

Using interior point methods for optimization in training very large scale Support Vector Machines

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joint work with Kristian Woodsend

## Outline

- Interior Point Methods for QP
- logarithmic barrier function
- complementarity conditions
- linear algebra
- Support Vector Machine training
- Quadratic Programming formulation
- specific features
- IPMs for SVM training
- separable formulations !!!
- linear and nonlinear kernels in SVMs
- Challenges remaining
- nonlinear kernels in SVMs
- indefinite kernels in SVMs
- Conclusions


## Part 1:

## Interior Point Methods for QP

## "Elements" of the IPM

What do we need to derive the Interior Point Method?

- logarithmic barriers.
- duality theory:

Lagrangian function; first order optimality conditions.

- Newton method.

Wright, Primal-Dual Interior-Point Methods, SIAM, 1997.
Andersen, Gondzio, Mészáros and Xu, Implementation of Interior Point Methods for Large Scale Linear Programming, in: Interior Point Methods in Mathematical Programming, T Terlaky (ed.), Kluwer Academic, 1996, pp. 189-252.

Montreal, 18 June 2009

## Logarithmic barrier

$-\ln v_{i}$
"replaces" the inequality $v_{i} \geq 0$.

Observe that

$$
\min \mathrm{e}^{-\sum_{i=1}^{n} \ln v_{i}} \Longleftrightarrow \max \prod_{i=1}^{n} v_{i}
$$

The minimization of $-\sum_{i=1}^{n} \ln v_{i}$ is equivalent to the maximization of the product of distances from all hyperplanes defining the positive orthant: it prevents all $v_{i}$ from approaching zero.

## Logarithmic barrier

Replace the primal QP

$$
\begin{array}{cc}
\min & c^{T} v+\frac{1}{2} v^{T} Q v \\
\text { s.t. } & A v=b, \\
& v \geq 0
\end{array}
$$

with the primal barrier program

$$
\begin{array}{lc}
\min & c^{T} v+\frac{1}{2} v^{T} Q v-\mu \sum_{j=1}^{n} \ln v_{j} \\
\text { s.t. } & A v=b .
\end{array}
$$

Lagrangian:

$$
L(v, \lambda, \mu)=c^{T} v+\frac{1}{2} v^{T} Q v-\lambda^{T}(A v-b)-\mu \sum_{j=1}^{n} \ln v_{j}
$$

Conditions for a stationary point of the Lagrangian

$$
\begin{aligned}
& \nabla_{v} L(v, \lambda, \mu)=c-A^{T} \lambda+Q v-\mu V^{-1} e=0 \\
& \nabla_{\lambda} L(v, \lambda, \mu)=\quad A v-b=0,
\end{aligned}
$$

where $V^{-1}=\operatorname{diag}\left\{v_{1}^{-1}, v_{2}^{-1}, \cdots, v_{n}^{-1}\right\}$.
Let us denote

$$
s=\mu V^{-1} e, \quad \text { i.e. } \quad V S e=\mu e
$$

The First Order Optimality Conditions are:

$$
\begin{aligned}
A v & =b, \\
A^{T} \lambda+s-Q v & =c \\
V S e & =\mu e \\
(v, s) & >0
\end{aligned}
$$

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## First Order Optimality Conditions

Active-set Method:

$$
\begin{aligned}
A v & =b \\
A^{T} \lambda+s-Q v & =c \\
V S e & =0 \\
v, s & \geq 0
\end{aligned}
$$

Interior Point Method:

$$
\begin{aligned}
A v & =b \\
A^{T} \lambda+s-Q v & =c \\
V S e & =\mu e \\
v, s & \geq 0
\end{aligned}
$$

## Complementarity $\quad v_{i} \cdot s_{i}=0 \quad \forall i=1,2, \ldots, n$.

Active-set Method makes a guess of optimal partition:
$\mathcal{A} \cup \mathcal{I}=\{1,2, \ldots, n\}$.
For active constraints $(i \in \mathcal{A}), v_{i}=0$ and

$$
v_{i} \cdot s_{i}=0 \quad \forall i \in \mathcal{A}
$$

For inactive constraints $(i \in \mathcal{I}), s_{i}=0$ hence

$$
v_{i} \cdot s_{i}=0 \quad \forall i \in \mathcal{I} .
$$

Interior Point Method uses $\varepsilon$-mathematics:
Replace $\quad v_{i} \cdot s_{i}=0 \quad \forall i=1,2, \ldots, n$
by $\quad v_{i} \cdot s_{i}=\mu \quad \forall i=1,2, \ldots, n$.
Force convergence $\mu \rightarrow 0$.
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## Apply Newton Method to the FOC

The first order optimality conditions for the barrier problem form a large system of nonlinear equations

$$
f(v, \lambda, s)=0
$$

where $f: \mathcal{R}^{2 n+m} \mapsto \mathcal{R}^{2 n+m}$ is a mapping defined as follows:

$$
f(v, \lambda, s)=\left[\begin{array}{r}
A v-b \\
A^{T} \lambda+s-Q v-c \\
V S e-\mu e
\end{array}\right]
$$

Actually, the first two terms of it are linear; only the last one, corresponding to the complementarity condition, is nonlinear.

## Newton Method (cont'd)

Note that

$$
\nabla f(v, \lambda, s)=\left[\begin{array}{rcc}
A & 0 & 0 \\
-Q & A^{T} & I \\
S & 0 & V
\end{array}\right]
$$

Thus, for a given point $(v, \lambda, s)$ we find the Newton direction ( $\Delta v, \Delta \lambda, \Delta s$ ) by solving the system of linear equations:

$$
\left[\begin{array}{rcc}
A & 0 & 0 \\
-Q & A^{T} & I \\
S & 0 & V
\end{array}\right] \cdot\left[\begin{array}{l}
\Delta v \\
\Delta \lambda \\
\Delta s
\end{array}\right]=\left[\begin{array}{l}
b-A v \\
c-A^{T} \lambda-s+Q v \\
\mu e-V S e
\end{array}\right]
$$

## Linear Algebra of IPM for QP

$$
\left[\begin{array}{ccc}
A & 0 & 0 \\
-Q & A^{T} & I \\
S & 0 & V
\end{array}\right]\left[\begin{array}{c}
\Delta v \\
\Delta \lambda \\
\Delta s
\end{array}\right]=\left[\begin{array}{c}
\xi_{p} \\
\xi_{d} \\
\xi_{\mu}
\end{array}\right]=\left[\begin{array}{c}
b-A v \\
c-A^{T} \lambda-s+Q v \\
\mu e-V S e
\end{array}\right]
$$

Use the third equation to eliminate

$$
\begin{aligned}
\Delta s & =V^{-1}\left(\xi_{\mu}-S \Delta v\right) \\
& =-V^{-1} S \Delta v+V^{-1} \xi_{\mu}
\end{aligned}
$$

from the second equation and get

$$
\left[\begin{array}{cc}
-Q-\Theta^{-1} & A^{T} \\
A & 0
\end{array}\right]\left[\begin{array}{l}
\Delta v \\
\Delta \lambda
\end{array}\right]=\left[\begin{array}{c}
\xi_{d}-V^{-1} \xi_{\mu} \\
\xi_{p}
\end{array}\right]
$$

where $\Theta=V S^{-1}$ is a diagonal scaling matrix.
$\Theta$ is always very ill-conditioned.
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## Augmented system

$$
\left[\begin{array}{cc}
-Q-\Theta^{-1} & A^{T} \\
A & 0
\end{array}\right]\left[\begin{array}{l}
\Delta v \\
\Delta \lambda
\end{array}\right]=\left[\begin{array}{l}
r \\
h
\end{array}\right]=\left[\begin{array}{c}
\xi_{d}-V^{-1} \xi_{\mu} \\
\xi_{p}
\end{array}\right] .
$$

Symmetric but indefinite linear system. In general, it may be difficult to solve.

## Separable Quadratic Programs

When matrix $Q$ is diagonal $(Q=D)$, the augmented system can be further reduced. Eliminate

$$
\Delta v=\left(D+\Theta^{-1}\right)^{-1}\left(A^{T} \Delta \lambda-r\right)
$$

to get normal equations (symmetric, positive definite system)

$$
\left(A\left(D+\Theta^{-1}\right)^{-1} A^{T}\right) \Delta \lambda=g=A\left(D+\Theta^{-1}\right)^{-1} r+h
$$

## Sparsity Issues in QP

Observation: the inverse of the sparse matrix may be dense. Example

$$
\begin{aligned}
{\left[\begin{array}{lllll}
{[ } & 1 & & \\
1 & 2 & 1 & \\
& 1 & 2 & 1 \\
& & 1 & 2 & 1 \\
& & 1 & 2
\end{array}\right]^{-1} } & =\left([ \begin{array} { l l l l l } 
{ 1 } & { } & { } & { } \\
{ 1 } & { 1 } & { } & { } \\
{ } & { } & { 1 } & { } & { } \\
{ } & { } & { 1 } & { 1 } & { } \\
{ } & { } & { 1 } & { 1 }
\end{array} ] \cdot \left[\begin{array}{llll}
1 & 1 & & \\
& 1 & 1 & \\
& 1 & 1 & \\
& & & 1 \\
\hline
\end{array}\right.\right. \\
& =\left[\begin{array}{rrrrr}
1 & -1 & 1 & -1 & 1 \\
& 1 & -1 & 1 & -1 \\
& & 1 & -1 & 1 \\
& & & 1 & -1 \\
& & & & 1
\end{array}\right] \cdot\left[\begin{array}{rrrrr}
1 & 1 \\
-1 & 1 & \\
1 & -1 & 1 & \\
-1 & 1 & -1 & 1 \\
1 & -1 & 1 & -1 & 1
\end{array}\right]=\left[\begin{array}{rrrr}
5 & -4 & 3 & -2 \\
-4 & 4 & -3 & 2 \\
3 & -3 & 3 & -2 \\
-2 & 2 & -2 & 2 \\
1 & -1 & 1 & -1
\end{array}\right.
\end{aligned}
$$

IPMs for QP:
Do not explicitly invert the matrix $Q+\Theta^{-1}$
to form $A\left(Q+\Theta^{-1}\right)^{-1} A^{T}$ unless $Q$ is diagonal.

## Interior Point Methods

Theory: IPMs converge in $\mathcal{O}(\sqrt{n})$ or $\mathcal{O}(n)$ iterations Practice: IPMs converge in $\mathcal{O}(\log n)$ iterations
... but one iteration may be expensive!
Suppose $A \in \mathcal{R}^{m \times n}$ is a dense matrix.
Major computational effort when solving separable QP (separable QP means that $Q=D$, diagonal).
build $H=A\left(Q+\Theta^{-1}\right)^{-1} A^{T} \quad \mathcal{O}\left(n m^{2}\right)$
compute Cholesky $H=L \Lambda L^{T} \quad \mathcal{O}\left(m^{3}\right)$
Recall $n \gg m$.

## Ill-conditioning of $\Theta=V S^{-1}$

For active constraints:

$$
\Theta_{j}=v_{j} / s_{j} \rightarrow 0
$$

$\Theta_{j}^{-1} \rightarrow \infty$;
For inactive constraints: $\quad \Theta_{j}=v_{j} / s_{j} \rightarrow \infty \quad \Theta_{j}^{-1} \rightarrow 0$.

Goldfarb and Scheinberg, A product form Cholesky factorization for handling dense columns in IPMs for linear programming, Mathematical Programming, 99(2004) 1-34.

Although $\tilde{\Theta}=\left(Q+\Theta^{-1}\right)^{-1}$ behaves badly, the Cholesky factorization $H=L \Lambda L^{T}$ behaves well:
$\Lambda$ captures instability (variability) of $\tilde{\Theta}$;
$L$ is well conditioned (bounded independently of $\tilde{\Theta}$ ).
Represent $L=L_{1} L_{2} \ldots L_{m}$, where $L_{i}$ has entries only in column $i$. Drawback: PFCF is sequential by nature.
Montreal, 18 June 2009

## Interior Point Methods: Summary

- Interior Point Methods for QP
- polynomial algorithms
- excellent practical behaviour
- competitive for small problems ( $\leq 1,000,000$ vars)
- beyond competition for large problems ( $\geq 1,000,000$ vars)
- Opportunities for SVM training with IPMs
- dense data
- very large size
- well-suited to parallelism


## Part 2:

## Support Vector Machine training

## Classification

We consider a set of points $X=\left\{x_{1}, x_{2}, \ldots, x_{n}\right\}, x_{i} \in \mathcal{R}^{m}$ to be classified into two subsest of "good" and "bad" ones. $X=G \cup B$ and $G \cap B=\emptyset$.

We look for a function $f: X \mapsto \mathcal{R}$ such that
$f(x) \geq 0$ if $x \in G$ and $f(x)<0$ if $x \in B$.

Usually $n \gg m$.

## Linear Classification

We consider a case when $f$ is a linear function:

$$
f(x)=w^{T} x+b
$$

where $w \in \mathcal{R}^{m}$ and $b \in \mathcal{R}$.
In other words we look for a hyperplane which separates "good" points from "bad" ones.

In such case the decision rule is given by $y=\operatorname{sgn}(f(x))$.
If $f\left(x_{i}\right) \geq 0$, then $y_{i}=+1$ and $x_{i} \in G$.
If $f\left(x_{i}\right)<0$, then $y_{i}=-1$ and $x_{i} \in B$.
We say that there is a linearly separable training sample

$$
S=\left(\left(x_{1}, y_{1}\right),\left(x_{2}, y_{2}\right), \ldots,\left(x_{n}, y_{n}\right)\right)
$$

## How does it work?

Given a linearly separable database (training sample)

$$
S=\left(\left(x_{1}, y_{1}\right),\left(x_{2}, y_{2}\right), \ldots,\left(x_{n}, y_{n}\right)\right)
$$

find a separating hyperplane

$$
w^{T} x+b=0
$$

which satisfies

$$
y_{i}\left(w^{T} x_{i}+b\right) \geq 1, \quad \forall i=1,2, \ldots, n
$$

Given a new (unclassified) point $x_{0}$, compute

$$
y_{0}=\operatorname{sgn}\left(w^{T} x_{0}+b\right)
$$

to decide whether $x_{0}$ is "good" or "bad".

## Separating Hyperplane

To guarantee a nonzero margin of separation we look for a hyperplane

$$
w^{T} x+b=0
$$

such that
$w^{T} x_{i}+b \geq 1$ for "good" points; $w^{T} x_{i}+b \leq-1$ for "bad" points.
This is equivalent to:
$\frac{w^{T} x_{i}}{\|w\|}+\frac{b}{\|w\|} \geq \frac{1}{\|w\|}$ for "good" points;
$\frac{w^{T} x_{i}}{\|w\|}+\frac{b}{\|w\|} \leq-\frac{1}{\|w\|}$ for "bad" points.
In this formualtion the normal vector of the separating hyperplane $\frac{w}{\|w\|}$ has unit length. In this case the margin between "good" and "bad" points is measured by $\frac{2}{\|w\|}$. This margin should be maximised.
This can be achieved by minimising the norm $\|w\|$.

## QP Formulation

Finding a separating hyperplane can be formulated as a quadratic programming problem:

$$
\begin{array}{cc}
\min & \frac{1}{2} w^{T} w \\
\text { s.t. } & y_{i}\left(w^{T} x_{i}+b\right) \geq 1, \quad \forall i=1,2, \ldots, n .
\end{array}
$$

In this formulation the Euclidean norm of $w$ is minimized.
This is clearly a convex optimization problem.
(We can minimize $\|w\|_{1}$ or $\|w\|_{\infty}$ and then the problem can be reformulated as an LP.)
Two major difficulties:

- Clusters may not be separable at all
$\longrightarrow$ minimize the error of misclassifications;
- Clusters may be separable by a nonlinear manifold $\longrightarrow$ find the right feature map.


## Difficult Cases

Nonseparable clusters:


Errors when defining clusters of good and bad points.
Minimize the global error of misclassifications: $\xi_{1}+\xi_{2}$.

Use nonlinear feature map:


## Linearly nonseparable case

If perfect linear separation is impossible then for each misclassified data we introduce a slack variable $\xi_{i}$ which measures the distance between the hyperplane and misclassified data.

Finding the best hyperplane can be formulated as a quadratic programming problem:

$$
\begin{array}{lcl}
\min & \frac{1}{2} w^{T} w+C \sum_{i=1}^{n} \xi_{i} & \\
\text { s.t. } & y_{i}\left(w^{T} x_{i}+b\right)+\xi_{i} \geq 1, & \forall i=1,2, \ldots, n, \\
& \xi_{i} \geq 0 & \forall i=1,2, \ldots, n,
\end{array}
$$

where $C(C>0)$ controls the penalisation for misclassifications.

We will derive the dual quadratic problem.
We associate Lagrange multipliers $z \in \mathcal{R}^{n}(z \geq 0)$ and $s \in \mathcal{R}^{n}(s \geq 0)$ with the constraints $y_{i}\left(w^{T} x_{i}+b\right)+\xi_{i} \geq 1$ and $\xi \geq 0$, and write the Lagrangian
$L(w, b, \xi, z, s)=\frac{1}{2} w^{T} w+C \sum_{i=1}^{n} \xi_{i}-\sum_{i=1}^{n} z_{i}\left(y_{i}\left(w^{T} x_{i}+b\right)+\xi_{i}-1\right)-s^{T} \xi$.

SVM community uses $\alpha$ instead of $z$.

## Dual Quadratic Problem

Stationarity conditions (with respect to all primal variables):

$$
\begin{aligned}
\nabla_{w} L(w, b, \xi, z, s) & =w-\sum_{i=1}^{n} y_{i} x_{i} z_{i}
\end{aligned}=0.0 .
$$

Substituting these equations into the Lagrangian function we get

$$
L(w, b, \xi, z, s)=\sum_{i=1}^{n} z_{i}-\frac{1}{2} \sum_{i, j=1}^{n} y_{i} y_{j}\left(x_{i}^{T} x_{j}\right) z_{i} z_{j}
$$

Hence the dual problem has the form:

$$
\begin{array}{ccl}
\max & \sum_{i=1}^{n} z_{i}-\frac{1}{2} \sum_{i, j=1}^{n} y_{i} y_{j}\left(x_{i}^{T} x_{j}\right) z_{i} z_{j} & \\
\text { s.t. } & \sum_{i=1}^{n} y_{i} z_{i}=0, & \forall i=1,2, \ldots, n, \\
& 0 \leq z_{i} \leq C, &
\end{array}
$$

SVM community uses $\alpha$ instead of $z$.

## Dual Quadratic Problem (continued)

Observe that the dual problem has a neat formulation in which only dual variables $z$ are present. (The primal variables $(w, b, \xi)$ do not appear in the dual.)

Define a dense matrix $Q \in \mathcal{R}^{n \times n}$ such that $q_{i j}=y_{i} y_{j}\left(x_{i}^{T} x_{j}\right)$.
Rewrite the (dual) quadratic program:

$$
\begin{array}{cc}
\max & e^{T} z-\frac{1}{2} z^{T} Q z \\
\text { s.t. } & y^{T} z=0 \\
& 0 \leq z \leq C e
\end{array}
$$

where $e$ is the vector of ones in $\mathcal{R}^{n}$.
The matrix $Q$ corresponds to a specific linear kernel function.
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## Dual Quadratic Problem (continued)

The primal problem is convex hence the dual problem must be well defined too. The dual problem is to maximise the concave function. We can prove it directly.

Lemma: The matrix $Q$ is positive semidefinite.
Proof: Define

$$
G=\left[y_{1} x_{1}\left|y_{2} x_{2}\right| \ldots \mid y_{n} x_{n}\right]^{T} \in \mathcal{R}^{n \times m}
$$

and observe that

$$
\left.Q=G G^{T} \quad \text { (i.e., } \quad q_{i j}=y_{i} y_{j}\left(x_{i}^{T} x_{j}\right)\right)
$$

For any $z \in \mathcal{R}^{n}$ we have

$$
z^{T} Q z=\left(z^{T} G\right)\left(G^{T} z\right)=\left\|G^{T} z\right\|^{2} \geq 0
$$

hence $Q$ is positive semidefinite.
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## Part 3:

IPMs for Support Vector Machine training

## Interior Point Methods in SVM Context

Fine and Scheinberg, Efficient SVM training using low-rank kernel representations, J. of Machine Learning Res., 2(2002) 243-264.

Ferris and Munson, Interior point methods for massive support vector machines, SIAM J. on Optimization, 13(2003) 783-804.

Woodsend and Gondzio, Exploiting separability in large-scale linear SVM training, Tech Rep MS-07-002, Edinburgh 2007. http://www.maths.ed.ac.uk/~gondzio/reports/wgSVM.html

Unified framework which includes:

- Classification ( $\ell_{1}$ and $\ell_{2}$ error)
- Universum SVM
- Ordinal Regression
- Regression

Reformulate QPs as separable.
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## IPMs for SVMs: Exploit separability

Key trick: represent $Q=F^{T} D F$, where $F \in \mathcal{R}^{k \times n}, k \ll n$. Introduce new variable $u=F z$.
Observe: $z^{T} Q z=z^{T} F^{T} D F z=u^{T} D u$.

$$
\begin{array}{cc}
\min & c^{T} z+\frac{1}{2} z^{T} Q z \\
\text { s.t. } & A z=b, \\
& z \geq 0 .
\end{array}
$$

$$
\begin{array}{cc}
\min & c^{T} z+\frac{1}{2} u^{T} D u \\
\text { s.t. } & A z=b, \\
& F z-u=0, \\
& z \geq 0 .
\end{array}
$$

non-separable QP
$m$ constraints
$n$ variables
separable QP
$m+k$ constraints
$n+k$ variables

Comparison: SVM-HOPDM vs other algorithms Data with 255 attributes. $C=1,10 \%$ misclassified.


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Comparison: SVM-HOPDM vs other algorithms
Data with 255 attributes. $C=100,10 \%$ misclassified.


Comparison: of training times using real-world data sets.
Each data set was trained using $C=1,10$ and 100 .
NC indicates that the method did not converge to a solution.

| $\begin{array}{\|ll} \hline \begin{array}{l} \text { Data set } \\ (n \times m) \end{array} & C \\ \hline \end{array}$ | $\begin{gathered} \text { SVM- } \\ \text { HOPDM } \end{gathered}$ | SVM ${ }^{\text {Iight }}$ | SVM ${ }^{\text {perf }}$ | $\begin{array}{r} \hline \text { LIB- } \\ \text { INEAR } \\ \hline \end{array}$ | LibSVM | SVMTorch | SVM-QP | $\begin{aligned} & \hline \hline \begin{array}{l} \text { SVM-Q } \\ \text { presolv } \end{array} \end{aligned}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Adult | 16.5 | 87.7 | 280.7 | 1.6 | 192.4 | 621.8 | 164.5 | 188. |
| $32561 \times 123 \quad 10$ | 26.5 | 1043.3 | 3628.0 | 9.3 | 857.7 | 5046.0 | 284.1 | 206. |
| 100 | 27.9 | 10447.4 | 29147.2 | 64.2 | 5572.1 | 44962.5 | 544.8 | 216 |
| Covtype 1 | 47.7 | 992.4 | 795.6 | 8.5 | 2085.8 | 2187.9 | 731.8 | 405 |
| $150000 \times 5410$ | 52.7 | 6021.2 | 12274.5 | 34.3 | 2516.7 | 10880.6 | 971.6 | 441. |
| 100 | 55.4 | 66263.8 | 58699.8 | 235.2 | 6588.0 | 74418.1 | 1581.8 | 457 |
| MNIST 1 | 79.6 | 262.9 | 754.1 | 9.3 | 197.1 | 660.1 | 233.0 | 1019 |
| $10000 \times 780 \quad 10$ | 83.4 | 3425.5 | 8286.8 | 65.4 | 1275.2 | 5748.1 | 349.4 | 110 |
| 100 | 86.2 | NC | 196789.0 | NC | 11456.4 | 54360.6 | 602.5 | 1267 |
| SensIT 1 | 55.2 | 913.5 | 8418.3 | 53.6 | 2542.0 | 2814.4 | 535.2 | 456 |
| $78823 \times 100 \quad 10$ | 60.1 | 7797.4 | $>125000$ | 369.1 | 7867.8 | 21127.8 | 875.4 | 470. |
| 100 | 63.6 | NC | $>125000$ | NC | 49293.7 | 204642.6 | 1650.1 | 489 |
| USPS | 13.2 | 15.0 | 40.9 | 4.4 | 10.4 | 7.7 | 51.2 | 117 |
| $7291 \times 256 \quad 10$ | 14.2 | 147.4 | 346.6 | 27.7 | 20.9 | 23.9 | 64.7 | 127. |
| 100 | 14.3 | 1345.2 | 2079.5 | NC | 93.8 | 142.4 | 86.9 | 143 |

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Computational effort of IPM-based SVM implementation:
build $H=A\left(Q+\Theta^{-1}\right)^{-1} A^{T} \quad \mathcal{O}\left(n m^{2}\right)$
compute Cholesky $H=L \Lambda L^{T} \quad \mathcal{O}\left(m^{3}\right)$

## Attempts to reduce this effort

Gertz and Griffin, SVM classifiers for large datasets, Tech Rep ANL/MCS-TM-289, Argonne National Lab, 2005.
$\longrightarrow$ use iterative method (preconditioned conjugate gradient).
Jung, O'Leary and Tits, Adaptive constraint reduction for training SVMs, Electronic Trans on Num Analysis 31(2008) 156-177.
$\longrightarrow$ use a subset of points $n_{1} \ll n$ mimic "active-set" strategy within IPM.

## Parallelism

Exploit bordered block-diagonal structure in augm. system Break $H$ into blocks:

$$
H=\left[\begin{array}{ccccc}
H_{1} & & & & A_{1}^{T} \\
& H_{2} & & & A_{2}^{T} \\
& & \ddots & & \vdots \\
& & & H_{p} & A_{p}^{T} \\
A_{1} & A_{2} & \ldots & A_{p} & 0
\end{array}\right],
$$

and decompose

$$
H=\left[\begin{array}{cccc}
L_{1} & & & \\
& \ddots & & \\
& & L_{p} & \\
L_{A_{1}} & \ldots & L_{A_{p}} & L_{0}
\end{array}\right]\left[\begin{array}{ccccc}
\Lambda_{1} & & & & \\
& \ddots & & \\
& & \Lambda_{p} & \\
& & & \Lambda_{0}
\end{array}\right]\left[\begin{array}{cccc}
L_{1}^{T} & & & L_{A_{1}}^{T} \\
& \cdots & & \vdots \\
& & L_{p}^{T} & L_{A_{p}}^{T} \\
& & & \\
& & & \\
0
\end{array}\right]
$$

## Parallelism (continued)

- Cholesky factor preserves block-structure:

$$
\begin{aligned}
H_{i} & =L_{i} \Lambda_{i} L_{i}^{T}, \quad L_{i}=I, \Lambda_{i}=H_{i}, \quad i=1 . . p \\
L_{A_{i}} & =A_{i} L_{i}^{-T} \Lambda_{i}^{-1}=A_{i} H_{i}^{-1}, \quad i=1 . . p \\
H_{0} & =-\sum_{i=1}^{p} A_{i} H_{i}^{-1} A_{i}^{T}=L_{0} \Lambda_{0} L_{0}^{T}
\end{aligned}
$$

- And the system $H\left[\begin{array}{l}\Delta v \\ \Delta \lambda\end{array}\right]=\left[\begin{array}{l}r \\ h\end{array}\right]$ is solved by

$$
\begin{aligned}
t_{i} & =L_{i}^{-1} r_{i}, i=1 . . p \\
t_{0} & =L_{0}^{-1}\left(h-\sum L_{A_{i}} t_{i}\right) \\
q_{i} & =\Lambda_{i}^{-1} t_{i}, i=0 . . p \\
\Delta \lambda & =L_{0}^{-T} q_{0} \\
\Delta v_{i} & =L_{i}^{-T}\left(q_{i}-L_{A_{i}}^{T} \Delta \lambda\right), \quad i=1 . . p
\end{aligned}
$$

- Operations (Cholesky, Solve, Product) performed on sub-blocks

Comparison: Parallel software

## PASCAL Large Scale Learning Challenge

http://largescale.first.fraunhofer.de/about/

| Data set | $n$ | $m$ |
| :--- | ---: | ---: |
| Alpha | 500000 | 500 |
| Beta | 500000 | 500 |
| Gamma | 500000 | 500 |
| Delta | 500000 | 500 |
| Espilon | 500000 | 2000 |
| Zeta | 500000 | 2000 |
| FD | 2560000 | 900 |
| OCR | 3500000 | 1156 |
| DNA | 6000000 | 800 |

OOPS Object-Oriented Parallel Solver http://www.maths.ed.ac.uk/~gondzio/parallel/solver.html

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| Dataset | \# cores | C | OOPS | PGPDT | PSVM | Milde |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Alpha | 16 | 1 | 39 | 3673 | 1684 | (80611) |
|  |  | 0.01 | 50 | 4269 | 4824 | (85120) |
| Beta | 16 | 1 | 120 | 5003 | 2390 | (83407) |
|  |  | 0.01 | 48 | 4738 | 4816 | (84194) |
| Gamma | 16 | 1 | 44 |  | 1685 | (83715) |
|  |  | 0.01 | 49 | 7915 | 4801 | (84445) |
| Delta | 16 |  | 40 |  | 1116 | (57631) |
|  |  | 0.01 | 46 | 9492 | 4865 | (84421) |
| Epsilon | 32 | 1 | 730 | - | 17436 | (58488) |
|  |  | 0.01 | 293 | - | 36319 | (56984) |
| Zeta | 32 | 1 | 544 | - | 14368 | (22814) |
|  |  | 0.01 | 297 | - | 37283 | (68059) |
| FD | 32 | 1 | 3199 | - |  | (39227) |
|  |  | 0.01 | 2152 | - |  | (52408) |
| OCR | 32 | 1 | 1361 | - |  | (58307) |
|  |  | 0.01 | 1330 | - | - | (36523) |
| DNA | 48 | 1 | 2668 | - |  |  |
|  |  | 0.01 | 6557 | - | - | 14821 |

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| Dataset C |  | OOPS |  |  | LibLinear |  | LaRank |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  | $n$ | \# cores | Time |  | Time |  | Time |
| Alpha | 0.01 | 500,000 | 16 | 39 | 500,000 | 147 | 500,000 | 3354 |
| Beta |  | 500,000 | 16 | 50 | 500,000 | 112 |  | 2474 |
| Beta | $\stackrel{1}{0.01}$ | 500,000 | 16 | 18 | 500,000 | 112 | 5 | 1880 |
| Gamma | ${ }_{0}^{1}$ | 500,000 | 16 | 44 | 500,000 | (8845) | 500,000 |  |
|  | 0.01 |  |  | 49 |  | 348 | 20318 |  |
| Delta | $1$ | 500,000 | 16 | 40 | 500,000 | 13266 | 500,000 | - |
| Epsilon |  | 500,000 | 32 | 46 730 | 250,000 | 429 | 500,000 |  |
|  | 0.01 | 50,000 |  | 293 | 250,000 | 265 |  | $\begin{aligned} & 5599 \\ & 2410 \\ & \hline \end{aligned}$ |
| Zeta | ${ }_{0}^{1} 01$ | 500,000 | 32 | $\begin{aligned} & 544 \\ & 297 \end{aligned}$ | 250,000 | $\begin{aligned} & 278 \\ & 248 \end{aligned}$ | 500,000 | - |
| FD |  | 2,560,000 | 32 | 3199 | 500,000 | $231$ | 500,000 | $\begin{array}{r} 1537 \\ 332 \end{array}$ |
| OCR |  | 3,500,000 | 32 | 1361 | 250,000 | 181 | 500,000 | $\begin{aligned} & 5695 \\ & 4266 \end{aligned}$ |
|  | 0.01 |  |  | 1330 |  | 121 |  |  |
| DNA |  | 6,000,000 | 48 | 2668 | 600,000 | 144 | $600,000$ | $\begin{aligned} & 300 \\ & 407 \end{aligned}$ |
|  | 0.01 |  |  | 6557 |  | 30 |  |  |

Accuracy measured using area under precision recall curve.
Evaluation results taken from PASCAL Challenge website.

| Dataset | OOPS | LibLinear | LaRank |
| :--- | :--- | :--- | :--- |
| Alpha | $\mathbf{0 . 1 3 4 5}$ | 0.1601 | 0.1606 |
| Beta | $\mathbf{0 . 4 9 8 8}$ | $\mathbf{0 . 4 9 8 8}$ | 0.5001 |
| Gamma | $\mathbf{0 . 1 1 7 4}$ | 0.1185 | 0.1187 |
| Delta | $\mathbf{0 . 1 3 4 4}$ | 0.1346 | 0.1355 |
| Epsilon | $\mathbf{0 . 0 3 4 1}$ | 0.4935 | 0.4913 |
| Zeta | $\mathbf{0 . 0 1 1 5}$ | 0.4931 | 0.4875 |
| FD | $\mathbf{0 . 2 2 7 4}$ | 0.2654 | 0.3081 |
| OCR | $\mathbf{0 . 1 5 9 5}$ | 0.1660 | 0.1681 |

## Nonlinear and/or Indefinite Kernels:

A kernel is a function $K$, such that for all $x_{i}, x_{j} \in X$

$$
K\left(x_{i}, x_{j}\right)=\left\langle\phi\left(x_{i}\right), \phi\left(x_{j}\right)\right\rangle,
$$

where $\phi$ is a mapping from $X$ to an (inner product) feature space $F$. We use $\langle.,$.$\rangle to denote a scalar product.$
Linear Kernel $K\left(x_{i}, x_{j}\right)=x_{i}^{T} x_{j}$.
Polynomial Kernel $\quad K\left(x_{i}, x_{j}\right)=\left(x_{i}^{T} x_{j}+1\right)^{d}$.
Gaussian Kernel $K\left(x_{i}, x_{j}\right)=e^{-\frac{\left\|x_{i}-x_{j}\right\|^{2}}{\sigma^{2}}}$.

## Nonlinear and/or Indefinite Kernels:

Kernels are in general dense matrices making large-scale SVM training computationally demanding (or impossible).

Challenge: How to approximate kernels?
Find $\tilde{Q}$ with "desirable" properties such that

$$
\text { distance }(Q, \tilde{Q})
$$

is minimized. The distance may be measured with a matrix norm (say, Frobenius) or a Bregman divergence.

Dhillon and Tropp, Matrix nearness problems with Bregman divergences, SIAM J. on Matrix An. \&́ Appl., 29(2007) 1120-1146.
Lanckriet, Cristianini, Bartlett, Ghaoui and Jordan, Learning the kernel matrix with semidefinite programming, Journal of Machine Learning Research 5 (2004), 27-72.

## IPM perspective: nonlinear/indefinite Kernels:

 Approximate kernel matrix $Q, Q_{i j}=K\left(x_{i}, x_{j}\right)$ using low rank outer product$$
Q \approx L \Lambda L^{T}+D
$$

where $L \in \mathcal{R}^{n \times k}, k \ll n$.

## Exploit separability within IPMs

 Augmented system becomes:

## Conclusions:

## Interior Point Methods

$\rightarrow$ are well-suited to large scale optimization

Support Vector Machine training
$\rightarrow$ requires a solution of very large optimization problem

IPMs provide an attractive approach to solve SVM training problems

## Thank you for your attention!

## Woodsend and Gondzio,

Exploiting separability in large-scale linear SVM training, Tech Rep MS-07-002, Edinburgh 2007. http://www.maths.ed.ac.uk/~gondzio/reports/wgSVM.html

## Woodsend and Gondzio,

 Hybrid MPI/OpenMP parallel linear SVM training, Tech Rep ERGO-09-001, Edinburgh, 2009.http://www.maths.ed.ac.uk/~gondzio/reports/wgHybridSVM.html
Montreal, 18 June 2009

