Linear models

Subhransu Maji

CMPSCI 670: Computer Vision

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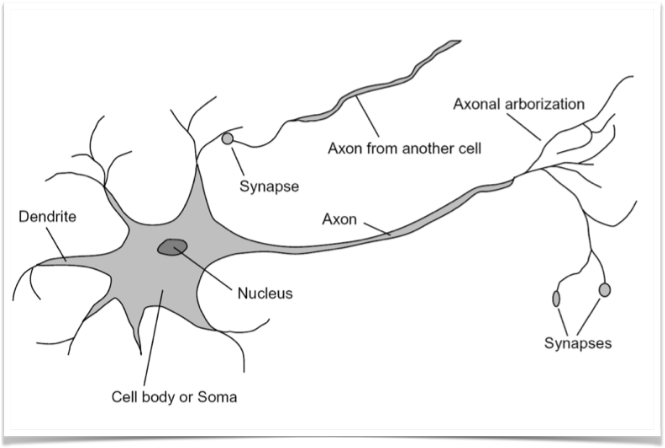
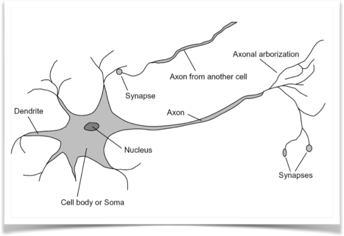
A neuron (or how our brains work)



Neuroscience 101

Perceptron

- Input are feature values
- Each feature has a weight
- Sum in the activation

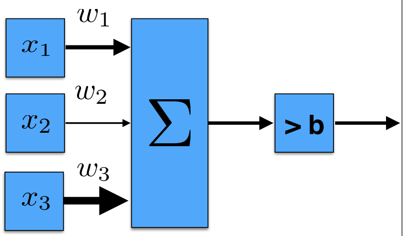


$$\text{activation}(\mathbf{w}, \mathbf{x}) = \sum_i w_i x_i = \mathbf{w}^T \mathbf{x}$$

- If the activation is:
  - > b, output *class 1*
  - otherwise, output *class 2*

$$\mathbf{x} \to (\mathbf{x}, 1)$$

$$\mathbf{w}^T \mathbf{x} + b \to (\mathbf{w}, b)^T (\mathbf{x}, 1)$$



Example: Spam

- Imagine 3 features (spam is “positive” class):
  - free (number of occurrences of “free”)
  - money (number of occurrences of “money”)
  - BIAS (intercept, always has value 1)

email	$\mathbf{x}$	$\mathbf{w}$	$\mathbf{w}^T\mathbf{x}$

“free money”	`BIAS  : 1`
	`free  : 1`
	`money : 1`
	`...`
		`BIAS  : -3`
		`free  :  4`
		`money :  2`
		`...`
			$(1)(-3)\ +$
			$(1)(4)\ +$
			$(1)(2)\ +$
			$\dots$
			$= 3$

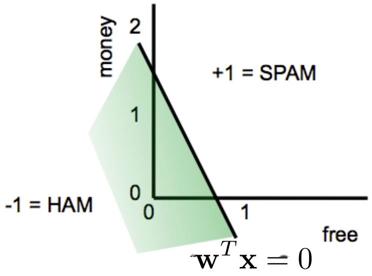
$$\mathbf{w}^T \mathbf{x} > 0 \to \text{SPAM!!}$$

Geometry of the perceptron

- In the space of feature vectors
  - examples are points (in D dimensions)
  - an weight vector is a hyperplane (a D-1 dimensional object)
  - One side corresponds to y=+1
  - Other side corresponds to y=-1
- Perceptrons are also called as linear classifiers

$\mathbf{w}$

```
BIAS  : -3
free  :  4
money :  2
...
```

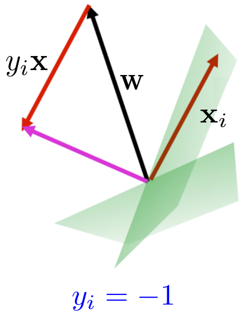


Learning a perceptron

Input: training data $(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \ldots, (\mathbf{x}_n, y_n)$

Perceptron training algorithm [Rosenblatt 57]

```
◆ Initialize $\mathbf{w} \leftarrow [0, \ldots, 0]$
◆ for iter = 1,…,T
    ▸ for i = 1,..,n
        • predict according to the current model
              $\hat{y}_i = \begin{cases} +1 & \text{if } \mathbf{w}^T\mathbf{x}_i > 0 \\ -1 & \text{if } \mathbf{w}^T\mathbf{x}_i \le 0 \end{cases}$
        • if $y_i = \hat{y}_i$ , no change
        • else, $\mathbf{w} \leftarrow \mathbf{w} + y_i\mathbf{x}_i$
```



error driven, online, activations increase for +, randomize

Properties of perceptrons

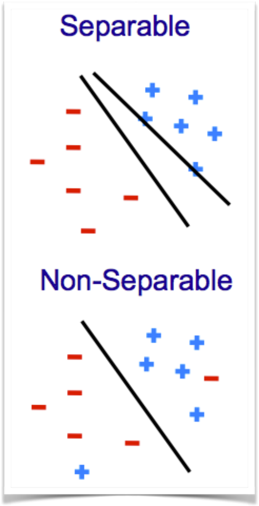
- **Separability:** some parameters will classify the training data perfectly
- **Convergence:** if the training data is separable then the perceptron training will eventually converge [Block 62, Novikoff 62]
- **Mistake bound:** the maximum number of mistakes is related to the margin

$$\text{assuming, } ||\mathbf{x}_i|| \le 1$$

$$\#\text{mistakes} < \frac{1}{\delta^2}$$

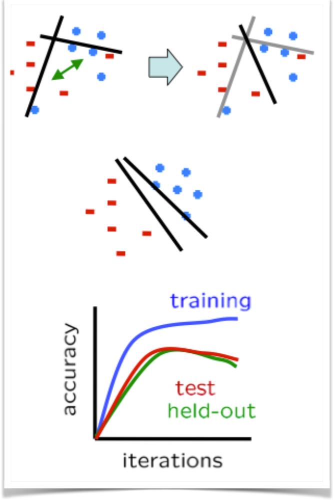
$$\delta = \max_{\mathbf{w}} \min_{(\mathbf{x}_i, y_i)} \left[y_i \mathbf{w}^T \mathbf{x}_i \right]$$

$$\text{such that, } ||\mathbf{w}|| = 1$$



Limitations of perceptrons

- **Convergence:** if the data isn't separable, the training algorithm may not terminate
  - noise can cause this
  - some simple functions are not separable (xor)
- **Mediocre generation:** the algorithm finds a solution that "barely" separates the data
- **Overtraining:** test/validation accuracy rises and then falls
  - Overtraining is a kind of overfitting



Overview

- Linear models
  - Perceptron: model and learning algorithm combined as one
  - Is there a better way to learn linear models?
- We will separate models and learning algorithms
  - Learning as optimization
  - Surrogate loss function
  - Regularization

    } model design
  - Gradient descent
  - Batch and online gradients
  - Subgradient descent

    } optimization
  - Support vector machines

Learning as optimization

$$\min_{\mathbf{w}} \sum_n \underset{\substack{\uparrow \\ \text{fewest mistakes}}}{\mathbf{1}[y_n \mathbf{w}^T \mathbf{x}_n < 0]}$$

- The perceptron algorithm will find an optimal **w** if the data is separable
  - efficiency depends on the margin and norm of the data
- However, if the data is not separable, optimizing this is NP-hard
  - i.e., there is no efficient way to minimize this unless **P=NP**

Learning as optimization

$$\min_{\mathbf{w}} \sum_n \underset{\substack{\uparrow \\ \text{fewest mistakes}}}{\mathbf{1}[y_n \mathbf{w}^T \mathbf{x}_n < 0]} + \overset{\substack{\text{hyperparameter} \\ \downarrow}}{\lambda} \underset{\substack{\nwarrow \\ \text{simpler model}}}{R(\mathbf{w})}$$

- In addition to minimizing training error, we want a simpler model
  - Remember our goal is to minimize generalization error
  - Recall the bias and variance tradeoff for learners
- We can add a regularization term *R(**w**)* that prefers simpler models
  - For example we may prefer decision trees of shallow depth
- Here λ is a hyperparameter of optimization problem

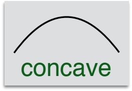
Learning as optimization

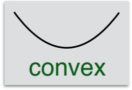
$$\min_{\mathbf{w}} \sum_n \underset{\substack{\uparrow \\ \text{fewest mistakes}}}{\mathbf{1}[y_n \mathbf{w}^T \mathbf{x}_n < 0]} + \overset{\substack{\text{hyperparameter} \\ \downarrow}}{\lambda} \underset{\substack{\nwarrow \\ \text{simpler model}}}{R(\mathbf{w})}$$

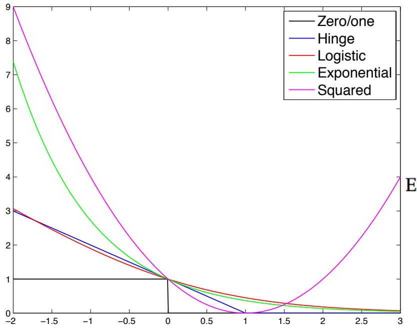
- The questions that remain are:
  - What are good ways to adjust the optimization problem so that there are efficient algorithms for solving it?
  - What are good regularizations *R(**w**)* for hyperplanes?
  - Assuming that the optimization problem can be adjusted appropriately, what algorithms exist for solving the regularized optimization problem?

Convex surrogate loss functions

- Zero/one loss is hard to optimize
  - Small changes in **w** can cause large changes in the loss
- Surrogate loss: replace Zero/one loss by a smooth function
  - Easier to optimize if the surrogate loss is convex
- Examples:







$$y = +1 \qquad \hat{y} \leftarrow \mathbf{w}^T\mathbf{x}$$

$$\text{Zero/one:} \quad \ell^{(0/1)}(y,\hat{y}) = \mathbf{1}[y\hat{y} \le 0]$$

$$\text{Hinge:} \quad \ell^{(\text{hin})}(y,\hat{y}) = \max\{0, 1 - y\hat{y}\}$$

$$\text{Logistic:} \quad \ell^{(\text{log})}(y,\hat{y}) = \frac{1}{\log 2}\log\left(1 + \exp[-y\hat{y}]\right)$$

$$\text{Exponential:} \quad \ell^{(\text{exp})}(y,\hat{y}) = \exp[-y\hat{y}]$$

$$\text{Squared:} \quad \ell^{(\text{sqr})}(y,\hat{y}) = (y - \hat{y})^2$$

Weight regularization

- What are good regularization functions *R(**w**)* for hyperplanes?
- We would like the weights —
  - To be small —
    - Change in the features cause small change to the score
    - Robustness to noise
  - To be sparse —
    - Use as few features as possible
    - Similar to controlling the depth of a decision tree
- This is a form of inductive bias

Weight regularization

- Just like the surrogate loss function, we would like *R(**w**)* to be convex
- Small weights regularization

$$R^{(\text{norm})}(\mathbf{w}) = \sqrt{\sum_d w_d^2} \qquad R^{(\text{sqrd})}(\mathbf{w}) = \sum_d w_d^2$$

- Sparsity regularization

$$R^{(\text{count})}(\mathbf{w}) = \sum_d \mathbf{1}[|w_d| > 0]$$

not convex

- Family of "p-norm" regularization

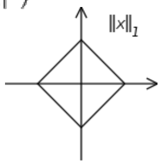
$$R^{(\text{p-norm})}(\mathbf{w}) = \left(\sum_d |w_d|^p\right)^{1/p}$$

Contours of p-norms

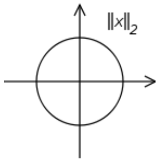
$$\|x\|_p = \left(|x_1|^p + |x_2|^p + \cdots + |x_n|^p\right)^{\frac{1}{p}}$$

convex for $p \ge 1$

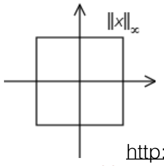
$$\|x\|_1 = \sum_{i=1}^{n} |x_i|$$



$$\|x\|_2 = \sqrt{\sum_{i=1}^{n} |x_i|^2}$$



$$\|x\|_\infty = \max_{i=1,\ldots,n} |x_i|$$



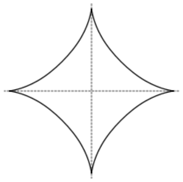
http://en.wikipedia.org/wiki/Lp_space

Contours of p-norms

$$\|x\|_p = (|x_1|^p + |x_2|^p + \cdots + |x_n|^p)^{\frac{1}{p}}$$

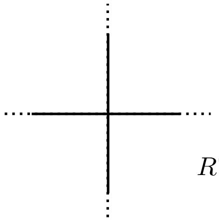
not convex for $0 \le p < 1$

$p = \frac{2}{3}$



Counting non-zeros:

$p = 0$



$$R^{(\text{count})}(\mathbf{w}) = \sum_d \mathbf{1}[|w_d| > 0]$$

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

General optimization framework

hyperparameter

$$\min_{\mathbf{w}} \sum_n \ell\left(y_n, \mathbf{w}^T \mathbf{x}_n\right) + \lambda R(\mathbf{w})$$

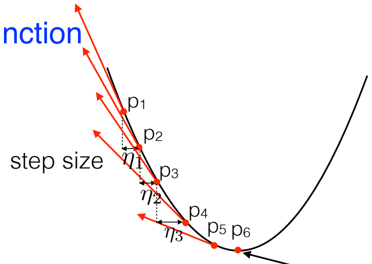
surrogate loss regularization

- Select a suitable:
  - convex surrogate loss
  - convex regularization
- Select the hyperparameter λ
- Minimize the regularized objective with respect to **w**
- This framework for optimization is called Tikhonov regularization or generally Structural Risk Minimization (SRM)

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

Optimization by gradient descent

Convex function



$$g^{(k)} \leftarrow \nabla_p F(p)|_{p_k}$$

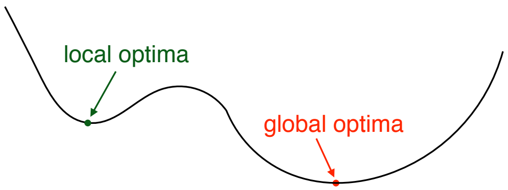
compute gradient at the current location

$$p_{k+1} \leftarrow p_k - \eta_k g^{(k)}$$

take a step down the gradient

local optima = global optima

Non-convex function

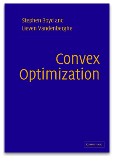


Choice of step size

- The step size is important —
  - too small: slow convergence
  - too large: no convergence
- A strategy is to use large step sizes initially and small step sizes later:

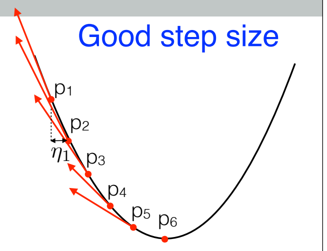
$$\eta_t \leftarrow \eta_0/(t_0 + t)$$

- There are methods that converge faster by adapting step size to the curvature of the function
  - Field of convex optimization

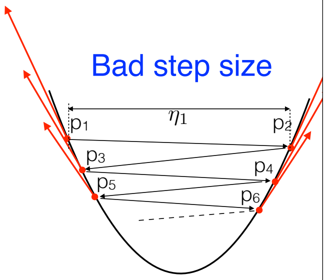


http://stanford.edu/~boyd/cvxbook/

Good step size



Bad step size



Example: Exponential loss

$$\mathcal{L}(\mathbf{w}) = \sum_n \exp(-y_n \mathbf{w}^T \mathbf{x}_n) + \frac{\lambda}{2}||\mathbf{w}||^2$$ objective

$$\frac{d\mathcal{L}}{d\mathbf{w}} = \sum_n -y_n \mathbf{x}_n \exp(-y_n \mathbf{w}^T \mathbf{x}_n) + \lambda \mathbf{w}$$ gradient

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \left(\sum_n -y_n \mathbf{x}_n \exp(-y_n \mathbf{w}^T \mathbf{x}_n) + \lambda \mathbf{w} \right)$$ update

loss term

$$\mathbf{w} \leftarrow \mathbf{w} + c y_n \mathbf{x}_n$$

↑

high for misclassified points

similar to the perceptron update rule!

regularization term

$$\mathbf{w} \leftarrow (1 - \eta\lambda)\mathbf{w}$$

shrinks weights towards zero

Batch and online gradients

$$\mathcal{L}(\mathbf{w}) = \sum_n \mathcal{L}_n(\mathbf{w})$$ objective

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \frac{d\mathcal{L}}{d\mathbf{w}}$$ gradient descent

batch gradient

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \left(\sum_n \frac{d\mathcal{L}_n}{d\mathbf{w}} \right)$$

↑

sum of n gradients

update weight after you see all points

online gradient

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \left(\frac{d\mathcal{L}_n}{d\mathbf{w}} \right)$$

↑

gradient at nth point

update weights after you see each point

Online gradients are the default method for multi-layer perceptrons

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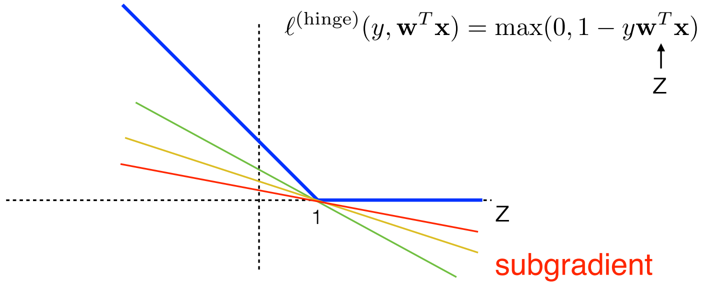
Subgradient



$$\ell^{(\text{hinge})}(y, \mathbf{w}^T \mathbf{x}) = \max(0, 1 - y\mathbf{w}^T \mathbf{x})$$

- The hinge loss is not differentiable at z=1
- Subgradient is any direction that is below the function
- For the hinge loss a possible subgradient is:

$$\frac{d\ell^{\text{hinge}}}{d\mathbf{w}} = \begin{cases} 0 & \text{if } y\mathbf{w}^T\mathbf{x} > 1 \\ -y\mathbf{x} & \text{otherwise} \end{cases}$$

Example: Hinge loss

$$\mathcal{L}(\mathbf{w}) = \sum_n \max(0, 1 - y_n \mathbf{w}^T \mathbf{x}_n) + \frac{\lambda}{2}||\mathbf{w}||^2$$ objective

$$\frac{d\mathcal{L}}{d\mathbf{w}} = \sum_n -\mathbf{1}[y_n \mathbf{w}^T \mathbf{x}_n \leq 1] y_n \mathbf{x}_n + \lambda \mathbf{w}$$ subgradient

$$\mathbf{w} \leftarrow \mathbf{w} - \eta \left(\sum_n -\mathbf{1}[y_n \mathbf{w}^T \mathbf{x}_n \leq 1] y_n \mathbf{x}_n + \lambda \mathbf{w} \right)$$ update

loss term

$$\mathbf{w} \leftarrow \mathbf{w} + \eta y_n \mathbf{x}_n$$

↑

only for points $y_n \mathbf{w}^T \mathbf{x}_n \leq 1$

perceptron update $y_n \mathbf{w}^T \mathbf{x}_n \leq 0$

regularization term

$$\mathbf{w} \leftarrow (1 - \eta\lambda)\mathbf{w}$$

shrinks weights towards zero

Example: Squared loss

$$\mathcal{L}(\mathbf{w}) = \sum_n \left(y_n - \mathbf{w}^T\mathbf{x}_n\right)^2 + \frac{\lambda}{2}||\mathbf{w}||^2$$

objective

$\big\downarrow$ matrix notation

$$\underbrace{\begin{bmatrix} x_{1,1} & x_{1,2} & \cdots & x_{1,D} \\ x_{2,1} & x_{2,2} & \cdots & x_{2,D} \\ \vdots & \vdots & \ddots & \vdots \\ x_{N,1} & x_{N,2} & \cdots & x_{N,D} \end{bmatrix}}_{\mathbf{X}} \underbrace{\begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_D \end{bmatrix}}_{w} = \underbrace{\begin{bmatrix} \sum_d x_{1,d}w_d \\ \sum_d x_{2,d}w_d \\ \vdots \\ \sum_d x_{N,d}w_d \end{bmatrix}}_{\hat{\mathbf{Y}}} \approx \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{bmatrix}}_{\hat{\mathbf{Y}}}$$

$\big\downarrow$ equivalent loss

$$\min_{w} \quad \mathcal{L}(w) = \frac{1}{2}||\mathbf{X}w - \mathbf{Y}||^2 + \frac{\lambda}{2}||w||^2$$

Example: Squared loss

$$\min_{w} \quad \mathcal{L}(w) = \frac{1}{2}||\mathbf{X}w - \mathbf{Y}||^2 + \frac{\lambda}{2}||w||^2$$

objective

$$\begin{aligned} \nabla_w \mathcal{L}(w) &= \mathbf{X}^\top(\mathbf{X}w - \mathbf{Y}) + \lambda w \\ &= \mathbf{X}^\top\mathbf{X}w - \mathbf{X}^\top\mathbf{Y} + \lambda w \\ &= \left(\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}\right)w - \mathbf{X}^\top\mathbf{Y} \end{aligned}$$

gradient

At optima the gradient=0

$$\begin{aligned} & \left(\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}\right)w - \mathbf{X}^\top\mathbf{Y} = 0 \\ \iff & \left(\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_D\right)w = \mathbf{X}^\top\mathbf{Y} \\ \iff & w = \left(\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_D\right)^{-1}\mathbf{X}^\top\mathbf{Y} \end{aligned}$$

exact closed-form solution

Matrix inversion vs. gradient descent

- Assume, we have D features and N points
- Overall time via matrix inversion
  - The closed form solution involves computing:

$$w = \left(\mathbf{X}^\top\mathbf{X} + \lambda\mathbf{I}_D\right)^{-1}\mathbf{X}^\top\mathbf{Y}$$

  - Total time is $O(D^2N + D^3 + DN)$, assuming $O(D^3)$ matrix inversion
  - If N > D, then total time is $O(D^2N)$
- Overall time via gradient descent
  - Gradient: $\dfrac{d\mathcal{L}}{d\mathbf{w}} = \sum_n -2(y_n - \mathbf{w}^T\mathbf{x}_n)\mathbf{x}_n + \lambda\mathbf{w}$
  - Each iteration: O(ND); T iterations: O(TND)
- Which one is faster?
  - Small problems D < 100: probably faster to run matrix inversion
  - Large problems D > 10,000: probably faster to run gradient descent

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Optimization for linear models

- Under suitable conditions*, provided you pick the step sizes appropriately, the convergence rate of gradient descent is O(1/N)
  - i.e., if you want a solution within 0.0001 of the optimal you have to run the gradient descent for N=1000 iterations.
- For linear models (hinge/logistic/exponential loss) and squared-norm regularization there are off-the-shelf solvers that are fast in practice: SVM$^{\text{perf}}$, LIBLINEAR, PEGASOS
  - SVM$^{\text{perf}}$, LIBLINEAR use a different optimization method

* the function is strongly convex: $f(y) \geq f(x) + \nabla f(x)^T(y - x) + \frac{m}{2}\|y - x\|_2^2$

Feature normalization

- Even if a feature is useful some normalization may be good
- Per-feature normalization
  - Centering $x_{n,d} \leftarrow x_{n,d} - \mu_d$
  - Variance scaling $x_{n,d} \leftarrow x_{n,d}/\sigma_d$
  - Absolute scaling $x_{n,d} \leftarrow x_{n,d}/r_d$

$$\mu_d = \frac{1}{N}\sum_n x_{n,d}$$

$$\sigma_d = \sqrt{\frac{1}{N}\sum_n (x_{n,d} - \mu_d)^2}$$

$$r_d = \max_n |x_{n,d}|$$

  - Non-linear transformation
    - square-root

$$x_{n,d} \leftarrow \sqrt{x_{n,d}}$$

(corrects for burstiness)

Caltech-101 image classification

41.6% linear
63.8% square-root

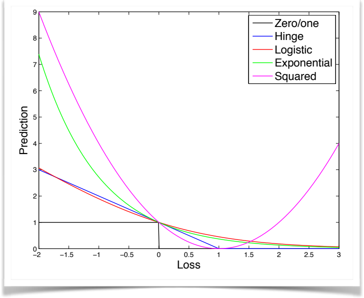
- Per-example normalization
  - fixed norm for each example $||\mathbf{x}|| = 1$

Slides credit

- Figures of various “p-norms” are from Wikipedia
  - http://en.wikipedia.org/wiki/Lp_space
- Some of the slides are based on CIML book by Hal Daume III

Appendix: code for surrogateLoss

Output



```
% Code to plot various loss functions
y1=1;
y2=linspace(-2,3,500);
zeroOneLoss = y1*y2 <=0;
hingeLoss = max(0, 1-y1*y2);
logisticLoss = log(1+exp(-y1*y2))/log(2);
expLoss = exp(-y1*y2);
squaredLoss = (y1-y2).^2;

% Plot them
figure(1); clf; hold on;
plot(y2, zeroOneLoss,’k-’,’LineWidth’,1);
plot(y2, hingeLoss,’b-’,’LineWidth’,1);
plot(y2, logisticLoss,’r-’,’LineWidth’,1);
plot(y2, expLoss,’g-’,’LineWidth’,1);
plot(y2, squaredLoss,’m-’,’LineWidth’,1);
ylabel(’Prediction’,’FontSize’,16);
xlabel(’Loss’,’FontSize’,16);
legend({’Zero/one’, ’Hinge’, ’Logistic’, ’Exponential’, ’Squared’}, ’Location’,↙
’NorthEast’, ’FontSize’,16);
box on;
```

Matlab code