LECTURE 16: LASSO AND COORDINATE DESCENT

STAT 598z: Introduction to computing for statistics

Vinayak Rao

Department of Statistics, Purdue University

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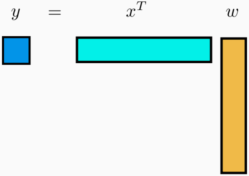
Problem: Given training data $(\mathrm{X}, \mathrm{y}) \equiv \{\mathrm{x}_i, y_i\}$,
minimize $\mathcal{L}(\mathrm{w}) = \frac{1}{2}(\mathrm{Y} - \mathrm{Xw})^2$



Bias-variance and regularization

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To reduce variance (i.e. sensitivity to small changes in training data) , add a penalty $\Omega(\mathsf{w})$:

$$\hat{\mathsf{w}} = \text{argmin } \mathcal{L}(\mathsf{w}) + \lambda\Omega(\mathsf{w})$$

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Ridge regression/L_2 regression:

- $\Omega(\mathsf{w}) = \|\mathsf{w}\|_2^2$
- $\hat{\mathsf{w}} = (\mathsf{X}^\top\mathsf{X} + \lambda\mathsf{I})^{-1}\mathsf{X}^\top\mathsf{y}$ (Shrinkage)

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LASSO:

- $\Omega(\mathsf{w}) = \|\mathsf{w}\|_1$
- Shrinkage and selection
  (w is sparse with some components equal to 0)
- No simple closed-form solution

Regularization as constrained optimization

$\text{argmin}(\mathbf{y} - \mathbf{X}^\top \mathbf{w})^2 + \lambda \|\mathbf{w}\|_2^2$ is equivalent to

$\text{argmin}(\mathbf{y} - \mathbf{X}^\top \mathbf{w})^2 \quad s.t. \; \|\mathbf{w}\|_2^2 \leq \gamma$

(Note: γ will depend on data)

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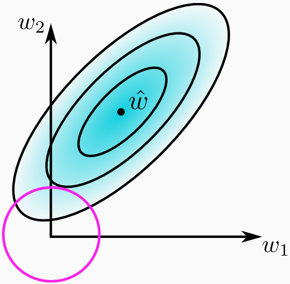
First problem: regularized optimization
Second problem: constrained optimization



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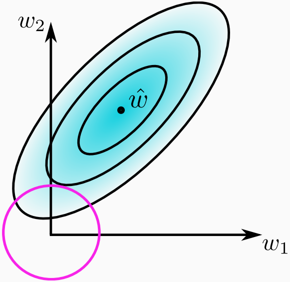

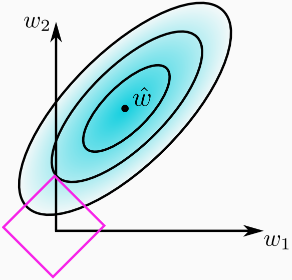

Lasso

$\text{argmin}(\mathbf{y} - \mathbf{X}^\top \mathbf{w})^2 \quad s.t.\ \|\mathbf{w}\|_1 \leq \gamma$

$\|\mathbf{w}\|_1 = \sum_{j=1}^{p} |w_j|$ is the ℓ_1-norm.

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Lasso: least absolute shrinkage and selection operator.

$$\hat{\mathbf{w}} = \text{argmin} \sum_{i=1}^{n} (y_i - \mathbf{x}_i^\top \mathbf{w})^2 + \lambda \|\mathbf{w}\|_1$$

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- Penalizes small w_j more than ridge regression.
- Tolerates larger w_j more than ridge regression.

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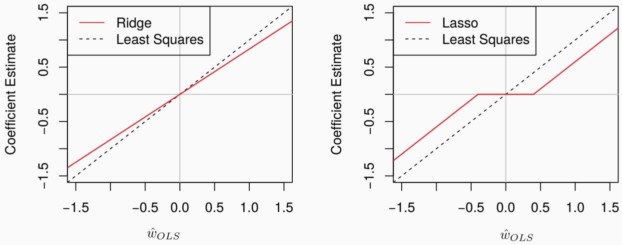
Result:

- $\hat{\mathbf{w}}_{LASSO}$ has some components *exactly* equal to zero.
- Performs feature selection.

The 1-D case



In the 1-d case, $(\mathbf{x}, \mathbf{y}) \equiv \{x_i, y_i\}$

Least-squares solution: $\hat{w}_{ols} = \frac{\mathbf{x}^\top \mathbf{y}}{\mathbf{x}^\top \mathbf{x}}$

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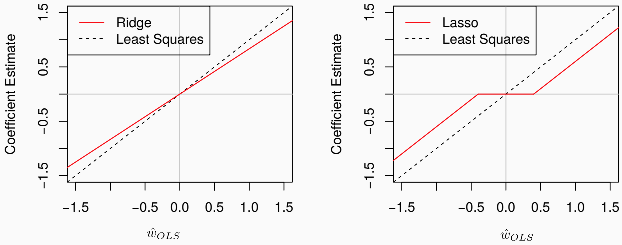

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Least-squares solution: $\hat{w}_{ols} = \frac{\mathbf{x}^\top \mathbf{y}}{\mathbf{x}^\top \mathbf{x}}$

Ridge regression solution: $\hat{w}_{ridge} = \frac{\mathbf{x}^\top \mathbf{x}}{\mathbf{x}^\top \mathbf{x} + \lambda}$

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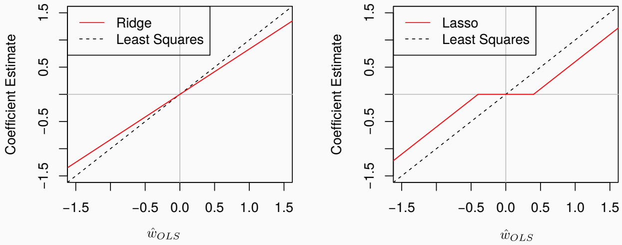

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LASSO solution?

Optimization in R

Use the `optim` function

Syntax:

```
optim(par, fn, gr = NULL, ...,
  method = c('Nelder-Mead', 'BFGS', 'CG', 'L-BFGS-B', 'SANN',
             'Brent'),
  lower = -Inf, upper = Inf,
  control = list(), hessian = FALSE)
```

`fn`: function to be optimized

`gr`: gradient function (calculate numerically if `NULL`)

`par`: initial value of parameter to be optimized (should be first argument of `fn`)

LASSO IN 1-D

$\hat{w} = \operatorname{argmin} \mathcal{L}(w) = \operatorname{argmin} \frac{1}{2}\sum_{i=1}^{n}(y_i - wx_i)^2 + \lambda|w|$

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-\sum_{i=1}^{n}y_ix_i + w\sum_{i=1}^{n}x_i^2 + \lambda\frac{\mathrm{d}|w|}{\mathrm{d}w} &= 0 \\
w = \frac{\sum_{i=1}^{n}y_ix_i - \lambda\frac{\mathrm{d}|w|}{\mathrm{d}w}}{\sum_{i=1}^{n}x_i^2}
\end{aligned}
$$

Subgradients

$$w = \frac{\sum_{i=1}^{n} y_i x_i - \lambda \frac{\mathrm{d}|w|}{\mathrm{d}w}}{\sum_{i=1}^{n} x_i^2} = \frac{\mathbf{y}^\top \mathbf{x} - \lambda \frac{\mathrm{d}|w|}{\mathrm{d}w}}{\mathbf{x}^\top \mathbf{x}} : \quad \text{What is } \frac{\mathrm{d}|w|}{\mathrm{d}w}?$$

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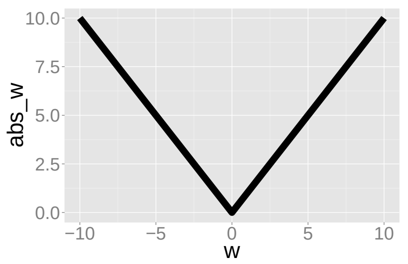

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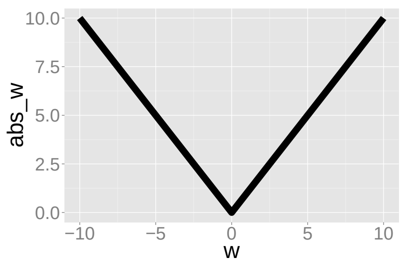

$$w > 0 \quad \leftrightarrow \frac{\mathrm{d}|w|}{\mathrm{d}w} = 1$$

$$w < 0 \quad \leftrightarrow \frac{\mathrm{d}|w|}{\mathrm{d}w} = -1$$

$$w = 0 \quad \leftrightarrow \frac{\mathrm{d}|w|}{\mathrm{d}w} \in (-1, 1)$$

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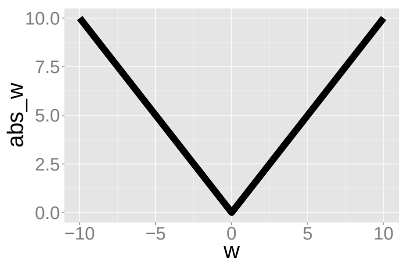
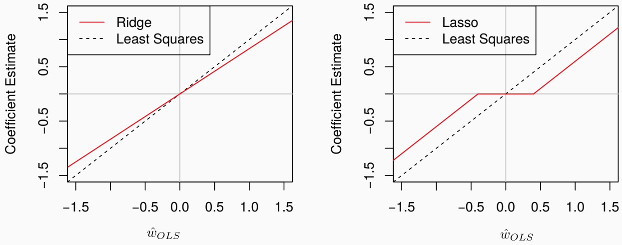


$$w > 0 \quad \leftrightarrow \frac{\mathrm{d}|w|}{\mathrm{d}w} = 1 \qquad\qquad w > 0 \quad \leftrightarrow w = \frac{\mathbf{y}^\top \mathbf{x} - \lambda}{\mathbf{x}^\top \mathbf{x}}$$

$$w < 0 \quad \leftrightarrow \frac{\mathrm{d}|w|}{\mathrm{d}w} = -1 \qquad\qquad w < 0 \quad \leftrightarrow w = \frac{\mathbf{y}^\top \mathbf{x} + \lambda}{\mathbf{x}^\top \mathbf{x}}$$

$$w = 0 \quad \leftrightarrow \frac{\mathrm{d}|w|}{\mathrm{d}w} \in (-1, 1) \qquad\qquad w = 0 \quad \leftrightarrow w = \text{otherwise}$$

The 1-D case



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First calculate: $\hat{w}_{ols} = \frac{\mathbf{y}^\top \mathbf{x}}{\mathbf{x}^\top \mathbf{x}}$

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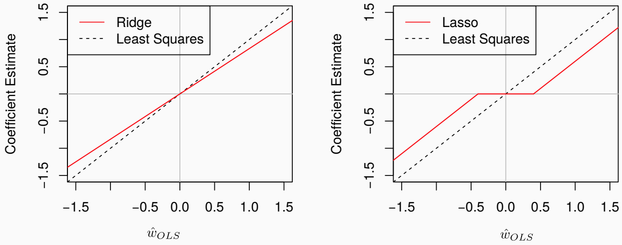

LASSO

First calculate: $\hat{w}_{ols} = \frac{\mathbf{y}^\top \mathbf{x}}{\mathbf{x}^\top \mathbf{x}}$

Soft threshold: $\hat{w}_{LASSO} = \text{sign}(\hat{w}_{ols})(|\hat{w}_{ols}| - \frac{\lambda}{\mathbf{x}^\top \mathbf{x}})_+$

(here $(x)_+ = x \textit{ if } x > 0, \textit{else } 0$)

Find $\mathbf{w}$ by coordinate descent

$$\mathcal{L}(\mathbf{w}) = \sum_{i=1}^{n} (y_i - \mathbf{w}^\top \mathbf{x}_i)^2 + \lambda \|\mathbf{w}\|_1 \tag{1}$$

$$\tag{3}$$

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$$= \sum_{i=1}^{n}(y_i - \sum_{j=1}^{p} w_j x_{ij})^2 + \lambda \sum_{j=1}^{p} |w_j| \tag{2}$$

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Lasso in higher (p) dimensions

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Here r_{id} is the residual of obs. i:

$$r_{id} = y_i - \sum_{j \neq d} w_j x_{ij}$$

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Eq(3) is just 1d LASSO! Can solve for w_d by soft-thresholding.

Repeat

Initialize $\mathbf{w}$ to some arbitrary value

For dimension d, calculate the residual $\mathbf{r}_d = (r_{1d}, \cdots, r_{nd})$, $r_{id} = y_i - \sum_{j \neq d} w_j x_{ij}$ for each observation i

Set $\hat{w}_{ols} = \frac{(\mathbf{x}_d)^\top \mathbf{r}_d}{(\mathbf{x}_d)^\top \mathbf{x}_d}$ where $\mathbf{x}_d$ is the dth column of $\mathbf{X}$ and we have:

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Repeat across dimensions d till convergence.

Co-ordinate descent

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Does this work?

Does co-ordinate descent work?

For convex differentiable functions: yes

Convex function f: local optimum is a global minimum.

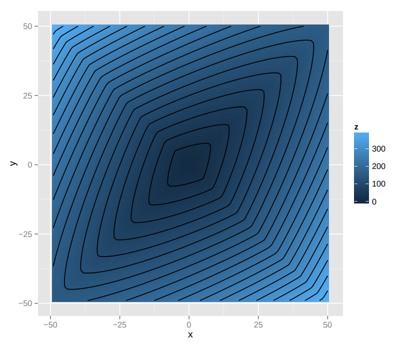
Local optimum for a differentiable function:

$$\nabla f(\mathrm{w}) = \left[\frac{\partial f}{\partial w_1}, \cdots, \frac{\partial f}{\partial w_p}\right] = 0$$

At a stationary point of coordinate descent, the RHS is true.

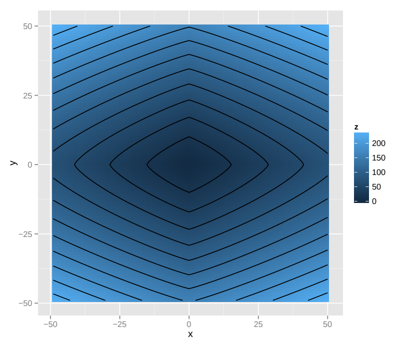
Does co-ordinate descent work?

For convex non-differentiable functions: in general, no!



Does co-ordinate descent work?

For functions of the form: $f(\mathbf{w}) = g(\mathbf{w}) + \sum_{i=1}^{p} h_i(w_i)$, where f is convex and differentiable, h_i's are convex but not differentiable: yes



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Obtains the solution $\hat{\mathrm{w}}$ for any λ

Can repeat for different λ's (though some ways are better).

Pathwise co-ordinate descent

We want $\hat{\mathbf{w}}$'s for a set of λ's

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Divide into equidistant grid points (typ. on logscale)

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Converges after a few sweeps

Repeat

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Repeat

This kind of a guided search is often faster, even if we just want one λ.