10-601 Introduction to Machine Learning

Machine Learning Department
School of Computer Science
Carnegie Mellon University

Kernels + Support Vector Machines (SVMs)

SVM Readings:
Murphy 14.5
Bishop 7.1
HTF 12 - 12.38
Mitchell --

Matt Gormley
Lecture 12
February 27, 2016

Reminders

- **Homework 4: Perceptron / Kernels / SVM**
  - Release: Wed, Feb. 22
  - Due: Fri, Mar. 03 at 11:59pm
- **Midterm Exam (Evening Exam)**
  - Tue, Mar. 07 at 7:00pm – 9:30pm
  - See Piazza for details about location
- **Grading**

9 days
for HW4

Outline

- **Kernels**
  - Kernel Perceptron
  - Kernel as a dot product
  - Gram matrix
  - Examples: Polynomial, RBF
- **Support Vector Machine (SVM)**
  - Background: Constrained Optimization, Linearly Separable, Margin
  - SVM Primal (Linearly Separable Case)
  - SVM Primal (Non-linearly Separable Case)
  - SVM Dual

Last Lecture

This Lecture

KERNELS

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**

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

Kernels

Whiteboard

- Kernel Perceptron
- Kernel as a dot product
- Gram matrix
- Examples: RBF kernel, string kernel

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, …

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

Example: Polynomial Kernel

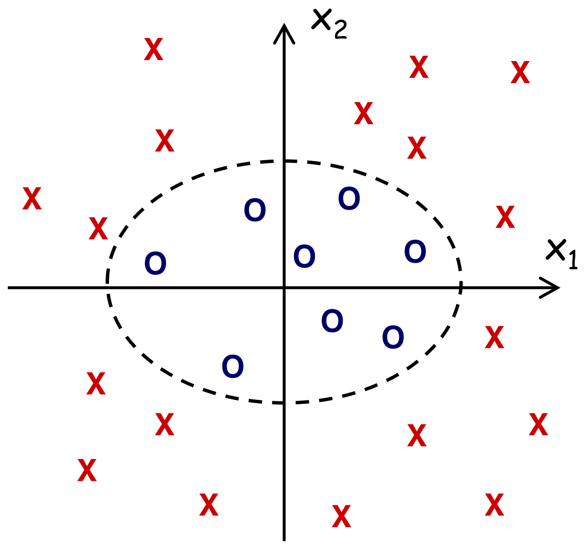
For n=2, d=2, the kernel $K(x,z) = (x \cdot z)^d$ corresponds to

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

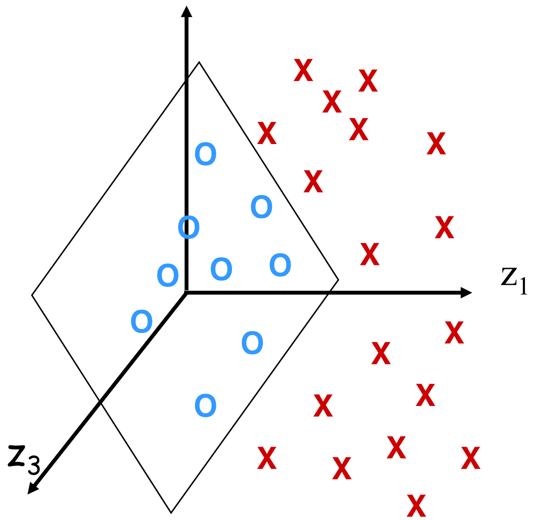
$$\phi(x) \cdot \phi(z) = \left(x_1^2, x_2^2, \sqrt{2}x_1x_2\right) \cdot (z_1^2, z_2^2, \sqrt{2}z_1z_2)$$

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

Original space



Φ-space



Slide from Nina Balcan

Example: Polynomial Kernel

Feature space can grow really large and really quickly….

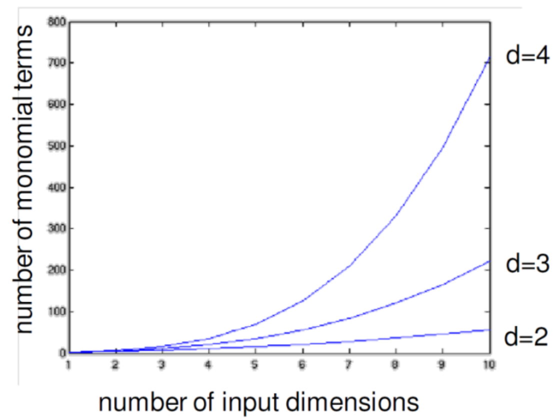
Crucial to think of ϕ as implicit, not explicit!!!!

Polynomial kernel degreee d, $k(x,z) = (x^\top z)^d = \phi(x) \cdot \phi(z)$

- $x_1^d, x_1 x_2 \ldots x_d, x_1^2 x_2 \ldots x_{d-1}$
- Total number of such feature is

$$\binom{d+n-1}{d} = \frac{(d+n-1)!}{d!\,(n-1)!}$$

- $d = 6, n = 100$, there are 1.6 billion terms



$O(n)$ computation!

$$k(x,z) = (x^\top z)^d = \phi(x) \cdot \phi(z)$$

Kernel Examples

Side Note: The feature space might not be unique!

Explicit representation #1:

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

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

$$= (x_1 z_1 + x_2 z_2)^2 = (x \cdot z)^2 = K(x, z)$$

Explicit representation #2:

$$\phi: R^2 \to R^4,\ (x_1, x_2) \to \Phi(x) = (x_1^2, x_2^2, x_1 x_2, x_2 x_1)$$

$$\phi(x) \cdot \phi(z) = (x_1^2, x_2^2, x_1 x_2, x_2 x_1) \cdot (z_1^2, z_2^2, z_1 z_2, z_2 z_1)$$

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

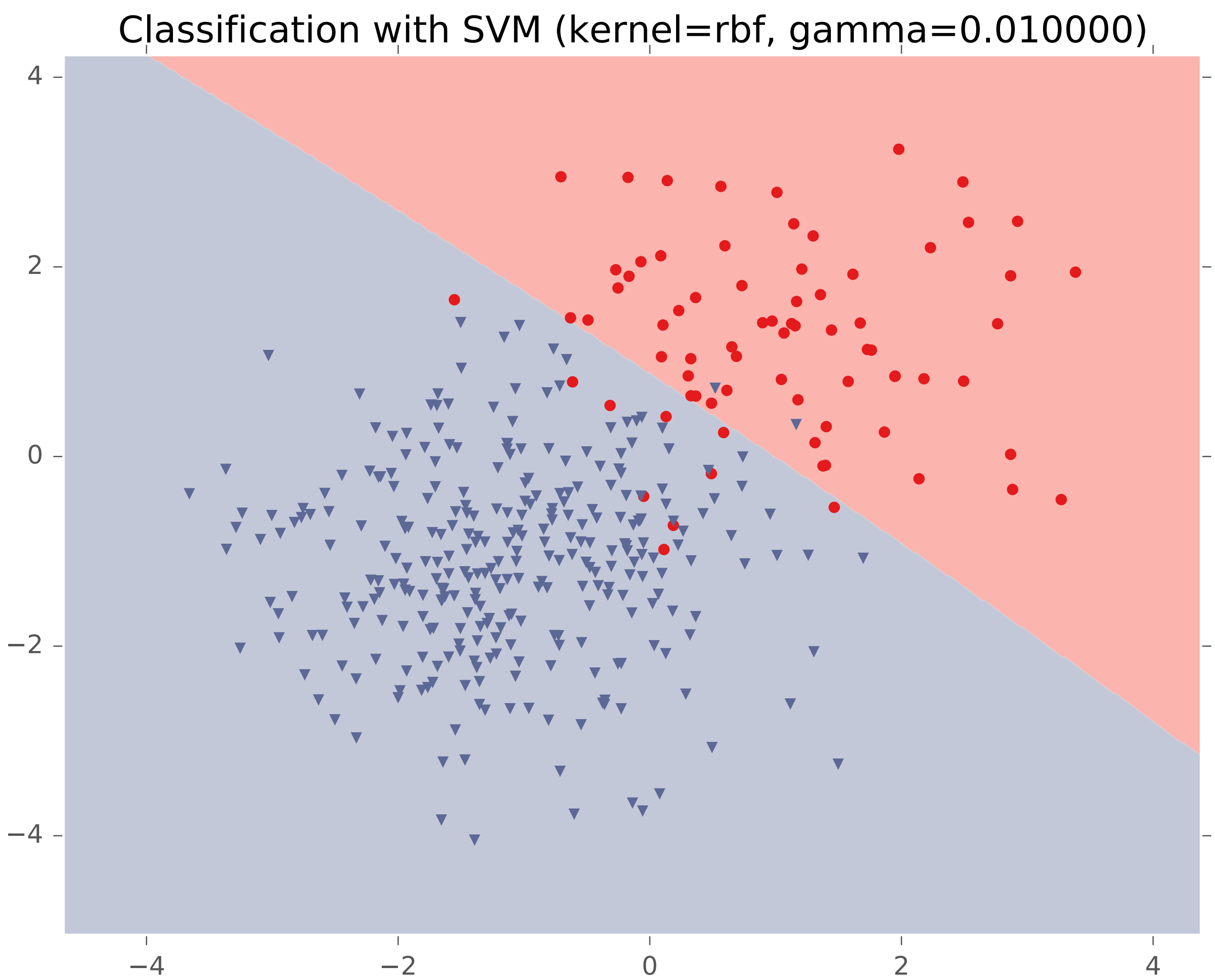
These two different feature representations correspond to the same kernel function!

Slide from Nina Balcan

Kernel Examples

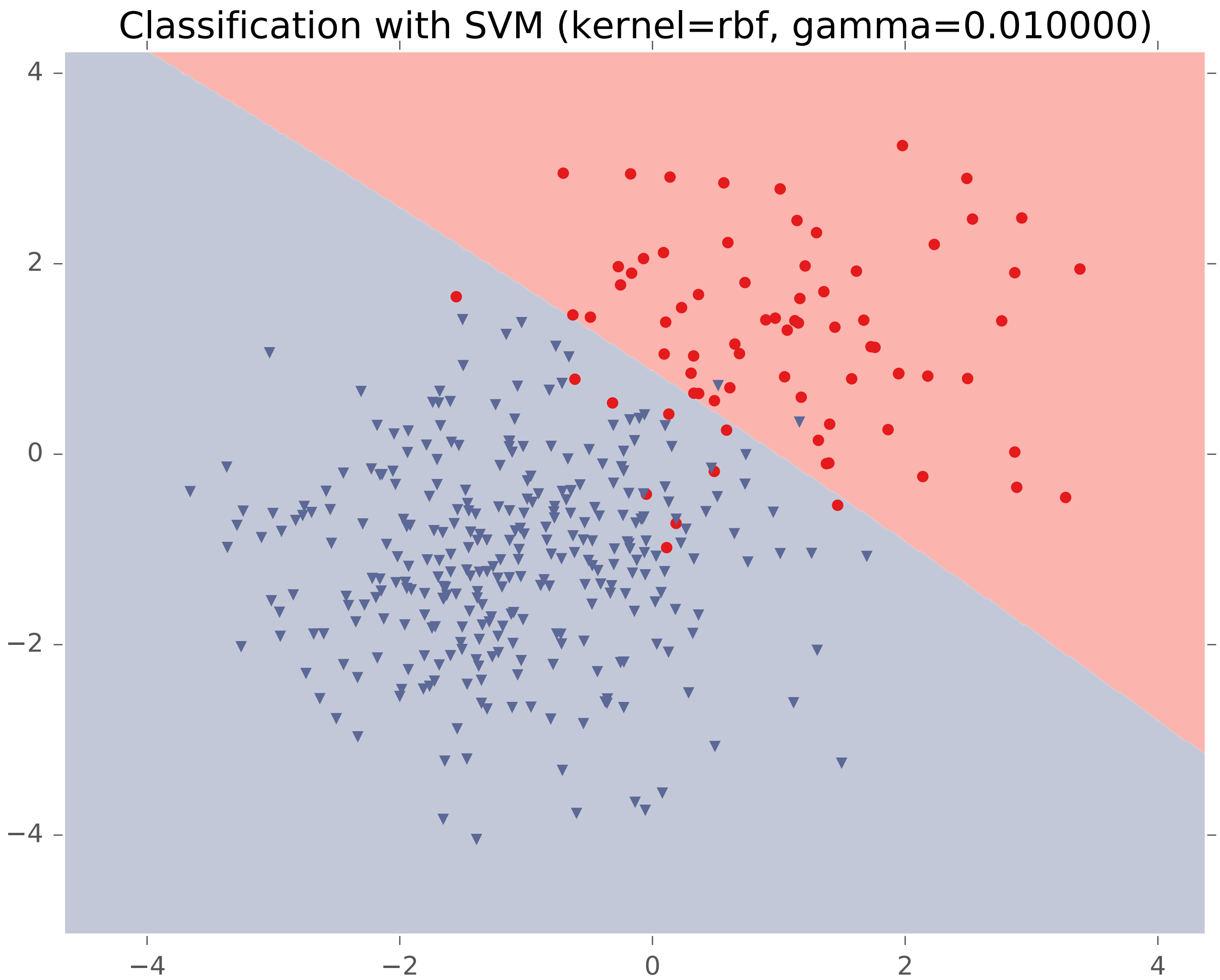
Name	Kernel Function (implicit dot product)	Feature Space (explicit dot product)
Linear	$K(\mathbf{x}, \mathbf{z}) = \mathbf{x}^T \mathbf{z}$	Same as original input space
Polynomial (v1)	$K(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^T \mathbf{z})^d$	All polynomials **of** degree d
Polynomial (v2)	$K(\mathbf{x}, \mathbf{z}) = (\mathbf{x}^T \mathbf{z} + 1)^d$	All polynomials **up to** degree d
Gaussian	$K(\mathbf{x}, \mathbf{z}) = \exp(-\frac{\|\|\mathbf{x} - \mathbf{z}\|\|_2^2}{2\sigma^2})$	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)

RBF Kernel Example



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

RBF Kernel Example



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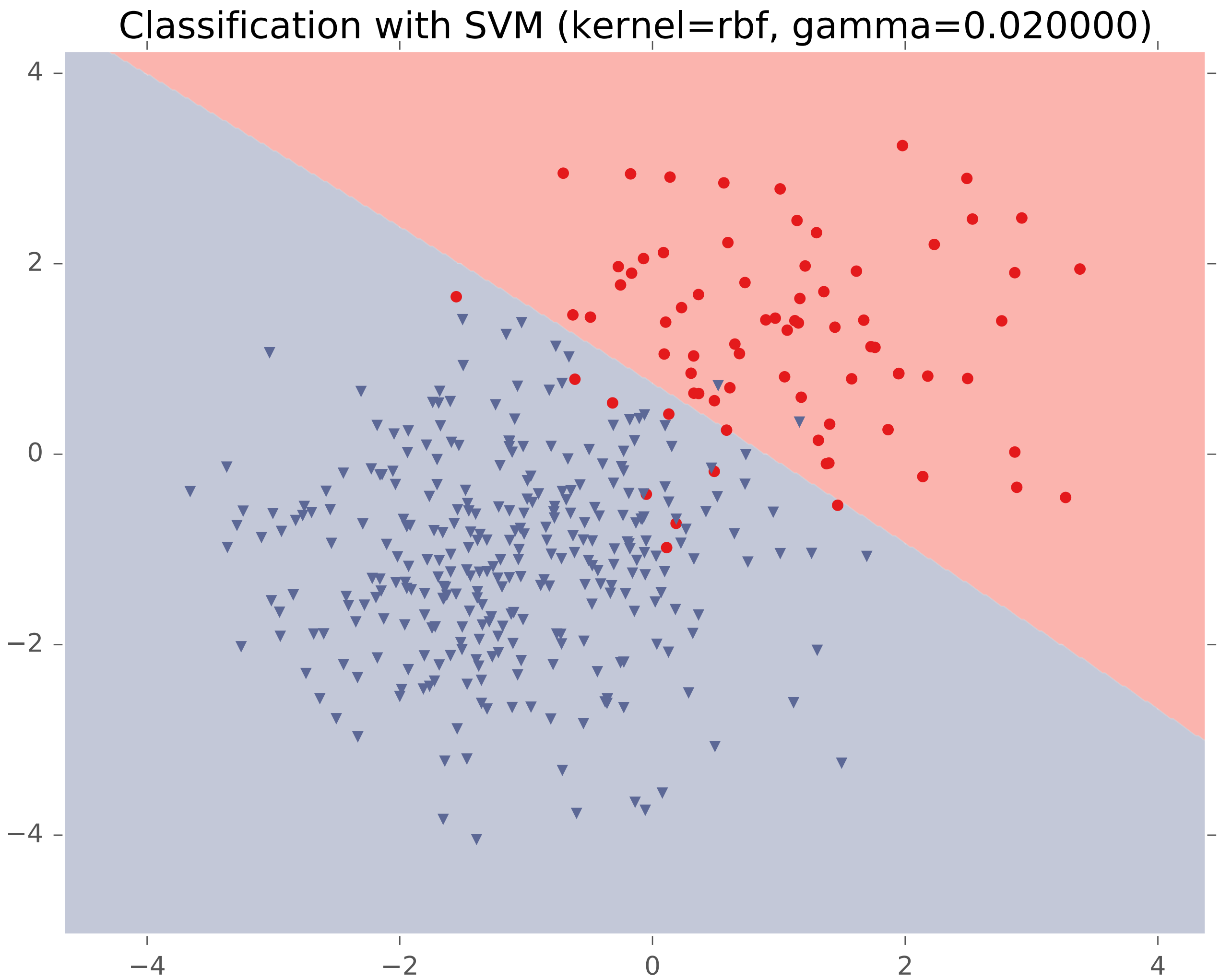

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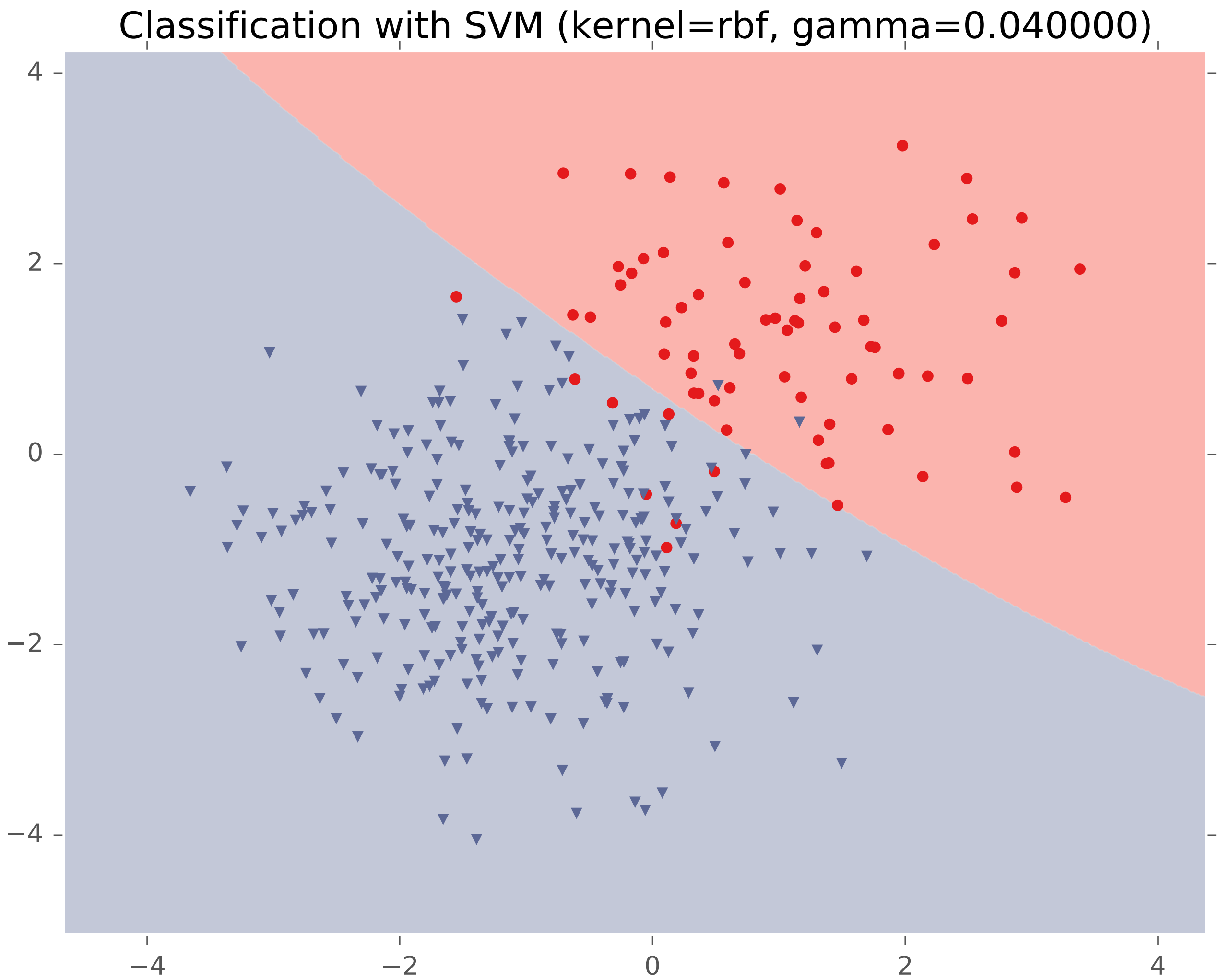

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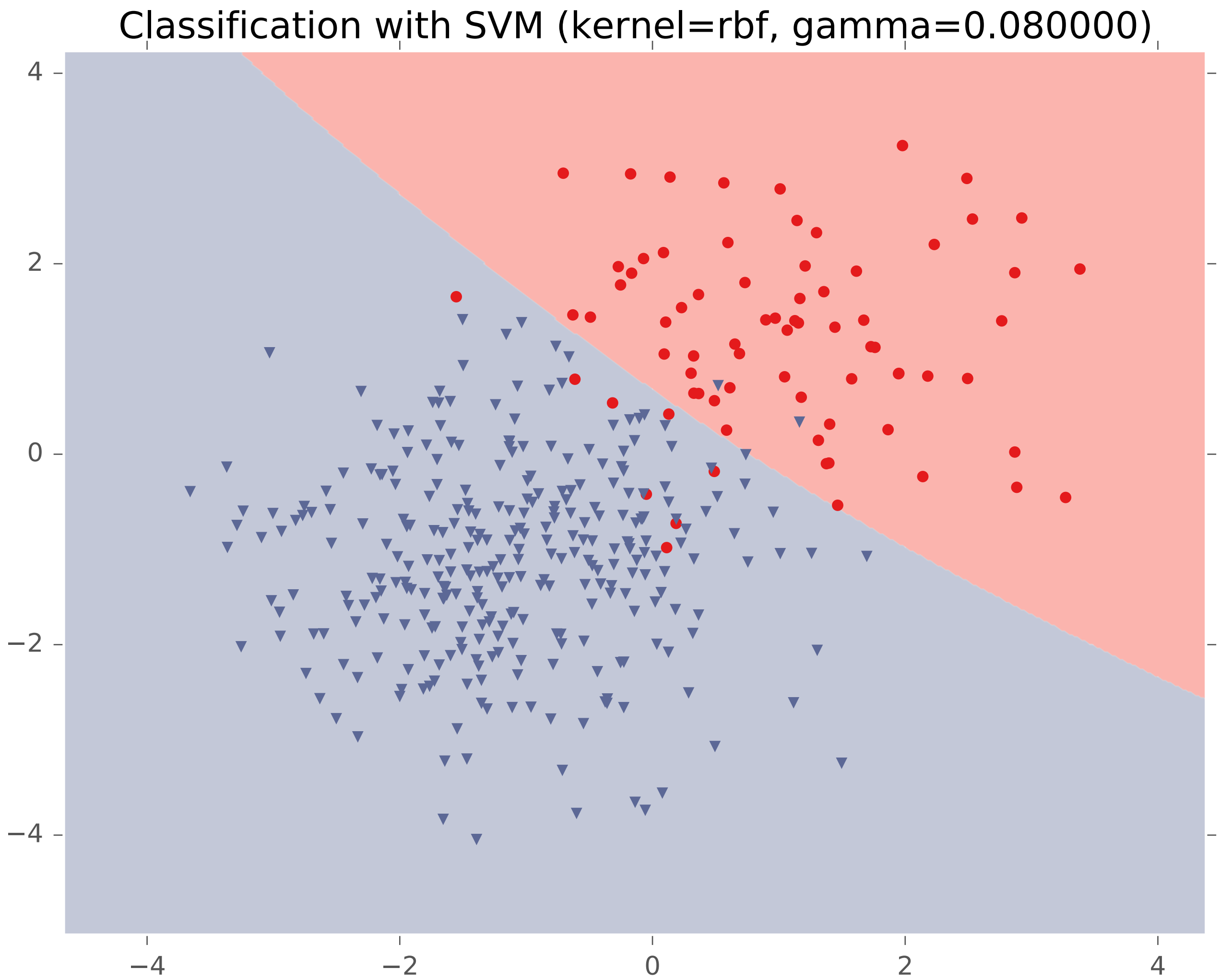

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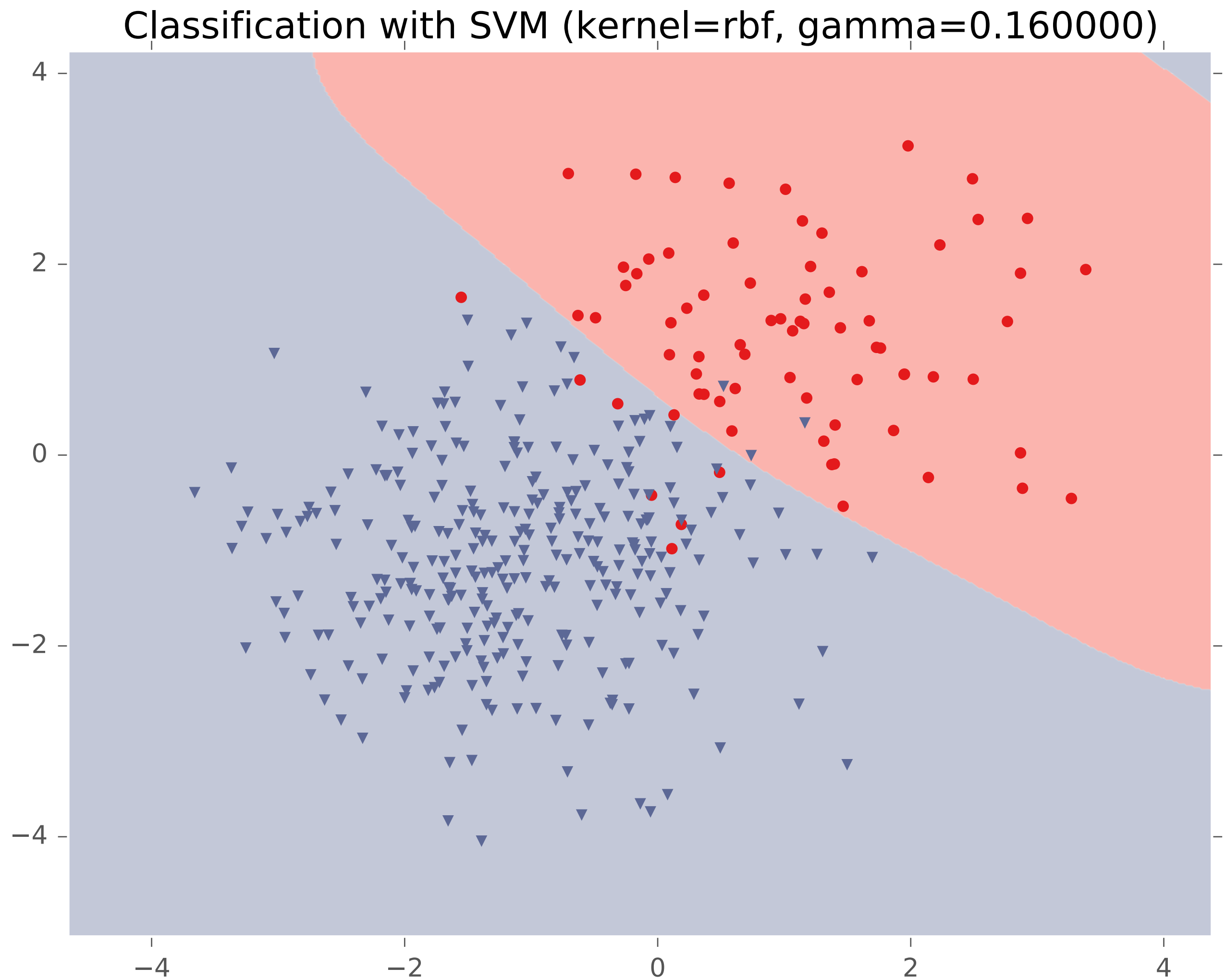
RBF Kernel Example



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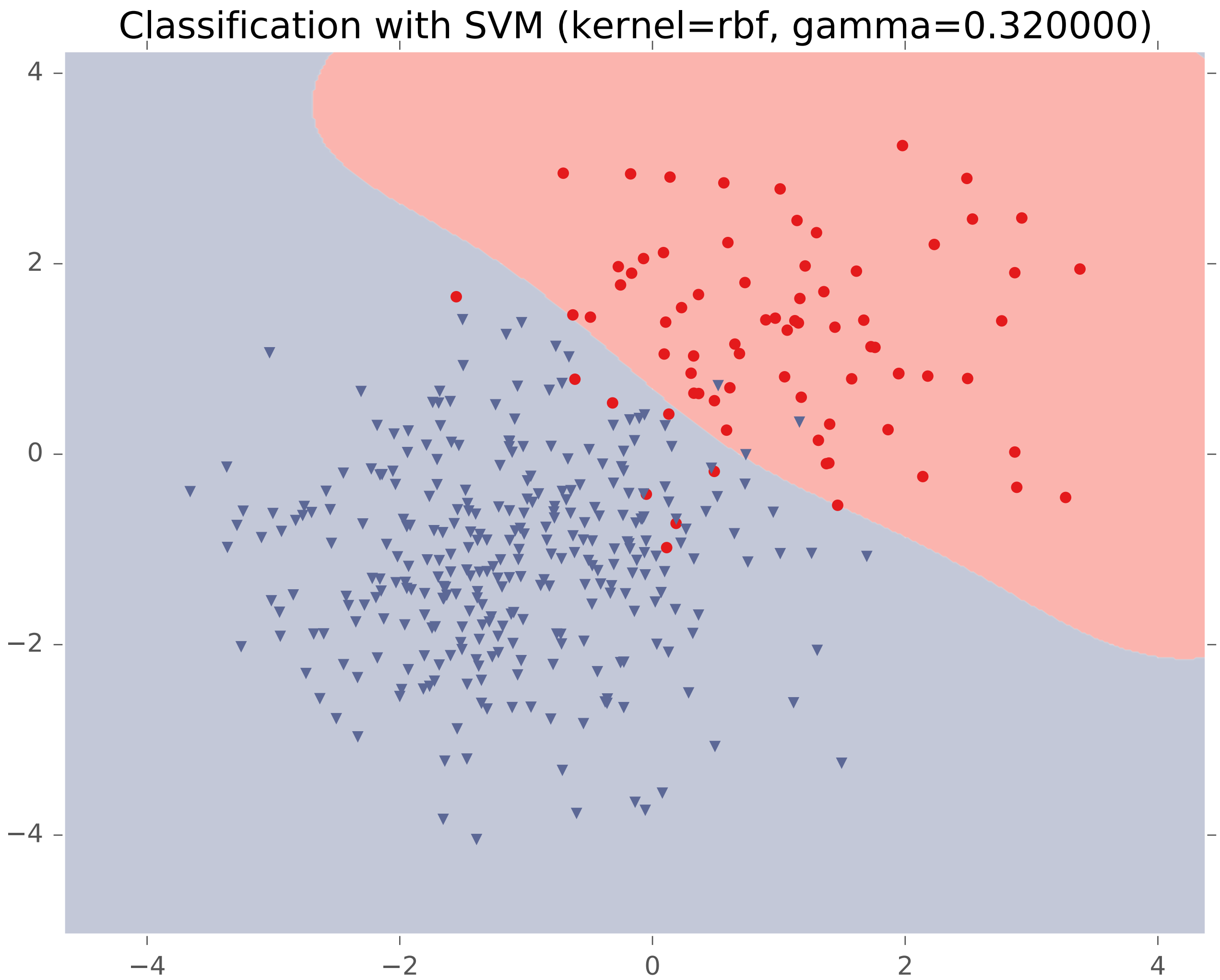
RBF Kernel Example



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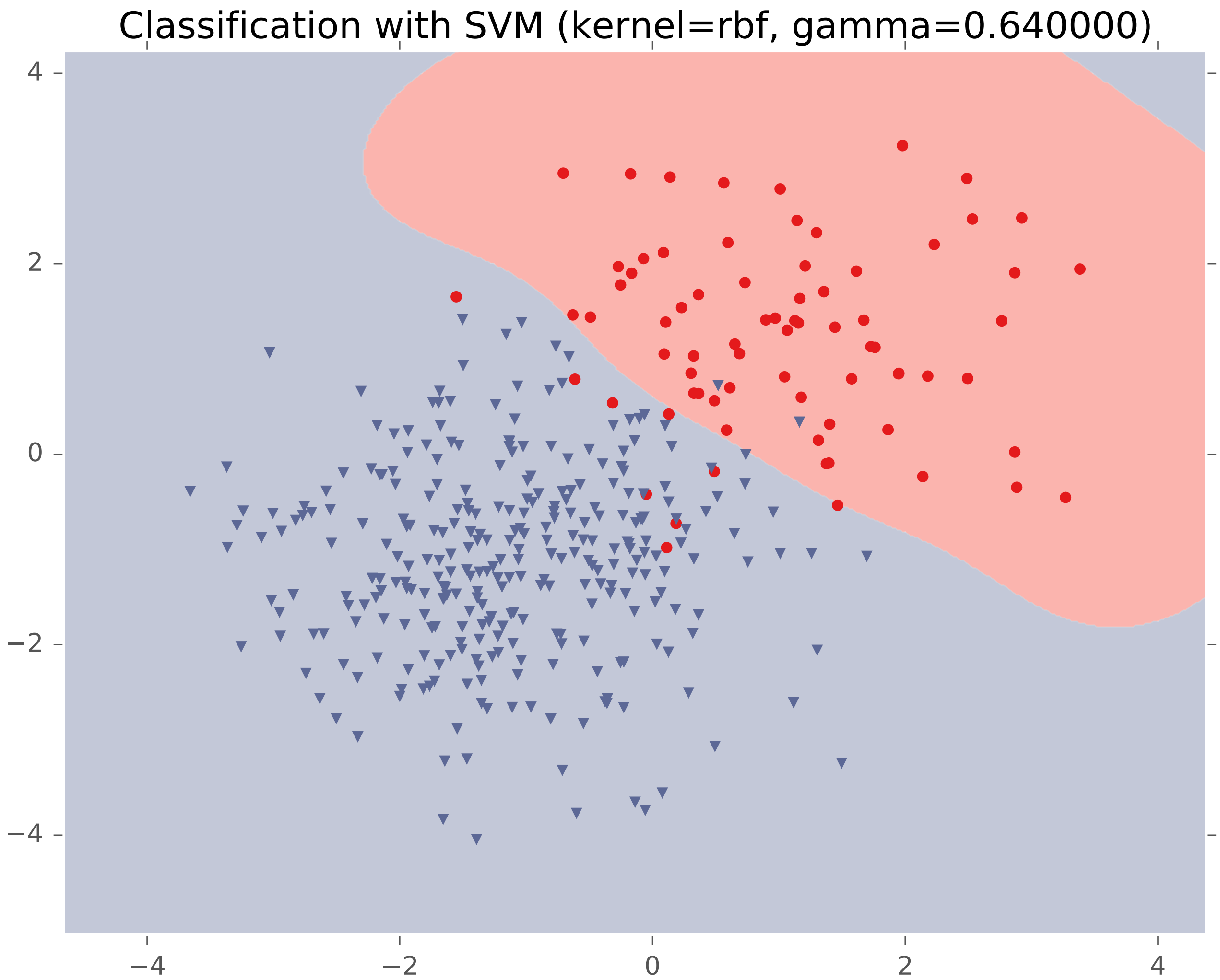

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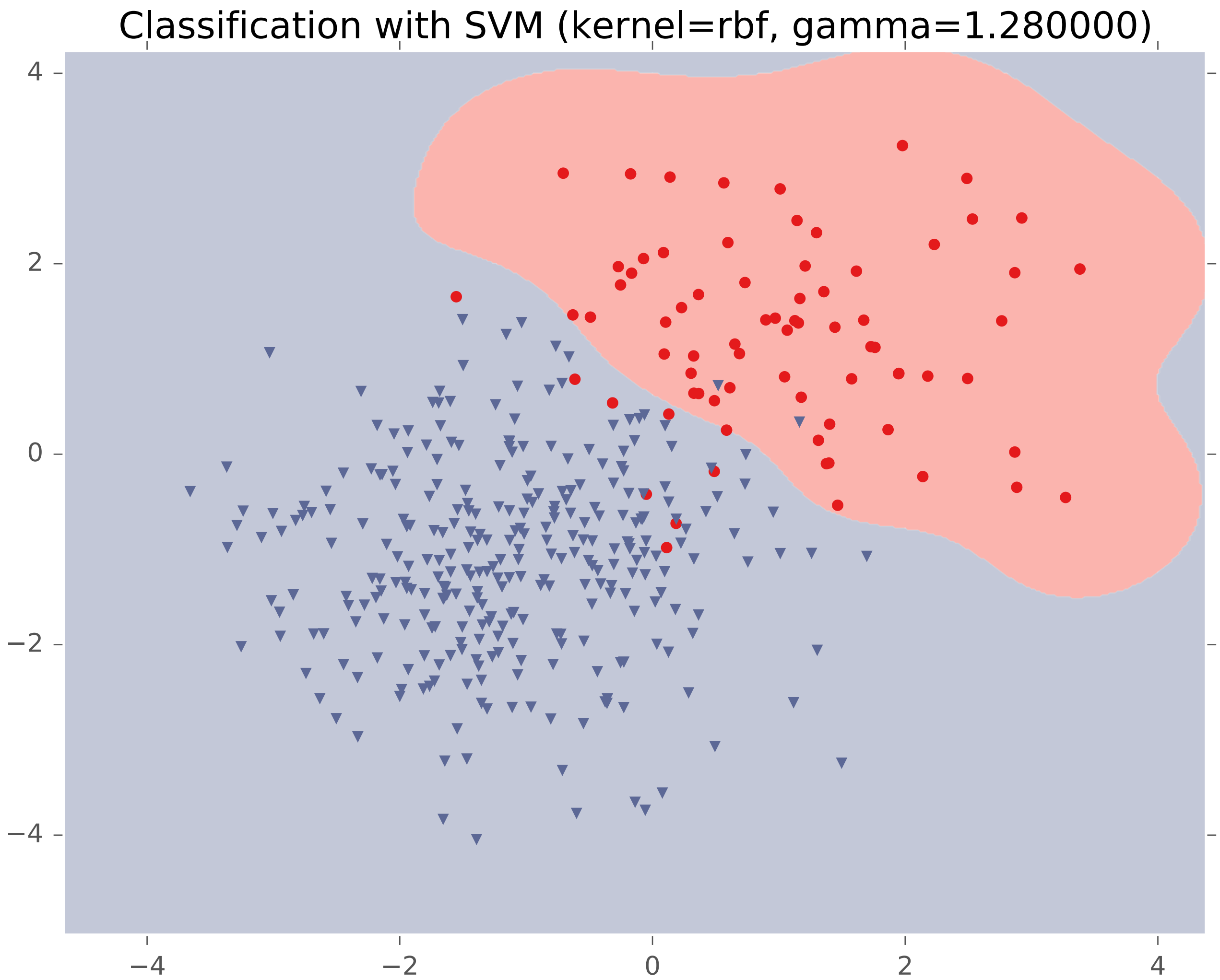

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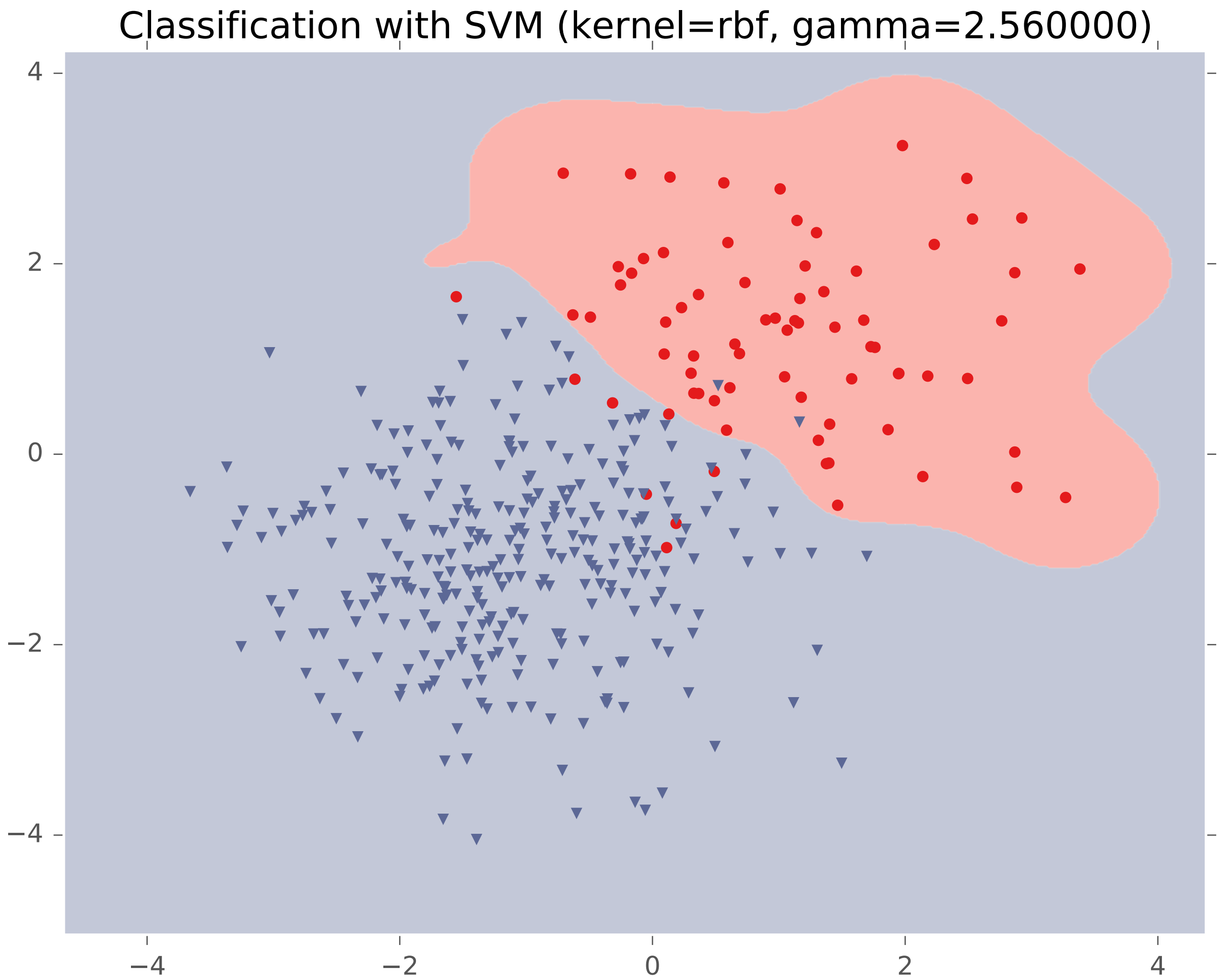

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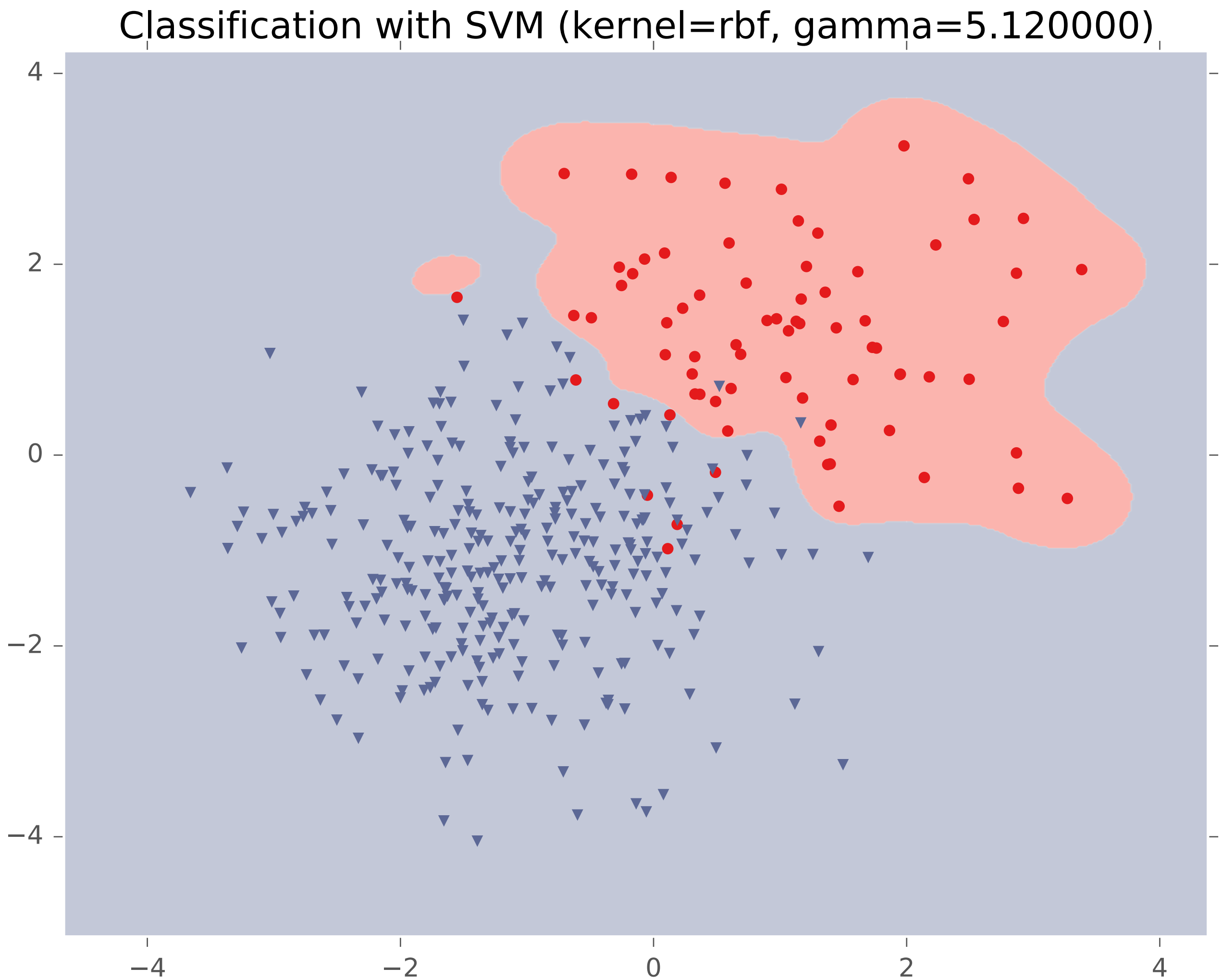

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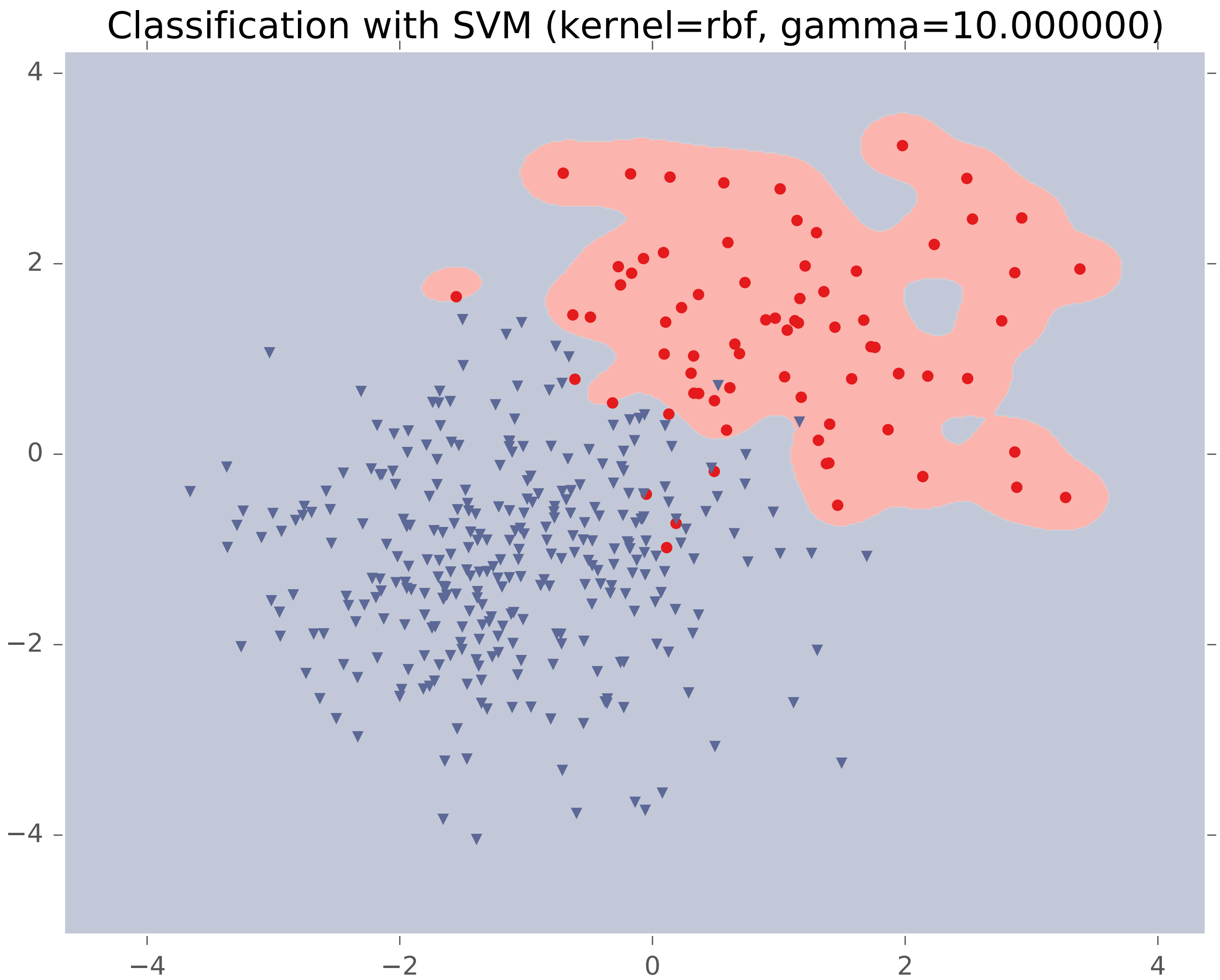
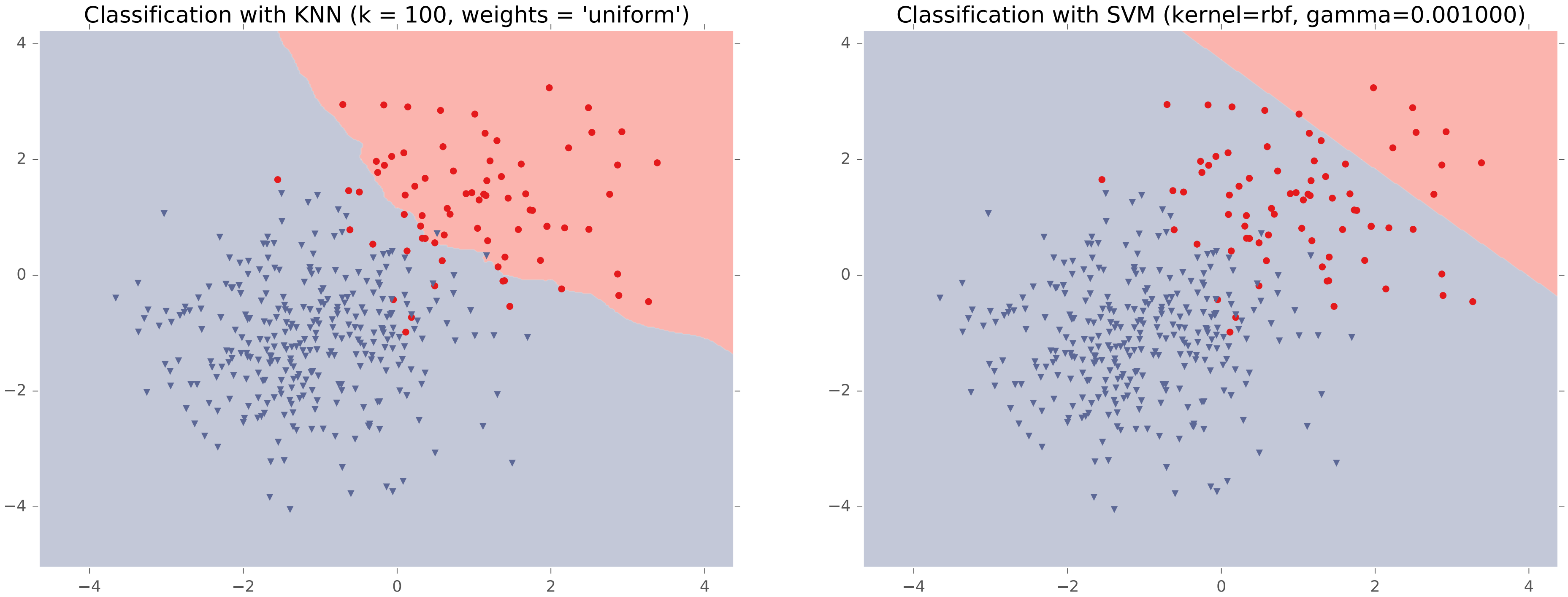
RBF Kernel Example



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

RBF Kernel Example

KNN vs. SVM



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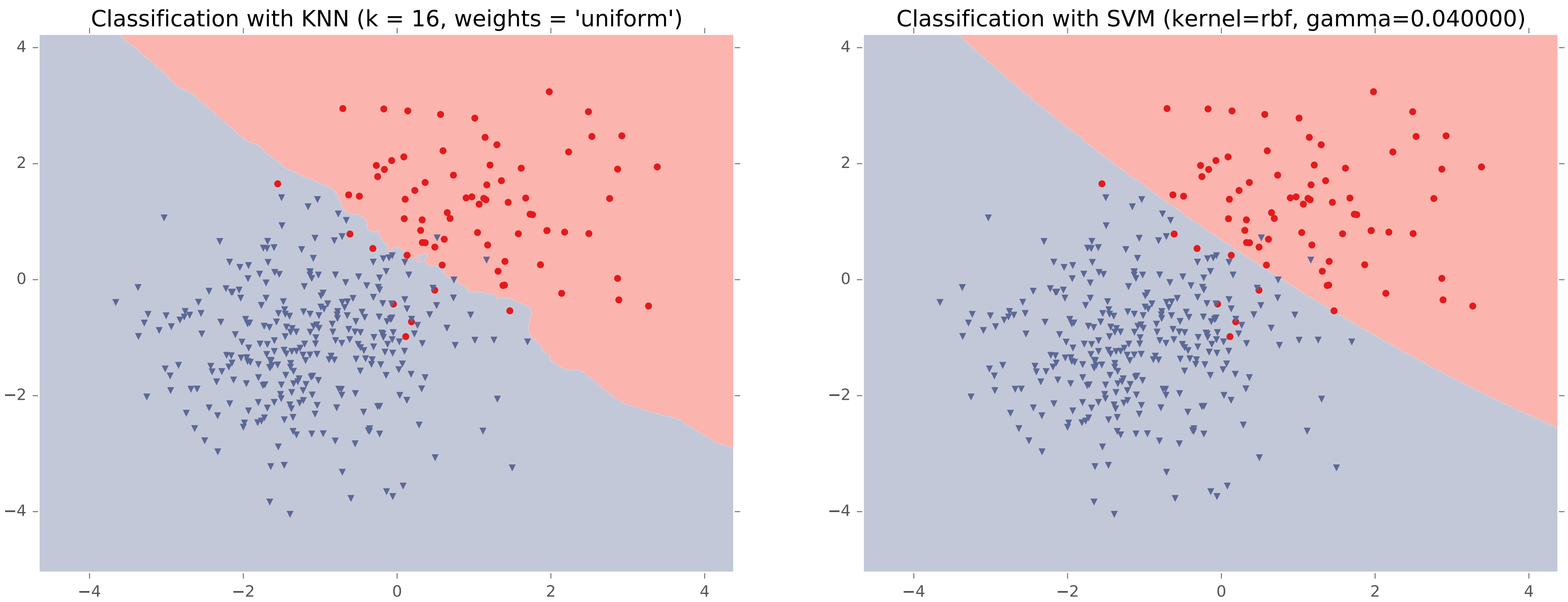
RBF Kernel Example

KNN vs. SVM



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RBF Kernel Example

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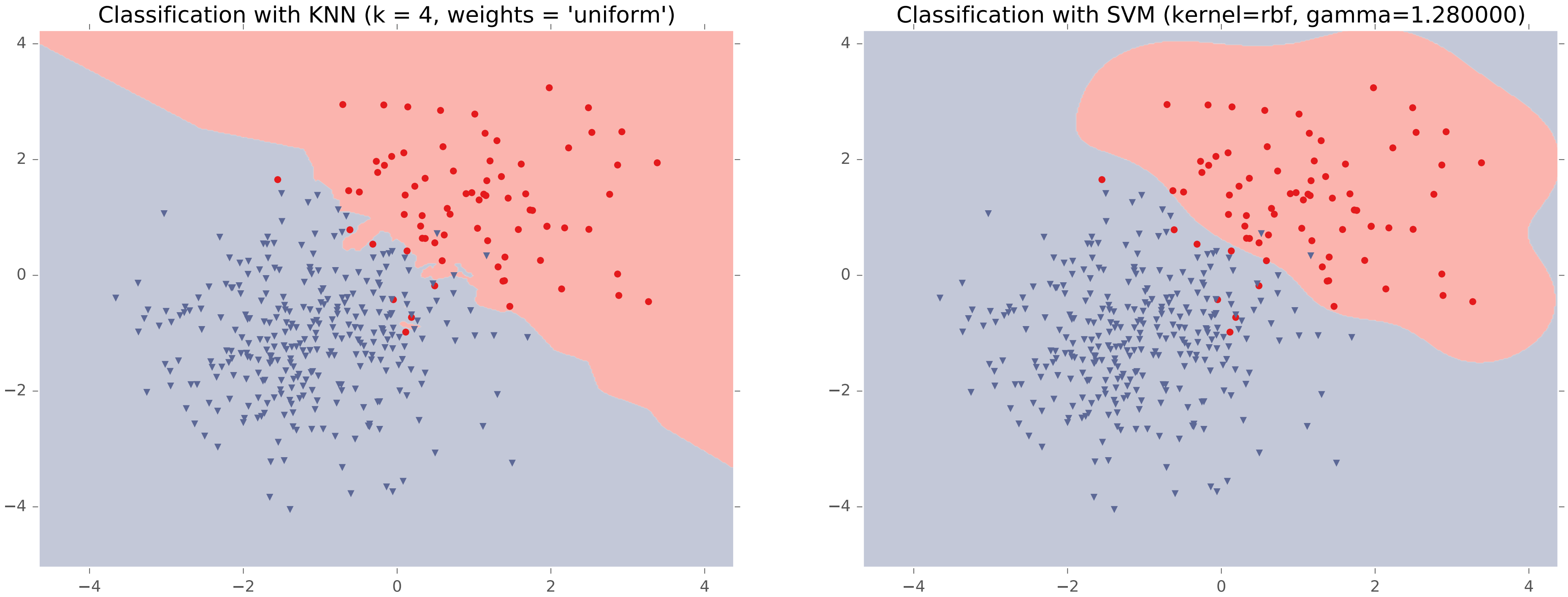

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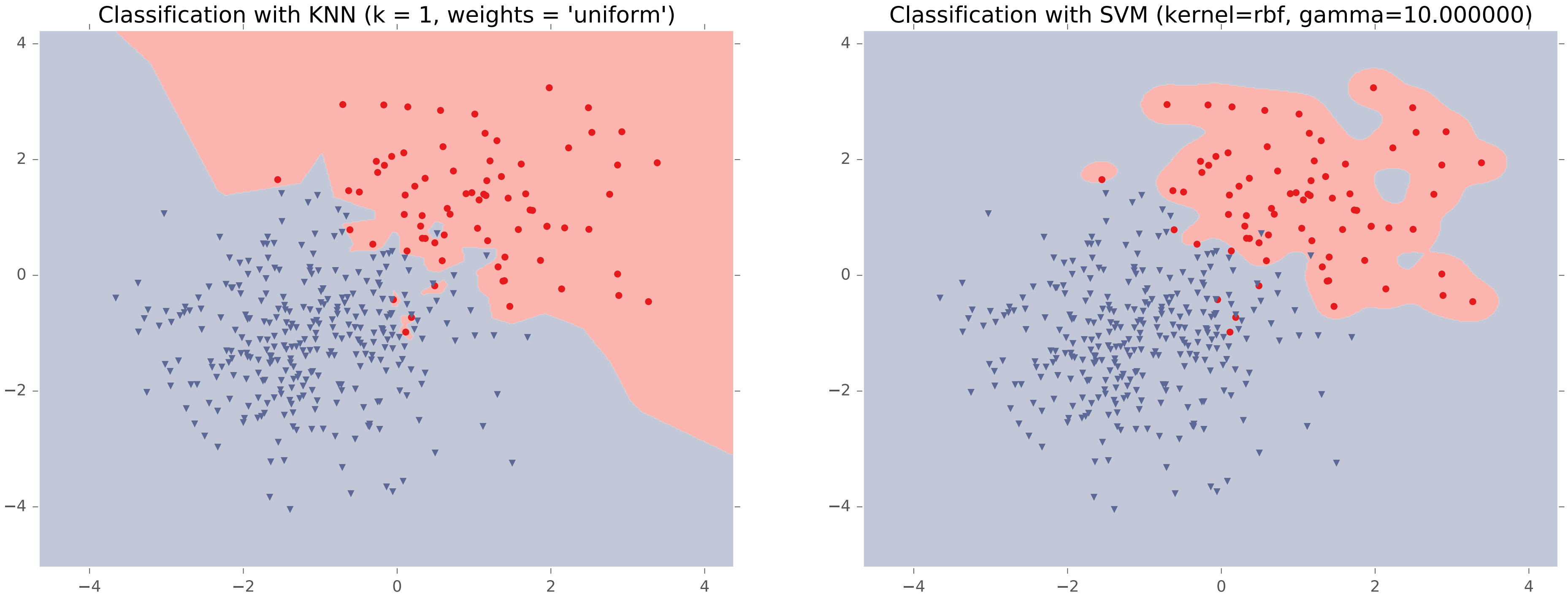
RBF Kernel Example

KNN vs. SVM



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

Example: String Kernel

Setup:

- Input instances **x** are strings of characters (e.g. $\mathbf{x}^{(3)}$ = [‘s’, ‘a’, ‘t’], $\mathbf{x}^{(7)}$ = [‘c’, ‘a’, ‘t’]
- Want indicator features for the presence / absence of each possible substring up to length K

Questions:

1. What is the best **runtime** of a single **Standard Perceptron** update?
2. What is the best **runtime** of a single **Kernel Perceptron** update?

Kernels: Discussion

- If all computations involving instances are in terms of inner products then:
  - Conceptually, work in a very high diml space and the alg's performance depends only on linear separability in that extended space.
  - Computationally, only need to modify the algo by replacing each $\mathrm{x} \cdot \mathrm{z}$ with a $\mathrm{K}(\mathrm{x}, \mathrm{z})$.

How to choose a kernel:

- Kernels often encode domain knowledge (e.g., string kernels)
- Use Cross-Validation to choose the parameters, e.g., σ for Gaussian Kernel $\mathrm{K}(\mathrm{x}, z) = \exp\left[-\frac{||x-z||^2}{2\,\sigma^2}\right]$
- Learn a good kernel; e.g., [Lanckriet-Cristianini-Bartlett-El Ghaoui-Jordan'04]

Slide from Nina Balcan

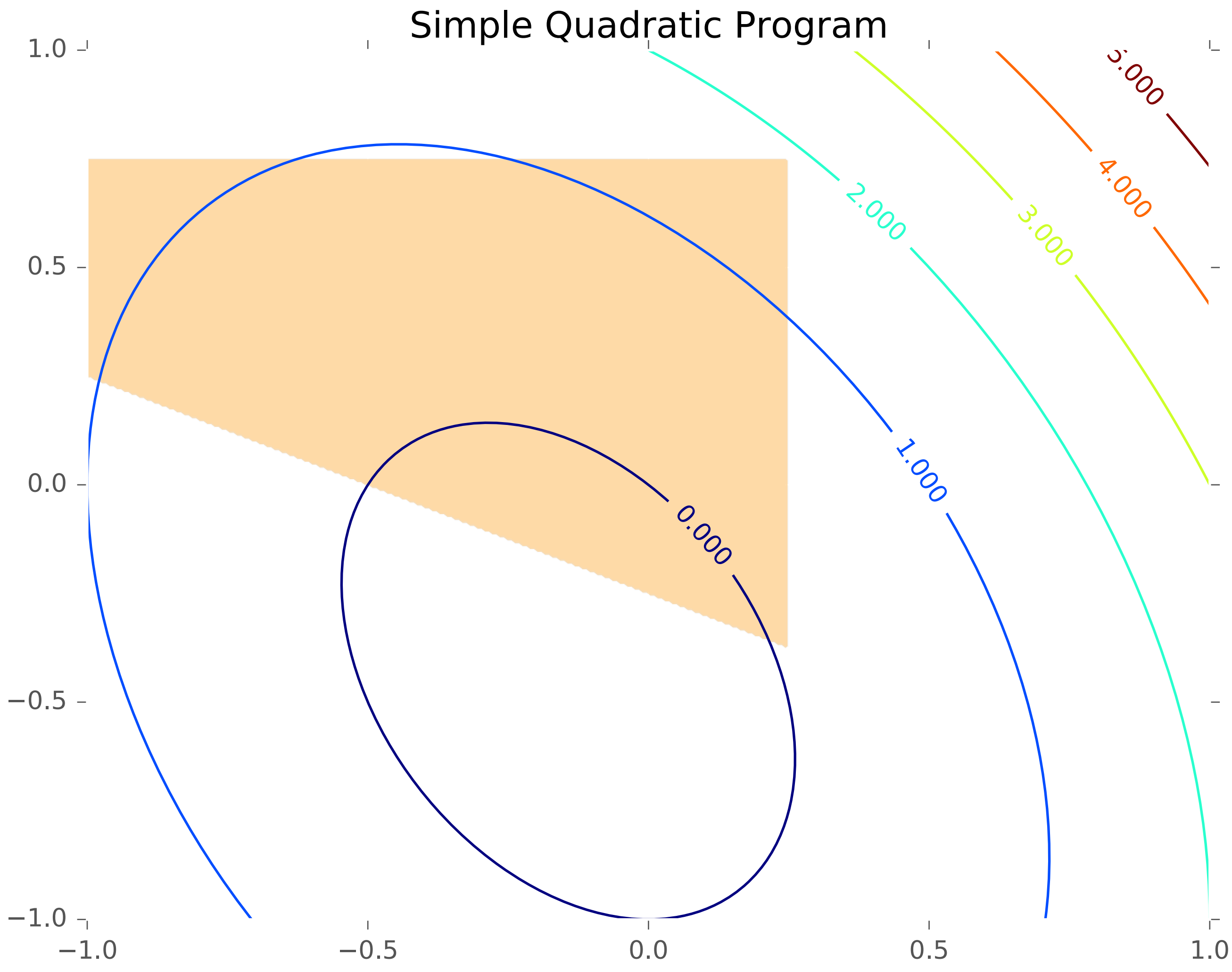
SUPPORT VECTOR MACHINE (SVM)

SVM: Optimization Background

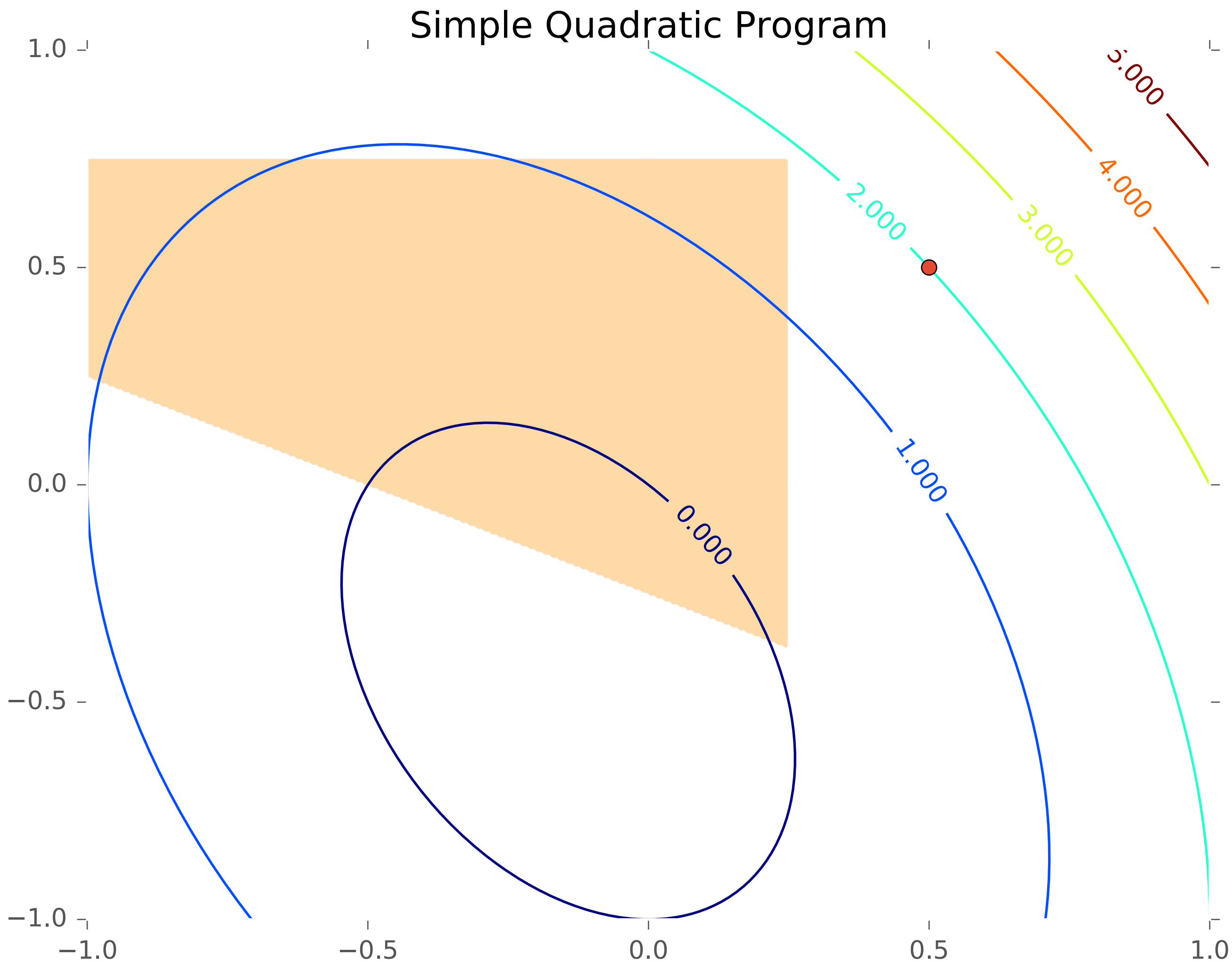
Whiteboard

- Constrained Optimization
- Linear programming
- Quadratic programming
- Example: 2D quadratic function with linear constraints

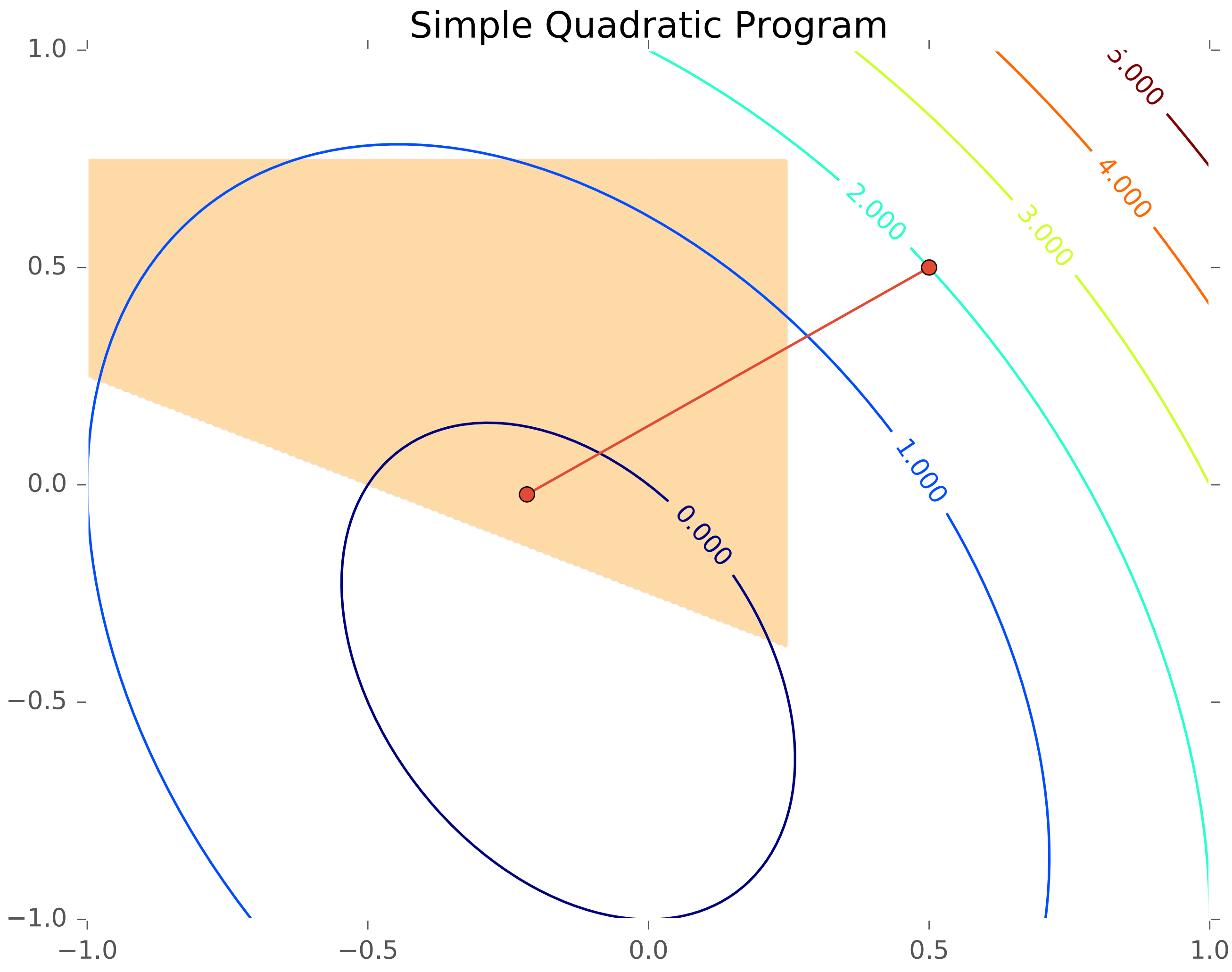
Quadratic Program



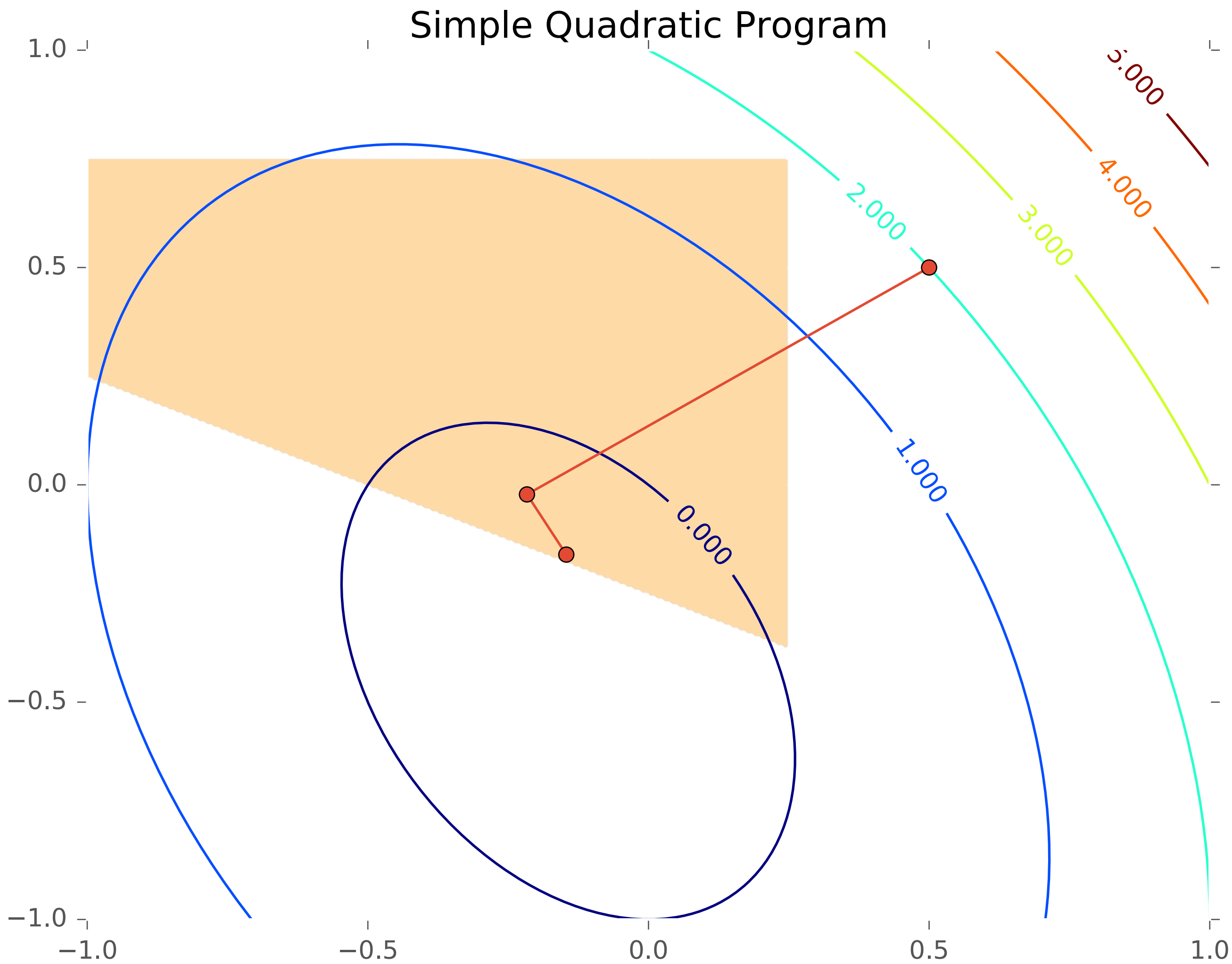
Quadratic Program



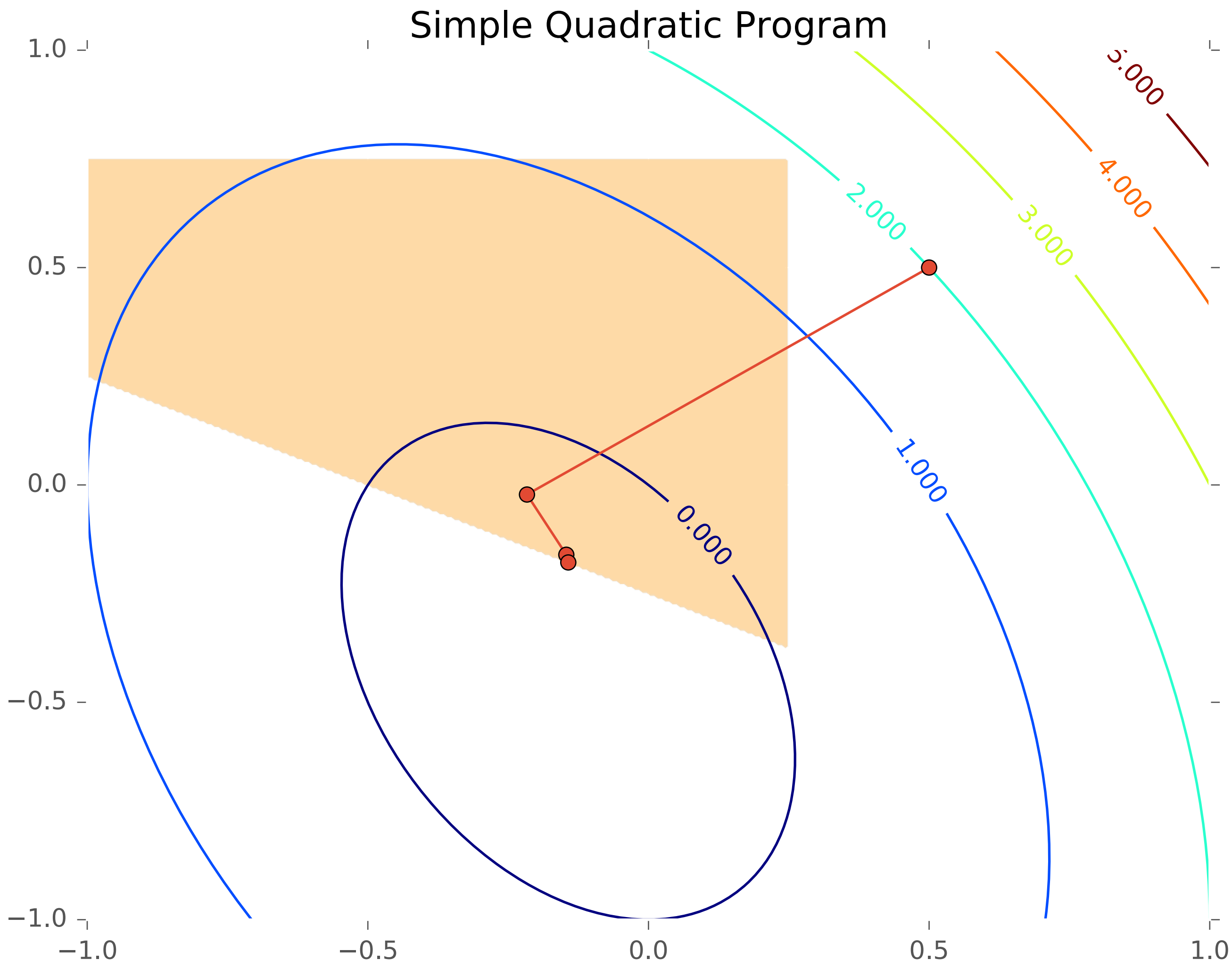
Quadratic Program



Quadratic Program



Quadratic Program

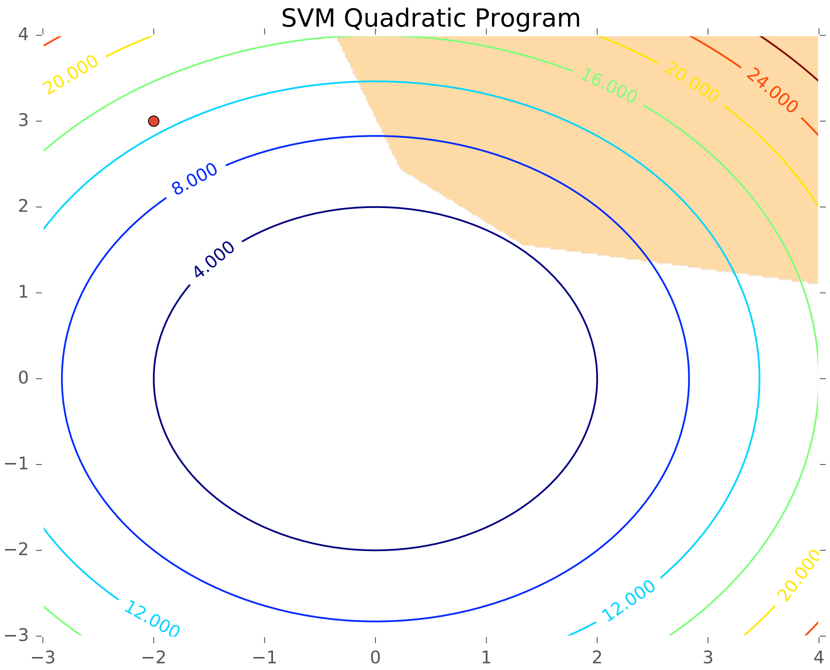


SVM

Whiteboard

- SVM Primal (Linearly Separable Case)
- SVM Primal (Non-linearly Separable Case)

SVM QP


SVM Quadratic Program
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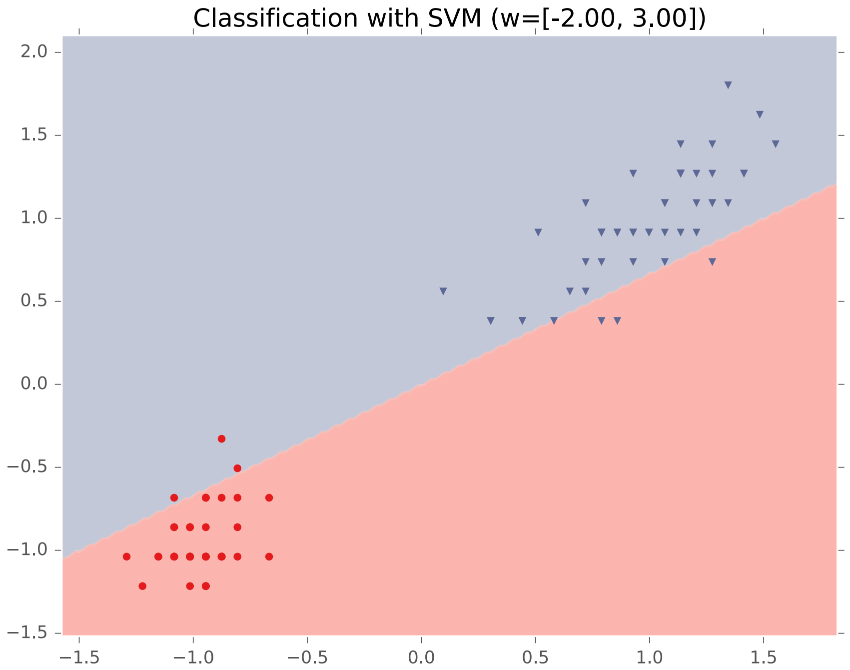
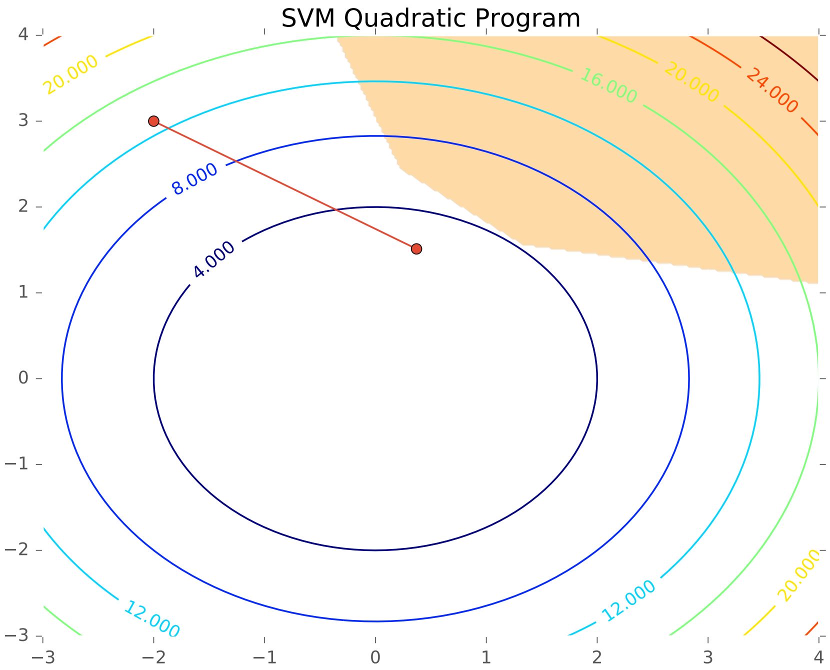

Classification with SVM (w=[-2.00, 3.00])

SVM QP


SVM Quadratic Program
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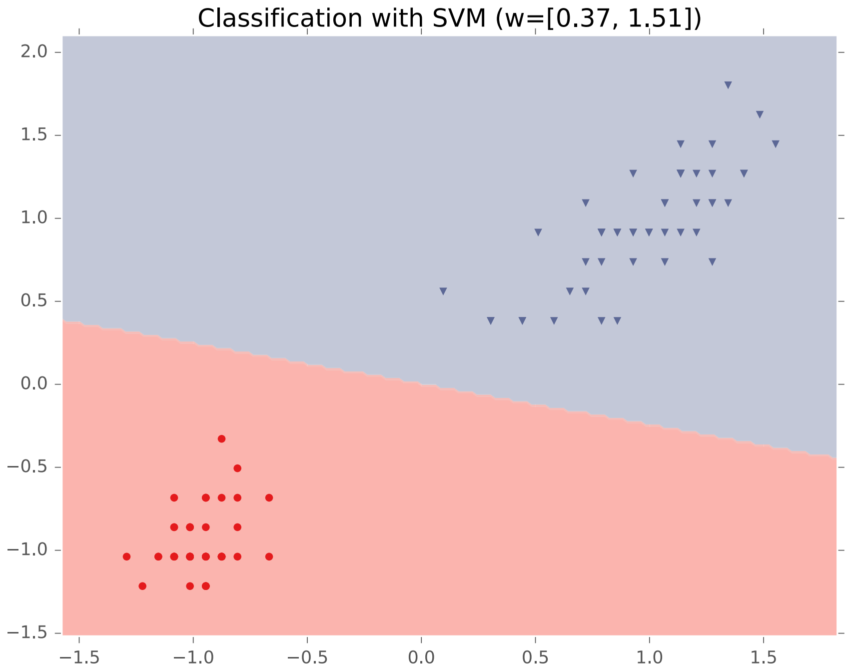
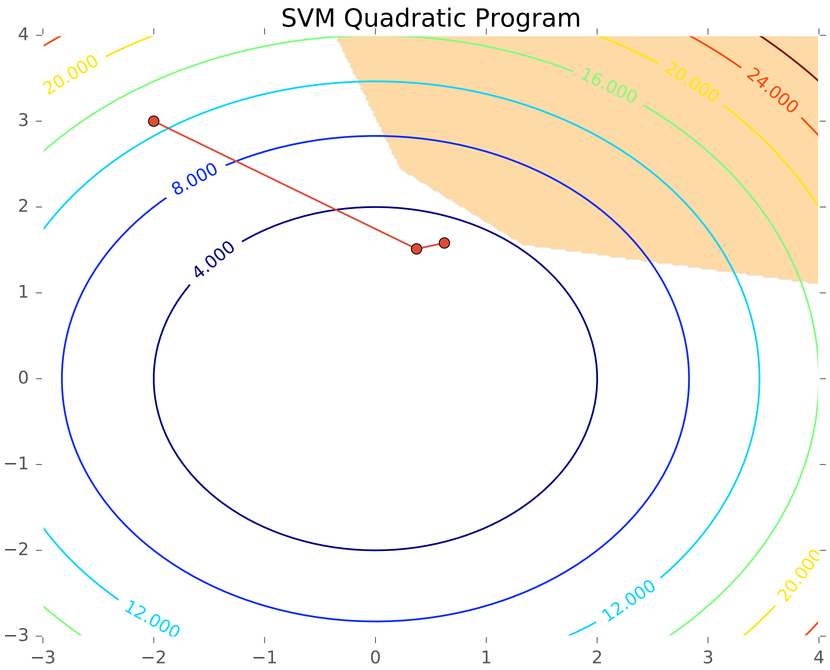

Classification with SVM (w=[0.37, 1.51])

SVM QP



SVM Quadratic Program
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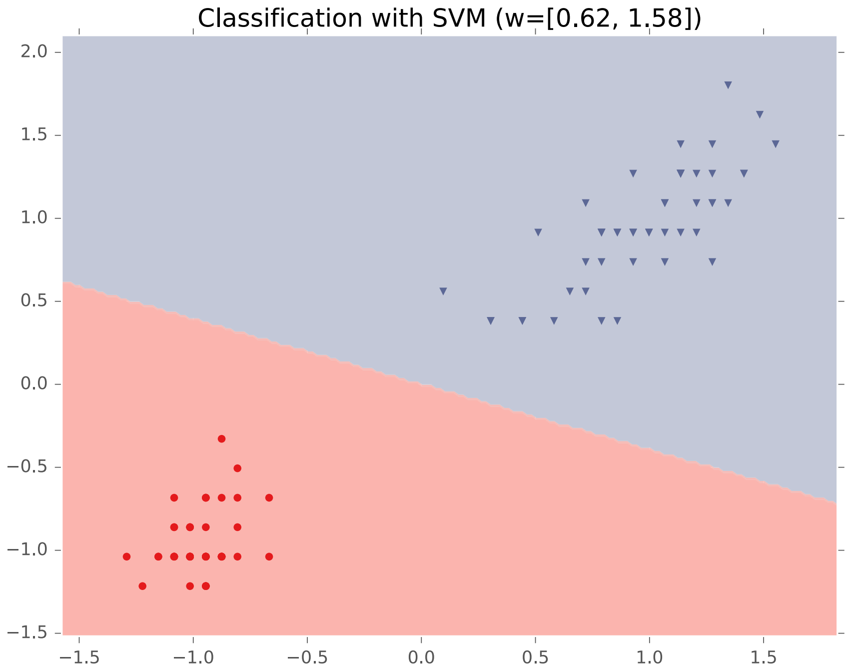
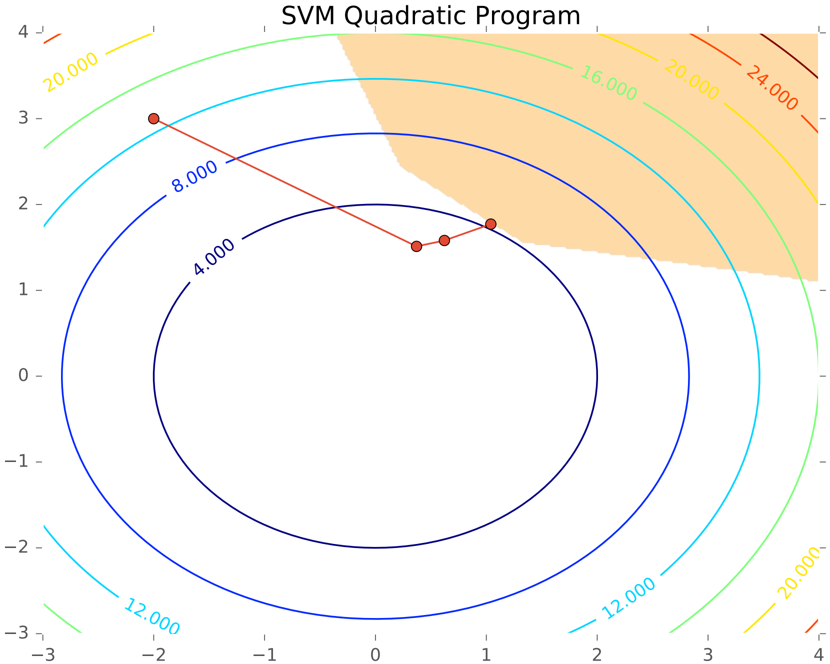


Classification with SVM (w=[0.62, 1.58])

SVM QP


SVM Quadratic Program
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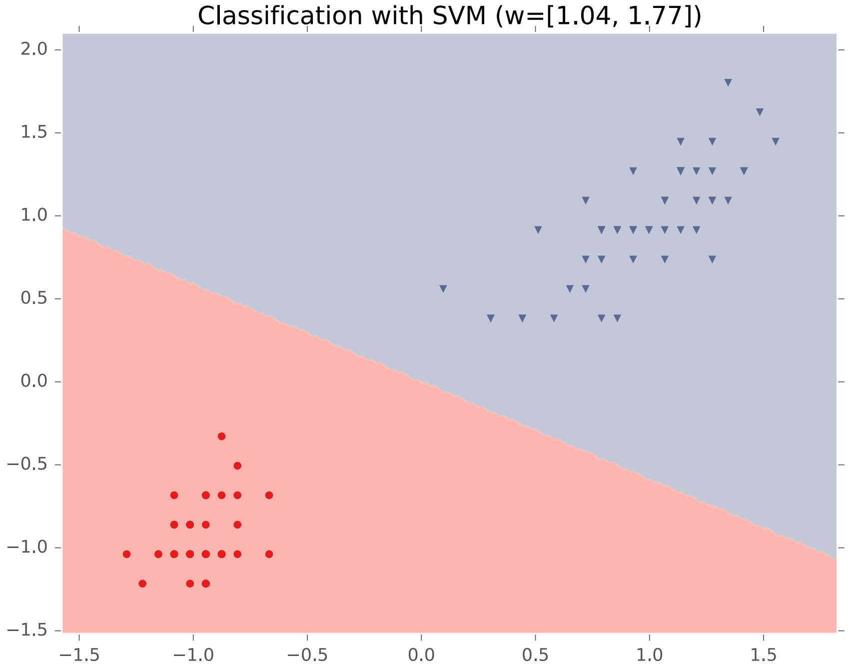
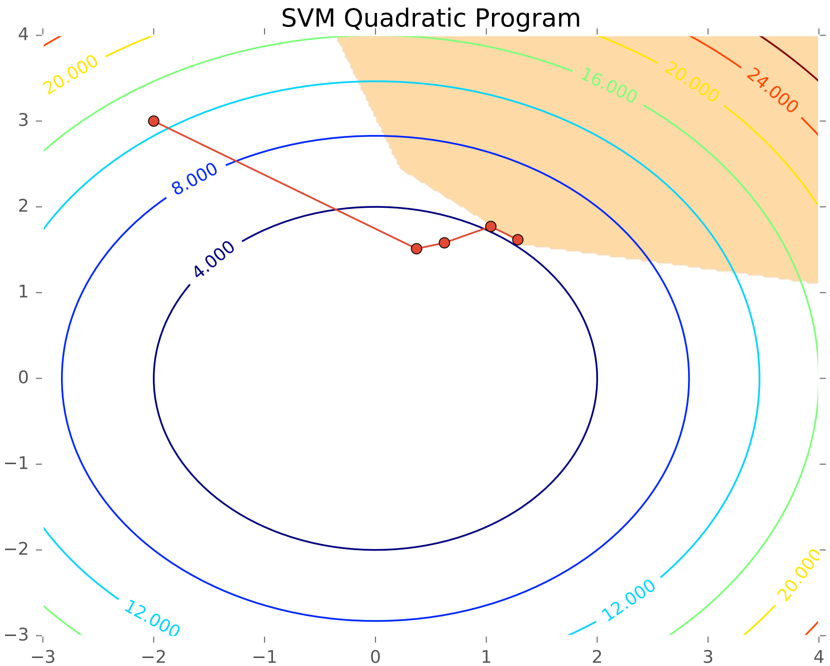

Classification with SVM (w=[1.04, 1.77])

SVM QP



SVM Quadratic Program
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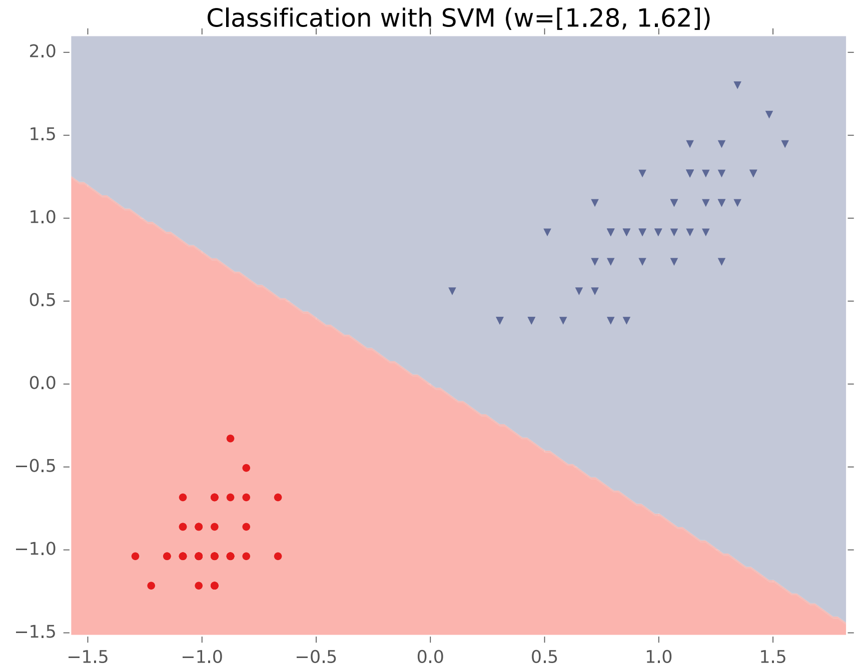
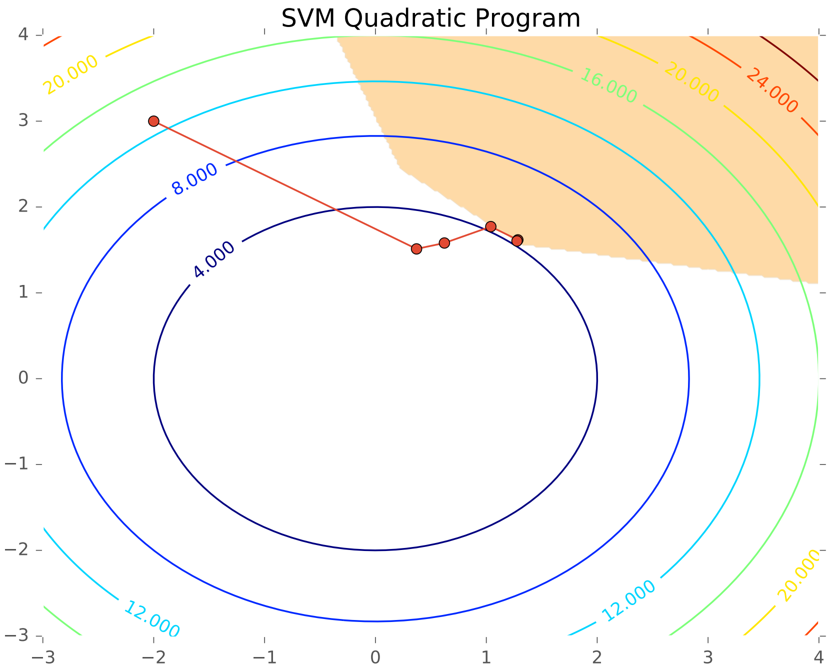


Classification with SVM (w=[1.28, 1.62])

SVM QP



SVM Quadratic Program
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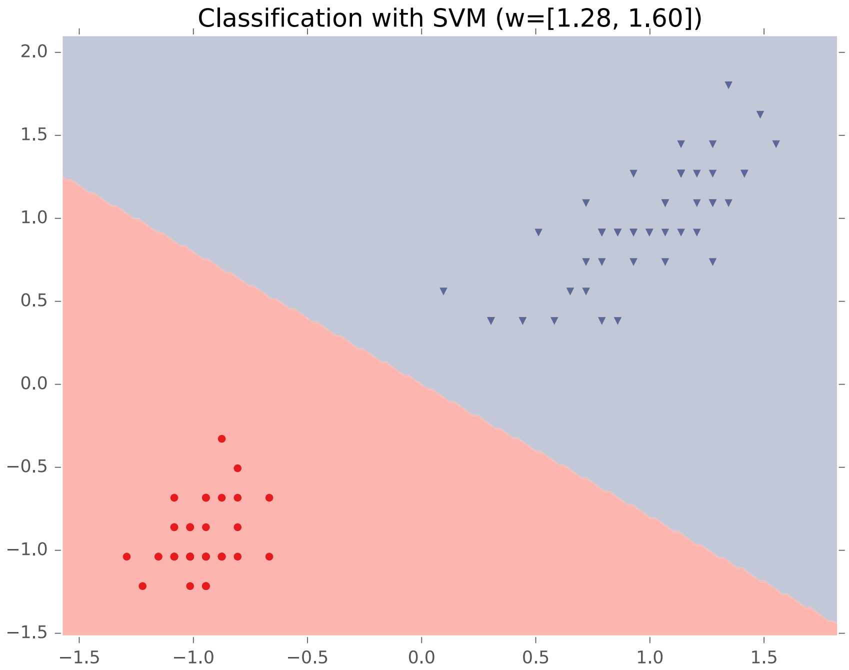


Classification with SVM (w=[1.28, 1.60])

Support Vector Machines (SVMs)

Input: S={(x_1, y_1), …,(x_m, y_m)};

Find $\text{argmin}_{w,\xi_1,\ldots,\xi_m} ||w||^2 + C \sum_i \xi_i$ s.t.:

- For all i, $y_i w \cdot x_i \geq 1 - \xi_i$

  $\xi_i \geq 0$

Primal form

Which is equivalent to:

Can be kernelized!!!

Input: S={(x_1, y_1), …,(x_m, y_m)};

Find $\text{argmin}_{\alpha} \frac{1}{2} \sum_i \sum_j y_i y_j \alpha_i \alpha_j x_i \cdot x_j - \sum_i \alpha_i$ s.t.:

- For all i, $0 \leq \alpha_i \leq C_i$

  $$\sum_i y_i \alpha_i = 0$$

Lagrangian Dual

Slide from Nina Balcan

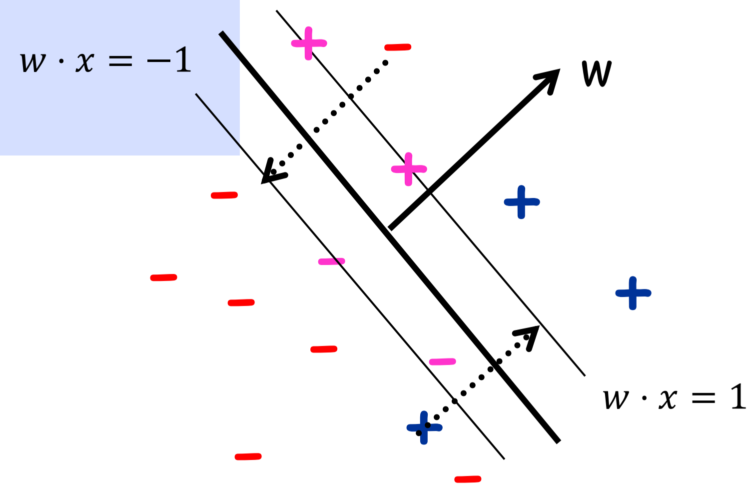
SVMs (Lagrangian Dual)

<u>Input</u>: $S=\{(x_1, y_1), \ldots,(x_m, y_m)\}$;

<u>Find</u> $\mathrm{argmin}_\alpha \frac{1}{2}\sum_i \sum_j y_i y_j \alpha_i \alpha_j x_i \cdot x_j - \sum_i \alpha_i$ s.t.:

- For all i, $0 \leq \alpha_i \leq C_i$

$$\sum_i y_i \alpha_i = 0$$



- Final classifier is: $w = \sum_i \alpha_i y_i x_i$
- The points x_i for which $\alpha_i \neq 0$ are called the "support vectors"

SVM 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**