

Iterative Runge-Kutta type Methods for Nonlinear ill-posed Problems and Applications

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Inverse Problems: developments in theory and applications

Contents

- 1 Inverse Ill-posed Problems
 - Brief Introduction
- 2 Runge-Kutta Iterative Regularization Methods
 - Padé Regularization for Linear Problems
 - Investigations of Nonlinear Problems
- 3 Application in Atmospheric Physics

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Asymptotic Regularization

Rewriting $Af = g^\epsilon$ to autonomous ODE

$$\dot{f}(t) = A^*(g^\epsilon - Af(t)), \quad f(t_0) = f_0, \quad \|g - g^\epsilon\| \leq \epsilon.$$

That kind of ODE has a **stationary state** $f_\infty = (f^+)$, which coincides with the **solution of Normal Eq.** $A^*Af_\infty = A^*g^\epsilon$. The regularization here consists in choosing a proper finite time t_{opt} .

Application to Nonlinear Problems $F(w) = g^\epsilon$

$$\dot{w}(t) = F'(w(t))^* [g^\epsilon - F(w(t))], \quad w(t_0) = w_0$$

Now, the problem obviously consists in solving those ODEs.

Tautenhahn U., On the asymptotical regularization of nonlinear ill-posed problems. *Inverse Problems*, 10(6):1405-18, 1994.

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ODE Solvers

Application of Runge-Kutta family to asymptotic regularization

Applying a RKM $\frac{c}{b^T} \left| \begin{array}{c} A \\ \hline \end{array} \right.$, i.e., a general s-stage method yields

$$f_{i+1} = r(-\tau_{i+1}A^*A)f_i + \tau_{i+1}t^{-1}(-\tau_{i+1}A^*A)A^*g^\varepsilon$$

with **rational functions** $r(s)$ and $t(s)$

A. Rieder, Runge-Kutta integrators yield optimal regularization schemes. *Inverse Problems*, **21(2005)**pp. 453-71.

Stability Function $r(s)$

Is a rational approximation to the exponential function, so we write $r(s) = p(s)/q(s)$ with polynomials $p(s)$ and $q(s)$.

If a Runge-Kutta method has the **stability function** $r(s)$ and is of consistency order ψ , then $r(s) = \exp(s) + O(t^{\psi+1})$ for $t \rightarrow 0$ holds.

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ODE Solvers

Main Goal: Fast Iterative Regularization Method

While in solving ODEs one main goal is maximal **consistency order**, for iteratively solving ill-posed problems it is **less important**.

Butcher Barriers

The classical Runge-Kutta method is a 4-stage method of order 4 and has the stability function $r(s) = \sum_{i=0}^4 \frac{s^i}{i!}$, but it does not exist an explicit RK method of order 5 with the stability function $r_*(s) = \sum_{i=0}^5 \frac{s^i}{i!}$ due to the **Butcher barrier**.

Padé approximations

But it is still possible to construct an iteration for ill-posed problems from this stability function. This leads to the **concept** of iterative regularization methods via **Padé approximations**.

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Padé Iterative Regularization

Preconditioner

Padé iteration is a generalization of the Landweber iteration with $T = I$ (Euler method) via preconditioners. Thus, our equation becomes

$$f_{i+1} = f_i + \tau T^{-1}(A^* g^\varepsilon - A^* A f_i),$$

with T an **invertible preconditioner**. For the Padé iteration, the preconditioner is defined via two polynomials. Those rational functions are rational approximations to the exponential function.

A. Kirsche and C.B., Rational approximation for ill-conditioned equation system *Appl. Math. Comput.* **171** (2005) 385–97.

Padé Iterative Regularization

Definition

Preconditioner for the (k, j) -Padé iteration method from the polynomials

$$p_{k,j}(s) = \sum_{i=0}^j \binom{k+j}{i}^{-1} \binom{j}{i} \frac{s^i}{i!} \quad \text{and} \quad q_{k,j}(s) = p_{j,k}(-s)$$

and

$$h_{k,j}(s) = \sum_{i=0}^{\max\{k,j\}-1} \frac{1}{i+1} \binom{j+k}{i+1}^{-1} \left[\binom{j}{i+1} - (-1)^{i+1} \binom{k}{i+1} \right] \frac{s^i}{i!}$$

Setting $t(s) = q(s)/h(s)$ and $T^{-1} = t^{-1}(-\tau A^* A)$, yields the iteration equation

$$f_{i+1} = f_i + \tau t^{-1}(-\tau A^* A)(A^* g^\varepsilon - A^* A f_i).$$

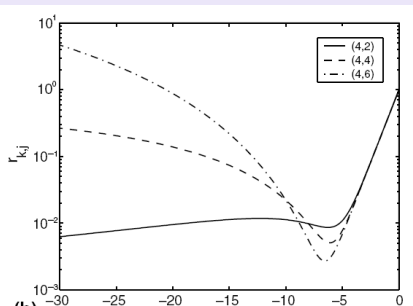
Padé Iterative Regularization

Convergence Properties

The (k, j) -Padé method has the following convergence behavior.

- i If $k \geq j$ then the (k, j) -Padé method converges **for all** stepsizes $\tau \in \mathbb{R}^+$.
- ii If $k < j$ then $\tau_1 \in \mathbb{R}^+$ exists such that for all $\tau < \tau_1$ the (k, j) -Padé method is convergent and for all $\tau \geq \tau_1$ the method is not convergent.
- iii If $k \leq j$ then a unique effective stepsize (relaxation parameter) τ_{eff} exists.
- iv If $k > j$ we have $\lim_{s \rightarrow -\infty} |r(s)| = 0$ and hence **no effective parameter τ_{eff} needs** to be determined.

Example



Polynomials of some (k,j) -Padé iteration methods and their optimal relaxation parameter

(k,j)	$q(x)$	$h(x)$	ω_{opt}
$(0,1)$	1	1	$\frac{2}{\lambda_1 + \lambda_m}$
$(0,2)$	1	$1 + \frac{1}{2}x$	$\frac{2}{\lambda_1 + \lambda_m}$
$(1,1)$	$1 - \frac{1}{2}x$	1	$\frac{2}{\sqrt{\lambda_1 \lambda_m}}$
$(1,2)$	$1 - \frac{1}{3}x$	$1 + \frac{1}{6}x$	$\frac{3}{2\lambda_1} \left(\frac{\sqrt{\lambda_1^2 + 10\lambda_1 \lambda_m + \lambda_m^2} - \lambda_1}{\lambda_m} - 1 \right)$
$(2,2)$	$1 - \frac{1}{2}x + \frac{1}{12}x^2$	1	$2\sqrt{\frac{3}{\lambda_1 \lambda_m}}$
$(2,1)$	$1 - \frac{2}{3}x + \frac{1}{6}x^2$	$1 - \frac{1}{6}x$	-

Convergence condition:

Spectral radius $\rho(r(-\tau A^* A)) < 1$

$\tau_{eff} = \operatorname{argmin} \rho(r(-\tau A^* A))$

Padé Iterative Regularization

Optimal Convergence Rate

Let X, Y be infinite dimensional separable Hilbert spaces and $A \in \mathcal{K}(X, Y)$, $k, j \in \mathbb{N}^+$, $g \in \mathcal{R}(A)$, $\|g - g^\varepsilon\|_Y \leq \varepsilon$, $\tau < \tau_1$ and $A^+g \in X_\mu = \mathcal{R}((K^*K)^\mu)$, $\mu > 0$.

Then the discrepancy principle applied to the (k, j) -Padé iteration method delivers a finite stopping index.

The Padé iteration method is **order optimal** for all $\mu \in (0, \infty)$ and has infinite qualification*.

$$\text{Filter: } F_i(\lambda) = \frac{1 - r_{k,j}(-\tau\lambda)^i}{\lambda}$$

The $(1, 0)$ -Padé and $(2, 1)$ -Padé methods proved to have good convergence properties.

* in classical sense

A. Kirsche and C.B., Padé iteration method for regularization *Appl. Math. Comput.* **180** (2006) 648–63.

Applying to nonlinear Problems $F(w) = g^\epsilon$

Runge-Kutta Family

Applying RKM $\begin{array}{c|c} c & A \\ \hline & b^T \end{array}$ we obtain

$$w_{n+1}^\epsilon = w_n^\epsilon + \tau_n \sum_{i=1}^s b_i F'(k_i)^* (g^\epsilon - F(k_i))$$

and

$$k_i = w_n^\epsilon + \tau_n \sum_{j=1}^s a_{ij} F'(k_j)^* (g^\epsilon - F(k_j)).$$

Define $z_i = k_i - w_n^\epsilon$. We approximate z_i by using Taylor's formula and the fact that $F'(\cdot)$ is a linear operator. We have

$$z_i \approx \tau_n \sum_{j=1}^s a_{ij} F'(w_n^\epsilon)^* (g^\epsilon - F(w_n^\epsilon)) - \tau_n \sum_{j=1}^s a_{ij} F'(w_n^\epsilon)^* F'(w_n^\epsilon) z_j.$$

Applying to nonlinear Problems

Family of iterative Regularization

With the notations $Z := (z_1 \dots z_s)^T$ and $S_n := F'(w_n^\epsilon)$ as well as the operators $\Pi_n := \delta + \tau_n A S_n^* S_n$ and $H_n := \delta + \tau_n A S_n S_n^*$ which are a linear ones we get

$$Z = \tau_n \Pi_n^{-1} A \mathbf{1} S_n^* (g^\epsilon - F(w_n^\epsilon)),$$

$$w_{n+1}^\epsilon = w_n^\epsilon + \tau_n b^T \mathbf{1} S_n^* (g^\epsilon - F(w_n^\epsilon)) - \tau_n b^T S_n^* S_n Z.$$

Finally,

$$w_{n+1}^\epsilon = w_n^\epsilon + \tau_n b^T \Pi_n^{-1} \mathbf{1} S_n^* (g^\epsilon - F(w_n^\epsilon)).$$

In particular, the well-known nonlinear Landweber and Levenberg-Marquardt methods correspond to the 1-stage explicit and implicit Euler method.

Convergence Behavior

Assumptions to the Operator

Local condition on F (as usual)

$$\|F(\tilde{w}) - F(w) - F'(w)(\tilde{w} - w)\|_Y \leq \eta \|F(\tilde{w}) - F(w)\|_Y \quad (1)$$

$w, \tilde{w} \in B_\rho(w_0) \subset \mathcal{D}(F)$ with $0 < \eta < (c_1^2 - \tau c_{a\tau}^2)/(2c_1) \leq 1/2$.

Upper and Lower Bounds

$$\frac{c_1}{\sqrt{2}} \|y\|_Y \leq \|b^T H_n^{-1} \mathbf{1} y\|_Y \leq c_1 \|y\|_Y, \quad (2)$$

$$\|b^T (A - I) S_n^* H_n^{-1} \mathbf{1} y\|_X \leq c_{a\tau} \|y\|_Y.$$

with $c_1 > 0, c_{a\tau} > 0$.

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Convergence Behavior

Hölder Source Condition

$$w^\dagger - w_0 = (F'(w^\dagger)^* F'(w^\dagger))^\gamma v, \quad 0 < \gamma \leq \frac{1}{2}, \quad \|v\| \text{ sufficiently small}$$

Note this is a particular case with $\varphi(t) = t^\gamma$ of a general source condition $w^\dagger - w_0 = \varphi(F'(w^\dagger)^* F'(w^\dagger))v$ with a continuous, strictly increasing **index function** φ with $\varphi(t) \rightarrow 0$ as $t \rightarrow 0^+$.

Others e.g.: $\varphi(t) = t^\gamma \ln^{-p}(\frac{1}{t})$ and $\varphi(t) = \exp(\frac{p}{t})$

- Mathè P, Pereverzev S V, Geometry of linear ill posed problems in variable Hilbert scales. *Inverse Problems* 19(2003) 789-803.
- Hofmann B, Mathè P, Analysis of profile functions for general linear regularization methods. *SIAM J. Numer. Anal.* 45(2007)1122-41.
- Hohage, T., Logarithmic convergence rates of the iteratively regularized Gauss - Newton method for an inverse potential and an inverse scattering problem *Inverse Problems*, 13(1997)1279-1299.

Convergence Behavior

a-posteriori PCR: Discrepancy principle

$$\|g^\epsilon - F(w_{n_*}^\epsilon)\|_Y \leq \mu\epsilon < \|g^\epsilon - F(w_n^\epsilon)\|_Y, \quad 0 \leq n < n_*,$$

$$\text{with } \mu \geq (2(\eta + 1)c_1) / (c_1(c_1 - 2\eta) - \tau c_{aT}^2) > 0$$

Convergence Theorem

It holds $\|w_* - w_{n+1}^\epsilon\|_X \leq \|w_* - w_n^\epsilon\|_X$, $0 \leq n < n_*$ (exists finitely).

If $\epsilon = 0$ then $\sum_{n=0}^{\infty} \|g - F(w_n)\|_Y^2 < \infty$.

If w^\dagger is the unique solution of minimal distance to w_0 and if $\mathcal{N}(F'(w^\dagger)) \subset \mathcal{N}(F'(w))$ for $w \in B_\rho(w_0)$ then $w_n \rightarrow w^\dagger$.

If $\epsilon > 0$ one gets $w_{n_*}^\epsilon \rightarrow w^\dagger$ as $\epsilon \rightarrow 0$.

C.B., P. Ponsawad, Iterative Runge-Kutta-type methods for nonlinear ill-posed problems.
Inverse Problems, 24(2008)(17pp).

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Convergence Rate Analysis first stage RKM

Adaption to $s = 1$

Applying RKM $\frac{c}{1} \left| \frac{a}{1} \right|$ with $a \in (3 - 2\sqrt{2}, 3 + 2\sqrt{2})$ then

$\mu \geq 8a(\eta + 1)/(4a(1 - 2\eta) - (1 - a)^2)$ and
 $\eta < (4a - (1 - a)^2)/(8a)$ since $c_{a\tau} \geq |1 - a|/(2\sqrt{\tau a})$ and $c_1 = 1$.
 Thus the stepsize parameter is not limited.

Usual Operator Assumptions

$\|F'(w)\|_Y \leq c_F < 1$ and $F'(w) = R_w F'(w^\dagger)$ hold for $w \in B_\rho(w_0)$.

Moreover, we assume $\|R_w - E\| \leq c_L \|w - w^\dagger\|$, $c_L > 0$, and
 $0 < c_R \leq |||R_w||| - |||E|||$.

We have $\|R_w\| \leq c_r$ since R_w is linear bounded.

Convergence Rate Analysis first stage RKM

Main Theorem: Order Optimal Rate

There exists a positive constant c_* , depending on γ only,

$$\|w^\dagger - w_k^\varepsilon\|_X \leq c_* \|v\|_X (k+1)^{-\gamma}$$

$\|g^\varepsilon - F(w_k^\varepsilon)\|_Y \leq 3c_* \|v\|_X (k+1)^{-\gamma-\frac{1}{2}}$ for $0 \leq k < k_*$ where k_* is the termination index. Moreover,

$$k_* \leq c_{**} (\|v\|_X / \varepsilon)^{2/(2\gamma+1)} \quad (3)$$

and

$$\|w^\dagger - w_{k_*}^\varepsilon\|_X \leq c_{***} \|v\|_X^{1/(2\gamma+1)} \varepsilon^{2\gamma/(2\gamma+1)}. \quad (4)$$

with $c_{**}, c_{***} > 0$ depending on $\gamma \in (0, \frac{1}{2}]$.

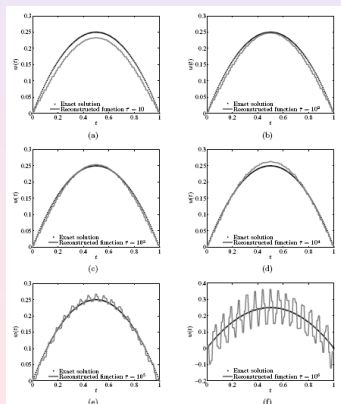
- P. Ponsawad and C.B., On the convergence rate analysis of the first stage Runge-Kutta-type regularization. *Inverse Problems*, 26(2010)(12pp).
- Hochbruck M, Hönl M and Ostermann A, A convergence analysis of the exponential Euler iteration for nonlinear ill posed problems. *Inverse Problems*, 25(2009)(18pp).

Example

Radau
Method

$[F(w)](s) = \exp \int_0^1 k(s, t)w(t)dt$
noisy data $g^\epsilon(s) = (s^4 - 2s^3 + s) / 12 + \epsilon \cos(100s)$
 $s \in [0, 1], \epsilon = 0.001, m = 65, \mu = 2.1, w_0(t) = 0$

$\bar{\tau}$	n_*	$[s_{n_*} - 1]s_{n_*}$	$[e_{n_*} - 1]e_{n_*}$
10	22	[1.0194]0.9259	[0.1156]0.1053
10^2	3	[1.1009]0.4702	[0.1245]0.0563
10^3	2	[1.0161]0.3178	[0.1139]0.0364
10^4	1	[-]0.4044	[-]0.0423
10^5	1	[-]0.3257	[-]0.0529
10^6	1	[-]0.3164	[-]0.4273



Example

Table 2. The termination index obtained by the iterative RK-type regularization methods. Here $\tau = 10$ and $\varepsilon = 2.8 \times 10^{-4}$.

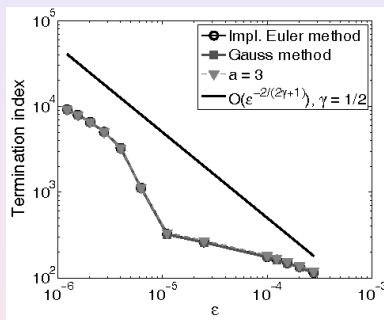
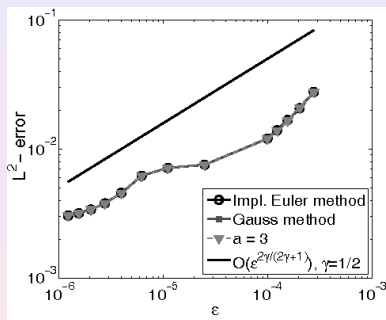
	c_{sc}	a								
		0.18	0.25	0.35	0.45	0.5	1	2	3	5
$\mu = 31$	0.8	10	10	10	10	10	10	11	12	14
	0.6	13	13	13	13	13	14	15	16	19
	0.1	76	77	77	78	78	82	90	98	113
	0.08	95	96	97	98	98	103	113	122	142
$\mu = 3.1$	0.8			37	37	38	39	43	47	
	0.6			50	50	50	53	58	63	
	0.1			303	306	307	323	354	385	
	0.08			379	383	385	404	443	482	

$$[F(w)](s) = \exp \int_0^1 k(s, t) w(t) dt \quad (5)$$

with the noisy data $g^\varepsilon(s) = (s^4 - 2s^3 + s) / 12 + \varepsilon \cos(100s)$, $s \in [0, 1]$ and the exact solution $w^\dagger(t) = t(1-t)$, $t \in [0, 1]$. The kernel function is given by

$$k(s, t) = \begin{cases} s(1-t) & \text{if } s < t; \\ t(1-s) & \text{if } t \leq s. \end{cases} \quad (6)$$

Example



We can see that the values of k_* and the L^2 -error do not fit to a perfect straight line because of random noise is involved in setting the perturbed data. However, the asymptotic behavior can be observed for both figures.

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Scattering and absorption of solar and infrared radiation
(Direct Aerosol Effect)

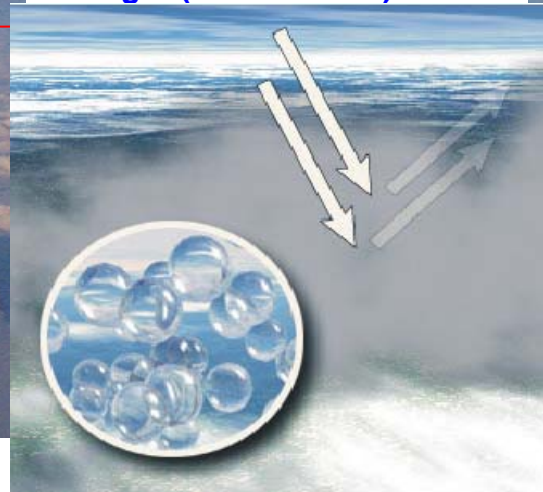
1. Why Aerosols are Important ?

observed aerosol layer in March 2000

Changes in clouds
(Indirect Aerosol Effect)

This cloud has only few cloud droplets, hence, reflects less sunlight (darker cloud).

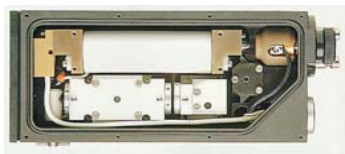
This cloud has more cloud droplets, hence, reflects more sunlight (lighter cloud).





2. Lidar System Set Up

NTUA 6-Wavelength Raman Lidar:
Member of EARLINET Lidar Network



→
→ 355, 532, and 1064 nm, 10 Hz repetition rate
→

Emission
(Nd:YAG laser)

Detection: Elastic: 355 , 532 , 1064 nm
+ Inelastic (Raman): 387nm (N₂) and 607nm (N₂)



3. Retrieval of Aerosol Optical Properties

Raman lidar equation:

$$P(\lambda_R, z) = P(\lambda_L) C_R O(z) \frac{\beta_R(\lambda_L, z)}{z^2} \exp \left\{ - \int_0^z [\alpha(\lambda_L, \zeta) + \alpha(\lambda_R, \zeta)] d\zeta \right\}$$

Numerical Derivative: (P. Pornsawad, C.B. , C. Ritter, *Appl. Opt.* 2008)

ill-posed Problem – very sensitive to data errors → **Regularization helps**

$$\alpha_{\text{aer}}(\lambda_L, z) = \frac{\frac{d}{dz} \ln \frac{N(z)}{z^2 P(\lambda_R, z)} - \alpha_{\text{mol}}(\lambda_L, z) - \alpha_{\text{mol}}(\lambda_R, z)}{1 + \left(\frac{\lambda_L}{\lambda_R} \right)^k}$$



$$\frac{d}{dz} \ln \left[\frac{N(z)}{z^2 P(\lambda_R, z)} \right]$$

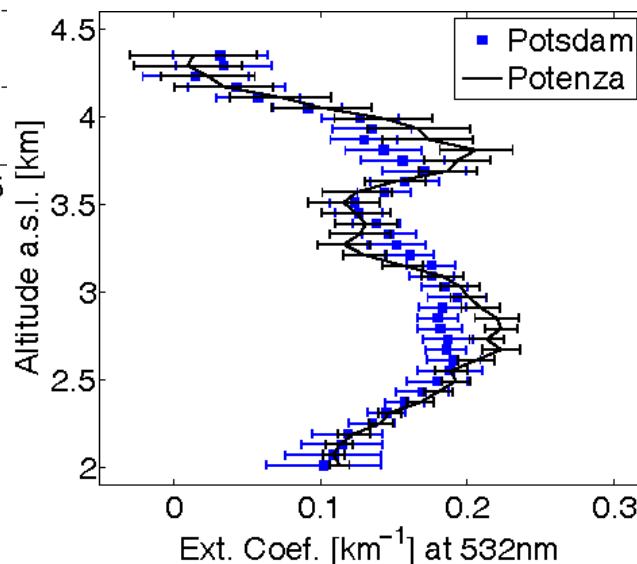
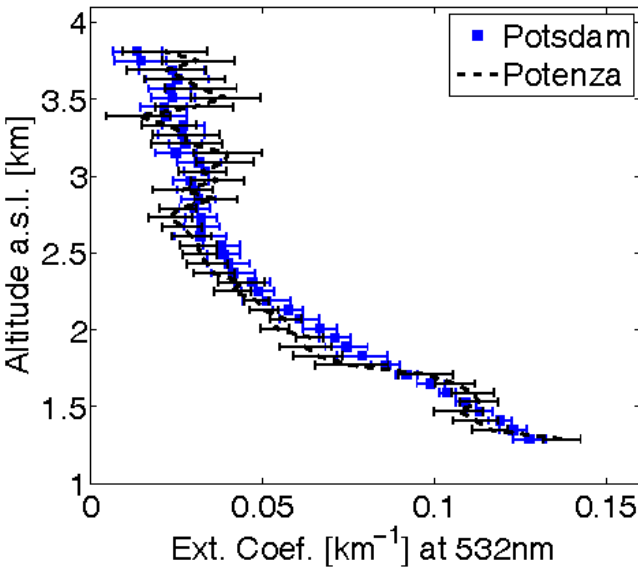
Transformation
Volterra integral eq.
(ill-posed)

$$\int_{z_1}^z x(z) dz = \ln \left[\frac{z_1^2 P(\lambda_R, z_1) N(z)}{z^2 P(\lambda_R, z) N(z_1)} \right]$$

for $z \in [z_1, z_n]$

Discretization
Collocation
Method

$$Ax^\varepsilon = y^\varepsilon, \|y - y^\varepsilon\| \leq \varepsilon$$



Potenza, Italy 40°36'N 15°44'E

26 May 2008 19:43 - 20:43 UTC
30 Aug 2007 18:06 - 18:18 UTC

Padé (1,0) – Iteration
with L-curve



4. Retrieval of Microphysical Properties

- ✓ Fredholm system of **two integral equations** of the first kind for the backscatter (π) and extinction (ext) coefficients:

$$\beta_{\text{aer}} \text{ or } \alpha_{\text{aer}} = \Gamma(\lambda) = \int_{r_{\text{min}}}^{r_{\text{max}}} K_{\pi/\text{ext}}^v(r, \lambda, m) v(r) dr = \int_{r_{\text{min}}}^{r_{\text{max}}} \frac{3}{4r} Q_{\pi/\text{ext}}(r, \lambda, m) v(r) dr$$

again an ill-posed problem

where (for homogeneous spheres)

$$Q_{\pi} = \frac{1}{k^2 r^2} \left| \sum_{n=1}^{\infty} (2n+1)(-1)^n (a_n - b_n) \right|^2, \quad Q_{\text{ext}} = \frac{2}{k^2 r^2} \sum_{n=1}^{\infty} (2n+1) \text{Re}(a_n + b_n)$$

→ **Regularization helps**

(C.B., *Appl. Opt.* 2001, 2006)
(C.B. et al., *JOSAA* 2005)

$\beta(\lambda)$:	aerosol backscatter coefficient
$\alpha(\lambda)$:	aerosol extinction coefficient
$v(r)$:	particle volume distribution
m :	refractive index
$Q(\lambda, r, m)$:	efficiency of sphere (backscatter or extinction)
$r_{\text{min}}, r_{\text{max}}$:	particle radius (realistic lower, upper limits)



5. Iterative Regularization by Adaptive Base Points

Integral Equations: $\Gamma(\lambda) = \int_{r_{\min}}^{r_{\max}} K_{\pi/ext}^v(r, \lambda, m) v(r) dr = \int_{r_{\min}}^{r_{\max}} \frac{3}{4r} Q_{\pi/ext}(r, \lambda, m) v(r) dr$
ill-posed



Discretization
by Collocation



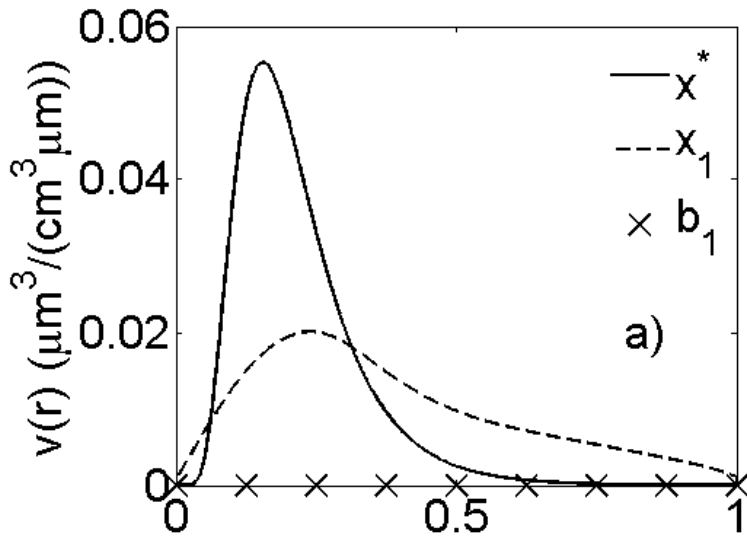
Using B splines of order 3 or 4

Linear Equation System:
ill-conditioned

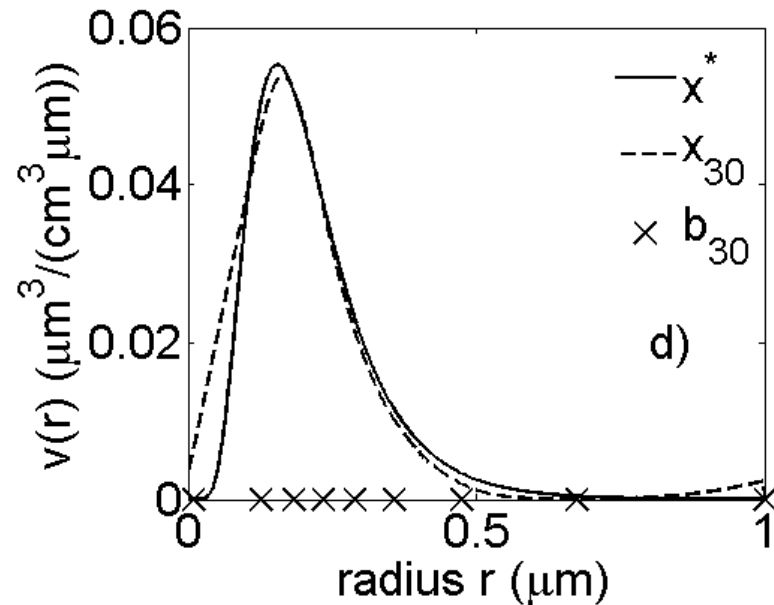
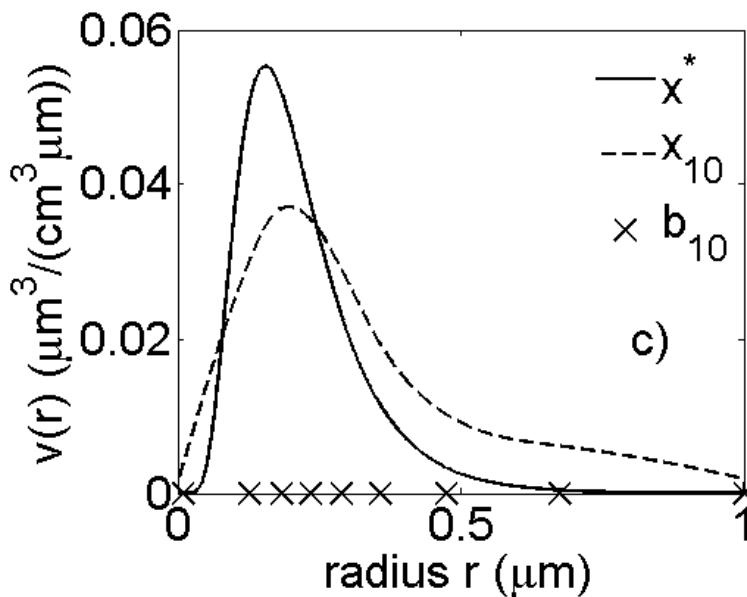
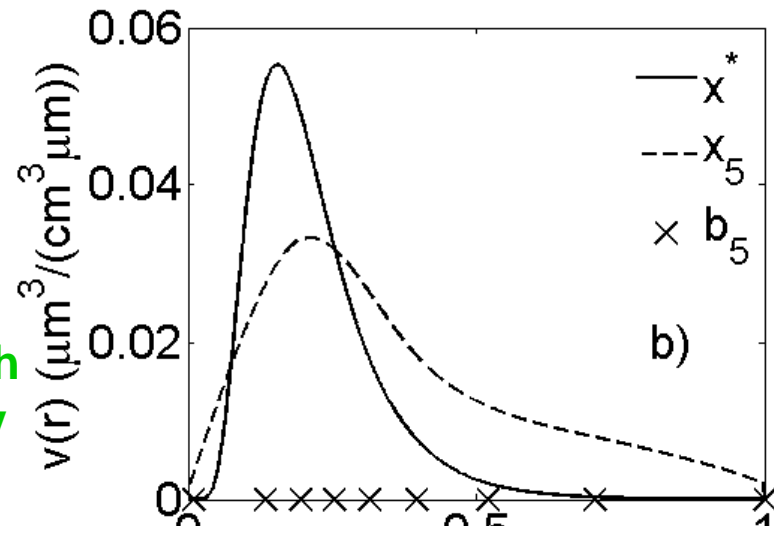
$$K^T K = K^T \Gamma$$

Solving by an iterative regularization method

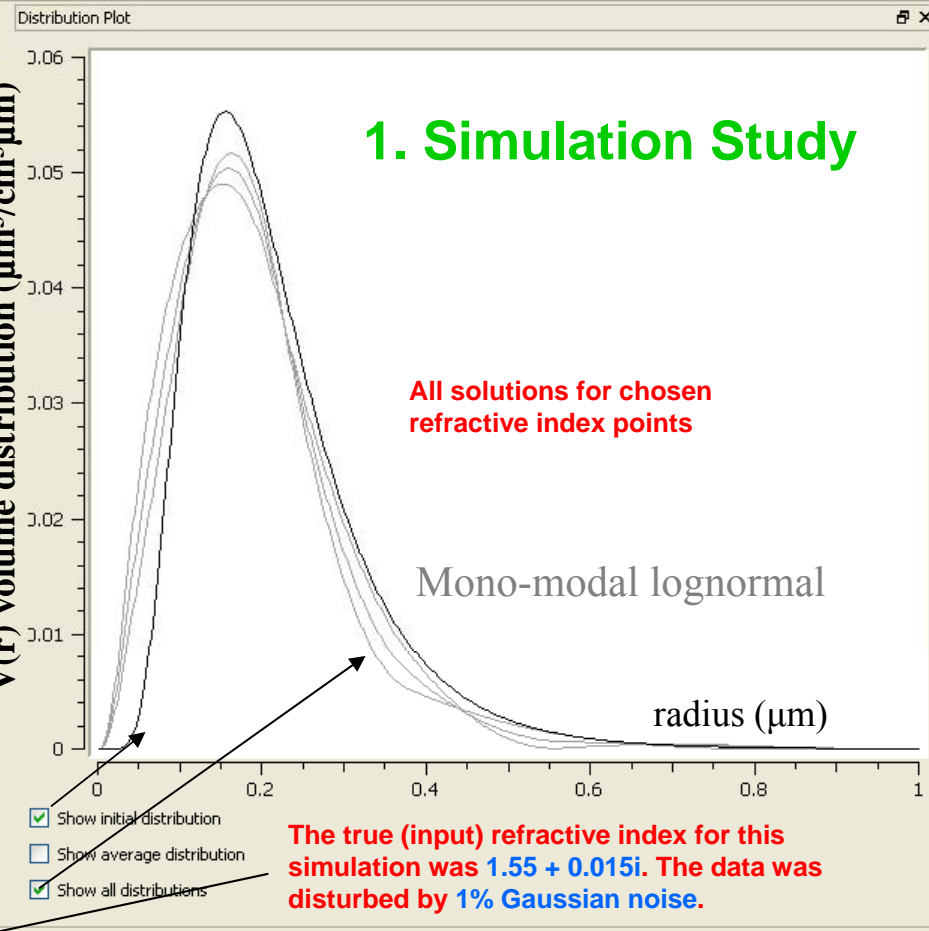
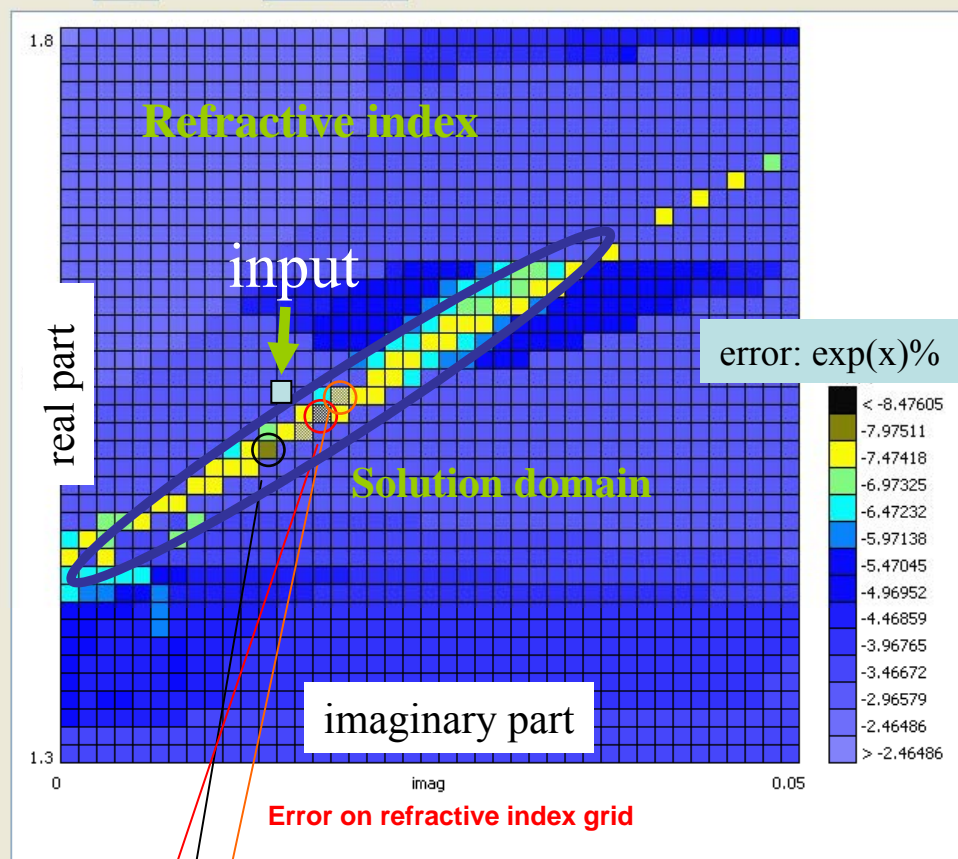
- Number of iteration steps serves as regularization parameter
- Using adaptive base points
- Non-negativity restriction by projection during iteration steps



Projected
Padé (2,1)
Iteration with
Discrepancy
Principle



Noise run: 1 Error type: absolute



1. Simulation Study

Details

Details

Average microphysical properties

	refindex real	refindex imag	effective radius	surface concentration	volume concentration	number concentration	SSA 355nm	SSA 532nm
average	1.5375	0.0175	0.138405	242165	11151.2	8.33232e+06	0.911403	0.919511
standard deviation	0.0125	0.00125	0.00487016	19441.7	502.537	1.94617e+06	0.00340592	0.00346967

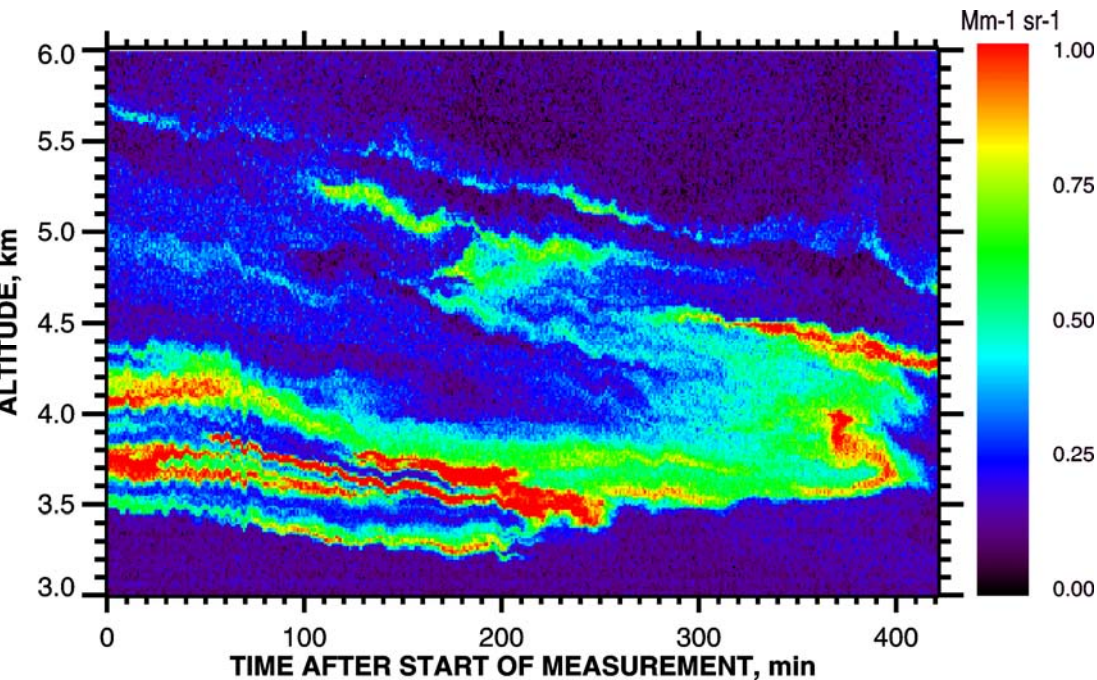
Tables containing the calculated microphysical properties for chosen refractive index points

Detailed results

refindex	deviation	effective radius	surface concentration	volume concentration	number concentration	B-Spline (deg,dim,cut)	integration range	SSA 355 nm	SSA 532 nm
{1.5375+0.0175i}	0.000208401	0.13845	241337	11137.7	8.24066e+06	3, 5, 1	0.001 ... 1	0.911465	0.919551
{1.525+0.01625i}	0.000251496	0.133512	262008	11660.4	1.03227e+07	3, 5, 1	0.001 ... 1	0.914778	0.922961
{1.55+0.01875i}	0.000252301	0.143252	223151	10655.6	6.4336e+06	3, 5, 1	0.001 ... 1	0.907967	0.916022



Case Study : Forest fire aerosols (29 06 07)



MODIS 290607



Aerosol backscatter coefficient @532 nm ($1/m \cdot sr$)

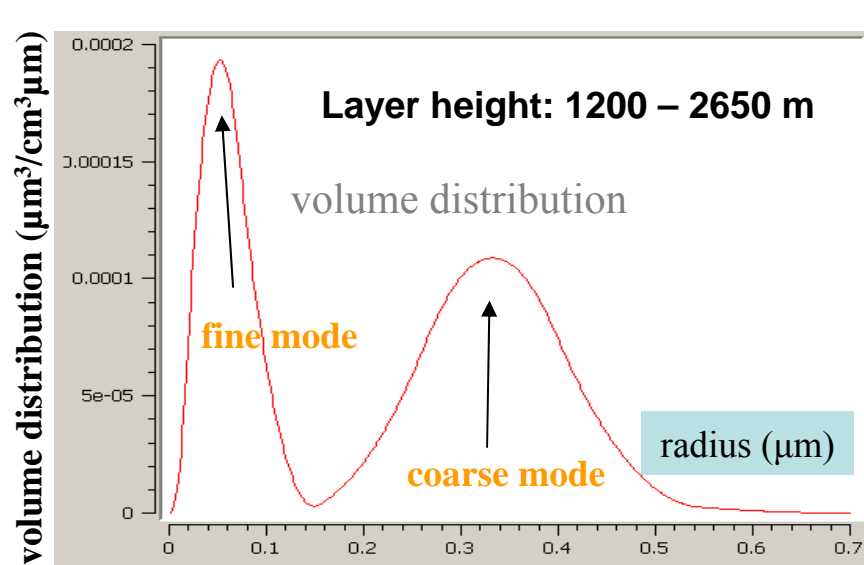
(Qualitative figure only)

(A. Papayannis et al, *Proc. 24. ILRC 2008*)

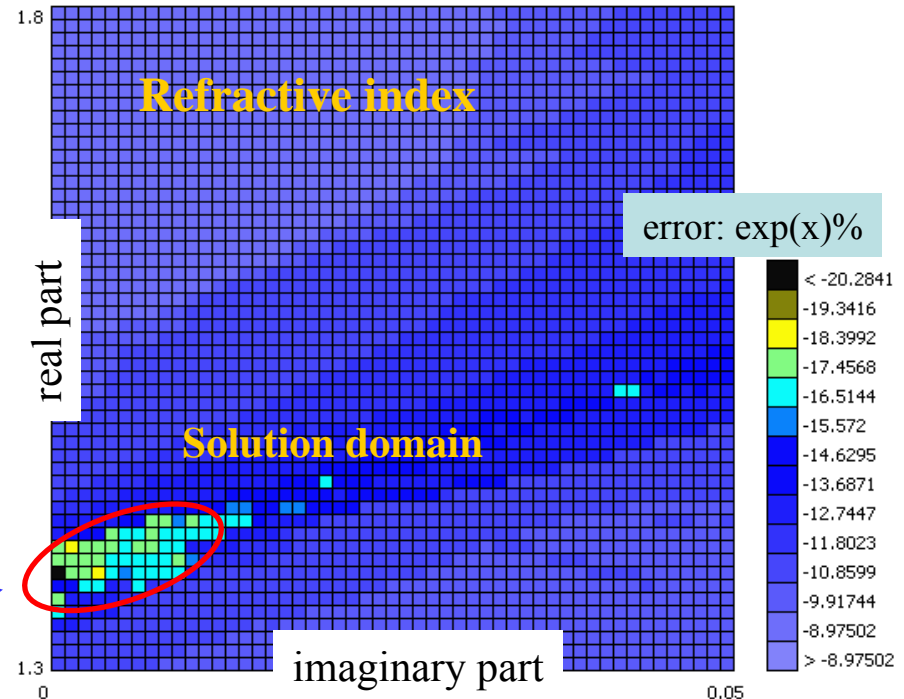


Case Study : Forest fire aerosols (29 06 07)

Output



A bimodal reconstruction has been calculated for the best data point.



The diagonal structure is an important feature meaning good measurement data.

Retrieved average microphysical properties (around the best point):

$$m=1.386(\pm 0.019)+0.006(\pm 0.004)i, r_{\text{eff}}=0.1\pm 0.023 (\mu\text{m})$$

$$\text{vol.conc.}=34.771\pm 5.873 (\mu\text{m}^3\text{cm}^{-3}), \text{surf.conc.}=1124.64\pm 472.43 (\mu\text{m}^2\text{cm}^{-3})$$

$$\text{SSA}(355\text{nm})=0.956\pm 0.029, \text{SSA}(532\text{nm})=0.938\pm 0.039$$

In good agreement with an additional chemical analysis.

A. Nenes and C. Fountoukis are acknowledged for the provision of the ISORROPIA II model.



Thank you very much for your interest and your attention.

