Pattern Information Processing: Robust Method

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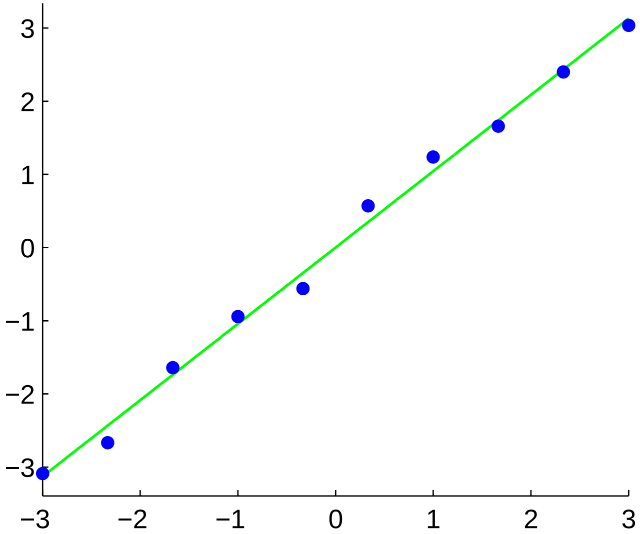
Outliers

- In practice, very large noise sometimes appears.
- Furthermore, irregular values can be observed by measurement trouble or by human error.
- Samples with such irregular values are called outliers.

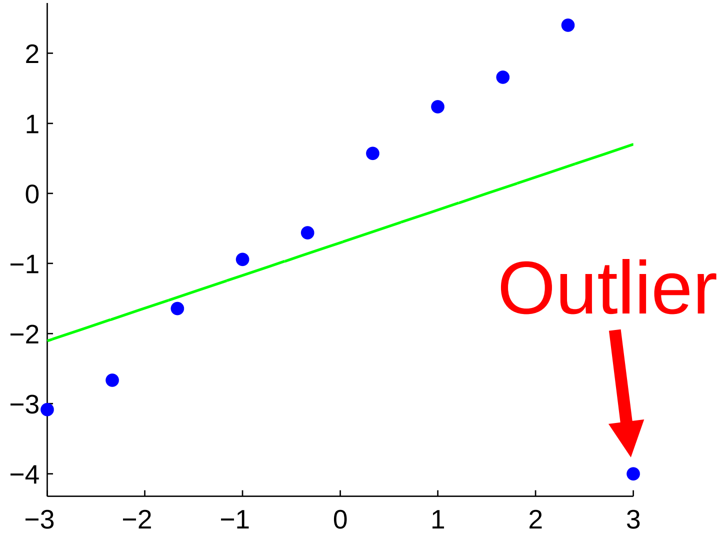
Outliers (cont.)

- LS criterion is sensitive to outliers.

$$\hat{f}(x) = \alpha_1 + \alpha_2 x$$



LS (without outlier)



LS (with outlier)

- Even a single outlier can corrupt the learning result badly!

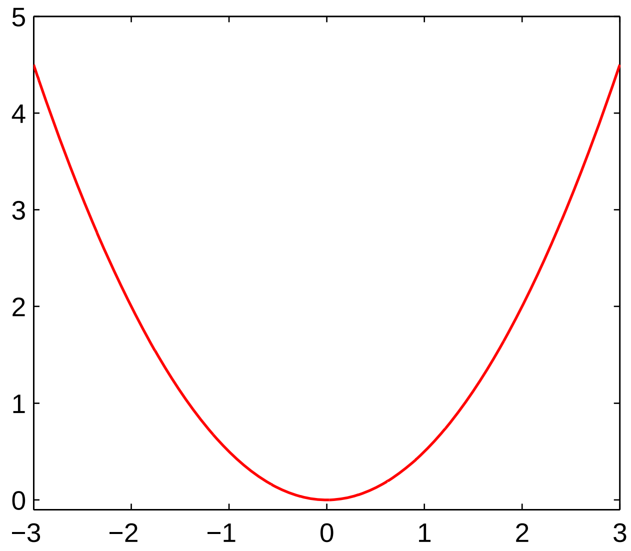
Today’s Plan

- Robust learning method
- How to obtain solutions
- Standard form of quadratic programs
- Robustness and sparseness

Quadratic Loss

$$J_{LS}(\boldsymbol{\alpha}) = \sum_{i=1}^{n} \left(\hat{f}(\boldsymbol{x}_i) - y_i \right)^2$$

- In LS, goodness-of-fit is measured by the squared loss.
- Therefore, even a single outlier has quadratic power to “pull” the learned function
- The solution will be robust if the effect of outliers are deemphasized.

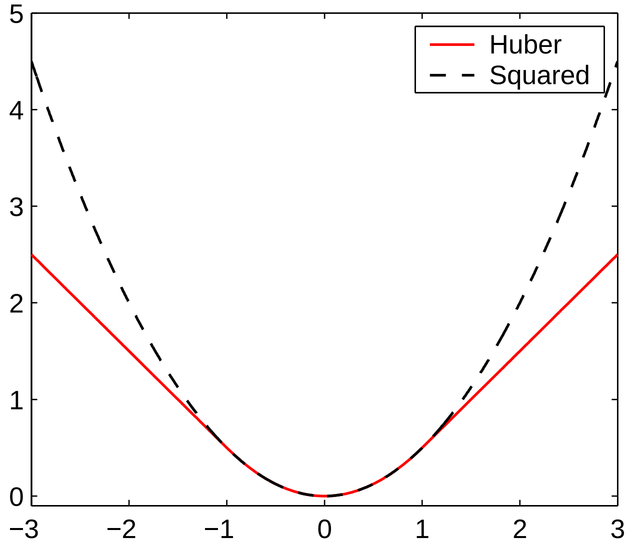


Huber's Robust Learning

$$\hat{\boldsymbol{\alpha}}_{Huber} = \underset{\boldsymbol{\alpha} \in \mathbb{R}^b}{\text{argmin}} \left[\sum_{i=1}^{n} \rho\left(\hat{f}(\boldsymbol{x}_i) - y_i \right) \right]$$

$$t > 0$$

$$\rho(y) = \begin{cases} \frac{1}{2} y^2 & (|y| \leq t) \\ t|y| - \frac{1}{2} t^2 & (|y| > t) \end{cases}$$



- Squared-loss for non-outliers with small errors.
- Linear penalty for outliers with large errors.

P. J. Huber, Robust Statistics, Wiley, New York, 1981.

How to Obtain Solutions

- How to deal with Huber’s loss?
- Use the following lemma:

Lemma

$$\rho(y) = \min_{v \in \mathbb{R}} g(v)$$

$$g(v) = \frac{1}{2}v^2 + t|y - v|$$

See:
Mangasarian & Musicant, Robust linear and support vector regression, IEEE Trans. Pattern Analysis and Machine Intelligence, 22(9), 950-955,2000

Proof of Lemma

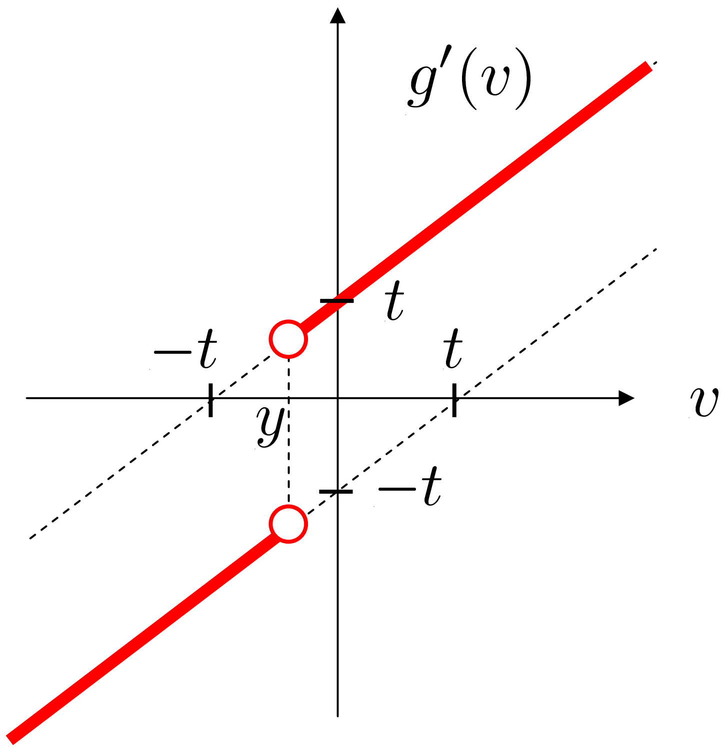
- Here, we give a non-constructive proof.
  - We explicitly compute $\min_{v \in \mathbb{R}} g(v)$ using $g'(v)$.

$$g(v) = \begin{cases} \frac{1}{2}v^2 + ty - tv & (v \leq y) \\ \frac{1}{2}v^2 - ty + tv & (v > y) \end{cases}$$

$$g'(v) = \begin{cases} v - t & (v < y) \\ v + t & (v > y) \end{cases}$$

Proof of Lemma (cont.)

- If $-t \le y \le t$, $g(v)$ is minimized at $v = y$.



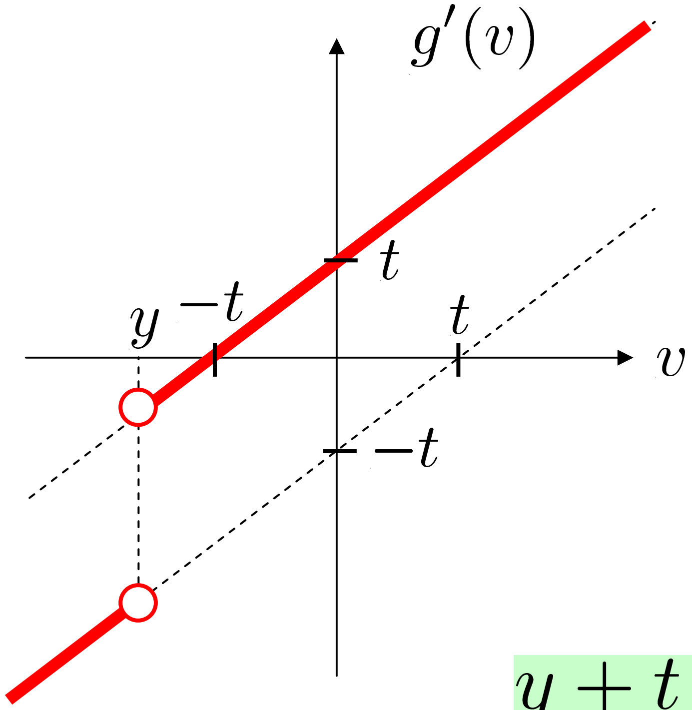
- Then

$$\min_{v\in\mathbb{R}} g(v) = g(y) = \frac{1}{2}y^2 = \rho(y)$$

Note: $g(v)$ is continuous

Proof of Lemma (cont.)

- If $y < -t$, $g(v)$ is minimized at $v = -t$.



$y + t < 0$

Then

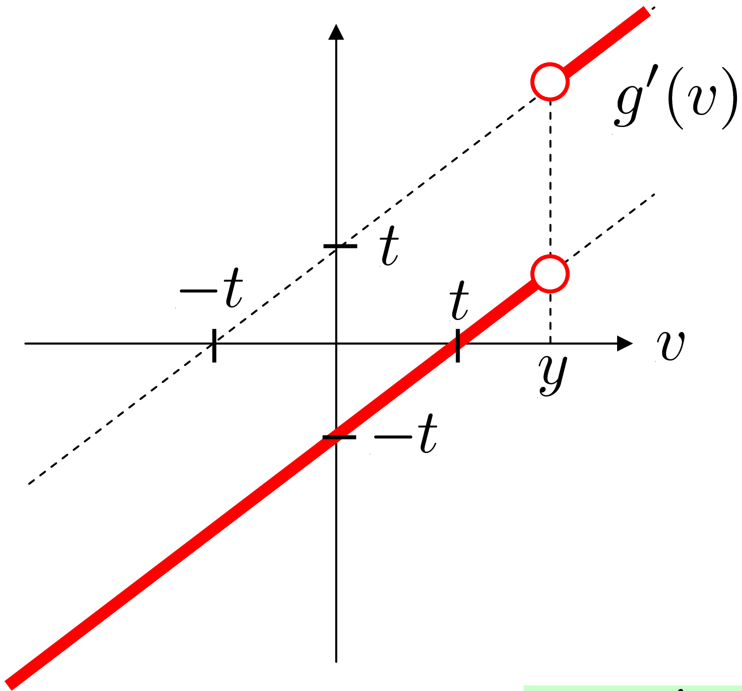
$$\min_{v \in \mathbb{R}} g(v) = g(-t) = \frac{1}{2}t^2 + t|y+t| = -ty - \frac{1}{2}t^2$$

$y < 0$

$$= t|y| - \frac{1}{2}t^2 = \rho(y)$$

Proof of Lemma (cont.)

- If $y > t$, $g(v)$ is minimized at $v = t$.



Then

$y - t > 0$

$$\min_{v \in \mathbb{R}} g(v) = g(t) = \frac{1}{2}t^2 + t|y - t| = ty - \frac{1}{2}t^2$$

$y > 0$

$$= t|y| - \frac{1}{2}t^2 = \rho(y)$$

Q.E.D.

How to Obtain Solutions (cont.)

- Using

$$\rho(y) = \min_{v \in \mathbb{R}} \left[\frac{1}{2} v^2 + t|y - v| \right]$$

we have

$$\hat{\boldsymbol{\alpha}}_{Huber} = \mathop{\mathrm{argmin}}_{\boldsymbol{\alpha} \in \mathbb{R}^b, \boldsymbol{v} \in \mathbb{R}^n} \left[\frac{1}{2} \|\boldsymbol{v}\|^2 + t \|\boldsymbol{X}\boldsymbol{\alpha} - \boldsymbol{y} - \boldsymbol{v}\|_1 \right]$$

$$\boldsymbol{X}_{i,j} = \varphi_j(\boldsymbol{x}_i)$$

$$\hat{\boldsymbol{\alpha}}_{Huber} \equiv \mathop{\mathrm{argmin}}_{\boldsymbol{\alpha} \in \mathbb{R}^b} \left[\sum_{i=1}^{n} \rho\left(\hat{f}(\boldsymbol{x}_i) - y_i \right) \right]$$

How to Obtain Solutions (cont.)

- Trick to avoid absolute value:

$$\|\boldsymbol{X}\boldsymbol{\alpha} - \boldsymbol{y} - \boldsymbol{v}\|_1 = \min_{\boldsymbol{u}\in\mathbb{R}^n} \left[\sum_{i=1}^{n} u_i\right]$$

$$\text{subject to } -\boldsymbol{u} \leq \boldsymbol{X}\boldsymbol{\alpha} - \boldsymbol{y} - \boldsymbol{v} \leq \boldsymbol{u}$$

- $\hat{\boldsymbol{\alpha}}_{Huber}$ is given as the solution of

$$\mathop{\mathrm{argmin}}_{\boldsymbol{\alpha}\in\mathbb{R}^b,\boldsymbol{u},\boldsymbol{v}\in\mathbb{R}^n} \left[\frac{1}{2}\|\boldsymbol{v}\|^2 + t\sum_{i=1}^{n} u_i\right]$$

$$\text{subject to } -\boldsymbol{u} \leq \boldsymbol{X}\boldsymbol{\alpha} - \boldsymbol{y} - \boldsymbol{v} \leq \boldsymbol{u}$$

Standard Form (Huber)

- Let $\boldsymbol{\beta} = \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{u} \\ \boldsymbol{v} \end{pmatrix}$

$$\boldsymbol{\Gamma}_{\boldsymbol{\alpha}} = (\boldsymbol{I}_b, \boldsymbol{O}_{b\times n}, \boldsymbol{O}_{b\times n})$$
$$\boldsymbol{\Gamma}_{\boldsymbol{u}} = (\boldsymbol{O}_{n\times b}, \boldsymbol{I}_n, \boldsymbol{O}_{n\times n})$$
$$\boldsymbol{\Gamma}_{\boldsymbol{v}} = (\boldsymbol{O}_{n\times b}, \boldsymbol{O}_{n\times n}, \boldsymbol{I}_n)$$

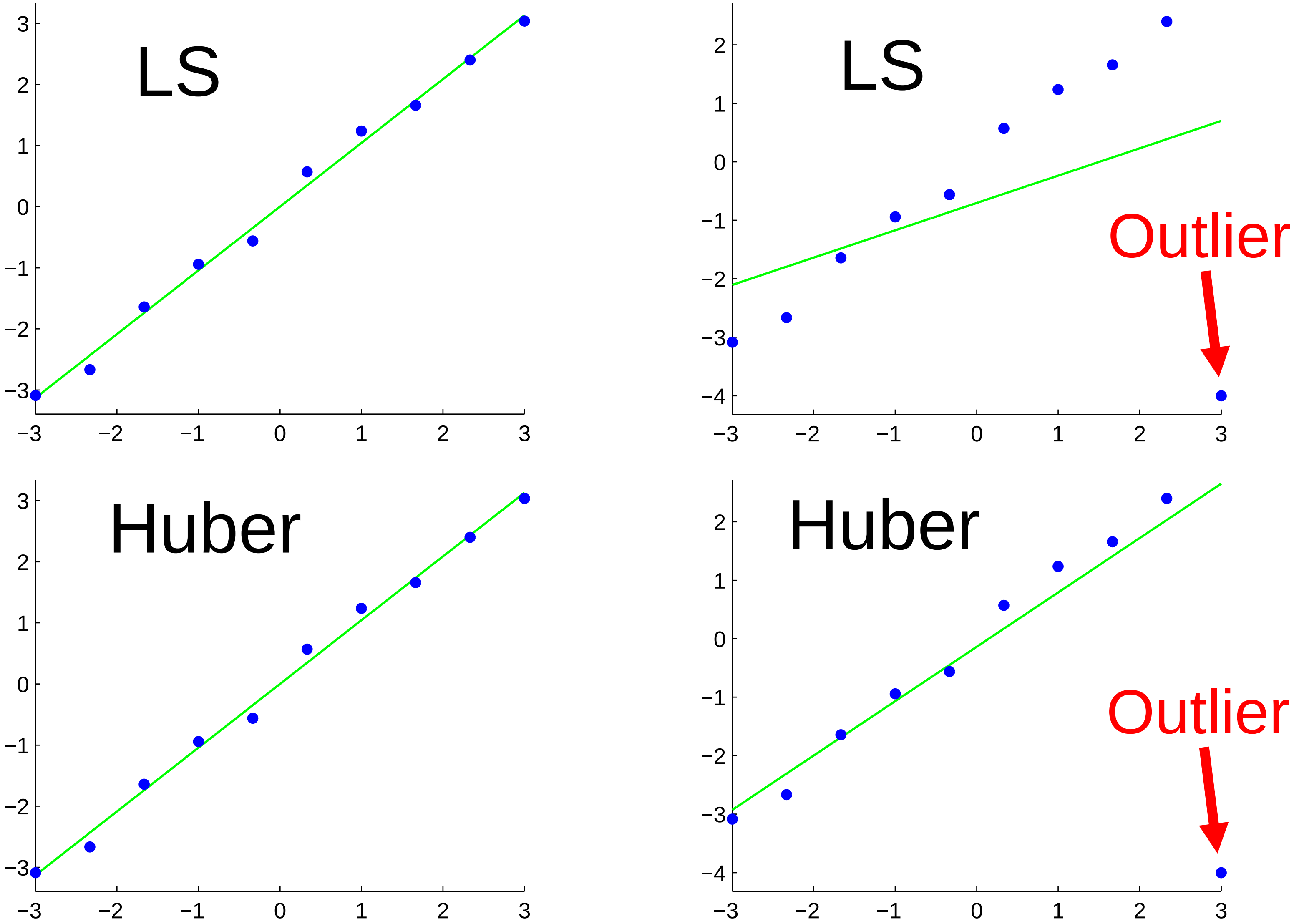
$$\Rightarrow \quad \boldsymbol{\alpha} = \boldsymbol{\Gamma}_{\boldsymbol{\alpha}}\boldsymbol{\beta} \qquad \boldsymbol{u} = \boldsymbol{\Gamma}_{\boldsymbol{u}}\boldsymbol{\beta} \qquad \boldsymbol{v} = \boldsymbol{\Gamma}_{\boldsymbol{v}}\boldsymbol{\beta}$$

- $\frac{1}{2}\|\boldsymbol{v}\|^2 + t\sum_{i=1}^{n} u_i = \frac{1}{2}\langle \boldsymbol{\Gamma}_{\boldsymbol{v}}^\top \boldsymbol{\Gamma}_{\boldsymbol{v}}\boldsymbol{\beta}, \boldsymbol{\beta}\rangle + \langle \boldsymbol{\beta}, t\boldsymbol{\Gamma}_{\boldsymbol{u}}^\top \mathbf{1}_n\rangle$
- $-\boldsymbol{u} \leq \boldsymbol{X}\boldsymbol{\alpha} - \boldsymbol{y} - \boldsymbol{v} \leq \boldsymbol{u}$

$$\Rightarrow \quad \begin{pmatrix} -\boldsymbol{u} - \boldsymbol{X}\boldsymbol{\alpha} + \boldsymbol{v} \\ \boldsymbol{X}\boldsymbol{\alpha} - \boldsymbol{v} - \boldsymbol{u} \end{pmatrix} \leq \begin{pmatrix} -\boldsymbol{y} \\ \boldsymbol{y} \end{pmatrix}$$

$$\Rightarrow \quad \begin{pmatrix} -\boldsymbol{X}\boldsymbol{\Gamma}_{\boldsymbol{\alpha}} - \boldsymbol{\Gamma}_{\boldsymbol{u}} + \boldsymbol{\Gamma}_{\boldsymbol{v}} \\ \boldsymbol{X}\boldsymbol{\Gamma}_{\boldsymbol{\alpha}} - \boldsymbol{\Gamma}_{\boldsymbol{u}} - \boldsymbol{\Gamma}_{\boldsymbol{v}} \end{pmatrix} \boldsymbol{\beta} \leq \begin{pmatrix} -\boldsymbol{y} \\ \boldsymbol{y} \end{pmatrix}$$

Example of Huber's Method



Robust and Sparse

- Huber's method does not generally provide a sparse solution.
- Combining Huber's loss with ℓ_1 constraint.

$$\hat{\boldsymbol{\alpha}}_{SparseHuber} = \mathop{\mathrm{argmin}}_{\boldsymbol{\alpha}\in\mathbb{R}^b} \left[\sum_{i=1}^{n} \rho\left(\hat{f}(\boldsymbol{x}_i) - y_i\right) \right]$$

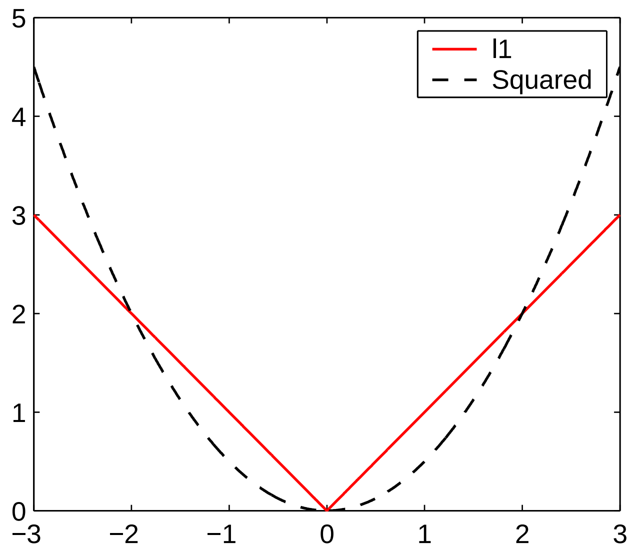
$$\text{subject to } \|\boldsymbol{\alpha}\|_1 \leq C$$

- Solving quadratic programming problem is computationally rather demanding.
- Is it possible to make it faster?

l1 Loss

- Quadratic term comes from Huber's loss.
- ℓ_1-loss is linear.

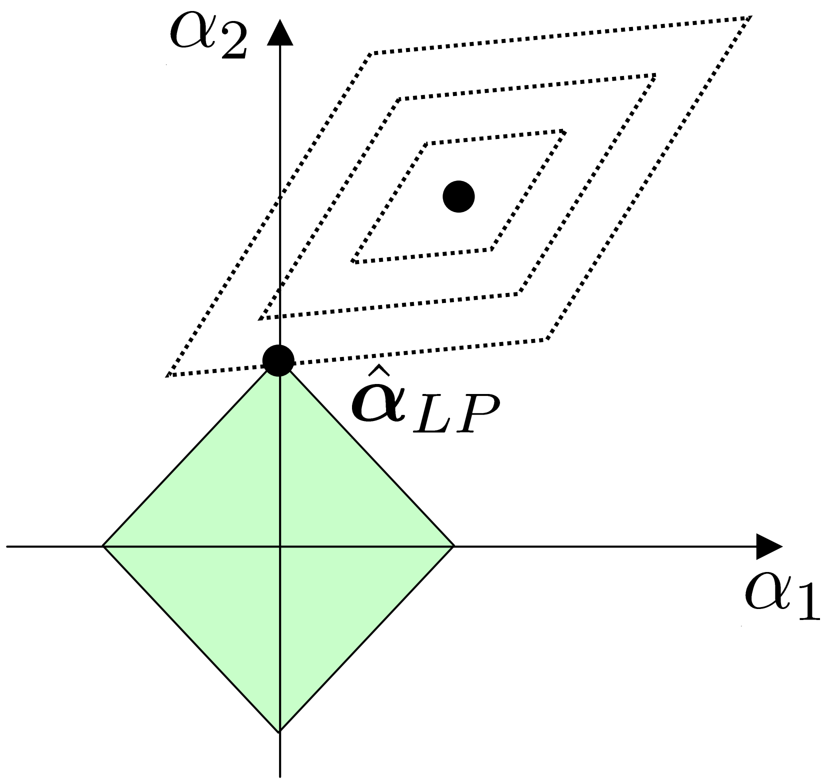
$$\sum_{i=1}^{n} \left| \hat{f}(\boldsymbol{x}_i) - y_i \right|$$



Linear Programming Learning

- Combine ℓ_1 loss with ℓ_1 regularizer:

$$\hat{\boldsymbol{\alpha}}_{LP} = \mathop{\mathrm{argmin}}_{\boldsymbol{\alpha}\in\mathbb{R}^b} \left[\sum_{i=1}^{n} \left| \hat{f}(\boldsymbol{x}_i) - y_i \right| + \lambda \sum_{i=1}^{b} |\alpha_i| \right]$$



How to Obtain Solutions

- Trick to avoid absolute value:

$$\|\boldsymbol{\alpha}\|_1 = \min_{\boldsymbol{u}\in\mathbb{R}^b} \left[\sum_{i=1}^{b} u_i\right]$$

$$\text{subject to } -\boldsymbol{u} \leq \boldsymbol{\alpha} \leq \boldsymbol{u},$$

- $\hat{\boldsymbol{\alpha}}_{LP}$ is given as the solution of

$$\underset{\boldsymbol{\alpha},\boldsymbol{u}\in\mathbb{R}^b,\boldsymbol{v}\in\mathbb{R}^n}{\text{argmin}} \left[\sum_{i=1}^{n} v_i + \lambda \sum_{i=1}^{b} u_i\right]$$

$$\text{subject to } -\boldsymbol{v} \leq \boldsymbol{X}\boldsymbol{\alpha} - \boldsymbol{y} \leq \boldsymbol{v}$$

$$-\boldsymbol{u} \leq \boldsymbol{\alpha} \leq \boldsymbol{u}$$

Linearly Constrained Linear Programming Problem

- Standard optimization software can solve the following form of linearly constrained linear programming problems.

$$\min_{\boldsymbol{\beta}} \langle \boldsymbol{\beta}, \boldsymbol{q} \rangle \quad \text{subject to } \boldsymbol{V}\boldsymbol{\beta} \leq \boldsymbol{v}$$
$$\boldsymbol{G}\boldsymbol{\beta} = \boldsymbol{g}$$

Standard Form (LP)

- Let $\boldsymbol{\beta} = \begin{pmatrix} \boldsymbol{\alpha} \\ \boldsymbol{u} \\ \boldsymbol{v} \end{pmatrix}$

$$\begin{aligned} \boldsymbol{\Gamma}_{\boldsymbol{\alpha}} &= (\boldsymbol{I}_b, \boldsymbol{O}_{b\times b}, \boldsymbol{O}_{b\times n}) \\ \boldsymbol{\Gamma}_{\boldsymbol{u}} &= (\boldsymbol{O}_{b\times b}, \boldsymbol{I}_b, \boldsymbol{O}_{b\times n}) \\ \boldsymbol{\Gamma}_{\boldsymbol{v}} &= (\boldsymbol{O}_{n\times b}, \boldsymbol{O}_{n\times b}, \boldsymbol{I}_n) \end{aligned}$$

$$\Rightarrow \quad \boldsymbol{\alpha} = \boldsymbol{\Gamma}_{\boldsymbol{\alpha}}\boldsymbol{\beta} \qquad \boldsymbol{u} = \boldsymbol{\Gamma}_{\boldsymbol{u}}\boldsymbol{\beta} \qquad \boldsymbol{v} = \boldsymbol{\Gamma}_{\boldsymbol{v}}\boldsymbol{\beta}$$

- $\displaystyle\sum_{i=1}^{n} v_i + \lambda \sum_{i=1}^{b} u_i = \langle \boldsymbol{\beta}, \boldsymbol{\Gamma}_{\boldsymbol{v}}^\top \mathbf{1}_n + \lambda \boldsymbol{\Gamma}_{\boldsymbol{u}}^\top \mathbf{1}_b \rangle$

- $-\boldsymbol{v} \leq \boldsymbol{X}\boldsymbol{\alpha} - \boldsymbol{y} \leq \boldsymbol{v} \qquad -\boldsymbol{u} \leq \boldsymbol{\alpha} \leq \boldsymbol{u}$

$$\Rightarrow \quad \begin{pmatrix} -\boldsymbol{X}\boldsymbol{\Gamma}_{\boldsymbol{\alpha}} - \boldsymbol{\Gamma}_{\boldsymbol{v}} \\ \boldsymbol{X}\boldsymbol{\Gamma}_{\boldsymbol{\alpha}} - \boldsymbol{\Gamma}_{\boldsymbol{v}} \\ -\boldsymbol{\Gamma}_{\boldsymbol{\alpha}} - \boldsymbol{\Gamma}_{\boldsymbol{u}} \\ \boldsymbol{\Gamma}_{\boldsymbol{\alpha}} - \boldsymbol{\Gamma}_{\boldsymbol{u}} \end{pmatrix} \boldsymbol{\beta} \leq \begin{pmatrix} -\boldsymbol{y} \\ \boldsymbol{y} \\ \mathbf{0}_b \\ \mathbf{0}_b \end{pmatrix}$$

Sparseness and Robustness

	Sparseness	Robustness	Optimization
ℓ_1 constrained LS	Yes	No	Quadratic
Huber's method	No	Yes	Quadratic
ℓ_1 constrained Huber	Yes	Yes	Quadratic
Linear programming	Yes	Yes	Linear

Homework

- For your own toy 1-dimensional data, perform simulations using
  - Linear/Gaussian kernel models
  - Huber/linear-programming learning

  and analyze the results, e.g., by changing
  - Target functions
  - Number of samples
  - Noise level

  Including outliers in the dataset would be essential for this homework.