Systematic Generation of Algorithms for Iterative Methods

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Introduction: The FLAME Project

- FLAME: Formal Linear Algebra Methods Environment.
- Goal: Automatic development of linear algebra libraries.
  - Automatic generation of algorithms (direct methods).

My thesis:

- Iterative methods.
- Preliminary results by Eijkhout et al., 2010.

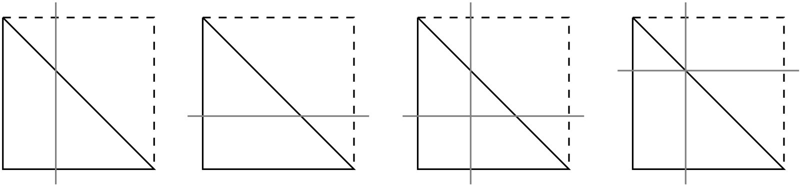
PME Generation: Input

Operation: Lower triangular linear system.

$$x := \Phi(A, b) \equiv \begin{cases} P_{\text{pre}} : \{\texttt{Input}[A] \wedge \texttt{Matrix}[A] \wedge \\ \qquad \texttt{NonSingular}[A] \wedge \\ \qquad \texttt{LowerTriangular}[A] \wedge \\ \qquad \texttt{Input}[b] \wedge \texttt{Vector}[b] \wedge \\ \qquad \texttt{Output}[x] \wedge \texttt{Vector}[x]\} \\ P_{\text{post}} : \{Ax = b\} \end{cases}$$

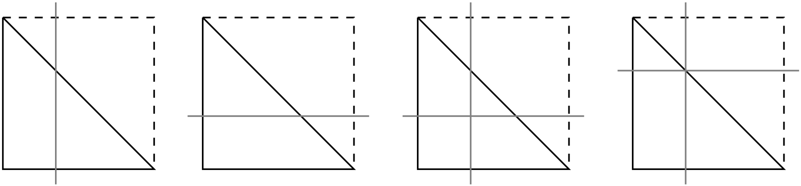
PME Generation: Initial Partitioning

$$P_{\text{post}} : \{Ax = b\}$$



PME Generation: Initial Partitioning

$$P_{\text{post}} : \{Ax = b\}$$



$$\left(\begin{array}{c|c} A_{TL} & 0 \\ \hline A_{BL} & A_{BR} \end{array}\right) \left(\begin{array}{c} x_T \\ \hline x_B \end{array}\right) = \left(\begin{array}{c} b_T \\ \hline b_B \end{array}\right)$$

PME Generation

$$\left(\begin{array}{c|c} A_{TL} & 0 \\ \hline A_{BL} & A_{BR} \end{array}\right)\left(\begin{array}{c} x_T \\ \hline x_B \end{array}\right) = \left(\begin{array}{c} b_T \\ \hline b_B \end{array}\right)$$

PME Generation

$$\left(\frac{A_{TL}x_T}{A_{BL}x_T + A_{BR}x_B}\right) = \left(\frac{b_T}{b_B}\right)$$

PME Generation

$$\left(\frac{A_{TL} x_T = b_T}{A_{BL} x_T + A_{BR} x_B = b_B} \right)$$

PME Generation

$$\left(\frac{x_T := \Phi\left(A_{TL}, b_T\right)}{A_{BL}x_T + A_{BR}x_B = b_B} \right)$$

PME Generation

$$\left(\frac{x_T := \Phi\left(A_{TL}, b_T\right)}{A_{BR} x_B = b_B - A_{BL} x_T} \right)$$

PME Generation

Partitioned Matrix Expression (PME):

$$\left(\frac{x_T := \Phi\left(A_{TL}, b_T\right)}{x_B := \Phi\left(A_{BR}, b_B - A_{BL} x_T\right)} \right)$$

Loop Invariant Identification

$\ldots$

$\{P_{inv}\}$

While G do

    $\{P_{inv}\}$

    $\ldots$

    $\{P_{inv}\}$

endwhile

$\{P_{inv} \wedge \neg G\}$

$\ldots$

Loop Invariant Identification

$$\left(\frac{x_T := \Phi\left(A_{TL}, b_T\right)}{x_B := \Phi\left(A_{BR}, b_B - A_{BL} x_T\right)} \right)$$

Loop Invariant Identification

$$\left(\frac{x_T := \Phi\left(A_{TL}, b_T\right)}{x_B := \Phi\left(A_{BR}, b_B - A_{BL}x_T\right)}\right)$$

1. $x_T := \Phi\left(A_{TL}, b_T\right)$
2. $b_B := b_B - A_{BL}x_T$
3. $x_B := \Phi\left(A_{BR}, b_B\right)$

Loop Invariant Identification

$$\left(\frac{x_T := \Phi\left(A_{TL}, b_T\right)}{x_B := \Phi\left(A_{BR}, b_B - A_{BL} x_T\right)} \right)$$

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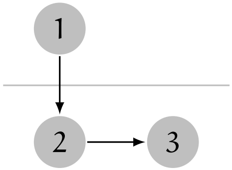

Loop Invariant Identification

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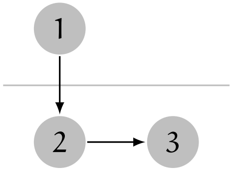

Loop invariant candidates: $\varnothing, \{1\}, \{1, 2\}, \{1, 2, 3\}$

Loop Invariant Identification

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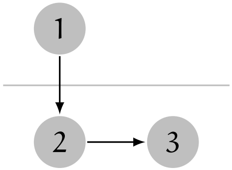

Loop invariant candidates: $\varnothing, \{1\}, \{1,2\}, \{1,2,3\}$
Feasible loop invariants: $\{1\}, \{1,2\}$

Algorithm Construction: Worksheet

Algorithm: ...
$\{ P_{\text{pre}} \}$
Partition
$\{ P_{\text{inv}} \}$
While G **do**
$\{(P_{\text{inv}}) \wedge (G)\}$
Repartition
$\{ P_{\text{before}} \}$
Update
$\{ P_{\text{after}} \}$
Continue with
$\{ P_{\text{inv}} \}$
endwhile
$\{(P_{\text{inv}}) \wedge \neg (G)\}$
$\{ P_{\text{post}} \}$

Algorithm Construction: Repartitioning

"Repartition" rule:

$$\left(\begin{array}{c|c} A_{TL} & 0 \\ \hline A_{BL} & A_{BR} \end{array}\right) \rightarrow \left(\begin{array}{c|c|c} A_{00} & 0 & 0 \\ \hline A_{10} & A_{11} & 0 \\ \hline A_{20} & A_{21} & A_{22} \end{array}\right)$$

"Continue with" rule:

$$\left(\begin{array}{c|c} A_{TL} & 0 \\ \hline A_{BL} & A_{BR} \end{array}\right) \leftarrow \left(\begin{array}{c|c|c} A_{00} & 0 & 0 \\ \hline A_{10} & A_{11} & 0 \\ \hline A_{20} & A_{21} & A_{22} \end{array}\right)$$

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P_{inv}:

$$\{x_T := \Phi\left(A_{TL}, b_T\right) \wedge b_B := b_B - A_{BL}x_T\}$$

Algorithm Construction

P_{before}

$$x_0 := \Phi\left(A_{00}, b_0\right)$$
$$b_1 := b_1 - A_{10}x_0$$
$$b_2 := b_2 - A_{20}x_0$$

P_{after}

$$x_0 := \Phi(A_{00}, b_0)$$
$$x_1 := \Phi(A_{11}, b_1 - A_{10}x_0)$$
$$b_2 := b_2 - A_{20}x_0 - A_{21}x_1$$

Algorithm Construction

P_{before}

$$x_0 := \Phi\left(A_{00}, b_0\right)$$
$$b_1 := b_1 - A_{10}x_0$$
$$b_2 := b_2 - A_{20}x_0$$

P_{after}

$$x_0 := \Phi(A_{00}, b_0)$$
$$x_1 := \Phi(A_{11}, b_1 - A_{10}x_0)$$
$$b_2 := b_2 - A_{20}x_0 - A_{21}x_1$$

Update:

$$x_1 := \Phi\left(A_{11}, b_1\right)$$

Algorithm Construction

P_{before}

$$
\begin{aligned}
x_0 &:= \Phi\left(A_{00}, b_0\right) \\
b_1 &:= b_1 - A_{10}x_0 \\
b_2 &:= b_2 - A_{20}x_0
\end{aligned}
$$

P_{after}

$$
\begin{aligned}
x_0 &:= \Phi(A_{00}, b_0) \\
x_1 &:= \Phi(A_{11}, b_1 - A_{10}x_0) \\
b_2 &:= b_2 - A_{20}x_0 - A_{21}x_1
\end{aligned}
$$

Update:

$$
\begin{aligned}
x_1 &:= \Phi\left(A_{11}, b_1\right) \\
b_2 &:= b_2 - A_{21}x_1
\end{aligned}
$$

Algorithm Construction

Algorithm: $x := \Phi(A, b)$

Partition $A \rightarrow \left(\begin{array}{c|c} A_{TL} & 0 \\ \hline A_{BL} & A_{BR} \end{array}\right)$

where A_{TL} is 0×0

While size$(A_{TL}) <$ size(A) **do**

Repartition

$$\left(\begin{array}{c|c} A_{TL} & 0 \\ \hline A_{BL} & A_{BR} \end{array}\right) \rightarrow \left(\begin{array}{c|c|c} A_{00} & 0 & 0 \\ \hline A_{10} & A_{11} & 0 \\ \hline A_{20} & A_{21} & A_{22} \end{array}\right)$$

where A is $k \times k$

Variant 1	Variant 2
$b_1 := b_1 - A_{10}x_0$	$x_1 := \Phi(A_{11}, b_1)$
$x_1 := \Phi(A_{11}, b_1)$	$b_2 := b_2 - A_{21}x_1$

Continue with

$$\left(\begin{array}{c|c} A_{TL} & 0 \\ \hline A_{BL} & A_{BR} \end{array}\right) \leftarrow \left(\begin{array}{c|c|c} A_{00} & 0 & 0 \\ \hline A_{10} & A_{11} & 0 \\ \hline A_{20} & A_{21} & A_{22} \end{array}\right)$$

endwhile

Iterative Methods

- Iterative methods for solving linear systems $Ax = b$.
- Initial guess x_0.
- Successively better solutions $x_1, x_2, \ldots$
- Convergence: $\|Ax_i - b\| < \varepsilon$.

Iterative Methods

- Iterative methods for solving linear systems $Ax = b$.
- Initial guess x_0.
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- Convergence: $\|Ax_i - b\| < \varepsilon$.

Matrix representation:

$$X = (x_0 \; x_1 \; x_2 \ldots)$$
$$R = (r_0 \; r_1 \; r_2 \ldots)$$

Matrix Representation

Operation: Symmetric conjugate gradient method.

P_{post} :

$$
\begin{aligned}
APD &= R\left(\underline{I} - \underline{J}\right) \\
P\left(I - U\right) &= \underline{R} \\
PD &= X\left(\underline{I} - \underline{J}\right) \\
\|Re_r\| &< \varepsilon
\end{aligned}
$$

Source: Eijkhout et al., 2010.

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\|Re_r\| &< \varepsilon
\end{aligned}
$$

$$\{R, U, P, D, X\} := \mathsf{CG}\left(A, Re_0, Xe_0\right)$$

Source: Eijkhout et al., 2010.

PME Generation: Initial Partitioning

$$\begin{aligned} APD &= R\left(\underline{I} - \underline{J}\right) \\ P\left(I - U\right) &= \underline{R} \\ PD &= X\left(\underline{I} - \underline{J}\right) \end{aligned}$$

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$$A \left(\begin{array}{c|c} P_L & p_R \end{array} \right) \left(\begin{array}{c|c} D_{TL} & 0 \\ \hline 0 & \delta_{BR} \end{array} \right) = \left(\begin{array}{c|c|c} R_L & r_R & r_+ \end{array} \right) \left(\begin{array}{c|c} I - J & 0 \\ \hline -e_r^T & 1 \\ \hline 0 & -1 \end{array} \right)$$

$$\left(\begin{array}{c|c} P_L & p_R \end{array} \right) \left(\begin{array}{c|c} I - U_{TL} & -u_{TR} \\ \hline 0 & 1 \end{array} \right) = \left(\begin{array}{c|c} R_L & r_R \end{array} \right)$$

$$\left(\begin{array}{c|c} P_L & p_R \end{array} \right) \left(\begin{array}{c|c} D_{TL} & 0 \\ \hline 0 & \delta_{BR} \end{array} \right) = \left(\begin{array}{c|c|c} X_L & x_R & x_+ \end{array} \right) \left(\begin{array}{c|c} I - J & 0 \\ \hline -e_r^T & 1 \\ \hline 0 & -1 \end{array} \right)$$

PME Generation

$$\left(\begin{array}{c|c} AP_L D_{TL} = R_L \left(I - J \right) - r_R e_r^T & Ap_R \delta_{BR} = r_R - r_+ \end{array} \right)$$

$$\left(\begin{array}{c|c} P_L \left(I - U_{TL} \right) = R_L & -P_L u_{TR} + p_R = r_R \end{array} \right)$$

$$\left(\begin{array}{c|c} P_L D_{TL} = X_L \left(I - J \right) - x_R e_r^T & p_R \delta_{BR} = x_R - x_+ \end{array} \right)$$

$$\begin{aligned} P_{\text{post}} : \\ APD &= R \left(\underline{I} - \underline{J} \right) \\ P \left(I - U \right) &= \underline{R} \\ PD &= X \left(\underline{I} - \underline{J} \right) \end{aligned}$$

PME Generation

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$$\left(\begin{array}{c|c} P_L D_{TL} = X_L (I - J) - x_R e_r^T & p_R \delta_{BR} = x_R - x_+ \end{array} \right)$$

$$AP_L D_{TL} = \left(\begin{array}{c|c} R_L & r_R \end{array} \right) \left(\frac{I - J}{-e_r^T} \right)$$

$$P_L (I - U_{TL}) = R_L$$

$$P_L D_{TL} = \left(\begin{array}{c|c} X_L & x_R \end{array} \right) \left(\frac{I - J}{-e_r^T} \right)$$

P_{post} :

$$APD = R \left(\underline{I} - \underline{J} \right)$$

$$P (I - U) = \underline{R}$$

$$PD = X \left(\underline{I} - \underline{J} \right)$$

PME Generation

$$\left(\; AP_L D_{TL} = R_L \left(I - J \right) - r_R e_r^T \;\middle|\; Ap_R \delta_{BR} = r_R - r_+ \; \right)$$

$$\left(\; P_L \left(I - U_{TL} \right) = R_L \;\middle|\; -P_L u_{TR} + p_R = r_R \; \right)$$

$$\left(\; P_L D_{TL} = X_L \left(I - J \right) - x_R e_r^T \;\middle|\; p_R \delta_{BR} = x_R - x_+ \; \right)$$

$$\{ \left(R_L \mid r_R \right), U_{TL}, P_L, D_{TL}, \left(X_L \mid x_R \right) \} := \mathbf{CG} \left(A, R_L e_0, X_L e_0 \right)$$

PME Generation

$$\left(\; A P_L D_{TL} = R_L\,(I - J) - r_R e_r^T \;\middle|\; A p_R \delta_{BR} = r_R - r_+ \; \right)$$

$$\left(\; P_L\,(I - U_{TL}) = R_L \;\middle|\; -P_L u_{TR} + p_R = r_R \; \right)$$

$$\left(\; P_L D_{TL} = X_L\,(I - J) - x_R e_r^T \;\middle|\; p_R \delta_{BR} = x_R - x_+ \; \right)$$

$$\{(R_L \mid r_R)\,, U_{TL}, P_L, D_{TL}, (X_L \mid x_R)\} := \mathbf{CG}\,(A, R_L e_0, X_L e_0)$$

$$-P_L u_{TR} + p_R = r_R$$

PME Generation

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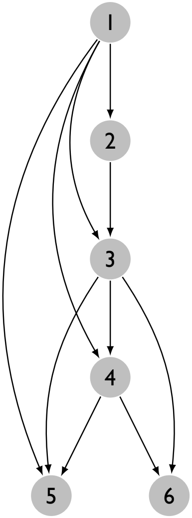
$$-P_L^T A P_L u_{TR} + P_L^T A p_R = P_L^T A r_R$$

PME Generation

PME:

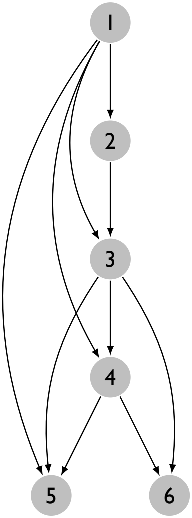
$$\begin{aligned}
\{(R_L \mid r_R), U_{TL}, P_L, D_{TL}, (X_L \mid x_R)\} &:= \mathbf{CG}(A, R_L e_0, X_L e_0) \\
u_{TR} &:= -\left(P_L^T A P_L\right)^{-1} P_L^T A r_R \\
p_R &:= r_R + P_L u_{TR} \\
\delta_{BR} &:= \frac{r_R^T r_R}{r_R^T A p_R} \\
r_+ &:= r_R - A p_R \delta_{BR} \\
x_+ &:= x_R - p_R \delta_{BR}
\end{aligned}$$

Loop Invariant Identification



1. $\{\ldots\} := \mathsf{CG}\,(A, R_L e_0, X_L e_0)$
2. $u_{TR} := -\left(P_L^T A P_L\right)^{-1} P_L^T A r_R$
3. $p_R := r_R + P_L u_{TR}$
4. $\delta_{BR} := \frac{r_R^T r_R}{r_R^T A p_R}$
5. $r_+ := r_R - A p_R \delta_{BR}$
6. $x_+ := x_R - p_R \delta_{BR}$

Loop Invariant Identification



1. $\{\ldots\} := \mathsf{CG}\,(A, R_L e_0, X_L e_0)$
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4. $\delta_{BR} := \frac{r_R^T r_R}{r_R^T A p_R}$
5. $r_+ := r_R - A p_R \delta_{BR}$
6. $x_+ := x_R - p_R \delta_{BR}$

We use $P_{\text{inv}} = \{1, 2, 3\}$

Loop Invariant Identification: Feasibility

Algorithm: $\ldots$
$\{ P_{pre} \}$
Partition
Preprocessing
$\{ P_{inv} \}$
While G **do**
$\{(P_{inv}) \wedge (G)\}$
Repartition
$\{ P_{before} \}$
Update
$\{ P_{after} \}$
Continue with
$\{ P_{inv} \}$
endwhile
$\{(P_{inv}) \wedge \neg (G)\}$
$\{ P_{post} \}$

Loop Invariant Identification: Feasibility

P_{post} :

$$\begin{aligned} APD &= R\left(\underline{I} - \underline{J}\right) \\ P\left(I - U\right) &= \underline{R} \\ PD &= X\left(\underline{I} - \underline{J}\right) \\ \|Re_r\| &< \varepsilon \end{aligned}$$

Loop Invariant Identification: Feasibility

P_{post} :

$$\begin{aligned} APD &= R\left(\underline{I} - \underline{J}\right) \\ P\,(I - U) &= \underline{R} \\ PD &= X\left(\underline{I} - \underline{J}\right) \\ \|Re_r\| &< \varepsilon \end{aligned}$$

Loop guard G: $\|r_R\| \geqslant \varepsilon$

Loop Invariant Identification: Feasibility

P_{post} :

$$
\begin{aligned}
APD &= R\left(\underline{I} - \underline{J}\right) \\
P\left(I - U\right) &= \underline{R} \\
PD &= X\left(\underline{I} - \underline{J}\right) \\
\|Re_r\| &< \varepsilon
\end{aligned}
$$

Loop guard G: $\|r_R\| \geqslant \varepsilon$

$$
R \rightarrow \left(\; R_L \;\middle|\; r_R \;\middle|\; r_+ \; \right)
$$

Loop Invariant Identification: Feasibility

$$P_{\text{inv}} \wedge \neg G \Rightarrow P_{\text{post}}$$

P_{inv}:

$$\begin{aligned}\{(R_L \mid r_R), U_{TL}, P_L, D_{TL}, (X_L \mid x_R)\} &:= \mathbf{CG}\left(A, R_L e_0, X_L e_0\right)\\ u_{TR} &:= -\left(P_L^T A P_L\right)^{-1} P_L^T A r_R\\ p_R &:= r_R + P_L u_{TR}\end{aligned}$$

$G : \|r_R\| \geqslant \varepsilon$

Loop Invariant Identification: Feasibility

$$P_{\text{inv}} \wedge \neg G \Rightarrow P_{\text{post}}$$

P_{inv}:

$$\begin{aligned} \{(R_L \mid r_R), U_{TL}, P_L, D_{TL}, (X_L \mid x_R)\} &:= \mathbf{CG}\,(A, R_L e_0, X_L e_0) \\ u_{TR} &:= -\left(P_L^T A P_L\right)^{-1} P_L^T A r_R \\ p_R &:= r_R + P_L u_{TR} \end{aligned}$$

$\neg G : \|r_R\| < \varepsilon$

Loop Invariant Identification: Feasibility

$$P_{\text{inv}} \wedge \neg G \Rightarrow P_{\text{post}}$$

P_{inv}:

$$\begin{aligned} \{(R_L \mid r_R), U_{TL}, P_L, D_{TL}, (X_L \mid x_R)\} &:= \mathbf{CG}\left(A, R_L e_0, X_L e_0\right) \\ u_{TR} &:= -\left(P_L^T A P_L\right)^{-1} P_L^T A r_R \\ p_R &:= r_R + P_L u_{TR} \end{aligned}$$

$\neg G : \|r_R\| < \varepsilon$

P_{post}:

$$\begin{aligned} \{R, U, P, D, X\} &:= \mathbf{CG}\left(A, Re_0, Xe_0\right) \\ \|Re_r\| &< \varepsilon \end{aligned}$$

Algorithm Construction: Repartitioning

"Repartition" rules:

$$\left(R_L \,\middle|\, r_R \,\middle|\, r_+ \right) \rightarrow \left(R_0 \,\middle|\, r_1 \,\middle|\, r_2 \right)$$

$$\left(\begin{array}{c|c} D_{TL} & 0 \\ \hline 0 & \delta_{BR} \end{array} \right) \rightarrow \left(\begin{array}{c|c} D_{00} & 0 \\ \hline 0 & \delta_{11} \end{array} \right)$$

"Continue with" rules:

$$\left(R_L \,\middle|\, r_R \,\middle|\, r_+ \right) \leftarrow \left(R_0 \,|\, r_1 \,\middle|\, r_2 \,\middle|\, r_3 \right)$$

$$\left(\begin{array}{c|c} D_{TL} & 0 \\ \hline 0 & \delta_{BR} \end{array} \right) \leftarrow \left(\begin{array}{c|c|c} D_{00} & 0 & 0 \\ \hline 0 & \delta_{11} & 0 \\ \hline 0 & 0 & \delta_{11} \end{array} \right)$$

Algorithm Construction

P_{before}

$$\begin{aligned}
\{(R_0 \mid r_1), U_{00}, P_0, D_{00}, (X_0 \mid x_1)\} &:= \mathsf{CG}\,(A, R_0 e_0, X_0 e_0) \\
u_{01} &:= -\left(P_0^T A P_0\right)^{-1} P_0^T A r_1 \\
p_1 &:= r_1 + P_0 u_{01}
\end{aligned}$$

Algorithm Construction

P_{after}:

$$\begin{aligned}
\{(R_0 \mid r_1), U_{00}, P_0, D_{00}, (X_0 \mid x_1)\} &:= \mathsf{CG}(A, R_0 e_0, X_0 e_0) \\
u_{01} &:= -\left(P_0^T A P_0\right)^{-1} P_0^T A r_1 \\
p_1 &:= r_1 + P_0 u_{01} \\
\delta_{11} &:= \frac{r_1^T r_1}{r_1^T A p_1} \\
r_2 &:= r_1 - A p_1 \delta_{11} \\
x_2 &:= x_1 - p_1 \delta_{11} \\
\nu_{12} &:= -\frac{p_1^T A r_2}{p_1^T A p_1} \\
p_2 &:= r_2 + p_1 \nu_{12}
\end{aligned}$$

Algorithm Construction

P_{after}:

$$\begin{aligned}
\{(R_0 \mid r_1), U_{00}, P_0, D_{00}, (X_0 \mid x_1)\} &:= \mathsf{CG}\,(A, R_0 e_0, X_0 e_0) \\
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\end{aligned}$$

Conclusion

Automatic derivation of algorithms for iterative methods.

- Automatic derivation of matrix properties.
- Provably correct algorithms.
- Families of algorithms.

Future work:

- Matrix representations.
- Stability analysis.
- Performance analysis.
- Implementation.

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Derivation of Properties

$$\begin{aligned} APD &= R\left(I - J\right) \\ P\left(I - U\right) &= R \end{aligned}$$

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`Diagonal`$[R^T R]$

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`Diagonal`$[R^T R]$

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\begin{aligned}
R^T AP &= R^T R\,(I - J)\,D^{-1} \\
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Derivation of Properties

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Derivation of Properties

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$$\begin{aligned} R^T AP &= R^T R\,(I - J)\,D^{-1} \\ R^T P &= R^T R\,(I - U)^{-1} \end{aligned}$$

$\texttt{UpperTriangular}[R^T P] \rightarrow \texttt{LowerTriangular}[P^T R]$

$$P^T AP = P^T R\,(I - J)\,D^{-1}$$

Loop Invariant Identification: Feasibility

Initially, R_L, P_L,... have size $n \times 0$.

$$
\begin{aligned}
\{(R_L \mid r_R), U_{TL}, P_L, D_{TL}, (X_L \mid x_R)\} &:= \mathsf{CG}(A, R_L e_0, X_L e_0) \\
u_{TR} &:= -\left(P_L^T A P_L\right)^{-1} P_L^T A r_R \\
p_R &:= r_R + P_L u_{TR}
\end{aligned}
$$

Loop Invariant Identification: Feasibility

Initially, R_L, P_L,... have size $n \times 0$.

$$\{r_R, \varnothing, \varnothing, \varnothing, x_R\} = \mathsf{CG}\left(A, r_R, x_R\right)$$

$$p_R = r_R$$

Loop Invariant Identification: Feasibility

Initially, R_L, P_L,... have size $n \times 0$.

$$\{r_R, \varnothing, \varnothing, \varnothing, x_R\} = \mathsf{CG}\left(A, r_R, x_R\right)$$

$$p_R = r_R$$

Preprocessing operation: $p_R := r_R$