Announcements

Assignments

- HW8: due Thu, 12/3, 11:59 pm
- HW9
  - Out Friday
  - Due Wed, 12/9, 11:59 pm
  - The two slip days are free (last possible submission Fri, 12/11, 11:59 pm)

Final Exam

- Mon, 12/14
- Stay tuned to Piazza for more details

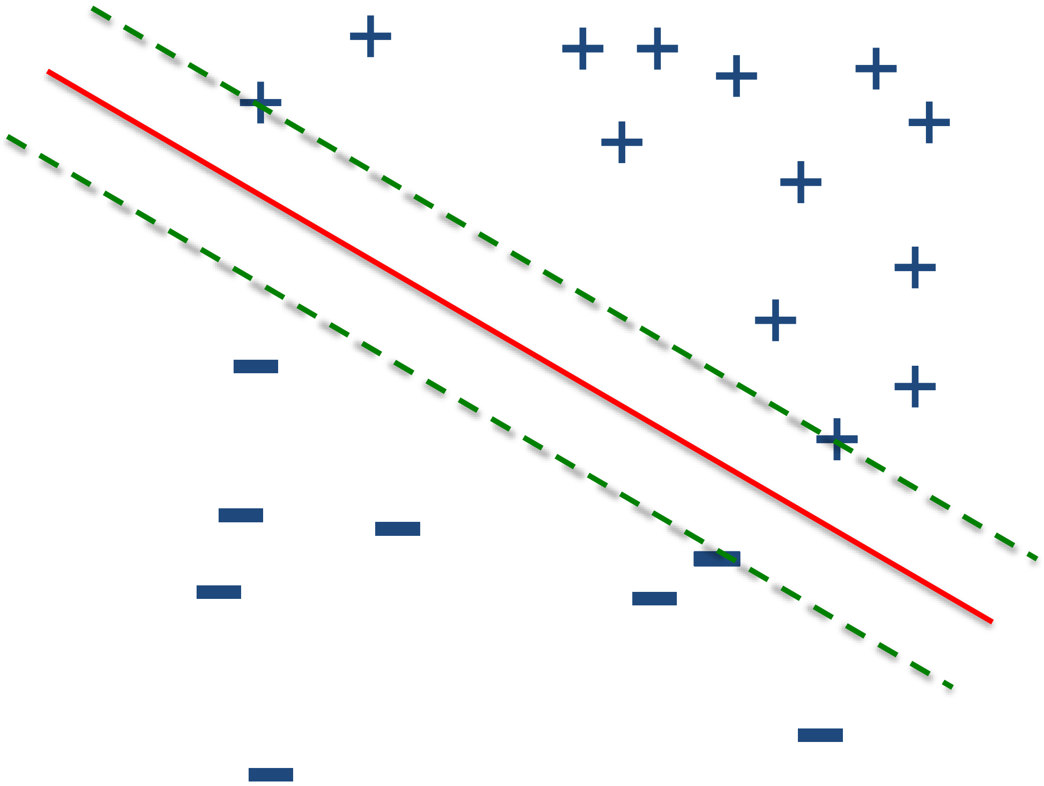
Introduction to Machine Learning

Support Vector Machines

Instructor: Pat Virtue

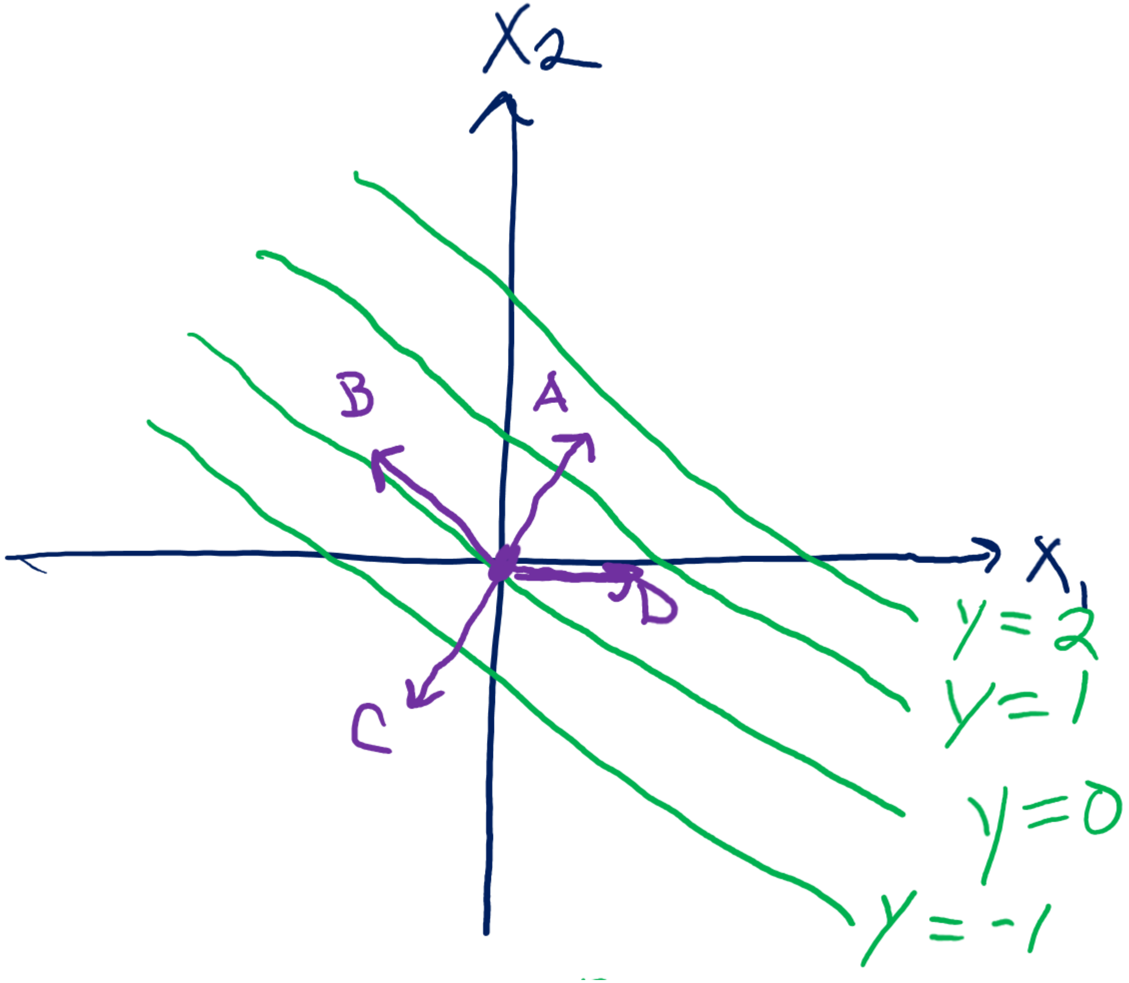
Support Vector Machines

Find linear separator with maximum margin



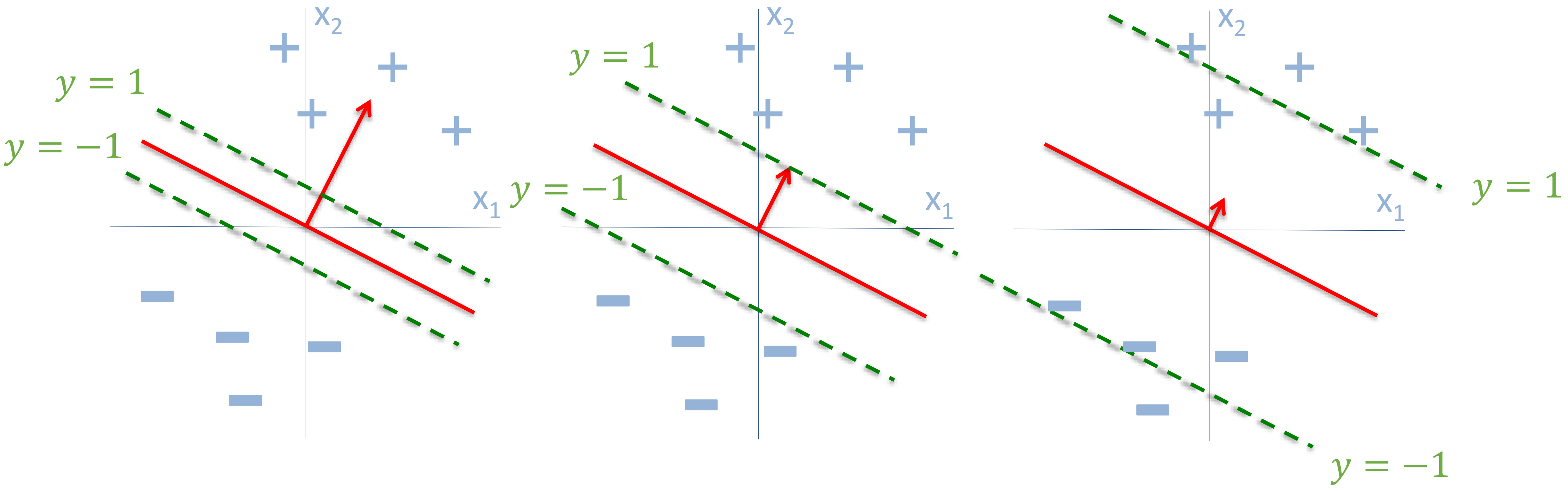
Previous Piazza Poll

As the magnitude of w increases, will the distance between the contour lines of $y = \boldsymbol{w}^T \boldsymbol{x} + b$ increase or decrease?



Support Vector Machines

Find linear separator with maximum margin



Linear Separability

Data

$$\mathcal{D} = \{\boldsymbol{x}^{(i)}, y^{(i)}\}_{i=1}^{N} \quad \boldsymbol{x} \in \mathbb{R}^M, \quad y \in \{-1, +1\}$$

Linearly separable iff:

$$\exists\, \boldsymbol{w}, b \qquad s.t. \quad \boldsymbol{w}^T \boldsymbol{x}^{(i)} + b > 0 \quad \text{if} \quad y^{(i)} = +1 \quad \text{and}$$

$$\boldsymbol{w}^T \boldsymbol{x}^{(i)} + b < 0 \quad \text{if} \quad y^{(i)} = -1$$

Linear Separability

Data

$$\mathcal{D} = \left\{\boldsymbol{x}^{(i)}, y^{(i)}\right\}_{i=1}^{N} \quad \boldsymbol{x} \in \mathbb{R}^M, \quad y \in \{-1, +1\}$$

Linearly separable iff:

$$\begin{aligned}
&\exists\, \boldsymbol{w}, b \quad && s.t. \quad \boldsymbol{w}^T\boldsymbol{x}^{(i)} + b > 0 \;\; \text{if} \;\; y^{(i)} = +1 \quad \text{and} \\
& && \quad \boldsymbol{w}^T\boldsymbol{x}^{(i)} + b < 0 \;\; \text{if} \;\; y^{(i)} = -1 \\
\Leftrightarrow\; &\exists\, \boldsymbol{w}, b && s.t. \quad y^{(i)}\left(\boldsymbol{w}^T\boldsymbol{x}^{(i)} + b\right) > 0 \\
\Leftrightarrow\; &\exists\, \boldsymbol{w}, b, c && s.t. \quad y^{(i)}\left(\boldsymbol{w}^T\boldsymbol{x}^{(i)} + b\right) \geq c \quad \text{and} \quad c > 0
\end{aligned}$$

Slide credit: CMU MLD Matt Gormley

Piazza Poll 1

Are these two statements equivalent?

$$\exists\, \boldsymbol{w}, b, c \quad s.t. \quad y^{(i)}\left(\boldsymbol{w}^T \boldsymbol{x}^{(i)} + b\right) \geq c \quad \text{and} \quad c > 0$$

$$\exists\, \boldsymbol{w}, b \qquad s.t. \quad y^{(i)}\left(\boldsymbol{w}^T \boldsymbol{x}^{(i)} + b\right) \geq 1$$

Linear Separability

Data

$$\mathcal{D} = \{\boldsymbol{x}^{(i)}, y^{(i)}\}_{i=1}^{N} \quad \boldsymbol{x} \in \mathbb{R}^M, \quad y \in \{-1, +1\}$$

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\Leftrightarrow\ & \exists\, \boldsymbol{w}, b \quad s.t. \quad && y^{(i)}\left(\boldsymbol{w}^T \boldsymbol{x}^{(i)} + b\right) > 0 \\
\Leftrightarrow\ & \exists\, \boldsymbol{w}, b, c \quad s.t. \quad && y^{(i)}\left(\boldsymbol{w}^T \boldsymbol{x}^{(i)} + b\right) \geq c \quad \text{and} \quad c > 0 \\
\Leftrightarrow\ & \exists\, \boldsymbol{w}, b \quad s.t. \quad && y^{(i)}\left(\boldsymbol{w}^T \boldsymbol{x}^{(i)} + b\right) \geq 1
\end{aligned}$$

Slide credit: CMU MLD Matt Gormley

Support Vector Machines

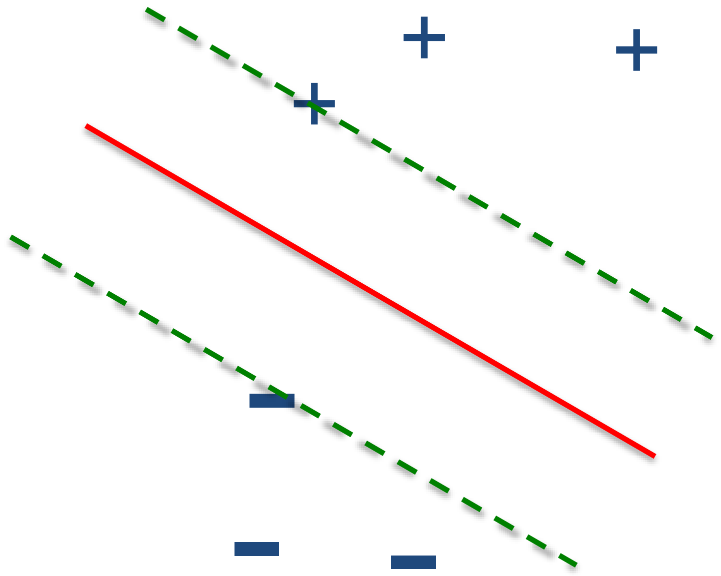
Find linear separator with maximum margin

Let $\boldsymbol{x}_+$ and $\boldsymbol{x}_-$ be hypothetical points on the +/- margin from the decision boundary

$$\exists\, \boldsymbol{w}, b \quad s.t.\quad y^{(i)}\left(\boldsymbol{w}^T\boldsymbol{x}^{(i)} + b\right) \geq 1$$

$$\Leftrightarrow\ \exists\, \boldsymbol{w}, b \quad s.t.\quad \boldsymbol{w}^T\boldsymbol{x}_+ + b \geq +1 \quad \text{and}$$

$$\boldsymbol{w}^T\boldsymbol{x}_- + b \leq -1$$



Consider the vector from $\boldsymbol{x}_-$ to $\boldsymbol{x}_+$ and its projection onto the vector $\boldsymbol{w}$:

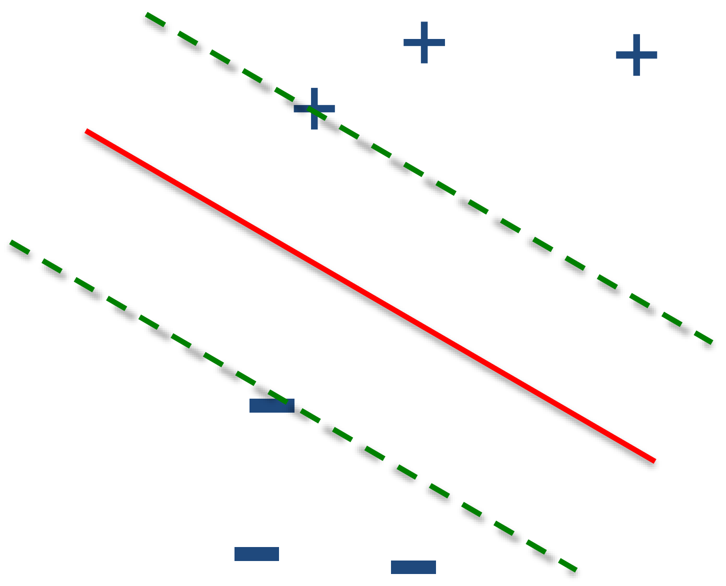
Support Vector Machines

$$width = \frac{\boldsymbol{w}^T}{\|\boldsymbol{w}\|_2}(\boldsymbol{x}_+ - \boldsymbol{x}_-)$$

Find linear separator with maximum margin

$$\max_{\boldsymbol{w},b} \quad \text{"width"}$$

$$\text{s.t.} \quad y^{(i)}\left(\boldsymbol{w}^T\boldsymbol{x}^{(i)} + b\right) \geq 1 \quad \forall\, i$$

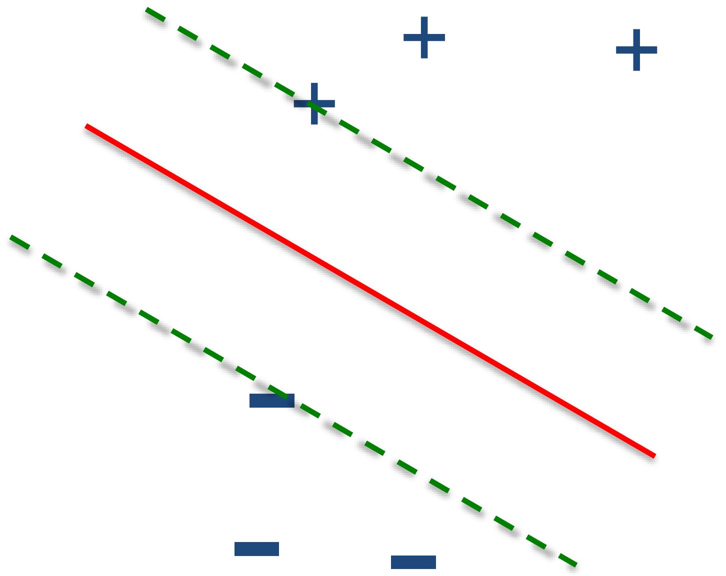


Support Vector Machines

$$\text{width} = \frac{2}{\|\boldsymbol{w}\|_2}$$

Find linear separator with maximum margin

$$\underset{\boldsymbol{w},b}{\operatorname{argmax}} \quad \text{width}$$



Support Vector Machines

$$\text{width} = \frac{2}{\|\boldsymbol{w}\|_2}$$

Find linear separator with maximum margin

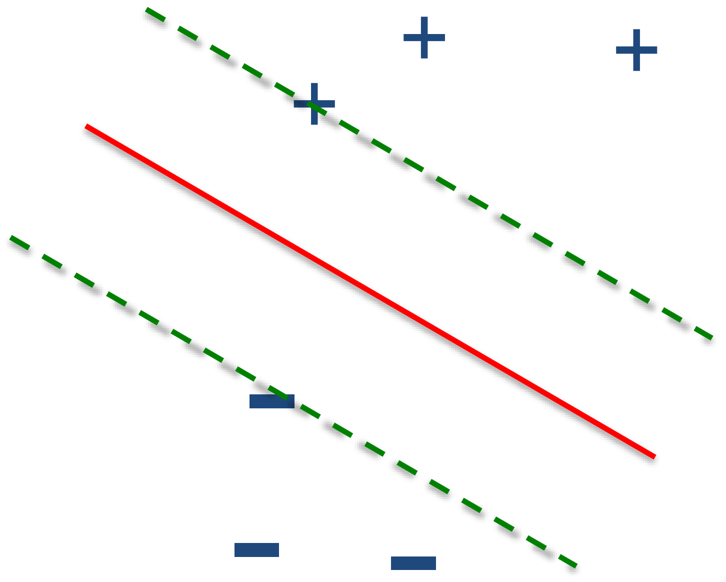
$$\underset{\boldsymbol{w},b}{\operatorname{argmax}} \quad \text{width}$$

$$\Leftrightarrow \underset{\boldsymbol{w},b}{\operatorname{argmax}} \quad \frac{2}{\|\boldsymbol{w}\|_2}$$

$$\Leftrightarrow \underset{\boldsymbol{w},b}{\operatorname{argmin}} \quad \frac{1}{2}\|\boldsymbol{w}\|_2$$

$$\Leftrightarrow \underset{\boldsymbol{w},b}{\operatorname{argmin}} \quad \frac{1}{2}\|\boldsymbol{w}\|_2^2$$

$$\Leftrightarrow \underset{\boldsymbol{w},b}{\operatorname{argmin}} \quad \frac{1}{2}\boldsymbol{w}^T\boldsymbol{w}$$



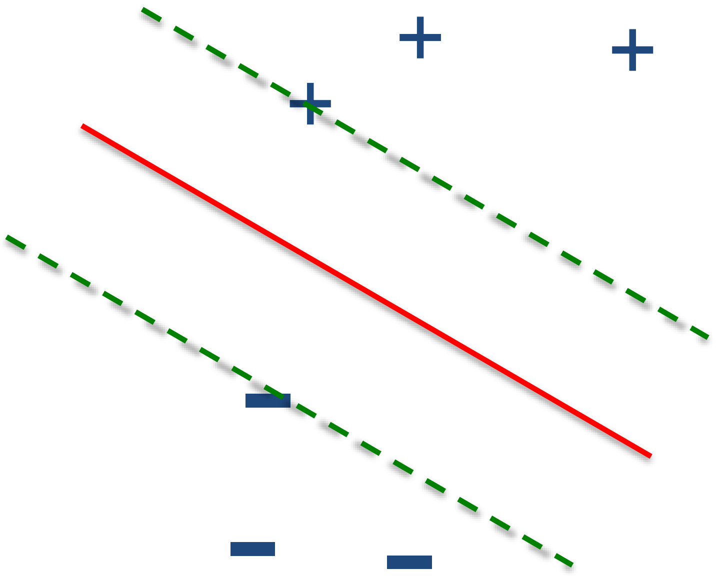
SVM Optimization

Quadratic Program

$$\min_{\boldsymbol{x}} \quad \boldsymbol{x}^T \boldsymbol{Q} \boldsymbol{x} + \boldsymbol{c}^T \boldsymbol{x}$$
$$\text{s.t.} \quad \boldsymbol{A}\boldsymbol{x} \preceq \boldsymbol{b}$$

Quadratic program!

$$\min_{\boldsymbol{w},b} \quad \frac{1}{2}\boldsymbol{w}^T\boldsymbol{w}$$
$$\text{s.t.} \quad y^{(i)}\left(\boldsymbol{w}^T\boldsymbol{x}^{(i)} + b\right) \geq 1 \quad \forall\, i$$

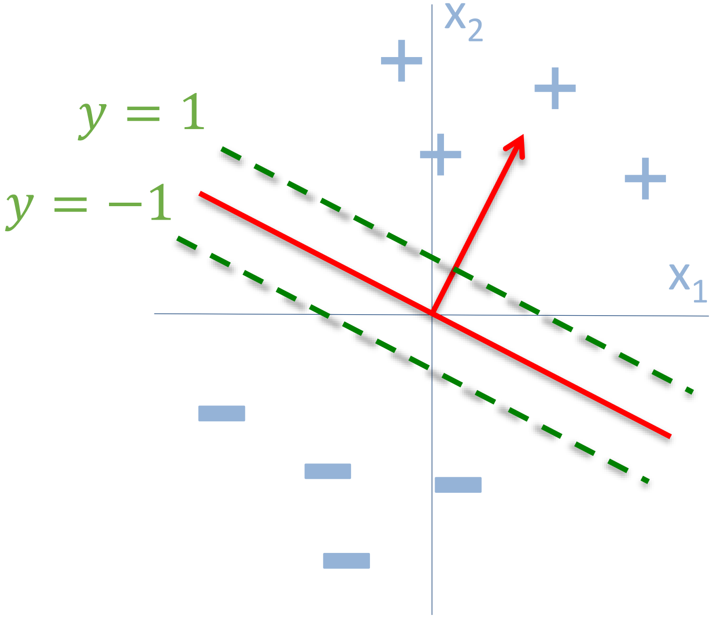


SVM Optimization

How did we go from maximizing margin to minimizing $||\boldsymbol{w}||_2$?

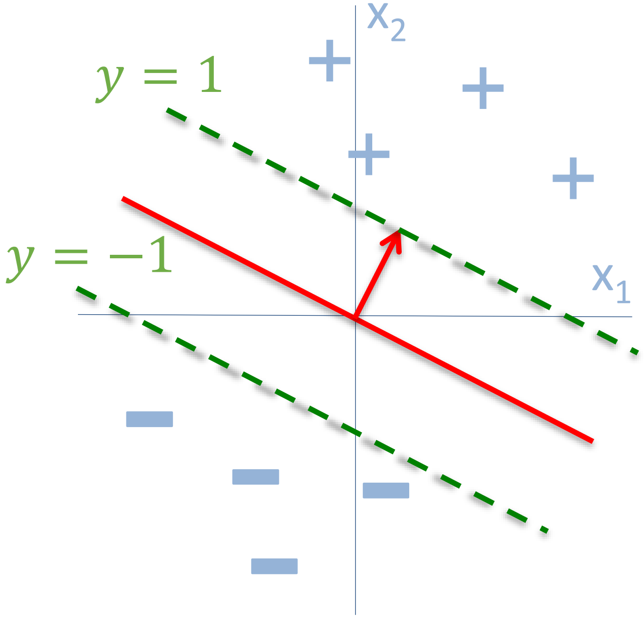
SVM Optimization

How did we go from maximizing margin to minimizing $\|\boldsymbol{w}\|_2$?



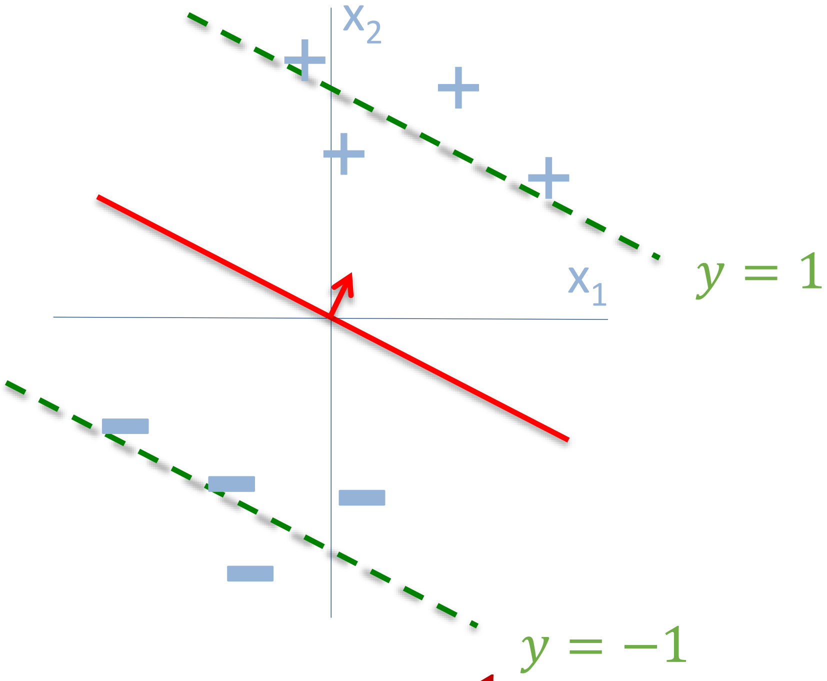
$$\|\boldsymbol{w}\|_2 = 2$$

$$\frac{1}{\|\boldsymbol{w}\|_2} = \frac{1}{2}$$



$$\|\boldsymbol{w}\|_2 = 1$$

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



$$\|\boldsymbol{w}\|_2 = \frac{1}{2}$$

$$\frac{1}{\|\boldsymbol{w}\|_2} = 2$$

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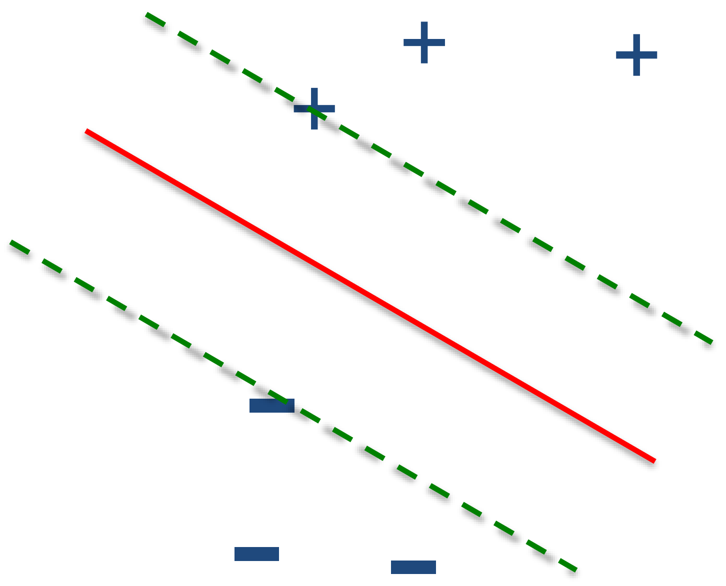

SVM Optimization

Quadratic program!

$$\min_{\boldsymbol{w},b} \quad \frac{1}{2}\|\boldsymbol{w}\|_2^2$$
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Quadratic Program

$$\min_{\boldsymbol{x}} \quad \boldsymbol{x}^T\boldsymbol{Q}\boldsymbol{x} + \boldsymbol{c}^T\boldsymbol{x}$$
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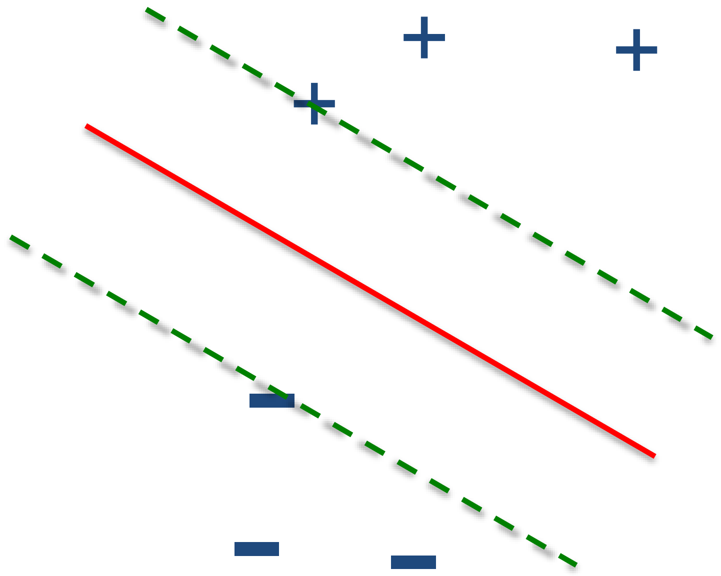


Constrained Optimization

Linear Program

$$\begin{aligned} \min_{\boldsymbol{x}} \quad & \boldsymbol{c}^T \boldsymbol{x} \\ \text{s.t.} \quad & \boldsymbol{A}\boldsymbol{x} \preceq \boldsymbol{b} \end{aligned}$$

Quadratic Program

$$\begin{aligned} \min_{\boldsymbol{x}} \quad & \boldsymbol{x}^T \boldsymbol{Q} \boldsymbol{x} + \boldsymbol{c}^T \boldsymbol{x} \\ \text{s.t.} \quad & \boldsymbol{A}\boldsymbol{x} \preceq \boldsymbol{b} \end{aligned}$$

Solvers

- Simplex
- Interior point methods

Solvers

- Conjugate gradient
- Ellipsoid method
- Interior point methods

Constrained Optimization

Linear Program

$$\min_{\boldsymbol{x}} \quad \boldsymbol{c}^T \boldsymbol{x}$$
$$\text{s.t.} \quad \boldsymbol{A}\boldsymbol{x} \preceq \boldsymbol{b}$$

Quadratic Program

$$\min_{\boldsymbol{x}} \quad \boldsymbol{x}^T \boldsymbol{Q} \boldsymbol{x} + \boldsymbol{c}^T \boldsymbol{x}$$
$$\text{s.t.} \quad \boldsymbol{A}\boldsymbol{x} \preceq \boldsymbol{b}$$

Solvers

- Simplex
- Interior point methods

Special Case

- If $\boldsymbol{Q}$ is positive-definite, the problem is convex
- $\boldsymbol{Q}$ is positive-definite if:
  $\boldsymbol{v}^T \boldsymbol{Q} \boldsymbol{v} > 0 \quad \forall\, \boldsymbol{v} \in \mathbb{R}^M \backslash \boldsymbol{0}$
- A symmetric $\boldsymbol{Q}$ is positive-definite if all of its eigenvalues are positive

Support Vector Machines

Next steps

- Different optimization formulation
  - Primal → dual
  - “Support vectors”
- Support non-linear classification
  - Feature maps
  - Kernel trick
- Support non-separable data
  - Hard-margin SVM → soft-margin SVM

Method of Lagrange Multipliers

Goal

$$\min_{\boldsymbol{x}} \quad f(\boldsymbol{x})$$
$$\text{s.t.} \quad g(\boldsymbol{x}) \leq c$$

Step 1: Construct Lagrangian

$$\mathcal{L}(\boldsymbol{x}, \lambda) = f(\boldsymbol{x}) + \lambda(g(\boldsymbol{x}) - c)$$

Step 2: Solve

$$\min_{\boldsymbol{x}} \quad \max_{\lambda \geq 0} \quad \mathcal{L}(\boldsymbol{x}, \lambda)$$

Find saddle point:

$$\nabla \mathcal{L}(\boldsymbol{x}, \lambda) \quad \text{s.t. } \lambda \geq 0$$

Equivalent to solving:

$$\nabla f(x) = \lambda \nabla g(x) \quad \text{s.t. } \lambda \geq 0$$

SVM Primal vs Dual

Construct Lagrangian

Primal

$$\min_{\boldsymbol{w},\boldsymbol{b}} \quad \frac{1}{2}\|\boldsymbol{w}\|_2^2$$

$$\text{s.t.} \quad y^{(i)}\left(\boldsymbol{w}^T\boldsymbol{x}^{(i)} + b\right) \geq 1 \quad \forall\, i$$

Lagrange Multipliers

$$\min_{\boldsymbol{x}} \; f(\boldsymbol{x}) \quad \text{s.t.} \quad g(\boldsymbol{x}) \leq c$$

Construct Lagrangian

$$\mathcal{L}(\boldsymbol{x},\lambda) = f(\boldsymbol{x}) + \lambda(g(\boldsymbol{x}) - c)$$

Solve: $\min\limits_{\boldsymbol{x}} \; \max\limits_{\lambda \geq 0} \; \mathcal{L}(\boldsymbol{x},\lambda)$

SVM Dual Optimization

$$\mathcal{L}(w, b, \boldsymbol{\alpha}) = \frac{1}{2}\boldsymbol{w}^T\boldsymbol{w} \ - \sum_i^N \alpha_i [\, y^{(i)}\left(\boldsymbol{w}^T\boldsymbol{x}^{(i)} + b\right) - 1]$$

SVM Dual Optimization

Dual

$$\max_{\boldsymbol{\alpha}} \quad \sum_i^N \alpha_i - \frac{1}{2}\sum_i^N \sum_j^N \alpha_i \alpha_j y^{(i)} y^{(j)} \boldsymbol{x}^{(i)T} \boldsymbol{x}^{(j)}$$

$$\text{s.t.} \quad \alpha_i \geq 0 \quad \forall\, i$$

$$\boldsymbol{w} = \sum_i^N \alpha_i y^{(i)} \boldsymbol{x}^{(i)}$$

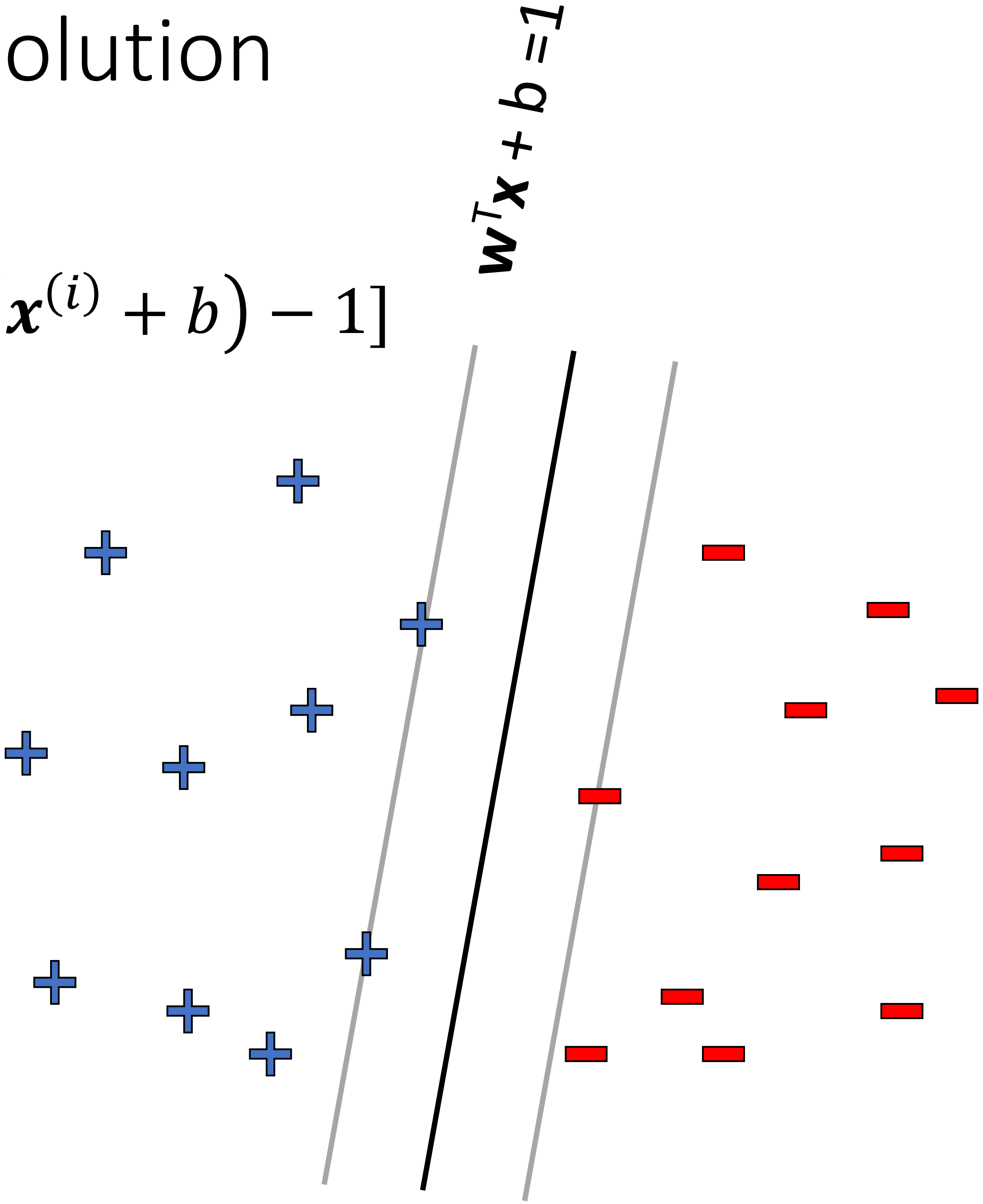
$b = y^{(k)} - \boldsymbol{w}^T \boldsymbol{x}^{(\boldsymbol{k})}$ for any k where $\alpha_k > 0$

Prediction

Dual SVM: Sparsity of dual solution

$$\min_{\boldsymbol{w},b} \max_{\boldsymbol{\alpha}\geq 0} \mathcal{L}(\boldsymbol{w}, b, \boldsymbol{\alpha})$$

$$\min_{\boldsymbol{w},b} \max_{\boldsymbol{\alpha}\geq 0} \frac{1}{2}\boldsymbol{w}^T\boldsymbol{w} - \sum_i^N \alpha_i [\, y^{(i)}(\boldsymbol{w}^T\boldsymbol{x}^{(i)} + b) - 1]$$



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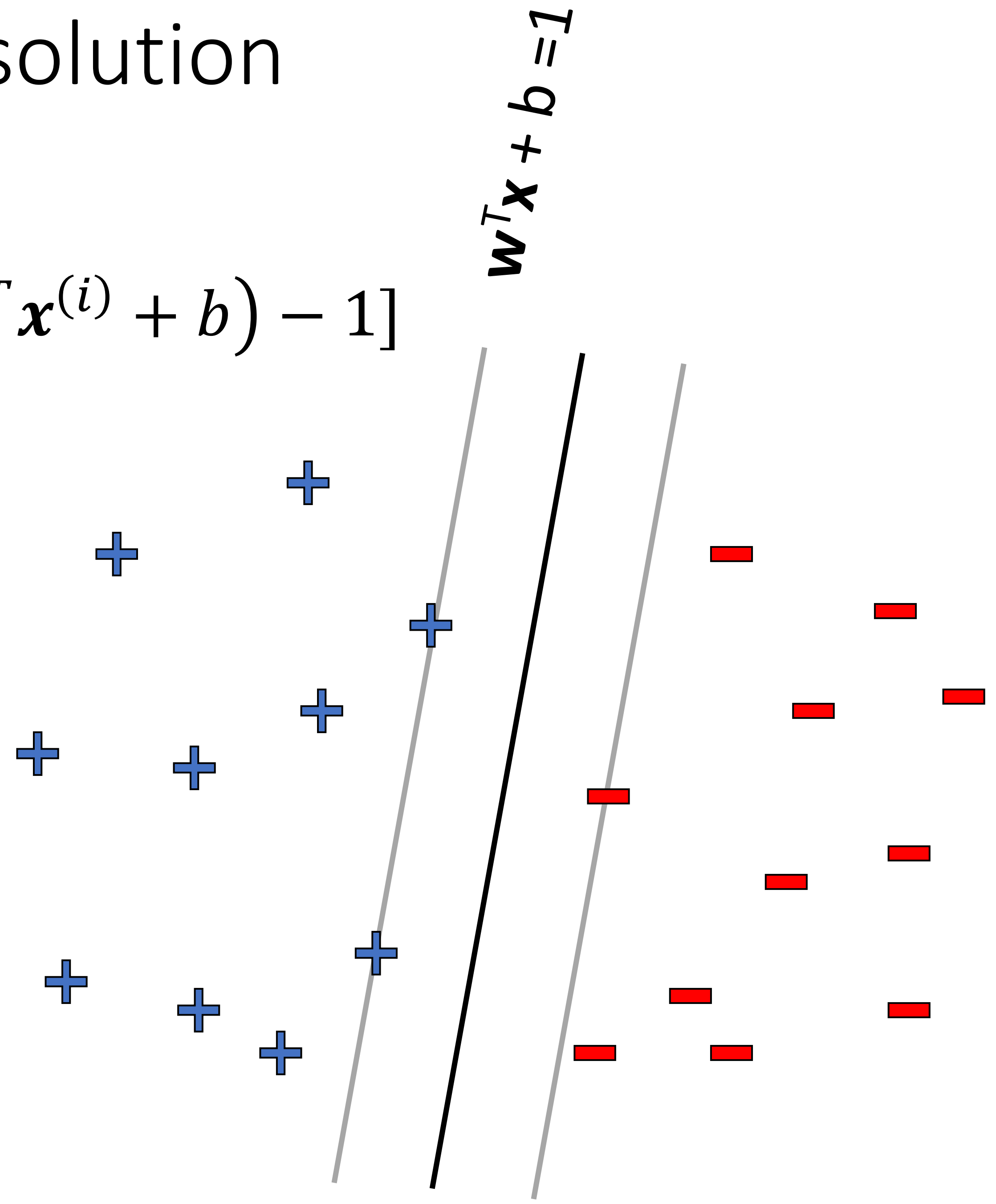
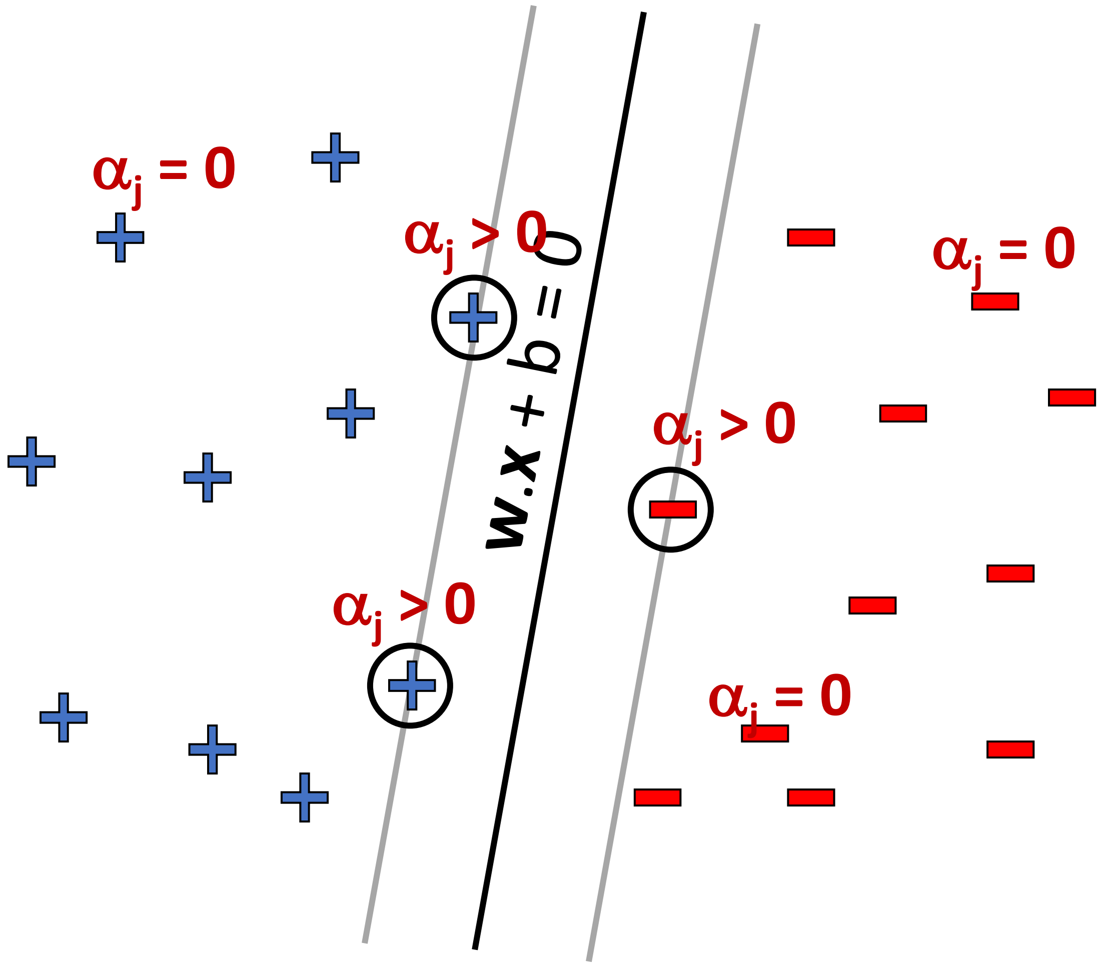


Dual SVM: Sparsity of dual solution



$$\mathbf{w} = \sum_j \alpha_j y_j \mathbf{x}_j$$

Only few α_js can be non-zero : where constraint is active and tight

$$(\mathbf{w}.\mathbf{x}_j + b)y_j = 1$$

Support vectors – training points j whose α_js are non-zero

Slide credit: CMU MLD Aarti Singh

Support Vector Machines

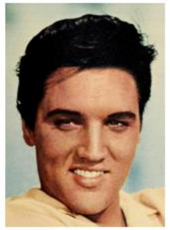
Next steps

- Different optimization formulation
  - Primal → dual
  - "Support vectors"
- Support non-linear classification
  - Feature maps
  - Kernel trick
- Support non-separable data
  - Hard-margin SVM → soft-margin SVM

Kernels: Motivation

Most real-world problems exhibit data that is not linearly separable.

Example: pixel representation for Facial Recognition:

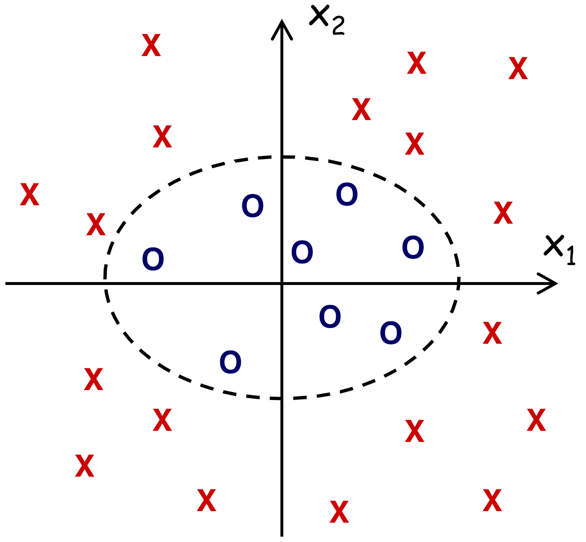
Q: When your data is **not linearly separable**, how can you still use a linear classifier?

A: Preprocess the data to produce **nonlinear features**

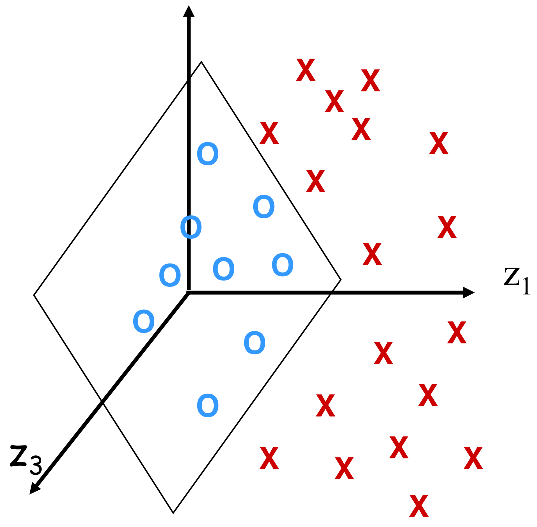
Example: Polynomial Kernel

https://www.youtube.com/watch?v=3liCbRZPrZA

Original space



Φ-space



Kernels: Motivation

- Motivation #1: Inefficient Features
  - Non-linearly separable data requires **high dimensional** representation
  - Might be **prohibitively expensive** to compute or store
- Motivation #2: Memory-based Methods
  - k-Nearest Neighbors (KNN) for facial recognition allows a **distance metric** between images -- no need to worry about linearity restriction at all

Kernel Methods

- **Key idea:**
  1. Rewrite the algorithm so that we only work with **dot products** $x^T z$ of feature vectors
  2. Replace the **dot products** $x^T z$ with a **kernel function** $k(x, z)$

- The kernel $k(x,z)$ can be **any** legal definition of a dot product:

  $$k(x, z) = \varphi(x)^T \varphi(z) \text{ for any function } \varphi: \mathcal{X} \rightarrow \mathbf{R}^D$$

  So we only compute the φ dot product **implicitly**

- This **"kernel trick"** can be applied to many algorithms:
  - classification: perceptron, SVM, …
  - regression: ridge regression, …
  - clustering: k-means, …

SVM: Kernel Trick

Hard-margin SVM (Primal)

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|_2^2$$

$$\text{s.t. } y^{(i)}(\mathbf{w}^T\mathbf{x}^{(i)} + b) \geq 1, \quad \forall i$$

Hard-margin SVM (Lagrangian Dual)

$$\max_{\boldsymbol{\alpha}} \sum_{i=1}^{N} \alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i \alpha_j y^{(i)} y^{(j)} \mathbf{x}^{(i)} \cdot \mathbf{x}^{(j)}$$

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

$$\sum_{i=1}^{N} \alpha_i y^{(i)} = 0$$

- Suppose we do some feature engineering
- Our feature function is ϕ
- We apply ϕ to each input vector **x**

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|_2^2$$

$$\text{s.t. } y^{(i)}(\mathbf{w}^T\phi\left(\mathbf{x}^{(i)}\right) + b) \geq 1, \quad \forall i$$

$$\max_{\boldsymbol{\alpha}} \sum_{i=1}^{N} \alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i \alpha_j y^{(i)} y^{(j)} \phi\left(\mathbf{x}^{(i)}\right) \cdot \phi\left(\mathbf{x}^{(j)}\right)$$

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SVM: Kernel Trick

Hard-margin SVM (Lagrangian Dual)

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

$$\sum_{i=1}^{N} \alpha_i y^{(i)} = 0$$

We could replace the dot product of the two feature vectors in the transformed space with a function k(x,z)
where $k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \phi\left(\mathbf{x}^{(i)}\right) \cdot \phi\left(\mathbf{x}^{(j)}\right)$

Slide credit: CMU MLD Matt Gormley

SVM: Kernel Trick

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$$\max_{\boldsymbol{\alpha}} \sum_{i=1}^{N} \alpha_i - \frac{1}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} \alpha_i \alpha_j y^{(i)} y^{(j)} \boxed{k(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})}$$

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

$$\sum_{i=1}^{N} \alpha_i y^{(i)} = 0$$

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Kernel Methods

Q: These are just non-linear features, right?

A: Yes, but…

Q: Can't we just compute the feature transformation φ explicitly?

A: That depends...

Q: So, why all the hype about the kernel trick?

A: Because the **explicit features** might either be **prohibitively expensive** to compute or **infinite length** vectors

Slide credit: CMU MLD Matt Gormley

Example: Polynomial Kernel

For n=2, d=2, the kernel $K(x, z) = (x \cdot z)^d$ corresponds to

$$\phi: R^2 \to R^3, (x_1, x_2) \to \Phi(x) = (x_1^2, x_2^2, \sqrt{2}x_1x_2)$$

$$\phi(x) \cdot \phi(z) = \left(x_1^2, x_2^2, \sqrt{2}x_1x_2\right) \cdot (z_1^2, z_2^2, \sqrt{2}z_1z_2)$$

$$= (x_1z_1 + x_2z_2)^2 = (x \cdot z)^2 = K(x, z)$$

Kernel Examples

Side Note: The feature space might not be unique!

Explicit representation #1:

$$\phi: \mathrm{R}^2 \to \mathrm{R}^3,\ (\mathrm{x}_1, \mathrm{x}_2) \to \Phi(\mathrm{x}) = (\mathrm{x}_1^2, \mathrm{x}_2^2, \sqrt{2}\mathrm{x}_1\mathrm{x}_2)$$

$$\phi(\mathrm{x}) \cdot \phi(z) = \left(\mathrm{x}_1^2, \mathrm{x}_2^2, \sqrt{2}\mathrm{x}_1\mathrm{x}_2\right) \cdot (z_1^2, z_2^2, \sqrt{2}z_1 z_2)$$

$$= (\mathrm{x}_1 z_1 + \mathrm{x}_2 z_2)^2 = (\mathrm{x} \cdot z)^2 = \mathrm{K}(\mathrm{x}, \mathrm{z})$$

Explicit representation #2:

$$\phi: \mathrm{R}^2 \to \mathrm{R}^4,\ (\mathrm{x}_1, \mathrm{x}_2) \to \Phi(\mathrm{x}) = (\mathrm{x}_1^2, \mathrm{x}_2^2, \mathrm{x}_1\mathrm{x}_2, \mathrm{x}_2\mathrm{x}_1)$$

$$\phi(\mathrm{x}) \cdot \phi(z) = (\mathrm{x}_1^2, \mathrm{x}_2^2, \mathrm{x}_1\mathrm{x}_2, \mathrm{x}_2\mathrm{x}_1) \cdot (\mathrm{z}_1^2, \mathrm{z}_2^2, \mathrm{z}_1\mathrm{z}_2, \mathrm{z}_2\mathrm{z}_1)$$

$$= (\mathrm{x} \cdot z)^2 = \mathrm{K}(\mathrm{x}, \mathrm{z})$$

These two different feature representations correspond to the same kernel function!

Slide credit: CMU MLD Nina Balcan

Kernel Examples

Name	Kernel Function (implicit dot product)	Feature Space (explicit dot product)
Linear	$K(\mathbf{x}, \mathbf{z}) = \mathbf{x}^T \mathbf{z}$	Same as original input space
Polynomial (v1)	$K(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^T \mathbf{z})^d$	All polynomials **of** degree d
Polynomial (v2)	$K(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^T \mathbf{z} + 1)^d$	All polynomials **up to** degree d
Gaussian (RBF)	$K(\mathbf{x}, \mathbf{z}) = \exp(-\frac{\|\|\mathbf{x} - \mathbf{z}\|\|_2^2}{2\sigma^2})$	Infinite dimensional space
Hyperbolic Tangent (Sigmoid) Kernel	$K(\mathbf{x}, \mathbf{z}) = \tanh(\alpha \mathbf{x}^T \mathbf{z} + c)$	(With SVM, this is equivalent to a 2-layer neural network)

Slide credit: CMU MLD Matt Gormley

Kernels: Mercer's Theorem

What functions are valid kernels that correspond to feature vectors $\varphi(\mathbf{x})$?

Answer: Mercer kernels for $k(\mathbf{x}, \mathbf{z})$ and
matrix K, where $K_{i,j} = k(x^{(i)}, x^{(j)})$

- $k(\mathbf{x}, \mathbf{z})$ is continuous
- K is symmetric
- K is positive semi-definite, i.e. $\mathbf{z}^T K \mathbf{z} \geq 0$ for all $\mathbf{z}$

Slide credit: CMU MLD Aarti Singh

SVMs with Kernels

- Choose a set of features and kernel function
- Solve dual problem to obtain support vectors α_i
- At classification time, compute:

$$\mathbf{w} \cdot \Phi(\mathbf{x}) = \sum_i \alpha_i y_i K(\mathbf{x}, \mathbf{x}_i)$$

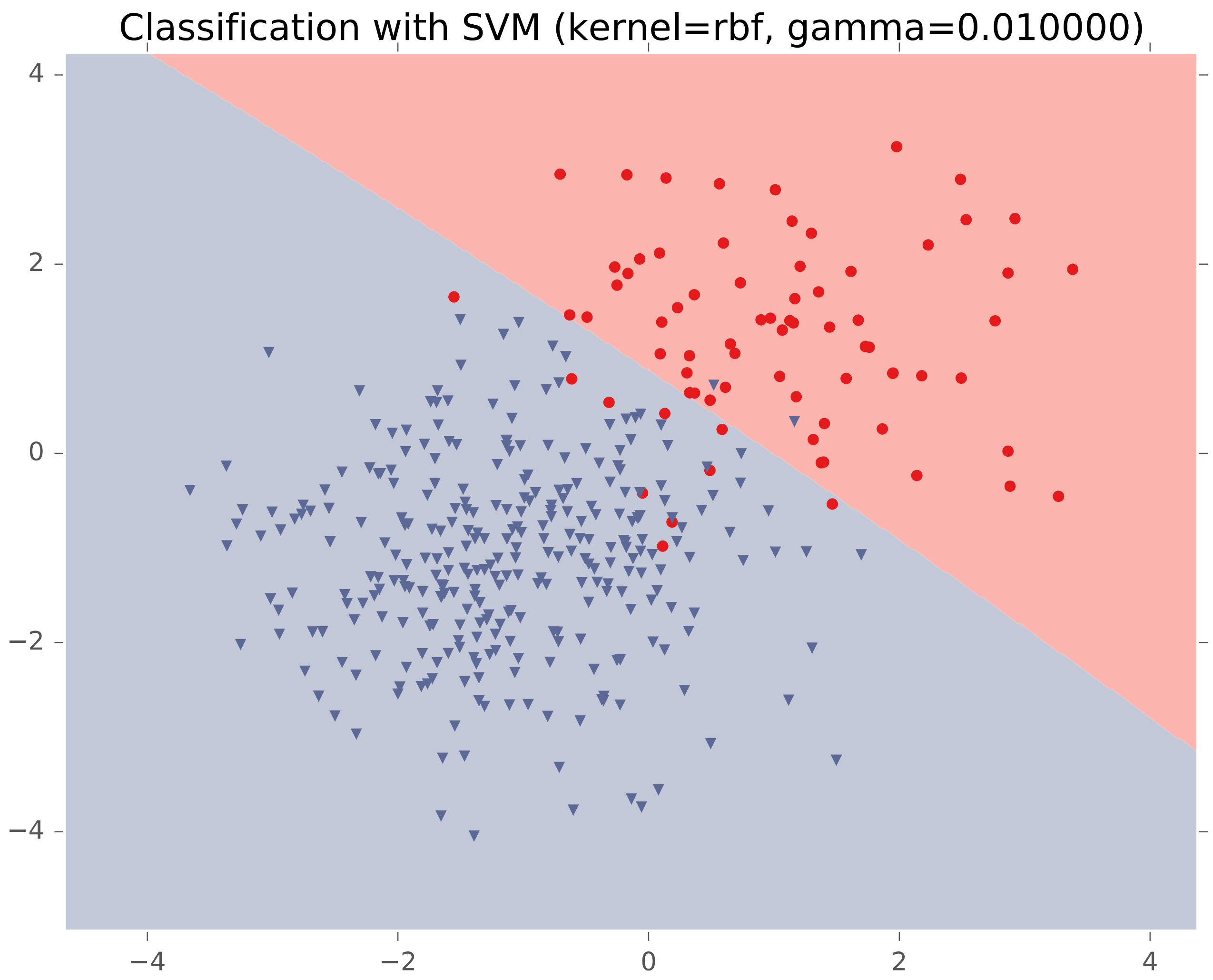
$$b = y_k - \sum_i \alpha_i y_i K(\mathbf{x}_k, \mathbf{x}_i)$$

for any k where $C > \alpha_k > 0$

Classify as

$$sign\left(\mathbf{w} \cdot \Phi(\mathbf{x}) + b\right)$$

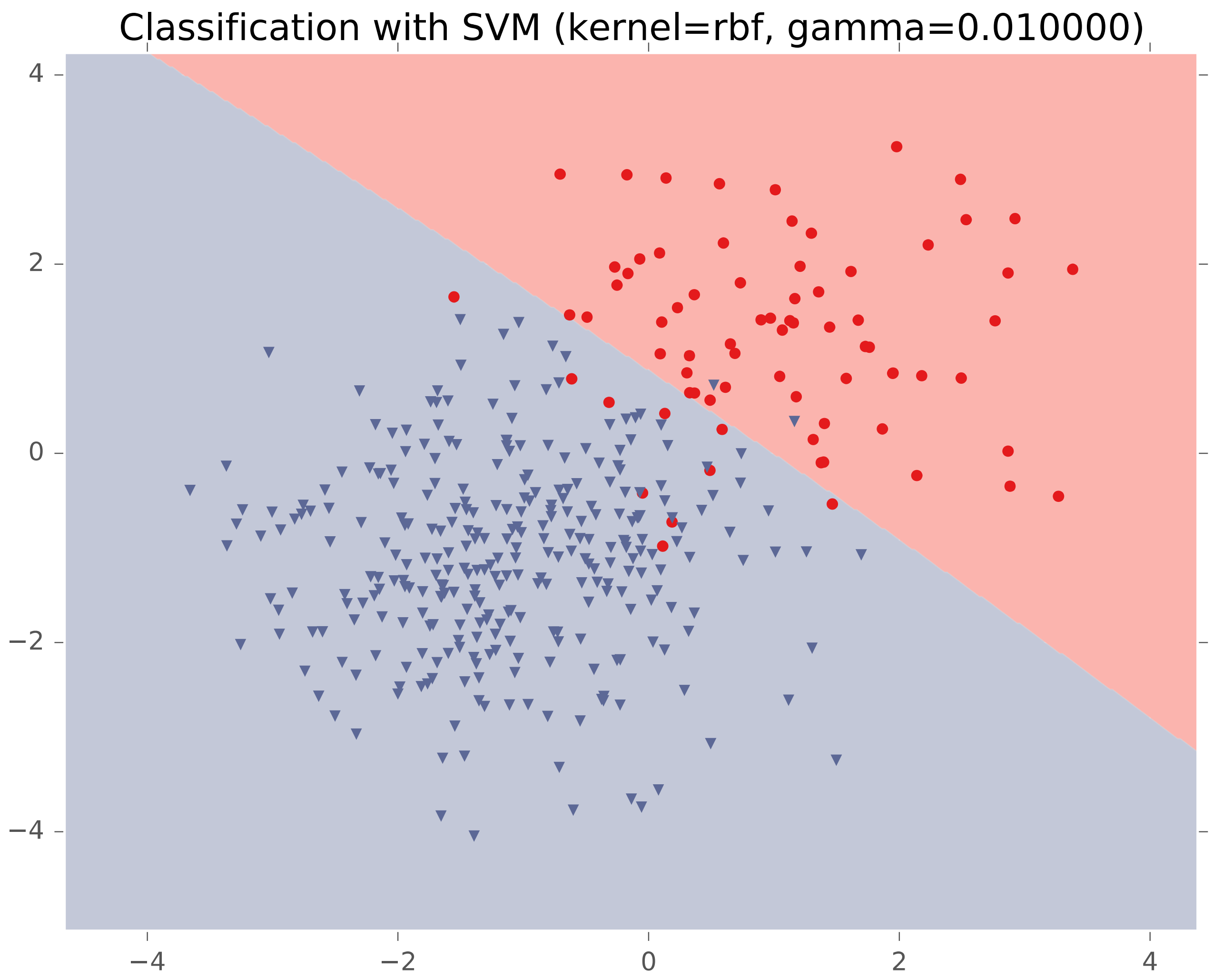
RBF Kernel Example



RBF Kernel: $K(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) = \exp(-\gamma ||\mathbf{x}^{(i)} - \mathbf{x}^{(j)}||_2^2)$

Slide credit: CMU MLD Matt Gormley

RBF Kernel Example



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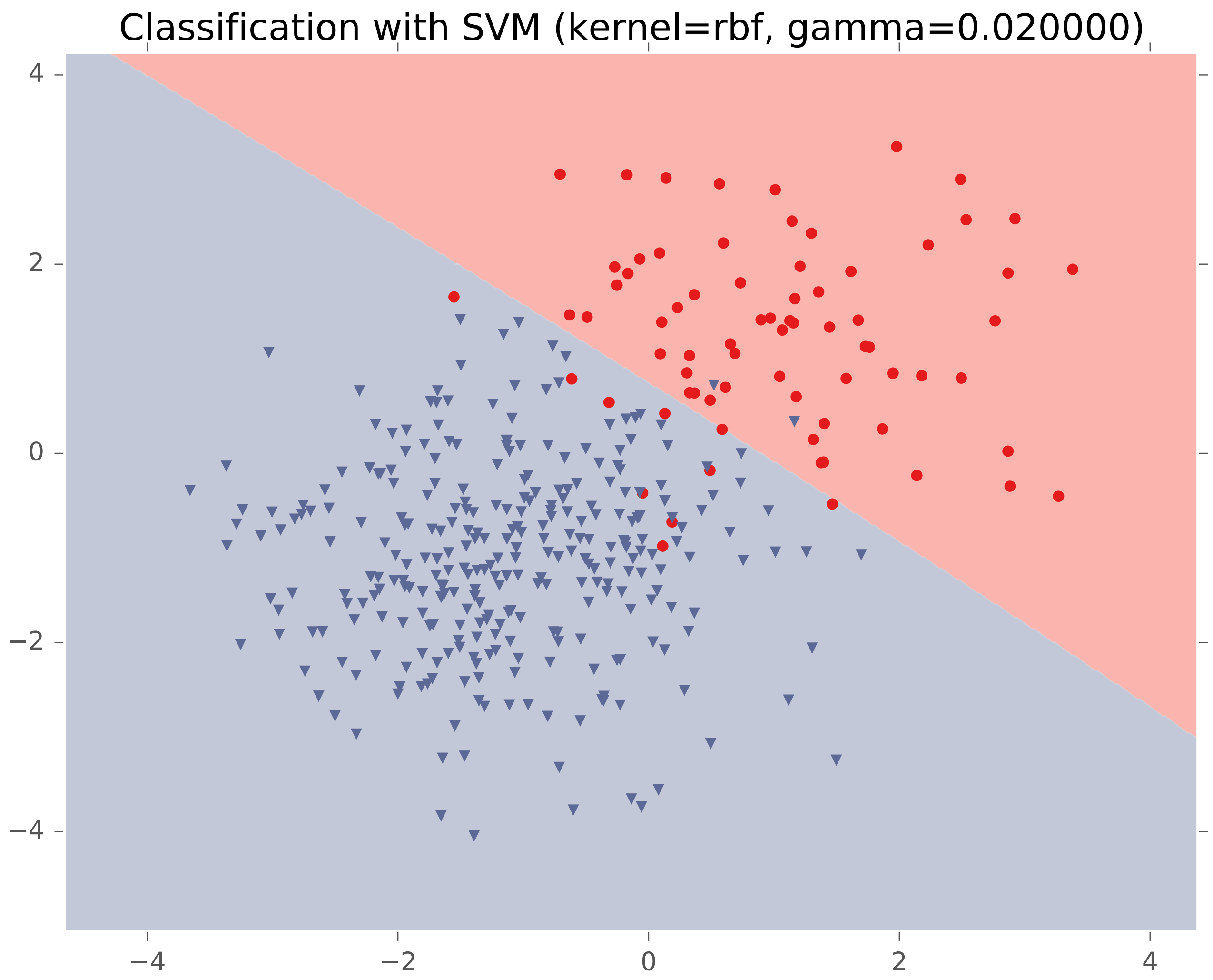

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Slide credit: CMU MLD Matt Gormley

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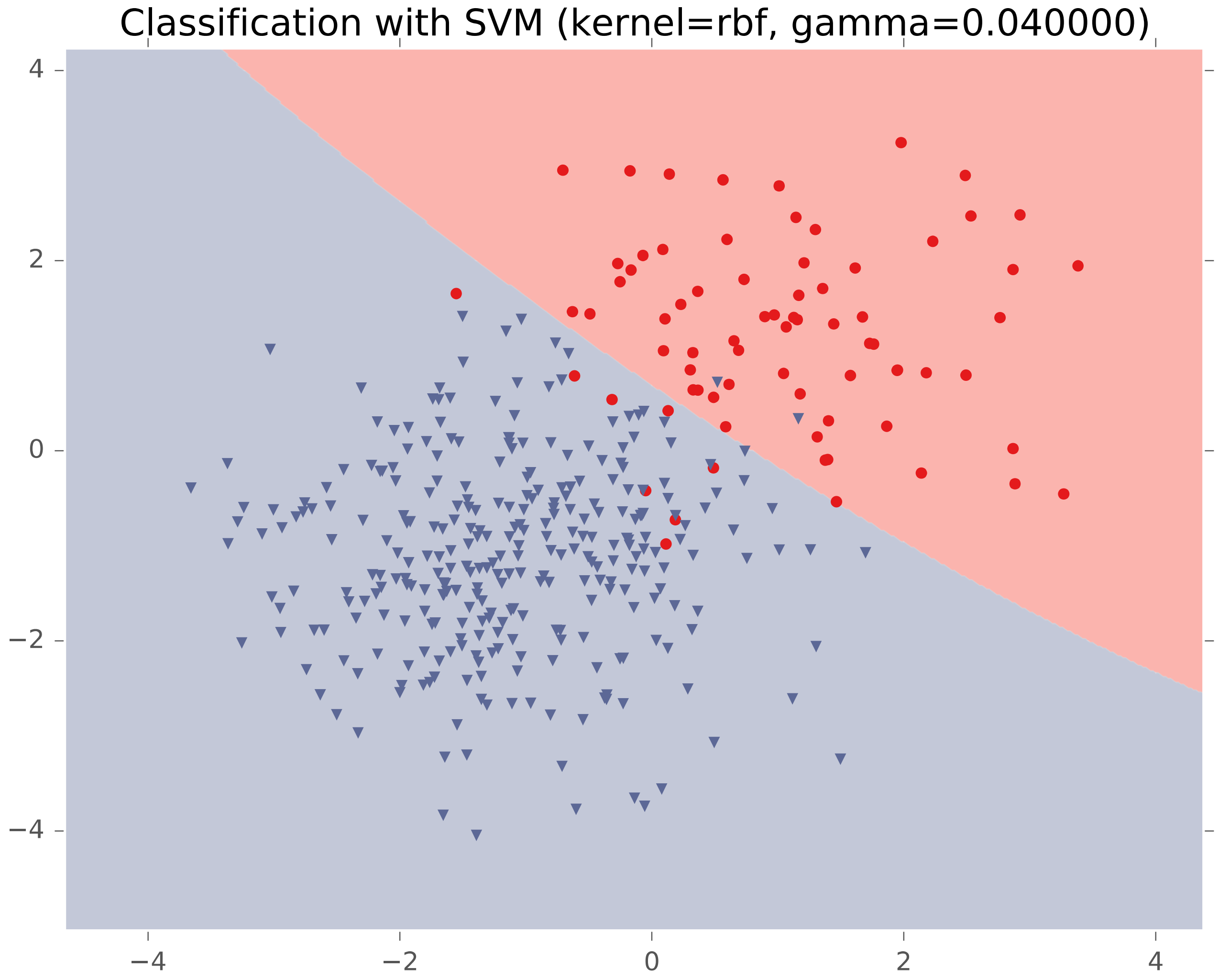

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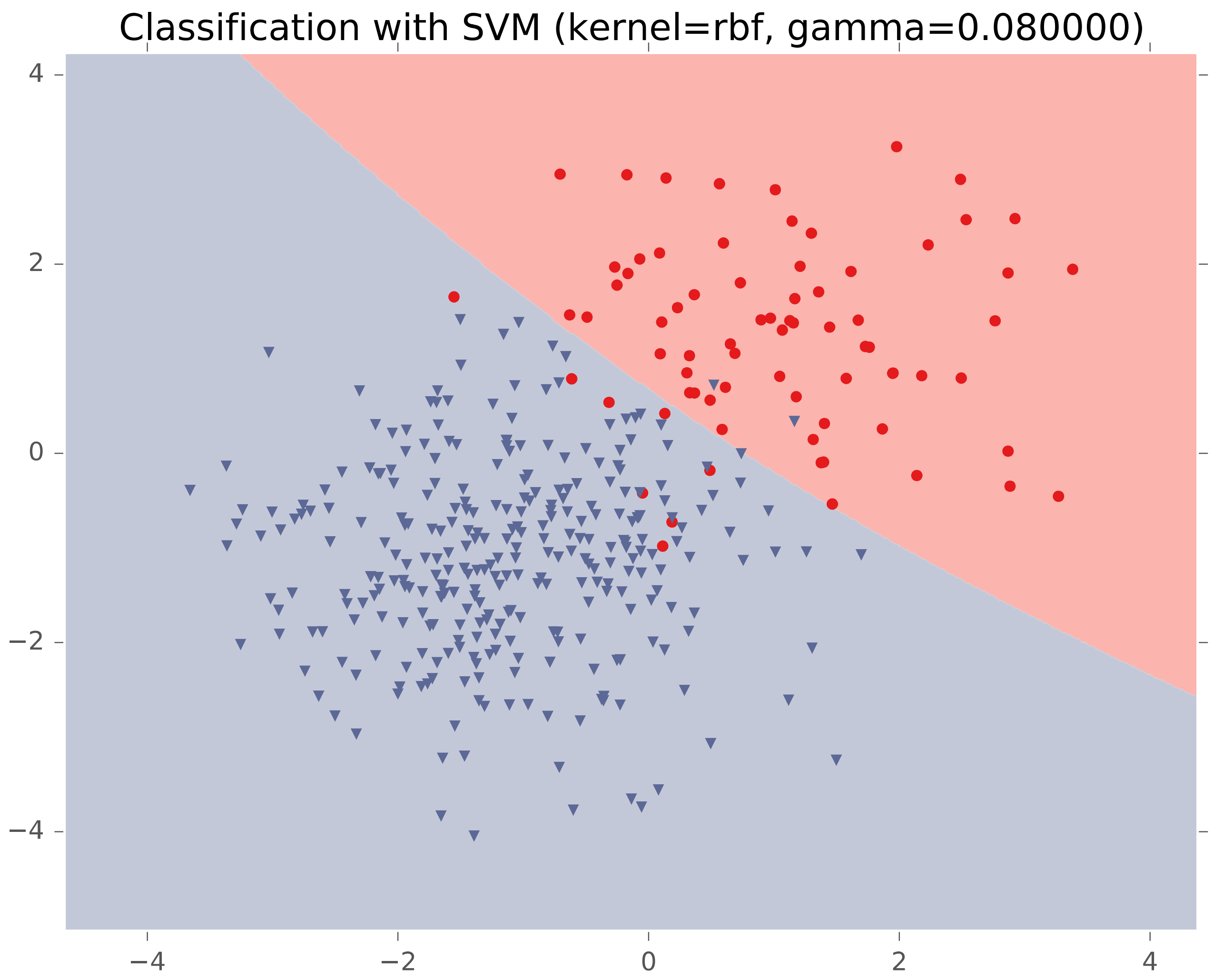

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Slide credit: CMU MLD Matt Gormley

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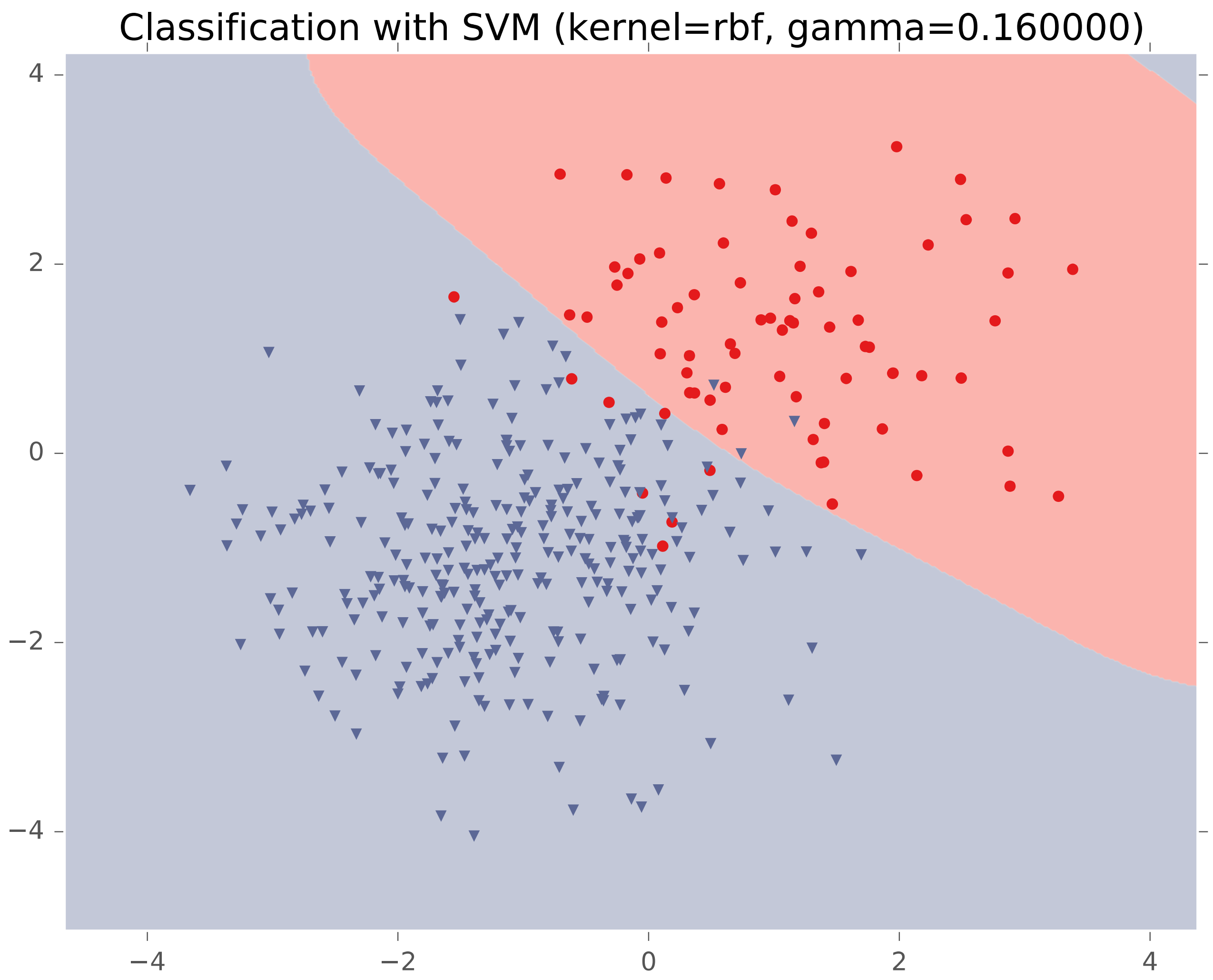

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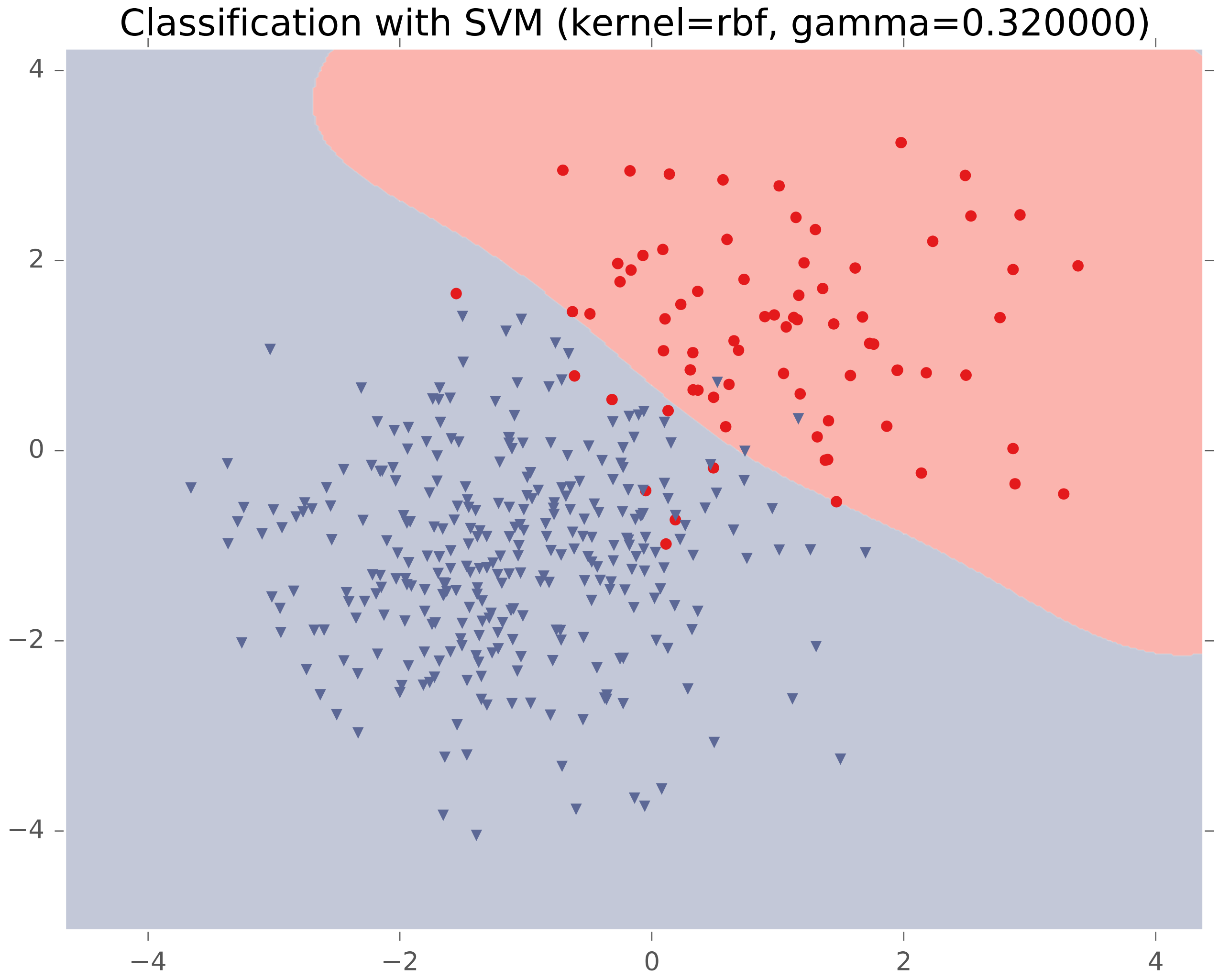

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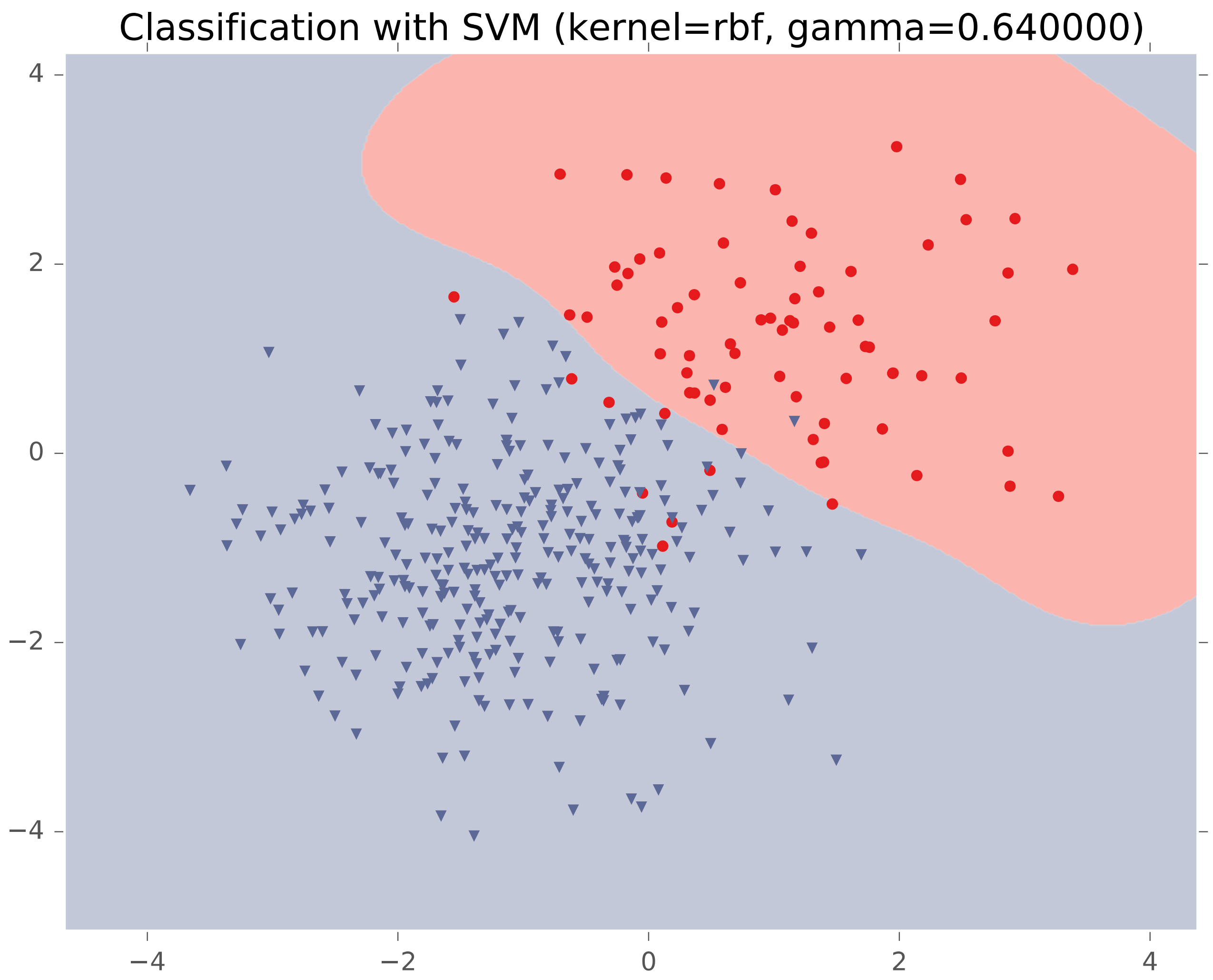

Slide credit: CMU MLD Matt Gormley

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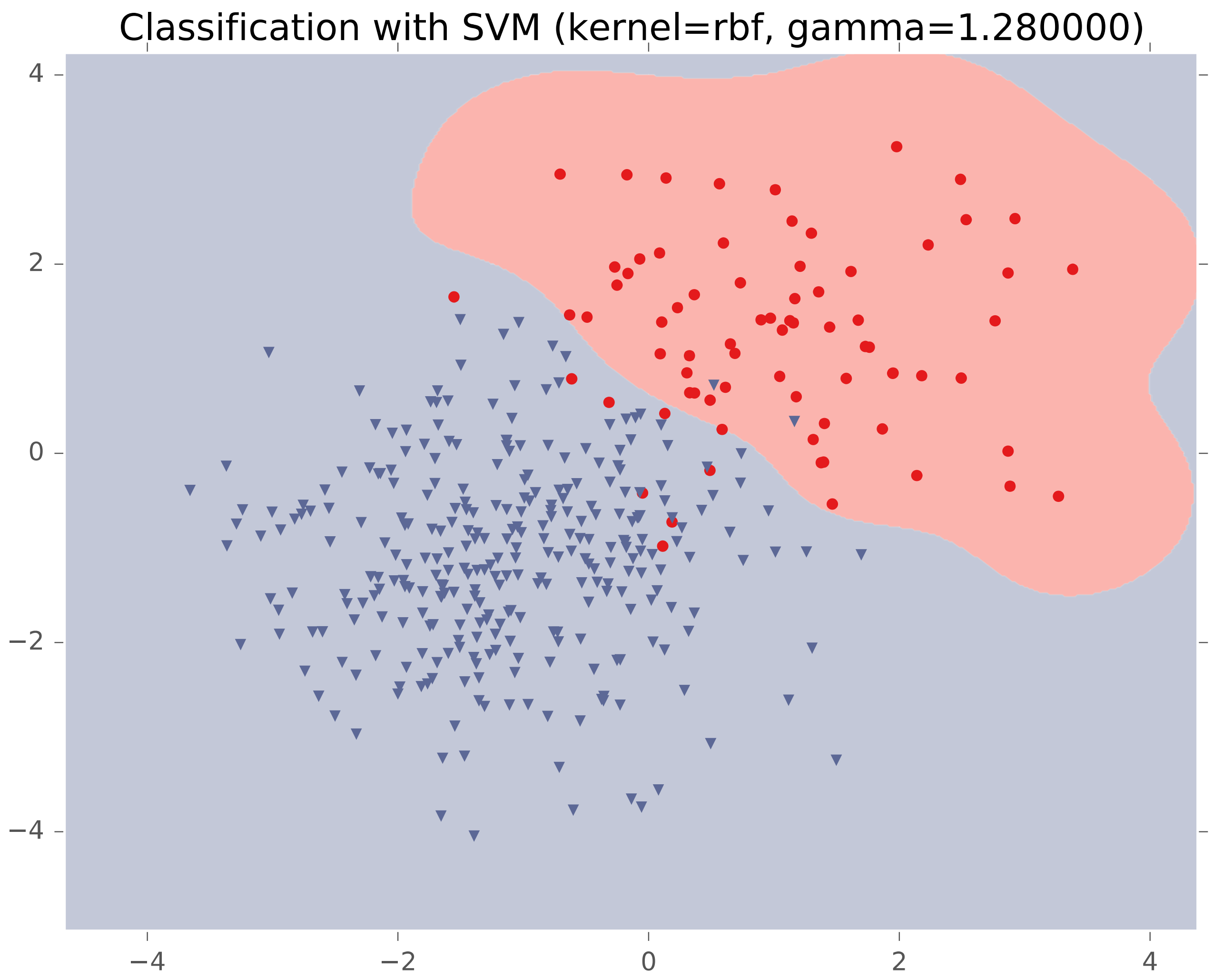
RBF Kernel Example



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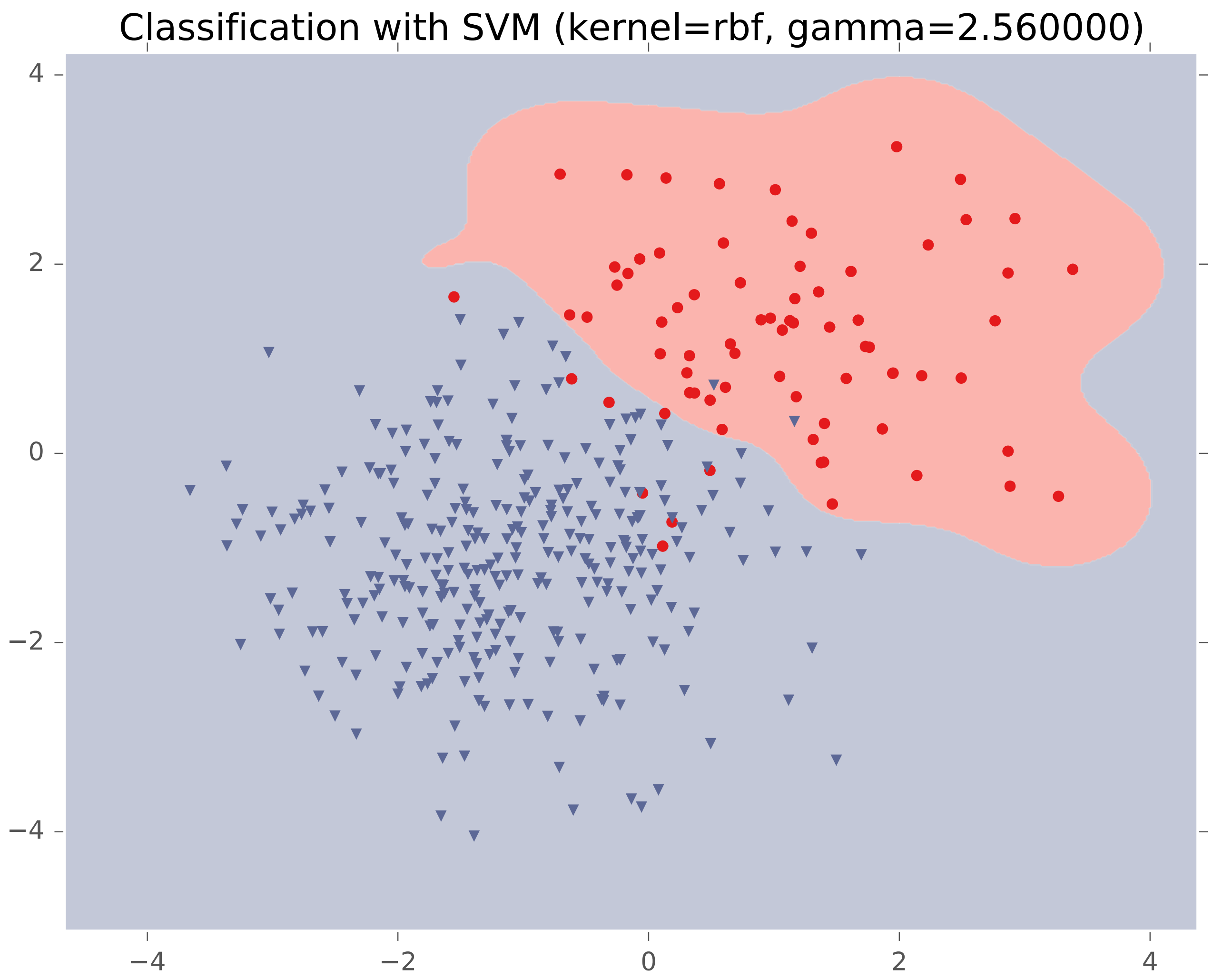

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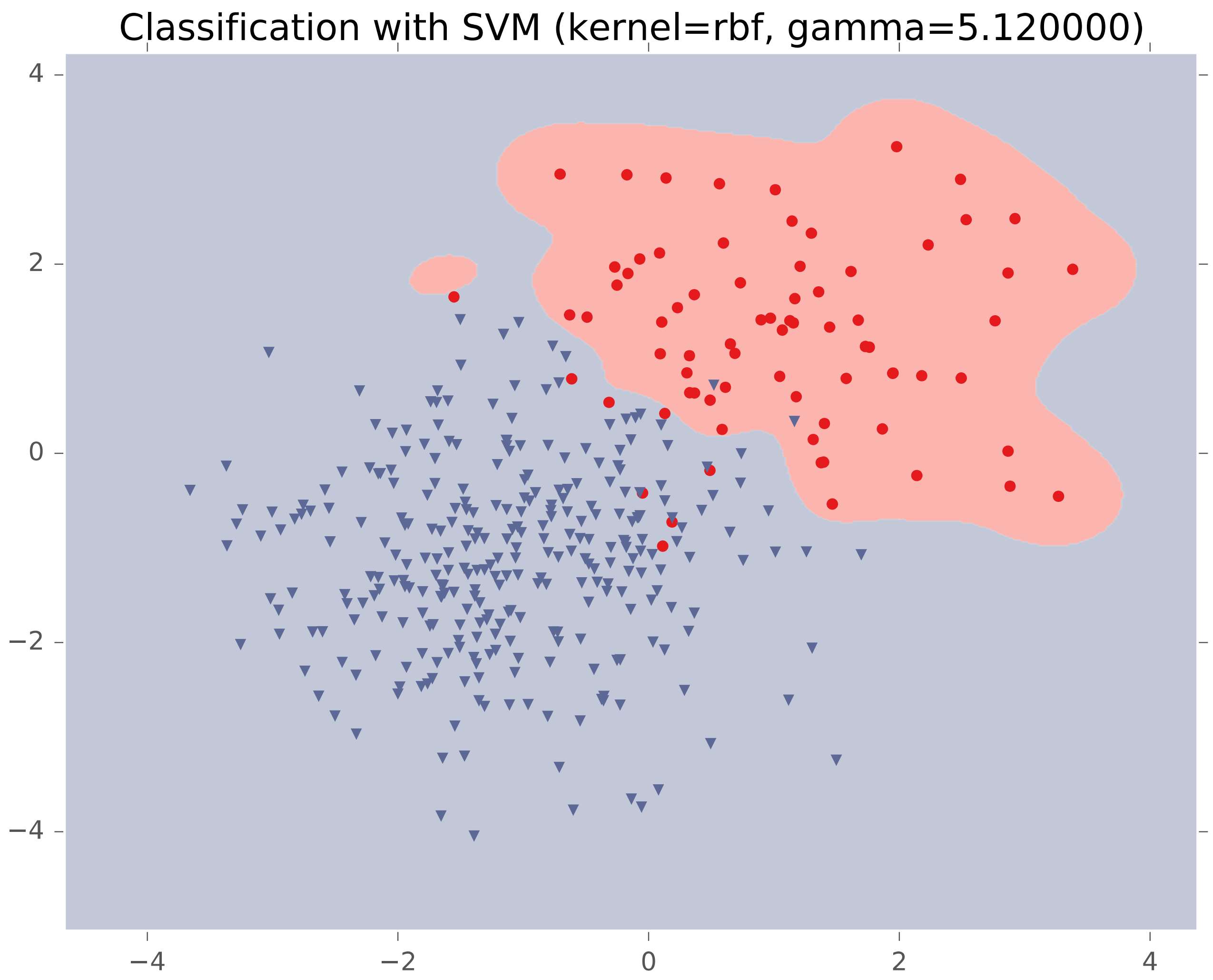

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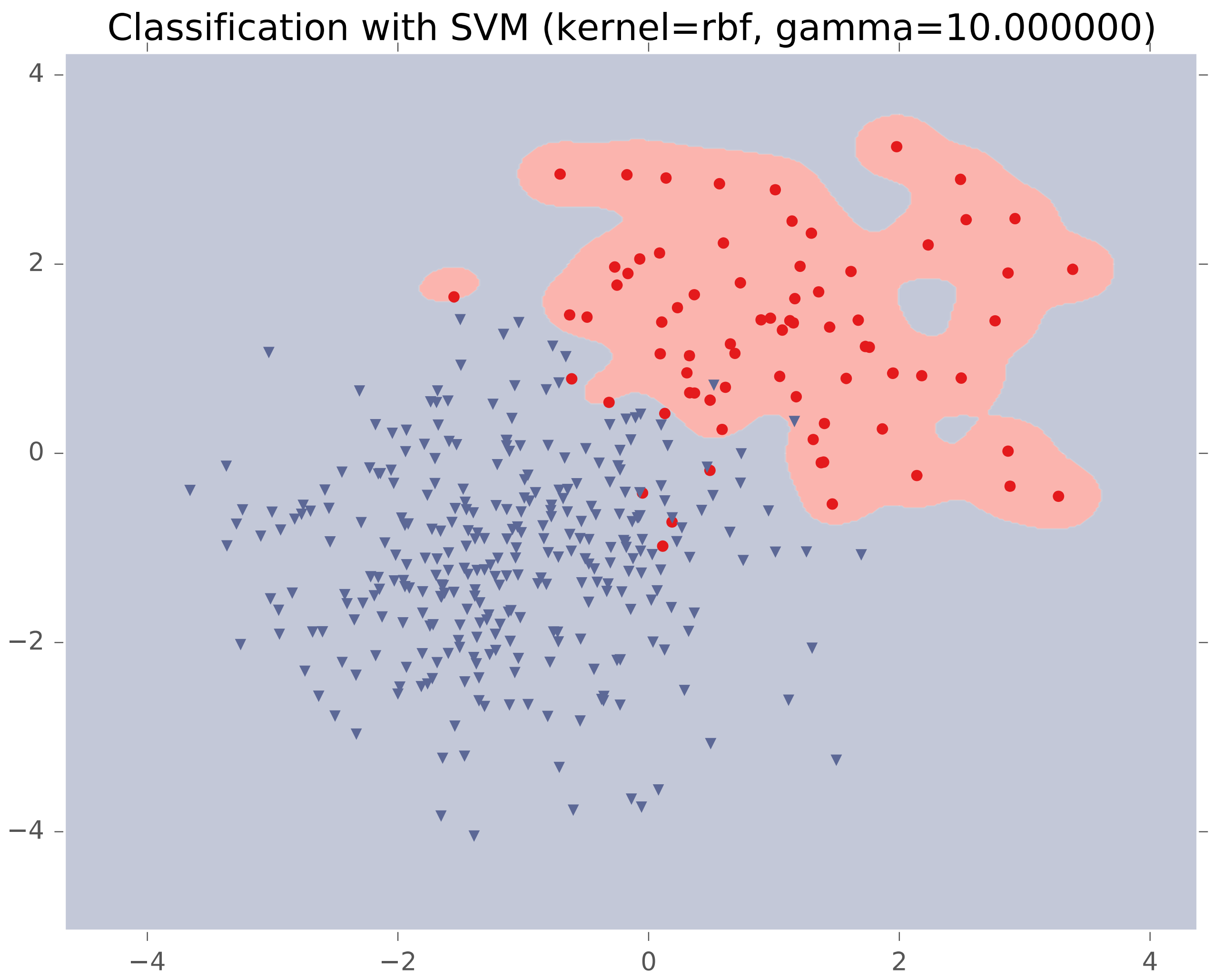

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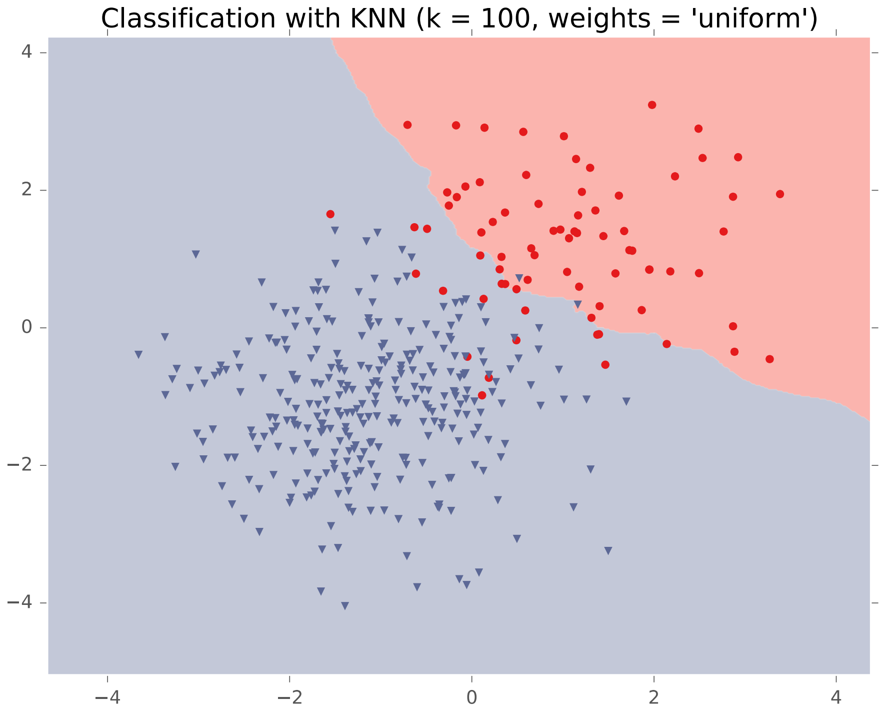
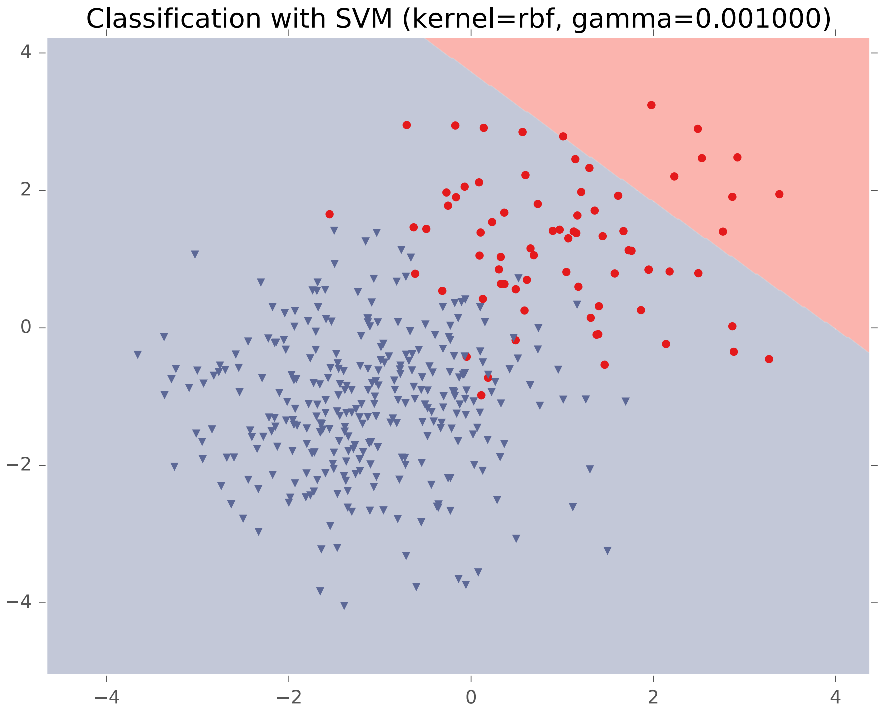
RBF Kernel Example

KNN vs. SVM





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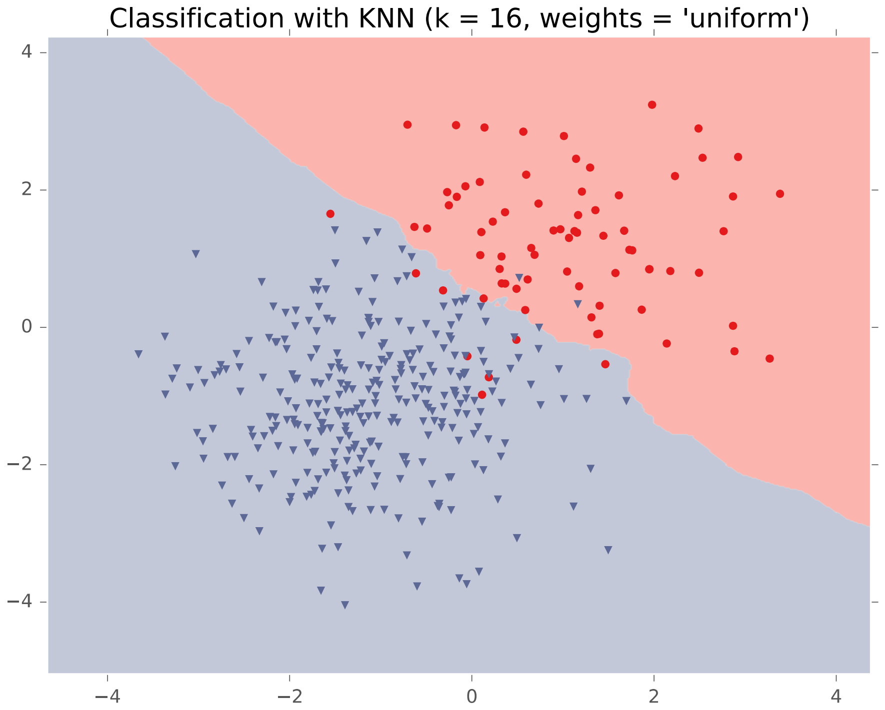
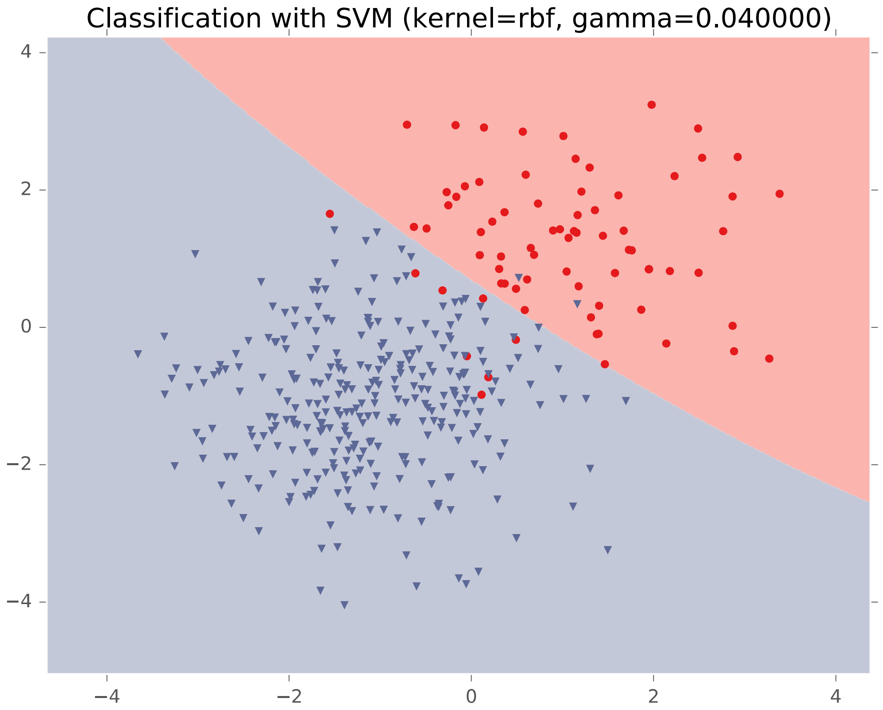
RBF Kernel Example

KNN vs. SVM





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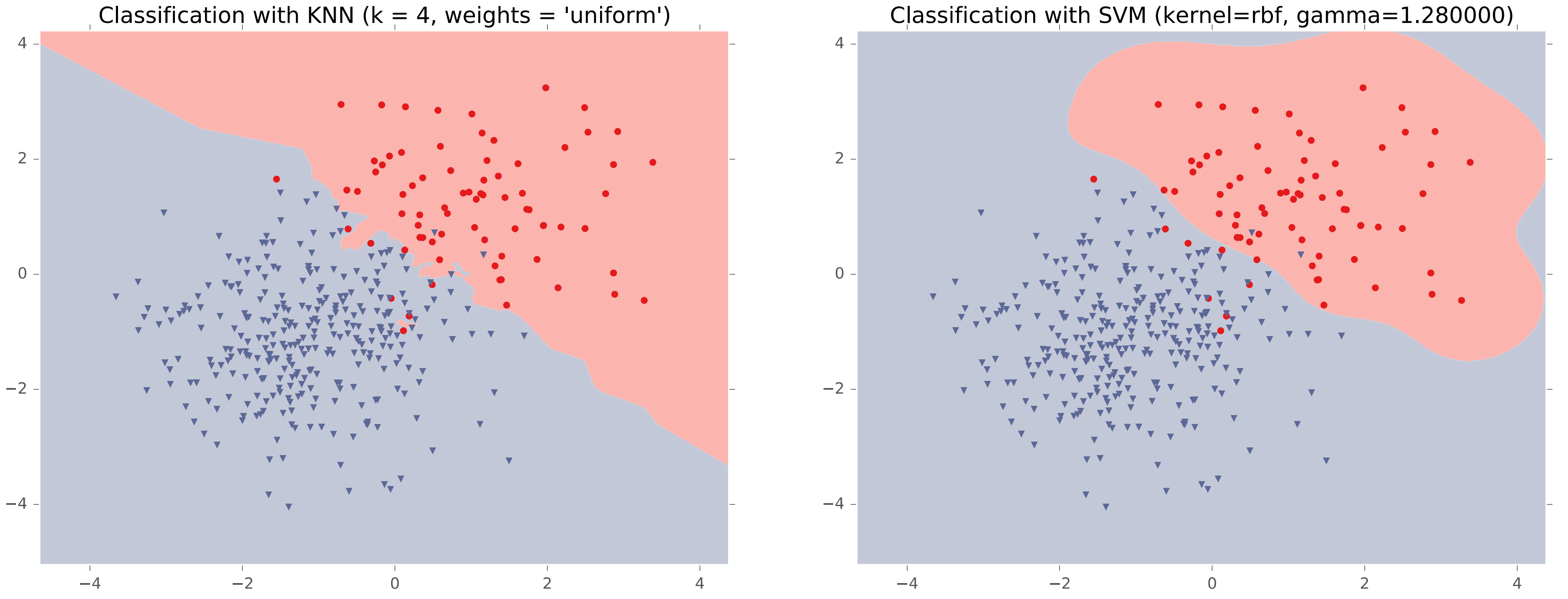

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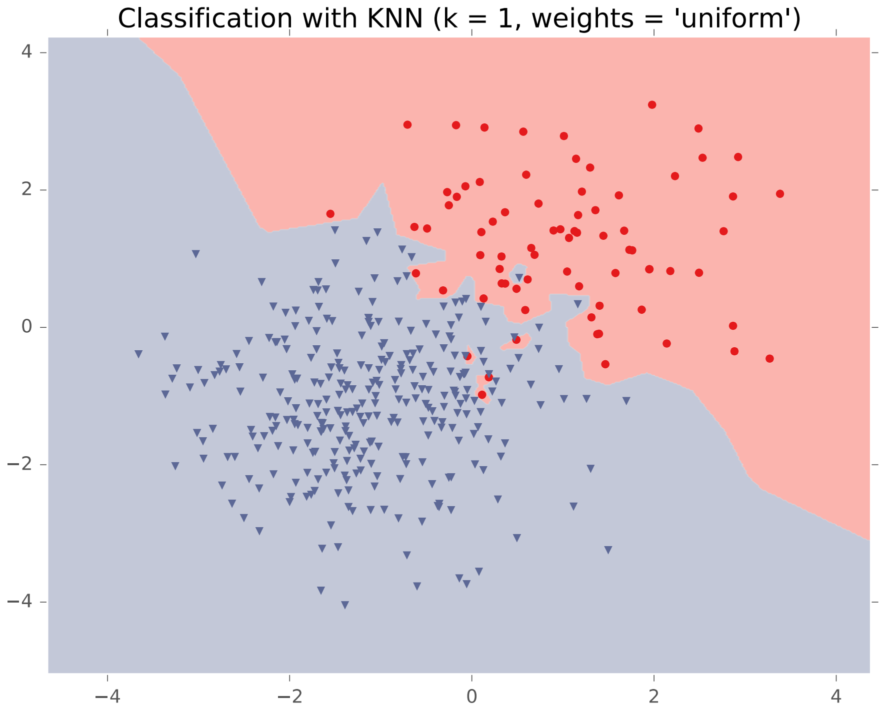

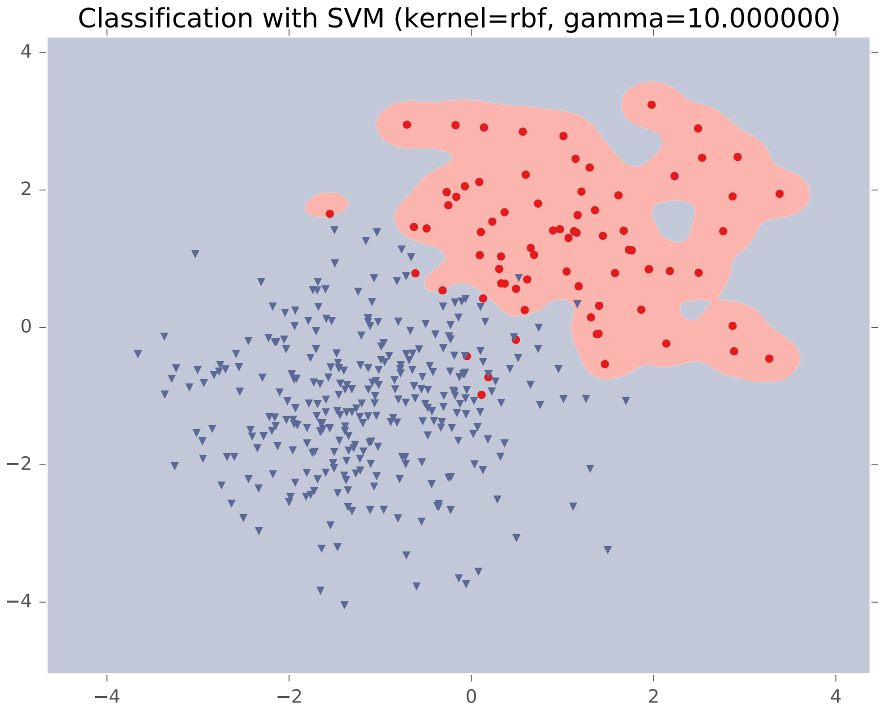

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Φ

Kernel Methods

- **Key idea:**
  1. Rewrite the algorithm so that we only work with **dot products** $x^T z$ of feature vectors
  2. Replace the **dot products** $x^T z$ with a **kernel function** $k(x, z)$

- The kernel $k(x,z)$ can be **any** legal definition of a dot product:

  $$k(x, z) = \varphi(x)^T \varphi(z) \text{ for any function } \varphi: \mathcal{X} \rightarrow \mathbf{R}^D$$

  So we only compute the φ dot product **implicitly**

- This **“kernel trick”** can be applied to many algorithms:
  - classification: perceptron, SVM, …
  - regression: ridge regression, …
  - clustering: k-means, …

SVM + Kernels: Takeaways

- Maximizing the margin of a linear separator is a **good training criteria**
- Support Vector Machines (SVMs) learn a **max-margin linear classifier**
- The SVM optimization problem can be solved with **black-box Quadratic Programming (QP) solvers**
- Learned decision boundary is defined by its **support vectors**
- Kernel methods allow us to work in a transformed feature space **without explicitly representing that space**
- The **kernel-trick** can be applied to **SVMs**, as well as many other algorithms

Support Vector Machines

Next steps

- Different optimization formulation
  - Primal → dual
  - “Support vectors”
- Support non-linear classification
  - Feature maps
  - Kernel trick
- Support non-separable data
  - Hard-margin SVM → soft-margin SVM

Support Vector Machines (SVMs)

Hard-margin SVM (Primal)

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|_2^2$$

$$\text{s.t. } y^{(i)}(\mathbf{w}^T\mathbf{x}^{(i)} + b) \geq 1, \quad \forall i = 1, \ldots, N$$

Hard-margin SVM (Lagrangian Dual)

$$\max_{\boldsymbol{\alpha}} \sum_{i=1}^{N} \alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i\alpha_j y^{(i)} y^{(j)} \mathbf{x}^{(i)} \cdot \mathbf{x}^{(j)}$$

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

$$\sum_{i=1}^{N} \alpha_i y^{(i)} = 0$$

- Instead of minimizing the primal, we can maximize the dual problem
- For the SVM, these two problems give the same answer (i.e. the minimum of one is the maximum of the other)
- *Definition*: **support vectors** are those points $x^{(i)}$ for which $\alpha^{(i)} \neq 0$

Soft-Margin SVM

Hard-margin SVM (Primal)

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|_2^2$$

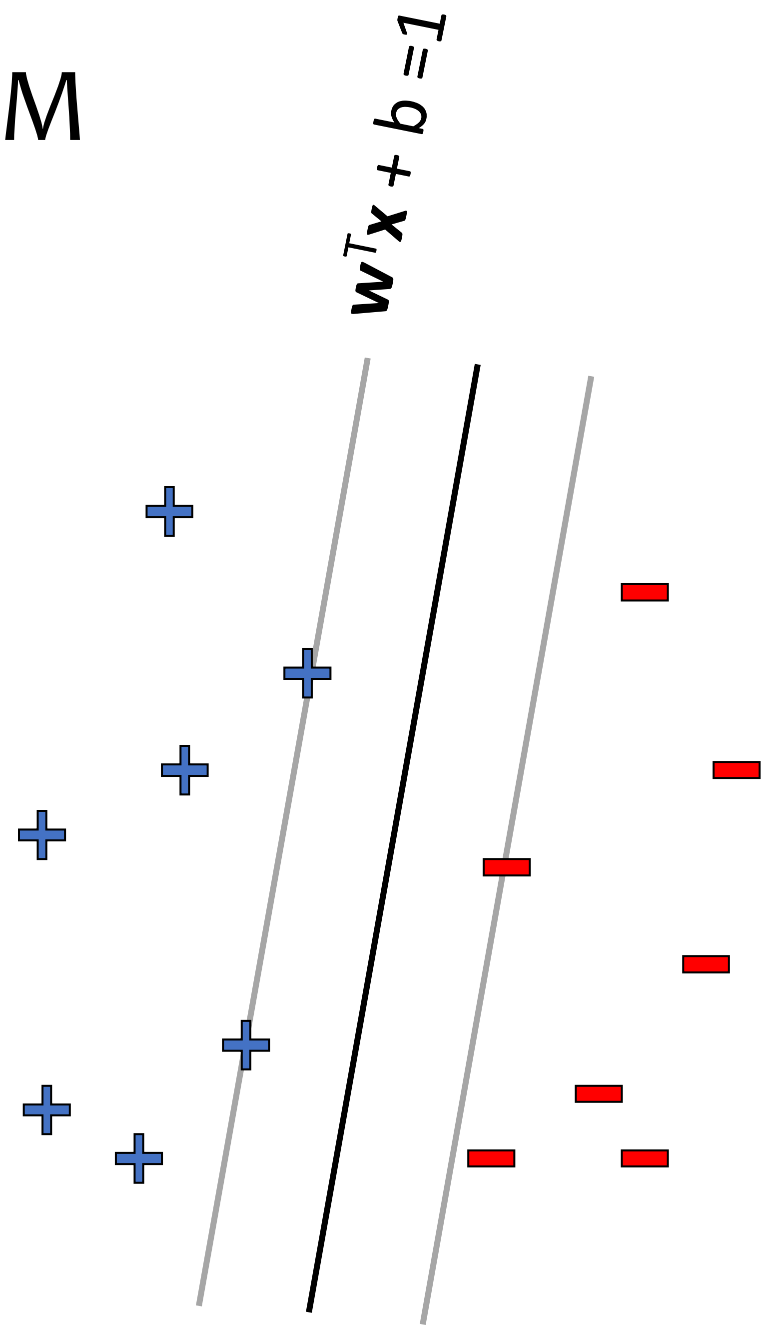
$$\text{s.t. } y^{(i)}(\mathbf{w}^T\mathbf{x}^{(i)} + b) \geq 1, \quad \forall i = 1, \ldots, N$$

Soft-margin SVM (Primal)

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|_2^2 + C\left(\sum_{i=1}^{N} e_i\right)$$

$$\text{s.t. } y^{(i)}(\mathbf{w}^T\mathbf{x}^{(i)} + b) \geq 1 - e_i, \quad \forall i = 1, \ldots, N$$

$$e_i \geq 0, \quad \forall i = 1, \ldots, N$$



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Soft-Margin SVM

Hard-margin SVM (Primal)

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|_2^2$$
$$\text{s.t. } y^{(i)}(\mathbf{w}^T\mathbf{x}^{(i)} + b) \geq 1, \quad \forall i = 1, \ldots, N$$

Hard-margin SVM (Lagrangian Dual)

$$\max_{\boldsymbol{\alpha}} \sum_{i=1}^{N} \alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i \alpha_j y^{(i)} y^{(j)} \mathbf{x}^{(i)} \cdot \mathbf{x}^{(j)}$$
$$\text{s.t. } \alpha_i \geq 0, \quad \forall i = 1, \ldots, N$$
$$\sum_{i=1}^{N} \alpha_i y^{(i)} = 0$$

Soft-margin SVM (Primal)

$$\min_{\mathbf{w},b} \frac{1}{2}\|\mathbf{w}\|_2^2 + C\left(\sum_{i=1}^{N} e_i\right)$$
$$\text{s.t. } y^{(i)}(\mathbf{w}^T\mathbf{x}^{(i)} + b) \geq 1 - e_i, \quad \forall i = 1, \ldots, N$$
$$e_i \geq 0, \quad \forall i = 1, \ldots, N$$

Soft-margin SVM (Lagrangian Dual)

$$\max_{\boldsymbol{\alpha}} \sum_{i=1}^{N} \alpha_i - \frac{1}{2}\sum_{i=1}^{N}\sum_{j=1}^{N} \alpha_i \alpha_j y^{(i)} y^{(j)} \mathbf{x}^{(i)} \cdot \mathbf{x}^{(j)}$$
$$\text{s.t. } 0 \leq \alpha_i \leq C, \quad \forall i = 1, \ldots, N$$
$$\sum_{i=1}^{N} \alpha_i y^{(i)} = 0$$

We can also work with the dual of the soft-margin SVM

Slide credit: CMU MLD Matt Gormley