15-830 – Machine Learning 3: Classification

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Classification

- **Regression:** predict continuous-valued outputs ($y_i \in \mathbb{R}$)
- **Classification:** predict discrete-valued outputs
  - Common case, binary classification: $y_i \in \{-1, 1\}$

- Binary classification: predictions have yes/no answers
  - Will the peak demand in be higher than 2GW tomorrow?
  - Will a wind turbine operate at max capacity in the next hour?
  - Will this electric line reach its maximum capacity?
  - Is the the device plugged into this outlet a refrigerator?
- Even when predicting a numerical quantity, what we really care about is often the answer to a yes/no question

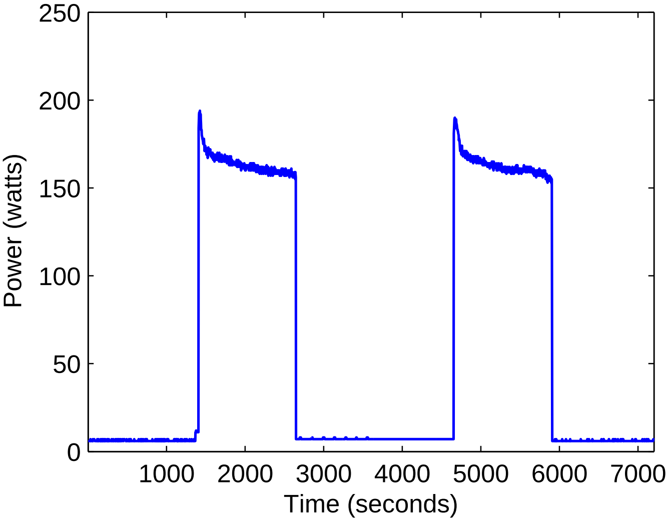
Understanding building energy consumption

Buildings (residential and commercial) account for 71% of electricity consumption [Source: US EIA]

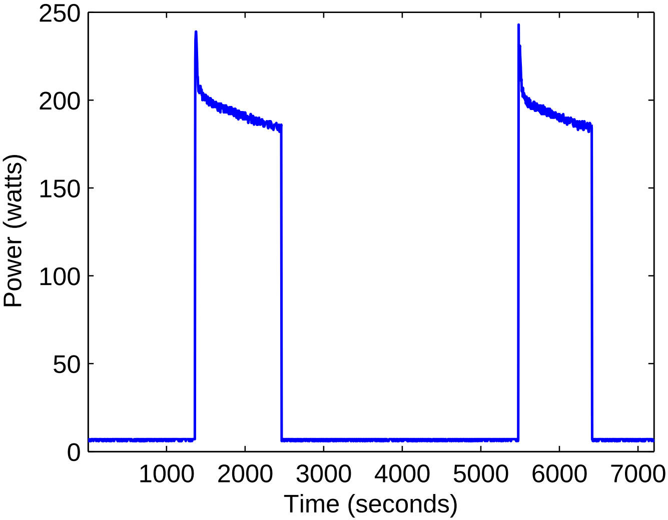
- The task: automatically identify appliances from their (individual) power signals

- Feedback about building energy consumption allows users to make more informed decisions

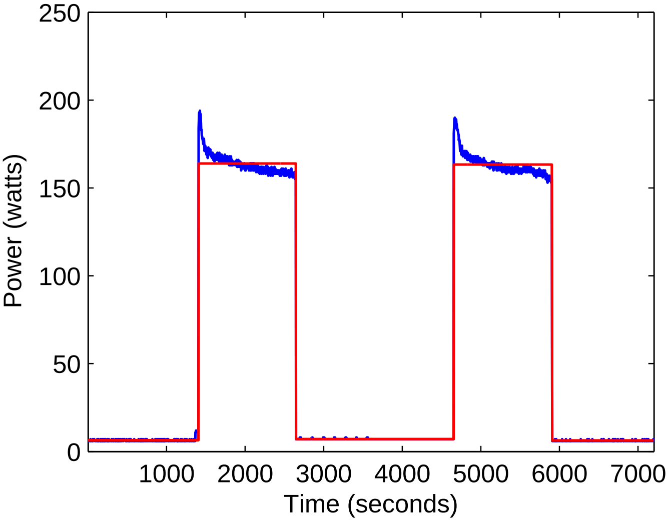
- Modified but similar techniques can be used to identify appliances from just *whole-building* energy signals



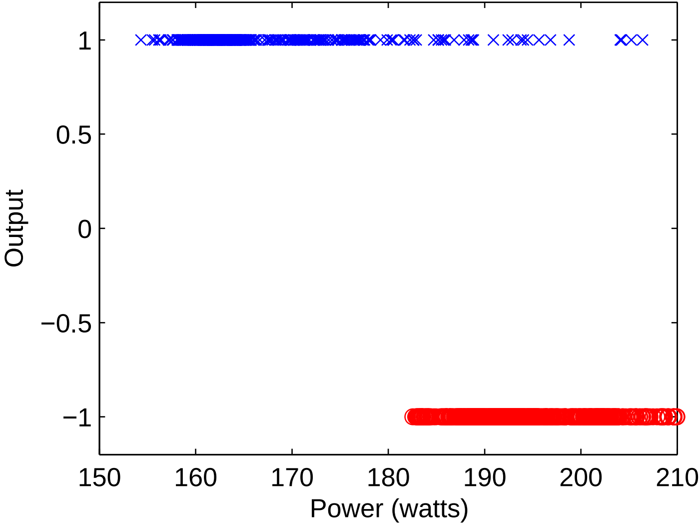
Power signal for refrigerator 1



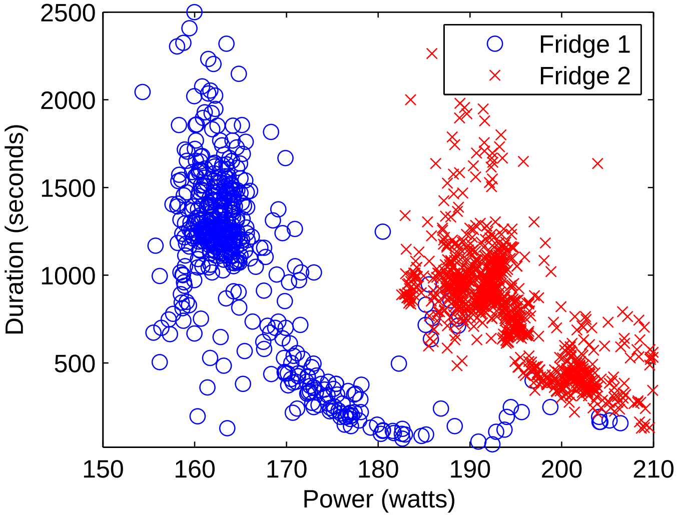
Power signal for refrigerator 2



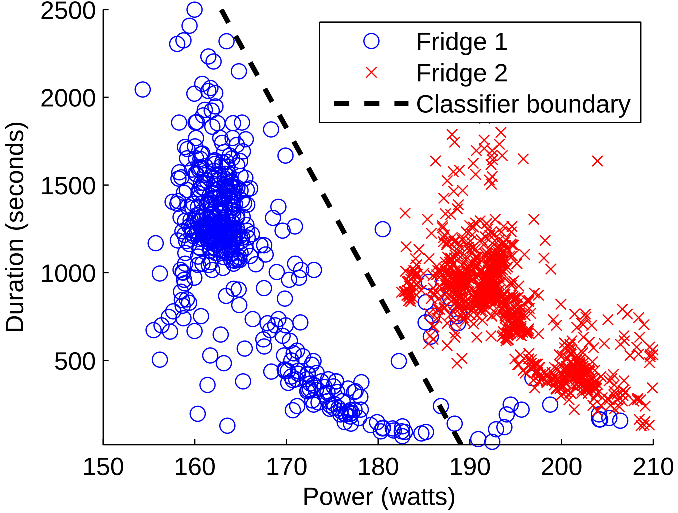
Constructing inputs from power signal



Classifying fridge 1 vs. fridge 2 using power as input



Classifying fridge 1 vs. fridge 2 using power and duration as inputs



Classification boundary from a linear classifier (here, a support vector machine)

Formal problem setting

- **Input**: $x_i \in \mathbb{R}^n, \;\; i = 1, \ldots, m$
- **Output**: $y_i \in \{-1, +1\}$ (binary classification task)
- **Feature mapping**: $\phi : \mathbb{R}^n \to \mathbb{R}^k$
- **Model Parameters**: $\theta \in \mathbb{R}^k$
- **Predicted output**: $\hat{y}_i \in \mathbb{R} = \theta^T \phi(x_i)$
  - Intuition: for $y = +1$ we want $\hat{y} > 0$, for $y = -1$, $\hat{y} < 0$

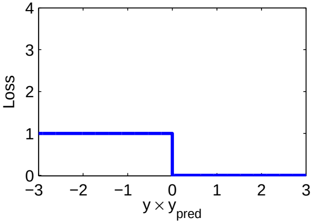
Loss functions

- Loss function: $\ell : \mathbb{R} \times \{-1, +1\} \to \mathbb{R}_+$
  - Again, $\ell(\hat{y}, y)$ measures how "good" the prediction is

- 0-1 Loss

$$\ell(\hat{y}, y) = \begin{cases} 0 & \text{if } y = +1 \text{ and } \hat{y} \geq 0 \text{, or if } y = -1 \text{ and } \hat{y} \leq 0 \\ 1 & \text{otherwise} \end{cases}$$

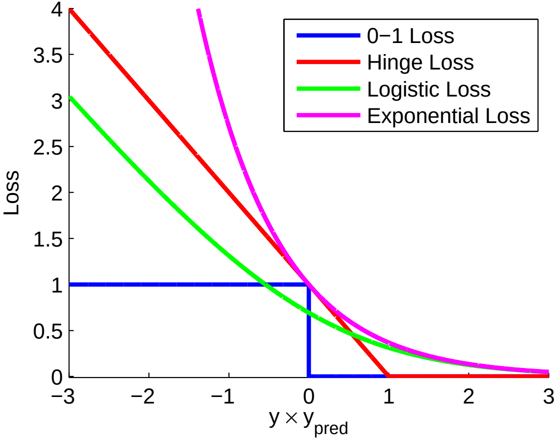
$$= \begin{cases} 0 & y \cdot \hat{y} \geq 0 \\ 1 & y \cdot \hat{y} < 0 \end{cases} \equiv \mathbf{1}\{y \cdot \hat{y} < 0\}$$



- Unfortunately, hard to optimize 0-1 loss

- Many other loss functions are used in practice

$$
\begin{aligned}
\text{Hinge loss:} \quad & \ell(\hat{y}, y) = \max\{1 - y \cdot \hat{y}, 0\} \\
\text{Squared hinge loss:} \quad & \ell(\hat{y}, y) = \max\{1 - y \cdot \hat{y}, 0\}^2 \\
\text{Logistic loss:} \quad & \ell(\hat{y}, y) = \log(1 + e^{-y \cdot \hat{y}}) \\
\text{Exponential loss:} \quad & \ell(\hat{y}, y) = e^{-y \cdot \hat{y}}
\end{aligned}
$$



Common loss functions for classification

Some typical classification algorithms

- Logistic Regression: minimize logistic loss

$$\underset{\theta}{\text{minimize}} \ \sum_{i=1}^{m} \log\left(1 + \exp\left(-y_i \cdot \theta^T \phi(x_i)\right)\right)$$

  – Probabilistic interpretation: $p(y_i = +1|x_i) = \frac{1}{1+\exp(-\theta^T \phi(x_i))}$

- Support vector machine (SVM): minimize (regularized) hinge loss

$$\underset{\theta}{\text{minimize}} \ \sum_{i=1}^{m} \max\left\{0, 1 - y_i \cdot \theta^T \phi(x_i)\right\} + \lambda\|\theta\|_2^2$$

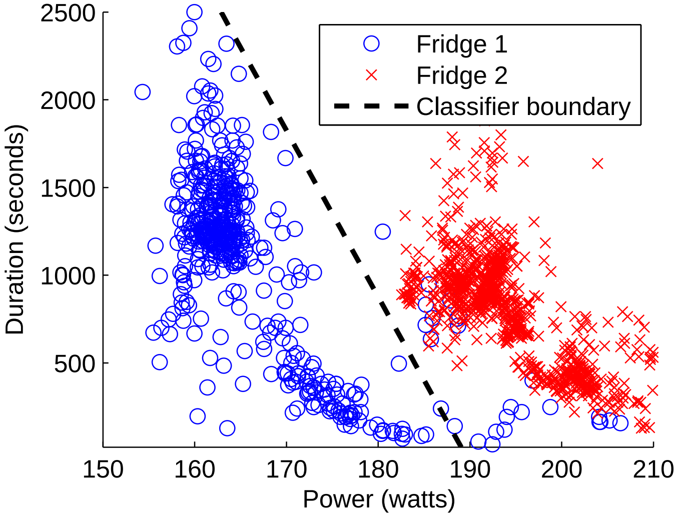
  – If you've seen SVMs before, you may have seen them described geometrically in terms of maximizing the margin of the linear classifier; that formulation is equivalent to the above

- YALMIP code for logistic regression

```
theta = sdpvar(n,1);
solvesdp([], sum(log(1+exp(-y.*(Phi*theta)))));
```

- YALMIP code for SVM

```
theta = sdpvar(n,1);
solvesdp([], sum(max(0,1-y.*(Phi*theta))) + ...
               lambda*norm(theta)^2);
```



Classification boundary from a support vector machine

Optimizing loss functions in classification

- YALMIP is great for rapid prototyping, and medium-size problems

- For larger problems, we might prefer specialized solution methods, like we used for least-squares

- Logistic regression:

$$J(\theta) = \sum_{i=1}^{m} \log\left(1 + \exp\left(-y_i \cdot \theta^T \phi(x_i)\right)\right)$$

  – Differentiable, but cannot analytically solve for $\nabla_\theta J(\theta) = 0$

Newton's method

- Newton's method is a *root-finding* algorithm
  - i.e., for some vector-input, vector output function $f : \mathbb{R}^n \to \mathbb{R}^n$, it finds $z \in \mathbb{R}^n$ such that $f(z) = 0$
- 1D case: $f : \mathbb{R} \to \mathbb{R}$
  - Given some initial z, repeat $z \leftarrow z - f(z)/f'(z)$;

- To extend to the multi-variate case, for a function $f : \mathbb{R}^n \to \mathbb{R}^m$ we'll define the *Jacobian* $D_z f(z)$,

$$D_z f(z) \in \mathbb{R}^{m \times n} = \begin{bmatrix} \frac{\partial f_1(z)}{\partial z_1} & \cdots & \frac{\partial f_1(z)}{\partial z_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m(z)}{\partial z_1} & \cdots & \frac{\partial f_m(z)}{\partial z_n} \end{bmatrix}$$

- Jacobian is like the gradient, but also defined for vector-valued functions
  - For scalar valued functions, $D_z f(z) \in \mathbb{R}^{1 \times n} = (\nabla_z f(z))^T$

- Multi-variate Newton's method: for $f : \mathbb{R}^n \to \mathbb{R}^n$

$$\text{Repeat: } z \leftarrow z - (D_z f(z))^{-1} f(z)$$

- Newton's method applied to optimization: apply Newton's method to find z such that $\nabla_z f(z) = 0$

- The *Hessian* is a matrix of second derivatives of a real-valued function $f : \mathbb{R}^n \to \mathbb{R}$

$$\nabla_z^2 f(z) \in \mathbb{R}^{n \times n} = \begin{bmatrix} \frac{\partial^2 f(z)}{\partial z_1^2} & \cdots & \frac{\partial^2 f(z)}{\partial z_1 \partial z_n} \\ \vdots & \ddots & \vdots \\ \frac{\partial^2 f(z)}{\partial z_n \partial z_1} & \cdots & \frac{\partial^2 f(z)}{\partial z_n^2} \end{bmatrix}$$

$$= D_z(\nabla_z f(z)) \text{ (Jacobian of the gradient)}$$

- Newton's method update:

$$\text{Repeat: } z \leftarrow z - (\nabla_z^2 f(z))^{-1} \nabla_z f(z)$$

- Logistic regression:

$$J(\theta) = \sum_{i=1}^{m} \log(1 + \exp(-y_i \cdot \theta^T \phi(x_i)))$$

- Gradient and Hessian given by:

$$\nabla_\theta J(\theta) = -\Phi^T Z y$$
$$\nabla_\theta^2 J(\theta) = \Phi^T Z (I - Z) \Phi$$

where

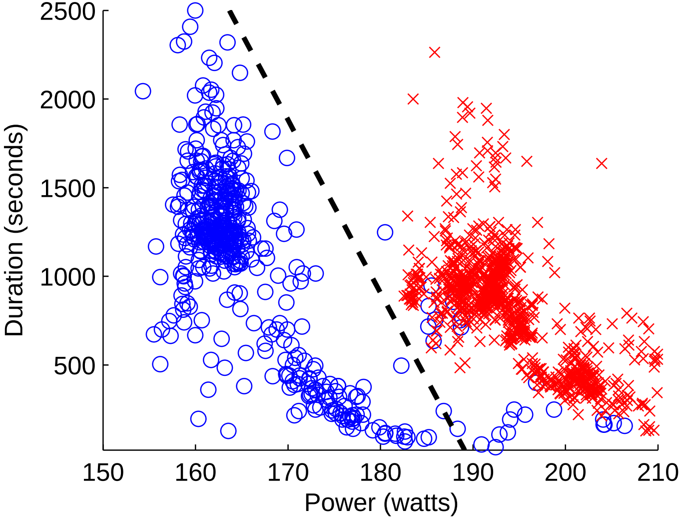
$$Z \in \mathbb{R}^{m \times m} \text{diagonal}, \quad Z_{ii} = \frac{1}{1 + \exp(y_i \cdot \theta^T \phi(x_i))}$$

- MATLAB code for logistic regression

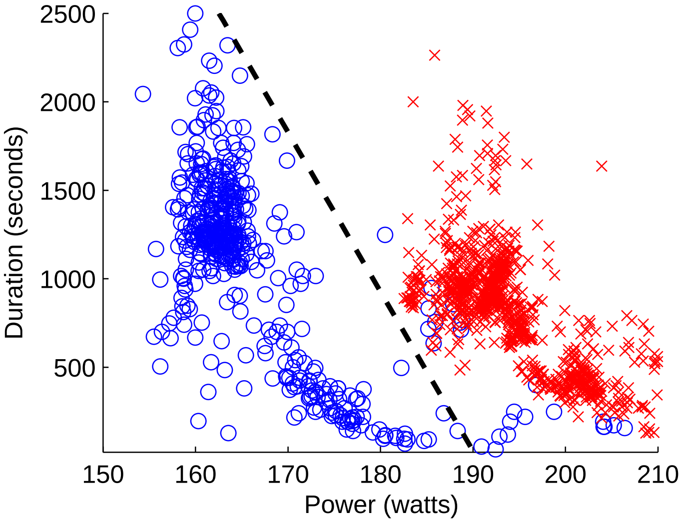
```
function theta = logreg(Phi,y)
k = size(Phi,2);
theta = zeros(k,1);
g = 1;

while (norm(g) > 1e-10)
  z = 1./(1 + exp(y.*(Phi*theta)));
  g = -Phi'*(z.*y);
  H = Phi'*diag(z.*(1-z))*Phi;
  theta = theta - H \ g;
end
```

- YALMIP code: 20.9 seconds, logreg.m: 0.016 seconds ($m = 300$, $n = 3$)

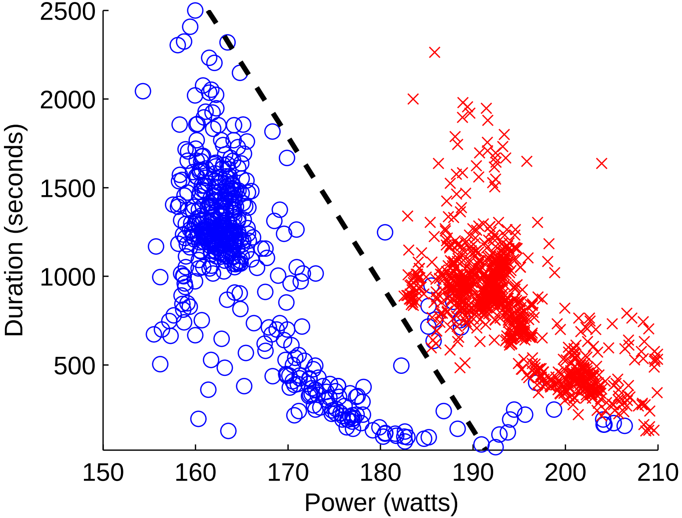
- SVMs are a bit harder to optimize with custom routines; lots of free libraries available (`libsvm`, `svm-light`)



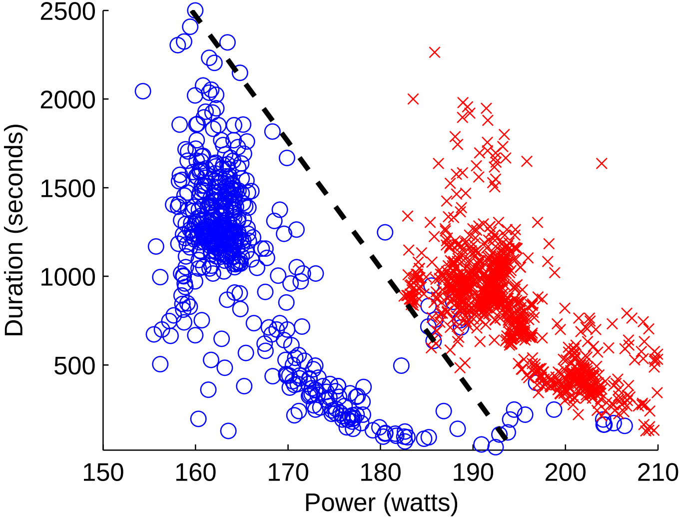
Newton's method, iteration 1



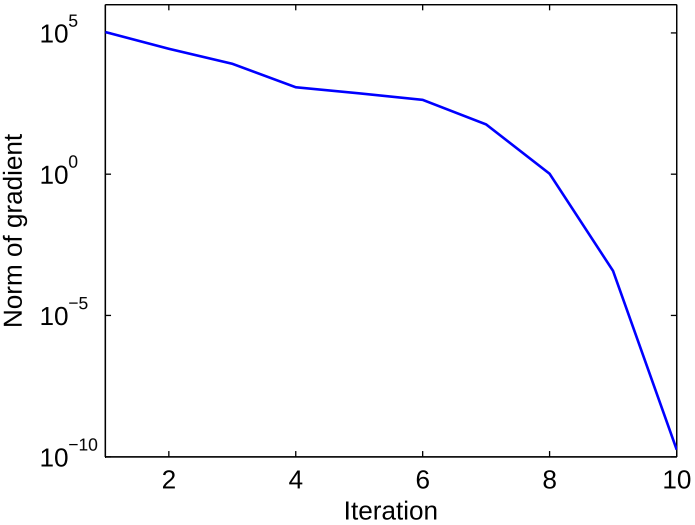
Newton's method, iteration 2



Newton's method, iteration 3



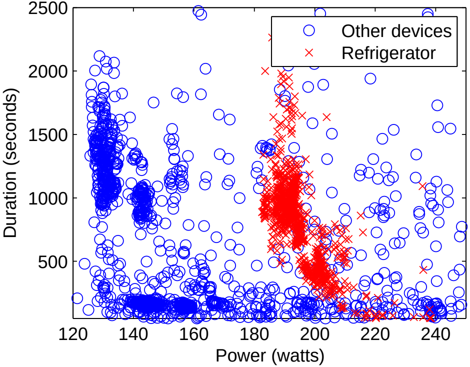
Newton's method, iteration 10



Progress of Newton's method

Non-linear classification

- Same idea as for linear regression: non-linear features, either explicit or using kernels



Classifying refrigerator vs. all other devices

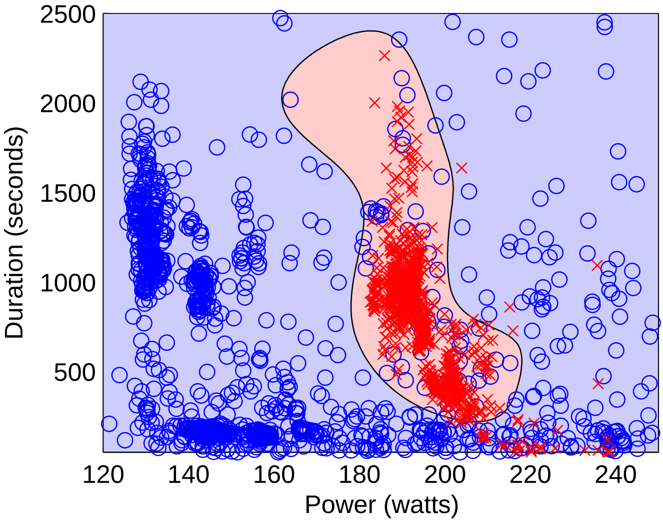
- Key component of kernels is still just the replacement

$$\theta = \sum_{j=1}^{m} \alpha_j \phi(x_j)$$

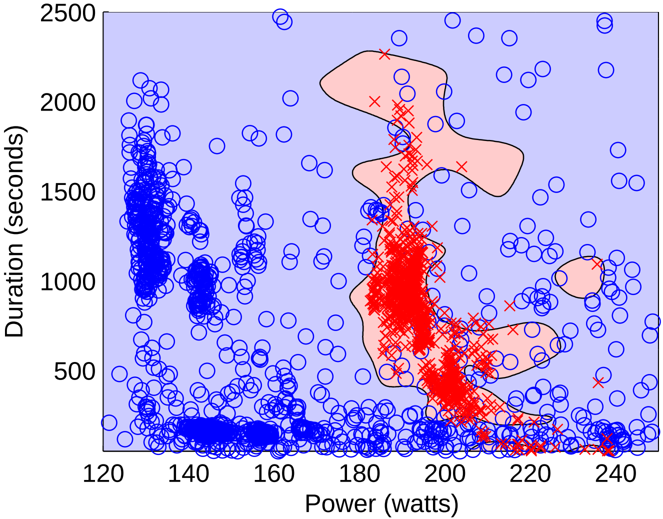
- YALMIP code for kernelized SVM:

```
K = (X*X' + 1).^d; % polynomial kernel
K = exp(-sqdist(X',X')/(2*sig^2)); % Gaussian kernel

alpha = sdpvar(m,1);
solvesdp([], lambda*alpha'*K*alpha + ...
         sum(max(1 - y.*(K*alpha), 0)));
```

- Can derive Newton's method for kernelized formulation as well



Kernelized SVM, Gaussian kernel



Kernelized SVM, Gassian kernel (smaller bandwidth)