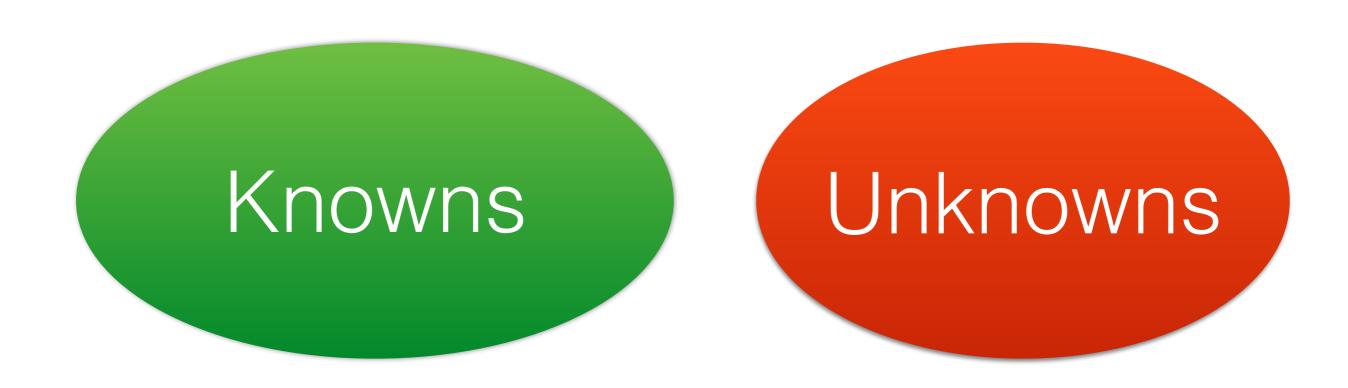
Selective Classification for Deep Neural Networks

Yonatan Geifman, Ran El-Yaniv

Motivation

- Would you let a 95% accuracy CNN examine your MRI scans?
- Would you let a 54% accuracy classifier invest your funds?
- Would you fall a sleep in a 99% accurate autonomous car?

Knowledge



Knowledge

Known knowns Known unknowns

Unknown unknowns

Statistical Learning

- Underlying unknown distribution P(X,Y)
- A labeled set $S_m = \{(x,y)\}^m \sim P$
- Our goal is to find $f \in \mathcal{F}$ that minimizes the risk:

$$R(f) \triangleq E_P[\ell(f(x), y)]$$

Selective Classification

• Selective Classifier is a pair (f,g)

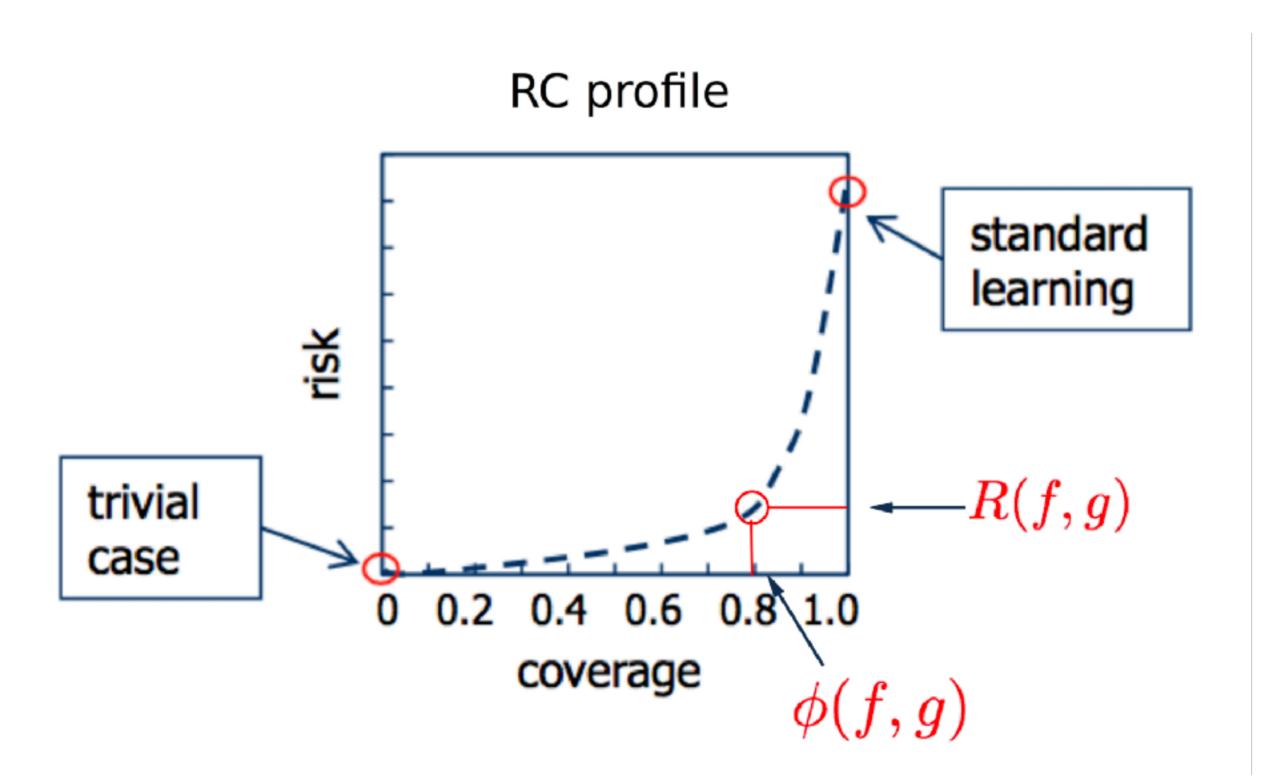
$$(f,g)(x) = \begin{cases} f(x), & \text{if } g(x) = 1; \\ \text{don't know}, & \text{if } g(x) = 0. \end{cases}$$

Coverage:

$$\phi(f,g) \triangleq E_P[g(x)]$$

• Risk: $R(f,g) \triangleq \frac{E_P[\ell(f(x),y)g(x)]}{\phi(f,g)}$.

Selective Classification



Related Areas

active learning

pointwisecompetitive selective

selective prediction

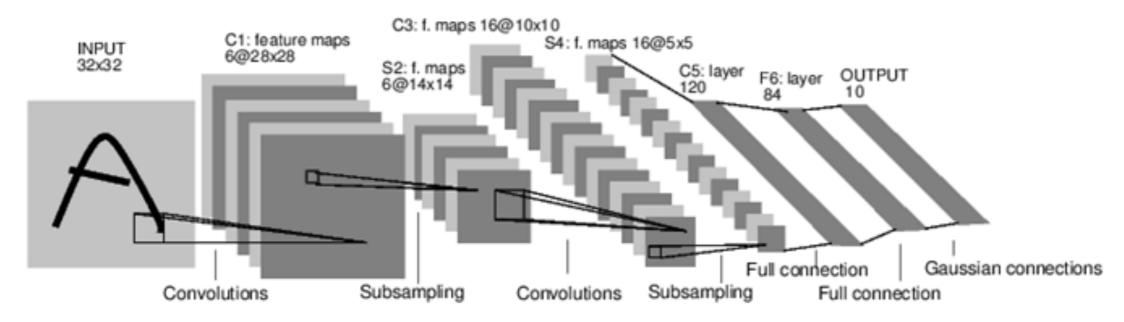
self-aware learning

classification with a reject option

confidence-rated prediction

Deep Neural Networks

- Multiple layers of processing units
- Feature representations learned at each layer
- Low level features to high level
- In this work we focus on convolutional neural networks



Confidence Rate Functions

• For a classifier f, We seek for a confidence rate function κ_f that reflects loss monotonicity

$$\kappa_f(x_1) \le \kappa_f(x_2) \iff \ell(f(x_1), y_1) \ge \ell(f(x_2), y_2)$$

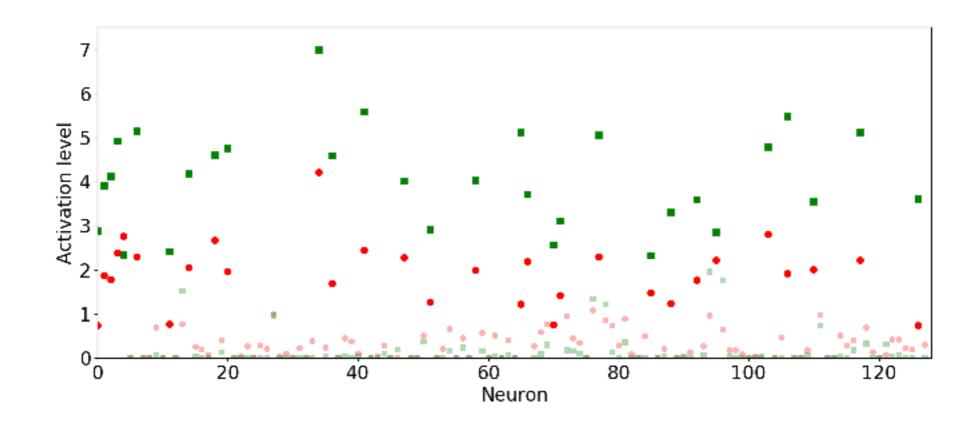
- We discuss two candidates:
 - SOFTMAX response
 - MC-Dropout

Confidence - Softmax Response

• Simply take κ to be the Softmax output

$$\kappa_f \triangleq \max_{j \in \mathcal{Y}} (f(x|j))$$

Motivation - MNIST activations:



Confidence - MC-Dropout

- Apply dropout at inference
- Estimate prediction variance over numerous (100) forward passes with dropout (p=0.5)
- Intuition kind of ensemble variance

Gal, Yarin, and Zoubin Ghahramani. "Dropout as a Bayesian approximation: Representing model uncertainty in deep learning."

Selection with Guaranteed Risk (SGR)

 A selective classifier obtained by thresholding the confidence rate function

$$g_{\theta}(x) \triangleq \begin{cases} 1, & \text{if } \kappa_f(x) \ge \theta; \\ 0, & \text{otherwise.} \end{cases}$$

• Given a training set S_m , a desired risk r^* , and a confidence parameter δ , our goal is to learn a selective classifier such that:

$$Pr_{S_m} \{ R(f, g) > r^* \} < \delta$$

Lemma 1 - Binomial Tail

• Let $B^*(\hat{r}_i, \delta, S_m)$ be the solution b of the following equation

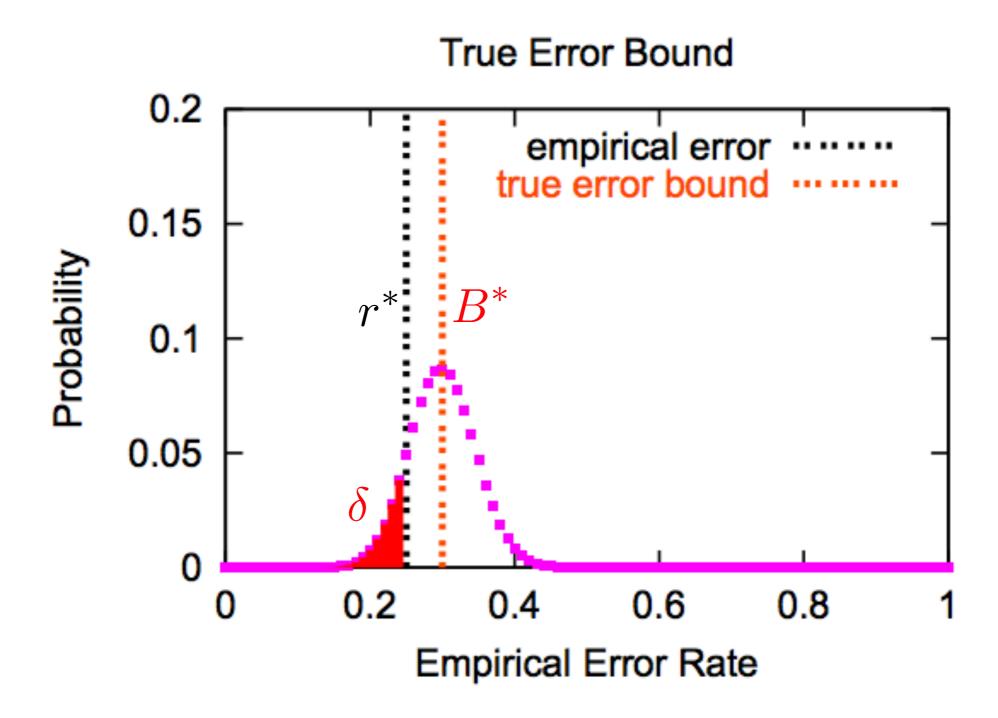
$$\sum_{j=0}^{m \cdot \hat{r}(f|S_m)} {m \choose j} b^j (1-b)^{m-j} = \delta.$$

Then

$$Pr_{S_m}\{R(f|P)>B^*(\hat{r}_i,\delta,S_m)\}<\delta$$

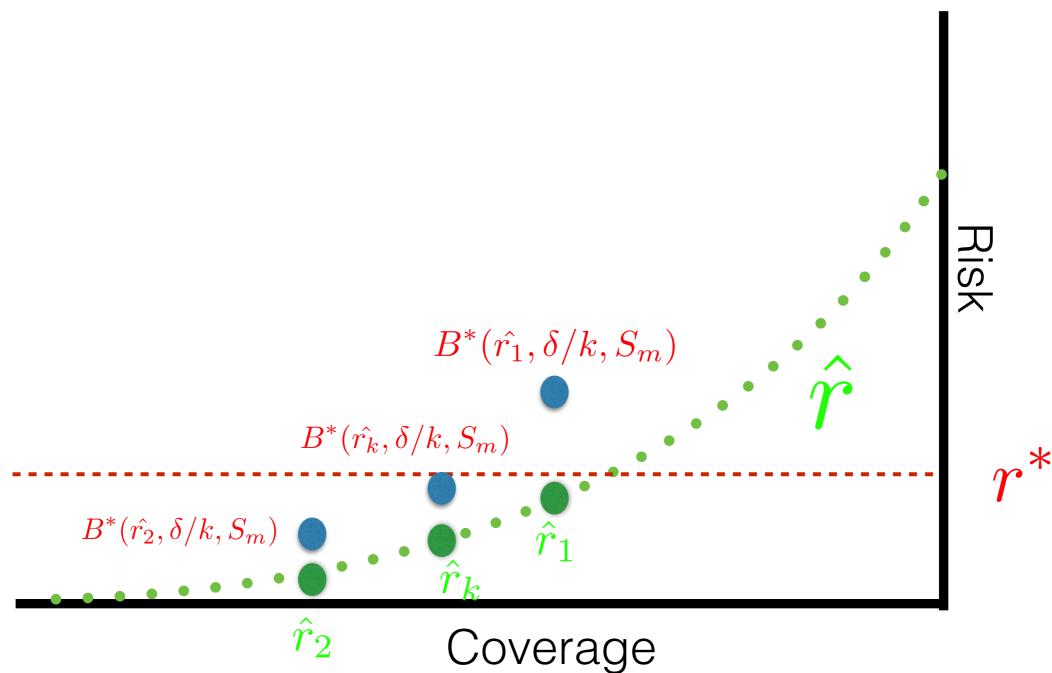
O. Gascuel and G. Caraux. Distribution-free performance bounds with the resubstitution error estimate.

Lemma 1 - Binomial Tail



Langford, John. "Tutorial on practical prediction theory for classification."

- For a given training set $S_m \sim P(X,Y)$, a desired risk r^* and a confidence parameter δ
- set $k = \lceil \log(m) \rceil$
- Use binary search to find $\hat{\theta} \in \{\kappa(x) : x \in S_m\}$ such that $B^*(\hat{r}_{\theta}, \delta/k, S_m) \leq r^*$



Algorithm 1 Selection with Guaranteed Risk (SGR)

16: Output- (f, g_k) and the bound b_k^* .

```
1: SGR(f, \kappa_f, \delta, r^*, S_m)
 2: Sort S_m according to \kappa_f(x_i), x_i \in S_m (and now assume w.l.o.g. that indices reflect this
    ordering).
 3: z_{\min} = 1; z_{\max} = m
 4: for i = 1 to k \triangleq \lceil \log_2 m \rceil do
      z = \lceil (z_{\min} + z_{\max})/2 \rceil
     \theta = \kappa_f(x_z)
       g_i = g_\theta \ \{ (\text{see } (3)) \}
     \hat{r}_i = \hat{r}(f, g_i | S_m)
    b_i^* = B^*(\hat{r}_i, \delta/\lceil \log_2 m \rceil, g_i(S_m)) {see Lemma 3.1 }
       if b_i^* < r^* then
10:
11:
        z_{\rm max} = z
        else
12:
13:
           z_{\min} = z
        end if
14:
15: end for
```

Theorem 1 - SGR Generalization bound

Theorem: For an application of SGR on $S_m \sim P(X, Y)$ with a given r^* and δ , the output (f, g_k) Satisfies

$$Pr_{S_m}\left\{R(f,g) > r^*\right\} < \delta$$

Theorem 1 - SGR Generalization bound - Proof Sketch

On each iteration

$$Pr_{S_m}\{R(f,g_i) > B^*(\hat{r}_i,\delta,S_m)\} < \delta/k$$

Due to the binary search

$$\exists i: B^*(\hat{r}_i, \delta, S_m) \leq r^*$$

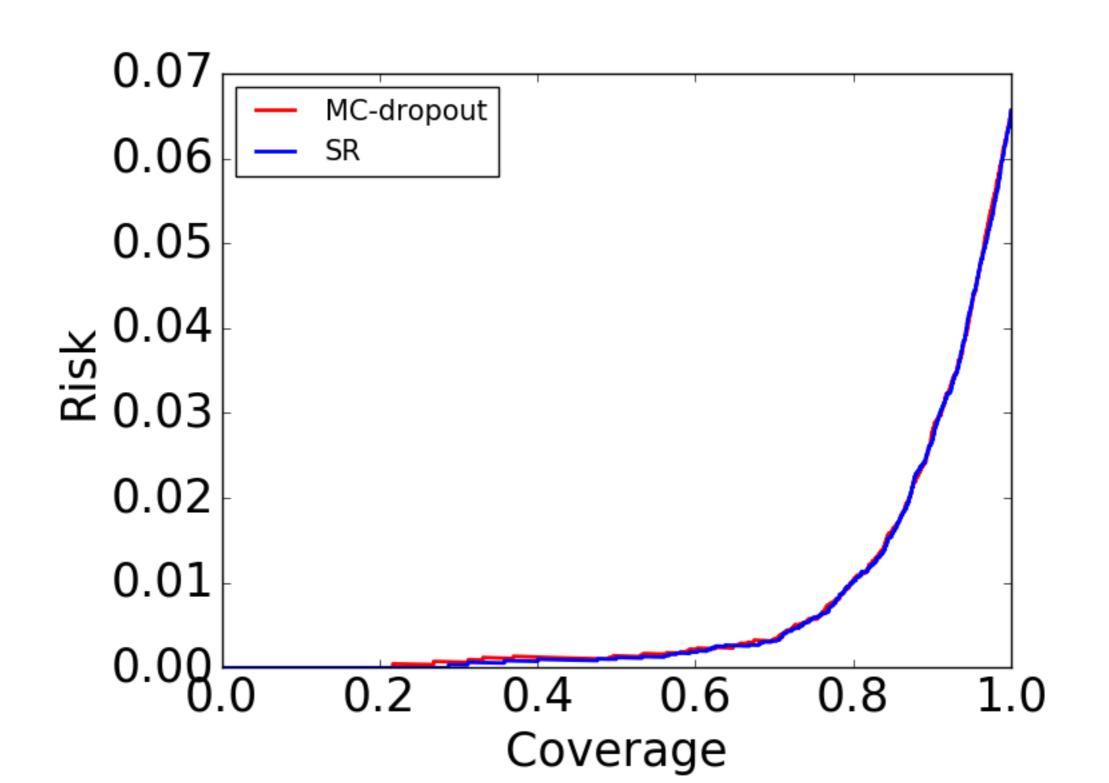
 An application of the union bound among iterations complete the proof

- A generalization bound for DNNs
- The tightest bound possible
- Can work on a pre-trained network

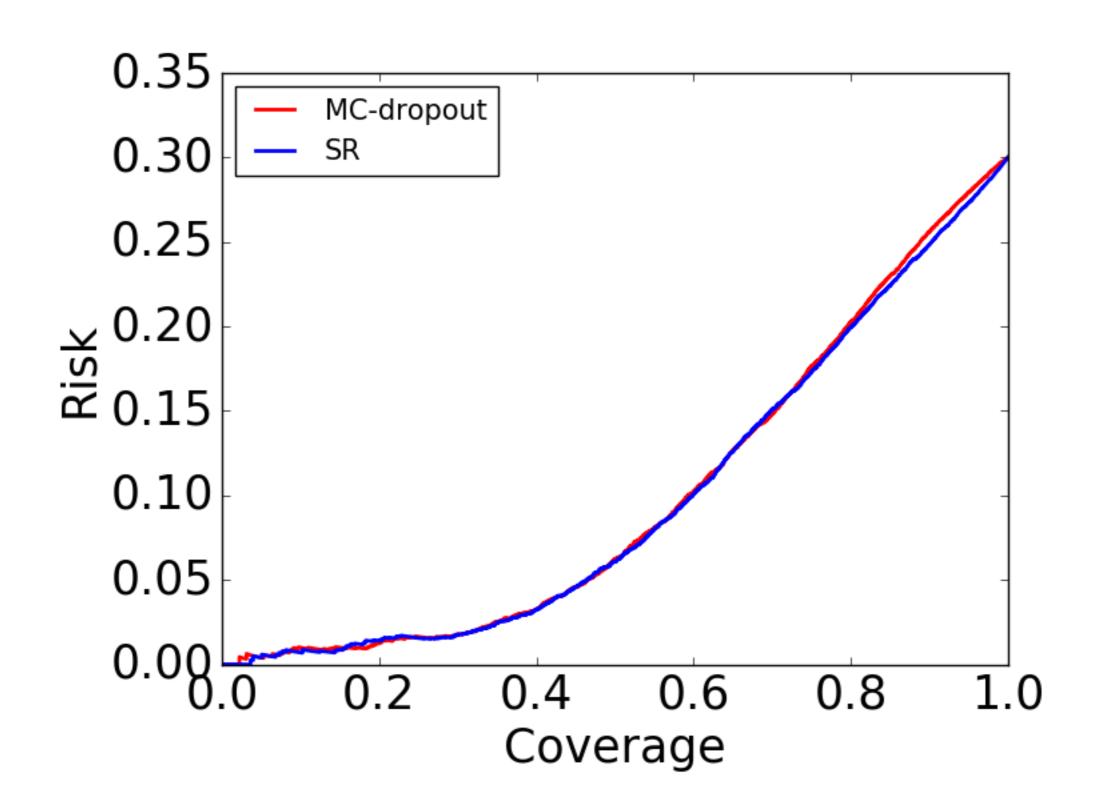
Experimental Setting

- Datasets:
 - CIFAR-10 VGG-16
 - CIFAR-100 VGG-16
 - IMAGENET VGG-16 + Resnet-50 (top1 and top 5)

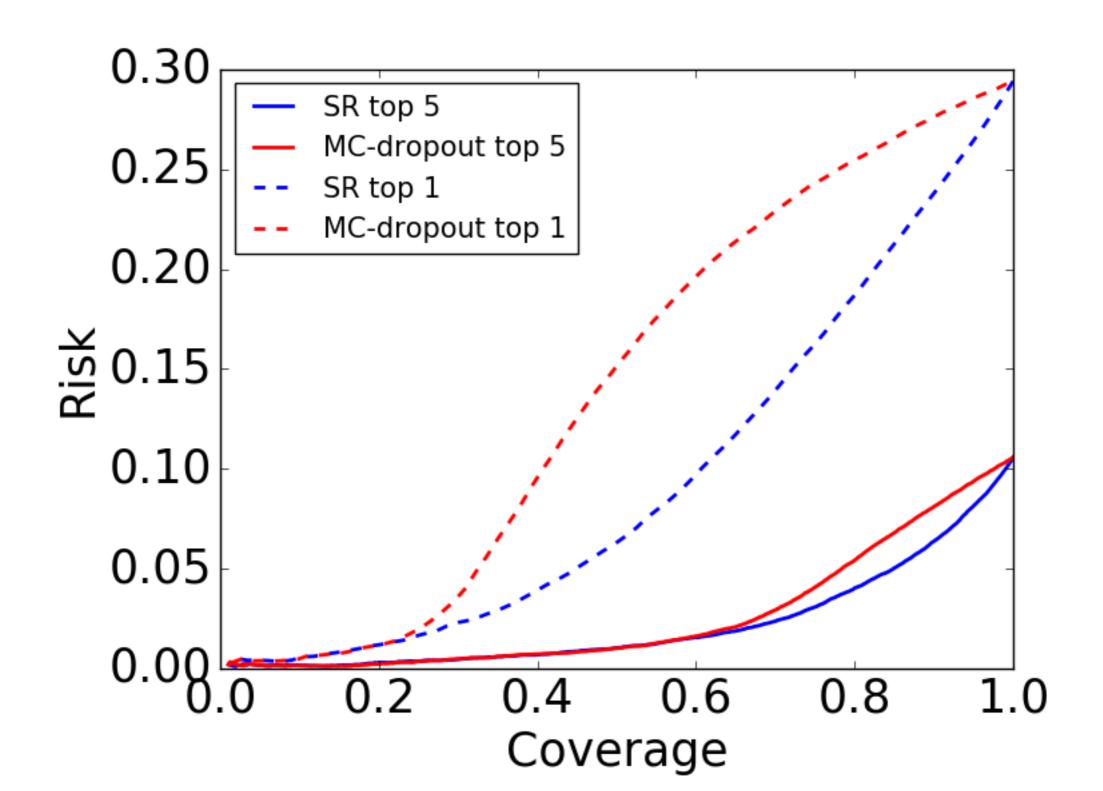
Experiments - RC-curve - CIFAR-10



Experiments - RC-curve - Cifar-100



Experiments - RC-curve Imagenet



Experiments - SGR

CIFAR-10 - VGG-16

Desired risk (r^*)	Train risk	Train coverage	Test risk	Test coverage	Risk bound (b^*)
0.01	0.0079	0.7822	0.0092	0.7856	0.0099
0.02	0.0160	0.8482	0.0149	0.8466	0.0199
0.03	0.0260	0.8988	0.0261	0.8966	0.0298
0.04	0.0362	0.9348	0.0380	0.9318	0.0399
0.05	0.0454	0.9610	0.0486	0.9596	0.0491
0.06	0.0526	0.9778	0.0572	0.9784	0.0600

• IMAGENET - top 5 with Resnet-50

Desired risk (r^*)	Train risk	Train coverage	Test risk	Test coverage	Risk bound(b^*)
0.01	0.0080	0.3796	0.0085	0.3807	0.0099
0.02	0.0181	0.5938	0.0189	0.5935	0.0200
0.03	0.0281	0.7122	0.0273	0.7096	0.0300
0.04	0.0381	0.8180	0.0358	0.8158	0.0400
0.05	0.0481	0.8856	0.0464	0.8846	0.0500
0.06	0.0581	0.9256	0.0552	0.9231	0.0600
0.07	0.0663	0.9508	0.0629	0.9484	0.0700

Future Work

- Optimal confidence rate function
- Selection with Guaranteed coverage
- Neyman-Pearson selective classification
- Learning the pair (f,g) together

Questions?