Warm up

Regrade requests submitted directly in Gradescope, do not email instructors.

1 float in NumPy = 8 bytes
$10^6 \approx 2^{20}$ bytes = 1 MB
$10^9 \approx 2^{30}$ bytes = 1 GB

```
# generate some nonsense data for an example
X = np.random.randn(n,d)
y = np.random.randn(n)
```

```
# generate the random features
G = np.random.randn(p, d)*np.sqrt(.1)
b = np.random.rand(p)*2*np.pi
```

```
# construct HTH
HTH = np.zeros((p,p))
HTy = np.zeros(p)
for i in range(n):
    hi = np.dot(X[i,:], G.T)+b
    HTH += np.outer(hi, hi)
    HTy += y[i]*hi
    if i % 1000==0: print(i)
```

```
H = np.dot(X, G.T) + b.T
HTH = np.dot(H.T, H)
HTy = np.dot(H.T, y)
```

```
# construct HTH
HTH = np.zeros((p,p))
HTy = np.zeros(p)
block = p
for i in range(int(np.ceil(n/block))+1):
    Hi = np.dot(X[i*block:min(n,(i+1)*block),:], G.T)+b
    HTH += np.dot(Hi.T, Hi)
    HTy += np.dot(Hi.T, y[i*block:min(n,(i+1)*block)])
```

```
w = np.linalg.solve(HTH + lam*np.eye(p), HTy)
```

For each block compute the memory required in terms of n, p, d.

If d << p << n, what is the most memory efficient program (blue, green, red)?

If you have unlimited memory, what do you think is the fastest program?

Gradient Descent

Machine Learning – CSE546
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October 18, 2016

Machine Learning Problems

- Have a bunch of iid data of the form:

$$\{(x_i, y_i)\}_{i=1}^n \qquad x_i \in \mathbb{R}^d \qquad y_i \in \mathbb{R}$$

- Learning a model's parameters:

$$\sum_{i=1}^n \ell_i(w)$$

Each $\ell_i(w)$ is convex.

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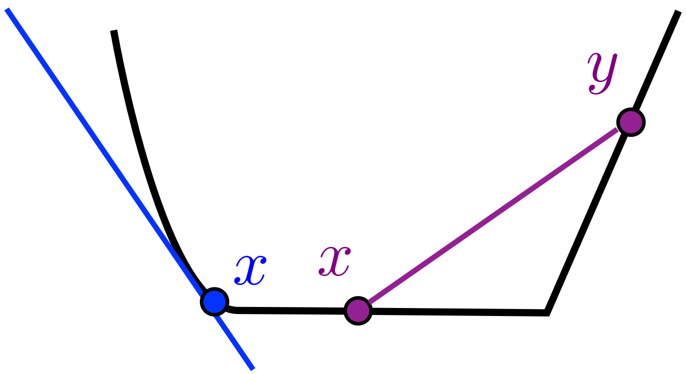

g is a subgradient at x if

$$f(y) \geq f(x) + g^T(y - x)$$

f convex:

$$f(\lambda x + (1-\lambda)y) \leq \lambda f(x) + (1-\lambda) f(y) \qquad \forall x, y, \lambda \in [0,1]$$

$$f(y) \geq f(x) + \nabla f(x)^T (y - x) \qquad \forall x, y$$

Machine Learning Problems

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- Learning a model's parameters:

  Each $\ell_i(w)$ is convex.

$$\sum_{i=1}^n \ell_i(w)$$

Logistic Loss: $\ell_i(w) = \log(1 + \exp(-y_i \, x_i^T w))$

Squared error Loss: $\ell_i(w) = (y_i - x_i^T w)^2$

Least squares

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How does software solve: $\frac{1}{2}||\mathrm{X}w - \mathrm{y}||_2^2$

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How does software solve: $\frac{1}{2}||\mathrm{X}w - \mathrm{y}||_2^2$

…its complicated:
(LAPACK, BLAS, MKL…)

Do you need high precision?
Is X column/row sparse?
Is $\widehat{w}_{LS}$ sparse?
Is $\mathrm{X}^T\mathrm{X}$ "well-conditioned"?
Can $\mathrm{X}^T\mathrm{X}$ fit in cache/memory?

Taylor Series Approximation

- Taylor series in one dimension:

$$f(x+\delta) = f(x) + f'(x)\delta + \tfrac{1}{2} f''(x)\delta^2 + \dots$$

- Gradient descent:

Taylor Series Approximation

- Taylor series in **d** dimensions:

$$f(x+v) = f(x) + \nabla f(x)^T v + \frac{1}{2} v^T \nabla^2 f(x) v + \dots$$

- Gradient descent:

Gradient Descent $f(w) = \frac{1}{2}||\mathrm{X}w - \mathrm{y}||_2^2$

$$w_{t+1} = w_t - \eta \nabla f(w_t)$$

$$\nabla f(w) =$$

Gradient Descent $f(w) = \frac{1}{2}||\mathrm{X}w - \mathrm{y}||_2^2$

$$w_{t+1} = w_t - \eta \nabla f(w_t)$$

$$\nabla f(w) = \mathbf{X}^T(\mathbf{X}w - y)$$

$$w_* = \arg\min_w f(w) \implies \nabla f(w_*) = 0$$

$$\begin{aligned} w_{t+1} - w_* &= w_t - w_* - \eta \nabla f(w_t) \\ &= w_t - w_* - \eta(\nabla f(w_t) - \nabla f(w_*)) \\ &= w_t - w_* - \eta \mathbf{X}^T\mathbf{X}(w_t - w_*) \\ &= (I - \eta \mathbf{X}^T\mathbf{X})(w_t - w_*) \\ &= (I - \eta \mathbf{X}^T\mathbf{X})^{t+1}(w_0 - w_*) \end{aligned}$$

Gradient Descent $f(w) = \frac{1}{2}||\mathrm{X}w - \mathrm{y}||_2^2$

$$w_{t+1} = w_t - \eta \nabla f(w_t)$$

$$(w_{t+1} - w_*) = (I - \eta \mathrm{X}^T \mathrm{X})(w_t - w_*)$$
$$= (I - \eta \mathrm{X}^T \mathrm{X})^{t+1}(w_0 - w_*)$$

Example: $\mathrm{X} = \begin{bmatrix} 10^{-3} & 0 \\ 0 & 1 \end{bmatrix}$ $\mathrm{y} = \begin{bmatrix} 10^{-3} \\ 1 \end{bmatrix}$ $w_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ $w_* =$

Gradient Descent $f(w) = \frac{1}{2}||Xw - y||_2^2$

$$w_{t+1} = w_t - \eta \nabla f(w_t)$$

$$(w_{t+1} - w_*) = (I - \eta X^T X)(w_t - w_*)$$
$$= (I - \eta X^T X)^{t+1}(w_0 - w_*)$$

Example: $X = \begin{bmatrix} 10^{-3} & 0 \\ 0 & 1 \end{bmatrix}$ $y = \begin{bmatrix} 10^{-3} \\ 1 \end{bmatrix}$ $w_0 = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ $w_* = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

$$X^T X = \begin{bmatrix} 10^{-6} & 0 \\ 0 & 1 \end{bmatrix}$$

Pick η such that
$\max\{|1 - \eta 10^{-6}|, |1 - \eta|\} < 1$

$$|w_{t+1,1} - w_{*,1}| = |1 - \eta 10^{-6}|^{t+1} |w_{0,1} - w_{*,1}| = |1 - \eta 10^{-6}|^{t+1}$$
$$|w_{t+1,2} - w_{*,2}| = |1 - \eta|^{t+1} |w_{0,2} - w_{*,2}| = |1 - \eta|^{t+1}$$

Taylor Series Approximation

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- Newton's method:

Taylor Series Approximation

- Taylor series in d dimensions:

$$f(x+v) = f(x) + \nabla f(x)^T v + \frac{1}{2} v^T \nabla^2 f(x) v + \dots$$

- Newton's method:

Newton's Method $f(w) = \frac{1}{2}||\mathrm{X}w - \mathrm{y}||_2^2$

$\nabla f(w) =$

$\nabla^2 f(w) =$

$v_t \text{ is solution to} : \nabla^2 f(w_t) v_t = -\nabla f(w_t)$

$w_{t+1} = w_t + \eta v_t$

Newton's Method $f(w) = \frac{1}{2}||\mathrm{X}w - \mathrm{y}||_2^2$

$$\nabla f(w) = \mathrm{X}^T(\mathrm{X}w - \mathrm{y})$$

$$\nabla^2 f(w) = \mathrm{X}^T\mathrm{X}$$

$$v_t \text{ is solution to} : \nabla^2 f(w_t) v_t = -\nabla f(w_t)$$

$$w_{t+1} = w_t + \eta v_t$$

For quadratics, Newton's method can converge in one step! (No surprise, why?)

$$\begin{aligned} w_1 &= w_0 - \eta(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T(\mathbf{X}w_0 - y) \\ &= (1-\eta)w_0 + \eta(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T y \\ &= (1-\eta)w_0 + \eta w_* \end{aligned}$$

In general, for w_t "close enough" to w_* one should use $\eta = 1$

General case

In general for Newton's method to achieve $f(w_t) - f(w_*) \leq \epsilon$:

So why are ML problems overwhelmingly solved by gradient methods?

Hint: v_t is solution to : $\nabla^2 f(w_t) v_t = -\nabla f(w_t)$

General Convex case $f(w_t) - f(w_*) \leq \epsilon$

Clean converge nice proofs: Bubeck

Newton's method:

$$t \approx \log(\log(1/\epsilon))$$

Gradient descent:

- f is *smooth* and *strongly convex:* $aI \preceq \nabla^2 f(w) \preceq bI$
- f is *smooth*: $\nabla^2 f(w) \preceq bI$
- f is potentially non-differentiable: $||\nabla f(w)||_2 \leq c$

Nocedal +Wright, Bubeck

Other: BFGS, Heavy-ball, BCD, SVRG, ADAM, Adagrad,…

Revisiting… Logistic Regression

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Loss function: Conditional Likelihood

- Have a bunch of iid data of the form: $\{(x_i, y_i)\}_{i=1}^n \quad x_i \in \mathbb{R}^d, \quad y_i \in \{-1, 1\}$

$$\widehat{w}_{MLE} = \arg\max_w \prod_{i=1}^n P(y_i|x_i, w) \qquad P(Y = y|x, w) = \frac{1}{1 + \exp(-y\, w^T x)}$$

$$f(w) = \arg\min_w \sum_{i=1}^n \log(1 + \exp(-y_i\, x_i^T w))$$

$$\nabla f(w) =$$

Stochastic Gradient Descent

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Stochastic Gradient Descent

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Each $\ell_i(w)$ is convex.

Gradient Descent:

$$w_{t+1} = w_t - \eta \nabla_w \left(\frac{1}{n}\sum_{i=1}^n \ell_i(w) \right) \Big|_{w=w_t}$$

Stochastic Gradient Descent

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Stochastic Gradient Descent:

$$w_{t+1} = w_t - \eta \nabla_w \ell_{I_t}(w) \Big|_{w=w_t}$$

I_t drawn uniform at random from $\{1, \dots, n\}$

$$\mathbb{E}[\nabla \ell_{I_t}(w)] =$$

Stochastic Gradient Descent

Theorem

Let $w_{t+1} = w_t - \eta \nabla_w \ell_{I_t}(w)\Big|_{w=w_t}$ $\quad$ I_t drawn uniform at random from $\{1,\dots,n\}$ $\quad$ so that

$$\mathbb{E}[\nabla \ell_{I_t}(w)] = \frac{1}{n}\sum_{i=1}^{n} \nabla \ell_i(w) =: \nabla \ell(w)$$

If $\|w_1 - w_0\|_2^2 \leq R$ and $\sup_w \max_i \|\nabla \ell_i(w)\|_2 \leq G$ then

$$\mathbb{E}[\ell(\bar{w}) - \ell(w_*)] \leq \frac{R}{2T\eta} + \frac{\eta G}{2} \leq \sqrt{\frac{RG}{T}}$$

$$\eta = \sqrt{\frac{R}{GT}}$$

$$\bar{w} = \frac{1}{T}\sum_{t=1}^{T} w_t$$

(In practice use last iterate)

Stochastic Gradient Descent

Proof

$$\mathbb{E}[||w_{t+1} - w_*||_2^2] = \mathbb{E}[||w_t - \eta \nabla \ell_{I_t}(w_t) - w_*||_2^2]$$

Stochastic Gradient Descent

Proof

$$\mathbb{E}[||w_{t+1} - w_*||_2^2] = \mathbb{E}[||w_t - \eta \nabla \ell_{I_t}(w_t) - w_*||_2^2]$$

$$= \mathbb{E}[||w_t - w_*||_2^2] - 2\eta \mathbb{E}[\nabla \ell_{I_t}(w_t)^T (w_t - w_*)] + \eta^2 \mathbb{E}[||\nabla \ell_{I_t}(w_t)||_2^2]$$

$$\leq \mathbb{E}[||w_t - w_*||_2^2] - 2\eta \mathbb{E}[\ell(w_t) - \ell(w_*)] + \eta^2 G$$

$$\mathbb{E}[\nabla \ell_{I_t}(w_t)^T (w_t - w_*)] = \mathbb{E}\left[\mathbb{E}[\nabla \ell_{I_t}(w_t)^T (w_t - w_*) | I_1, w_1, \dots, I_{t-1}, w_{t-1}]\right]$$

$$= \mathbb{E}\left[\nabla \ell(w_t)^T (w_t - w_*)\right]$$

$$\geq \mathbb{E}\left[\ell(w_t) - \ell(w_*)\right]$$

$$\sum_{t=1}^{T} \mathbb{E}[\ell(w_t) - \ell(w_*)] \leq \frac{1}{2\eta}\left(\mathbb{E}[||w_1 - w_*||_2^2] - \mathbb{E}[||w_{T+1} - w_*||_2^2] + T\eta^2 G\right)$$

$$\leq \frac{R}{2\eta} + \frac{T\eta G}{2}$$

Stochastic Gradient Descent

Proof

Jensen's inequality:
For any random $Z \in \mathbb{R}^d$ and convex function $\phi : \mathbb{R}^d \to \mathbb{R}$, $\phi(\mathbb{E}[Z]) \leq \mathbb{E}[\phi(Z)]$

$$\mathbb{E}[\ell(\bar{w}) - \ell(w_*)] \leq \frac{1}{T}\sum_{t=1}^{T}\mathbb{E}[\ell(w_t) - \ell(w_*)]$$

$$\bar{w} = \frac{1}{T}\sum_{t=1}^{T} w_t$$

Stochastic Gradient Descent

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$$\mathbb{E}[\ell(\bar{w}) - \ell(w_*)] \leq \frac{R}{2T\eta} + \frac{\eta G}{2} \leq \sqrt{\frac{RG}{T}}$$

$$\eta = \sqrt{\frac{R}{GT}}$$

Stochastic Gradient Descent: A Learning perspective

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October 18, 2016

Learning Problems as Expectations

- Minimizing loss in training data:
  - Given dataset:
    - Sampled iid from some distribution p(**x**) on features:
  - Loss function, e.g., hinge loss, logistic loss,…
  - We often minimize loss in training data:

$$\ell_{\mathcal{D}}(\mathbf{w}) = \frac{1}{N}\sum_{j=1}^{N} \ell(\mathbf{w}, \mathbf{x}^j)$$

- However, we should really minimize expected loss on all data:

$$\ell(\mathbf{w}) = E_{\mathbf{x}}\left[\ell(\mathbf{w}, \mathbf{x})\right] = \int p(\mathbf{x})\ell(\mathbf{w}, \mathbf{x})d\mathbf{x}$$

- So, we are approximating the integral by the average on the training data

Gradient descent in Terms of Expectations

- "True" objective function:

$$\ell(\mathbf{w}) = E_{\mathbf{x}}\left[\ell(\mathbf{w}, \mathbf{x})\right] = \int p(\mathbf{x})\ell(\mathbf{w}, \mathbf{x})d\mathbf{x}$$

- Taking the gradient:

- "True" gradient descent rule:

- How do we estimate expected gradient?

SGD: Stochastic Gradient Descent

- "True" gradient: $$\nabla \ell(\mathbf{w}) = E_{\mathbf{x}}\left[\nabla \ell(\mathbf{w}, \mathbf{x})\right]$$
- Sample based approximation:
- What if we estimate gradient with just one sample???
  - Unbiased estimate of gradient
  - Very noisy!
  - Also called stochastic gradient descent
    - Among many other names
  - VERY useful in practice!!!

Perceptron

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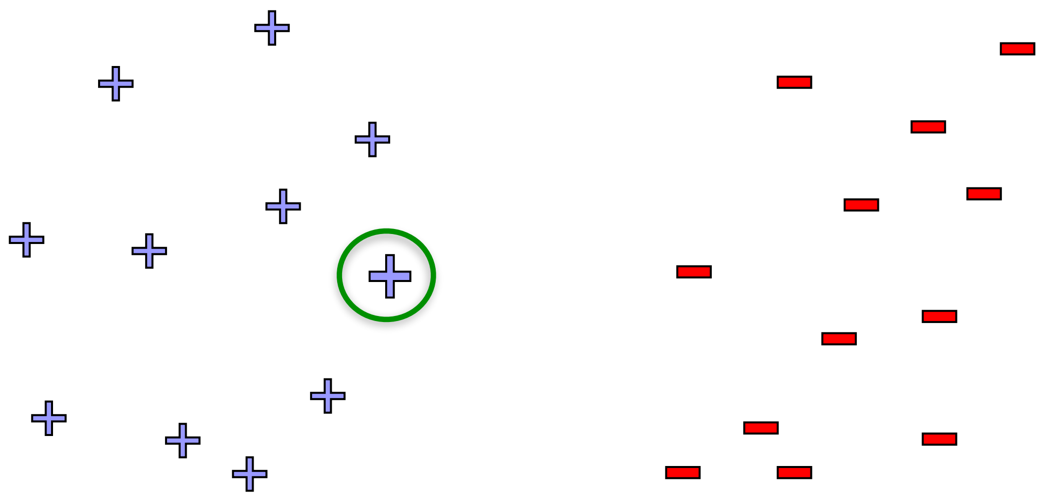
Online learning

- Click prediction for ads is a streaming data task:
  - User enters query, and ad must be selected
    - Observe $\mathbf{x}^j$, and must predict y^j
  - User either clicks or doesn't click on ad
    - Label y^j is revealed afterwards
      - Google gets a reward if user clicks on ad
  - Update model for next time

Online classification



New point arrives at time k

The Perceptron Algorithm [Rosenblatt ‘58, ‘62]

- Classification setting: y in {-1,+1}
- Linear model
  - Prediction:
- Training:
  - Initialize weight vector:
  - At each time step:
    - Observe features:
    - Make prediction:
    - Observe true class:
    - Update model:
      - If prediction is not equal to truth

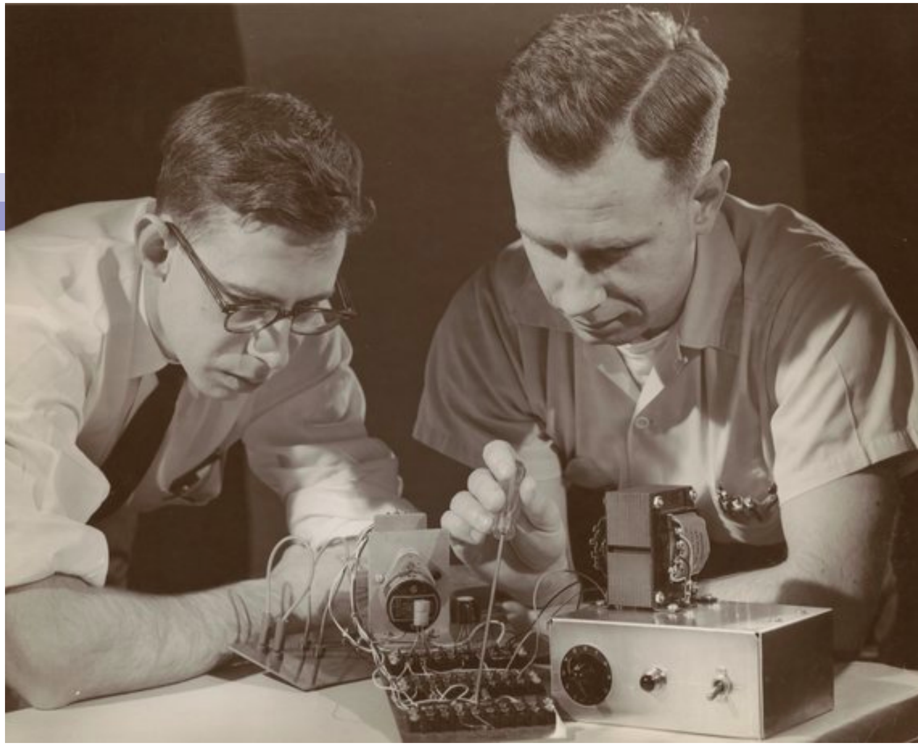
The Perceptron Algorithm [Rosenblatt '58, '62]

- Classification setting: y in {-1,+1}
- Linear model
  - Prediction: $\text{sign}(w^T x_i + b)$

- Training:
  - Initialize weight vector: $w_0 = 0, b_0 = 0$
  - At each time step:
    - Observe features: x_k
    - Make prediction: $\text{sign}(x_k^T w_k + b_k)$
    - Observe true class: y_k

    - Update model:
      - If prediction is not equal to truth

$$\begin{bmatrix} w_{k+1} \\ b_{k+1} \end{bmatrix} = \begin{bmatrix} w_k \\ b_k \end{bmatrix} + y_k \begin{bmatrix} x_k \\ 1 \end{bmatrix}$$

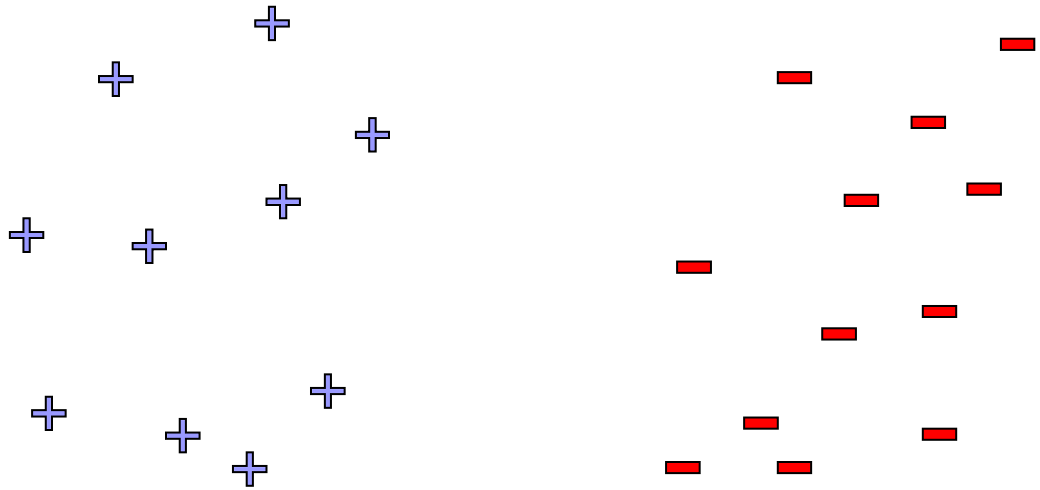


Rosenblatt 1957

"the embryo of an electronic computer that [the Navy] expects will be able to walk, talk, see, write, reproduce itself and be conscious of its existence."

The New York Times, 1958

Linear Separability



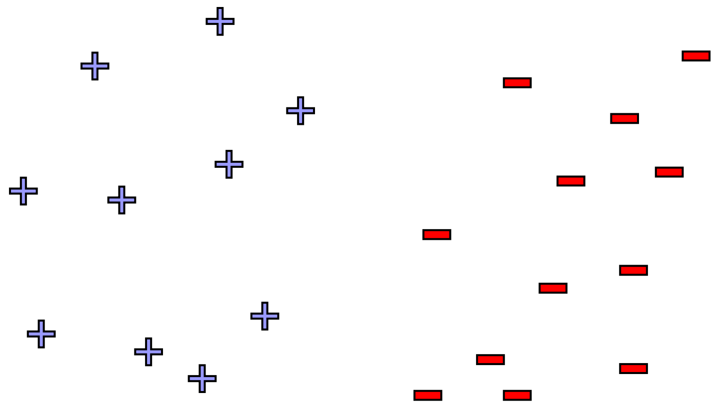
- Perceptron guaranteed to converge if
  - Data linearly separable:

Perceptron Analysis: Linearly Separable Case

- Theorem [Block, Novikoff]:
  - Given a sequence of labeled examples:
  - Each feature vector has bounded norm:
  - If dataset is linearly separable:
- Then the number of mistakes made by the online perceptron on any such sequence is bounded by

Beyond Linearly Separable Case

- Perceptron algorithm is super cool!
  - No assumption about data distribution!
    - Could be generated by an oblivious adversary, no need to be iid
  - Makes a fixed number of mistakes, and it's done for ever!
    - Even if you see infinite data



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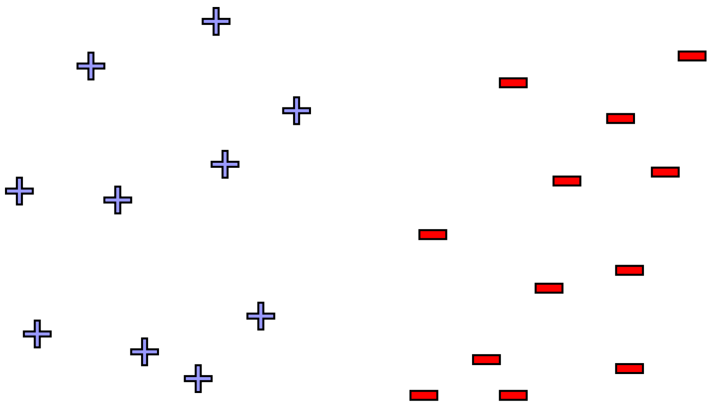

- Perceptron is useless in practice!
  - Real world not linearly separable
  - If data not separable, cycles forever and hard to detect
  - Even if separable may not give good generalization accuracy (small margin)

What is the Perceptron Doing???

- When we discussed logistic regression:
  - Started from maximizing conditional log-likelihood
- When we discussed the Perceptron:
  - Started from description of an algorithm
- What is the Perceptron optimizing????

Support Vector Machines

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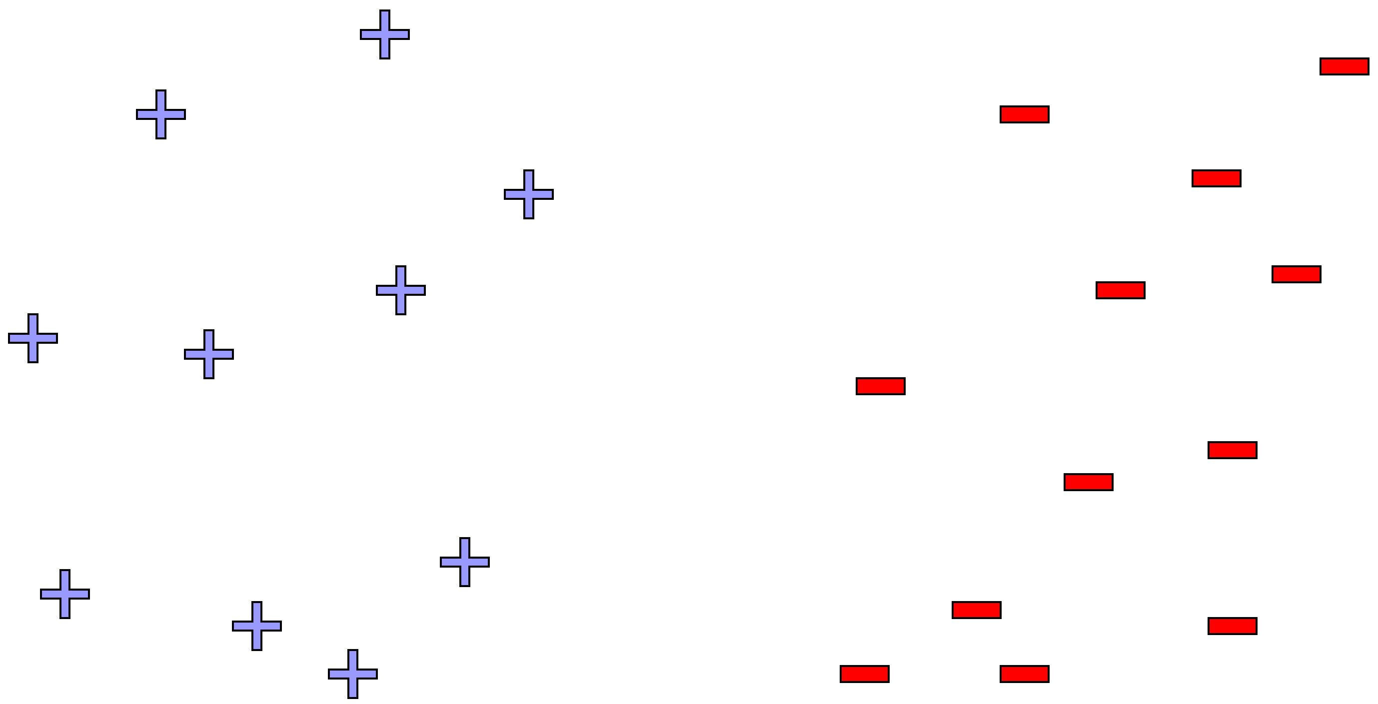
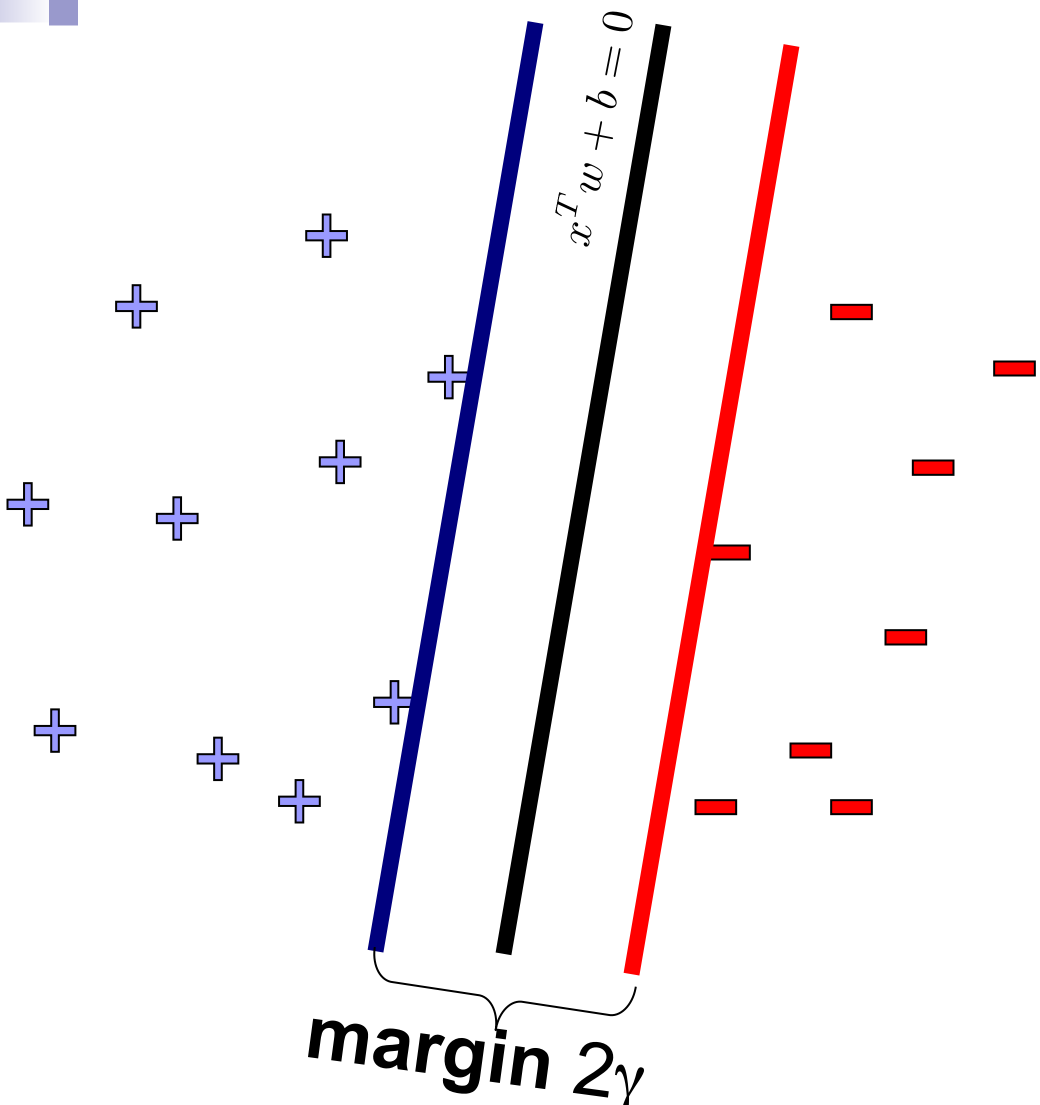
Linear classifiers – Which line is better?



Pick the one with the largest margin!



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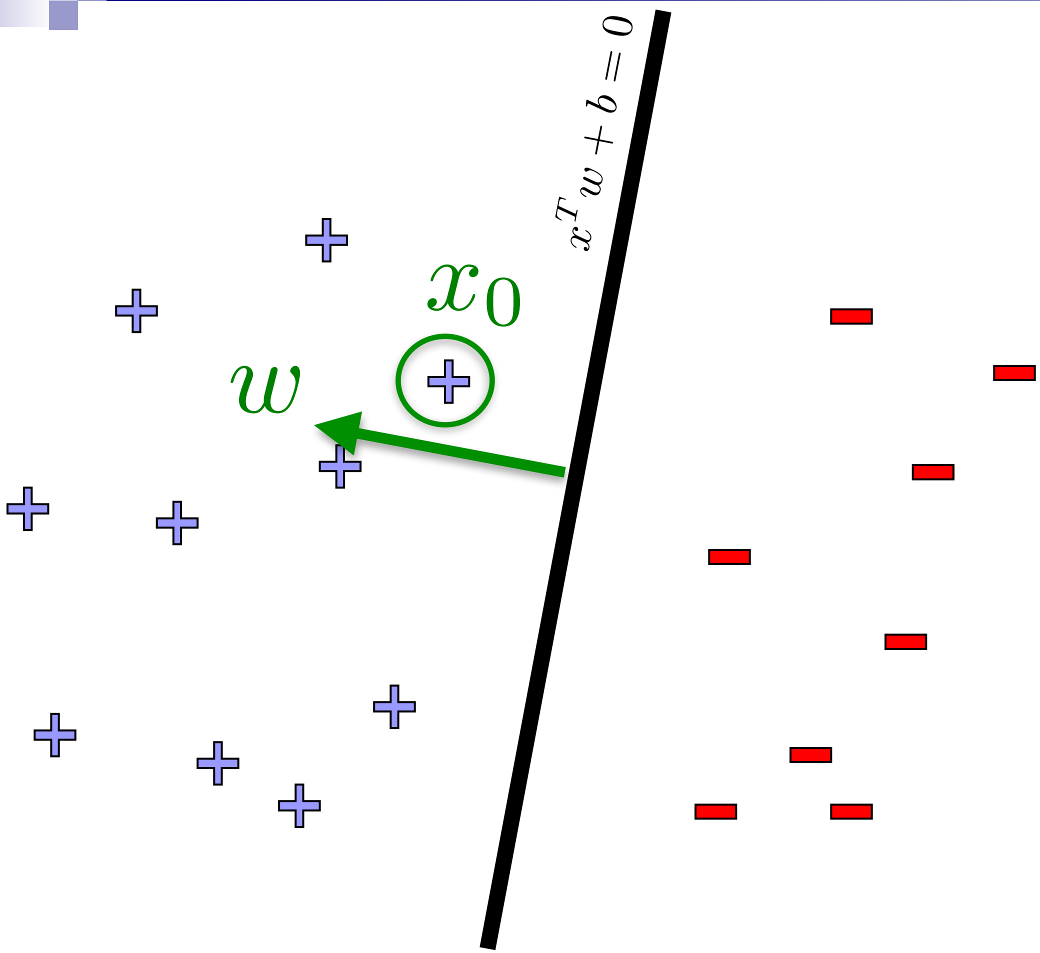
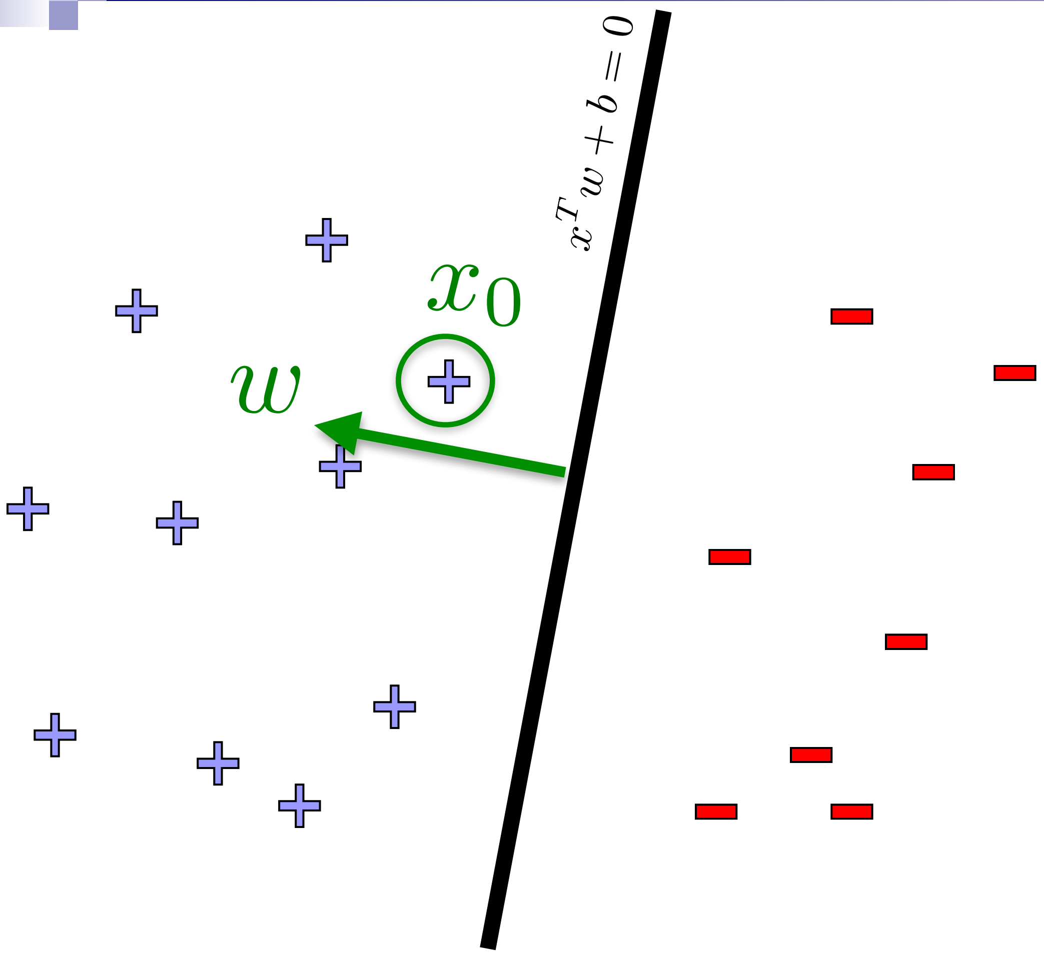


Distance from x_0 to hyperplane defined by $x^T w + b = 0$?

Pick the one with the largest margin!



Distance from x_0 to hyperplane defined by $x^T w + b = 0$?

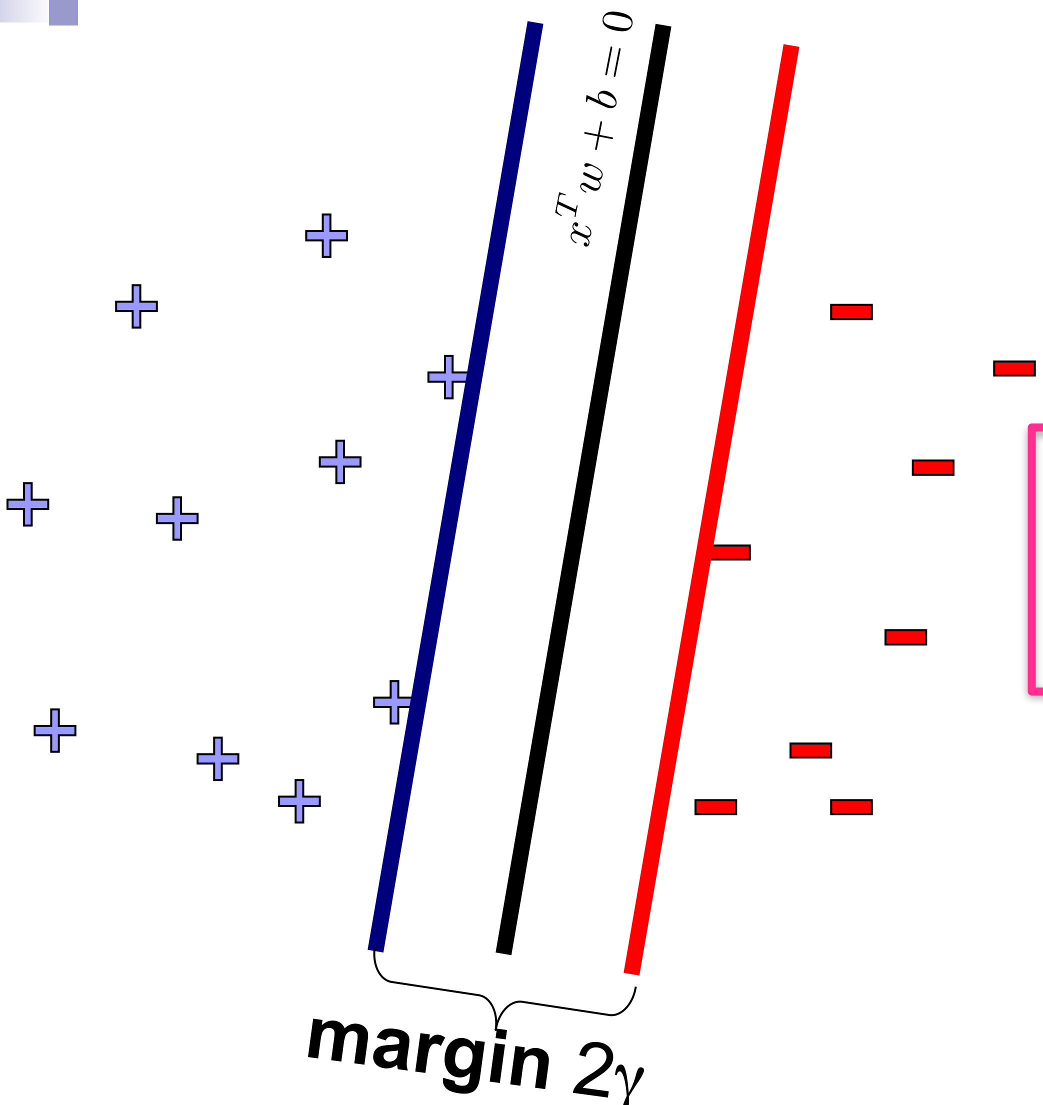
If $\widetilde{x}_0$ is the projection of x_0 onto the hyperplane then

$$||x_0 - \widetilde{x}_0||_2 = |(x_0^T - \widetilde{x}_0)^T \frac{w}{||w||_2}|$$

$$= \frac{1}{||w||_2} |x_0^T w - \widetilde{x}_0^T w|$$

$$= \frac{1}{||w||_2} |x_0^T w + b|$$

Pick the one with the largest margin!



Distance of x_0 from hyperplane $x^T w + b$:

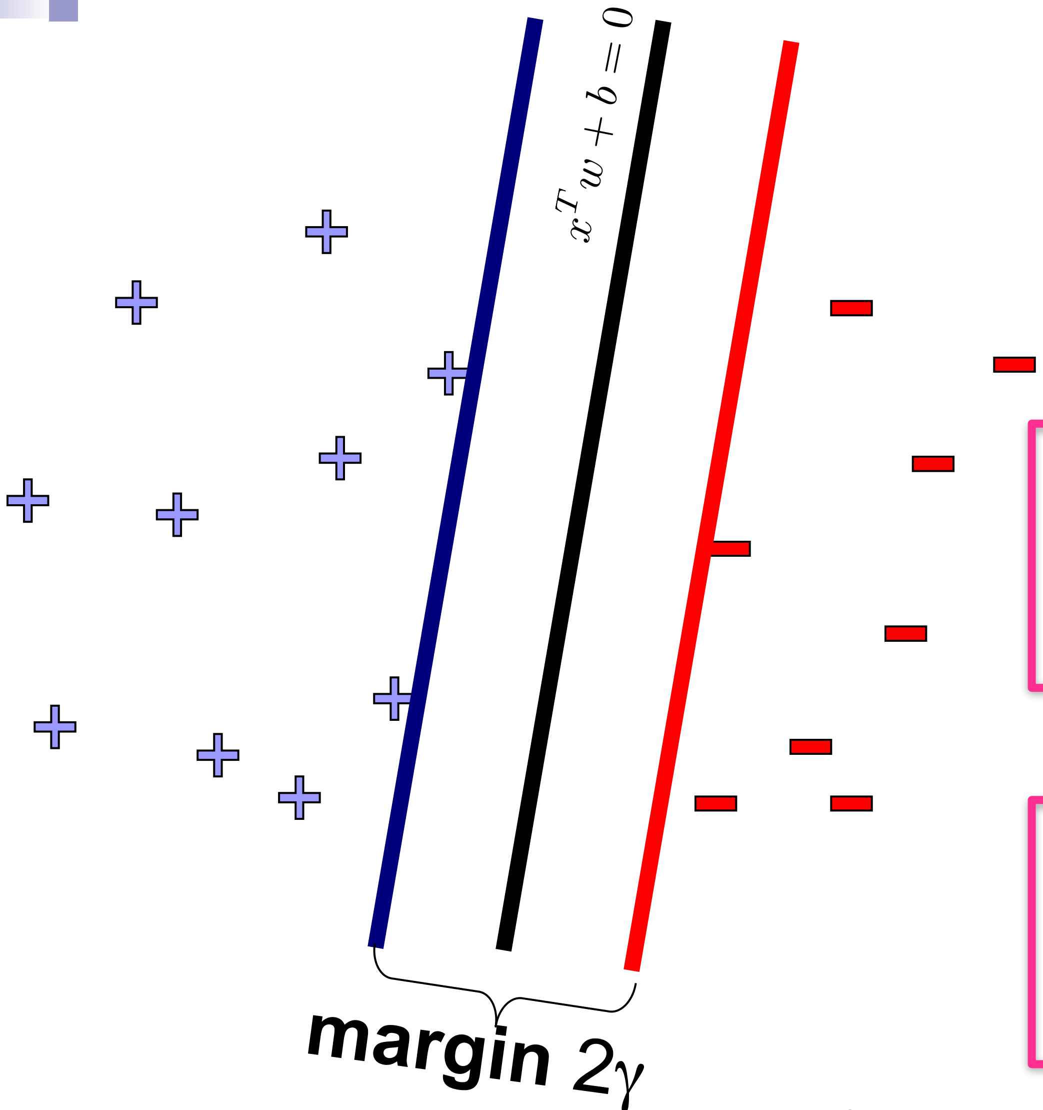
$$\frac{1}{||w||_2}(x_0^T w + b)$$

Optimal Hyperplane

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

$$\text{subject to } \frac{1}{||w||_2} y_i (x_i^T w + b) \geq \gamma \quad \forall i$$

Pick the one with the largest margin!



Distance of x_0 from hyperplane $x^Tw + b$:

$$\frac{1}{||w||_2}(x_0^Tw + b)$$

Optimal Hyperplane

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

$$\text{subject to } \frac{1}{||w||_2} y_i(x_i^Tw + b) \geq \gamma \quad \forall i$$

Optimal Hyperplane (reparameterized)

$$\min_{w,b} ||w||_2^2$$

$$\text{subject to } y_i(x_i^Tw + b) \geq 1 \quad \forall i$$

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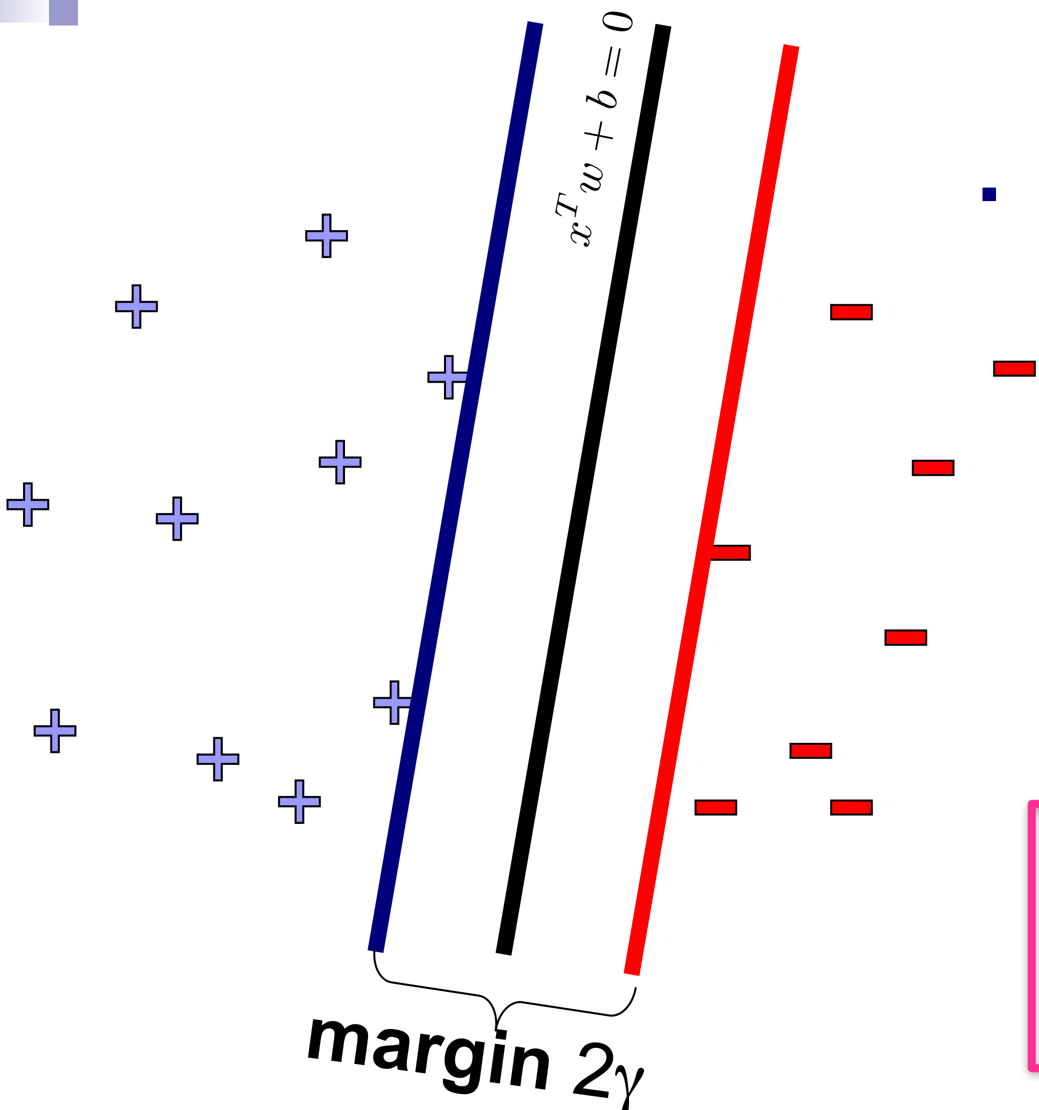

- Solve efficiently by many methods, e.g.,
  - quadratic programming (QP)
    - Well-studied solution algorithms
  - Stochastic gradient descent
  - Coordinate descent (in the dual)

Optimal Hyperplane (reparameterized)

$$\min_{w,b} ||w||_2^2$$

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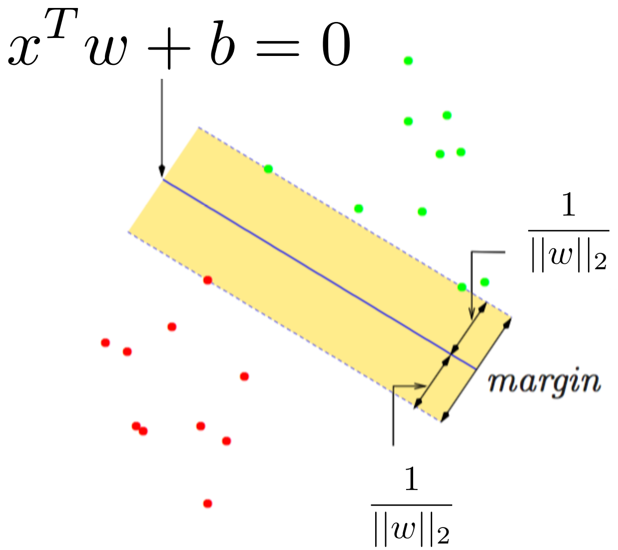
What if the data is still not linearly separable?



- If data is linearly separable

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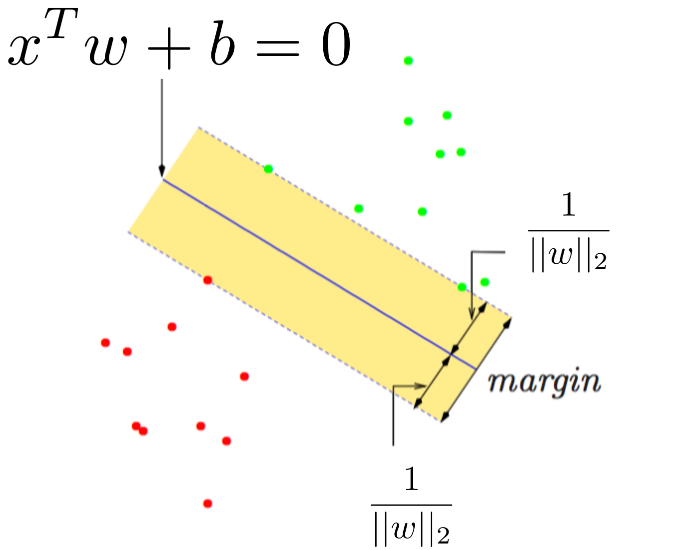

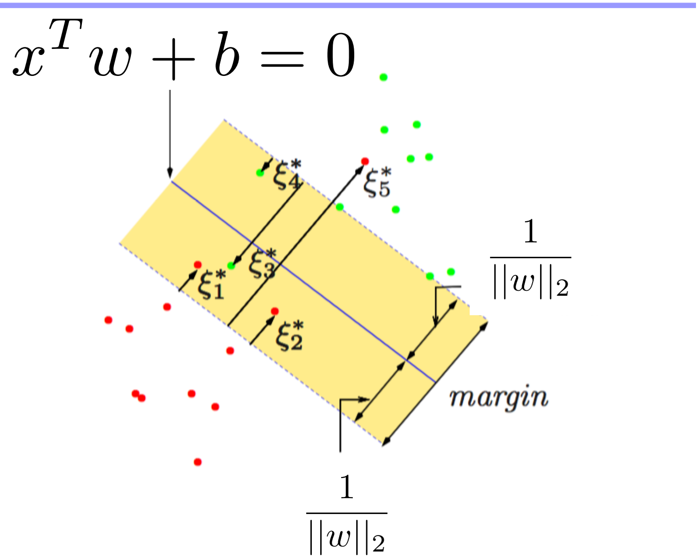

- If data is linearly separable

$$\min_{w,b} ||w||_2^2$$

$$y_i(x_i^T w + b) \geq 1 \quad \forall i$$

- If data is not linearly separable, some points don't satisfy margin constraint:

$$\min_{w,b} ||w||_2^2$$

$$y_i(x_i^T w + b) \geq 1 - \xi_i \quad \forall i$$

$$\xi_i \geq 0, \sum_{j=1}^{n} \xi_j \leq \nu$$

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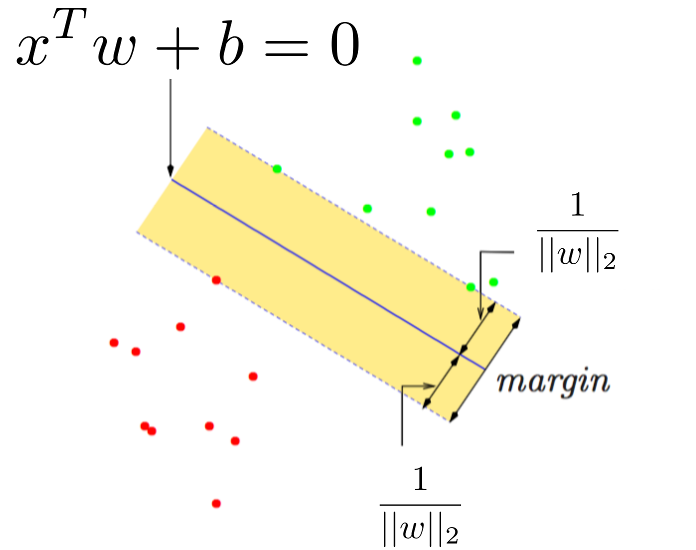

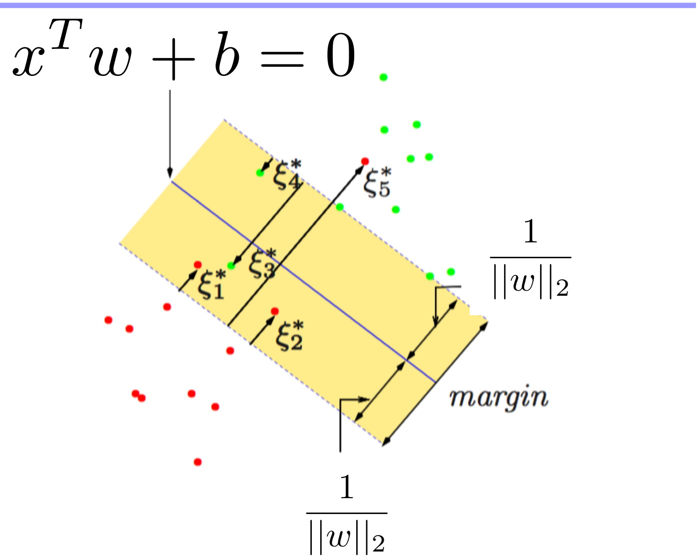

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- What are "support vectors?"

SVM as penalization method

- Original quadratic program with linear constraints:

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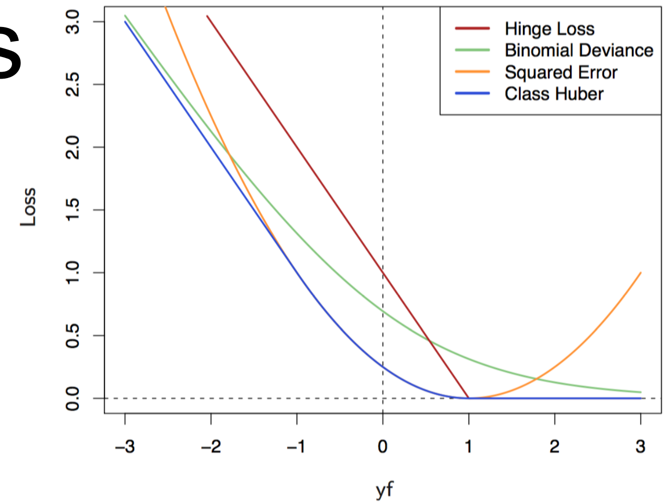
- Using same constrained convex optimization trick as for lasso:

For any $\nu \geq 0$ there exists a $\lambda \geq 0$ such that the solution the following solution is equivalent:

$$\sum_{i=1}^n \max\{0, 1 - y_i(b + x_i^T w)\} + \lambda ||w||_2^2$$

Machine Learning Problems



- Have a bunch of iid data of the form:

$$\{(x_i, y_i)\}_{i=1}^n \qquad x_i \in \mathbb{R}^d \qquad y_i \in \mathbb{R}$$

- Learning a model's parameters: $\sum_{i=1}^n \ell_i(w)$

Each $\ell_i(w)$ is convex.

Hinge Loss: $\ell_i(w) = \max\{0, 1 - y_i x_i^T w\}$

Logistic Loss: $\ell_i(w) = \log(1 + \exp(-y_i\, x_i^T w))$

Squared error Loss: $\ell_i(w) = (y_i - x_i^T w)^2$

How do we solve for *w*? The last two lectures!

Perceptron is optimizing what?

Perceptron update rule:

$$\begin{bmatrix} w_{k+1} \\ b_{k+1} \end{bmatrix} = \begin{bmatrix} w_k \\ b_k \end{bmatrix} + y_k \begin{bmatrix} x_k \\ 1 \end{bmatrix} \mathbf{1}\{y_i(b + x_i^T w) < 0\}$$

SVM objective:

$$\sum_{i=1}^{n} \max\{0, 1 - y_i(b + x_i^T w)\} + \lambda ||w||_2^2 \; = \sum_{i=1}^{n} \ell_i(w, b)$$

$$\nabla_w \ell_i(w,b) = \begin{cases} -x_i y_i + \frac{2\lambda}{n} w & \text{if } y_i(b + x_i^T w) < 1 \\ 0 & \text{otherwise} \end{cases}$$

$$\nabla_b \ell_i(w,b) = \begin{cases} -y_i & \text{if } y_i(b + x_i^T w) < 1 \\ 0 & \text{otherwise} \end{cases}$$

Perceptron is just SGD on SVM with $\lambda = 0$, $\eta = 1$!

SVMs vs logistic regression

- We often want probabilities/confidences, logistic wins here?

SVMs vs logistic regression

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- No! Perform isotonic regression or non-parametric bootstrap for probability calibration. Predictor gives some score, how do we transform that score to a probability?

SVMs vs logistic regression

- We often want probabilities/confidences, logistic wins here?
- No! Perform isotonic regression or non-parametric bootstrap for probability calibration. Predictor gives some score, how do we transform that score to a probability?

- For classification loss, logistic and svm are comparable
- Multiclass setting:
  - Softmax naturally generalizes logistic regression
  - SVMs have
- What about good old least squares?

What about multiple classes?