

Machine Learning

Support Vector Machines

Algorithm: Perceptron

- Initialize w and η
- On each round
 - Receive example x
 - Predict $\hat{y} = \text{sign}(w \cdot x)$
 - Receive correct label $y \in \{+1,-1\}$
 - Suffer loss $\ell_{0/1}(\mathbf{y},\hat{\mathbf{y}})$
 - Update w: $W^{j+1} = W^j + \eta y_i x_i$

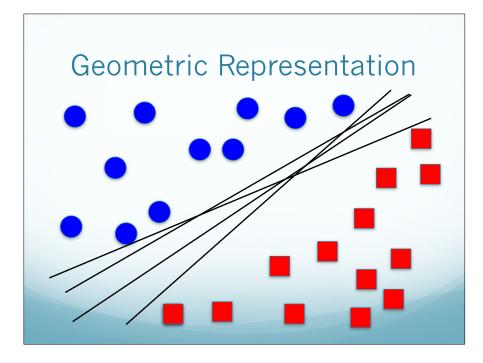
Perceptron

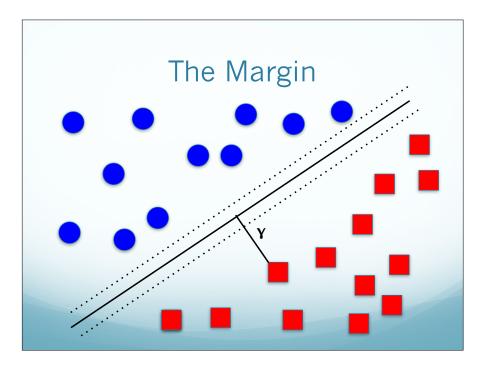
Fitting a function to data

- Fitting: Stochastic gradient descent
- Function: 0/1 loss with linear function
- Data: Update using a single example at a time

Questions

- Perceptron picks one separating hyperplane (of many)
 - What would we do if we saw all of the data (batch)?
 - We'd pick the best separating hyperplane!
- Which separating hyperplane is the best?
 - Let's look at the geometric model
- Better solutions for non-linear data?





Functional Margin

• Prediction and y should agree to get large margin

$$\hat{\gamma}^i = y_i(w^T x + b)$$

• What if we double w?

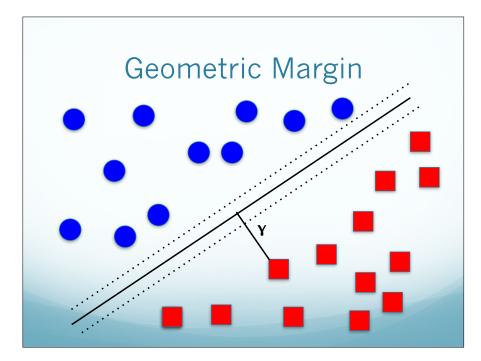
$$\hat{\gamma}^i = y_i (2w^T x + 2b)$$

- Doubles margin, but no practical change
 - We will address this in a moment

Functional Margin of Data

- Given a training set of size N:
 - Smallest margin

$$\hat{\gamma} = \min_{i=1,\dots,N} \hat{\gamma}^i$$



Geometric Margin

- Size of γ?
- $\frac{w}{||w||}$ is a unit length vector pointing in the direction of w
- ullet γ intersects with the decision boundary at

$$x_i - \gamma^i \cdot \frac{w}{||w||}$$

and points on the boundary must give a prediction of 0

 $\gamma^{i} = y_{i} \left(\left(\frac{w}{||w||} \right)^{T} x_{i} + \frac{b}{||w||} \right)$

if ||w|| = 1 then functional = geometric margin

Max-Margin Principle

- Assuming the observed data is linearly separable
- Select the hyperplane that separates the data with the maximal margin
- Why?
 - New examples are likely to be close to old examples
 - Gives the best generalization error on new data

Maximum Geometric Margin

$$\max_{\substack{\gamma, w, b \\ \gamma, w, b}} \gamma$$

$$s.t. \ y_i(w^T x_i + b) \ge \gamma, i = 1, \dots, N$$

$$||w|| = 1$$

- Every training instance has margin at least γ
- ||w|| constraint means geometric = functional margin
- Problem: ||w|| constraint is non-convex!

Maximum Geometric Margin

- Functional and geometric related by $\gamma = \frac{\hat{\gamma}}{||w||}$ $\max_{\hat{\gamma},w,b} \frac{\hat{\gamma}}{||w||}$
 - s.t. $y_i(w^T x_i + b) \ge \hat{\gamma}, i = 1, \dots, N$

Maximum Geometric Margin

- Recall: we can arbitrarily scale w!
 - ullet Arbitrarily set $\,\gamma=1\,$

$$\min_{w,b} \quad \frac{1}{2} ||w||^2$$
 s.t. $y_i(w^T x_i + b) \ge 1, i = 1, ..., N$

- min ||w||² same as max 1/||w||
- Quadratic program (QP): quadratic objective with linear constraints

Support Vector Machines Fitting a function to data

- Fitting: Batch optimization method: QP solver
- Function: hyperplane with functional margin >= 1
 - New loss function?
- Data: Train in batch mode

SVM vs. Logistic Regression

- Both minimize the empirical loss with some regularization
 - SVM:

$$\frac{1}{n} \sum_{i=1}^{n} (1 - y_i [w \cdot x_i])^+ + \lambda \frac{1}{2} ||w||^2$$

• Logistic:

$$\frac{1}{n} \sum_{i=1}^{n} \underbrace{-\log g(y_i[w \cdot x_i])}_{-P(y_i|x_i,w)} + \lambda \frac{1}{2} ||w||^2$$

- (z)⁺ indicates only positive values
- $g(z) = (1+exp(-z))^{-1}$ is the logistic function

Loss Function

Both minimize

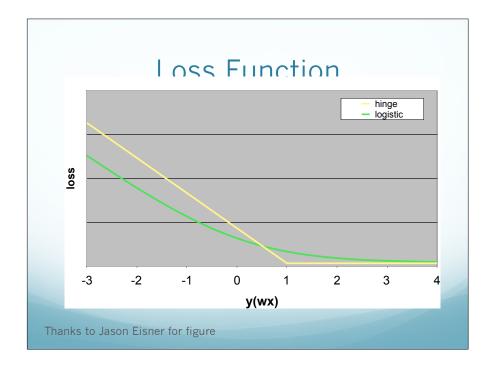
$$\frac{1}{n}\sum_{i=1}^n \ell(\mathbf{y}_i[\mathbf{w}\cdot\mathbf{x}_i]) + \lambda \frac{1}{2} \|\mathbf{w}\|^2$$

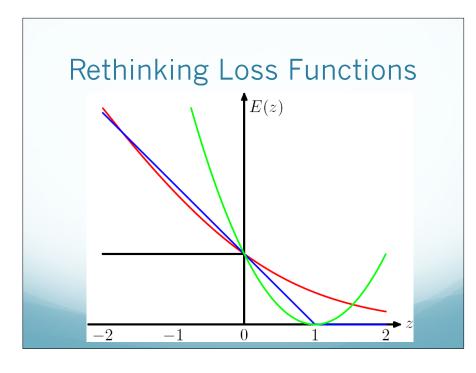
- Different loss functions
- SVM: Hinge Loss

$$\ell(\mathbf{w}, \mathbf{x}, \mathbf{y}) = \max (0, 1 - \mathbf{y}[\mathbf{w} \cdot \mathbf{x}])$$

Logistic regression: Logistic loss

$$\ell(\textbf{\textit{w}}, \textbf{\textit{x}}, \textbf{\textit{y}}) = \log (1 + \exp\{-\textbf{\textit{y}}[\textbf{\textit{w}} \cdot \textbf{\textit{x}}]\})$$





Perceptron: How to Update?

- How do we update w to improve our loss?
- Define an error function based on 0/1 loss

$$L_w(y) = \sum_{i}^{N} max(0, -y_i w \cdot x_i)$$

• What is the difference?

Rethinking Loss Functions E(z) -2 -1 0 1 2

The Perceptron Connection

- SVM minimizes the Perceptron but goes further
- Perceptron gives local updates, SVM gives global updates
- SVM is more aggressive: max-margin principle
- Could we apply max-margin to online learning?
 - Yes! Perceptron with margin
 - Other methods as well

Support Vector Machines Fitting a function to data

- Fitting: Batch optimization method
- Function: select hyperplane that ensures a fixed margin, L2 regularization
 - Loss: hinge loss
- Data: Train in batch mode

Another Formulation

Dual Formulation

- The primal and dual formulations are complimentary
 Solving one will give the solution for the other
- Primal problem: objective function is a combination of the m variables
 - Minimize the objective function
 - Solution is a vector of m values that minimize function
- Dual problem: objective function is a combination of n variables
 - Maximize the objective function
 - Solution is a vector of n values called the dual variables

SVM Solution

Select αs that maximize

$$\sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} \mathbf{y}_i \mathbf{y}_j \alpha_i \alpha_j (\mathbf{x}_i \mathbf{x}_j^T)$$

such that $\alpha_i \ge 0$ and $\sum_{i=1}^n \alpha_i y_i = 0$

Predictions for new examples

$$\mathbf{X}^T \cdot \mathbf{W} = \mathbf{X}^T \cdot \sum_{i=1}^n [\alpha_i \mathbf{y}_i \mathbf{X}_i] = \sum_{i=1}^n \alpha_i \mathbf{y}_i (\mathbf{X}^T \cdot \mathbf{X}_i)$$

New Approach

Fitting a function to data

- Fitting: Maximize objective in the dual using a QP solver
- Function: max margin linear classifier

$$\hat{y} = \operatorname{sign}(\mathbf{x}^T \cdot \mathbf{w}) = \operatorname{sign}(\sum_{i=1}^n \alpha_i y_i (\mathbf{x}^T \cdot \mathbf{x}_i))$$

• Data: Train in batch mode

Dual vs. Primal Formulation

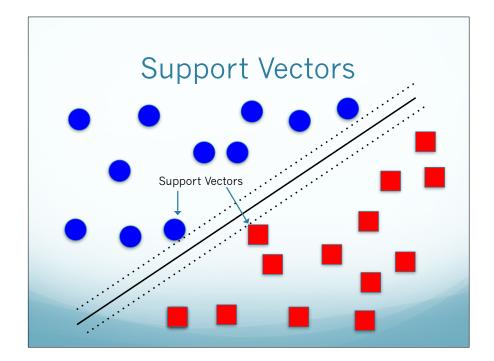
- In the primal we have M variables to solve
 - Solve for the vector **w** (length of features)
- In the dual we have N variables to solve
 - ullet Solve for the vector $oldsymbol{lpha}$ (length of examples)
- When to use the primal?
 - Lots of examples without many features
- When to use the dual?
 - Lots of features without many examples
 - Some other reasons (we'll talk about later)

Support Vectors

- Why is it called support vector machine?
- Only some of the α s will be non-zero
 - All misclassified examples will be support vectors

$$\sum_{i=1}^{n} \alpha_{i} \mathbf{y}_{i} (\mathbf{x}^{T} \cdot \mathbf{x}_{i})$$

- Only these vector support the hyperplane
- These are the vectors closest to the hyperplane
- These are called "support vectors"



By the Way

- We represented w in terms of the input X
- w is a linear combination of the inputs
 - Before: prediction was linear combination of w and x

$$W = \sum_{i=1}^{n} [\alpha_{i} y_{i} x_{i}]$$

- The same is true of Perceptron
 - If we store the support examples



Non-Separable Data

- But not all data is linearly separable
 - Previous solution: add a unique feature to every example to make it separable
- What will SVMs do?
 - The regularization forces the weights to be small
 - But it must still find a max margin solution
 - Result: even with significant regularization, still leads to over-fitting

Slack Variables

$$\min_{\mathbf{w}} \frac{1}{2} \|\mathbf{w}\|^2 + C \sum_{i=1}^n \xi_i$$

such that $(\mathbf{w} \mathbf{x}_i) \mathbf{y}_i + \xi_i \ge 1$, $\forall i$
 $\xi_i \ge 0$, $\forall i$

- We can always satisfy the margin using ξ
 - We want these ξs to be small
 - Trade off parameter C (similar to λ before)
- ξs are called slack variables
 - The cut the margin some "slack"

Non-Separable Solution

- Similar form to the separable solution
- Extra term added to objective

Bias vs. Variance

- Smaller C means more slack (larger ξ)
 - More training examples are wrong
 - More bias (less variance) in the output
- Larger C means less slack (smaller ξ)
 - Better fit to the data
 - Less bias (more variance) in the output
- For non-separable data we can't learn a perfect separator so we don't want to try too hard
 - Finding the right balance is a tradeoff

Lingering Questions

- What would we do if we saw all of the data (batch)?
 - We'd pick the best separating hyperplane!
- Which separating hyperplane is the best?
 - The maximum margin separator
 - Use a quadratic regularizer on the weights
- What can we do for non-linear data?
 - It's not separable, use slack variables
 - Can we do better?

Next Time

Kernel Methods and Non-Linear Support Vector Machines