Caltech

Machine Learning & Data Mining

CS/CNS/EE 155

Lecture 4:

Regularization, Sparsity & Lasso

Recap: Complete Pipeline

$$S = \left\{(x_i, y_i)\right\}_{i=1}^{N}$$

Training Data

$$f(x \mid w, b) = w^T x - b$$

Model Class(es)

$$L(a,b) = (a-b)^2$$

Loss Function

$$\underset{w,b}{\operatorname{argmin}} \sum_{i=1}^{N} L\big(y_i, f(x_i \mid w, b)\big)$$

SGD!

Cross Validation & Model Selection

Profit!

Different Model Classes?

- Option 1: SVMs vs ANNs vs LR vs LS
- Option 2: Regularization

$$\underset{w,b}{\operatorname{argmin}} \sum_{i=1}^{N} L\left(y_i, f(x_i \mid w, b)\right)$$

SGD!

Cross Validation & Model Selection

Notation Part 1

- L0 Norm (not actually a norm)
  - # of non-zero entries

$$\|w\|_0 = \sum_d 1_{[w_d \neq 0]}$$

- L1 Norm
  - Sum of absolute values

$$|w| = \|w\|_1 = \sum_d |w_d|$$

- L2 Norm & Squared L2 Norm
  - Sum of squares
  - Sqrt(sum of squares)

$$\|w\| = \sqrt{\sum_d w_d^2} \equiv \sqrt{w^T w}$$

$$\|w\|^2 = \sum_d w_d^2 \equiv w^T w$$

- L-infinity Norm
  - Max absolute value

$$\|w\|_\infty = \lim_{p \to \infty} \sqrt[p]{\sum_d |w_d|^p} = \max_d |w_d|$$

Notation Part 2

- Minimizing Squared Loss
  - Regression
  - Least-Squares

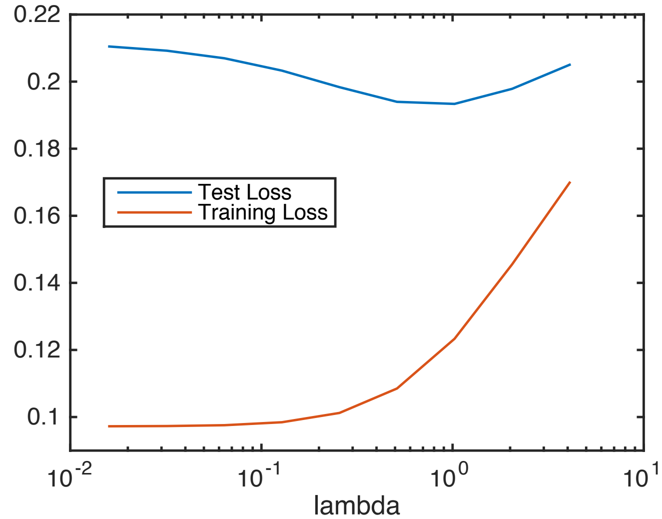
$$\operatorname*{argmin}_{w} \sum_{i} \left(y_i - w^T x_i + b \right)^2$$

  - (Unless Otherwise Stated)
    - E.g., Logistic Regression = Log Loss

Ridge Regression

$$\underset{w,b}{\operatorname{argmin}} \underbrace{\lambda w^T w}_{\text{Regularization}} + \underbrace{\sum_i \left(y_i - w^T x_i + b\right)^2}_{\text{Training Loss}}$$

- aka L2-Regularized Regression
- Trades off model complexity vs training loss
- Each choice of λ a "model class"
  - Will discuss the further later



$$\underset{w,b}{\operatorname{argmin}} \lambda w^T w + \sum_i \left(y_i - w^T x_i + b\right)^2$$

Larger Lambda

w		b
0.7401	0.2441	-0.1745
0.7122	0.2277	-0.1967
0.6197	0.1765	-0.2686
0.4124	0.0817	-0.4196
0.1801	0.0161	-0.5686
	⋮	
0.0001	0.0000	-0.6666

	Person	Age>10	Male?	Height > 55"
Train	Alice	1	0	1
	Bob	0	1	0
	Carol	0	0	0
	Dave	1	1	1
	Erin	1	0	1
	Frank	0	1	1
Test	Gena	0	0	0
	Harold	1	1	1
	Irene	1	0	0
	John	0	1	1
	Kelly	1	0	1
	Larry	1	1	1

Updated Pipeline

$$S = \left\{(x_i, y_i)\right\}_{i=1}^{N}$$

Training Data

$$f(x \mid w, b) = w^T x - b$$

Model Class

$$L(a,b) = (a-b)^2$$

Loss Function

$$\underset{w,b}{\operatorname{argmin}}\ \lambda w^T w + \sum_{i=1}^{N} L\big(y_i, f(x_i \mid w, b)\big)$$

Choosing λ!

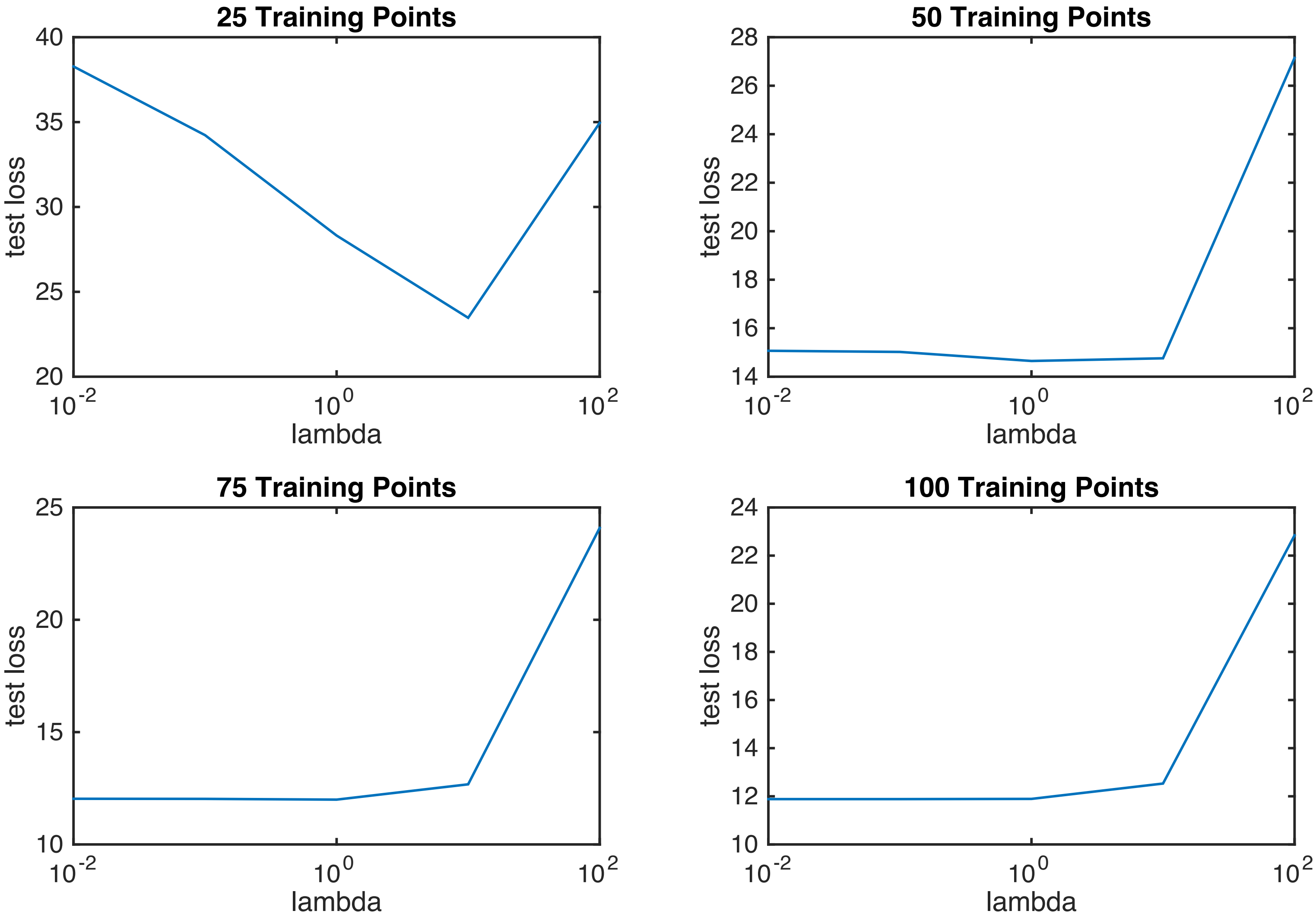
Cross Validation & Model Selection

Profit!

	Person	Age>10	Male ?	Height > 55”	Model Score w/ Increasing Lambda				
Train	Alice	1	0	1	0.91	0.89	0.83	0.75	0.67
	Bob	0	1	0	0.42	0.45	0.50	0.58	0.67
	Carol	0	0	0	0.17	0.26	0.42	0.50	0.67
	Dave	1	1	1	1.16	1.06	0.91	0.83	0.67
	Erin	1	0	1	0.91	0.89	0.83	0.79	0.67
	Frank	0	1	1	0.42	0.45	0.50	0.54	0.67
Test	Gena	0	0	0	0.17	0.27	0.42	0.50	0.67
	Harold	1	1	1	1.16	1.06	0.91	0.83	0.67
	Irene	1	0	0	0.91	0.89	0.83	0.79	0.67
	John	0	1	1	0.42	0.45	0.50	0.54	0.67
	Kelly	1	0	1	0.91	0.89	0.83	0.79	0.67
	Larry	1	1	1	1.16	1.06	0.91	0.83	0.67

Best test error

Choice of Lambda Depends on Training Size



25 dimensional space
Randomly generated linear response function + noise

Recap: Ridge Regularization

- Ridge Regression:
  - L2 Regularized Least-Squares

$$\underset{w,b}{\operatorname{argmin}} \lambda w^T w + \sum_i \left(y_i - w^T x_i + b \right)^2$$

- Large λ ➔ more stable predictions
  - Less likely to overfit to training data
  - Too large λ ➔ underfit
- Works with other loss
  - Hinge Loss, Log Loss, etc.

Aside: Stochastic Gradient Descent

$$\underset{w,b}{\operatorname{argmin}}\ \lambda\|w\|^2 + \sum_{i=1}^{N} L\big(y_i, f(x_i \mid w, b)\big)$$

$$\tilde{L}(w,b) = \sum_{i=1}^{N}\left[\frac{1}{N}\lambda\|w\|^2 + L_i(w,b)\right]$$

$$\frac{1}{N}\tilde{L}(w,b) = \mathrm{E}_i\left[\tilde{L}_i(w,b)\right]$$

Do SGD on this

Model Class Interpretation

$$\underset{w,b}{\operatorname{argmin}} \lambda w^T w + \sum_{i=1}^{N} L\left(y_i, f(x_i \mid w, b)\right)$$

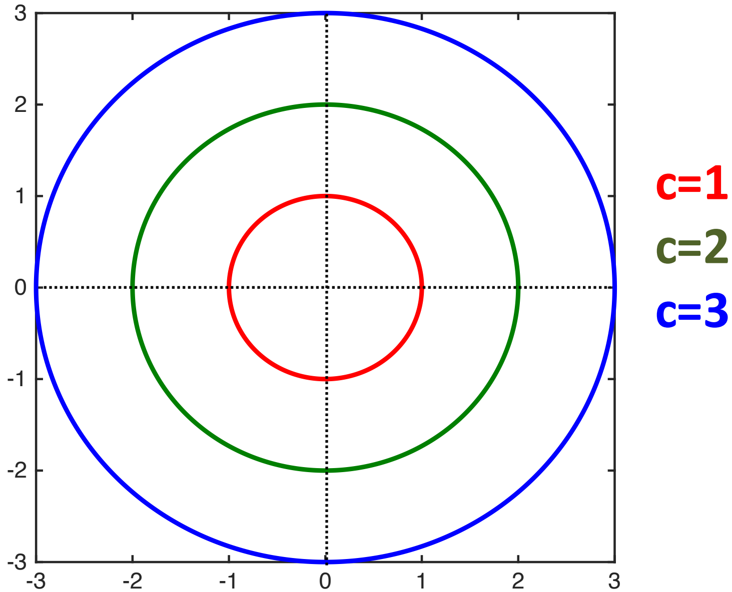
- This is not a model class!
  - At least not what we've discussed...

- An optimization procedure
  - Is there a connection?

Norm Constrained Model Class

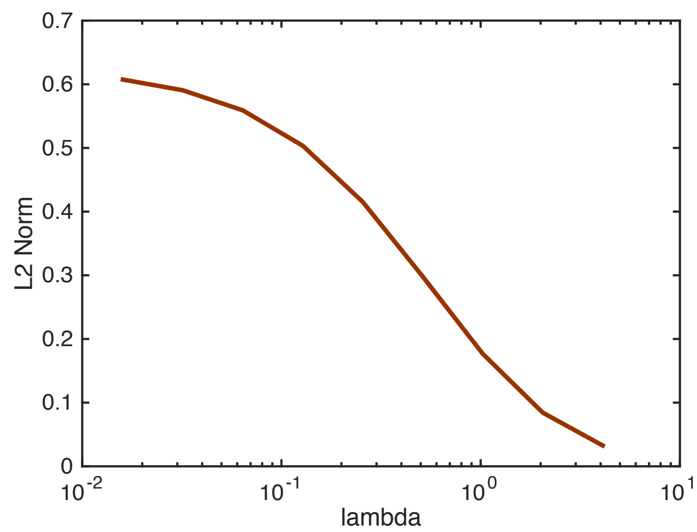
$$f(x \mid w, b) = w^T x - b \qquad \text{s.t. } w^T w \le c \equiv \|w\|^2 \le c$$

Visualization



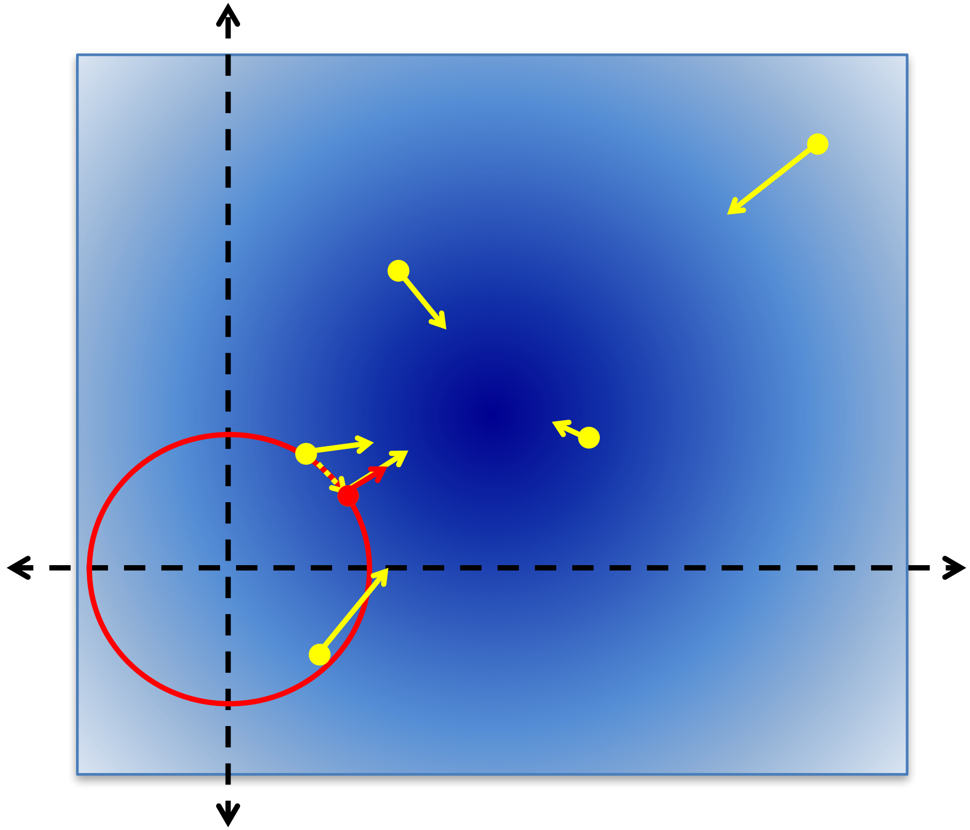
Seems to correspond to lambda...

$$\underset{w,b}{\operatorname{argmin}}\ \lambda w^T w + \sum_{i=1}^{N} L\big(y_i, f(x_i \mid w, b)\big)$$



Lagrange Multipliers

$$\underset{w}{\operatorname{argmin}} L(y,w) \equiv \left(y - w^T x\right)^2$$



- Optimality Condition:
  - Gradients aligned!
  - Constraint Boundary
  - Loss

$$\exists \lambda \geq 0 : \left(\partial_w L(y,w) = -\lambda \partial_w w^T w\right) \wedge \left(w^T w \leq c\right)$$

Omitting b &
1 training data
for simplicity

http://en.wikipedia.org/wiki/Lagrange_multiplier

Norm Constrained Model Class Training:

$$\underset{w}{\operatorname{argmin}}\, L(y,w) \equiv \left(y - w^T x\right)^2 \qquad \text{s.t. } w^T w \le c$$

Omitting b & 1 training data for simplicity

Two Conditions Must Be Satisfied At Optimality ⇔.

Observation about Optimality:

$$\exists \lambda \ge 0 : \left(\partial_w L(y,w) = -\lambda \partial_w w^T w\right) \wedge \left(w^T w \le c\right)$$

Lagrangian:

$$\underset{w,\lambda}{\operatorname{argmin}}\, \Lambda(w,\lambda) = \left(y - w^T x\right)^2 + \lambda\left(w^T w - c\right)$$

Claim: Solving Lagrangian Solves Norm-Constrained Training Problem

Optimality Implication of Lagrangian:

$$\partial_w \Lambda(w,\lambda) = -2x\left(y - w^T x\right)^T + 2\lambda w \equiv 0$$

$$\rightarrow 2x(y - w^T x)^T = -2\lambda w$$

Satisfies First Condition!

http://en.wikipedia.org/wiki/Lagrange_multiplier

Norm Constrained Model Class Training:

$$\underset{w}{\operatorname{argmin}}\, L(y,w) \equiv \left(y - w^T x\right)^2 \qquad \text{s.t. } w^T w \leq c$$

Omitting b & 1 training data for simplicity

Two Conditions Must Be Satisfied At Optimality ⇔.

Observation about Optimality:

$$\exists \lambda \geq 0 : \left(\partial_w L(y,w) = -\lambda \partial_w w^T w\right) \wedge \left(w^T w \leq c\right)$$

Lagrangian:

$$\underset{w,\lambda}{\operatorname{argmin}}\, \Lambda(w,\lambda) = \left(y - w^T x\right)^2 + \lambda\left(w^T w - c\right)$$

Claim: Solving Lagrangian Solves Norm-Constrained Training Problem

Optimality Implication of Lagrangian:

Satisfies 2nd Condition!

$$\partial_\lambda \Lambda(w,\lambda) = \begin{cases} 0 & \text{if } w^T w < c \\ w^T w - c & \text{if } w^T w \geq c \end{cases} \equiv 0 \;\rightarrow\; w^T w \leq c$$

http://en.wikipedia.org/wiki/Lagrange_multiplier

Norm Constrained Model Class Training:

$$\underset{w}{\operatorname{argmin}}\, L(y,w) \equiv \left(y - w^T x\right)^2 \qquad \text{s.t. } w^T w \leq c$$

L2 Regularized Training:

$$\underset{w}{\operatorname{argmin}}\, \lambda w^T w + \left(y - w^T x\right)^2$$

Lagrangian:

$$\underset{w,\lambda}{\operatorname{argmin}}\, \Lambda(w,\lambda) = \left(y - w^T x\right)^2 + \lambda\left(w^T w - c\right)$$

- Lagrangian = Norm Constrained Training:

$$\exists \lambda \geq 0 : \left(\partial_w L(y,w) = -\lambda \partial_w w^T w\right) \wedge \left(w^T w \leq c\right)$$

- Lagrangian = L2 Regularized Training:
  - Hold λ fixed
  - **Equivalent to solving Norm Constrained!**
  - **For some c**

Omitting b & 1 training data for simplicity

http://en.wikipedia.org/wiki/Lagrange_multiplier

Recap #2: Ridge Regularization

- Ridge Regression:
  - L2 Regularized Least-Squares = Norm Constrained Model

$$\underset{w,b}{\operatorname{argmin}}\, \lambda w^T w + L(w) \quad \equiv \quad \underset{w,b}{\operatorname{argmin}}\, L(w) \text{ s.t. } w^T w \le c$$

- Large λ ➔ more stable predictions
  - Less likely to overfit to training data
  - Too large λ ➔ underfit
- Works with other loss
  - Hinge Loss, Log Loss, etc.

Hallucinating Data Points

$$\underset{w}{\operatorname{argmin}}\, \lambda w^T w + \sum_{i=1}^{N}\left(y_i - w^T x_i\right)^2 \qquad \partial_w = 2\lambda w - 2\sum_{i=1}^{N} x\left(y_i - w^T x_i\right)^T$$

- Instead hallucinate D data points?

$$\left\{\left(\sqrt{\lambda} e_d, 0\right)\right\}_{d=1}^{D}$$

$$\underset{w}{\operatorname{argmin}} \sum_{d=1}^{D}\left(0 - w^T \sqrt{\lambda} e_d\right)^2 + \sum_{i=1}^{N}\left(y_i - w^T x_i\right)^2$$

Unit vector along d-th Dimension

$$e_d = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

$$\partial_w = 2\underbrace{\sum_{d=1}^{D}\sqrt{\lambda} e_d \left(w^T \sqrt{\lambda} e_d\right)^T}_{} - 2\sum_{i=1}^{N} x\left(y_i - w^T x_i\right)^T$$

$$= 2\sum_{d=1}^{D}\lambda e_d^T w = 2\sum_{d=1}^{D}\lambda w_d = 2\lambda w$$

Identical to Regularization!

Omitting b & for simplicity

Extension: Multi-task Learning

- 2 prediction tasks:
  - Spam filter for Alice
  - Spam filter for Bob

- Limited training data for both…
  - … but Alice is similar to Bob

Extension: Multi-task Learning

- Two Training Sets
  - N relatively small

$$S^{(1)} = \left\{ (x_i^{(1)}, y_i^{(1)}) \right\}_{i=1}^{N}$$

$$S^{(2)} = \left\{ (x_i^{(2)}, y_i^{(2)}) \right\}_{i=1}^{N}$$

- **Option 1:** Train Separately

$$\underset{w}{\operatorname{argmin}}\, \lambda w^T w + \sum_{i=1}^{N} \left(y_i^{(1)} - w^T x_i^{(1)} \right)^2$$

$$\underset{v}{\operatorname{argmin}}\, \lambda v^T v + \sum_{i=1}^{N} \left(y_i^{(2)} - v^T x_i^{(2)} \right)^2$$

Both models have high error.

Omitting b & for simplicity

Extension: Multi-task Learning

- Two Training Sets
  - N relatively small

$$S^{(1)} = \left\{ (x_i^{(1)}, y_i^{(1)}) \right\}_{i=1}^{N}$$

$$S^{(2)} = \left\{ (x_i^{(2)}, y_i^{(2)}) \right\}_{i=1}^{N}$$

- **Option 2:** Train Jointly

$$\operatorname*{argmin}_{w,v} \lambda w^T w + \sum_{i=1}^{N} \left(y_i^{(1)} - w^T x_i^{(1)} \right)^2$$
$$+ \lambda v^T v + \sum_{i=1}^{N} \left(y_i^{(2)} - v^T x_i^{(2)} \right)^2$$

Doesn't accomplish anything!
(w & v don't depend on each other)

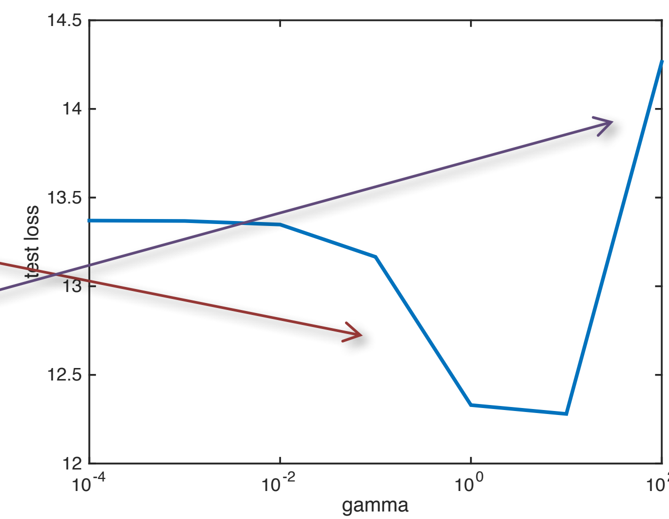
Omitting b &
for simplicity

Multi-task Regularization

$$\underset{w,v}{\operatorname{argmin}} \underbrace{\lambda w^T w + \lambda v^T v}_{\text{Standard Regularization}} + \underbrace{\gamma (w - v)^T (w - v)}_{\text{Multi-task Regularization}} + \underbrace{\sum_{i=1}^{N} \left(y_i^{(1)} - w^T x_i^{(1)} \right)^2 + \sum_{i=1}^{N} \left(y_i^{(2)} - v^T x_i^{(2)} \right)^2}_{\text{Training Loss}}$$

- Prefer w & v to be “close”
  - Controlled by γ
  - Tasks similar
    - Larger γ helps!
  - Tasks not identical
    - γ not too large

Test Loss (Task 2)



Lasso

L1-Regularized Least-Squares

L1 Regularized Least Squares

$$\underset{w}{\operatorname{argmin}}\, \lambda |w| + \sum_{i=1}^{N} \left(y_i - w^T x_i \right)^2 \qquad \underset{w}{\operatorname{argmin}}\, \lambda \|w\|^2 + \sum_{i=1}^{N} \left(y_i - w^T x_i \right)^2$$

- L2:

$w = \sqrt{2}$ vs $w = 1$

=

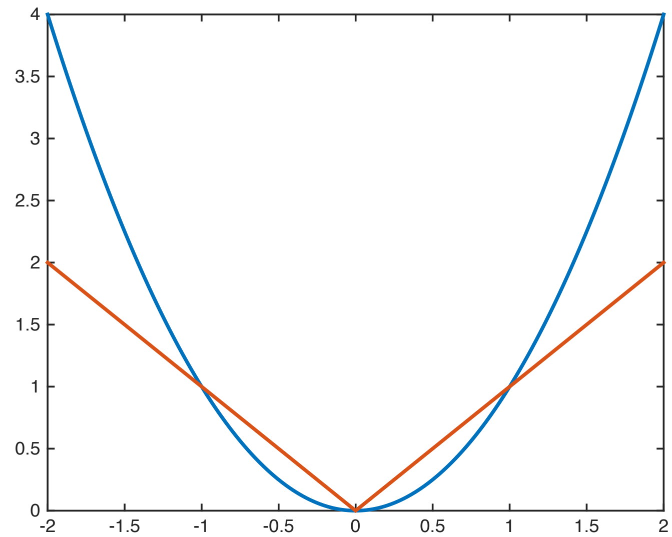
$w = 1$ vs $w = 0$

- L1:

$w = 2$ vs $w = 1$

=

$w = 1$ vs $w = 0$



Omitting b & for simplicity

Aside: Subgradient (sub-differential)

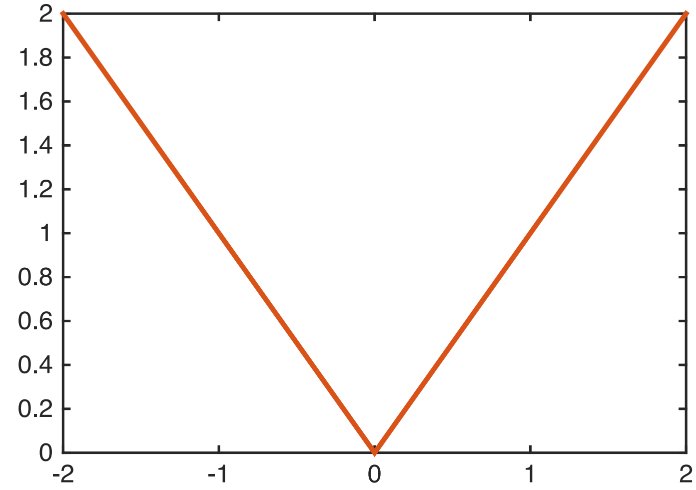
$$\nabla_a R(a) = \left\{ c \,\middle|\, \forall a' : R(a') - R(a) \geq c(a' - a) \right\}$$

- Differentiable: $\nabla_a R(a) = \partial_a R(a)$

- L1:

$$\nabla_{w_d} |w| \begin{cases} -1 & \text{if} \quad w_d < 0 \\ +1 & \text{if} \quad w_d > 0 \\ [-1,+1] & \text{if} \quad w_d = 0 \end{cases}$$

Continuous range for w=0!



Omitting b &
for simplicity

L1 Regularized Least Squares

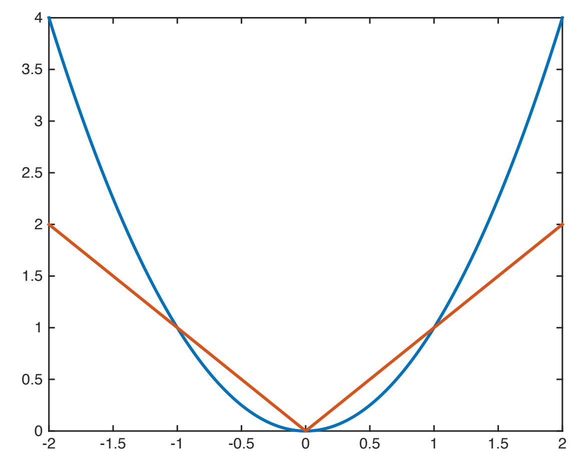
$$\underset{w}{\operatorname{argmin}} \lambda |w| + \sum_{i=1}^{N} \left(y_i - w^T x_i\right)^2 \qquad \underset{w}{\operatorname{argmin}} \lambda \|w\|^2 + \sum_{i=1}^{N} \left(y_i - w^T x_i\right)^2$$

- L2:

$$\nabla_{w_d} \|w\|^2 = 2w_d$$

- L1:

$$\nabla_{w_d} |w| \begin{cases} -1 & \text{if} \quad w_d < 0 \\ +1 & \text{if} \quad w_d > 0 \\ [-1,+1] & \text{if} \quad w_d = 0 \end{cases}$$



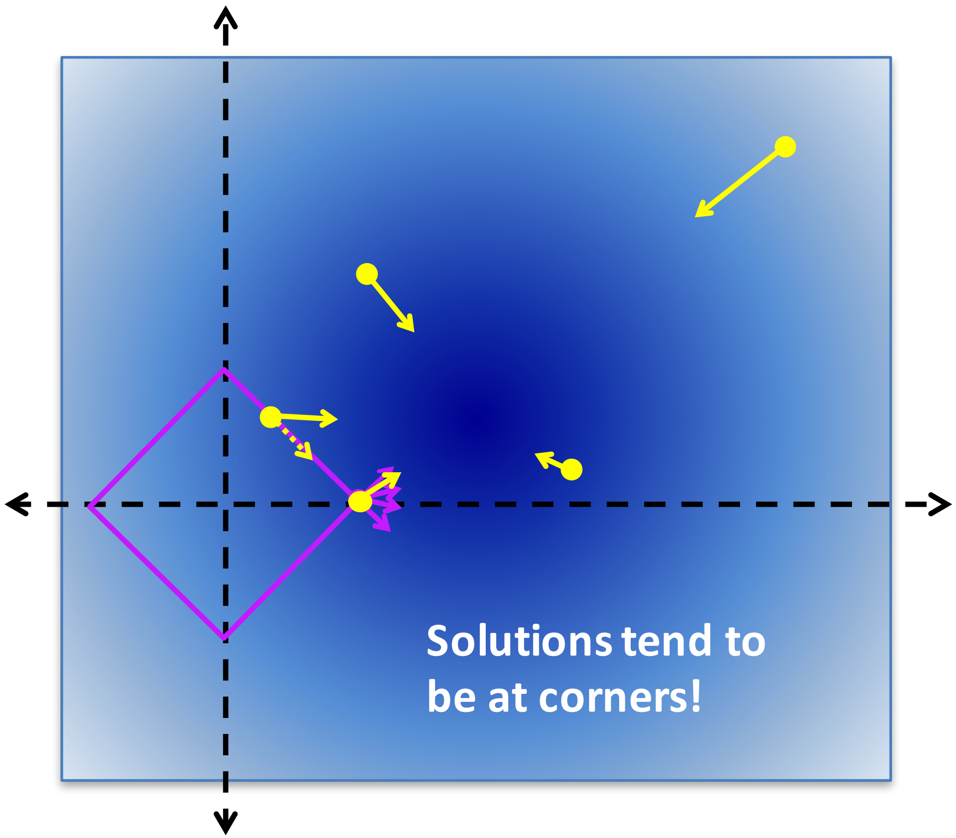
Omitting b &
for simplicity

Lagrange Multipliers

$$\underset{w}{\operatorname{argmin}} L(y,w) \equiv \left(y - w^T x\right)^2$$

$$\text{s.t. } |w| \le c$$

$$\nabla_{w_d} |w| \begin{cases} -1 & \text{if} \quad w_d < 0 \\ +1 & \text{if} \quad w_d > 0 \\ \left[-1,+1\right] & \text{if} \quad w_d = 0 \end{cases}$$



$$\exists \lambda \ge 0 : \left(\partial_w L(y,w) \in -\lambda \nabla_w |w|\right) \wedge \left(|w| \le c\right)$$

Omitting b & 1 training data for simplicity

http://en.wikipedia.org/wiki/Lagrange_multiplier

Sparsity

- w is sparse if mostly 0's:
  – Small L0 Norm

$$\|w\|_0 = \sum_d 1_{[w_d \neq 0]}$$

- Why not L0 Regularization?
  – **Not continuous!**

$$\underset{w}{\operatorname{argmin}} \lambda \|w\|_0 + \sum_{i=1}^{N} \left(y_i - w^T x_i\right)^2$$

- L1 induces sparsity
  – And is continuous!

$$\underset{w}{\operatorname{argmin}} \lambda |w| + \sum_{i=1}^{N} \left(y_i - w^T x_i\right)^2$$

Omitting b &
for simplicity

Why is Sparsity Important?

- Computational / Memory Efficiency
  - Store 1M numbers in array
  - Store 2 numbers per non-zero
    - (Index, Value) pairs
    - E.g., [(50,1), (51,1)]
  - Dot product more efficient: $w^T x$

$$\begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

- Sometimes true w is sparse
  - Want to recover non-zero dimensions

Lasso Guarantee

$$\underset{w}{\operatorname{argmin}} \lambda|w| + \sum_{i=1}^{N}\left(y_i - w^T x_i + b\right)^2$$

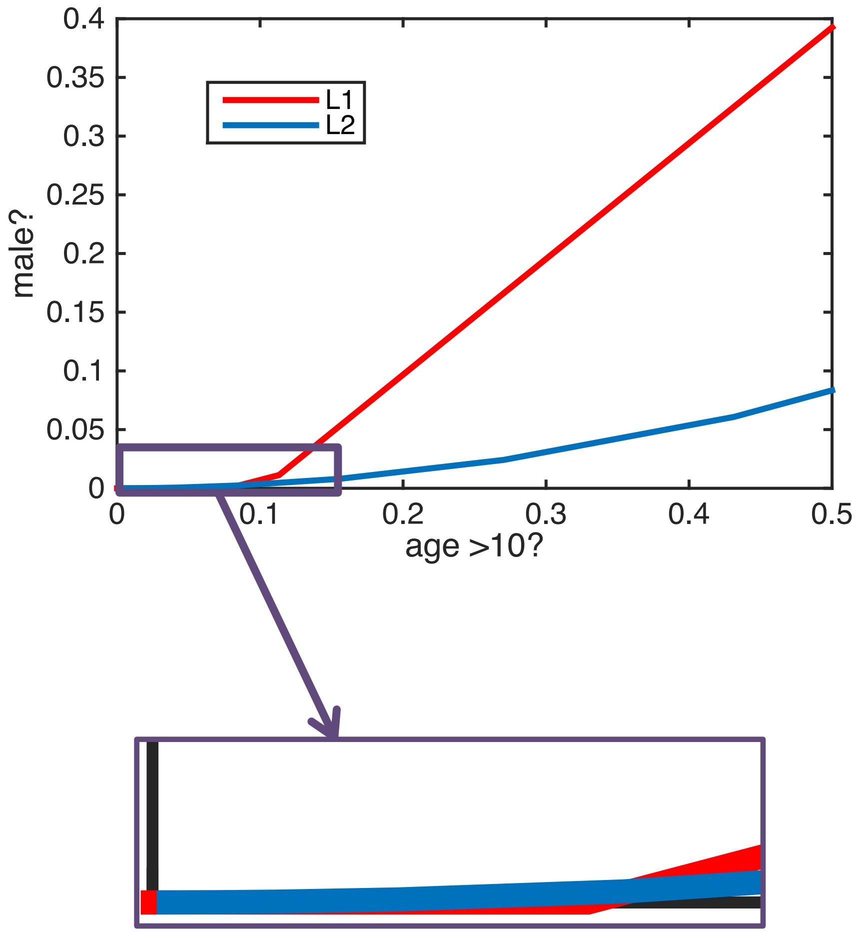
- Suppose data generated as: $y_i \sim Normal\left(w_*^T x_i, \sigma^2\right)$
- Then if: $\lambda > \frac{2}{\kappa}\sqrt{\frac{2\sigma^2 \log D}{N}}$
- With high probability (increasing with N):

$Supp(w) \subseteq Supp(w_*)$ **High Precision Parameter Recovery**

$\forall d : |w_d| \geq \lambda c \rightarrow Supp(w) = Supp(w_*)$ **Sometimes High Recall**

$$Supp(w_*) = \{d | w_{*,d} \neq 0\}$$

See also: https://www.cs.utexas.edu/~pradeepr/courses/395T-LT/filez/highdimII.pdf
http://www.eecs.berkeley.edu/~wainwrig/Papers/Wai_SparseInfo09.pdf



Magnitude of the two weights.
(As regularization shrinks)

Person	Age>10	Male?	Height > 55”
Alice	1	0	1
Bob	0	1	0
Carol	0	0	0
Dave	1	1	1
Erin	1	0	1
Frank	0	1	1
Gena	0	0	0
Harold	1	1	1
Irene	1	0	0
John	0	1	1
Kelly	1	0	1
Larry	1	1	1

Aside: Optimizing Lasso

- Solving Lasso gives sparse model
  - Will stochastic gradient descent find it?
- **No!**
  - Hard to hit exactly 0 with gradient descent
- **Solution:** Iterative Soft Thresholding
  - Intuition: if gradient update passes 0, clamp at 0

https://blogs.princeton.edu/imabandit/2013/04/11/orf523-ista-and-fista/

Recap: Lasso vs Ridge

- Model Assumptions
  - Lasso learns sparse weight vector
- Predictive Accuracy
  - Lasso often not as accurate
  - **Re-run Least Squares on dimensions selected by Lasso**
- Ease of Inspection
  - Sparse w's easier to inspect
- Ease of Optimization
  - Lasso somewhat trickier to optimize

Recap: Regularization

- L2

$$\underset{w}{\operatorname{argmin}}\, \lambda \|w\|^2 + \sum_{i=1}^{N} \left(y_i - w^T x_i \right)^2$$

- L1 (Lasso)

$$\underset{w}{\operatorname{argmin}}\, \lambda |w| + \sum_{i=1}^{N} \left(y_i - w^T x_i \right)^2$$

- Multi-task

$$\underset{w,v}{\operatorname{argmin}}\, \lambda w^T w + \lambda v^T v + \gamma (w - v)^T (w - v)$$

$$+ \sum_{i=1}^{N} \left(y_i^{(1)} - w^T x_i^{(1)} \right)^2 + \sum_{i=1}^{N} \left(y_i^{(2)} - v^T x_i^{(2)} \right)^2$$

- **[Insert Yours Here!]**

Omitting b &
for simplicity

Recap: Updated Pipeline

$$S = \{(x_i, y_i)\}_{i=1}^{N}$$

Training Data

$$f(x \mid w, b) = w^T x - b$$

Model Class

$$L(a, b) = (a - b)^2$$

Loss Function

$$\underset{w,b}{\operatorname{argmin}}\ \lambda w^T w + \sum_{i=1}^{N} L\big(y_i, f(x_i \mid w, b)\big)$$

Choosing λ!

Cross Validation & Model Selection

Profit!

Next Lectures

- Decision Trees
- Bagging
- Random Forests
- Boosting
- Ensemble Selection

- **Recitation tonight: Linear Algebra**