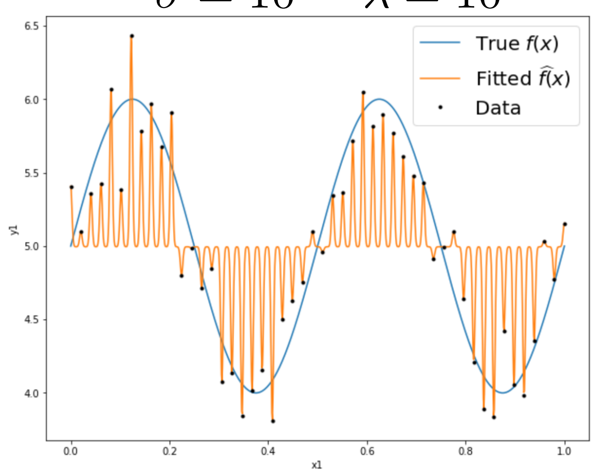
$\sigma = 10^{-1} \quad \lambda = 10^{-4}$



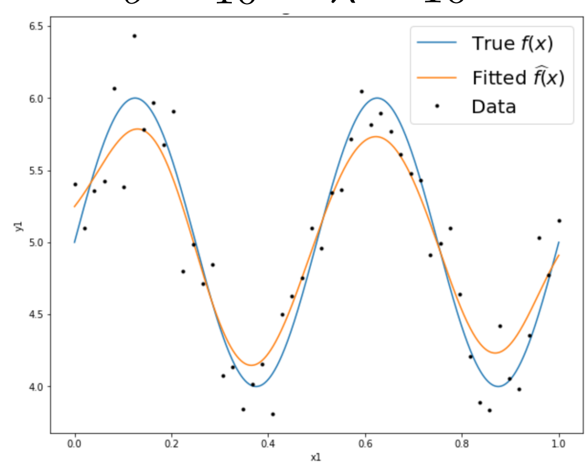
$\sigma = 10^{-0} \quad \lambda = 10^{-4}$



$\sigma = 10^{-3} \quad \lambda = 10^{-4}$



$\sigma = 10^{-1} \quad \lambda = 10^{-0}$

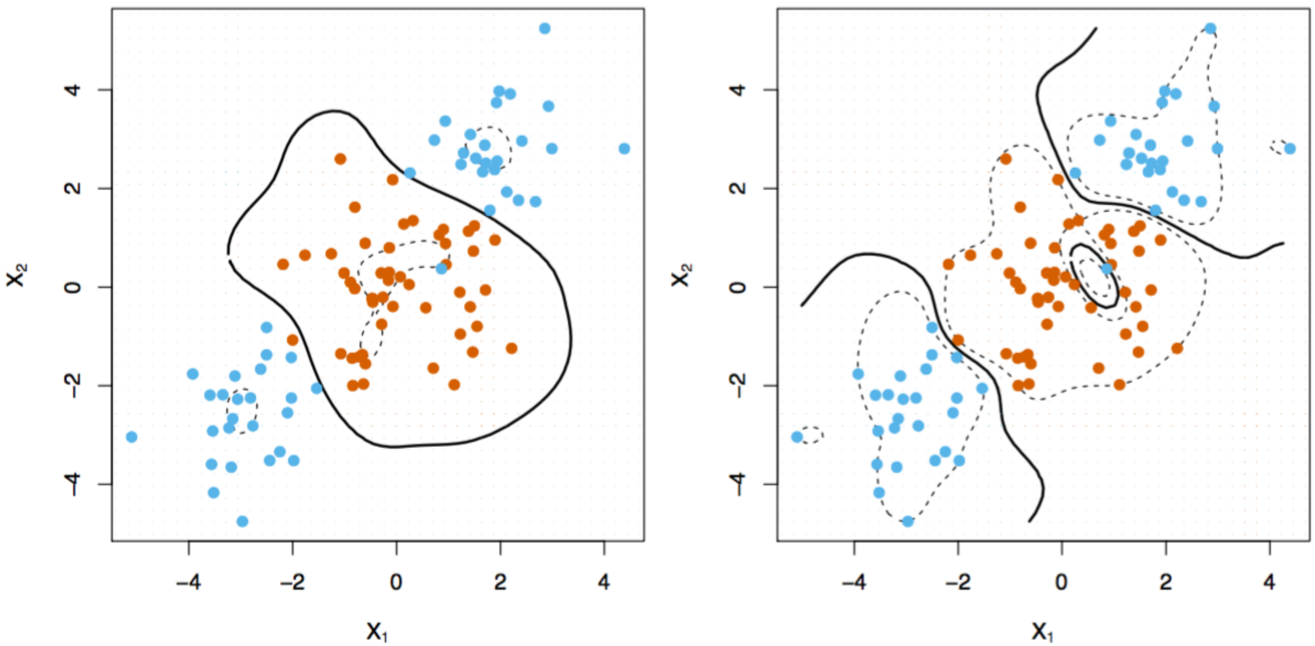


$$\widehat{f}(x) = \sum_{i=1}^{n} \widehat{\alpha}_i K(x_i, x)$$

RBF kernel and random features

$$\widehat{w} = \sum_{i=1}^{n} \max\{0, 1 - y_i(b + x_i^T w)\} + \lambda ||w||_2^2$$

$$\min_{\alpha,b} \sum_{i=1}^{n} \max\{0, 1 - y_i(b + \sum_{j=1}^{n} \alpha_j \langle x_i, x_j \rangle)\} + \lambda \sum_{i,j=1}^{n} \alpha_i \alpha_j \langle x_i, x_j \rangle$$



RBF kernel and random features

$$K(\mathbf{u}, \mathbf{v}) = \exp\left(-\frac{||\mathbf{u} - \mathbf{v}||_2^2}{2\sigma^2}\right)$$

If n is very large, allocating an n-by-n matrix is tough.

RBF kernel and random features

$$K(\mathbf{u}, \mathbf{v}) = \exp\left(-\frac{||\mathbf{u}-\mathbf{v}||_2^2}{2\sigma^2}\right)$$

If n is very large, allocating an n-by-n matrix is tough.

$$2\cos(\alpha)\cos(\beta) = \cos(\alpha+\beta) + \cos(\alpha-\beta)$$
$$e^{jz} = \cos(z) + j\sin(z)$$

$$\phi(x) = \begin{bmatrix} \sqrt{2}\cos(w_1^T x + b_1) \\ \vdots \\ \sqrt{2}\cos(w_p^T x + b_p) \end{bmatrix}$$

$$w_k \sim \mathcal{N}(0, 2\gamma\, I)$$
$$b_k \sim \text{uniform}(0, \pi)$$

[Rahimi, Recht NIPS 2007]
"NIPS Test of Time Award, 2018"

String Kernels

Example from Efron and Hastie, 2016

Amino acid sequences of different lengths:

x1

IPTSALVKETLALLSTHRTLLIANETLRIPVPVHKNHQLCTEEIFQGIGTLESQTVQGGTV
ERLFKNLSLIKKYIDGQKKKCGEERRRVNQFLDY**LQE**FLGVMNTEWI

x2

PHRRDLCSRSIWLARKIRSDLTALTESYVKHQGLWSELTEAER**LQE**NLQAYRTFHVLLA
RLLEDQQVHFTPTEGDFHQAIHTLLLQVAAFAYQIEELMILLEYKIPRNEADGMLFEKK
LWGLKV**LQE**LSQWTVRSIHDLRFISSHQTGIP

All subsequences of length 3 (of possible 20 amino acids) $20^3 = 8{,}000$

$$h^3_{\text{LQE}}(x_1) = 1 \text{ and } h^3_{\text{LQE}}(x_2) = 2.$$

Fixed Feature V.S. Learned Feature