First and Second Order Taylor Approximations for Radiancies

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1 Gradients, Jacobians, and Hessians

Gradient vector of $I_l : \mathbb{R}^Q \to \mathbb{R}$ is given as

$$\nabla I_l(\mathbf{f}) \;\; = \;\; \left[\begin{array}{ccc} \dfrac{\partial I_l}{\partial f_1} & \cdots & \dfrac{\partial I_l}{\partial f_Q} \end{array} \right]. \tag{1}$$

Jacobian matrix of $I : \mathbb{R}^Q \to \mathbb{R}^L$ is given as

$$J I(\mathbf{f}) \;\; = \;\; \left[\begin{array}{ccc} \dfrac{\partial I_1}{\partial f_1} & \cdots & \dfrac{\partial I_1}{\partial f_Q} \\ \vdots & & \vdots \\ \dfrac{\partial I_L}{\partial f_1} & \cdots & \dfrac{\partial I_L}{\partial f_Q} \end{array} \right]. \tag{2}$$

Hessian matrix of $I_l : \mathbb{R}^Q \to \mathbb{R}$ is given as

$$H I_l(\mathbf{f}) \;\; = \;\; J(\nabla I_l(\mathbf{f})) \;\; = \;\; \left[\begin{array}{c} \nabla\left(\dfrac{\partial I_l}{\partial f_1}\right) \\ \vdots \\ \nabla\left(\dfrac{\partial I_l}{\partial f_Q}\right) \end{array} \right] \;\; = \;\; \left[\begin{array}{ccc} \dfrac{\partial^2 I_l}{\partial f_1 \partial f_1} & \cdots & \dfrac{\partial^2 I_l}{\partial f_Q \partial f_1} \\ \vdots & & \vdots \\ \dfrac{\partial^2 I_l}{\partial f_1 \partial f_Q} & \cdots & \dfrac{\partial^2 I_l}{\partial f_Q \partial f_Q} \end{array} \right]. \tag{3}$$

Since I is a function from $\mathbb{R}^Q \to \mathbb{R}^L$, i.e.

$$I(\mathbf{f}) = (I_1, I_2, \ldots, I_L),$$

then the array of second partial derivatives is not a two-dimensional matrix of size $Q \times Q$, but rather a tensor of order 3, with dimensions $L \times Q \times Q$.

2 Sensitivity Measurements

Denote $\mathbf{f}^*$ be an unperturbed state vector, for which the radiance $I_l(\mathbf{f}^*)$ at level L, as well as gradient vector $\nabla I_l(\mathbf{f}^*)$ and Hessian matrix $HI_l(\mathbf{f}^*)$ had been calculated. Let $\mathbf{f}$ denote the perturbed state vector, with perturbation defined as $\triangle \mathbf{f} = \mathbf{f} - \mathbf{f}^*$.

Accuracy of an $n-th$ order Taylor expansion can be assessed via calculating $I_l(\mathbf{f})$ analytically, and comparing the result with an approximation $I_l^{approx}(\mathbf{f})$ obtained using the Taylor expansion.

2.1 First-Order Model

The accuracy of the first order Taylor expansion can be determined by comparing how similar $I_l(\mathbf{f})$ is to the result obtained with the first order Taylor polynomial:

$$I_l(\mathbf{f}) \approx I_l(\mathbf{f}^*) + \sum_{q=1}^{Q} \frac{\partial I_l}{\partial f_q}(\mathbf{f}^*) \cdot (f_q - f_q^*).$$

This can be written in matrix notation:

$$I(\mathbf{f}) \approx I(\mathbf{f}^*) + JI(\mathbf{f}^*) \cdot (\mathbf{f} - \mathbf{f}^*)$$

or

$$I(\mathbf{f}^* + \triangle \mathbf{f}) \approx I(\mathbf{f}^*) + JI(\mathbf{f}^*) \cdot \triangle \mathbf{f}.$$

2.2 Second-Order Model

The accuracy of the second order Taylor expansion can be determined using

$$I_l(\mathbf{f}) \approx I_l(\mathbf{f}^*) + \sum_{q=1}^{Q} \frac{\partial I_l}{\partial f_q}(\mathbf{f}^*) \cdot (f_q - f_q^*) + \frac{1}{2} \sum_{q,\tilde{q}=1}^{Q} \frac{\partial^2 I_l}{\partial f_q \partial f_{\tilde{q}}}(\mathbf{f}^*) \cdot (f_q - f_q^*) \cdot (f_{\tilde{q}} - f_{\tilde{q}}^*),$$

or

$$I_l(\mathbf{f}) \approx I_l(\mathbf{f}^*) + \nabla I_l(\mathbf{f}^*) \cdot \triangle \mathbf{f} + \frac{1}{2}(\triangle \mathbf{f})^t \cdot HI_l(\mathbf{f}^*) \cdot \triangle \mathbf{f}.$$

This can not be directly reformulated in *full* matrix notation. However, we could generalize hessian matrix H to $\hat{H}$ and write:

$$I(\mathbf{f}) \approx I(\mathbf{f}^*) + JI(\mathbf{f}^*) \cdot (\mathbf{f} - \mathbf{f}^*) + \frac{1}{2}(\mathbf{f} - \mathbf{f}^*)^t \cdot \hat{H}I(\mathbf{f}^*) \cdot (\mathbf{f} - \mathbf{f}^*).$$

2.2.1 Numerical Computations

Denote $\triangle\mathbf{f} = \mathbf{f} - \mathbf{f}^*$.

The **first order** sensitivity measurement can be tested approximating $I_l(\mathbf{f})$ as:

$$I_l^{approx}(\mathbf{f}) = I_l(\mathbf{f}^*) + \nabla I_l(\mathbf{f}^*) \cdot \triangle\mathbf{f},$$

for $l = 1, \ldots, L$.

The **second order** sensitivity measurement can be tested with

$$I_l^{approx}(\mathbf{f}) = I_l(\mathbf{f}^*) + \nabla I_l(\mathbf{f}^*) \cdot \triangle\mathbf{f} + \frac{1}{2}(\triangle\mathbf{f})^t \cdot HI_l(\mathbf{f}^*) \cdot \triangle\mathbf{f}.$$

In the experiments below, $\nabla I_l(\mathbf{f}^*)$ was obtained *analytically* for both mixing ratio and temperature state vectors, in both first-order and second-order cases. For mixing ratios, $HI_l(\mathbf{f}^{O_3*})$ was obtained either *analytically* or *numerically*. For temperature, $HI_l(\mathbf{f}^{T*})$ was obtained *numerically*.

The L_∞, L_1, and L_2 norms on errors between the exact radiance $I(\mathbf{f})$ and its approximation $I^{approx}(\mathbf{f})$ are given as:

$$||I(\mathbf{f}) - I^{approx}(\mathbf{f})||_\infty \quad = \quad \max_l |I_l(\mathbf{f}) - I_l^{approx}(\mathbf{f})|$$

$$||I(\mathbf{f}) - I^{approx}(\mathbf{f})||_1 \quad = \quad \sum_{l=1}^{L} |I_l(\mathbf{f}) - I_l^{approx}(\mathbf{f})|$$

$$||I(\mathbf{f}) - I^{approx}(\mathbf{f})||_2 \quad = \quad \left(\sum_{l=1}^{L} |I_l(\mathbf{f}) - I_l^{approx}(\mathbf{f})|^2 \right)^{\frac{1}{2}}$$

Table 1: L_∞ norm

	$\nu_1 = 234709.8550$	$\nu_2 = 235309.855$	$\nu_3 = 235509.855$	$\nu_4 = 235659.855$	$\nu_5 = 235709.855$
$\mathbf{f}^{O_3}$, 1st order	0.047641	0.18545	0.31660	0.24590	3.2225
$\mathbf{f}^{O_3}$, 2nd order H numerical	0.00056974	0.0033343	0.0081745	0.0094711	0.20130
$\mathbf{f}^{O_3}$, 2nd order H analytical	0.00056974	0.0033343	0.0081742	0.0094665	0.20125
$\mathbf{f}^{T}$, 1st order	2.4617	2.8695	3.5324	4.8195	2.2144
$\mathbf{f}^{T}$, 2nd order H numerical	0.65547	0.66530	0.64894	0.58542	0.26306

Table 2: L_1 norm
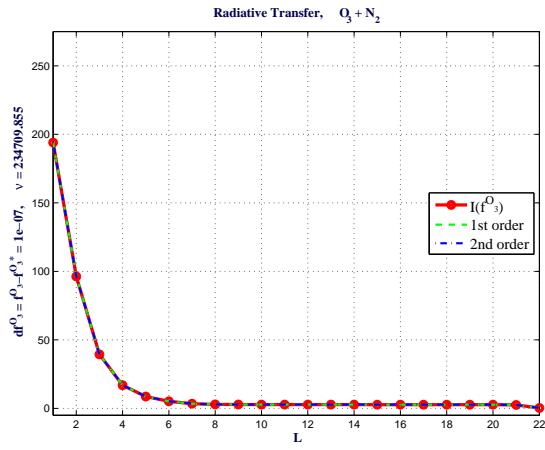
	$\nu_1 = 234709.8550$	$\nu_2 = 235309.855$	$\nu_3 = 235509.855$	$\nu_4 = 235659.855$	$\nu_5 = 235709.855$
$\mathbf{f}^{O_3}$, 1st order	0.099391	0.46032	0.88068	0.77977	25.884
$\mathbf{f}^{O_3}$, 2nd order H numerical	0.00094000	0.0079154	0.020786	0.027963	1.3724
$\mathbf{f}^{O_3}$, 2nd order H analytical	0.00094000	0.0079152	0.020784	0.027923	1.3720
$\mathbf{f}^{T}$, 1st order	4.6970	5.3108	5.9812	27.177	11.452
$\mathbf{f}^{T}$, 2nd order H numerical	1.1046	1.1405	1.6347	1.9412	1.7328

Table 3: L_2 norm
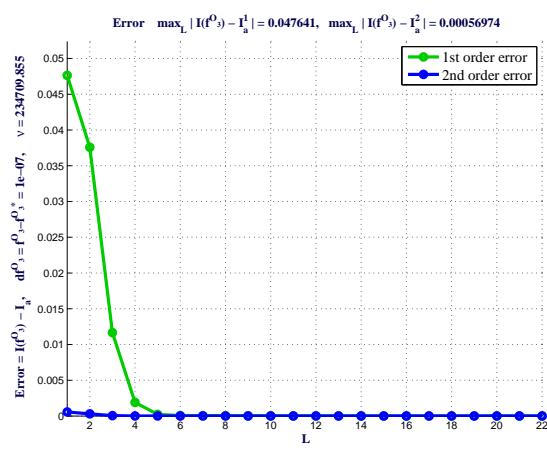
	$\nu_1 = 234709.8550$	$\nu_2 = 235309.855$	$\nu_3 = 235509.855$	$\nu_4 = 235659.855$	$\nu_5 = 235709.855$
$\mathbf{f}^{O_3}$, 1st order	0.061821	0.25454	0.45740	0.37598	7.5943
$\mathbf{f}^{O_3}$, 2nd order H numerical	0.00064711	0.0046358	0.011305	0.014099	0.42816
$\mathbf{f}^{O_3}$, 2nd order H analytical	0.00064710	0.0046358	0.011304	0.014087	0.42806
$\mathbf{f}^{T}$, 1st order	2.7136	3.0899	3.7292	10.604	4.0330
$\mathbf{f}^{T}$, 2nd order H numerical	0.69588	0.72608	0.80568	0.84050	0.52705

Accuracy comparisons of first and second order Taylor approximations for Radiances. *Mixing Ratios* **Gradients were obtained** *analytically* **and** *Mixing Ratios* **Hessians were obtained** *numerically.*
**(Part 1 of 2)**
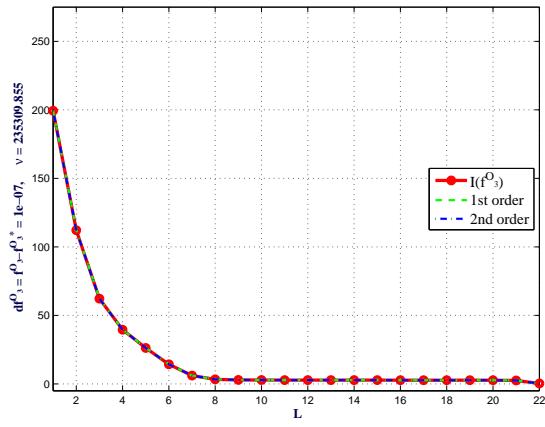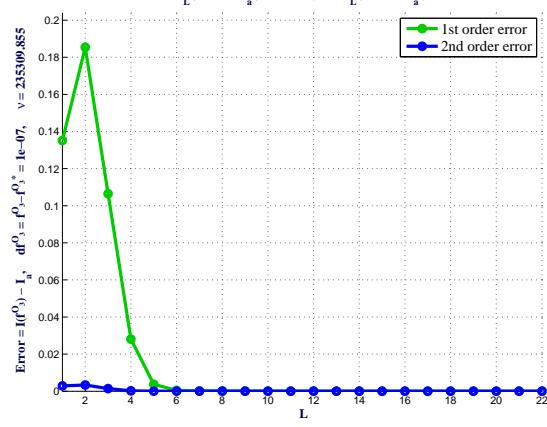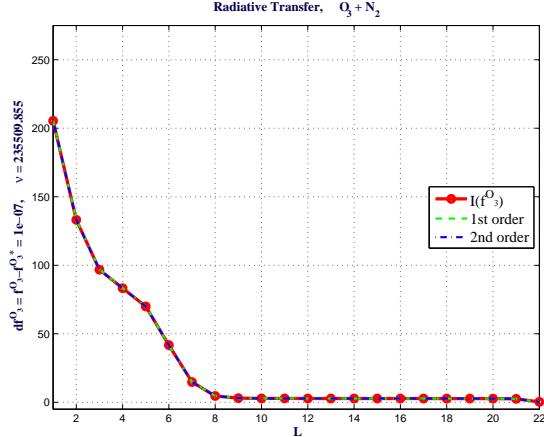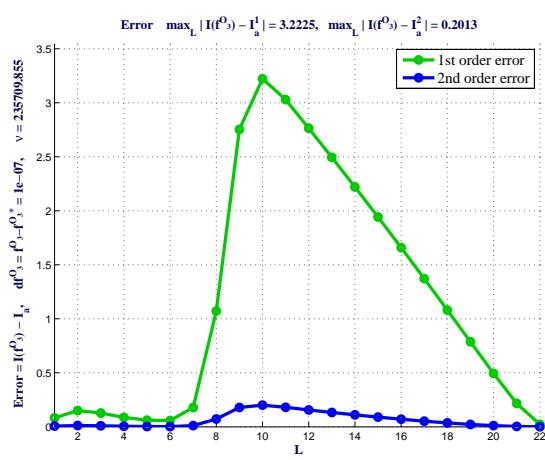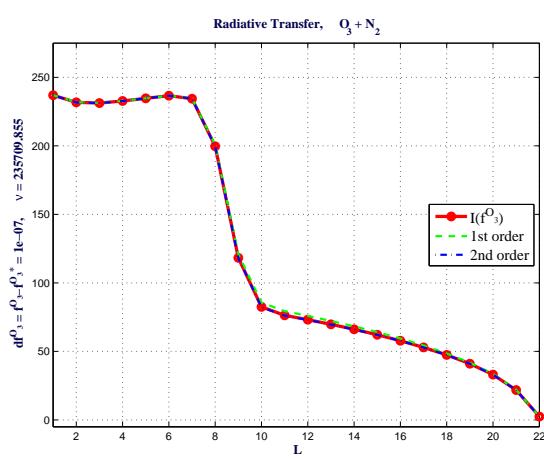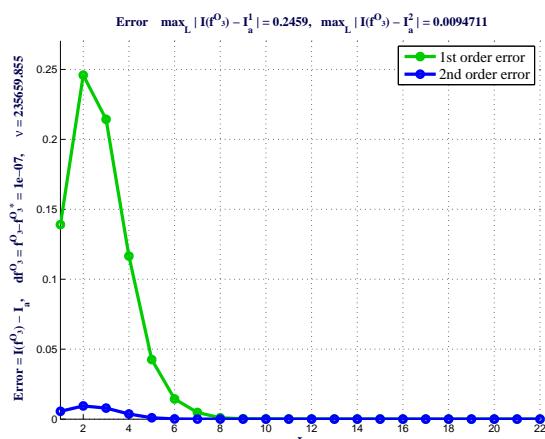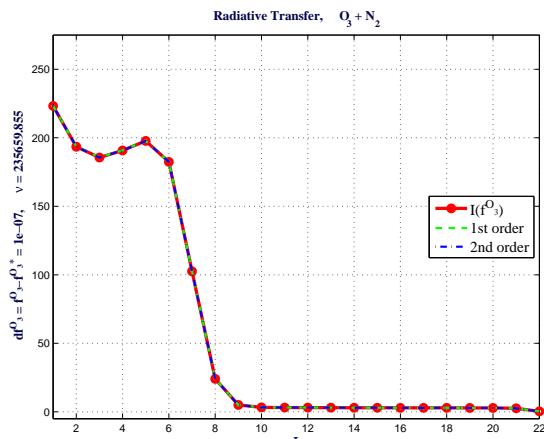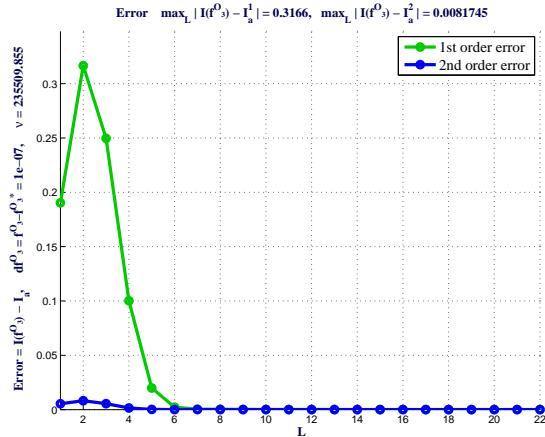
Antenna Radiances

**Errors**
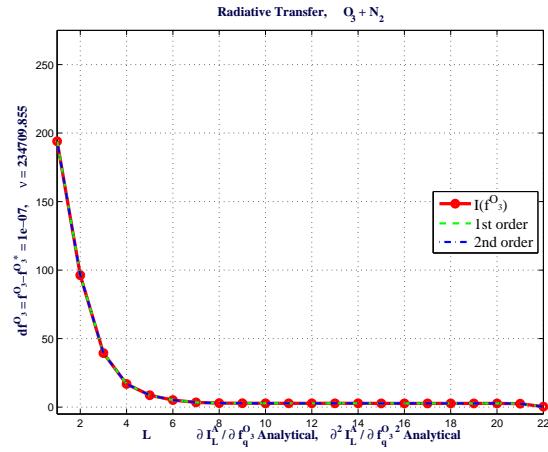
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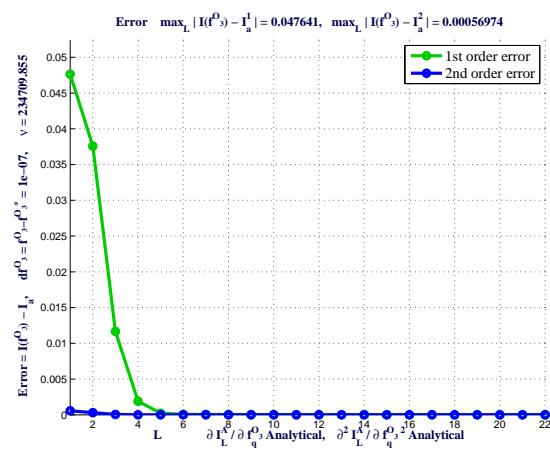
Errors

Accuracy comparisons of first and second order Taylor approximations for Radiances. *Mixing Ratios* Gradients and *Mixing Ratios* Hessians were obtained *analytically*.

(Part 1 of 2)
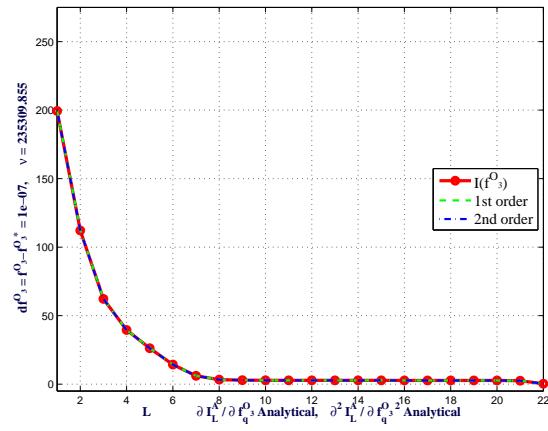
### Antenna Radiances
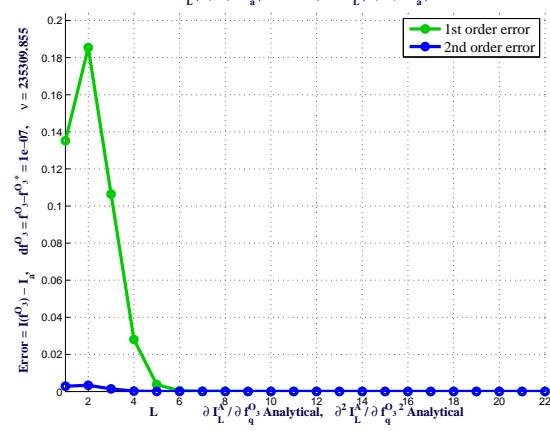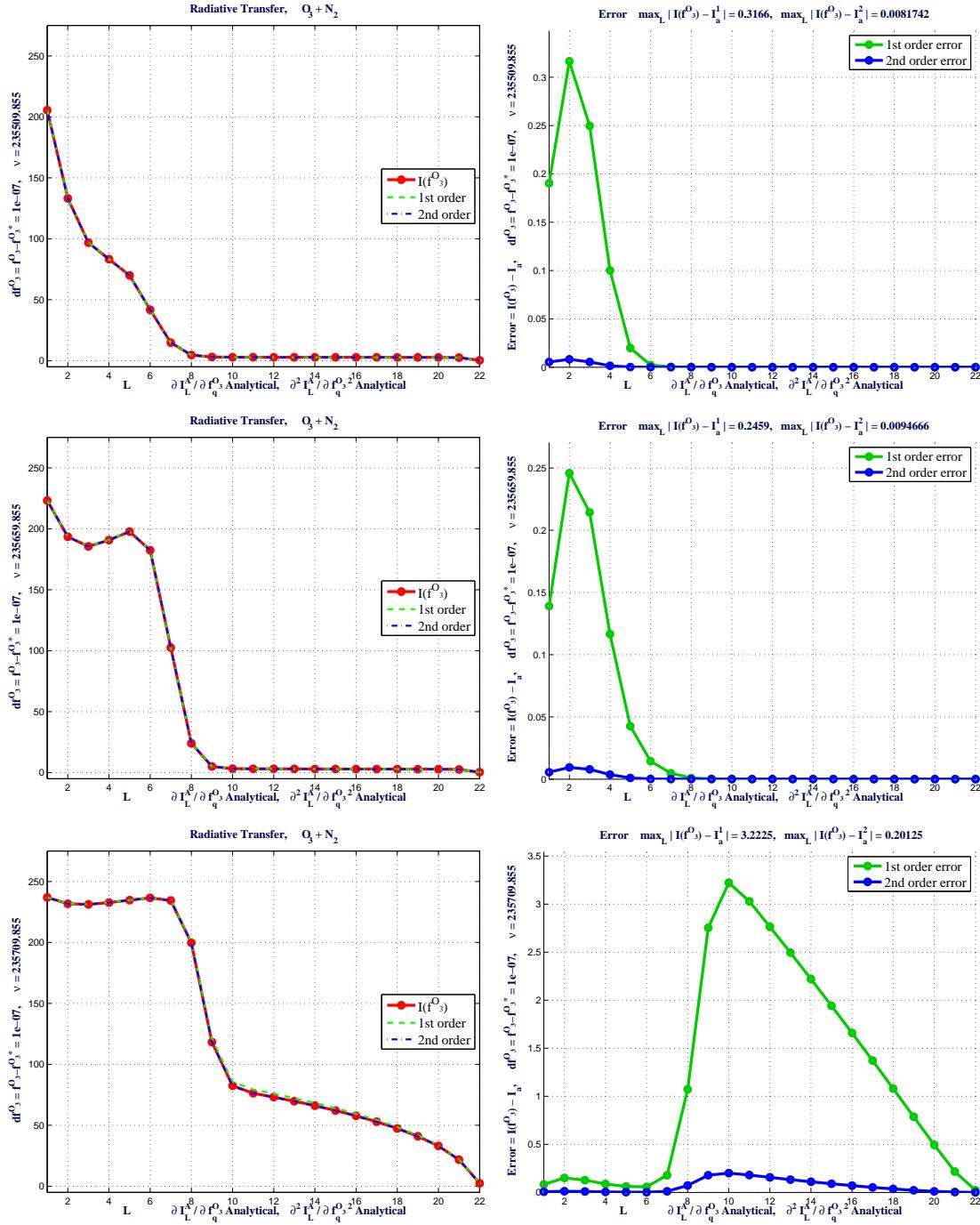
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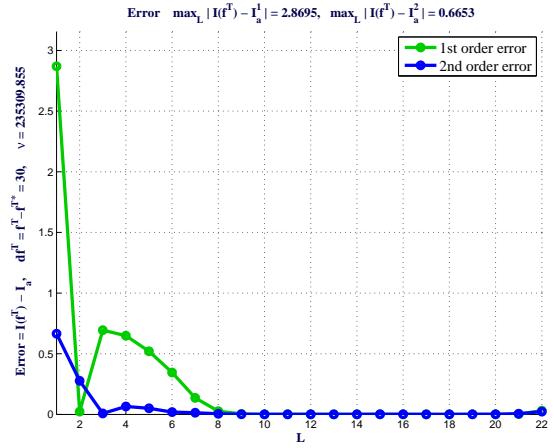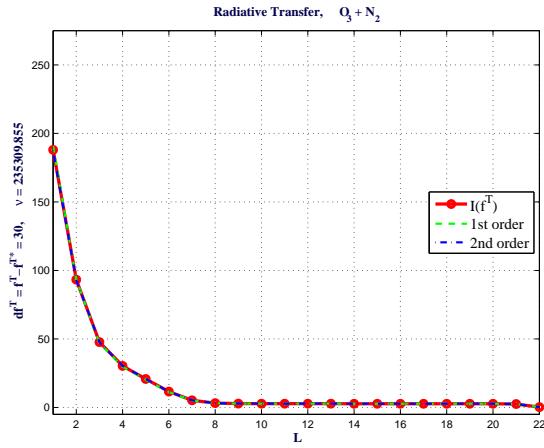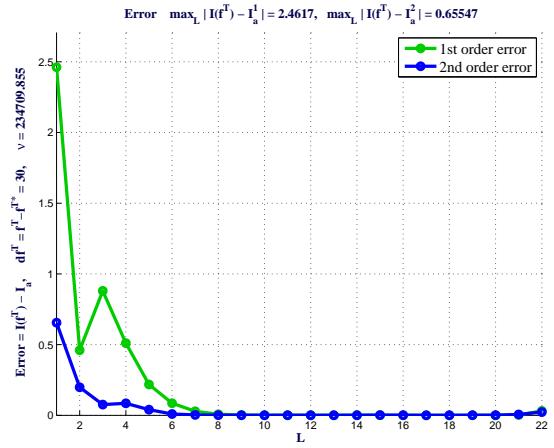
Errors

**Accuracy comparisons of first and second order Taylor approximations for Radiances.** *Temperature* **Gradients were obtained** *analytically* **and** *Temperature* **Hessians were obtained** *numerically.* **(Part 1 of 2)**

Antenna Radiances

Errors

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