

## Who can solve this system of equations?



## Before going any further, just a word about the terminology and concepts <br> Previous example can be looked at as solving an optimization problem

$$
\min _{x} J=\frac{1}{2}\left[\begin{array}{ll}
x_{1} & x_{2}
\end{array}\right]\left[\begin{array}{cc}
4 & -1 \\
-1 & 4
\end{array}\right]\left[\begin{array}{l}
x_{1} \\
x_{2}
\end{array}\right]-\left[\begin{array}{ll}
5 & -5
\end{array}\right]\left[\begin{array}{l}
x_{1} \\
x_{2}
\end{array}\right], \text { s.t. } \quad x_{i} \geq 0, \quad i=1,2
$$

taking the derivative of $J, \mathbf{g}=\partial \mathbf{J} / \partial \mathbf{x}$, one obtains the gradient $\mathbf{g}$

$$
\mathbf{g}=\left[\begin{array}{cc}
4 & -1 \\
-1 & 4
\end{array}\right]\left[\begin{array}{l}
x_{1} \\
x_{2}
\end{array}\right]-\left[\begin{array}{c}
5 \\
-5
\end{array}\right], \text { or } g_{1}=4 x_{1}-x_{2}-5, g_{2}=-x_{1}+4 x_{2}+5
$$

The above is same as solving a system of equations

$$
\begin{aligned}
& 4 x_{1}-x_{2}=5 \\
& -x_{1}+4 x_{2}=-5, \quad \text { s.t. } \quad x_{i} \geq 0, \quad i=1,2
\end{aligned}
$$

For which the errors in solutions can be expressed as

$$
e_{1}=5-4 x_{1}+x_{2}, \quad e_{2}=-5+x_{1}-4 x_{2}
$$



Imagine now that your problem is posed as

$$
\begin{array}{lcc}
2 x_{1}-1.2 x_{2}+\cdots-1.5 x_{999,999}+1.1 x_{1,000,000}=1 \\
\vdots & \vdots & \vdots \\
1.1 x_{1}+1.9 x_{2}-\cdots+1.2 x_{999,999}+2 x_{1,000,000}=1 \\
\text { s.t. } & x_{i} \geq 0, & i=1,2,3, \cdots, 1,000,000
\end{array}
$$

This kind of tasks is what VCU's
Learning Algorithms and Applications Laboratory (LAAL) is trying to solve with both decent accuracy and decent CPU time

## Motivations for this work

## Solve $\mathbf{A x}=\mathbf{b}$ for $\mathbf{x}$

- No direct solution for either small/medium linear systems with constraints or the huge ones either with or without constraints.
- Such problems arise in modern machine learning (ML) i.e., data mining (DM) with millions of records as well as in almost all the other areas of modern science and engineering.

Definition of HUGE linear systems:
Huge $=$ when system matrix A can't be stored and operated with / on / in a computer memory

> Remark
> In both cases mentioned, direct calculations of $\mathbf{x}$ (either by Gaussian elimination, or by inversion, or by LU, QR, Cholesky i.e., by any other factorization) are not feasible/possible and we must resort to the iterative solutions!

## One more remark

ML is not the first scientific field facing humongous number of equations Many other areas have been doing it for decades e.g., Solving PDEs.

- What is so particular about (L1 and L2) SVM models?
$-1^{\text {st }}$ system of equation is not sparse. In fact, it is always extremely dense. It often has a system matrix with a high condition number, say $>10^{8}$ i.e., system is very ill-conditioned
$2^{\text {nd }}$ system matrix is both symmetric \& positive definite $3^{\text {rd }}$
- for L1 SVMs, constraints are usually box constraints accompanied by 1 only equality constraint
- for L2 SVMs, constraints are just nonnegative ones.

In both cases, constraints make solution x to be sparse

- The last three facts are very different in respect to the classic huge linear system of equations originating from PDE solving
- They exclude all the conclusions about what iterative method is possibly the best
- One of the basic advices was that the Conjugate-Gradient method is The Tool It is not for our very dense systems!!!

Hence, we have to invent something better, more suitable, for the new problem setting.

Welcome to the Good Old Iterative Methods Ready for Renewal

- Jacobi
- Gauss-Seidel
- Successive Over Relaxation
- Steepest Descent
- Conjugate gradient
- Active-Set Approaches
- etc, ...

For a dense, symmetric positive definite (SPD), systems we have shown that actually only Gauss-Seidel and its SOR can be efficient

- Jacobi -
- Gauss-Seidel
- Successive Over Relaxation
- Steopest Descent
- Conjugate gradient
- Active-Set Approaches

As for the strikings shown, see the papers from Zigic-Kecman in 2013 \& 2014

## SVMs \& Linear System of Equations

For L1-SVM, learning means solving the QP problem below
$\underset{\alpha}{\arg \min } L_{d}=\frac{1}{2} \sum_{i, j=1}^{n} y_{i} y_{j} \alpha_{i} \alpha_{j} K\left(\mathbf{x}_{i}, \mathbf{x}_{j}\right)-\sum_{i=1}^{n} \alpha_{i}$
s.t. $C \geq \alpha_{i} \geq 0, \quad i=1, n \quad n$ inequality constraints
$\sum_{i}^{n} \alpha_{i} y_{i}=0 \quad 1$ only equality constraint
${ }^{\circ} \mathrm{C} \geq \alpha_{i} \geq 0$. These are known as the BOX constraints.
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## Iterative Single Data Algorithm ISDA

- Between 2002 and 2005 I have, jointly with then PhD students and Drs. Huang and Vogt today, developed ISDA algorithm. We have shown that ISDA is actually equal to
- 1 - SMO* without bias term,
- 2 - Kernel AdaTron algorithm
'smo $=$ Sequential minimal opimization and that all the three approaches are actually Gauss-Seidel methods for solving linear systems of equations under the given SVMs' constraints.
*SMO, developed by Dr. Platt at Microsoft Research, is the world most used (i.e., the working horse) algorithm for training SVMs


## ISDA

- ISDA is quite The Algorithm, competing with and (often) beating the best methods for training SVMs.
- This is why in its newest releases in 2014 MATLAB has (out of few dozens SVM algorithms proposed) implemented our ISDA (together with SMO) as the default algorithm for training large SVMs.

Check fitcsvm.m at Mathworks (MATLAB)

Fine, but if my students and I had already invented it, developed it and implemented it what is this seminar then about?

- Well, it's about what comes in next 34 slides.
- In essence, the story is as follows:

Zigic, Strack, and Kecman have invented and recently proposed a novel DL2 SVM model for very large ML tasks which literally cries for an even more efficient training algorithm than ISDA

- While searching for it, l've got some new insights which I want to share with you today ${ }_{1653}$

The novel SVM model dubbed Direct L2 SVM Algorithm (DL2 SVM) boiles down to solving this problem:

$$
\mathrm{Hx}=1 \quad \text { subject to } x_{i} \geq 0, i=1, \ldots, n
$$

and, this is a very well known
NONNEGATIVE (least squares) PROBLEM
See papers from Zigic-Kecman in 2013 \& 2014

How to solve a system of linear
equations having muuuuuuge
symmetric positive definite matrix H and (possibly) some constraints
???

Well, let's go back to the


Good Old Gauss-Seidel iterative method for solving a system of linear equations having the SPD matrix H $\mathrm{Hx}=\mathrm{b}$
$h_{11} x_{1}+h_{12} x_{2}+h_{13} x_{3}+\ldots+h_{1 n} x_{n}=b_{1}$
$h_{21} x_{1}+h_{22} x_{2}+h_{23} x_{3}+\ldots+h_{2 n} x_{n}=b_{2}$ $\vdots$
$h_{n 1} x_{1}+h_{n 2} x_{2}+h_{n 3} x_{3}+\ldots+h_{n n} x_{n}=b_{n}$

See the rewritten $i$-th equation $f_{i}$ and it's derivative $\partial f_{i} / \partial x_{i}$ below - we'll need it soon $f_{i}=h_{i 1} x_{1}+h_{i 2} x_{2}+\ldots+h_{i i} x_{i}+\ldots+h_{i n} x_{n}-b_{i}=0, \quad \frac{\partial f_{i}}{\partial x_{i}}=h_{i i}$

## Gauss-Seidel

Start with any $\mathbf{x}=\left[\begin{array}{llllll}x_{1} & x_{2} & x_{3} & \ldots & x_{n-1} & x_{n}\end{array}\right]^{t}$. Usually, $\mathbf{x}=\mathbf{0}$ !

$$
\begin{aligned}
& x_{1}=\frac{b_{1}-h_{12} x_{2}-h_{13} x_{3} \ldots \ldots-h_{1 n} x_{n}}{h_{11}} \leftarrow \begin{array}{r}
\text { Repeat until } \\
\text { stopping } \\
\text { criterion is } \\
\text { satisfied }
\end{array} \\
& x_{2}=\frac{b_{2}-h_{21} x_{1}-h_{23} x_{3} \ldots \ldots-h_{2 n} x_{n}}{h_{22}} \vdots \\
& \vdots \\
& x_{n-1}=\frac{b_{n-1}-h_{n-1,1} x_{1}-h_{n-1,2} x_{2} \ldots \ldots-h_{n-1, n-2} x_{n-2}-h_{n-1, n} x_{n}}{h_{n-1, n-1}} \\
& x_{n}=\frac{b_{n}-h_{n 1} x_{1}-h_{n 2} x_{2}-\ldots \ldots-h_{n, n-1} x_{n-1}}{h_{n n}}
\end{aligned}
$$

## Gauss-Seidel

Let's rewrite the last equation as


## Newton-Raphson

Fine, but how are the G-S \& N-R methods related?
In order to find the roots of some $f(x)$, or for what value of $x$ the function $f(x)$ will equal zero, Newton-Raphson method proposes the iterative scheme below

$$
x=x-\frac{f(x)}{f^{\prime}(x)}
$$



In our case $f(x)=g=H x-b$ and $f=H$, and when working with matrices division is a multiplication by an inverse. With this in mind, the last equation becomes

$$
x=x-H^{-1}(H x-b)=x-H^{-1} g
$$

Writing the equation above component-wise one would get the expressions on previous slide.

Gauss-Seidel's \& Newton-Raphson's geometries when optimizing along a single coordinate


Well, comparing slides 25 \& 26 one can say that Newton-Raphson method, even without knowing it, was used for iterative solving of linear system of equations hidden in the Gauss-Seidel method! It seems nobody has taken to much care about it?!
The reason for such a "neglect" is due to the fact that Newton, i.e. Newton-Raphson, method is tied with the root finding in (a system of) NL equation(s) so deeply and strongly up
that some books on linear algebra don't mention Newton-Raphson method whatsoever e.g., the book from
R. Varga (on Matrix iterative methods), B. Noble, J. Dieudonne, S. Roman, K. Kuttler, ..., and many other books

QQ I can't believe it

## Gauss-Seidel \& Newton-Raphson

Let's show it analytically too!


## Gauss-Seidel \& Newton-Raphson

G-S procedure must not update the variables in a cyclic order (starting with the $1^{\text {st }}$ eq., ending with the last one and repeating those sweeps).

A more efficient way is to update the variable having the largest absolute value of a gradient vector. This corresponds to selecting the variable with the biggest absolute error.

In ML this variable is called the worst violator. Such a choice ensures the fastest convergence to the minimum value of the (hyper)quadrics J .


## Gauss-Seidel \& Newton-Raphson

The key proposal of the seminar is an Expansion of G-S i.e., N-R, over The Subspace Spanned by $k$ Worst Violators

Remind, in each iteration step G-S updates 1 variable only!
Idea, why don't we choose 2 worst violators/errors, or 3, or more, say $k$, and update them in a single $N-R$ step?

In other words - why not to perform the updates as given on the slide 26 but written for $k$ coordinates below

$$
x_{k}=x_{k}-H_{k}^{-1} g_{k}
$$

Index $k$ denotes that $k$ worst violating variables are being updated In a geometric sense, we are finding the $k$ optimal values of $x$ defining the minimum of the elliptic paraboloid over a $k$
dimensional subspace spanned by the $k$ worst violators. $\quad 30153$

## Gauss-Seidel \& Newton-Raphson

The difference between G-S and $\mathbf{N}-\mathbf{R}$ for $k=2$ can be readily seen in the figure below.


## Gauss-Seidel \& Newton-Raphson

$H$ is SPD matrix and the solution must be same for any $k$ we choose, meaning accuracy must be 'equal' for any chosen $k$.

Hence, the basic issue when using $k$ violators is the speed or, the CPU time needed to find the solution.
Well, there is a tradeoff here:
An increase in $k$ reduces the number of sweeps through the datasets but the calculations are more complex because:
first, instead of finding a single worst violator with a cost of $\mathrm{O}\{n\}$, we have to find $k$ of them. This costs $k O\{n\}$ and,
second, in each Newton-Raphson iteration step we must solve a system of $k$ equations which costs $\sim O\left\{k^{3}\right\}$.
At the moment we have only experimental answers which support using more violators. How many, hard to tell right now, or, $k=$ ?
Novel Iterative Algorithm for Solving SPD System of Linear Equations - Pseudocode
$\mathrm{x}=0$ (put, any other good guess helps too )
$\mathrm{g}=-\mathrm{b} \quad(\mathrm{f} \mathrm{x} \neq 0, \mathrm{~g}=\mathrm{Hx}-\mathrm{b}) \quad \mathrm{x}_{\text {old }}=\mathrm{x}, \quad$ err $=1$
stopping $=0.001$ (or, use other metrics here )
while err > stopping
find indices vector I of $k$ worst violators in $\mathrm{g} \quad \begin{aligned} & \text { Selection of a } k \text {-dim subspace }\end{aligned}$ calculate $\mathrm{H}_{k}(\mathbb{I})$ and $\mathrm{g}_{k}()$
$\left.\mathbf{x}_{k} \mathbf{l}\right)=\mathbf{x}_{k}()-\mathrm{H}_{k}^{-1} \mathbf{g}_{k} \longrightarrow$ Only $k$ components of vector ensure $x_{k}$ )satisfies given constraints

err $=\frac{\left\|\mathbf{x}-\mathbf{x}_{\text {old }}\right\|}{\|\mathbf{x}\|}$ or, any other suitable metrics ) columns of H given by I is updated.
$\mathbf{X}_{\text {old }}=\mathbf{X}$
end
$\mathrm{g}=\mathrm{r}$ (residual, error) in a classic numerical algebra literature! 34/53

## Remark on the Successive Over-Relaxation (SOR)

- I am sure that the proposed model must also work with the SOR, which is given below. (However, I didn't check it and this claim asks for some investigations).

$$
x_{k}=x_{k}-\omega H_{k}^{-1} g_{k}=x_{k}-\omega \Delta x
$$

As always, the tricky part will be to pick up a correct value for $\omega$ !
and, because $\mathrm{H}_{k}$ is an SPD matrix,
$\Delta x$ can be found quicker by using Cholesky decomposition. This may bring a 'significant' CPU time speedup (up to 3 times).

Replacing the Calculation of an Inverse of a Matrix $\mathbf{H}_{k}$ Note that the update step

$$
\mathbf{x}(\mathbf{I})=\mathbf{x}(\mathrm{I})-\mathbf{H}_{k}^{-1} \mathbf{g}_{k}
$$

can also be rewritten as

$$
\mathbf{x}(\mathrm{I})=\mathbf{x}(\mathrm{I})-\Delta \mathbf{x}
$$

where $\Delta x$ is a solution of the equation

$$
\mathbf{H}_{k} \Delta \mathbf{x}=\mathbf{g}_{k}
$$

Remark on the number of violators $k$ used

My, the very first and thus the wildest, guess is to pickup $k$ according to the memory size.

Use the highest possible $k$ which still enables both the storing of the ( $k, k$ ) matrix $\mathbf{H}_{k}$ and the calculation of the updates by performing $\mathbf{H}_{k}^{-1} \mathbf{g}_{k}$ within the memory .

## Let's Christen The Algorithm

There is a good habit in both all times and all civilizations which goes as: soon after a baby's born give him/her the name

Being The Very Humble Person I'll name the approach proposed just Recman Algorithom


## Let's Position the Proposed Method i.e., Let's Compare It with Other Algorithms

Well, depending upon $k$, it is somewhere
in between Gauss-Seidel and an exact, one step, solution with the fleur of Newton-Raphson, and a scent of a Block G-S $\square$ meaning For
$k=1, \quad$ it's a pure Gauss-Seidel Method
$k=n, \quad$ it's a pure $N-R$ having a, one step, exact solution which is, however, prohibitive when dealing with huge matrices H. $x=x-H^{-1}(H x-b)=H^{-1} b$
$1<k<n$, the proposed method is original, working in a $\boldsymbol{k}$-dimensional subspace of $\boldsymbol{k}$ worst violators, finding there a local $\mathbf{x}_{k-o p t}$ in a single step, and iteratively approaching the global optimal solution $\mathbf{x}_{o p t}$. $39 / 53$

## The Proposed Algorithm Falls Into the Category of Projection Methods such as

- Galerkin, Kaczmarz, Cimmino, G-S, Block G-S Richardson, Southwell (these are different methods, but sometimes 'equal', i.e., similar, too) - Conjugate Gradient i.e Krylov Subspace Methods
- ABS (named after Abaffy, Broyden and Spedicato), Row projection methods, Steepest Descent
Block G-S is different because it works with predetermined blocks \& it is cyclic => block G-S algorithm is entirely different (but similar in the spirit). For its cyclic nature, I expect it to be much slower too. Note also that block G-S (usually) assumes knowing the whole matrix $\mathbf{H}$

If interested, check Brezinski's book, "Projection Methods for Systems of Equations" North-Holland, 1997 \& Hackbusch's, Iterative Solution of Large Sparse Systems of Equations, Springer, 199440/53

## Experimental Results

are finally in order - for linear systems without constraints (the solution vector $\mathrm{X}_{\text {opt }}$ is dense) and for different both
sizes
from $n=100$ to $n=10,000$

## \&

condition numbers
from $\sim 2$ to $10^{8}$

Gauss-Seidel \& Newton-Raphson i.e., the Proposed Method in $k$-dimensional subspace of $k$ worst violators (coordinates)

Some experimental runs

$$
n=100
$$






Gauss-Seidel \& Newton-Raphson i.e., the Proposed Method in $k$-dimensional subspace of $k$ worst violators (coordinates)

Some experimental runs

$$
n=4,000
$$



Gauss-Seidel \& Newton-Raphson i.e., the Proposed Method in $k$-dimensional subspace of $k$ worst violators (coordinates)

Some experimental runs. Note, here we have $k=.25$ too

$$
n=5,000
$$



## Gauss-Seidel \& Newton-Raphson i.e., the Proposed Method in $k$-dimensional subspace of $k$ worst violators (coordinates)

Some experimental runs

$$
n=10,000
$$



## Basic Remarks and Comments

1) Solving LARGE systems is possible only with iterative algorithms
2) All the results shown are WITHOUT CONSTRAINTS, hence, no sparseness in a solution vector $\mathbf{x}$ whatsoever
3) Results may be different for SVM tasks or, when solving any other linear system of equations with constraints
4) It is highly recommended to use more violators. Value of $\boldsymbol{k}$ is ???
5) The bigger the system, the higher the speed up
6) The proposed method using $\boldsymbol{k}$ worst violators, is the strongest candidate method for HUGE SVM classification tasks, i.e. HUGE linear system of equations with nonnegativity, and other, constraints
7) Whether the last claim is true is under an investigation for DL2 SVMs by LAAL's PhD student Ljiljana Zigic
8) Warning - implementation of a proposed method when having constraints is a particularly challenging research task because

There Is No King's Way to Algorithms Implementations Eithewis3

## Basic Remarks and Comments

9) I didn't check it, but I believe that the algorithm on slide 35 converges whenever the G-S does. Hence, the question whether a symmetry and positive definiteness is required for a proposed method should be investigated in more details
10) Sure, the proposed algorithm shown here for a linear system can also (but, for issues of convergence, with a lot of caution) be applied for a system of nonlinear equations as follows:
do the Gauss-Newton algorithm along the lines of the pseudocode for the proposed method on the slide 35, meaning don't build Jacobian for all F(x). Go in chunks of $k$. It may be faster, but be aware that the proposed method converges because our linear system is a symmetric positive definite one
With nonlinear systems there will be many additional issues and convergence is generally not quite guaranteed! 5153

## Wait, wait, wait

This is not the end of the story yet !!!
This was just what I was doing lately. Vojo's stuff! So, forget it !
The Very Big and The True Story of The Day Is

- each of you is facing some problem you have to solve
- look at it, see what is in the very root of your problem
- find out was there anybody else who was facing it, or who was doing similar stuff (remind, this is a heavy digging)
If there is nobody, check it twice. After checking it $2^{\text {nd }}$ time, check it one more time (l mean, check it indeed) just to be sure. (As for me, I believe, your problem, possibly disguised, has already been solved).
If, after all the thorough checking, there was nobody who was entertaining your problem, think about your problem again
- Is it right?
- Is it properly posed
- Is it novel?
» Is your advisor 'pleased' about your PhD topic?
If All the Answers are Positive You Are at the Blessed Spot!
The Whole Big World is Waiting for Your Solutions and The Fame Is in Front of You!!!


