Fréchet derivatives under various parameterizations using chain rule

for LEGO module m_parameterization.f90

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Overview

Physical meaning of symbols uniformly used in this code:

vp	P-wave velocity
vs	S-wave velocity
sp =1/vp	P-wave slowness
sps=vs/vp	inv Vp-Vs ratio
ip =vp*rho	P-wave (acoustic) impedance
rho	density
kpa=rho*vp^2	bulk modulus
lda=rho*(vp^2-2vs^2)	1st Lamé parameter
mu =rho*vs^2	2nd Lamé parameter, shear modulus

Overview

Considered parameterizations

SITUATION	PARAMETERIZATION	ALLOWED PARAMETERS
WaveEquation	moduli-density	kpa (or lda mu) rho
I/O models	velocities-density	vp vs rho
seismic	velocities-impedance	vp vs ip
tomography	slowness-density	sp sps rho
optimization	can be any of above	

Source-Destination trilogy:

$$\boxed{\text{model m} \xrightarrow{\textit{FWD}} \text{WaveEq lm} \xrightarrow{\textit{PARAMETERIZATION}} \text{optim x,g} \xrightarrow{\textit{FWD}} \text{model m}}$$

- model m $\rightarrow$ WaveEq lm depending on field.
- WaveEq produces gkpa (or glda, gmu) and grho under moduli-density parameterization.
- then m_parameterization.f90 converts them to another parameterization for optim x,g, which can be any of parameterization

ACTIVE versus PASSIVE

- Active parameters will be converted to optim x via feature scaling (e.g. (par-par_min)/(par_max-par_min)), and will be updated by optimization methods.
  - Mono-parameter inversion: 1 active parameter.
  - Multi-parameter inversion: >1 active parameters.
    - Scaling in m_linesearch.f90 depends only on the 1st active parameters (no matter of it's velocity or not).
    - Output of inversion results has same sequence of active parameters listed in setup.in
- Passive parameters will NOT be converted to optim x, and will NOT be updated by optimization methods.
- However, they may still be updated according to user-specified empirical law (e.g. Gardner), which serves as hard constraints between parameters.
  - User has to modified the code where necessary to insert such a law as symbolic computation is not straightforward in fortran
  - Such a law may change the optim g for active parameters.

velocities-density

velocities-impedance

slowness-density

PARAMETERIZATION velocities-density

isotropic ACoustic

$$\begin{cases} \kappa = \rho V_P^2 \\ \rho_0 = \rho \end{cases}$$

$$\begin{aligned}
\nabla_{V_P} &= \nabla_\kappa \frac{\partial \kappa}{\partial V_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_P} \\
&= \nabla_\kappa 2\rho V_P \\
\nabla_\rho &= \nabla_\kappa \frac{\partial \kappa}{\partial \rho} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial \rho} \\
&= \nabla_\kappa V_P^2 + \nabla_{\rho_0}
\end{aligned}$$

$$\begin{cases} V_P = \sqrt{\frac{\kappa}{\rho_0}} \\ \rho = \rho_0 \end{cases}$$

$$\begin{aligned}
\nabla_\kappa &= \nabla_{V_P} \frac{\partial V_P}{\partial \kappa} + \nabla_\rho \frac{\partial \rho}{\partial \kappa} \\
&= \nabla_{V_P} \frac{1}{2\rho_0} \sqrt{\frac{\rho_0}{\kappa}} \\
&= \nabla_{V_P} 0.5 \rho_0^{-0.5} \kappa^{-0.5} \\
\nabla_{\rho_0} &= \nabla_{V_P} \frac{\partial V_P}{\partial \rho_0} + \nabla_\rho \frac{\partial \rho}{\partial \rho_0} \\
&= \nabla_{V_P} \left(-\frac{\kappa}{2\rho_0^2} \sqrt{\frac{\rho_0}{\kappa}} \right) + \nabla_\rho \\
&= \nabla_{V_P} \left(-0.5 \rho_0^{-1.5} \kappa^{0.5} \right) + \nabla_\rho
\end{aligned}$$

PARAMETERIZATION velocities-density + PASSIVE gardner

isotropic ACoustic

$$\boxed{\rho = aV_P^b}$$

$$\begin{cases} \kappa = \rho V_P^2 = aV_P^{b+2} \\ \rho_0 = \rho = aV_P^b \end{cases}$$

$$V_P = \left(\frac{\kappa}{a}\right)^{\frac{1}{b+2}}$$

$$\begin{aligned} \nabla_{V_P} &= \nabla_\kappa \frac{\partial \kappa}{\partial V_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_P} \\ &= \nabla_\kappa a(b+2)V_P^{b+1} + \nabla_{\rho_0} abV_P^{b-1} \\ &= \left(\nabla_\kappa \frac{b+2}{b} V_P^2 + \nabla_{\rho_0}\right) abV_P^{b-1} \end{aligned}$$

$$\begin{aligned} \nabla_\kappa &= \nabla_{V_P} \frac{\partial V_P}{\partial \kappa} \\ &= \nabla_{V_P} \frac{1}{a(b+2)} \left(\frac{\kappa}{a}\right)^{-\frac{b+1}{b+2}} \end{aligned}$$

PARAMETERIZATION velocities-density

isotropic P-SV

$$\begin{cases} \lambda = \rho(V_P^2 - 2V_S^2) \\ \mu = \rho V_S^2 \\ \rho_0 = \rho \end{cases}$$

$$\begin{cases} V_P = \sqrt{\frac{\lambda+2\mu}{\rho_0}} \\ V_S = \sqrt{\frac{\mu}{\rho_0}} \\ \rho = \rho_0 \end{cases}$$

$$\begin{aligned}
\nabla_{V_P} &= \nabla_\lambda \frac{\partial \lambda}{\partial V_P} + \nabla_\mu \frac{\partial \mu}{\partial V_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_P} \\
&= \nabla_\lambda 2\rho V_P \\
\nabla_{V_S} &= \nabla_\lambda \frac{\partial \lambda}{\partial V_S} + \nabla_\mu \frac{\partial \mu}{\partial V_S} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_S} \\
&= \nabla_\lambda (-4)\rho V_S + \nabla_\mu 2\rho V_S \\
&= (-\nabla_\lambda 2 + \nabla_\mu) 2\rho V_S \\
\nabla_\rho &= \nabla_\lambda \frac{\partial \lambda}{\partial \rho} + \nabla_\mu \frac{\partial \mu}{\partial \rho} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial \rho} \\
&= \nabla_\lambda (V_P^2 - 2V_S^2) + \nabla_\mu V_S^2 + \nabla_{\rho_0}
\end{aligned}$$

$$\begin{aligned}
\nabla_\lambda &= \nabla_{V_P} \frac{\partial V_P}{\partial \lambda} + \nabla_{V_S} \frac{\partial V_S}{\partial \lambda} + \nabla_\rho \frac{\partial \rho}{\partial \lambda} \\
&= \dots \\
\nabla_\mu &= \nabla_{V_P} \frac{\partial V_P}{\partial \mu} + \nabla_{V_S} \frac{\partial V_S}{\partial \mu} + \nabla_\rho \frac{\partial \rho}{\partial \mu} \\
&= \dots \\
\nabla_{\rho_0} &= \nabla_{V_P} \frac{\partial V_P}{\partial \rho_0} + \nabla_{V_S} \frac{\partial V_S}{\partial \rho_0} + \nabla_\rho \frac{\partial \rho}{\partial \rho_0} \\
&= \dots
\end{aligned}$$

PARAMETERIZATION velocities-density + PASSIVE gardner

isotropic P-SV

$$\boxed{\rho = aV_P^b}$$

$$\begin{cases} \lambda = \rho(V_P^2 - 2V_S^2) = aV_P^{b+2} - 2aV_P^b V_S^2 \\ \mu = \rho V_S^2 = aV_P^b V_S^2 \\ \rho_0 = \rho = aV_P^b \end{cases}$$

$$\begin{aligned}
\nabla_{V_P} &= \nabla_\lambda \frac{\partial \lambda}{\partial V_P} + \nabla_\mu \frac{\partial \mu}{\partial V_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_P} \\
&= \nabla_\lambda \left(a(b+2)V_P^{b+1} - 2abV_P^{b-1}V_S^2 \right) + \nabla_\mu abV_P^{b-1}V_S^2 + \nabla_{\rho_0} abV_P^{b-1} \\
&= \left(\nabla_\lambda \left(\frac{b+2}{b} V_P^2 - 2V_S^2 \right) + \nabla_\mu V_S^2 + \nabla_{\rho_0} \right) abV_P^{b-1} \\
\nabla_{V_S} &= \nabla_\lambda \frac{\partial \lambda}{\partial V_S} + \nabla_\mu \frac{\partial \mu}{\partial V_S} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_S} \\
&= \nabla_\lambda(-4aV_P^b V_S) + \nabla_\mu 2aV_P^b V_S \\
&= (\nabla_\lambda(-2) + \nabla_\mu)\, 2aV_P^b V_S
\end{aligned}$$

velocities-density

velocities-impedance

slowness-density

PARAMETERIZATION velocities-impedance

isotropic ACoustic

$$\boxed{I_P = V_P \rho}$$

$$\left\{ \begin{array}{l} \kappa = \rho V_P^2 = V_P I_P \\ \rho_0 = \rho = \frac{I_P}{V_P} \end{array} \right.$$

$$\begin{array}{rcl} \nabla_{V_P} & = & \nabla_\kappa \dfrac{\partial \kappa}{\partial V_P} + \nabla_{\rho_0} \dfrac{\partial \rho_0}{\partial V_P} \\ & = & \nabla_\kappa I_P + \nabla_{\rho_0}(-I_P V_P^{-2}) \\ \nabla_{I_P} & = & \nabla_\kappa \dfrac{\partial \kappa}{\partial I_P} + \nabla_{\rho_0} \dfrac{\partial \rho_0}{\partial I_P} \\ & = & \nabla_\kappa V_P + \nabla_{\rho_0} V_P^{-1} \end{array}$$

$$\left\{ \begin{array}{l} V_P = \sqrt{\frac{\kappa}{\rho_0}} \\ I_P = \sqrt{\kappa \rho_0} \end{array} \right.$$

$$\begin{array}{rcl} \nabla_\kappa & = & \nabla_{V_P} \dfrac{\partial V_P}{\partial \kappa} + \nabla_{I_P} \dfrac{\partial I_P}{\partial \kappa} \\ & = & \nabla_{V_P} \dfrac{1}{2\rho_0} \sqrt{\dfrac{\rho_0}{\kappa}} + \nabla_{I_P} \dfrac{\rho_0}{2\sqrt{\kappa \rho_0}} \\ & = & \nabla_{V_P} 0.5 \rho_0^{-0.5} \kappa^{-0.5} + \nabla_{I_P} 0.5 \rho_0^{0.5} \kappa^{-0.5} \\ & = & (\nabla_{V_P} + \nabla_{I_P} \rho_0)\, 0.5 \rho_0^{-0.5} \kappa^{-0.5} \\ \nabla_{\rho_0} & = & \nabla_{V_P} \dfrac{\partial V_P}{\partial \rho_0} + \nabla_{I_P} \dfrac{\partial I_P}{\partial \rho_0} \\ & = & \nabla_{V_P} \dfrac{-\kappa}{2\rho_0^2} \sqrt{\dfrac{\rho_0}{\kappa}} + \nabla_{I_P} \dfrac{\kappa}{2\sqrt{\kappa \rho_0}} \\ & = & \nabla_{V_P} (-0.5) \rho_0^{-1.5} \kappa^{0.5} + \nabla_{I_P} 0.5 \rho_0^{-0.5} \kappa^{0.5} \\ & = & \left(-\nabla_{V_P} \rho_0^{-1} + \nabla_{I_P}\right) 0.5 \rho_0^{-0.5} \kappa^{0.5} \end{array}$$

PARAMETERIZATION velocities-impedance

isotropic P-SV

$$\begin{cases} \lambda = \rho(V_P^2 - 2V_S^2) = V_P I_P - \frac{2V_S^2 I_P}{V_P} \\ \mu = \rho V_S^2 = \frac{V_S^2 I_P}{V_P} \\ \rho_0 = \rho = \frac{I_P}{V_P} \end{cases}$$

$$\begin{aligned}
\nabla_{V_P} &= \nabla_\lambda \frac{\partial \lambda}{\partial V_P} + \nabla_\mu \frac{\partial \mu}{\partial V_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_P} \\
&= \nabla_\lambda \left(I_P + \frac{2V_S^2 I_P}{V_P^2} \right) + \nabla_\mu \left(-\frac{V_S^2 I_P}{V_P^2} \right) + \nabla_{\rho_0} \left(-\frac{I_P}{V_P^2} \right) \\
&= \nabla_\lambda \left(I_P + \frac{2V_S^2 I_P}{V_P^2} \right) + \nabla_\mu \left(-\frac{V_S^2 I_P}{V_P^2} \right) + \nabla_{\rho_0} \left(-\frac{I_P}{V_P^2} \right) \\
&= \left(\nabla_\lambda (V_P^2 + 2V_S^2) - \nabla_\mu V_S^2 - \nabla_{\rho_0} \right) \frac{I_P}{V_P^2} \\
\nabla_{V_S} &= \nabla_\lambda \frac{\partial \lambda}{\partial V_S} + \nabla_\mu \frac{\partial \mu}{\partial V_S} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial V_S} \\
&= \nabla_\lambda \frac{-4V_S I_P}{V_P} + \nabla_\mu \frac{2V_S I_P}{V_P} \\
&= (-2\nabla_\lambda + \nabla_\mu) \frac{2V_S I_P}{V_P}
\end{aligned}$$

PARAMETERIZATION velocities-impedance

isotropic P-SV *continued*

$$\begin{cases} \lambda = \rho(V_P^2 - 2V_S^2) = V_P I_P - \frac{2V_S^2 I_P}{V_P} \\ \mu = \rho V_S^2 = \frac{V_S^2 I_P}{V_P} \\ \rho_0 = \rho = \frac{I_P}{V_P} \end{cases}$$

$$\begin{aligned} \nabla_{I_P} &= \nabla_\lambda \frac{\partial \lambda}{\partial I_P} + \nabla_\mu \frac{\partial \mu}{\partial I_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial I_P} \\ &= \nabla_\lambda \left(V_P - \frac{2V_S^2}{V_P} \right) + \nabla_\mu \frac{V_S^2}{V_P} + \nabla_{\rho_0} \frac{1}{V_P} \\ &= \left(\nabla_\lambda (V_P^2 - 2V_S^2) + \nabla_\mu V_S^2 + \nabla_{\rho_0} \right) \frac{1}{V_P} \end{aligned}$$

velocities-density

velocities-impedance

slowness-density

PARAMETERIZATION slowness-density

isotropic ACoustic

$$\boxed{S_P = 1/V_P}$$

$$\begin{cases} \kappa = \rho V_P^2 = \rho S_P^{-2} \\ \rho_0 = \rho \end{cases}$$

$$\begin{aligned}
\nabla_{S_P} &= \nabla_\kappa \frac{\partial \kappa}{\partial S_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial S_P} \\
&= \nabla_\kappa (-2\rho S_P^{-3}) \\
\nabla_\rho &= \nabla_\kappa \frac{\partial \kappa}{\partial \rho} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial \rho} \\
&= \nabla_\kappa S_P^{-2} + \nabla_{\rho_0}
\end{aligned}$$

$$\begin{cases} S_P = \sqrt{\frac{\rho_0}{\kappa}} \\ \rho = \rho_0 \end{cases}$$

$$\begin{aligned}
\nabla_\kappa &= \nabla_{S_P} \frac{\partial S_P}{\partial \kappa} + \nabla_\rho \frac{\partial \rho}{\partial \kappa} \\
&= \nabla_{S_P} \left(\frac{1}{2} \sqrt{\frac{\kappa}{\rho_0}} \frac{-\rho_0}{\kappa^2} \right) \\
&= \nabla_{S_P} (-0.5) \rho_0^{0.5} \kappa^{-1.5} \\
\nabla_{\rho_0} &= \nabla_{S_P} \frac{\partial S_P}{\partial \rho_0} + \nabla_\rho \frac{\partial \rho}{\partial \rho_0} \\
&= \nabla_{S_P} \left(\frac{1}{2} \sqrt{\frac{\kappa}{\rho_0}} \frac{1}{\kappa} \right) + \nabla_\rho \\
&= \nabla_{S_P} 0.5 \rho_0^{-0.5} \kappa^{-0.5} + \nabla_\rho
\end{aligned}$$

PARAMETERIZATION slowness-density + PASSIVE gardner

isotropic ACoustic

$$\boxed{\rho = a S_P^{-b}}$$

$$\begin{cases} \kappa = \rho V_P^2 = a S_P^{-b-2} \\ \rho_0 = \rho = a S_P^{-b} \end{cases}$$

$$\begin{aligned} \nabla_{S_P} &= \nabla_\kappa \frac{\partial \kappa}{\partial S_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial S_P} \\ &= \nabla_\kappa a(-b-2) S_P^{-b-3} \\ &\quad + \nabla_{\rho_0} (-ab) S_P^{-b-1} \\ &= -\left(\nabla_\kappa a(b+2) + \nabla_{\rho_0} ab S_P^2\right) S_P^{-b-3} \end{aligned}$$

$$S_P = \left(\frac{\kappa}{a}\right)^{-\frac{1}{b+2}}$$

$$\begin{aligned} \nabla_\kappa &= \nabla_{S_P} \frac{\partial S_P}{\partial \kappa} \\ &= \nabla_{S_P} \frac{-1}{a(b+2)} \left(\frac{\kappa}{a}\right)^{-\frac{b+3}{b+2}} \end{aligned}$$

PARAMETERIZATION slowness-density

isotropic P-SV

$$\boxed{S_{PS} = V_S / V_P = V_S S_P}$$

$$\begin{cases} \lambda = \rho(V_P^2 - 2V_S^2) = \rho S_P^{-2}(1 - 2S_{PS}^2) \\ \mu = \rho V_S^2 = \rho (S_{PS}/S_P)^2 \\ \rho_0 = \rho \end{cases}$$

$$\begin{aligned}
\nabla_{S_P} &= \nabla_\lambda \frac{\partial \lambda}{\partial S_P} + \nabla_\mu \frac{\partial \mu}{\partial S_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial S_P} \\
&= \nabla_\lambda \rho(-2) S_P^{-3}(1 - 2S_{PS}^2) + \nabla_\mu \rho S_{PS}^2 (-2) S_P^{-3} \\
&= \left(\nabla_\lambda (1 - 2S_{PS}^2) + \nabla_\mu S_{PS}^2 \right) (-2) \rho S_P^{-3} \\
\nabla_{S_{PS}} &= \nabla_\lambda \frac{\partial \lambda}{\partial S_{PS}} + \nabla_\mu \frac{\partial \mu}{\partial S_{PS}} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial S_{PS}} \\
&= \nabla_\lambda \rho S_P^{-2}(-4) S_{PS} + \nabla_\mu 2\rho S_{PS}/S_P^2 \\
&= (-\nabla_\lambda 2 + \nabla_\mu)\, 2\rho S_{PS} S_P^{-2} \\
\nabla_\rho &= \nabla_\lambda \frac{\partial \lambda}{\partial \rho} + \nabla_\mu \frac{\partial \mu}{\partial \rho} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial \rho} \\
&= \nabla_\lambda S_P^{-2}(1 - 2S_{PS}^2) + \nabla_\mu (S_{PS}/S_P)^2 + \nabla_{\rho_0} \\
&= \left(\nabla_\lambda (1 - 2S_{PS}^2) + \nabla_\mu S_{PS} \right) S_P^{-2} + \nabla_{\rho_0}
\end{aligned}$$

PARAMETERIZATION slowness-density + PASSIVE gardner

isotropic P-SV

$$\boxed{S_{PS} = V_S S_P ; \rho = a S_P^{-b}}$$

$$\begin{cases} \lambda = \rho S_P^{-2}(1 - 2S_{PS}^2) = a S_P^{-b-2}(1 - 2S_{PS}^2) \\ \mu = \rho (S_{PS}/S_P)^2 = a S_P^{-b-2} S_{PS}^2 \\ \rho_0 = a S_P^{-b} \end{cases}$$

$$\begin{aligned}
\nabla_{S_P} &= \nabla_\lambda \frac{\partial \lambda}{\partial S_P} + \nabla_\mu \frac{\partial \mu}{\partial S_P} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial S_P} \\
&= \nabla_\lambda a(-b-2) S_P^{-b-3}(1 - 2S_{PS}^2) \\
&\quad + \nabla_\mu a(-b-2) S_P^{-b-3} S_{PS}^2 + \nabla_{\rho_0} a(-b) S_P^{-b-1} \\
&= \left(\nabla_\lambda (b+2)(1 - 2S_{PS}^2) + \nabla_\mu (b+2) S_{PS}^2 + \nabla_{\rho_0} b S_P^2 \right) (-a) S_P^{-b-3} \\
\nabla_{S_{PS}} &= \nabla_\lambda \frac{\partial \lambda}{\partial S_{PS}} + \nabla_\mu \frac{\partial \mu}{\partial S_{PS}} + \nabla_{\rho_0} \frac{\partial \rho_0}{\partial S_{PS}} \\
&= \nabla_\lambda a S_P^{-b-2}(-4) S_{PS} + \nabla_\mu a S_P^{-b-2} 2 S_{PS} \\
&= (-\nabla_\lambda 2 + \nabla_\mu) 2a S_P^{-b-2} S_{PS}
\end{aligned} \tag{1}$$