Variable Selection Using Regularized Loss Functions

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Logistic Regression

- Binary classification: classes y=1 and y=-1 (not 0)

$$P(y=1|\mathbf{x}) = \frac{\exp(w_0 + \sum_i w_i x_i)}{1+\exp(w_0 + \sum_i w_i x_i)} = \frac{1}{1+\exp(-\mathbf{w}^T\mathbf{x})}$$

$$P(y=-1|\mathbf{x}) = \frac{1}{1+\exp(w_0 + \sum_i w_i x_i)} = \frac{1}{1+\exp(\mathbf{w}^T\mathbf{x})}$$

- Hence

$$P(y|\mathbf{x}) = \frac{1}{1+\exp(-y\mathbf{w}^T\mathbf{x})}$$

- Conditional negative log likelihood for training examples (x_j, y_j):

$$L(\mathbf{w}) = \frac{1}{N}\sum_{j=1}^{N} \ln(1+e^{-y_j\mathbf{w}^T\mathbf{x}_j})$$

Variable Selection

- Why Variable Selection
  - Simpler model= better prediction accuracy
  - Occam's razor again
  - Can have many features e.g. 100000.
  - Computationally more efficient.

- Negative log likelihood + penalty

$$L(\mathbf{w}) = \frac{1}{N}\sum_{j=1}^{N} \ln(1 + e^{-y_j \mathbf{w}^T \mathbf{x}_j}) + \lambda \underbrace{\sum_{i=1}^{p} \rho(w_i)}_{\text{Penalty}}$$

  - Penalty = Sparsifying effect

Variable Selection

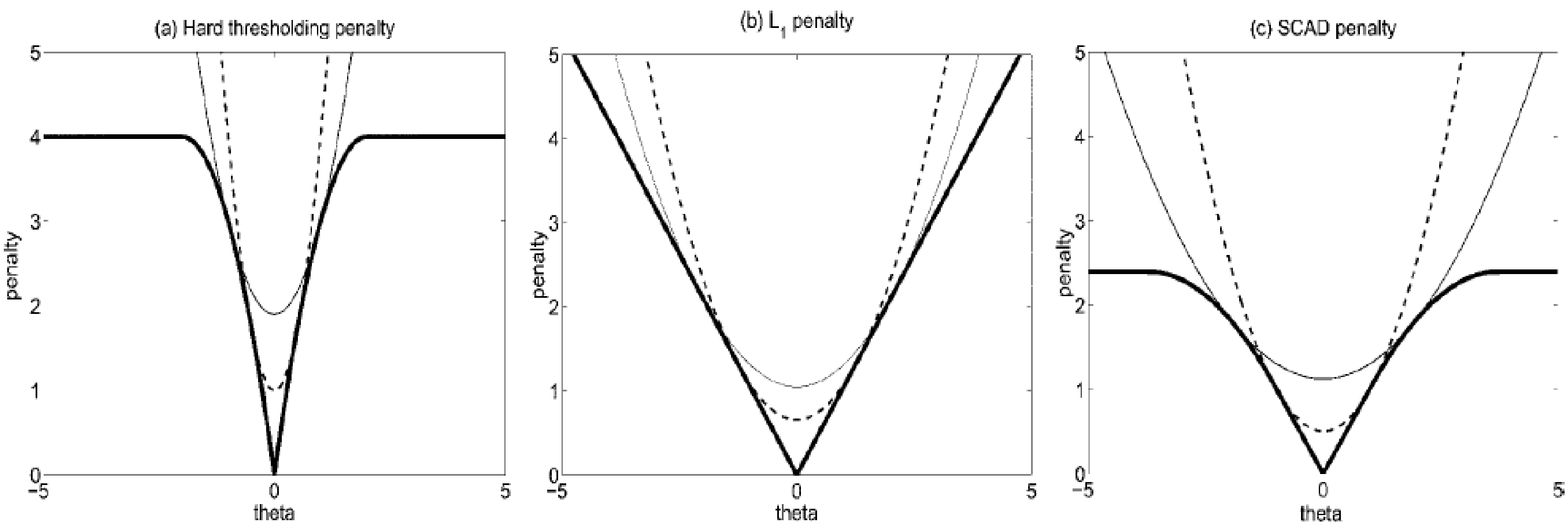
- Regularized logistic loss:

$$L(\mathbf{w}) = \frac{1}{N}\sum_{j=1}^{N} \ln(1 + e^{-y_j \mathbf{w}^T \mathbf{x}_j}) + \lambda \sum_{i=1}^{p} \rho(w_i)$$

Logistic Loss

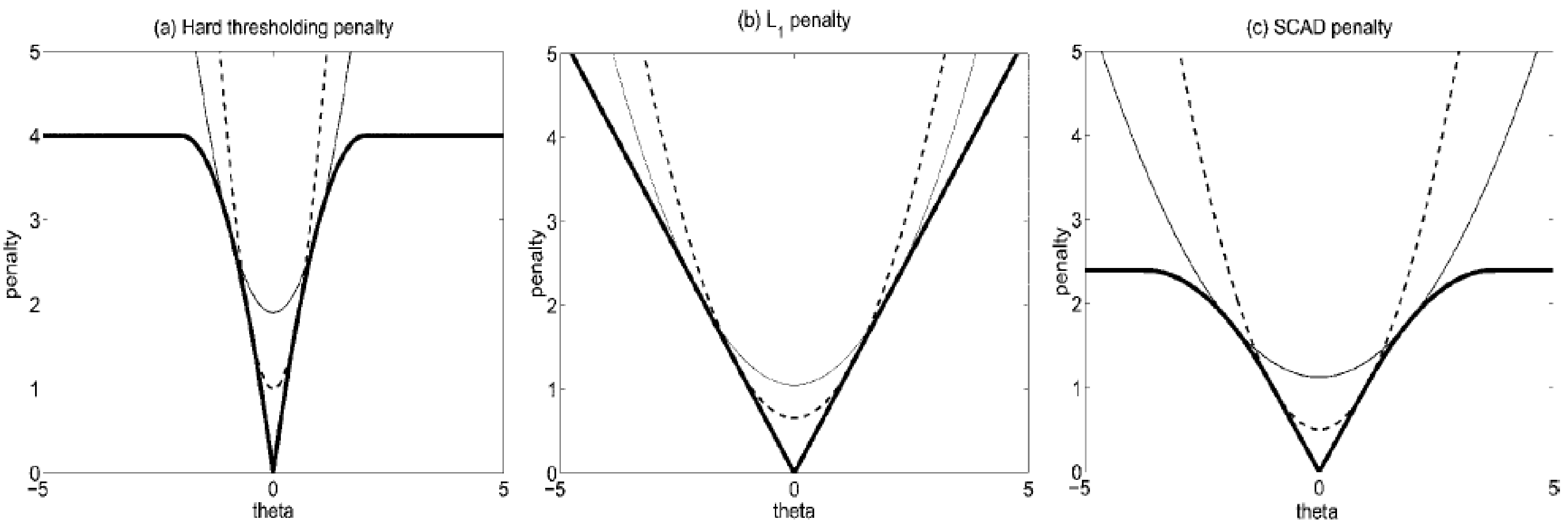
Penalty

- Sparsifying penalty functions ρ must be singular at origin

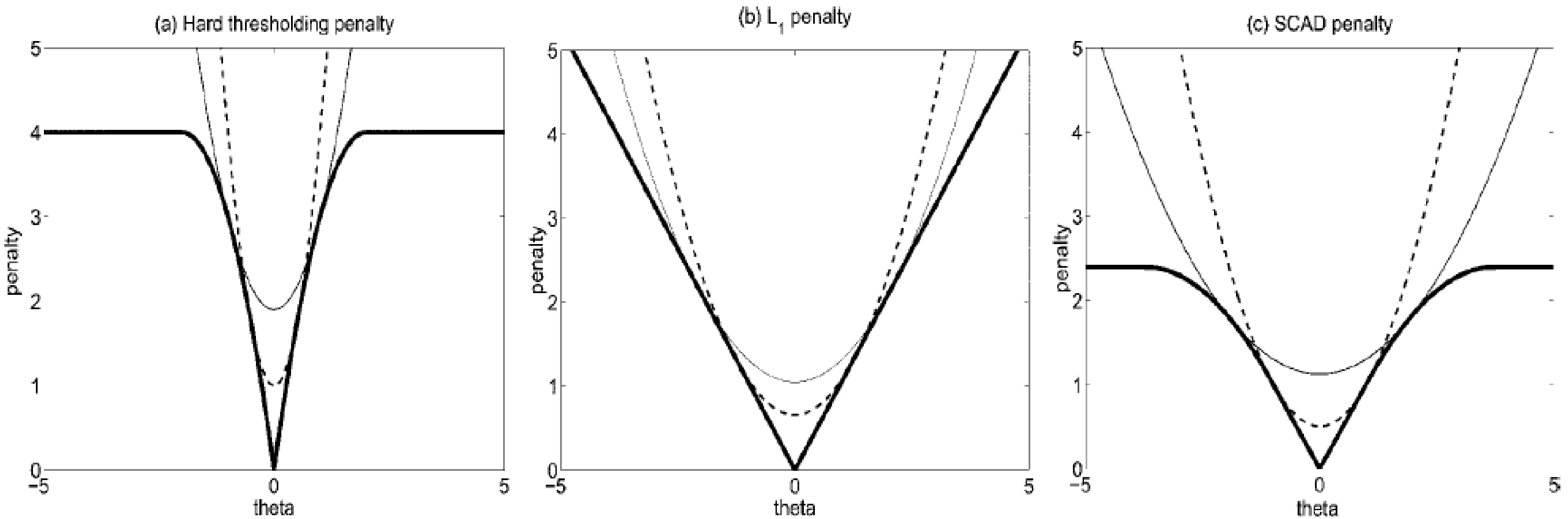


Variable Selection

- Sparsifying penalty functions
  - Hard thresholding $\rho_\lambda(x) = \begin{cases} \lambda^2 - (|x| - \lambda)^2 & \text{if } |x| < \lambda \\ \lambda^2 & \text{else} \end{cases}$
  - L1 penalty $\rho(x) = |x|$
  - Smoothly clipped absolute deviation (SCAD) penalty
- L_2 penalty to avoid overfitting $\rho(x) = x^2$



Penalty Functions



- The L_1 penalty biases coefficients (makes them smaller)
- The other penalties result in non-convex optimization
  - Suboptimal result
  - Computationally intensive

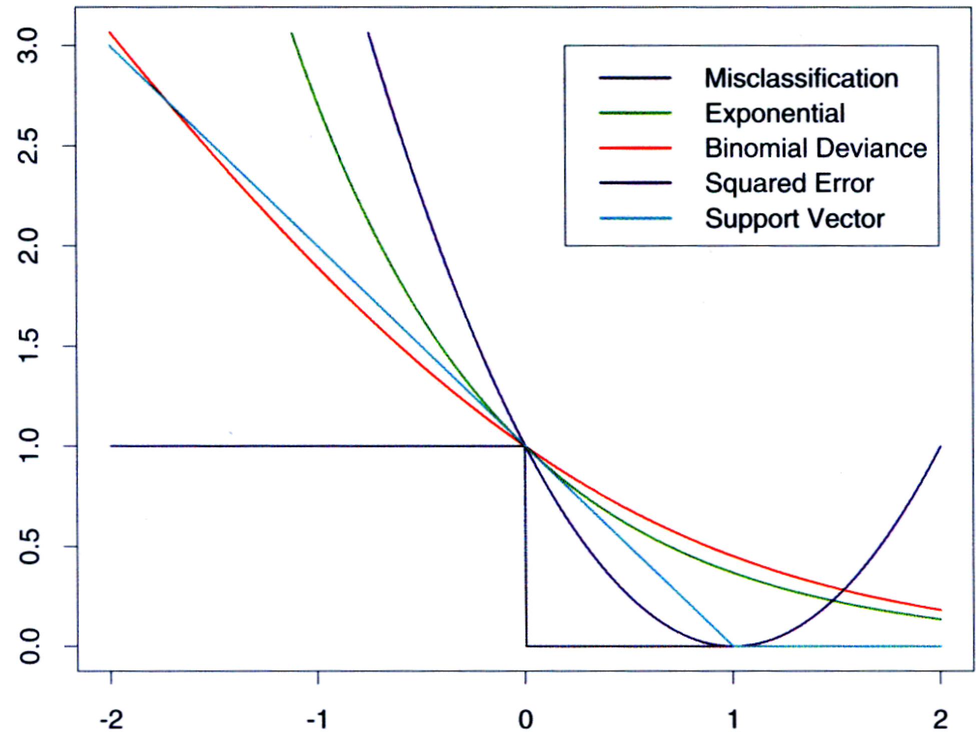
Regularized Loss Functions

- More generally:

$$L(\mathbf{w}) = \frac{1}{N}\sum_{j=1}^{N} f(\mathbf{w}^T\mathbf{x}_j, y_j) + \lambda \sum_{i=1}^{p} \rho(w_i)$$

- Loss functions f
  - Logistic (binomial deviance)
    $f(x,y) = \log_2(1+e^{-xy})$
  - Exponential loss
    $f(x,y) = e^{-xy}$
  - Square loss
    $f(x,y) = (x-y)^2$
  - Hinge (SVM) loss

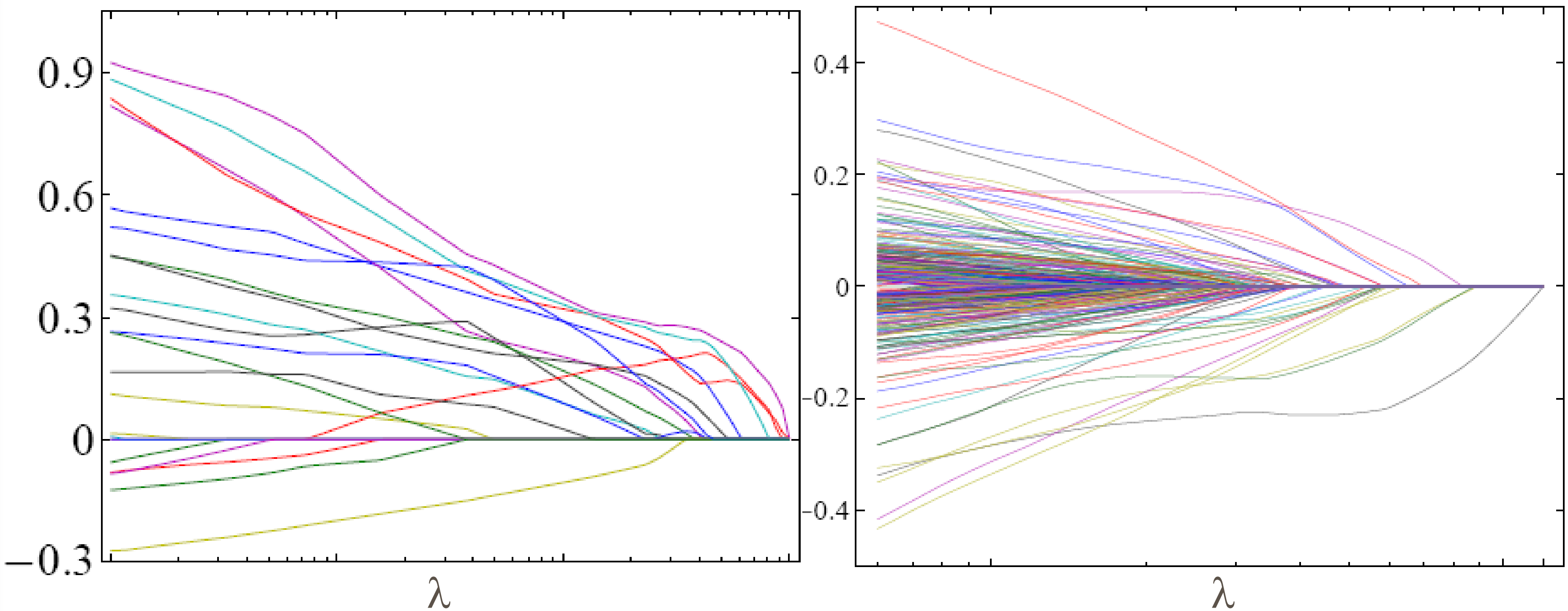
$$f(x,y) = \begin{cases} 1 - xy & \text{if } xy < 1 \\ 0 & \text{else} \end{cases}$$



Learning with Regularized Loss Functions

- Convex Optimization
  - Any convex loss with L_1 or L_2 penalty
  - E.g:
    - Logistic loss with L_1 penalty (Boyd 2007)
    - SVM (Hinge loss with L_2 penalty)
  - Can be slow
- Analytical:
  - Least Angle Regression (LARS) (Efron et al, 2004) for Square loss with L_1 penalty
  - For other combinations, see Rosset & Zhu, 2007
  - Faster but only defined for some combinations Loss/Penalty
- Greedy:
  - Grafting (Perking et al, 2003)
    - Keeps a set F of nonzero weights w_i
    - Adds variables to F based on a gradient criterion
    - Gradient descent using the weights in F only
    - Fast but can be suboptimal

Regularization Path



- Graph of the weights vs. λ
- In some cases it is piecewise linear
  - Can be obtained using the LARS algorithm

TISP – Thresholding-based Iterative Selection Procedure

- Penalized Regression:

$$L(\mathbf{w}) = \frac{1}{N}\sum_{j=1}^{N} \|\mathbf{w}^T\mathbf{x}_j - y_j\|^2 + \lambda \sum_{i=1}^{p} \rho(w_i)$$

- Algorithm iterates:

$$\mathbf{w}^{(t+1)} = \Theta(\mathbf{w}^{(t)} + \eta(X^T\mathbf{y} - X^T X\mathbf{w}^{(t)}), \lambda)$$

where η could be 1/N and the thresholding operator Θ is connected to ρ through

$$\rho(x) = \int_0^{|x|} [\sup\{t, \Theta(t,\lambda) \le u\} - u] du$$

She, EJS 2009

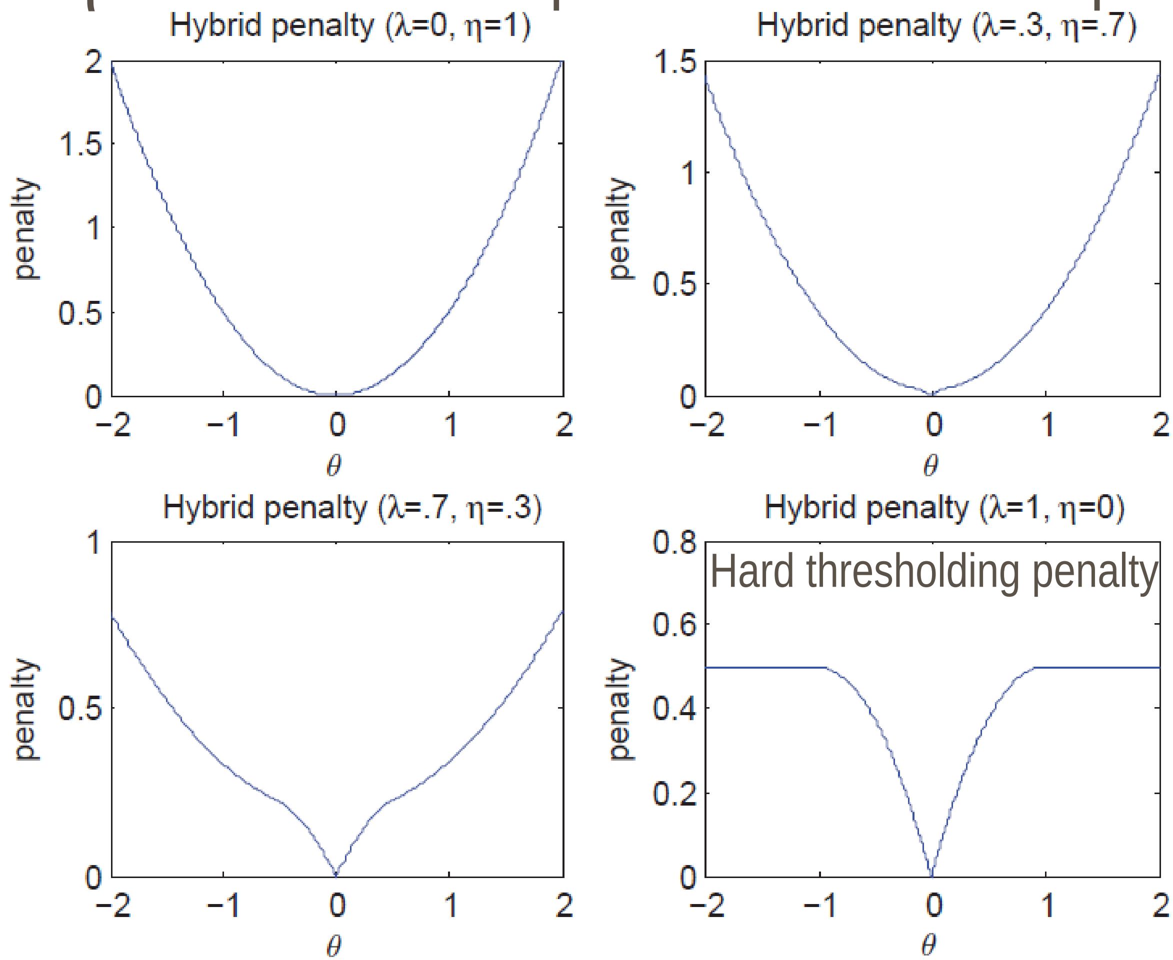
TISP

She, EJS 2009

- Example of thresholding operator:

$$\Theta(x,\lambda,\eta) = \begin{cases} 0 & \text{if } |x| \le \lambda \\ \frac{x}{1+\eta} & \text{if } |x| > \lambda \end{cases}$$

parameter η controls the shape of its associated penalty ρ



TISP for Classification

- Penalized logistic regression:

$$L(\mathbf{w}) = \frac{1}{N}\sum_{j=1}^{N} \ln(1 + e^{-y_j^* \mathbf{w}^T \mathbf{x}_j}) + \lambda \sum_{i=1}^{p} \rho(w_i)$$

y_j^* take values -1 and 1

- Algorithm iterates (y_j are 0 or 1):

$$\mathbf{w}^{(t+1)} = \Theta(\mathbf{w}^{(t)} + \eta' X^T \left[\mathbf{y} - \frac{1}{1 + \exp(-X\mathbf{w}^{(t)})}\right], \lambda)$$

where learning rate η' could be 1/N

She, CSDA 2012

Discussion Points

- Why do we want to do variable selection
- Why would we want a convex penalized loss?
- Which penalized loss function is convex?
  - What problems does it have?
- How to optimize a convex loss function?
- Which of the loss functions in slide 7 are convex?
- What is the regularization path?
- How does TISP work?

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