ECE 5984: Introduction to Machine Learning

Topics:
- SVM
  - SVM dual & kernels
  - Multi-class SVMs

Readings: Barber 17.5

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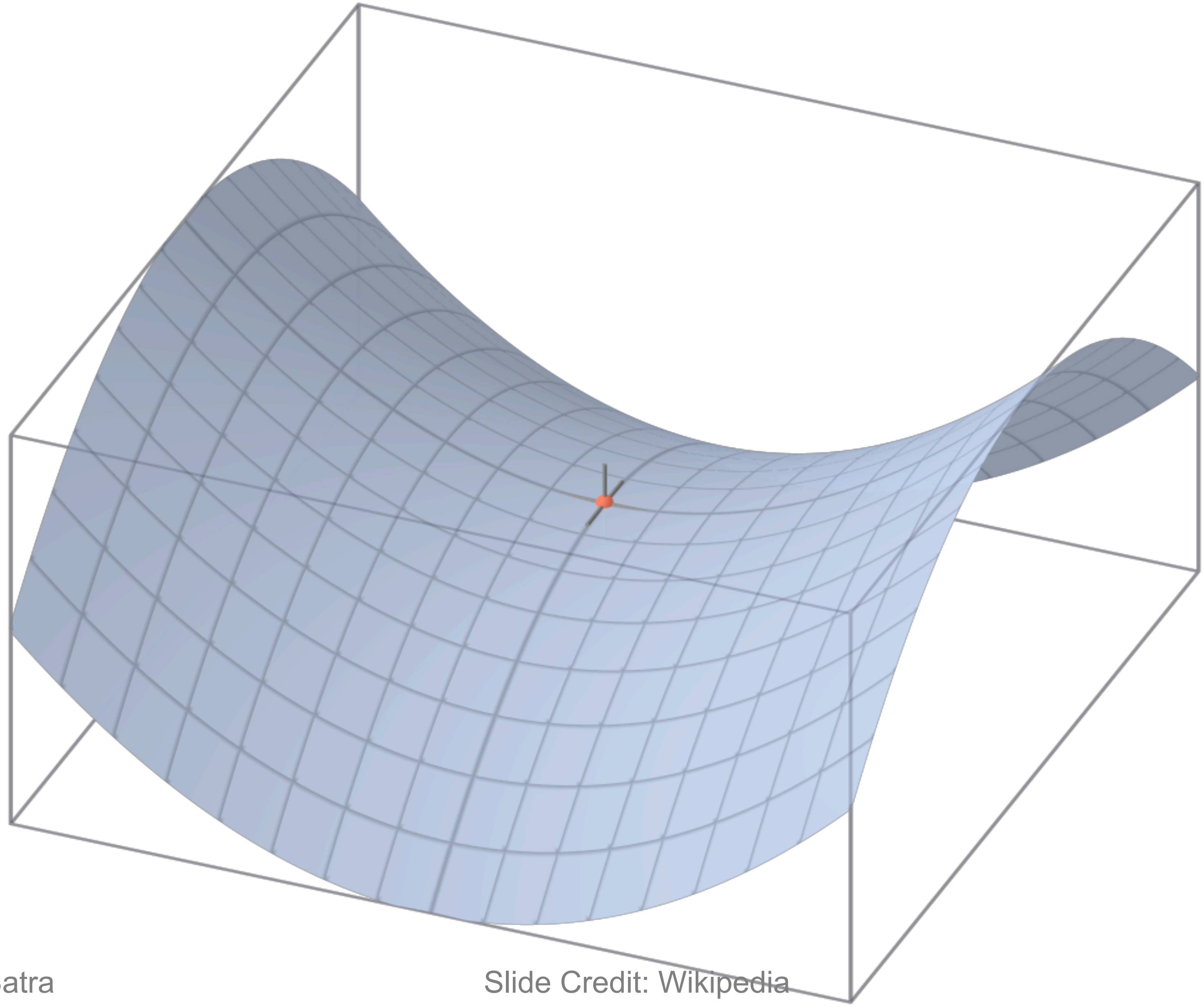
Lagrangian Duality

- On paper

Saddle Points



Dual SVM derivation (1) – the linearly separable case

$$\text{minimize}_{\mathbf{w},b} \quad \frac{1}{2}\mathbf{w}.\mathbf{w}$$

$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq 1, \ \forall j$$

Dual SVM derivation (1) – the linearly separable case

$$L(\mathbf{w},\alpha) = \frac{1}{2}\mathbf{w}.\mathbf{w} - \sum_j \alpha_j \left[\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j - 1\right]$$
$$\alpha_j \geq 0, \ \ \forall j$$

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

Dual SVM formulation – the linearly separable case

$$\text{maximize}_\alpha \quad \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \mathbf{x}_j$$

$$\sum_i \alpha_i y_i = 0$$

$$\alpha_i \geq 0$$

$$\boxed{\begin{array}{l} \mathbf{w} = \sum_i \alpha_i y_i \mathbf{x}_i \\ \\ b = y_k - \mathbf{w}.\mathbf{x}_k \\ \text{for any } k \text{ where } \alpha_k > 0 \end{array}}$$

Dual SVM formulation – the non-separable case

$$\text{minimize}_{\mathbf{w},b} \quad \frac{1}{2}\mathbf{w}.\mathbf{w} + C\sum_j \xi_j$$
$$\left(\mathbf{w}.\mathbf{x}_j + b\right) y_j \geq 1 - \xi_j, \ \forall j$$
$$\xi_j \geq 0, \ \forall j$$

Dual SVM formulation – the non-separable case

$$\text{maximize}_\alpha \quad \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \mathbf{x}_j$$

$$\sum_i \alpha_i y_i = 0$$

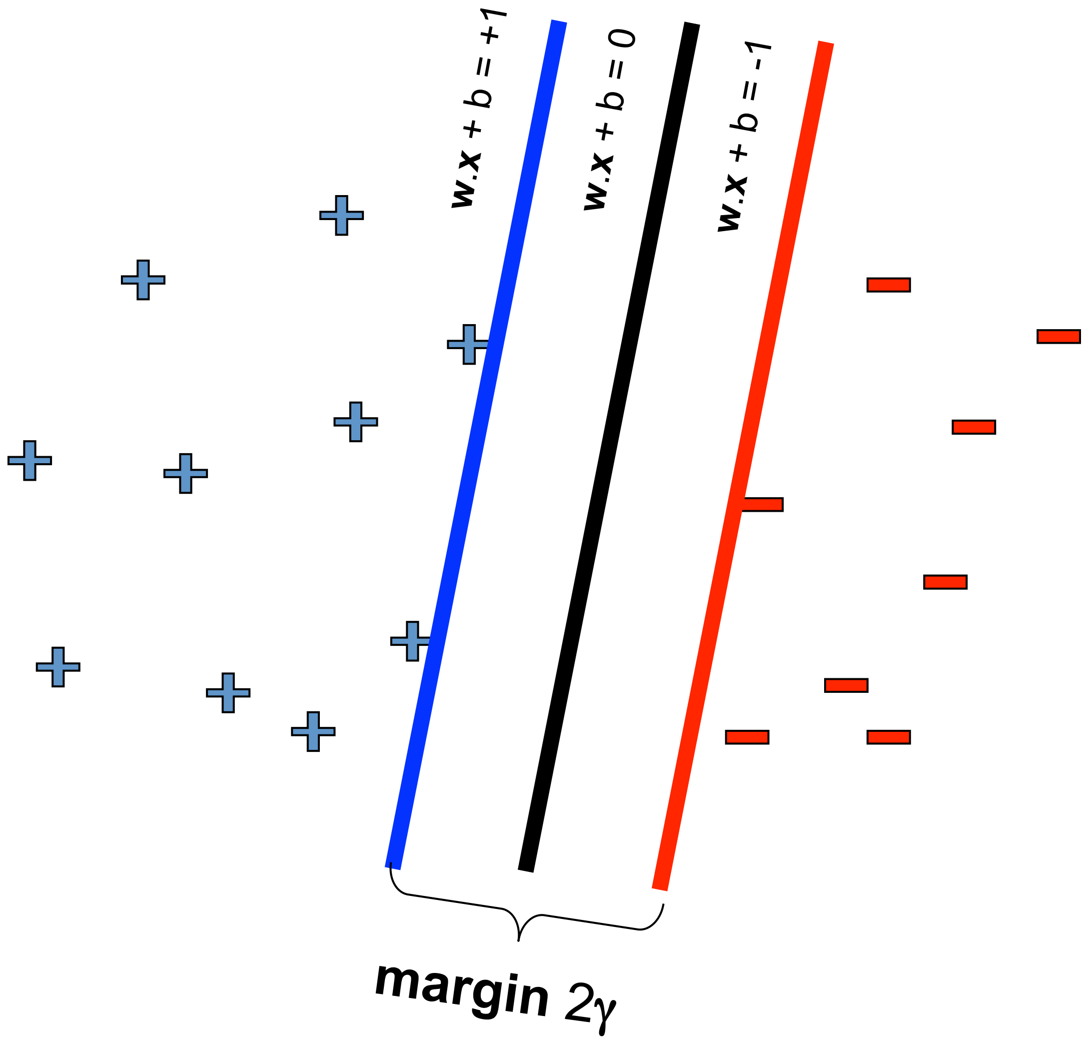
$$C \geq \alpha_i \geq 0$$

$$\boxed{\begin{array}{c} \mathbf{w} = \sum_i \alpha_i y_i \mathbf{x}_i \\ \\ b = y_k - \mathbf{w}.\mathbf{x}_k \\ \text{for any } k \text{ where } C > \alpha_k > 0 \end{array}}$$

Why did we learn about the dual SVM?

- Builds character!
- Exposes structure about the problem
- There are some quadratic programming algorithms that can solve the dual faster than the primal
- The “**kernel trick**”!!!

Dual SVM interpretation: Sparsity



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

Dual formulation only depends on dot-products, not on **w**!

$$\text{maximize}_\alpha \quad \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j \mathbf{x}_i \mathbf{x}_j$$

$$\sum_i \alpha_i y_i = 0$$
$$C \geq \alpha_i \geq 0$$

$$\text{maximize}_\alpha \quad \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

$$K(\mathbf{x}_i, \mathbf{x}_j) = \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_j)$$
$$\sum_i \alpha_i y_i = 0$$
$$C \geq \alpha_i \geq 0$$

Dot-product of polynomials

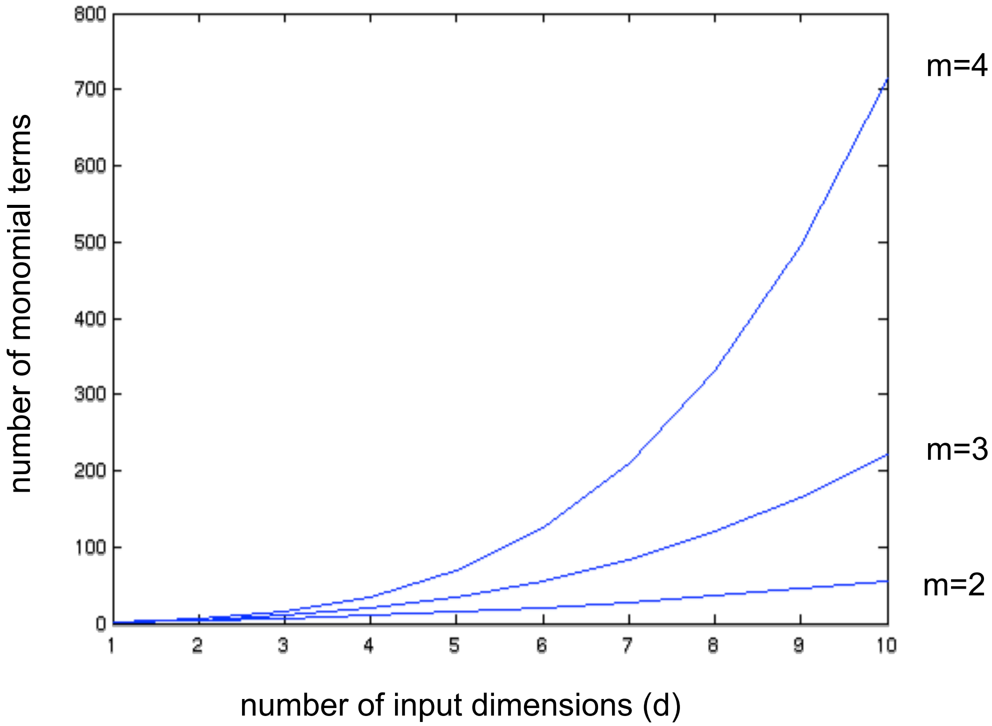
$\Phi(\mathbf{u}) =$ Vector of Monomials of degree m

Higher order polynomials

$$\#\text{terms} = D = \binom{m+d-1}{m} = \frac{(m+d-1)!}{m!(d-1)!}$$

d – input features

m – degree of polynomial



grows fast!

m = 6, d = 100

D = about 1.6 billion terms

Common kernels

- Polynomials of degree d

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

- Polynomials of degree up to d

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

- Gaussian kernel / Radial Basis Function

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

- Sigmoid

$$K(\mathbf{u},\mathbf{v}) = \tanh(\eta\mathbf{u}\cdot\mathbf{v}+\nu)$$

Kernel Demo

- Demo
  - http://www.eee.metu.edu.tr/~alatan/Courses/Demo/AppletSVM.html

What is a kernel?

- k: X x X → R

- Any measure of "similarity" between two inputs

- Mercer Kernel / Positive Semi-Definite Kernel
  - Often just called "kernel"

How to Check if a Function is a Kernel

Problem:

- Checking if a given $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ fulfills the conditions for a kernel is *difficult*:
- We need to prove or disprove

$$\sum_{i,j=1}^{n} t_i k(x_i, x_j) t_j \geq 0.$$

for *any set* $x_1, \ldots, x_n \in \mathcal{X}$ *and any* $t \in \mathbb{R}^n$ *for any* $n \in \mathbb{N}$.

Workaround:

- It is easy to *construct* functions k that are positive definite kernels.

Constructing Kernels

1) We can *construct kernels from scratch*:

- For any $\varphi : \mathcal{X} \to \mathbb{R}^m$, $k(x, x') = \langle \varphi(x), \varphi(x') \rangle_{\mathbb{R}^m}$ is a kernel.

Constructing Kernels

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- For any $\varphi : \mathcal{X} \to \mathbb{R}^m$, $k(x, x') = \langle \varphi(x), \varphi(x') \rangle_{\mathbb{R}^m}$ is a kernel.
- If $d : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a *distance function*, i.e.
  - $d(x, x') \geq 0$ for all $x, x' \in \mathcal{X}$,
  - $d(x, x') = 0$ only for $x = x'$,
  - $d(x, x') = d(x', x)$ for all $x, x' \in \mathcal{X}$,
  - $d(x, x') \leq d(x, x'') + d(x'', x')$ for all $x, x', x'' \in \mathcal{X}$,

  then $k(x, x') := \exp(-d(x, x'))$ is a kernel.

Slide Credit: Blaschko & Lampert

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2) We can *construct kernels from other kernels*:

- if k is a kernel and $\alpha > 0$, then αk and $k + \alpha$ are kernels.
- if k_1, k_2 are kernels, then $k_1 + k_2$ and $k_1 \cdot k_2$ are kernels.

Slide Credit: Blaschko & Lampert

Finally: the "kernel trick"!

$$\text{maximize}_\alpha \quad \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i\alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

$$K(\mathbf{x}_i, \mathbf{x}_j) = \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_j)$$

$$\sum_i \alpha_i y_i = 0$$

$$C \geq \alpha_i \geq 0$$

- Never represent features explicitly
  - Compute dot products in closed form
- Constant-time high-dimensional dot-products for many classes of features
- Very interesting theory – Reproducing Kernel Hilbert Spaces

$$\boxed{\begin{array}{c} \mathbf{w} = \sum_i \alpha_i y_i \mathbf{x}_i \\[2ex] b = y_k - \mathbf{w}.\mathbf{x}_k \\ \text{for any } k \text{ where } C > \alpha_k > 0 \end{array}}$$

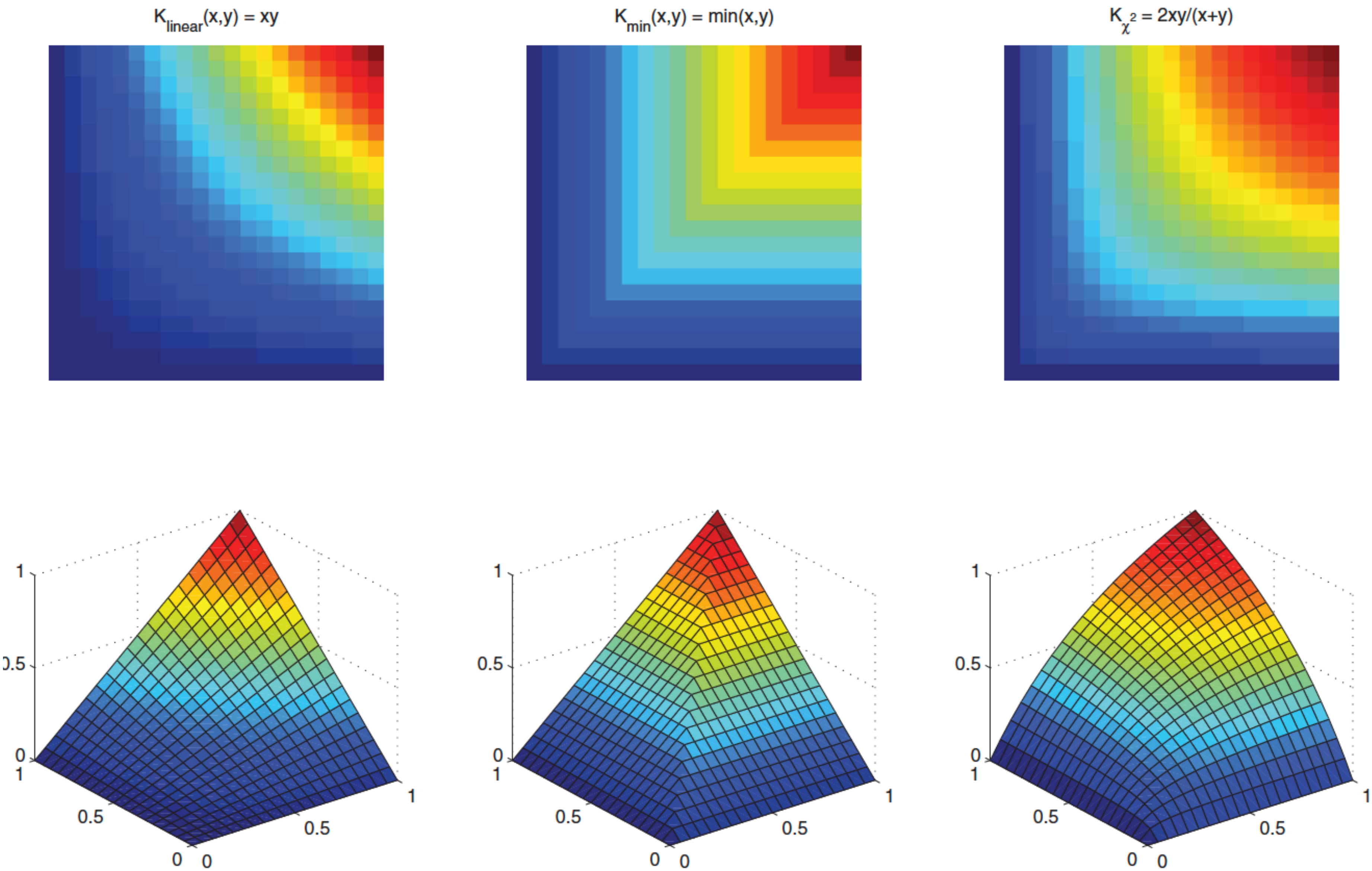
Kernels in Computer Vision

- Features x = histogram (of color, texture, etc)

- Common Kernels
  - Intersection Kernel
  - Chi-square Kernel

$$K_{\text{intersect}}(\boldsymbol{u}, \boldsymbol{v}) = \sum_i \min(u_i, v_i)$$

$$K_{\chi^2}(\boldsymbol{u}, \boldsymbol{v}) = \sum_i \frac{2u_i v_i}{u_i + v_i}$$


K_linear(x,y) = xy
K_min(x,y) = min(x,y)
K_χ2 = 2xy/(x+y)
1
0.5
0
1
0.5
0
0
0.5
1

What about at classification time

- For a new input **x**, if we need to represent Φ(**x**), we are in trouble!
- Recall classifier: sign(**w**.Φ(**x**)+b)

- Using kernels we are fine!

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

Kernels in logistic regression

$$P(Y=1 \mid x, \mathbf{w}) = \frac{1}{1+e^{-(\mathbf{w}\cdot\Phi(\mathbf{x})+b)}}$$

- Define weights in terms of support vectors:

$$\mathbf{w} = \sum_i \alpha_i \Phi(\mathbf{x}_i)$$

$$\begin{aligned} P(Y=1 \mid x, \mathbf{w}) &= \frac{1}{1+e^{-(\sum_i \alpha_i \Phi(\mathbf{x}_i)\cdot\Phi(\mathbf{x})+b)}} \\ &= \frac{1}{1+e^{-(\sum_i \alpha_i K(\mathbf{x},\mathbf{x}_i)+b)}} \end{aligned}$$

- Derive simple gradient descent rule on α_i

Kernels

- Kernel Logistic Regression
- Kernel Least Squares
- Kernel PCA …