Quantification and Visualization of Uncertainties in CT Reconstruction

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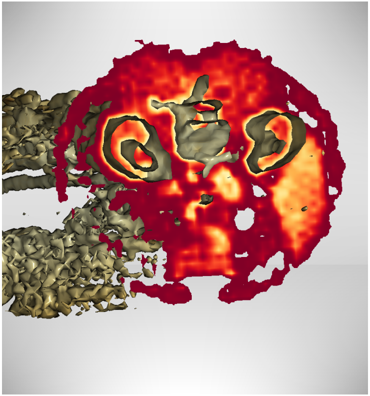
on behalf of the
SIVERT research training group
and the Bergen pCT collaboration



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The SIVERT Research Training Group

Safe and intelligent visualization and realtime-reconstruction techniques for pCT

The SIVERT project aims to contribute to improving particle therapy using **pCT**, with the goal of moving this technology closer to clinical use. Towards this goal, intelligent **machine learning techniques** and **visualization methods** are investigated and developed to advance the heretofore prototypical approaches towards increased speed and **safety**.
`https://sivert.info`

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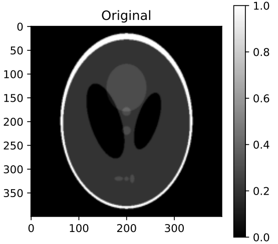
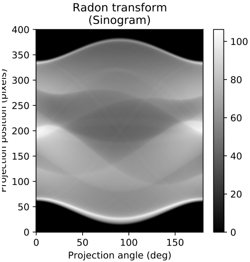
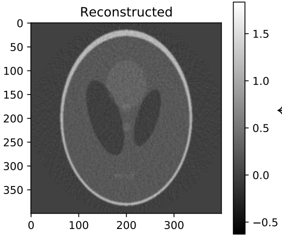
How sure can we be about the CT output?

the patient

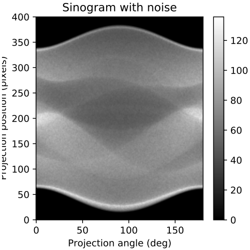




signal that the ideal CT device would measure:
xCT: sinogram
pCT: tracks



CT output



actually measured signal

Outline

1a. Uncertainties relate to derivatives.

1b. How to compute derivatives of computer programs.

2. Visualization of uncertain isocontours.

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1a. Uncertainties relate to derivatives.

1b. How to compute derivatives of computer programs.

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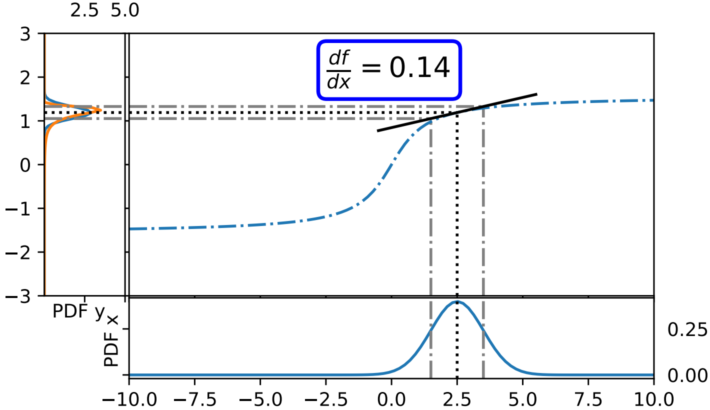
Uncertainty amplification ↔ derivatives

Question: $Y = f(X)$ maps Gaussian $X \sim N(\mu_X, \sigma_X^2)$ to $Y = ?$
Answer: Approximate $Y \sim N(\mu_Y, \sigma_Y^2)$ with

$$\mu_Y = f(\mu_X), \quad \sigma_Y^2 = \frac{\mathrm{d}f}{\mathrm{d}x}\Big|_{x=\mu_X}^2 \cdot \sigma_X^2.$$



... if the tangent is a good approximation.

$f = \arctan$

$\mu_X = 2.5$
$\sigma_X^2 = 1.0$

$\mu_X = 0.0$
$\sigma_X^2 = 3.0$

Uncertainty amplification $\leftrightarrow$ derivatives

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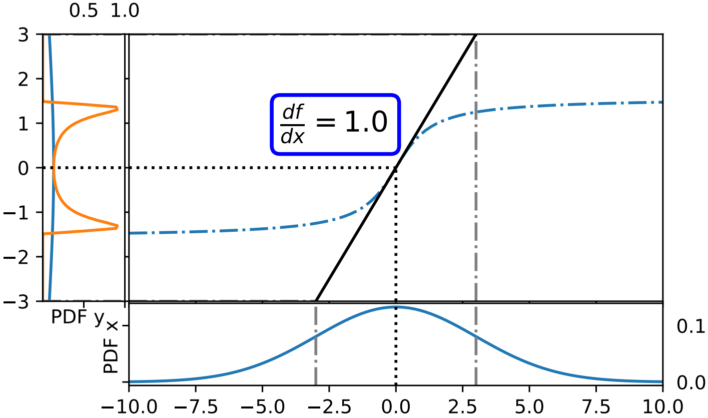

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Uncertainty amplification $\leftrightarrow$ derivatives

Question: $Y = f(X)$ with multi-dimensional $X \sim N(\mu_X, \Sigma_X)$?
Answer: Approximate $Y \sim N(\mu_Y, \Sigma_Y)$ with

$$\mu_Y = f(\mu_X), \quad \Sigma_Y = f'(\mu_X) \cdot \Sigma_X \cdot f'(\mu_X)^\top.$$

Question: How to compute the Jacobian $f'(x) = (\frac{\partial y_i}{\partial x_j})_{i,j}$?

Outline

1a. Uncertainties relate to derivatives.

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Question: How to compute the Jacobian $f'(x) = (\frac{\partial y_i}{\partial x_j})_{i,j}$?

Answer:

- Finite Difference Quotients: e. g. $\frac{\partial y_i}{\partial x_j} \approx \frac{y_i(x+h\cdot \mathrm{e}_i)-y_i(x)}{h}$
- Apply differentiation rules by hand.
- *Automatic Differentiation*:
  The program is a sequence of elementary operations, for which we know *exact* differentiation rules.

Forward-mode AD

	value	$\frac{\partial \text{ value}}{\partial \text{ input}}$

a		
b		
c		

a		
b		
c		

a		
b		
c		

```
a = 3. is an input;

b = 2. * a;

c = a * b;

c is an output;
```

Forward-mode AD

	value	$\frac{\partial \text{ value}}{\partial \text{ input}}$

a	3.	1.
b		
c		

a		
b		
c		

a		
b		
c		

```
a = 3. is an input;

b = 2. * a;

c = a * b;

c is an output;
```

Forward-mode AD

	value	$\frac{\partial \textbf{ value}}{\partial \textbf{ input}}$
a	3.	1.
b		
c		

a	3.	1.
b	6.	2.
c		

a		
b		
c		

```
a = 3. is an input;

b = 2. * a;

c = a * b;

c is an output;
```

Forward-mode AD

	value	$\frac{\partial\,\textbf{value}}{\partial\,\textbf{input}}$
a	3.	1.
b		
c		

a	3.	1.
b	6.	2.
c		

a	3.	1.
b	6.	2.
c	18.	12.

```
a = 3. is an input;

b = 2. * a;

c = a * b;

c is an output;
```

Forward-mode AD

	value	$\frac{\partial \text{ value}}{\partial \text{ input}}$

a	3.	1.
b		
c		

```
a = 3. is an input;
```

a	3.	1.
b	6.	2.
c		

```
b = 2. * a;
```

a	3.	1.
b	6.	2.
c	18.	12.

```
c = a * b;
```

```
c is an output;
```

Check: at $a = 3$, $2a^2 = 18$ and $4a = 12$.

Implementation by Operator Overloading

Forward-mode AD

- Replace type `double` of **value**s by a class which stores $\boxed{\textbf{value} \mid \frac{\partial\,\textbf{value}}{\partial\,\textbf{input}}}$.
- Overload `operator*`, `sin`, ... to compute $\frac{\partial\,\textbf{value}}{\partial\,\textbf{input}}$ alongside **value**, according to differentiation rules.
- Time complexity: $\mathcal{O}(\text{primal} \cdot \#\text{inputs})$
- Space complexity: $\mathcal{O}(\text{primal})$ possible

Reverse-mode AD

...

CoDiPack

Many implementations of forward and reverse AD exist. We chose CoDiPack[1]:
https://www.scicomp.uni-kl.de/software/codi.

```
#include <iostream>
#include "codi.hpp"

int main(int nargs, char** args) {
  codi::RealForward x = 4.0, y;
  x.setGradient(1.0);

  y = x * x + 1;

  std::cout << "f(4.0) = " << y << "\n";
  std::cout << "df/dx(4.0) = " << y.getGradient() << "\n";
}
```

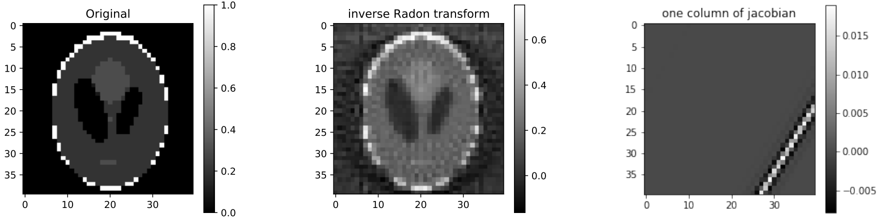
[1] M. Sagebaum, T. Albring, N. R. Gauger: High-Performance Derivative Computations using CoDiPack. *ACM Trans. Math. Softw. 45*(4), 2019.

Is that everything to bear in mind?

In general, we just have to replace `double` by a `codi`-type everywhere, including numerical libraries etc.

But: Concerning **iterative numerical algorithms** like DROP-TVS, adjustments will be necessary.

Filtered Back-Projection derivative:
Already implemented and verified against Tensorflow.



Original, FBP-reconstructed image and one column of the Jacobian of the FBP-reconstruction.

Uncertainty Quantification Wrap-Up

- We can propagate **uncertainties through complex algorithms**, e. g. CT reconstruction,
- approximately, by propagating **normal distributions** $N(\mu, \Sigma)$ **through linearizations**.
- Linearizations can be formed by **Automatic Differentiation**.

Outline

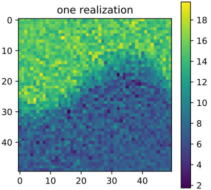
1a. Uncertainties relate to derivatives.

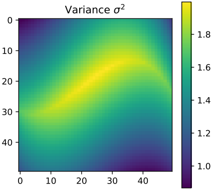
1b. How to compute derivatives of computer programs.

2. Visualization of uncertain isocontours.

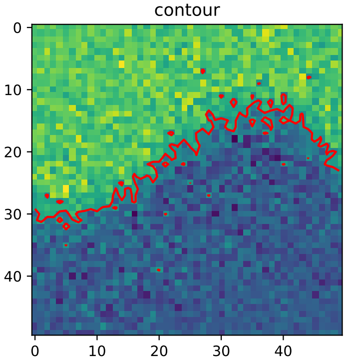
Uncertain isocontours

At each **grid point x**, besides the **realization** $f_{\text{recon}}(\mathbf{x})$ we get a **variance** $\sigma_{\text{AD}}(\mathbf{x})^2$ through AD.





How certain is the isocontour $\{\mathbf{x} : f(\mathbf{x}) = \theta\}$?



Uncertain isocontours

Model the true value at $\mathbf{x}$ as

$$f_{\text{true}}(\mathbf{x}) \sim N(f_{\text{recon}}(\mathbf{x}), \sigma_{\text{AD}}(x)^2).$$

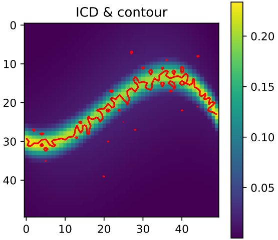
To mark the uncertainty of the contour $\{\mathbf{x} : f(\mathbf{x}) = \theta\}$, color every $\mathbf{x}$ by

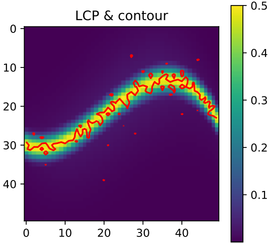
- the "**Isocontour Density**" (**ICD**):

$$\text{Prob. density of } f_{\text{true}}(\mathbf{x}) = \theta.$$

- the "**Level-Crossing Probability**" (**LCP**):

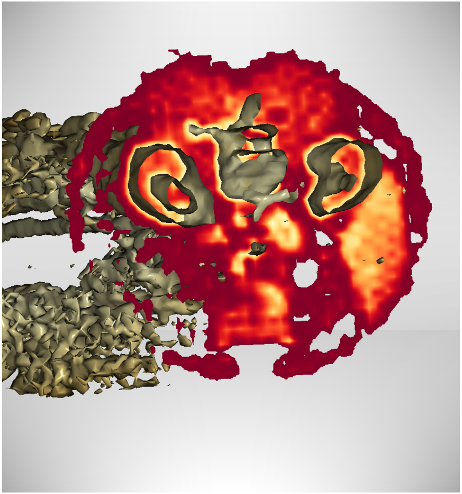
$$2 \cdot (\text{Prob. of } f_{\text{true}}(\mathbf{x}) < \theta) \cdot (\text{Prob. of } f_{\text{true}}(\mathbf{x}) > \theta).$$





K. Pöthkow, H.-C. Hege: Positional Uncertainty of Isocontours: Condition Analysis and Probabilistic Measures. *IEEE Trans. Vis. Comput. Graph. 17*(10), 2011.

Results



X-ray CT from the CHAOS dataset[1], reconstructed via FBP in Tensorflow.

We assumed that the covariance between two sinogram pixels decreased exponentially with their distance.

Contour surface at threshold
$\theta = 125\ 133\ 137$.

Axial plane:
ICD/LCP colouring at $\theta = 137$,
yellow = high ICD/LCP.

Contact:
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[1]A. E. Kavur, M. A. Selver et al: CHAOS – Combined (CT-MR) Healthy Abdominal Organ Segmentation Challenge Data (Version v1.03). 2019. Zenodo, http://doi.org/10.5281/zenodo.3362844

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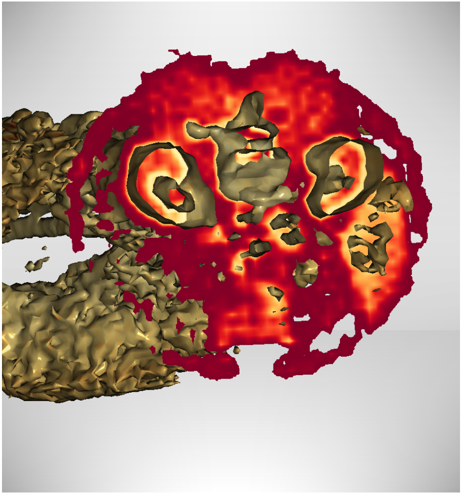

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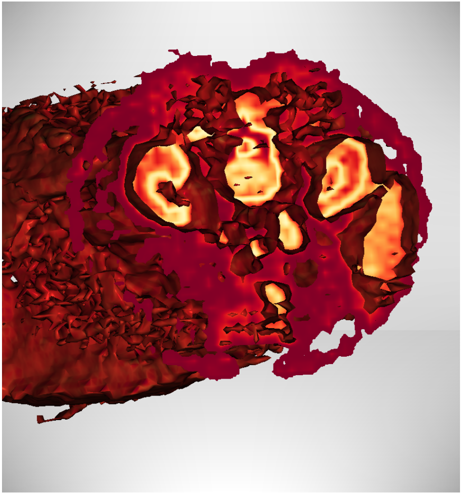

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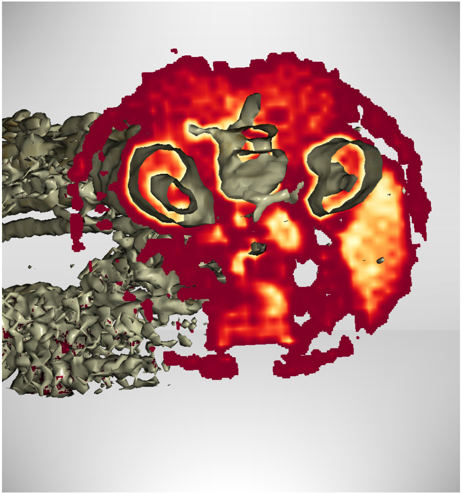

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The Bergen pCT Collaboration and SIVERT Research Training Group

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- Saint Petersburg State University, Saint Petersburg, Russia
- Utrecht University, Netherlands
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