Exploiting Large Sample Size to Reduce Statistical Risk and Computational Cost

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March 26, 2018
18.898G Midterm Presentation

Designing Statistical Estimators That Balance Sample Size, Risk, and Computational Cost

John J. Bruer, Joel A. Tropp, Volkan Cevher, and Stephen R. Becker

[1] Paper from 2015
By people in Caltech, EPFL & UCBoulder

Motivation: Data as a Computational Resource?

- Many problems nowadays involve massive data sets.
- Surprisingly, increase in data size doesn't always lead to higher computational cost. SVM example in 2008 [2]
- This paper proposes an approach to:
 - systematically take advantage of large sample size in solving statistical problems through convex optimization.
 - by using extra samples for smoothing in the dual domain.

Roadmap

1. Define the regression problem, risk (R), and statistical dimension of descent cone (δ)

Regularized Linear Regression Problem

$$\boldsymbol{b} = \boldsymbol{A}\boldsymbol{x}^{\natural} + \boldsymbol{v}.$$

```
x^{
abla} \in \mathbb{R}^d, d parameters of a statistical model b \in \mathbb{R}^m m observations A \in \mathbb{R}^{m \times d} m d-dimensional inputs v \in \mathbb{R}^m i.i.d. zero-mean noise
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 m observations

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 m d-dimensional inputs

$$\boldsymbol{v} \in \mathbb{R}^m$$
 i.i.d. zero-mean noise

$$\widehat{x} := \underset{x}{\arg \min} f(x)$$

$$\text{subject to} \quad ||Ax - b|| \le \sqrt{m \cdot R_{\max}} =: \epsilon$$

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abla} \in \mathbb{R}^d$, d parameters of a statistical model $b \in \mathbb{R}^m$ m observations $A \in \mathbb{R}^{m \times d}$ m d-dimensional inputs $v \in \mathbb{R}^m$ i.i.d. zero-mean noise

$$f: \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$$
 Convex regularizer function, i.e. L1 norm

$$\widehat{x} := \underset{x}{\arg\min} f(x)$$

subject to
$$||Ax - b|| \le \sqrt{m \cdot R_{\text{max}}} =: \epsilon$$

 R_{max} Maximal empirical risk that's tolerated

Statistical and Empirical Risk

$$R(\widehat{x}) = \frac{1}{m} \|A\widehat{x} - Ax^{\sharp}\|^2$$

Average squared prediction error for sample size m

$$\mathbb{E}_{\boldsymbol{v}}[R(\widehat{\boldsymbol{x}})]$$

Statistical risk of estimate \widehat{x}

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 Empirical risk of estimate \widehat{x}

Statistical Dimension of Descent Cone

Definition III.1 (Descent cone). The *descent cone* of a proper convex function $f: \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$ at the point $\mathbf{x} \in \mathbb{R}^d$ is the convex cone

$$\mathcal{D}(f; \mathbf{x}) := \bigcup_{\tau > 0} \left\{ \mathbf{y} \in \mathbb{R}^d : f(\mathbf{x} + \tau \mathbf{y}) \le f(\mathbf{x}) \right\}.$$

= set of directions that decrease f locally at \mathbf{x}

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Definition III.2 (Statistical dimension [3, Def. 2.1]). Let $C \in \mathbb{R}^d$ be a closed convex cone. Its *statistical dimension* $\delta(C)$ is defined as

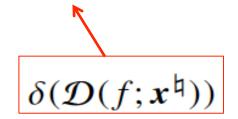
$$\delta(C) := \mathbb{E}_{\boldsymbol{g}} \left[\| \mathbf{\Pi}_{C}(\boldsymbol{g}) \|^{2} \right],$$

 $g \in \mathbb{R}^d$ i.i.d Gaussian noise

 $\Pi_{\mathcal{C}}$ Projection onto C

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- 1. Define the regression problem, risk (R), and statistical dimension of descent cone (δ)
- 2. Show relationship between R, sample size (m), and δ

If **A** has orthonormal rows, σ is standard deviation of \boldsymbol{v} , \mathbf{x}^* is minimizer of our regression problem, and \mathbf{c}_1 , \mathbf{c}_2 are some constants:

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• Whenever $m < \delta$,

$$\max_{\sigma>0} \frac{\mathbb{E}_{\boldsymbol{v}}\left[R(\boldsymbol{x}^{\star}) \mid \boldsymbol{A}\right]}{\sigma^2} = 1,$$

and

$$\lim_{\sigma \to 0} \frac{\mathbb{E}_{\boldsymbol{v}} \left[\widehat{R}(\boldsymbol{x}^{\star}) \mid \boldsymbol{A} \right]}{\sigma^2} = 0,$$

with probability $1 - c_1 \exp(-c_2(m-\delta)^2/d)$.

• Whenever $m > \delta$,

$$\left| \max_{\sigma > 0} \frac{\mathbb{E}_{\boldsymbol{v}} \left[R(\boldsymbol{x}^{\star}) \mid \boldsymbol{A} \right]}{\sigma^2} - \frac{\delta}{m} \right| \leq t m^{-1} \sqrt{d},$$

and

$$\left|\lim_{\sigma\to 0}\frac{\mathbb{E}_{\boldsymbol{v}}\left[\widehat{R}(\boldsymbol{x}^{\star})\mid \boldsymbol{A}\right]}{\sigma^{2}}-\left(1-\frac{\delta}{m}\right)\right|\leq tm^{-1}\sqrt{d},$$

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The probabilities are taken over A.

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Worst-case statistical risk (R) can be bounded!

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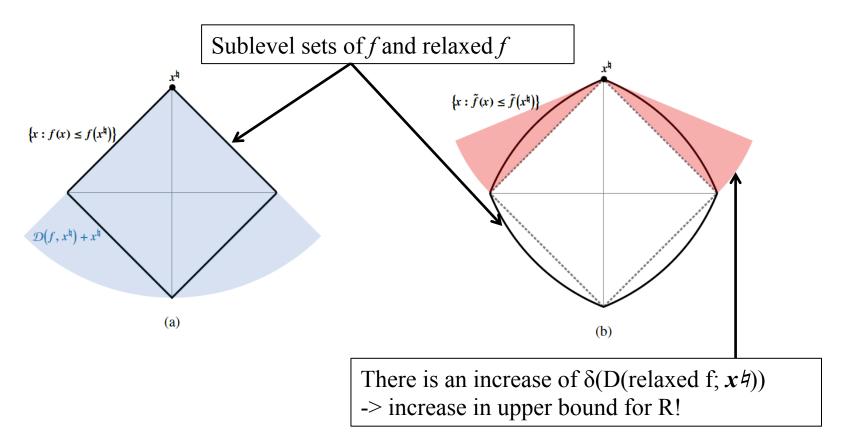
When $m < \delta$, R is constant -> statistical accuracy doesn't improve with m.

But after phase transition, worst-case risk decreases at 1/m. That matches with our intuition.

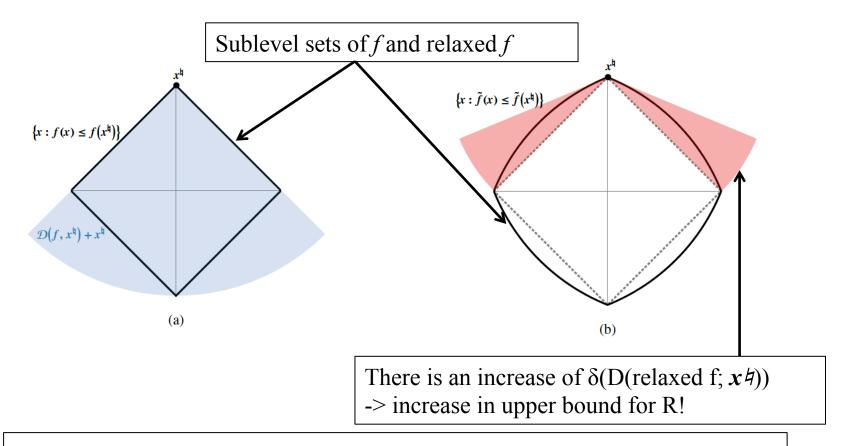
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- 3. Show geometric relationship between relaxing f, δ , and R

Geometry of relaxing f and increasing δ



Geometry of relaxing f and increasing δ



Relaxing f could help with optimization, BUT it decreases statistical accuracy. Note that if we smooth f directly, D(smoothed f; $x \not = 0$) becomes half-space and we lose control of δ . -> we start thinking about the dual problem.

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- 1. Define the regression problem, risk (R), and statistical dimension of descent cone (δ)
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- 4. Define strong convexity, Lipschitz gradient, and dual problem

Strong Convexity and Lipschitz gradient

Definition IV.1 (Strong convexity). A function $f_{\mu} : \mathbb{R}^d \to \mathbb{R}$ is μ -strongly convex if there exists a positive constant μ such that the function

$$\mathbf{x} \mapsto f_{\mu}(\mathbf{x}) - \frac{\mu}{2} \|\mathbf{x}\|^2,$$

is convex.

"More convex" functions have higher μ

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is convex.

"More convex" functions have higher μ

Definition IV.2 (Lipschitz gradient). A function $g: \mathbb{R}^m \to \mathbb{R}$ has an *L-Lipschitz gradient* if there exists a positive constant L such that

$$\|\nabla g(z_1) - \nabla g(z_2)\| \le L \|z_1 - z_2\|,$$

for all vectors $z_1, z_2 \in \mathbb{R}^m$.

Smoother functions have lower L

Duality of Convexity and Smoothing

Fact IV.3 (The duality between convexity and smoothing [18, Prop. 12.60]). *If the proper closed convex function* $f_{\mu} \colon \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$ is μ -strongly convex, then its convex conjugate $f_{\mu}^* \colon \mathbb{R}^d \to \mathbb{R} \cup \{+\infty\}$ is differentiable and ∇f_{μ}^* is $\frac{1}{\mu}$ -Lipschitz, where $f_{\mu}^*(\mathbf{x}^*) = -\inf_{\mathbf{x} \in \mathbb{R}^d} \left\{ f_{\mu}(\mathbf{x}) - \langle \mathbf{x}^*, \mathbf{x} \rangle \right\}$.

Higher μ -> more convex f_{μ} -> smoother conjugate f_{μ} *

Convex conjugate f_{μ}^* is also differentiable.

Dual Problem of Our Regression

Primal:
$$\widehat{x}_{\mu} := \underset{x}{\arg\min} f_{\mu}(x)$$
 subject to $||Ax - b|| \le \epsilon$.

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$$\widehat{x}_{\mu} := \arg\min_{x} f_{\mu}(x)$$
 subject to $\|Ax - b\| \le \epsilon$.

Dual: $\max g_{\mu}(z) := \inf_{z} \left\{ f_{\mu}(x) - \langle z, Ax - b \rangle - \epsilon \|z\| \right\}$

$$-> g_{\mu}(z) = \inf_{x} \left\{ f_{\mu}(x) - \langle A^{T}z, x \rangle \right\} + \langle z, b \rangle - \epsilon ||z||$$

$$= \underbrace{-f_{\mu}^{*}(A^{T}z) + \langle z, b \rangle}_{\text{smooth } \tilde{g}_{\mu}(z)} - \epsilon ||z||,$$

$$= \underbrace{-f_{\mu}^{*}(A^{T}z) + \langle z, b \rangle}_{h(z) \text{ non-smooth}}$$

Dual Problem of Our Regression

$$\widehat{x}_{\mu} := \underset{x}{\arg \min} f_{\mu}(x)$$
 subject to $||Ax - b|| \le \epsilon$.

maximize
$$g_{\mu}(z) := \inf_{x} \left\{ f_{\mu}(x) - \langle z, Ax - b \rangle - \epsilon ||z|| \right\}$$

$$= \inf_{\mathbf{x}} \left\{ f_{\mu}(\mathbf{x}) - \langle \mathbf{A}^T \mathbf{z}, \mathbf{x} \rangle \right\} + \langle \mathbf{z}, \mathbf{b} \rangle - \epsilon \|\mathbf{z}\|$$

$$= -f_{\mu}^* (\mathbf{A}^T \mathbf{z}) + \langle \mathbf{z}, \mathbf{b} \rangle - \epsilon \|\mathbf{z}\|,$$
smooth $\tilde{g}_{\mu}(\mathbf{z})$

$$h(\mathbf{z}) \text{ non-smooth}$$

Gradient of dual problem:

$$\nabla \tilde{g}_{\mu}(z) = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}_{z},$$

$$\boldsymbol{x}_{z} := \arg\min_{\boldsymbol{x}} \left\{ f_{\mu}(\boldsymbol{x}) - \langle \boldsymbol{A}^{T}\boldsymbol{z}, \ \boldsymbol{x} \rangle \right\}$$

Subgradient of $h(\mathbf{z}) = \varepsilon \mathbf{z}/||\mathbf{z}||$ if $\mathbf{z} \neq 0$, $\{\mathbf{y}| ||\mathbf{y}|| \leq 1\}$ if $\mathbf{z} = 0$

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- 5. Show relationship between dual-smoothing, computational cost, and risk

Algorithm 1. **Auslender–Teboulle**

```
Input: measurement matrix A, observed vector b, parameter \epsilon

1: z_0 \leftarrow 0, \overline{z}_0 \leftarrow z_0, \theta_0 \leftarrow 1

2: for k = 0, 1, 2, ... do

3: y_k \leftarrow (1 - \theta_k)z_k + \theta_k \overline{z}_k

4: x_k \leftarrow \arg\min_{x} \{f(x) + \langle y_k, b - Ax \rangle\}

5: \overline{z}_{k+1} \leftarrow \operatorname{Shrink} \left(\overline{z}_k - (b - Ax_k)/(L_{\mu} \cdot \theta), \epsilon/(L_{\mu} \cdot \theta)\right)

6: z_{k+1} \leftarrow (1 - \theta_k)z_k + \theta_k \overline{z}_{k+1}

7: \theta_{k+1} \leftarrow 2/(1 + (1 + 4/\theta_k^2)^{1/2})

8: end for
```

Algorithm 1. Auslender–Teboulle

Input: measurement matrix A, observed vector b, parameter ϵ

- 1: $z_0 \leftarrow \mathbf{0}, \, \overline{z}_0 \leftarrow z_0, \, \theta_0 \leftarrow 1$ 2: **for** $k = 0, 1, 2, \dots$ **do** $\mathbf{u}_{k} \leftarrow (1 - \theta_{k}) \mathbf{z}_{k} + \theta_{k} \overline{\mathbf{z}}_{k}$ 3:
- $x_k \leftarrow \arg\min_{\mathbf{x}} \{ f(\mathbf{x}) + \langle \mathbf{y}_k, \mathbf{b} A\mathbf{x} \rangle \}$
- $\overline{z}_{k+1} \leftarrow \text{Shrink}\left(\overline{z}_k (b Ax_k)/(L_{\mu} \cdot \theta), \epsilon/(L_{\mu} \cdot \theta)\right)$
- $z_{k+1} \leftarrow (1 \theta_k) z_k + \theta_k \overline{z}_{k+1} \\ \theta_{k+1} \leftarrow 2/(1 + (1 + 4/\theta_k^2)^{1/2})$
- 8: end for

Shrink
$$(z,t) = \max \left\{ 1 - \frac{t}{\|z\|}, 0 \right\} \cdot z.$$

$$\bar{z}_{k+1} \leftarrow \underset{z \in \mathbb{R}^m}{\min} \left\{ \tilde{g}_{\mu}(z_k) + \langle -\nabla \tilde{g}_{\mu}(z_k), z - z_k \rangle + \frac{1}{2} L_{\mu} \theta_k \|z - \bar{z}_k\|^2 + h(z) \right\}$$

Algorithm 1. Auslender–Teboulle

Input: measurement matrix A, observed vector b, parameter ϵ

If line 4 costs little, then per iteration, cost will be O(md), for matrix multiplications with A

Assuming dual-smoothing method + iterative first-order algorithm,

Theorem IV.5 (Primal feasibility gap). Assume that the regularizer f_{μ} in the linear regression problem (7) is μ -strongly convex. Apply Algorithm 1 to the corresponding dual problem (8), and let z^* be the optimal dual point. For any $k \geq 0$,

$$|||Ax_k - b|| - \epsilon| \le \frac{2||A||^2 ||z^*||}{\mu k}.$$
 (11)

If μ is large, upper bound for duality gap is lower.

Or for fixed $||Ax-b|| = \sqrt{(mR)}$ and ε , if μ is large, iteration k can be smaller.

Designing Statistical Estimators That Balance Sample Size, Risk, and Computational Cost

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$$= m = R = O(kmd)$$

... using μ , dual-smoothing parameter

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How to relax regularizer f

Turn convex f into strongly convex f_{μ} $f_{\mu}(\mathbf{x}) := f(\mathbf{x}) + \frac{\mu}{2} \|\mathbf{x}\|^2$.

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Upper bound on number of iterations for convergence:

$$k \le \frac{2 \|z^*\|}{\gamma \mu \sigma \sqrt{m - \delta}}.$$

If μ is higher, δ increases too, so there's probably an upper bound to how much we can increase μ before k stops decreasing.

If μ is constant, computational cost O(kmd) is proportional to \sqrt{m} .

Summary so far:

• δ is proportional to μ (geometric intuition)

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$$k \le \frac{2 \|z^*\|}{\gamma \mu \sigma \sqrt{m - \delta}}.$$

$$\frac{\delta\left(\mathcal{D}(f_{\mu}; \boldsymbol{x}^{\natural})\right)}{m} = \frac{\overline{\delta}}{\overline{m} + (m - \overline{m})^{\alpha}} \begin{vmatrix} \alpha = 1 \\ \alpha = -\infty \end{vmatrix}$$

$$\alpha = 1$$
:

$$\alpha = -\infty$$
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Baseline δ from small baseline value for μ

$$\frac{\delta \left(\mathcal{D}(f_{\mu}; \boldsymbol{x}^{\natural}) \right)}{m} = \frac{\overline{\delta}}{\overline{m} + (m - \overline{m})^{\alpha}} \qquad \alpha = 1:$$

$$\alpha = -\infty:$$
Baseline sample size m

$$\alpha \text{ in } (-\infty, 1):$$

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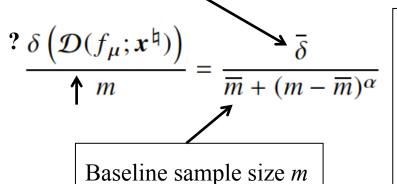
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?
$$\frac{\delta \left(\mathcal{D}(f_{\mu}; \boldsymbol{x}^{\natural}) \right)}{\uparrow m} = \frac{1}{\overline{m} + (m - \overline{m})^{\alpha}}$$
 $\alpha = 1$:
$$\alpha = -\infty$$
:
Baseline sample size m α in $(-\infty, 1)$:

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Baseline δ from small baseline value for μ



 $\alpha = 1$: μ is constant; δ is constant; R falls; cost increases

$$\alpha = -\infty$$
:

 α in $(-\infty,1)$:

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Baseline δ from small baseline value for μ

$$\frac{? \delta \left(\mathcal{D}(f_{\mu}; x^{\natural}) \right)}{\uparrow m} = \frac{\sqrt{\delta}}{\overline{m} + (m - \overline{m})^{\alpha}}$$
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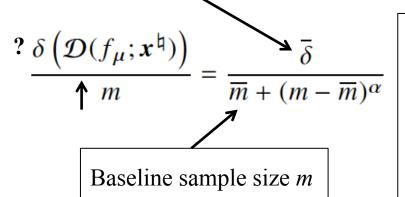
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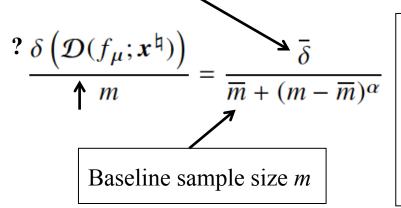
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 α in (- ∞ ,1): balance!

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Baseline δ from small baseline value for μ



 $\alpha = 1$: μ is constant; δ is constant; R falls; cost increases

 $\alpha = -\infty$: μ increases; δ increases; R is constant; cost decreases

 α in (- ∞ ,1): balance!

"When we have excess samples in the data set, we can exploit them to decrease the statistical risk of our estimator or to lower the computational cost through additional smoothing. A tradeoff arises from the balance between these two competing interests."

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- 1. Define the regression problem, risk (R), and statistical dimension of descent cone (δ)
- 2. Show relationship between risk, sample size (m), and δ
- 3. Show geometric relationship between relaxed f, δ , and R
- 4. Define strong convexity, Lipschitz gradient, and dual problem
- 5. Show relationship between smoothing, computational cost, and risk
- 6. Describe smoothing approach
- 7. Results on simulations

LASSO

$$\widehat{x}_{\mu} := \underset{x}{\operatorname{arg min}} f_{\mu}(x)$$
 subject to $||Ax - b|| \le \epsilon$.

$$f_{\mu}(\mathbf{x}) = \|\mathbf{x}\|_{\ell_1} + \frac{\mu}{2} \|\mathbf{x}\|^2$$

Proposition VI.1 (Statistical dimension bound for the dual-smoothed ℓ_1 norm). Let $\mathbf{x} \in \mathbb{R}^d$ be s-sparse, and define the normalized sparsity $\rho := s/d$. Let f_{μ} be as in (13). Then

$$\frac{\delta\left(\mathcal{D}(f_{\mu};\boldsymbol{x})\right)}{d} \leq \psi(\rho),$$

where $\psi: [0,1] \to \mathbb{R}$ is the function given by

$$\psi(\rho) = \inf_{\tau \ge 0} \left\{ \rho \left[1 + \tau^2 (1 + \mu \|\mathbf{x}\|_{\ell_{\infty}})^2 \right] + (1 - \rho) \sqrt{\frac{2}{\pi}} \int_{-\infty}^{\infty} (u - \tau)^2 e^{-u^2/2} du \right\}.$$

Some complicated looking value for upper bound of δ .

We just need to notice μ there.

LASSO

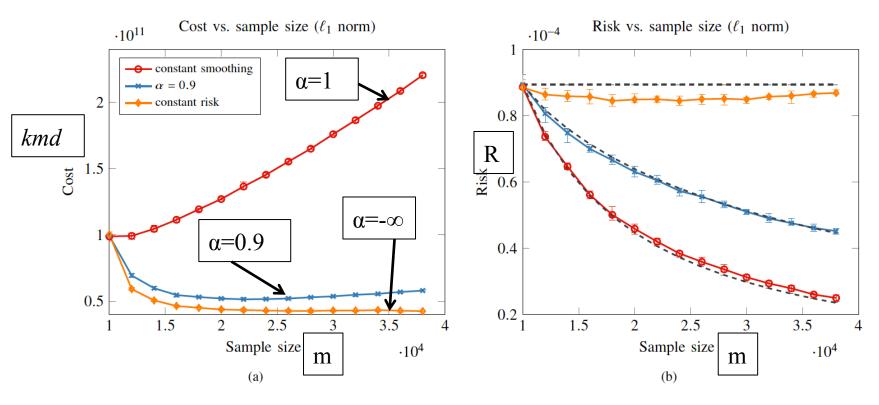
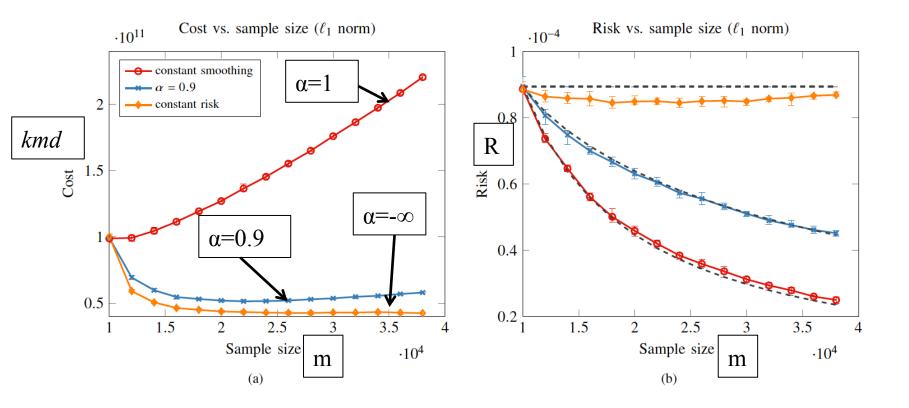


Fig. 2. **Sparse vector regression experiment.** The panels show (a) the average computational cost and (b) the estimated statistical risk over 10 random trials of the dual-smoothed sparse vector regression problem with ambient dimension $d=40\,000$, normalized sparsity $\rho=5\%$, and noise level $\sigma=0.01$ for various sample sizes m. The red curve (circles) represents using a fixed smoothing parameter $\mu=0.1$, the orange curve (diamonds) results from adjusting the smoothing parameter μ to maintain the baseline risk, and the blue curve (crosses) uses the balanced scheme (12) with scaling parameter $\alpha=0.9$. For all schemes, the baseline smoothing parameter $\mu=0.1$, and the baseline sample size $m=10\,000$. The error bars indicate the minimum and maximum observed values. The dashed black lines show the predicted risk based on Proposition VI.1 and Fact III.3.

LASSO



 $\alpha = 1$: μ is constant; δ is constant; **R falls; cost increases** $\alpha = -\infty$: μ increases; δ increases; **R is constant; cost decreases** α in $(-\infty,1)$: *balance!*

Low-Rank Matrix Regression

$$\widehat{x}_{\mu} := \underset{x}{\arg\min} f_{\mu}(x)$$
 subject to $||Ax - b|| \le \epsilon$.

$$f_{\mu}(X) = ||X||_* + \frac{\mu}{2} ||X||_{\mathrm{F}}^2$$

$$\begin{split} \psi(\rho) &:= \inf_{0 \leq \tau \leq 2} \left\{ \rho + (1 - \rho) \left[\rho \left(1 + \tau^2 (1 + \mu) \|X\| \right)^2 \right) \right. \\ &+ \frac{(1 - \rho)}{12\pi} \left[24(1 + \tau^2) \cos^{-1}(\tau/2) - \tau (26 + \tau^2) \sqrt{4 - \tau^2} \right] \right] \right\}. \end{split}$$

Again, we have some complicated looking upper bound for δ .

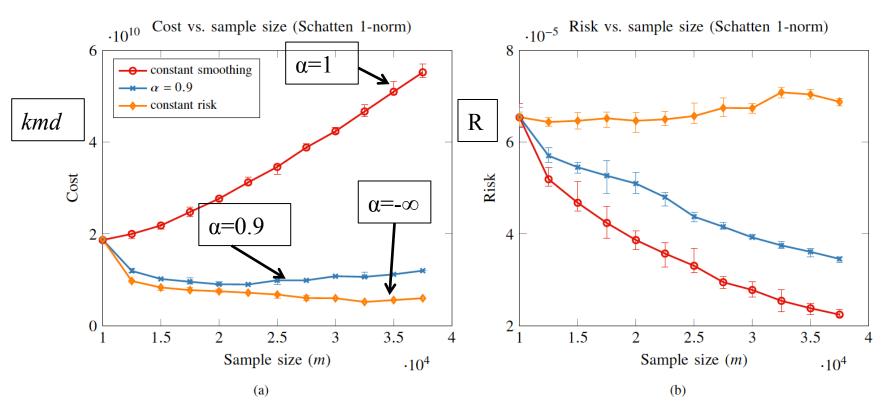


Fig. 3. Low-rank matrix regression experiment. The panels show (a) the average computational cost and (b) the estimated statistical risk over 10 random trials of the dual-smoothed low-rank matrix regression problem with ambient dimension $d=200\times200$, normalized rank $\rho=5\%$, and noise level $\sigma=0.01$ for various sample sizes m. The red curve (circles) represents using a fixed smoothing parameter $\mu=0.1$, the orange curve (diamonds) results from adjusting the smoothing parameter μ to maintain the baseline risk, and the blue curve (crosses) uses the balanced scheme (12) with scaling parameter $\alpha=0.9$. For all schemes, the baseline smoothing parameter $\mu=0.1$, and the baseline sample size $m=10\,000$. The error bars indicate the minimum and maximum observed values.

Image Interpolation

minimize
$$\|\mathcal{W}(X)\|_{\ell_1} + \frac{\mu}{2} \|\mathcal{W}(X)\|^2$$

subject to $\mathcal{A}(X) = b$,

W is 2D discrete cosine transformation (DCT) operator. We expect this to be sparse for natural images.

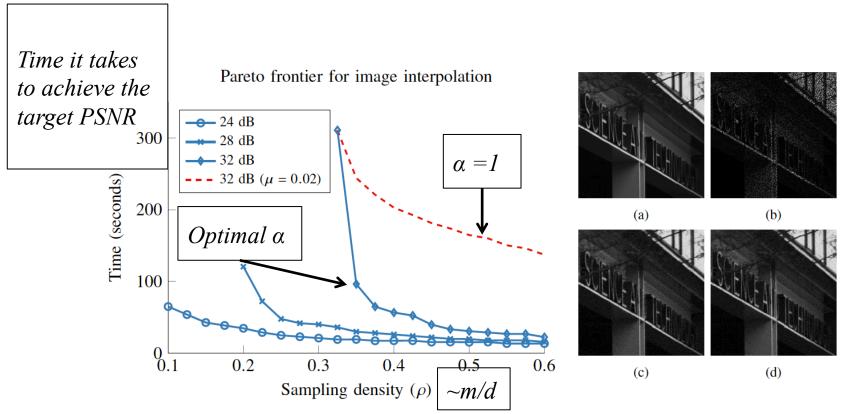


Fig. 4. **Image interpolation.** The graph shows the observed Pareto frontier in our image interpolation experiment where we treat the sampling density ρ and computational time as the two resources that we trade off. The solid blue lines give the Pareto frontiers achieved by aggressively smoothing the problem as we increase the sampling density ρ . These frontiers correspond to three different accuracy levels of the reconstructed images given as a peak signal-to-noise-ratio (PSNR). The dashed red line shows the frontier achieved for 32 dB PSNR accuracy with a fixed smoothing parameter $\mu = 0.02$ as sampling density ρ increases. Our aggressive smoothing outperforms the constant smoothing by a large margin. The grid of images shows 450×450 pixel patches of: (a) the original image, (b) the original image subsampled at $\rho = 40\%$, (c) the reconstructed image with $\rho = 40\%$ and $\mu = 0.32$ (32.2 dB PSNR). The shown reconstructions are of the same quality despite the differing values of μ .

Peak signal to noise ratio
$$PSNR(X_k) = 10 \cdot \log_{10} \left(\frac{d_1 d_2}{\|X_k - X^{\natural}\|_F} \right)$$
,

couple of comments...

- Why not use the actual time taken instead of *kmd* in the numerical simulations? Or does that even matter?
- To use phase transition theorem, measurement matrix A had to have orthonormal rows; is that restriction costly in any way?
- They mention the possibility of tuning μ to meet target R. That would be really interesting to see.

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