Stochastic Optimization for Spectral Risk Measures

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Stochastic Programming is the prevailing model for machine learning.

$$\min_{w \in \mathbb{R}^d} \mathbb{E}_{Z \sim P}[\ell(w, Z)]$$

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model parameters

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data generating distribution

data instance

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$$\min_{w \in \mathbb{R}^d} \mathbb{E}_{Z \sim P}[\ell(w, Z)]$$

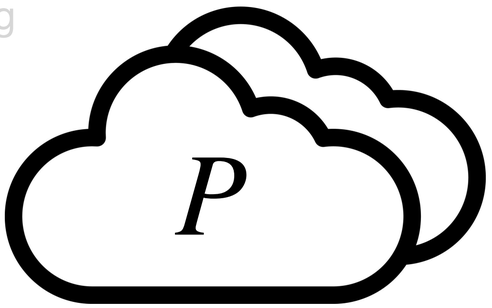
loss function

Stochastic Programming is the prevailing model for machine learning.

$$\min_{w \in \mathbb{R}^d} \mathbb{E}_{Z \sim P}[\ell(w, Z)]$$

$$\approx$$

Training



$$\xrightarrow{Z_1, \ldots, Z_n} \min_{w \in \mathbb{R}^d} \sum_{i=1}^{n} \frac{1}{n} \ell(w, Z_i)$$

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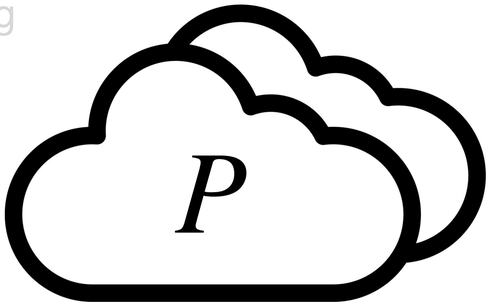
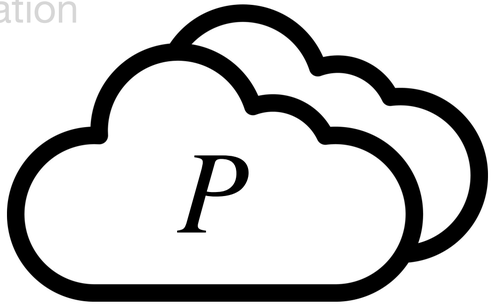


$Z_1, \ldots, Z_n$

$$\min_{w \in \mathbb{R}^d} \sum_{i=1}^{n} \frac{1}{n} \ell(w, Z_i)$$

$w^\star$

Evaluation



Z

Cost incurred:

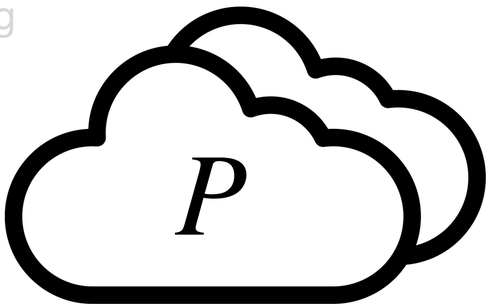
$$\ell(w^\star, Z)$$

This formulation may not agree with modern practice.

$$\min_{w \in \mathbb{R}^d} \mathbb{E}_{Z \sim P}[\ell(w, Z)]$$

$$\approx$$

Training



$Z_1, \ldots, Z_n$

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$w^\star$

Evaluation

Z

Accuracy, fairness, worst-case error, etc.

Distributionally robust objectives explicitly account for subpopulation shifts.

$$\min_{w \in \mathbb{R}^d} \max_{q \in \mathcal{U}} \sum_{i=1}^{n} q_i \ell(w, Z_i) - \nu D(q \| \mathbf{1}_n / n)$$

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ambiguity set of possible distributions, i.e. each $q_i \geq 0$ and $\sum_{i=1}^{n} q_i = 1$

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shift cost

deviation of q from original distribution

Spectral risk measures are generated by letting $\mathcal{U}$ be a permutahedron in $\mathbb{R}^n$.

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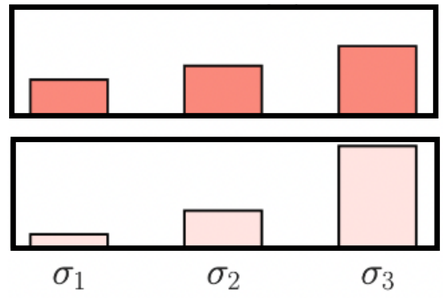
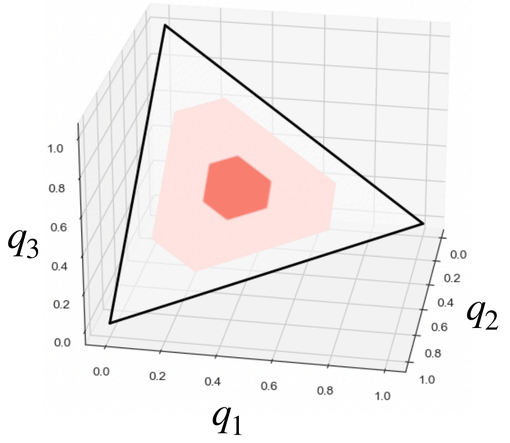
Example for $n = 3$

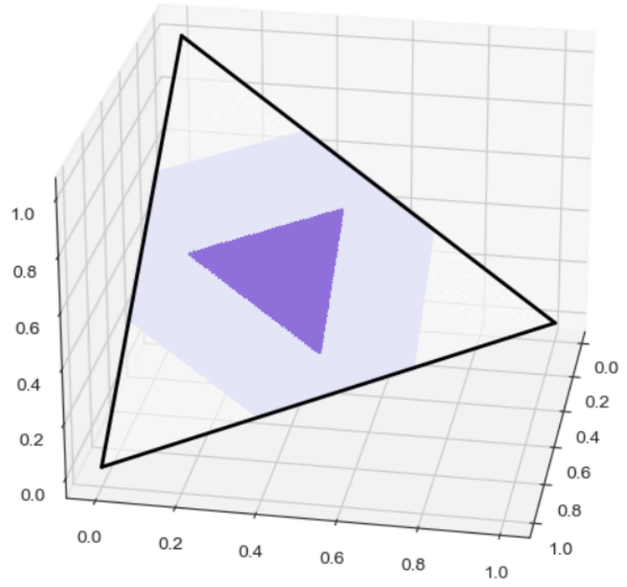


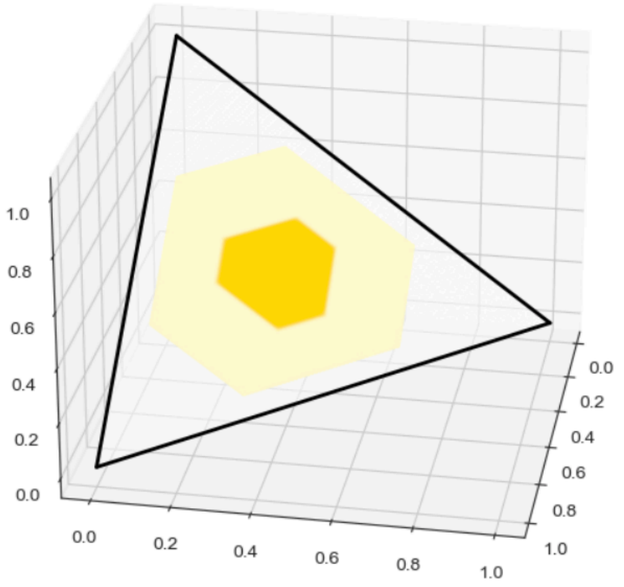


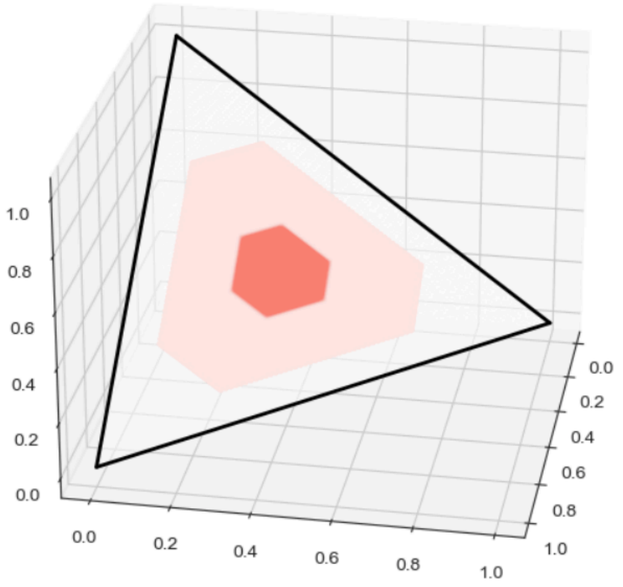
Spectral Risk Measure

Specify hyperparameter $\sigma = (\sigma_1, \ldots, \sigma_n)$ such that $\sigma_1 \leq \ldots \leq \sigma_n$ and $\sum_{i=1}^{n} \sigma_i = 1$, and use ambiguity set $\mathcal{P}(\sigma)$ by

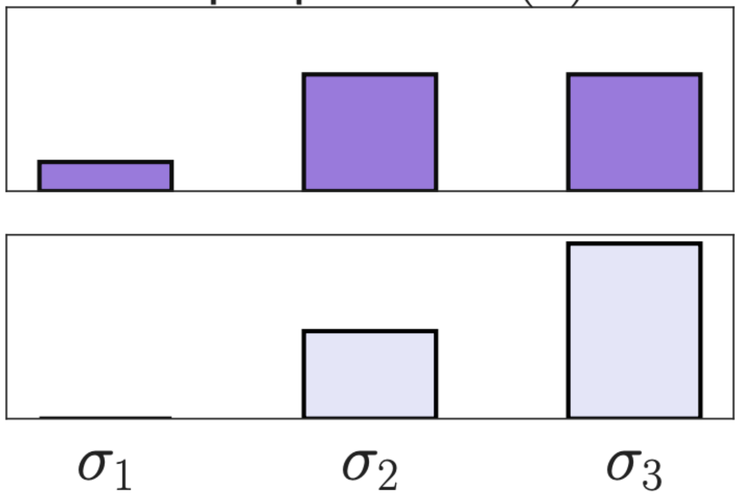
$$\mathcal{P}(\sigma) = \text{ConvexHull}\{(\sigma_{\pi(1)}, \ldots, \sigma_{\pi(n)}) : \pi \textbf{ is a permutation on } [n]\}$$



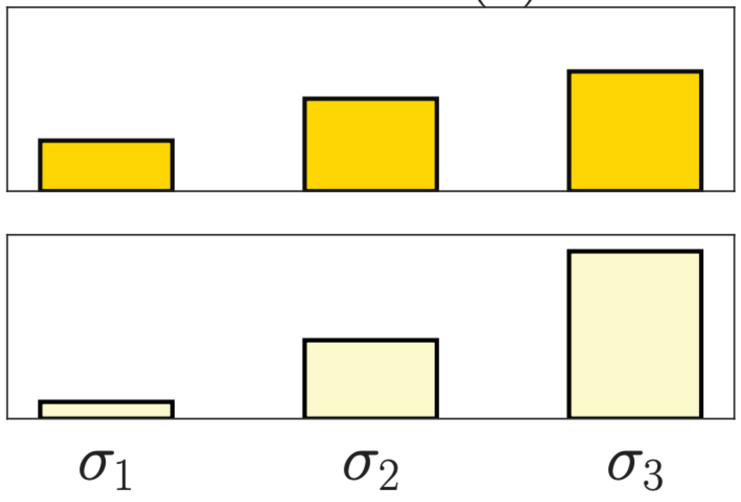




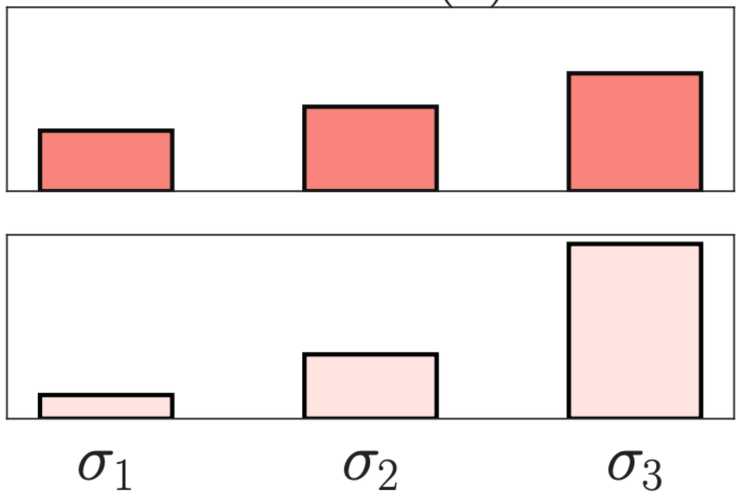
Superquantile $\mathcal{P}(\sigma)$



Extremile $\mathcal{P}(\sigma)$



ESRM $\mathcal{P}(\sigma)$



Stochastic optimization is an essential ingredient for ERM, but implementing these algorithms for SRMs is a key challenge.

$$w_{t+1} = w_t - \eta_t g_t$$

stepsize sequence

stochastic gradient estimate that only depends on $O(1)$ calls to oracles $\{\ell(\cdot, Z_i), \nabla\ell(\cdot, Z_i)\}_{i=1}^n$

Notation

$R =$ objective function

$P_n =$ sampling distribution used for g_t (e.g. mini-batch sampling)

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$$w_{t+1} = w_t - \eta_t g_t$$

Bias

$$\mathbb{E}_{P_n}[g_t] - \nabla R(w_t)$$

Variance

$$\mathbb{E}_{P_n}\|g_t - \mathbb{E}[g_t]\|_2^2$$

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Problem in ERM as well, usually handled by decreasing learning rate or variance-reduced methods.

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$$w_{t+1} = w_t - \eta_t g_t$$

Unbiased estimates are used in ERM, but this is impossible for SRMs, resulting in poor convergence.

Bias

$$\mathbb{E}_{P_n}[g_t] - \nabla R(w_t)$$

Variance

$$\mathbb{E}_{P_n}\|g_t - \mathbb{E}[g_t]\|_2^2$$

Is there an optimizer that converges to the spectral risk minimizer using only $O(1)$ oracle calls per iterate?

Quantitative Finance & Econometrics

Alternative risk measures (functionals of the loss distribution) and their axiomatic properties are well-studied.

He, 2018; Rockafellar 2007; Cotter, 2006; Acerbi, 2002; Daouia, 2019

Statistics

When $\nu = 0$, SRMs reduce to linear combinations of order statistics, or L-estimators.

Huber, 2009; Shorack, 2017

Spectral Risk Objectives in Machine Learning

Many recent examples of spectral risk-based objectives have appeared in ML, with focus on the superquantile.

Maurer, 2021; Laguel, 2021; Khim, 2020; Holland, 2022

Distributionally Robust Optimization Methods

Optimization approaches rely on full-batch gradient descent, biased SGD, or saddle-point formulations.

Levy 2020; Yu 2022; Yang 2020; Palaniappan, 2016; Kawaguchi & Lu, 2020;

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Contributions

1. Characterize the smoothness properties of the objective as a function of the underlying losses.
2. Quantify the bias of current stochastic approaches.
3. Propose LSVRG, a stochastic optimization algorithm and establish its linear convergence rate.
4. Demonstrate superior convergence of LSVRG experimentally via numerical evaluations.

Outline

Properties of SRM Objective

Bias and Variance of Current Methods

LSVRG Algorithm

Theoretical Guarantees

Numerical Performance

Conclusion & Future Work

$$R(w) := \max_{q \in \mathscr{P}(\sigma)} q^\top \ell(w) - \nu n \|q - \mathbf{1}_n/n\|_2^2 + \frac{\mu}{2}\|w\|_2^2$$

$D_{\chi^2}(q\|\mathbf{1}_n/n) = n\|q - \mathbf{1}_n/n\|_2^2.$

strongly convex regularizer

$$R(w) := \max_{q \in \mathscr{P}(\sigma)} q^\top \ell(w) - \nu n \|q - \mathbf{1}_n/n\|_2^2 + \frac{\mu}{2}\|w\|_2^2$$

$\ell(w) := (\ell_1(w), \ldots, \ell_n(w)) \in \mathbb{R}^n$

$\ell_i(w) := \ell_i(w, Z_i) \quad i = 1, \ldots, n\,.$

$$R(w) := h_\nu(\ell(w)) + \frac{\mu}{2}\|w\|_2^2$$

$$h_\nu(l) := \max_{q \in \mathcal{P}(\sigma)} q^\top l - \nu n \|q - \mathbf{1}_n/n\|_2^2,\ l \in \mathbb{R}^n$$

$$\ell : \mathbb{R}^d \to \mathbb{R}^n$$

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$$h_\nu : \mathbb{R}^n \to \mathbb{R}$$

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$$h_\nu(l) := \max_{q \in \mathcal{P}(\sigma)} q^\top l - \nu n \|q - \mathbf{1}_n/n\|_2^2,\ l \in \mathbb{R}^n$$

Assumptions

Each loss $\ell_i : \mathbb{R}^d \to \mathbb{R}$ is convex, G-Lipschitz continuous, and L-smooth, i.e. $w \mapsto \nabla \ell(w)$ is well-defined and L-Lipschitz continuous w.r.t. $\|\cdot\|_2$.

The regularization parameter μ and shift cost ν satisfy $\mu > 0$ and $\nu > 0$.

Proposition 1

$$\nabla h_\nu(l) = q^*(l) := \operatorname{argmax}_{q \in \mathcal{P}(\sigma)} q^\top l - \nu n \|q - \mathbf{1}_n/n\|_2^2$$

$$\begin{aligned}\nabla R(w) &= \nabla \ell(w)^\top q^*(\ell(w)) + \mu w \\ &= \sum_{i=1}^{n} q_i^*(\ell(w))(\nabla \ell_i(w) + \mu w)\,.\end{aligned}$$

The gradient of $R(w) := h_\nu(\ell(w)) + \frac{\mu}{2}\|w\|_2^2$ is a weighted average of the gradients of individual (regularized) losses, weighed by the "most unfavorable" distribution shift $q^*(\ell(w))$.

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One could construct an unbiased estimator of $\nabla R(w)$… if $q^*(\ell(w))$ was known!

Proposition 2

The map $l \mapsto q^*(l)$ is
$(2n\nu)^{-1}$-Lipschitz continuous.

The map $w \mapsto \nabla R(w)$ is
$(L + \mu + G^2/(2\nu))$-Lipschitz continuous.

In other words, R is $(L + \mu + G^2/(2\nu))$-smooth.

Increasing the shift cost ν improves the conditioning of the objective, just like a typical regularization parameter.

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Stochastic Gradient Descent

Choose mini-batch size $m < n$ such that m divides n, and define the "binned" spectrum $\hat{\sigma} = (\hat{\sigma}_1, \ldots, \hat{\sigma}_n) \in \mathbb{R}^m$ by:

$$\hat{\sigma}_j = \sigma_{(j-1)n/m} + \ldots \sigma_{jn/m} \, .$$

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Sample mini-batch $S_m = (i_1, \ldots, i_m)$ uniformly without replacement from $\{1, \ldots, n\}$ and define the gradient estimate

$$g_t := \nabla \left\{ \max_{\rho \in \mathscr{P}(\hat{\sigma})} \sum_{j=1}^{m} \rho_j \ell_{i_j}(w_t) - \nu n \|\rho - \mathbf{1}_n/n\|_2^2 + \frac{\mu}{2} \|w_t\|_2^2 \right\}$$

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Perform the update:

$$w_{t+1} = w_t - \eta_t g_t$$

Notation

$R =$ objective function

$P_n =$ sampling distribution used for g_t (e.g. mini-batch sampling)

$$\bar{w}_t = \frac{1}{t}\sum_{k=1}^{t} w_k$$

$$w^\star = \operatorname{argmin}_w R(w)$$

$$B_\mu = \sup_{i,w:\|w\|_2 \le G/\mu} \ell_i(w)$$

Proposition 3

The output of SGD with stepsize sequence $\eta_t = 1/(\mu t)$ achieves

$$\mathbb{E}_{P_n^t}[R(\bar{w}_t)] - R(w^\star) \lesssim B_\mu \sqrt{\frac{1}{m}\left(1 - \frac{m}{n}\right)} + \frac{G^2 \ln t}{\mu t}$$

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bias term

optimization term for surrogate objective

$$\hat{R}(w) = \mathbb{E}_{P_n}\left[\max_{\rho \in \mathcal{P}(\hat{\sigma})} \sum_{j=1}^{m} \rho_j \ell_{i_j}(w) - \nu n \|\rho - \mathbf{1}_n/n\|_2^2\right] + \frac{\mu}{2}\|w\|_2^2$$

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Bias bound cannot be decreased using shift cost ν or learning rate η_t, but can using regularization μ .

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Variance is simply handled with $\|g_t\|_2^2 \le G^2$ in the optimization term.

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LSVRG

Choose an epoch length $N > 0$, and at the start of each epoch, store a checkpoint iterate $\bar{w}$ along with $\bar{q} := q^*(\ell(\bar{w}))$ and

$$\nabla R(\bar{w}) = \sum_{i1=}^{n} \bar{q}_i(\nabla \ell_i(\bar{w}) + \mu \bar{w}).$$

At iterate t, sample i_t uniformly from $\{1, \ldots, n\}$ and compute

$$g_t := n\bar{q}_{i_t}(\nabla \ell_{i_t}(w_t) + \mu w_t) - n\bar{q}_{i_t} \nabla \ell_{i_t}(\bar{w}) + \sum_{i=1}^{n} \bar{q}_i \nabla \ell_i(\bar{w}) .$$

zero-mean term used for variance reduction

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Still biased, but bias decreases asymptotically.

$$\mathbb{E}_{P_n}[n\bar{q}_{i_t} \nabla \ell_i(w_t)] = \sum_{i=1}^{n} \bar{q}_i \nabla \ell_i(w) \neq \sum_{i=1}^{n} q_i^*(\ell(w_t)) \nabla \ell_i(w)$$

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Perform the update:

$$w_{t+1} = w_t - \eta g_t$$

constant stepsize, as update direction combines bias reduction and variance reduction

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$P_n =$ sampling distribution used for g_t (e.g. mini-batch sampling)

$w^\star = \operatorname{argmin}_w R(w)$

$\kappa = n\sigma_n L/\mu + 1$

Theorem 1

Assume that $\nu \geq O(G^2/\mu)$. The output of LSVRG with epoch length $N = O(n + \kappa)$ and stepsize $\eta = O(1/(N\mu))$ achieves

$$\mathbb{E}_{P_n^t}\|w_t - w^\star\|_2^2 \lesssim 2^{-\frac{t}{4(n+8\kappa)}}$$

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condition number and sample size decoupled, as in variance-reduced algorithms for ERM

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Proof proceeds by considering the saddle-point formulation $\Phi(w, q) = q^\top \ell(w) - \nu n\|q - \mathbf{1}_n/n\|_2^2$ such that $R(w) = \max_q \Phi(w, q)$. We then view each epoch as alternating (exact) maximization steps and (inexact) minimization steps.

Outline

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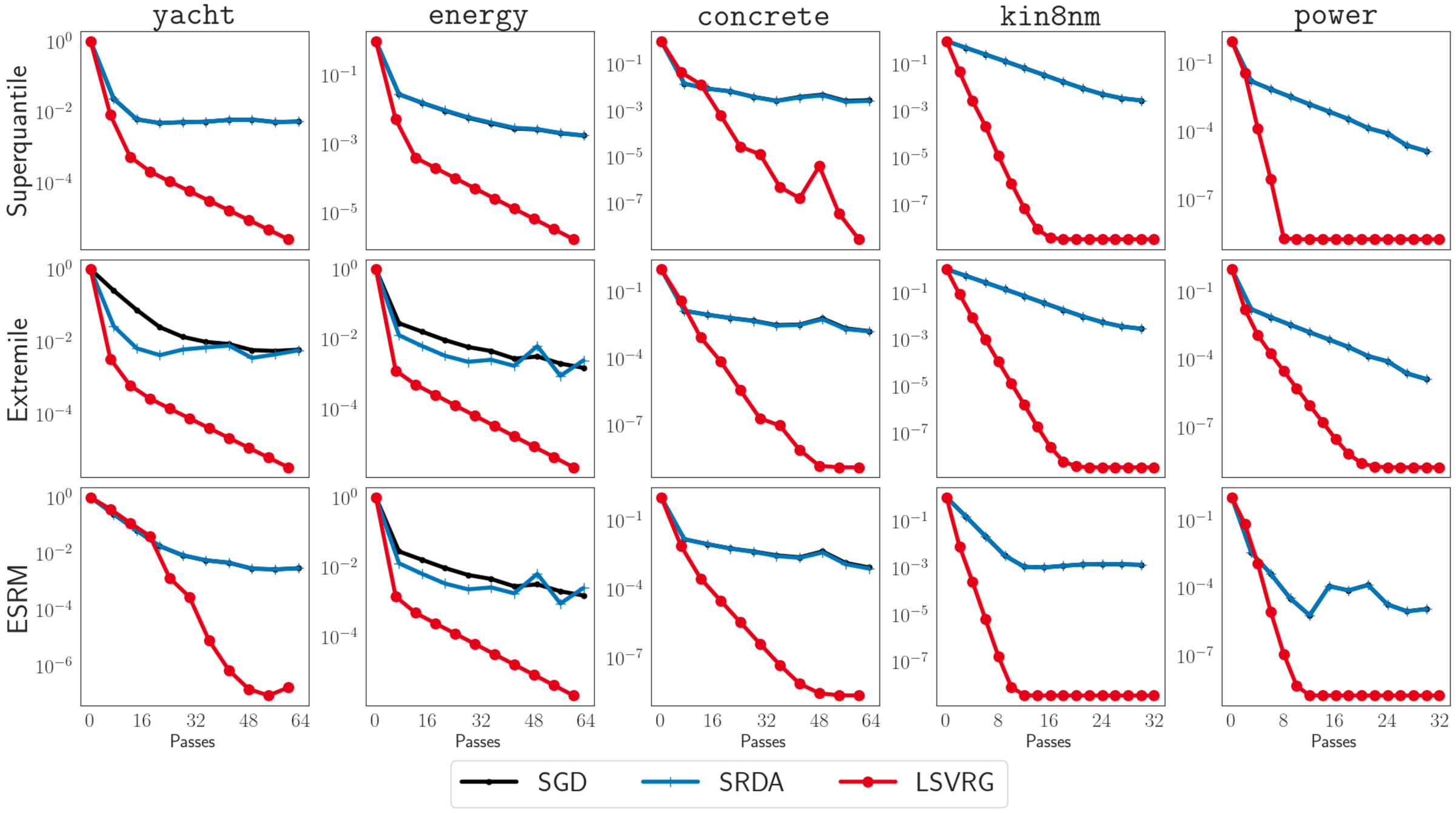
Regression Benchmarks

- We consider five regression tasks, for which we use squared loss under a linear prediction model.
- Datasets are labeled as *yacht*, *energy*, *concrete*, *kin8nm*, and *power*.
- Main metric is training suboptimality $(R(w_t) - R(w^\star))/(R(w_0) - R(w^\star))$.
- Baselines are stochastic gradient descent (SGD), and stochastic regularized dual averaging (SRDA).


yacht
energy
concrete
kin8nm
power
Superquantile
Extremile
ESRM
Passes
SGD
SRDA
LSVRG

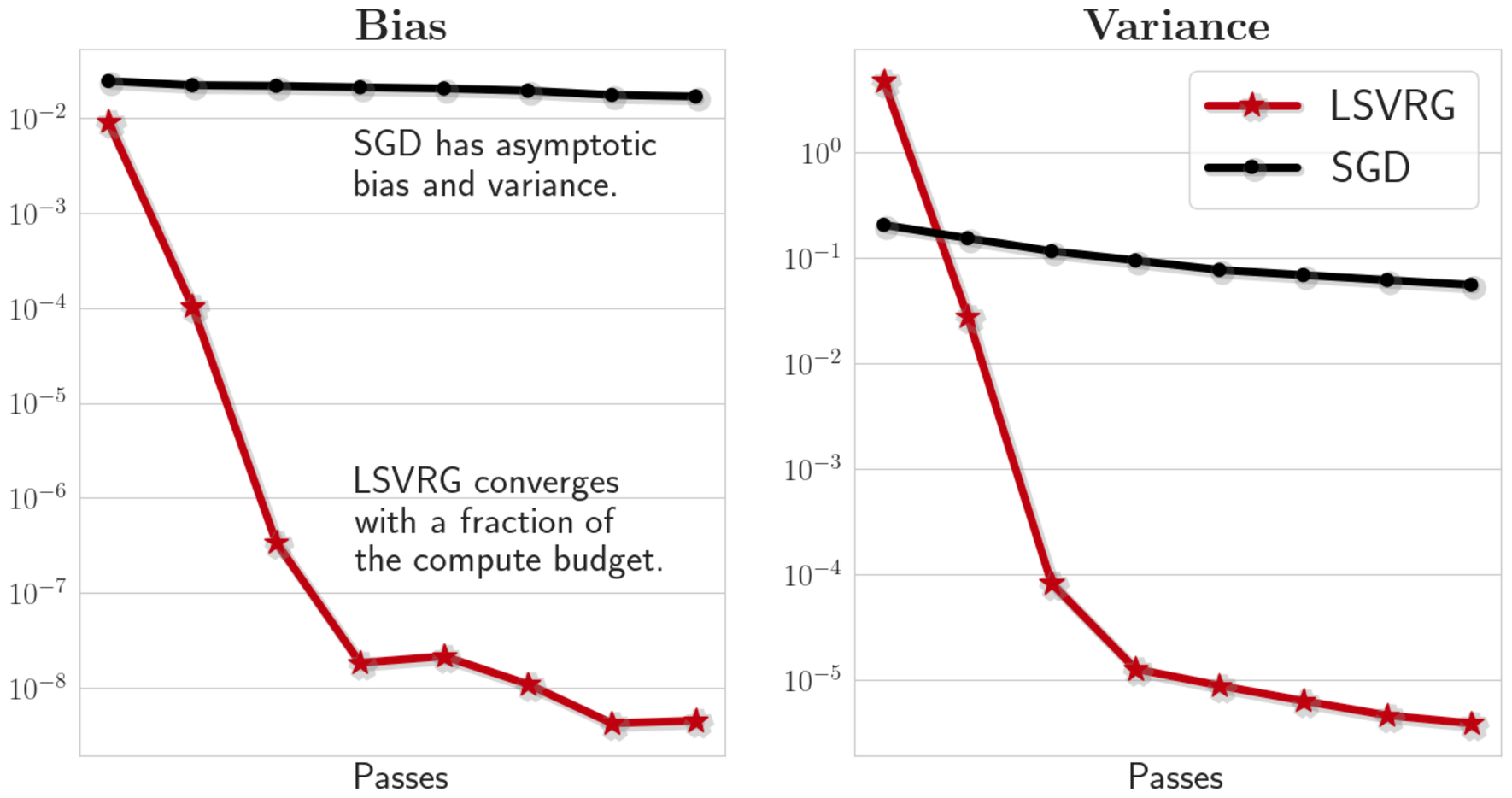
Bias

$$\|\mathbb{E}_{P_n}[g_t] - \nabla R(w_t)\|_2^2$$

Variance

$$\mathbb{E}_{P_n}\|g_t - \mathbb{E}[g_t]\|_2^2$$

Superquantile on `yacht` Benchmark



Classification Benchmarks

- We consider two classification tasks, for which we use cross entropy loss under a multinomial logistic regression model.

- Datasets considered are:

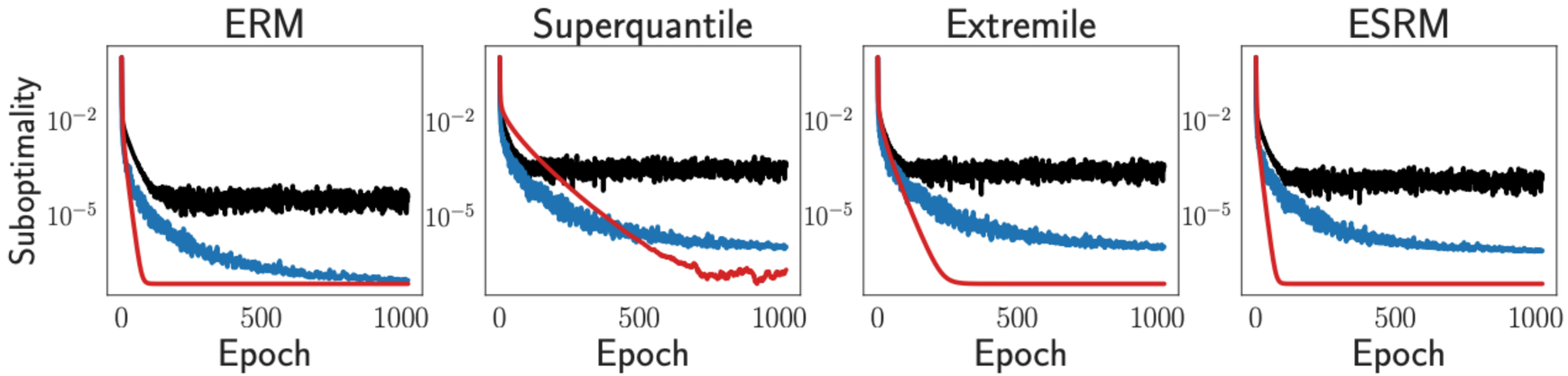
    - *emotion*, in which the task is to classify the emotional sentiment of natural language passages from BERT features, and

    - iwildcam, in which the task is to classify the flora and fauna captured in wilderness images from ResNet50 features.

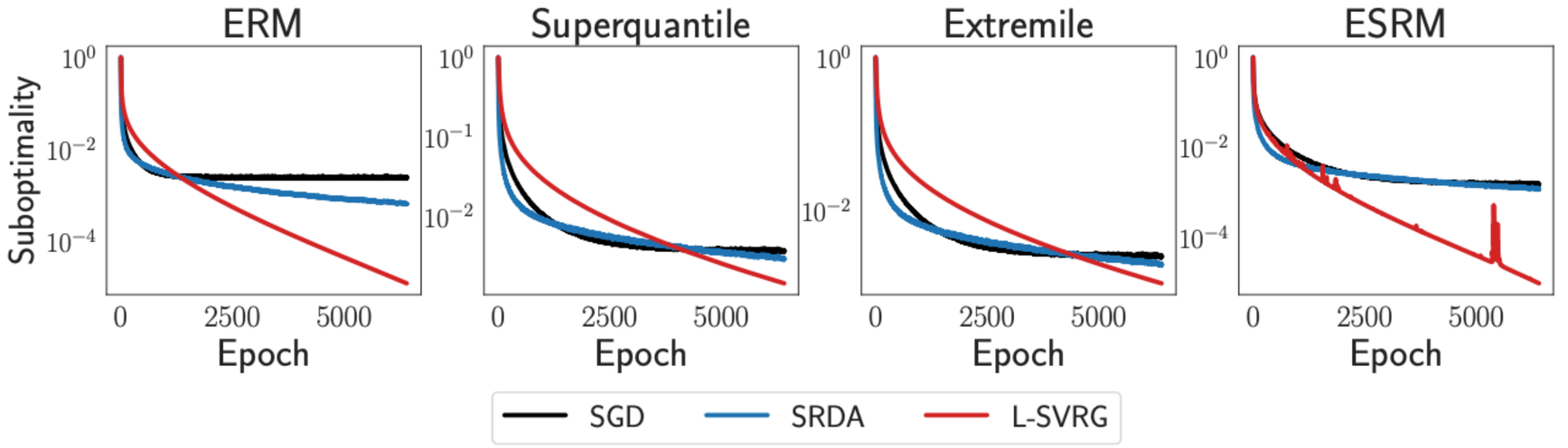
- Main metric is training suboptimality $(R(w_t) - R(w^\star))/(R(w_0) - R(w^\star))$.

- Baselines are stochastic gradient descent (SGD), and stochastic regularized dual averaging (SRDA).

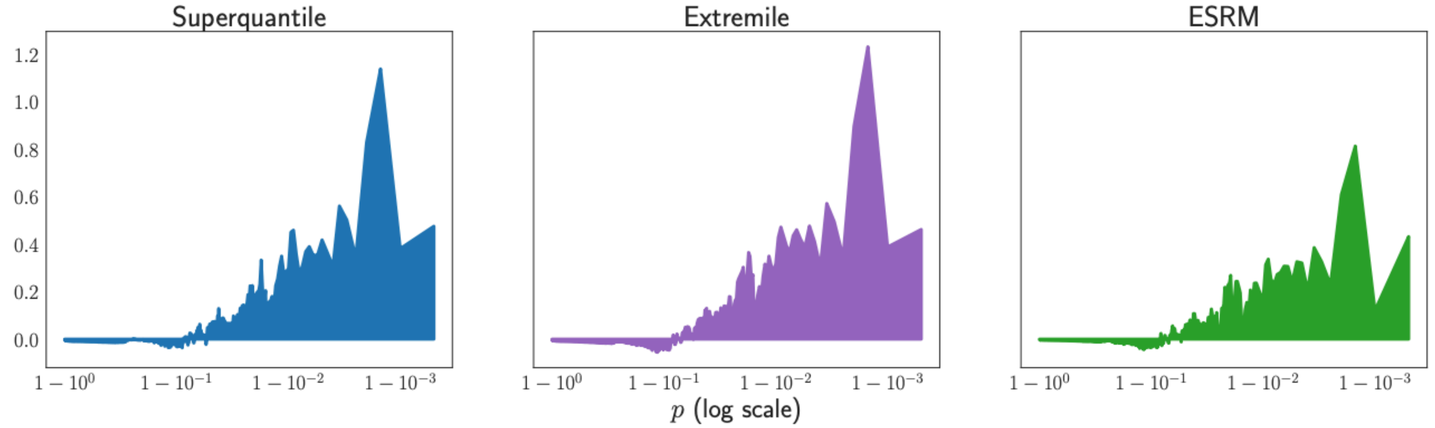
emotion



iwildcam



emotion



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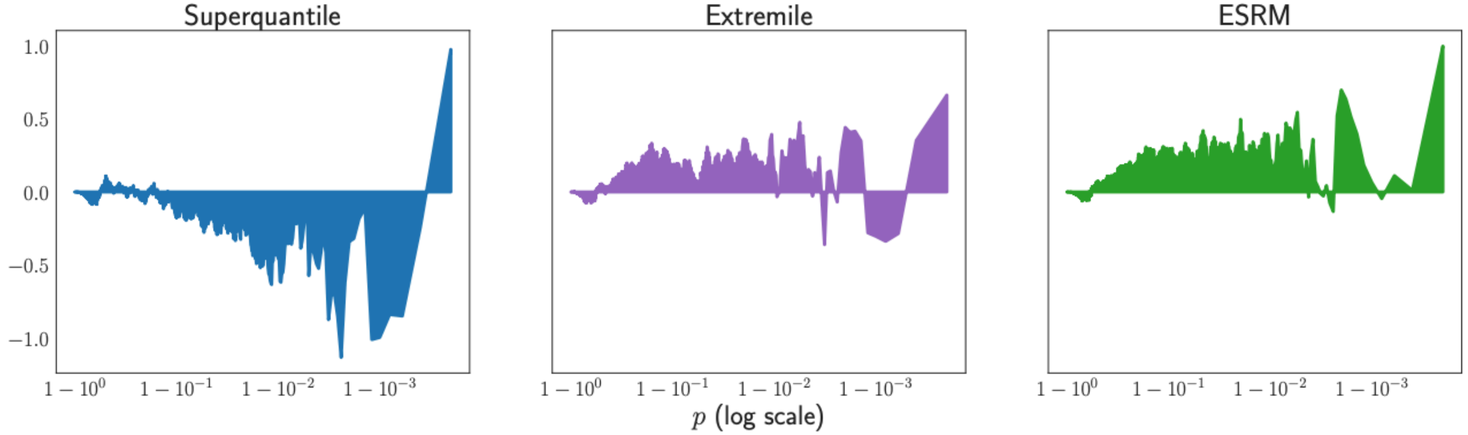
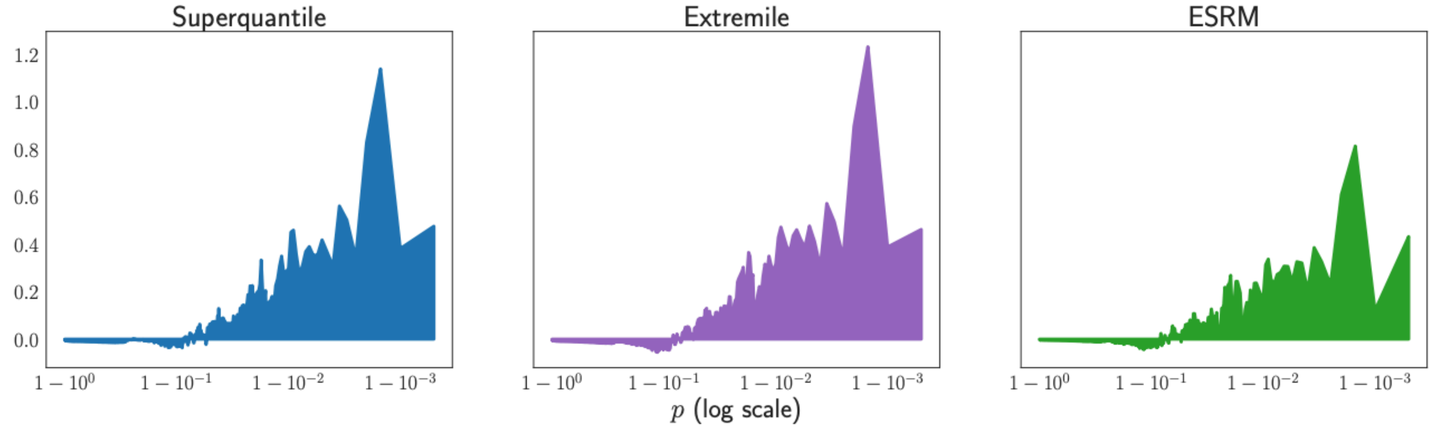


***y*-axis:** Test loss of ERM minimizer minus test loss of spectral risk minimizer (with LSVRG).

emotion



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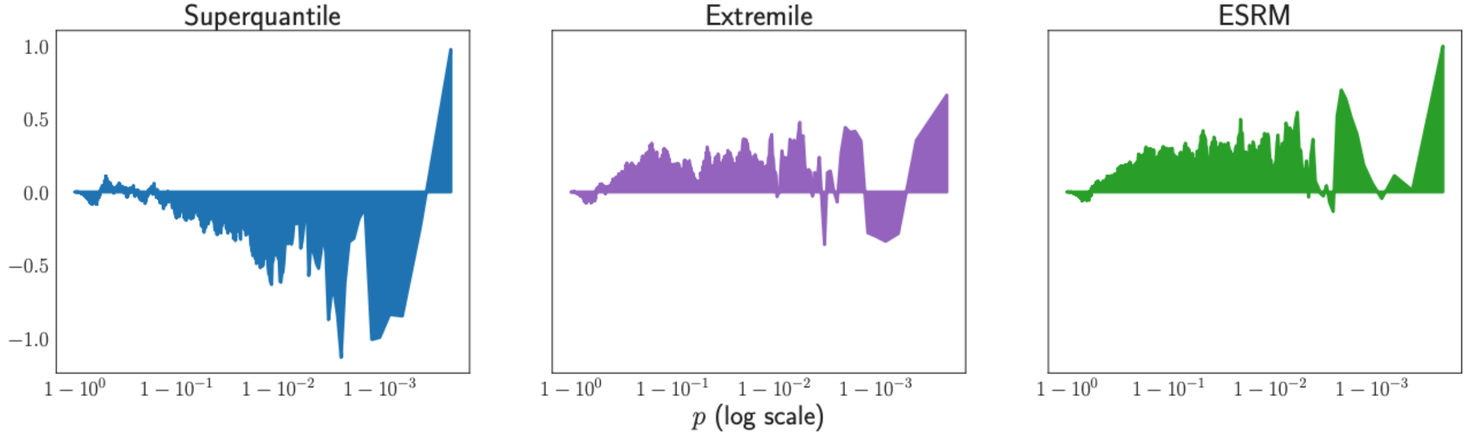
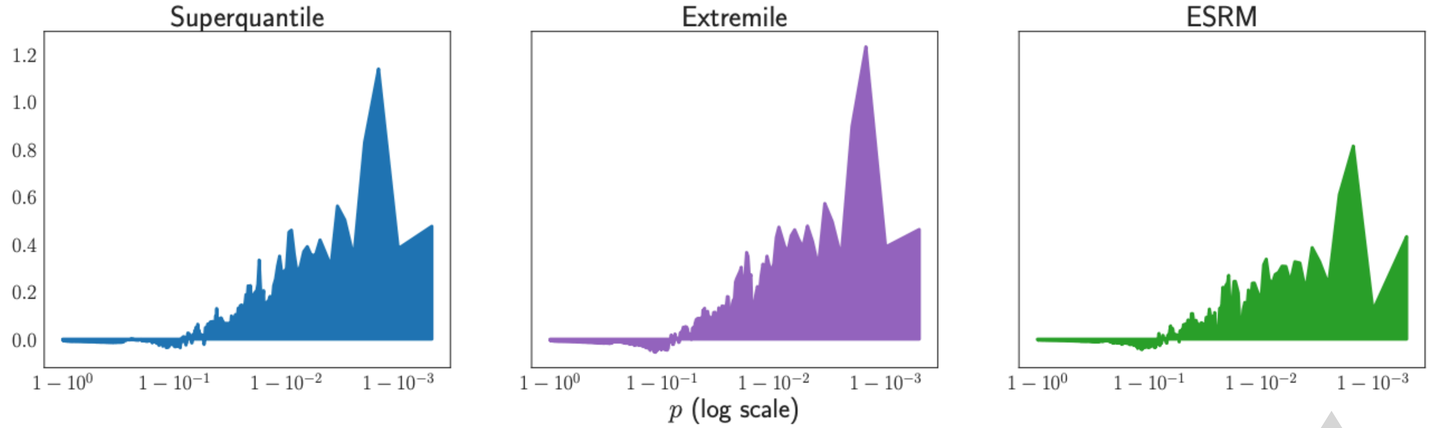


emotion



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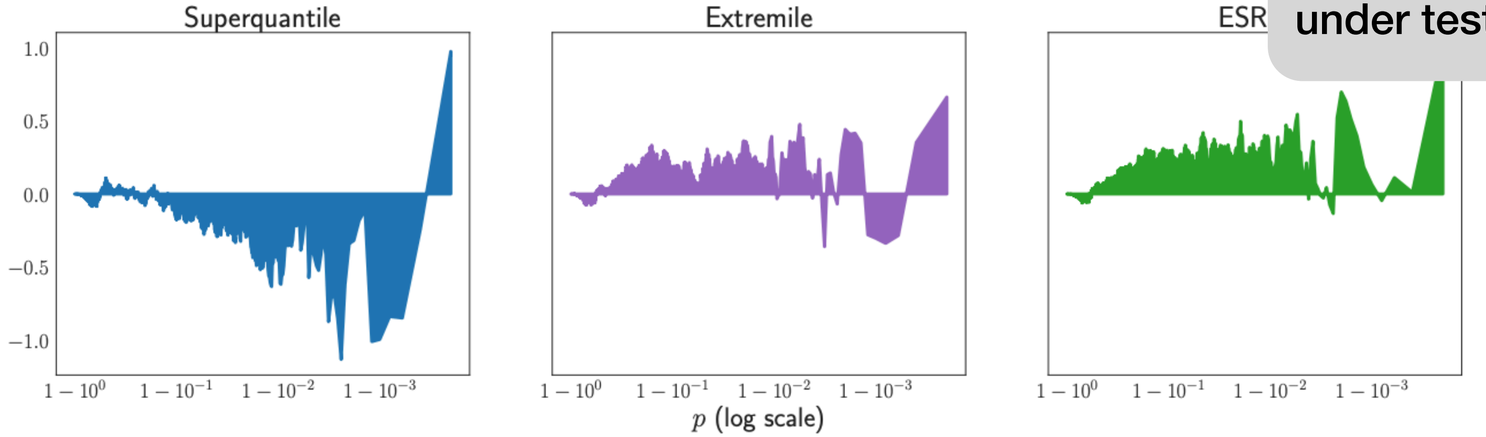
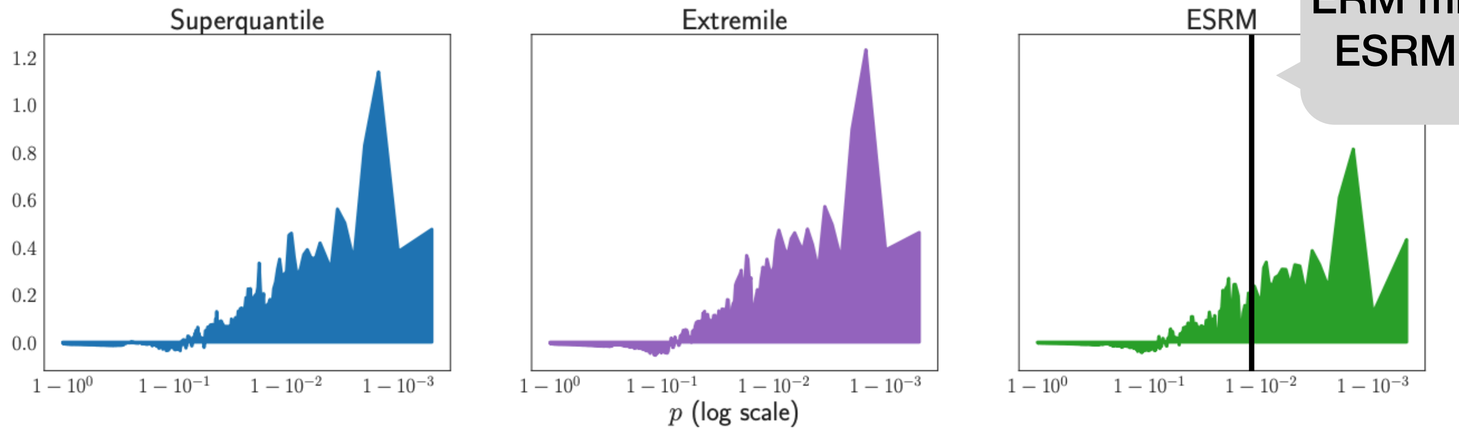


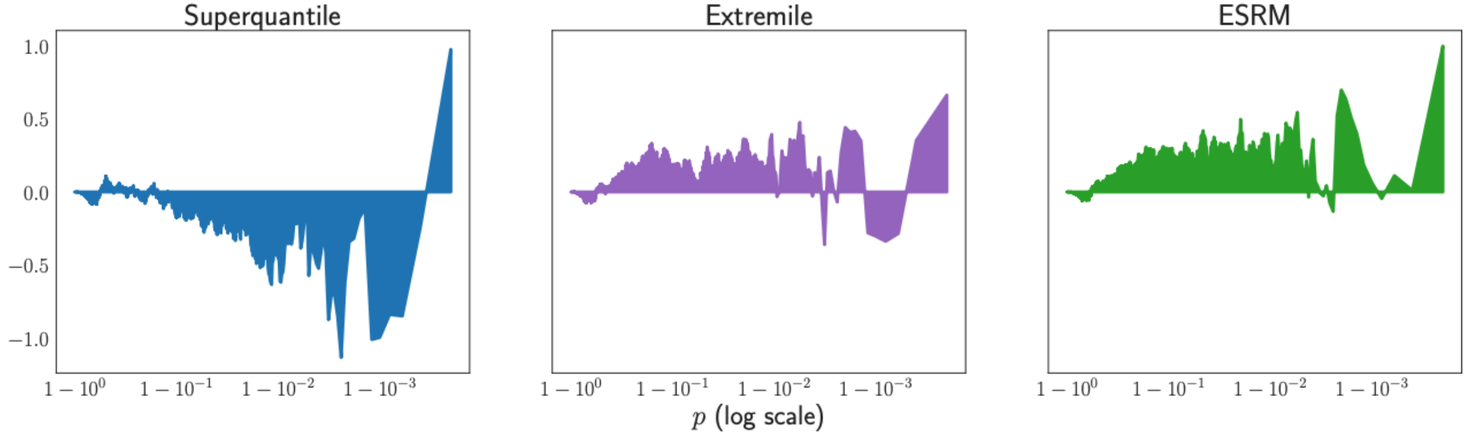
***x*-axis:** Probability of observing a lower loss under test distribution.

emotion



Difference in 0.99-quantile of ERM minimizer's test loss and ESRM minimizer's test loss.

iwildcam



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Summary

- We present a stochastic algorithm to optimize spectral risks measures of the empirical loss distribution that:
    - finds an exact minimizer/is asymptotically unbiased
    - makes $O(1)$ calls to a function/gradient oracle per update, and
    - outperforms out-of-the-box convex optimizers on real data.
- Future work includes extensions to the non-convex setting and exploring statistical properties of learned minimizers.

Thank you!