CS184A/284A
AI in Biology and Medicine

SVM

Machine Learning

Support Vector Machines

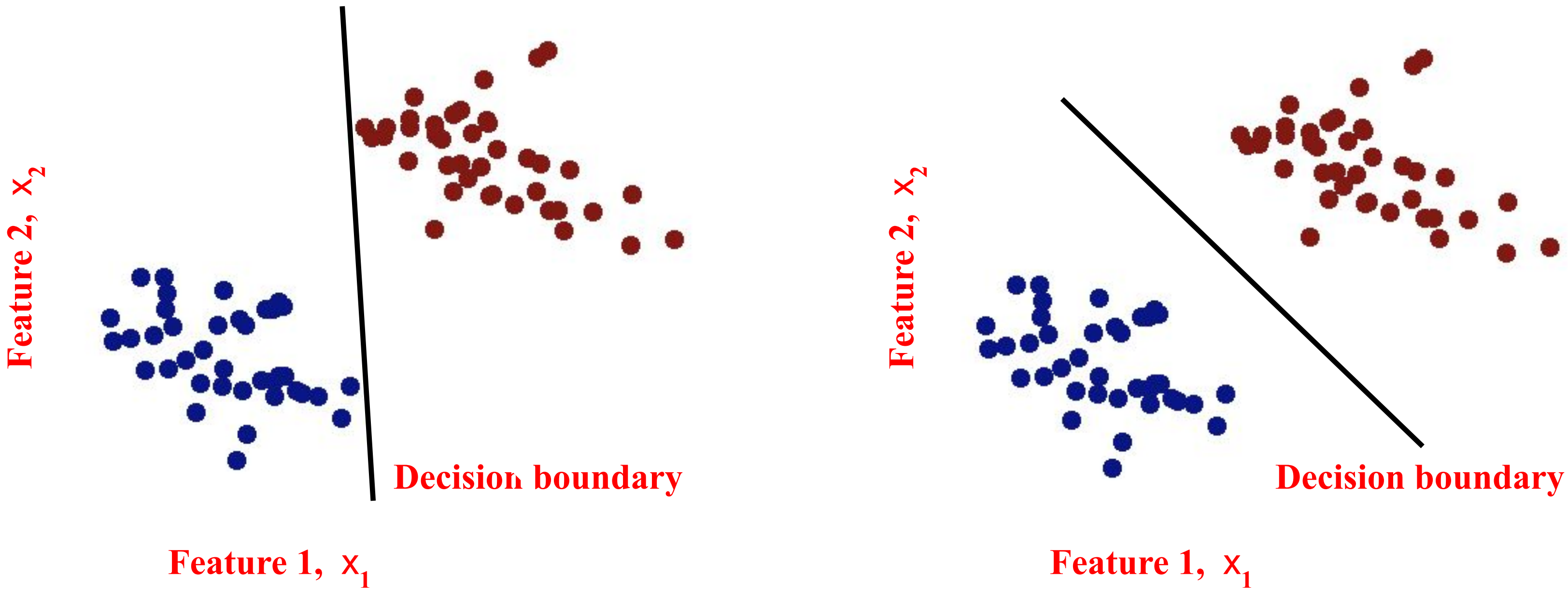
Lagrangian and Dual

The Kernel Trick

Linear classifiers

- Which decision boundary is "better"?
  - Both have zero training error (perfect training accuracy)
  - But, one of them seems intuitively better…

- How can we quantify "better",
  and learn the "best" parameter settings?

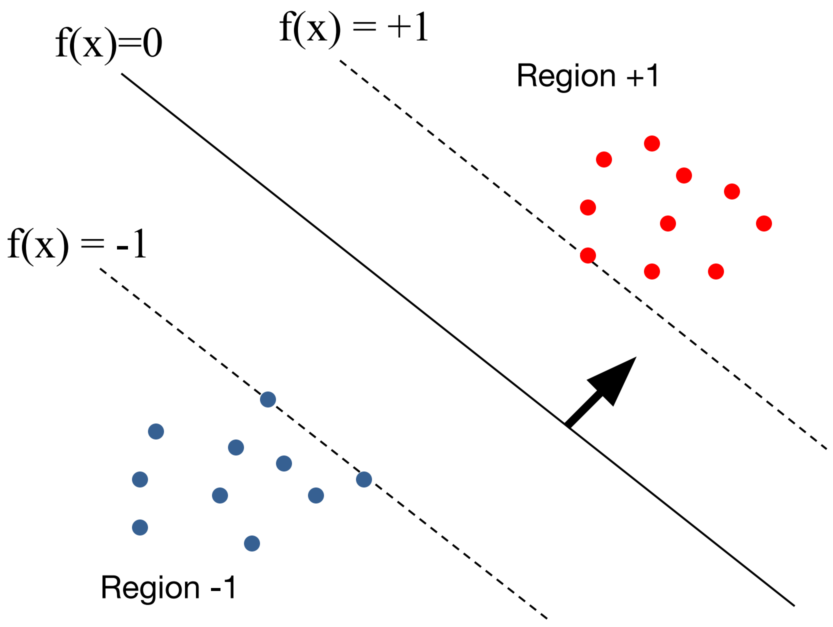


One possible answer…

Notation change!

$$\theta_0 + \theta_1 x_1 + \theta_2 x_2 + \ldots$$
$$\Downarrow$$
$$b + w_1 x_1 + w_2 x_2 + \ldots$$

- Maybe we want to maximize our "margin"
- To optimize, relate to model parameters
- Remove "scale invariance"
  - Define class +1 in some region, class –1 in another
  - Make those regions as far apart as possible



We could define such a function:

f(x) = w*x + b

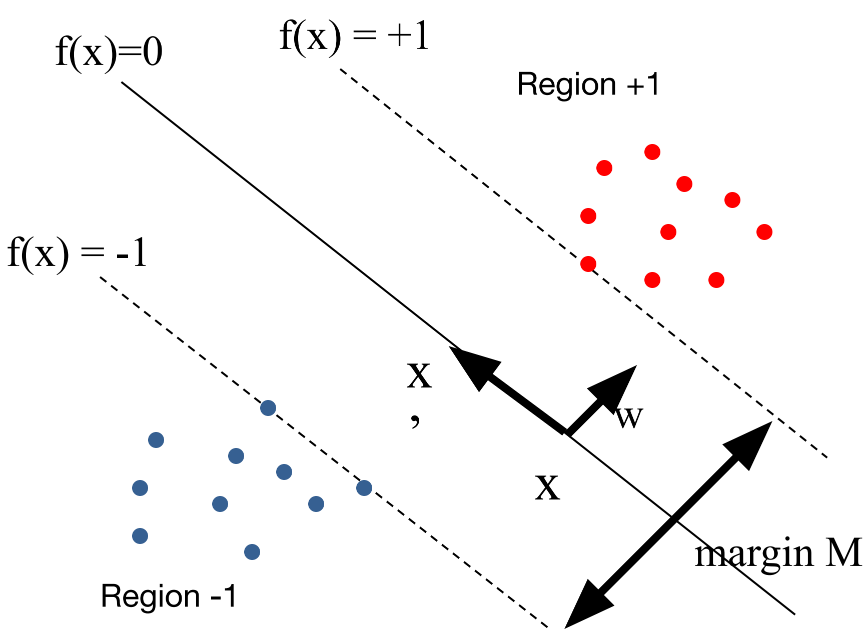
f(x) > +1 in region +1
f(x) < –1 in region –1

Passes through zero in center…

"Support vectors" – data points on margin

Computing the margin width

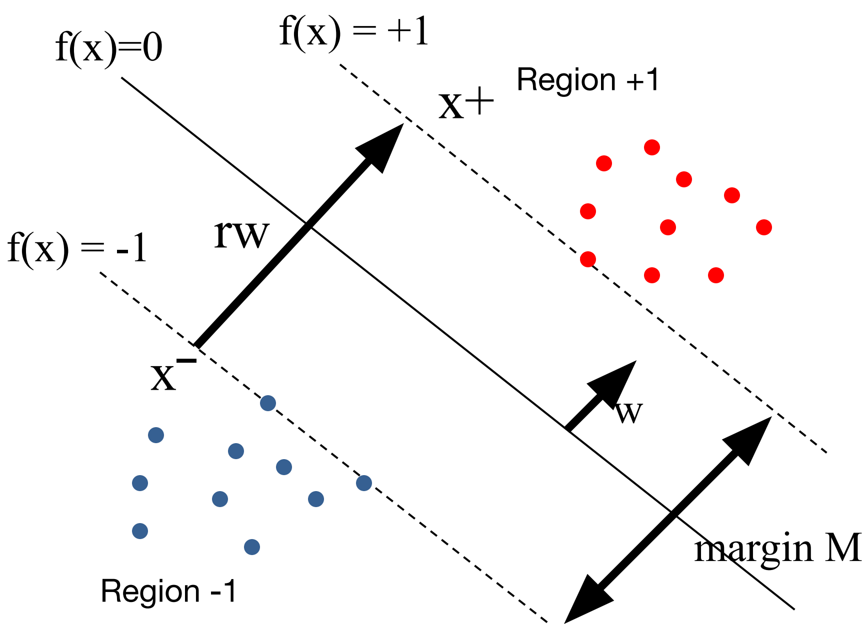
- Vector **w**=[w_1 w_2 …] is perpendicular to the boundaries (why?)
- w x + b = 0 & w x' + b = 0 => w · (x'-x) = 0 : orthogonal



Computing the margin width

- Vector **w**=[w_1 w_2 …] is perpendicular to the boundaries
- Choose $\mathbf{x}^-$ st $f(\mathbf{x}^-) = -1$; let $\mathbf{x}^+$ be the closest point with $f(\mathbf{x}^+) = +1$
  - $\mathbf{x}^+ = \mathbf{x}^- + r * \mathbf{w}$ (why?)
- Closest two points on the margin also satisfy

$$w \cdot x^- + b = -1 \qquad\qquad w \cdot x^+ + b = +1$$



Computing the margin width

- Vector $\underline{w}=[w_1\ w_2\ \ldots]$ is perpendicular to the boundaries
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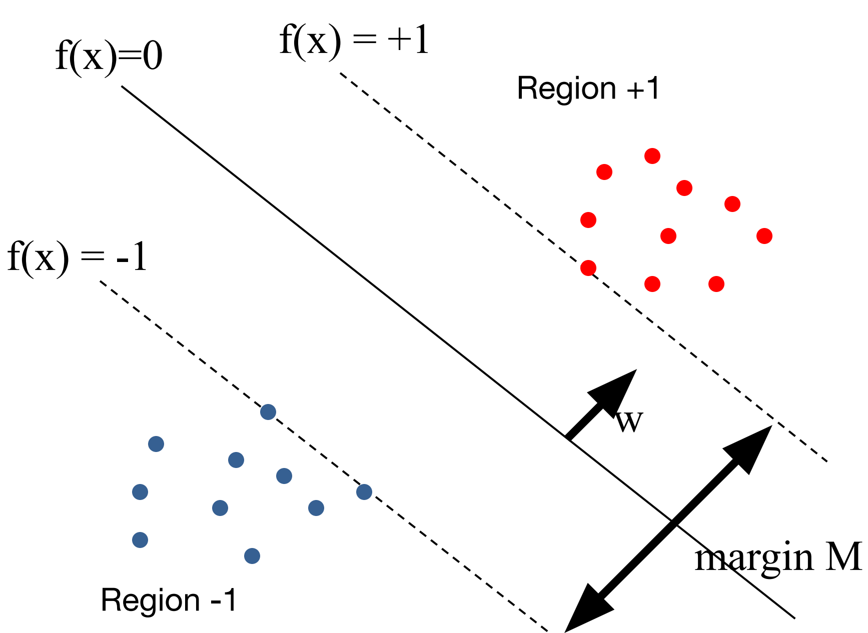


$$w \cdot (x^- + rw) + b = +1$$
$$\Rightarrow \quad r\|w\|^2 + w \cdot x^- + b = +1$$
$$\Rightarrow \quad r\|w\|^2 - 1 = +1$$
$$\Rightarrow \quad r = \frac{2}{\|w\|^2}$$

$$M = \|x^+ - x^-\| = \|rw\|$$
$$= \frac{2}{\|w\|^2}\|w\| = \frac{2}{\sqrt{w^T w}}$$

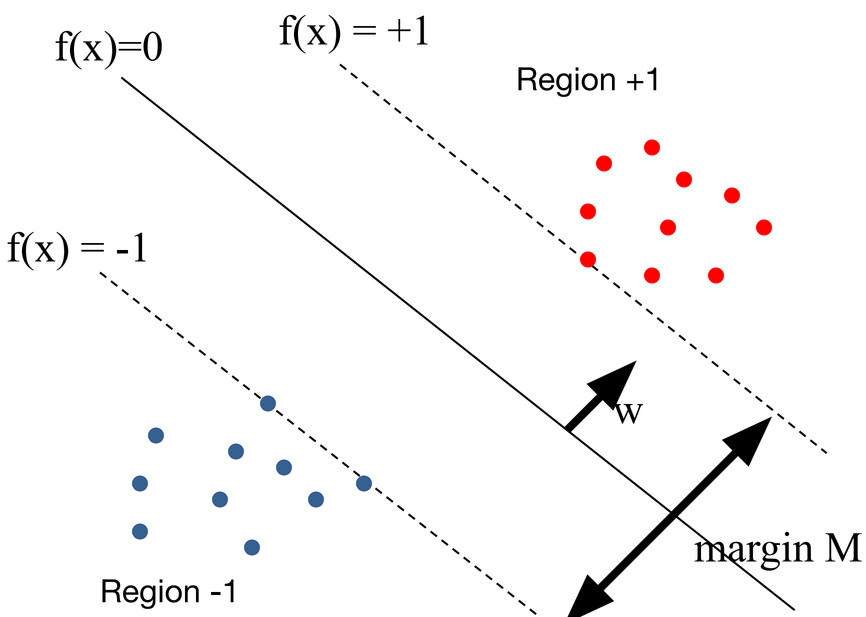
Maximum margin classifier

- Constrained optimization
  - Get all data points correct
  - Maximize the margin

$$w^* = \arg\max_w \frac{2}{\sqrt{w^T w}}$$

such that "all data on the correct side of the margin"

This is an example of a quadratic program: quadratic cost function, linear constraints



Primal problem:

$$w^* = \arg\min_w \sum_j w_j^2$$

s.t.

$$y^{(i)} = +1 \Rightarrow \quad w \cdot x^{(i)} + b \geq +1$$

$$y^{(i)} = -1 \Rightarrow \quad w \cdot x^{(i)} + b \leq -1$$

(m constraints)

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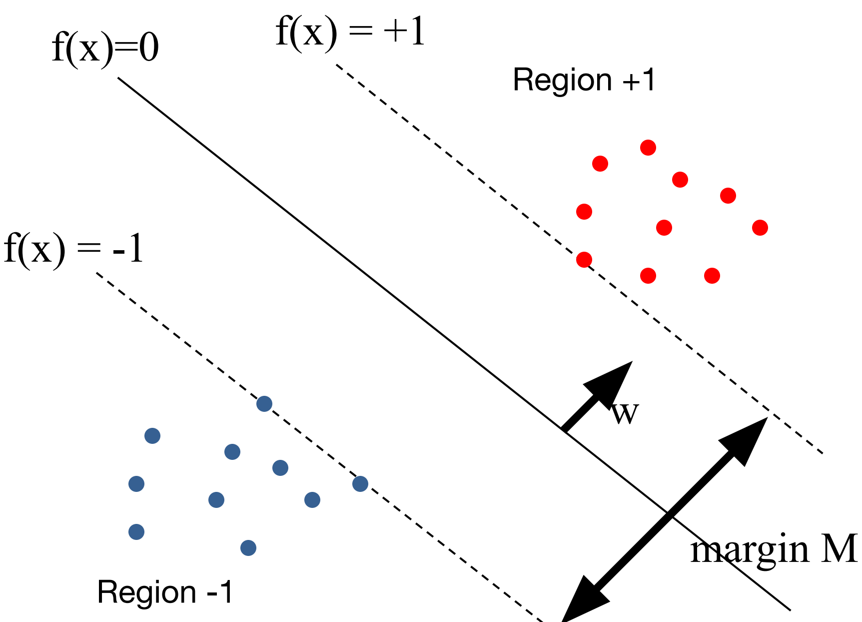

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A 1D Example

- Suppose we have three data points

  x = -3, y = -1

  x = -1, y = -1

  x = 2, y = 1

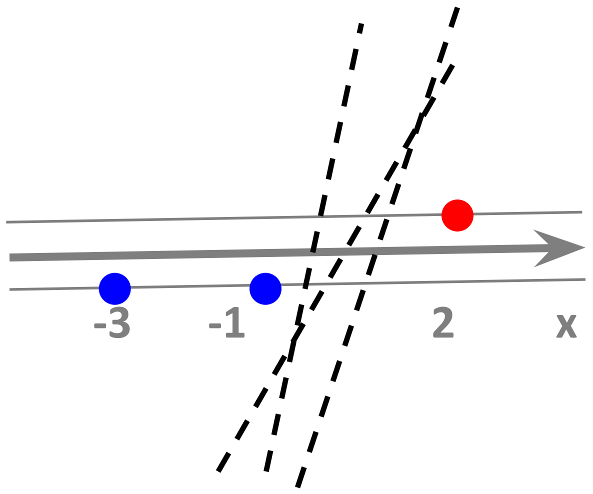
- Many separating perceptrons, T[ax+b]
  - Anything with ax+b = 0 between -1 and 2

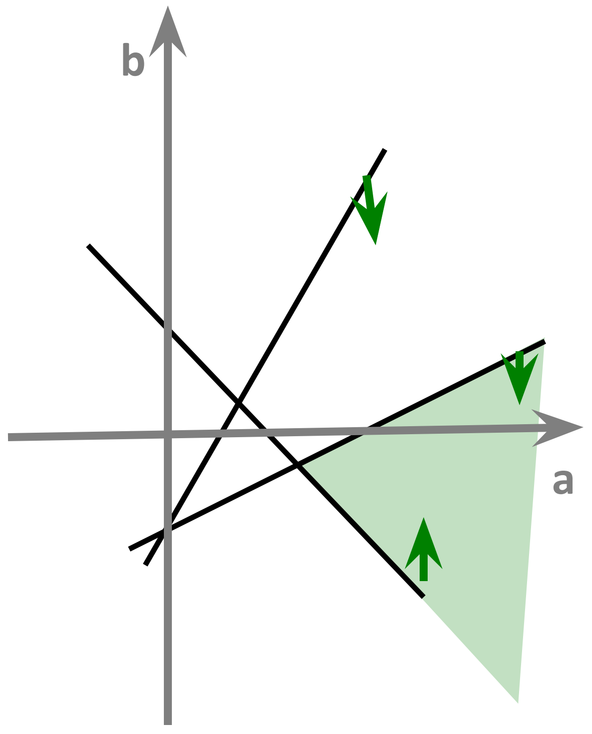
- We can write the margin constraints

  a (-3) + b < -1   => b < 3a - 1

  a (-1) + b < -1   => b <   a - 1

  a (2) + b > +1   => b > -2a + 1





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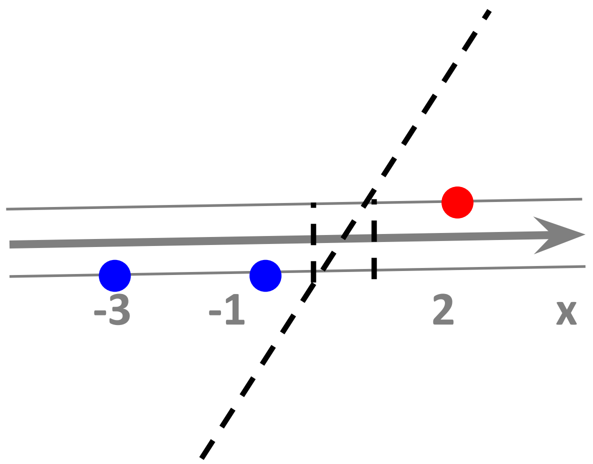
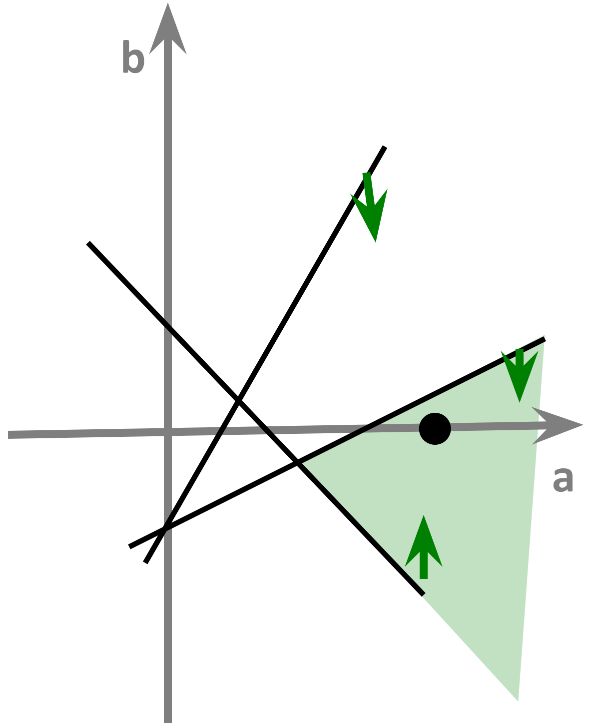
- Ex: a = 1, b = 0





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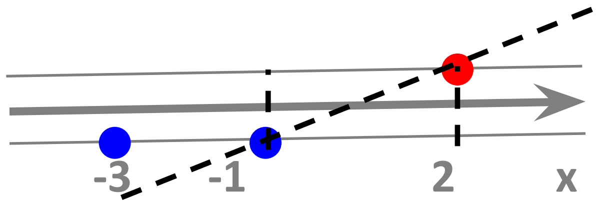

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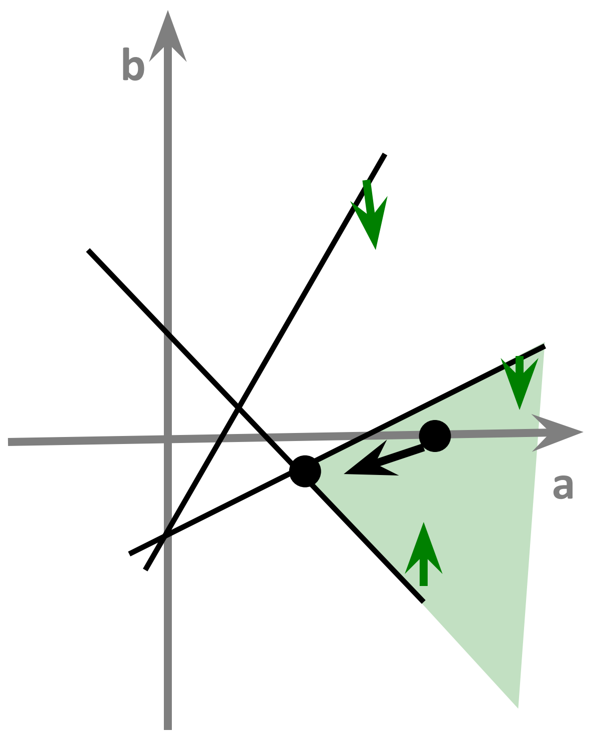
- Ex: a = 1, b = 0
- Minimize ||a|| => a = .66, b = -.33
  - Two data on the margin; constraints "tight"



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Lagrangian optimization

- Want to optimize constrained system:

$\theta = (w,b)$

$$\underbrace{w^* = \arg\min_{w,b} \sum_j w_j^2}_{f(\theta)} \qquad s.t. \qquad \underbrace{1 - y^{(i)}(w \cdot x^{(i)} + b) \leq 0}_{g_i(\theta) \leq 0}$$

- Introduce Lagrange multipliers α (one per constraint)

$$\theta^* = \arg\min_{\theta} \max_{\alpha \geq 0} f(\theta) + \sum_i \alpha_i \, g_i(\theta)$$

  - Can optimize θ, α jointly over a simpler constraint set (initialization easy)
  - For inner max:

$$g_i(\theta) \leq 0 \; : \quad \alpha_i = 0$$
$$g_i(\theta) > 0 \; : \quad \alpha_i \to +\infty$$

  - Any optimum of the original problem is a saddle point of the new
  - KKT complementary slackness:

$$\alpha_i > 0 \;\Rightarrow\; g_i(\theta) = 0$$

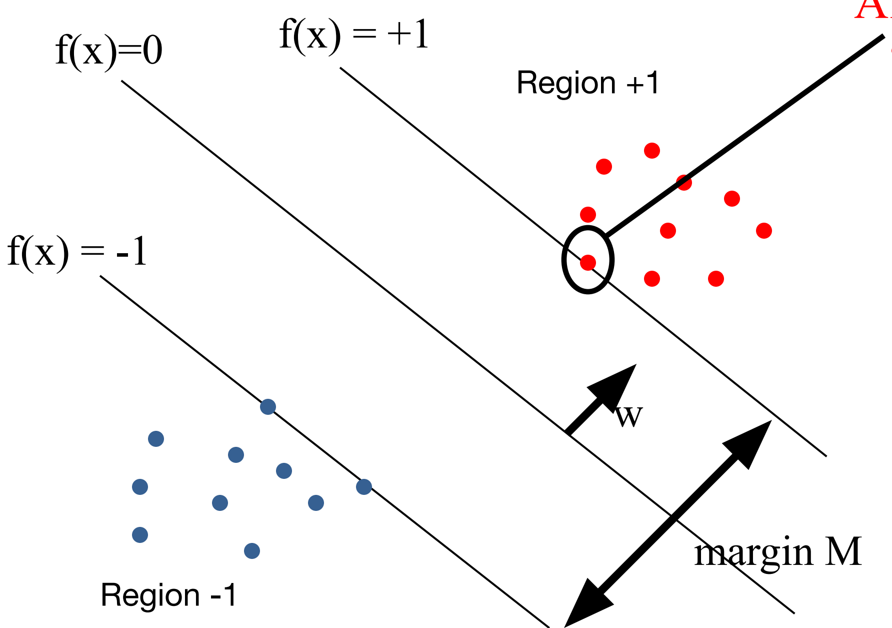
Notes on Lagrangian optimization

- Equivalence if alpha fully optimized
- Simple to initialize to valid point
  - Gi may be unsatisfied => if so, penalty grows, encouraging theta to satisfy
- Visualization; valid region?

Optimization

- Use Lagrange multipliers
  - Enforce inequality constraints

$$w^* = \arg\min_w \max_{\alpha \geq 0} \frac{1}{2} \sum_j w_j^2 + \sum_i \alpha_i (1 - y^{(i)} (w \cdot x^{(i)} + b))$$



Alphas > 0 only on the margin: "support vectors"

Stationary conditions wrt w:

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

and since any support vector has y = wx + b,

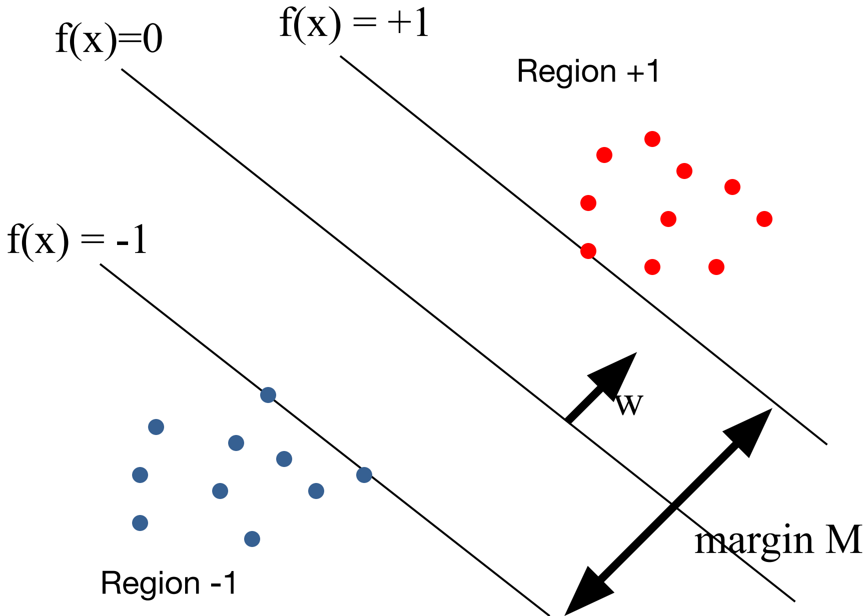
$$b = \frac{1}{Nsv} \sum_{i \in SV} (y^{(i)} - w \cdot x^{(i)})$$

Dual form

- Use Lagrange multipliers
  - Enforce inequality constraints
  - Use solution w* to write solely in terms of alphas:

$$\max_{\alpha \geq 0} \sum_i \left[\alpha_i - \frac{1}{2} \sum_j \alpha_i \alpha_j \, y^{(i)} y^{(j)} \, (x^{(i)} \cdot x^{(j)}) \right]$$

$$\text{s.t.} \quad \sum_i \alpha_i y^{(i)} = 0 \qquad \text{(since derivative wrt b = 0)}$$



Another quadratic program:
optimize m vars with 1+m (simple) constraints
cost function has m^2 dot products

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

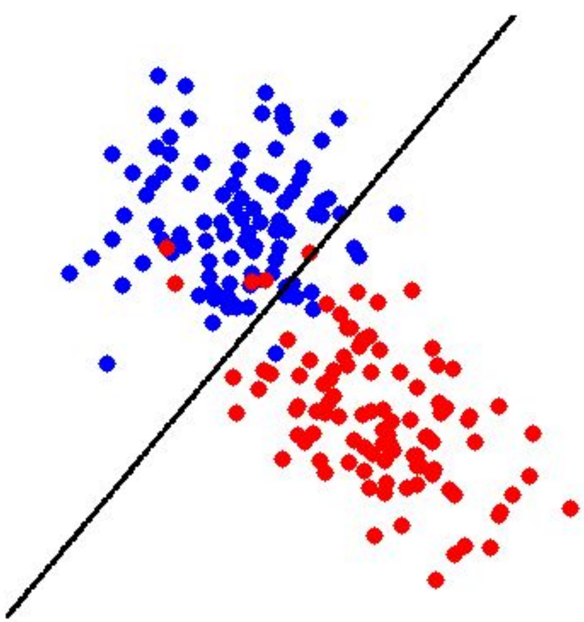
$$b = \frac{1}{Nsv} \sum_{i \in SV} (y^{(i)} - w \cdot x^{(i)})$$

Maximum margin classifier

- What if the data are not linearly separable?
  - Want a large "margin": Want low error:

$$\min_w \sum_j w_j^2 \qquad\qquad \min_w \sum_i J(y^{(i)}\ ,\ w \cdot x^{(i)} + b)$$

  - "Soft margin" : introduce slack variables for violated constraints



$$w^* = \arg\min_{w,\epsilon} \sum_j w_j^2 + R \sum_i \epsilon^{(i)}$$

$s.t$

$$y^{(i)}(\,w^T x^{(i)} + b\,) \geq +1 - \epsilon^{(i)}$$ (violate margin by ^{2})

$$\epsilon^{(i)} \geq 0$$

Assigns "cost" R proportional to distance from margin

Another quadratic program!

Soft margin SVM

- Large margin vs. Slack variables
- R large = hard margin
- R smaller
  - A few wrong predictions; boundary farther from rest

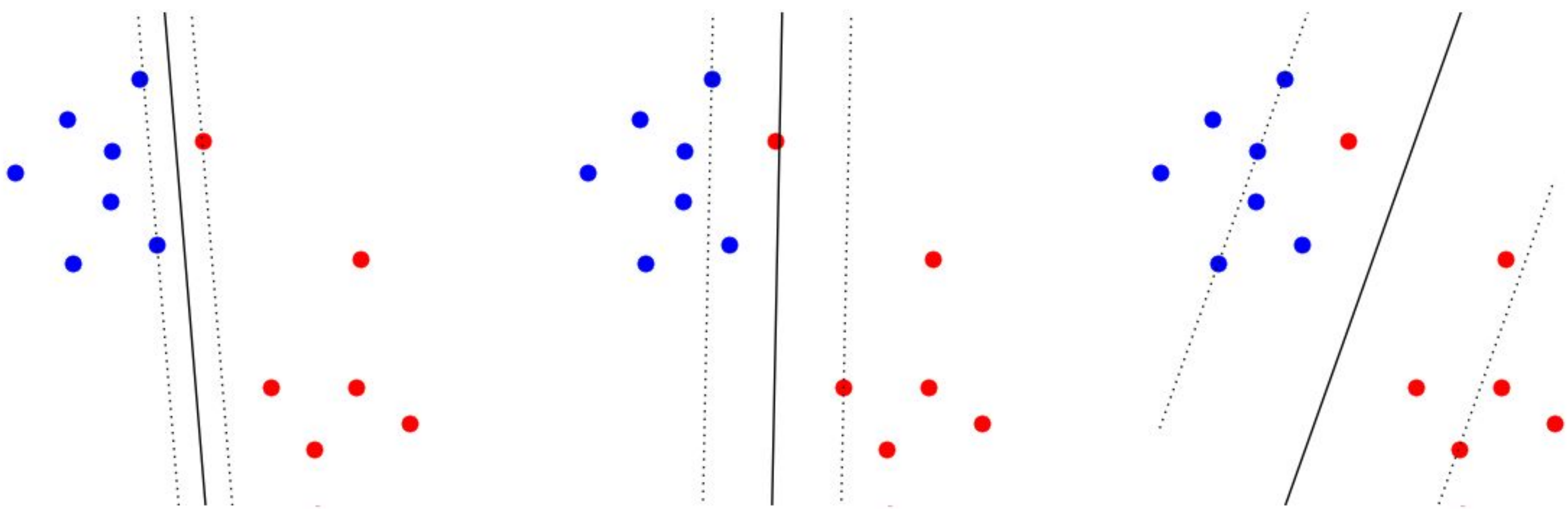
$$w^* = \arg\min_{w,\epsilon} \sum_j w_j^2 + R \sum_i \epsilon^{(i)}$$

$s.t.$

$$y^{(i)}(w^T x^{(i)} + b) \ge +1 - \epsilon^{(i)}$$

$$\epsilon^{(i)} \ge 0$$

$R = R_0$ $\quad$ $R = 10^{-2} R_0$ $\quad$ $R = 10^{-4} R_0$



Maximum margin classifier

- Soft margin optimization:
  - For *any* weights w,

  we can choose ε to satisfy constraints

$$w^* = \arg\min_{w,\epsilon} \sum_j w_j^2 + R \sum_i \epsilon^{(i)}$$

$$y^{(i)} \left(w^T x^{(i)} + b \right) \ge +1 - \epsilon^{(i)}$$

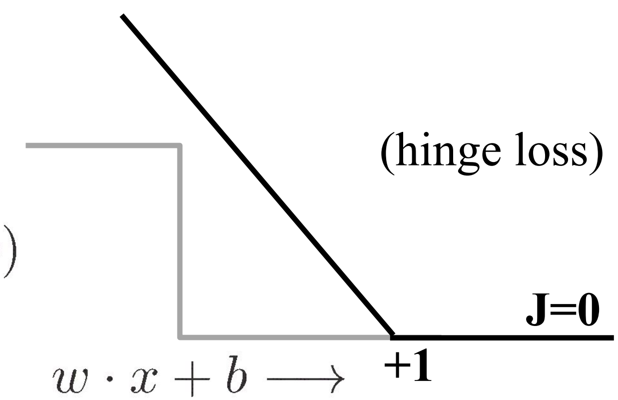
  - Write ε* as a function of w (call this J) and optimize directly

- J = distance from the “correct” place

$$J_i = \max[\, 0 \,,\, 1 - y^{(i)} (w \cdot x^{(i)} + b) \,]$$

$$w^* = \arg\min_{w} \frac{1}{R} \sum_j w_j^2 + \sum_i J_i(y^{(i)} \,,\; w \cdot x^{(i)} + b)$$

(L2 regularization on the weights)



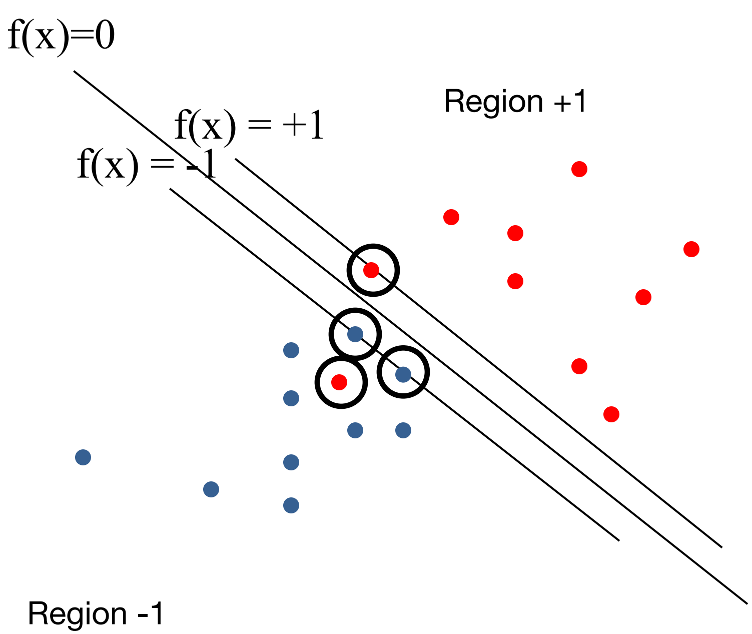
Dual form

- Soft margin dual:

$$\max_{0\leq\alpha\leq R} \sum_i \alpha_i - \frac{1}{2}\sum_j \alpha_i\alpha_j\, y^{(i)}y^{(j)}\, \overbrace{x^{(i)}\cdot x^{(j)}}^{K_{ij}})$$

K_{ij} measures "similarity" of x_i and x_j (their dot product)

$$\text{s.t. } \sum_i \alpha_i y^{(i)} = 0$$



Support vectors now data on or past margin…

Prediction:

$$\hat{y} = w^* \cdot x + b = \sum_i \alpha_i y^{(i)} x^{(i)} \cdot x + b$$

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

$$b = \dots$$

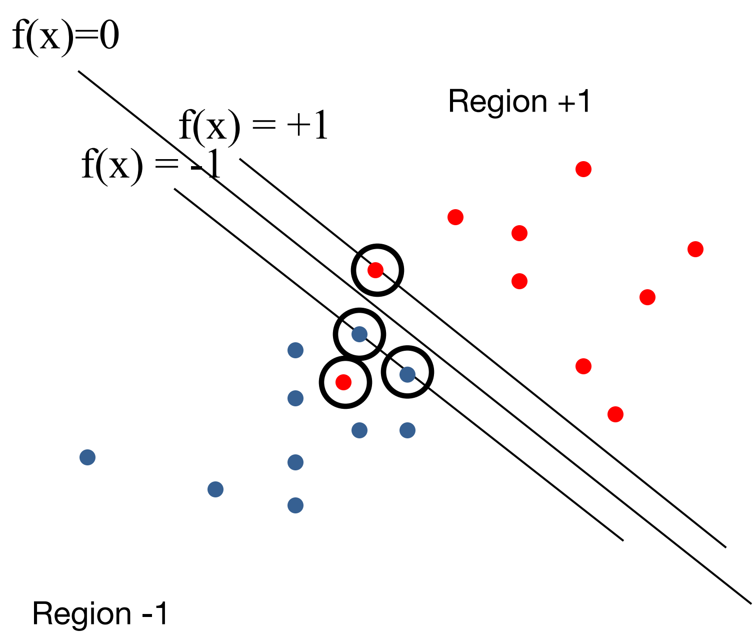
More complicated; can solve e.g. using any $\alpha \in (0,R)$

Support Vectors

The *support vectors* are data points i with non-zero weight α_i:

- Points with minimum margin (on optimized boundary)
- Points which violate margin constraint, but are still correctly classified
- Points which are misclassified

For all other training data, features have *no impact* on learned weight vector



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$$b = \ldots$$

More complicated; can solve e.g. using any α ∈ (0,R)

Multi-class SVMs

- Use standard multi-class linear prediction, 0/1 loss:

$$\hat{y} = f(x;\theta) = \arg\max_y \ \theta \cdot \Phi(x,y)$$

$$\Phi(x,y) = [\ \mathbb{1}[y=0]\,\Phi(x)\ ,\ \mathbb{1}[y=1]\,\Phi(x)\ ,\ \ldots\ ]$$

- Hinge-like loss / slack variable optimization:

$$w^* = \arg\min_{w,b,\epsilon} \sum_j w_j^2 + R \sum_i \epsilon^{(i)}$$

$$w^T \Phi(x^{(i)}, y^{(i)}) - w^T \Phi(x^{(i)}, y) \geq 1 - \epsilon^{(i)} \qquad \forall y \neq y^{(i)}$$

- Can introduce class-specific loss function: $\Delta(y, \hat{y})$

$$w^T \Phi(x^{(i)}, y^{(i)}) - w^T \Phi(x^{(i)}, y) \geq \Delta(y^{(i)}, y) - \epsilon^{(i)} \qquad \forall y \neq y^{(i)}$$

  - Reduces to earlier form for 0/1 loss: $\Delta(y, \hat{y}) = \mathbb{1}[y \neq \hat{y}]$
  - Again, can optimize as QP (e.g., SMO) or hinge-like loss (e.g., SGD)

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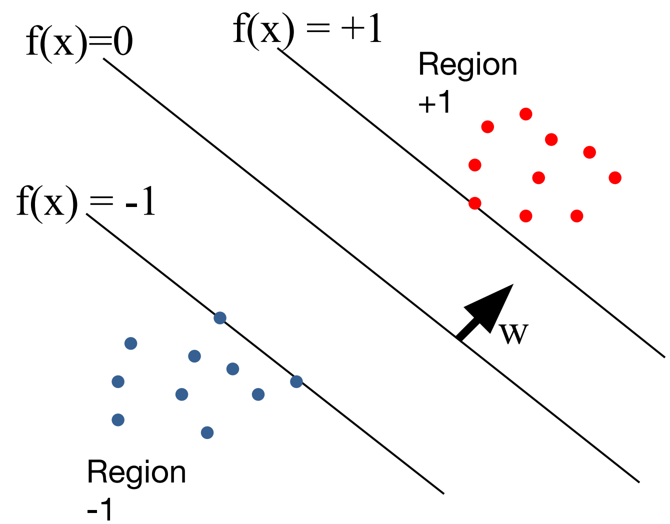
Linear SVMs

- So far, looked at linear SVMs:
  - Expressible as linear weights "w"
  - Linear decision boundary



- Dual optimization for a linear SVM:

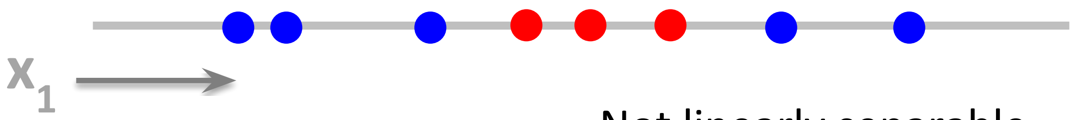
$$\max_{0 \le \alpha \le R} \sum_i \alpha_i - \frac{1}{2} \sum_j \alpha_i \alpha_j \, y^{(i)} y^{(j)} \left(x^{(i)} \cdot x^{(j)} \right) \qquad \text{s.t.} \ \sum_i \alpha_i y^{(i)} = 0$$

- Depend on pairwise dot products:
  - Kij measures "similarity", e.g., 0 if orthogonal $K_{ij} = x^{(i)} \cdot x^{(j)}$

Adding features

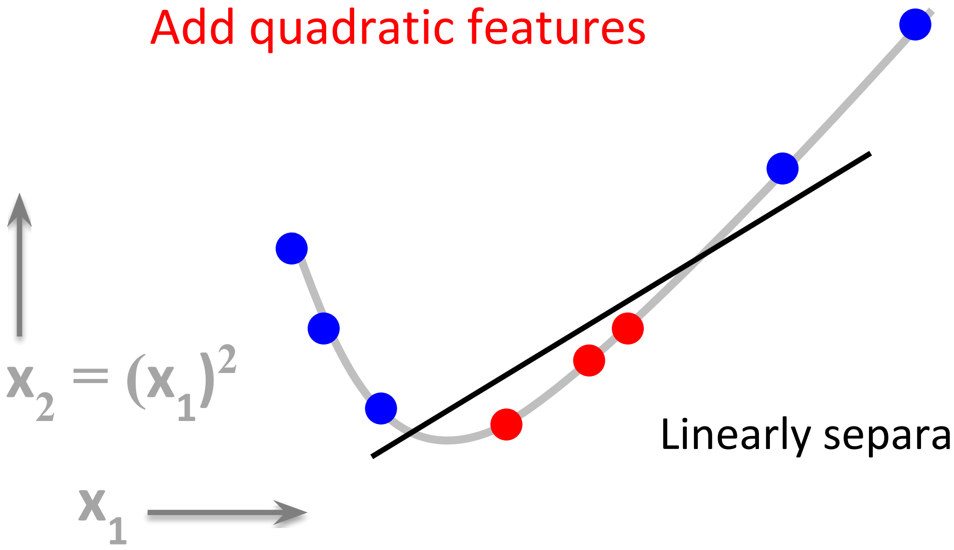
- Linear classifier can't learn some functions

1D example:



Not linearly separable

Add quadratic features



Linearly separable in new features…

Adding features

- Recall: feature function Phi(x)
  - Predict using some transformation of original features

$$\hat{y}(x) = \text{sign}\big[\, w \cdot \Phi(x) + b \,\big]$$

- Dual form of SVM optimization is:

$$\max_{0 \le \alpha \le R} \sum_i \alpha_i - \frac{1}{2} \sum_j \alpha_i \alpha_j \, y^{(i)} y^{(j)} \, \Phi(x^{(i)}) \Phi(x^{(j)})^T \quad \text{s.t.} \; \sum_i \alpha_i y^{(i)} = 0$$

- For example, quadratic (polynomial) features:

$$\Phi(x) = \big(1 \;\; \sqrt{2}x_1 \;\; \sqrt{2}x_2 \;\; \cdots \;\; x_1^2 \;\; x_2^2 \;\; \cdots \;\; \sqrt{2}x_1 x_2 \;\; \sqrt{2}x_1 x_3 \;\; \cdots\big)$$

  - Ignore root-2 scaling for now…
  - Expands “x” to length $O(n^2)$

Implicit features

- Need $\Phi(x^{(i)})\Phi(x^{(j)})^T$

$$\Phi(x) = \left(1 \ \sqrt{2}x_1 \ \sqrt{2}x_2 \ \cdots \ x_1^2 \ x_2^2 \ \cdots \ \sqrt{2}x_1x_2 \ \sqrt{2}x_1x_3 \ \cdots\right)$$

$$\Phi(a) = \left(1 \ \sqrt{2}a_1 \ \sqrt{2}a_2 \ \cdots \ a_1^2 \ a_2^2 \ \cdots \ \sqrt{2}a_1a_2 \ \sqrt{2}a_1a_3 \ \cdots\right)$$

$$\Phi(b) = \left(1 \ \sqrt{2}b_1 \ \sqrt{2}b_2 \ \cdots \ b_1^2 \ b_2^2 \ \cdots \ \sqrt{2}b_1b_2 \ \sqrt{2}b_1b_3 \ \cdots\right)$$

$$\Phi(a)^T\Phi(b) = 1 + \sum_j 2a_jb_j + \sum_j a_j^2b_j^2 + \sum_j \sum_{k>j} 2a_ja_kb_jb_k + \ldots$$

$$= (1 + \sum_j a_jb_j)^2$$

$$= K(a,b)$$

Can evaluate dot product in only O(n) computations!

Mercer Kernels

- If K(x,x') satisfies Mercer's condition:

$$\int_a \int_b K(a,b)\, g(a)\, g(b)\, da\, db \;\geq 0$$

For all datasets X:

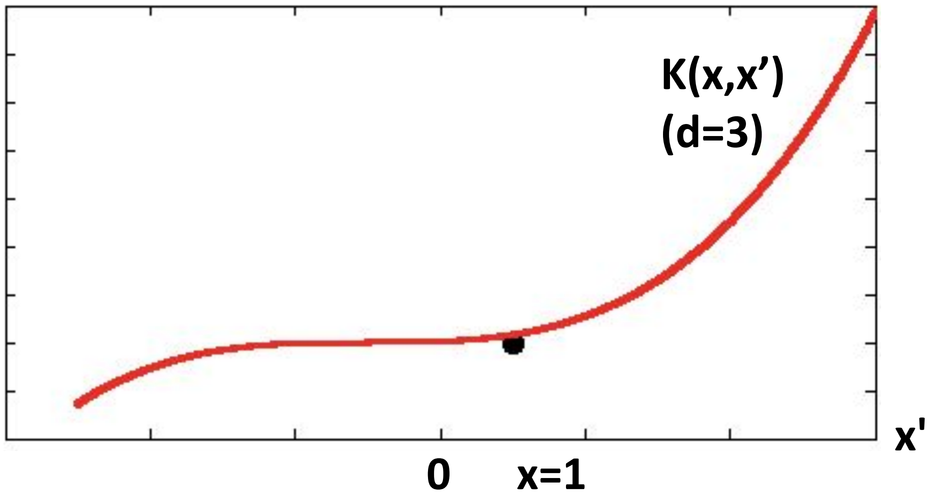
$$g^T \cdot K \cdot g \;\geq 0$$

- Then, $K(a,b) = \Phi(a) \cdot \Phi(b)$ for some $\Phi(x)$

- Notably, Phi may be hard to calculate
  - May even be infinite dimensional!
  - Only matters that K(x,x') is easy to compute:
  - Computation always stays O(m^2)

Common kernel functions

- Some commonly used kernel functions & their shape:
- Polynomial $K(a,b) = (1 + \sum_j a_j b_j)^d$



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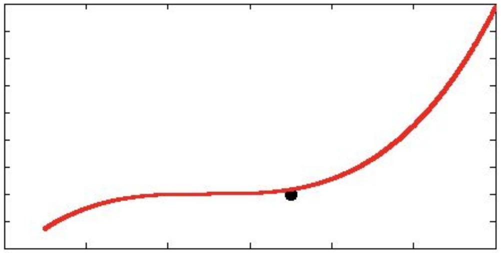
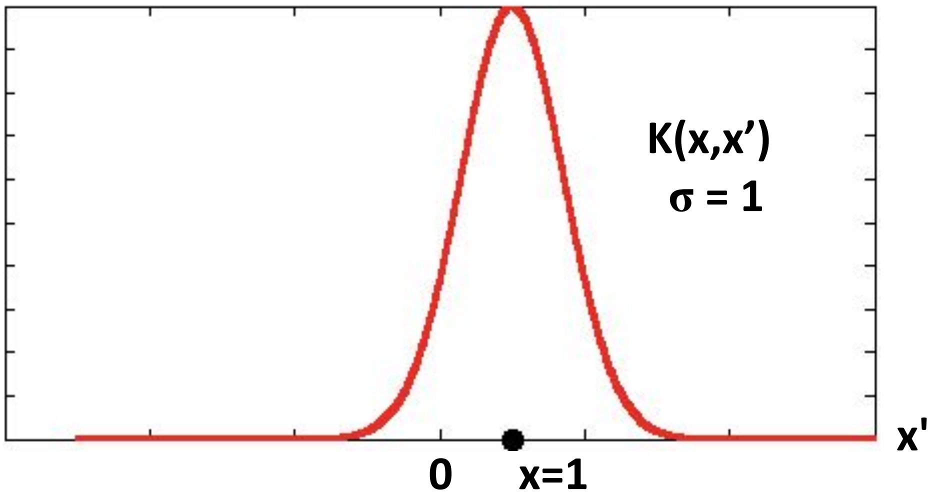


- Radial Basis Functions

$$K(a,b) = \exp(-(a-b)^2/2\sigma^2)$$



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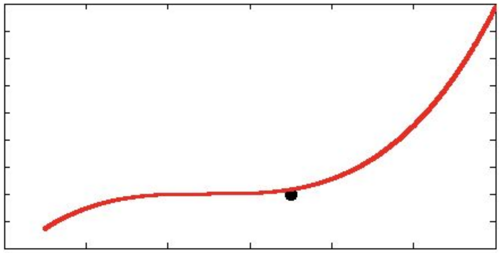

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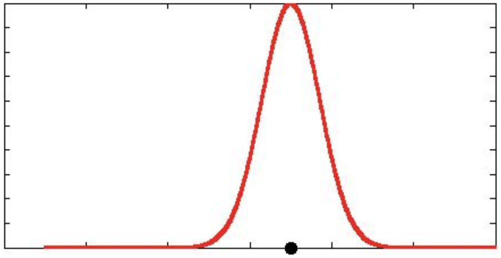
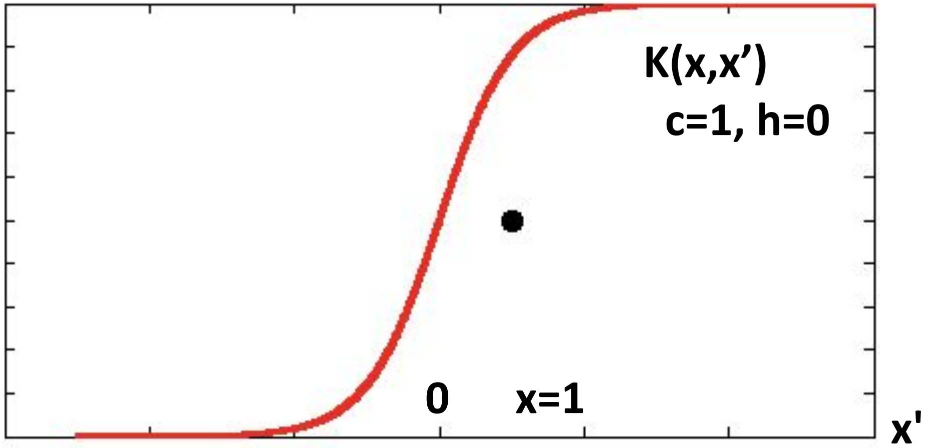


- Saturating, sigmoid-like:

$$K(a,b) = \tanh(ca^T b + h)$$



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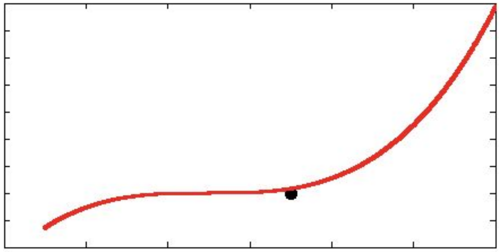
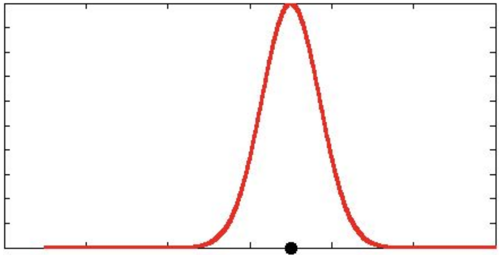
- Some commonly used kernel functions & their shape:
- Polynomial $K(a,b) = (1 + \sum_j a_j b_j)^d$



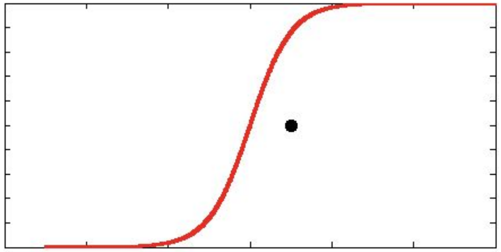
- Radial Basis Functions

$$K(a,b) = \exp(-(a-b)^2/2\sigma^2)$$



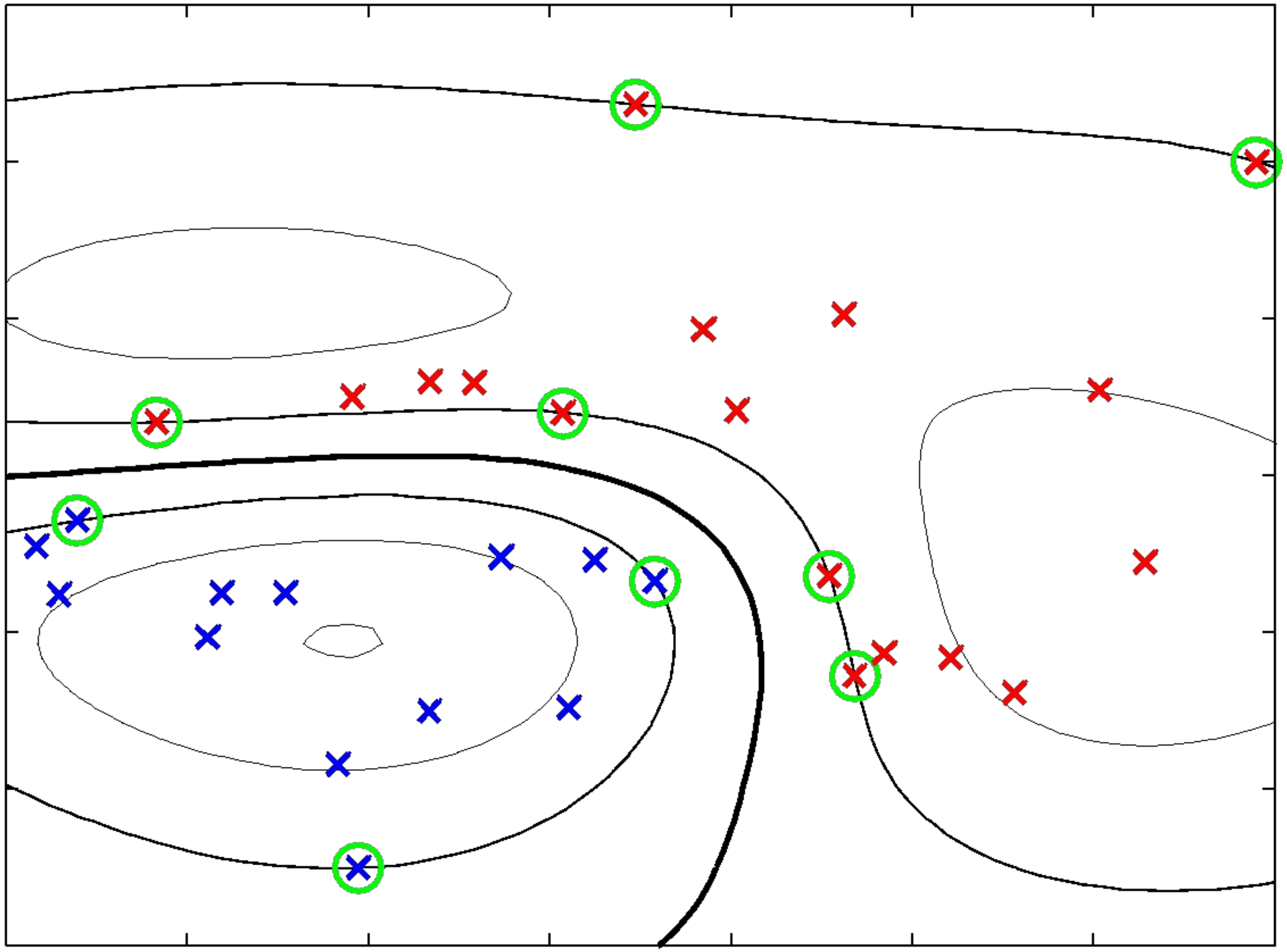
- Saturating, sigmoid-like:

$$K(a,b) = \tanh(ca^T b + h)$$



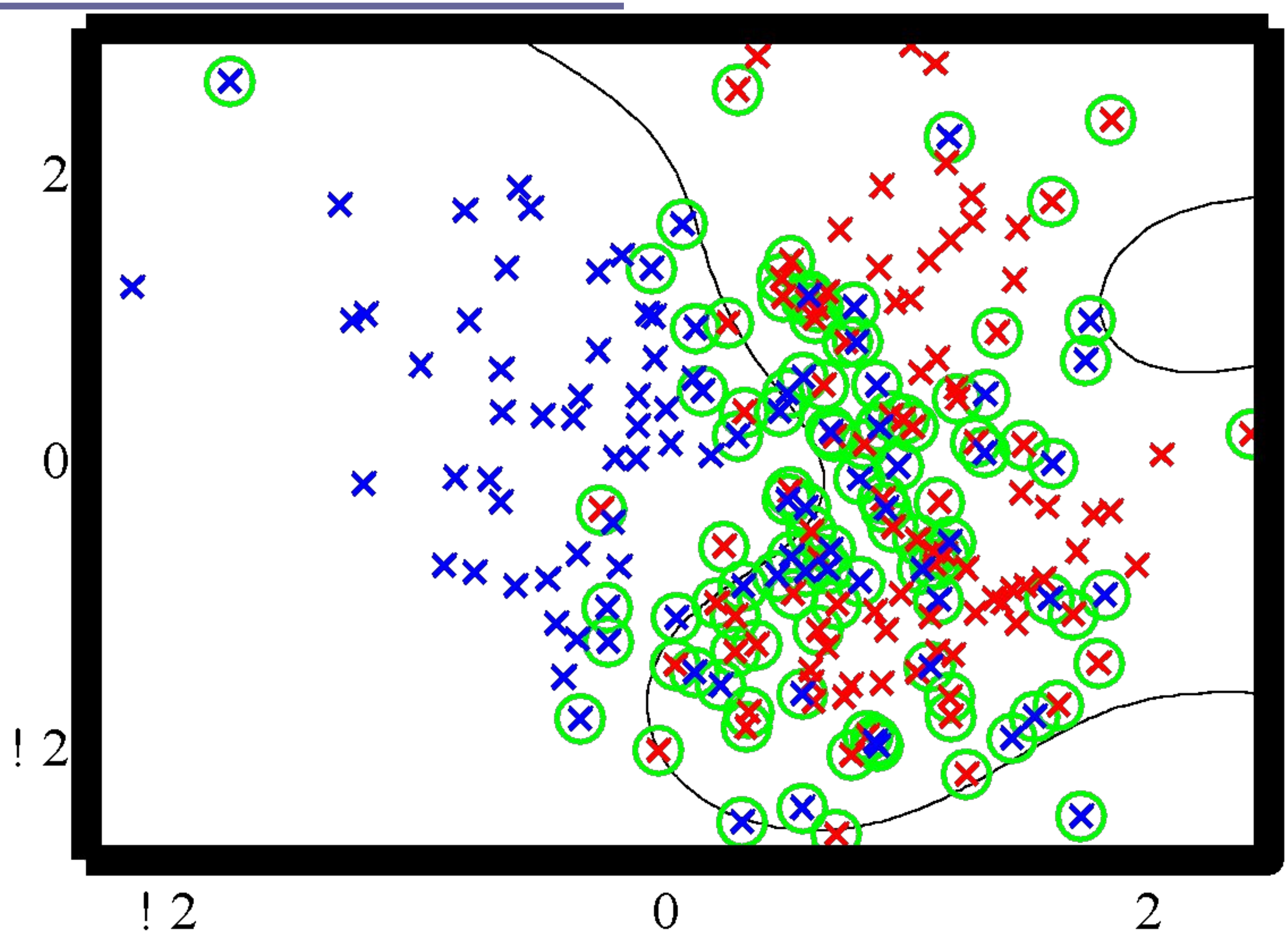
- Many for special data types:
  - String similarity for text, genetics
- In practice, may not even be Mercer kernels…

Support Vectors for Kernel SVMs



Support vectors (green) for data separable by radial basis function kernels, and non-linear margin boundaries

How Many Support Vectors?



Only need to evaluate kernel at support vectors, not all training data. But there may still be a lot of support vectors.

Kernel SVMs

- Linear SVMs
  - Can represent classifier using (w,b) = n+1 parameters
  - Or, represent using support vectors, $x^{(i)}$
- Kernelized?
  - K(x,x') may correspond to high (infinite?) dimensional Phi(x)
  - Typically more efficient to remember the SVs
  - "Instance based" – save data, rather than parameters
- Contrast:
  - Linear SVM: identify *features* with linear relationship to target
  - Kernel SVM: identify *similarity measure* between data

(Sometimes one may be easier; sometimes the other!)

Kernel Least-squares Linear Regression

- Recall L2-regularized linear regression:

$$\theta = y\,X(X^T X + \alpha I)^{-1}$$

$$\Rightarrow \theta\,(X^T X + \alpha I) = y\,X \xrightarrow{\text{Rearranging,}} \alpha\theta = (y - \theta\,X^T)\,X$$

Define:

$$r = \frac{1}{\alpha}(y - \theta\,X^T) \longrightarrow \underline{\theta} = rX$$

$$\alpha\,r = \underline{y} - \underline{\theta}\,\underline{X}^T = \underline{y} - r\,X X^T$$

Gram matrix: m x m,

$$K_{ij} = \langle x^{(i)}, x^{(j)} \rangle$$

Rearrange & solve for r:

$$r = (XX^T + \alpha I)^{-1} y = (K + \alpha I)^{-1} y$$

Linear prediction:

$$\tilde{y} = \langle \theta, \tilde{x} \rangle = rX\,(\tilde{x})^T = \sum_j r_j \langle x^{(j)}, \tilde{x} \rangle = \sum_j r_j K(x^{(j)}, \tilde{x})$$

Now just replace K(x,x') with your desired kernel function!

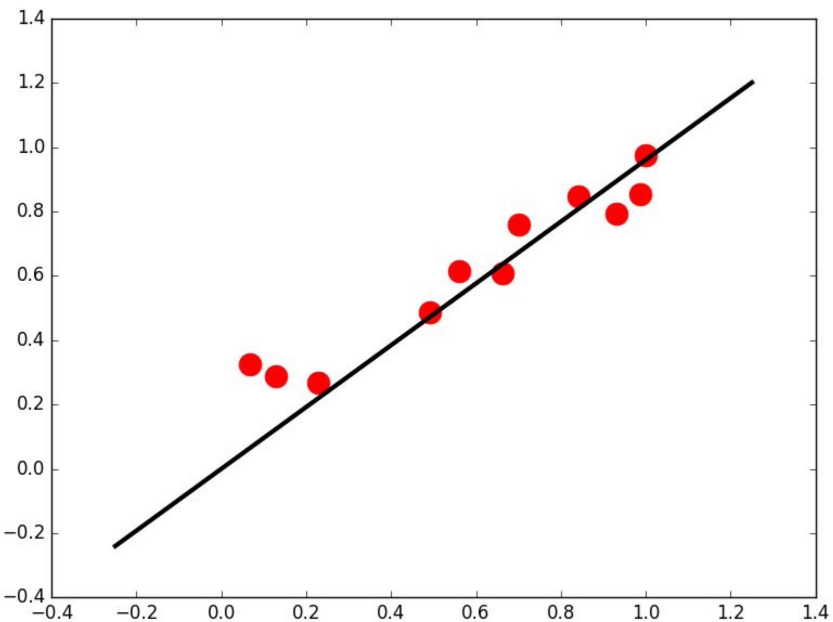
Example: Kernel Linear Regression

- K: MxM

$$r = (K + \alpha I)^{-1} y \qquad \tilde{y} = \sum_j r_j K(x^{(j)}, \tilde{x})$$

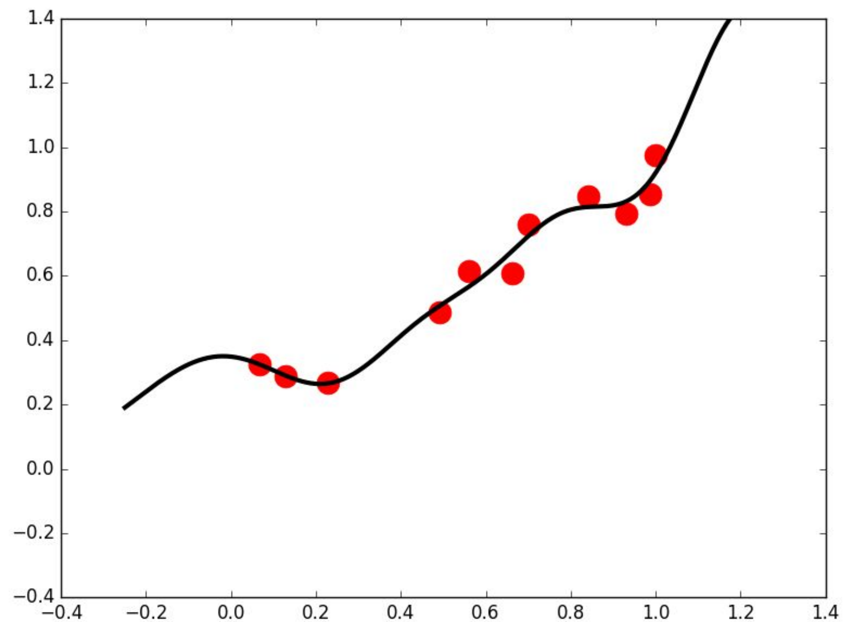
Linear kernel:

$$K(x, x') = x^T \cdot x'$$



Gaussian (RBF) kernel:

$$K(x, x') = \exp(-\gamma(x - x')^2)$$



Summary

- Support vector machines
- “Large margin” for separable data
  - Primal QP: maximize margin subject to linear constraints
  - Lagrangian optimization simplifies constraints
  - Dual QP: m variables; involves m^2 dot product
- “Soft margin” for non-separable data
  - Primal form: regularized hinge loss
  - Dual form: m-dimensional QP
- Kernels
  - Dual form involves only pairwise similarity
  - Mercer kernels: dot products in implicit high-dimensional space