Frontiers of Machine Learning

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Aims:

The lectures are intended to give a personal perspective on machine learning and pattern analysis and current frontiers. We will cover:

- What is Pattern Analysis?
- Example of linear pattern functions
- Non-linearity though the kernel approach
- Approaches to deeper learning and complex applications

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Pattern Analysis

- Data can exhibit regularities that may not be immediately apparent
  - exact patterns – eg motions of planets
  - complex patterns – eg genes in DNA
  - probabilistic patterns – eg market research
- Detecting patterns makes it possible to understand and/or exploit the regularities to make predictions
- Pattern analysis is the study of automatic detection of patterns in data

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Defining patterns

- Exact patterns: non-trivial function f such that

$$f(\mathbf{x}) = 0 \quad \text{for all } \mathbf{x}$$

- Approximate patterns: f such that

$$f(\mathbf{x}) \approx 0 \quad \text{for all } \mathbf{x}$$

- Statistical patterns: f such that

$$\mathbb{E}_{\mathbf{x}\sim\mathcal{D}}[f(\mathbf{x})] \approx 0$$

where $\mathcal{D}$ is the distribution generating $\mathbf{x}$.

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Pattern analysis algorithms

We would like algorithms to be:

- Computationally efficient – running time polynomial in the size of the data – often needs to be of a low degree
- Robust – able to handle noisy data, eg examples misclassified, noisy sensors or outputs only to a certain accuracy
- Statistical stability – able to distinguish between chance patterns and those characteristic of the underlying source of the data

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Brief Historical Perspective

- Machine learning using neural like structures first considered seriously in 1960s with such systems as the Perceptron
  - Linear patterns
  - Simple learning algorithm
  - shown to be limited in complexity
- Resurrection of ideas in more powerful multi-layer perceptrons in 1980s
  - networks of perceptrons with continuous activation functions
  - very slow learning
  - no statistical analysis

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Kernel methods

Kernel methods (re)introduced in 1990s with Support Vector Machines

- Linear functions but in high dimensional spaces equivalent to non-linear functions in the input space
- Statistical analysis showing large margin can overcome curse of dimensionality
- Extensions rapidly introduced for many other tasks other than classification

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Kernel methods approach

- Data embedded into a Euclidean feature space
- Linear relations are sought among the images of the data
- Algorithms implemented so that only require inner products between vectors
- Embedding designed so that inner products of images of two points can be computed directly by an efficient 'short-cut' known as the kernel.

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Worked example: Ridge Regression

Consider the problem of finding a homogeneous real-valued linear function

$$g(\mathbf{x}) = \langle \mathbf{w}, \mathbf{x} \rangle = \mathbf{x}'\mathbf{w} = \sum_{i=1}^{n} w_i x_i,$$

that best interpolates a given training set

$$S = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$$

of points $\mathbf{x}_i$ from $X \subseteq \mathbb{R}^n$ with corresponding labels y_i in $Y \subseteq \mathbb{R}$.

Possible pattern function

- Measures discrepancy between function output and correct output – squared to ensure always positive:

$$f_g((\mathbf{x}, y)) = (g(\mathbf{x}) - y)^2$$

Note that the pattern function f_g is not itself a linear function, but a simple functional of the linear functions g.

- We introduce notation: matrix $\mathbf{X}$ has rows the m examples of S. Hence we can write

$$\xi = \mathbf{y} - \mathbf{X}\mathbf{w}$$

for the vector of differences between $g(\mathbf{x}_i)$ and y_i.

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Optimising the choice of g

Need to ensure flexibility of g is controlled – controlling the norm of $\mathbf{w}$ proves effective:

$$\min_{\mathbf{w}} \mathcal{L}_\lambda(\mathbf{w}, S) = \min_{\mathbf{w}} \lambda \|\mathbf{w}\|^2 + \|\xi\|^2,$$

where we can compute

$$\begin{aligned} \|\xi\|^2 &= \langle \mathbf{y} - \mathbf{X}\mathbf{w}, \mathbf{y} - \mathbf{X}\mathbf{w} \rangle \\ &= \mathbf{y}'\mathbf{y} - 2\mathbf{w}'\mathbf{X}'\mathbf{y} + \mathbf{w}'\mathbf{X}'\mathbf{X}\mathbf{w} \end{aligned}$$

Setting derivative of $\mathcal{L}_\lambda(\mathbf{w}, S)$ equal to 0 gives

$$\mathbf{X}'\mathbf{X}\mathbf{w} + \lambda\mathbf{w} = \left(\mathbf{X}'\mathbf{X} + \lambda\mathbf{I}_n\right)\mathbf{w} = \mathbf{X}'\mathbf{y}$$

Primal solution

We get the primal solution weight vector:

$$\mathbf{w} = \left(\mathbf{X}'\mathbf{X} + \lambda \mathbf{I}_n\right)^{-1} \mathbf{X}'\mathbf{y}$$

and regression function

$$g(\mathbf{x}) = \mathbf{x}'\mathbf{w} = \mathbf{x}' \left(\mathbf{X}'\mathbf{X} + \lambda \mathbf{I}_n\right)^{-1} \mathbf{X}'\mathbf{y}$$

Dual solution

A dual solution should involve only computation of inner products – this is achieved by expressing the weight vector as a linear combination of the training examples:

$$\mathbf{X}'\mathbf{X}\mathbf{w} + \lambda\mathbf{w} = \mathbf{X}'\mathbf{y} \quad \text{implies}$$

$$\mathbf{w} = \frac{1}{\lambda}\left(\mathbf{X}'\mathbf{y} - \mathbf{X}'\mathbf{X}\mathbf{w}\right) = \mathbf{X}'\frac{1}{\lambda}\left(\mathbf{y} - \mathbf{X}\mathbf{w}\right) = \mathbf{X}'\alpha,$$

where

$$\alpha = \frac{1}{\lambda}\left(\mathbf{y} - \mathbf{X}\mathbf{w}\right) \tag{1}$$

or equivalently

$$\mathbf{w} = \sum_{i=1}^{m} \alpha_i \mathbf{x}_i$$

Dual solution

Substituting $\mathbf{w} = \mathbf{X}'\alpha$ into equation (1) we obtain:

$$\lambda\alpha = \mathbf{y} - \mathbf{X}\mathbf{X}'\alpha$$

implying

$$\left(\mathbf{X}\mathbf{X}' + \lambda\mathbf{I}_m\right)\alpha = \mathbf{y}$$

This gives the dual solution:

$$\alpha = \left(\mathbf{X}\mathbf{X}' + \lambda\mathbf{I}_m\right)^{-1}\mathbf{y}$$

and regression function

$$g(\mathbf{x}) = \mathbf{x}'\mathbf{w} = \mathbf{x}'\mathbf{X}'\alpha = \sum_{i=1}^{m}\alpha_i\langle\mathbf{x}, \mathbf{x}_i\rangle$$

Key ingredients of dual solution

Step 1: Compute

$$\alpha = (\mathbf{K} + \lambda \mathbf{I}_m)^{-1} \mathbf{y}$$

where $\mathbf{K} = \mathbf{X}\mathbf{X}'$ that is $\mathbf{K}_{ij} = \langle \mathbf{x}_i, \mathbf{x}_j \rangle$

Step 2: Evaluate on new point $\mathbf{x}$ by

$$g(\mathbf{x}) = \sum_{i=1}^{m} \alpha_i \langle \mathbf{x}, \mathbf{x}_i \rangle$$

Important observation: Both steps only involve inner products between datapoints

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Applying the 'kernel trick'

Since the computation only involves inner products, we can substitute for all occurrences of $\langle \cdot, \cdot \rangle$ a kernel function κ that computes:

$$\kappa(\mathbf{x}, \mathbf{z}) = \langle \phi(\mathbf{x}), \phi(\mathbf{z}) \rangle$$

and we obtain an algorithm for ridge regression in the feature space F defined by the mapping

$$\phi : \mathbf{x} \longmapsto \phi(\mathbf{x}) \in F$$

Note if ϕ is the identity we remain linear in the input space.

A simple kernel example

The simplest non-trivial kernel function is the quadratic kernel:

$$\kappa(\mathbf{x}, \mathbf{z}) = \langle \mathbf{x}, \mathbf{z} \rangle^2$$

involving just one extra operation. But surprisingly this kernel function now corresponds to a complex feature mapping:

$$\begin{aligned} \kappa(\mathbf{x}, \mathbf{z}) &= (\mathbf{x}'\mathbf{z})^2 = \mathbf{z}'(\mathbf{x}\mathbf{x}')\mathbf{z} \\ &= \langle \mathrm{vec}(\mathbf{z}\mathbf{z}'), \mathrm{vec}(\mathbf{x}\mathbf{x}') \rangle \end{aligned}$$

where $\mathrm{vec}(A)$ stacks the columns of the matrix A on top of each other. Hence, κ corresponds to the feature mapping

$$\phi : \mathbf{x} \longmapsto \mathrm{vec}(\mathbf{x}\mathbf{x}')$$

Implications of the kernel trick

- Consider for example computing a regression function over 1000 images represented by pixel vectors – say $32 \times 32 = 1024$.
- By using the quadratic kernel we implement the regression function in a $1,000,000$ dimensional space
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Implications of kernel algorithms

- Can perform linear regression in very high-dimensional (even infinite dimensional) spaces efficiently.
- This is equivalent to performing non-linear regression in the original input space: for example quadratic kernel leads to solution of the form

$$g(\mathbf{x}) = \sum_{i=1}^{m} \alpha_i \langle \mathbf{x}_i, \mathbf{x} \rangle^2$$

that is a quadratic polynomial function of the components of the input vector $\mathbf{x}$.

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Theories of learning

- Basic approach of SLT is to view learning from a statistical viewpoint.
- Aim of any theory is to model real/ artificial phenomena so that we can better understand/ predict/ exploit them.
- SLT is just one approach to understanding/ predicting/ exploiting learning systems, others include Bayesian inference, inductive inference, statistical physics, traditional statistical analysis.

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Theories of learning cont.

- Each theory makes assumptions about the phenomenon of learning and based on these derives predictions of behaviour as well as algorithms that aim at optimising the predictions.
- Each theory has strengths and weaknesses – the better it captures the key details of real world system, the better the theory and the better the chances of it making accurate predictions and driving good algorithms.

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General statistical considerations

- Statistical models (not including Bayesian) begin with an assumption that the data is generated by an underlying distribution $\mathcal{D}$ typically not given explicitly to the learner.
- If we are trying to classify cancerous tissue from healthy tissue, there are two distributions, one for cancerous cells and one for healthy ones.

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General statistical considerations cont.

- Usually the distribution subsumes the processes of the natural/artificial world that we are studying.
- Rather than accessing the distribution directly, statistical learning typically assumes that we are given a 'training sample' or 'training set'

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Generalisation of a learner

- Assume that we have a learning algorithm $\mathcal{A}$ that chooses a function $\mathcal{A}_{\mathcal{F}}(S)$ from a function space $\mathcal{F}$ in response to the training set S.
- From a statistical point of view the quantity of interest is the random variable:

$$\epsilon(S, \mathcal{A}, \mathcal{F}) = \mathbb{E}_{(\mathbf{x},y)\sim\mathcal{D}}\left[\ell(\mathcal{A}_{\mathcal{F}}(S), \mathbf{x}, y)\right],$$

where ℓ is a 'loss' function that measures the discrepancy between $\mathcal{A}_{\mathcal{F}}(S)(\mathbf{x})$ and y.

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- For example, in the case of classification ℓ is 1 if the two disagree and 0 otherwise, while for regression it could be the square of the difference between $\mathcal{A}_{\mathcal{F}}(S)(\mathbf{x})$ and y.
- We refer to the random variable $\epsilon(S, \mathcal{A}, \mathcal{F})$ as the generalisation of the learner.

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Example of Generalisation I

- We consider the Breast Cancer dataset from the UCI repository.
- Use the simple Parzen window classifier described by the weight vector

$$\mathbf{w}^+ - \mathbf{w}^-$$

where $\mathbf{w}^+$ is the average of the positive training examples and $\mathbf{w}^-$ is average of negative training examples. Threshold is set so hyperplane bisects the line joining these two points.

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Example of Generalisation II

- Given a size m of the training set, by repeatedly drawing random training sets S we estimate the distribution of

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  by using the test set error as a proxy for the true generalisation.
- We plot the histogram and the average of the distribution for various sizes of training set – initially the whole dataset gives a single value if we use training and test as all the examples, but then we plot for training set sizes:

$$342, 273, 205, 137, 68, 34, 27, 20, 14, 7.$$

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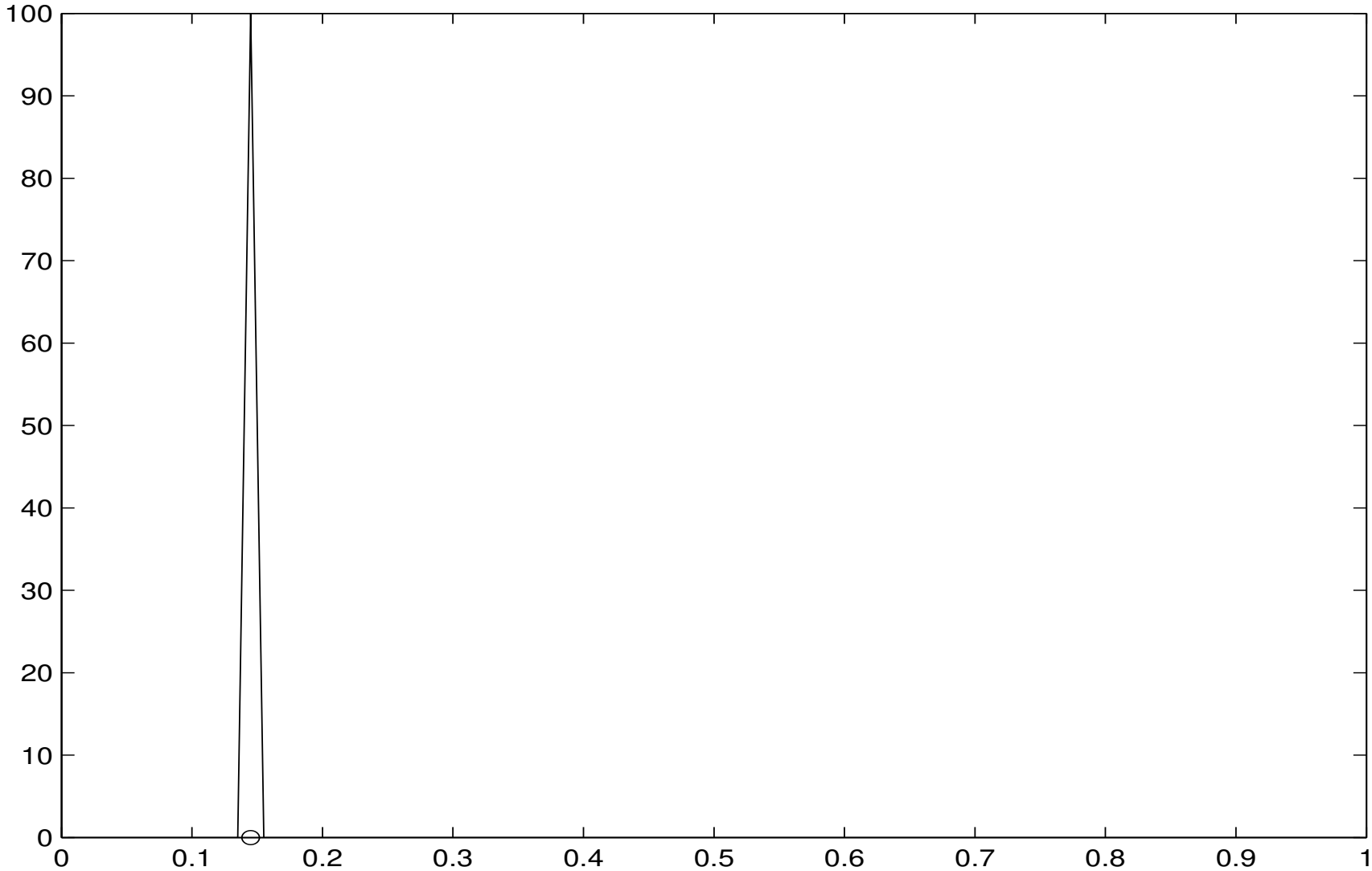
Example of Generalisation III

- Since the expected classifier is in all cases the same:

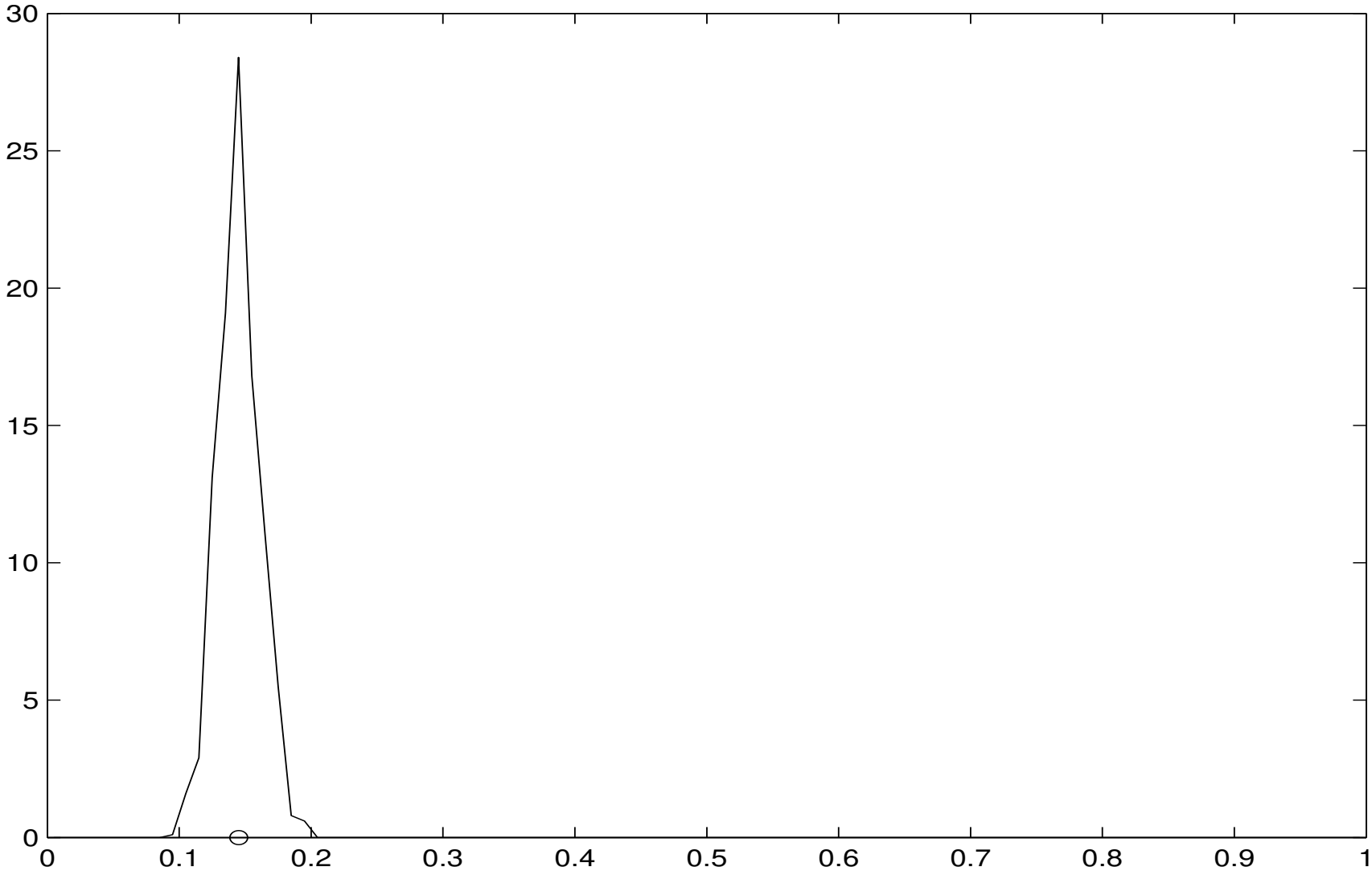
$$\begin{aligned}\mathbb{E}\left[\mathcal{A}_{\mathcal{F}}(S)\right] &= \mathbb{E}_S\left[\mathbf{w}_S^+ - \mathbf{w}_S^-\right] \\ &= \mathbb{E}_S\left[\mathbf{w}_S^+\right] - \mathbb{E}_S\left[\mathbf{w}_S^-\right] \\ &= \mathbb{E}_{y=+1}\left[\mathbf{x}\right] - \mathbb{E}_{y=-1}\left[\mathbf{x}\right],\end{aligned}$$

we do not expect large differences in the average of the distribution, though the non-linearity of the loss function means they won't be the same exactly.

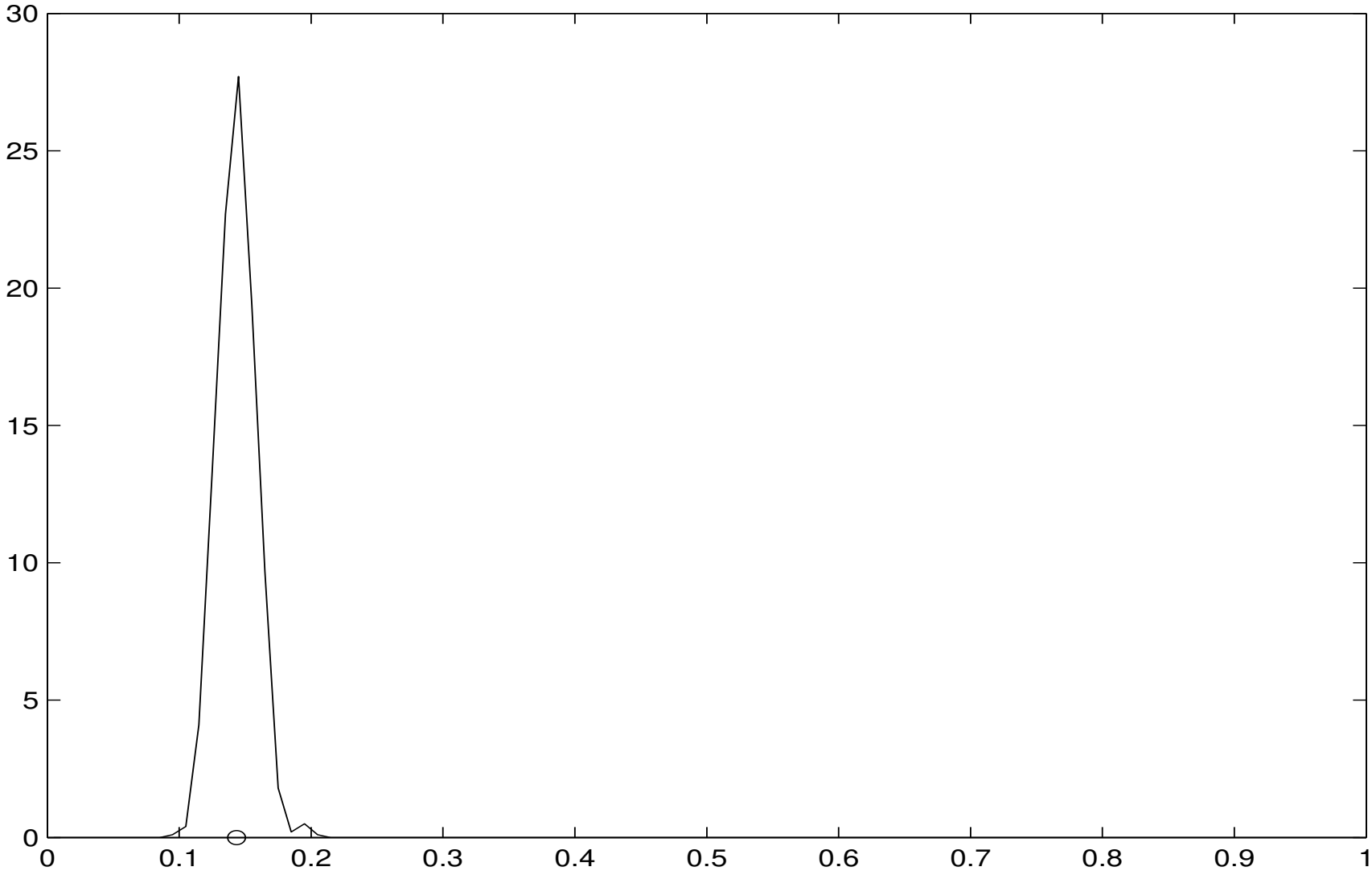
Error distribution: full dataset



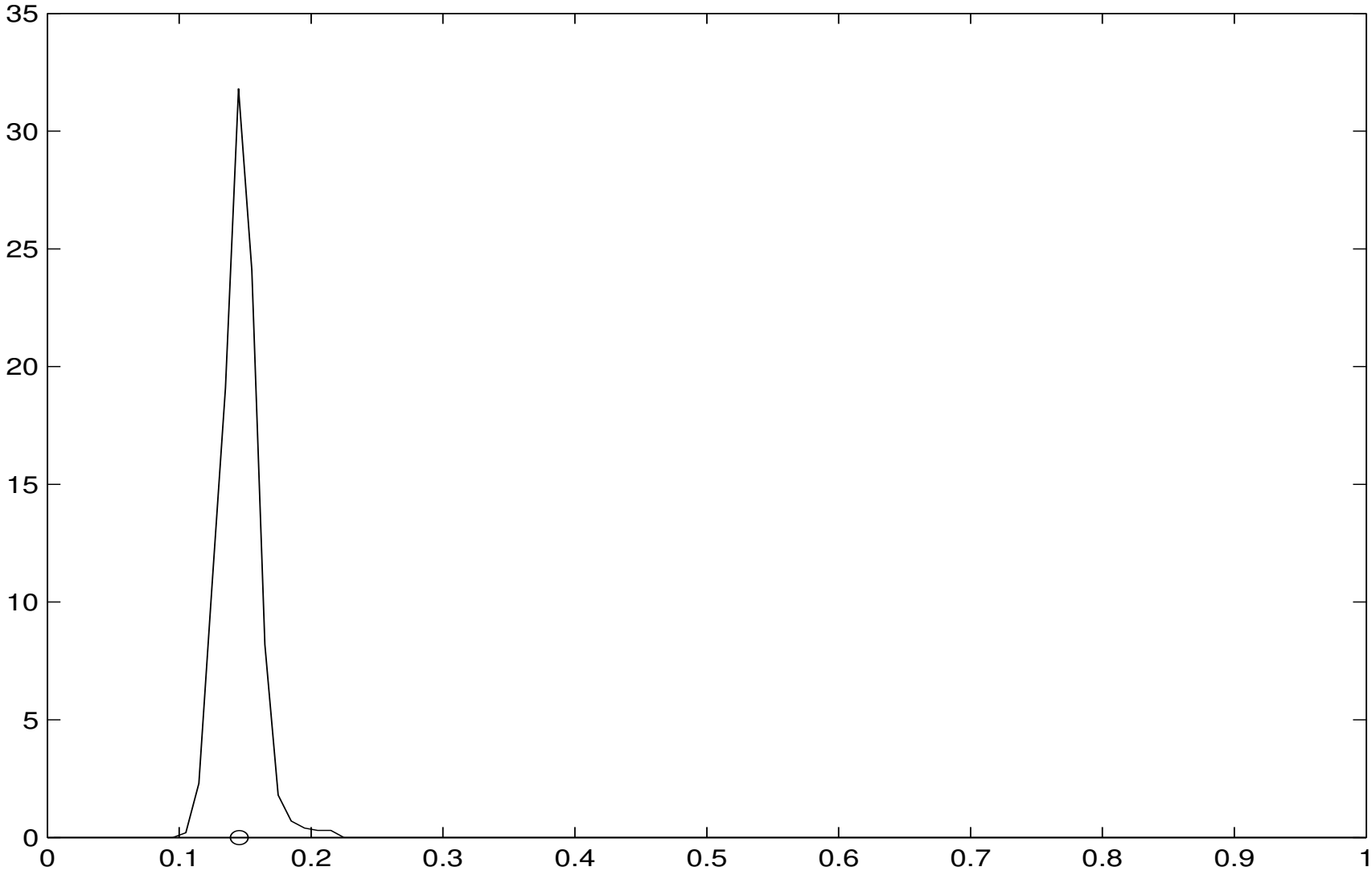
Error distribution: dataset size: 342



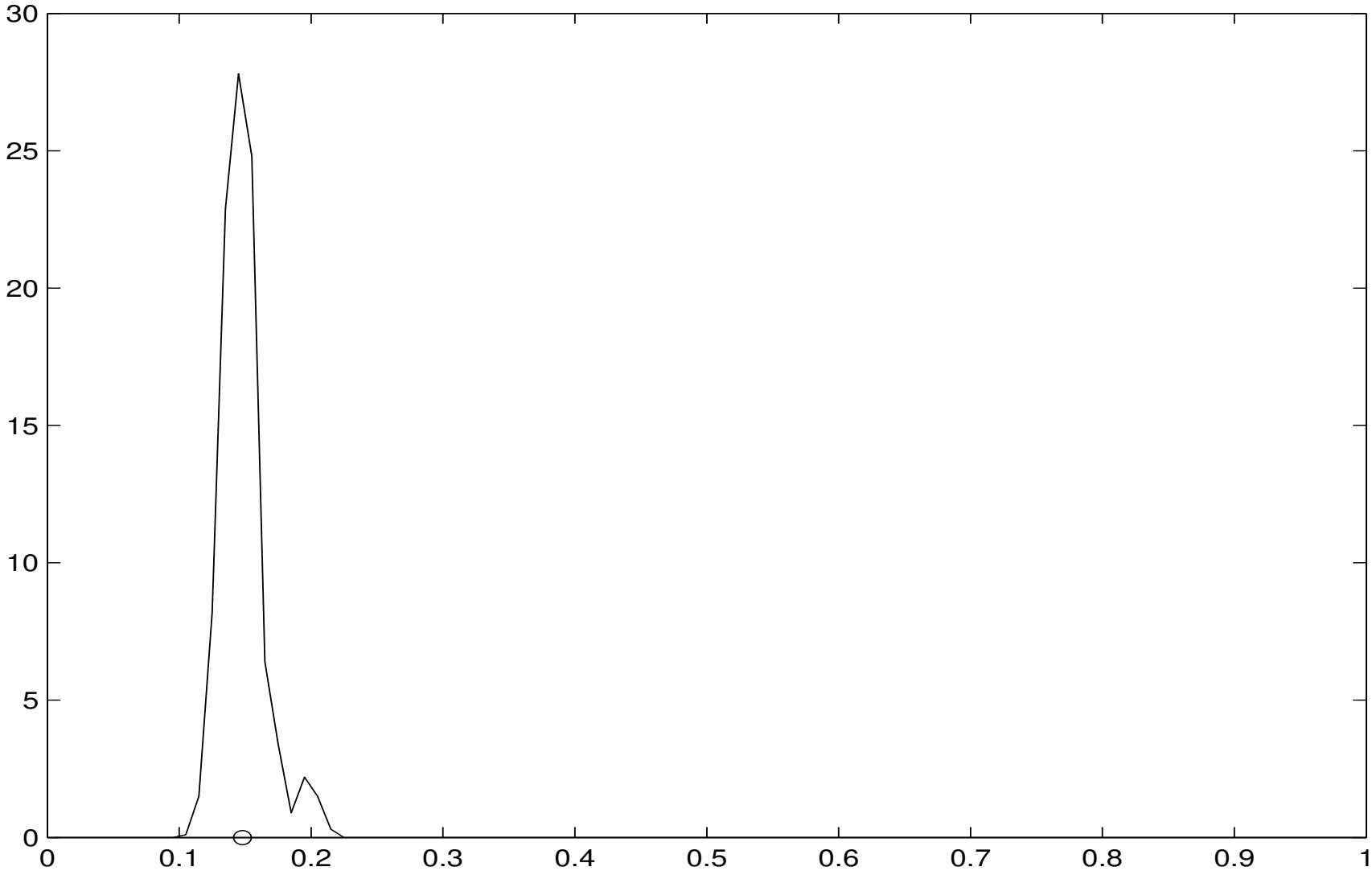
Error distribution: dataset size: 273



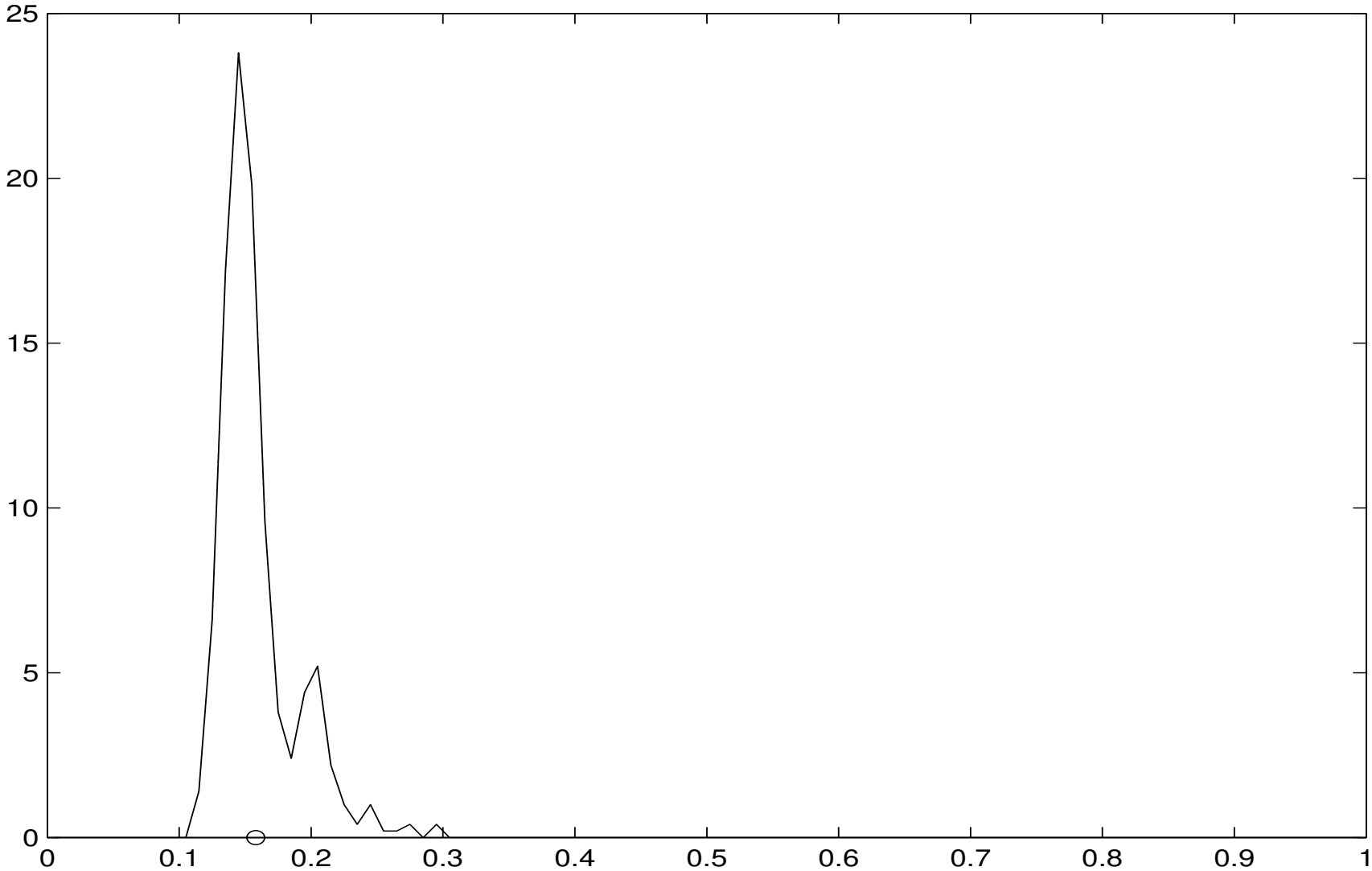
Error distribution: dataset size: 205



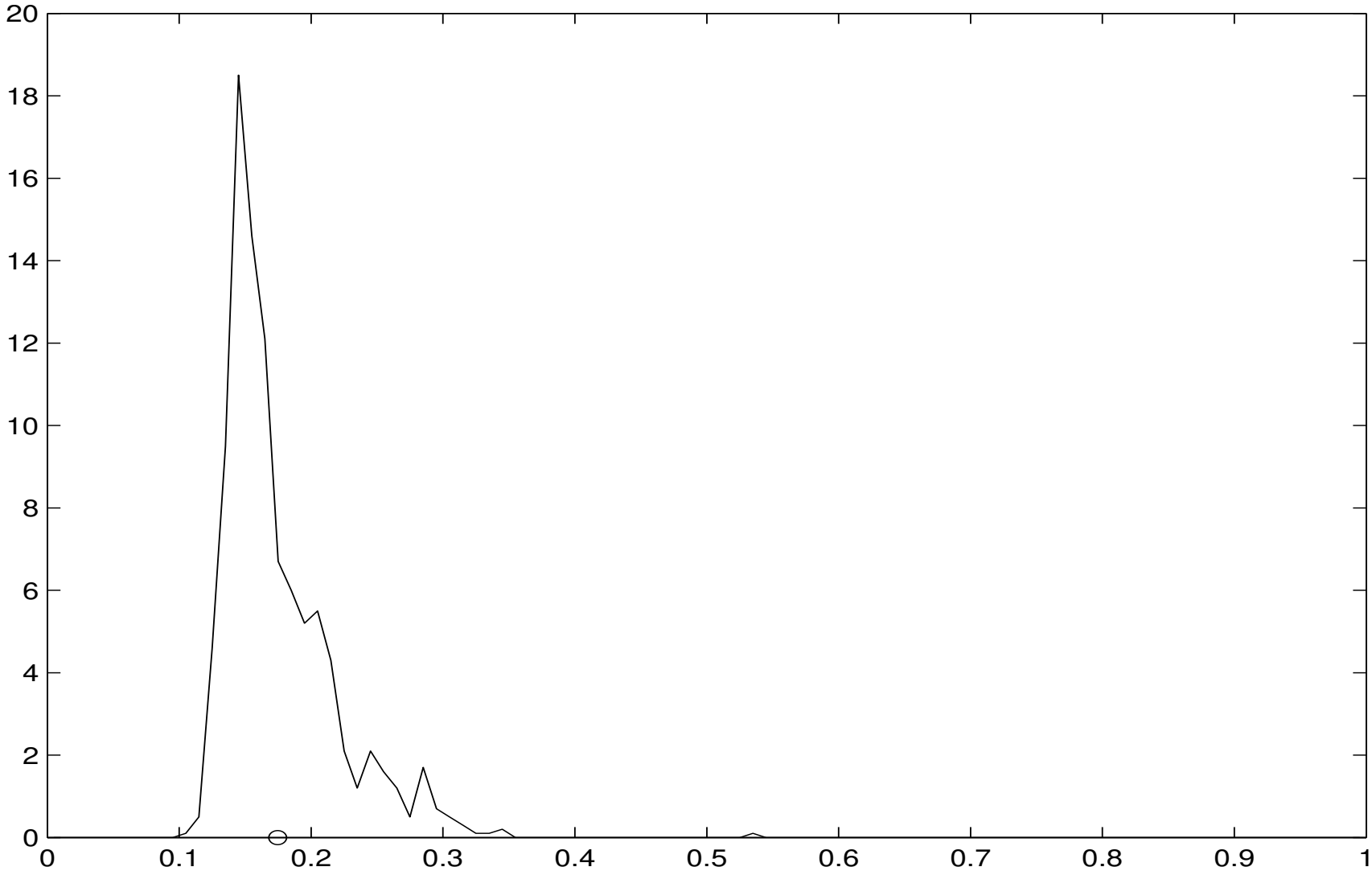
Error distribution: dataset size: 137



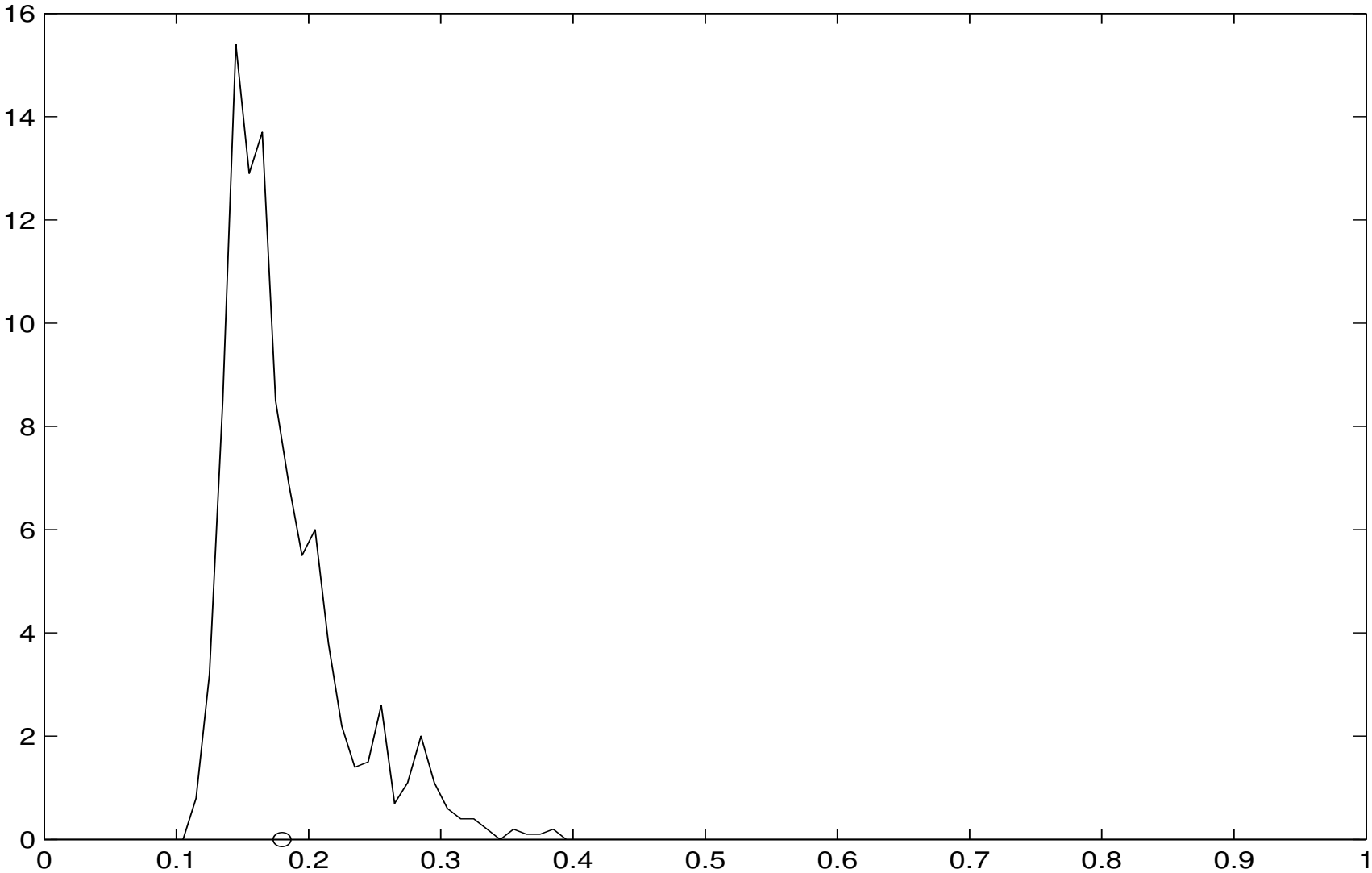
Error distribution: dataset size: 68



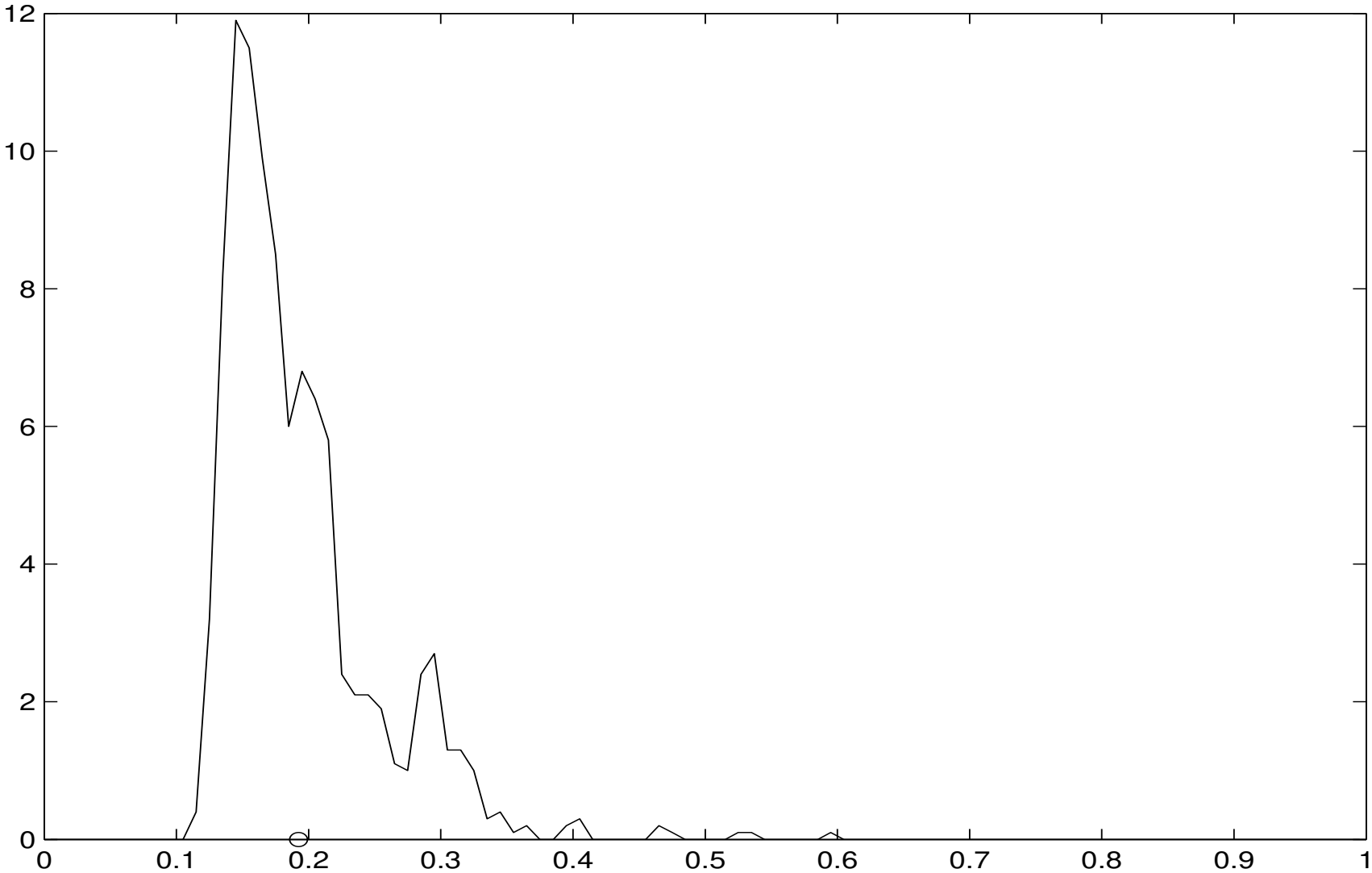
Error distribution: dataset size: 34



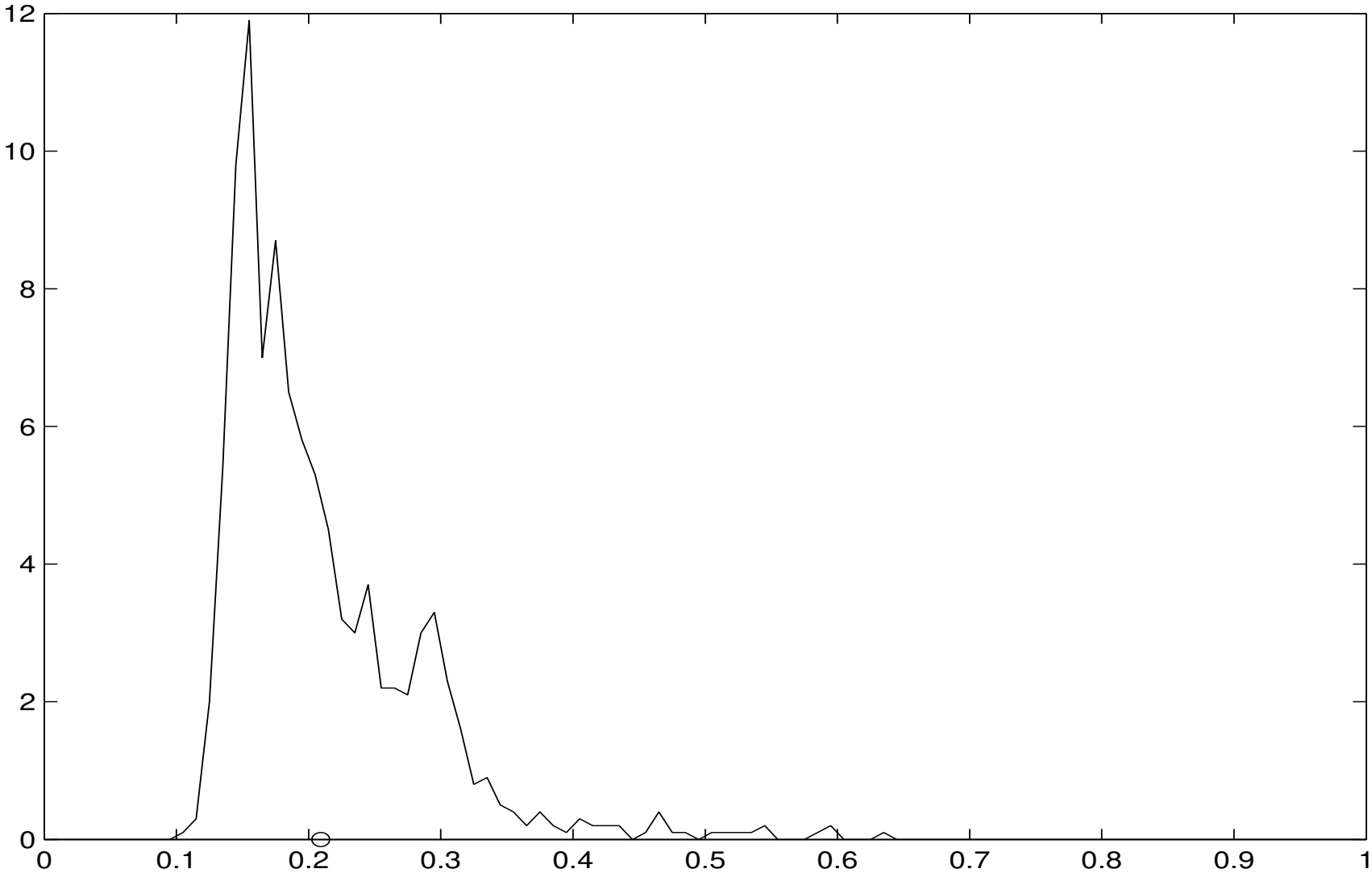
Error distribution: dataset size: 27



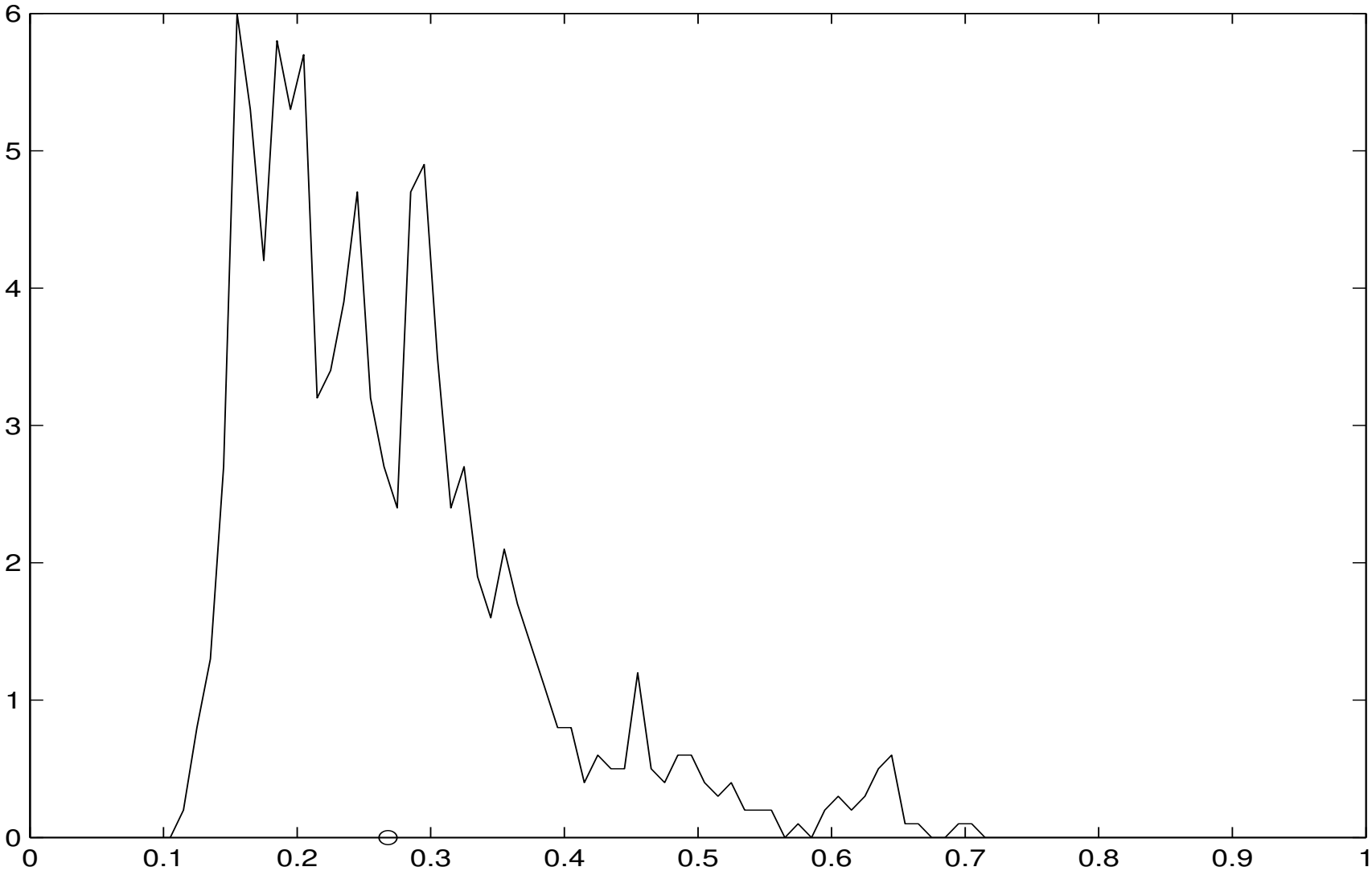
Error distribution: dataset size: 20



Error distribution: dataset size: 14



Error distribution: dataset size: 7



Expected versus confident bounds

- For a finite sample the generalisation $\epsilon(S, \mathcal{A}, \mathcal{F})$ has a distribution depending on the algorithm, function class and sample size m.
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Concentration inequalities

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Concentration inequalities cont.

- As an example consider the mean of a sample of m 1-dimensional random variables $X_1, \ldots, X_m$:

$$S_m = \frac{1}{m} \sum_{i=1}^{m} X_i.$$

- Hoeffding's inequality states that if $X_i \in [a_i, b_i]$

$$P\{|S_m - \mathbb{E}[S_m]| \geq \epsilon\} \leq 2 \exp\left(-\frac{2m^2\epsilon^2}{\sum_{i=1}^{m}(b_i - a_i)^2}\right)$$

Note how the probability falls off exponentially with the distance from the mean and with the number of variables.

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McDiarmid's inequality

Theorem

Let $X_1, \ldots, X_n$ be independent random variables taking values in a set A, and assume that $f : A^n \to \mathbb{R}$ satisfies

$$\sup_{x_1,\ldots,x_n,\hat{x}_i \in A} |f(x_1, \ldots, x_n) - f(x_1, \ldots, \hat{x}_i, x_{i+1}, \ldots, x_n)| \leq c_i,$$

for $1 \leq i \leq n$. Then for all $\epsilon > 0$,

$$P\left\{f\left(X_1, \ldots, X_n\right) - \mathbb{E}f\left(X_1, \ldots, X_n\right) \geq \epsilon\right\} \leq \exp\left(\frac{-2\epsilon^2}{\sum_{i=1}^n c_i^2}\right)$$

- Hoeffding is a special case when $f(x_1, \ldots, x_n) = S_n$

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Using McDiarmid

- By setting the right hand side equal to δ, we can always invert McDiarmid to get a high confidence bound: with probability at least $1 - \delta$

$$f(X_1, \ldots, X_n) < \mathbb{E}f(X_1, \ldots, X_n) + \sqrt{\frac{\sum_{i=1}^n c_i^2}{2} \log \frac{1}{\delta}}$$

- If $c_i = c/n$ for each i this reduces to

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Rademacher complexity

The Rademacher complexity provides a way of measuring the complexity of a function class $\mathcal{F}$ by testing how well on average it can align with random noise:

$$R_m(\mathcal{F}) = \mathbb{E}_{S\sigma}\left[\sup_{f\in\mathcal{F}}\left|\frac{2}{m}\sum_{i=1}^{m}\sigma_i f\left(\mathbf{z}_i\right)\right|\right].$$

is known as the Rademacher complexity of the function class $\mathcal{F}$ where $\sigma_i, i = 1, m$ are uniformly random $+1, -1$ valued variables.

Main Rademacher theorem

The main theorem of Rademacher complexity: with probability at least $1-\delta$ over random samples S of size m, every $f \in \mathcal{F}$ satisfies

$$\mathbb{E}\left[f(\mathbf{z})\right] \leq \hat{\mathbb{E}}\left[f(\mathbf{z})\right] + R_m(\mathcal{F}) + \sqrt{\frac{\ln(1/\delta)}{2m}}$$

- Note that Rademacher complexity gives the expected value of the maximal correlation with random noise – a very natural measure of capacity.
- Note that the Rademacher complexity is distribution dependent since it involves an expectation over the choice of sample – this might seem hard to compute.

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Empirical Rademacher theorem

- Since the empirical Rademacher complexity

$$\hat{R}_m(\mathcal{F}) = \mathbb{E}_\sigma \left[\sup_{f \in \mathcal{F}} \left| \frac{2}{m} \sum_{i=1}^{m} \sigma_i f(\mathbf{z}_i) \right| \middle| \mathbf{z}_1, \ldots, \mathbf{z}_m \right]$$

  is concentrated, we can make a further application of McDiarmid to obtain with probability at least $1 - \delta$

$$\mathbb{E}_{\mathcal{D}}[f(\mathbf{z})] \leq \hat{\mathbb{E}}[f(\mathbf{z})] + \hat{R}_m(\mathcal{F}) + 3\sqrt{\frac{\ln(2/\delta)}{2m}}.$$

Application to large margin classification

- Rademacher complexity comes into its own for analysing Support Vector Machines as well as Boosting algorithms.

Rademacher complexity for SVMs

- The Rademacher complexity of a class of linear functions with bounded 2-norm:

$$\left\{\mathbf{x} \to \sum_{i=1}^{m} \alpha_i \kappa(\mathbf{x}_i, \mathbf{x}) \colon \alpha' \mathbf{K} \alpha \leq B^2\right\} \subseteq$$
$$\subseteq \{\mathbf{x} \to \langle \mathbf{w}, \phi(\mathbf{x}) \rangle : \|\mathbf{w}\| \leq B\}$$
$$= \mathcal{F}_B,$$

where we assume a kernel defined feature space with

$$\langle \phi(\mathbf{x}), \phi(\mathbf{z}) \rangle = \kappa(\mathbf{x}, \mathbf{z}).$$

Rademacher complexity of $\mathcal{F}_B$

The following derivation gives the result

$$\begin{aligned}
\hat{R}_m(\mathcal{F}_B) &= \mathbb{E}_\sigma \left[\sup_{f \in \mathcal{F}_B} \left| \frac{2}{m} \sum_{i=1}^{m} \sigma_i f(\mathbf{x}_i) \right| \right] \\
&= \mathbb{E}_\sigma \left[\sup_{\|\mathbf{w}\| \leq B} \left| \left\langle \mathbf{w}, \frac{2}{m} \sum_{i=1}^{m} \sigma_i \phi(\mathbf{x}_i) \right\rangle \right| \right] \\
&\leq \frac{2B}{m} \mathbb{E}_\sigma \left[\left\| \sum_{i=1}^{m} \sigma_i \phi(\mathbf{x}_i) \right\| \right] \\
&= \frac{2B}{m} \mathbb{E}_\sigma \left[\left(\left\langle \sum_{i=1}^{m} \sigma_i \phi(\mathbf{x}_i), \sum_{j=1}^{m} \sigma_j \phi(\mathbf{x}_j) \right\rangle \right)^{1/2} \right] \\
&\leq \frac{2B}{m} \left(\mathbb{E}_\sigma \left[\sum_{i,j=1}^{m} \sigma_i \sigma_j \kappa(\mathbf{x}_i, \mathbf{x}_j) \right] \right)^{1/2} = \frac{2B}{m} \sqrt{\sum_{i=1}^{m} \kappa(\mathbf{x}_i, \mathbf{x}_i)}
\end{aligned}$$

Support Vector Machines (SVM)

- SVM seeks linear function in a feature space defined implicitly via a kernel κ:

$$\kappa(\mathbf{x}, \mathbf{z}) = \langle \phi(\mathbf{x}), \phi(\mathbf{z}) \rangle$$

  that optimises a bound on the generalisation.

- The first step is to introduce a loss function which upper bounds the discrete loss

$$P(y \neq \text{sgn}(g(\mathbf{x}))) = \mathbb{E}\left[\mathcal{H}(-yg(\mathbf{x}))\right],$$

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Margins in SVMs

- Critical to the bound will be the margin of the classifier

$$\gamma(\mathbf{x}, y) = yg(\mathbf{x}) = y(\langle \mathbf{w}, \phi(\mathbf{x}) \rangle + b) :$$

positive if correctly classified, and measures distance from the separating hyperplane when the weight vector is normalised.

- The margin of a linear function g is

$$\gamma(g) = \min_i \gamma(\mathbf{x}_i, y_i)$$

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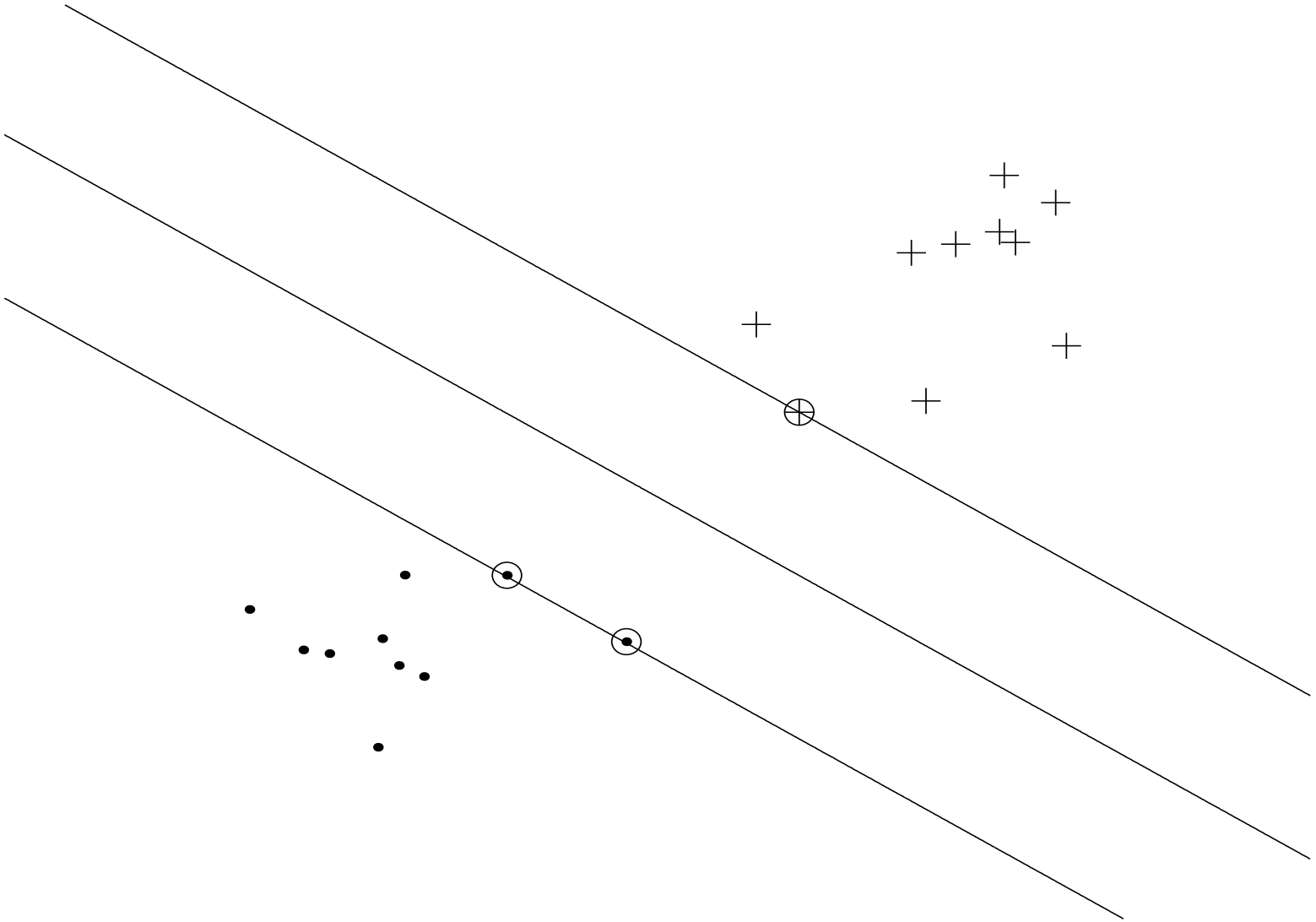

Applying the Rademacher theorem

- Consider the loss function $\mathcal{A} : \mathbb{R} \to [0, 1]$, given by

$$\mathcal{A}(a) = \begin{cases} 1, & \text{if } a > 0; \\ 1 + a/\gamma, & \text{if } -\gamma \leq a \leq 0; \\ 0, & \text{otherwise.} \end{cases}$$

- By the Rademacher Theorem and since the loss function $\mathcal{A}$ dominates $\mathcal{H}$, we have that

$$\begin{aligned} \mathbb{E}\left[\mathcal{H}(-yg(\mathbf{x}))\right] &\leq \mathbb{E}\left[\mathcal{A}(-yg(\mathbf{x}))\right] \\ &\leq \hat{\mathbb{E}}\left[\mathcal{A}(-yg(\mathbf{x}))\right] + \\ &\quad \hat{R}_m(\mathcal{A} \circ \mathcal{F}) + 3\sqrt{\frac{\ln(2/\delta)}{2m}}. \end{aligned}$$

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Empirical loss and slack variables

- But the function $\mathcal{A}(-y_i g(\mathbf{x}_i)) \leq \xi_i/\gamma$, for $i = 1, \ldots, m$, and so

$$\mathbb{E}\left[\mathcal{H}(-yg(\mathbf{x}))\right] \leq \frac{1}{m\gamma}\sum_{i=1}^{m}\xi_i + \hat{R}_m(\mathcal{A}\circ\mathcal{F}) + 3\sqrt{\frac{\ln(2/\delta)}{2m}}.$$

- The final missing ingredient to complete the bound is to bound $\hat{R}_m(\mathcal{A}\circ\mathcal{F})$ in terms of $\hat{R}_m(\mathcal{F})$.
- This can be obtained in terms of the maximal slope of the function $\mathcal{A}$: $\hat{R}_m(\mathcal{A}\circ\mathcal{F}) \leq \frac{2}{\gamma}\hat{R}_m(\mathcal{F})$.

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Final SVM bound

- Assembling the result we obtain:

$$P(y \neq \mathrm{sgn}(g(\mathbf{x}))) = \mathbb{E}\left[\mathcal{H}(-yg(\mathbf{x}))\right]$$
$$\leq \frac{1}{m\gamma}\sum_{i=1}^{m}\xi_i + \frac{4}{m\gamma}\sqrt{\sum_{i=1}^{m}\kappa(\mathbf{x}_i,\mathbf{x}_i)} + 3\sqrt{\frac{\ln(2/\delta)}{2m}}$$

- Note that for the Gaussian kernel this reduces to

$$P(y \neq \mathrm{sgn}(g(\mathbf{x}))) \leq \frac{1}{m\gamma}\sum_{i=1}^{m}\xi_i + \frac{4}{\sqrt{m}\gamma} + 3\sqrt{\frac{\ln(2/\delta)}{2m}}$$

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Applying to 1-norm SVMs

We take the following formulation of the 1-norm SVM to optimise the bound:

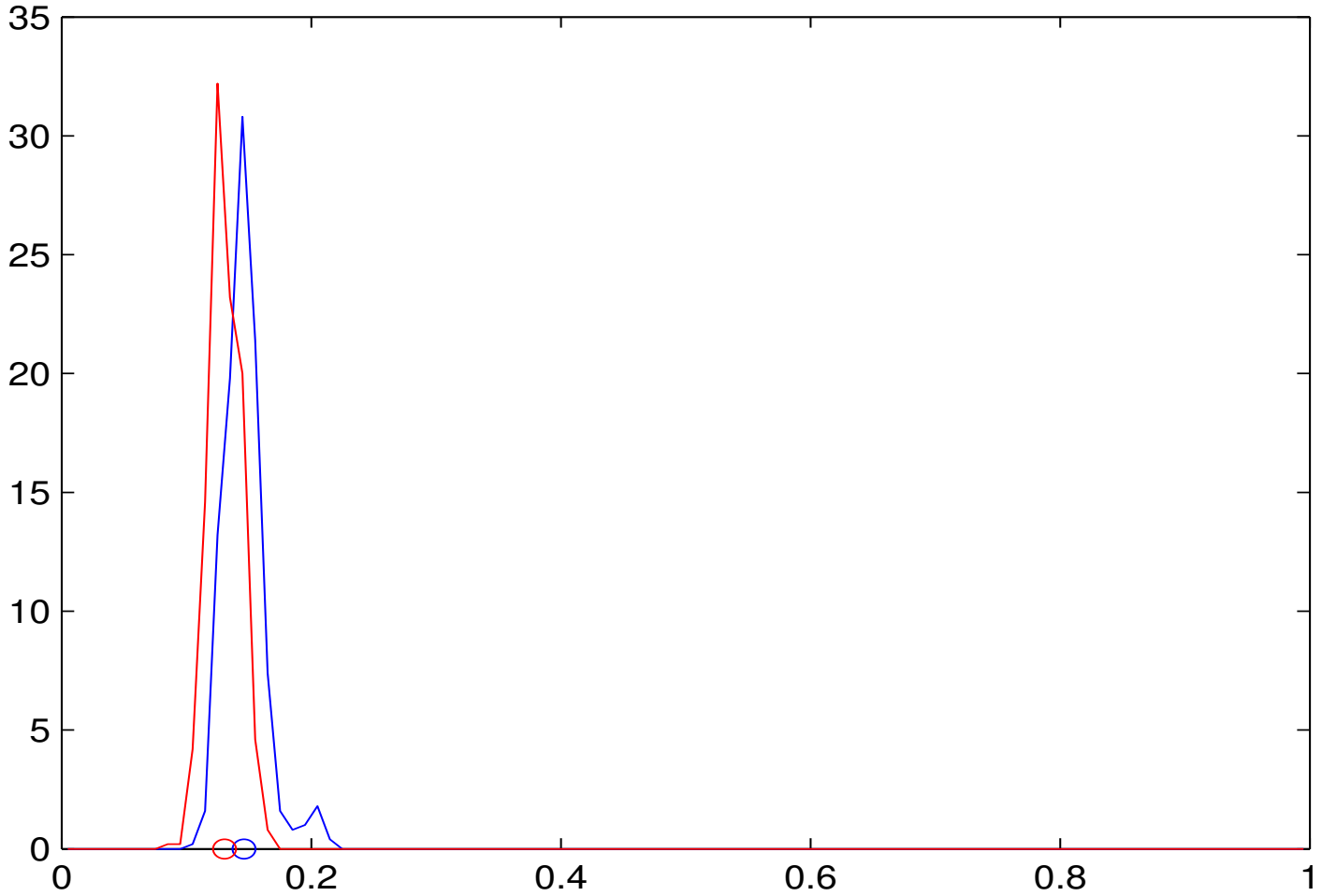
$$\begin{array}{ll} \min_{\mathbf{w},b,\gamma,\xi} & -\gamma + C\sum_{i=1}^{m}\xi_i \\ \text{subject to} & y_i\left(\langle \mathbf{w}, \phi\left(\mathbf{x}_i\right)\rangle + b\right) \geq \gamma - \xi_i,\ \xi_i \geq 0, \\ & i = 1, \ldots, m, \text{ and } \|\mathbf{w}\|^2 = 1. \end{array} \tag{2}$$

Note that

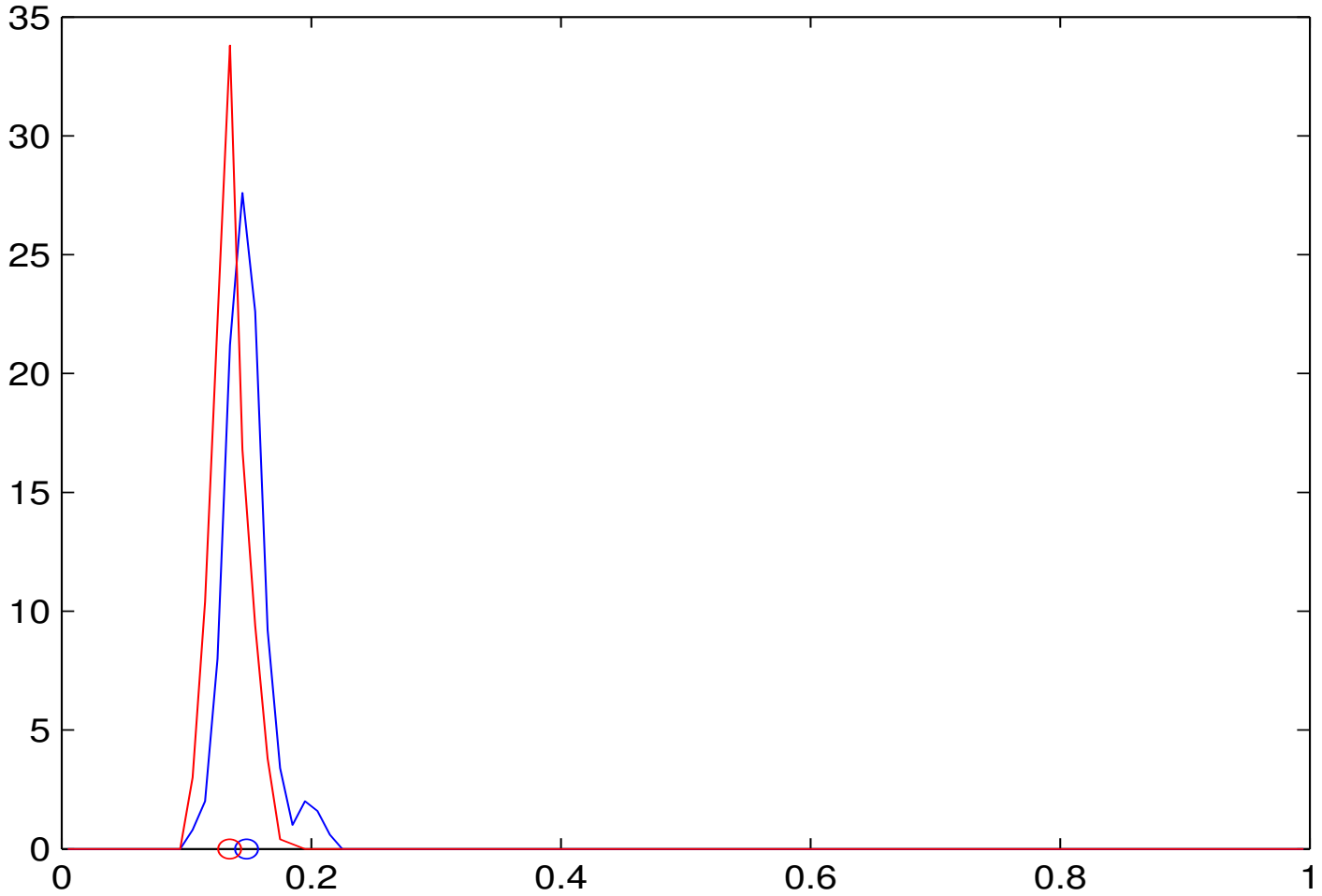
$$\xi_i = \left(\gamma - y_i g(\mathbf{x}_i)\right)_+,$$

where $g(\cdot) = \langle \mathbf{w}, \phi(\cdot)\rangle + b$.

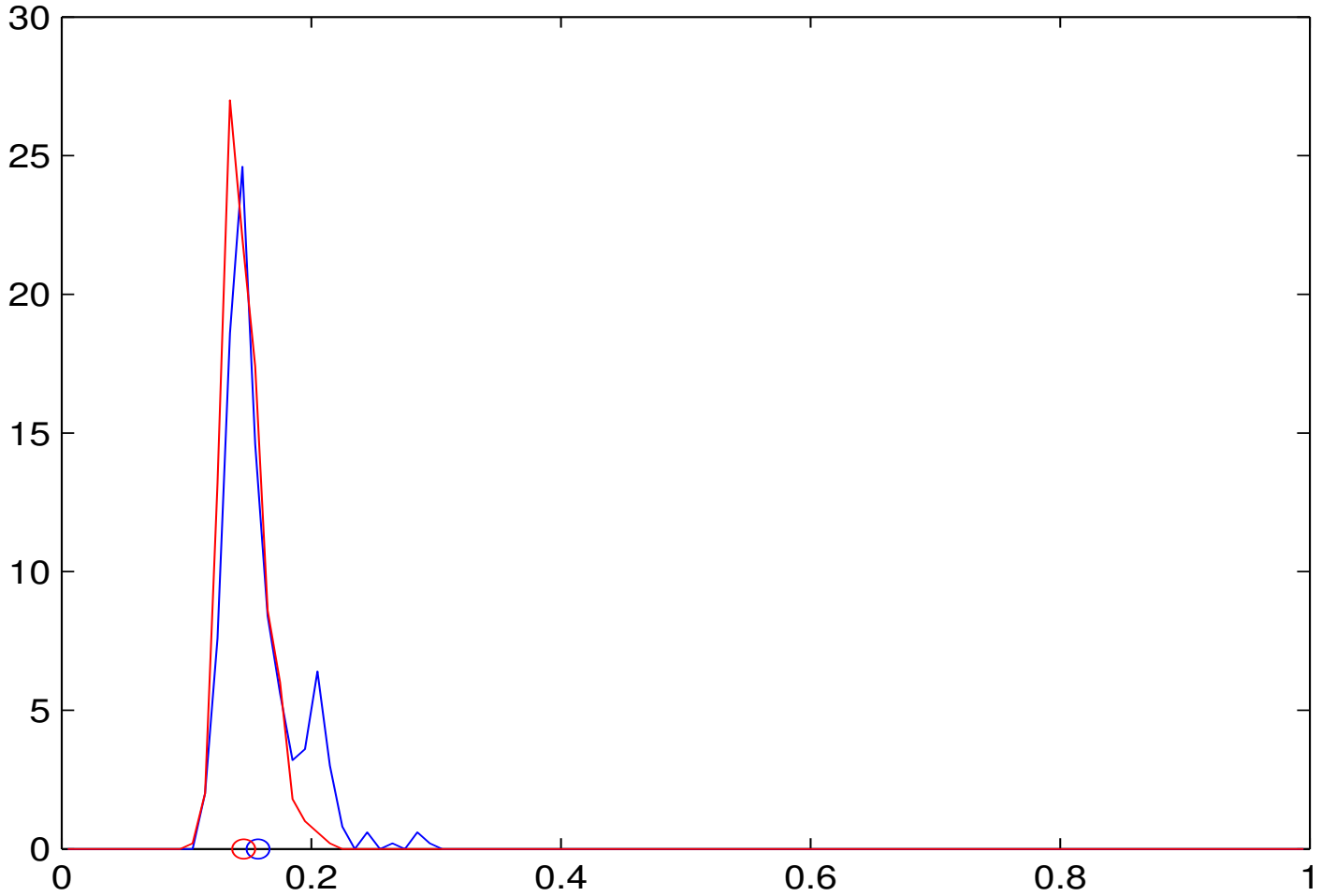
Error distribution: dataset size: 205



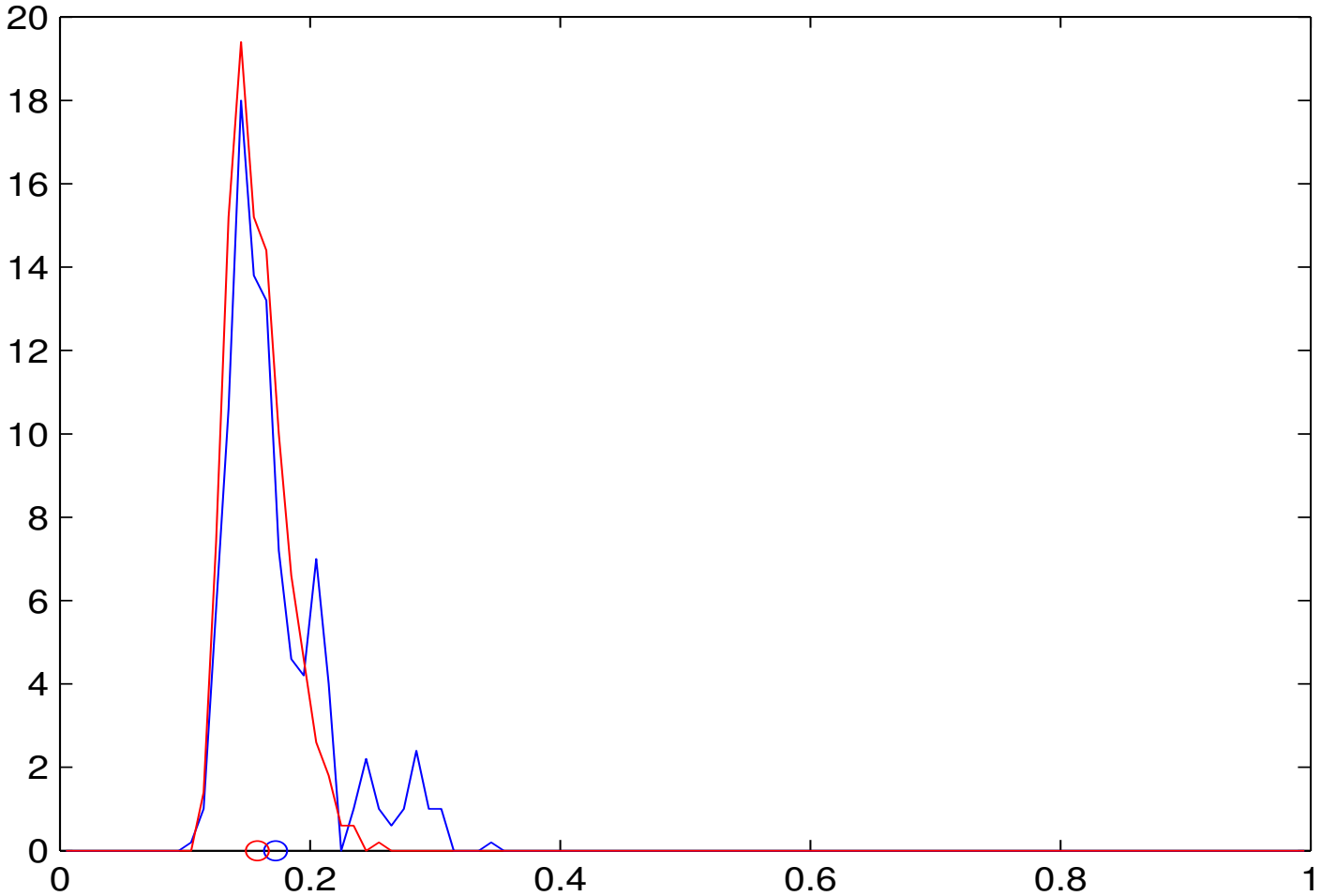
Error distribution: dataset size: 137



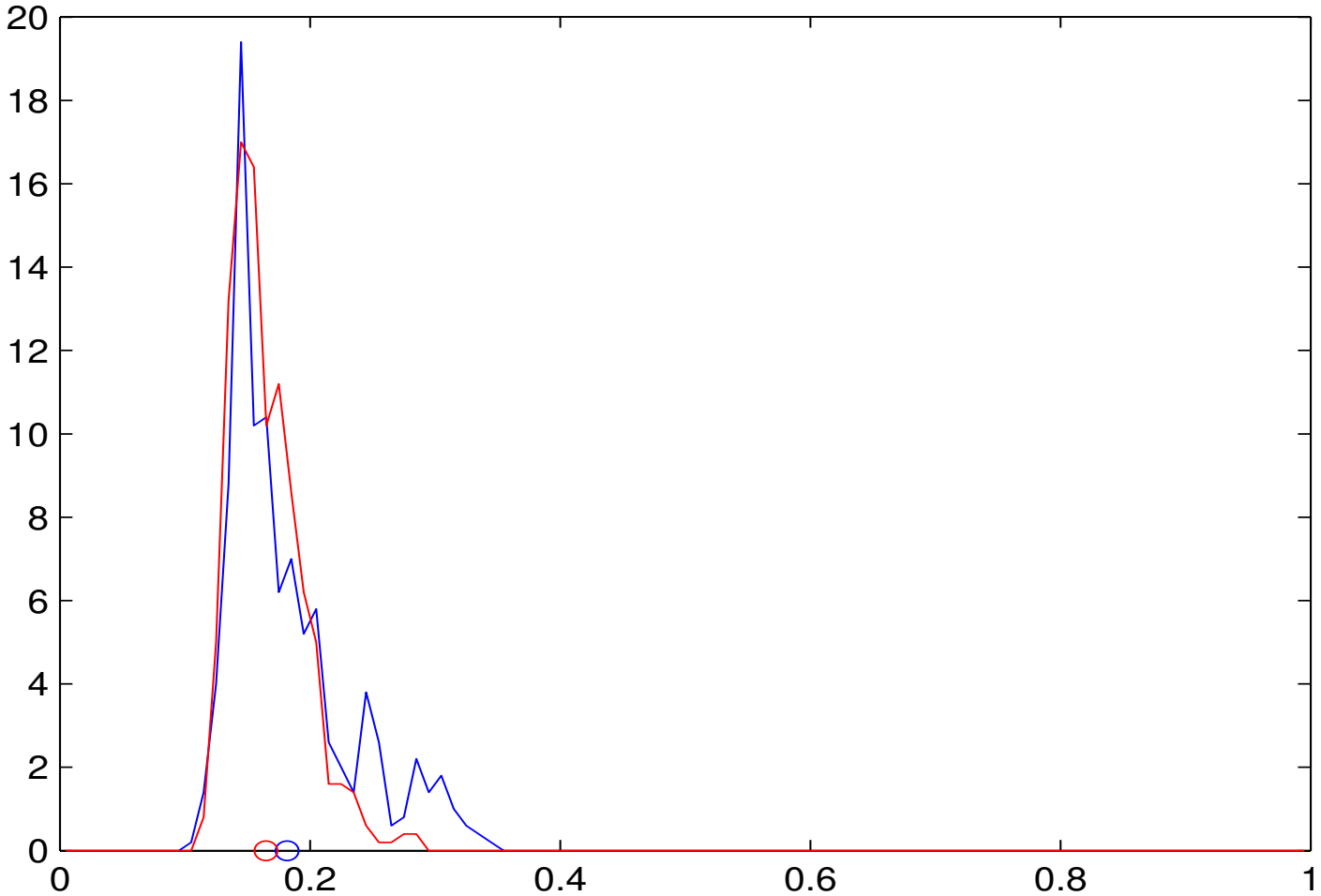
Error distribution: dataset size: 68



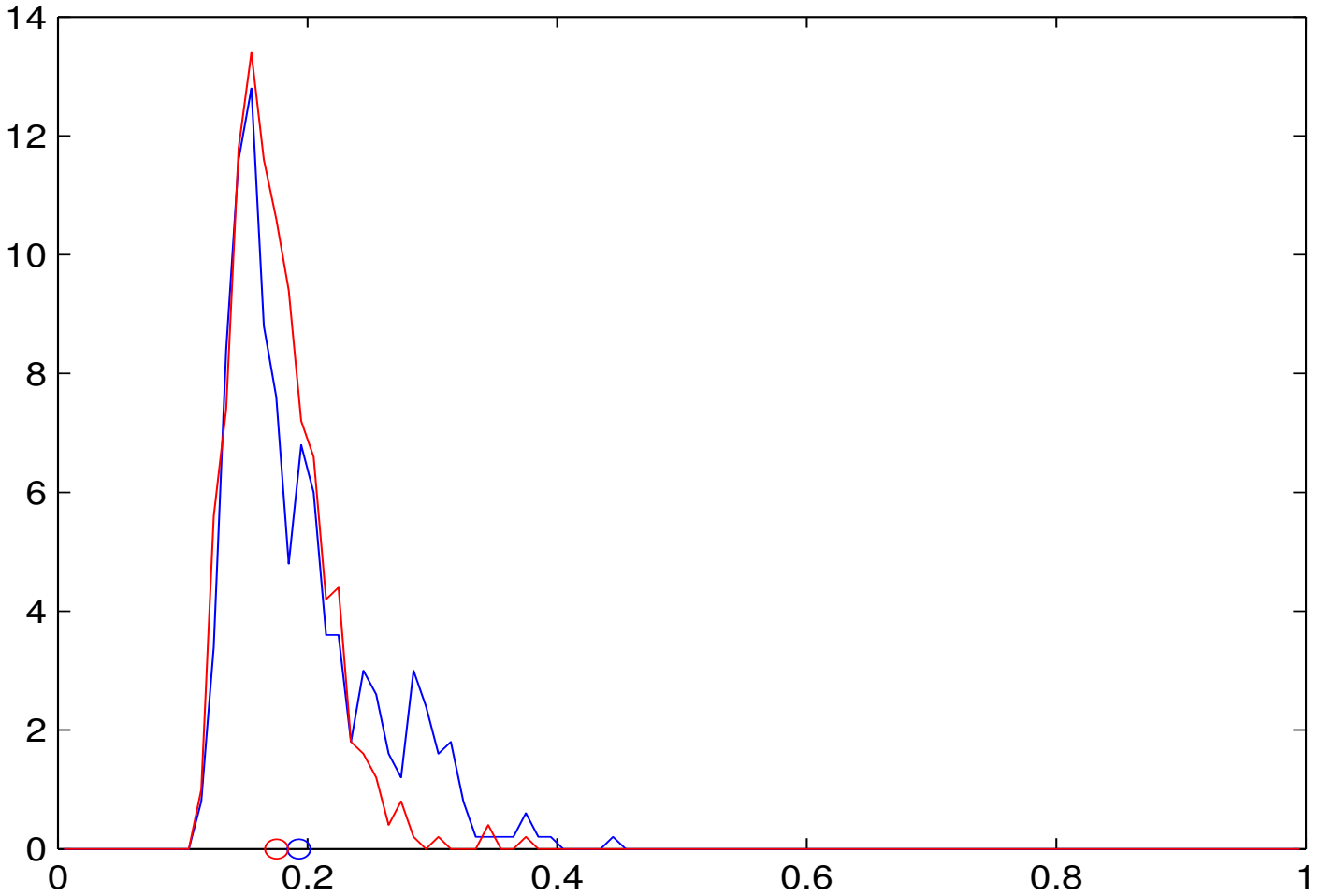
Error distribution: dataset size: 34



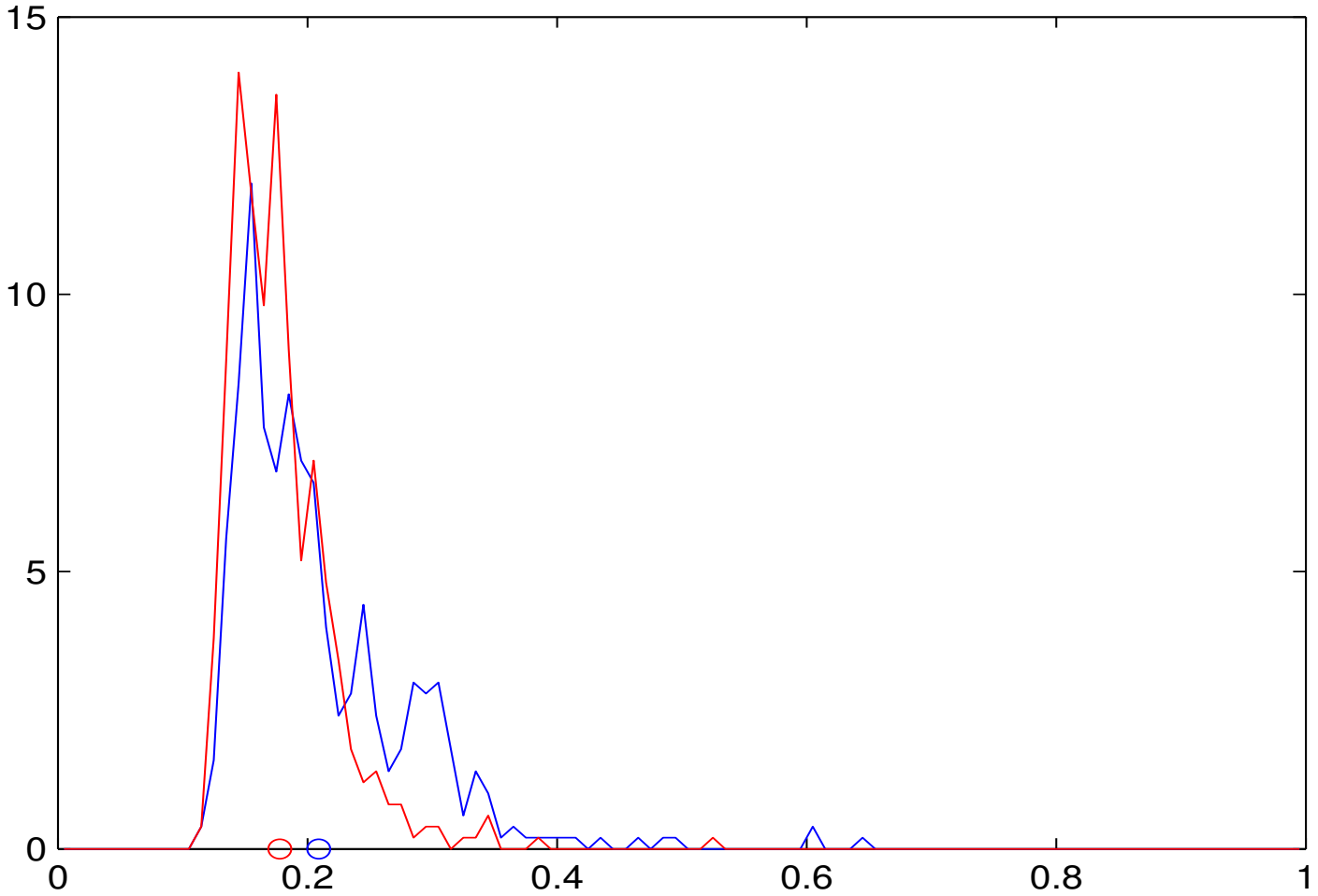
Error distribution: dataset size: 27



Error distribution: dataset size: 20



Error distribution: dataset size: 14



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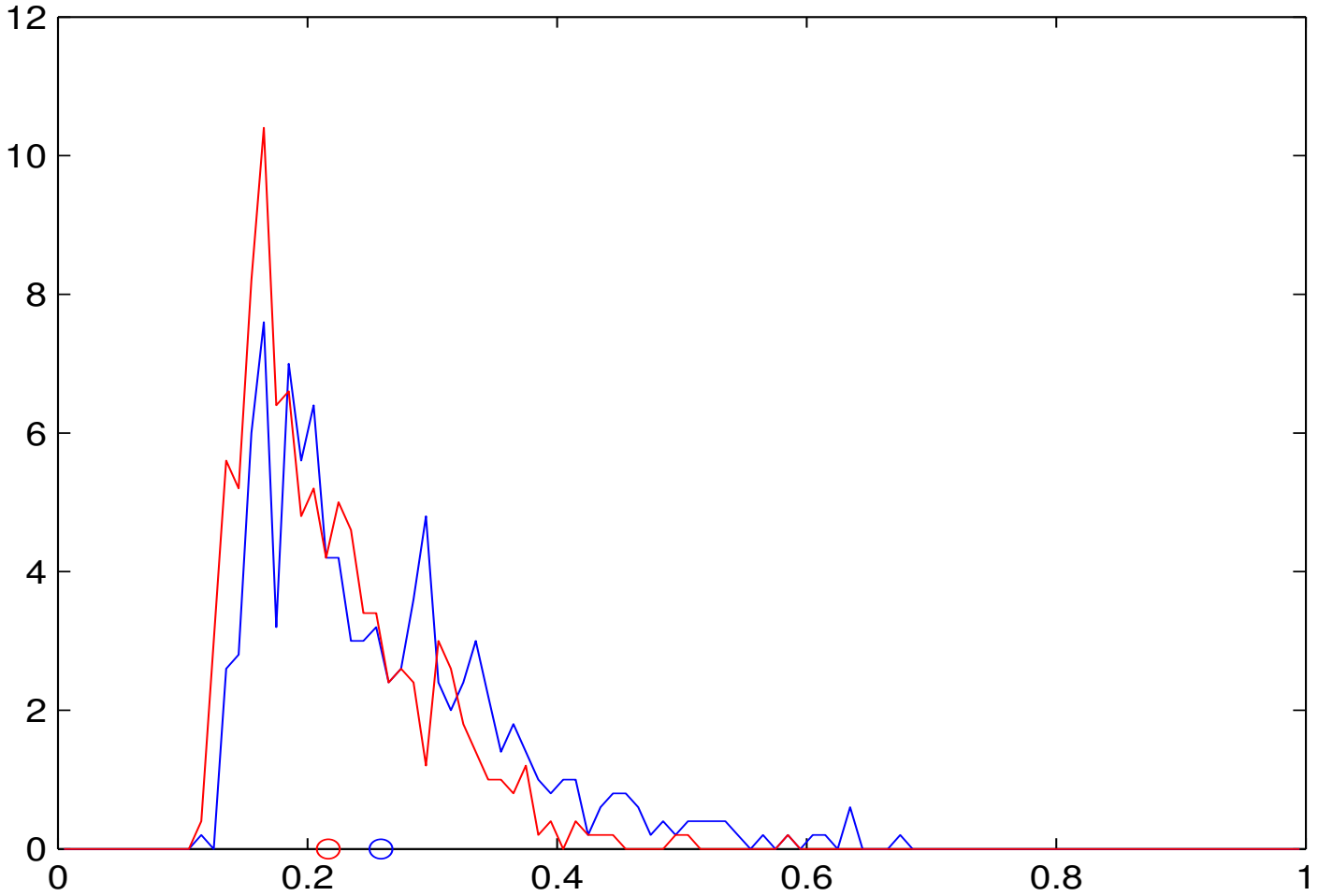


Dual form of the SVM problem

Forming the Lagrangian $L(\mathbf{w}, b, \gamma, \xi, \alpha, \beta, \lambda)$:

$$-\gamma + C\sum_{i=1}^{m}\xi_i - \sum_{i=1}^{m}\alpha_i\left[y_i(\langle\phi(\mathbf{x}_i), \mathbf{w}\rangle + b) - \gamma + \xi_i\right]$$
$$-\sum_{i=1}^{m}\beta_i\xi_i + \lambda\left(\|\mathbf{w}\|^2 - 1\right)$$

with $\alpha_i \geq 0$ and $\beta_i \geq 0$.

Dual form of the SVM problem

Taking derivatives gives:

$$\begin{aligned}
\frac{\partial L(\mathbf{w}, b, \gamma, \xi, \alpha, \beta, \lambda)}{\partial \mathbf{w}} &= 2\lambda \mathbf{w} - \sum_{i=1}^{m} y_i \alpha_i \phi(\mathbf{x}_i) = \mathbf{0}, \\
\frac{\partial L(\mathbf{w}, b, \gamma, \xi, \alpha, \beta, \lambda)}{\partial \xi_i} &= C - \alpha_i - \beta_i = 0, \\
\frac{\partial L(\mathbf{w}, b, \gamma, \xi, \alpha, \beta, \lambda)}{\partial b} &= \sum_{i=1}^{m} y_i \alpha_i = 0, \\
\frac{\partial L(\mathbf{w}, b, \gamma, \xi, \alpha, \beta, \lambda)}{\partial \gamma} &= 1 - \sum_{i=1}^{m} \alpha_i = 0.
\end{aligned}$$

Dual form of the SVM problem

$$L(\alpha, \lambda) = -\frac{1}{4\lambda} \sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \kappa(\mathbf{x}_i, \mathbf{x}_j) - \lambda,$$

which, again optimising with respect to λ, gives

$$\lambda^* = \frac{1}{2} \left(\sum_{i,j=1}^{m} y_i y_j \alpha_i \alpha_j \kappa(\mathbf{x}_i, \mathbf{x}_j) \right)^{1/2}$$

Dual form of the SVM problem

equivalent to maximising

$$L(\alpha) = -\sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j \kappa(\mathbf{x}_i, \mathbf{x}_j),$$

subject to the constraints

$$0 \leq \alpha_i \leq C, \quad \sum_{i=1}^{m} \alpha_i = 1 \quad \sum_{i=1}^{m} y_i \alpha_i = 0$$

to give solution

$$\alpha_i^*, i = 1, \ldots, m$$

Dual form of the SVM problem

Kuhn-Tucker conditions:

$$\begin{aligned} \alpha_i \left[y_i (\langle \phi(\mathbf{x}_i), \mathbf{w} \rangle + b) - \gamma + \xi_i \right] &= 0 \\ \beta_i \xi_i &= 0 \end{aligned}$$

These imply:

- $\alpha_i \neq 0$ only if

$$y_i (\langle \phi(\mathbf{x}_i), \mathbf{w} \rangle + b) = \gamma - \xi_i$$

  these correspond to support vectors – their margins are less than or equal to γ.
- $\xi_i \neq 0$ only if $\beta_i = 0$ implying that $\alpha_i = C$, i.e. for $0 < \alpha_i < C$ margin is exactly γ.

Dual form of the SVM problem

The solution can then be computed as:

$$\begin{aligned}
\text{choose} \quad & i, j \text{ such that } -C < \alpha_i^* y_i < 0 < \alpha_j^* y_j < C \\
b^* &= -0.5 \left(\sum_{k=1}^{m} \alpha_k^* y_k \kappa(\mathbf{x}_k, \mathbf{x}_i) + \sum_{k=1}^{m} \alpha_k^* y_k \kappa(\mathbf{x}_k, \mathbf{x}_j) \right) \\
f(\cdot) &= \operatorname{sgn} \left(\sum_{j=1}^{m} \alpha_j^* y_j \kappa(\mathbf{x}_j, \cdot) + b^* \right);
\end{aligned}$$

Dual form of the SVM problem

We can compute the margin as follows:

$$\begin{aligned}\lambda^* &= \frac{1}{2}\left(\sum_{i,j=1}^{m} y_i y_j \alpha_i^* \alpha_j^* \kappa(\mathbf{x}_i, \mathbf{x}_j)\right)^{1/2} \\ \gamma^* &= (2\lambda^*)^{-1}\left(\sum_{k=1}^{m} \alpha_k^* y_k \kappa(\mathbf{x}_k, \mathbf{x}_j) + b^*\right)\end{aligned}$$

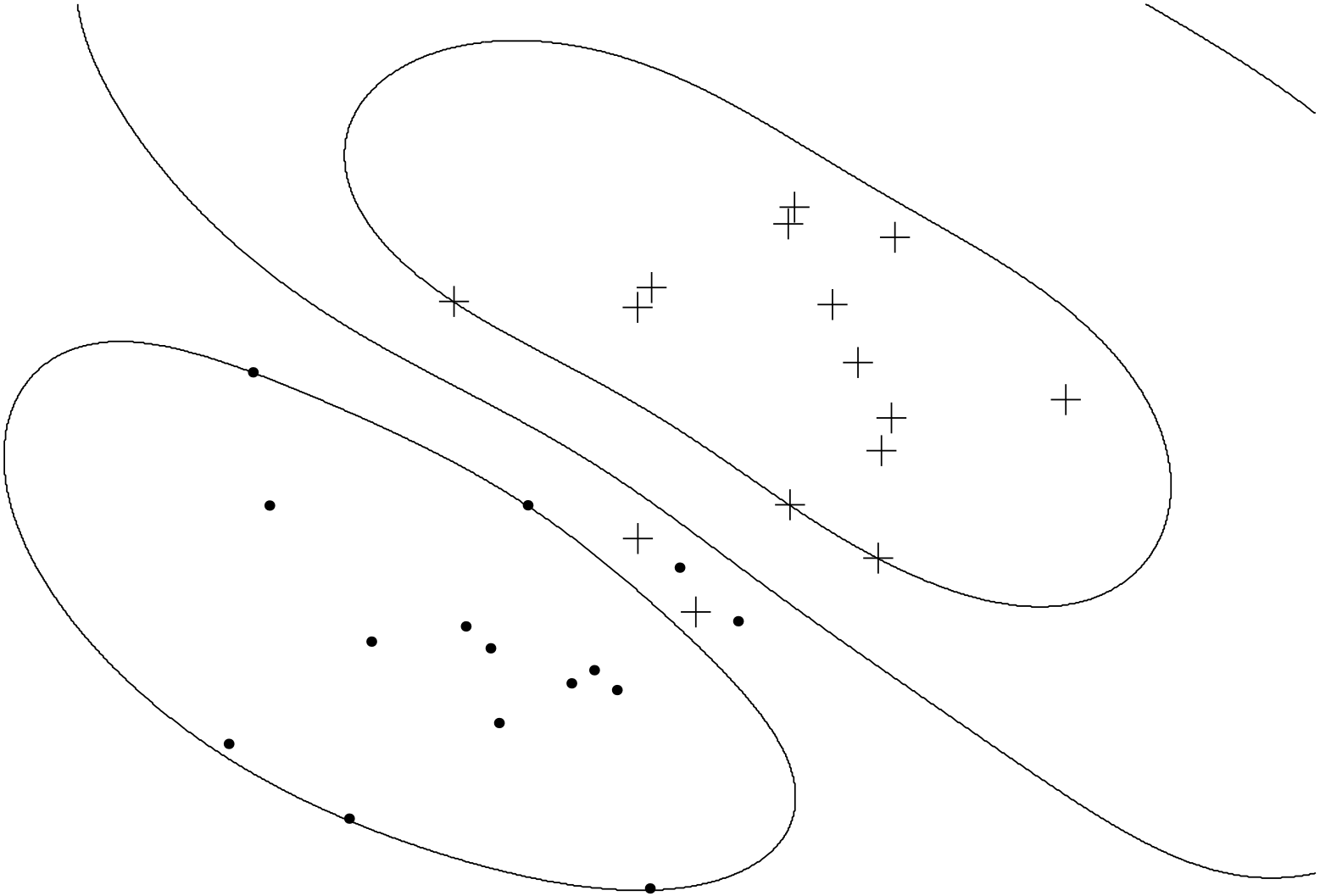
Similarly we can compute

$$\sum_{i=1}^{m} \xi_i = \frac{-2\lambda^* + \gamma^*}{C}$$

if we wish to compute the value of the bound.

Dual form of the SVM problem

Decision boundary and γ margin for 1-norm svm with a gaussian kernel:



Dual form of the SVM problem

- Have introduced a slightly non-standard version of the SVM but makes ν-SVM very simple to define.
- Consider expressing $C = 1/(\nu m)$:
  - implies $0 \leq \alpha_i \leq 1/(\nu m)$
  - if $\xi > 0$ then $\alpha_i = 1/(\nu m)$, but $\sum_{i=1}^{m} \alpha_i = 1$ so at most νm inputs can have this hold.
  - equally at least νm inputs have $\alpha_i \neq 0$
- Hence, ν can be seen as the fraction of 'support vectors', a natural measure of the noise in the data.

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Alternative form of the SVM problem

Note more traditional form of the dual SVM optimisation:

$$L(\alpha) = \sum_{i=1}^{m} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{m} \alpha_i \alpha_j y_i y_j \kappa(\mathbf{x}_i, \mathbf{x}_j).$$

with constraints

$$0 \leq \alpha_i \leq C, \qquad \sum_{i=1}^{m} y_i \alpha_i = 0$$

Alternative form of the SVM problem

- Arises from considering renormalising so that output at margin is 1 and minimising the weight vector.
- The values of the regularisation parameter C do not correspond.
- Has advantage of simple kernel adatron algorithm if we consider the case of fixing $b = 0$ which removes the constraint $\sum_{i=1}^{m} \alpha_i y_i = 0$, so can perform gradient descent on individual α_i independently.
- SMO algorithm performs the update on pairs of α_i, α_j to ensure constraints remain satisfied.

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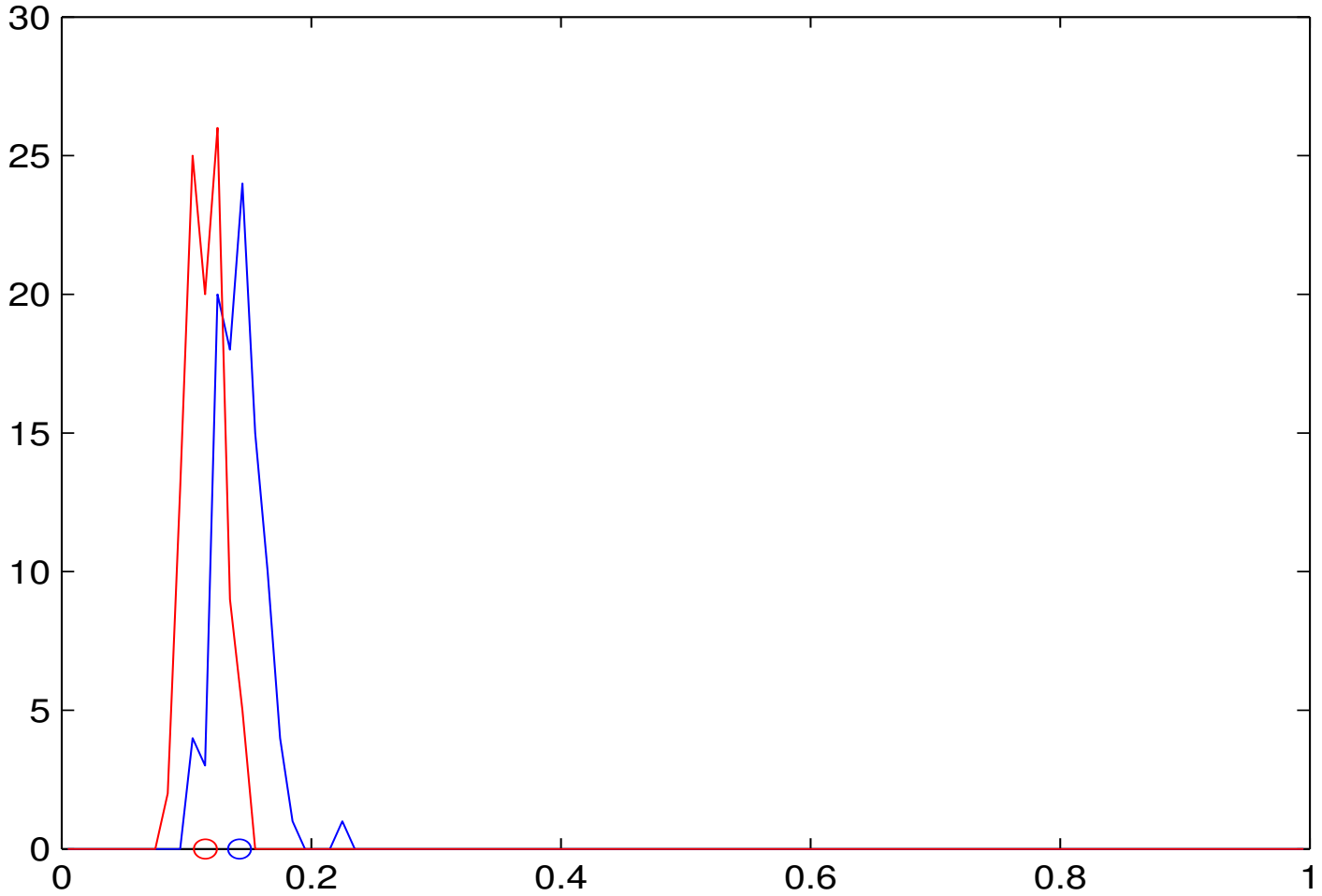
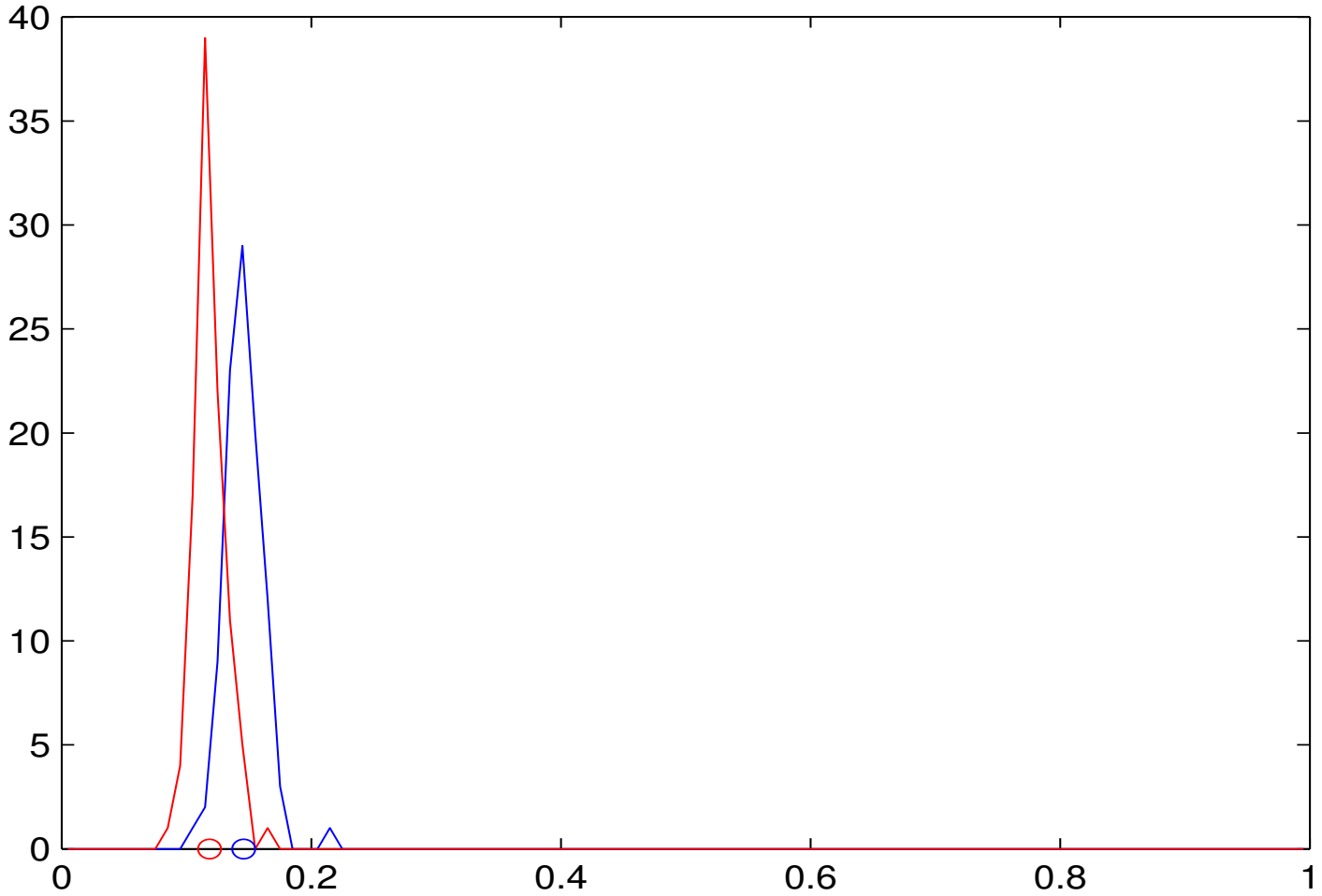
Error distribution: dataset size: 342



Error distribution: dataset size: 273



Linear programming machine

- Boosting leverages a large class H of 'weak learners' only able to classify slightly above 50% accuracy to build a (small) linear combination that performs very accurately.
- Some questions about why it works so well
- Seeks linear function in a feature space defined explicitly and can use the 1-norm to keep most coefficients zero.

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Linear programming boosting

- Very slight generalisation considers the features as a set $\mathbf{H}_{ij}$ of 'weak' learners (and includes the constant function as one weak learner and negative of each weak learner):

$$\begin{aligned} \min_{\mathbf{a},\xi} \quad & \|\mathbf{a}\|_1 + C\sum_{i=1}^m \xi_i \\ \text{subject to} \quad & y_i\mathbf{H}_i\mathbf{a} \geq 1-\xi_i,\ \xi_i \geq 0,\ a_i \geq 0 \\ & i = 1,\ldots,m. \end{aligned}$$

where $\mathbf{a}$ is the vector of coefficients.

Final Boosting bound

- Applying a similar strategy for Boosting with the 1-norm of the slack variables we arrive at Linear programming boosting that minimises

$$\sum_h a_h + C \sum_{i=1}^m \xi_i,$$

where $\xi_i = (1 - y_i \sum_h a_h h(\mathbf{x}_i))_+$ and $a_h \geq 0$.

- with corresponding bound:

$$\begin{aligned} P(y \neq \text{sgn}(g(\mathbf{x}))) &= \mathbb{E}[\mathcal{H}(-yg(\mathbf{x}))] \\ &\leq \frac{1}{m} \sum_{i=1}^m \xi_i + \hat{R}(H) \sum_h a_h + 3\sqrt{\frac{\ln(2/\delta)}{2m}} \end{aligned}$$

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Alternative version

- Can explicitly optimise margin with 1-norm fixed:

$$\begin{aligned} \max_{\rho,\mathbf{a},\xi} \quad & \rho - D\sum_{i=1}^{m}\xi_i \\ \text{subject to} \quad & y_i\mathbf{H}_i\mathbf{a} \geq \rho - \xi_i,\ \xi_i \geq 0, a_j \geq 0 \\ & \sum_{j=1}^{N} a_j = 1. \end{aligned}$$

- Dual has the following form:

$$\begin{aligned} \min_{\beta,\mathbf{u}} \quad & \beta \\ \text{subject to} \quad & \sum_{i=1}^{m} u_i y_i \mathbf{H}_{ij} \leq \beta,\ j = 1,\ldots,N, \\ & \sum_{i=1}^{m} u_i = 1,\ 0 \leq u_i \leq D. \end{aligned}$$

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Column generation

Can solve the dual linear programme using an iterative method:

1. initialise $u_i = 1/m, i = 1, \ldots, m$, $\beta = \infty$, $J = \emptyset$
2. choose $j^\star$ that maximises $f(j) = \sum_{i=1}^{m} u_i y_i \mathbf{H}_{ij}$
3. if $f(j^\star) \leq \beta$ solve primal restricted to J and exit
4. $J = J \cup \{j^\star\}$
5. Solve dual restricted to set J to give u_i, β
6. Go to 2

- Note that u_i is a distribution on the examples
- Each j added acts like an additional weak learner
- $f(j)$ is simply the weighted classification accuracy
- Hence gives 'boosting' algorithm - with previous weights updated satisfying error bound
- Guaranteed convergence and soft stopping criterion

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Multiple kernel learning

- MKL puts a 1-norm constraint on a linear combination of kernels:

$$\left\{ \kappa(\mathbf{x}, \mathbf{z}) = \sum_{t=1}^{N} z_t \kappa_t(\mathbf{x}, \mathbf{z}) : z_t \geq 0, \sum_{t=1}^{N} z_t = 1 \right\}$$

  and trains an SVM while optimizing z_t – a convex problem,

- equivalent to performing Linear Programming boosting over the (infinite) set of functions

$$\mathcal{F} = \bigcup_{t=1}^{N} \mathcal{F}_t$$

  where $\mathcal{F}_t = \{\mathbf{x} \to \langle \mathbf{w}, \phi_t(\mathbf{x}) \rangle : \|\mathbf{w}\| \leq 1\}$.

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Multiple kernel learning

- The corresponding Rademacher bound gives

$$P(y \neq \mathrm{sgn}(g(\mathbf{x}))) \leq \frac{1}{m\gamma}\sum_{i=1}^{m}\xi_i + \frac{1}{\gamma}\hat{R}_m\left(\bigcup_{t=1}^{N}\mathcal{F}_t\right) + 3\sqrt{\frac{\ln(2/\delta)}{2m}}$$

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Bounding MKL

- First further applications of McDiarmid gives with probability $1-\delta_0$ of a random selection of σ^*:

$$\hat{R}_m(\mathcal{F}) \leq \frac{2}{m} \sup_{f\in\mathcal{F}} \sum_{i=1}^{m} \sigma_i^* f(\mathbf{x}_i) + 4\sqrt{\frac{\ln(1/\delta_t)}{2m}}$$

and

$$\frac{2}{m} \sup_{f\in\mathcal{F}_t} \sum_{i=1}^{m} \sigma_i^* f(\mathbf{x}_i) \leq \hat{R}_m(\mathcal{F}_t) + 4\sqrt{\frac{\ln(1/\delta_t)}{2m}}$$

with probability $1-\delta_t$

Bounding MKL

- Hence taking $\delta_t = \delta/2(N+1)$ for $t = 0, \ldots, N$

$$\hat{R}_m\left(\mathcal{F} = \bigcup_{t=1}^{N} \mathcal{F}_t\right)$$

$$\leq \frac{2}{m} \sup_{f \in \mathcal{F}} \sum_{i=1}^{m} \sigma_i^* f(\mathbf{x}_i) + 4\sqrt{\frac{\ln(2(N+1)/\delta)}{2m}}$$

$$\leq \frac{2}{m} \max_{1 \leq t \leq N} \sup_{f \in \mathcal{F}_t} \sum_{i=1}^{m} \sigma_i^* f(\mathbf{x}_i) + 4\sqrt{\frac{\ln(2(N+1)/\delta)}{2m}}$$

$$\leq \frac{2}{m} \max_{1 \leq t \leq N} \hat{R}_m(\mathcal{F}_t) + 8\sqrt{\frac{\ln(2(N+1)/\delta)}{2m}}$$

with probability $1 - \delta/2$.

Bounding MKL

- This gives an overall bound on the generalisation of MKL of

$$P(y \neq \mathrm{sgn}(g(\mathbf{x}))) \leq \frac{1}{m\gamma}\sum_{i=1}^{m}\xi_i + \frac{2}{\gamma m}\max_{1\leq t\leq N}\mathrm{tr}(\mathbf{K}_t) + \frac{8}{\gamma}\sqrt{\frac{\ln(2(N+1)/\delta)}{2m}} + 3\sqrt{\frac{\ln(4/\delta)}{2m}}$$

  where $\mathbf{K}_t$ is the t-th kernel matrix.

- Bound gives only a logarithmic dependence on the number of kernels.

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Experimental results with large-scale MKL

- Vedaldi et al. have applied to the PASCAL Visual Objects Challenge (VOC 2007) data and
  - improvements over the winners of the challenge in 17 out of the 20 categories
  - in more than half of the categories the increase in average precision was over 25%
  - have also scaled effectively to millions of kernels

$\star$ A. Vedaldi, V. Gulshan, M. Varma and A. Zisserman. Multiple kernels for object detection. In Proceedings CVPR, Kyoto, Japan, September 2009.

Linear Programming MKL

- Column generation gives efficient MKL if we can pick the best weak learner in each $\mathcal{F}_t$ efficiently:

$$\begin{aligned}
\sup_{f\in\mathcal{F}_t}\sum_{i=1}^{m}u_i y_i f(\mathbf{x}_i) &= \sup_{\mathbf{w}:\|\mathbf{w}\|\le 1}\sum_{i=1}^{m}u_i y_i \langle \mathbf{w}, \phi_t(\mathbf{x}_i)\rangle \\
&= \sup_{\mathbf{w}:\|\mathbf{w}\|\le 1}\left\langle \mathbf{w}, \sum_{i=1}^{m}u_i y_i \phi_t(\mathbf{x}_i)\right\rangle \\
&= \left\|\sum_{i=1}^{m}u_i y_i \phi_t(\mathbf{x}_i)\right\| \\
&= \sqrt{\mathbf{u}'\mathbf{Y}\mathbf{K}_t\mathbf{Y}\mathbf{u}} =: N_t
\end{aligned}$$

easily computable from the kernel matrices (note that $\mathbf{u}$ is sparse after first iteration and can also be chosen sparse at the start).

Linear Programming MKL

- The optimal weak learner from $\mathcal{F}_t$ is realised by the weight vector that achieves the supremum

$$\mathbf{w} = \frac{\sum_{i=1}^{m} u_i y_i \phi_t(\mathbf{x}_i)}{\|\sum_{i=1}^{m} u_i y_i \phi_t(\mathbf{x}_i)\|}$$

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Frontiers of Machine Learning

- Deep learning has (re-)emerged as having important research and commercial value
- Deep belief networks and related approaches have led this charge
- Kernels are sometimes referred to as 'shallow'
- Now consider:
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  - possible integration of kernel and deep methods

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Why Shallow Learning?

- Kernels learn non-linear functions in the input space so would appear to be as flexible as deep learning systems
- However, they actually implement linear functions in the kernel defined feature space:

$$\mathbf{x} \longmapsto_{\text{fixed}} \phi(\mathbf{x}) \longmapsto_{\text{learned}} \langle \mathbf{w}, \phi(\mathbf{x}) \rangle$$

  so that the learning (of $\mathbf{w}$) only occurs in one 'layer'.
- This is contrasted with deep learning where parameters are spread across several layers typically with non-linear transfer functions
  - Learning of the deeper layers is often unsupervised with the final classifier trained with the earlier layers fixed
  - Hence, we are effectively pre-learning a representation – this would be analogous to learning the kernel

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What happens in practice?

- In practice we typically do perform some learning of the kernel:
  - fix some hyper-parameters via some heuristic (e.g. width σ of a Gaussian kernel)
  - use cross-validation to adapt the hyperparameter to optimise performance of the task (classification, regression, etc)
- In some respects this undermines the more principled approach espoused by kernel methods based on generalisation bounds:
  - standard generalisation bounds no longer apply if we choose the feature space based on the training data
  - even test set bounds will be invalidated if we include the testing data in the representation learning phase
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Kernel defined features spaces

- Kernels define a feature space implicitly via a function $\kappa(\cdot,\cdot)$ that computes an inner product:
  - symmetric:

$$\kappa(\mathbf{x},\mathbf{z}) = \langle\phi(\mathbf{x}),\phi(\mathbf{z})\rangle = \langle\phi(\mathbf{z}),\phi(\mathbf{x})\rangle = \kappa(\mathbf{z},\mathbf{x})$$

  - kernel matrices are positive semi-definite:

$$\begin{aligned}\mathbf{u}'\mathbf{K}\mathbf{u} &= \sum_{i,j=1}^{m} u_i u_j \langle\phi(\mathbf{x}_i),\phi(\mathbf{x}_j)\rangle \\ &= \left\langle \sum_{i=1}^{m} u_i\phi(\mathbf{x}_i), \sum_{j=1}^{m} u_j\phi(\mathbf{x}_j)\right\rangle \\ &= \left\| \sum_{i=1}^{m} u_i\phi(\mathbf{x}_i)\right\|^2 \geq 0\end{aligned}$$

Kernel functions

- These two properties are all that is required for a kernel function to be valid: symmetric and every kernel matrix is psd.
- Implies that we can define kernels on virtually any objects provided these properties are satisfied, eg documents, graphs, networks, etc.
- Many standard linear algorithms can be implemented in the kernel defined feature space using a dual representation of the weight vectors – typically requires regularisation of the 2-norm
- Examples: ridge regression, PCA, CCA, SVMs, etc.

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Generating the feature space

Proof outline:

- Define feature space as class of functions:

$$\mathcal{F} = \left\{ \sum_{i=1}^{m} \alpha_i \kappa(\mathbf{x}_i, \cdot) \; : \; m \in \mathbb{N}, \; \mathbf{x}_i \in X, \; \alpha_i \in \mathbb{R}, \; i = 1, \ldots, m \right\}$$

- Linear space with inner product defined by $\langle \kappa(\mathbf{x}, \cdot), \kappa(\mathbf{z}, \cdot) \rangle = \kappa(\mathbf{x}, \mathbf{z})$
- embedding given by

$$\mathbf{x} \longmapsto \kappa(\mathbf{x}, \cdot)$$

- Note reproducing property: for a function $f \in \mathcal{F}$

$$f(\mathbf{x}) = \langle f, \kappa(\mathbf{x}, \cdot) \rangle$$

so called *Reproducing Kernel Hilbert Space (RKHS)*

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Mean Embeddings

- If there is a distribution $\mathcal{D}$ on the input space it defines a point $\mu_{\mathcal{D}}$ in the feature space:

$$\mu_{\mathcal{D}} = \mathbb{E}_{\mathbf{x}\sim\mathcal{D}}[\phi(\mathbf{x})]$$

- and its empirical counterpart for a finite sample S:

$$\hat{\mu}_S = \mathbb{E}_{\mathbf{x}\sim S}[\phi(\mathbf{x})] = \hat{\mathbb{E}}[\phi(\mathbf{x})]$$

- Surprisingly, despite their being no restriction on the dimensionality of $\mathcal{F}$, if $\mathcal{D}$ has support in the R ball, with probability at least $1-\delta$ over an iid sample S

$$\|\mu_{\mathcal{D}} - \hat{\mu}_S\| \leq \frac{R}{\sqrt{m}}\left(2 + \sqrt{2\ln\frac{1}{\delta}}\right)$$

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- Since $\mathcal{F}$ is a space of functions, using the reproducing property we can also estimate expectations for $f \in \mathcal{F}$

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- similarly for its empirical counterpart and furthermore we can bound the error of the empirical estimate:

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Conditional Mean Embeddings

- It is natural to ask if we can generalise these ideas to conditional distributions $P(X|Y)$
- Now the distribution and hence mean embedding is a function of Y

$$\mu_{P(X|Y)} = \mu(Y) \in \mathcal{F}$$

- Hence $\mu : Y \longrightarrow \mathcal{F}$ can be viewed as a regressor, albeit into a Hilbert space.

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- Reinforcement Learning models agents that learn through acting in an environment and receiving reward
- AKA Markov Decision Processes:
  - set of states $\mathcal{S}$
  - set of actions $\mathcal{A}$
  - Markov transition kernel $P(s'|s,a)$
  - reward function $r : \mathcal{S} \times \mathcal{A} \to [0,1])$
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Experience in RL

- Agent experience: $\xi = (S_1, A_1, S_2, A_2, \ldots)$
- $S_1 \sim P_1$, $A_t \sim \pi(S_t)$, $S_{t+1} \sim P(\cdot|S_t, A_t)$
- Expected return:

$$J(\pi) = \mathbb{E}\left[\sum_{t=1}^{\infty} \gamma^{t-1} r(S_t, A_t)|\pi\right]$$

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Linear representations of the Value function

- Can assume a linear form for V^π:

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- Recall if $V(s) = \langle v, \phi(s) \rangle$ then

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- We learn regressor $\hat{\mu}$ using training loss

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- so reduced to finite MDP
- Size of the MDP rapidly becomes infeasible - so now turn to methods to control the number of states

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- Solution has the form $\hat{\mu}(s,a) = \sum_{i=1}^{m} \alpha_i(s,a)\phi(s_i')$
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Greedy compression set

`augmentCompressionSet`$(\mathcal{C}, \delta, \mathcal{P})$

Input: Initial compression set $\mathcal{C} = c_1, ..., c_m$, candidates $\mathcal{P} = s'_1, ..., s'_n$, tolerance δ

for $j = 1, 2, ..., n$ **do**

if $\min_{\boldsymbol{b} \in \mathbb{R}^m, ||\boldsymbol{b}||_1 \leq 1} || \sum_{i=1}^m b_i \phi(c_i) - \phi(s'_j) ||_{\mathcal{F}} > \delta$ **then**

Augment compression set: $\mathcal{C} \leftarrow \mathcal{C} \cup s'_j$, $m \leftarrow m + 1$

end if

end for

- For learning the α coefficients:

$$\alpha_j(s, a) = \sum_{i=1}^{m} K((s, a), (s_i, a_i)) W_{ij}$$

we have a regression problem – again with high complexity – turn to matching pursuit

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Matching pursuit

- Matching pursuit greedily chooses training examples that determine directions in feature space that are well-suited to some task and then deflates
- Analysis combining sparse reconstruction with generalisation error bounds gives first bounds on performance in learnt subspace
- Allows different criteria for selection to be implemented in one framework, eg sparse PCA, classification, regression, canonical correlation analysis, etc. and all come with bounds

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Matching pursuit for KCCA

Require: two views $\mathbf{K}_x$, $\mathbf{K}_y$ and sparsity parameter $k > 0$.

1: initialise index vector $\mathbf{i} = [\,]$ and an all one vector $\mathbf{1}$.

2: **for** $i = 1$ to k **do**

3: set $\mathbf{i}_i$ to index of $\max_i \frac{\mathbf{K}_x[:,i]'\mathbf{K}_y[:,i]}{\sqrt{\mathbf{K}_x^2[i,i]\mathbf{K}_y^2[i,i]}}$

4: set $\boldsymbol{\tau}_x = \mathbf{K}_x[:,\mathbf{i}_i]$ and $\boldsymbol{\tau}_y = \mathbf{K}_y[:,\mathbf{i}_i]$ to deflate kernel matrices:

$$\mathbf{K}_x = \mathbf{K}_x - \frac{\boldsymbol{\tau}_x\left(\boldsymbol{\tau}_x'\mathbf{K}_x\right)}{\boldsymbol{\tau}_x'\boldsymbol{\tau}_x}$$

$$\mathbf{K}_y = \mathbf{K}_y - \frac{\boldsymbol{\tau}_y\left(\boldsymbol{\tau}_y'\mathbf{K}_y\right)}{\boldsymbol{\tau}_y'\boldsymbol{\tau}_y}$$

5: **end for**

6: solve KCCA on points indexed by final $\mathbf{i}$ to find $\tilde{\boldsymbol{\alpha}}_x$ and $\tilde{\boldsymbol{\alpha}}_y$ the duals of the projection vectors.

Matching pursuit bound plot

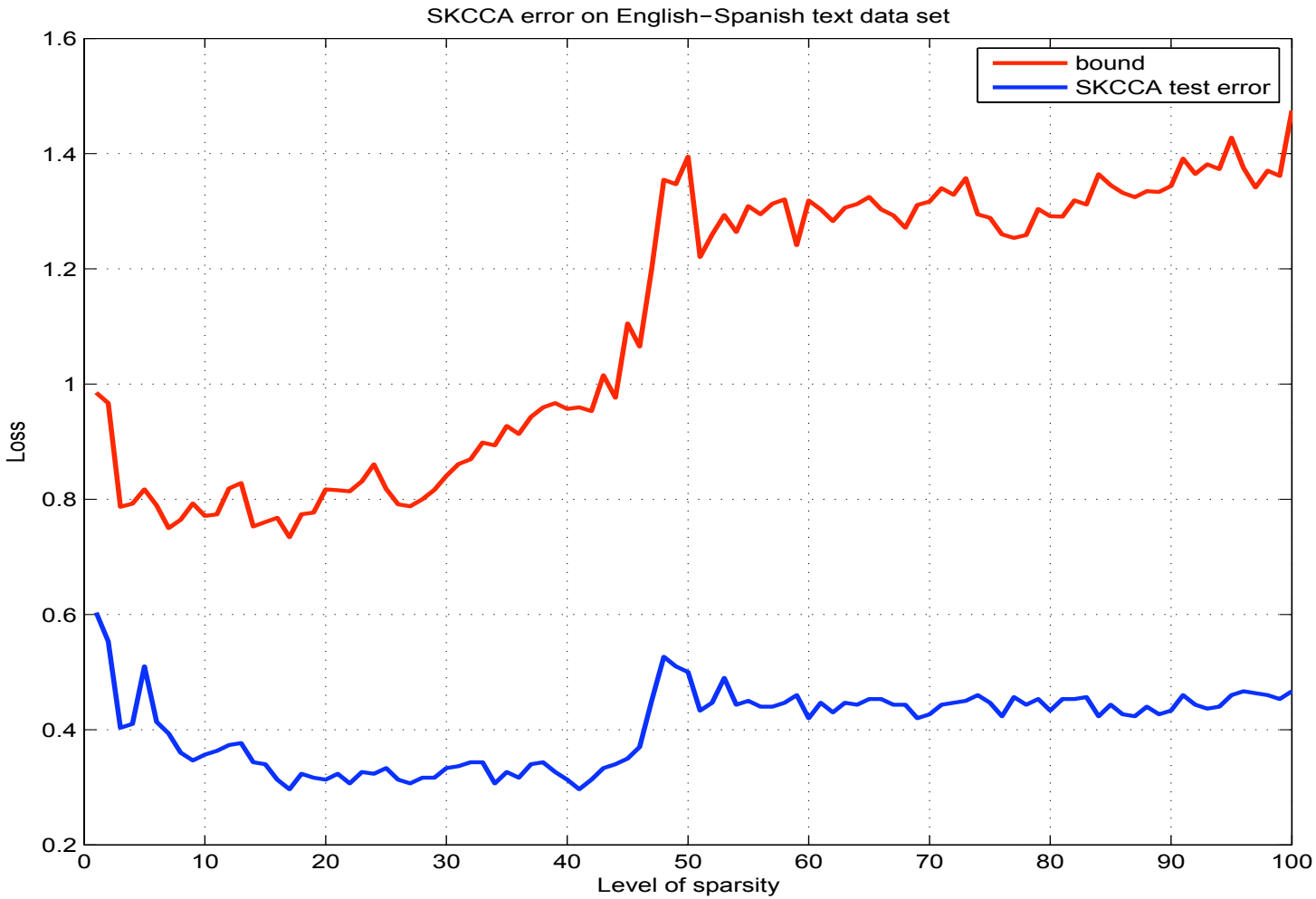


Figure: Bound plot for sparse KCCA using 1-dimension.

Policy iteration with Compressed kernel CMEs

for $k = 1, 2, \ldots$ **do**

$\mathcal{C}_k = \text{augmentCompressionSet}(\mathcal{C}_{k-1}, \{s'_i\}_{i=n_{k-1}+1}^{n_k}, \delta)$.

$\mathcal{G}_k = \mathcal{B}_{k-1} \cup \{K(\cdot, (s_i, a_i))\}_{i=n_{k-1}+1}^{n_k}$

Sparse basis selection: Learn sparse basis $\mathcal{B}_k = \{K(\cdot, (\hat{s}_\ell, \hat{a}_\ell))\}_{\ell=1}^{d_k}$, $d_k \leq d$ from candidates $\mathcal{G}_k$ using matching pursuit; Set $\psi_\ell^k(\cdot) = K((\hat{s}_\ell, \hat{a}_\ell), \cdot)$,

$\mathbf{\Psi}_k = \left(\psi^k(s_1, a_1), \ldots, \psi^k(s_{n_k}, a_{n_k})\right)^\top$.

$\mathbf{W}_k^{CMP} = (\mathbf{\Psi}_k^\top \mathbf{\Psi}_k + \lambda \mathbf{K})^{-1} \mathbf{\Psi}_k^\top \mathbf{L}^{DC} (\mathbf{L}^{CC})^{-1}$.

for $\ell = 1, 2, \ldots, J$ **do**

Policy evaluation: Using finite pseudo-MDP dynamics $\alpha^{PCMP}(c_j, a)$ for $a \in \mathcal{A}$, $c_j \in \mathcal{C}$ solve approximate Bellman Equation to obtain estimate $\hat{V}_\ell$ of V^{π_k} at the compression points $c_j \in \mathcal{C}$. Set

$\hat{Q}_\ell(s, a) = r(s, a) + \gamma \sum_{j=1}^{|\mathcal{C}_k|} \alpha_j^{PCMP}(s, a) \hat{V}_\ell(c_j)$.

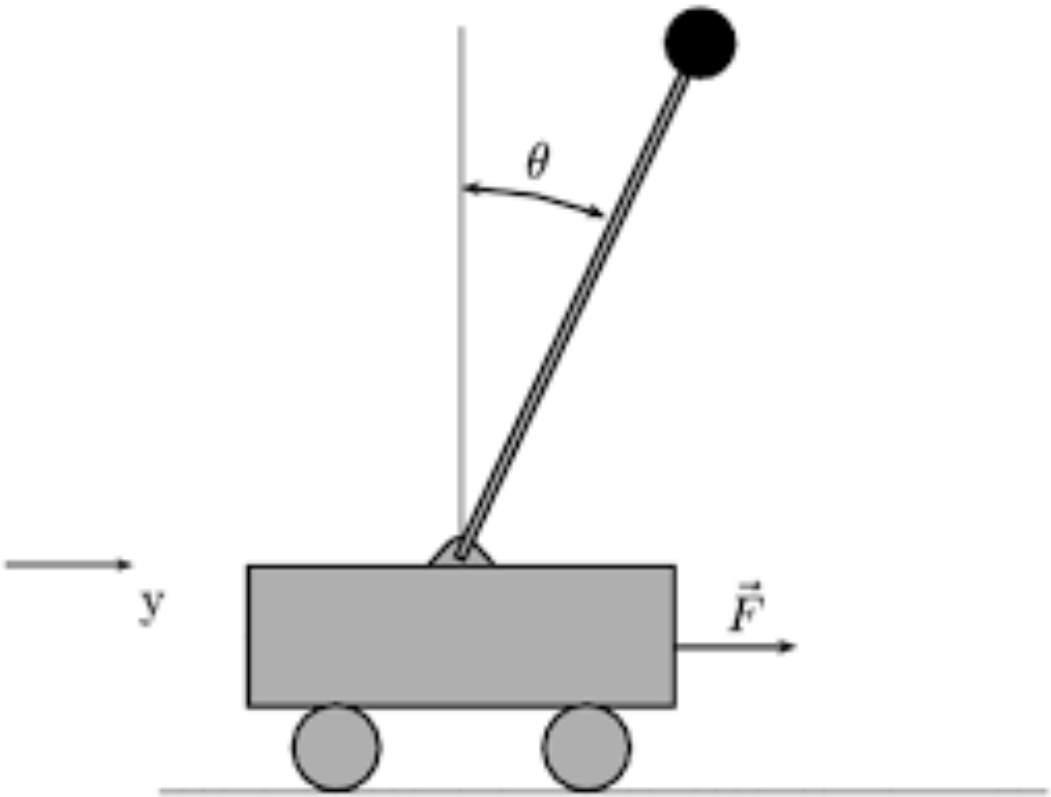
Policy improvement: $\pi_k \leftarrow \text{greedy}(\hat{Q}_\ell)$.

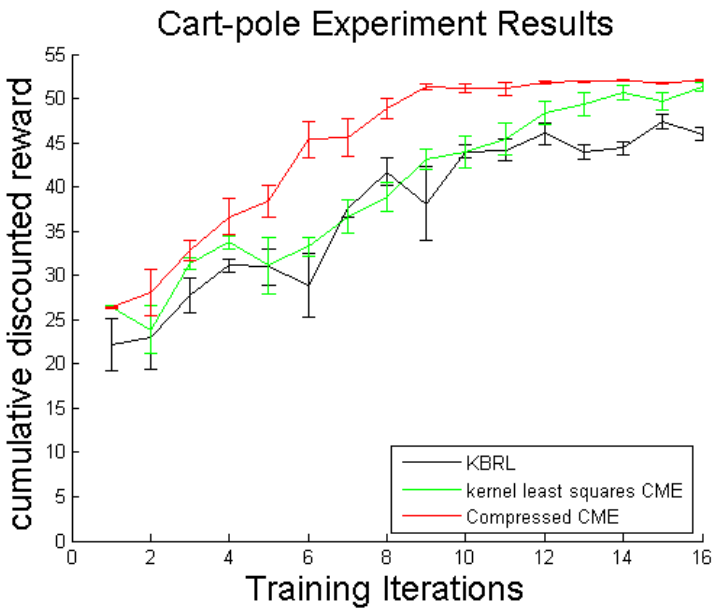
end for

Experiments: Cart-pole benchmark

Simulated under-actuated cart-pole swing-up benchmark problem

- $\mathcal{S} = \mathbb{R}^2$, $s = (\theta, \dot{\theta})$, $\mathcal{A} = [-50, 50]$, horizontal force in newtons





Experiments: Quadrocopter Simulator

Simulator calibrated to model the dynamics of Pelican^{TM} quadrocopter platforms
$\mathcal{S} \subset \mathbb{R}^{13}$, $s = (x, y, z, \theta\, \phi, \psi, \dot{x}, \dot{y}, \dot{z}, \dot{\theta}, \dot{\phi}, \dot{\psi}, F)$
$\mathcal{A} \subset \mathbb{R}^3$ represents desired velocity vectors, PID controller translates into low level commands
Tasks:

- Navigation: platform must navigate to point
- Holding pattern: platform must stay in circle and maintain minimum velocity

Experiments: Quadrocopter Results

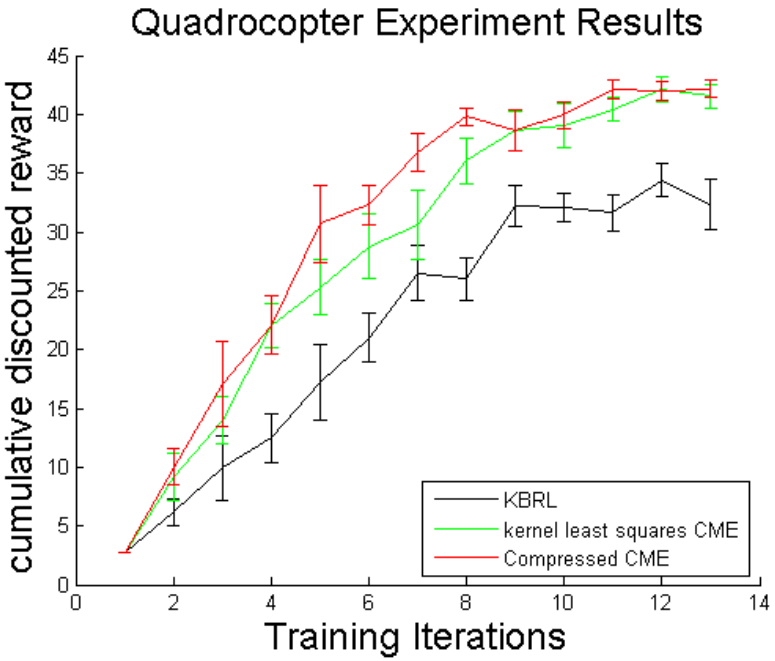


Figure: Quadrocopter tasks: navigation and holding pattern

RKHS controller **better in high-dim. state-space**

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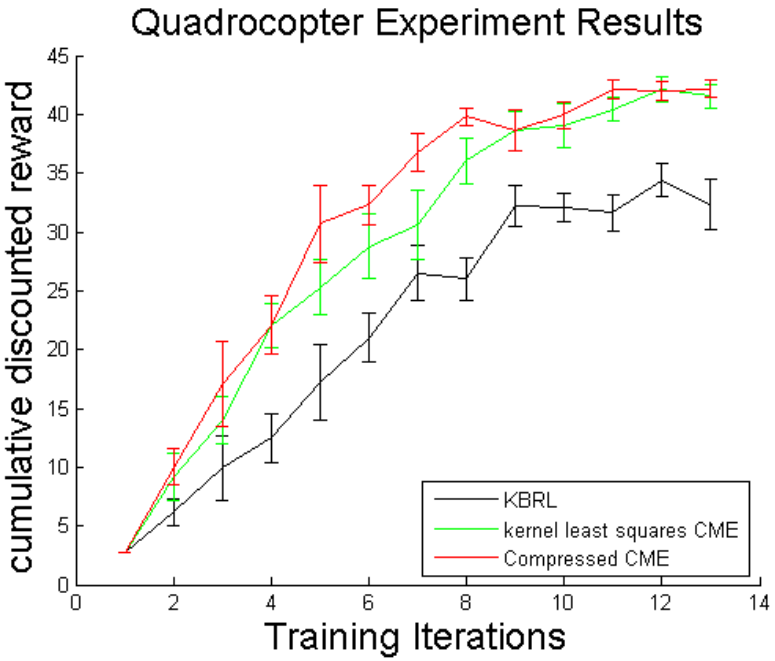

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Deep Learning models

- Deep learning models allow learning more complex models through multiple layers of parameters
- This means that the optimisation space is no longer convex and typically the problem is cast as seeking a local minimum through (stochastic) gradient descent
- Remarkably the generalisation performance does not seem to be adversely affected by using such flexible models
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Motivation

- Stochastic Gradient Descent uses mini-batches to derive noisy gradient estimates
- Simplest approach is average of gradients, but can include longer averages
- Conjugate gradient methods exploit second order information
- Can more be extracted from mini-batch gradients exploiting the fact that they represent an i.i.d. sample of the data distribution?

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Key idea

- View weight update direction as a classifier of the mini-batch: correct classification if reducing its error, incorrect if increasing its error
- This is ignoring second order effects: i.e. for small weight updates will hold

$$f^j(\mathbf{w} + \delta\mathbf{w}, \mathbf{x}_i) \approx f^j(\mathbf{w}, \mathbf{x}_i) + \langle \delta\mathbf{w}, \nabla f^j(\mathbf{w}, \mathbf{x}_i) \rangle$$

- Have a target reduction of ϵ
- In order to minimise second order effects, we need to choose a minimum norm update that has the desired error reductions
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Update optimisation to choose $\delta\mathbf{w}$

1: Minimise $\frac{1}{2}\|\delta\mathbf{w}\|^2 + C\sum_{i=1}^{\ell}\sum_{j=1}^{K}\xi_{ij}$
2: Subject to: $y_{ij}\langle\delta\mathbf{w}, \nabla f^j(\mathbf{w}, \mathbf{x}_i)\rangle \geq \epsilon - \xi_{ij}$ $\xi_{ij} \geq 0$, $i = 1, \ldots, \ell; j = 1, \ldots, K$

this is an SVM optimisation (with target margin ϵ).

The dual optimisation is

1: Max $\epsilon\sum_{ij}\alpha_{ij} - \frac{1}{2}\sum_{ijkl}\alpha_{ij}\alpha_{kl}\kappa((\mathbf{x}_i, j), (\mathbf{x}_k, l))$
2: Subject to: $C \geq \alpha_{ij} \geq 0$

where $\kappa((\mathbf{x}_i, j), (\mathbf{x}_k, l)) = \langle\nabla f^j(\mathbf{w}, \mathbf{x}_i), \nabla f^l(\mathbf{w}, \mathbf{x}_k)\rangle$

Analysis

- Since data generated iid, can use generalisation bounds to analyse the effects of the weight update
- The following bound holds

$$\mathbb{E}_{\mathcal{D}}[(\epsilon - y_j\langle \delta\mathbf{w}, \nabla f^j(\mathbf{w}, \mathbf{x})\rangle)_+] \leq A = \frac{1}{\ell\epsilon}\sum_{ij}\xi_{ij} + \frac{4\|\delta\mathbf{w}\|}{\epsilon\ell}\sqrt{\mathrm{tr}(\mathbf{K})} + 3\sqrt{\frac{\ln(2/\delta)}{2\ell}}$$

- Hence, ignoring second order effects, for an $\eta\delta\mathbf{w}$ weight update, the average hinge loss across the whole training (and test) set will with high probability reduce by at least

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Optimization

$\eta = 0.1$; $r = 1.0$; $\ell =$ initial batch size
for $i \in [1, 2, \cdots, num\_iter]$ **do**
  $\mathcal{B}_s \leftarrow$ generateMinibatches($\mathcal{D}$, ℓ)
  $\delta \mathbf{w} \leftarrow$ trainMinibatch($\mathcal{B}_s$, $\mathcal{C}$, r)
  bound_term $= \|\delta \mathbf{w}\| \sqrt{tr(\mathbf{K})}/\ell$
  while bound_term $>$ threshold **do**
    $\ell \leftarrow 2 * \ell$ #minibatch size
    $r \leftarrow 0.1 * r$ #SVM Regularizer
    $\mathcal{B}_s \leftarrow$ generateMinibatches($\mathcal{D}$, ℓ)
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    bound_term $= \|\delta \mathbf{w}\| \sqrt{tr(\mathbf{K})}/\ell$
  end while
  $\mathbf{w} \leftarrow \mathbf{w} + \eta * \delta \mathbf{w}$
end for

Datasets

- MNIST: It consists of images of handwritten digits in binary. It has a training set of 60,000 examples, and a test set of 10,000 examples.
- CIFAR-10: It consists of 60000 32x32 colour images in 10 classes, with 6000 images per class.

Convergence

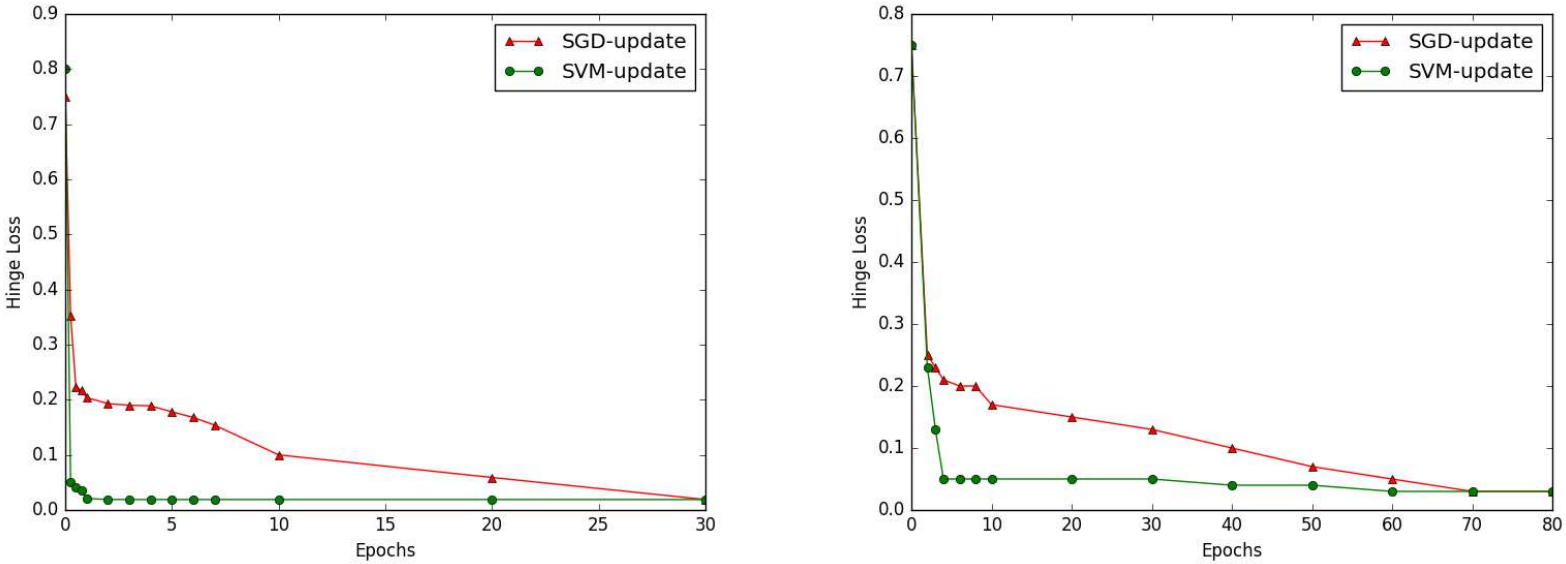

Figure: **Left**: MNIST & **Right**: CIFAR. We plot the hinge loss over train set versus epochs.

Accuracy

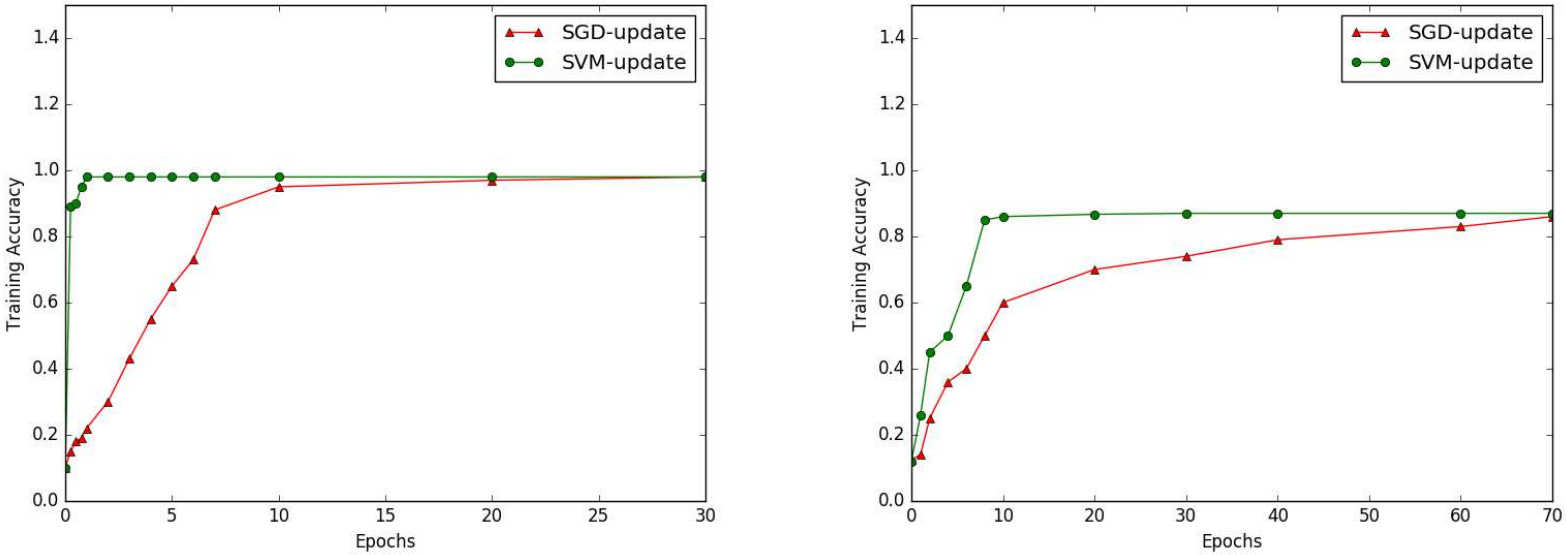

Figure: **Left**: MNIST & **Right**: CIFAR. We plot the training accuracy over the entire train set versus epochs.

Generalization

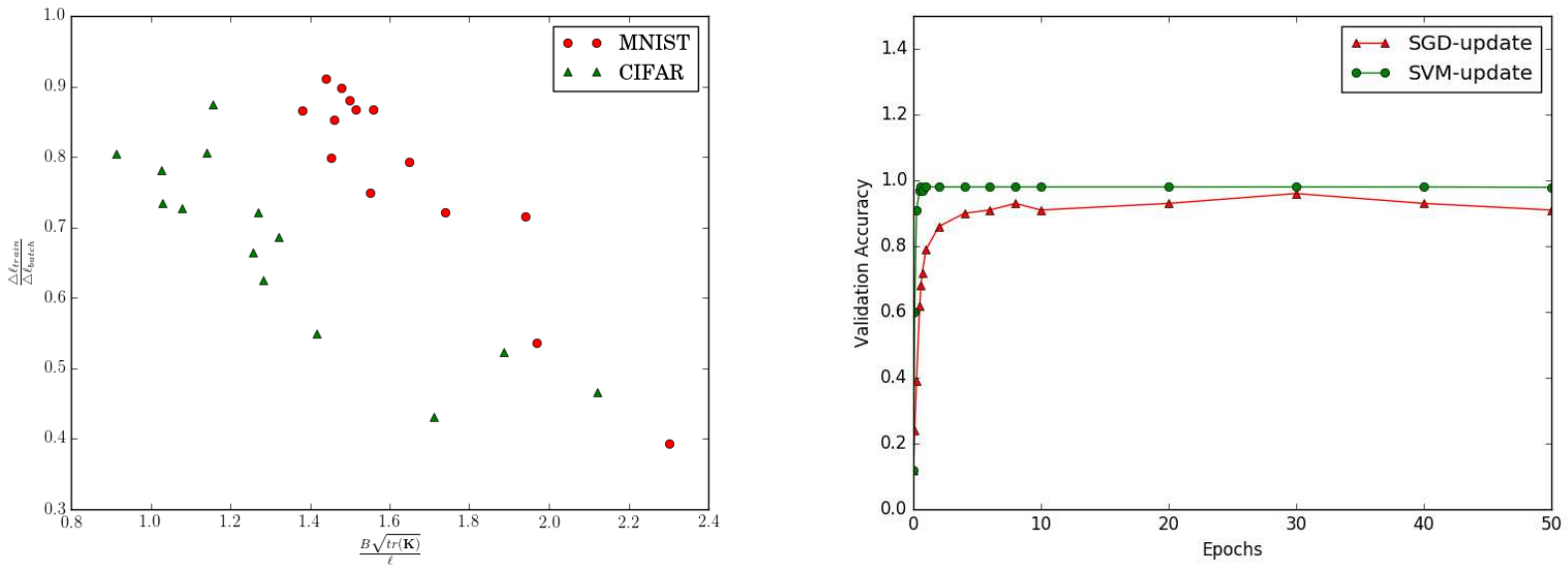

Figure: **Left**: We see that the ratio of decrease in loss over train set and mini-batch decreases with increase in the bound, implying that the updates become less generalized. **Right**: We observe that the validation accuracy initially increases and then stabilizes for mnist using our algorithm, as opposed to sgd.

Robustness: Adversarial Noise

Norm	MNIST		CIFAR	
	sgd-based	svm-based	sgd-based	svm-based
frobenius	5.12	7.32	7.95	9.25
infinity	5.90	8.11	6.50	8.57
nuclear	7.29	8.11	8.50	9.12
1-norm	6.23	7.59	7.40	9.10

Table: We give details of the additive adversarial noise learned for **left**: MNIST and **right**: CIFAR using traditional back-propagation and svm-based updates. Additive adversarial noise is the minimum amount of noise to be added to images such that the network misclassifies them.

Summary and Conclusions

- Introduction to pattern analysis and machine learning through the perspective of kernel methods
- Emphasis on the need to assess and improve generalisation: analysis provided through Radmacher Complexity
- Attempts to use principled methods for complex tasks such as Reinforcement Learning have met with considerable success
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